



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 03:25 PM EDT

PDB ID : 9Z33 / pdb_00009z33
Title : RT XFEL structure of dark-stable state of Photosystem II (0F, S1 rich) at 1.97 Angstrom obtained from anomalous data at 9.5 keV
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Minnetian, N.M.; Zhang, M.
Deposited on : 2025-11-05
Resolution : 1.97 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:

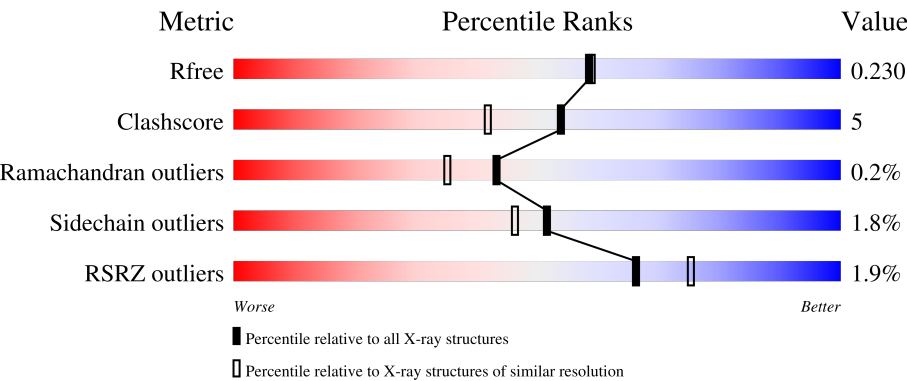
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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.



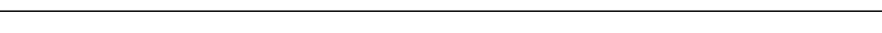
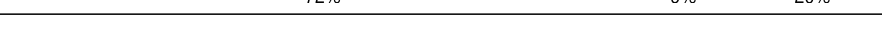
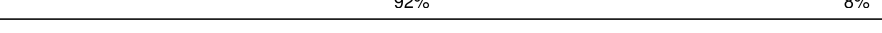
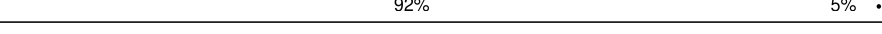
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	89%8%
1	a	344	86%10%
2	B	510	92%7%
2	b	510	93%6%

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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
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 52714 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			
1	a	334	Total	C	N	O	S	0	0	0
			2619	1714	431	459	15			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	1	0
			3426	2249	571	593	13			
3	c	451	Total	C	N	O	S	0	2	0
			3500	2290	587	610	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			
4	d	341	Total	C	N	O	S	0	1	0
			2723	1804	444	463	12			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			505	335	82	85	3			
7	h	63	Total	C	N	O	S	0	0	0
			493	327	80	83	3			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

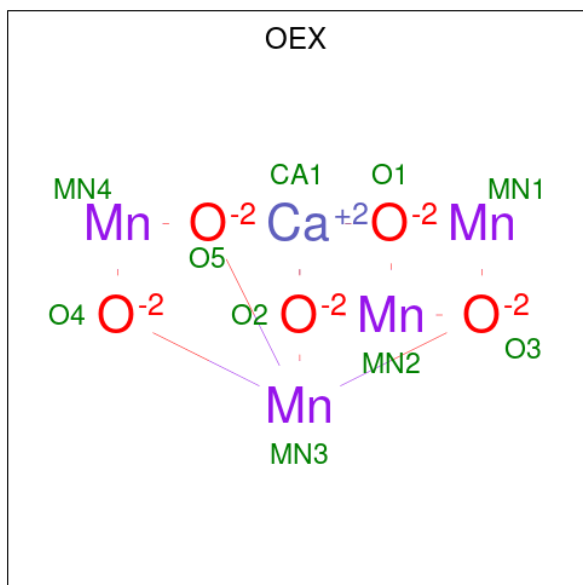
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	28	Total	C	N	O	0	0	0
			221	151	38	32			

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

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



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

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

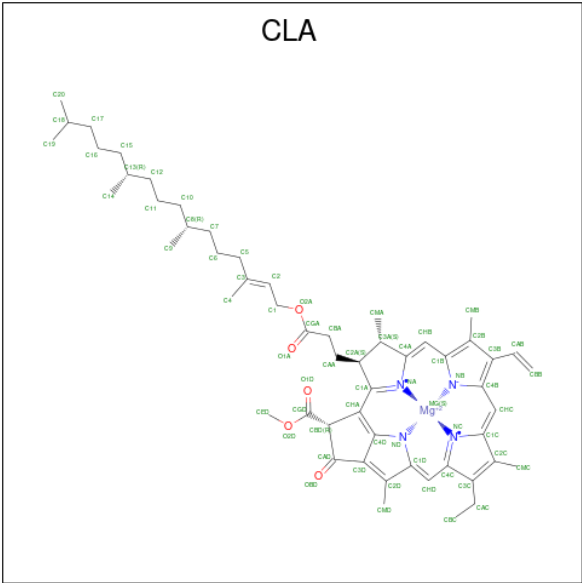
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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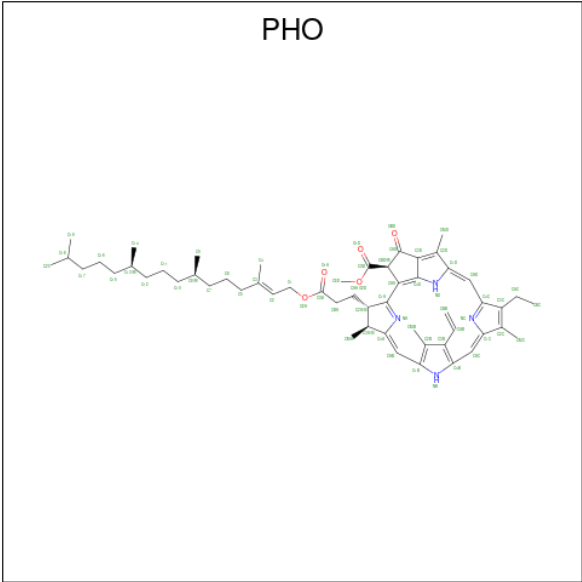
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N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

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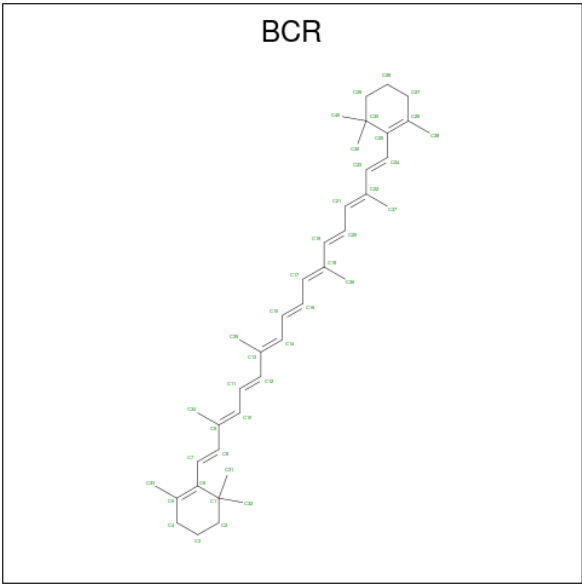
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



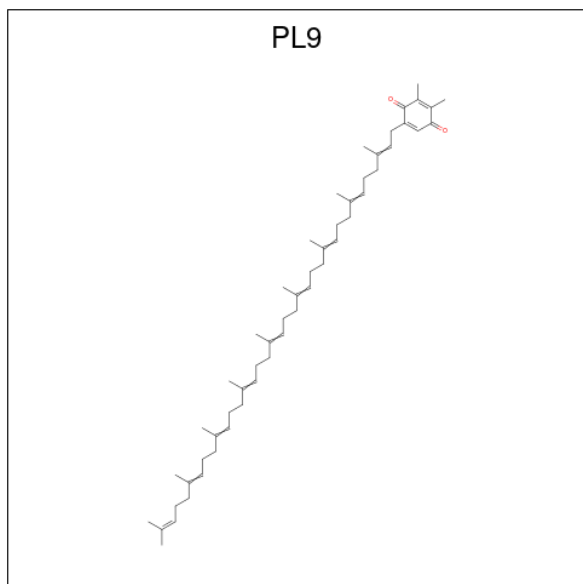
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



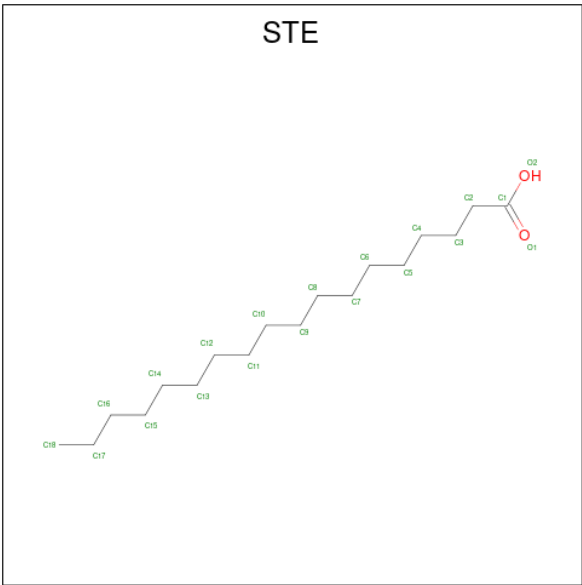
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 28 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	C	0	0
			9	9		
28	A	1	Total	C	0	0
			8	8		
28	A	1	Total	C	0	0
			17	17		
28	A	1	Total	C	0	0
			11	11		
28	B	1	Total	C	0	0
			17	15		
				O		
			2			
28	B	1	Total	C	0	0
			14	12		
				O		
			2			
28	B	1	Total	C	0	0
			18	16		
				O		
			2			
28	B	1	Total	C	0	0
			12	10		
				O		
			2			
28	B	1	Total	C	0	0
			15	15		
28	C	1	Total	C	0	0
			14	12		
				O		
			2			
28	C	1	Total	C	0	0
			5	5		
28	C	1	Total	C	0	0
			7	7		
28	C	1	Total	C	0	0
			10	10		
28	C	1	Total	C	0	0
			12	10		
				O		
			2			

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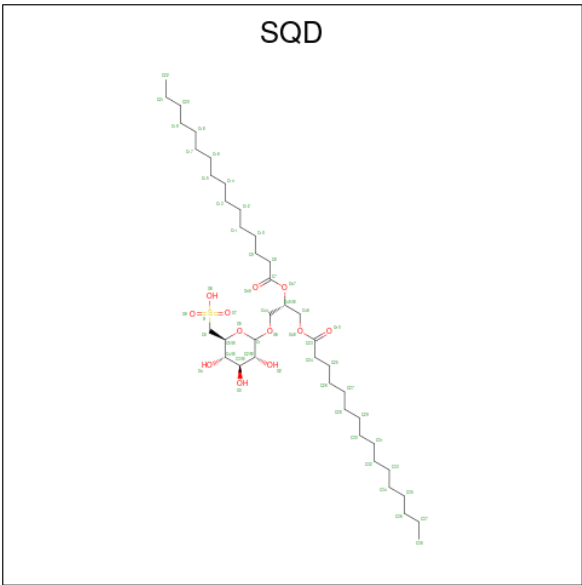
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C 16 16	0	0
28	C	1	Total C 14 14	0	0
28	D	1	Total C O 20 18 2	0	0
28	E	1	Total C O 12 10 2	0	0
28	E	1	Total C 12 12	0	0
28	E	1	Total C O 20 18 2	0	0
28	H	1	Total C 18 18	0	0
28	H	1	Total C 9 9	0	0
28	I	1	Total C O 17 15 2	0	0
28	I	1	Total C O 15 13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

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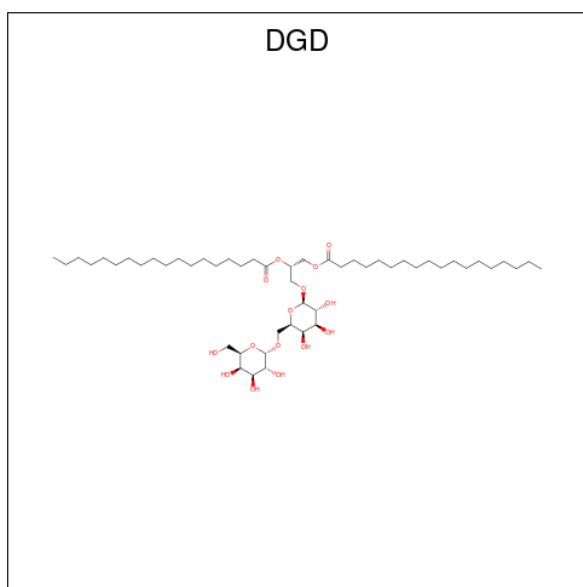
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	b	1	Total C 11 11	0	0
28	c	1	Total C 13 13	0	0
28	c	1	Total C 18 18	0	0
28	d	1	Total C O 20 18 2	0	0
28	d	1	Total C O 20 18 2	0	0
28	d	1	Total C O 20 18 2	0	0
28	d	1	Total C 10 10	0	0
28	d	1	Total C O 14 12 2	0	0
28	e	1	Total C 9 9	0	0
28	e	1	Total C 8 8	0	0
28	e	1	Total C 9 9	0	0
28	e	1	Total C O 13 11 2	0	0
28	i	1	Total C O 12 10 2	0	0
28	i	1	Total C 6 6	0	0
28	j	1	Total C O 12 10 2	0	0
28	j	1	Total C 16 16	0	0
28	m	1	Total C O 12 10 2	0	0
28	m	1	Total C 18 18	0	0
28	t	1	Total C 10 10	0	0
28	z	1	Total C 9 9	0	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



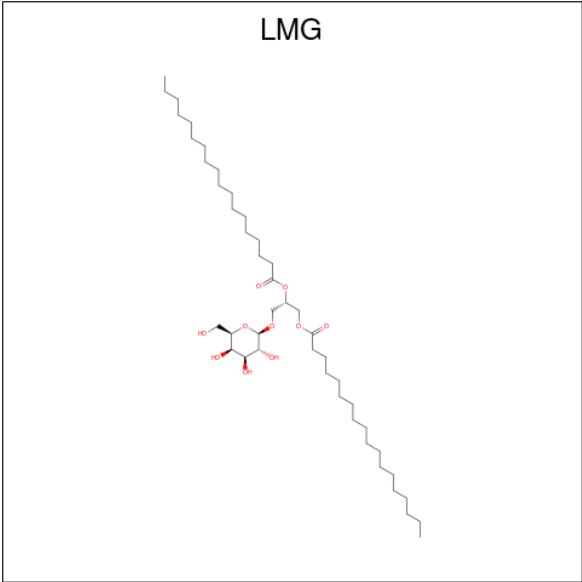
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O	S	0	0
			43	30	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			36	25	10	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O	S	0	0
			49	36	12	1		
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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

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



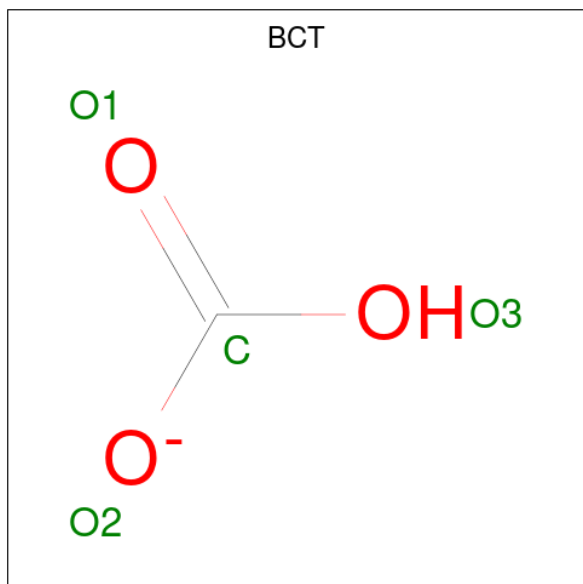
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			45	35	10		
31	B	1	Total	C	O	0	0
			51	41	10		
31	C	1	Total	C	O	0	0
			36	26	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			50	40	10		
31	D	1	Total	C	O	0	0
			51	41	10		
31	a	1	Total	C	O	0	0
			55	45	10		
31	a	1	Total	C	O	0	0
			49	39	10		
31	b	1	Total	C	O	0	0
			51	41	10		
31	b	1	Total	C	O	0	0
			55	45	10		
31	c	1	Total	C	O	0	0
			30	25	5		
31	c	1	Total	C	O	0	0
			46	36	10		
31	c	1	Total	C	O	0	0
			48	38	10		

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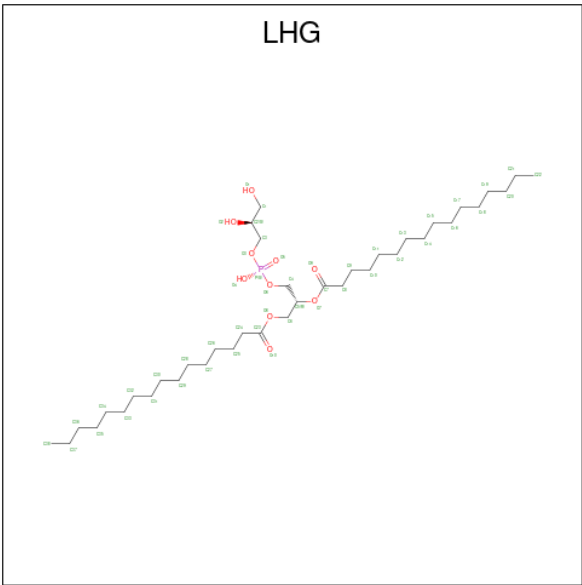
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	d	1	Total	C	O	0	0
			44	34	10		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



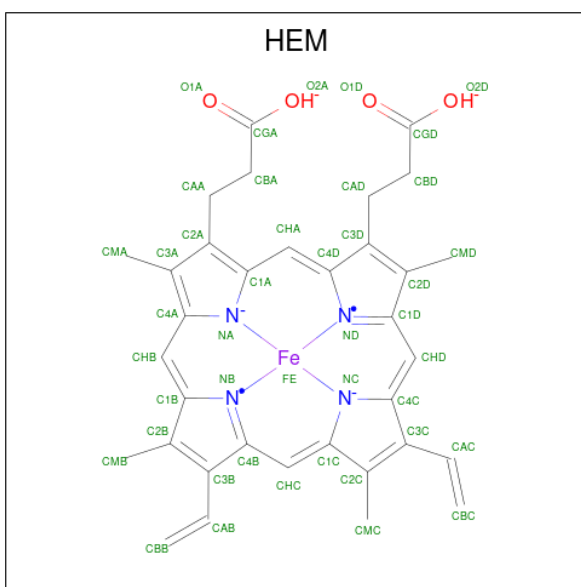
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			4	1	3		
32	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



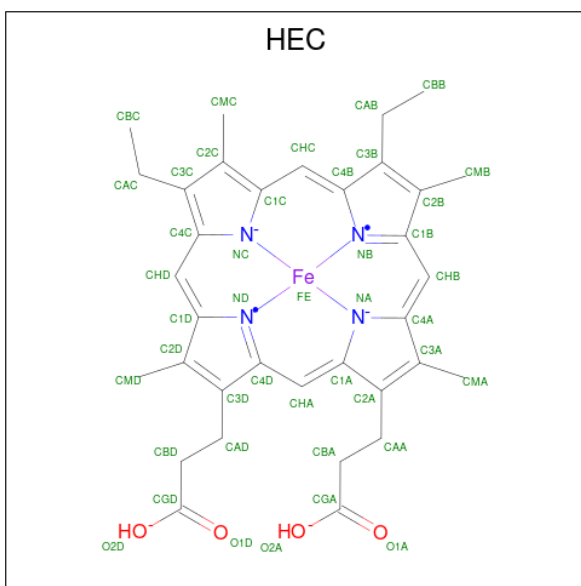
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			47	36	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	E	1	Total	C	O	P	0	0
			49	38	10	1		
33	L	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			39	28	10	1		
33	d	1	Total	C	O	P	0	0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

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



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	145	Total O 145 145	0	0
36	B	247	Total O 247 247	0	0
36	C	192	Total O 192 192	0	0
36	D	144	Total O 144 144	0	0
36	E	27	Total O 27 27	0	0
36	F	9	Total O 9 9	0	0
36	H	35	Total O 35 35	0	0
36	I	14	Total O 14 14	0	0
36	J	12	Total O 12 12	0	0
36	K	3	Total O 3 3	0	0
36	L	14	Total O 14 14	0	0
36	M	8	Total O 8 8	0	0
36	O	111	Total O 111 111	0	0
36	T	8	Total O 8 8	0	0
36	U	60	Total O 60 60	0	0
36	V	80	Total O 80 80	0	0
36	Y	3	Total O 3 3	0	0
36	X	10	Total O 10 10	0	0
36	Z	8	Total O 8 8	0	0
36	R	1	Total O 1 1	0	0
36	a	120	Total O 120 120	0	0

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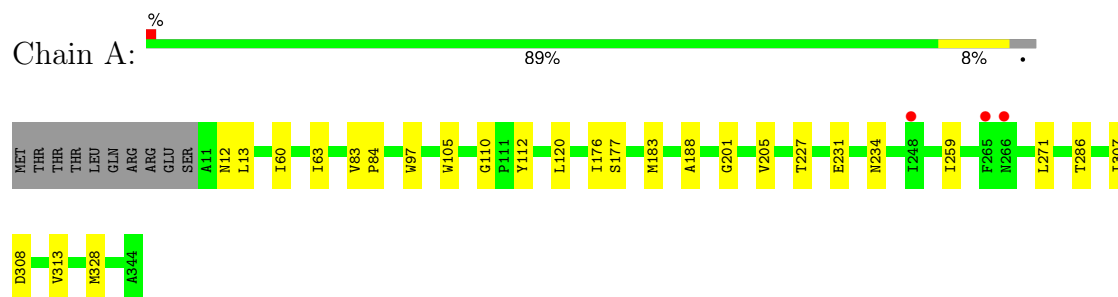
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	b	231	Total 231	O 231	0	0
36	c	178	Total 178	O 178	0	0
36	d	145	Total 145	O 145	0	0
36	e	19	Total 19	O 19	0	0
36	f	10	Total 10	O 10	0	0
36	h	20	Total 20	O 20	0	0
36	i	8	Total 8	O 8	0	0
36	j	9	Total 9	O 9	0	0
36	k	5	Total 5	O 5	0	0
36	l	18	Total 18	O 18	0	0
36	m	10	Total 10	O 10	0	0
36	o	131	Total 131	O 131	0	0
36	t	8	Total 8	O 8	0	0
36	u	62	Total 62	O 62	0	0
36	v	56	Total 56	O 56	0	0
36	y	3	Total 3	O 3	0	0
36	x	5	Total 5	O 5	0	0
36	z	7	Total 7	O 7	0	0

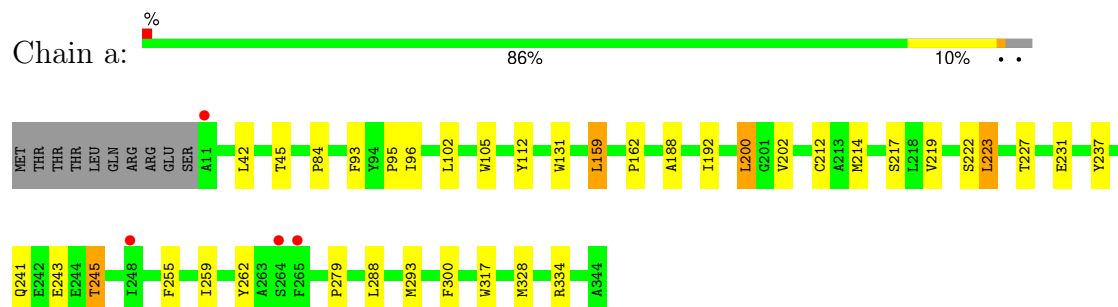
3 Residue-property plots [i](#)

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

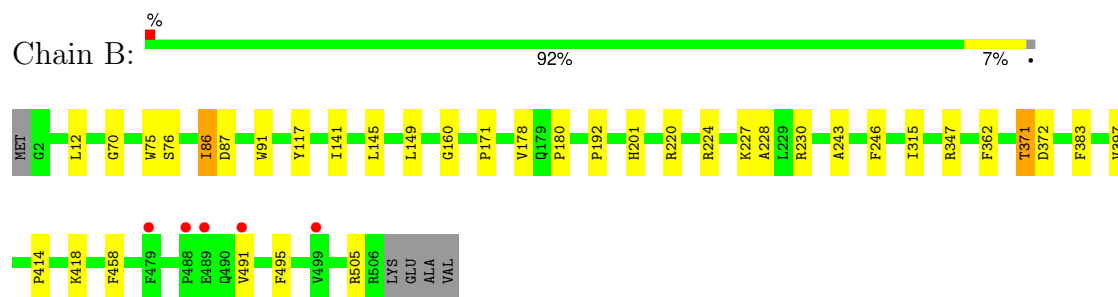
- Molecule 1: Photosystem II protein D1 1



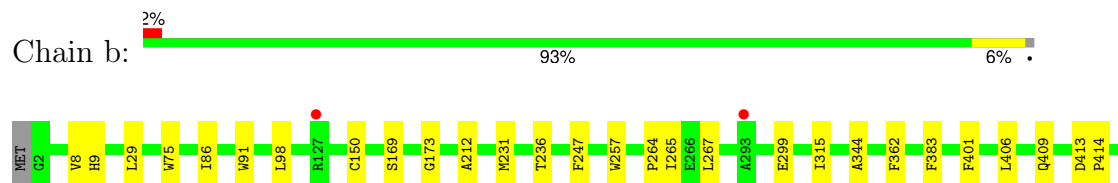
- Molecule 1: Photosystem II protein D1 1

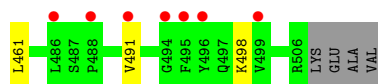


- Molecule 2: Photosystem II CP47 reaction center protein



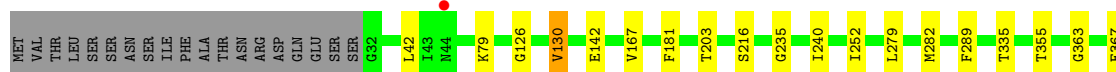
- Molecule 2: Photosystem II CP47 reaction center protein





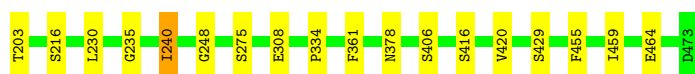
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 90% 5% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 8% .



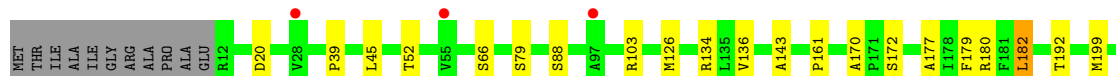
- Molecule 4: Photosystem II D2 protein

Chain D: 87% 10% .



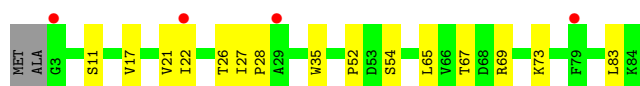
- Molecule 4: Photosystem II D2 protein

Chain d: 86% 10% . .

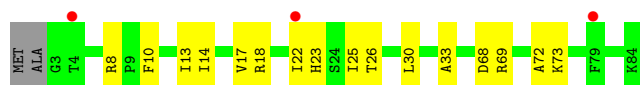
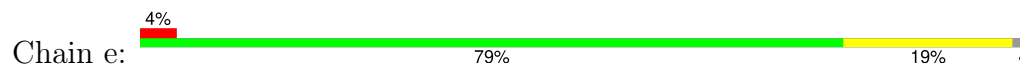


- Molecule 5: Cytochrome b559 subunit alpha

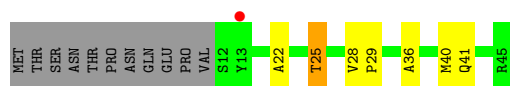
Chain E: 5% 80% 18% .



- Molecule 5: Cytochrome b559 subunit alpha



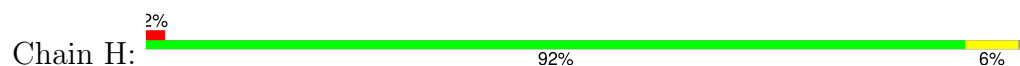
- Molecule 6: Cytochrome b559 subunit beta



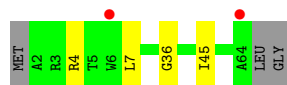
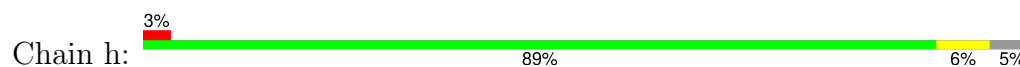
- Molecule 6: Cytochrome b559 subunit beta



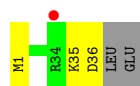
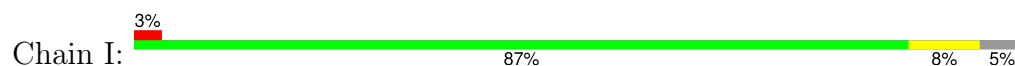
- Molecule 7: Photosystem II reaction center protein H



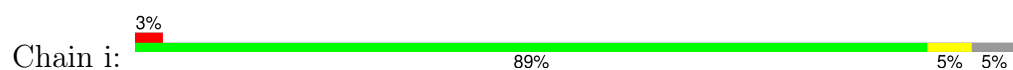
- Molecule 7: Photosystem II reaction center protein H



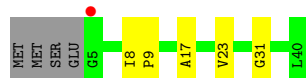
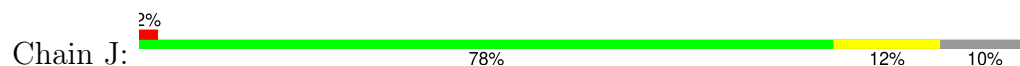
- Molecule 8: Photosystem II reaction center protein I



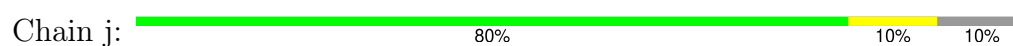
- Molecule 8: Photosystem II reaction center protein I



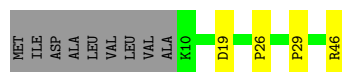
- Molecule 9: Photosystem II reaction center protein J



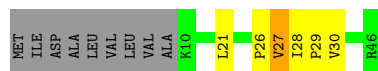
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



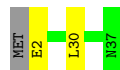
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  81% 8% 8%



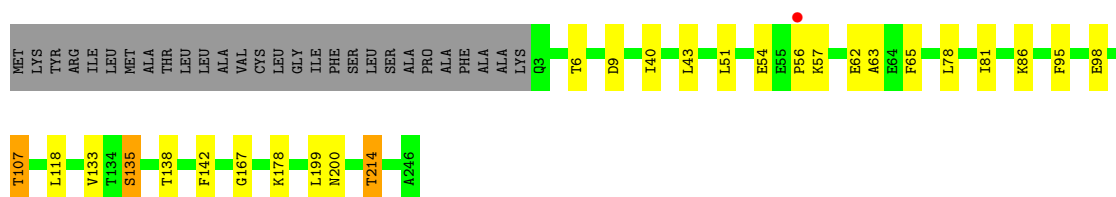
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 14% 11%



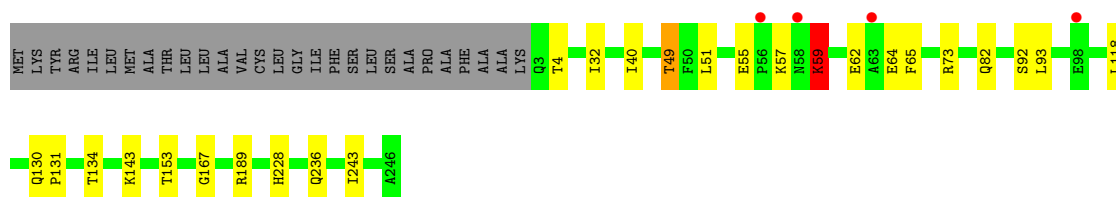
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  80% 9% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  80% 9% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 78% 12% 6%

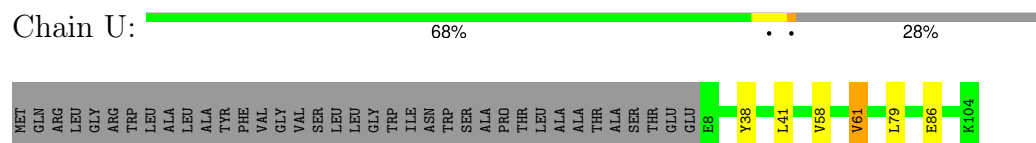


- Molecule 14: Photosystem II reaction center protein T

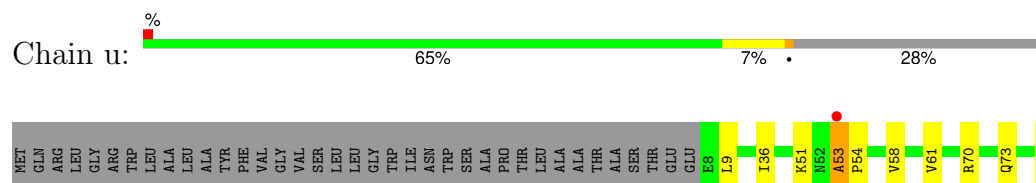
Chain t:  6% 88% 6% 6%



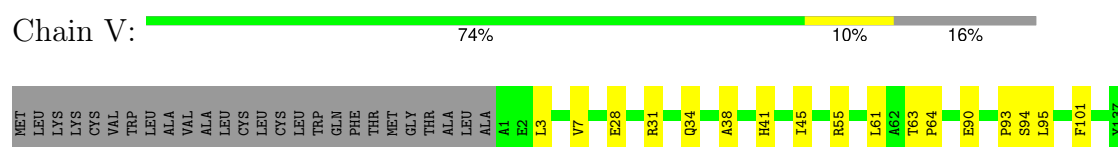
- Molecule 15: Photosystem II 12 kDa extrinsic protein



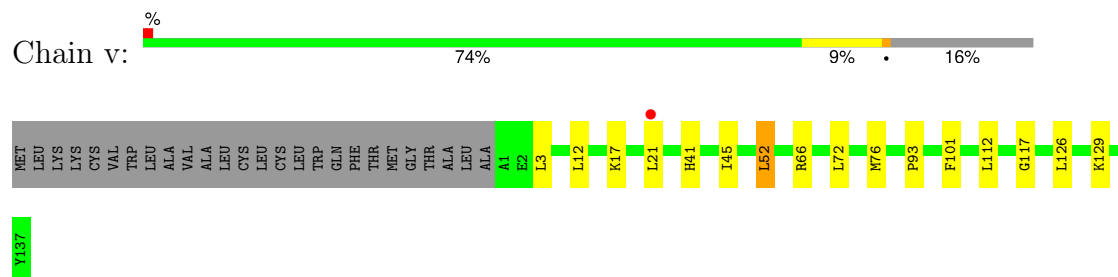
- Molecule 15: Photosystem II 12 kDa extrinsic protein



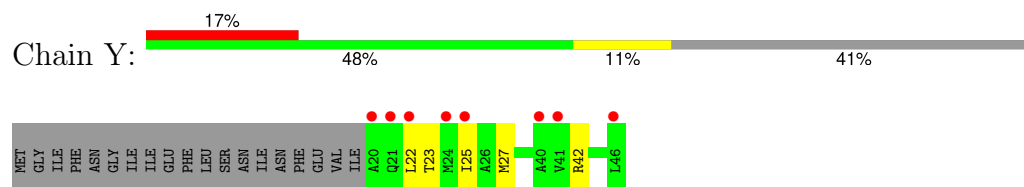
- Molecule 16: Cytochrome c-550



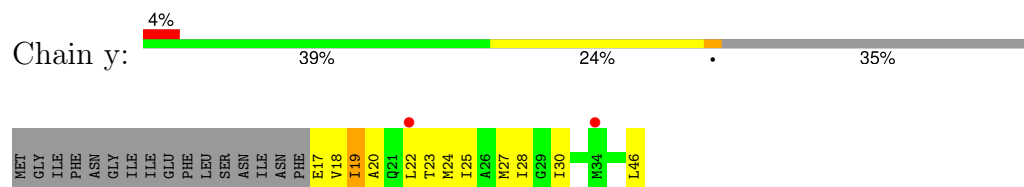
- Molecule 16: Cytochrome c-550



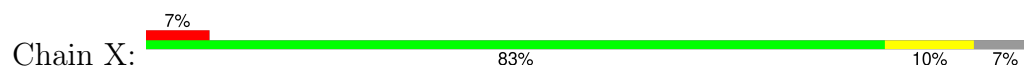
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

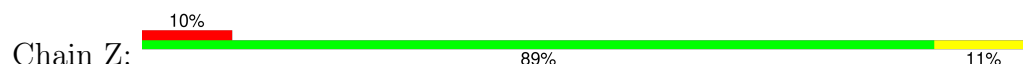




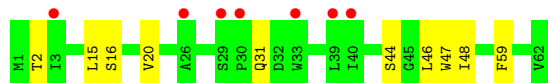
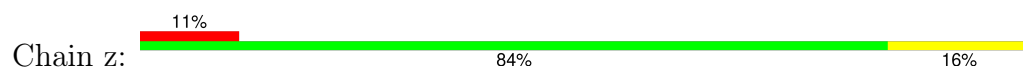
- Molecule 18: Photosystem II reaction center X protein



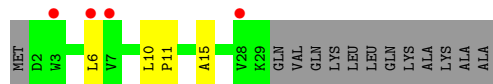
- Molecule 19: Photosystem II reaction center protein Z



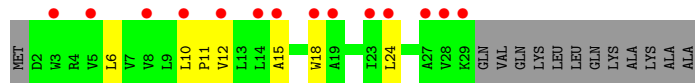
- Molecule 19: Photosystem II reaction center protein Z



- 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	117.48Å 222.57Å 308.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.14 – 1.97 35.14 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.14-1.97) 82.7 (35.14-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.26 (at 1.97Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.194 , 0.230 0.194 , 0.230	Depositor DCC
R_{free} test set	5025 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52714	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: PHO, FME, LMG, DGD, SQD, FE2, STE, HEM, CLA, BCR, BCT, OEX, LHG, CL, HEC, PL9

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	0.37	0/2707	0.52	0/3692
1	a	0.34	0/2704	0.51	0/3688
2	B	0.32	0/4166	0.47	0/5675
2	b	0.30	0/4127	0.46	0/5623
3	C	0.32	0/3539	0.46	0/4819
3	c	0.29	0/3619	0.45	0/4926
4	D	0.34	0/2812	0.50	0/3832
4	d	0.32	0/2821	0.48	0/3844
5	E	0.24	0/688	0.42	0/940
5	e	0.22	0/683	0.39	0/932
6	F	0.23	0/284	0.37	0/387
6	f	0.22	0/284	0.46	0/387
7	H	0.29	0/517	0.43	0/705
7	h	0.26	0/505	0.42	0/689
8	I	0.27	0/293	0.42	0/396
8	i	0.32	0/293	0.38	0/396
9	J	0.27	0/263	0.42	0/356
9	j	0.22	0/263	0.37	0/356
10	K	0.27	0/303	0.40	0/416
10	k	0.24	0/303	0.36	0/416
11	L	0.35	0/311	0.44	0/422
11	l	0.29	0/303	0.42	0/412
12	M	0.31	0/249	0.49	0/341
12	m	0.29	0/244	0.48	0/334
13	O	0.29	0/1904	0.51	0/2585
13	o	0.29	0/1905	0.51	0/2583
14	T	0.36	0/257	0.49	0/349
14	t	0.28	0/255	0.41	0/346
15	U	0.28	0/785	0.43	0/1064
15	u	0.28	0/785	0.47	0/1064
16	V	0.30	0/1085	0.53	0/1473
16	v	0.25	0/1085	0.40	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.20	0/197	0.31	0/264
17	y	0.18	0/219	0.33	0/294
18	X	0.23	0/284	0.35	0/384
18	x	0.20	0/289	0.32	0/391
19	Z	0.21	0/490	0.40	0/669
19	z	0.18	0/488	0.36	0/666
20	R	0.19	0/227	0.35	0/313
20	r	0.18	0/227	0.31	0/313
All	All	0.30	0/42763	0.46	0/58215

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	0	2519	16	0
1	a	2619	0	2510	27	0
2	B	4016	0	3883	30	0
2	b	3984	0	3842	25	0
3	C	3426	0	3353	14	0
3	c	3500	0	3426	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2717	0	2621	26	0
4	d	2723	0	2627	29	0
5	E	666	0	651	10	0
5	e	664	0	648	16	0
6	F	275	0	282	5	0
6	f	275	0	282	9	0
7	H	505	0	528	4	0
7	h	493	0	514	3	0
8	I	296	0	311	2	0
8	i	296	0	311	2	0
9	J	257	0	268	4	0
9	j	257	0	268	4	0
10	K	293	0	305	1	0
10	k	293	0	305	4	0
11	L	304	0	316	3	0
11	l	296	0	304	0	0
12	M	256	0	269	4	0
12	m	251	0	267	4	0
13	O	1870	0	1830	16	0
13	o	1874	0	1846	15	0
14	T	258	0	261	4	0
14	t	256	0	256	1	0
15	U	774	0	773	4	0
15	u	774	0	773	6	0
16	V	1064	0	1073	10	0
16	v	1064	0	1073	10	0
17	Y	196	0	217	3	0
17	y	218	0	241	8	0
18	X	281	0	312	3	0
18	x	286	0	314	1	0
19	Z	479	0	516	5	0
19	z	477	0	509	7	0
20	R	221	0	238	2	0
20	r	221	0	238	5	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	184	0	192	7	0
24	B	1035	0	1139	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	839	0	922	14	0
24	D	195	0	216	6	0
24	a	260	0	288	7	0
24	b	1035	0	1139	26	0
24	c	839	0	919	30	0
24	d	130	0	144	3	0
25	A	128	0	148	1	0
25	a	64	0	74	0	0
25	d	64	0	74	2	0
26	A	40	0	56	0	0
26	B	120	0	168	3	0
26	C	120	0	168	3	0
26	D	40	0	56	1	0
26	H	40	0	56	2	0
26	K	40	0	56	1	0
26	T	40	0	56	2	0
26	a	40	0	56	1	0
26	b	120	0	168	2	0
26	c	80	0	112	3	0
26	d	40	0	56	1	0
26	h	40	0	56	2	0
26	k	80	0	112	3	0
26	t	40	0	56	3	0
27	A	55	0	80	5	0
27	D	55	0	80	0	0
27	a	55	0	80	6	0
27	d	55	0	80	2	0
28	A	45	0	83	4	0
28	B	76	0	116	3	0
28	C	78	0	126	3	0
28	D	20	0	35	1	0
28	E	44	0	74	2	0
28	H	27	0	52	3	0
28	I	32	0	48	2	0
28	J	12	0	16	0	0
28	K	14	0	27	1	0
28	M	40	0	67	1	0
28	Z	17	0	33	1	0
28	a	12	0	16	0	0
28	b	73	0	127	5	0
28	c	31	0	57	3	0
28	d	84	0	144	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	e	39	0	67	1	0
28	i	18	0	24	4	0
28	j	28	0	47	1	0
28	m	30	0	51	0	0
28	t	10	0	16	0	0
28	z	9	0	14	1	0
29	A	95	0	124	3	0
29	B	54	0	78	2	0
29	D	36	0	46	0	0
29	a	108	0	156	4	0
29	b	49	0	65	2	0
29	f	41	0	49	3	0
30	A	66	0	96	4	0
30	C	186	0	246	4	0
30	H	62	0	82	1	0
30	c	186	0	246	4	0
30	h	62	0	82	0	0
31	B	96	0	132	5	0
31	C	132	0	172	4	0
31	D	101	0	142	10	0
31	a	104	0	154	6	0
31	b	106	0	158	4	0
31	c	124	0	172	5	0
31	d	44	0	58	0	0
32	D	4	0	1	0	0
32	d	4	0	1	0	0
33	D	145	0	215	11	0
33	E	49	0	74	4	0
33	L	49	0	74	1	0
33	a	39	0	51	2	0
33	d	98	0	148	2	0
33	e	42	0	57	1	0
33	l	49	0	74	2	0
34	F	43	0	30	2	0
34	e	43	0	30	4	0
35	V	43	0	30	0	0
35	v	43	0	30	1	0
36	A	145	0	0	3	0
36	B	247	0	0	4	0
36	C	192	0	0	3	0
36	D	144	0	0	5	0
36	E	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	F	9	0	0	0	0
36	H	35	0	0	0	0
36	I	14	0	0	0	0
36	J	12	0	0	2	0
36	K	3	0	0	0	0
36	L	14	0	0	0	0
36	M	8	0	0	0	0
36	O	111	0	0	4	0
36	R	1	0	0	0	0
36	T	8	0	0	0	0
36	U	60	0	0	1	0
36	V	80	0	0	5	0
36	X	10	0	0	0	0
36	Y	3	0	0	1	0
36	Z	8	0	0	1	0
36	a	120	0	0	1	0
36	b	231	0	0	8	0
36	c	178	0	0	8	0
36	d	145	0	0	1	0
36	e	19	0	0	0	0
36	f	10	0	0	1	0
36	h	20	0	0	0	0
36	i	8	0	0	2	0
36	j	9	0	0	0	0
36	k	5	0	0	0	0
36	l	18	0	0	0	0
36	m	10	0	0	0	0
36	o	131	0	0	2	0
36	t	8	0	0	0	0
36	u	62	0	0	0	0
36	v	56	0	0	0	0
36	x	5	0	0	0	0
36	y	3	0	0	0	0
36	z	7	0	0	2	0
All	All	52714	0	52200	500	0

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

All (500) 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)
24:b:615:CLA:H72	24:b:616:CLA:HBB1	1.53	0.90
24:C:513:CLA:H202	28:C:528:STE:H172	1.62	0.82
28:A:617:STE:H162	28:A:618:STE:H122	1.61	0.82
31:c:518:LMG:H122	31:c:518:LMG:H302	1.64	0.79
13:O:200:ASN:HD22	13:O:214:THR:HG22	1.52	0.75
24:C:502:CLA:H61	24:C:512:CLA:H42	1.69	0.75
1:A:176:ILE:O	36:A:701:HOH:O	2.05	0.74
24:a:608:CLA:H111	24:a:608:CLA:H52	1.71	0.73
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.71	0.72
4:D:181:PHE:O	36:D:501:HOH:O	2.08	0.72
13:O:56:PRO:HD3	13:O:63:ALA:HB2	1.71	0.72
24:c:501:CLA:H192	24:c:507:CLA:HBB1	1.71	0.71
2:b:91:TRP:HE1	28:b:623:STE:H32	1.55	0.70
34:F:101:HEM:HBC2	34:F:101:HEM:HHH	1.74	0.70
3:c:180:MET:HE1	31:c:523:LMG:HC72	1.75	0.69
30:A:615:DGD:HBE1	28:I:102:STE:H121	1.76	0.68
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.75	0.67
3:c:118:HIS:HA	36:c:630:HOH:O	1.94	0.67
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.78	0.66
24:B:604:CLA:H43	24:B:605:CLA:H2	1.78	0.66
30:A:615:DGD:HD5	2:b:75:TRP:HB3	1.78	0.66
3:c:378:ASN:HD21	13:o:82:GLN:HE22	1.41	0.65
4:D:184:PHE:HB3	36:D:501:HOH:O	1.95	0.64
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.62	0.64
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.79	0.64
2:B:371:THR:HG23	2:B:372:ASP:O	1.97	0.64
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.79	0.64
5:e:30:LEU:HD23	20:r:12:VAL:HG12	1.81	0.63
26:B:617:BCR:H383	29:B:623:SQD:H112	1.80	0.62
2:B:227:LYS:HE3	31:B:620:LMG:O3	1.99	0.62
28:M:103:STE:H81	28:b:621:STE:H71	1.80	0.62
2:b:406:LEU:HB2	36:b:701:HOH:O	1.99	0.62
24:c:503:CLA:H203	24:c:510:CLA:HAB	1.82	0.62
36:B:713:HOH:O	11:L:2:GLU:HG2	1.98	0.62
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.82	0.61
3:c:170:ILE:HD11	31:c:523:LMG:H381	1.81	0.61
31:C:522:LMG:H381	30:C:523:DGD:HB52	1.82	0.61
34:e:102:HEM:HHH	34:e:102:HEM:HBC2	1.82	0.61
24:A:606:CLA:H152	27:A:611:PL9:H23	1.83	0.61
33:D:411:LHG:H341	33:D:411:LHG:H142	1.82	0.61
27:d:406:PL9:H201	33:l:101:LHG:H202	1.82	0.61
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:ALA:HB2	31:D:407:LMG:H322	1.83	0.60
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.83	0.60
29:A:613:SQD:H131	33:D:411:LHG:H172	1.84	0.60
24:c:501:CLA:C3D	24:c:503:CLA:H2	2.31	0.60
34:e:102:HEM:HHC	34:e:102:HEM:HBB2	1.83	0.60
4:D:181:PHE:C	36:D:501:HOH:O	2.44	0.59
26:D:405:BCR:H23C	26:D:405:BCR:H392	1.84	0.59
27:A:611:PL9:H361	6:F:25:THR:HG21	1.85	0.59
5:e:17:VAL:H	9:j:7:ARG:HD2	1.68	0.59
24:b:603:CLA:H2	24:b:605:CLA:H91	1.85	0.59
24:C:507:CLA:H192	28:C:529:STE:H82	1.85	0.58
31:D:407:LMG:H301	31:D:407:LMG:H112	1.84	0.58
18:X:25:PHE:O	18:X:29:ILE:HG12	2.04	0.58
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.85	0.58
6:F:22:ALA:O	6:F:25:THR:HG22	2.03	0.58
24:D:402:CLA:HHC	24:D:402:CLA:HBB1	1.85	0.57
26:C:521:BCR:HC8	26:C:521:BCR:H321	1.85	0.57
5:e:18:ARG:HH12	6:f:15:ILE:HD12	1.69	0.57
26:T:101:BCR:H311	26:T:101:BCR:HC8	1.85	0.57
1:a:214:MET:HE1	1:a:255:PHE:CE1	2.40	0.57
16:V:55:ARG:HD3	36:V:333:HOH:O	2.04	0.57
2:b:212:ALA:HA	36:b:911:HOH:O	2.04	0.57
26:d:405:BCR:H403	26:d:405:BCR:H23C	1.85	0.57
1:a:84:PRO:HA	1:a:112:TYR:CG	2.40	0.56
28:b:627:STE:H171	28:d:410:STE:H61	1.86	0.56
2:b:98:LEU:HD11	24:b:606:CLA:H152	1.87	0.56
2:B:149[A]:LEU:HD21	24:B:606:CLA:HBB2	1.86	0.56
1:a:300:PHE:HZ	30:c:521:DGD:HB61	1.71	0.56
33:E:101:LHG:H271	33:E:101:LHG:H322	1.88	0.56
5:E:35:TRP:HE1	28:E:104:STE:H141	1.71	0.56
17:y:19:ILE:O	17:y:23:THR:HG22	2.06	0.56
5:e:68:ASP:O	5:e:72:ALA:HB2	2.06	0.56
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.88	0.56
3:c:406:SER:HA	3:c:420:VAL:HG23	1.87	0.55
33:D:410:LHG:H321	14:T:21:ILE:HD11	1.89	0.55
2:b:264:PRO:HG2	2:b:267:LEU:HD22	1.89	0.55
2:B:227:LYS:HD3	31:D:407:LMG:H302	1.88	0.55
15:U:58:VAL:O	15:U:61:VAL:HG22	2.07	0.55
4:d:192:THR:HG23	24:d:403:CLA:HBC2	1.88	0.55
6:f:18:VAL:HG22	29:f:101:SQD:H272	1.88	0.55
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:745:HOH:O	13:O:107:THR:HG21	2.07	0.55
27:a:610:PL9:H48	4:d:39:PRO:HG3	1.89	0.55
2:B:91:TRP:HE1	28:B:622:STE:H32	1.72	0.55
26:H:101:BCR:HC8	26:H:101:BCR:H331	1.88	0.55
26:T:101:BCR:H382	26:T:101:BCR:H23C	1.88	0.55
2:B:495:PHE:HD2	2:B:505:ARG:HH12	1.55	0.54
24:b:610:CLA:HBB1	26:h:101:BCR:HC21	1.88	0.54
24:b:609:CLA:H2	36:b:752:HOH:O	2.06	0.54
26:t:101:BCR:HC8	26:t:101:BCR:H311	1.89	0.54
24:C:513:CLA:HBA2	28:C:518:STE:H42	1.89	0.54
28:D:413:STE:H102	18:X:16:SER:HB3	1.90	0.54
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.90	0.54
3:c:42:LEU:HD21	24:c:511:CLA:H2A	1.90	0.54
17:y:17:GLU:HB3	17:y:19:ILE:HG22	1.89	0.54
24:b:615:CLA:H2	24:b:616:CLA:HBB2	1.89	0.53
33:D:411:LHG:H171	33:D:411:LHG:H322	1.90	0.53
28:i:102:STE:H112	36:i:208:HOH:O	2.08	0.53
16:V:90:GLU:HG2	36:V:351:HOH:O	2.08	0.53
24:c:509:CLA:HMA1	36:c:641:HOH:O	2.08	0.53
3:C:406:SER:HA	3:C:420:VAL:HG23	1.89	0.53
4:d:279:LEU:HD22	25:d:402:PHO:HBC3	1.90	0.53
13:o:57:LYS:HE2	36:o:340:HOH:O	2.08	0.53
24:B:615:CLA:H162	7:H:7:LEU:HD21	1.90	0.53
1:a:217:SER:HA	4:d:272:LEU:HD12	1.91	0.53
3:c:166:ILE:HG21	24:c:512:CLA:H202	1.91	0.53
4:D:32:TRP:CD1	31:D:407:LMG:H171	2.44	0.53
1:A:177:SER:C	36:A:701:HOH:O	2.51	0.52
15:U:86:GLU:HG3	36:U:248:HOH:O	2.08	0.52
24:c:513:CLA:HBA2	28:c:516:STE:H121	1.92	0.52
3:c:45:LEU:HA	3:c:139:THR:HG22	1.92	0.52
4:d:134:ARG:HG2	28:d:407:STE:H41	1.92	0.52
10:k:27:VAL:O	10:k:30:VAL:HG22	2.08	0.52
9:J:17:ALA:HB3	36:J:208:HOH:O	2.09	0.52
2:B:117:TYR:HA	11:L:1:MET:HE1	1.92	0.52
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.91	0.52
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.92	0.51
3:c:94:THR:HB	36:c:601:HOH:O	2.10	0.51
2:B:230:ARG:NH2	31:B:620:LMG:HC5	2.25	0.51
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.45	0.51
4:D:283:ALA:HA	36:D:502:HOH:O	2.11	0.51
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.92	0.51
24:b:601:CLA:H42	36:b:727:HOH:O	2.11	0.51
12:m:17:VAL:HB	12:m:18:PRO:HD3	1.93	0.51
19:Z:47:TRP:CD2	28:Z:101:STE:H171	2.45	0.51
1:A:63:ILE:HB	3:C:335:THR:HG21	1.92	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.46	0.51
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.93	0.51
5:e:33:ALA:HB2	20:r:11:PRO:HG2	1.91	0.51
3:C:79:LYS:HD3	36:C:618:HOH:O	2.09	0.51
3:c:121:SER:HB3	26:c:514:BCR:H16C	1.92	0.51
5:e:26:THR:HA	20:r:15:ALA:HB1	1.93	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.50
24:b:615:CLA:H112	24:b:616:CLA:H102	1.92	0.50
16:V:94:SER:HB2	36:V:301:HOH:O	2.11	0.50
17:Y:42:ARG:HB3	36:Y:102:HOH:O	2.11	0.50
24:B:607:CLA:H91	24:B:613:CLA:H202	1.92	0.50
2:B:86:ILE:HG12	2:B:87:ASP:N	2.26	0.50
2:B:224:ARG:HD3	31:D:407:LMG:H292	1.93	0.50
1:A:97:TRP:HA	8:I:1:FME:HG2	1.94	0.50
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.50
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.94	0.50
16:v:12:LEU:HD23	16:v:17:LYS:HD3	1.93	0.50
19:z:46:LEU:HB3	36:z:201:HOH:O	2.12	0.50
28:A:618:STE:H112	28:A:618:STE:H183	1.92	0.49
4:d:79:SER:HA	4:d:172:SER:HB3	1.93	0.49
4:d:199:MET:HG2	27:d:406:PL9:H321	1.94	0.49
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.94	0.49
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.12	0.49
2:b:498:LYS:HD2	4:d:20:ASP:HA	1.93	0.49
3:c:429:SER:HB3	30:c:520:DGD:HBT2	1.93	0.49
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.95	0.49
16:V:28:GLU:CD	16:V:31:ARG:HH12	2.20	0.49
24:b:602:CLA:H43	7:h:45:ILE:HG22	1.95	0.49
8:i:3:THR:HG23	28:i:101:STE:H62	1.94	0.49
5:E:26:THR:HA	20:R:15:ALA:HB1	1.94	0.49
13:o:228:HIS:HD2	36:o:301:HOH:O	1.95	0.49
3:C:181:PHE:HE2	31:C:517:LMG:H292	1.77	0.49
1:a:212:CYS:HB2	4:d:211:CYS:HB2	1.94	0.49
17:y:20:ALA:O	17:y:24:MET:HG2	2.13	0.49
27:A:611:PL9:H271	33:E:101:LHG:H202	1.95	0.49
1:a:227:THR:HB	1:a:231:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:412:STE:H121	18:x:16:SER:HB3	1.94	0.49
4:d:241:GLU:CD	4:d:241:GLU:H	2.19	0.48
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.47	0.48
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.95	0.48
1:A:227:THR:HB	1:A:231:GLU:HG3	1.95	0.48
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.95	0.48
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.95	0.48
3:C:252:ILE:HB	36:C:652:HOH:O	2.13	0.48
24:c:506:CLA:H13	24:c:506:CLA:H102	1.57	0.48
26:b:617:BCR:H322	31:b:622:LMG:H111	1.94	0.48
26:C:521:BCR:HC32	26:K:101:BCR:H343	1.95	0.48
4:D:152:VAL:HG22	24:D:403:CLA:HED1	1.94	0.48
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.95	0.48
24:c:508:CLA:H92	24:c:510:CLA:H52	1.94	0.48
24:B:615:CLA:H2	24:B:616:CLA:HBB2	1.96	0.48
3:C:429:SER:HB3	30:C:524:DGD:HBT1	1.96	0.48
4:D:282:SER:OG	24:D:403:CLA:HED2	2.13	0.48
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.49	0.48
36:c:732:HOH:O	4:d:230:SER:HB2	2.14	0.48
25:d:402:PHO:H3A	24:d:403:CLA:H142	1.96	0.48
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.96	0.48
2:B:12:LEU:HB2	24:B:612:CLA:HMC2	1.96	0.48
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.48	0.47
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.96	0.47
24:B:610:CLA:HHC	24:B:610:CLA:HBB1	1.96	0.47
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.47
4:D:194:ASN:HA	4:D:295:SER:OG	2.15	0.47
5:E:17:VAL:O	5:E:21:VAL:HG23	2.14	0.47
31:c:518:LMG:H292	31:c:518:LMG:HC92	1.49	0.47
29:B:623:SQD:H342	29:B:623:SQD:H152	1.95	0.47
2:b:257:TRP:CE2	4:d:291:LEU:HD12	2.50	0.47
4:d:267:LEU:C	4:d:267:LEU:HD23	2.39	0.47
20:r:6:LEU:O	20:r:10:LEU:HG	2.14	0.47
24:a:608:CLA:H61	24:a:608:CLA:H41	1.77	0.47
3:c:91:HIS:C	36:c:601:HOH:O	2.58	0.47
36:C:721:HOH:O	28:K:102:STE:H71	2.14	0.47
31:D:407:LMG:H352	31:D:407:LMG:H162	1.95	0.47
5:E:65:LEU:O	5:E:67:THR:HG23	2.15	0.47
28:I:102:STE:H22	24:b:606:CLA:H192	1.96	0.47
1:a:200:LEU:HD21	30:c:521:DGD:HBH1	1.96	0.47
2:b:98:LEU:HB2	36:b:925:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:524:DGD:HB32	30:C:524:DGD:HB61	1.72	0.47
10:K:26:PRO:O	10:K:29:PRO:HD2	2.15	0.47
15:u:70:ARG:HH11	15:u:73:GLN:HE21	1.62	0.47
2:B:149[B]:LEU:HD11	24:B:604:CLA:H162	1.95	0.47
2:B:171:PRO:HA	7:H:65:LEU:HD12	1.96	0.47
1:a:131:TRP:CH2	24:c:505:CLA:HAA2	2.50	0.47
2:B:458:PHE:HB3	24:B:604:CLA:HBC2	1.97	0.46
24:B:613:CLA:H143	24:B:613:CLA:H111	1.81	0.46
29:a:613:SQD:H122	29:a:613:SQD:H152	1.56	0.46
28:c:517:STE:H121	19:z:59:PHE:HE1	1.80	0.46
25:A:608:PHO:HBC2	25:A:608:PHO:HHD	1.96	0.46
29:f:101:SQD:H341	29:f:101:SQD:H371	1.61	0.46
2:b:231:MET:HE2	24:b:610:CLA:HMC2	1.96	0.46
2:b:247:PHE:HE1	24:b:602:CLA:H102	1.79	0.46
13:o:143:LYS:HB2	13:o:143:LYS:HE2	1.60	0.46
28:B:627:STE:H121	28:B:627:STE:H92	1.45	0.46
4:D:269:PHE:CG	33:D:412:LHG:HC12	2.49	0.46
6:F:36:ALA:O	6:F:40:MET:HG3	2.16	0.46
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.98	0.46
3:c:121:SER:HB2	36:c:630:HOH:O	2.14	0.46
19:z:47:TRP:CD2	28:z:101:STE:H71	2.50	0.46
24:B:601:CLA:C3	28:H:103:STE:H162	2.45	0.46
24:C:509:CLA:H93	24:C:509:CLA:H112	1.73	0.46
24:c:511:CLA:H171	19:z:20:VAL:HA	1.98	0.46
24:c:504:CLA:H92	24:c:504:CLA:H62	1.77	0.46
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.97	0.46
2:B:414:PRO:O	2:B:418:LYS:HG3	2.15	0.46
19:Z:44:SER:O	19:Z:48:ILE:HG13	2.16	0.46
33:a:612:LHG:H242	33:a:612:LHG:H272	1.60	0.46
24:B:601:CLA:H51	28:H:103:STE:H183	1.98	0.46
24:B:606:CLA:H93	24:B:606:CLA:H112	1.68	0.46
2:b:299:GLU:HG3	36:b:891:HOH:O	2.15	0.46
28:d:414:STE:H42	28:d:414:STE:H72	1.70	0.46
13:o:40:ILE:HD13	13:o:243:ILE:HG12	1.97	0.46
24:b:609:CLA:HBC3	36:b:911:HOH:O	2.16	0.45
24:c:509:CLA:HHB	36:c:641:HOH:O	2.15	0.45
13:o:130:GLN:H	13:o:130:GLN:NE2	2.14	0.45
5:e:23:HIS:HA	5:e:26:THR:OG1	2.16	0.45
17:y:46:LEU:HD23	17:y:46:LEU:HA	1.77	0.45
28:A:618:STE:H151	28:A:618:STE:H121	1.63	0.45
24:c:504:CLA:H91	24:c:508:CLA:H171	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:409:GLN:HE21	2:b:409:GLN:HB3	1.60	0.45
24:b:613:CLA:H13	31:b:622:LMG:H241	1.98	0.45
4:d:126:MET:HE3	4:d:143:ALA:O	2.15	0.45
1:A:183:MET:HA	24:A:605:CLA:HMD1	1.99	0.45
2:B:141:ILE:O	2:B:145:LEU:HG	2.15	0.45
24:B:614:CLA:H171	31:B:621:LMG:H421	1.97	0.45
24:c:509:CLA:H161	24:c:509:CLA:H141	1.81	0.45
14:T:1:FME:HCN	28:b:621:STE:H102	1.98	0.45
6:f:36:ALA:O	6:f:40:MET:HG3	2.17	0.45
28:j:102:STE:H41	28:j:102:STE:H71	1.72	0.45
2:B:230:ARG:HH22	31:B:620:LMG:HC5	1.81	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.17	0.45
1:a:214:MET:HB3	1:a:214:MET:HE3	1.56	0.45
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.52	0.45
24:B:601:CLA:H152	24:B:601:CLA:H111	1.69	0.45
30:H:102:DGD:HB21	30:H:102:DGD:HB51	1.80	0.45
24:b:611:CLA:H72	24:b:611:CLA:H112	1.70	0.45
16:v:41:HIS:HA	16:v:45:ILE:O	2.17	0.45
2:B:86:ILE:HD12	36:B:778:HOH:O	2.17	0.45
33:l:101:LHG:H271	12:m:22:LEU:HD21	1.97	0.45
24:B:614:CLA:H13	24:B:614:CLA:H172	1.38	0.44
36:B:816:HOH:O	7:H:45:ILE:HG23	2.18	0.44
24:A:609:CLA:H61	24:A:609:CLA:H41	1.68	0.44
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.99	0.44
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.29	0.44
13:o:59:LYS:H	13:o:59:LYS:HG3	1.53	0.44
24:B:611:CLA:H72	24:B:611:CLA:H112	1.64	0.44
3:C:216:SER:HB2	31:C:522:LMG:HC72	1.99	0.44
31:a:615:LMG:H182	36:i:208:HOH:O	2.17	0.44
2:b:257:TRP:CZ2	4:d:291:LEU:HD12	2.53	0.44
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.81	0.44
3:c:95:LEU:HD21	24:c:501:CLA:OBD	2.17	0.44
24:c:508:CLA:H91	24:c:508:CLA:H111	1.72	0.44
10:k:26:PRO:O	10:k:29:PRO:HD2	2.18	0.44
15:u:51:LYS:HB2	15:u:51:LYS:HE2	1.55	0.44
3:C:363:GLY:O	3:C:367:GLU:HG2	2.17	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.44
24:c:501:CLA:C2D	24:c:503:CLA:H2	2.47	0.44
24:B:613:CLA:H171	26:B:618:BCR:H312	1.98	0.44
13:O:98:GLU:HB3	36:O:401:HOH:O	2.17	0.44
3:c:134:ILE:HD12	24:c:511:CLA:H43	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:413:STE:H102	28:d:413:STE:H131	1.73	0.44
5:e:17:VAL:HB	9:j:7:ARG:HH11	1.83	0.44
5:e:30:LEU:HD11	34:e:102:HEM:HBB2	1.98	0.44
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.99	0.44
16:V:95:LEU:N	36:V:301:HOH:O	2.50	0.44
4:D:23:LYS:HZ1	31:D:407:LMG:H151	1.83	0.44
27:a:610:PL9:H471	29:f:101:SQD:H342	2.00	0.44
24:b:614:CLA:H61	24:b:614:CLA:H93	1.65	0.44
9:j:18:GLY:O	9:j:21:VAL:HG22	2.18	0.44
1:A:271:LEU:HD11	27:A:611:PL9:HC71	2.00	0.44
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.99	0.44
29:a:614:SQD:H1	36:a:765:HOH:O	2.17	0.44
2:B:201:HIS:HB2	24:B:602:CLA:CHB	2.48	0.44
26:H:101:BCR:H331	26:H:101:BCR:C8	2.47	0.44
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.99	0.44
1:a:202:VAL:HG11	24:a:606:CLA:C3D	2.48	0.44
31:a:615:LMG:O8	31:a:615:LMG:C10	2.66	0.44
17:y:27:MET:O	17:y:30:ILE:HG22	2.18	0.44
1:A:307:ILE:HG22	1:A:313:VAL:HA	2.00	0.43
24:B:616:CLA:H11	24:B:616:CLA:H51	1.75	0.43
33:E:101:LHG:HC92	33:E:101:LHG:H121	1.93	0.43
29:a:613:SQD:H292	29:a:613:SQD:H261	1.65	0.43
24:b:612:CLA:H8	24:b:612:CLA:H122	1.75	0.43
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.00	0.43
24:A:605:CLA:HBD	24:D:402:CLA:HAC2	1.99	0.43
24:C:505:CLA:H162	24:C:505:CLA:H193	1.81	0.43
31:D:408:LMG:H161	31:D:408:LMG:H191	1.75	0.43
1:a:334:ARG:HD3	4:d:320:LEU:HD13	2.00	0.43
29:b:620:SQD:H223	29:b:620:SQD:H191	1.74	0.43
30:c:519:DGD:HB51	30:c:519:DGD:HB22	1.93	0.43
10:k:21:LEU:HD21	26:k:101:BCR:HC31	1.99	0.43
14:t:18:PHE:HB2	26:t:101:BCR:HC8	1.99	0.43
15:u:36:ILE:HD13	16:v:52:LEU:HD13	2.01	0.43
28:b:627:STE:H162	28:d:410:STE:H71	1.99	0.43
3:c:455:PHE:HD2	8:i:33:LYS:HG3	1.83	0.43
28:c:517:STE:H172	28:c:517:STE:H141	1.74	0.43
5:e:25:ILE:HD13	20:r:18:TRP:NE1	2.33	0.43
13:o:62:GLU:HG3	13:o:64:GLU:HG3	2.00	0.43
3:C:410:VAL:HG22	3:C:413[B]:GLU:HG2	1.99	0.43
31:C:526:LMG:H332	31:C:526:LMG:H202	2.00	0.43
27:a:610:PL9:H302	4:d:45:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:509:CLA:H3A	24:c:509:CLA:HBA1	1.88	0.43
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.47	0.43
16:v:66:ARG:O	16:v:72:LEU:HG	2.17	0.43
24:D:402:CLA:H162	24:D:402:CLA:H192	1.63	0.43
24:B:607:CLA:H141	24:B:607:CLA:H161	1.69	0.43
16:v:126:LEU:HB3	16:v:129:LYS:HB2	2.00	0.43
24:A:606:CLA:H202	24:A:606:CLA:H161	1.75	0.43
24:a:611:CLA:H152	33:d:409:LHG:H223	2.01	0.43
31:b:624:LMG:HC92	36:b:861:HOH:O	2.17	0.43
6:f:26:LEU:O	6:f:29:PRO:HD2	2.19	0.43
31:D:407:LMG:H131	31:D:407:LMG:HC5	2.01	0.43
29:a:613:SQD:H141	29:a:613:SQD:H172	1.66	0.43
5:E:54:SER:HB2	5:E:83:LEU:HD13	2.00	0.43
19:Z:39:LEU:HD23	19:Z:39:LEU:HA	1.85	0.43
3:c:131:TYR:OH	24:c:513:CLA:HED2	2.19	0.43
4:D:79:SER:HA	4:D:172:SER:HB3	2.00	0.43
7:H:34:PHE:CZ	28:H:103:STE:H51	2.54	0.43
7:h:4:ARG:HE	7:h:4:ARG:HB3	1.66	0.43
28:i:101:STE:H61	28:i:101:STE:H32	1.48	0.43
1:A:201:GLY:HA3	1:A:286:THR:HB	2.01	0.42
13:O:178:LYS:HE3	13:O:178:LYS:HB2	1.42	0.42
1:a:262:TYR:HB3	33:e:103:LHG:C23	2.49	0.42
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.01	0.42
28:d:410:STE:H92	36:d:586:HOH:O	2.19	0.42
19:z:16:SER:O	19:z:20:VAL:HG23	2.19	0.42
27:A:611:PL9:H401	27:A:611:PL9:H422	1.72	0.42
3:C:126:GLY:O	3:C:130:VAL:HG13	2.20	0.42
24:C:504:CLA:H62	24:C:504:CLA:H41	1.88	0.42
24:C:511:CLA:H143	19:Z:20:VAL:HG13	2.01	0.42
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.01	0.42
33:a:612:LHG:H311	33:a:612:LHG:H352	2.00	0.42
5:e:10:PHE:O	5:e:14:ILE:HG12	2.18	0.42
26:k:102:BCR:H20C	26:k:102:BCR:H361	1.93	0.42
1:A:60:ILE:HB	1:A:83:VAL:CG1	2.50	0.42
16:V:41:HIS:HA	16:V:45:ILE:O	2.19	0.42
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.54	0.42
24:b:616:CLA:H91	24:b:616:CLA:H112	1.76	0.42
24:c:508:CLA:H152	24:c:508:CLA:H112	1.76	0.42
24:c:510:CLA:HAA1	36:c:641:HOH:O	2.19	0.42
4:d:103:ARG:HG3	5:e:73:LYS:HG3	2.01	0.42
2:B:75:TRP:HB3	31:a:615:LMG:HC8	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:HIS:HE1	4:D:80:THR:O	2.03	0.42
4:D:131:GLU:O	4:D:135:LEU:HG	2.19	0.42
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.01	0.42
33:L:101:LHG:H311	12:M:21:PHE:CD2	2.54	0.42
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.00	0.42
13:O:54:GLU:HB2	36:O:338:HOH:O	2.19	0.42
13:O:133:VAL:HG12	13:O:135:SER:H	1.83	0.42
26:a:609:BCR:H20C	26:a:609:BCR:H361	1.88	0.42
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.55	0.42
2:b:344:ALA:HB2	2:b:401:PHE:CE1	2.54	0.42
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.42
13:o:92:SER:HB3	13:o:131:PRO:HA	2.01	0.42
31:B:620:LMG:H172	4:D:127:LEU:HD13	2.01	0.42
3:C:167:VAL:HG13	24:C:512:CLA:H61	2.00	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.20	0.42
24:c:512:CLA:H142	24:c:512:CLA:H112	1.78	0.42
4:D:266:TRP:CD1	33:D:410:LHG:HC31	2.55	0.42
33:D:411:LHG:H102	33:D:411:LHG:H132	1.82	0.42
13:O:86:LYS:HB2	13:O:86:LYS:HE3	1.75	0.42
18:X:8:LYS:HB2	18:X:8:LYS:HE3	1.91	0.42
24:c:505:CLA:H112	24:c:505:CLA:H72	1.75	0.42
2:b:29:LEU:HD23	29:b:620:SQD:H223	2.01	0.42
3:c:459:ILE:HG21	3:c:464:GLU:HG3	2.02	0.42
26:c:514:BCR:H24C	26:c:514:BCR:H371	1.86	0.42
28:d:410:STE:H61	28:d:410:STE:H31	1.70	0.42
28:i:101:STE:H61	28:i:101:STE:H91	1.52	0.42
16:v:3:LEU:HD12	16:v:3:LEU:HA	1.92	0.42
24:A:605:CLA:H191	33:D:410:LHG:H331	2.01	0.42
19:Z:62:VAL:HG22	36:Z:204:HOH:O	2.19	0.42
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.55	0.42
27:a:610:PL9:HC2	27:a:610:PL9:HC8	1.84	0.42
24:b:603:CLA:H143	24:b:603:CLA:H111	1.81	0.42
3:c:275:SER:HB3	24:c:509:CLA:HED3	2.01	0.42
24:d:404:CLA:H152	7:h:36:GLY:HA3	2.02	0.42
24:A:605:CLA:H192	24:A:605:CLA:H161	1.82	0.41
29:A:614:SQD:H162	29:A:614:SQD:H192	1.71	0.41
24:B:614:CLA:H62	24:B:614:CLA:H41	1.69	0.41
33:D:411:LHG:H151	33:D:411:LHG:H121	1.71	0.41
13:O:54:GLU:HA	36:O:320:HOH:O	2.19	0.41
14:T:29:ILE:HG22	14:T:30:THR:HG23	2.02	0.41
24:c:503:CLA:H142	24:c:503:CLA:H111	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:510:CLA:H201	31:c:522:LMG:H382	2.01	0.41
33:D:412:LHG:H111	33:D:412:LHG:H141	1.90	0.41
1:a:102:LEU:HB2	31:a:615:LMG:H112	2.02	0.41
31:b:622:LMG:H322	31:b:622:LMG:H291	1.85	0.41
26:k:101:BCR:H321	26:k:101:BCR:HC8	2.02	0.41
30:A:615:DGD:HB91	30:A:615:DGD:HB51	2.02	0.41
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.21	0.41
24:a:605:CLA:CBD	24:a:611:CLA:HAC2	2.51	0.41
5:e:8:ARG:HG2	5:e:13:ILE:HG13	2.02	0.41
33:E:101:LHG:H292	33:E:101:LHG:H262	1.94	0.41
24:a:611:CLA:HBB1	24:a:611:CLA:HMB1	2.02	0.41
3:c:56:HIS:HA	3:c:59:LEU:HD12	2.02	0.41
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.55	0.41
28:A:618:STE:H183	28:A:618:STE:H151	1.67	0.41
2:B:192:PRO:HD3	36:B:877:HOH:O	2.20	0.41
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.55	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.97	0.41
2:B:149[B]:LEU:HD11	24:B:604:CLA:H13	2.02	0.41
24:C:507:CLA:H203	24:C:507:CLA:H161	1.85	0.41
1:a:102:LEU:H	31:a:615:LMG:C12	2.33	0.41
1:a:245:THR:HB	4:d:265:ARG:HE	1.86	0.41
1:a:279:PRO:HG2	4:d:212:ALA:HB2	2.01	0.41
2:b:98:LEU:CD1	24:b:606:CLA:H152	2.50	0.41
2:b:247:PHE:CE1	24:b:602:CLA:H102	2.55	0.41
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.02	0.41
17:y:17:GLU:HG2	17:y:18:VAL:H	1.85	0.41
24:C:505:CLA:HBC2	26:C:515:BCR:H341	2.02	0.41
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.51	0.41
16:V:34:GLN:HA	16:V:38:ALA:HB2	2.03	0.41
6:f:21:VAL:O	6:f:25:THR:HG23	2.21	0.41
1:A:234:ASN:HD21	33:D:412:LHG:HC11	1.85	0.41
24:B:609:CLA:H112	24:B:609:CLA:H91	1.83	0.41
31:D:407:LMG:H122	36:D:508:HOH:O	2.21	0.41
9:J:8:ILE:HA	9:J:9:PRO:HD3	1.98	0.41
16:V:61:LEU:HD23	16:V:61:LEU:HA	1.84	0.41
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.56	0.41
1:a:159:LEU:C	1:a:162:PRO:HD2	2.46	0.41
1:a:219:VAL:O	1:a:223:LEU:HD13	2.21	0.41
27:a:610:PL9:H372	6:f:22:ALA:HA	2.03	0.41
31:a:615:LMG:H131	31:a:615:LMG:H181	2.02	0.41
24:b:614:CLA:H62	24:b:614:CLA:H41	1.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:230:LEU:HD23	3:c:230:LEU:HA	1.85	0.41
4:d:52:THR:O	4:d:66:SER:HA	2.21	0.41
5:e:18:ARG:O	5:e:22:ILE:HD12	2.21	0.41
26:h:101:BCR:H24C	26:h:101:BCR:H371	1.90	0.41
13:o:189:ARG:HD2	15:u:9:LEU:HD22	2.03	0.41
16:v:21:LEU:HD11	16:v:117:GLY:HA3	2.03	0.41
26:B:617:BCR:H333	12:M:13:LEU:HD12	2.02	0.41
4:D:272:LEU:C	4:D:272:LEU:HD23	2.46	0.41
34:F:101:HEM:HBB2	34:F:101:HEM:HMB1	2.03	0.41
16:v:41:HIS:CD2	35:v:201:HEC:NB	2.88	0.41
24:B:606:CLA:ND	28:B:622:STE:H61	2.36	0.40
11:L:14:ARG:HB3	14:T:25:GLU:HG2	2.03	0.40
2:b:413:ASP:HA	2:b:414:PRO:HD3	1.87	0.40
2:b:461:LEU:HD21	4:d:284:ILE:HD11	2.02	0.40
24:b:610:CLA:H203	24:b:610:CLA:H162	1.65	0.40
24:b:613:CLA:H121	24:b:613:CLA:H162	1.67	0.40
24:b:613:CLA:H203	33:d:408:LHG:H202	2.03	0.40
9:j:18:GLY:O	9:j:22:ILE:HG13	2.22	0.40
2:B:220:ARG:HD2	2:B:220:ARG:HA	1.90	0.40
9:J:23:VAL:HG23	36:J:202:HOH:O	2.21	0.40
13:O:178:LYS:HE3	36:O:305:HOH:O	2.21	0.40
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.56	0.40
6:f:19:ARG:O	6:f:23:VAL:HG13	2.21	0.40
29:A:613:SQD:H461	4:D:232:PHE:CE2	2.56	0.40
16:V:28:GLU:HG2	36:V:334:HOH:O	2.21	0.40
1:a:45:THR:HG23	24:a:611:CLA:H201	2.03	0.40
5:e:30:LEU:HD11	34:e:102:HEM:CBB	2.51	0.40
28:e:106:STE:H51	28:e:106:STE:H82	1.75	0.40
10:k:28:ILE:HD11	17:y:28:ILE:HD13	2.03	0.40
26:t:101:BCR:H23C	26:t:101:BCR:H382	2.03	0.40
17:y:22:LEU:HA	17:y:25:ILE:HG22	2.04	0.40
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.91	0.40
2:B:347:ARG:O	2:B:397:VAL:HA	2.22	0.40
24:C:504:CLA:H101	30:C:525:DGD:HBH1	2.02	0.40
5:E:11:SER:HB3	28:E:103:STE:H122	2.03	0.40
2:b:150:CYS:HB2	24:b:603:CLA:CMC	2.52	0.40
6:f:44:GLN:HB3	36:f:206:HOH:O	2.21	0.40
19:z:44:SER:O	19:z:48:ILE:HG13	2.21	0.40
1:A:308:ASP:HB2	5:E:52:PRO:O	2.22	0.40
30:A:615:DGD:HBT1	8:I:1:FME:HCN	2.03	0.40
4:D:56:THR:HG22	36:E:204:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.03	0.40
4:D:152:VAL:HG13	24:D:403:CLA:CED	2.52	0.40
27:a:610:PL9:H172	27:a:610:PL9:H151	1.87	0.40
26:b:617:BCR:H24C	26:b:617:BCR:H371	1.84	0.40
24:c:505:CLA:HBC2	26:c:515:BCR:H341	2.04	0.40
24:c:509:CLA:HMB1	24:c:509:CLA:HBB1	2.02	0.40
19:z:15:LEU:HD11	36:z:201:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	328 (99%)	3 (1%)	1 (0%)	36	27
1	a	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	36	27
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	504/510 (99%)	494 (98%)	10 (2%)	0	100	100
3	C	441/461 (96%)	432 (98%)	8 (2%)	1 (0%)	43	35
3	c	451/461 (98%)	441 (98%)	9 (2%)	1 (0%)	43	35
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	233 (96%)	7 (3%)	3 (1%)	10	3
13	o	242/272 (89%)	234 (97%)	6 (2%)	2 (1%)	16	7
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	0	1 (4%)	2	0
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	4
16	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	18	9
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	55 (92%)	4 (7%)	1 (2%)	7	1
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	24 (92%)	2 (8%)	0	100	100
All	All	5231/5700 (92%)	5108 (98%)	110 (2%)	13 (0%)	43	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	64	PRO
3	C	416	SER

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Mol	Chain	Res	Type
3	c	416	SER
19	z	2	THR
13	O	57	LYS
15	u	53	ALA
13	O	62	GLU
13	o	59	LYS
13	o	73	ARG
13	O	138	THR
1	A	259	ILE
14	t	29	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	267 (99%)	3 (1%)	65	61
1	a	269/280 (96%)	261 (97%)	8 (3%)	36	27
2	B	408/407 (100%)	403 (99%)	5 (1%)	63	58
2	b	403/407 (99%)	398 (99%)	5 (1%)	63	58
3	C	345/362 (95%)	339 (98%)	6 (2%)	53	48
3	c	354/362 (98%)	349 (99%)	5 (1%)	59	54
4	D	276/283 (98%)	274 (99%)	2 (1%)	76	73
4	d	277/283 (98%)	270 (98%)	7 (2%)	42	33
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	29
5	e	71/73 (97%)	71 (100%)	0	100	100
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	20
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	44
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	5
10	k	30/37 (81%)	29 (97%)	1 (3%)	33	23
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	8
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	5
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	20
13	O	206/228 (90%)	201 (98%)	5 (2%)	43	35
13	o	207/228 (91%)	201 (97%)	6 (3%)	37	28
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	19
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	83 (99%)	1 (1%)	63	58
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	58
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	48
16	v	117/138 (85%)	116 (99%)	1 (1%)	70	67
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	13
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	24
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	44
19	z	51/52 (98%)	50 (98%)	1 (2%)	48	42
20	R	22/33 (67%)	21 (96%)	1 (4%)	24	13
20	r	22/33 (67%)	21 (96%)	1 (4%)	24	13
All	All	4321/4654 (93%)	4243 (98%)	78 (2%)	51	46

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	205	VAL

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Mol	Chain	Res	Type
2	B	76	SER
2	B	86	ILE
2	B	315	ILE
2	B	362	PHE
2	B	371	THR
3	C	130	VAL
3	C	142	GLU
3	C	240	ILE
3	C	289	PHE
3	C	355	THR
3	C	416	SER
4	D	43	LEU
4	D	154	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
8	I	35	LYS
8	I	36	ASP
10	K	19	ASP
10	K	46	ARG
12	M	9	ILE
12	M	20	VAL
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	214	THR
14	T	30	THR
15	U	61	VAL
16	V	3	LEU
16	V	7	VAL
19	Z	3	ILE
20	R	6	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	222	SER
1	a	223	LEU
1	a	243	GLU
1	a	245	THR
1	a	288	LEU
2	b	86	ILE

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Mol	Chain	Res	Type
2	b	169	SER
2	b	236	THR
2	b	315	ILE
2	b	362	PHE
3	c	99	VAL
3	c	121	SER
3	c	124	VAL
3	c	216	SER
3	c	240	ILE
4	d	182	LEU
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
7	h	7	LEU
10	k	27	VAL
11	l	2	GLU
11	l	30	LEU
12	m	13	LEU
13	o	4	THR
13	o	49	THR
13	o	55	GLU
13	o	59	LYS
13	o	118	LEU
13	o	134	THR
15	u	61	VAL
16	v	52	LEU
17	y	19	ILE
18	x	2	THR
19	z	31	GLN
20	r	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	181	ASN
1	A	234	ASN
1	A	261	GLN
1	A	338	ASN

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Mol	Chain	Res	Type
2	B	282	GLN
2	B	338	GLN
2	B	497	GLN
3	C	373	ASN
3	C	415	ASN
4	D	61	HIS
13	O	61	GLN
13	O	130	GLN
13	O	155	ASN
13	O	196	GLN
13	O	200	ASN
13	O	219	GLN
13	O	231	HIS
15	U	37	GLN
15	U	78	ASN
17	Y	45	ASN
19	Z	6	GLN
20	R	22	ASN
1	a	165	GLN
1	a	234	ASN
1	a	296	ASN
2	b	14	ASN
2	b	338	GLN
2	b	394	GLN
2	b	409	GLN
3	c	311	GLN
3	c	378	ASN
3	c	382	ASN
4	d	186	GLN
7	h	59	ASN
10	k	40	GLN
12	m	32	GLN
13	o	36	GLN
13	o	58	ASN
13	o	61	GLN
13	o	88	ASN
13	o	130	GLN
13	o	132	ASN
13	o	155	ASN
15	u	73	GLN
16	v	78	ASN
17	y	45	ASN

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Mol	Chain	Res	Type
18	x	33	GLN
19	z	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	t	1	14	8,9,10	0.55	0	8,9,11	0.92	0
12	FME	M	1	12	8,9,10	0.50	0	8,9,11	0.96	0
8	FME	i	1	8	8,9,10	0.51	0	8,9,11	0.74	0
12	FME	m	1	12	8,9,10	0.37	0	8,9,11	0.92	0
14	FME	T	1	14	8,9,10	0.57	0	8,9,11	0.81	0
8	FME	I	1	8	8,9,10	0.52	0	8,9,11	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	I	1	8	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	1	0
8	I	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 211 ligands modelled in this entry, 6 are monoatomic - leaving 205 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
28	STE	d	407	-	19,19,19	0.65	0	19,19,19	1.00	1 (5%)
24	CLA	b	606	2	69,73,73	1.30	8 (11%)	82,113,113	1.47	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	614	2	69,73,73	1.17	5 (7%)	82,113,113	1.32	8 (9%)
24	CLA	b	612	2	69,73,73	1.15	8 (11%)	82,113,113	1.31	10 (12%)
29	SQD	a	614	-	52,54,54	1.63	8 (15%)	62,65,65	1.55	9 (14%)
26	BCR	c	515	-	41,41,41	0.41	0	56,56,56	0.75	1 (1%)
26	BCR	h	101	-	41,41,41	0.45	0	56,56,56	0.78	2 (3%)
24	CLA	C	501	3	69,73,73	1.47	7 (10%)	82,113,113	1.39	6 (7%)
30	DGD	C	525	-	63,63,67	0.58	1 (1%)	77,77,81	0.79	0
24	CLA	b	602	2	69,73,73	1.30	9 (13%)	82,113,113	1.39	9 (10%)
31	LMG	B	621	-	51,51,55	0.46	0	59,59,63	0.85	2 (3%)
24	CLA	c	506	3	69,73,73	1.15	6 (8%)	82,113,113	1.22	6 (7%)
28	STE	b	625	-	15,15,19	0.72	0	15,15,19	1.07	1 (6%)
24	CLA	B	613	2	69,73,73	1.19	8 (11%)	82,113,113	1.36	8 (9%)
28	STE	b	621	-	15,15,19	0.36	0	14,14,19	0.81	0
26	BCR	C	514	-	41,41,41	0.31	0	56,56,56	0.65	0
30	DGD	H	102	-	63,63,67	0.58	0	77,77,81	0.89	3 (3%)
33	LHG	e	103	-	41,41,48	0.58	0	44,47,54	0.58	0
26	BCR	H	101	-	41,41,41	0.44	0	56,56,56	1.00	5 (8%)
28	STE	d	412	-	19,19,19	0.64	0	19,19,19	0.91	0
28	STE	E	102	-	11,11,19	0.73	0	11,11,19	1.21	2 (18%)
24	CLA	b	616	2	64,68,73	1.27	9 (14%)	76,107,113	1.46	8 (10%)
24	CLA	C	512	3	69,73,73	1.37	10 (14%)	82,113,113	1.38	9 (10%)
28	STE	j	102	-	15,15,19	0.38	0	14,14,19	0.73	0
33	LHG	l	101	-	48,48,48	0.47	0	51,54,54	0.59	0
28	STE	z	101	-	8,8,19	0.38	0	7,7,19	0.62	0
28	STE	d	414	-	13,13,19	0.68	0	13,13,19	1.10	0
26	BCR	b	619	-	41,41,41	0.38	0	56,56,56	0.88	1 (1%)
30	DGD	c	521	-	63,63,67	0.54	0	77,77,81	0.82	3 (3%)
28	STE	d	413	-	9,9,19	0.38	0	8,8,19	0.67	0
25	PHO	A	608	-	58,69,69	2.08	9 (15%)	55,99,99	1.81	10 (18%)
28	STE	C	528	-	15,15,19	0.35	0	14,14,19	0.77	0
28	STE	A	618	-	10,10,19	0.34	0	9,9,19	0.74	0
24	CLA	b	615	2	69,73,73	1.31	9 (13%)	82,113,113	1.36	9 (10%)
24	CLA	c	502	3	69,73,73	1.27	6 (8%)	82,113,113	1.34	7 (8%)
28	STE	B	624	-	13,13,19	0.65	0	13,13,19	1.16	0
24	CLA	D	404	4	69,73,73	1.18	10 (14%)	82,113,113	1.23	7 (8%)
28	STE	i	102	-	5,5,19	0.39	0	4,4,19	0.51	0
26	BCR	C	521	-	41,41,41	0.36	0	56,56,56	0.79	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	a	612	-	38,38,48	0.55	0	41,44,54	0.58	0
24	CLA	b	613	2	69,73,73	1.24	9 (13%)	82,113,113	1.43	9 (10%)
24	CLA	B	616	2	64,68,73	1.40	6 (9%)	76,107,113	1.50	9 (11%)
33	LHG	d	409	-	48,48,48	0.56	0	51,54,54	0.65	1 (1%)
24	CLA	a	608	1	69,73,73	1.23	7 (10%)	82,113,113	1.25	9 (10%)
24	CLA	d	404	4	69,73,73	1.30	8 (11%)	82,113,113	1.18	8 (9%)
28	STE	B	626	-	11,11,19	0.74	0	11,11,19	1.16	1 (9%)
28	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.81	0
30	DGD	C	524	-	63,63,67	0.56	0	77,77,81	0.69	0
31	LMG	b	624	-	55,55,55	0.44	0	63,63,63	0.93	4 (6%)
29	SQD	b	620	-	47,49,54	1.65	11 (23%)	57,60,65	1.82	11 (19%)
24	CLA	B	601	36	69,73,73	1.31	7 (10%)	82,113,113	1.42	4 (4%)
24	CLA	b	614	2	69,73,73	1.29	8 (11%)	82,113,113	1.31	6 (7%)
28	STE	e	106	-	12,12,19	0.66	0	12,12,19	1.31	2 (16%)
24	CLA	C	513	3	69,73,73	1.37	7 (10%)	82,113,113	1.32	9 (10%)
28	STE	C	516	-	13,13,19	0.77	0	13,13,19	1.00	0
24	CLA	c	511	3	69,73,73	1.48	7 (10%)	82,113,113	1.43	9 (10%)
31	LMG	D	407	-	50,50,55	0.50	0	58,58,63	1.18	5 (8%)
24	CLA	C	504	36	63,67,73	1.30	8 (12%)	74,105,113	1.33	9 (12%)
28	STE	B	627	-	14,14,19	0.40	0	13,13,19	0.67	0
28	STE	e	105	-	8,8,19	0.33	0	7,7,19	0.73	0
30	DGD	c	520	-	63,63,67	0.58	0	77,77,81	0.83	5 (6%)
28	STE	m	102	-	17,17,19	0.35	0	16,16,19	0.82	0
24	CLA	B	611	2	69,73,73	1.15	8 (11%)	82,113,113	1.44	8 (9%)
31	LMG	C	522	-	48,48,55	0.46	0	56,56,63	0.66	1 (1%)
31	LMG	a	616	-	49,49,55	0.53	0	57,57,63	0.82	2 (3%)
31	LMG	C	526	-	48,48,55	0.47	0	56,56,63	0.60	0
28	STE	H	104	-	8,8,19	0.36	0	7,7,19	0.72	0
24	CLA	b	610	36	69,73,73	1.20	7 (10%)	82,113,113	1.28	8 (9%)
29	SQD	B	623	-	52,54,54	1.57	9 (17%)	62,65,65	1.81	13 (20%)
24	CLA	A	606	36	69,73,73	1.22	6 (8%)	82,113,113	1.35	6 (7%)
26	BCR	b	618	-	41,41,41	0.39	0	56,56,56	0.90	1 (1%)
25	PHO	A	607	-	58,69,69	1.97	10 (17%)	55,99,99	1.66	7 (12%)
28	STE	c	516	-	12,12,19	0.35	0	11,11,19	0.79	0
28	STE	c	517	-	17,17,19	0.39	0	16,16,19	0.72	0
24	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.46	10 (12%)
31	LMG	D	408	-	51,51,55	0.48	0	59,59,63	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	J	101	-	11,11,19	0.72	0	11,11,19	1.18	0
28	STE	e	104	-	7,7,19	0.36	0	6,6,19	0.67	0
24	CLA	a	606	36	69,73,73	1.21	10 (14%)	82,113,113	1.36	6 (7%)
30	DGD	C	523	-	63,63,67	0.61	0	77,77,81	0.92	3 (3%)
24	CLA	c	509	3	69,73,73	1.21	7 (10%)	82,113,113	1.41	8 (9%)
33	LHG	d	408	-	48,48,48	0.52	0	51,54,54	0.62	0
28	STE	A	612	-	8,8,19	0.38	0	7,7,19	0.67	0
30	DGD	c	519	-	63,63,67	0.65	0	77,77,81	0.83	1 (1%)
28	STE	a	617	-	11,11,19	0.78	0	11,11,19	1.03	0
26	BCR	K	101	-	41,41,41	0.39	0	56,56,56	0.98	1 (1%)
25	PHO	a	607	-	58,69,69	2.05	9 (15%)	55,99,99	1.58	11 (20%)
24	CLA	B	615	2	69,73,73	1.41	8 (11%)	82,113,113	1.32	6 (7%)
31	LMG	b	622	-	51,51,55	0.49	0	59,59,63	0.84	2 (3%)
24	CLA	D	403	4	69,73,73	1.13	8 (11%)	82,113,113	1.32	8 (9%)
24	CLA	B	602	2	69,73,73	1.19	7 (10%)	82,113,113	1.27	8 (9%)
24	CLA	c	513	3	69,73,73	1.23	9 (13%)	82,113,113	1.20	7 (8%)
33	LHG	D	410	-	48,48,48	0.58	0	51,54,54	0.63	1 (1%)
28	STE	b	626	-	9,9,19	0.35	0	8,8,19	0.76	0
26	BCR	c	514	-	41,41,41	0.34	0	56,56,56	0.46	0
24	CLA	a	605	1	69,73,73	1.37	8 (11%)	82,113,113	1.33	8 (9%)
24	CLA	D	402	36	69,73,73	1.43	8 (11%)	82,113,113	1.37	6 (7%)
24	CLA	c	505	3	69,73,73	1.26	8 (11%)	82,113,113	1.44	8 (9%)
24	CLA	c	504	36	64,68,73	1.16	7 (10%)	76,107,113	1.34	10 (13%)
24	CLA	b	601	36	69,73,73	1.27	7 (10%)	82,113,113	1.39	5 (6%)
26	BCR	a	609	-	41,41,41	0.41	0	56,56,56	0.81	1 (1%)
27	PL9	a	610	-	55,55,55	0.92	2 (3%)	68,69,69	1.57	11 (16%)
24	CLA	C	502	3	69,73,73	1.27	7 (10%)	82,113,113	1.26	6 (7%)
32	BCT	D	401	22	3,3,3	0.77	0	2,3,3	2.19	1 (50%)
28	STE	B	625	-	17,17,19	0.62	0	17,17,19	1.19	0
24	CLA	b	611	2	69,73,73	1.32	8 (11%)	82,113,113	1.28	9 (10%)
26	BCR	C	515	-	41,41,41	0.37	0	56,56,56	0.84	2 (3%)
24	CLA	B	612	2	69,73,73	1.12	6 (8%)	82,113,113	1.39	9 (10%)
31	LMG	a	615	-	55,55,55	0.50	0	63,63,63	1.25	8 (12%)
26	BCR	t	101	-	41,41,41	0.47	0	56,56,56	1.18	4 (7%)
24	CLA	c	503	3	69,73,73	1.28	9 (13%)	82,113,113	1.44	7 (8%)
24	CLA	B	608	2	69,73,73	1.18	6 (8%)	82,113,113	1.34	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	k	101	-	41,41,41	0.39	0	56,56,56	0.81	1 (1%)
24	CLA	C	509	3	69,73,73	1.24	10 (14%)	82,113,113	1.23	6 (7%)
28	STE	K	102	-	13,13,19	0.32	0	12,12,19	0.87	0
28	STE	d	410	-	19,19,19	0.60	0	19,19,19	0.98	0
28	STE	t	102	-	9,9,19	0.40	0	8,8,19	0.66	0
28	STE	m	101	-	11,11,19	0.76	0	11,11,19	1.35	2 (18%)
24	CLA	C	511	3	69,73,73	1.45	10 (14%)	82,113,113	1.44	5 (6%)
29	SQD	A	613	-	50,52,54	1.54	8 (16%)	60,63,65	1.99	11 (18%)
33	LHG	L	101	-	48,48,48	0.52	0	51,54,54	0.72	1 (1%)
24	CLA	C	506	3	69,73,73	1.26	7 (10%)	82,113,113	1.28	6 (7%)
33	LHG	D	412	-	48,48,48	0.57	0	51,54,54	0.64	0
24	CLA	b	603	2	69,73,73	1.28	7 (10%)	82,113,113	1.36	10 (12%)
26	BCR	b	617	-	41,41,41	0.41	0	56,56,56	0.83	2 (3%)
32	BCT	d	401	22	3,3,3	0.77	0	2,3,3	2.40	2 (100%)
24	CLA	c	507	36	69,73,73	1.32	8 (11%)	82,113,113	1.33	5 (6%)
24	CLA	B	610	36	69,73,73	1.30	9 (13%)	82,113,113	1.34	9 (10%)
27	PL9	A	611	-	55,55,55	0.77	1 (1%)	68,69,69	1.54	8 (11%)
24	CLA	B	603	2	69,73,73	1.17	5 (7%)	82,113,113	1.33	9 (10%)
28	STE	E	103	-	11,11,19	0.35	0	10,10,19	0.72	0
29	SQD	D	409	-	34,36,54	1.46	5 (14%)	42,45,65	1.64	9 (21%)
21	OEX	A	601	3,1,36	0,14,14	-	-	-	-	-
31	LMG	d	411	-	44,44,55	0.56	0	52,52,63	0.77	2 (3%)
26	BCR	A	610	-	41,41,41	0.38	0	56,56,56	0.80	1 (1%)
24	CLA	b	605	2	69,73,73	1.33	7 (10%)	82,113,113	1.42	10 (12%)
26	BCR	B	617	-	41,41,41	0.44	0	56,56,56	0.73	1 (1%)
30	DGD	A	615	-	67,67,67	0.51	0	81,81,81	0.91	4 (4%)
28	STE	C	520	-	9,9,19	0.41	0	8,8,19	0.63	0
25	PHO	d	402	-	58,69,69	2.18	9 (15%)	55,99,99	1.73	10 (18%)
33	LHG	E	101	-	48,48,48	0.54	0	51,54,54	0.56	0
35	HEC	v	201	16	50,50,50	1.64	6 (12%)	68,82,82	1.29	7 (10%)
31	LMG	c	522	-	46,46,55	0.48	0	54,54,63	0.72	2 (3%)
28	STE	E	104	-	19,19,19	0.63	0	19,19,19	1.06	1 (5%)
28	STE	D	413	-	19,19,19	0.63	0	19,19,19	1.07	0
24	CLA	B	604	2	69,73,73	1.33	7 (10%)	82,113,113	1.51	8 (9%)
24	CLA	C	505	3	69,73,73	1.28	6 (8%)	82,113,113	1.36	6 (7%)
24	CLA	b	604	2	69,73,73	1.15	7 (10%)	82,113,113	1.51	10 (12%)
28	STE	M	102	-	9,9,19	0.33	0	8,8,19	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	B	620	-	45,45,55	0.52	0	53,53,63	0.97	3 (5%)
24	CLA	B	607	36	69,73,73	1.11	5 (7%)	82,113,113	1.28	6 (7%)
29	SQD	f	101	-	39,41,54	1.66	7 (17%)	49,52,65	1.74	11 (22%)
31	LMG	c	518	-	29,29,55	0.40	0	31,31,63	0.68	1 (3%)
24	CLA	B	609	2	69,73,73	1.26	6 (8%)	82,113,113	1.33	6 (7%)
28	STE	A	616	-	7,7,19	0.32	0	6,6,19	0.79	0
28	STE	b	623	-	19,19,19	0.62	0	19,19,19	1.09	0
24	CLA	c	508	3	68,72,73	1.23	7 (10%)	80,111,113	1.24	9 (11%)
24	CLA	A	605	1	69,73,73	1.24	6 (8%)	82,113,113	1.28	5 (6%)
28	STE	Z	101	-	16,16,19	0.39	0	15,15,19	0.69	0
34	HEM	e	102	6,5	50,50,50	1.56	8 (16%)	67,82,82	1.36	11 (16%)
24	CLA	b	608	2	69,73,73	1.29	10 (14%)	82,113,113	1.43	12 (14%)
27	PL9	D	406	-	55,55,55	1.04	4 (7%)	68,69,69	1.53	12 (17%)
24	CLA	b	607	36	69,73,73	1.24	6 (8%)	82,113,113	1.25	5 (6%)
24	CLA	c	512	3	69,73,73	1.25	7 (10%)	82,113,113	1.36	7 (8%)
24	CLA	a	611	36	69,73,73	1.32	6 (8%)	82,113,113	1.34	8 (9%)
29	SQD	a	613	-	52,54,54	1.54	7 (13%)	62,65,65	1.93	12 (19%)
30	DGD	h	102	-	63,63,67	0.55	0	77,77,81	1.00	6 (7%)
35	HEC	V	201	16	50,50,50	1.78	8 (16%)	68,82,82	1.41	10 (14%)
28	STE	C	519	-	6,6,19	0.37	0	5,5,19	0.61	0
24	CLA	c	501	3	69,73,73	1.13	6 (8%)	82,113,113	1.36	5 (6%)
24	CLA	B	605	2	69,73,73	1.20	7 (10%)	82,113,113	1.40	5 (6%)
28	STE	M	101	-	14,14,19	0.67	0	14,14,19	1.23	2 (14%)
28	STE	j	101	-	11,11,19	0.75	0	11,11,19	1.16	1 (9%)
28	STE	C	529	-	13,13,19	0.36	0	12,12,19	0.77	0
28	STE	e	101	-	8,8,19	0.38	0	7,7,19	0.64	0
28	STE	C	518	-	4,4,19	0.39	0	3,3,19	0.44	0
28	STE	C	527	-	11,11,19	0.71	0	11,11,19	1.31	1 (9%)
27	PL9	d	406	-	55,55,55	0.99	3 (5%)	68,69,69	1.55	13 (19%)
24	CLA	C	510	3	69,73,73	1.24	8 (11%)	82,113,113	1.37	7 (8%)
26	BCR	k	102	-	41,41,41	0.41	0	56,56,56	0.78	1 (1%)
28	STE	A	617	-	16,16,19	0.37	0	15,15,19	0.72	0
31	LMG	C	517	-	35,35,55	0.51	0	43,43,63	1.39	6 (13%)
26	BCR	D	405	-	41,41,41	0.42	0	56,56,56	0.97	1 (1%)
28	STE	B	622	-	16,16,19	0.66	0	16,16,19	1.16	0
24	CLA	C	503	3	69,73,73	1.38	9 (13%)	82,113,113	1.52	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	I	101	-	16,16,19	0.71	0	16,16,19	1.02	1 (6%)
34	HEM	F	101	6,5	50,50,50	1.49	8 (16%)	67,82,82	1.21	8 (11%)
24	CLA	C	507	36	69,73,73	1.16	6 (8%)	82,113,113	1.45	6 (7%)
26	BCR	T	101	-	41,41,41	0.48	0	56,56,56	0.99	3 (5%)
24	CLA	b	609	2	69,73,73	1.19	6 (8%)	82,113,113	1.32	8 (9%)
24	CLA	c	510	3	69,73,73	1.25	8 (11%)	82,113,113	1.21	8 (9%)
28	STE	b	627	-	10,10,19	0.35	0	9,9,19	0.71	0
33	LHG	D	411	-	46,46,48	0.55	0	49,52,54	0.63	0
26	BCR	B	619	-	41,41,41	0.42	0	56,56,56	1.01	3 (5%)
28	STE	I	102	-	14,14,19	0.67	0	14,14,19	1.13	1 (7%)
29	SQD	A	614	-	41,43,54	1.72	8 (19%)	51,54,65	1.51	8 (15%)
24	CLA	A	609	1	58,62,73	1.21	5 (8%)	68,99,113	1.37	9 (13%)
24	CLA	B	606	2	69,73,73	1.47	6 (8%)	82,113,113	1.43	9 (10%)
31	LMG	c	523	-	48,48,55	0.47	0	56,56,63	0.72	0
24	CLA	d	403	4	69,73,73	1.10	6 (8%)	82,113,113	1.25	7 (8%)
26	BCR	d	405	-	41,41,41	0.52	0	56,56,56	1.03	4 (7%)
28	STE	i	101	-	11,11,19	0.75	0	11,11,19	1.11	1 (9%)
21	OEX	a	601	3,1,36	0,14,14	-	-	-	-	-
26	BCR	B	618	-	41,41,41	0.41	0	56,56,56	0.90	1 (1%)
28	STE	M	103	-	14,14,19	0.34	0	13,13,19	0.83	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
28	STE	d	407	-	-	11/17/17/17	-
24	CLA	b	606	2	-	13/39/115/115	-
24	CLA	B	614	2	-	15/39/115/115	-
24	CLA	b	612	2	-	5/39/115/115	-
29	SQD	a	614	-	-	23/49/69/69	0/1/1/1
26	BCR	c	515	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	501	3	-	1/39/115/115	-
30	DGD	C	525	-	-	10/51/91/95	0/2/2/2
24	CLA	b	602	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	B	621	-	-	16/46/66/70	0/1/1/1
24	CLA	c	506	3	-	18/39/115/115	-
28	STE	b	625	-	-	7/13/13/17	-
24	CLA	B	613	2	-	14/39/115/115	-
28	STE	b	621	-	-	10/13/13/17	-
26	BCR	C	514	-	-	4/29/63/63	0/2/2/2
30	DGD	H	102	-	-	20/51/91/95	0/2/2/2
33	LHG	e	103	-	-	18/46/46/53	-
26	BCR	H	101	-	-	4/29/63/63	0/2/2/2
28	STE	d	412	-	-	12/17/17/17	-
28	STE	E	102	-	-	6/9/9/17	-
24	CLA	b	616	2	-	5/33/109/115	-
24	CLA	C	512	3	-	8/39/115/115	-
28	STE	j	102	-	-	7/13/13/17	-
33	LHG	l	101	-	-	18/53/53/53	-
28	STE	z	101	-	-	3/6/6/17	-
28	STE	d	414	-	-	8/11/11/17	-
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
30	DGD	c	521	-	-	17/51/91/95	0/2/2/2
28	STE	d	413	-	-	2/7/7/17	-
25	PHO	A	608	-	-	2/37/103/103	0/5/6/6
28	STE	C	528	-	-	8/13/13/17	-
28	STE	A	618	-	-	7/8/8/17	-
24	CLA	b	615	2	-	7/39/115/115	-
24	CLA	c	502	3	-	8/39/115/115	-
28	STE	B	624	-	-	5/11/11/17	-
24	CLA	D	404	4	-	9/39/115/115	-
28	STE	i	102	-	-	1/3/3/17	-
26	BCR	C	521	-	-	6/29/63/63	0/2/2/2
33	LHG	a	612	-	-	9/43/43/53	-
24	CLA	b	613	2	-	10/39/115/115	-
24	CLA	B	616	2	-	10/33/109/115	-
33	LHG	d	409	-	-	11/53/53/53	-
24	CLA	a	608	1	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	404	4	-	10/39/115/115	-
28	STE	B	626	-	-	5/9/9/17	-
28	STE	H	103	-	-	7/15/15/17	-
30	DGD	C	524	-	-	21/51/91/95	0/2/2/2
31	LMG	b	624	-	-	25/50/70/70	0/1/1/1
29	SQD	b	620	-	-	22/44/64/69	0/1/1/1
24	CLA	B	601	36	-	20/39/115/115	-
24	CLA	b	614	2	-	15/39/115/115	-
28	STE	e	106	-	-	4/10/10/17	-
24	CLA	C	513	3	-	10/39/115/115	-
28	STE	C	516	-	-	4/11/11/17	-
24	CLA	c	511	3	-	6/39/115/115	-
31	LMG	D	407	-	-	20/45/65/70	0/1/1/1
24	CLA	C	504	36	-	7/32/108/115	-
28	STE	B	627	-	-	8/12/12/17	-
28	STE	e	105	-	-	4/6/6/17	-
30	DGD	c	520	-	-	17/51/91/95	0/2/2/2
28	STE	m	102	-	-	13/15/15/17	-
24	CLA	B	611	2	-	5/39/115/115	-
31	LMG	C	522	-	-	12/43/63/70	0/1/1/1
31	LMG	a	616	-	-	15/44/64/70	0/1/1/1
31	LMG	C	526	-	-	16/43/63/70	0/1/1/1
28	STE	H	104	-	-	3/6/6/17	-
24	CLA	b	610	36	-	5/39/115/115	-
29	SQD	B	623	-	-	27/49/69/69	0/1/1/1
24	CLA	A	606	36	-	8/39/115/115	-
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	PHO	A	607	-	-	0/37/103/103	0/5/6/6
28	STE	c	516	-	-	6/10/10/17	-
28	STE	c	517	-	-	7/15/15/17	-
24	CLA	C	508	3	-	4/39/115/115	-
31	LMG	D	408	-	-	17/46/66/70	0/1/1/1
28	STE	J	101	-	-	7/9/9/17	-
28	STE	e	104	-	-	4/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	606	36	-	7/39/115/115	-
30	DGD	C	523	-	-	22/51/91/95	0/2/2/2
24	CLA	c	509	3	-	16/39/115/115	-
33	LHG	d	408	-	-	16/53/53/53	-
28	STE	A	612	-	-	3/6/6/17	-
30	DGD	c	519	-	-	24/51/91/95	0/2/2/2
28	STE	a	617	-	-	3/9/9/17	-
26	BCR	K	101	-	-	3/29/63/63	0/2/2/2
25	PHO	a	607	-	-	1/37/103/103	0/5/6/6
24	CLA	B	615	2	-	14/39/115/115	-
31	LMG	b	622	-	-	19/46/66/70	0/1/1/1
24	CLA	D	403	4	-	6/39/115/115	-
24	CLA	B	602	2	-	4/39/115/115	-
24	CLA	c	513	3	-	11/39/115/115	-
33	LHG	D	410	-	-	18/53/53/53	-
28	STE	b	626	-	-	5/7/7/17	-
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
24	CLA	a	605	1	-	3/39/115/115	-
24	CLA	D	402	36	-	5/39/115/115	-
24	CLA	c	505	3	-	12/39/115/115	-
24	CLA	c	504	36	-	9/33/109/115	-
24	CLA	b	601	36	-	14/39/115/115	-
26	BCR	a	609	-	-	0/29/63/63	0/2/2/2
27	PL9	a	610	-	-	19/53/73/73	0/1/1/1
24	CLA	C	502	3	-	12/39/115/115	-
28	STE	B	625	-	-	9/15/15/17	-
24	CLA	b	611	2	-	10/39/115/115	-
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	CLA	B	612	2	-	10/39/115/115	-
31	LMG	a	615	-	-	28/50/70/70	0/1/1/1
26	BCR	t	101	-	-	8/29/63/63	0/2/2/2
24	CLA	c	503	3	-	10/39/115/115	-
24	CLA	B	608	2	-	1/39/115/115	-
26	BCR	k	101	-	-	7/29/63/63	0/2/2/2
24	CLA	C	509	3	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	K	102	-	-	5/11/11/17	-
28	STE	d	410	-	-	9/17/17/17	-
28	STE	t	102	-	-	4/7/7/17	-
28	STE	m	101	-	-	4/9/9/17	-
24	CLA	C	511	3	-	4/39/115/115	-
29	SQD	A	613	-	-	22/47/67/69	0/1/1/1
33	LHG	L	101	-	-	10/53/53/53	-
24	CLA	C	506	3	-	8/39/115/115	-
33	LHG	D	412	-	-	16/53/53/53	-
24	CLA	b	603	2	-	10/39/115/115	-
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
24	CLA	c	507	36	-	8/39/115/115	-
24	CLA	B	610	36	-	5/39/115/115	-
27	PL9	A	611	-	-	19/53/73/73	0/1/1/1
24	CLA	B	603	2	-	12/39/115/115	-
28	STE	E	103	-	-	4/9/9/17	-
29	SQD	D	409	-	-	14/28/48/69	0/1/1/1
31	LMG	d	411	-	-	7/39/59/70	0/1/1/1
26	BCR	A	610	-	-	0/29/63/63	0/2/2/2
24	CLA	b	605	2	-	1/39/115/115	-
26	BCR	B	617	-	-	1/29/63/63	0/2/2/2
30	DGD	A	615	-	-	20/55/95/95	0/2/2/2
28	STE	C	520	-	-	6/7/7/17	-
25	PHO	d	402	-	-	4/37/103/103	0/5/6/6
33	LHG	E	101	-	-	24/53/53/53	-
35	HEC	v	201	16	1/1/3/7	4/14/54/54	-
31	LMG	c	522	-	-	13/41/61/70	0/1/1/1
28	STE	E	104	-	-	7/17/17/17	-
28	STE	D	413	-	-	7/17/17/17	-
24	CLA	B	604	2	-	8/39/115/115	-
24	CLA	C	505	3	-	8/39/115/115	-
24	CLA	b	604	2	-	7/39/115/115	-
28	STE	M	102	-	-	3/7/7/17	-
31	LMG	B	620	-	-	13/40/60/70	0/1/1/1
24	CLA	B	607	36	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	f	101	-	-	18/36/56/69	0/1/1/1
31	LMG	c	518	-	-	8/31/31/70	-
24	CLA	B	609	2	-	1/39/115/115	-
28	STE	A	616	-	-	3/5/5/17	-
28	STE	b	623	-	-	11/17/17/17	-
24	CLA	c	508	3	-	8/38/114/115	-
24	CLA	A	605	1	-	4/39/115/115	-
28	STE	Z	101	-	-	7/14/14/17	-
34	HEM	e	102	6,5	-	6/14/54/54	-
24	CLA	b	608	2	-	3/39/115/115	-
27	PL9	D	406	-	-	5/53/73/73	0/1/1/1
24	CLA	b	607	36	-	15/39/115/115	-
24	CLA	c	512	3	-	18/39/115/115	-
24	CLA	a	611	36	-	3/39/115/115	-
29	SQD	a	613	-	-	22/49/69/69	0/1/1/1
30	DGD	h	102	-	-	18/51/91/95	0/2/2/2
35	HEC	V	201	16	1/1/3/7	5/14/54/54	-
28	STE	C	519	-	-	3/4/4/17	-
24	CLA	c	501	3	-	3/39/115/115	-
24	CLA	B	605	2	-	10/39/115/115	-
28	STE	M	101	-	-	9/12/12/17	-
28	STE	j	101	-	-	4/9/9/17	-
28	STE	C	529	-	-	4/11/11/17	-
28	STE	e	101	-	-	1/6/6/17	-
28	STE	C	518	-	-	0/2/2/17	-
28	STE	C	527	-	-	4/9/9/17	-
27	PL9	d	406	-	-	10/53/73/73	0/1/1/1
24	CLA	C	510	3	-	5/39/115/115	-
26	BCR	k	102	-	-	2/29/63/63	0/2/2/2
28	STE	A	617	-	-	10/14/14/17	-
31	LMG	C	517	-	-	15/30/50/70	0/1/1/1
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
28	STE	B	622	-	-	7/14/14/17	-
24	CLA	C	503	3	-	5/39/115/115	-
28	STE	I	101	-	-	10/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HEM	F	101	6,5	-	3/14/54/54	-
24	CLA	C	507	36	-	7/39/115/115	-
26	BCR	T	101	-	-	7/29/63/63	0/2/2/2
24	CLA	b	609	2	-	9/39/115/115	-
24	CLA	c	510	3	-	6/39/115/115	-
28	STE	b	627	-	-	4/8/8/17	-
33	LHG	D	411	-	-	15/51/51/53	-
26	BCR	B	619	-	-	3/29/63/63	0/2/2/2
28	STE	I	102	-	-	4/12/12/17	-
29	SQD	A	614	-	-	12/38/58/69	0/1/1/1
24	CLA	A	609	1	-	2/26/102/115	-
24	CLA	B	606	2	-	13/39/115/115	-
31	LMG	c	523	-	-	14/43/63/70	0/1/1/1
24	CLA	d	403	4	-	9/39/115/115	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
28	STE	i	101	-	-	6/9/9/17	-
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
28	STE	M	103	-	-	8/12/12/17	-

All (659) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	PHO	C3B-C4B	9.59	1.51	1.41
25	d	402	PHO	C1B-C2B	9.49	1.49	1.39
25	A	608	PHO	C1B-C2B	8.86	1.49	1.39
25	a	607	PHO	C1B-C2B	8.85	1.49	1.39
25	A	608	PHO	C3B-C4B	8.73	1.50	1.41
25	a	607	PHO	C3B-C4B	8.20	1.49	1.41
24	B	606	CLA	MG-NA	8.07	2.25	2.06
25	A	607	PHO	C3B-C4B	7.82	1.49	1.41
25	A	607	PHO	C1B-C2B	7.74	1.48	1.39
35	V	201	HEC	C3D-C2D	7.53	1.53	1.36
24	C	501	CLA	MG-NA	7.40	2.23	2.06
35	v	201	HEC	C3D-C2D	7.34	1.52	1.36
24	c	511	CLA	MG-NA	6.69	2.22	2.06
24	B	616	CLA	MG-NA	6.21	2.21	2.06
24	a	611	CLA	MG-NA	6.18	2.20	2.06
24	b	606	CLA	MG-NA	5.91	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	MG-NA	5.45	2.19	2.06
24	C	505	CLA	MG-NA	5.44	2.19	2.06
24	b	605	CLA	MG-NA	5.43	2.19	2.06
35	V	201	HEC	FE-ND	5.41	2.11	1.94
24	D	402	CLA	MG-NB	5.34	2.16	2.05
24	B	604	CLA	MG-NA	5.33	2.18	2.06
24	C	511	CLA	MG-NA	5.33	2.18	2.06
34	e	102	HEM	FE-NA	5.23	2.12	1.95
24	C	513	CLA	MG-NA	5.22	2.18	2.06
34	F	101	HEM	FE-NC	5.21	2.12	1.95
24	b	611	CLA	MG-NA	5.18	2.18	2.06
24	c	510	CLA	MG-NA	5.07	2.18	2.06
24	b	615	CLA	MG-NA	5.02	2.18	2.06
24	d	404	CLA	MG-ND	-4.90	1.96	2.05
24	B	615	CLA	MG-NA	4.87	2.17	2.06
24	A	605	CLA	MG-NA	4.85	2.17	2.06
24	a	605	CLA	MG-NA	4.84	2.17	2.06
29	B	623	SQD	O48-C23	4.83	1.47	1.33
29	a	614	SQD	O48-C23	4.76	1.47	1.33
29	f	101	SQD	O48-C23	4.72	1.47	1.33
24	C	512	CLA	MG-NC	4.69	2.17	2.06
24	B	608	CLA	MG-NA	4.65	2.17	2.06
24	C	503	CLA	MG-NA	4.64	2.17	2.06
29	D	409	SQD	O48-C23	4.64	1.46	1.33
29	A	614	SQD	O48-C23	4.61	1.46	1.33
29	A	613	SQD	O48-C23	4.61	1.46	1.33
24	C	508	CLA	MG-NA	4.51	2.17	2.06
24	a	608	CLA	C1D-ND	4.51	1.43	1.37
29	a	613	SQD	O48-C23	4.51	1.46	1.33
25	A	608	PHO	C1D-C2D	4.50	1.44	1.39
24	D	402	CLA	MG-NA	4.48	2.16	2.06
24	B	603	CLA	MG-NA	4.45	2.16	2.06
27	d	406	PL9	C3-C4	-4.34	1.42	1.49
24	C	506	CLA	MG-NC	4.33	2.16	2.06
24	c	502	CLA	MG-NA	4.30	2.16	2.06
24	b	603	CLA	MG-NA	4.27	2.16	2.06
34	e	102	HEM	FE-NB	4.23	2.07	1.94
24	C	502	CLA	MG-NA	4.23	2.16	2.06
24	C	504	CLA	MG-NA	4.19	2.16	2.06
24	C	501	CLA	C1D-ND	4.18	1.43	1.37
29	b	620	SQD	O48-C23	4.10	1.45	1.33
27	a	610	PL9	C7-C3	-4.09	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	607	PHO	C1D-C2D	4.09	1.44	1.39
24	b	609	CLA	MG-NA	4.08	2.16	2.06
25	a	607	PHO	C1D-C2D	4.07	1.44	1.39
24	c	507	CLA	MG-NA	4.03	2.15	2.06
35	V	201	HEC	FE-NB	4.01	2.07	1.94
24	B	610	CLA	MG-NA	4.00	2.15	2.06
24	B	614	CLA	MG-NA	3.99	2.15	2.06
24	b	608	CLA	MG-NA	3.96	2.15	2.06
24	C	513	CLA	MG-ND	3.96	2.13	2.05
24	B	602	CLA	C1D-ND	3.93	1.43	1.37
24	c	512	CLA	MG-NB	3.93	2.13	2.05
24	a	608	CLA	MG-ND	-3.93	1.98	2.05
24	c	505	CLA	MG-NA	3.91	2.15	2.06
25	d	402	PHO	C1D-C2D	3.91	1.43	1.39
29	b	620	SQD	O47-C7	3.89	1.45	1.34
24	B	616	CLA	C1D-ND	3.87	1.42	1.37
29	a	613	SQD	O47-C45	-3.83	1.37	1.46
24	b	614	CLA	MG-NA	3.82	2.15	2.06
29	a	614	SQD	O5-C1	3.82	1.51	1.41
24	a	605	CLA	C1D-ND	3.81	1.42	1.37
24	b	604	CLA	MG-NA	3.78	2.15	2.06
24	B	604	CLA	C1D-ND	3.76	1.42	1.37
24	b	614	CLA	C4B-NB	3.75	1.42	1.37
24	b	610	CLA	C1D-ND	3.74	1.42	1.37
29	f	101	SQD	O47-C7	3.74	1.44	1.34
24	b	616	CLA	C1D-ND	3.74	1.42	1.37
24	D	404	CLA	C1D-ND	3.73	1.42	1.37
24	c	509	CLA	C1D-ND	3.69	1.42	1.37
24	B	605	CLA	C1D-ND	3.69	1.42	1.37
25	a	607	PHO	C4D-CHA	3.67	1.45	1.39
24	c	502	CLA	C1D-ND	3.67	1.42	1.37
24	c	507	CLA	MG-NB	-3.67	1.98	2.05
24	b	614	CLA	C1D-ND	3.65	1.42	1.37
24	B	609	CLA	C1D-ND	3.64	1.42	1.37
24	c	507	CLA	C1D-ND	3.64	1.42	1.37
24	B	610	CLA	C4B-NB	3.63	1.42	1.37
24	b	603	CLA	C1D-ND	3.63	1.42	1.37
24	c	511	CLA	C1D-ND	3.63	1.42	1.37
24	b	602	CLA	MG-ND	-3.62	1.98	2.05
24	C	509	CLA	MG-NB	-3.62	1.98	2.05
24	D	402	CLA	C1D-ND	3.62	1.42	1.37
24	B	606	CLA	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	MG-NB	-3.60	1.98	2.05
35	v	201	HEC	FE-NA	3.60	2.07	1.95
29	A	613	SQD	O47-C45	-3.59	1.38	1.46
27	D	406	PL9	C3-C4	-3.59	1.43	1.49
24	a	611	CLA	C1D-ND	3.58	1.42	1.37
24	C	502	CLA	C1D-ND	3.58	1.42	1.37
24	c	502	CLA	MG-NB	-3.57	1.98	2.05
29	A	614	SQD	O47-C45	-3.57	1.38	1.46
34	F	101	HEM	FE-NB	3.57	2.05	1.94
24	c	513	CLA	C1D-ND	3.57	1.42	1.37
24	c	501	CLA	C1D-ND	3.57	1.42	1.37
24	C	503	CLA	C1D-ND	3.56	1.42	1.37
24	b	612	CLA	C1D-ND	3.56	1.42	1.37
24	b	613	CLA	C1D-ND	3.55	1.42	1.37
24	b	607	CLA	MG-NA	3.54	2.14	2.06
24	B	613	CLA	C1D-ND	3.54	1.42	1.37
24	b	602	CLA	C1D-ND	3.54	1.42	1.37
24	b	607	CLA	C1D-ND	3.54	1.42	1.37
24	c	508	CLA	C1D-ND	3.53	1.42	1.37
24	c	503	CLA	MG-NA	3.51	2.14	2.06
29	a	614	SQD	O47-C7	3.51	1.44	1.34
24	C	508	CLA	C1D-ND	3.51	1.42	1.37
24	B	601	CLA	C1D-ND	3.50	1.42	1.37
24	d	404	CLA	C1D-ND	3.48	1.42	1.37
24	b	601	CLA	C4B-NB	3.48	1.42	1.37
24	c	504	CLA	C4B-NB	3.48	1.42	1.37
24	B	615	CLA	MG-NC	3.48	2.14	2.06
24	B	614	CLA	C1D-ND	3.46	1.42	1.37
24	b	613	CLA	C4B-NB	3.46	1.42	1.37
29	a	614	SQD	O47-C45	-3.45	1.38	1.46
24	C	512	CLA	MG-NB	3.45	2.12	2.05
24	b	608	CLA	MG-NB	3.45	2.12	2.05
24	B	610	CLA	C1D-ND	3.45	1.42	1.37
24	A	606	CLA	MG-NA	3.45	2.14	2.06
24	A	605	CLA	C1D-ND	3.45	1.42	1.37
24	B	615	CLA	C1D-ND	3.44	1.42	1.37
24	C	511	CLA	C1D-ND	3.44	1.42	1.37
25	d	402	PHO	C4D-CHA	3.44	1.44	1.39
29	B	623	SQD	O47-C45	-3.44	1.38	1.46
24	b	607	CLA	MG-ND	-3.42	1.99	2.05
29	B	623	SQD	O47-C7	3.42	1.43	1.34
24	B	615	CLA	MG-NB	3.41	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	MG-NA	3.38	2.14	2.06
24	C	510	CLA	C1D-ND	3.38	1.42	1.37
24	C	509	CLA	C1D-ND	3.38	1.42	1.37
24	b	601	CLA	C1D-ND	3.37	1.42	1.37
24	B	601	CLA	C4B-NB	3.36	1.42	1.37
24	b	605	CLA	C4B-NB	3.36	1.42	1.37
24	b	615	CLA	C1D-ND	3.36	1.42	1.37
24	b	602	CLA	MG-NB	3.35	2.12	2.05
29	A	614	SQD	O5-C1	3.34	1.50	1.41
24	c	511	CLA	MG-ND	-3.32	1.99	2.05
24	A	606	CLA	C1D-ND	3.32	1.42	1.37
24	B	607	CLA	C1D-ND	3.32	1.42	1.37
35	v	201	HEC	FE-ND	3.32	2.05	1.94
24	C	511	CLA	C1B-C2B	3.31	1.50	1.43
24	B	601	CLA	MG-NB	-3.31	1.99	2.05
24	C	506	CLA	C4B-NB	3.30	1.42	1.37
24	B	603	CLA	C1D-ND	3.30	1.42	1.37
24	C	506	CLA	C1D-ND	3.30	1.42	1.37
29	b	620	SQD	O5-C1	3.30	1.50	1.41
24	B	612	CLA	C1D-ND	3.28	1.42	1.37
24	a	606	CLA	MG-NC	3.27	2.14	2.06
24	b	601	CLA	MG-NA	3.27	2.14	2.06
24	B	613	CLA	MG-NA	3.26	2.14	2.06
24	b	605	CLA	C1B-C2B	3.26	1.50	1.43
24	B	615	CLA	C4B-NB	3.26	1.42	1.37
24	D	403	CLA	MG-NC	3.26	2.14	2.06
24	c	503	CLA	C1D-ND	3.26	1.42	1.37
24	B	615	CLA	C1B-C2B	3.25	1.50	1.43
24	d	404	CLA	C4B-NB	3.25	1.42	1.37
24	C	507	CLA	C1B-C2B	3.23	1.50	1.43
24	C	513	CLA	C1D-ND	3.23	1.42	1.37
24	C	507	CLA	MG-NA	3.22	2.13	2.06
24	c	512	CLA	C1D-ND	3.21	1.42	1.37
24	a	606	CLA	C1D-ND	3.21	1.42	1.37
24	A	609	CLA	C1D-ND	3.19	1.42	1.37
29	D	409	SQD	C24-C23	3.18	1.59	1.50
24	B	611	CLA	C4B-NB	3.18	1.42	1.37
25	A	607	PHO	C4D-CHA	3.17	1.44	1.39
24	b	615	CLA	C4B-NB	3.17	1.42	1.37
24	B	602	CLA	C4B-NB	3.17	1.42	1.37
24	c	513	CLA	MG-NC	3.16	2.13	2.06
24	C	512	CLA	C1D-ND	3.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C1B-C2B	3.14	1.50	1.43
24	C	510	CLA	C1B-C2B	3.14	1.50	1.43
24	b	609	CLA	C1D-ND	3.14	1.42	1.37
24	a	611	CLA	C1B-C2B	3.13	1.50	1.43
29	f	101	SQD	O47-C45	-3.13	1.39	1.46
29	a	613	SQD	O47-C7	3.13	1.43	1.34
24	C	505	CLA	C1D-ND	3.12	1.42	1.37
24	B	601	CLA	C1B-C2B	3.11	1.50	1.43
29	A	613	SQD	C24-C23	3.10	1.59	1.50
29	a	614	SQD	C24-C23	3.10	1.59	1.50
24	c	505	CLA	MG-ND	3.10	2.11	2.05
24	c	511	CLA	C4B-NB	3.10	1.41	1.37
24	A	605	CLA	C1B-C2B	3.10	1.50	1.43
24	D	402	CLA	C3B-C4B	3.09	1.51	1.42
24	b	601	CLA	C1B-C2B	3.09	1.50	1.43
24	C	511	CLA	C4B-NB	3.08	1.41	1.37
24	C	503	CLA	C1B-C2B	3.08	1.50	1.43
29	b	620	SQD	C24-C23	3.08	1.59	1.50
24	b	604	CLA	C1D-ND	3.07	1.41	1.37
34	e	102	HEM	CAC-C3C	3.07	1.55	1.47
24	c	509	CLA	C1B-C2B	3.07	1.50	1.43
24	B	614	CLA	C4B-NB	3.06	1.41	1.37
24	b	602	CLA	C1B-C2B	3.06	1.50	1.43
27	d	406	PL9	C6-C1	-3.06	1.43	1.48
24	b	611	CLA	MG-ND	3.05	2.11	2.05
24	c	506	CLA	C4B-NB	3.05	1.41	1.37
24	d	403	CLA	C1D-ND	3.05	1.41	1.37
24	b	611	CLA	C1B-C2B	3.04	1.50	1.43
24	C	508	CLA	C1B-C2B	3.04	1.50	1.43
24	C	513	CLA	C1B-C2B	3.04	1.50	1.43
24	b	605	CLA	MG-ND	3.03	2.11	2.05
24	B	605	CLA	C4B-NB	3.03	1.41	1.37
29	A	614	SQD	C24-C23	3.03	1.59	1.50
24	a	605	CLA	C1B-C2B	3.03	1.50	1.43
24	c	507	CLA	C1B-C2B	3.01	1.50	1.43
24	C	502	CLA	C4B-NB	3.01	1.41	1.37
29	B	623	SQD	C24-C23	3.00	1.59	1.50
24	B	612	CLA	C4B-NB	3.00	1.41	1.37
29	A	613	SQD	O47-C7	3.00	1.42	1.34
24	c	503	CLA	C1B-C2B	2.99	1.50	1.43
24	c	513	CLA	C1B-C2B	2.99	1.50	1.43
24	b	609	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	C1D-ND	2.99	1.41	1.37
24	B	604	CLA	C4B-NB	2.99	1.41	1.37
24	B	611	CLA	C1B-C2B	2.98	1.50	1.43
24	C	511	CLA	MG-NB	-2.97	1.99	2.05
34	F	101	HEM	CAC-C3C	2.97	1.55	1.47
29	a	613	SQD	C24-C23	2.97	1.59	1.50
29	A	614	SQD	O47-C7	2.96	1.42	1.34
24	C	511	CLA	MG-ND	2.96	2.11	2.05
24	C	512	CLA	C4B-NB	2.96	1.41	1.37
24	B	601	CLA	MG-NA	2.95	2.13	2.06
24	B	602	CLA	MG-NA	2.95	2.13	2.06
29	f	101	SQD	O5-C1	2.94	1.49	1.41
24	b	606	CLA	C1D-ND	2.94	1.41	1.37
24	C	507	CLA	C1D-ND	2.94	1.41	1.37
24	C	504	CLA	C4B-NB	2.93	1.41	1.37
24	C	510	CLA	CHC-C1C	2.93	1.44	1.38
24	a	605	CLA	MG-NB	2.93	2.11	2.05
24	C	506	CLA	C1B-C2B	2.93	1.50	1.43
24	C	503	CLA	MG-NB	2.93	2.11	2.05
24	c	505	CLA	C4B-NB	2.92	1.41	1.37
29	a	613	SQD	O5-C1	2.92	1.49	1.41
24	c	512	CLA	C1B-C2B	2.92	1.50	1.43
24	b	612	CLA	C4B-NB	2.92	1.41	1.37
24	C	501	CLA	C4B-NB	2.91	1.41	1.37
29	f	101	SQD	C24-C23	2.91	1.59	1.50
24	c	503	CLA	C4B-NB	2.91	1.41	1.37
34	e	102	HEM	FE-ND	2.91	2.03	1.94
24	b	614	CLA	CHC-C1C	2.91	1.44	1.38
29	b	620	SQD	O47-C45	-2.90	1.39	1.46
24	B	605	CLA	MG-NC	2.90	2.13	2.06
24	c	513	CLA	C4B-NB	2.90	1.41	1.37
24	D	402	CLA	C1B-C2B	2.90	1.49	1.43
35	V	201	HEC	FE-NC	2.90	2.04	1.95
24	c	510	CLA	C1D-ND	2.89	1.41	1.37
24	B	606	CLA	C1B-C2B	2.89	1.49	1.43
24	A	606	CLA	CHC-C1C	2.89	1.44	1.38
24	B	603	CLA	C1B-C2B	2.89	1.49	1.43
24	B	606	CLA	C4B-NB	2.89	1.41	1.37
24	b	615	CLA	C1B-C2B	2.89	1.49	1.43
24	d	404	CLA	C1B-C2B	2.88	1.49	1.43
24	C	503	CLA	C4B-NB	2.87	1.41	1.37
24	c	505	CLA	CHC-C1C	2.87	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	MG-NA	2.87	2.13	2.06
24	b	616	CLA	MG-NA	2.86	2.13	2.06
24	b	608	CLA	CHC-C1C	2.86	1.44	1.38
24	C	509	CLA	MG-NA	2.86	2.13	2.06
24	c	509	CLA	C4B-NB	2.86	1.41	1.37
24	c	504	CLA	C1D-ND	2.85	1.41	1.37
24	c	507	CLA	C4B-NB	2.85	1.41	1.37
35	v	201	HEC	FE-NB	2.85	2.03	1.94
24	c	501	CLA	C1B-C2B	2.85	1.49	1.43
24	a	605	CLA	MG-NC	2.84	2.13	2.06
24	A	606	CLA	C4B-NB	2.84	1.41	1.37
24	B	605	CLA	MG-NA	2.84	2.13	2.06
24	b	608	CLA	C3B-C4B	2.84	1.51	1.42
25	A	607	PHO	C3D-C4D	2.84	1.45	1.41
24	b	603	CLA	C4B-NB	2.84	1.41	1.37
24	B	605	CLA	CHC-C1C	2.84	1.44	1.38
24	c	506	CLA	C1D-ND	2.84	1.41	1.37
24	b	616	CLA	C1B-C2B	2.83	1.49	1.43
24	b	605	CLA	CHC-C1C	2.83	1.44	1.38
24	c	508	CLA	CHC-C1C	2.83	1.44	1.38
29	B	623	SQD	O5-C1	2.83	1.49	1.41
24	b	612	CLA	C1B-C2B	2.83	1.49	1.43
24	C	502	CLA	C1B-C2B	2.83	1.49	1.43
24	b	611	CLA	C4B-NB	2.82	1.41	1.37
24	c	503	CLA	MG-NB	2.82	2.11	2.05
24	A	609	CLA	C4B-NB	2.81	1.41	1.37
24	B	616	CLA	C1B-C2B	2.81	1.49	1.43
24	B	610	CLA	MG-ND	-2.80	2.00	2.05
34	F	101	HEM	CAB-C3B	2.80	1.54	1.47
24	a	606	CLA	C4B-NB	2.80	1.41	1.37
24	B	607	CLA	C1B-C2B	2.80	1.49	1.43
24	C	513	CLA	C4B-NB	2.79	1.41	1.37
25	A	608	PHO	C4D-CHA	2.78	1.43	1.39
24	C	504	CLA	C1D-ND	2.78	1.41	1.37
24	b	608	CLA	C1B-C2B	2.78	1.49	1.43
24	c	508	CLA	C4B-NB	2.78	1.41	1.37
24	B	605	CLA	C1B-C2B	2.78	1.49	1.43
24	c	508	CLA	C1B-C2B	2.78	1.49	1.43
24	C	511	CLA	MG-NC	2.78	2.12	2.06
24	b	605	CLA	C3B-C4B	2.77	1.50	1.42
24	C	503	CLA	MG-NC	2.77	2.12	2.06
24	b	610	CLA	MG-NC	2.76	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	C1D-ND	2.76	1.41	1.37
24	b	613	CLA	MG-NA	2.76	2.12	2.06
24	b	613	CLA	MG-NC	2.76	2.12	2.06
24	c	510	CLA	C4B-NB	2.75	1.41	1.37
27	a	610	PL9	C53-C6	-2.75	1.45	1.50
24	B	604	CLA	MG-NC	2.75	2.12	2.06
24	c	505	CLA	C1B-C2B	2.75	1.49	1.43
24	B	608	CLA	C1D-ND	2.75	1.41	1.37
24	b	607	CLA	C1B-C2B	2.75	1.49	1.43
24	B	613	CLA	C1B-C2B	2.73	1.49	1.43
24	c	511	CLA	C1B-C2B	2.73	1.49	1.43
24	D	403	CLA	MG-NB	2.73	2.11	2.05
24	b	610	CLA	C4B-NB	2.73	1.41	1.37
24	c	509	CLA	MG-NC	2.73	2.12	2.06
24	C	512	CLA	C1B-C2B	2.73	1.49	1.43
24	B	609	CLA	C1B-C2B	2.73	1.49	1.43
25	d	402	PHO	CMC-C2C	-2.72	1.46	1.50
24	D	404	CLA	C1B-C2B	2.72	1.49	1.43
24	b	608	CLA	C1D-ND	2.71	1.41	1.37
24	c	504	CLA	C1B-C2B	2.71	1.49	1.43
24	C	508	CLA	C4B-NB	2.71	1.41	1.37
34	e	102	HEM	CAB-C3B	2.71	1.54	1.47
24	B	607	CLA	MG-NA	2.70	2.12	2.06
24	c	501	CLA	MG-NA	2.70	2.12	2.06
24	c	506	CLA	MG-NC	2.70	2.12	2.06
24	C	505	CLA	C4B-NB	2.70	1.41	1.37
24	a	606	CLA	C1B-C2B	2.70	1.49	1.43
29	D	409	SQD	O5-C1	2.70	1.48	1.41
24	B	605	CLA	C3B-C4B	2.69	1.50	1.42
24	C	510	CLA	C4B-NB	2.69	1.41	1.37
24	C	504	CLA	C3B-C4B	2.68	1.50	1.42
24	a	608	CLA	C1B-C2B	2.68	1.49	1.43
24	B	610	CLA	C1B-C2B	2.68	1.49	1.43
24	c	506	CLA	C1B-C2B	2.68	1.49	1.43
25	A	608	PHO	CMC-C2C	-2.67	1.46	1.50
25	A	607	PHO	CMC-C2C	-2.67	1.46	1.50
24	c	510	CLA	C1B-C2B	2.67	1.49	1.43
25	A	607	PHO	CBD-CGD	-2.67	1.49	1.52
24	C	509	CLA	C1B-C2B	2.67	1.49	1.43
24	B	608	CLA	C4B-NB	2.66	1.41	1.37
24	c	512	CLA	CHC-C1C	2.65	1.43	1.38
24	b	615	CLA	MG-NB	2.64	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	MG-NC	2.64	2.12	2.06
24	C	502	CLA	C3B-C4B	2.64	1.50	1.42
24	a	605	CLA	CHC-C1C	2.64	1.43	1.38
24	D	404	CLA	C4B-NB	2.63	1.41	1.37
24	C	501	CLA	C3B-C4B	2.63	1.50	1.42
24	c	512	CLA	C4B-NB	2.63	1.41	1.37
24	C	501	CLA	C1B-C2B	2.62	1.49	1.43
24	b	609	CLA	C1B-C2B	2.62	1.49	1.43
24	B	608	CLA	C1B-C2B	2.61	1.49	1.43
24	C	504	CLA	C1B-C2B	2.61	1.49	1.43
24	C	511	CLA	C3B-C4B	2.60	1.50	1.42
24	b	606	CLA	C1B-C2B	2.60	1.49	1.43
24	c	508	CLA	MG-NA	2.60	2.12	2.06
24	B	604	CLA	CHC-C1C	2.59	1.43	1.38
24	C	507	CLA	C4B-NB	2.59	1.41	1.37
24	A	606	CLA	C1B-C2B	2.59	1.49	1.43
24	B	610	CLA	C3B-C4B	2.59	1.50	1.42
24	b	611	CLA	CHC-C1C	2.59	1.43	1.38
24	B	602	CLA	C1B-C2B	2.58	1.49	1.43
24	b	616	CLA	C4B-NB	2.58	1.41	1.37
24	b	610	CLA	C1B-C2B	2.58	1.49	1.43
24	B	616	CLA	C4B-NB	2.58	1.41	1.37
25	d	402	PHO	CMD-C2D	-2.58	1.46	1.51
29	A	614	SQD	O9-S	2.58	1.52	1.45
24	A	609	CLA	MG-NB	2.58	2.10	2.05
24	b	607	CLA	C4B-NB	2.57	1.41	1.37
24	D	403	CLA	C1B-C2B	2.57	1.49	1.43
24	B	613	CLA	C4B-NB	2.57	1.41	1.37
24	c	505	CLA	C3B-C4B	2.56	1.50	1.42
24	B	614	CLA	CHC-C1C	2.55	1.43	1.38
24	b	603	CLA	C1B-C2B	2.55	1.49	1.43
24	b	608	CLA	C4B-NB	2.55	1.41	1.37
24	c	502	CLA	C1B-C2B	2.55	1.49	1.43
24	B	611	CLA	MG-NB	2.54	2.10	2.05
24	B	604	CLA	C1B-C2B	2.54	1.49	1.43
34	F	101	HEM	FE-NA	2.54	2.03	1.95
24	c	513	CLA	C3B-C4B	2.53	1.50	1.42
24	a	605	CLA	C4B-NB	2.53	1.41	1.37
24	b	604	CLA	C1B-C2B	2.53	1.49	1.43
24	c	508	CLA	C3B-C4B	2.53	1.50	1.42
24	C	505	CLA	CHC-C1C	2.52	1.43	1.38
24	b	601	CLA	CHC-C1C	2.52	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	608	PHO	CMD-C2D	-2.52	1.46	1.51
24	C	509	CLA	C4B-NB	2.52	1.41	1.37
24	C	512	CLA	C3B-C4B	2.52	1.50	1.42
24	B	609	CLA	C4B-NB	2.52	1.41	1.37
24	A	605	CLA	C3B-C4B	2.52	1.50	1.42
24	B	610	CLA	MG-NC	-2.51	2.00	2.06
29	a	614	SQD	O7-S	2.51	1.52	1.45
29	A	613	SQD	O5-C1	2.51	1.48	1.41
24	d	403	CLA	C1B-C2B	2.51	1.49	1.43
24	C	512	CLA	MG-NA	2.50	2.12	2.06
24	b	615	CLA	C3B-C4B	2.50	1.50	1.42
24	c	510	CLA	CHC-C1C	2.50	1.43	1.38
24	a	606	CLA	CHC-C1C	2.49	1.43	1.38
24	c	513	CLA	CHC-C1C	2.49	1.43	1.38
24	C	502	CLA	CHC-C1C	2.49	1.43	1.38
24	C	508	CLA	C3B-C4B	2.47	1.49	1.42
24	C	502	CLA	MG-ND	-2.47	2.00	2.05
24	C	508	CLA	C1D-C2D	2.47	1.50	1.45
35	V	201	HEC	CMB-C2B	2.47	1.55	1.50
24	b	602	CLA	C4B-NB	2.46	1.41	1.37
24	D	402	CLA	CHC-C1C	2.46	1.43	1.38
24	c	503	CLA	CHC-C1C	2.46	1.43	1.38
24	C	501	CLA	CHC-C1C	2.46	1.43	1.38
27	A	611	PL9	C53-C6	-2.45	1.45	1.50
24	b	604	CLA	C4B-NB	2.45	1.41	1.37
27	D	406	PL9	C6-C1	-2.45	1.44	1.48
24	c	503	CLA	MG-NC	2.45	2.12	2.06
24	c	513	CLA	MG-NA	2.45	2.12	2.06
24	a	611	CLA	C3B-C4B	2.45	1.49	1.42
24	c	511	CLA	CHC-C1C	2.45	1.43	1.38
24	A	606	CLA	C3B-C4B	2.45	1.49	1.42
25	A	608	PHO	C4D-ND	-2.44	1.34	1.38
24	b	606	CLA	MG-NC	2.44	2.12	2.06
25	a	607	PHO	C3D-C4D	2.44	1.44	1.41
24	B	611	CLA	C1D-ND	2.44	1.41	1.37
25	d	402	PHO	C4D-ND	-2.44	1.34	1.38
24	B	615	CLA	CHC-C1C	2.44	1.43	1.38
29	a	614	SQD	O9-S	2.43	1.52	1.45
24	C	503	CLA	C3B-C4B	2.43	1.49	1.42
24	c	512	CLA	C3B-C4B	2.43	1.49	1.42
24	C	510	CLA	MG-NA	2.43	2.12	2.06
24	d	403	CLA	MG-NC	2.43	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	601	CLA	C3B-C4B	2.43	1.49	1.42
24	c	509	CLA	CHC-C1C	2.43	1.43	1.38
24	b	602	CLA	CMD-C2D	-2.43	1.45	1.50
24	B	615	CLA	CMB-C2B	-2.42	1.45	1.50
29	b	620	SQD	O9-S	2.42	1.51	1.45
24	C	512	CLA	CHC-C1C	2.42	1.43	1.38
29	A	614	SQD	O7-S	2.42	1.51	1.45
24	C	510	CLA	C3B-C4B	2.41	1.49	1.42
24	b	612	CLA	CHC-C1C	2.41	1.43	1.38
25	A	607	PHO	C4D-ND	-2.41	1.34	1.38
24	a	605	CLA	C3B-C4B	2.41	1.49	1.42
24	b	613	CLA	CHC-C1C	2.41	1.43	1.38
29	b	620	SQD	O7-S	2.40	1.51	1.45
24	b	614	CLA	C1B-C2B	2.40	1.48	1.43
29	f	101	SQD	O9-S	2.40	1.51	1.45
24	D	403	CLA	C1D-ND	2.40	1.41	1.37
24	b	606	CLA	C3B-C4B	2.39	1.49	1.42
24	B	602	CLA	MG-NC	2.39	2.12	2.06
29	f	101	SQD	O7-S	2.39	1.51	1.45
24	C	503	CLA	CHC-C1C	2.39	1.43	1.38
24	b	604	CLA	C3B-C4B	2.39	1.49	1.42
24	D	403	CLA	C3B-C4B	2.38	1.49	1.42
24	b	606	CLA	C4B-NB	2.38	1.41	1.37
24	c	502	CLA	C4B-NB	2.38	1.41	1.37
24	d	403	CLA	C3B-C4B	2.38	1.49	1.42
24	C	505	CLA	C3B-C4B	2.38	1.49	1.42
24	B	611	CLA	MG-NA	2.37	2.11	2.06
24	c	503	CLA	C3B-C4B	2.37	1.49	1.42
24	a	606	CLA	MG-ND	2.36	2.10	2.05
24	C	506	CLA	C3B-C4B	2.36	1.49	1.42
24	A	609	CLA	C1B-C2B	2.36	1.48	1.43
29	a	614	SQD	O5-C5	2.36	1.50	1.44
24	C	513	CLA	C3B-C4B	2.36	1.49	1.42
24	d	404	CLA	C3B-C4B	2.36	1.49	1.42
24	C	504	CLA	CHC-C1C	2.35	1.43	1.38
25	A	607	PHO	C3B-C2B	-2.35	1.37	1.40
24	C	506	CLA	CHC-C1C	2.35	1.43	1.38
24	B	611	CLA	C1D-C2D	2.34	1.50	1.45
24	A	609	CLA	CHC-C1C	2.34	1.43	1.38
24	a	606	CLA	C3B-C4B	2.34	1.49	1.42
24	B	606	CLA	CHC-C1C	2.33	1.43	1.38
24	B	606	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C3B-C4B	2.33	1.49	1.42
24	C	507	CLA	CHC-C1C	2.33	1.43	1.38
24	b	616	CLA	C3B-C4B	2.32	1.49	1.42
24	b	606	CLA	CHC-C1C	2.32	1.43	1.38
24	d	403	CLA	C4B-NB	2.31	1.40	1.37
24	b	605	CLA	C1D-ND	2.31	1.40	1.37
24	b	614	CLA	C3B-C4B	2.31	1.49	1.42
24	B	602	CLA	CHC-C1C	2.31	1.43	1.38
24	B	612	CLA	CHC-C1C	2.30	1.43	1.38
24	b	616	CLA	MG-NB	2.30	2.10	2.05
24	B	603	CLA	C3B-C4B	2.30	1.49	1.42
24	b	603	CLA	MG-ND	-2.30	2.01	2.05
24	c	506	CLA	CHC-C1C	2.30	1.43	1.38
25	A	607	PHO	CMD-C2D	-2.30	1.47	1.51
24	b	604	CLA	CHC-C1C	2.29	1.43	1.38
24	c	505	CLA	CMB-C2B	-2.29	1.46	1.50
24	b	609	CLA	CHC-C1C	2.29	1.43	1.38
24	b	602	CLA	C3B-C4B	2.29	1.49	1.42
24	D	404	CLA	MG-NA	2.28	2.11	2.06
24	C	510	CLA	CMD-C2D	-2.28	1.46	1.50
24	b	616	CLA	CHC-C1C	2.28	1.43	1.38
25	a	607	PHO	CMC-C2C	-2.28	1.47	1.50
25	A	608	PHO	CMB-C2B	-2.28	1.47	1.51
24	D	404	CLA	MG-ND	-2.27	2.01	2.05
24	c	506	CLA	C3B-C4B	2.27	1.49	1.42
24	B	607	CLA	C4B-NB	2.27	1.40	1.37
34	e	102	HEM	C3B-C2B	-2.27	1.32	1.37
24	b	610	CLA	C3B-C4B	2.27	1.49	1.42
24	D	403	CLA	CHC-C1C	2.27	1.43	1.38
24	c	501	CLA	C4B-NB	2.26	1.40	1.37
24	c	509	CLA	C3B-C4B	2.26	1.49	1.42
24	c	510	CLA	CMB-C2B	-2.26	1.46	1.50
35	V	201	HEC	CAC-C3C	2.26	1.56	1.51
24	a	608	CLA	MG-NA	2.25	2.11	2.06
24	b	602	CLA	MG-NA	2.25	2.11	2.06
24	d	404	CLA	MG-NA	2.25	2.11	2.06
24	c	513	CLA	CMB-C2B	-2.25	1.46	1.50
24	b	613	CLA	C1B-C2B	2.25	1.48	1.43
24	C	503	CLA	C1D-C2D	2.25	1.49	1.45
24	B	604	CLA	C3B-C4B	2.24	1.49	1.42
29	B	623	SQD	O9-S	2.24	1.51	1.45
24	a	611	CLA	C1D-C2D	2.24	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	601	CLA	C3B-C4B	2.24	1.49	1.42
24	a	611	CLA	CHC-C1C	2.24	1.43	1.38
24	B	613	CLA	CHC-C1C	2.24	1.43	1.38
25	a	607	PHO	CMB-C2B	-2.23	1.47	1.51
24	b	609	CLA	C3B-C4B	2.23	1.49	1.42
24	c	507	CLA	CHC-C1C	2.23	1.43	1.38
27	d	406	PL9	C53-C6	-2.23	1.46	1.50
24	B	602	CLA	C3B-C4B	2.23	1.49	1.42
24	c	503	CLA	CMC-C2C	-2.22	1.46	1.50
24	b	612	CLA	C3B-C4B	2.22	1.49	1.42
24	a	608	CLA	CHC-C4B	-2.22	1.34	1.39
24	b	611	CLA	CMD-C2D	-2.21	1.46	1.50
24	D	404	CLA	CMC-C2C	-2.21	1.46	1.50
27	D	406	PL9	C46-C44	-2.21	1.46	1.51
24	B	609	CLA	C3B-C4B	2.21	1.49	1.42
24	b	603	CLA	CMD-C2D	-2.20	1.46	1.50
24	c	504	CLA	CHC-C1C	2.20	1.42	1.38
29	a	613	SQD	O7-S	2.20	1.51	1.45
24	b	615	CLA	CHC-C1C	2.19	1.42	1.38
24	B	612	CLA	C1B-C2B	2.19	1.48	1.43
24	C	508	CLA	CHC-C1C	2.19	1.42	1.38
24	D	402	CLA	C4B-NB	2.19	1.40	1.37
24	b	612	CLA	C1B-NB	-2.19	1.35	1.37
24	c	511	CLA	C3B-C4B	2.19	1.49	1.42
24	C	507	CLA	C3B-C4B	2.19	1.49	1.42
24	A	605	CLA	CHC-C1C	2.19	1.42	1.38
24	b	608	CLA	MG-NC	-2.18	2.01	2.06
24	b	613	CLA	CMB-C2B	-2.18	1.46	1.50
24	b	613	CLA	C3B-C4B	2.18	1.49	1.42
24	b	615	CLA	CMB-C2B	-2.18	1.46	1.50
24	B	613	CLA	C3B-C4B	2.17	1.49	1.42
24	C	504	CLA	CMB-C2B	-2.17	1.46	1.50
29	B	623	SQD	C8-C7	2.17	1.57	1.50
24	B	601	CLA	CHC-C1C	2.17	1.42	1.38
29	b	620	SQD	O6-C44	2.17	1.47	1.43
25	A	608	PHO	C3D-C4D	2.17	1.44	1.41
29	b	620	SQD	C44-C45	2.16	1.57	1.50
24	c	504	CLA	C3B-C4B	2.16	1.49	1.42
24	c	510	CLA	C3B-C4B	2.16	1.49	1.42
24	a	608	CLA	C4B-NB	2.15	1.40	1.37
24	B	607	CLA	MG-NC	2.15	2.11	2.06
24	B	614	CLA	C1B-C2B	2.15	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	CMD-C2D	-2.15	1.46	1.50
35	v	201	HEC	CMD-C2D	2.15	1.55	1.50
24	C	513	CLA	CHC-C1C	2.15	1.42	1.38
24	b	604	CLA	MG-NB	2.15	2.10	2.05
24	b	611	CLA	C3B-C4B	2.15	1.49	1.42
24	B	603	CLA	C4B-NB	2.15	1.40	1.37
29	a	613	SQD	O9-S	2.15	1.51	1.45
24	C	512	CLA	CMB-C2B	-2.15	1.46	1.50
24	C	511	CLA	CHC-C1C	2.15	1.42	1.38
29	D	409	SQD	O7-S	2.15	1.51	1.45
24	b	615	CLA	CMD-C2D	-2.15	1.46	1.50
29	b	620	SQD	O5-C5	2.14	1.49	1.44
24	C	508	CLA	MG-NC	2.14	2.11	2.06
35	v	201	HEC	CMA-C3A	2.14	1.55	1.50
24	c	504	CLA	CMD-C2D	-2.14	1.46	1.50
24	B	612	CLA	C3B-C4B	2.14	1.49	1.42
24	D	404	CLA	C3B-C4B	2.13	1.49	1.42
24	C	504	CLA	MG-ND	2.13	2.10	2.05
24	b	614	CLA	MG-ND	-2.13	2.01	2.05
24	a	608	CLA	C3B-C4B	2.13	1.48	1.42
24	b	610	CLA	CHC-C1C	2.12	1.42	1.38
24	d	404	CLA	CMB-C2B	-2.12	1.46	1.50
24	c	507	CLA	C3D-C4D	2.12	1.49	1.44
24	c	509	CLA	MG-ND	-2.12	2.01	2.05
24	c	512	CLA	CMD-C2D	-2.12	1.46	1.50
24	D	402	CLA	C3C-C2C	2.12	1.41	1.36
29	D	409	SQD	O9-S	2.12	1.51	1.45
34	e	102	HEM	CMA-C3A	2.11	1.55	1.50
34	F	101	HEM	FE-ND	2.11	2.01	1.94
24	b	608	CLA	C3C-C2C	2.11	1.41	1.36
24	B	608	CLA	C3B-C4B	2.10	1.48	1.42
24	B	611	CLA	CMD-C2D	-2.10	1.46	1.50
24	D	404	CLA	CMD-C2D	-2.10	1.46	1.50
24	b	613	CLA	CMD-C2D	-2.10	1.46	1.50
24	d	403	CLA	CMB-C2B	-2.10	1.46	1.50
24	A	605	CLA	C4B-NB	2.10	1.40	1.37
25	a	607	PHO	C4D-ND	-2.10	1.35	1.38
34	e	102	HEM	C2A-C3A	-2.10	1.33	1.38
34	F	101	HEM	CMC-C2C	2.09	1.55	1.50
27	D	406	PL9	C52-C5	-2.09	1.46	1.50
24	B	616	CLA	MG-ND	2.09	2.09	2.05
24	b	616	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	CMB-C2B	-2.08	1.46	1.50
24	D	403	CLA	C4B-NB	2.08	1.40	1.37
29	A	614	SQD	O5-C5	2.08	1.49	1.44
24	c	502	CLA	C3B-C4B	2.08	1.48	1.42
24	b	606	CLA	MG-ND	2.08	2.09	2.05
24	c	501	CLA	MG-NB	-2.08	2.01	2.05
24	C	501	CLA	CMD-C2D	-2.07	1.46	1.50
24	b	612	CLA	CMC-C2C	-2.07	1.46	1.50
24	a	606	CLA	CMD-C2D	-2.07	1.46	1.50
24	C	510	CLA	C3D-C4D	2.07	1.48	1.44
24	c	501	CLA	CHC-C4B	-2.07	1.34	1.39
30	C	525	DGD	O2G-C2G	-2.07	1.41	1.46
24	a	606	CLA	CMB-C2B	-2.07	1.46	1.50
29	A	613	SQD	O9-S	2.07	1.50	1.45
24	B	608	CLA	CHC-C1C	2.06	1.42	1.38
24	B	613	CLA	CMB-C2B	-2.06	1.46	1.50
24	C	508	CLA	MG-NB	2.06	2.09	2.05
24	B	610	CLA	C1D-C2D	2.05	1.49	1.45
24	B	616	CLA	CMC-C2C	-2.05	1.46	1.50
29	b	620	SQD	C8-C7	2.05	1.56	1.50
25	a	607	PHO	CMD-C2D	-2.05	1.47	1.51
24	C	506	CLA	MG-NA	2.04	2.11	2.06
24	C	511	CLA	CMC-C2C	-2.04	1.46	1.50
24	b	601	CLA	CMD-C2D	-2.04	1.46	1.50
24	b	602	CLA	CHC-C1C	2.04	1.42	1.38
24	c	508	CLA	CMD-C2D	-2.04	1.46	1.50
24	b	608	CLA	CMD-C2D	-2.04	1.46	1.50
29	A	613	SQD	C8-C7	2.04	1.56	1.50
24	D	403	CLA	CMD-C2D	-2.04	1.46	1.50
24	d	404	CLA	CHC-C1C	2.04	1.42	1.38
24	D	404	CLA	CHC-C1C	2.04	1.42	1.38
24	B	611	CLA	CHC-C1C	2.03	1.42	1.38
24	C	509	CLA	C3D-C4D	2.03	1.48	1.44
24	c	507	CLA	C3B-C4B	2.02	1.48	1.42
24	C	509	CLA	CHC-C1C	2.02	1.42	1.38
24	C	509	CLA	O2D-CGD	2.02	1.38	1.33
35	V	201	HEC	CMC-C2C	2.02	1.54	1.50
34	F	101	HEM	CMD-C2D	2.02	1.54	1.50
24	b	616	CLA	CMC-C2C	-2.02	1.46	1.50
35	V	201	HEC	CMD-C2D	2.01	1.54	1.50
24	B	610	CLA	CHC-C1C	2.01	1.42	1.38
29	B	623	SQD	C46-C45	2.01	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	CMD-C2D	-2.01	1.46	1.50
24	c	510	CLA	CMD-C2D	-2.01	1.46	1.50
29	A	613	SQD	C46-C45	2.01	1.57	1.50
24	c	513	CLA	CMD-C2D	-2.01	1.46	1.50
25	d	402	PHO	CAC-C3C	-2.01	1.48	1.51
24	D	404	CLA	CMB-C2B	-2.01	1.46	1.50
24	C	509	CLA	CMD-C2D	-2.01	1.46	1.50
24	b	603	CLA	C3B-C4B	2.01	1.48	1.42
24	B	613	CLA	MG-NC	2.01	2.11	2.06
24	B	609	CLA	CHC-C1C	2.01	1.42	1.38
24	a	606	CLA	MG-NA	2.01	2.11	2.06
25	d	402	PHO	C3D-C4D	2.00	1.44	1.41
29	B	623	SQD	O7-S	2.00	1.50	1.45

All (853) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	601	CLA	C4A-NA-C1A	9.14	110.85	106.68
24	C	511	CLA	C4A-NA-C1A	8.90	110.74	106.68
24	B	604	CLA	C4A-NA-C1A	8.56	110.59	106.68
24	b	606	CLA	C4A-NA-C1A	8.41	110.52	106.68
24	C	503	CLA	C4A-NA-C1A	8.37	110.50	106.68
24	b	601	CLA	C4A-NA-C1A	8.32	110.47	106.68
24	C	507	CLA	C4A-NA-C1A	8.18	110.41	106.68
24	B	606	CLA	C4A-NA-C1A	8.09	110.37	106.68
24	c	503	CLA	C4A-NA-C1A	7.92	110.29	106.68
24	c	511	CLA	C4A-NA-C1A	7.72	110.20	106.68
24	B	616	CLA	C4A-NA-C1A	7.63	110.16	106.68
24	C	508	CLA	C4A-NA-C1A	7.53	110.12	106.68
24	C	510	CLA	C4A-NA-C1A	7.51	110.11	106.68
24	B	605	CLA	C4A-NA-C1A	7.41	110.06	106.68
24	c	505	CLA	C4A-NA-C1A	7.30	110.01	106.68
29	a	613	SQD	O6-C1-C2	7.30	119.36	108.27
29	A	613	SQD	O6-C1-C2	7.28	119.33	108.27
24	c	507	CLA	C4A-NA-C1A	7.22	109.97	106.68
24	c	509	CLA	C4A-NA-C1A	7.14	109.94	106.68
24	B	608	CLA	C4A-NA-C1A	7.13	109.93	106.68
24	C	501	CLA	C4A-NA-C1A	7.11	109.92	106.68
24	B	615	CLA	C4A-NA-C1A	7.10	109.92	106.68
29	a	613	SQD	C1-O5-C5	-7.06	99.94	113.72
24	b	615	CLA	C4A-NA-C1A	7.00	109.87	106.68
24	D	402	CLA	C4A-NA-C1A	6.99	109.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	607	PHO	C4D-CHA-CBD	-6.97	105.11	108.45
24	C	505	CLA	C4A-NA-C1A	6.87	109.81	106.68
27	A	611	PL9	C7-C3-C4	6.80	122.51	116.91
24	B	609	CLA	C4A-NA-C1A	6.78	109.77	106.68
24	B	611	CLA	C4A-NA-C1A	6.78	109.77	106.68
24	b	604	CLA	C4A-NA-C1A	6.69	109.73	106.68
24	c	502	CLA	C4A-NA-C1A	6.66	109.72	106.68
25	a	607	PHO	C4D-CHA-CBD	-6.62	105.28	108.45
24	c	501	CLA	C4A-NA-C1A	6.57	109.68	106.68
24	b	613	CLA	C4A-NA-C1A	6.56	109.67	106.68
24	B	607	CLA	C4A-NA-C1A	6.51	109.65	106.68
24	A	605	CLA	C4A-NA-C1A	6.48	109.63	106.68
29	b	620	SQD	O6-C1-C2	6.44	118.06	108.27
24	C	506	CLA	C4A-NA-C1A	6.41	109.61	106.68
25	d	402	PHO	C4D-CHA-CBD	-6.39	105.39	108.45
24	a	605	CLA	C4A-NA-C1A	6.29	109.55	106.68
24	a	606	CLA	C4A-NA-C1A	6.26	109.53	106.68
24	b	616	CLA	C4A-NA-C1A	6.23	109.52	106.68
24	b	609	CLA	C4A-NA-C1A	6.21	109.51	106.68
24	b	607	CLA	C4A-NA-C1A	6.21	109.51	106.68
24	a	611	CLA	C4A-NA-C1A	6.18	109.50	106.68
24	b	602	CLA	C4A-NA-C1A	6.18	109.50	106.68
24	C	513	CLA	C4A-NA-C1A	6.15	109.49	106.68
24	B	612	CLA	C4A-NA-C1A	5.96	109.40	106.68
24	D	403	CLA	C4A-NA-C1A	5.95	109.39	106.68
24	C	509	CLA	C4A-NA-C1A	5.94	109.39	106.68
24	c	506	CLA	C4A-NA-C1A	5.93	109.39	106.68
24	B	613	CLA	C4A-NA-C1A	5.93	109.38	106.68
24	b	605	CLA	C4A-NA-C1A	5.91	109.37	106.68
24	c	512	CLA	C4A-NA-C1A	5.85	109.35	106.68
24	b	611	CLA	C4A-NA-C1A	5.84	109.34	106.68
24	C	512	CLA	C4A-NA-C1A	5.82	109.33	106.68
24	d	403	CLA	C4A-NA-C1A	5.81	109.33	106.68
25	A	608	PHO	CBC-CAC-C3C	5.79	121.16	112.87
24	c	513	CLA	C4A-NA-C1A	5.76	109.31	106.68
35	V	201	HEC	C1D-ND-C4D	5.69	111.94	105.21
24	c	504	CLA	C4A-NA-C1A	5.66	109.26	106.68
24	b	614	CLA	C4A-NA-C1A	5.65	109.26	106.68
29	A	613	SQD	C1-C2-C3	-5.58	98.27	110.01
24	C	504	CLA	C4A-NA-C1A	5.54	109.21	106.68
24	A	609	CLA	C4A-NA-C1A	5.46	109.17	106.68
24	b	603	CLA	C4A-NA-C1A	5.44	109.16	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	C4A-NA-C1A	5.42	109.15	106.68
24	b	608	CLA	C4A-NA-C1A	5.37	109.13	106.68
27	a	610	PL9	C7-C3-C4	5.36	121.32	116.91
24	B	614	CLA	C4A-NA-C1A	5.25	109.08	106.68
24	B	613	CLA	C1-C2-C3	-5.02	117.97	126.20
24	b	610	CLA	C4A-NA-C1A	5.00	108.96	106.68
25	A	608	PHO	C4D-CHA-CBD	-4.98	106.06	108.45
29	A	613	SQD	C1-O5-C5	-4.96	104.03	113.72
24	b	612	CLA	C4A-NA-C1A	4.96	108.94	106.68
35	v	201	HEC	C1D-ND-C4D	4.94	111.06	105.21
24	C	502	CLA	C4A-NA-C1A	4.93	108.93	106.68
24	B	602	CLA	C4A-NA-C1A	4.91	108.92	106.68
24	c	508	CLA	C4A-NA-C1A	4.88	108.90	106.68
24	A	606	CLA	C4A-NA-C1A	4.84	108.89	106.68
29	B	623	SQD	O7-S-C6	4.77	113.88	106.76
29	B	623	SQD	O6-C1-C2	4.75	115.49	108.27
25	A	607	PHO	CMA-C3A-C4A	-4.70	104.49	114.61
27	a	610	PL9	C7-C3-C2	-4.66	117.90	123.39
29	a	614	SQD	O47-C7-C8	4.65	121.55	111.48
24	B	603	CLA	C4A-NA-C1A	4.65	108.80	106.68
29	B	623	SQD	O47-C7-C8	4.53	121.29	111.48
24	D	404	CLA	C4A-NA-C1A	4.50	108.73	106.68
24	d	404	CLA	C4A-NA-C1A	4.50	108.73	106.68
31	C	517	LMG	C4-C3-C2	4.50	118.73	110.83
27	d	406	PL9	C7-C3-C4	4.47	120.59	116.91
25	A	608	PHO	O1D-CGD-CBD	4.46	131.49	124.72
27	A	611	PL9	C7-C3-C2	-4.44	118.15	123.39
25	a	607	PHO	CMA-C3A-C4A	-4.42	105.09	114.61
29	B	623	SQD	C1-O5-C5	-4.41	105.10	113.72
25	d	402	PHO	O1D-CGD-CBD	4.37	131.36	124.72
24	A	606	CLA	O2D-CGD-O1D	-4.34	115.40	123.85
24	D	402	CLA	C3B-C4B-NB	-4.33	106.67	110.53
24	C	501	CLA	C3B-C4B-NB	-4.32	106.68	110.53
29	A	613	SQD	O9-S-C6	4.31	113.19	106.76
29	a	614	SQD	O7-S-C6	4.30	113.18	106.76
29	D	409	SQD	O6-C1-C2	4.26	114.75	108.27
29	f	101	SQD	O6-C1-C2	4.26	114.75	108.27
29	b	620	SQD	O47-C7-C8	4.24	120.66	111.48
24	C	502	CLA	O2D-CGD-O1D	-4.23	115.61	123.85
31	a	615	LMG	O1-C1-C2	4.22	114.69	108.27
29	f	101	SQD	O9-S-O7	-4.20	100.16	113.82
29	A	613	SQD	O47-C7-C8	4.14	120.43	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C3B-C4B-NB	-4.12	106.86	110.53
27	D	406	PL9	C7-C3-C4	4.11	120.29	116.91
24	a	608	CLA	C4A-NA-C1A	4.10	108.55	106.68
25	d	402	PHO	C1-C2-C3	-4.09	119.49	126.20
24	c	501	CLA	O2D-CGD-O1D	-4.07	115.92	123.85
24	b	616	CLA	O2D-CGD-O1D	-4.05	115.96	123.85
24	c	505	CLA	C3B-C4B-NB	-4.05	106.92	110.53
24	b	614	CLA	C1-C2-C3	-4.04	119.58	126.20
24	B	610	CLA	C4A-NA-C1A	4.02	108.51	106.68
29	D	409	SQD	O8-S-C6	4.00	113.69	105.97
24	c	509	CLA	O2A-CGA-O1A	-3.97	113.69	123.63
25	A	608	PHO	O2D-CGD-O1D	-3.96	116.14	123.85
25	A	608	PHO	C1-C2-C3	-3.95	119.72	126.20
27	d	406	PL9	C37-C38-C39	-3.95	118.59	127.62
29	A	614	SQD	O47-C7-C8	3.95	120.02	111.48
24	D	404	CLA	O2D-CGD-O1D	-3.94	116.18	123.85
24	b	603	CLA	O2D-CGD-O1D	-3.94	116.18	123.85
27	a	610	PL9	C7-C8-C9	-3.91	120.09	126.83
24	b	604	CLA	C1-C2-C3	-3.91	119.80	126.20
24	B	614	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
24	b	608	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
24	a	608	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
24	A	606	CLA	C3B-C4B-NB	-3.86	107.08	110.53
27	D	406	PL9	C7-C8-C9	-3.86	120.18	126.83
24	B	610	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
24	C	513	CLA	O2D-CGD-O1D	-3.82	116.42	123.85
29	f	101	SQD	O7-S-C6	3.81	112.45	106.76
24	b	612	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
24	C	501	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
29	b	620	SQD	O7-S-C6	3.71	112.29	106.76
24	a	606	CLA	C3B-C4B-NB	-3.69	107.24	110.53
24	b	614	CLA	C3B-C4B-NB	-3.69	107.24	110.53
24	b	608	CLA	C3B-C4B-NB	-3.68	107.24	110.53
24	A	606	CLA	O2D-CGD-CBD	3.67	117.64	111.23
31	D	407	LMG	O6-C1-C2	-3.67	102.84	110.37
29	a	614	SQD	O9-S-O7	-3.64	101.97	113.82
24	c	505	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
31	B	621	LMG	C8-O7-C10	3.62	126.46	117.80
24	b	606	CLA	O2D-CGD-O1D	-3.62	116.81	123.85
24	b	615	CLA	C3B-C4B-NB	-3.61	107.31	110.53
24	B	611	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
29	b	620	SQD	O9-S-O7	-3.60	102.13	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	SQD	O9-S-C6	3.59	112.11	106.76
26	B	619	BCR	C29-C30-C25	3.57	115.63	110.44
24	B	614	CLA	C3B-C4B-NB	-3.57	107.34	110.53
24	b	602	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
24	b	613	CLA	O2D-CGD-O1D	-3.57	116.91	123.85
24	C	510	CLA	C3B-C4B-NB	-3.56	107.35	110.53
29	A	613	SQD	O9-S-O7	-3.55	102.26	113.82
26	A	610	BCR	C2-C1-C6	3.55	115.60	110.44
24	B	603	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
29	A	614	SQD	O5-C5-C4	3.55	116.09	109.70
24	c	512	CLA	C1-C2-C3	-3.53	120.41	126.20
24	B	602	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
29	A	614	SQD	O6-C1-C2	3.53	113.64	108.27
24	b	605	CLA	C1-C2-C3	-3.53	120.41	126.20
24	B	612	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	A	607	PHO	CMB-C2B-C3B	3.52	131.72	124.68
24	c	504	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
24	B	610	CLA	CHB-C4A-NA	3.52	129.48	124.40
24	B	610	CLA	O2A-CGA-O1A	-3.50	114.87	123.63
29	B	623	SQD	O48-C23-C24	3.49	122.48	111.83
29	f	101	SQD	C1-O5-C5	-3.49	106.91	113.72
31	C	517	LMG	O6-C5-C4	3.49	115.98	109.70
31	b	624	LMG	C8-O7-C10	3.48	126.13	117.80
29	b	620	SQD	C1-C2-C3	-3.48	102.68	110.01
24	C	508	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
24	a	605	CLA	C3B-C4B-NB	-3.46	107.44	110.53
25	A	608	PHO	CMB-C2B-C3B	3.45	131.58	124.68
31	a	615	LMG	C1-C2-C3	-3.42	102.82	110.01
29	a	613	SQD	C1-C2-C3	-3.42	102.82	110.01
24	d	403	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
24	b	601	CLA	C3B-C4B-NB	-3.41	107.49	110.53
24	b	611	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
26	d	405	BCR	C30-C25-C26	-3.40	117.98	122.64
31	D	407	LMG	O6-C5-C4	3.40	115.82	109.70
24	b	608	CLA	CHB-C4A-NA	3.39	129.30	124.40
24	b	603	CLA	O2D-CGD-CBD	3.39	117.15	111.23
24	a	606	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
24	b	606	CLA	C3B-C4B-NB	-3.38	107.52	110.53
29	f	101	SQD	O9-S-C6	3.37	111.79	106.76
29	b	620	SQD	O5-C5-C4	3.36	115.75	109.70
29	a	614	SQD	C3-C4-C5	3.34	116.29	110.23
24	b	605	CLA	O2D-CGD-O1D	-3.33	117.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	517	LMG	C8-O7-C10	3.33	125.77	117.80
24	b	601	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
24	b	610	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
24	b	602	CLA	CHB-C4A-NA	3.32	129.20	124.40
30	A	615	DGD	C3G-O3G-C1D	3.32	120.92	113.80
24	B	610	CLA	C1-C2-C3	-3.30	120.78	126.20
24	C	507	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
24	b	605	CLA	C3B-C4B-NB	-3.30	107.59	110.53
24	b	606	CLA	O2D-CGD-CBD	3.30	116.99	111.23
27	d	406	PL9	C7-C3-C2	-3.29	119.51	123.39
24	a	611	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
24	A	609	CLA	CHB-C4A-NA	3.29	129.14	124.40
24	c	512	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
29	a	613	SQD	O9-S-O7	-3.27	103.17	113.82
24	D	403	CLA	C3B-C4B-NB	-3.27	107.61	110.53
24	C	505	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
31	D	407	LMG	C1-C2-C3	-3.24	103.19	110.01
29	D	409	SQD	O9-S-C6	3.23	111.58	106.76
24	a	606	CLA	O2D-CGD-CBD	3.23	116.87	111.23
24	a	606	CLA	CHB-C4A-NA	3.23	129.06	124.40
24	b	616	CLA	O2D-CGD-CBD	3.22	116.86	111.23
25	A	608	PHO	C2B-C1B-NB	-3.22	107.10	109.43
34	F	101	HEM	CBD-CAD-C3D	-3.22	103.64	112.53
24	B	606	CLA	C3B-C4B-NB	-3.21	107.66	110.53
29	a	613	SQD	O47-C7-C8	3.21	118.42	111.48
27	D	406	PL9	C37-C38-C39	-3.21	120.28	127.62
27	D	406	PL9	C7-C3-C2	-3.20	119.61	123.39
29	B	623	SQD	C3-C4-C5	3.20	116.04	110.23
25	d	402	PHO	CMB-C2B-C3B	3.20	131.08	124.68
24	b	604	CLA	C3B-C4B-NB	-3.19	107.68	110.53
24	B	616	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
24	C	501	CLA	O2D-CGD-CBD	3.18	116.80	111.23
24	b	613	CLA	CMB-C2B-C1B	-3.17	120.59	125.42
24	C	512	CLA	C1-C2-C3	-3.17	121.01	126.20
24	D	403	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
24	c	512	CLA	CHB-C4A-NA	3.15	128.95	124.40
24	c	505	CLA	O2D-CGD-CBD	3.14	116.72	111.23
24	c	506	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
24	B	608	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
24	c	511	CLA	C3B-C4B-NB	-3.13	107.73	110.53
24	a	608	CLA	O2D-CGD-CBD	3.13	116.71	111.23
29	A	613	SQD	O8-S-C6	3.13	112.02	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	C3B-C4B-NB	-3.13	107.74	110.53
24	C	512	CLA	C3B-C4B-NB	-3.13	107.74	110.53
24	b	616	CLA	C1-C2-C3	-3.12	121.08	126.20
24	a	605	CLA	O2A-CGA-O1A	-3.12	115.82	123.63
31	D	407	LMG	O1-C1-C2	3.12	113.01	108.27
24	B	602	CLA	O2D-CGD-CBD	3.11	116.67	111.23
29	A	614	SQD	O9-S-O7	-3.11	103.72	113.82
24	b	613	CLA	C3B-C4B-NB	-3.09	107.77	110.53
24	b	604	CLA	CHB-C4A-NA	3.08	128.85	124.40
29	B	623	SQD	O9-S-O7	-3.08	103.80	113.82
24	d	404	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
24	C	504	CLA	C3B-C4B-NB	-3.07	107.78	110.53
24	c	512	CLA	C3B-C4B-NB	-3.07	107.79	110.53
29	B	623	SQD	O5-C5-C4	3.06	115.21	109.70
24	B	603	CLA	O2A-CGA-O1A	-3.05	115.99	123.63
24	C	507	CLA	CHB-C4A-NA	3.05	128.81	124.40
24	B	610	CLA	C3B-C4B-NB	-3.05	107.81	110.53
25	d	402	PHO	O2D-CGD-O1D	-3.05	117.92	123.85
27	D	406	PL9	C27-C28-C29	-3.05	120.65	127.62
24	c	508	CLA	C3B-C4B-NB	-3.04	107.82	110.53
29	f	101	SQD	O5-C5-C4	3.03	115.16	109.70
24	c	502	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
24	B	609	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
24	b	611	CLA	C3B-C4B-NB	-3.03	107.83	110.53
24	b	602	CLA	O2D-CGD-CBD	3.02	116.52	111.23
31	b	624	LMG	C3-C4-C5	-3.02	104.75	110.23
24	B	611	CLA	CHB-C4A-NA	3.02	128.76	124.40
24	c	503	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	c	501	CLA	O2D-CGD-CBD	3.01	116.49	111.23
24	B	601	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
26	t	101	BCR	C38-C26-C25	2.99	127.74	124.48
24	b	604	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
24	c	507	CLA	C3B-C4B-NB	-2.98	107.87	110.53
24	D	403	CLA	O2A-CGA-O1A	-2.98	116.17	123.63
24	c	510	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	a	610	PL9	C22-C23-C24	-2.98	120.81	127.62
24	C	506	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
24	c	511	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
24	c	502	CLA	C1-C2-C3	-2.98	121.32	126.20
24	b	608	CLA	O2D-CGD-CBD	2.96	116.41	111.23
25	a	607	PHO	CMB-C2B-C3B	2.96	130.60	124.68
24	B	603	CLA	O2D-CGD-CBD	2.96	116.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
24	B	602	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
24	A	605	CLA	O2A-CGA-O1A	-2.95	116.26	123.63
24	b	603	CLA	C3B-C4B-NB	-2.94	107.90	110.53
24	C	512	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
24	b	610	CLA	C1-C2-C3	-2.93	121.39	126.20
24	c	508	CLA	O2A-CGA-O1A	-2.93	116.29	123.63
30	A	615	DGD	C2G-O2G-C1B	2.93	124.80	117.80
24	b	612	CLA	O1D-CGD-CBD	2.92	130.29	124.52
24	B	604	CLA	C3B-C4B-NB	-2.92	107.92	110.53
24	B	612	CLA	C11-C12-C13	-2.92	106.25	115.97
29	D	409	SQD	O9-S-O7	-2.92	104.33	113.82
25	A	608	PHO	CMA-C3A-C4A	-2.91	108.34	114.61
30	C	523	DGD	C3D-C4D-C5D	-2.91	104.96	110.23
24	b	616	CLA	CHB-C4A-NA	2.90	128.58	124.40
31	B	620	LMG	O3-C3-C2	-2.89	103.56	110.38
24	D	403	CLA	CHB-C4A-NA	2.89	128.57	124.40
24	C	502	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	b	607	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
34	e	102	HEM	CBD-CAD-C3D	-2.89	104.55	112.53
24	B	608	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	C	511	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
31	C	517	LMG	C7-O1-C1	2.88	119.96	113.80
24	a	611	CLA	O2D-CGD-CBD	2.87	116.26	111.23
24	b	614	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
30	C	523	DGD	C6D-O5D-C1E	2.87	119.95	113.80
26	B	619	BCR	C24-C23-C22	2.87	130.47	126.23
24	B	606	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
24	D	402	CLA	CHB-C4A-NA	2.86	128.53	124.40
24	B	614	CLA	C1-C2-C3	-2.86	121.51	126.20
32	D	401	BCT	O2-C-O1	2.86	126.99	119.68
24	a	608	CLA	C1-C2-C3	-2.86	121.52	126.20
24	b	612	CLA	C1-C2-C3	-2.86	121.52	126.20
24	B	616	CLA	C1-C2-C3	-2.85	121.52	126.20
24	b	612	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
24	B	612	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
31	B	620	LMG	C4-C3-C2	2.85	115.83	110.83
24	B	602	CLA	O2A-CGA-O1A	-2.85	116.51	123.63
30	h	102	DGD	O6E-C5E-C4E	2.84	114.82	109.70
31	a	615	LMG	O6-C1-C2	-2.84	104.53	110.37
29	a	613	SQD	O48-C23-C24	2.84	120.49	111.83
24	b	610	CLA	CHB-C4A-NA	2.84	128.50	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	606	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
29	a	613	SQD	C44-O6-C1	-2.83	107.72	113.80
26	C	515	BCR	C2-C1-C6	2.83	114.55	110.44
27	d	406	PL9	C40-C39-C41	2.83	120.13	115.23
24	B	601	CLA	C3B-C4B-NB	-2.82	108.01	110.53
24	B	602	CLA	C3B-C4B-NB	-2.82	108.01	110.53
24	C	504	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
31	B	621	LMG	O1-C7-C8	-2.82	103.96	110.82
30	h	102	DGD	C6D-C5D-C4D	2.82	117.98	112.07
24	b	607	CLA	C3B-C4B-NB	-2.82	108.02	110.53
29	a	613	SQD	O8-S-C6	2.81	111.41	105.97
24	C	512	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	a	611	CLA	C3B-C4B-NB	-2.81	108.02	110.53
24	B	612	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
29	b	620	SQD	O5-C1-C2	-2.79	104.63	110.37
24	c	507	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
24	B	604	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
24	A	609	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
31	b	622	LMG	C1-C2-C3	-2.79	104.14	110.01
24	b	615	CLA	CHB-C4A-NA	2.78	128.42	124.40
26	H	101	BCR	C29-C30-C25	2.78	114.48	110.44
29	A	614	SQD	O7-S-C6	2.78	110.91	106.76
24	C	510	CLA	CHB-C4A-NA	2.78	128.41	124.40
24	A	609	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	D	404	CLA	CHB-C4A-NA	2.78	128.41	124.40
25	d	402	PHO	CMA-C3A-C4A	-2.77	108.64	114.61
24	B	612	CLA	C1-C2-C3	-2.77	121.66	126.20
24	B	615	CLA	C3B-C4B-NB	-2.77	108.06	110.53
24	b	604	CLA	O2D-CGD-CBD	2.77	116.07	111.23
24	c	510	CLA	C3B-C4B-NB	-2.76	108.06	110.53
27	D	406	PL9	C42-C43-C44	-2.76	121.30	127.62
24	c	503	CLA	C3B-C4B-NB	-2.76	108.07	110.53
24	A	605	CLA	C3B-C4B-NB	-2.76	108.07	110.53
24	b	615	CLA	C7-C6-C5	-2.76	105.92	113.26
24	d	403	CLA	C3B-C4B-NB	-2.75	108.07	110.53
24	b	610	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
24	B	614	CLA	O2D-CGD-CBD	2.74	116.02	111.23
27	A	611	PL9	O2-C1-C2	-2.74	115.60	121.83
24	c	504	CLA	O2D-CGD-CBD	2.74	116.02	111.23
24	d	403	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
24	c	513	CLA	C3B-C4B-NB	-2.73	108.09	110.53
30	H	102	DGD	C1E-O6E-C5E	2.73	119.06	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	614	SQD	O48-C23-C24	2.73	120.16	111.83
24	c	508	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
25	A	607	PHO	CMA-C3A-C2A	-2.73	103.59	114.13
24	b	602	CLA	C1-C2-C3	-2.72	121.73	126.20
24	C	510	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	C	505	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	T	101	BCR	C38-C26-C27	-2.72	107.79	113.60
27	D	406	PL9	C22-C23-C24	-2.72	121.40	127.62
24	D	404	CLA	O2D-CGD-CBD	2.72	115.98	111.23
31	a	615	LMG	C7-O1-C1	2.72	119.62	113.80
27	d	406	PL9	C7-C8-C9	-2.71	122.15	126.83
24	C	508	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	b	622	LMG	O1-C7-C8	-2.71	104.22	110.82
29	A	613	SQD	O48-C23-C24	2.71	120.11	111.83
24	b	604	CLA	C6-C7-C8	-2.71	106.95	115.97
24	b	616	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	c	509	CLA	CHB-C4A-NA	2.71	128.31	124.40
27	a	610	PL9	C40-C39-C41	2.71	119.93	115.23
25	d	402	PHO	CAA-C2A-C3A	-2.71	105.69	113.00
34	e	102	HEM	CBA-CAA-C2A	-2.71	105.05	112.53
29	f	101	SQD	O5-C1-C2	-2.70	104.83	110.37
24	b	610	CLA	CAA-CBA-CGA	-2.70	105.55	113.21
24	b	608	CLA	O2A-CGA-O1A	-2.69	116.89	123.63
24	b	609	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	B	615	CLA	CHB-C4A-NA	2.69	128.28	124.40
29	D	409	SQD	O5-C1-C2	-2.68	104.86	110.37
24	C	501	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
24	C	506	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	D	402	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
24	b	605	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
24	B	608	CLA	O2D-CGD-CBD	2.68	115.91	111.23
24	C	503	CLA	CHB-C4A-NA	2.67	128.26	124.40
27	d	406	PL9	C20-C19-C21	2.67	119.87	115.23
24	b	609	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
24	C	512	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
29	a	613	SQD	O7-S-C6	2.66	110.73	106.76
31	a	615	LMG	C8-O7-C10	2.66	124.15	117.80
24	B	609	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
24	C	512	CLA	CHB-C4A-NA	2.65	128.23	124.40
29	f	101	SQD	O47-C7-C8	2.65	120.68	110.93
24	B	609	CLA	C3B-C4B-NB	-2.65	108.16	110.53
24	b	613	CLA	O2D-CGD-CBD	2.65	115.86	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
24	B	604	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
24	B	616	CLA	CMB-C2B-C1B	-2.64	121.39	125.42
24	b	612	CLA	CHB-C4A-NA	2.64	128.21	124.40
35	V	201	HEC	C4B-NB-C1B	2.64	108.33	105.21
30	h	102	DGD	C1E-O6E-C5E	2.64	118.87	113.72
31	D	407	LMG	C8-O7-C10	2.63	124.09	117.80
24	B	613	CLA	C3B-C4B-NB	-2.63	108.18	110.53
26	H	101	BCR	C16-C17-C18	-2.63	123.59	127.28
30	h	102	DGD	O3D-C3D-C2D	-2.62	104.20	110.38
24	B	603	CLA	CHD-C1D-ND	-2.62	121.11	124.80
24	c	509	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
24	B	614	CLA	CHB-C4A-NA	2.62	128.18	124.40
24	C	508	CLA	CHD-C1D-ND	-2.62	121.12	124.80
30	H	102	DGD	C6D-C5D-C4D	2.61	117.55	112.07
25	A	607	PHO	C1-C2-C3	-2.61	121.91	126.20
24	c	501	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
29	b	620	SQD	O2-C2-C1	2.61	116.30	110.08
24	B	606	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
24	b	603	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
24	B	611	CLA	C1-C2-C3	-2.60	121.93	126.20
24	C	513	CLA	CHD-C1D-ND	-2.60	121.14	124.80
24	C	503	CLA	C7-C6-C5	-2.60	106.33	113.26
24	B	611	CLA	O2D-CGD-CBD	2.60	115.78	111.23
34	e	102	HEM	C3B-C2B-C1B	2.60	108.36	106.41
24	B	605	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
29	A	613	SQD	C44-O6-C1	-2.60	108.23	113.80
27	D	406	PL9	C40-C39-C41	2.59	119.73	115.23
24	A	609	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
24	C	512	CLA	O2D-CGD-CBD	2.59	115.76	111.23
29	D	409	SQD	O48-C23-C24	2.59	119.73	111.83
24	A	606	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
24	c	506	CLA	C3B-C4B-NB	-2.59	108.22	110.53
27	a	610	PL9	O2-C1-C2	-2.59	115.95	121.83
26	B	617	BCR	C29-C30-C25	2.58	114.19	110.44
27	d	406	PL9	C22-C23-C24	-2.58	121.72	127.62
27	d	406	PL9	O1-C4-C3	-2.57	118.02	120.73
24	C	510	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
35	v	201	HEC	CBD-CAD-C3D	-2.57	105.44	112.53
24	c	513	CLA	O2A-CGA-O1A	-2.56	117.21	123.63
27	d	406	PL9	C32-C33-C34	-2.56	121.76	127.62
24	c	509	CLA	C3B-C4B-NB	-2.56	108.24	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
24	B	611	CLA	CHD-C1D-ND	-2.55	121.21	124.80
24	B	616	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
24	B	612	CLA	O2A-CGA-O1A	-2.54	117.26	123.63
24	b	616	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
24	d	404	CLA	CHB-C4A-NA	2.54	128.07	124.40
24	B	613	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
24	c	502	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
35	V	201	HEC	CBD-CAD-C3D	-2.53	105.55	112.53
24	c	501	CLA	CHB-C4A-NA	2.53	128.05	124.40
24	B	612	CLA	CMB-C2B-C3B	2.53	132.49	126.55
24	C	503	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	c	502	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	C	503	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
31	d	411	LMG	O3-C3-C4	2.52	116.31	110.38
31	B	620	LMG	C9-C8-C7	2.52	117.66	111.78
24	b	605	CLA	CHD-C1D-ND	-2.52	121.26	124.80
24	b	612	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
24	c	508	CLA	C1-C2-C3	-2.51	122.08	126.20
34	e	102	HEM	CAB-C3B-C2B	-2.51	120.27	128.43
34	e	102	HEM	C3B-C4B-NB	-2.51	107.67	109.47
24	C	502	CLA	O1D-CGD-CBD	2.51	129.46	124.52
24	B	612	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	C	511	CLA	C3B-C4B-NB	-2.50	108.30	110.53
24	B	614	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
24	b	604	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
24	c	512	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
24	B	615	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
24	c	505	CLA	C1-C2-C3	-2.50	122.11	126.20
24	a	608	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
24	B	608	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	B	611	CLA	C3B-C4B-NB	-2.48	108.31	110.53
24	B	603	CLA	C3B-C4B-NB	-2.48	108.31	110.53
26	b	618	BCR	C15-C14-C13	-2.48	123.80	127.28
24	b	608	CLA	CHD-C4C-NC	2.48	128.08	124.23
26	a	609	BCR	C2-C1-C6	2.48	114.04	110.44
24	b	601	CLA	CHB-C4A-NA	2.48	127.98	124.40
24	b	603	CLA	CHC-C4B-NB	2.48	127.77	124.05
32	d	401	BCT	O2-C-O1	2.48	126.02	119.68
24	B	608	CLA	CHD-C1D-ND	-2.48	121.32	124.80
30	A	615	DGD	O5D-C1E-C2E	2.48	112.03	108.27
34	e	102	HEM	CHC-C1C-NC	2.47	127.15	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	409	SQD	C1-O5-C5	-2.47	108.89	113.72
29	a	613	SQD	O9-S-C6	2.47	110.44	106.76
26	b	617	BCR	C33-C5-C6	-2.47	121.79	124.48
24	b	611	CLA	O2D-CGD-CBD	2.47	115.55	111.23
35	v	201	HEC	C2A-C1A-NA	-2.47	107.94	110.32
27	A	611	PL9	C40-C39-C41	2.47	119.51	115.23
24	C	513	CLA	C3B-C4B-NB	-2.46	108.33	110.53
29	B	623	SQD	C25-C24-C23	-2.46	104.69	113.69
24	A	609	CLA	O2D-CGD-CBD	2.46	115.53	111.23
24	b	605	CLA	CHD-C4C-NC	2.46	128.04	124.23
24	D	403	CLA	C4-C3-C5	2.45	119.48	115.23
24	C	504	CLA	CHD-C4C-NC	2.45	128.03	124.23
24	B	602	CLA	CMB-C2B-C3B	2.45	132.30	126.55
24	C	508	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
24	b	603	CLA	CMB-C2B-C1B	-2.44	121.71	125.42
24	c	502	CLA	O2D-CGD-CBD	2.44	115.49	111.23
25	d	402	PHO	C2B-C1B-NB	-2.44	107.67	109.43
24	b	614	CLA	CHB-C4A-NA	2.44	127.91	124.40
24	a	611	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
24	a	605	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
26	C	515	BCR	C32-C1-C6	-2.43	106.43	110.24
25	d	402	PHO	CBC-CAC-C3C	2.43	116.35	112.87
24	B	605	CLA	CAA-CBA-CGA	-2.43	106.32	113.21
29	a	614	SQD	C4-C3-C2	2.43	115.09	110.83
24	A	605	CLA	CHB-C4A-NA	2.43	127.90	124.40
24	b	613	CLA	CHB-C4A-NA	2.43	127.90	124.40
25	a	607	PHO	O2A-CGA-O1A	-2.42	117.57	123.63
24	D	402	CLA	O2D-CGD-CBD	2.42	115.46	111.23
24	C	503	CLA	O1D-CGD-CBD	2.42	129.28	124.52
24	C	511	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	C	513	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
34	F	101	HEM	C4D-ND-C1D	2.41	108.06	105.21
24	b	613	CLA	C1-C2-C3	-2.41	122.24	126.20
24	C	501	CLA	CHB-C1B-NB	2.41	127.67	124.05
24	B	616	CLA	O2D-CGD-CBD	2.41	115.44	111.23
24	c	507	CLA	CHC-C4B-NB	2.41	127.67	124.05
24	A	605	CLA	O1D-CGD-CBD	2.41	129.27	124.52
24	B	613	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
24	B	611	CLA	CHD-C1D-C2D	2.40	130.49	125.49
27	A	611	PL9	C27-C28-C29	-2.40	122.13	127.62
35	V	201	HEC	CMD-C2D-C1D	2.39	128.78	125.03
24	C	504	CLA	CHD-C1D-ND	-2.39	121.44	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	e	106	STE	C3-C2-C1	-2.39	108.27	114.51
24	c	503	CLA	C7-C6-C5	-2.39	106.89	113.26
24	c	504	CLA	C3B-C4B-NB	-2.39	108.40	110.53
31	d	411	LMG	O3-C3-C2	-2.38	104.76	110.38
25	A	607	PHO	CBC-CAC-C3C	2.38	116.28	112.87
27	A	611	PL9	O2-C1-C6	2.38	124.27	120.48
29	A	613	SQD	O5-C1-C2	-2.38	105.48	110.37
35	v	201	HEC	CAD-CBD-CGD	-2.38	107.36	113.67
24	a	608	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
29	a	613	SQD	C3-C4-C5	2.37	114.53	110.23
24	C	507	CLA	C2A-C1A-CHA	2.37	127.98	123.87
24	B	604	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	C	508	CLA	CHD-C1D-C2D	2.37	130.41	125.49
24	C	506	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
26	D	405	BCR	C23-C22-C21	-2.36	115.29	119.01
26	h	101	BCR	C2-C1-C6	2.36	113.87	110.44
25	a	607	PHO	CMA-C3A-C2A	-2.36	105.00	114.13
27	D	406	PL9	O1-C4-C3	-2.36	118.24	120.73
31	a	616	LMG	C3-C4-C5	-2.36	105.96	110.23
30	h	102	DGD	C3D-C4D-C5D	-2.35	105.96	110.23
24	B	610	CLA	CHD-C1D-ND	-2.35	121.49	124.80
24	c	505	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	d	402	PHO	O2A-CGA-O1A	-2.35	117.75	123.63
24	c	506	CLA	CHB-C4A-NA	2.35	127.79	124.40
24	B	615	CLA	C16-C15-C13	-2.35	108.16	115.97
24	b	609	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
24	C	505	CLA	C1-C2-C3	-2.34	122.36	126.20
24	c	504	CLA	CHB-C4A-NA	2.34	127.78	124.40
28	j	101	STE	O2-C1-C2	2.34	121.39	114.00
31	a	615	LMG	O7-C8-C9	2.34	116.73	108.34
24	B	604	CLA	C1-O2A-CGA	-2.34	110.99	116.65
35	V	201	HEC	C3B-C4B-NB	-2.34	107.61	110.17
24	A	606	CLA	CHB-C4A-NA	2.33	127.77	124.40
27	D	406	PL9	C20-C19-C21	2.33	119.27	115.23
30	c	521	DGD	C3G-O3G-C1D	2.33	118.79	113.80
24	B	604	CLA	O2D-CGD-CBD	2.32	115.29	111.23
24	d	403	CLA	CHB-C4A-NA	2.32	127.75	124.40
27	d	406	PL9	C42-C43-C44	-2.32	122.32	127.62
29	b	620	SQD	O48-C23-C24	2.32	118.90	111.83
32	d	401	BCT	O3-C-O1	-2.32	113.75	119.68
24	b	615	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
28	m	101	STE	C3-C2-C1	-2.31	108.47	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	624	LMG	O3-C3-C4	2.31	115.83	110.38
24	C	512	CLA	CMB-C2B-C3B	2.31	131.99	126.55
24	B	606	CLA	O2D-CGD-CBD	2.31	115.27	111.23
24	b	602	CLA	C3B-C4B-NB	-2.31	108.47	110.53
26	b	617	BCR	C15-C14-C13	-2.31	124.04	127.28
24	b	612	CLA	C11-C12-C13	-2.31	108.29	115.97
24	b	607	CLA	CHC-C4B-NB	2.31	127.51	124.05
24	c	504	CLA	C1-C2-C3	-2.31	122.41	126.20
24	b	608	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
27	d	406	PL9	C27-C28-C29	-2.30	122.35	127.62
24	c	513	CLA	CHB-C4A-NA	2.30	127.72	124.40
24	a	611	CLA	CMB-C2B-C3B	2.30	131.96	126.55
24	b	611	CLA	CHD-C1D-C2D	2.30	130.27	125.49
24	c	504	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
30	h	102	DGD	O3D-C3D-C4D	2.30	115.80	110.38
31	a	615	LMG	C9-O8-C28	2.30	125.52	117.12
24	C	513	CLA	O2D-CGD-CBD	2.30	115.24	111.23
24	b	611	CLA	CHD-C1D-ND	-2.30	121.57	124.80
24	C	509	CLA	CHB-C4A-NA	2.29	127.71	124.40
28	d	407	STE	O2-C1-C2	2.29	121.24	114.00
24	a	608	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	D	403	CLA	O2D-CGD-CBD	2.29	115.23	111.23
31	C	517	LMG	O4-C4-C5	2.29	114.96	109.32
24	B	606	CLA	C1-C2-C3	-2.29	122.45	126.20
24	a	611	CLA	C1-C2-C3	-2.29	122.45	126.20
27	a	610	PL9	C37-C38-C39	-2.28	122.40	127.62
27	a	610	PL9	O2-C1-C6	2.28	124.11	120.48
26	b	619	BCR	C2-C1-C6	2.28	113.75	110.44
24	C	506	CLA	CHB-C4A-NA	2.28	127.69	124.40
24	C	509	CLA	C3B-C4B-NB	-2.28	108.50	110.53
29	A	614	SQD	O8-S-C6	2.28	110.37	105.97
24	c	503	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
27	d	406	PL9	C8-C7-C3	2.28	117.92	112.03
24	c	507	CLA	CHB-C4A-NA	2.28	127.68	124.40
24	D	404	CLA	CMB-C2B-C3B	2.28	131.90	126.55
24	B	616	CLA	CHC-C4B-NB	2.27	127.46	124.05
24	C	504	CLA	CHB-C4A-NA	2.27	127.68	124.40
28	M	101	STE	C3-C2-C1	-2.27	108.58	114.51
26	k	102	BCR	C7-C8-C9	-2.27	122.88	126.23
24	b	613	CLA	CMB-C2B-C3B	2.27	131.88	126.55
26	K	101	BCR	C33-C5-C6	2.27	126.96	124.48
29	A	614	SQD	O48-C23-C24	2.27	118.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	405	BCR	C38-C26-C27	-2.27	108.76	113.60
24	c	503	CLA	C4-C3-C5	2.27	119.16	115.23
24	B	607	CLA	CHC-C4B-NB	2.27	127.45	124.05
26	d	405	BCR	C15-C14-C13	2.26	130.45	127.28
24	D	404	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
26	t	101	BCR	C12-C13-C14	-2.26	115.46	119.01
24	C	504	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
24	C	510	CLA	CMB-C2B-C3B	2.26	131.86	126.55
33	d	409	LHG	O4-P-O5	2.26	122.94	112.44
27	a	610	PL9	C32-C33-C34	-2.25	122.46	127.62
24	C	510	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
24	B	607	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
34	F	101	HEM	CHC-C4B-NB	2.25	126.84	124.42
24	B	603	CLA	CHC-C4B-NB	2.25	127.42	124.05
24	b	606	CLA	CHB-C1B-NB	2.24	127.42	124.05
27	D	406	PL9	C12-C13-C14	-2.24	122.49	127.62
24	d	403	CLA	O2D-CGD-CBD	2.24	115.15	111.23
24	D	403	CLA	C6-C5-C3	2.24	118.93	113.47
27	d	406	PL9	C12-C13-C14	-2.24	122.50	127.62
24	C	507	CLA	C3B-C4B-NB	-2.24	108.53	110.53
24	b	606	CLA	C1-C2-C3	-2.24	122.53	126.20
24	c	504	CLA	CHD-C1D-ND	-2.24	121.65	124.80
29	f	101	SQD	C46-C45-C44	-2.24	106.57	111.78
29	f	101	SQD	O48-C23-C24	2.23	118.63	111.83
30	c	520	DGD	C6E-C5E-C4E	-2.23	107.55	113.02
35	V	201	HEC	C1D-C2D-C3D	-2.23	104.64	106.98
24	b	609	CLA	CHB-C4A-NA	2.23	127.61	124.40
24	b	603	CLA	CHB-C1B-NB	2.23	127.39	124.05
34	e	102	HEM	C4D-ND-C1D	2.23	107.84	105.21
29	a	614	SQD	O9-S-C6	2.23	110.08	106.76
29	D	409	SQD	O4-C4-C3	-2.23	105.13	110.38
24	a	611	CLA	CHB-C4A-NA	2.22	127.61	124.40
29	A	614	SQD	C3-C4-C5	2.22	114.26	110.23
26	t	101	BCR	C15-C14-C13	2.22	130.39	127.28
24	b	612	CLA	CMB-C2B-C3B	2.22	131.77	126.55
24	b	608	CLA	CMB-C2B-C3B	2.22	131.76	126.55
24	d	404	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
24	b	610	CLA	O1D-CGD-CBD	2.21	128.88	124.52
35	v	201	HEC	CBA-CAA-C2A	-2.21	106.42	112.53
24	B	607	CLA	CHB-C4A-NA	2.21	127.58	124.40
29	D	409	SQD	O5-C5-C4	2.21	113.68	109.70
30	c	520	DGD	O6E-C5E-C4E	2.21	113.67	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	CMB-C2B-C3B	2.20	131.73	126.55
24	B	601	CLA	CHB-C4A-NA	2.20	127.58	124.40
24	b	613	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
28	I	102	STE	O2-C1-C2	2.20	120.95	114.00
26	T	101	BCR	C39-C30-C25	-2.20	106.79	110.24
24	c	509	CLA	C16-C15-C13	-2.20	108.66	115.97
34	F	101	HEM	CHD-C4C-C3C	2.20	128.91	125.21
27	A	611	PL9	C35-C34-C36	2.19	119.03	115.23
29	A	613	SQD	O47-C7-O49	-2.18	118.60	123.70
31	b	624	LMG	C9-C8-C7	2.18	116.88	111.78
24	B	616	CLA	CHB-C1B-NB	2.18	127.32	124.05
25	a	607	PHO	O2D-CGD-O1D	-2.18	119.60	123.85
24	a	608	CLA	CMB-C2B-C3B	2.18	131.68	126.55
24	D	402	CLA	C7-C6-C5	-2.18	107.45	113.26
24	b	605	CLA	CHB-C1B-NB	2.18	127.32	124.05
24	b	603	CLA	CMB-C2B-C3B	2.18	131.67	126.55
28	B	626	STE	O2-C1-C2	2.17	120.85	114.00
28	e	106	STE	O2-C1-C2	2.17	120.85	114.00
24	c	511	CLA	CHA-C1A-NA	-2.17	121.48	126.39
24	c	509	CLA	O2A-CGA-CBA	2.17	118.44	111.83
31	C	522	LMG	O1-C1-C2	2.17	111.56	108.27
24	C	509	CLA	C1-C2-C3	-2.17	122.65	126.20
24	b	609	CLA	CHD-C1D-ND	-2.17	121.75	124.80
24	b	607	CLA	CHB-C4A-NA	2.16	127.52	124.40
28	b	625	STE	O2-C1-C2	2.16	120.83	114.00
24	c	510	CLA	O1D-CGD-CBD	2.16	128.78	124.52
27	a	610	PL9	O1-C4-C3	-2.16	118.45	120.73
24	B	606	CLA	CHB-C1B-NB	2.16	127.29	124.05
24	d	404	CLA	O2D-CGD-CBD	2.16	115.00	111.23
35	v	201	HEC	C1D-C2D-C3D	-2.16	104.71	106.98
24	c	508	CLA	O2D-CGD-CBD	2.16	115.00	111.23
27	A	611	PL9	C22-C23-C24	-2.16	122.69	127.62
30	c	520	DGD	C3D-C4D-C5D	-2.15	106.33	110.23
26	H	101	BCR	C33-C5-C6	2.15	126.83	124.48
24	a	605	CLA	CHB-C4A-NA	2.15	127.51	124.40
24	A	609	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
24	C	513	CLA	CHD-C1D-C2D	2.15	129.96	125.49
24	c	510	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
24	c	510	CLA	CHB-C4A-NA	2.15	127.50	124.40
29	a	614	SQD	C9-C8-C7	-2.15	105.83	113.69
27	a	610	PL9	C20-C19-C21	2.15	118.95	115.23
24	b	615	CLA	CED-O2D-CGD	2.14	120.78	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	L	101	LHG	C9-C8-C7	2.14	121.55	113.69
30	c	521	DGD	C6D-O5D-C1E	2.14	118.39	113.80
24	B	609	CLA	C7-C6-C5	-2.14	107.56	113.26
24	b	609	CLA	C7-C6-C5	-2.14	107.56	113.26
24	B	613	CLA	CED-O2D-CGD	2.14	120.76	115.92
24	B	615	CLA	CHC-C4B-NB	2.14	127.25	124.05
24	C	513	CLA	CHB-C4A-NA	2.13	127.48	124.40
28	M	101	STE	O2-C1-C2	2.13	120.73	114.00
24	c	511	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
24	D	404	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
24	B	607	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	C	517	LMG	C3-C4-C5	2.13	114.09	110.23
24	B	602	CLA	CHB-C1B-NB	2.12	127.23	124.05
24	c	506	CLA	CAC-C3C-C4C	2.12	127.55	124.79
24	b	612	CLA	C3B-C4B-NB	-2.12	108.64	110.53
31	a	615	LMG	O8-C9-C8	2.12	114.51	108.40
28	I	101	STE	O2-C1-C2	2.12	120.70	114.00
24	B	610	CLA	O1D-CGD-CBD	2.12	128.70	124.52
24	b	611	CLA	CHB-C4A-NA	2.12	127.45	124.40
28	E	104	STE	O2-C1-C2	2.11	120.68	114.00
33	D	410	LHG	O4-P-O5	2.11	122.28	112.44
24	c	502	CLA	CHB-C1B-NB	2.11	127.22	124.05
24	b	609	CLA	CMB-C2B-C3B	2.11	131.52	126.55
24	B	603	CLA	CHD-C1D-C2D	2.11	129.88	125.49
24	C	502	CLA	O2D-CGD-CBD	2.11	114.92	111.23
26	d	405	BCR	C40-C30-C25	2.11	113.55	110.24
24	b	605	CLA	CHD-C1D-C2D	2.11	129.87	125.49
24	B	606	CLA	CGD-CBD-CAD	-2.11	104.02	110.85
24	A	609	CLA	CMB-C2B-C3B	2.11	131.51	126.55
26	H	101	BCR	C2-C1-C6	2.11	113.50	110.44
24	c	511	CLA	C2A-C1A-CHA	2.10	127.52	123.87
24	b	604	CLA	C11-C10-C8	-2.10	108.97	115.97
24	C	509	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
24	c	511	CLA	C1-C2-C3	-2.10	122.75	126.20
24	c	511	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
29	a	614	SQD	O5-C1-C2	2.10	114.69	110.37
29	b	620	SQD	O48-C23-O10	-2.10	118.37	123.63
24	B	610	CLA	O2D-CGD-CBD	2.10	114.90	111.23
35	V	201	HEC	CHB-C1B-NB	2.10	126.68	124.42
24	c	511	CLA	CHB-C1B-NB	2.10	127.20	124.05
24	c	503	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	B	605	CLA	C16-C15-C13	-2.10	108.99	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	607	PHO	OBD-CAD-C3D	2.10	131.16	127.89
35	V	201	HEC	C3D-C4D-ND	-2.10	108.33	110.35
24	d	404	CLA	CMB-C2B-C3B	2.10	131.48	126.55
26	T	101	BCR	C30-C25-C24	-2.09	109.97	115.65
26	B	618	BCR	C16-C17-C18	2.09	130.21	127.28
25	a	607	PHO	C1-C2-C3	-2.09	122.77	126.20
24	b	611	CLA	C11-C12-C13	-2.09	109.01	115.97
24	B	607	CLA	C3B-C4B-NB	-2.09	108.66	110.53
24	C	509	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
24	d	404	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
24	c	513	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
34	F	101	HEM	C2A-C1A-NA	-2.09	107.83	110.15
30	c	521	DGD	C3D-C4D-C5D	-2.09	106.45	110.23
24	B	604	CLA	C2D-C1D-ND	-2.09	108.06	110.13
25	A	608	PHO	C3B-C4B-NB	-2.09	106.10	107.46
34	F	101	HEM	C2D-C1D-ND	-2.09	107.49	109.90
25	a	607	PHO	OBD-CAD-CBD	-2.09	122.76	125.82
28	m	101	STE	O2-C1-C2	2.08	120.58	114.00
24	b	615	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	B	613	CLA	CHB-C4A-NA	2.08	127.40	124.40
28	C	527	STE	O2-C1-C2	2.08	120.57	114.00
24	C	508	CLA	C1-C2-C3	-2.08	122.79	126.20
24	b	602	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
35	v	201	HEC	CHA-C4D-ND	2.08	126.66	124.42
24	b	608	CLA	CHD-C1D-ND	-2.08	121.88	124.80
24	c	510	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
24	b	602	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
34	e	102	HEM	C2D-C1D-ND	-2.07	107.50	109.90
24	c	512	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	c	518	LMG	C8-O7-C10	2.07	122.75	117.80
25	A	608	PHO	CMA-C3A-C2A	-2.07	106.13	114.13
24	a	605	CLA	CMB-C2B-C3B	2.07	131.42	126.55
24	b	616	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
24	C	504	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
25	a	607	PHO	O1D-CGD-CBD	2.07	127.86	124.72
24	b	604	CLA	C11-C12-C13	-2.07	109.09	115.97
24	c	509	CLA	C1-O2A-CGA	-2.07	111.65	116.65
24	c	510	CLA	CHD-C1D-ND	-2.07	121.89	124.80
24	C	508	CLA	O2D-CGD-CBD	2.07	114.84	111.23
24	C	508	CLA	CHB-C4A-NA	2.06	127.38	124.40
31	c	522	LMG	O4-C4-C5	2.06	114.41	109.32
28	E	102	STE	O2-C1-C2	2.06	120.52	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	101	HEM	CBA-CAA-C2A	-2.06	106.83	112.53
24	b	605	CLA	CHA-C1A-NA	-2.06	121.72	126.39
26	h	101	BCR	C33-C5-C6	2.06	126.73	124.48
34	F	101	HEM	O2D-CGD-CBD	2.06	120.50	114.00
24	C	502	CLA	CHB-C1B-NB	2.06	127.13	124.05
26	k	101	BCR	C23-C22-C21	-2.06	115.78	119.01
24	c	513	CLA	O1D-CGD-CBD	2.05	128.57	124.52
24	b	608	CLA	C6-C7-C8	-2.05	109.14	115.97
25	a	607	PHO	C2B-C1B-NB	-2.05	107.94	109.43
24	a	605	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
24	d	404	CLA	C3B-C4B-NB	-2.05	108.70	110.53
24	b	615	CLA	C11-C12-C13	-2.05	109.14	115.97
34	e	102	HEM	CHD-C4C-C3C	2.05	128.67	125.21
26	c	515	BCR	C11-C10-C9	-2.05	124.40	127.28
24	C	506	CLA	C1-C2-C3	-2.05	122.84	126.20
35	V	201	HEC	CHA-C4D-ND	2.05	126.62	124.42
29	B	623	SQD	O9-S-C6	2.05	109.81	106.76
24	B	603	CLA	C4-C3-C5	2.04	118.78	115.23
24	C	508	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
35	V	201	HEC	CAD-CBD-CGD	-2.04	108.25	113.67
30	C	523	DGD	O2E-C2E-C3E	2.04	115.19	110.38
24	C	504	CLA	CHB-C1B-NB	2.04	127.11	124.05
24	c	505	CLA	C1D-ND-C4D	2.04	107.74	106.31
24	B	609	CLA	O1D-CGD-CBD	2.04	128.54	124.52
24	C	507	CLA	CHA-C1A-NA	-2.04	121.77	126.39
25	a	607	PHO	OBD-CAD-C3D	2.04	131.07	127.89
24	b	601	CLA	O1D-CGD-CBD	2.04	128.54	124.52
29	B	623	SQD	C1-C2-C3	-2.04	105.73	110.01
24	c	508	CLA	CHD-C1D-ND	-2.03	121.94	124.80
29	B	623	SQD	C9-C8-C7	-2.03	106.24	113.69
24	d	403	CLA	C1-C2-C3	-2.03	122.87	126.20
24	b	611	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
24	b	615	CLA	C1-C2-C3	-2.03	122.87	126.20
30	c	520	DGD	C3G-O3G-C1D	2.03	118.15	113.80
24	c	505	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
30	c	520	DGD	O2D-C2D-C1D	-2.03	105.23	110.08
24	a	608	CLA	CHA-C1A-NA	-2.03	121.79	126.39
27	D	406	PL9	C8-C7-C3	2.03	117.28	112.03
29	a	613	SQD	C9-C8-C7	-2.03	106.25	113.69
24	B	606	CLA	CHB-C4A-NA	2.03	127.33	124.40
28	E	102	STE	C3-C2-C1	-2.03	109.21	114.51
26	C	521	BCR	C2-C1-C6	2.03	113.39	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
29	f	101	SQD	C3-C4-C5	2.03	113.90	110.23
24	C	505	CLA	O1D-CGD-CBD	2.02	128.51	124.52
34	e	102	HEM	C4C-NC-C1C	2.02	109.12	105.82
24	b	608	CLA	CHD-C4C-C3C	-2.02	121.82	124.77
34	e	102	HEM	C3C-C2C-C1C	2.02	108.96	107.05
24	a	605	CLA	C4-C3-C5	2.02	118.74	115.23
24	c	508	CLA	CHD-C4C-NC	2.02	127.36	124.23
29	B	623	SQD	C46-C45-C44	-2.02	107.08	111.78
24	B	614	CLA	CED-O2D-CGD	2.02	120.49	115.92
30	c	519	DGD	C3D-C4D-C5D	-2.02	106.57	110.23
26	B	619	BCR	C33-C5-C6	-2.02	122.28	124.48
26	t	101	BCR	C24-C25-C26	2.02	126.20	121.56
30	H	102	DGD	O3D-C3D-C2D	-2.02	105.62	110.38
24	A	609	CLA	C1-C2-C3	-2.01	122.90	126.20
24	B	608	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
24	c	504	CLA	CMB-C2B-C3B	2.01	131.28	126.55
24	C	511	CLA	O2D-CGD-CBD	2.01	114.75	111.23
26	H	101	BCR	C16-C15-C14	-2.01	119.40	123.52
31	a	616	LMG	O3-C3-C4	2.01	115.12	110.38
24	C	505	CLA	C11-C12-C13	-2.01	109.29	115.97
30	A	615	DGD	C3G-C2G-C1G	-2.01	107.10	111.78
31	c	522	LMG	C4-C3-C2	2.01	114.36	110.83
24	c	506	CLA	O1D-CGD-CBD	2.01	128.48	124.52
28	i	101	STE	O2-C1-C2	2.01	120.34	114.00
24	B	613	CLA	C6-C7-C8	-2.01	109.30	115.97
24	b	606	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
24	b	602	CLA	CMB-C2B-C3B	2.00	131.26	126.55
24	b	603	CLA	CHA-C4D-ND	2.00	136.68	132.55
24	C	513	CLA	CMB-C2B-C1B	-2.00	122.37	125.42

All (2) chirality outliers are listed below:

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

All (1770) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	606	CLA	C2B-C3B-CAB-CBB
24	A	606	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	A	609	CLA	C2-C3-C5-C6
24	A	609	CLA	C4-C3-C5-C6
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	601	CLA	C3A-C2A-CAA-CBA
24	B	601	CLA	CBA-CGA-O2A-C1
24	B	601	CLA	O1A-CGA-O2A-C1
24	B	606	CLA	C2B-C3B-CAB-CBB
24	B	606	CLA	C4B-C3B-CAB-CBB
24	B	610	CLA	C14-C13-C15-C16
24	B	613	CLA	C11-C12-C13-C14
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C11-C10-C8-C9
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	C2-C3-C5-C6
24	C	507	CLA	C4-C3-C5-C6
24	a	606	CLA	C4B-C3B-CAB-CBB
24	b	606	CLA	C14-C13-C15-C16
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	C11-C10-C8-C9
24	c	506	CLA	C12-C13-C15-C16
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	508	CLA	C11-C10-C8-C9
24	c	512	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
25	A	608	PHO	C4C-C3C-CAC-CBC
26	C	521	BCR	C1-C6-C7-C8
26	C	521	BCR	C5-C6-C7-C8
26	C	521	BCR	C21-C22-C23-C24
26	C	521	BCR	C37-C22-C23-C24
26	K	101	BCR	C7-C8-C9-C10
26	T	101	BCR	C23-C24-C25-C26
26	b	617	BCR	C5-C6-C7-C8
26	d	405	BCR	C21-C22-C23-C24
26	d	405	BCR	C37-C22-C23-C24
26	k	101	BCR	C1-C6-C7-C8
26	k	101	BCR	C5-C6-C7-C8
26	k	101	BCR	C17-C18-C19-C20
26	k	101	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
26	k	101	BCR	C21-C22-C23-C24
26	k	102	BCR	C7-C8-C9-C10
26	k	102	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C12-C13-C14
27	A	611	PL9	C27-C28-C29-C30
27	A	611	PL9	C27-C28-C29-C31
27	A	611	PL9	C29-C31-C32-C33
27	A	611	PL9	C37-C38-C39-C40
27	A	611	PL9	C37-C38-C39-C41
27	A	611	PL9	C38-C39-C41-C42
27	D	406	PL9	C32-C33-C34-C35
27	D	406	PL9	C32-C33-C34-C36
27	D	406	PL9	C47-C48-C49-C50
27	a	610	PL9	C7-C8-C9-C11
27	a	610	PL9	C35-C34-C36-C37
29	A	614	SQD	O6-C44-C45-O47
29	A	614	SQD	O5-C5-C6-S
29	B	623	SQD	C2-C1-O6-C44
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
29	B	623	SQD	O49-C7-O47-C45
29	B	623	SQD	C8-C7-O47-C45
29	D	409	SQD	C45-C44-O6-C1
29	D	409	SQD	O5-C1-O6-C44
29	a	613	SQD	O6-C44-C45-O47
29	a	614	SQD	O6-C44-C45-O47
29	a	614	SQD	O5-C5-C6-S
29	a	614	SQD	C5-C6-S-O7
29	a	614	SQD	C5-C6-S-O8
29	b	620	SQD	C8-C7-O47-C45
29	f	101	SQD	C2-C1-O6-C44
29	f	101	SQD	O5-C1-O6-C44
29	f	101	SQD	C8-C7-O47-C45
29	f	101	SQD	O10-C23-O48-C46
31	C	517	LMG	C2-C1-O1-C7
31	C	522	LMG	O9-C10-O7-C8
31	C	526	LMG	C11-C10-O7-C8
31	D	407	LMG	O6-C1-O1-C7
31	D	407	LMG	C11-C10-O7-C8
31	c	518	LMG	C29-C28-O8-C9
33	D	410	LHG	C3-O3-P-O4
33	D	410	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
33	D	410	LHG	C3-O3-P-O6
33	E	101	LHG	C3-O3-P-O4
33	E	101	LHG	C3-O3-P-O5
33	E	101	LHG	O9-C7-O7-C5
33	d	408	LHG	O1-C1-C2-C3
33	d	409	LHG	C3-O3-P-O5
33	e	103	LHG	O1-C1-C2-O2
33	e	103	LHG	O1-C1-C2-C3
33	e	103	LHG	C3-O3-P-O4
33	e	103	LHG	C3-O3-P-O6
33	e	103	LHG	O6-C4-C5-O7
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
24	D	403	CLA	O1D-CGD-O2D-CED
24	D	403	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	CBD-CGD-O2D-CED
31	c	518	LMG	O10-C28-O8-C9
27	D	406	PL9	C47-C48-C49-C51
27	a	610	PL9	C47-C48-C49-C51
29	f	101	SQD	C24-C23-O48-C46
31	B	620	LMG	O10-C28-O8-C9
31	a	615	LMG	O10-C28-O8-C9
24	B	614	CLA	C13-C15-C16-C17
29	b	620	SQD	O49-C7-O47-C45
29	f	101	SQD	O49-C7-O47-C45
31	C	526	LMG	O9-C10-O7-C8
31	D	407	LMG	O9-C10-O7-C8
24	b	604	CLA	C3-C5-C6-C7
31	B	620	LMG	C29-C28-O8-C9
31	C	522	LMG	C11-C10-O7-C8
33	E	101	LHG	C8-C7-O7-C5
25	A	608	PHO	C2C-C3C-CAC-CBC
24	B	605	CLA	C4-C3-C5-C6
24	B	614	CLA	C4-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	a	608	CLA	C4-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
24	c	507	CLA	C4-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	a	608	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	c	507	CLA	C2-C3-C5-C6
27	d	406	PL9	C38-C39-C41-C42
31	b	624	LMG	O10-C28-O8-C9
24	B	616	CLA	C3-C5-C6-C7
24	b	614	CLA	C3-C5-C6-C7
24	b	615	CLA	C3-C5-C6-C7
29	D	409	SQD	C24-C23-O48-C46
31	a	615	LMG	C29-C28-O8-C9
33	L	101	LHG	C7-C8-C9-C10
27	a	610	PL9	C22-C23-C24-C26
27	a	610	PL9	C47-C48-C49-C50
24	B	607	CLA	C3-C5-C6-C7
24	C	509	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	CBD-CGD-O2D-CED
33	a	612	LHG	C24-C25-C26-C27
33	D	410	LHG	O2-C2-C3-O3
24	B	616	CLA	CBA-CGA-O2A-C1
29	B	623	SQD	C24-C23-O48-C46
30	H	102	DGD	C4E-C5E-C6E-O5E
30	h	102	DGD	C4E-C5E-C6E-O5E
24	b	607	CLA	CBD-CGD-O2D-CED
30	h	102	DGD	O6E-C5E-C6E-O5E
31	b	624	LMG	C29-C28-O8-C9
24	B	605	CLA	C2-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
24	B	616	CLA	O1A-CGA-O2A-C1
29	D	409	SQD	O10-C23-O48-C46
31	b	624	LMG	O6-C5-C6-O5
27	A	611	PL9	C9-C11-C12-C13
27	A	611	PL9	C24-C26-C27-C28
27	A	611	PL9	C34-C36-C37-C38
27	D	406	PL9	C44-C46-C47-C48
27	a	610	PL9	C24-C26-C27-C28
27	a	610	PL9	C44-C46-C47-C48
28	B	627	STE	C9-C10-C11-C12
24	b	601	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	O1D-CGD-O2D-CED
30	C	523	DGD	O6E-C5E-C6E-O5E
29	b	620	SQD	O5-C1-O6-C44
31	a	616	LMG	O6-C1-O1-C7
31	b	624	LMG	O6-C1-O1-C7
30	H	102	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
30	A	615	DGD	C2A-C1A-O1G-C1G
31	B	621	LMG	C29-C28-O8-C9
31	C	517	LMG	C29-C28-O8-C9
24	b	606	CLA	CBD-CGD-O2D-CED
24	c	511	CLA	CBD-CGD-O2D-CED
29	B	623	SQD	O10-C23-O48-C46
30	A	615	DGD	O1A-C1A-O1G-C1G
30	A	615	DGD	CCA-CDA-CEA-CFA
24	c	501	CLA	CBD-CGD-O2D-CED
28	d	410	STE	C5-C6-C7-C8
24	B	615	CLA	C3-C5-C6-C7
28	A	618	STE	C12-C13-C14-C15
29	a	613	SQD	C12-C13-C14-C15
30	c	519	DGD	C2B-C3B-C4B-C5B
31	b	622	LMG	C34-C35-C36-C37
31	C	517	LMG	O10-C28-O8-C9
33	D	410	LHG	C1-C2-C3-O3
24	c	506	CLA	CBA-CGA-O2A-C1
29	b	620	SQD	C24-C23-O48-C46
31	a	615	LMG	C15-C16-C17-C18
25	d	402	PHO	CBD-CGD-O2D-CED
29	A	614	SQD	C16-C17-C18-C19
33	D	411	LHG	C12-C13-C14-C15
30	H	102	DGD	C7B-C8B-C9B-CAB
24	c	509	CLA	CBD-CGD-O2D-CED
24	B	606	CLA	C11-C12-C13-C14
24	B	615	CLA	C6-C7-C8-C9
24	C	503	CLA	C11-C10-C8-C9
24	C	509	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C10-C8-C9
24	a	606	CLA	C11-C12-C13-C14
24	a	608	CLA	C11-C12-C13-C14
24	b	601	CLA	C11-C10-C8-C9
24	b	603	CLA	C11-C12-C13-C14
24	b	606	CLA	C11-C10-C8-C9
24	b	610	CLA	C14-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C9
24	b	615	CLA	C6-C7-C8-C9
24	c	509	CLA	C11-C12-C13-C14
24	c	510	CLA	C11-C10-C8-C9
24	c	512	CLA	C6-C7-C8-C9
24	c	512	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	b	624	LMG	C4-C5-C6-O5
29	D	409	SQD	C2-C1-O6-C44
31	D	407	LMG	C2-C1-O1-C7
31	a	616	LMG	C2-C1-O1-C7
31	b	624	LMG	C2-C1-O1-C7
29	D	409	SQD	C23-C24-C25-C26
29	a	613	SQD	C14-C15-C16-C17
24	c	506	CLA	O1A-CGA-O2A-C1
29	b	620	SQD	O10-C23-O48-C46
26	B	619	BCR	C7-C8-C9-C34
26	K	101	BCR	C7-C8-C9-C34
26	T	101	BCR	C37-C22-C23-C24
26	d	405	BCR	C36-C18-C19-C20
26	k	101	BCR	C37-C22-C23-C24
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C12-C13-C35
24	B	613	CLA	C8-C10-C11-C12
31	D	408	LMG	C16-C17-C18-C19
31	c	523	LMG	C11-C10-O7-C8
31	d	411	LMG	C28-C29-C30-C31
30	c	521	DGD	C8B-C9B-CAB-CBB
33	D	412	LHG	C11-C12-C13-C14
35	V	201	HEC	C2C-C3C-CAC-CBC
27	a	610	PL9	C22-C23-C24-C25
27	a	610	PL9	C32-C33-C34-C35
24	B	607	CLA	C13-C15-C16-C17
24	B	615	CLA	C15-C16-C17-C18
24	C	506	CLA	C13-C15-C16-C17
24	c	509	CLA	C10-C11-C12-C13
30	c	519	DGD	O6E-C5E-C6E-O5E
24	B	613	CLA	C11-C10-C8-C7
24	B	603	CLA	C4-C3-C5-C6
29	a	613	SQD	C9-C10-C11-C12
29	a	613	SQD	C7-C8-C9-C10
31	D	407	LMG	C10-C11-C12-C13
26	t	101	BCR	C13-C14-C15-C16
27	A	611	PL9	C19-C21-C22-C23
28	B	622	STE	C1-C2-C3-C4
28	C	516	STE	C1-C2-C3-C4
28	a	617	STE	C1-C2-C3-C4
29	A	613	SQD	C7-C8-C9-C10
30	C	523	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
30	c	521	DGD	C1A-C2A-C3A-C4A
31	C	526	LMG	C28-C29-C30-C31
31	c	522	LMG	C28-C29-C30-C31
31	B	621	LMG	O10-C28-O8-C9
24	a	606	CLA	C15-C16-C17-C18
24	c	502	CLA	C13-C15-C16-C17
24	c	512	CLA	C2A-CAA-CBA-CGA
24	A	606	CLA	C15-C16-C17-C18
24	C	503	CLA	C5-C6-C7-C8
24	C	509	CLA	C10-C11-C12-C13
24	D	404	CLA	C10-C11-C12-C13
24	b	614	CLA	C5-C6-C7-C8
31	B	620	LMG	O6-C5-C6-O5
33	E	101	LHG	C23-C24-C25-C26
24	b	613	CLA	CBD-CGD-O2D-CED
31	a	615	LMG	O6-C1-O1-C7
28	d	410	STE	C3-C4-C5-C6
31	a	616	LMG	C29-C30-C31-C32
24	B	603	CLA	C8-C10-C11-C12
24	B	614	CLA	C8-C10-C11-C12
24	C	506	CLA	C8-C10-C11-C12
24	b	607	CLA	C8-C10-C11-C12
24	b	607	CLA	C10-C11-C12-C13
24	b	608	CLA	C8-C10-C11-C12
24	c	503	CLA	C8-C10-C11-C12
30	H	102	DGD	CCA-CDA-CEA-CFA
33	d	408	LHG	O2-C2-C3-O3
31	a	615	LMG	C10-C11-C12-C13
33	l	101	LHG	C7-C8-C9-C10
24	B	601	CLA	C5-C6-C7-C8
24	C	510	CLA	C10-C11-C12-C13
24	c	506	CLA	C10-C11-C12-C13
24	B	609	CLA	C13-C15-C16-C17
24	C	508	CLA	C15-C16-C17-C18
24	c	503	CLA	C10-C11-C12-C13
28	b	621	STE	C5-C6-C7-C8
30	C	524	DGD	C4A-C5A-C6A-C7A
30	c	521	DGD	CAB-CBB-CCB-CDB
24	C	509	CLA	O1D-CGD-O2D-CED
24	C	513	CLA	O1D-CGD-O2D-CED
24	b	611	CLA	C13-C15-C16-C17
24	b	616	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	c	502	CLA	C15-C16-C17-C18
24	c	506	CLA	C15-C16-C17-C18
30	c	520	DGD	C3B-C4B-C5B-C6B
28	A	617	STE	C7-C8-C9-C10
28	i	101	STE	C3-C4-C5-C6
24	C	507	CLA	C5-C6-C7-C8
31	a	616	LMG	C10-C11-C12-C13
31	c	523	LMG	O9-C10-O7-C8
33	d	408	LHG	C1-C2-C3-O3
24	b	606	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C10-C11-C12-C13
24	b	601	CLA	C10-C11-C12-C13
24	b	605	CLA	C5-C6-C7-C8
24	b	616	CLA	C8-C10-C11-C12
24	c	503	CLA	C15-C16-C17-C18
24	c	505	CLA	C13-C15-C16-C17
24	c	513	CLA	C13-C15-C16-C17
28	d	414	STE	C1-C2-C3-C4
24	C	509	CLA	C13-C15-C16-C17
24	b	606	CLA	C15-C16-C17-C18
24	B	601	CLA	C13-C15-C16-C17
24	C	506	CLA	C15-C16-C17-C18
24	b	601	CLA	C15-C16-C17-C18
24	b	611	CLA	C8-C10-C11-C12
30	c	519	DGD	C1B-C2B-C3B-C4B
24	b	609	CLA	C15-C16-C17-C18
24	b	607	CLA	O1D-CGD-O2D-CED
24	D	404	CLA	C16-C17-C18-C19
33	D	411	LHG	C32-C33-C34-C35
24	B	615	CLA	C5-C6-C7-C8
26	T	101	BCR	C7-C8-C9-C34
29	a	613	SQD	C26-C27-C28-C29
31	c	523	LMG	C13-C14-C15-C16
26	d	405	BCR	C17-C18-C19-C20
26	t	101	BCR	C7-C8-C9-C10
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C5-C6-C7-C8
33	D	410	LHG	O1-C1-C2-C3
33	D	411	LHG	O1-C1-C2-C3
33	D	412	LHG	O1-C1-C2-C3
33	a	612	LHG	O1-C1-C2-C3
29	b	620	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
24	B	603	CLA	C16-C17-C18-C20
24	C	510	CLA	C16-C17-C18-C19
24	C	512	CLA	C16-C17-C18-C20
24	C	513	CLA	C16-C17-C18-C19
24	c	506	CLA	C16-C17-C18-C20
24	d	403	CLA	C16-C17-C18-C19
30	C	524	DGD	C3B-C4B-C5B-C6B
30	c	521	DGD	C6B-C7B-C8B-C9B
24	B	612	CLA	C13-C15-C16-C17
24	B	603	CLA	C2-C3-C5-C6
35	V	201	HEC	C4C-C3C-CAC-CBC
24	C	511	CLA	CBD-CGD-O2D-CED
24	B	606	CLA	C16-C17-C18-C19
24	B	616	CLA	C11-C12-C13-C14
24	C	513	CLA	C16-C17-C18-C20
24	b	611	CLA	C16-C17-C18-C20
24	d	403	CLA	C16-C17-C18-C20
24	B	614	CLA	C15-C16-C17-C18
28	E	104	STE	C11-C10-C9-C8
28	H	103	STE	C3-C4-C5-C6
28	M	103	STE	C9-C10-C11-C12
33	a	612	LHG	C25-C26-C27-C28
28	A	617	STE	C9-C10-C11-C12
28	i	101	STE	C6-C7-C8-C9
28	j	102	STE	C6-C7-C8-C9
29	D	409	SQD	C25-C26-C27-C28
29	b	620	SQD	C13-C14-C15-C16
30	c	521	DGD	C4B-C5B-C6B-C7B
31	B	620	LMG	C32-C33-C34-C35
31	C	526	LMG	C30-C31-C32-C33
31	D	408	LMG	C17-C18-C19-C20
33	D	410	LHG	C16-C17-C18-C19
33	D	410	LHG	C17-C18-C19-C20
33	E	101	LHG	C17-C18-C19-C20
33	e	103	LHG	C13-C14-C15-C16
28	d	407	STE	C2-C3-C4-C5
28	e	105	STE	C13-C14-C15-C16
28	m	102	STE	C4-C5-C6-C7
31	b	622	LMG	C16-C17-C18-C19
31	c	522	LMG	C36-C37-C38-C39
28	B	625	STE	C12-C13-C14-C15
28	B	627	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	E	104	STE	C3-C4-C5-C6
28	M	103	STE	C6-C7-C8-C9
28	Z	101	STE	C6-C7-C8-C9
28	e	106	STE	C3-C4-C5-C6
29	a	614	SQD	C18-C19-C20-C21
31	B	621	LMG	C39-C40-C41-C42
31	a	615	LMG	C35-C36-C37-C38
31	d	411	LMG	C33-C34-C35-C36
33	a	612	LHG	C34-C35-C36-C37
33	d	408	LHG	C28-C29-C30-C31
33	l	101	LHG	C16-C17-C18-C19
33	l	101	LHG	C27-C28-C29-C30
33	D	412	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
28	E	104	STE	C4-C5-C6-C7
30	c	521	DGD	C4A-C5A-C6A-C7A
33	D	411	LHG	C16-C17-C18-C19
33	D	412	LHG	C31-C32-C33-C34
33	l	101	LHG	C17-C18-C19-C20
24	B	615	CLA	C4B-C3B-CAB-CBB
24	b	601	CLA	C4B-C3B-CAB-CBB
24	c	505	CLA	C4B-C3B-CAB-CBB
28	C	520	STE	C7-C8-C9-C10
24	B	601	CLA	C16-C17-C18-C20
24	B	603	CLA	C16-C17-C18-C19
24	b	602	CLA	C16-C17-C18-C19
24	b	613	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C19
24	b	601	CLA	O1D-CGD-O2D-CED
28	A	616	STE	C12-C13-C14-C15
28	A	618	STE	C11-C12-C13-C14
28	M	103	STE	C11-C12-C13-C14
29	b	620	SQD	C29-C30-C31-C32
31	c	523	LMG	C15-C16-C17-C18
24	D	404	CLA	C5-C6-C7-C8
31	a	615	LMG	C11-C10-O7-C8
24	b	606	CLA	C6-C7-C8-C10
24	b	613	CLA	C11-C10-C8-C7
24	c	503	CLA	C6-C7-C8-C10
28	d	414	STE	C5-C6-C7-C8
29	a	614	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	c	522	LMG	C39-C40-C41-C42
24	c	513	CLA	C8-C10-C11-C12
28	Z	101	STE	C11-C12-C13-C14
28	c	517	STE	C9-C10-C11-C12
29	a	613	SQD	C11-C12-C13-C14
30	C	523	DGD	CBB-CCB-CDB-CEB
30	h	102	DGD	C7B-C8B-C9B-CAB
33	L	101	LHG	C11-C10-C9-C8
24	c	512	CLA	C3A-C2A-CAA-CBA
28	b	623	STE	C5-C6-C7-C8
30	C	524	DGD	C6B-C7B-C8B-C9B
30	C	524	DGD	CCA-CDA-CEA-CFA
24	D	402	CLA	C13-C15-C16-C17
24	a	605	CLA	C15-C16-C17-C18
28	B	622	STE	C10-C11-C12-C13
29	f	101	SQD	C33-C34-C35-C36
24	B	601	CLA	C16-C17-C18-C19
24	b	611	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C20
28	a	617	STE	C6-C7-C8-C9
30	c	519	DGD	C2A-C3A-C4A-C5A
30	h	102	DGD	C2B-C3B-C4B-C5B
33	D	410	LHG	C18-C19-C20-C21
33	E	101	LHG	C28-C29-C30-C31
28	j	102	STE	C5-C6-C7-C8
30	H	102	DGD	C7A-C8A-C9A-CAA
33	e	103	LHG	C17-C18-C19-C20
24	c	511	CLA	O1D-CGD-O2D-CED
31	b	622	LMG	C29-C28-O8-C9
30	A	615	DGD	C1G-C2G-C3G-O3G
28	B	624	STE	C6-C7-C8-C9
28	C	520	STE	C5-C6-C7-C8
28	c	517	STE	C12-C13-C14-C15
30	c	520	DGD	CCB-CDB-CEB-CFB
31	B	621	LMG	C32-C33-C34-C35
31	D	407	LMG	C35-C36-C37-C38
31	D	408	LMG	C13-C14-C15-C16
33	l	101	LHG	C29-C30-C31-C32
28	E	104	STE	C9-C10-C11-C12
28	d	407	STE	C14-C15-C16-C17
28	d	412	STE	C3-C4-C5-C6
28	m	102	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	C11-C12-C13-C14
29	a	613	SQD	C31-C32-C33-C34
29	a	614	SQD	C31-C32-C33-C34
29	f	101	SQD	C32-C33-C34-C35
30	h	102	DGD	C8B-C9B-CAB-CBB
31	B	620	LMG	C33-C34-C35-C36
31	C	526	LMG	C37-C38-C39-C40
31	b	624	LMG	C32-C33-C34-C35
33	D	412	LHG	C9-C10-C11-C12
33	E	101	LHG	C24-C25-C26-C27
28	I	101	STE	C7-C8-C9-C10
29	A	613	SQD	C30-C31-C32-C33
31	D	407	LMG	C39-C40-C41-C42
33	d	408	LHG	C17-C18-C19-C20
28	M	103	STE	C13-C14-C15-C16
28	b	625	STE	C11-C10-C9-C8
28	d	414	STE	C6-C7-C8-C9
28	j	101	STE	C4-C5-C6-C7
29	D	409	SQD	C31-C32-C33-C34
28	C	529	STE	C7-C8-C9-C10
28	M	101	STE	C7-C8-C9-C10
28	m	102	STE	C11-C10-C9-C8
29	b	620	SQD	C16-C17-C18-C19
30	h	102	DGD	C7A-C8A-C9A-CAA
31	B	620	LMG	C34-C35-C36-C37
31	a	615	LMG	C32-C33-C34-C35
33	D	411	LHG	C11-C12-C13-C14
33	D	411	LHG	C29-C30-C31-C32
33	l	101	LHG	C34-C35-C36-C37
27	d	406	PL9	C42-C43-C44-C45
24	a	606	CLA	C2B-C3B-CAB-CBB
24	b	601	CLA	C2B-C3B-CAB-CBB
26	H	101	BCR	C5-C6-C7-C8
26	b	617	BCR	C1-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C30
26	t	101	BCR	C1-C6-C7-C8
26	t	101	BCR	C23-C24-C25-C26
28	B	627	STE	C10-C11-C12-C13
28	J	101	STE	C5-C6-C7-C8
28	e	101	STE	C13-C14-C15-C16
30	H	102	DGD	C4B-C5B-C6B-C7B
31	B	621	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
31	D	407	LMG	C30-C31-C32-C33
31	c	523	LMG	C37-C38-C39-C40
33	e	103	LHG	C8-C7-O7-C5
29	D	409	SQD	O6-C44-C45-C46
24	b	610	CLA	C15-C16-C17-C18
28	b	621	STE	C11-C12-C13-C14
31	b	624	LMG	C20-C21-C22-C23
31	d	411	LMG	C36-C37-C38-C39
28	d	410	STE	C9-C10-C11-C12
31	C	522	LMG	C35-C36-C37-C38
31	D	408	LMG	C39-C40-C41-C42
31	a	615	LMG	C29-C30-C31-C32
28	I	101	STE	C1-C2-C3-C4
29	B	623	SQD	C23-C24-C25-C26
28	J	101	STE	C6-C7-C8-C9
28	b	621	STE	C4-C5-C6-C7
30	A	615	DGD	C9B-CAB-CBB-CCB
30	C	525	DGD	C3A-C4A-C5A-C6A
27	a	610	PL9	C4-C3-C7-C8
28	B	625	STE	C6-C7-C8-C9
28	C	528	STE	C7-C8-C9-C10
28	H	104	STE	C14-C15-C16-C17
33	D	410	LHG	C11-C10-C9-C8
31	a	615	LMG	O9-C10-O7-C8
28	e	105	STE	C14-C15-C16-C17
29	A	613	SQD	C15-C16-C17-C18
31	C	526	LMG	C12-C13-C14-C15
33	D	412	LHG	C13-C14-C15-C16
33	d	408	LHG	C9-C10-C11-C12
27	A	611	PL9	C28-C29-C31-C32
24	C	510	CLA	C16-C17-C18-C20
28	C	528	STE	C5-C6-C7-C8
28	K	102	STE	C10-C11-C12-C13
33	D	412	LHG	C17-C18-C19-C20
33	e	103	LHG	C24-C25-C26-C27
28	B	625	STE	C5-C6-C7-C8
28	d	410	STE	C7-C8-C9-C10
28	d	414	STE	C2-C3-C4-C5
28	j	102	STE	C4-C5-C6-C7
29	a	613	SQD	C16-C17-C18-C19
33	D	410	LHG	C14-C15-C16-C17
31	d	411	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
28	b	623	STE	C4-C5-C6-C7
28	c	516	STE	C2-C3-C4-C5
31	C	526	LMG	C15-C16-C17-C18
31	a	615	LMG	C31-C32-C33-C34
28	B	627	STE	C3-C4-C5-C6
30	H	102	DGD	C5B-C6B-C7B-C8B
30	c	520	DGD	C8A-C9A-CAA-CBA
30	h	102	DGD	CCA-CDA-CEA-CFA
31	c	522	LMG	C29-C30-C31-C32
24	C	509	CLA	C8-C10-C11-C12
28	K	102	STE	C12-C13-C14-C15
30	C	523	DGD	CCA-CDA-CEA-CFA
30	H	102	DGD	C5A-C6A-C7A-C8A
31	D	408	LMG	C12-C13-C14-C15
28	M	103	STE	C11-C10-C9-C8
33	D	412	LHG	C28-C29-C30-C31
28	A	612	STE	C4-C5-C6-C7
28	c	516	STE	C7-C8-C9-C10
29	A	614	SQD	C10-C11-C12-C13
31	B	621	LMG	C37-C38-C39-C40
31	C	517	LMG	C16-C17-C18-C19
33	D	412	LHG	C12-C13-C14-C15
24	B	615	CLA	C16-C17-C18-C20
24	c	503	CLA	C16-C17-C18-C20
31	b	622	LMG	C11-C10-O7-C8
28	C	516	STE	C3-C4-C5-C6
28	C	527	STE	C2-C3-C4-C5
28	c	517	STE	C5-C6-C7-C8
29	A	613	SQD	C11-C10-C9-C8
24	C	502	CLA	C15-C16-C17-C18
24	C	505	CLA	C15-C16-C17-C18
31	C	517	LMG	C11-C12-C13-C14
31	c	518	LMG	C11-C12-C13-C14
33	D	411	LHG	C14-C15-C16-C17
28	d	407	STE	C5-C6-C7-C8
31	B	621	LMG	C15-C16-C17-C18
33	l	101	LHG	C11-C12-C13-C14
29	f	101	SQD	C25-C26-C27-C28
30	C	523	DGD	C6A-C7A-C8A-C9A
28	E	102	STE	C1-C2-C3-C4
26	B	619	BCR	C7-C8-C9-C10
30	C	524	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
31	a	615	LMG	C8-C7-O1-C1
28	m	102	STE	C6-C7-C8-C9
33	d	409	LHG	C9-C10-C11-C12
24	B	611	CLA	C16-C17-C18-C20
24	b	609	CLA	C16-C17-C18-C19
24	b	609	CLA	C16-C17-C18-C20
28	B	622	STE	C5-C6-C7-C8
30	A	615	DGD	C8B-C9B-CAB-CBB
30	h	102	DGD	CAA-CBA-CCA-CDA
33	d	408	LHG	C25-C26-C27-C28
33	l	101	LHG	C10-C11-C12-C13
24	c	505	CLA	C4-C3-C5-C6
28	B	625	STE	C11-C12-C13-C14
28	I	102	STE	C4-C5-C6-C7
33	L	101	LHG	C17-C18-C19-C20
29	a	613	SQD	C15-C16-C17-C18
33	D	412	LHG	C25-C26-C27-C28
24	B	613	CLA	C10-C11-C12-C13
24	c	505	CLA	C5-C6-C7-C8
29	B	623	SQD	C10-C11-C12-C13
31	D	408	LMG	C28-C29-C30-C31
30	C	524	DGD	CDB-CEB-CFB-CGB
24	c	509	CLA	O1D-CGD-O2D-CED
30	c	520	DGD	CAA-CBA-CCA-CDA
31	a	616	LMG	C14-C15-C16-C17
24	b	613	CLA	C15-C16-C17-C18
24	B	615	CLA	C16-C17-C18-C19
24	C	512	CLA	C16-C17-C18-C19
24	D	404	CLA	C16-C17-C18-C20
28	K	102	STE	C7-C8-C9-C10
28	Z	101	STE	C5-C6-C7-C8
29	B	623	SQD	C9-C10-C11-C12
31	b	622	LMG	O10-C28-O8-C9
27	d	406	PL9	C47-C48-C49-C51
31	B	620	LMG	C29-C30-C31-C32
33	D	410	LHG	C15-C16-C17-C18
33	D	412	LHG	C23-C24-C25-C26
33	e	103	LHG	C7-C8-C9-C10
30	c	520	DGD	C4E-C5E-C6E-O5E
24	c	512	CLA	C13-C15-C16-C17
24	d	404	CLA	C5-C6-C7-C8
29	A	613	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	c	508	CLA	CBD-CGD-O2D-CED
28	A	617	STE	C4-C5-C6-C7
28	A	618	STE	C14-C15-C16-C17
28	B	624	STE	C11-C10-C9-C8
28	B	625	STE	C9-C10-C11-C12
28	M	101	STE	C4-C5-C6-C7
28	b	626	STE	C4-C5-C6-C7
29	a	613	SQD	C13-C14-C15-C16
28	b	623	STE	C9-C10-C11-C12
28	c	516	STE	C5-C6-C7-C8
30	H	102	DGD	C3B-C4B-C5B-C6B
30	c	519	DGD	CBA-CCA-CDA-CEA
31	B	620	LMG	C11-C12-C13-C14
24	B	616	CLA	C8-C10-C11-C12
30	C	523	DGD	C5B-C6B-C7B-C8B
31	D	407	LMG	C13-C14-C15-C16
31	a	615	LMG	C13-C14-C15-C16
29	A	614	SQD	C14-C15-C16-C17
30	C	524	DGD	C7B-C8B-C9B-CAB
24	B	606	CLA	C16-C17-C18-C20
24	B	616	CLA	C11-C12-C13-C15
28	d	407	STE	C7-C8-C9-C10
28	m	102	STE	C2-C3-C4-C5
29	B	623	SQD	C17-C18-C19-C20
30	A	615	DGD	C2A-C3A-C4A-C5A
30	c	519	DGD	C7A-C8A-C9A-CAA
31	b	624	LMG	C12-C13-C14-C15
28	J	101	STE	C4-C5-C6-C7
28	b	621	STE	C12-C13-C14-C15
29	D	409	SQD	C33-C34-C35-C36
24	C	506	CLA	C2-C3-C5-C6
29	A	613	SQD	C12-C13-C14-C15
29	B	623	SQD	C13-C14-C15-C16
29	b	620	SQD	C28-C29-C30-C31
30	c	519	DGD	C3A-C4A-C5A-C6A
31	D	407	LMG	C14-C15-C16-C17
25	d	402	PHO	O1D-CGD-O2D-CED
30	A	615	DGD	C7B-C8B-C9B-CAB
28	e	104	STE	C11-C12-C13-C14
28	H	103	STE	C5-C6-C7-C8
28	d	410	STE	C4-C5-C6-C7
30	H	102	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
28	d	407	STE	C4-C5-C6-C7
28	z	101	STE	C4-C5-C6-C7
30	c	519	DGD	C9A-CAA-CBA-CCA
31	D	408	LMG	C33-C34-C35-C36
33	D	410	LHG	O1-C1-C2-O2
24	d	404	CLA	C3-C5-C6-C7
30	h	102	DGD	CDA-CEA-CFA-CGA
28	D	413	STE	C4-C5-C6-C7
29	A	613	SQD	C16-C17-C18-C19
31	C	522	LMG	C12-C13-C14-C15
24	c	503	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	c	513	CLA	C1A-C2A-CAA-CBA
24	B	606	CLA	C8-C10-C11-C12
24	D	402	CLA	C15-C16-C17-C18
24	b	604	CLA	C8-C10-C11-C12
29	a	613	SQD	C27-C28-C29-C30
30	C	523	DGD	C9A-CAA-CBA-CCA
31	a	615	LMG	C11-C12-C13-C14
33	d	408	LHG	C12-C13-C14-C15
24	C	504	CLA	C11-C12-C13-C14
28	E	103	STE	C10-C11-C12-C13
28	c	516	STE	C6-C7-C8-C9
31	b	624	LMG	C21-C22-C23-C24
24	C	512	CLA	C8-C10-C11-C12
30	h	102	DGD	C5B-C6B-C7B-C8B
24	B	604	CLA	C11-C10-C8-C7
24	B	612	CLA	C12-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C15
24	C	506	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	D	403	CLA	C12-C13-C15-C16
24	D	404	CLA	C11-C10-C8-C7
24	a	608	CLA	C6-C7-C8-C10
24	b	601	CLA	C11-C10-C8-C7
24	b	606	CLA	C12-C13-C15-C16
24	b	611	CLA	C12-C13-C15-C16
24	b	614	CLA	C12-C13-C15-C16
24	b	615	CLA	C6-C7-C8-C10
24	c	506	CLA	C11-C12-C13-C15
24	d	403	CLA	C6-C7-C8-C10
28	B	627	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	c	521	DGD	CBB-CCB-CDB-CEB
24	B	611	CLA	C16-C17-C18-C19
24	c	508	CLA	C8-C10-C11-C12
24	B	612	CLA	C10-C11-C12-C13
24	C	508	CLA	C10-C11-C12-C13
24	c	505	CLA	C2-C3-C5-C6
27	d	406	PL9	C13-C14-C16-C17
28	I	102	STE	C6-C7-C8-C9
30	h	102	DGD	CBB-CCB-CDB-CEB
31	c	522	LMG	O6-C5-C6-O5
31	C	522	LMG	C36-C37-C38-C39
31	c	523	LMG	C29-C30-C31-C32
24	b	610	CLA	C2A-CAA-CBA-CGA
24	B	613	CLA	C14-C13-C15-C16
24	B	614	CLA	C14-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C14
24	C	507	CLA	C11-C10-C8-C9
24	b	607	CLA	C6-C7-C8-C9
24	c	506	CLA	C6-C7-C8-C9
24	c	506	CLA	C11-C12-C13-C14
24	d	404	CLA	C14-C13-C15-C16
28	E	104	STE	C10-C11-C12-C13
28	M	101	STE	C9-C10-C11-C12
29	a	614	SQD	C17-C18-C19-C20
30	A	615	DGD	C4A-C5A-C6A-C7A
31	b	624	LMG	C29-C30-C31-C32
28	a	617	STE	C4-C5-C6-C7
29	b	620	SQD	C12-C13-C14-C15
30	C	523	DGD	CCB-CDB-CEB-CFB
30	C	524	DGD	CAB-CBB-CCB-CDB
31	D	407	LMG	C16-C17-C18-C19
33	E	101	LHG	C12-C13-C14-C15
24	b	614	CLA	C10-C11-C12-C13
24	c	501	CLA	O1D-CGD-O2D-CED
28	d	413	STE	C10-C11-C12-C13
33	e	103	LHG	O9-C7-O7-C5
24	B	606	CLA	C10-C11-C12-C13
29	B	623	SQD	O6-C44-C45-C46
31	D	407	LMG	O1-C7-C8-C9
33	e	103	LHG	C4-C5-C6-O8
29	A	613	SQD	C24-C25-C26-C27
29	a	613	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C9-C10-C11-C12
28	Z	101	STE	C2-C3-C4-C5
30	C	523	DGD	CDB-CEB-CFB-CGB
28	d	414	STE	C11-C10-C9-C8
24	c	503	CLA	C16-C17-C18-C19
28	d	412	STE	C5-C6-C7-C8
29	A	613	SQD	C13-C14-C15-C16
29	A	613	SQD	C32-C33-C34-C35
33	D	411	LHG	C24-C25-C26-C27
31	a	616	LMG	C17-C18-C19-C20
31	a	616	LMG	C33-C34-C35-C36
31	b	624	LMG	C11-C12-C13-C14
33	E	101	LHG	C32-C33-C34-C35
24	b	613	CLA	O1D-CGD-O2D-CED
31	c	523	LMG	O6-C5-C6-O5
28	M	102	STE	C4-C5-C6-C7
31	b	624	LMG	C13-C14-C15-C16
24	C	506	CLA	C4-C3-C5-C6
27	d	406	PL9	C28-C29-C31-C32
24	c	508	CLA	C5-C6-C7-C8
28	e	104	STE	C12-C13-C14-C15
30	c	520	DGD	C6B-C7B-C8B-C9B
31	D	408	LMG	O6-C5-C6-O5
30	c	519	DGD	O6D-C5D-C6D-O5D
24	a	608	CLA	C5-C6-C7-C8
28	M	101	STE	C11-C10-C9-C8
24	B	601	CLA	C2A-CAA-CBA-CGA
28	E	102	STE	C4-C5-C6-C7
28	b	623	STE	C10-C11-C12-C13
24	b	603	CLA	C8-C10-C11-C12
24	c	507	CLA	C5-C6-C7-C8
24	c	508	CLA	C10-C11-C12-C13
28	M	101	STE	C5-C6-C7-C8
30	C	524	DGD	CAA-CBA-CCA-CDA
28	I	102	STE	C5-C6-C7-C8
29	b	620	SQD	C18-C19-C20-C21
30	A	615	DGD	C5A-C6A-C7A-C8A
31	c	522	LMG	C34-C35-C36-C37
24	b	607	CLA	CBA-CGA-O2A-C1
24	B	604	CLA	O2A-C1-C2-C3
28	B	627	STE	C7-C8-C9-C10
28	b	623	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	b	624	LMG	C30-C31-C32-C33
28	D	413	STE	C9-C10-C11-C12
28	b	621	STE	C9-C10-C11-C12
30	H	102	DGD	CAA-CBA-CCA-CDA
30	c	519	DGD	C6A-C7A-C8A-C9A
31	b	622	LMG	C33-C34-C35-C36
31	c	518	LMG	C15-C16-C17-C18
31	c	522	LMG	C38-C39-C40-C41
31	c	523	LMG	C30-C31-C32-C33
33	D	410	LHG	C11-C12-C13-C14
29	A	614	SQD	C11-C10-C9-C8
24	b	606	CLA	C10-C11-C12-C13
28	D	413	STE	C12-C13-C14-C15
31	D	408	LMG	C38-C39-C40-C41
31	b	624	LMG	C39-C40-C41-C42
28	e	106	STE	C11-C10-C9-C8
28	m	102	STE	C1-C2-C3-C4
28	A	616	STE	C11-C12-C13-C14
30	c	521	DGD	C3A-C4A-C5A-C6A
28	C	529	STE	C6-C7-C8-C9
28	d	412	STE	C7-C8-C9-C10
30	A	615	DGD	C9A-CAA-CBA-CCA
33	D	412	LHG	C24-C25-C26-C27
24	c	503	CLA	C3-C5-C6-C7
28	C	528	STE	C14-C15-C16-C17
29	A	613	SQD	C28-C29-C30-C31
29	a	614	SQD	C9-C10-C11-C12
30	C	524	DGD	C5B-C6B-C7B-C8B
30	c	521	DGD	C2A-C3A-C4A-C5A
31	D	408	LMG	C37-C38-C39-C40
28	t	102	STE	C1-C2-C3-C4
28	B	625	STE	C4-C5-C6-C7
33	L	101	LHG	C27-C28-C29-C30
29	A	613	SQD	O6-C44-C45-O47
30	A	615	DGD	O2G-C2G-C3G-O3G
31	C	517	LMG	O7-C8-C9-O8
33	e	103	LHG	O2-C2-C3-O3
30	A	615	DGD	C7A-C8A-C9A-CAA
31	B	620	LMG	C31-C32-C33-C34
31	a	615	LMG	C17-C18-C19-C20
31	a	615	LMG	C23-C24-C25-C26
30	H	102	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
28	C	528	STE	C4-C5-C6-C7
28	d	407	STE	C13-C14-C15-C16
29	f	101	SQD	C29-C30-C31-C32
31	B	621	LMG	C36-C37-C38-C39
24	b	601	CLA	C3-C5-C6-C7
33	l	101	LHG	C14-C15-C16-C17
24	B	610	CLA	C15-C16-C17-C18
24	c	509	CLA	C13-C15-C16-C17
24	c	506	CLA	C2-C1-O2A-CGA
28	M	101	STE	C6-C7-C8-C9
28	K	102	STE	C14-C15-C16-C17
28	b	621	STE	C3-C4-C5-C6
28	m	102	STE	C15-C16-C17-C18
29	A	614	SQD	C19-C20-C21-C22
28	t	102	STE	C7-C8-C9-C10
30	C	523	DGD	O6D-C5D-C6D-O5D
28	H	103	STE	C6-C7-C8-C9
24	b	606	CLA	O1D-CGD-O2D-CED
24	A	605	CLA	C13-C15-C16-C17
24	b	607	CLA	C16-C17-C18-C20
24	c	509	CLA	C16-C17-C18-C20
30	C	524	DGD	C4B-C5B-C6B-C7B
24	b	604	CLA	C4-C3-C5-C6
24	c	509	CLA	C4-C3-C5-C6
27	a	610	PL9	C12-C11-C9-C10
28	A	617	STE	C2-C3-C4-C5
33	D	411	LHG	C10-C11-C12-C13
28	C	520	STE	C6-C7-C8-C9
28	b	625	STE	C9-C10-C11-C12
29	A	614	SQD	C9-C10-C11-C12
31	D	407	LMG	C17-C18-C19-C20
33	E	101	LHG	C10-C11-C12-C13
33	l	101	LHG	C12-C13-C14-C15
31	b	622	LMG	O9-C10-O7-C8
24	B	601	CLA	C11-C10-C8-C9
24	B	604	CLA	C11-C10-C8-C9
24	B	604	CLA	C14-C13-C15-C16
24	B	605	CLA	C6-C7-C8-C9
24	B	612	CLA	C14-C13-C15-C16
24	B	616	CLA	C6-C7-C8-C9
24	C	505	CLA	C11-C12-C13-C14
24	C	506	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	513	CLA	C11-C10-C8-C9
24	D	404	CLA	C11-C10-C8-C9
24	a	608	CLA	C6-C7-C8-C9
24	b	614	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C9
24	d	403	CLA	C6-C7-C8-C9
24	d	404	CLA	C11-C12-C13-C14
31	C	522	LMG	C29-C30-C31-C32
24	B	603	CLA	C15-C16-C17-C18
24	B	605	CLA	C8-C10-C11-C12
24	B	615	CLA	C13-C15-C16-C17
33	a	612	LHG	C2-C3-O3-P
28	H	103	STE	C1-C2-C3-C4
24	C	502	CLA	C4B-C3B-CAB-CBB
24	B	603	CLA	C10-C11-C12-C13
29	B	623	SQD	C19-C20-C21-C22
29	a	614	SQD	C35-C36-C37-C38
28	j	101	STE	C7-C8-C9-C10
31	b	622	LMG	C36-C37-C38-C39
28	z	101	STE	C3-C4-C5-C6
29	D	409	SQD	C27-C28-C29-C30
29	b	620	SQD	C26-C27-C28-C29
33	e	103	LHG	O6-C4-C5-C6
29	a	614	SQD	C24-C25-C26-C27
30	c	519	DGD	CAA-CBA-CCA-CDA
33	E	101	LHG	C25-C26-C27-C28
28	C	519	STE	C2-C3-C4-C5
28	b	625	STE	C11-C12-C13-C14
33	D	411	LHG	C15-C16-C17-C18
24	B	604	CLA	C11-C12-C13-C15
24	B	604	CLA	C12-C13-C15-C16
24	B	613	CLA	C11-C12-C13-C15
24	B	613	CLA	C12-C13-C15-C16
24	B	615	CLA	C6-C7-C8-C10
24	B	615	CLA	C11-C12-C13-C15
24	B	616	CLA	C6-C7-C8-C10
24	C	502	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C10-C8-C7
24	C	513	CLA	C11-C10-C8-C7
24	a	606	CLA	C12-C13-C15-C16
24	a	608	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	b	601	CLA	C6-C7-C8-C10
24	b	607	CLA	C6-C7-C8-C10
24	b	616	CLA	C11-C10-C8-C7
24	c	504	CLA	C11-C10-C8-C7
24	c	506	CLA	C6-C7-C8-C10
24	d	404	CLA	C11-C12-C13-C15
24	d	404	CLA	C12-C13-C15-C16
24	c	504	CLA	C8-C10-C11-C12
28	K	102	STE	C5-C6-C7-C8
28	A	617	STE	C13-C14-C15-C16
29	a	614	SQD	C7-C8-C9-C10
31	C	522	LMG	C19-C20-C21-C22
29	a	613	SQD	C33-C34-C35-C36
30	C	523	DGD	CAB-CBB-CCB-CDB
28	A	612	STE	C3-C4-C5-C6
24	c	509	CLA	C2-C3-C5-C6
33	E	101	LHG	C29-C30-C31-C32
33	l	101	LHG	C26-C27-C28-C29
24	B	604	CLA	C10-C11-C12-C13
31	D	407	LMG	C29-C28-O8-C9
26	C	514	BCR	C11-C12-C13-C35
28	I	102	STE	C9-C10-C11-C12
28	d	413	STE	C12-C13-C14-C15
24	b	607	CLA	O1A-CGA-O2A-C1
28	I	101	STE	C2-C3-C4-C5
28	H	104	STE	C10-C11-C12-C13
31	a	616	LMG	C16-C17-C18-C19
33	a	612	LHG	C23-C24-C25-C26
28	C	516	STE	C9-C10-C11-C12
29	b	620	SQD	C25-C26-C27-C28
31	b	622	LMG	C17-C18-C19-C20
28	A	618	STE	C13-C14-C15-C16
28	Z	101	STE	C9-C10-C11-C12
28	b	623	STE	C3-C4-C5-C6
29	A	613	SQD	O6-C44-C45-C46
29	A	614	SQD	O6-C44-C45-C46
31	C	517	LMG	C7-C8-C9-O8
31	C	526	LMG	O1-C7-C8-C9
31	a	616	LMG	C7-C8-C9-O8
33	E	101	LHG	C4-C5-C6-O8
28	J	101	STE	C7-C8-C9-C10
28	M	101	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C18-C19-C20-C21
24	A	605	CLA	C15-C16-C17-C18
24	B	616	CLA	C5-C6-C7-C8
28	b	625	STE	C4-C5-C6-C7
28	m	102	STE	C11-C12-C13-C14
28	m	102	STE	C14-C15-C16-C17
31	b	624	LMG	C15-C16-C17-C18
28	b	627	STE	C9-C10-C11-C12
30	c	519	DGD	C6B-C7B-C8B-C9B
27	d	406	PL9	C30-C29-C31-C32
28	C	519	STE	C3-C4-C5-C6
27	a	610	PL9	C42-C43-C44-C45
24	b	607	CLA	C16-C17-C18-C19
24	c	509	CLA	C16-C17-C18-C19
24	c	511	CLA	C16-C17-C18-C19
28	e	104	STE	C14-C15-C16-C17
26	D	405	BCR	C23-C24-C25-C26
24	B	611	CLA	C8-C10-C11-C12
29	B	623	SQD	C35-C36-C37-C38
28	B	625	STE	C1-C2-C3-C4
31	b	622	LMG	C40-C41-C42-C43
28	b	621	STE	C10-C11-C12-C13
24	B	606	CLA	C5-C6-C7-C8
28	B	625	STE	C7-C8-C9-C10
29	f	101	SQD	C27-C28-C29-C30
24	c	511	CLA	C16-C17-C18-C20
24	B	606	CLA	C15-C16-C17-C18
24	b	615	CLA	C13-C15-C16-C17
31	C	526	LMG	O1-C7-C8-O7
31	a	615	LMG	O7-C8-C9-O8
31	b	624	LMG	O1-C7-C8-O7
33	E	101	LHG	C15-C16-C17-C18
33	a	612	LHG	C29-C30-C31-C32
30	C	523	DGD	C4E-C5E-C6E-O5E
31	D	408	LMG	C10-C11-C12-C13
24	b	611	CLA	C4-C3-C5-C6
28	E	103	STE	C12-C13-C14-C15
28	d	412	STE	C14-C15-C16-C17
29	b	620	SQD	C27-C28-C29-C30
30	C	525	DGD	C3B-C4B-C5B-C6B
31	c	522	LMG	C33-C34-C35-C36
33	L	101	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	e	103	LHG	C15-C16-C17-C18
24	c	506	CLA	C8-C10-C11-C12
28	C	519	STE	C4-C5-C6-C7
28	e	106	STE	C4-C5-C6-C7
31	b	622	LMG	C18-C19-C20-C21
33	d	408	LHG	C32-C33-C34-C35
33	d	409	LHG	C12-C13-C14-C15
33	d	409	LHG	C34-C35-C36-C37
24	b	602	CLA	C16-C17-C18-C20
24	b	613	CLA	C16-C17-C18-C19
28	t	102	STE	C2-C3-C4-C5
30	h	102	DGD	CDB-CEB-CFB-CGB
29	A	614	SQD	C23-C24-C25-C26
30	c	520	DGD	C1B-C2B-C3B-C4B
24	d	403	CLA	C3-C5-C6-C7
25	d	402	PHO	C3-C5-C6-C7
24	B	604	CLA	C11-C12-C13-C14
24	a	606	CLA	C14-C13-C15-C16
24	a	608	CLA	C14-C13-C15-C16
24	b	601	CLA	C6-C7-C8-C9
24	b	615	CLA	C11-C10-C8-C9
30	A	615	DGD	C5B-C6B-C7B-C8B
24	a	605	CLA	C2C-C3C-CAC-CBC
24	D	404	CLA	C8-C10-C11-C12
29	b	620	SQD	C15-C16-C17-C18
31	C	522	LMG	O6-C1-O1-C7
29	a	613	SQD	C18-C19-C20-C21
30	C	524	DGD	C2A-C3A-C4A-C5A
24	B	610	CLA	C16-C17-C18-C19
28	m	102	STE	C9-C10-C11-C12
31	a	616	LMG	C40-C41-C42-C43
33	d	409	LHG	C19-C20-C21-C22
30	c	519	DGD	C4D-C5D-C6D-O5D
28	b	623	STE	C2-C3-C4-C5
28	b	626	STE	C5-C6-C7-C8
28	A	618	STE	C11-C10-C9-C8
31	a	616	LMG	C20-C21-C22-C23
31	C	517	LMG	C10-C11-C12-C13
29	B	623	SQD	C33-C34-C35-C36
30	C	524	DGD	C7A-C8A-C9A-CAA
26	h	101	BCR	C9-C10-C11-C12
26	k	101	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
30	h	102	DGD	O2G-C1B-C2B-C3B
27	a	610	PL9	C33-C34-C36-C37
29	A	613	SQD	C26-C27-C28-C29
29	b	620	SQD	C7-C8-C9-C10
24	c	512	CLA	C15-C16-C17-C18
24	d	404	CLA	C8-C10-C11-C12
27	d	406	PL9	C42-C43-C44-C46
28	b	623	STE	C11-C10-C9-C8
29	B	623	SQD	C25-C26-C27-C28
28	b	626	STE	C7-C8-C9-C10
28	E	102	STE	C6-C7-C8-C9
29	f	101	SQD	C34-C35-C36-C37
24	B	611	CLA	C15-C16-C17-C18
24	B	601	CLA	C11-C10-C8-C7
24	B	603	CLA	C11-C10-C8-C7
24	B	605	CLA	C11-C10-C8-C7
24	B	612	CLA	C11-C12-C13-C15
24	C	508	CLA	C12-C13-C15-C16
24	b	603	CLA	C12-C13-C15-C16
24	b	614	CLA	C11-C12-C13-C15
24	b	615	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
24	c	509	CLA	C11-C12-C13-C15
24	c	513	CLA	C12-C13-C15-C16
31	a	615	LMG	C28-C29-C30-C31
28	b	625	STE	C2-C3-C4-C5
29	f	101	SQD	C31-C32-C33-C34
30	c	520	DGD	CBA-CCA-CDA-CEA
28	c	517	STE	C4-C5-C6-C7
24	b	601	CLA	C8-C10-C11-C12
31	d	411	LMG	C15-C16-C17-C18
26	T	101	BCR	C21-C22-C23-C24
30	C	524	DGD	C5D-C6D-O5D-C1E
30	c	520	DGD	C2G-C3G-O3G-C1D
30	c	520	DGD	C5D-C6D-O5D-C1E
28	B	627	STE	C4-C5-C6-C7
24	C	513	CLA	C8-C10-C11-C12
30	A	615	DGD	C6A-C7A-C8A-C9A
31	B	621	LMG	C34-C35-C36-C37
33	d	409	LHG	C28-C29-C30-C31
27	d	406	PL9	C15-C14-C16-C17
24	b	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	B	626	STE	C7-C8-C9-C10
31	b	622	LMG	C32-C33-C34-C35
31	a	615	LMG	C9-C8-O7-C10
31	b	624	LMG	C9-C8-O7-C10
33	D	411	LHG	C27-C28-C29-C30
31	a	615	LMG	C40-C41-C42-C43
29	f	101	SQD	C24-C25-C26-C27
28	b	627	STE	C15-C16-C17-C18
31	c	523	LMG	C16-C17-C18-C19
29	a	613	SQD	O6-C44-C45-C46
29	a	614	SQD	O6-C44-C45-C46
31	a	616	LMG	O1-C7-C8-C9
34	F	101	HEM	C4C-C3C-CAC-CBC
34	e	102	HEM	C4B-C3B-CAB-CBB
34	e	102	HEM	C4C-C3C-CAC-CBC
24	A	606	CLA	C16-C17-C18-C20
24	B	607	CLA	C16-C17-C18-C19
24	d	404	CLA	C16-C17-C18-C19
24	b	609	CLA	C13-C15-C16-C17
33	d	409	LHG	C26-C27-C28-C29
24	C	505	CLA	C8-C10-C11-C12
24	b	602	CLA	C3-C5-C6-C7
29	f	101	SQD	O6-C44-C45-O47
31	D	407	LMG	O1-C7-C8-O7
31	D	407	LMG	O7-C8-C9-O8
24	b	612	CLA	C10-C11-C12-C13
24	A	606	CLA	C11-C12-C13-C14
24	B	603	CLA	C11-C10-C8-C9
24	B	605	CLA	C11-C10-C8-C9
24	B	607	CLA	C14-C13-C15-C16
24	b	606	CLA	C11-C12-C13-C14
24	b	613	CLA	C11-C12-C13-C14
24	c	506	CLA	C11-C10-C8-C9
28	b	623	STE	C7-C8-C9-C10
30	C	523	DGD	CBA-CCA-CDA-CEA
24	c	505	CLA	CBA-CGA-O2A-C1
28	d	412	STE	C2-C3-C4-C5
30	A	615	DGD	CAB-CBB-CCB-CDB
33	l	101	LHG	C15-C16-C17-C18
28	A	618	STE	C9-C10-C11-C12
28	b	625	STE	C5-C6-C7-C8
29	a	614	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	b	620	SQD	C10-C11-C12-C13
31	c	522	LMG	C35-C36-C37-C38
33	E	101	LHG	C13-C14-C15-C16
28	H	104	STE	C12-C13-C14-C15
30	C	524	DGD	C9B-CAB-CBB-CCB
31	a	615	LMG	C22-C23-C24-C25
31	c	518	LMG	C32-C33-C34-C35
33	a	612	LHG	C27-C28-C29-C30
30	C	523	DGD	C4D-C5D-C6D-O5D
28	j	102	STE	C11-C12-C13-C14
33	d	409	LHG	C15-C16-C17-C18
24	c	508	CLA	O1D-CGD-O2D-CED
30	c	519	DGD	CDB-CEB-CFB-CGB
30	A	615	DGD	C2B-C1B-O2G-C2G
24	B	605	CLA	C16-C17-C18-C19
24	B	614	CLA	C16-C17-C18-C19
24	B	612	CLA	C8-C10-C11-C12
30	c	521	DGD	C2B-C3B-C4B-C5B
31	b	624	LMG	C37-C38-C39-C40
31	c	523	LMG	C36-C37-C38-C39
28	E	102	STE	C5-C6-C7-C8
28	C	520	STE	C9-C10-C11-C12
28	D	413	STE	C11-C12-C13-C14
24	b	613	CLA	C5-C6-C7-C8
28	d	410	STE	C12-C13-C14-C15
24	B	610	CLA	C16-C17-C18-C20
24	B	614	CLA	C16-C17-C18-C20
31	D	408	LMG	C11-C12-C13-C14
33	l	101	LHG	C30-C31-C32-C33
33	L	101	LHG	C19-C20-C21-C22
30	h	102	DGD	C1A-C2A-C3A-C4A
31	D	407	LMG	O10-C28-O8-C9
30	H	102	DGD	C9A-CAA-CBA-CCA
28	E	104	STE	C2-C3-C4-C5
24	c	504	CLA	C11-C12-C13-C15
28	d	410	STE	C15-C16-C17-C18
24	c	505	CLA	O1A-CGA-O2A-C1
33	d	408	LHG	C15-C16-C17-C18
24	B	601	CLA	C4B-C3B-CAB-CBB
24	C	504	CLA	C4B-C3B-CAB-CBB
24	C	511	CLA	O1D-CGD-O2D-CED
24	B	607	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	CAA-CBA-CGA-O2A
31	C	517	LMG	C14-C15-C16-C17
31	C	526	LMG	C19-C20-C21-C22
29	a	613	SQD	C25-C26-C27-C28
28	i	101	STE	C2-C3-C4-C5
28	H	103	STE	C11-C10-C9-C8
30	A	615	DGD	O1B-C1B-O2G-C2G
24	B	613	CLA	C6-C7-C8-C10
24	C	504	CLA	C11-C10-C8-C7
24	C	505	CLA	C12-C13-C15-C16
24	a	606	CLA	C11-C12-C13-C15
24	b	602	CLA	C11-C10-C8-C7
24	b	603	CLA	C6-C7-C8-C10
24	b	604	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C15
24	b	614	CLA	C11-C10-C8-C7
24	c	507	CLA	C11-C12-C13-C15
24	c	510	CLA	C11-C10-C8-C7
28	E	103	STE	C7-C8-C9-C10
31	D	407	LMG	C32-C33-C34-C35
31	D	408	LMG	C36-C37-C38-C39
24	c	504	CLA	C11-C12-C13-C14
24	c	510	CLA	C16-C17-C18-C19
28	i	102	STE	C7-C8-C9-C10
31	C	522	LMG	C16-C17-C18-C19
28	d	412	STE	C11-C10-C9-C8
31	b	622	LMG	C38-C39-C40-C41
28	C	528	STE	C12-C13-C14-C15
28	C	529	STE	C11-C10-C9-C8
31	b	622	LMG	C12-C13-C14-C15
24	b	601	CLA	C13-C15-C16-C17
29	B	623	SQD	C45-C46-O48-C23
29	A	613	SQD	C33-C34-C35-C36
33	D	411	LHG	C2-C3-O3-P
24	a	611	CLA	C16-C17-C18-C19
28	b	621	STE	C6-C7-C8-C9
29	a	613	SQD	C24-C25-C26-C27
24	C	508	CLA	C6-C7-C8-C9
24	b	603	CLA	C6-C7-C8-C9
24	c	511	CLA	C11-C10-C8-C9
24	c	513	CLA	C14-C13-C15-C16
33	a	612	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	c	505	CLA	C15-C16-C17-C18
28	Z	101	STE	C10-C11-C12-C13
26	C	514	BCR	C19-C20-C21-C22
24	B	603	CLA	C13-C15-C16-C17
24	c	505	CLA	C8-C10-C11-C12
31	B	621	LMG	C16-C17-C18-C19
30	C	525	DGD	CAA-CBA-CCA-CDA
28	j	101	STE	C2-C3-C4-C5
29	D	409	SQD	C24-C25-C26-C27
29	b	620	SQD	O47-C45-C46-O48
31	a	616	LMG	O1-C7-C8-O7
31	a	616	LMG	O7-C8-C9-O8
33	E	101	LHG	O7-C5-C6-O8
33	e	103	LHG	O7-C5-C6-O8
28	e	105	STE	C11-C12-C13-C14
31	D	408	LMG	C30-C31-C32-C33
28	C	520	STE	C3-C4-C5-C6
29	b	620	SQD	C19-C20-C21-C22
24	a	611	CLA	C16-C17-C18-C20
31	a	615	LMG	C7-C8-C9-O8
31	b	624	LMG	O1-C7-C8-C9
29	D	409	SQD	C29-C30-C31-C32
31	a	615	LMG	C36-C37-C38-C39
30	C	524	DGD	CBB-CCB-CDB-CEB
24	B	601	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
28	C	516	STE	C11-C10-C9-C8
24	D	402	CLA	C16-C17-C18-C19
31	C	526	LMG	C11-C12-C13-C14
31	c	523	LMG	C39-C40-C41-C42
24	c	509	CLA	C8-C10-C11-C12
28	E	103	STE	C11-C10-C9-C8
28	b	627	STE	C10-C11-C12-C13
24	B	601	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	513	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
26	K	101	BCR	C13-C14-C15-C16
33	E	101	LHG	C3-O3-P-O6
33	E	101	LHG	C4-O6-P-O5
28	b	626	STE	C3-C4-C5-C6
28	d	407	STE	C9-C10-C11-C12
24	B	615	CLA	C2B-C3B-CAB-CBB
24	c	505	CLA	C2B-C3B-CAB-CBB
26	T	101	BCR	C23-C24-C25-C30
26	t	101	BCR	C23-C24-C25-C30
28	A	617	STE	C11-C12-C13-C14
28	d	412	STE	C4-C5-C6-C7
28	e	106	STE	C7-C8-C9-C10
28	c	516	STE	C4-C5-C6-C7
28	A	617	STE	C5-C6-C7-C8
28	Z	101	STE	C12-C13-C14-C15
30	C	525	DGD	C5A-C6A-C7A-C8A
28	c	517	STE	C7-C8-C9-C10
24	c	510	CLA	C16-C17-C18-C20
25	d	402	PHO	C2C-C3C-CAC-CBC
31	C	517	LMG	C7-C8-O7-C10
31	C	522	LMG	C9-C8-O7-C10
33	E	101	LHG	C6-C5-O7-C7
27	A	611	PL9	C40-C39-C41-C42
24	C	511	CLA	C8-C10-C11-C12
24	b	604	CLA	C15-C16-C17-C18
33	E	101	LHG	C16-C17-C18-C19
24	B	607	CLA	C16-C17-C18-C20
24	B	613	CLA	C16-C17-C18-C19
24	C	505	CLA	C16-C17-C18-C19
31	D	408	LMG	C20-C21-C22-C23
24	B	613	CLA	C11-C10-C8-C9
24	C	502	CLA	C14-C13-C15-C16
24	D	404	CLA	C14-C13-C15-C16
24	b	604	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C14
24	b	608	CLA	C11-C12-C13-C14
24	b	614	CLA	C11-C10-C8-C9
24	c	504	CLA	C6-C7-C8-C9
24	c	505	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	A	606	CLA	C6-C7-C8-C10
24	B	601	CLA	C11-C12-C13-C15
24	B	614	CLA	C12-C13-C15-C16
24	C	509	CLA	C12-C13-C15-C16
24	b	602	CLA	C11-C12-C13-C15
24	b	606	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C10-C8-C7
24	a	608	CLA	C15-C16-C17-C18
28	C	527	STE	C1-C2-C3-C4
31	B	620	LMG	C30-C31-C32-C33
33	d	408	LHG	C10-C11-C12-C13
24	c	512	CLA	C3-C5-C6-C7
28	A	618	STE	C15-C16-C17-C18
29	B	623	SQD	C29-C30-C31-C32
30	c	519	DGD	CDA-CEA-CFA-CGA
33	L	101	LHG	C35-C36-C37-C38
30	c	520	DGD	C2E-C1E-O5D-C6D
24	B	614	CLA	CBD-CGD-O2D-CED
31	B	620	LMG	C35-C36-C37-C38
33	L	101	LHG	C14-C15-C16-C17
24	B	613	CLA	C16-C17-C18-C20
35	v	201	HEC	C2C-C3C-CAC-CBC
28	j	102	STE	C10-C11-C12-C13
30	c	519	DGD	C9B-CAB-CBB-CCB
31	c	523	LMG	O7-C8-C9-O8
30	c	520	DGD	O6E-C5E-C6E-O5E
30	c	521	DGD	C5B-C6B-C7B-C8B
28	B	626	STE	C2-C3-C4-C5
30	C	525	DGD	C7B-C8B-C9B-CAB
31	b	622	LMG	C19-C20-C21-C22
31	d	411	LMG	C30-C31-C32-C33
28	C	528	STE	C11-C12-C13-C14
29	a	614	SQD	C16-C17-C18-C19
24	A	605	CLA	C2C-C3C-CAC-CBC
29	A	613	SQD	C23-C24-C25-C26
31	a	615	LMG	C24-C25-C26-C27
26	D	405	BCR	C7-C8-C9-C34
26	H	101	BCR	C7-C8-C9-C34
24	b	610	CLA	C16-C17-C18-C20
28	e	104	STE	C15-C16-C17-C18
31	b	624	LMG	C8-C7-O1-C1
31	b	624	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
26	C	521	BCR	C13-C14-C15-C16
24	b	609	CLA	C4-C3-C5-C6
24	C	513	CLA	C10-C11-C12-C13
33	d	409	LHG	C17-C18-C19-C20
31	B	621	LMG	C21-C22-C23-C24
31	C	517	LMG	O9-C10-O7-C8
24	b	603	CLA	C14-C13-C15-C16
24	b	613	CLA	C11-C10-C8-C9
33	d	408	LHG	C29-C30-C31-C32
28	A	612	STE	C6-C7-C8-C9
28	b	627	STE	C11-C12-C13-C14
24	c	502	CLA	C4B-C3B-CAB-CBB
30	A	615	DGD	CDB-CEB-CFB-CGB
33	D	411	LHG	C34-C35-C36-C37
28	d	407	STE	C12-C13-C14-C15
24	b	615	CLA	C8-C10-C11-C12
30	C	525	DGD	O6D-C5D-C6D-O5D
30	C	524	DGD	C2E-C1E-O5D-C6D
24	b	609	CLA	C3-C5-C6-C7
26	D	405	BCR	C19-C20-C21-C22
24	B	605	CLA	C16-C17-C18-C20
28	M	102	STE	C5-C6-C7-C8
29	a	614	SQD	C32-C33-C34-C35
28	M	103	STE	C14-C15-C16-C17
29	A	613	SQD	C10-C11-C12-C13
29	A	613	SQD	C14-C15-C16-C17
24	B	606	CLA	C12-C13-C15-C16
24	b	603	CLA	C11-C12-C13-C15
24	b	609	CLA	C11-C12-C13-C15
24	c	505	CLA	C11-C12-C13-C15
30	h	102	DGD	C9B-CAB-CBB-CCB
29	a	614	SQD	C26-C27-C28-C29
30	c	520	DGD	C9A-CAA-CBA-CCA
33	D	412	LHG	C11-C10-C9-C8
24	B	614	CLA	O1D-CGD-O2D-CED
31	B	620	LMG	C12-C13-C14-C15
28	D	413	STE	C3-C4-C5-C6
28	I	101	STE	C5-C6-C7-C8
28	b	626	STE	C2-C3-C4-C5
27	d	406	PL9	C40-C39-C41-C42
28	t	102	STE	C4-C5-C6-C7
30	c	521	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
31	C	522	LMG	C40-C41-C42-C43
28	m	101	STE	C6-C7-C8-C9
33	L	101	LHG	C5-C6-O8-C23
30	H	102	DGD	C9B-CAB-CBB-CCB
30	h	102	DGD	CBA-CCA-CDA-CEA
24	B	616	CLA	C10-C11-C12-C13
29	a	614	SQD	C12-C13-C14-C15
30	c	519	DGD	C4E-C5E-C6E-O5E
24	C	503	CLA	C15-C16-C17-C18
28	A	616	STE	C13-C14-C15-C16
30	c	521	DGD	CAA-CBA-CCA-CDA
35	V	201	HEC	CAD-CBD-CGD-O2D
35	v	201	HEC	CAD-CBD-CGD-O2D
24	c	512	CLA	C4-C3-C5-C6
27	a	610	PL9	C45-C44-C46-C47
28	E	104	STE	C6-C7-C8-C9
24	B	602	CLA	C13-C15-C16-C17
28	M	101	STE	O2-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O1D
28	I	101	STE	O1-C1-C2-C3
24	C	511	CLA	C11-C10-C8-C9
24	a	611	CLA	C14-C13-C15-C16
24	b	602	CLA	C6-C7-C8-C9
24	b	609	CLA	C14-C13-C15-C16
24	c	507	CLA	C14-C13-C15-C16
24	c	513	CLA	C11-C12-C13-C14
31	b	622	LMG	C13-C14-C15-C16
28	j	101	STE	C5-C6-C7-C8
30	H	102	DGD	CAB-CBB-CCB-CDB
33	D	411	LHG	C13-C14-C15-C16
29	B	623	SQD	C44-C45-O47-C7
29	B	623	SQD	C46-C45-O47-C7
29	f	101	SQD	C44-C45-O47-C7
29	f	101	SQD	C46-C45-O47-C7
31	B	621	LMG	C7-C8-O7-C10
33	E	101	LHG	C4-C5-O7-C7
31	c	522	LMG	C10-C11-C12-C13
33	d	408	LHG	C24-C25-C26-C27
31	b	624	LMG	C33-C34-C35-C36
29	a	614	SQD	C23-C24-C25-C26
30	H	102	DGD	C2B-C3B-C4B-C5B
29	a	614	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	C	526	LMG	C17-C18-C19-C20
31	b	622	LMG	C35-C36-C37-C38
33	d	408	LHG	C16-C17-C18-C19
28	I	101	STE	O2-C1-C2-C3
28	d	407	STE	O2-C1-C2-C3
28	m	101	STE	O2-C1-C2-C3
24	c	511	CLA	C1A-C2A-CAA-CBA
28	c	517	STE	C14-C15-C16-C17
31	C	517	LMG	C17-C18-C19-C20
28	M	101	STE	O1-C1-C2-C3
28	d	407	STE	O1-C1-C2-C3
31	B	621	LMG	C30-C31-C32-C33
30	c	520	DGD	C3A-C4A-C5A-C6A
24	B	601	CLA	C2B-C3B-CAB-CBB
24	C	504	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C5-C6-C7-C8
26	H	101	BCR	C23-C24-C25-C26
26	d	405	BCR	C23-C24-C25-C26
31	C	517	LMG	C11-C10-O7-C8
28	b	623	STE	C6-C7-C8-C9
30	A	615	DGD	C4B-C5B-C6B-C7B
28	I	101	STE	C12-C13-C14-C15
31	d	411	LMG	C37-C38-C39-C40
34	e	102	HEM	CAD-CBD-CGD-O1D
24	D	404	CLA	C4-C3-C5-C6
28	m	101	STE	C3-C4-C5-C6
28	H	103	STE	C7-C8-C9-C10
29	A	613	SQD	C9-C10-C11-C12
33	d	408	LHG	C33-C34-C35-C36
28	B	624	STE	O1-C1-C2-C3
28	i	101	STE	O2-C1-C2-C3
28	m	101	STE	O1-C1-C2-C3
34	F	101	HEM	CAD-CBD-CGD-O1D
24	C	512	CLA	C10-C11-C12-C13
24	B	601	CLA	C6-C7-C8-C10
24	B	602	CLA	C11-C12-C13-C15
24	C	510	CLA	C12-C13-C15-C16
24	c	502	CLA	C12-C13-C15-C16
27	a	610	PL9	C39-C41-C42-C43
24	c	501	CLA	C2A-CAA-CBA-CGA
24	c	509	CLA	C2A-CAA-CBA-CGA
28	D	413	STE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	a	613	SQD	O47-C45-C46-O48
30	C	524	DGD	C9A-CAA-CBA-CCA
28	m	102	STE	C7-C8-C9-C10
30	C	525	DGD	CDB-CEB-CFB-CGB
24	b	601	CLA	C16-C17-C18-C20
31	c	523	LMG	C32-C33-C34-C35
33	e	103	LHG	C1-C2-C3-O3
28	d	414	STE	C4-C5-C6-C7
24	d	403	CLA	C4-C3-C5-C6
24	c	512	CLA	C2-C3-C5-C6
27	A	611	PL9	C33-C34-C36-C37
28	I	101	STE	C6-C7-C8-C9
33	D	412	LHG	C26-C27-C28-C29
24	c	504	CLA	O1D-CGD-O2D-CED
28	C	528	STE	C3-C4-C5-C6
24	b	614	CLA	C8-C10-C11-C12
28	B	624	STE	O2-C1-C2-C3
30	c	519	DGD	CCB-CDB-CEB-CFB
28	M	103	STE	C12-C13-C14-C15
24	b	608	CLA	C13-C15-C16-C17
31	a	615	LMG	C38-C39-C40-C41
30	C	524	DGD	C8B-C9B-CAB-CBB
33	D	412	LHG	C29-C30-C31-C32
35	V	201	HEC	CAD-CBD-CGD-O1D
24	c	506	CLA	C14-C13-C15-C16
33	D	410	LHG	C26-C27-C28-C29
33	E	101	LHG	C27-C28-C29-C30
29	B	623	SQD	C34-C35-C36-C37
24	B	611	CLA	C10-C11-C12-C13
30	c	520	DGD	CCA-CDA-CEA-CFA
27	A	611	PL9	C15-C14-C16-C17
28	E	102	STE	O2-C1-C2-C3
28	i	101	STE	O1-C1-C2-C3
24	b	604	CLA	C2-C3-C5-C6
24	c	506	CLA	C13-C15-C16-C17
30	C	523	DGD	C2A-C1A-O1G-C1G
34	e	102	HEM	CAD-CBD-CGD-O2D
31	a	615	LMG	C30-C31-C32-C33
27	A	611	PL9	C39-C41-C42-C43
27	a	610	PL9	C14-C16-C17-C18
31	c	523	LMG	C7-C8-C9-O8
28	B	622	STE	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	c	510	CLA	C5-C6-C7-C8
30	H	102	DGD	C8A-C9A-CAA-CBA
27	A	611	PL9	C20-C19-C21-C22
27	d	406	PL9	C45-C44-C46-C47
28	d	414	STE	O2-C1-C2-C3
24	A	605	CLA	C4C-C3C-CAC-CBC
30	H	102	DGD	O1B-C1B-C2B-C3B
28	m	102	STE	C13-C14-C15-C16
28	M	102	STE	C1-C2-C3-C4
28	I	101	STE	C3-C4-C5-C6
24	b	606	CLA	C4B-C3B-CAB-CBB
24	b	611	CLA	O1A-CGA-O2A-C1
24	c	512	CLA	O1A-CGA-O2A-C1
28	J	101	STE	O2-C1-C2-C3
28	j	102	STE	C14-C15-C16-C17
24	c	512	CLA	CBA-CGA-O2A-C1
31	C	526	LMG	O10-C28-O8-C9
24	a	605	CLA	C4C-C3C-CAC-CBC
24	b	603	CLA	C16-C17-C18-C20
27	a	610	PL9	C17-C18-C19-C21
28	C	528	STE	C6-C7-C8-C9
28	d	407	STE	C15-C16-C17-C18
28	B	626	STE	O2-C1-C2-C3
34	F	101	HEM	CAD-CBD-CGD-O2D
33	D	412	LHG	C7-C8-C9-C10
30	c	521	DGD	C5A-C6A-C7A-C8A
33	l	101	LHG	O6-C4-C5-C6
35	v	201	HEC	C4C-C3C-CAC-CBC
31	c	518	LMG	O7-C8-C9-O8
31	B	620	LMG	C28-C29-C30-C31
24	b	609	CLA	C2-C3-C5-C6
30	C	523	DGD	O6E-C1E-O5D-C6D
30	c	519	DGD	O6E-C1E-O5D-C6D
24	b	610	CLA	C12-C13-C15-C16
28	H	103	STE	C13-C14-C15-C16
33	D	411	LHG	C25-C26-C27-C28
28	J	101	STE	O1-C1-C2-C3
28	C	520	STE	C11-C10-C9-C8
28	d	412	STE	C13-C14-C15-C16
31	a	615	LMG	C12-C13-C14-C15
24	B	613	CLA	C6-C7-C8-C9
24	b	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	c	521	DGD	O6D-C5D-C6D-O5D
29	A	614	SQD	C45-C44-O6-C1
24	d	403	CLA	C2-C1-O2A-CGA
24	B	606	CLA	C3-C5-C6-C7
24	d	404	CLA	C16-C17-C18-C20
28	i	101	STE	C7-C8-C9-C10
30	H	102	DGD	CDA-CEA-CFA-CGA
31	c	522	LMG	C17-C18-C19-C20
31	C	526	LMG	C29-C28-O8-C9
29	B	623	SQD	C7-C8-C9-C10
28	B	626	STE	O1-C1-C2-C3
33	D	410	LHG	C33-C34-C35-C36
29	A	613	SQD	O10-C23-O48-C46
31	b	624	LMG	C14-C15-C16-C17
30	C	525	DGD	CCB-CDB-CEB-CFB
28	E	102	STE	O1-C1-C2-C3
24	B	608	CLA	C15-C16-C17-C18
28	B	622	STE	O1-C1-C2-C3
28	d	414	STE	O1-C1-C2-C3
33	l	101	LHG	C24-C25-C26-C27
34	e	102	HEM	CAA-CBA-CGA-O2A
30	C	525	DGD	C4B-C5B-C6B-C7B
30	C	523	DGD	CDA-CEA-CFA-CGA
30	c	520	DGD	O6E-C1E-O5D-C6D
24	b	611	CLA	CBA-CGA-O2A-C1
28	B	622	STE	C4-C5-C6-C7
29	f	101	SQD	O6-C44-C45-C46
30	c	521	DGD	O1G-C1G-C2G-C3G
31	D	407	LMG	C7-C8-C9-O8
28	d	412	STE	C6-C7-C8-C9
30	C	523	DGD	O1A-C1A-O1G-C1G
29	A	613	SQD	C25-C26-C27-C28
27	A	611	PL9	C12-C11-C9-C10
27	A	611	PL9	C45-C44-C46-C47
30	c	521	DGD	C7A-C8A-C9A-CAA
28	D	413	STE	C7-C8-C9-C10
30	C	524	DGD	CBA-CCA-CDA-CEA
30	c	519	DGD	CAB-CBB-CCB-CDB
33	D	410	LHG	C32-C33-C34-C35
28	C	527	STE	C5-C6-C7-C8
29	D	409	SQD	O48-C23-C24-C25
33	d	409	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	C11-C12-C13-C14
24	C	502	CLA	C11-C12-C13-C14
24	C	504	CLA	C11-C10-C8-C9
24	C	505	CLA	C14-C13-C15-C16
24	D	402	CLA	C11-C12-C13-C14
24	c	507	CLA	C11-C12-C13-C14
24	C	502	CLA	C16-C17-C18-C20
29	B	623	SQD	C18-C19-C20-C21
28	j	102	STE	C12-C13-C14-C15
33	e	103	LHG	C18-C19-C20-C21
31	a	616	LMG	C32-C33-C34-C35
29	B	623	SQD	C16-C17-C18-C19
24	C	512	CLA	C2A-CAA-CBA-CGA
24	B	603	CLA	C11-C12-C13-C15
24	B	603	CLA	C12-C13-C15-C16
24	B	614	CLA	C11-C12-C13-C15
24	B	615	CLA	C11-C10-C8-C7
24	C	502	CLA	C11-C12-C13-C15
24	C	503	CLA	C11-C10-C8-C7
24	D	402	CLA	C11-C12-C13-C15
24	b	612	CLA	C11-C10-C8-C7
24	c	508	CLA	C11-C12-C13-C15
24	c	512	CLA	C6-C7-C8-C10
24	B	612	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C2B-C3B-CAB-CBB
24	D	403	CLA	C2B-C3B-CAB-CBB
24	b	606	CLA	C2B-C3B-CAB-CBB
24	c	502	CLA	C2B-C3B-CAB-CBB
24	c	513	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
26	B	619	BCR	C1-C6-C7-C8
26	C	514	BCR	C23-C24-C25-C26
26	C	521	BCR	C23-C24-C25-C30
26	D	405	BCR	C23-C24-C25-C30
26	T	101	BCR	C1-C6-C7-C8
28	A	617	STE	C11-C10-C9-C8
31	b	622	LMG	C21-C22-C23-C24
24	B	613	CLA	C2-C1-O2A-CGA
24	A	606	CLA	C16-C17-C18-C19
28	d	410	STE	C13-C14-C15-C16
28	B	622	STE	C12-C13-C14-C15
27	a	610	PL9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
29	a	613	SQD	O47-C7-C8-C9
31	c	522	LMG	O7-C10-C11-C12
29	A	613	SQD	C24-C23-O48-C46
24	b	612	CLA	C8-C10-C11-C12
30	C	523	DGD	C7A-C8A-C9A-CAA
31	D	408	LMG	C31-C32-C33-C34
28	A	617	STE	C15-C16-C17-C18
28	d	412	STE	O2-C1-C2-C3
28	b	625	STE	C6-C7-C8-C9
31	a	615	LMG	C42-C43-C44-C45
24	C	502	CLA	O1A-CGA-O2A-C1
27	A	611	PL9	C4-C3-C7-C8
31	C	517	LMG	O7-C10-C11-C12
31	c	518	LMG	O8-C28-C29-C30
31	B	621	LMG	C22-C23-C24-C25
29	B	623	SQD	C14-C15-C16-C17
27	a	610	PL9	C23-C24-C26-C27
28	I	101	STE	C10-C11-C12-C13
28	d	410	STE	C6-C7-C8-C9
24	b	602	CLA	C14-C13-C15-C16
24	b	607	CLA	C14-C13-C15-C16
24	c	503	CLA	C11-C10-C8-C9
24	d	404	CLA	C6-C7-C8-C9
28	m	102	STE	C10-C11-C12-C13
29	b	620	SQD	C44-C45-C46-O48
28	b	621	STE	C13-C14-C15-C16
30	C	525	DGD	C2A-C3A-C4A-C5A
30	c	519	DGD	C5A-C6A-C7A-C8A
24	a	608	CLA	C13-C15-C16-C17
24	C	503	CLA	C1A-C2A-CAA-CBA
24	D	403	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C4B-C3B-CAB-CBB
31	D	408	LMG	C22-C23-C24-C25
30	C	524	DGD	O6E-C1E-O5D-C6D
24	c	510	CLA	CAA-CBA-CGA-O2A
30	C	523	DGD	O2G-C1B-C2B-C3B
30	c	519	DGD	C8A-C9A-CAA-CBA
26	C	514	BCR	C11-C12-C13-C14
26	D	405	BCR	C7-C8-C9-C10
26	H	101	BCR	C7-C8-C9-C10
26	T	101	BCR	C7-C8-C9-C10
31	B	621	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
33	d	409	LHG	C14-C15-C16-C17
30	H	102	DGD	C3A-C4A-C5A-C6A
24	B	610	CLA	C2A-CAA-CBA-CGA
24	C	501	CLA	C2A-CAA-CBA-CGA
30	C	523	DGD	C3B-C4B-C5B-C6B
35	V	201	HEC	C2B-C3B-CAB-CBB
34	e	102	HEM	CAA-CBA-CGA-O1A
24	B	613	CLA	CAA-CBA-CGA-O2A
28	A	617	STE	C6-C7-C8-C9
29	a	614	SQD	C5-C6-S-O9
28	e	105	STE	C10-C11-C12-C13
30	h	102	DGD	O1B-C1B-C2B-C3B
28	M	103	STE	C7-C8-C9-C10
24	B	606	CLA	C11-C12-C13-C15
24	C	509	CLA	C11-C12-C13-C15
24	C	510	CLA	C11-C10-C8-C7
24	b	602	CLA	C12-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C10
24	c	503	CLA	C11-C10-C8-C7
24	c	508	CLA	C11-C10-C8-C7
28	c	517	STE	C13-C14-C15-C16
29	a	614	SQD	C34-C35-C36-C37
31	b	622	LMG	C39-C40-C41-C42
33	D	410	LHG	C25-C26-C27-C28
31	C	522	LMG	C17-C18-C19-C20
28	C	529	STE	C5-C6-C7-C8
24	B	614	CLA	C2A-CAA-CBA-CGA
28	d	412	STE	O1-C1-C2-C3
31	D	407	LMG	C4-C5-C6-O5
28	b	621	STE	C7-C8-C9-C10
24	B	601	CLA	C4-C3-C5-C6
29	a	613	SQD	O49-C7-C8-C9
28	d	412	STE	C12-C13-C14-C15
24	C	513	CLA	C13-C15-C16-C17
31	C	517	LMG	O9-C10-C11-C12
24	C	502	CLA	CBA-CGA-O2A-C1
24	b	613	CLA	CAA-CBA-CGA-O2A
24	c	509	CLA	CAA-CBA-CGA-O1A
31	c	518	LMG	O10-C28-C29-C30
28	J	101	STE	C2-C3-C4-C5
24	C	509	CLA	C5-C6-C7-C8
24	C	512	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	b	603	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C6-C7-C8-C9
24	B	605	CLA	C14-C13-C15-C16
24	B	612	CLA	C11-C12-C13-C14
24	C	509	CLA	C14-C13-C15-C16
24	b	611	CLA	C14-C13-C15-C16
24	b	612	CLA	C11-C10-C8-C9
24	c	502	CLA	C14-C13-C15-C16
24	c	513	CLA	C11-C10-C8-C9
28	c	516	STE	C9-C10-C11-C12
24	b	612	CLA	C3-C5-C6-C7
31	C	526	LMG	O7-C10-C11-C12
28	z	101	STE	C1-C2-C3-C4
28	B	625	STE	C2-C3-C4-C5
24	B	612	CLA	CAA-CBA-CGA-O2A
31	B	621	LMG	O8-C28-C29-C30
24	b	603	CLA	C10-C11-C12-C13
24	C	505	CLA	CBD-CGD-O2D-CED
31	c	522	LMG	O9-C10-C11-C12
24	B	602	CLA	C15-C16-C17-C18
29	b	620	SQD	C45-C44-O6-C1
30	h	102	DGD	C2G-C3G-O3G-C1D
24	a	608	CLA	O1A-CGA-O2A-C1
24	A	606	CLA	C13-C15-C16-C17
28	C	527	STE	C4-C5-C6-C7
29	a	613	SQD	C28-C29-C30-C31
30	C	523	DGD	O1B-C1B-C2B-C3B
29	a	614	SQD	C15-C16-C17-C18
28	B	626	STE	C5-C6-C7-C8
24	b	616	CLA	CAD-CBD-CGD-O2D
25	a	607	PHO	CAD-CBD-CGD-O2D
28	B	624	STE	C3-C4-C5-C6
30	c	520	DGD	O6D-C5D-C6D-O5D
31	b	624	LMG	C17-C18-C19-C20
24	C	506	CLA	C2-C1-O2A-CGA
24	D	403	CLA	C2-C1-O2A-CGA
24	c	512	CLA	C2-C1-O2A-CGA
28	b	623	STE	C14-C15-C16-C17
24	B	612	CLA	CAA-CBA-CGA-O1A
24	b	607	CLA	C15-C16-C17-C18
24	B	605	CLA	C13-C15-C16-C17
30	c	519	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
29	A	614	SQD	C7-C8-C9-C10
31	C	526	LMG	O9-C10-C11-C12
28	B	627	STE	C1-C2-C3-C4
30	c	519	DGD	C4B-C5B-C6B-C7B

There are no ring outliers.

151 monomers are involved in 262 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	407	STE	1	0
24	b	606	CLA	3	0
24	B	614	CLA	3	0
24	b	612	CLA	1	0
29	a	614	SQD	1	0
26	c	515	BCR	1	0
26	h	101	BCR	2	0
30	C	525	DGD	1	0
24	b	602	CLA	3	0
31	B	621	LMG	1	0
24	c	506	CLA	1	0
24	B	613	CLA	3	0
28	b	621	STE	2	0
30	H	102	DGD	1	0
33	e	103	LHG	1	0
26	H	101	BCR	2	0
28	d	412	STE	1	0
24	b	616	CLA	4	0
24	C	512	CLA	2	0
28	j	102	STE	1	0
33	l	101	LHG	2	0
28	z	101	STE	1	0
28	d	414	STE	1	0
30	c	521	DGD	2	0
28	d	413	STE	1	0
25	A	608	PHO	1	0
28	C	528	STE	1	0
28	A	618	STE	4	0
24	b	615	CLA	3	0
28	i	102	STE	1	0
26	C	521	BCR	2	0
33	a	612	LHG	2	0
24	b	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	616	CLA	2	0
33	d	409	LHG	1	0
24	a	608	CLA	2	0
24	d	404	CLA	1	0
28	H	103	STE	3	0
30	C	524	DGD	2	0
31	b	624	LMG	1	0
29	b	620	SQD	2	0
24	B	601	CLA	3	0
24	b	614	CLA	2	0
28	e	106	STE	1	0
24	C	513	CLA	2	0
24	c	511	CLA	3	0
31	D	407	LMG	9	0
24	C	504	CLA	2	0
28	B	627	STE	1	0
30	c	520	DGD	1	0
24	B	611	CLA	1	0
31	C	522	LMG	2	0
31	C	526	LMG	1	0
24	b	610	CLA	3	0
29	B	623	SQD	2	0
24	A	606	CLA	2	0
28	c	516	STE	1	0
28	c	517	STE	2	0
31	D	408	LMG	1	0
24	a	606	CLA	1	0
30	C	523	DGD	1	0
24	c	509	CLA	6	0
33	d	408	LHG	1	0
30	c	519	DGD	1	0
26	K	101	BCR	1	0
24	B	615	CLA	2	0
31	b	622	LMG	3	0
24	D	403	CLA	3	0
24	B	602	CLA	1	0
24	c	513	CLA	2	0
33	D	410	LHG	3	0
26	c	514	BCR	2	0
24	a	605	CLA	1	0
24	D	402	CLA	3	0
24	c	505	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	504	CLA	2	0
24	b	601	CLA	1	0
26	a	609	BCR	1	0
27	a	610	PL9	6	0
24	C	502	CLA	1	0
24	b	611	CLA	1	0
26	C	515	BCR	1	0
24	B	612	CLA	1	0
31	a	615	LMG	6	0
26	t	101	BCR	3	0
24	c	503	CLA	4	0
26	k	101	BCR	2	0
24	C	509	CLA	2	0
28	K	102	STE	1	0
28	d	410	STE	4	0
24	C	511	CLA	2	0
29	A	613	SQD	2	0
33	L	101	LHG	1	0
33	D	412	LHG	3	0
24	b	603	CLA	3	0
26	b	617	BCR	2	0
24	c	507	CLA	1	0
24	B	610	CLA	1	0
27	A	611	PL9	5	0
28	E	103	STE	1	0
24	b	605	CLA	1	0
26	B	617	BCR	2	0
30	A	615	DGD	4	0
25	d	402	PHO	2	0
33	E	101	LHG	4	0
35	v	201	HEC	1	0
31	c	522	LMG	1	0
28	E	104	STE	1	0
28	D	413	STE	1	0
24	B	604	CLA	4	0
24	C	505	CLA	2	0
31	B	620	LMG	4	0
24	B	607	CLA	2	0
29	f	101	SQD	3	0
31	c	518	LMG	2	0
24	B	609	CLA	1	0
28	b	623	STE	1	0

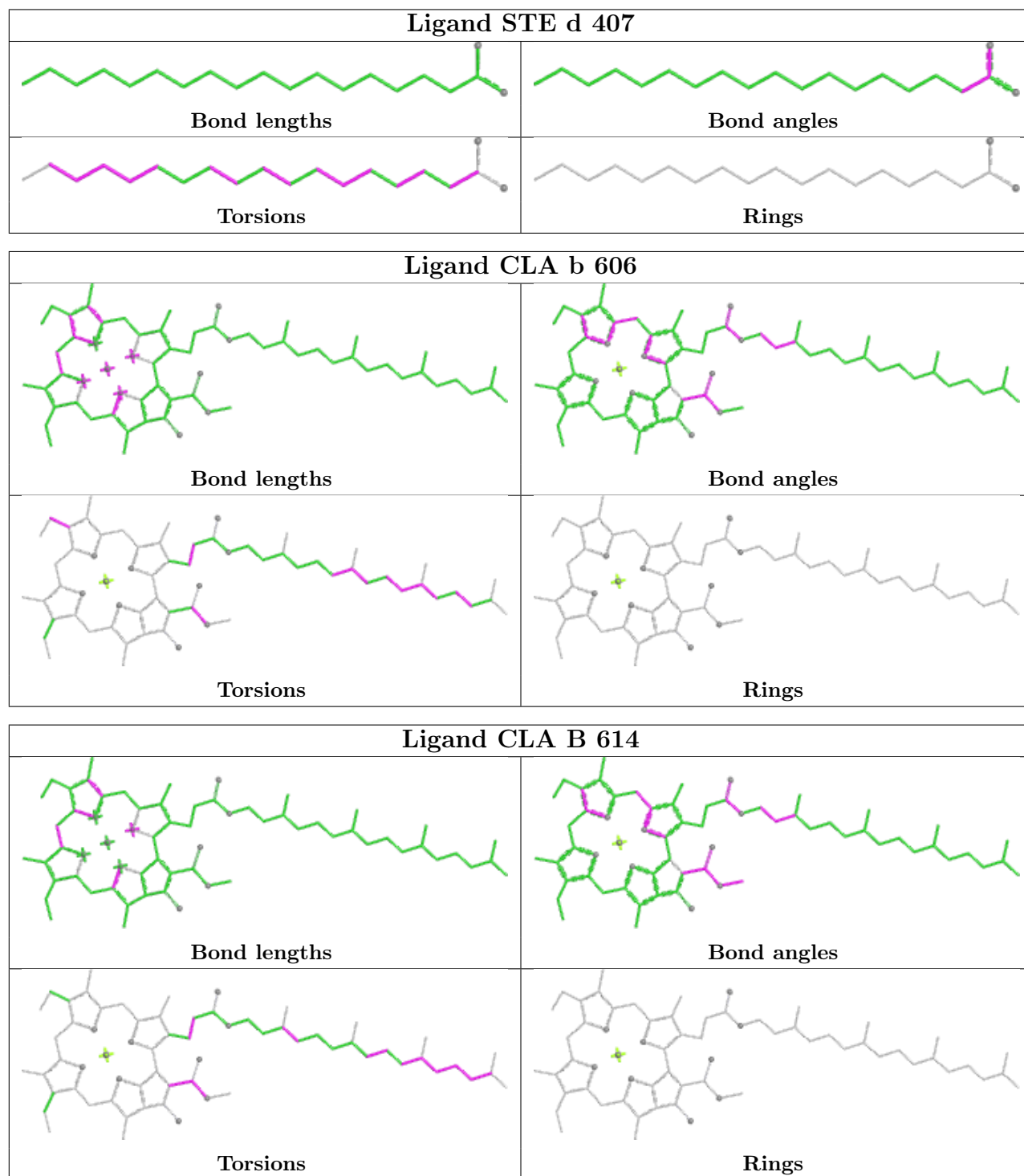
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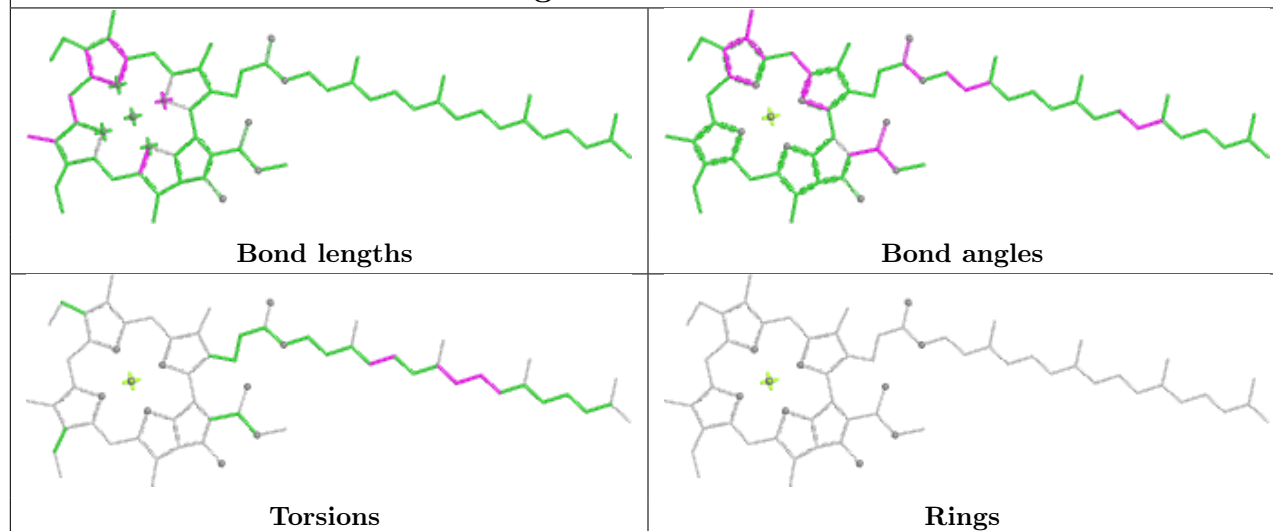
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	508	CLA	4	0
24	A	605	CLA	4	0
28	Z	101	STE	1	0
34	e	102	HEM	4	0
24	c	512	CLA	2	0
24	a	611	CLA	4	0
29	a	613	SQD	3	0
24	c	501	CLA	4	0
24	B	605	CLA	1	0
28	C	529	STE	1	0
28	C	518	STE	1	0
27	d	406	PL9	2	0
26	k	102	BCR	1	0
28	A	617	STE	1	0
31	C	517	LMG	1	0
26	D	405	BCR	1	0
28	B	622	STE	2	0
34	F	101	HEM	2	0
24	C	507	CLA	2	0
26	T	101	BCR	2	0
24	b	609	CLA	2	0
24	c	510	CLA	4	0
28	b	627	STE	2	0
33	D	411	LHG	5	0
28	I	102	STE	2	0
29	A	614	SQD	1	0
24	A	609	CLA	1	0
24	B	606	CLA	3	0
31	c	523	LMG	2	0
24	d	403	CLA	2	0
26	d	405	BCR	1	0
28	i	101	STE	3	0
26	B	618	BCR	1	0
28	M	103	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

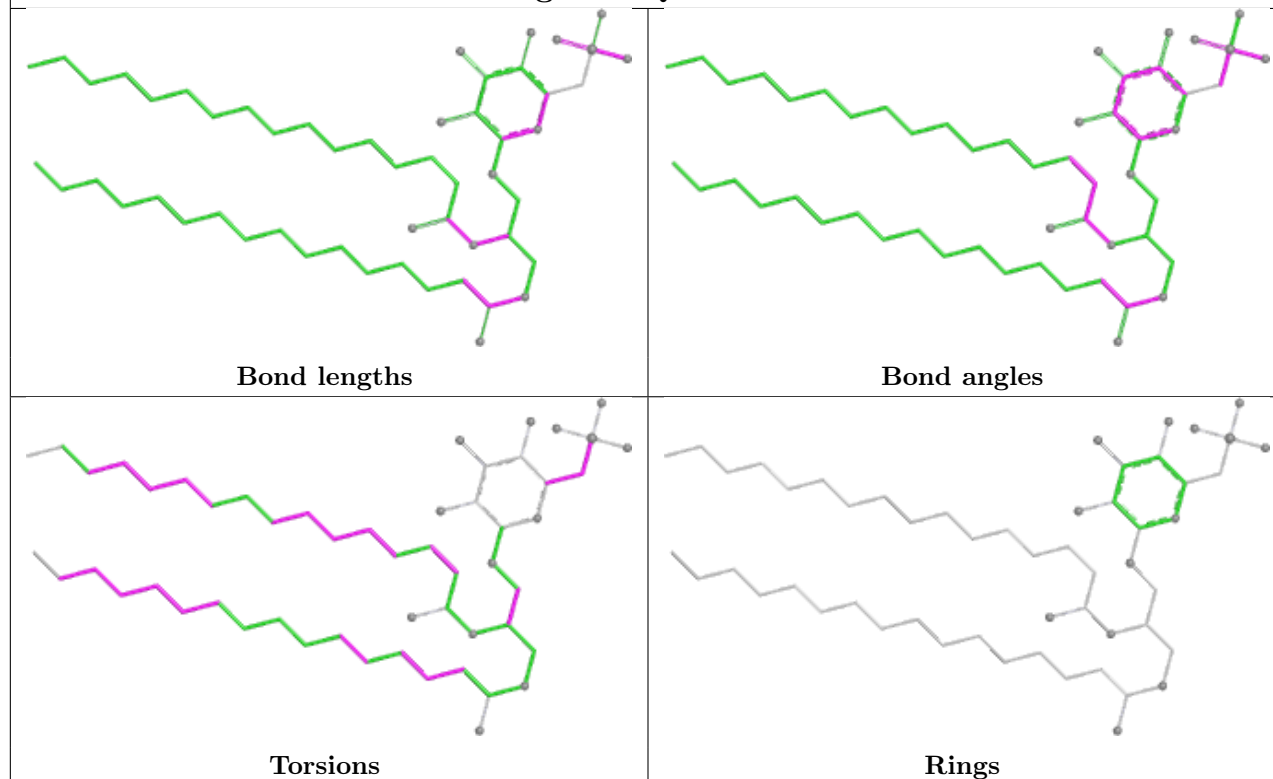
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



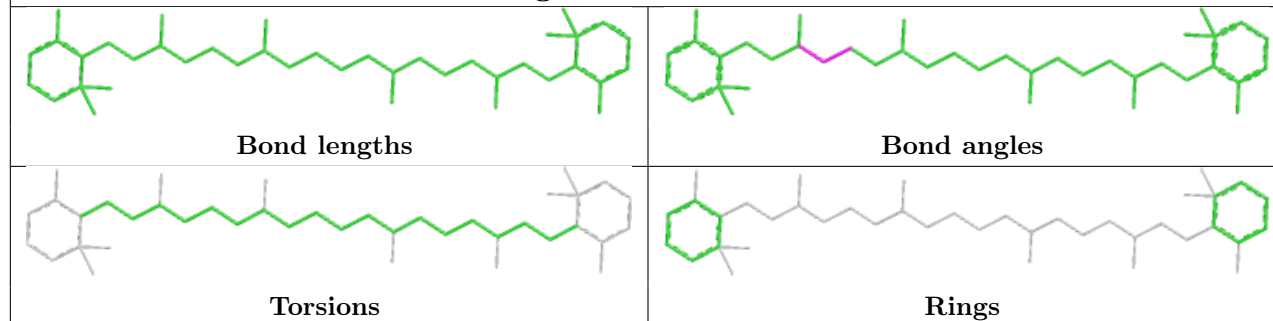
Ligand CLA b 612



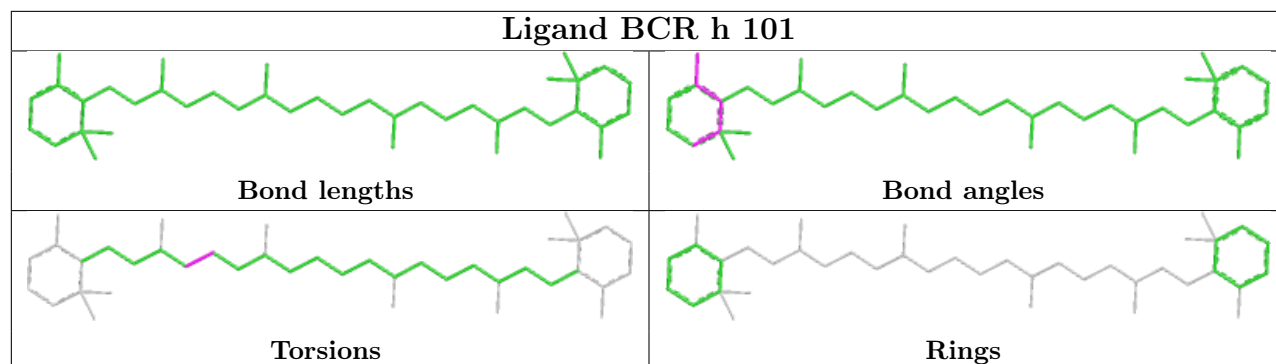
Ligand SQD a 614



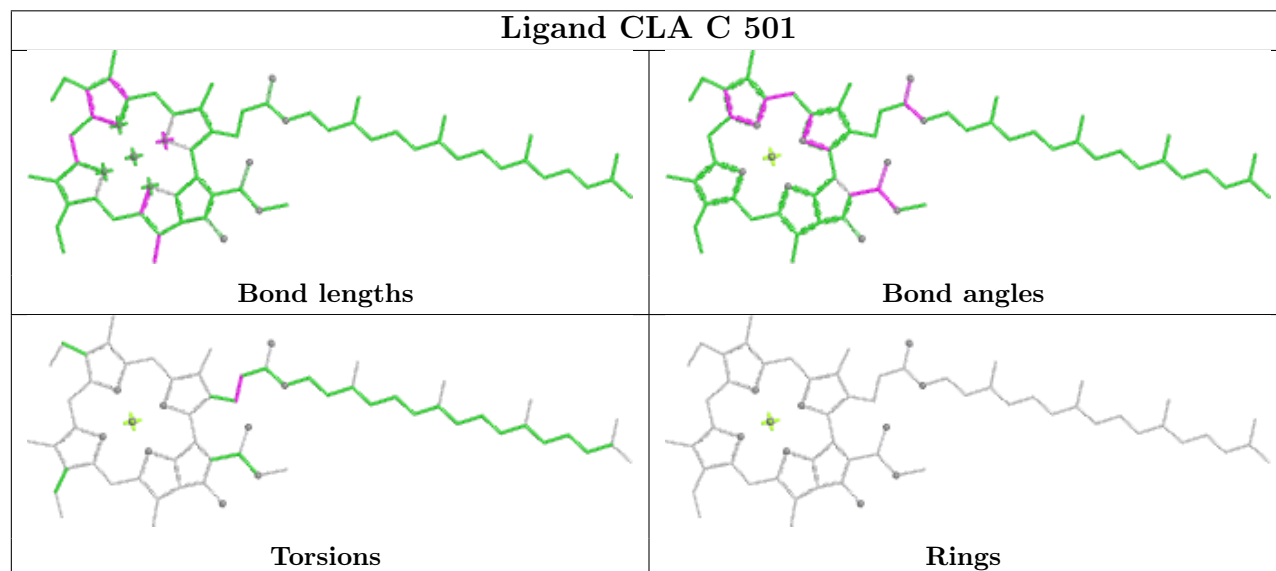
Ligand BCR c 515



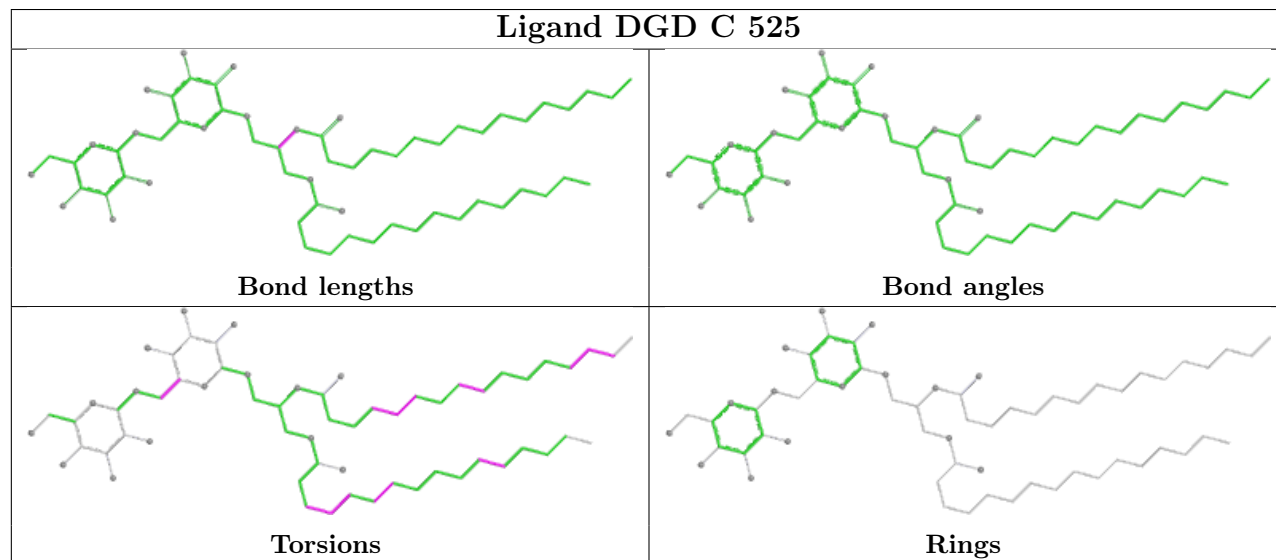
Ligand BCR h 101



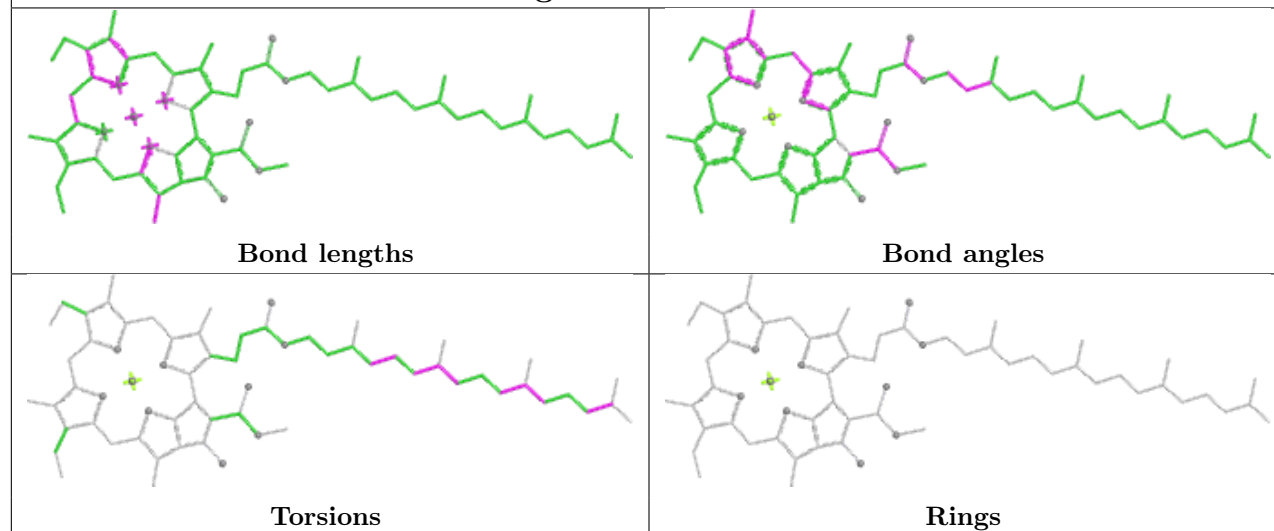
Ligand CLA C 501



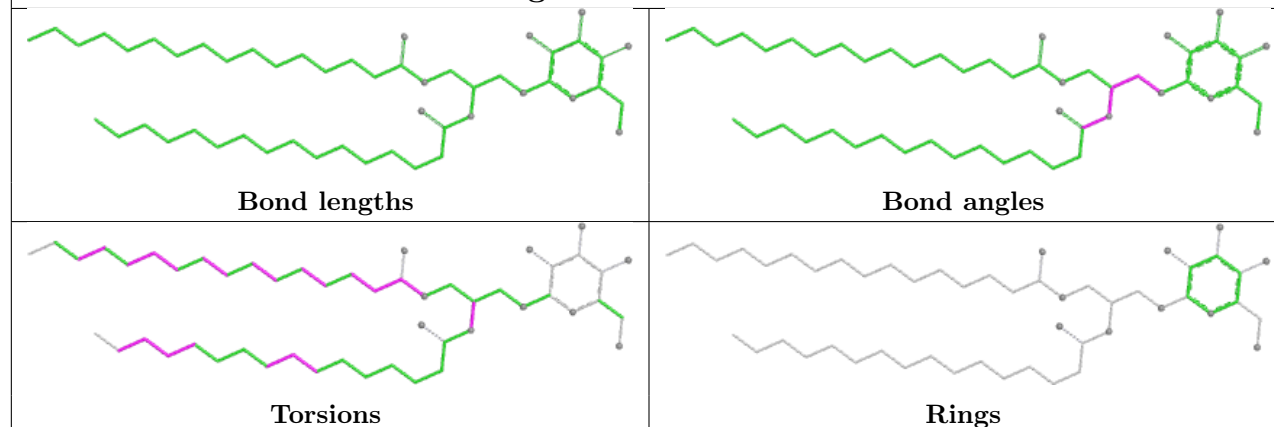
Ligand DGD C 525



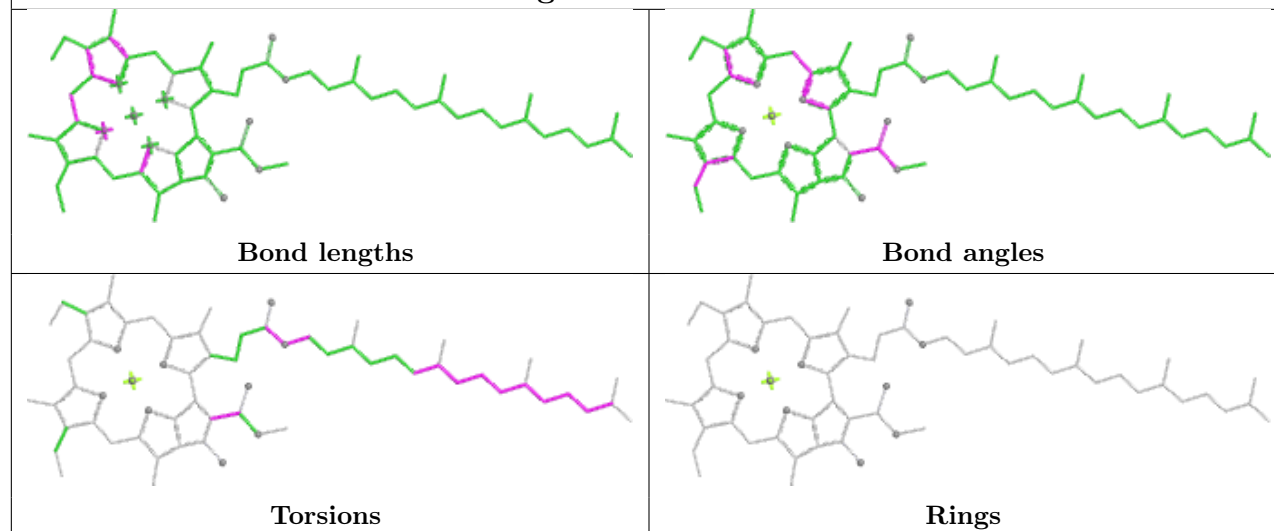
Ligand CLA b 602

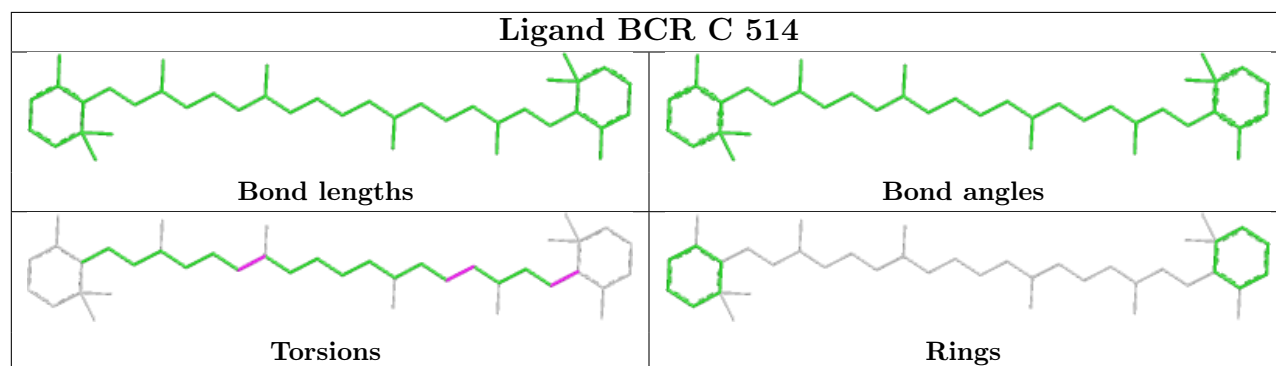
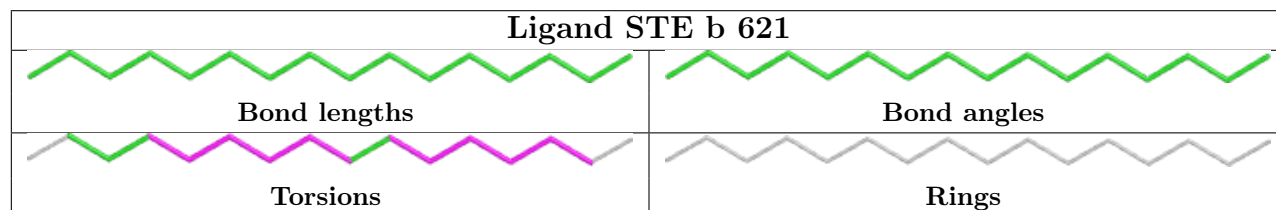
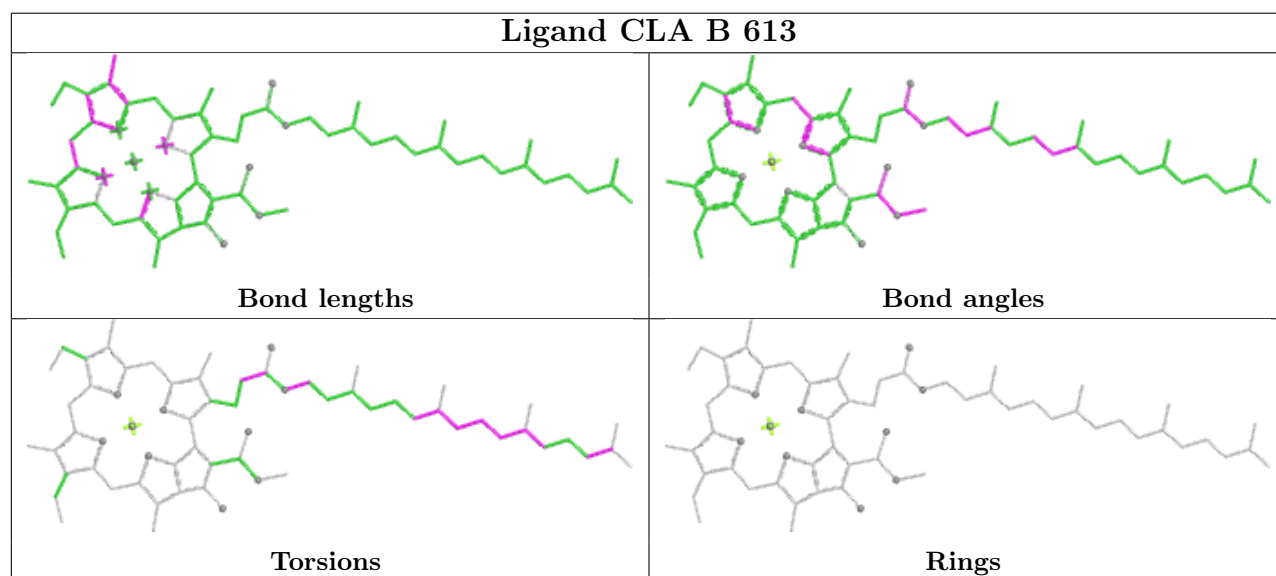
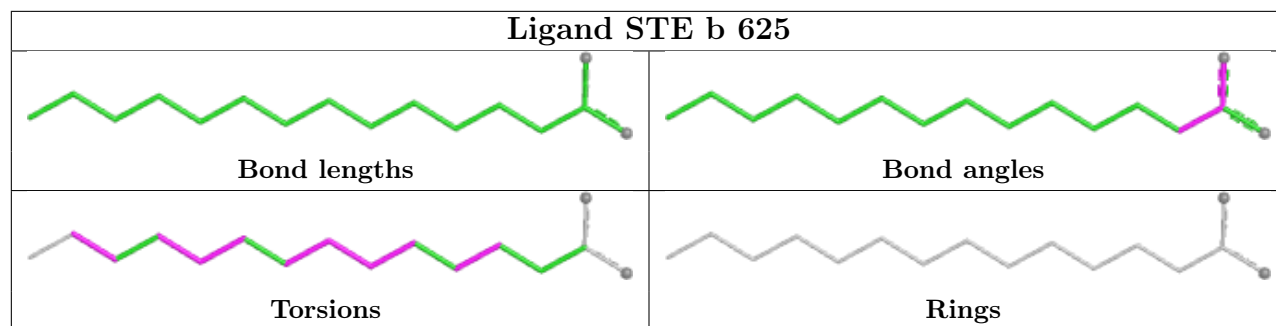


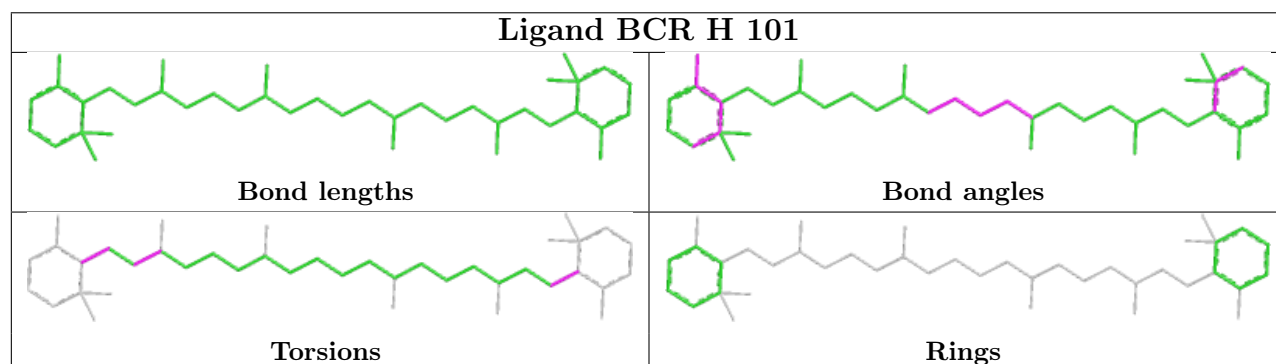
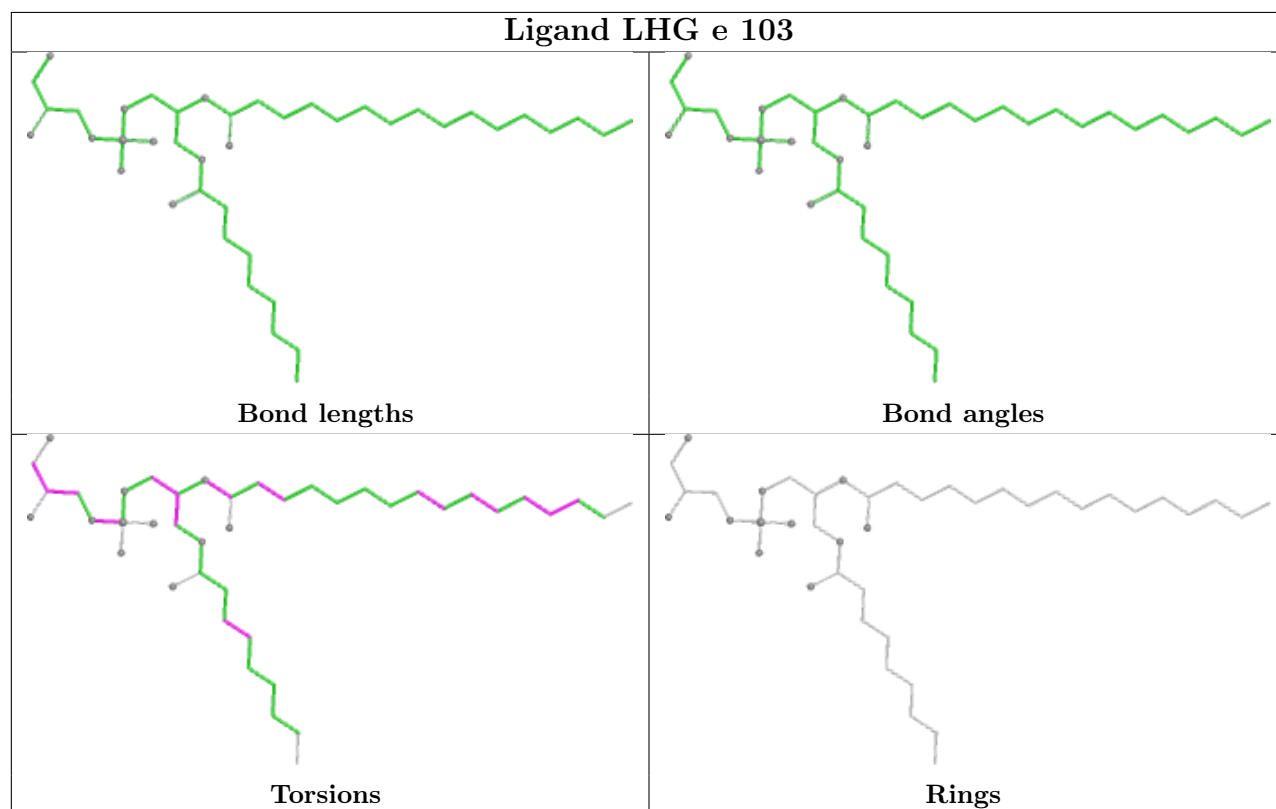
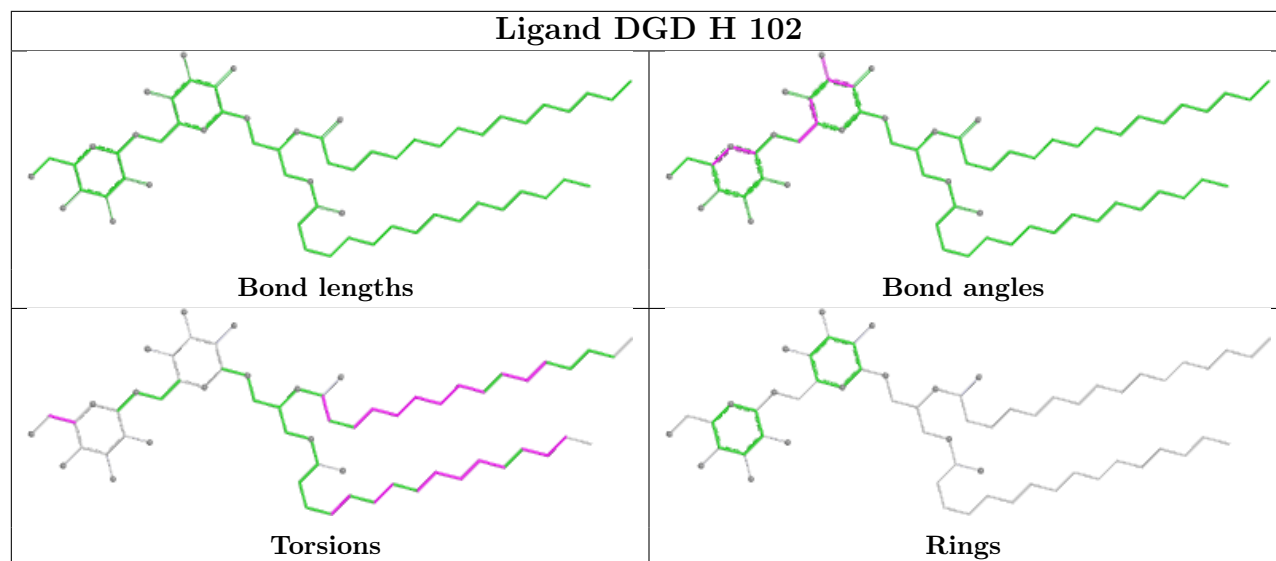
Ligand LMG B 621

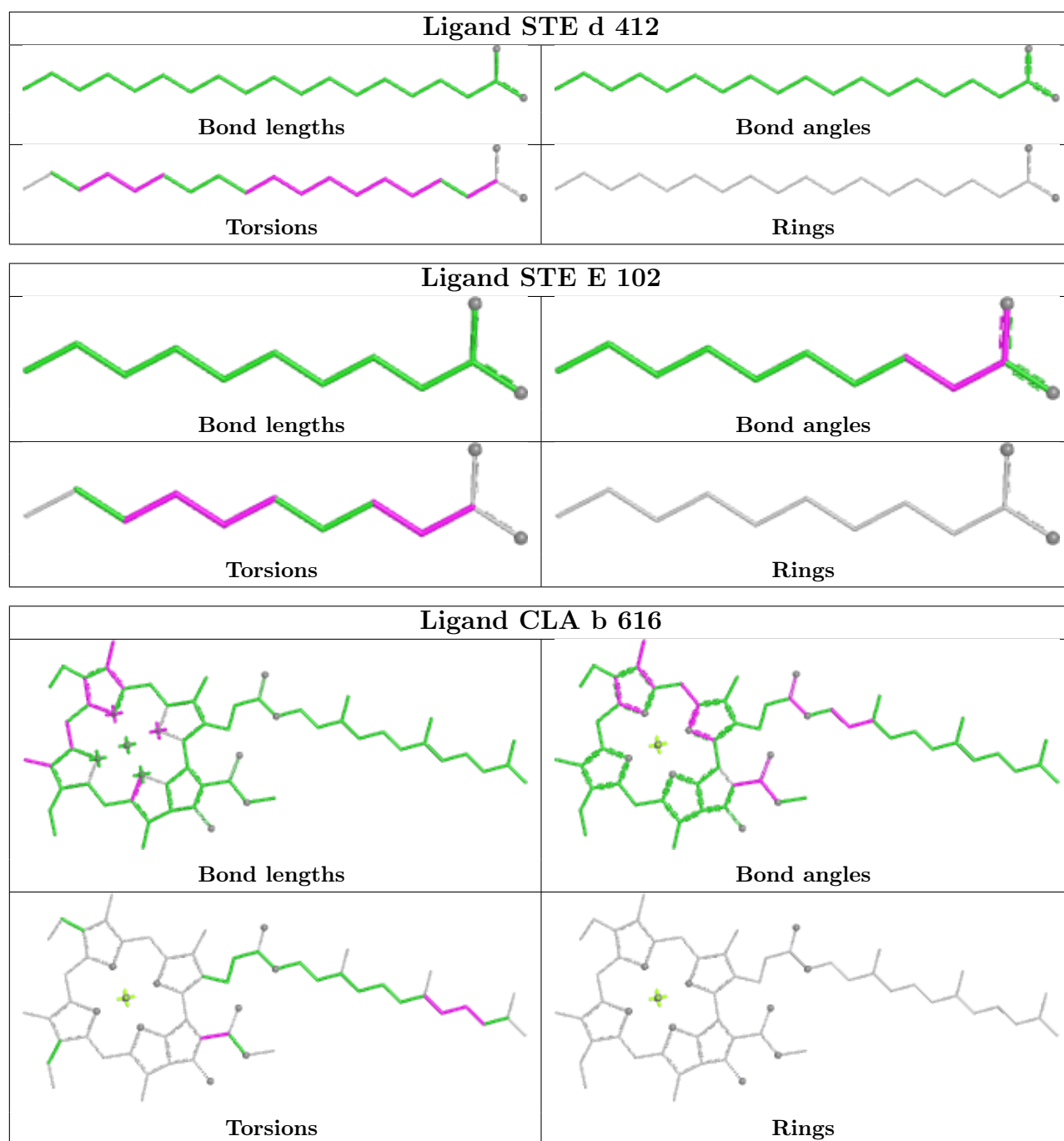


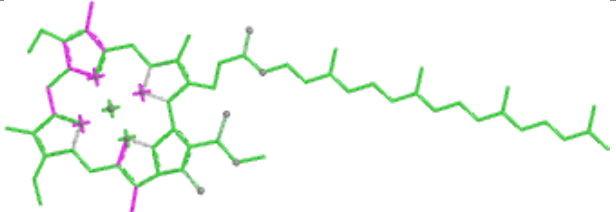
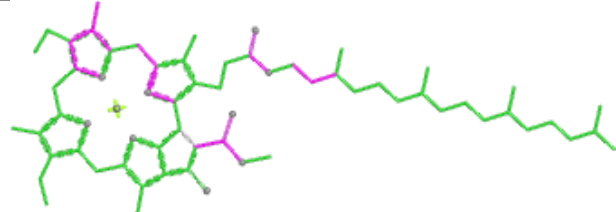
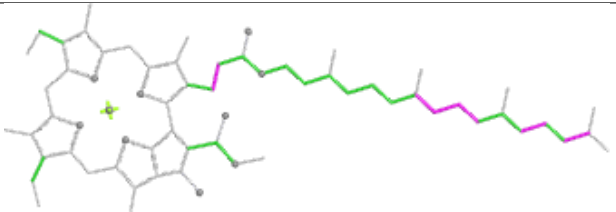
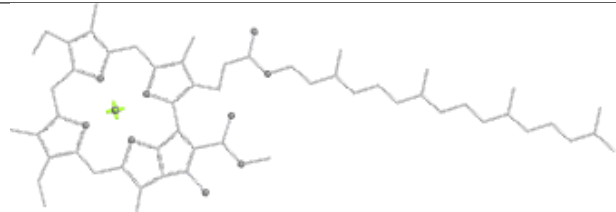
Ligand CLA c 506



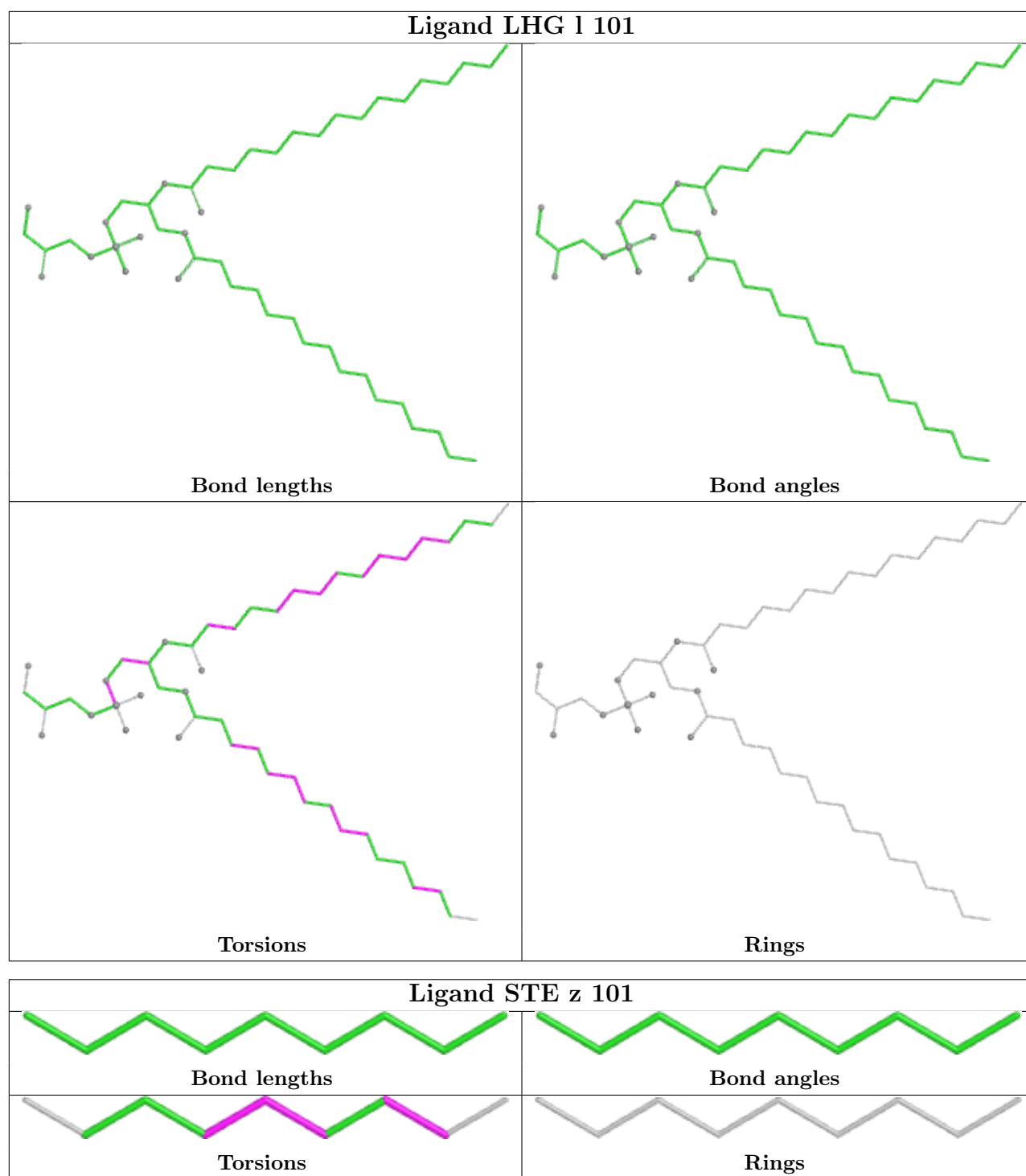


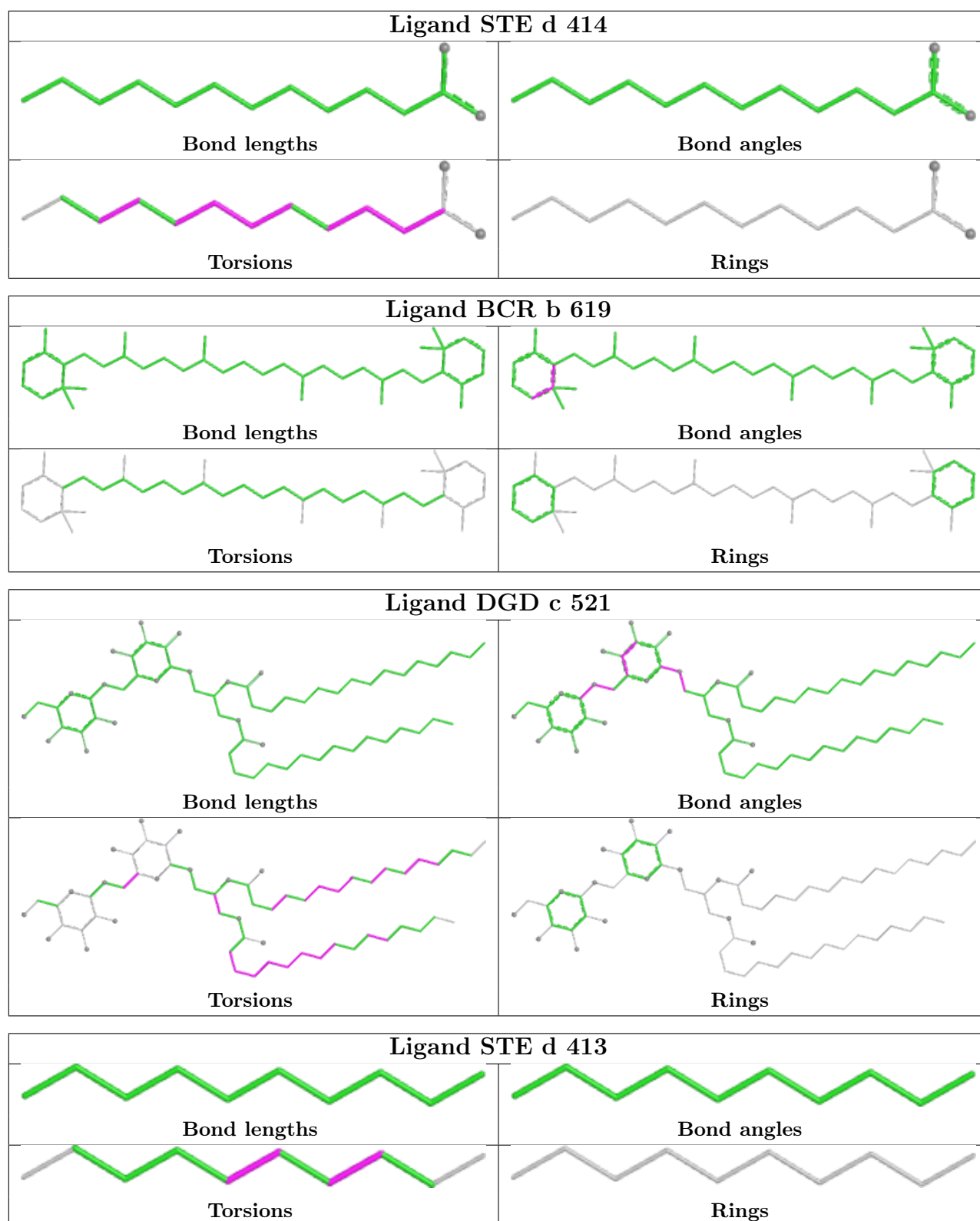


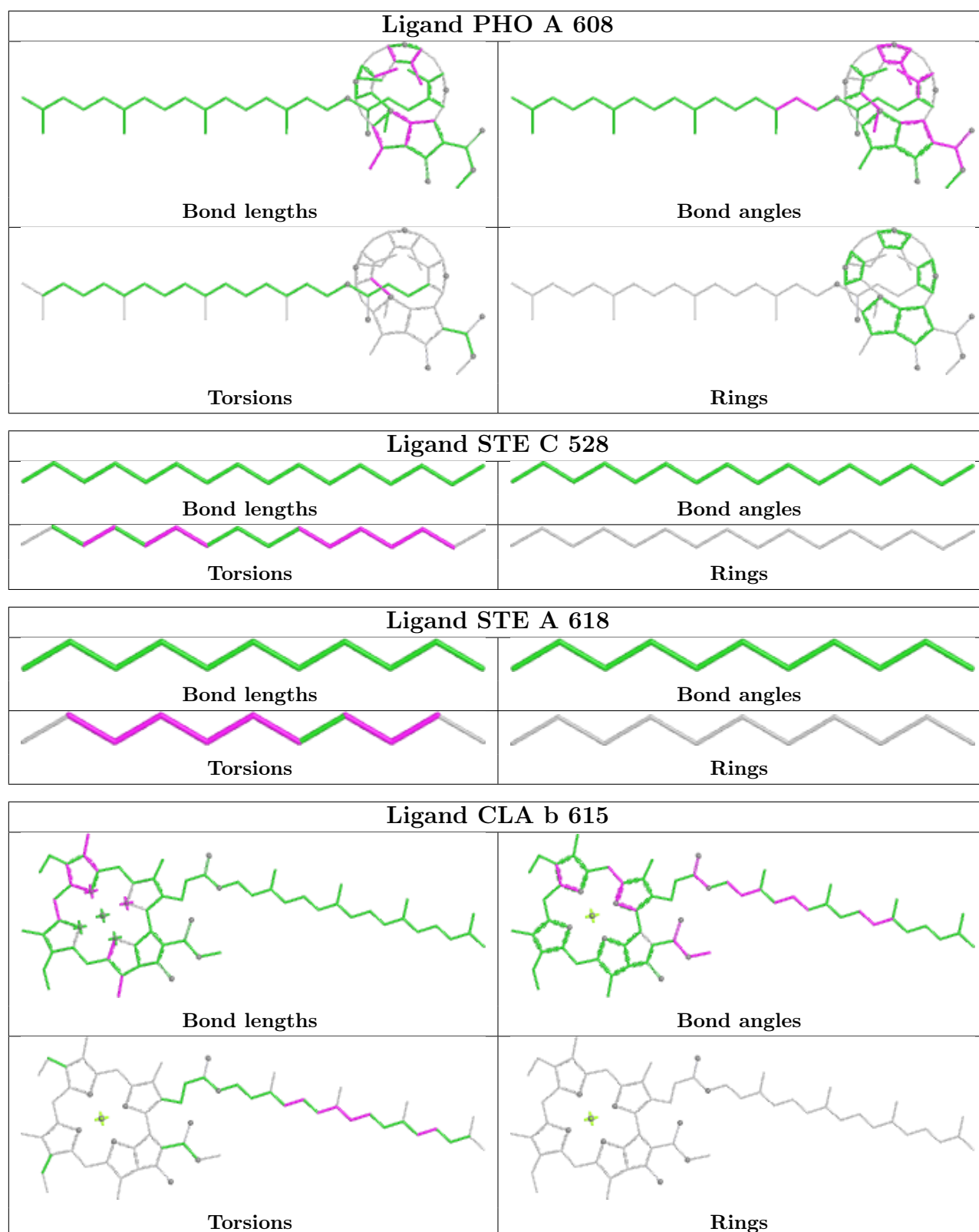


Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

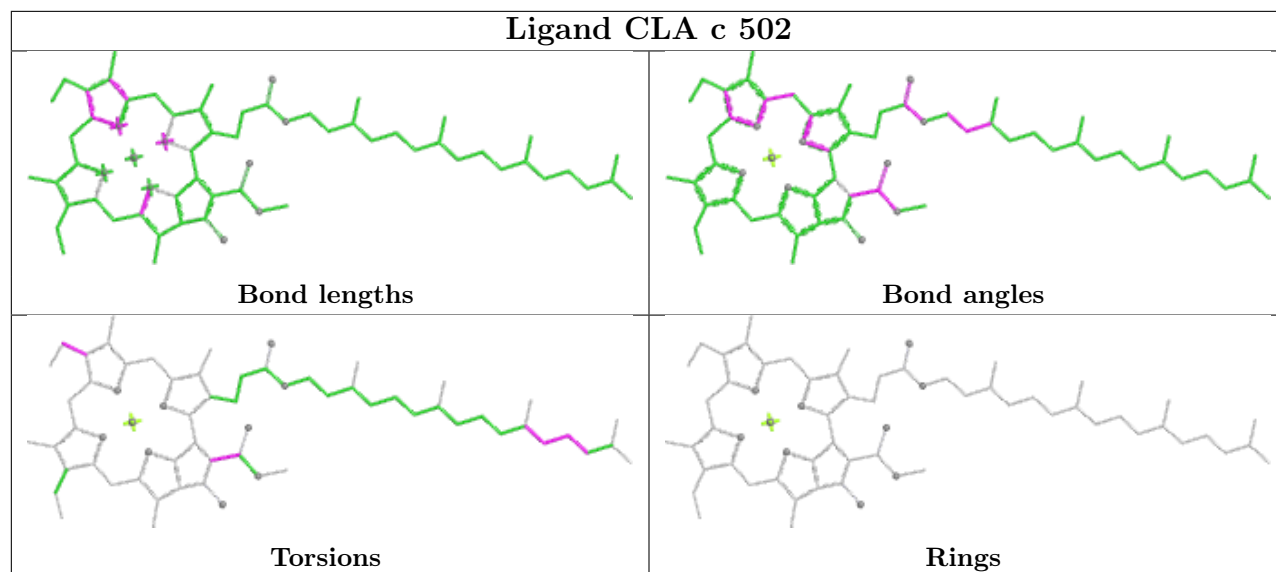
Ligand STE j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



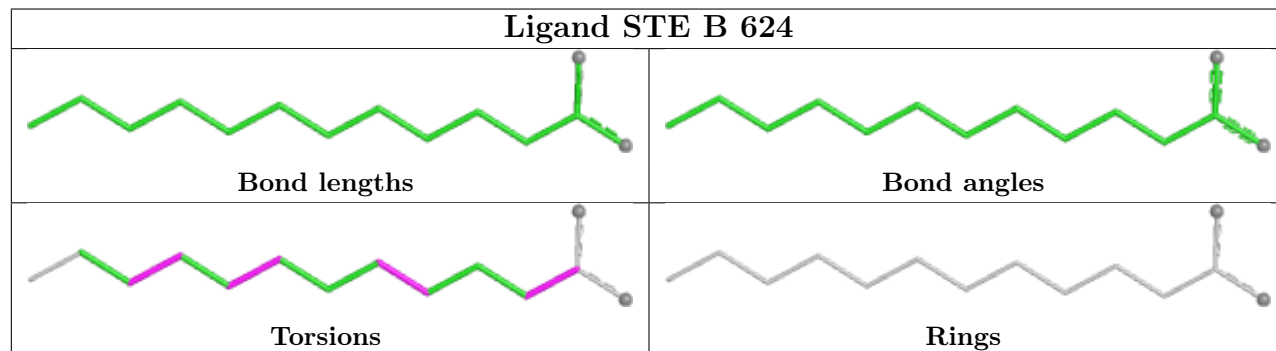




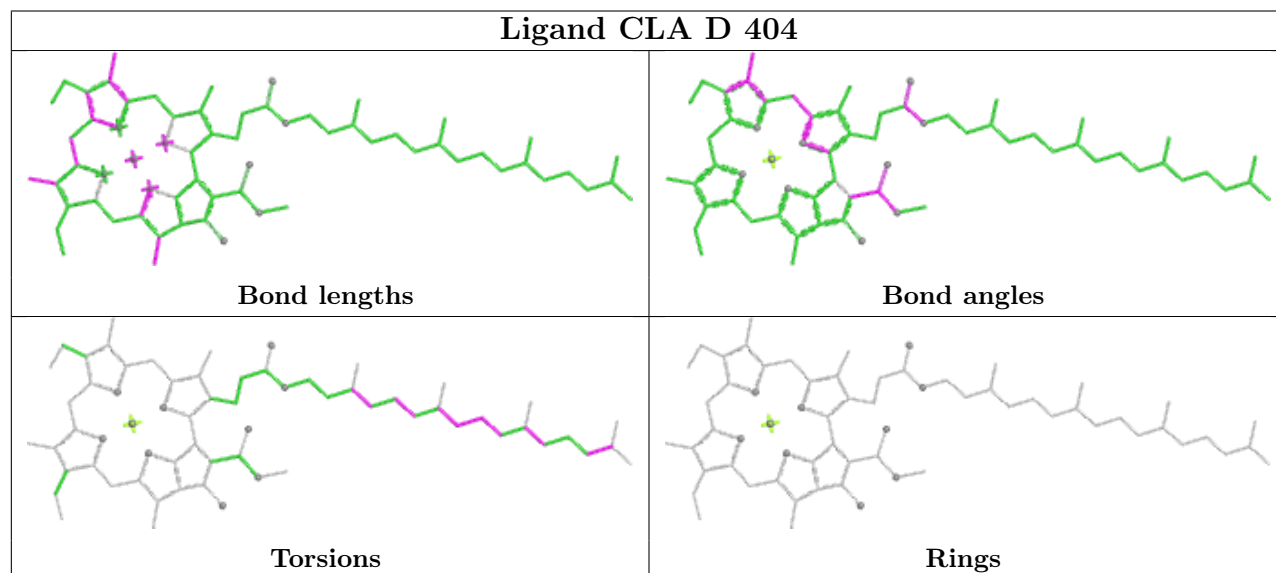
Ligand CLA c 502

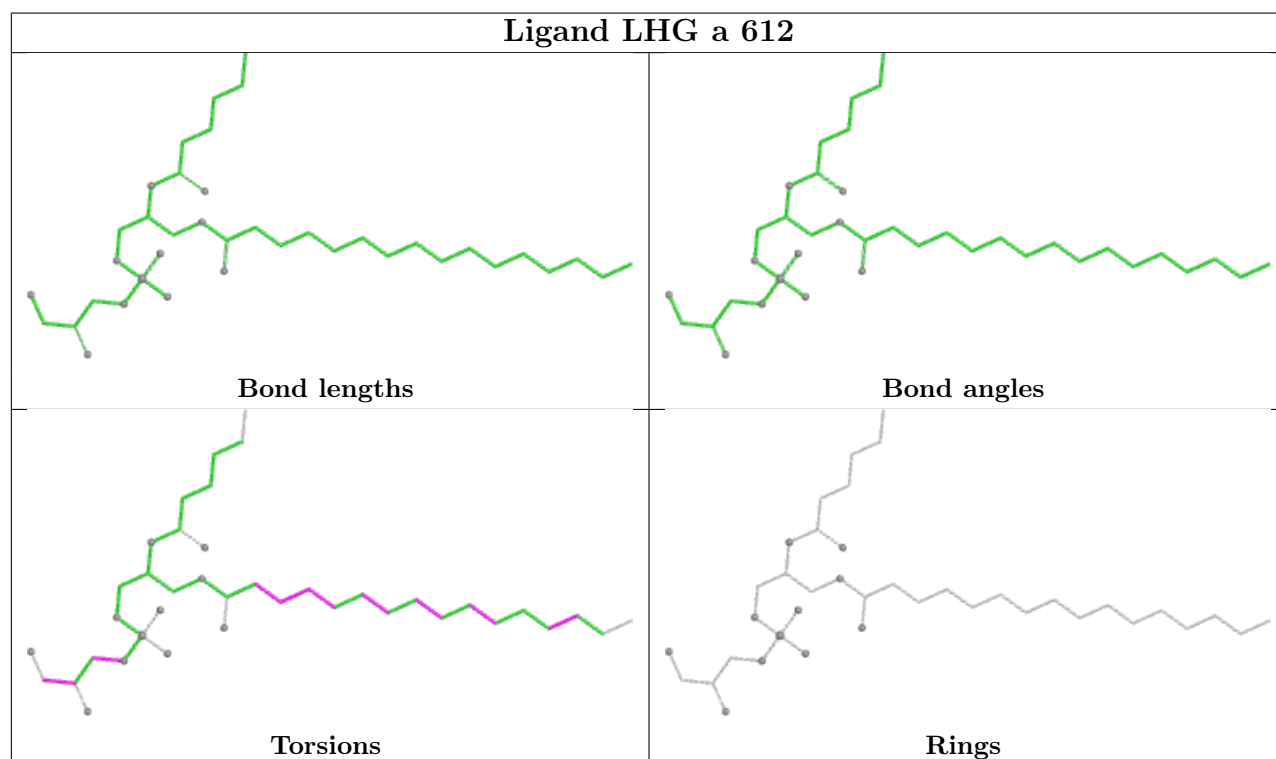
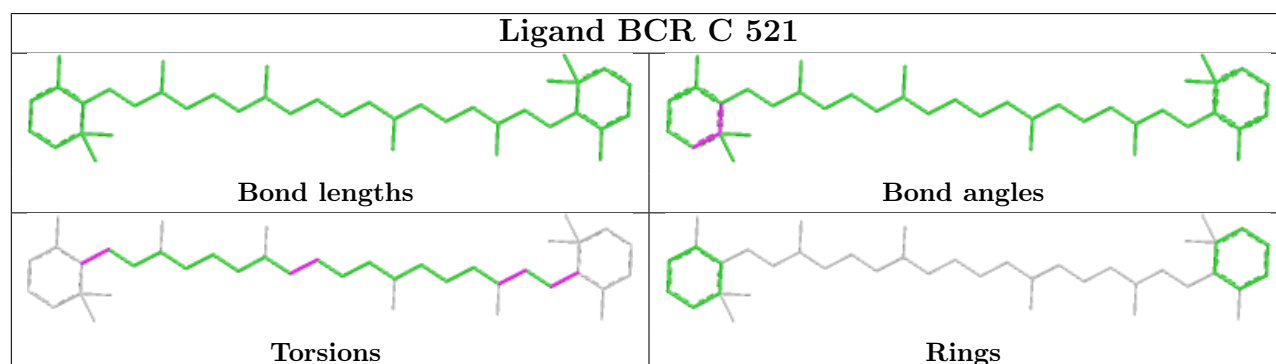
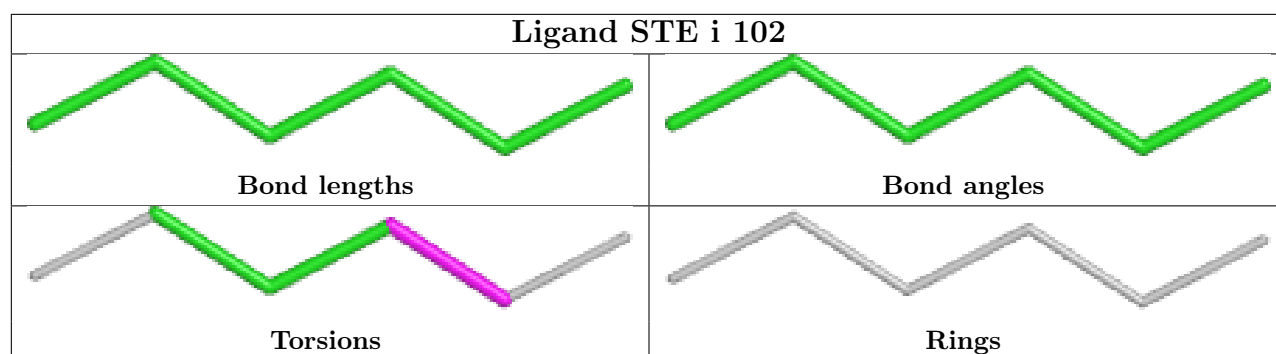


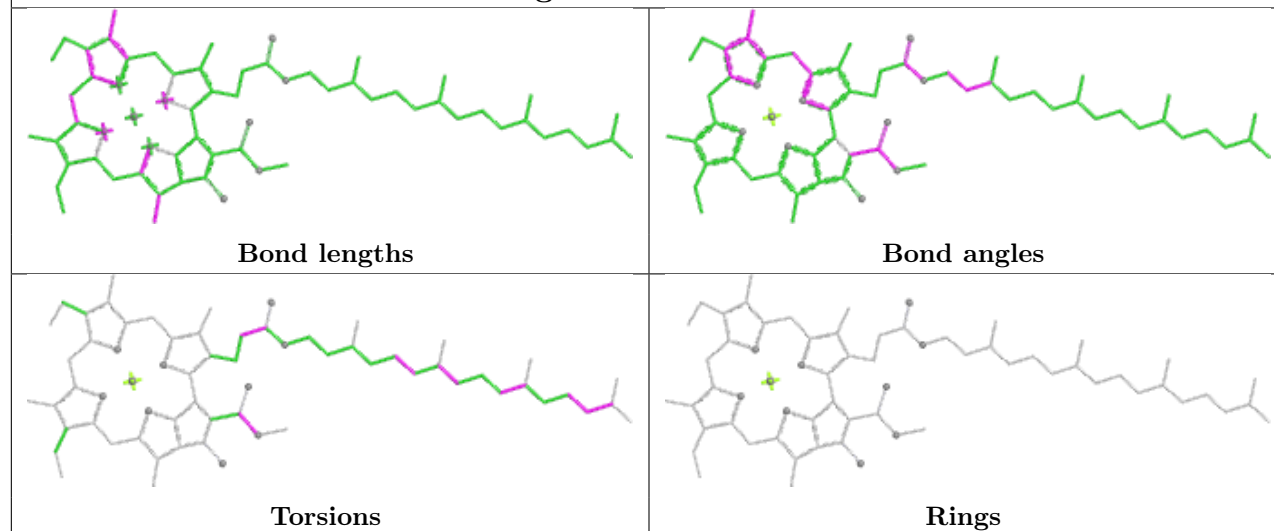
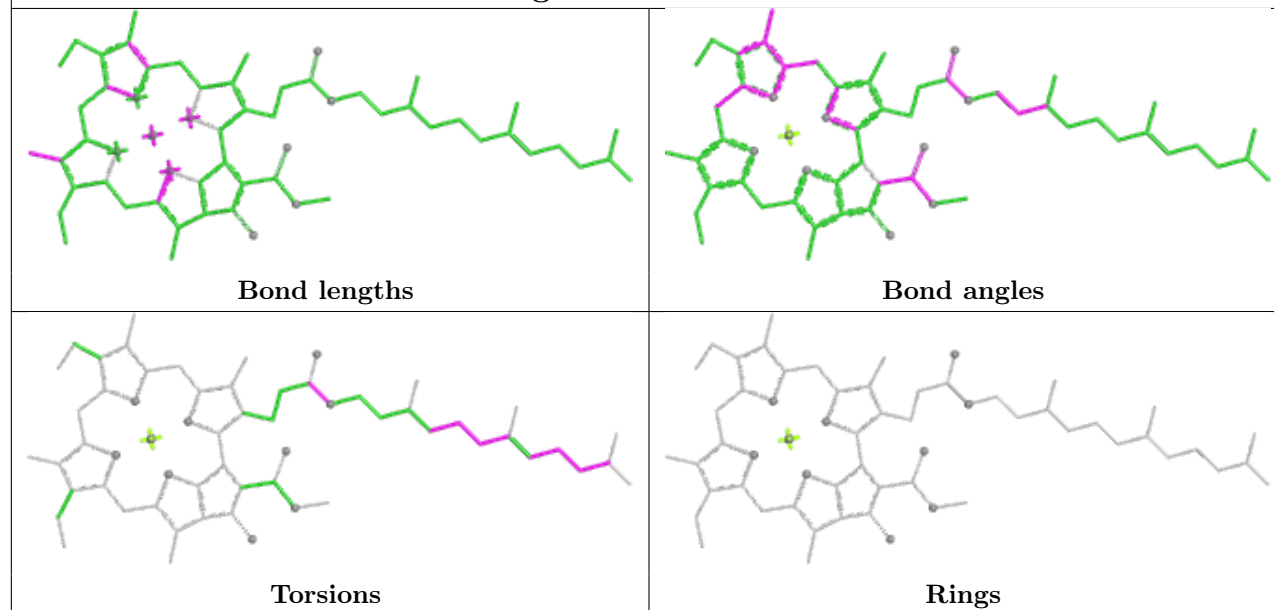
Ligand STE B 624

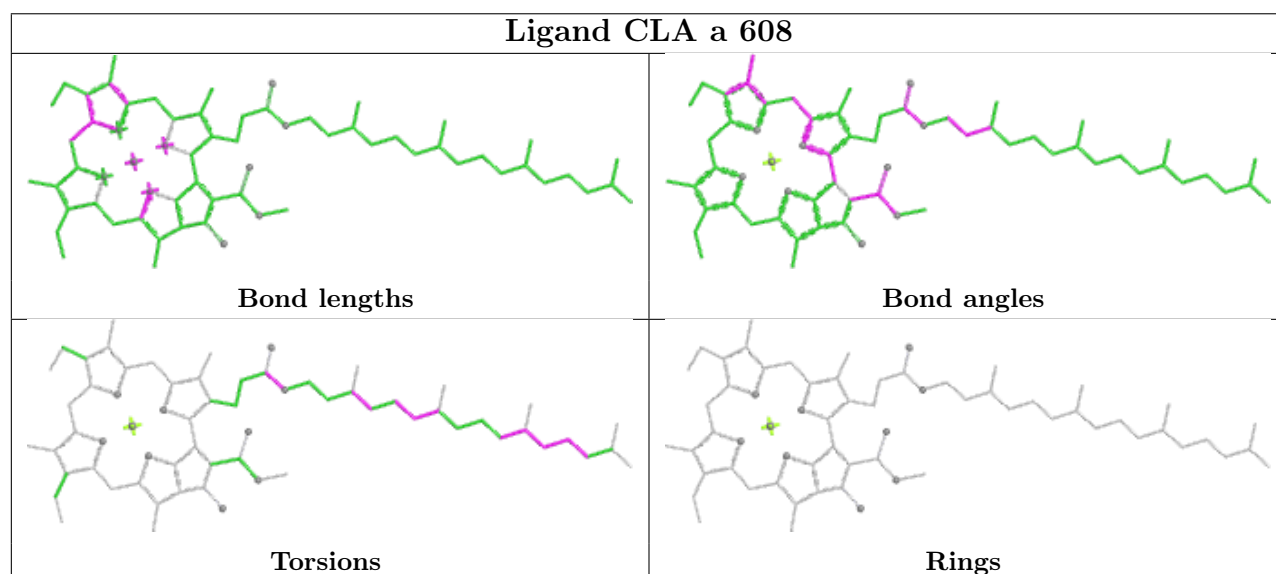
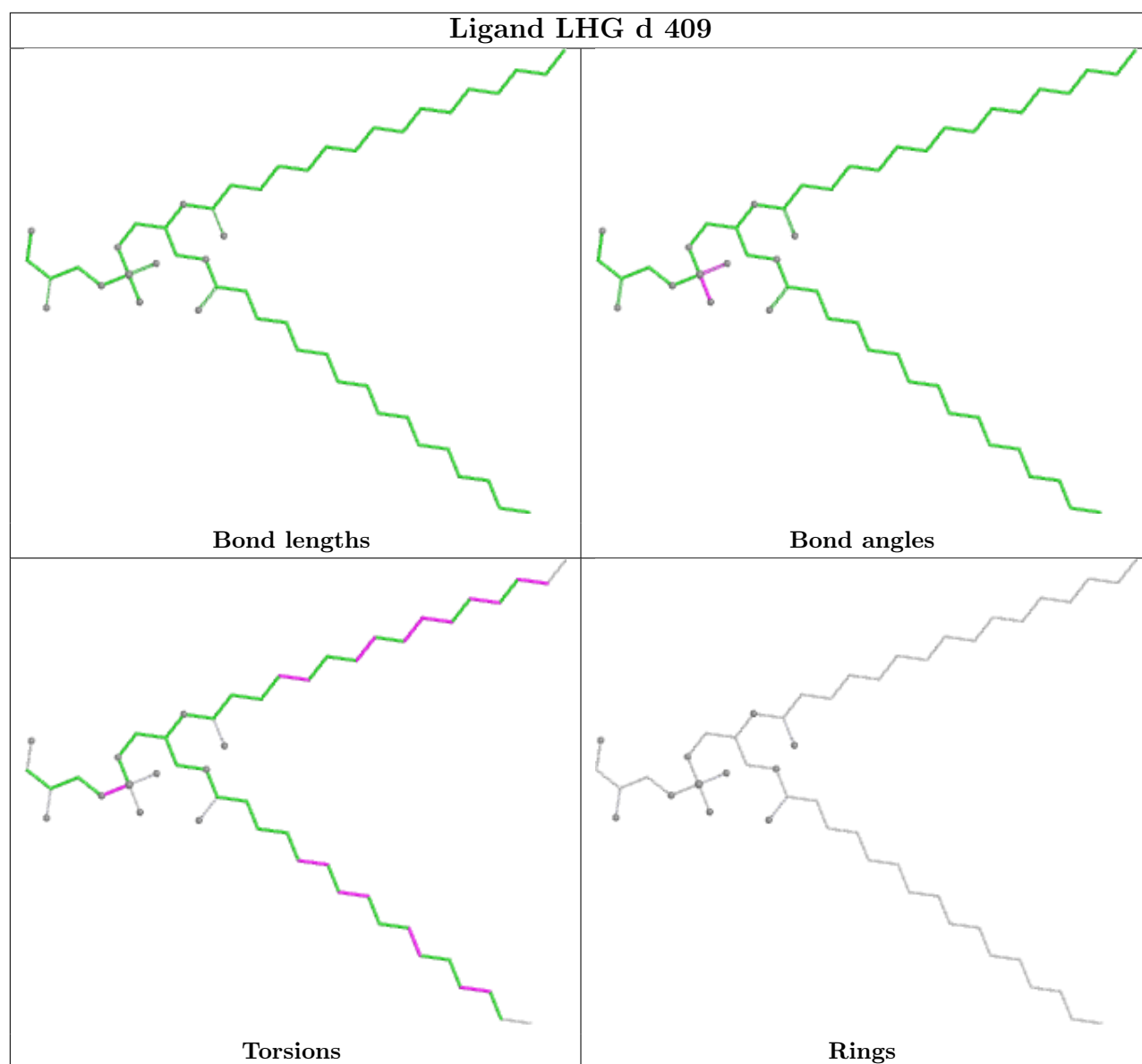


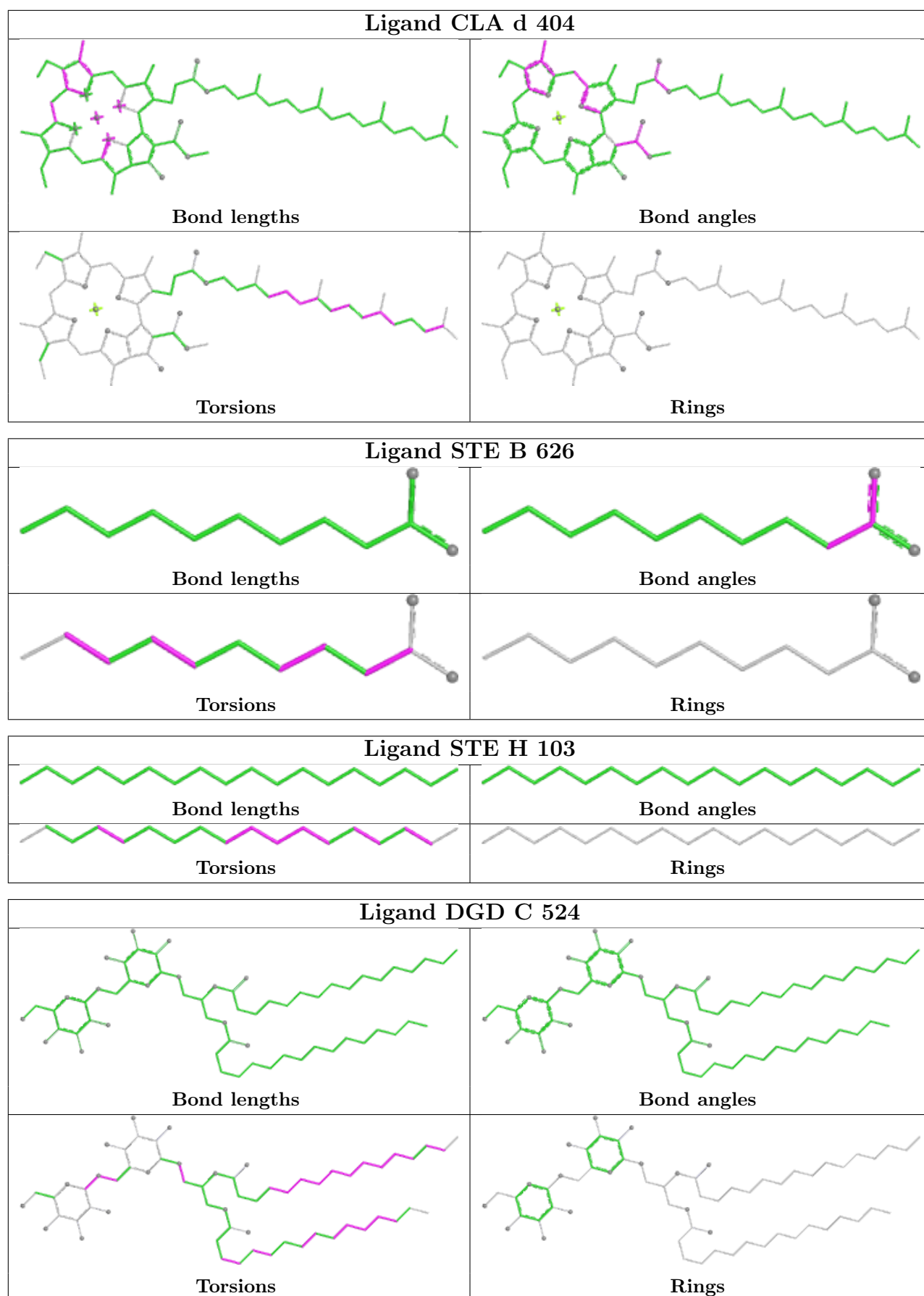
Ligand CLA D 404

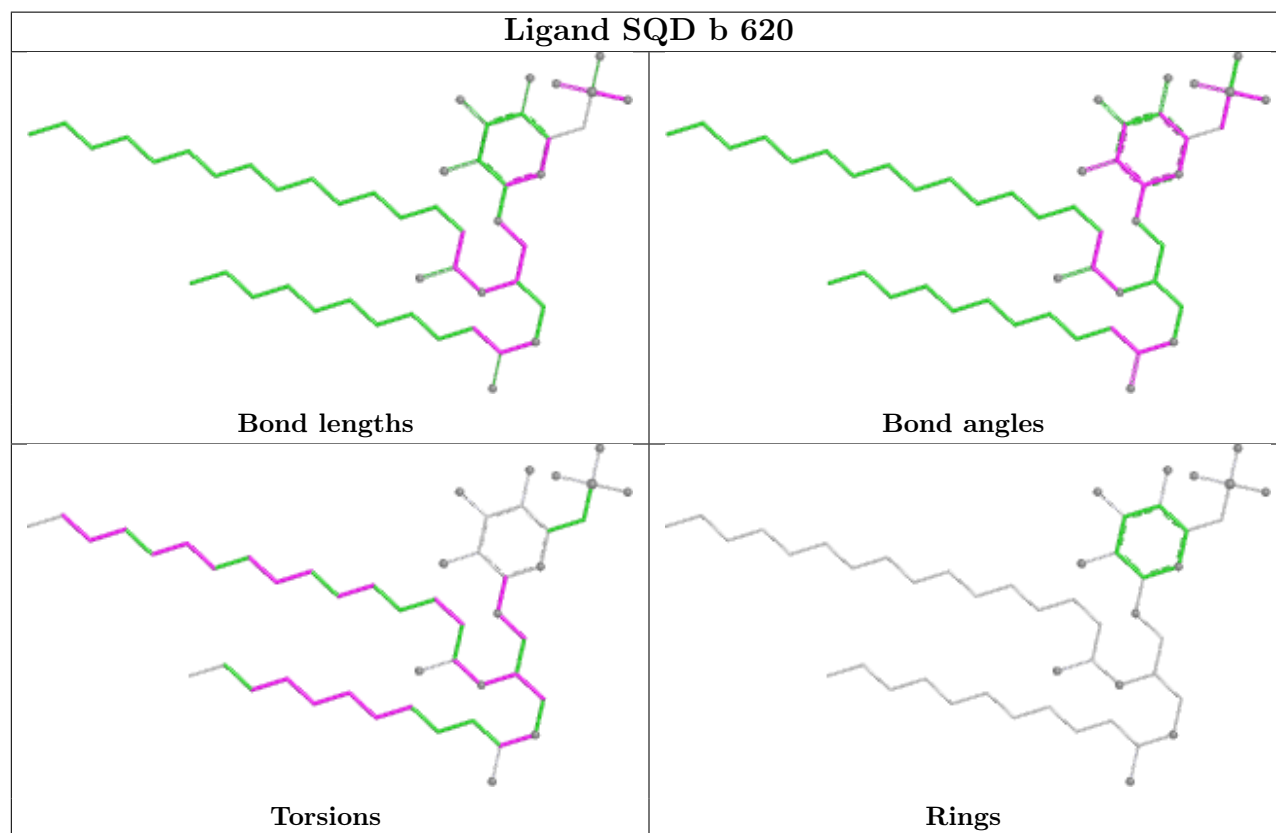
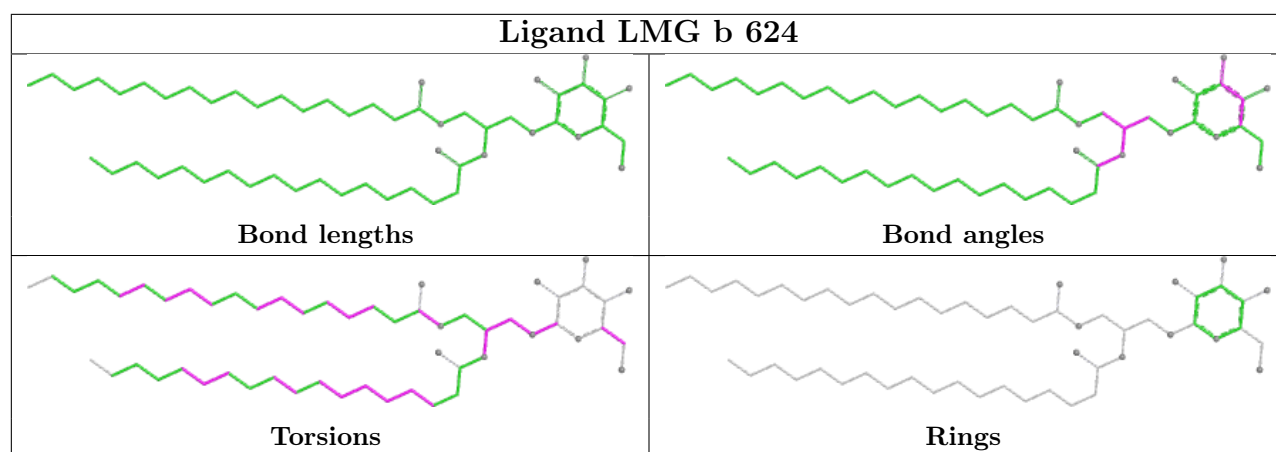




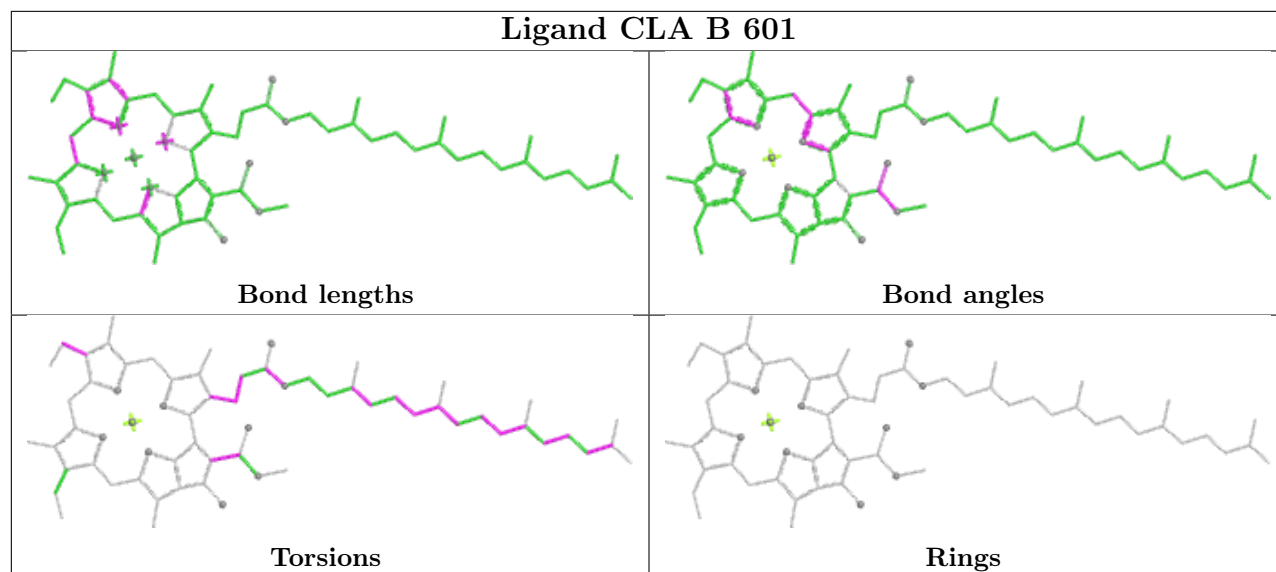
Ligand CLA b 613**Ligand CLA B 616**



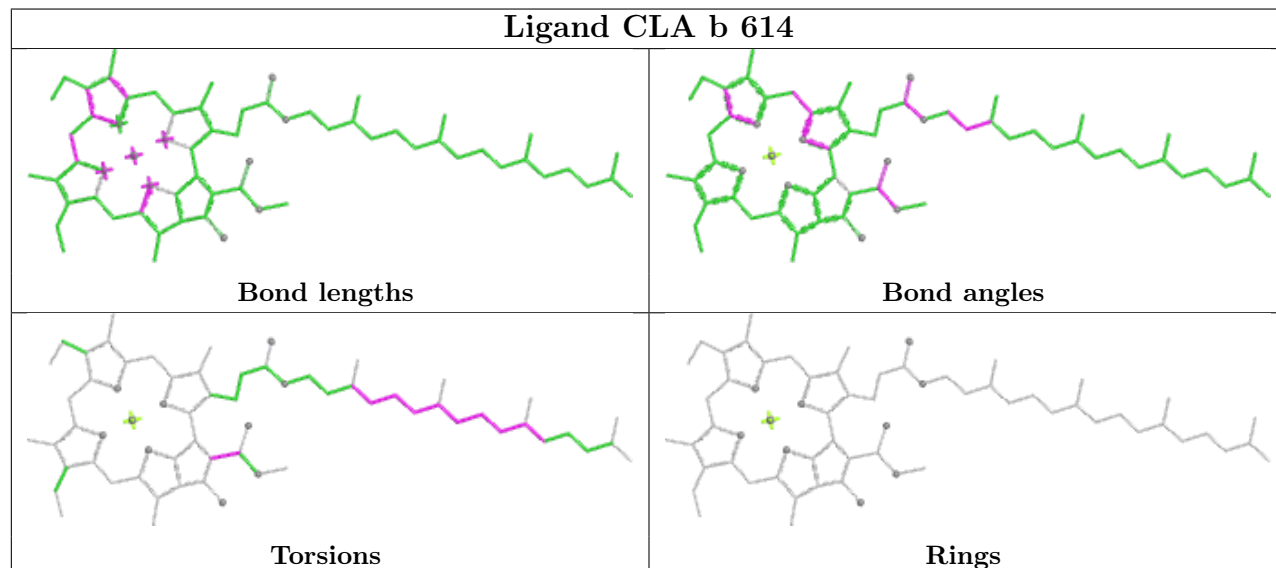




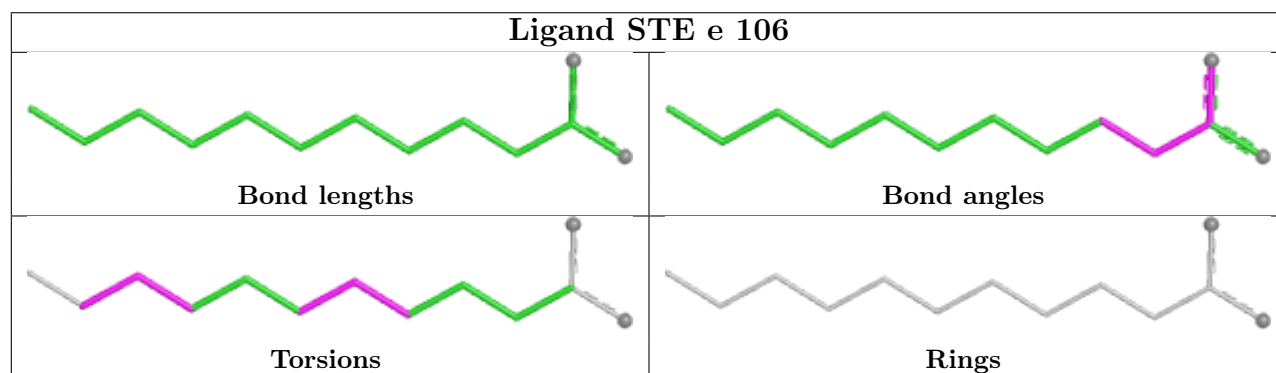
Ligand CLA B 601



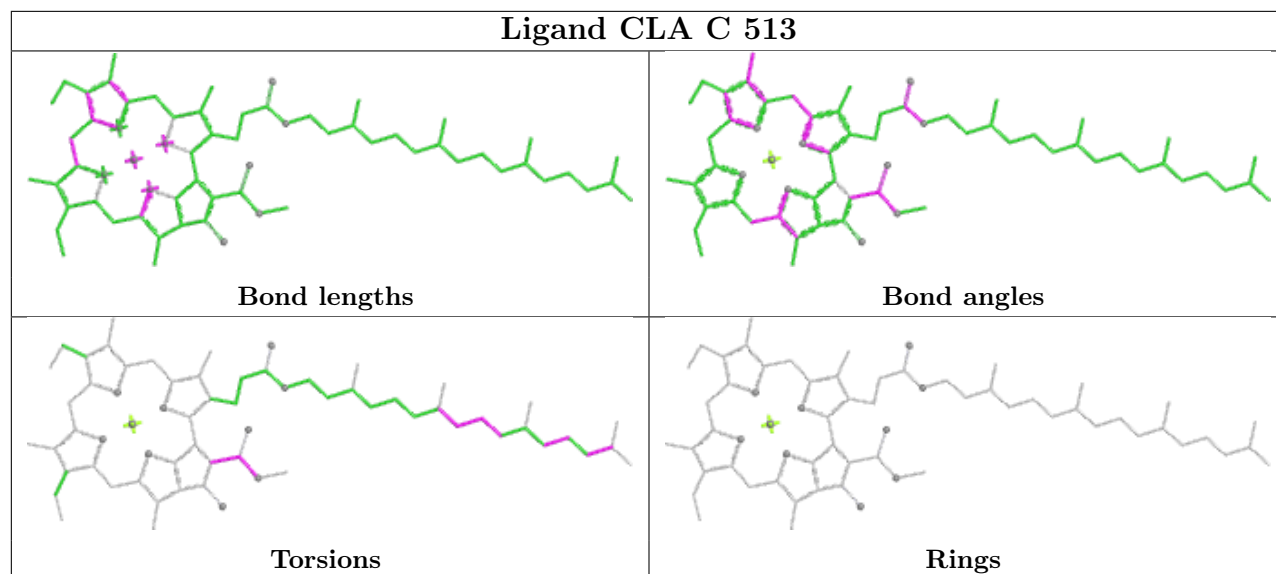
Ligand CLA b 614



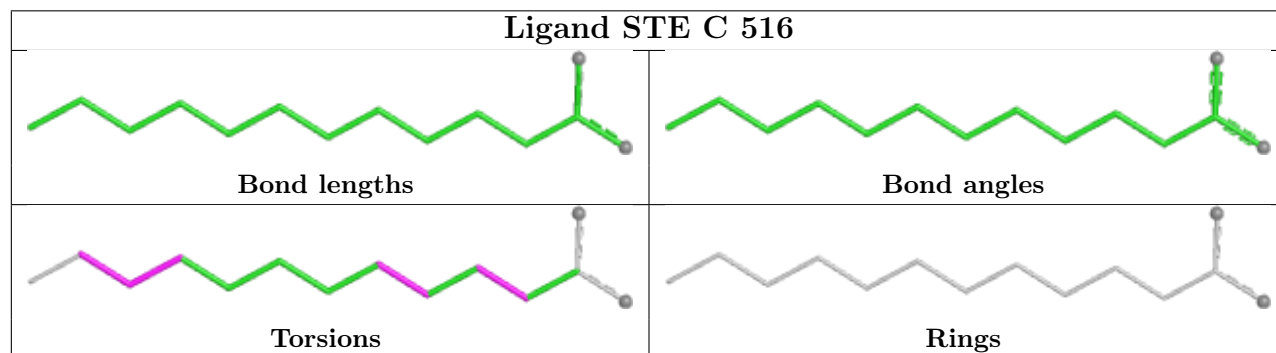
Ligand STE e 106



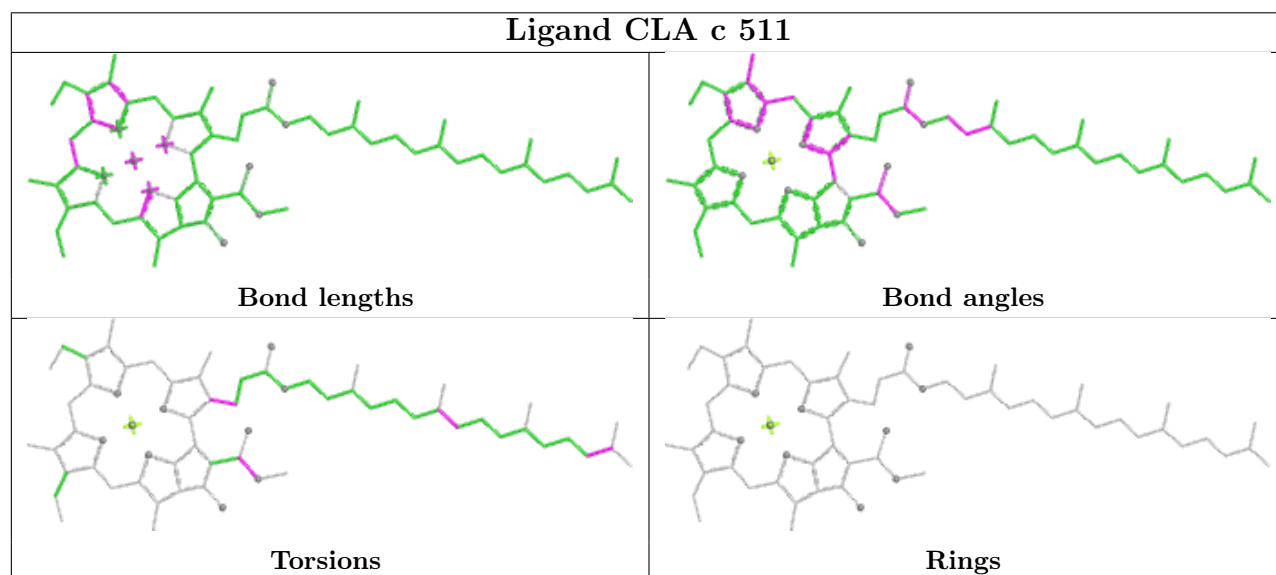
Ligand CLA C 513

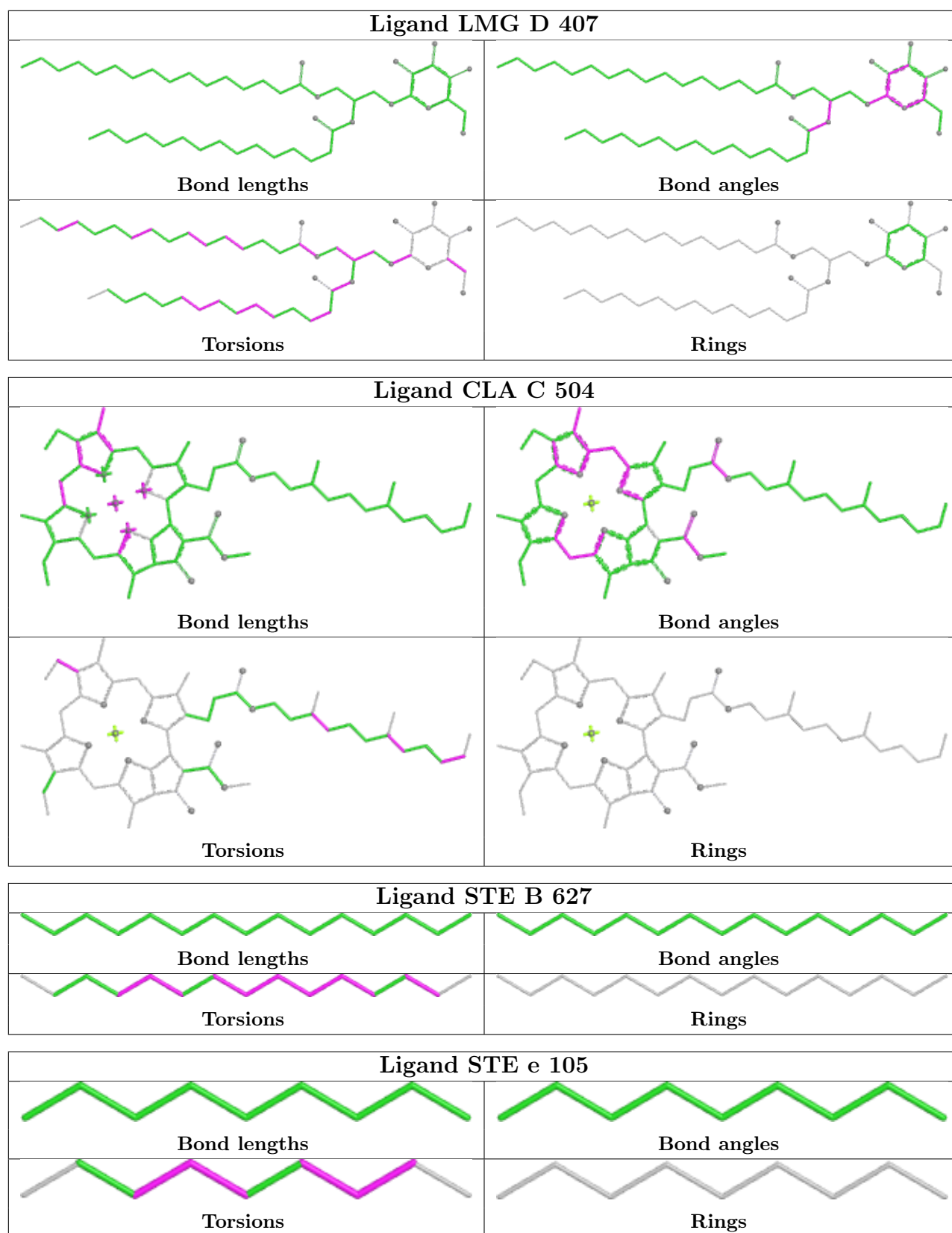


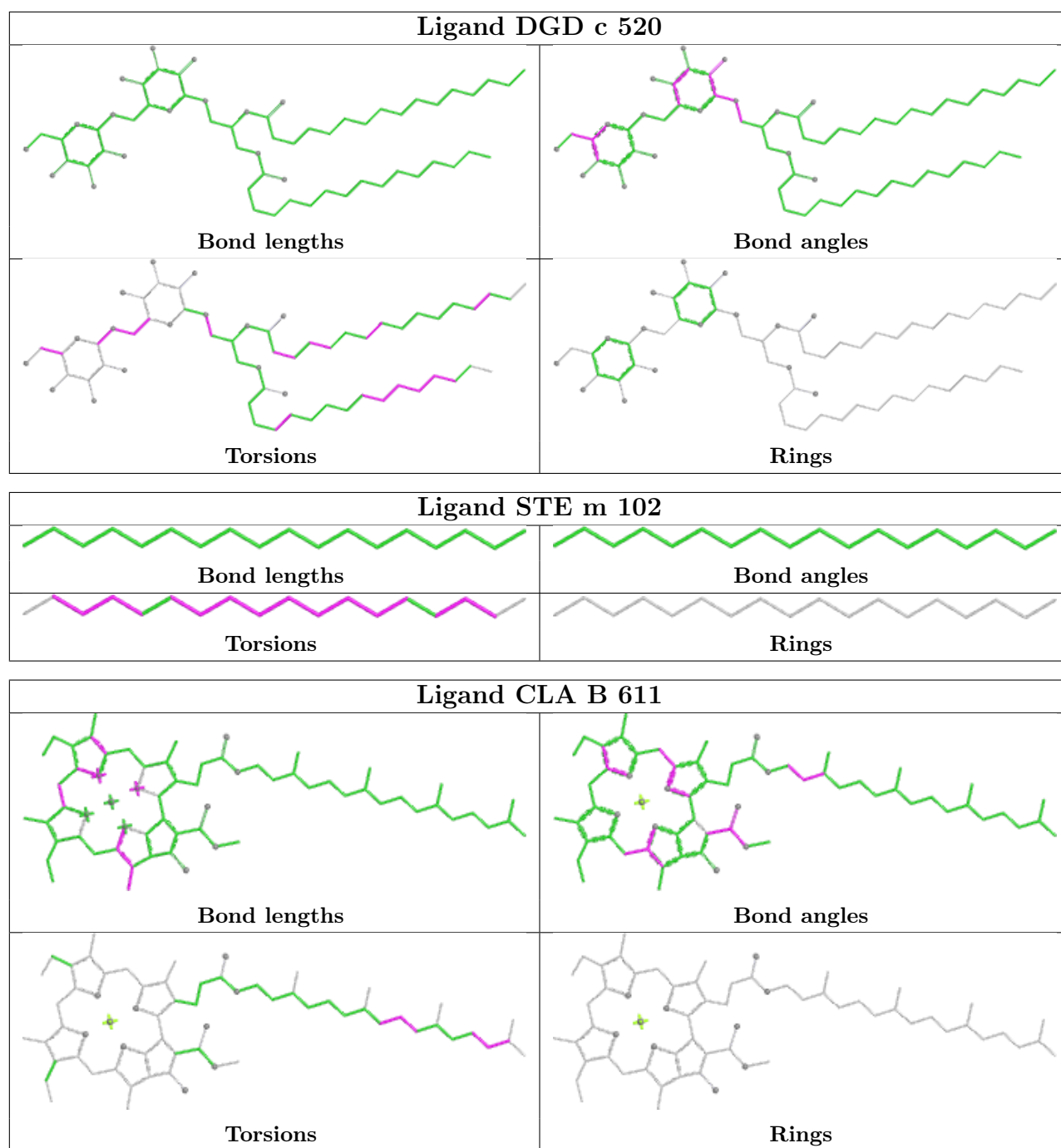
Ligand STE C 516

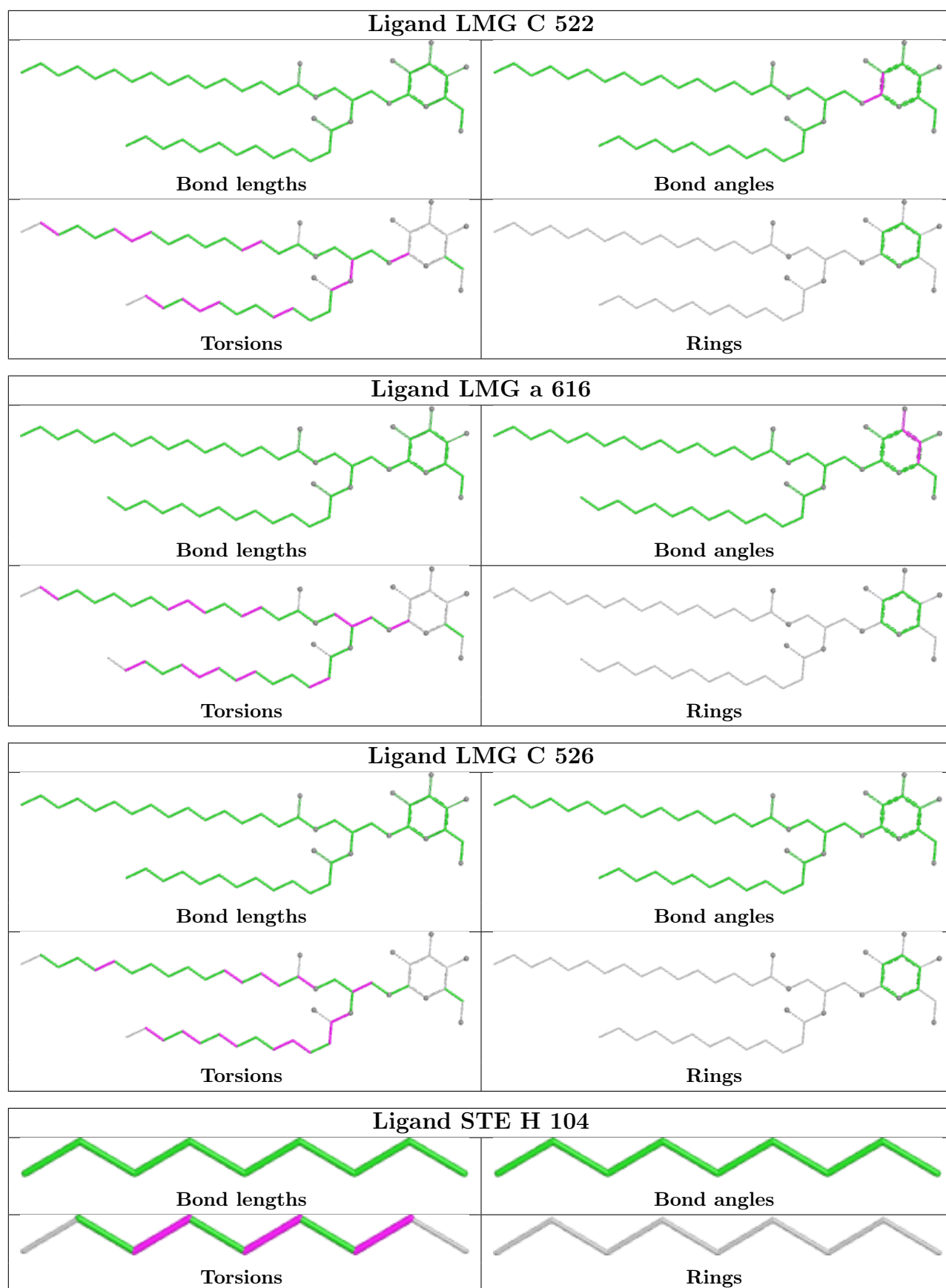


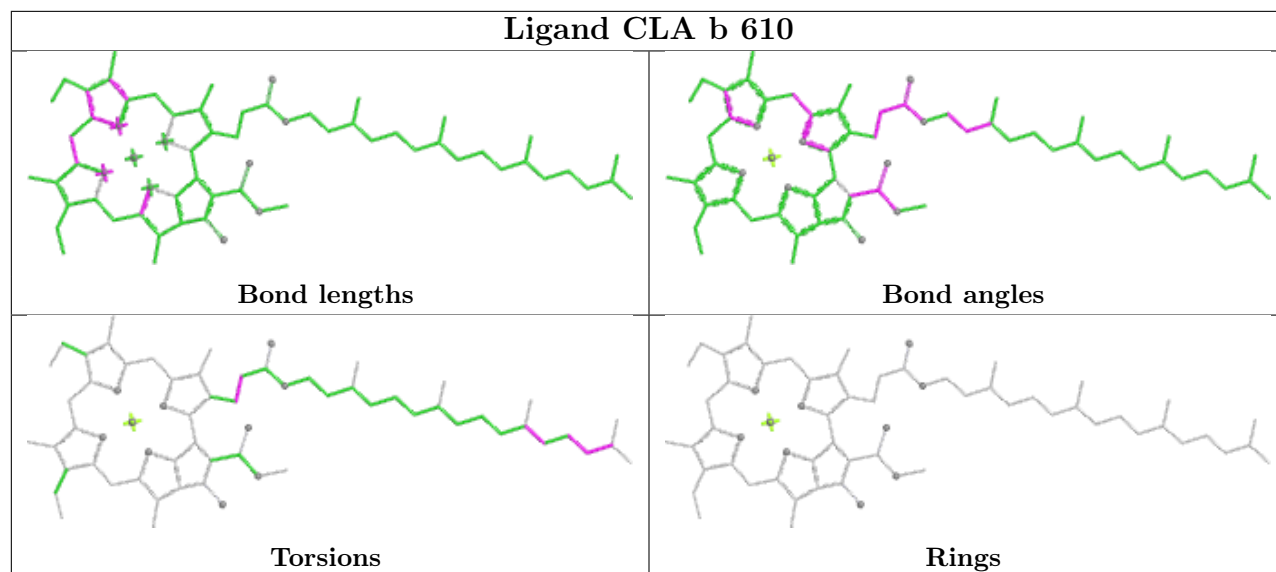
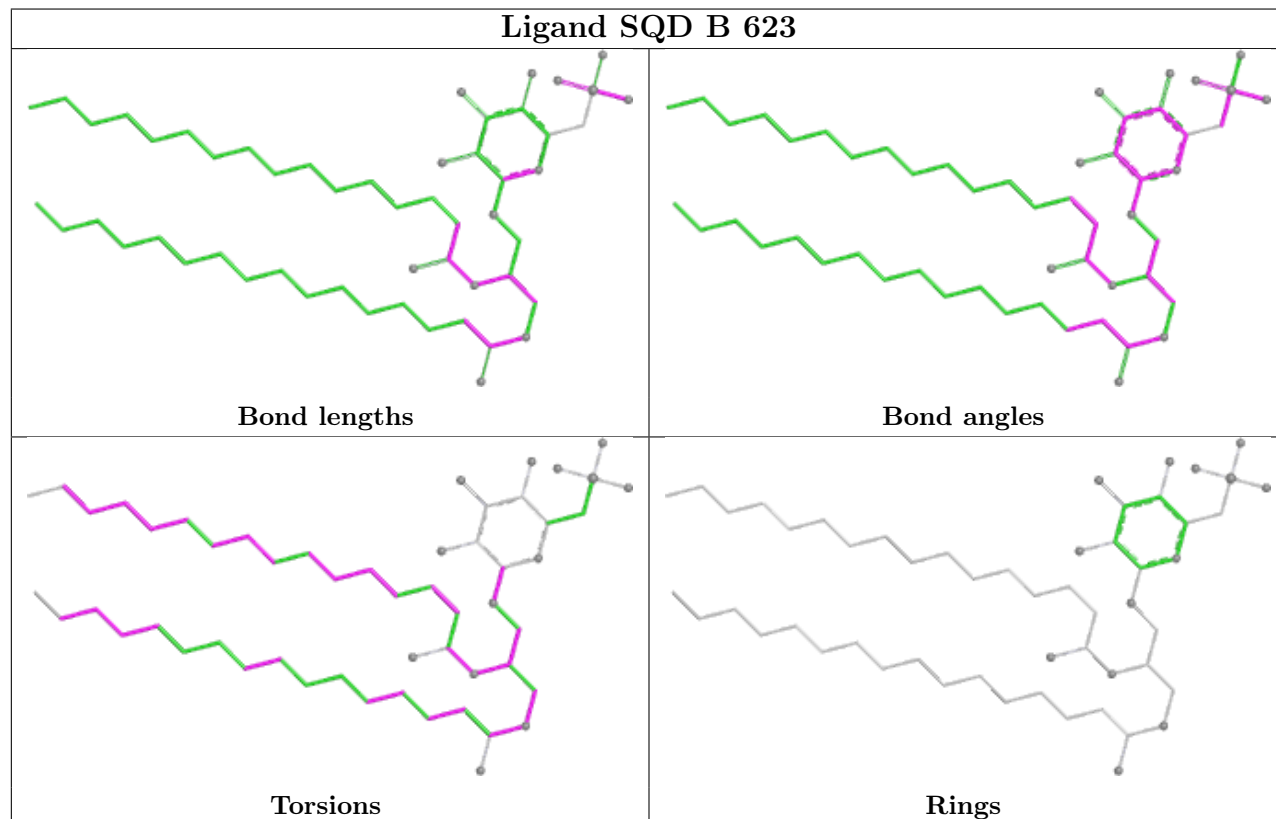
Ligand CLA c 511

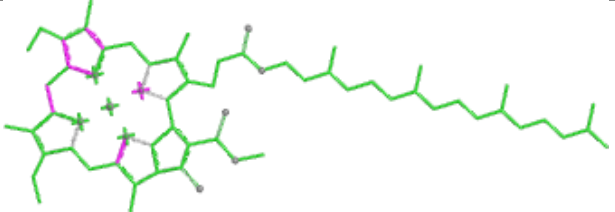
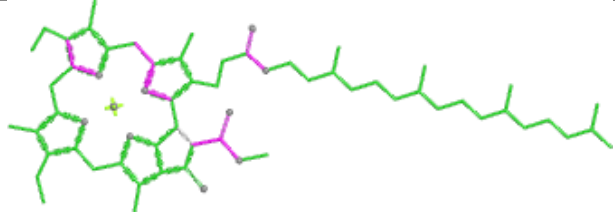
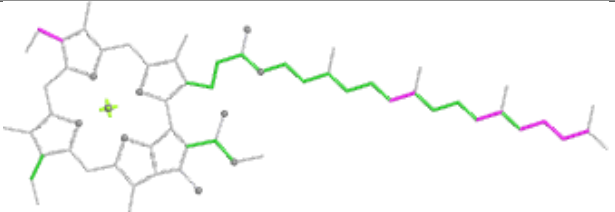
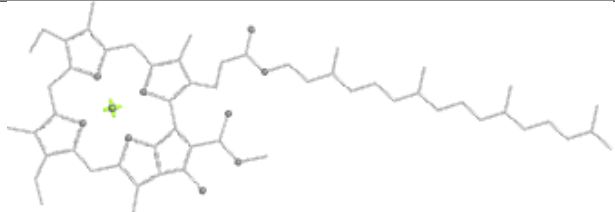
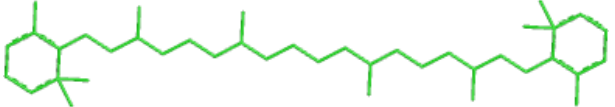
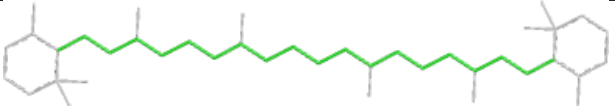
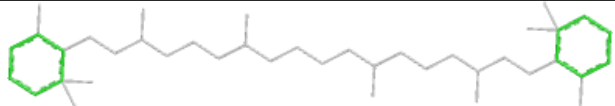
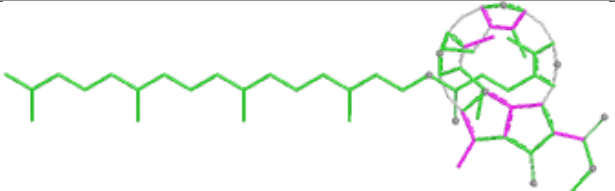
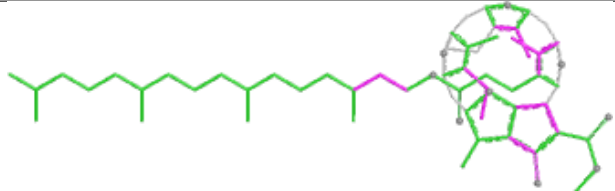
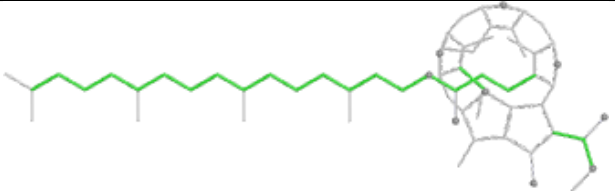
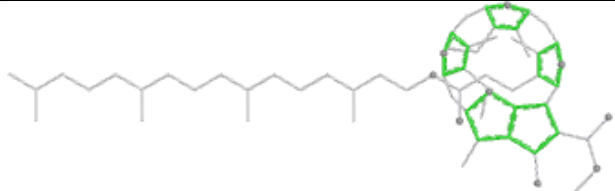


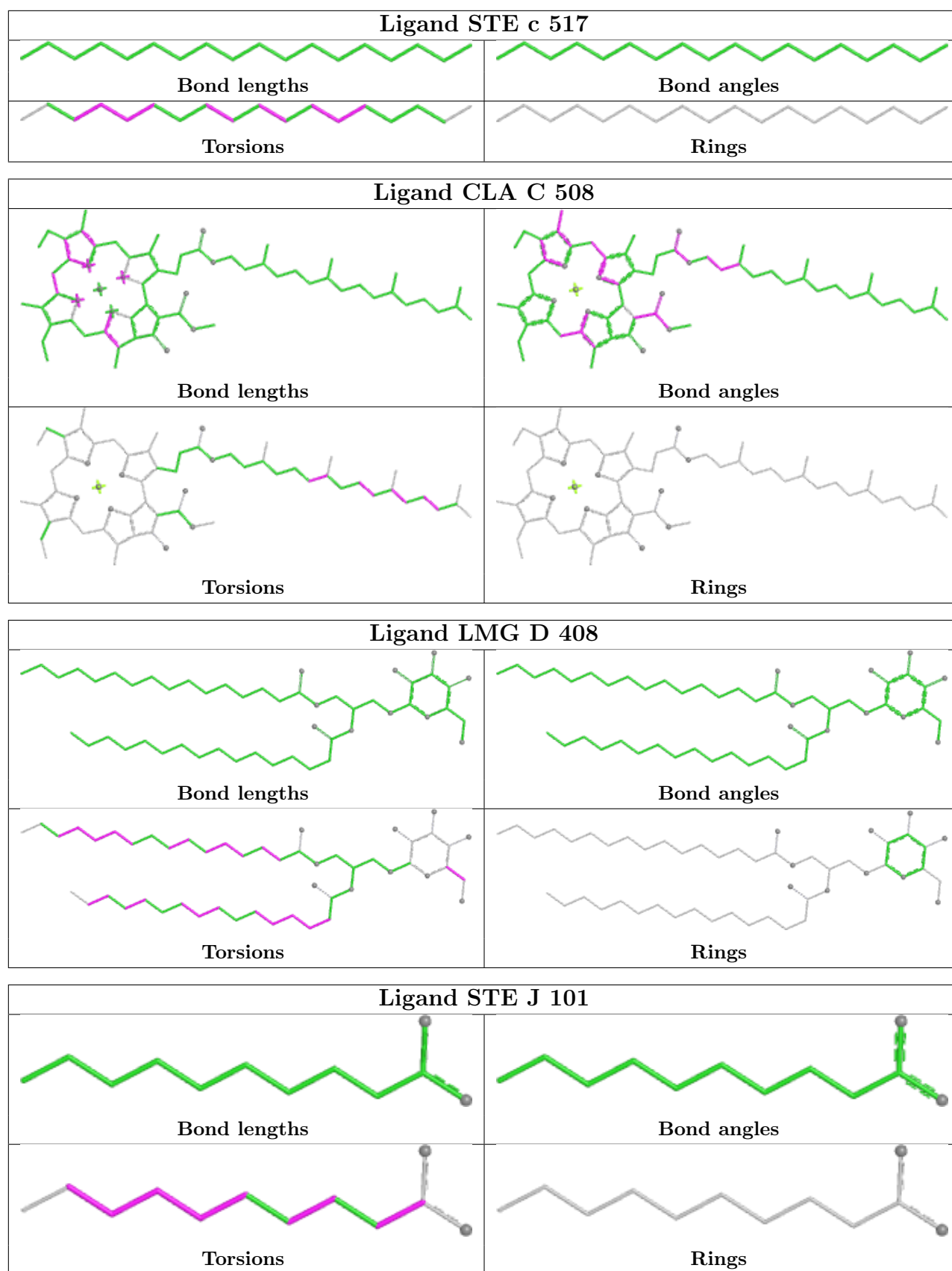


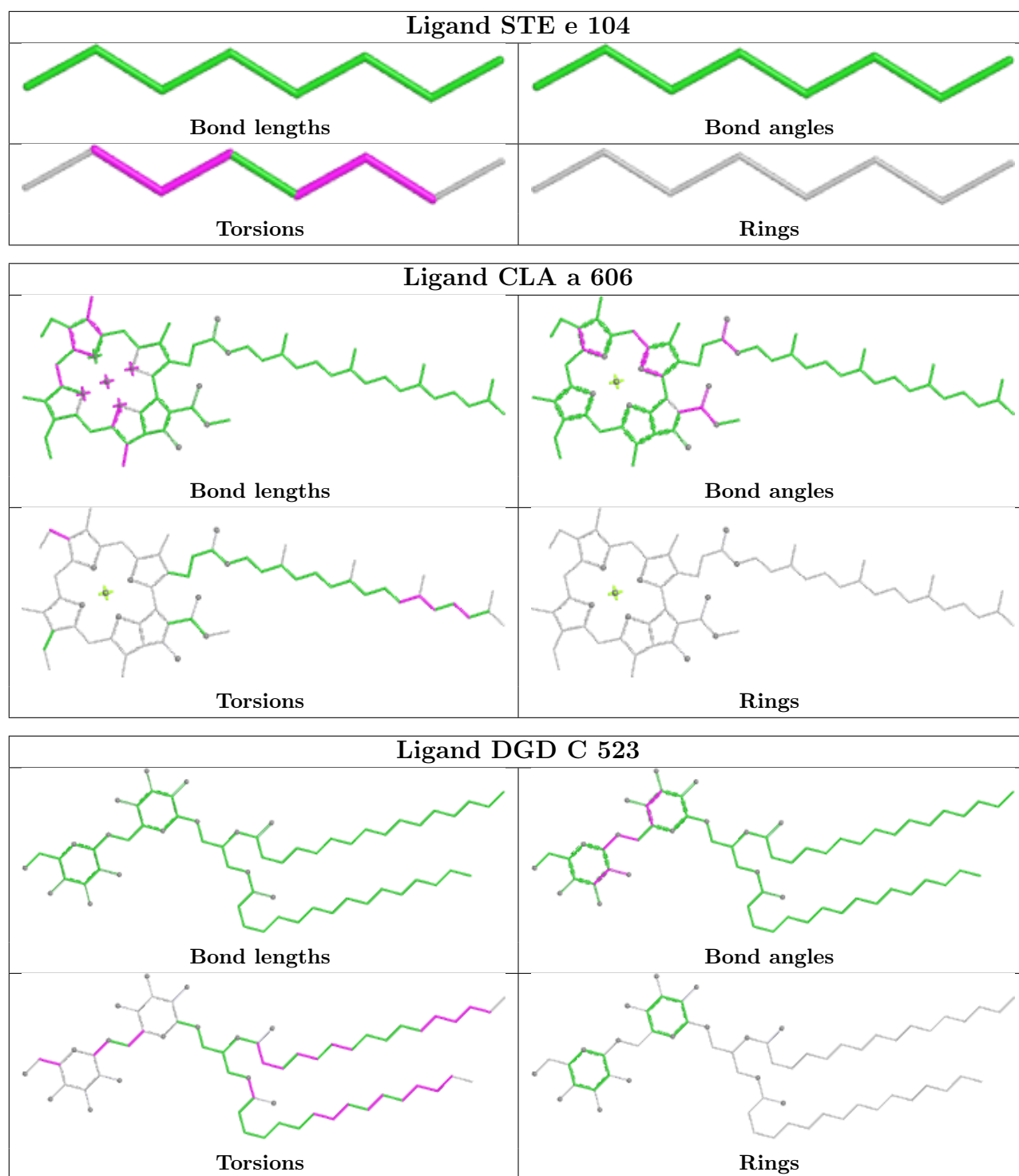


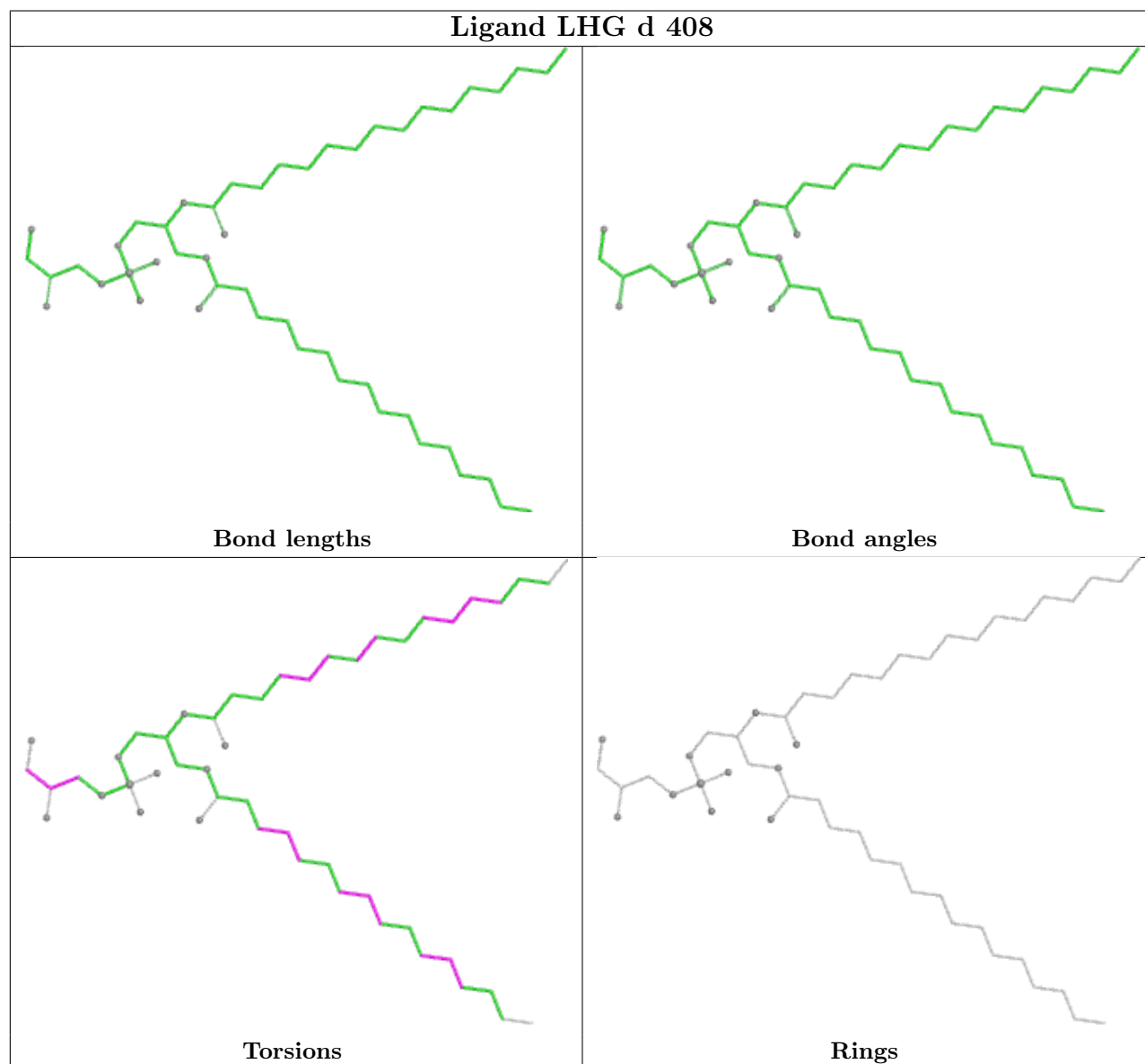
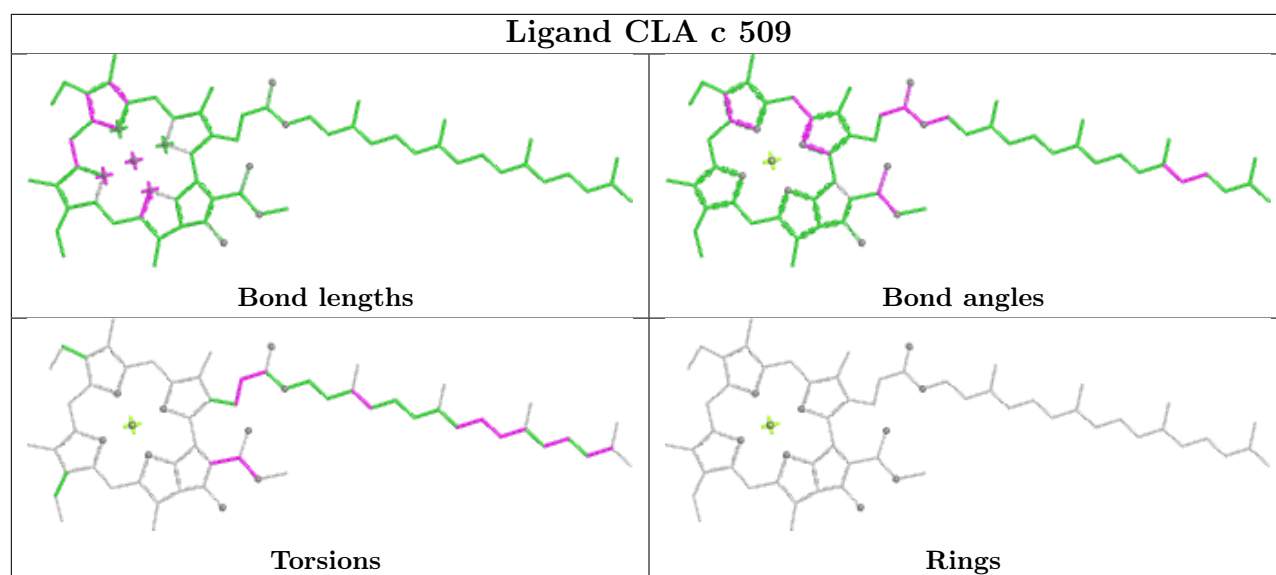


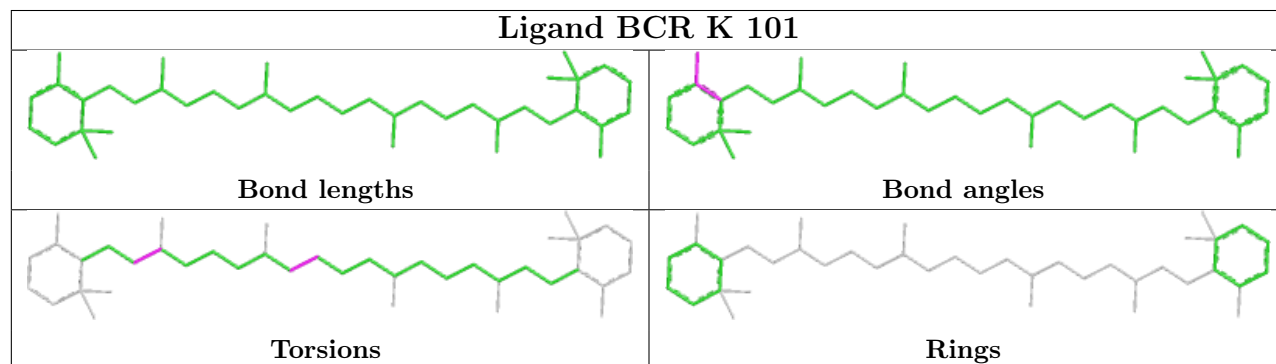
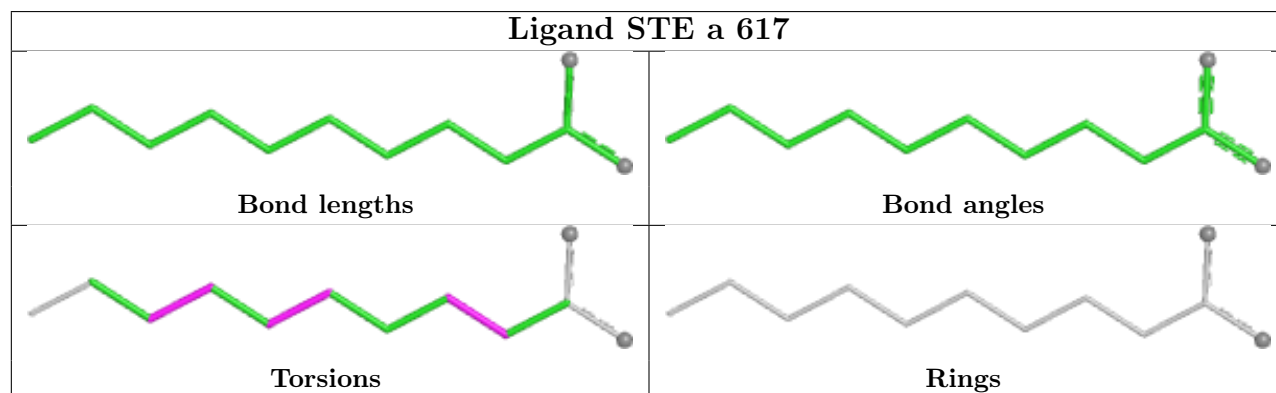
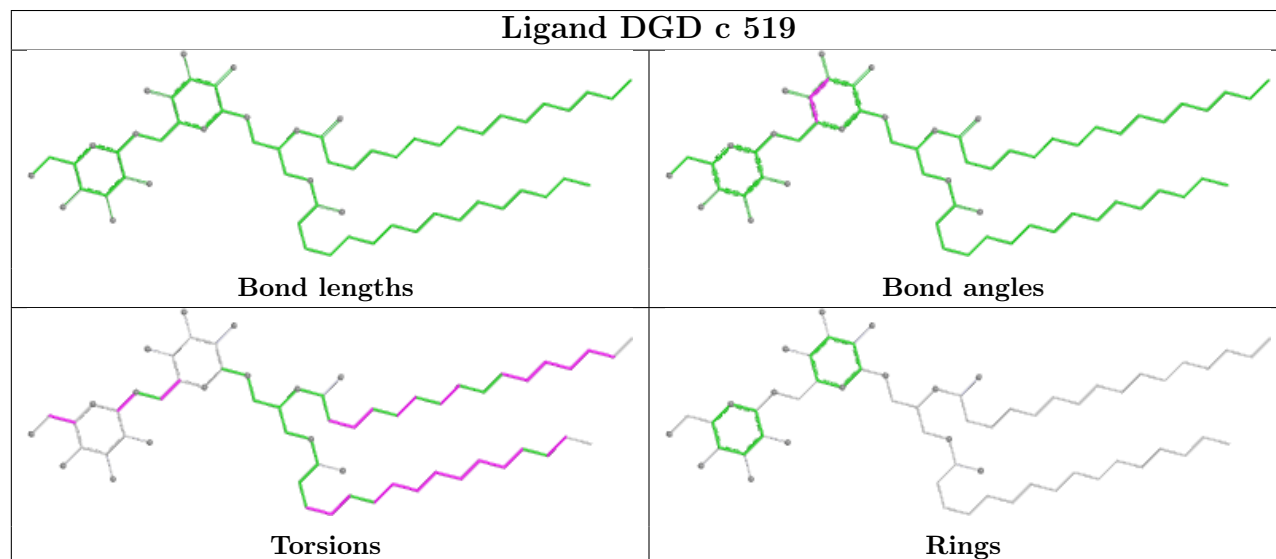
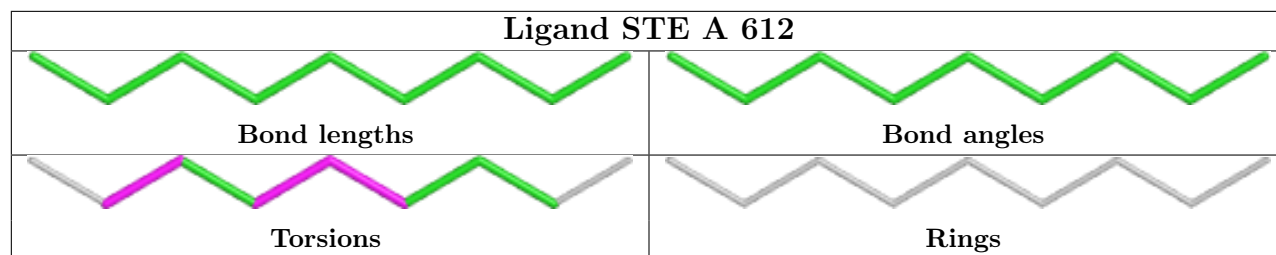
Ligand CLA b 610**Ligand SQD B 623**

Ligand CLA A 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO A 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE c 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

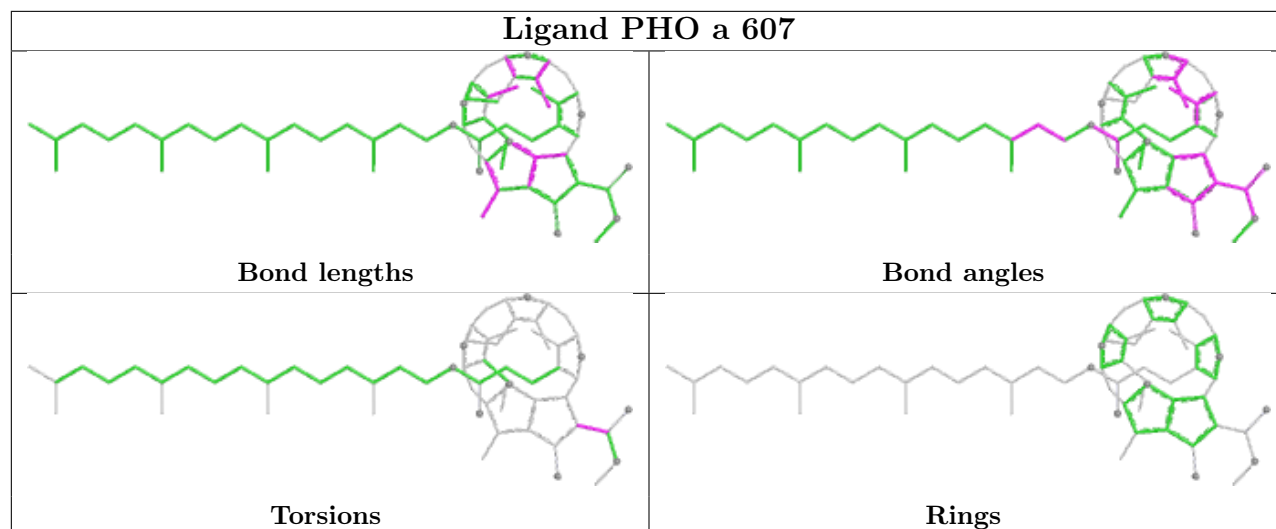




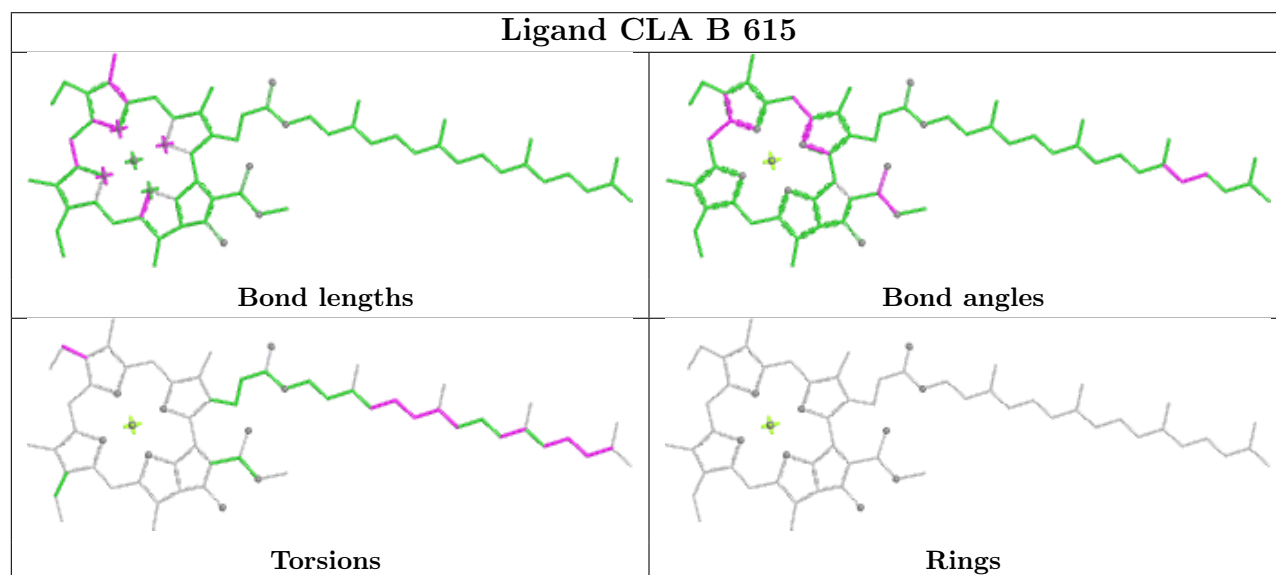




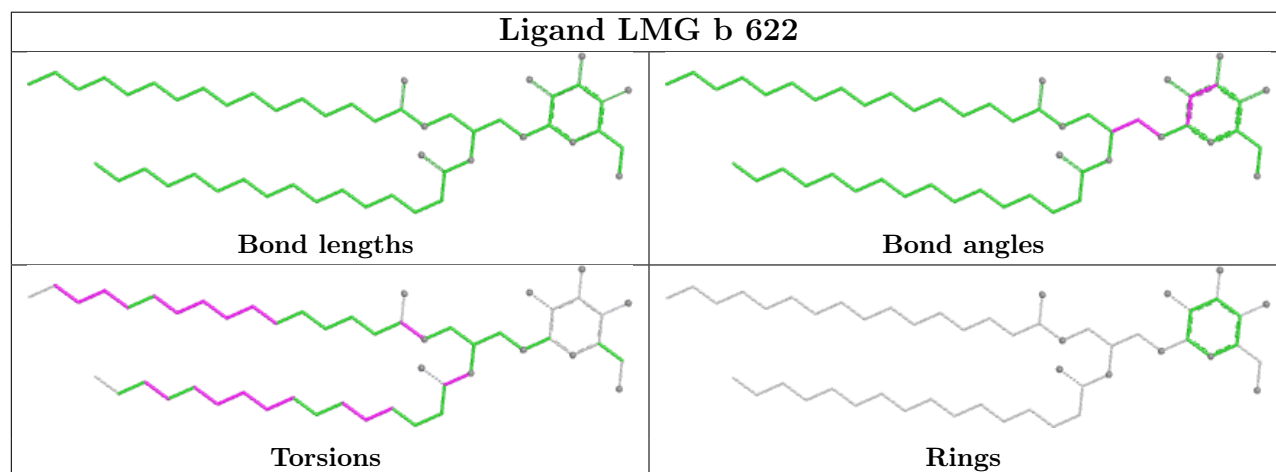
Ligand PHO a 607



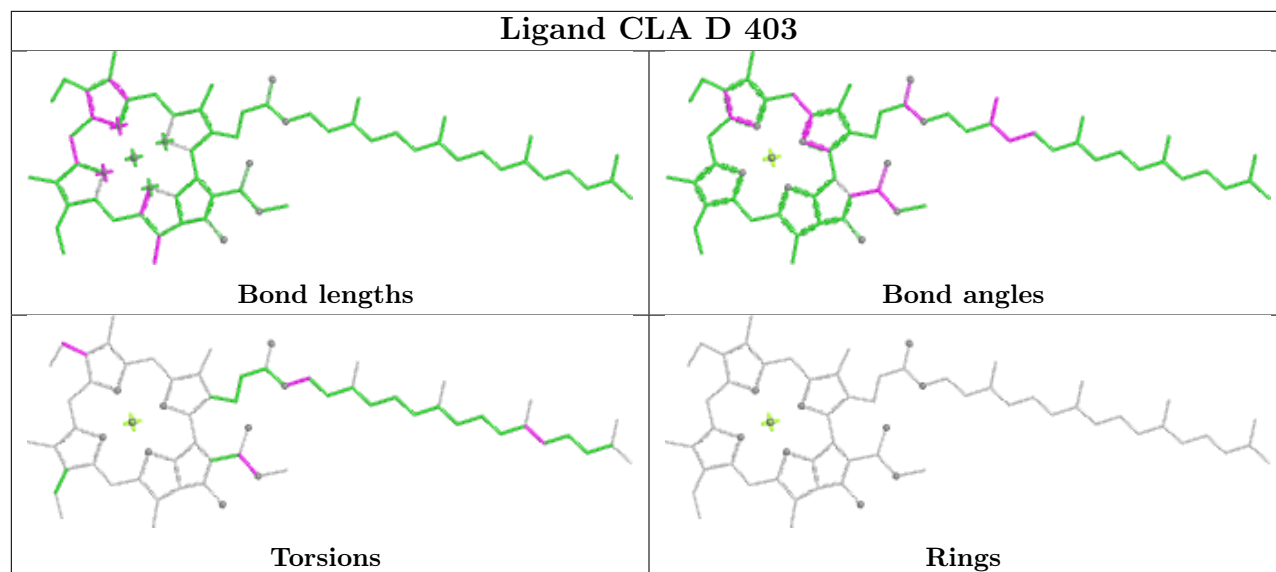
Ligand CLA B 615



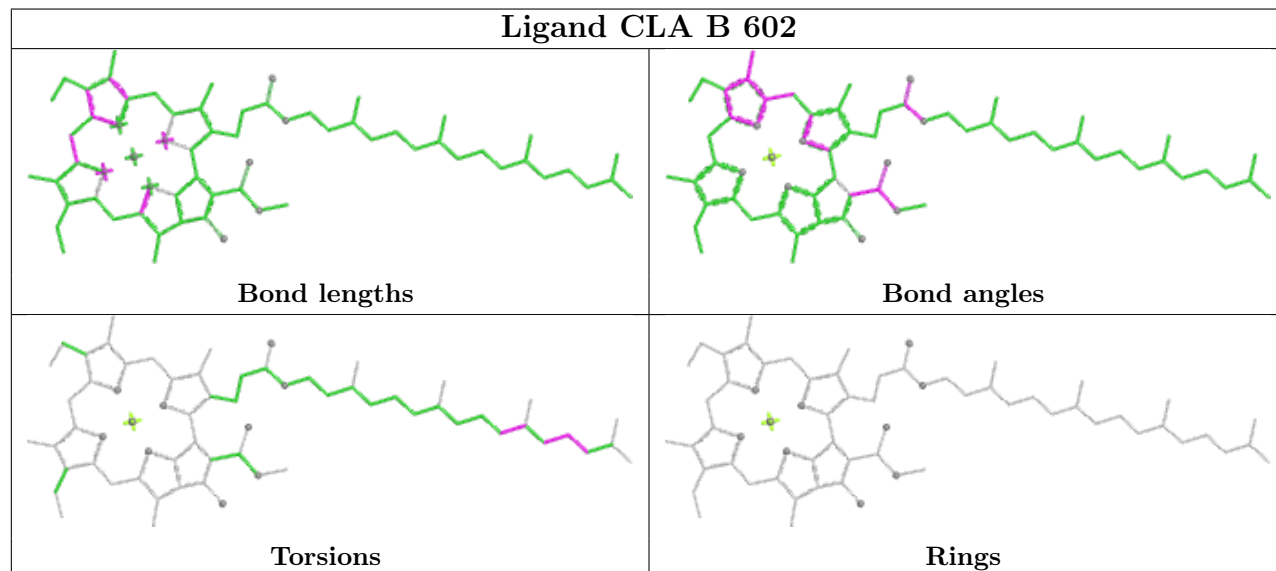
Ligand LMG b 622



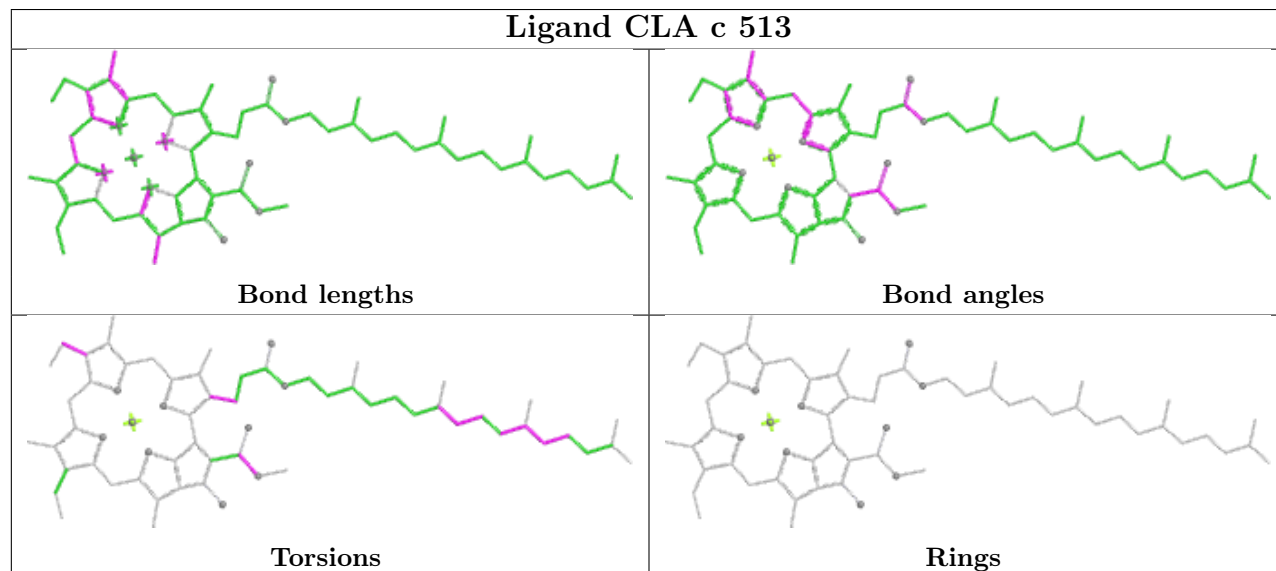
Ligand CLA D 403

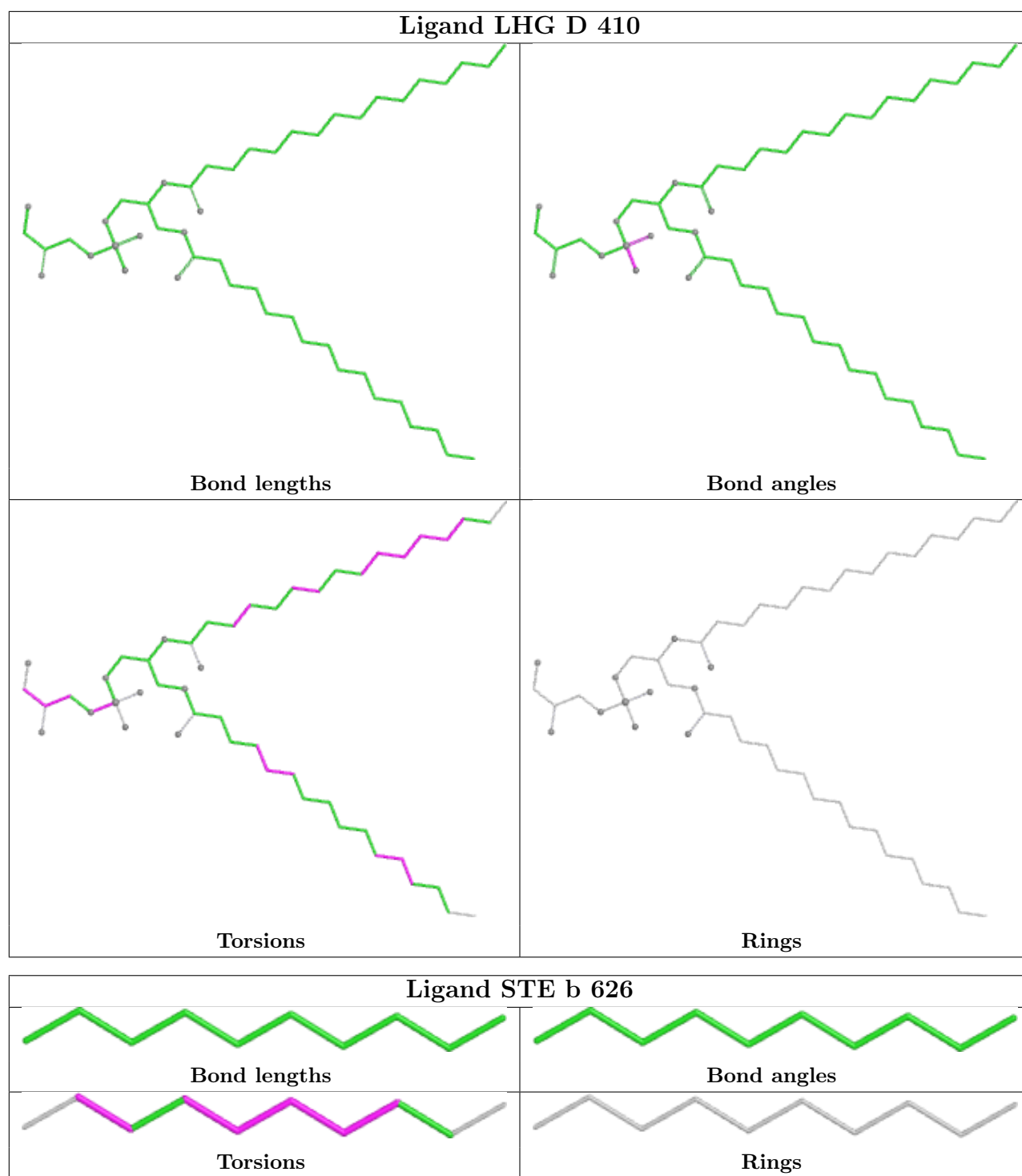


Ligand CLA B 602

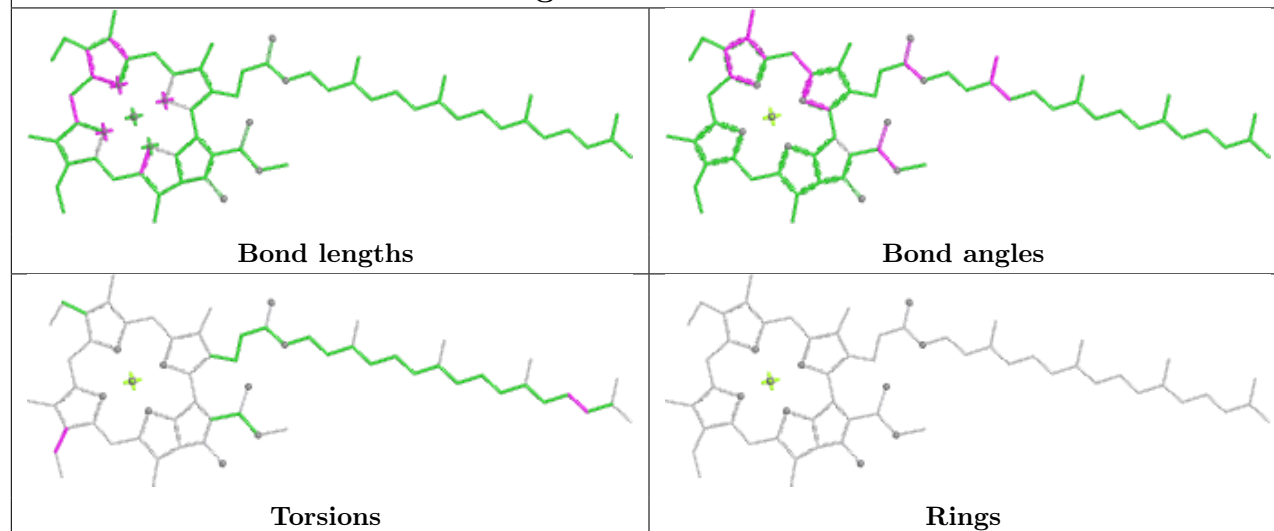


Ligand CLA c 513

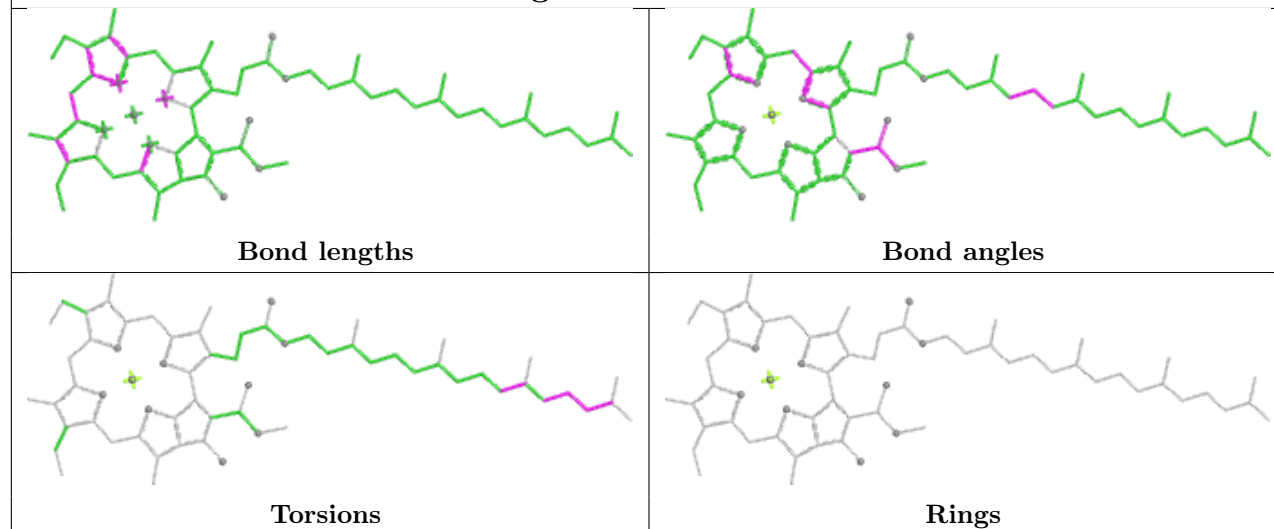




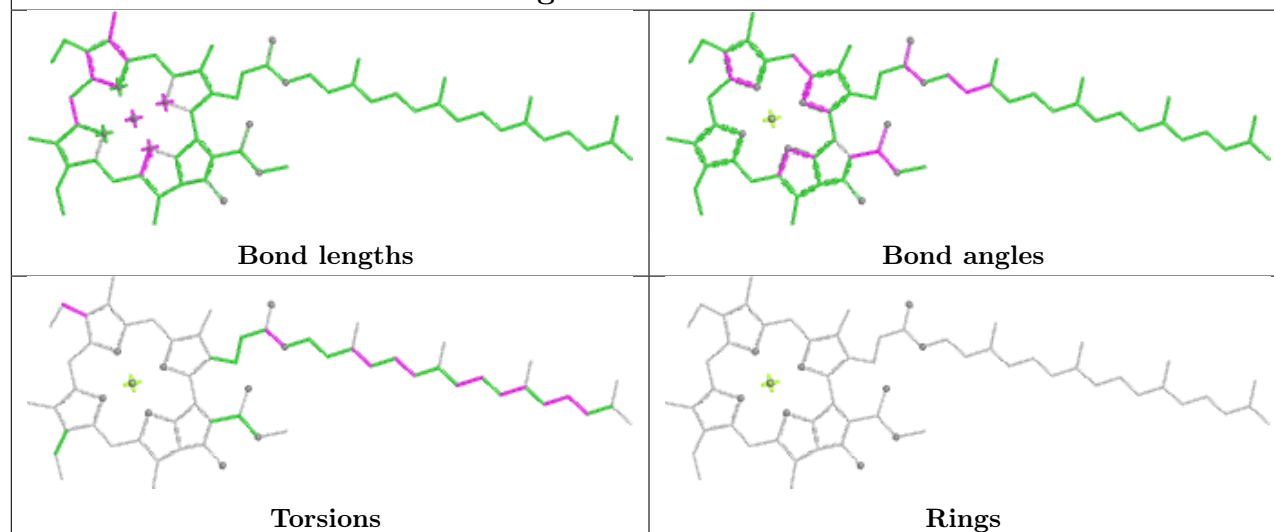
Ligand CLA a 605

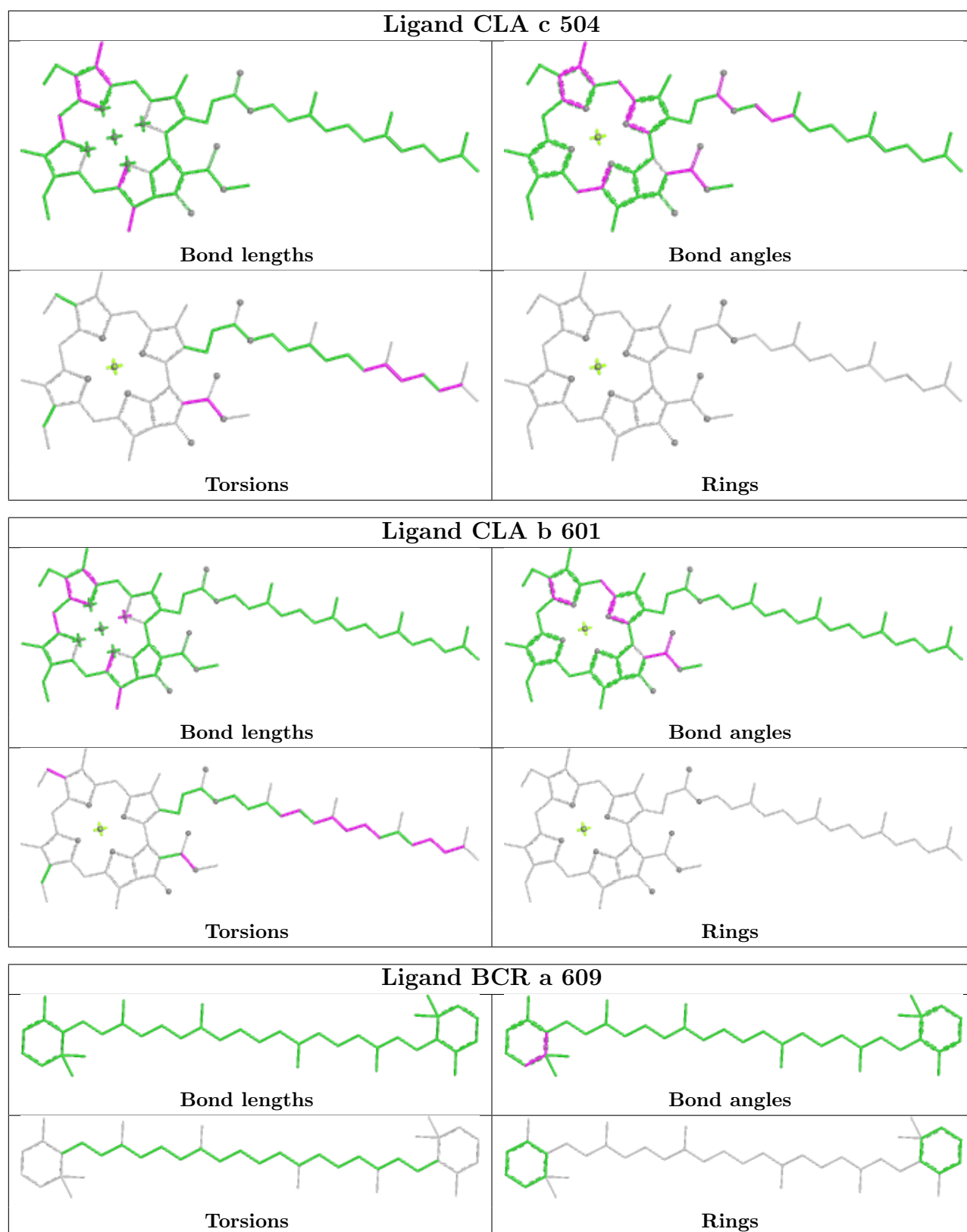


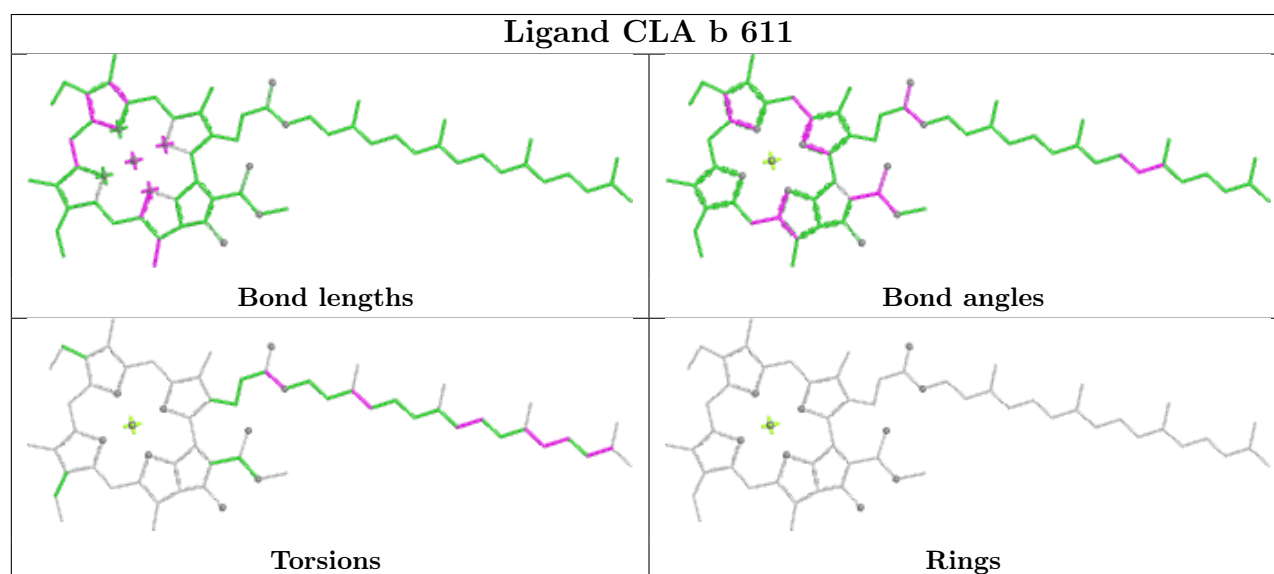
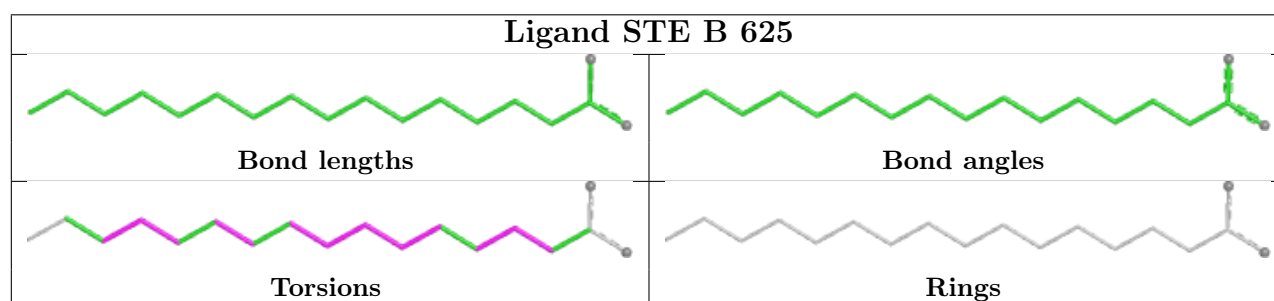
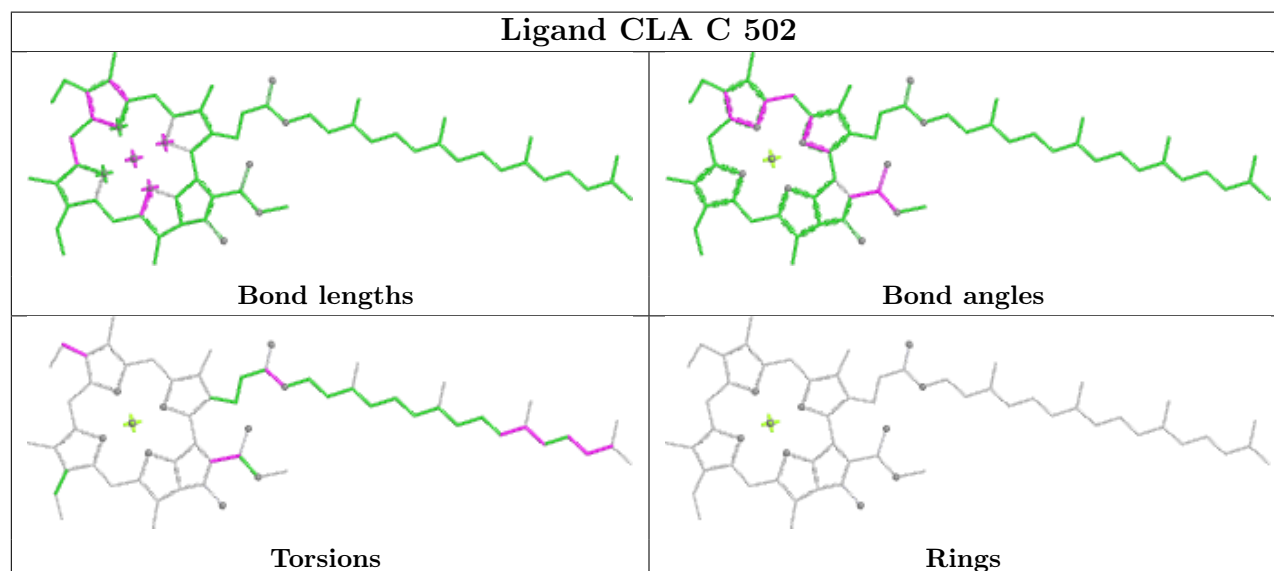
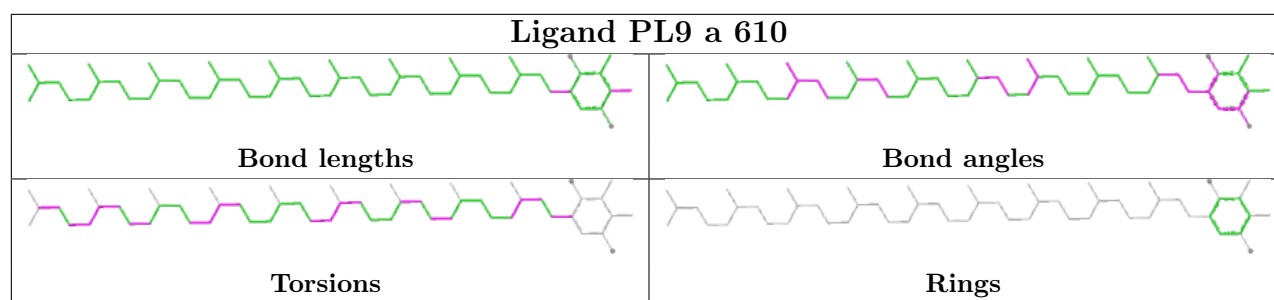
Ligand CLA D 402

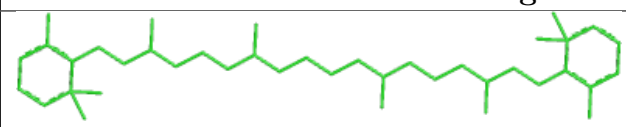
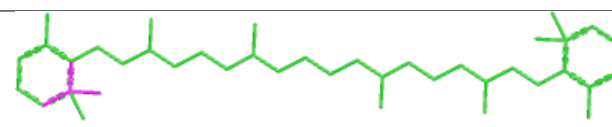
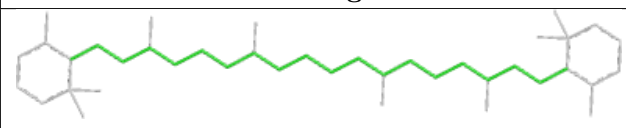
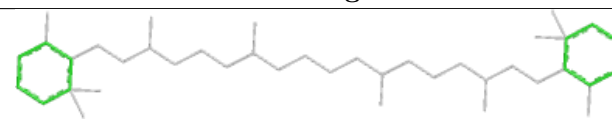


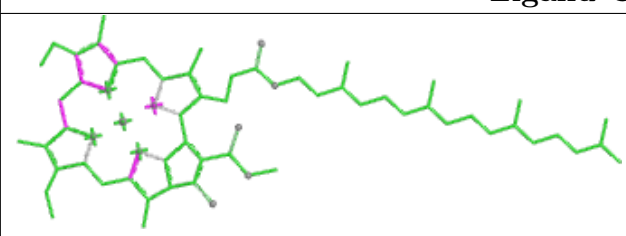
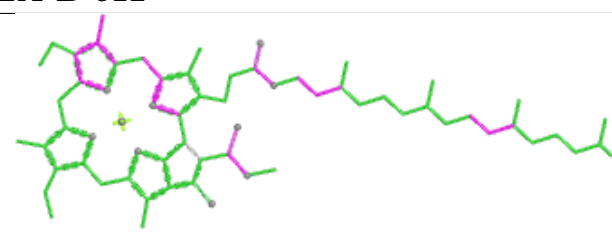
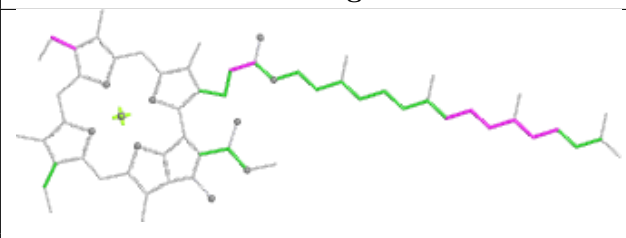
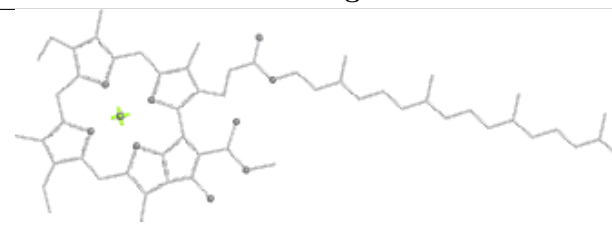
Ligand CLA c 505

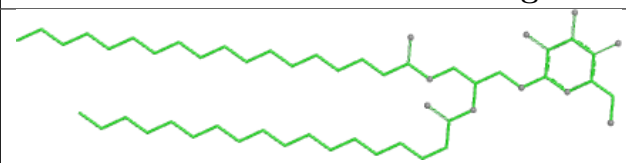
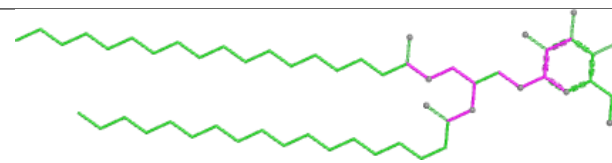
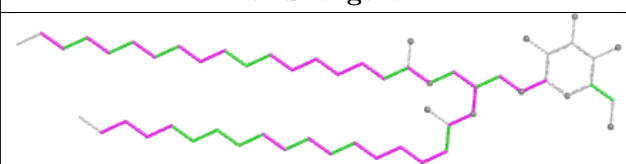
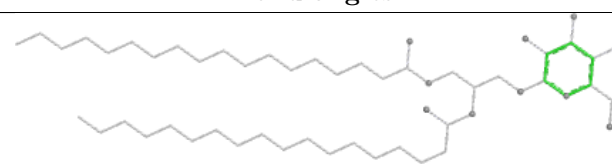


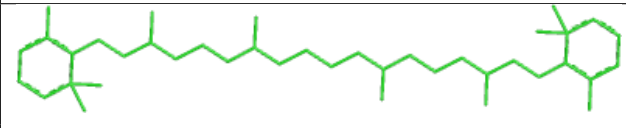
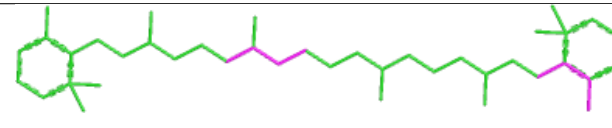
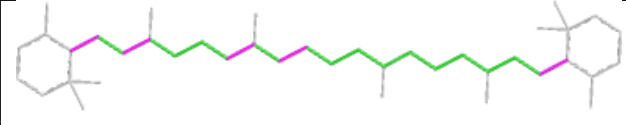
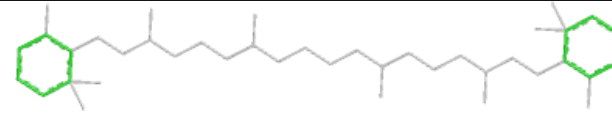


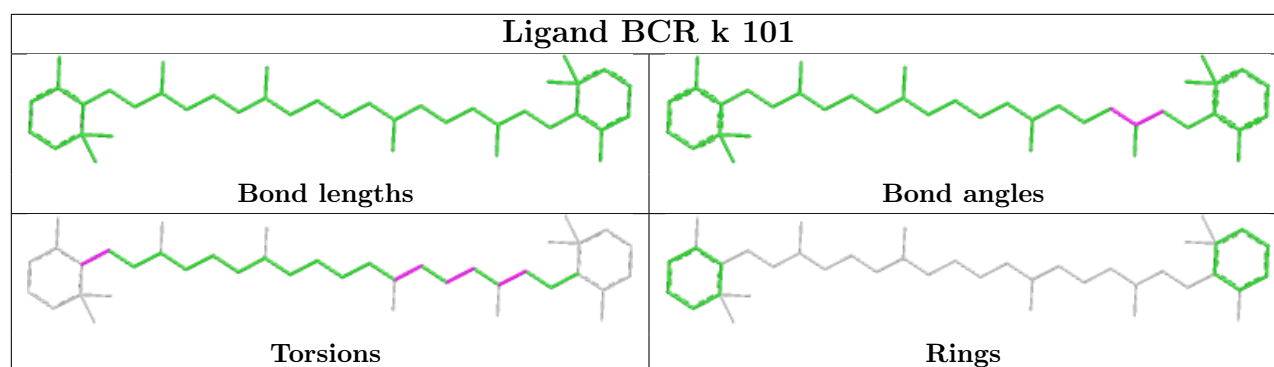
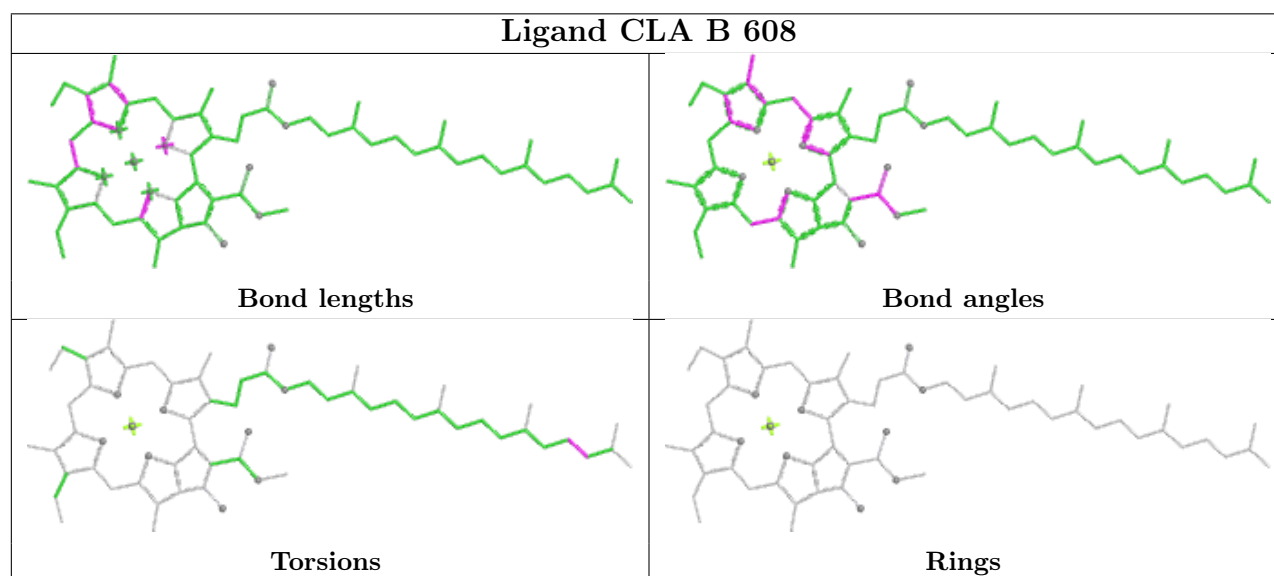
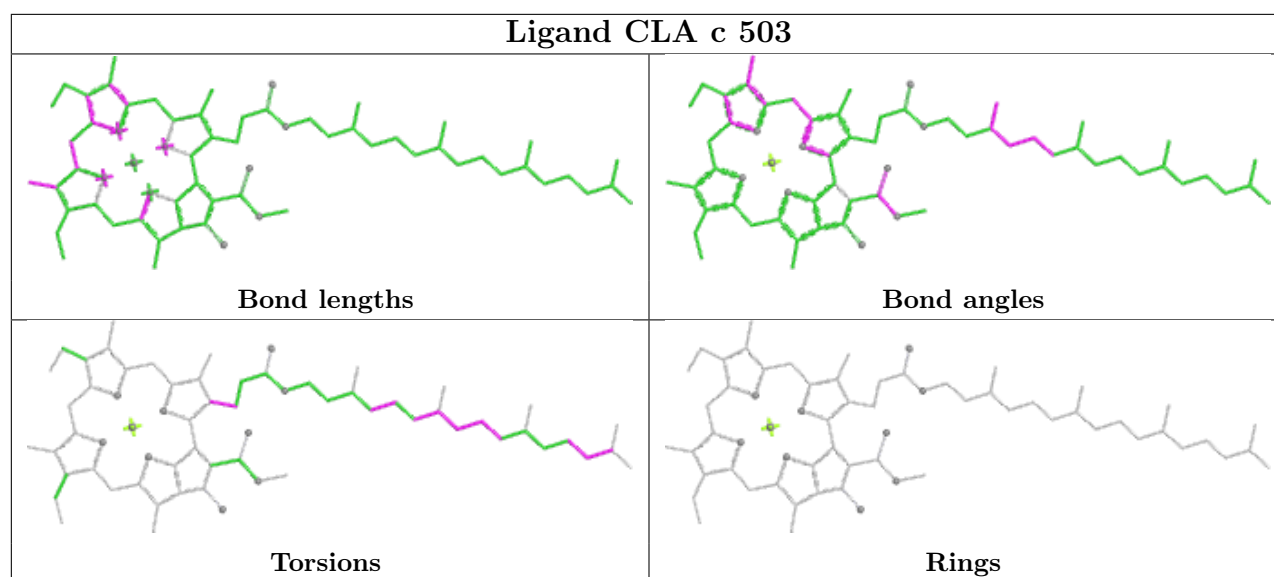


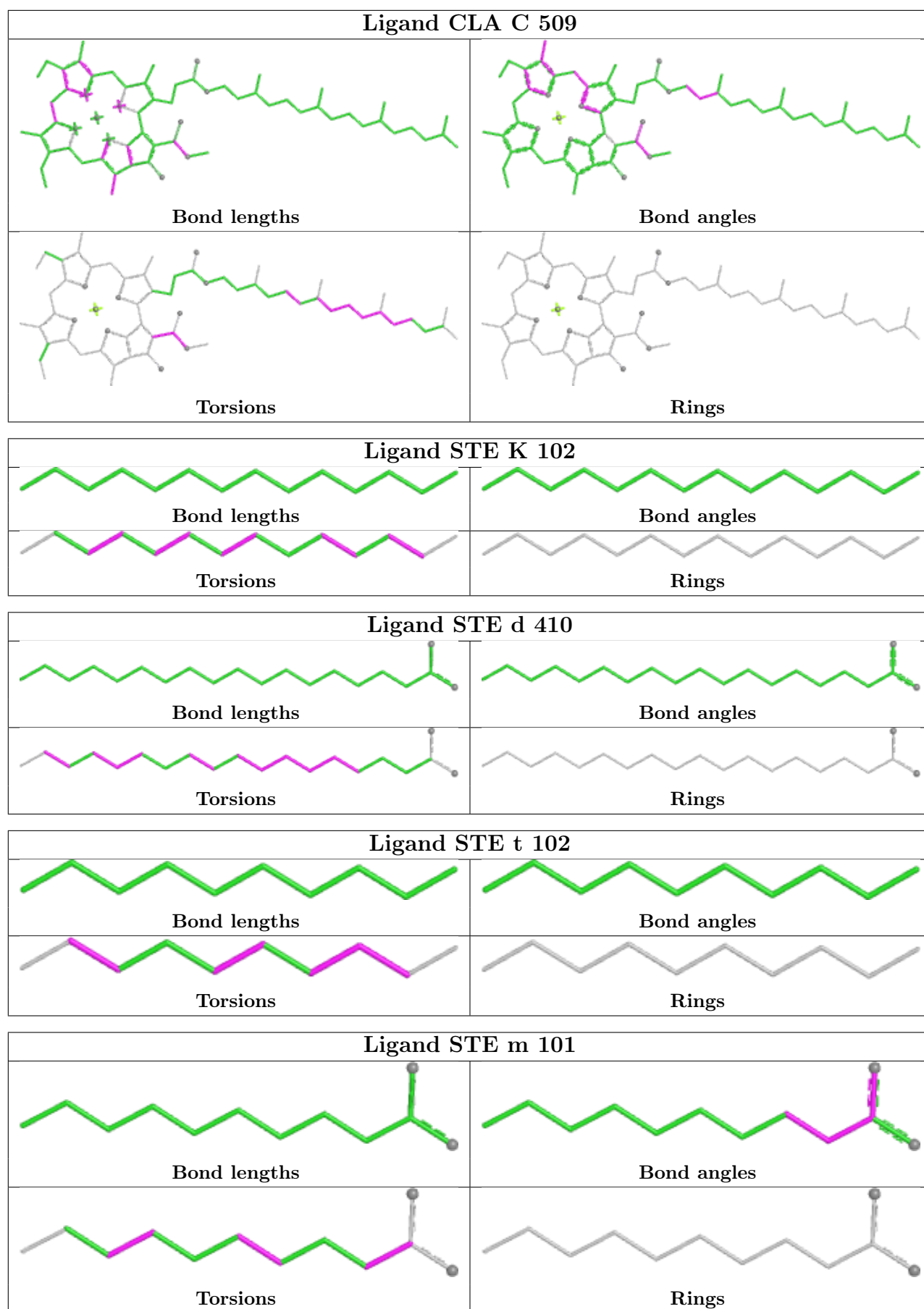
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

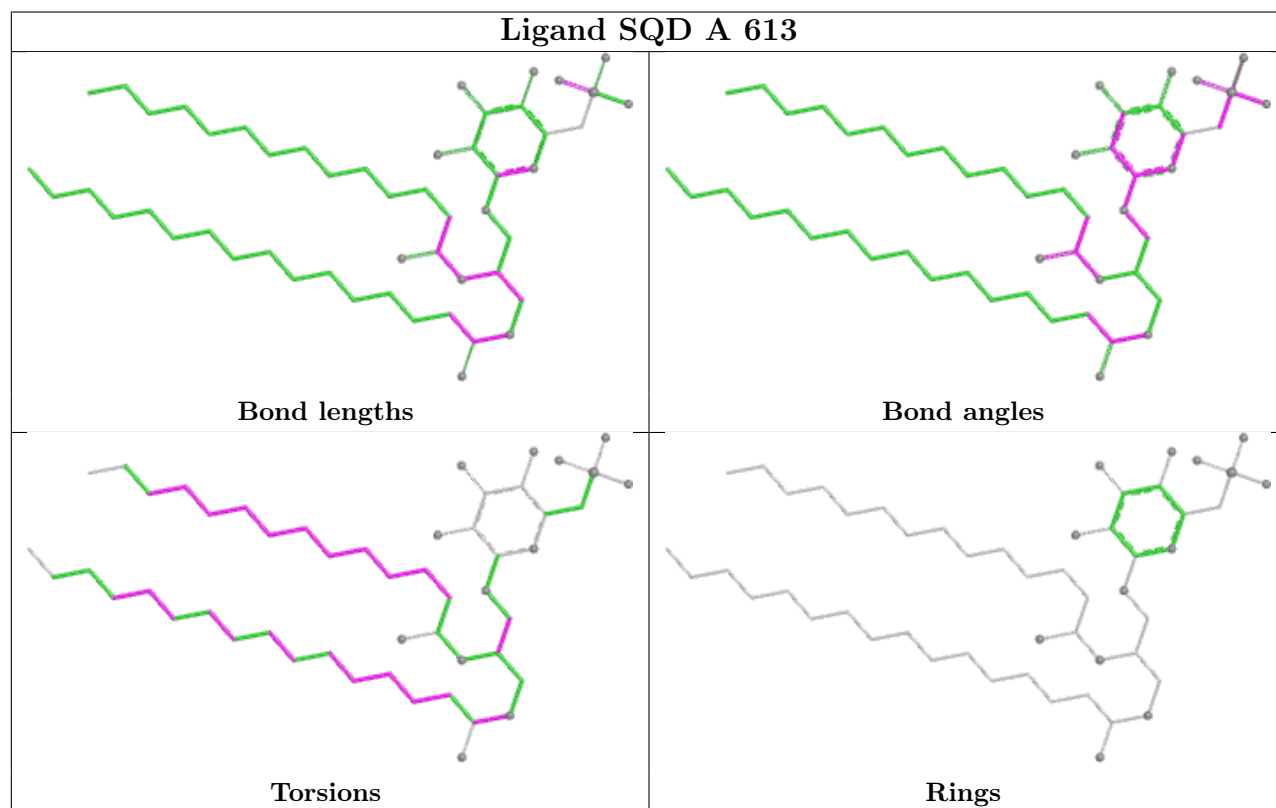
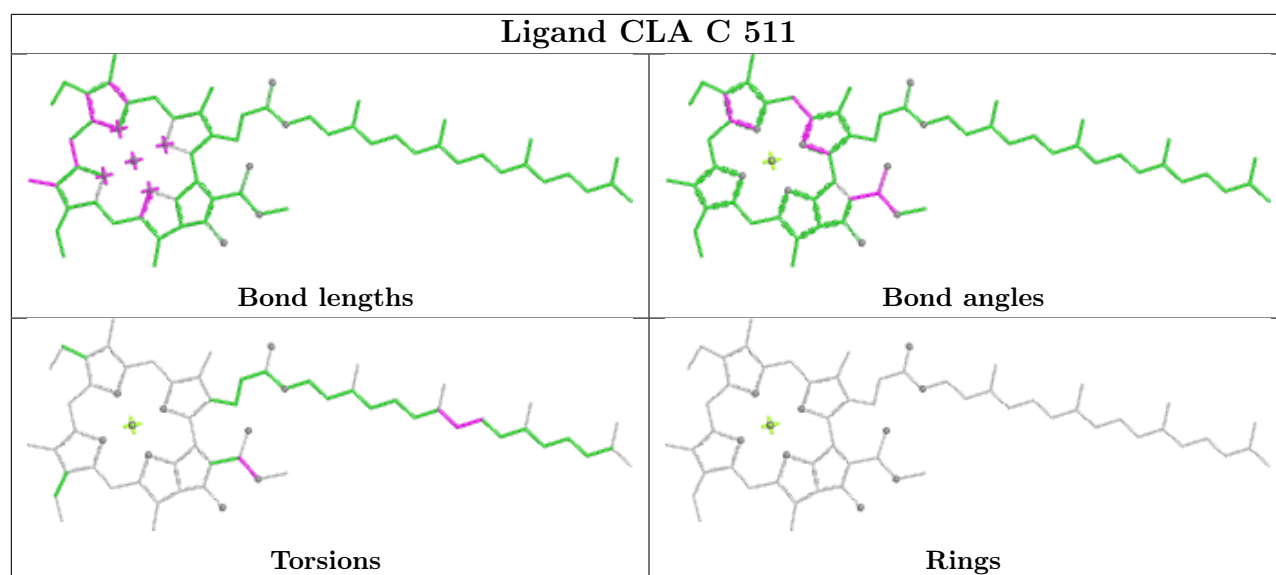
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

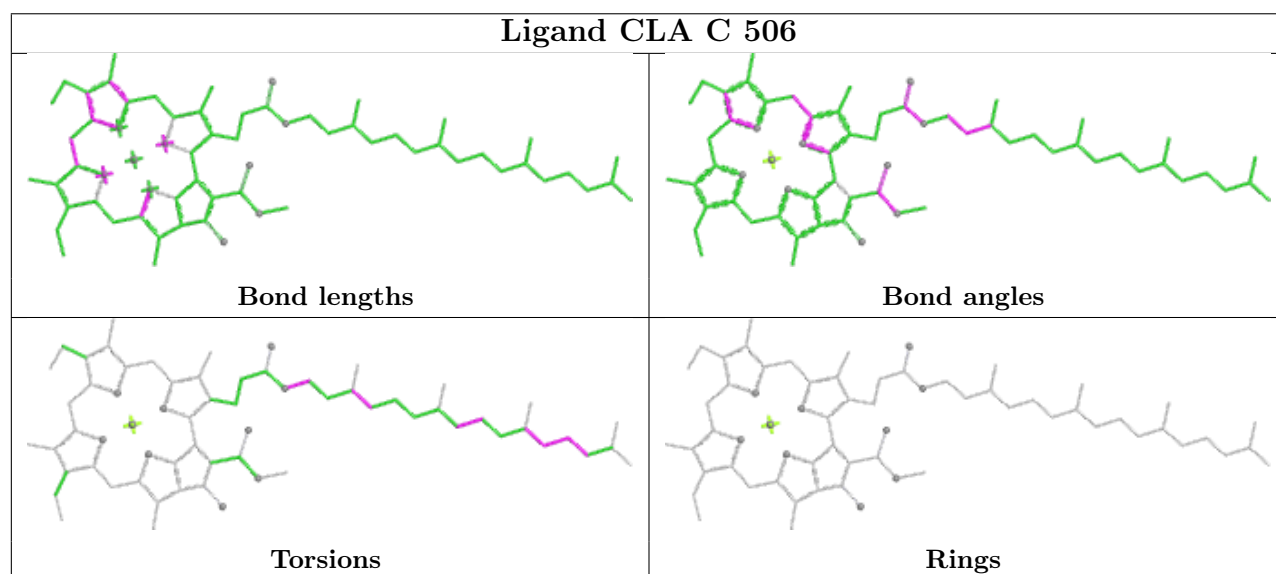
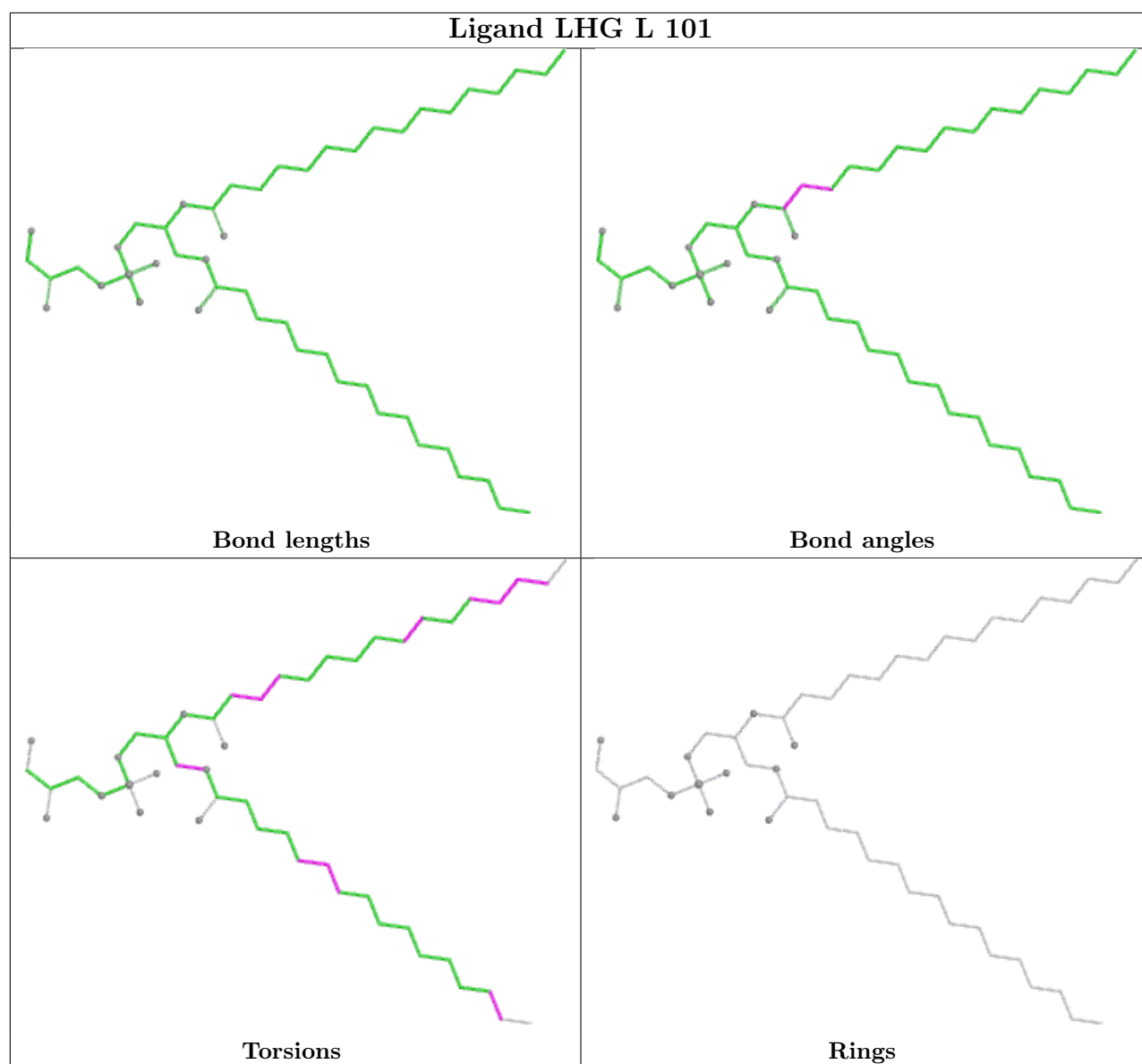
Ligand LMG a 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

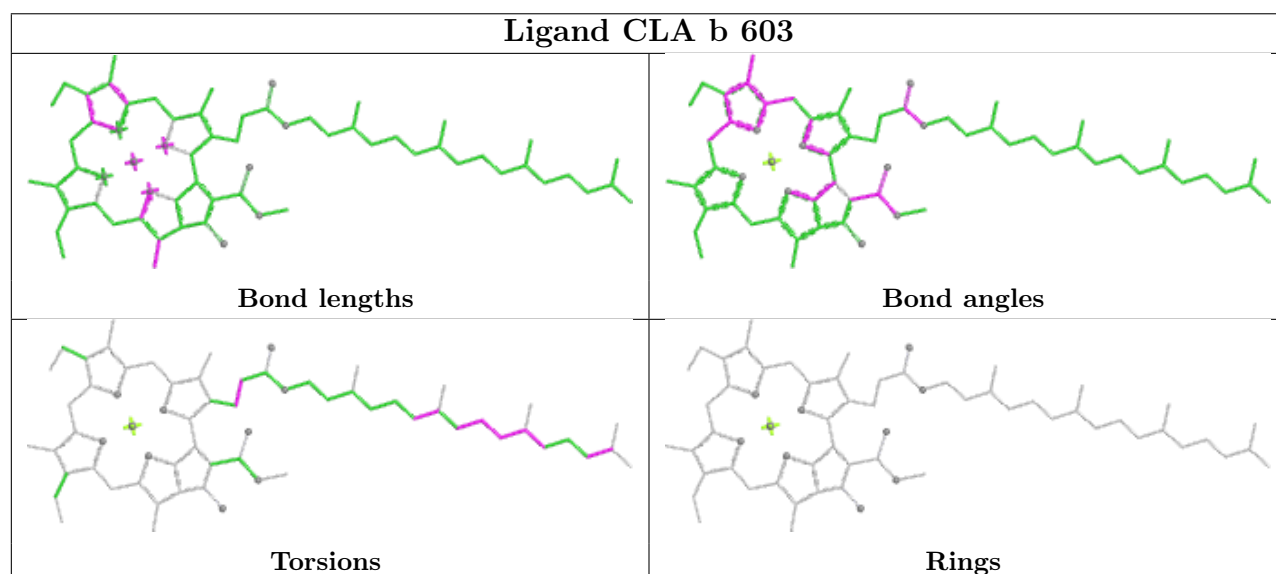
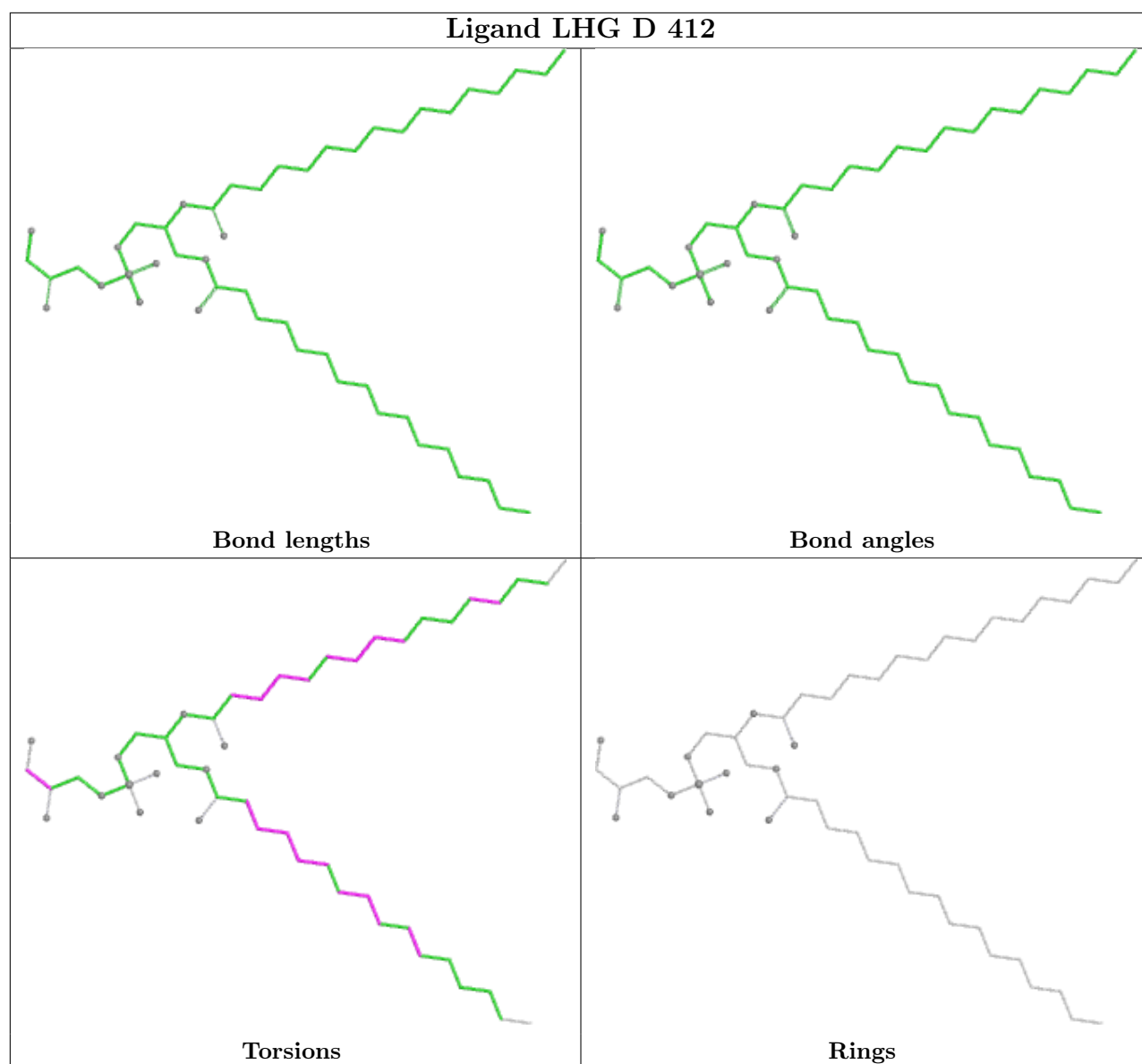
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



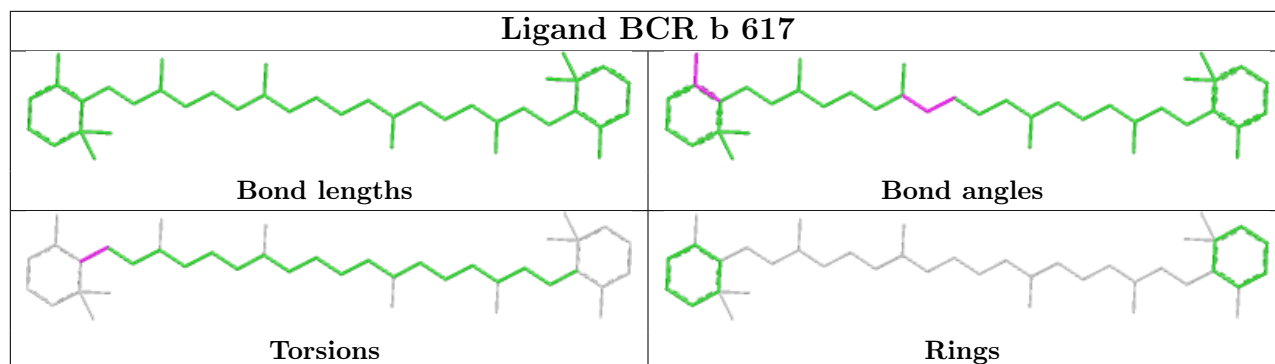




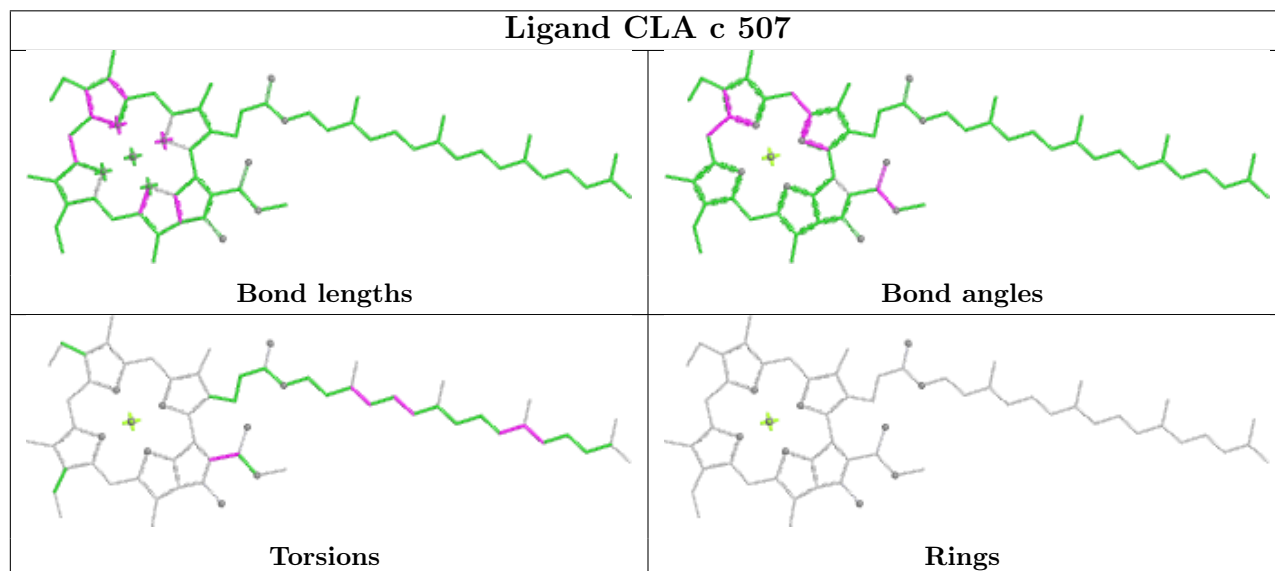




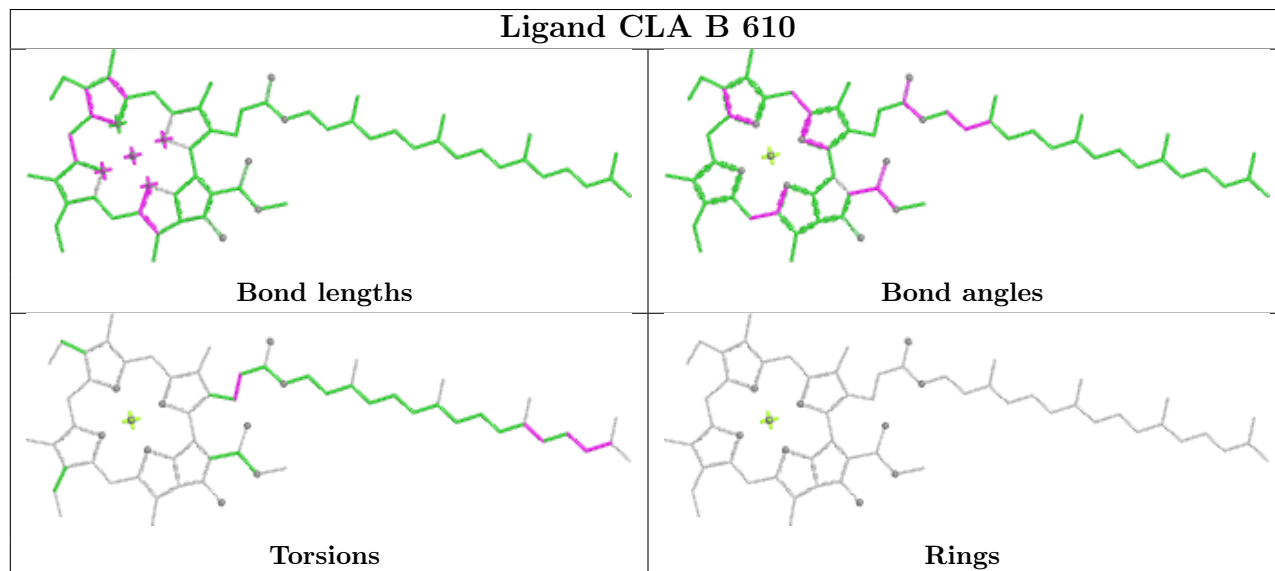
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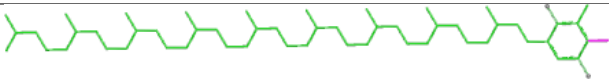
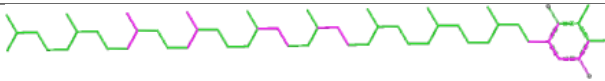
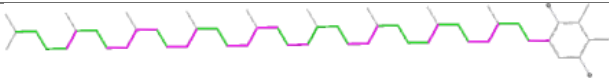
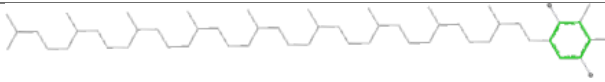


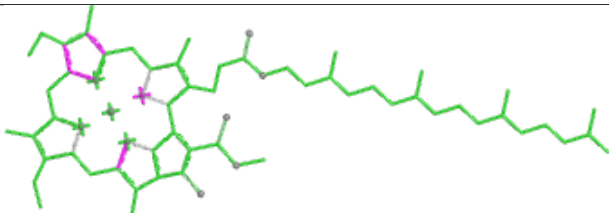
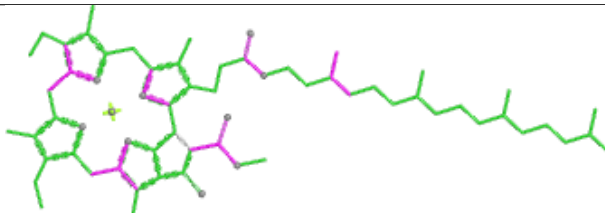
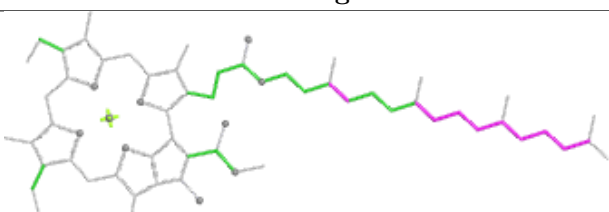
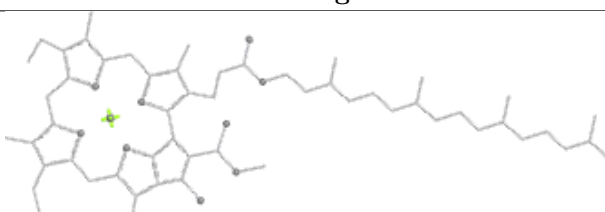
Ligand CLA c 507



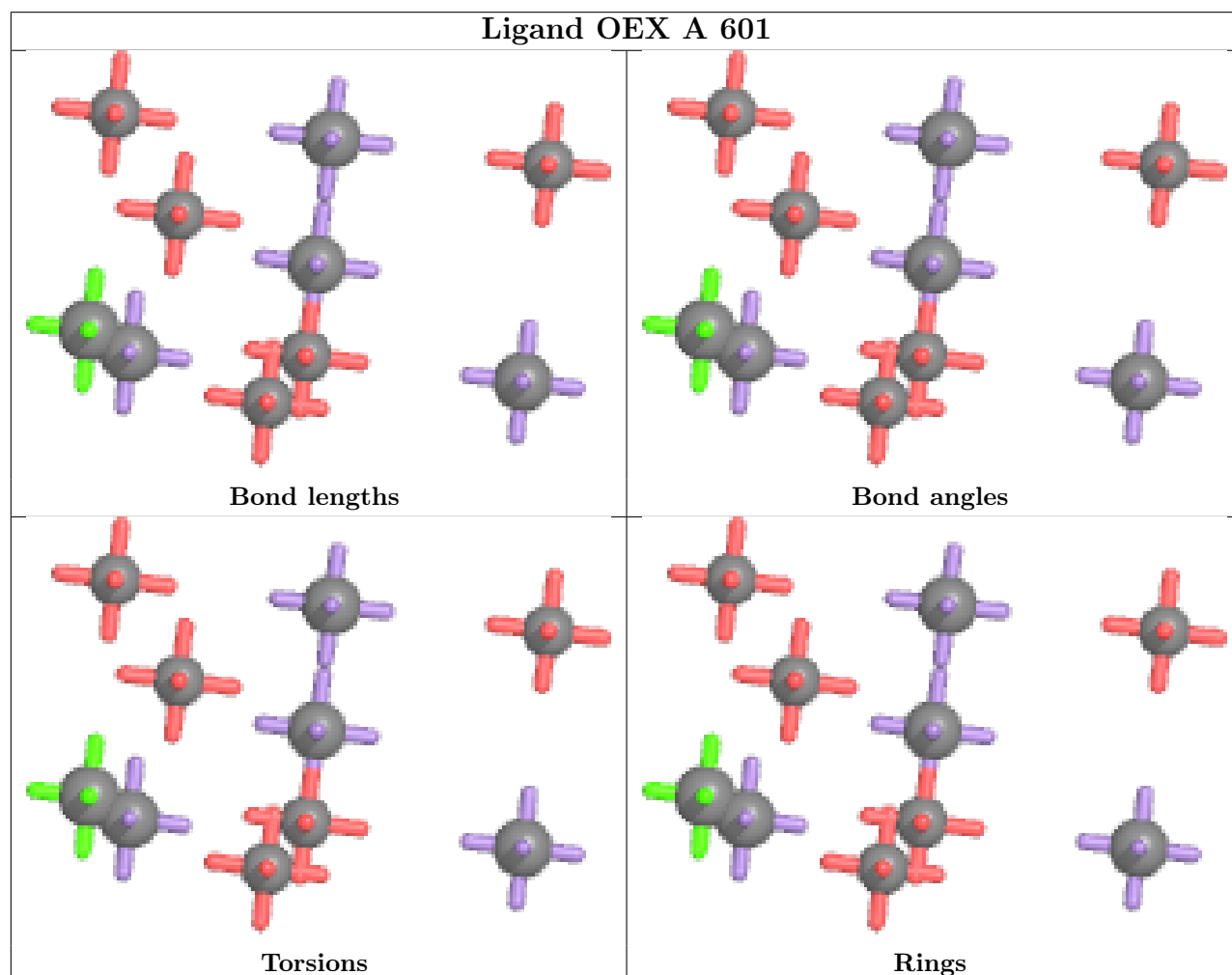
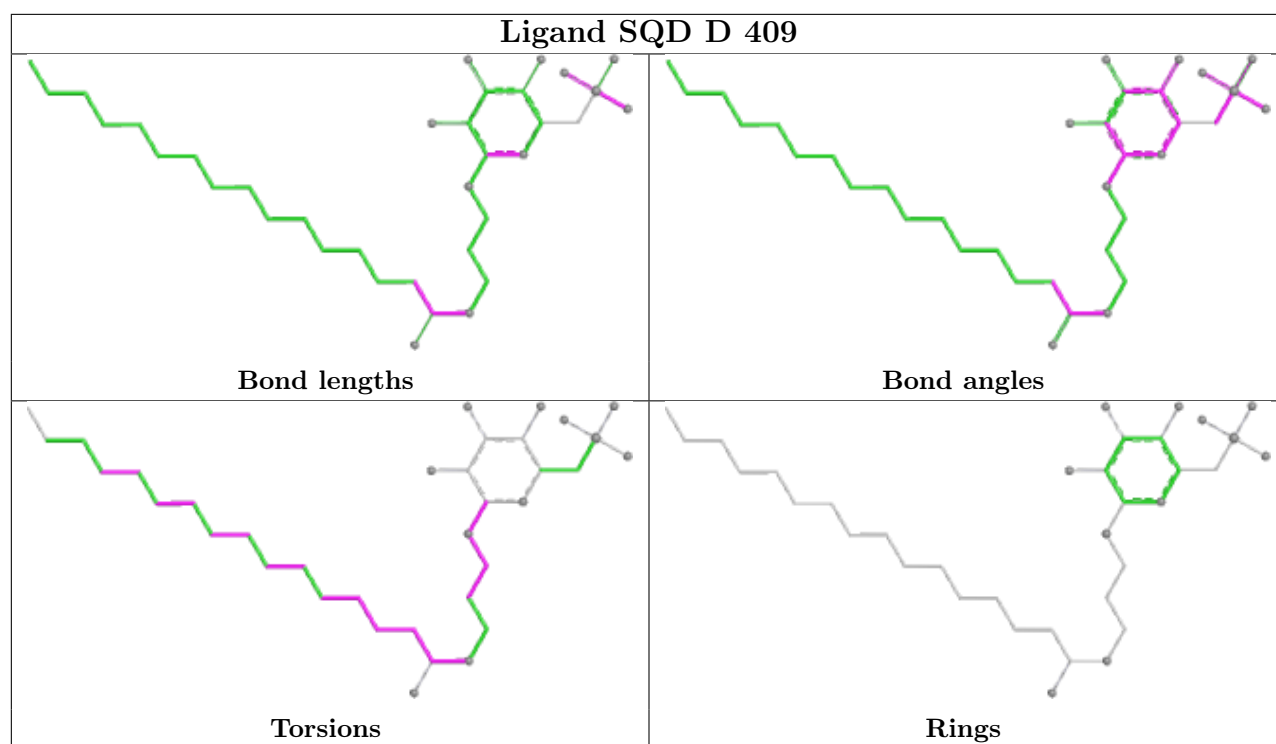
Ligand CLA B 610

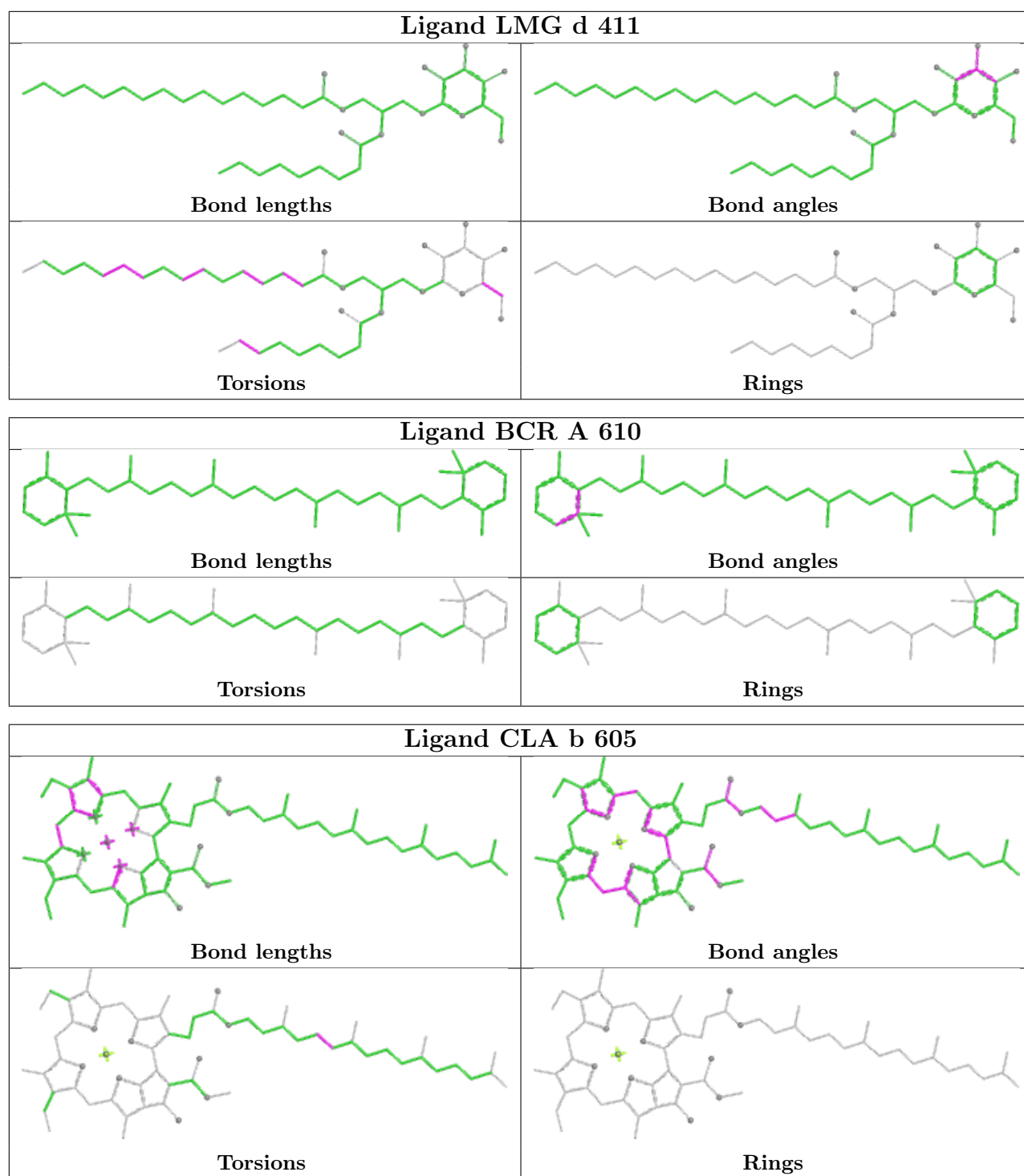


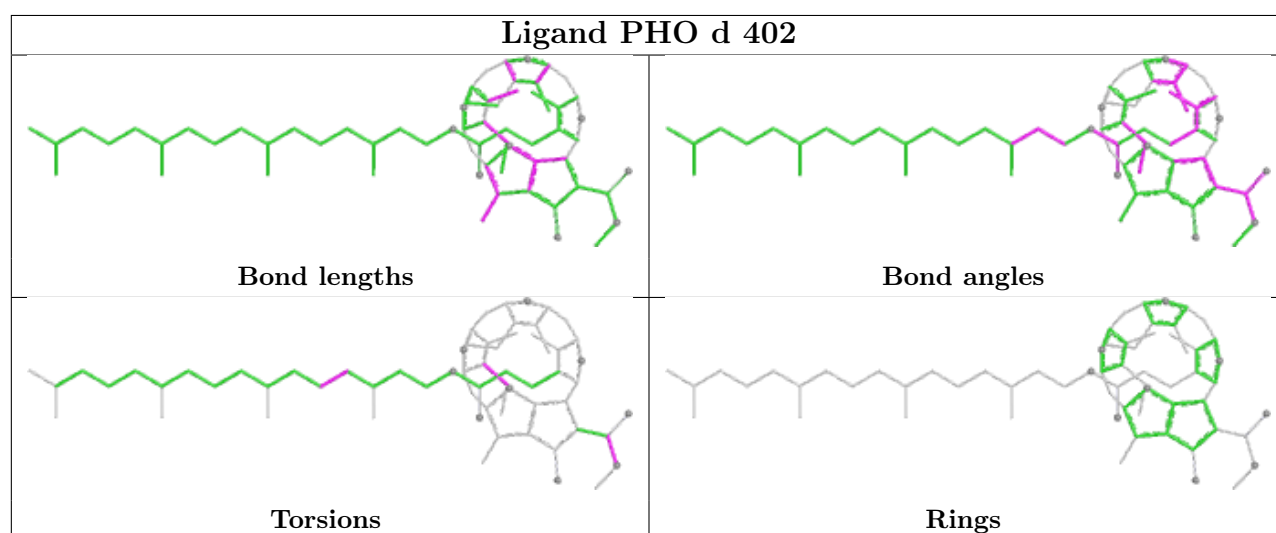
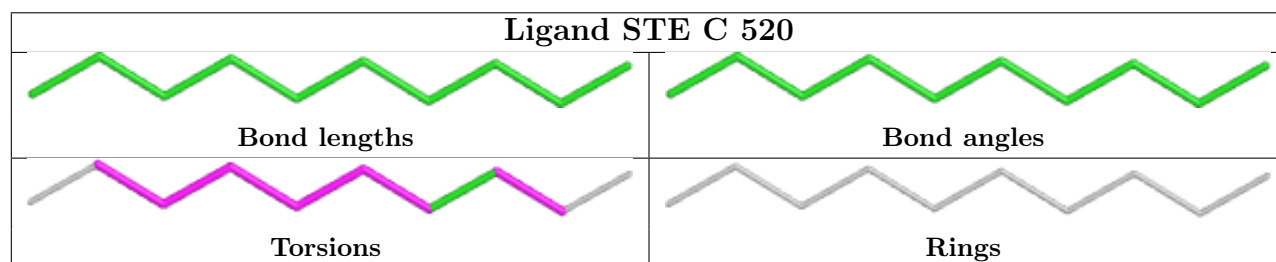
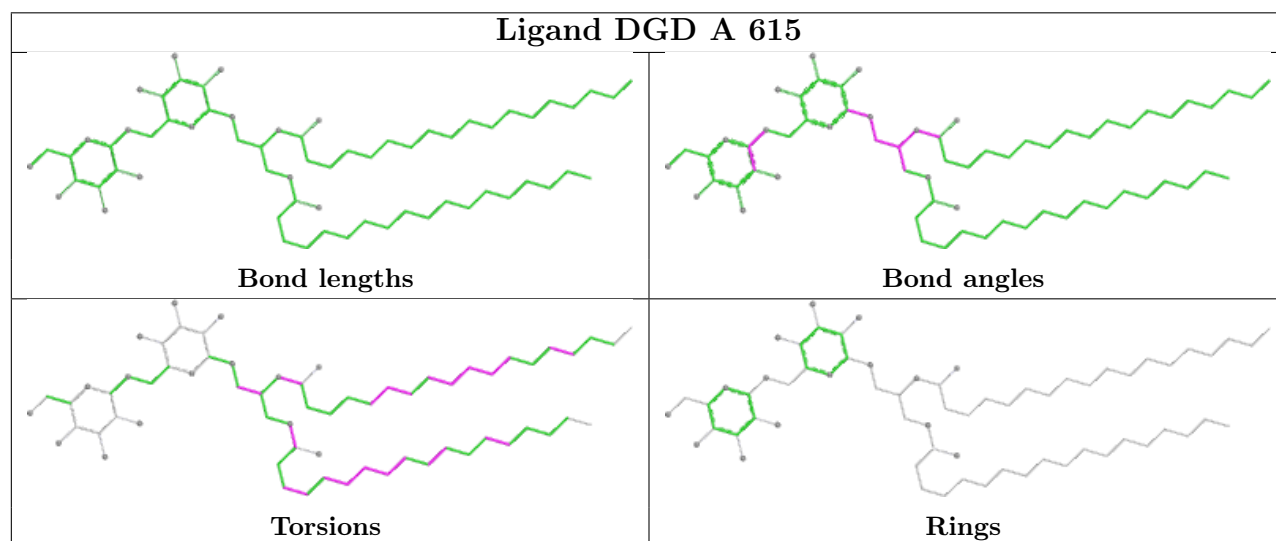
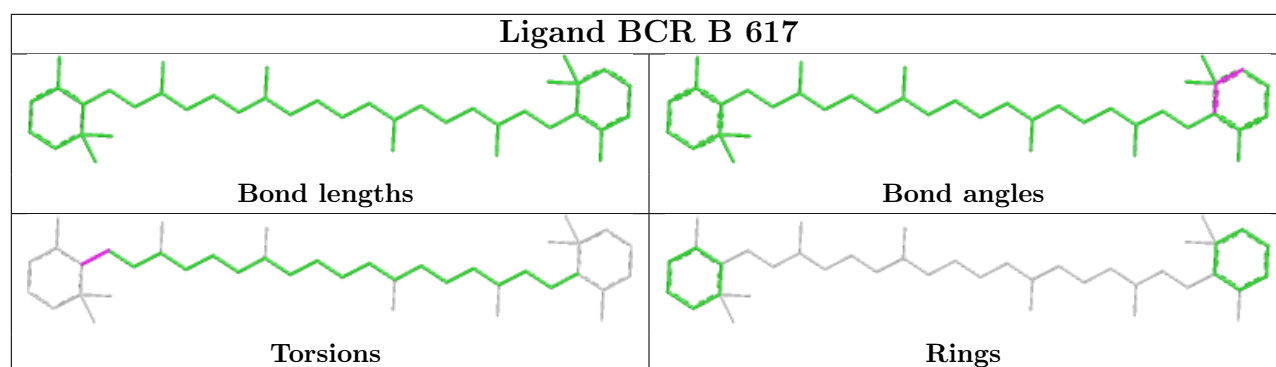
Ligand PL9 A 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

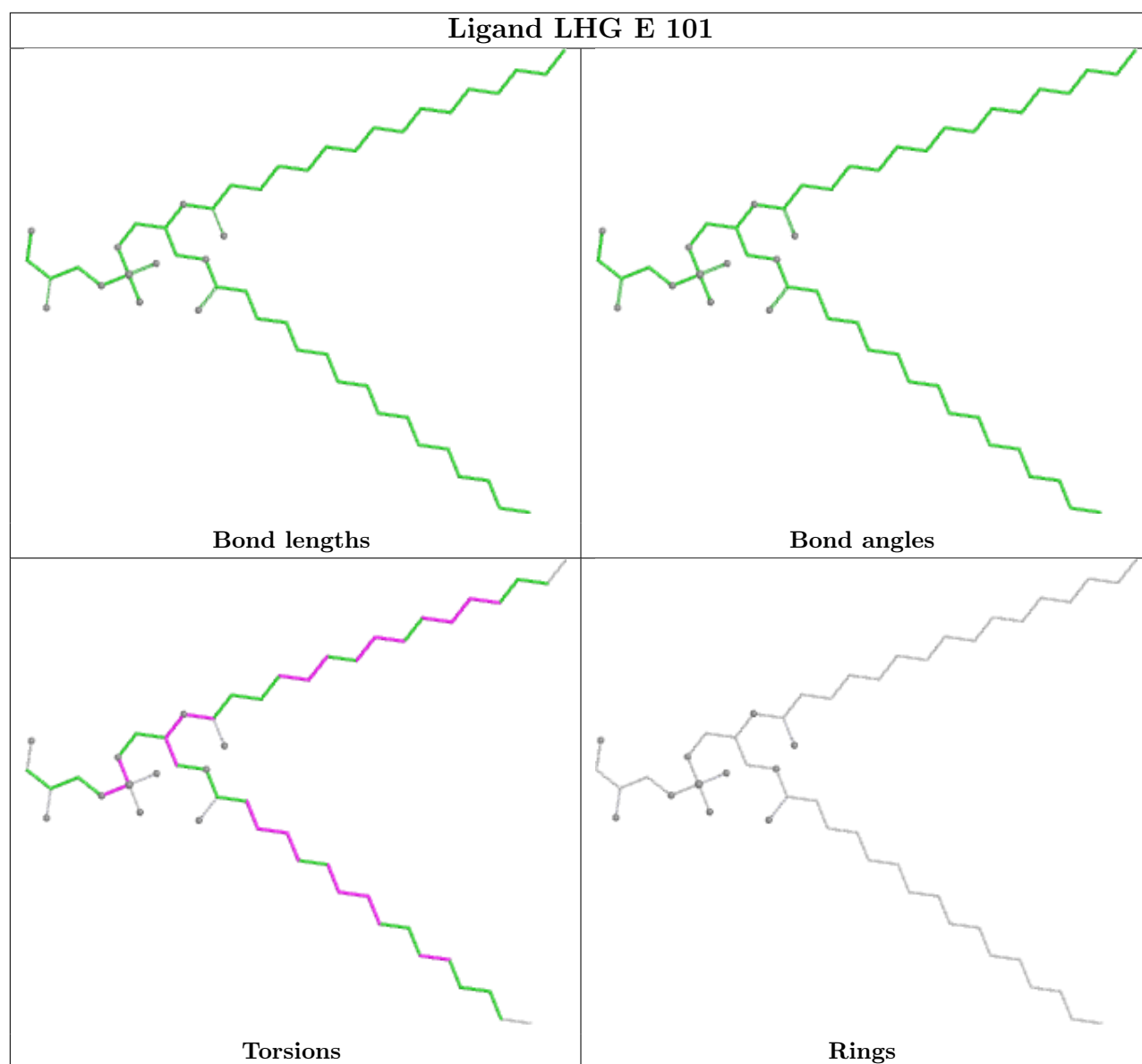
Ligand CLA B 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE E 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

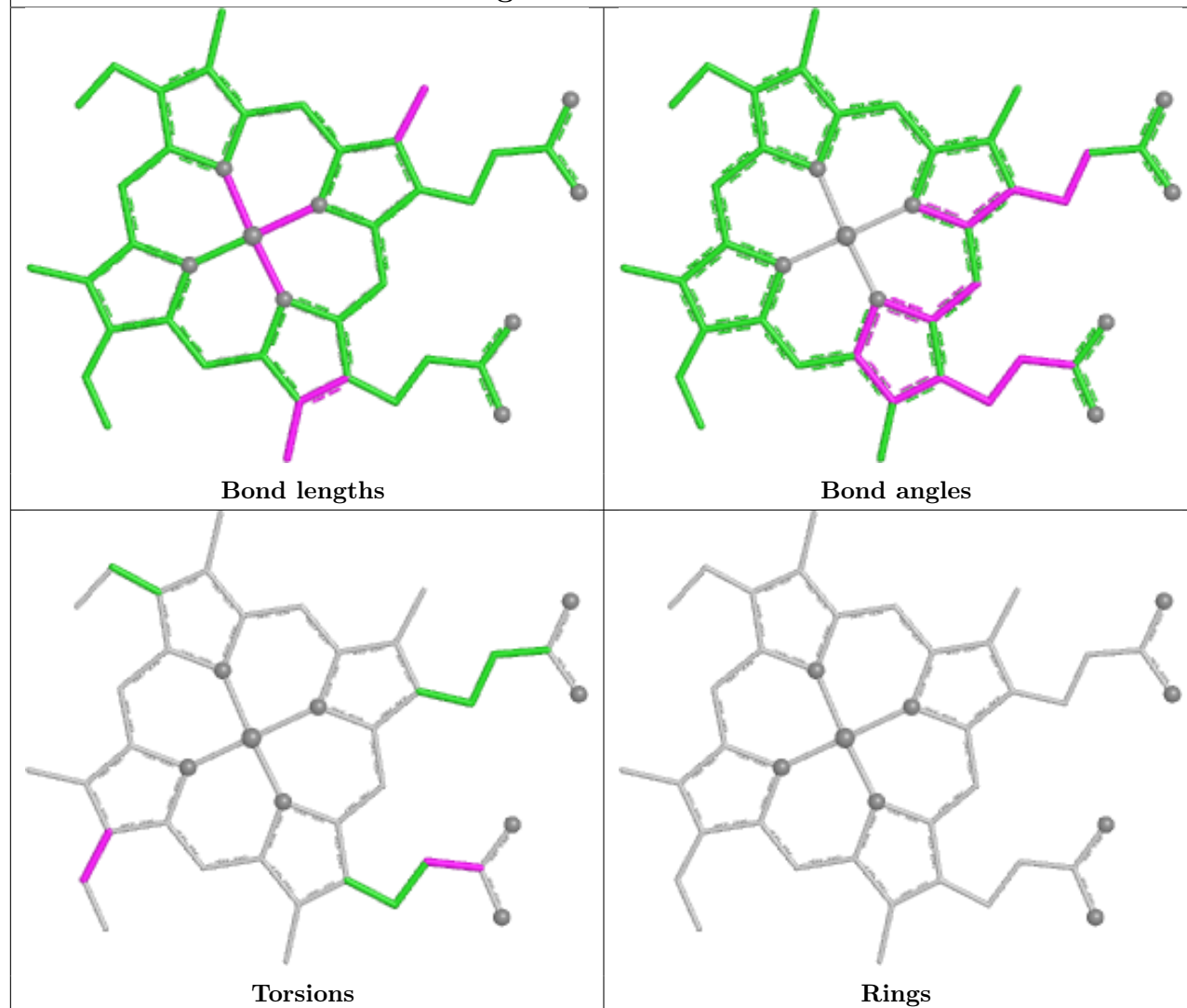




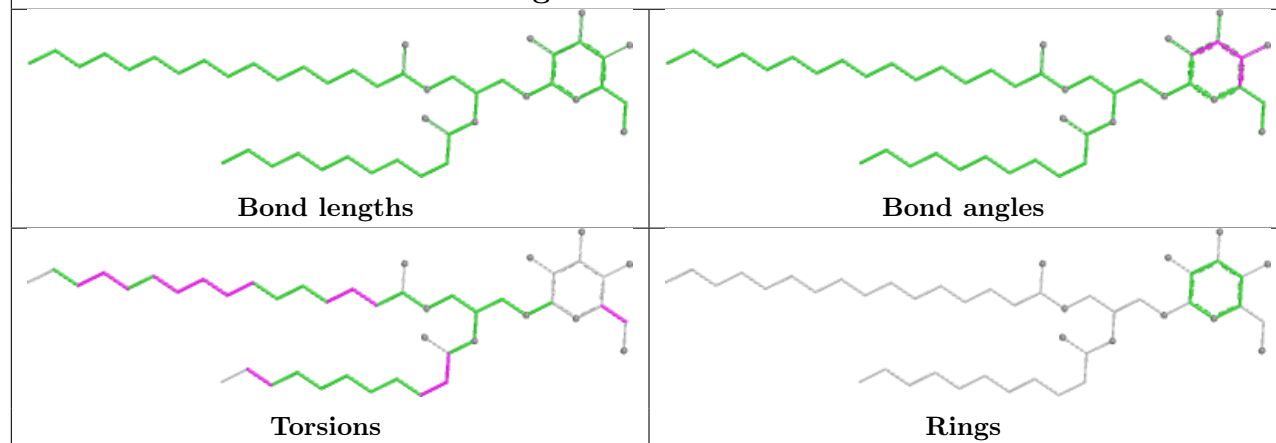


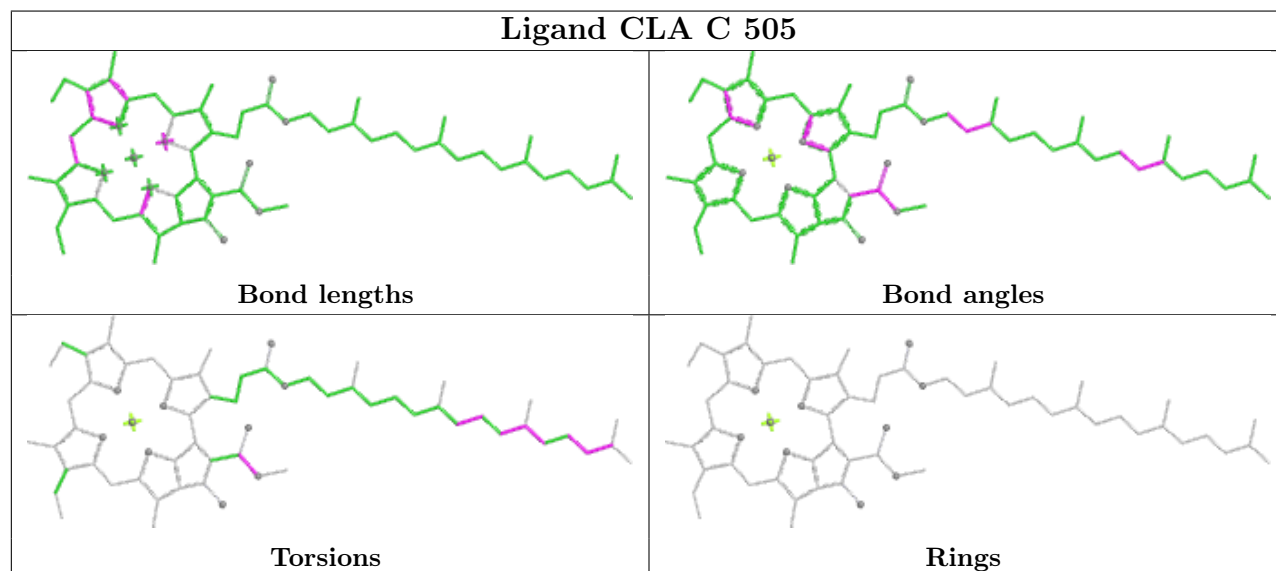
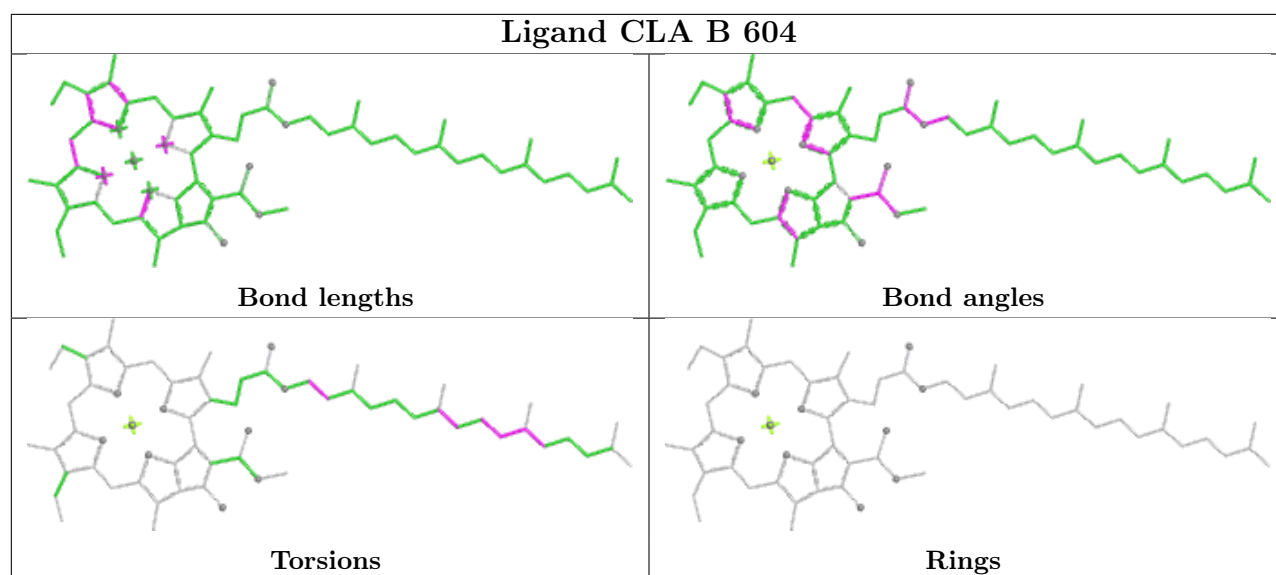
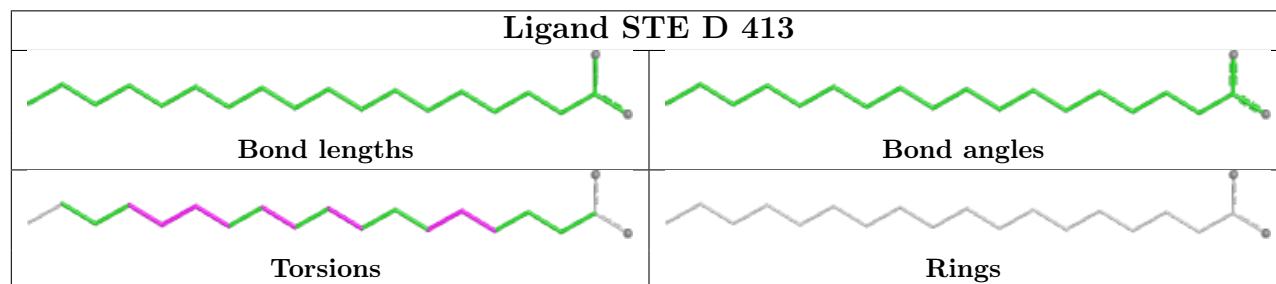
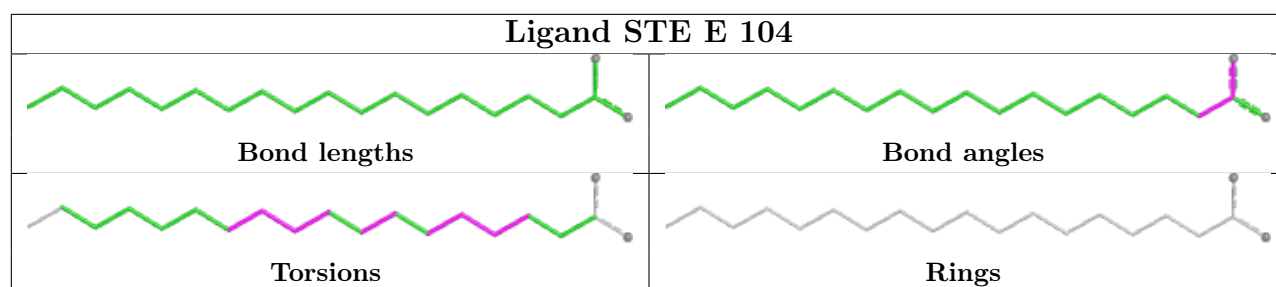


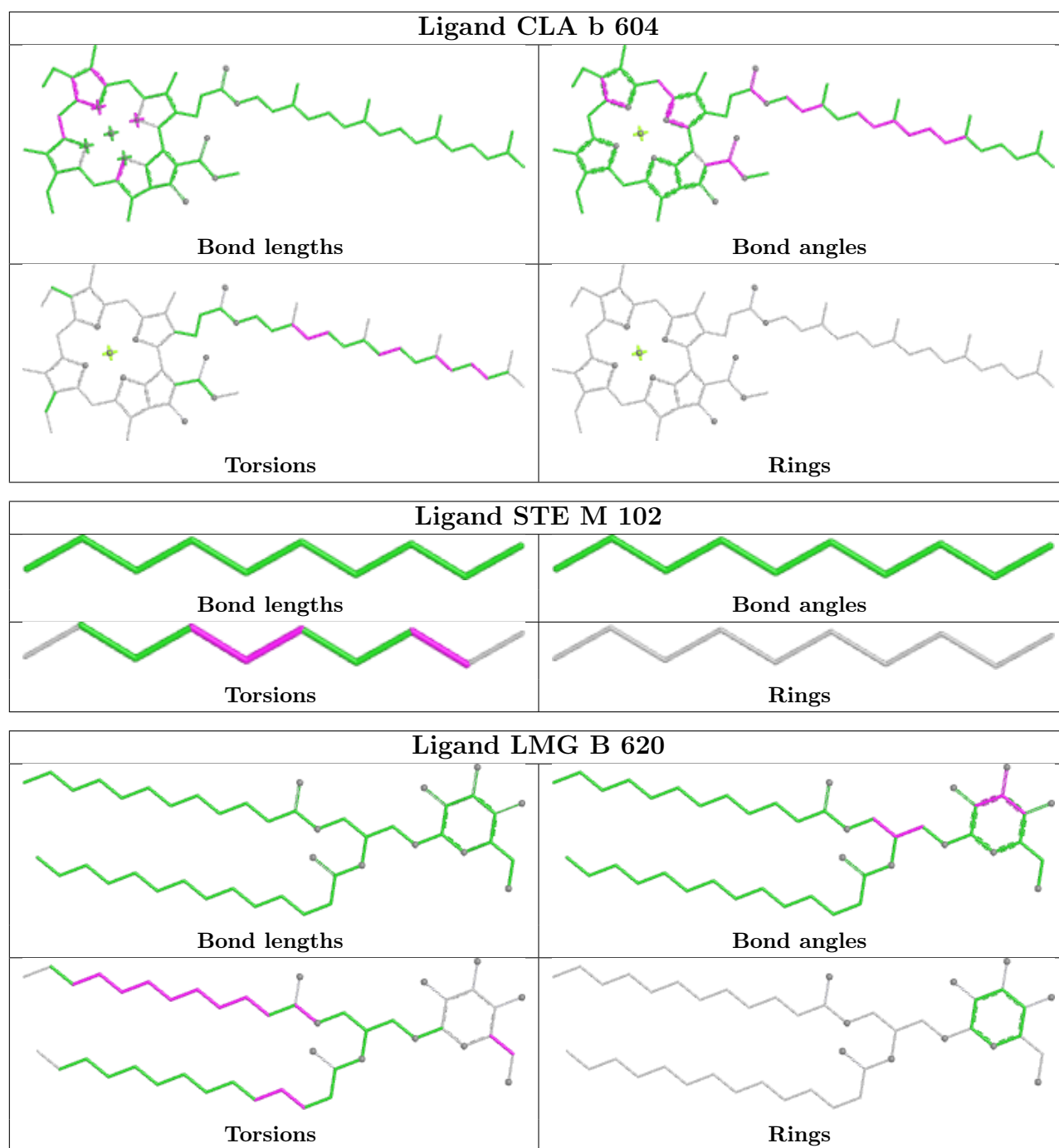
Ligand HEC v 201

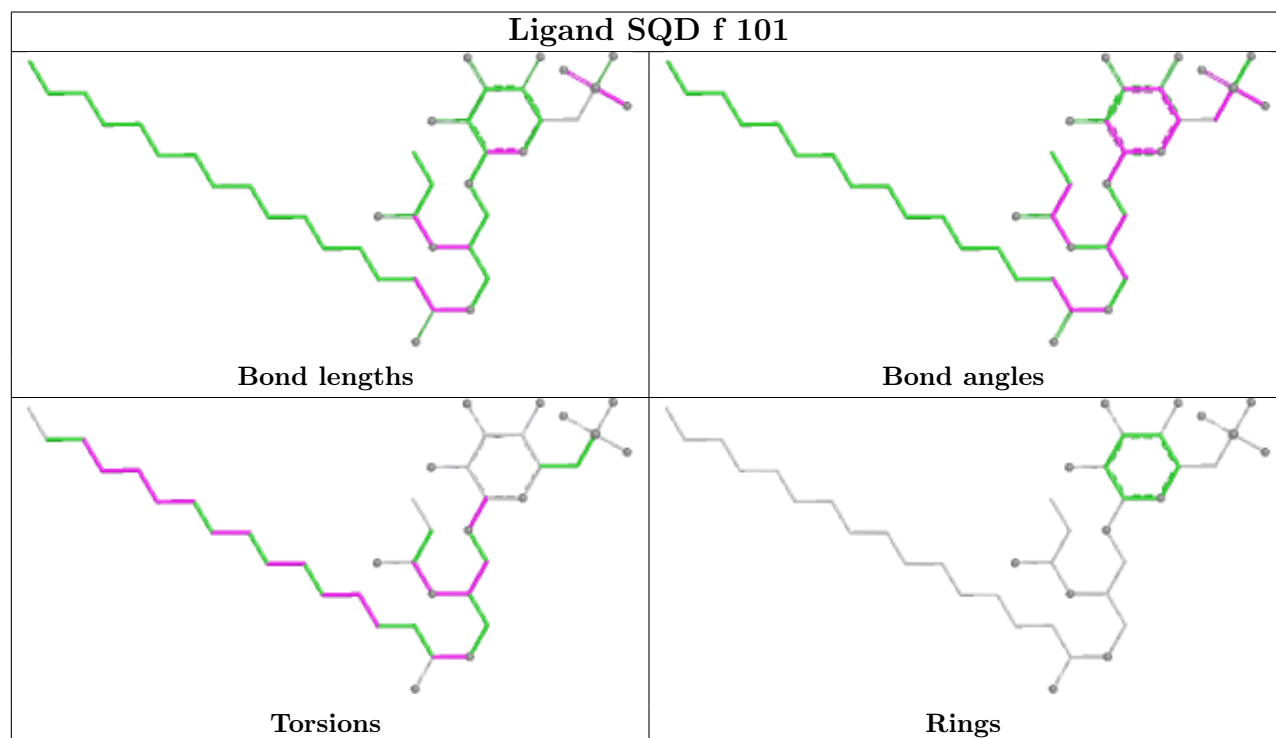
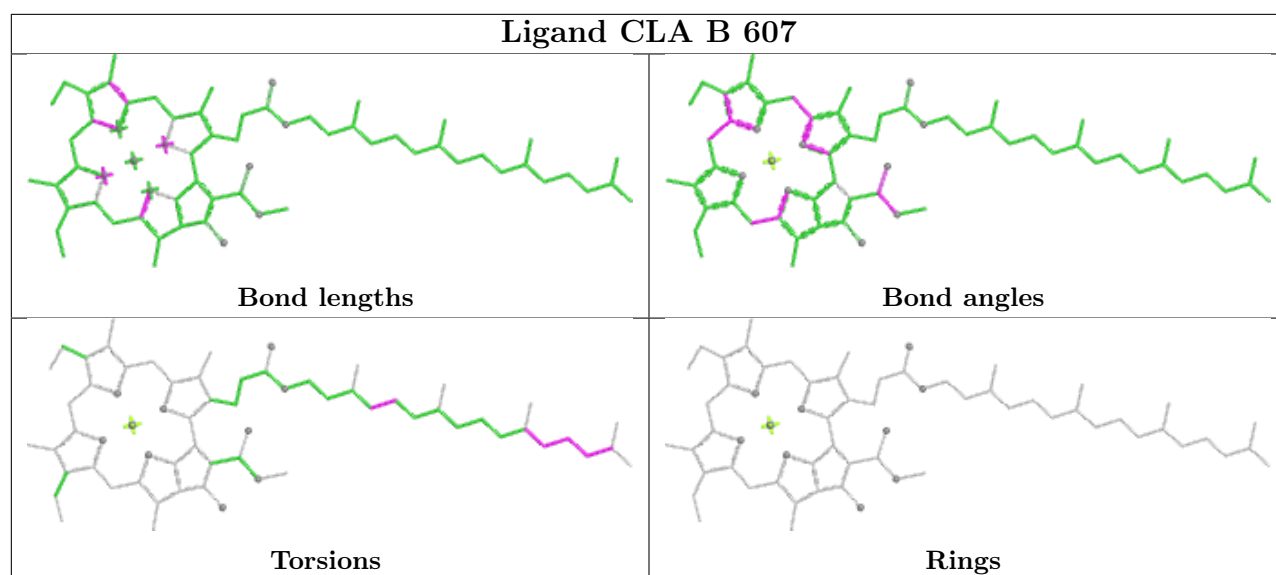


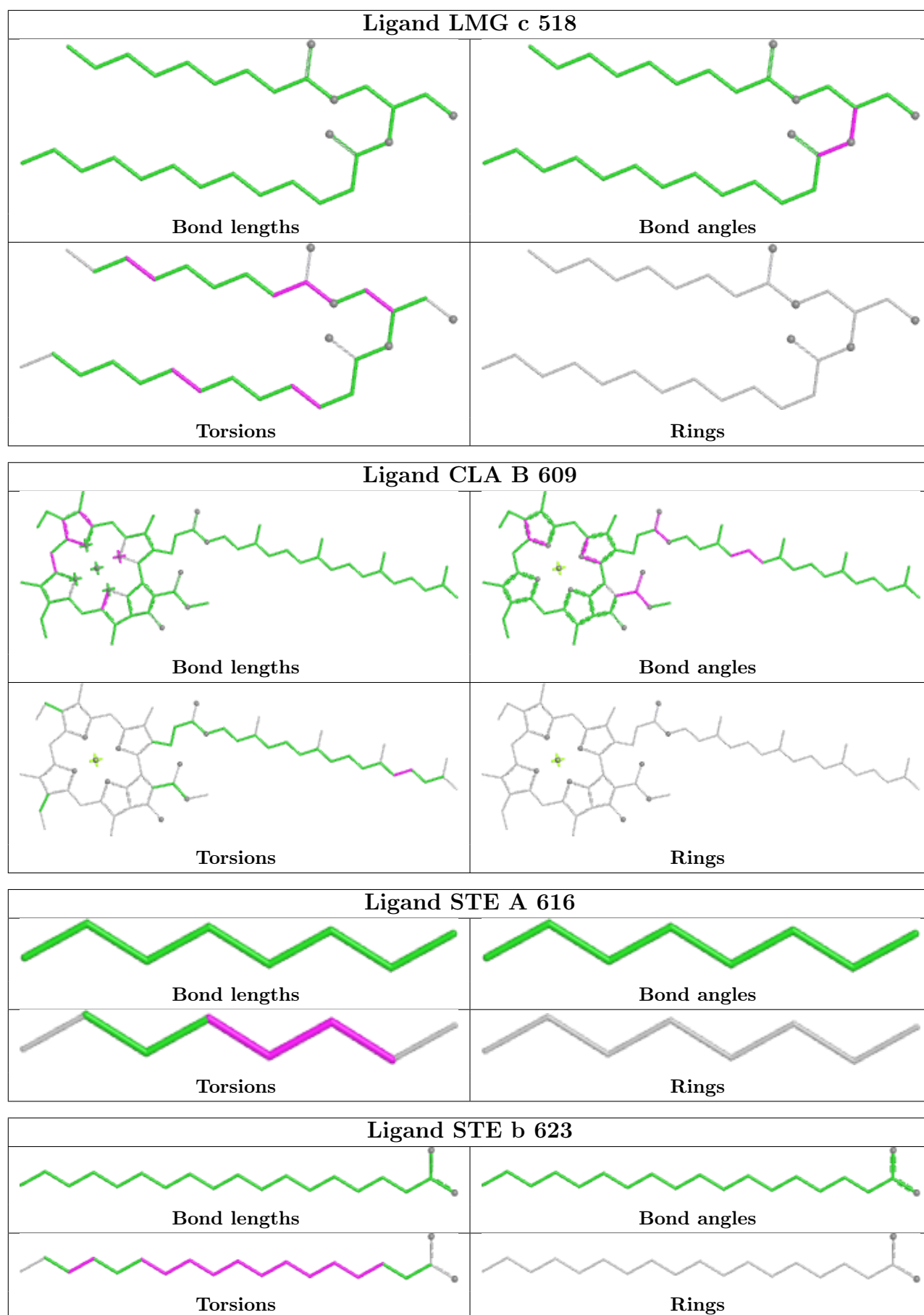
Ligand LMG c 522

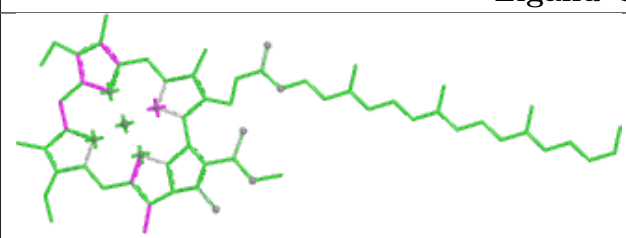
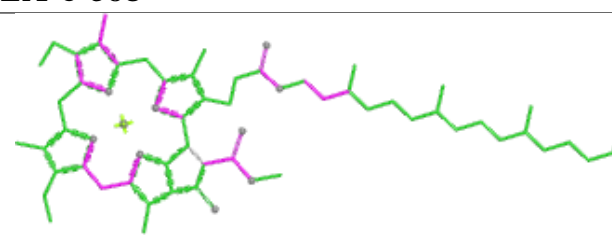
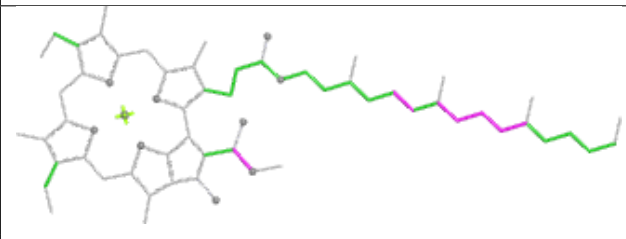
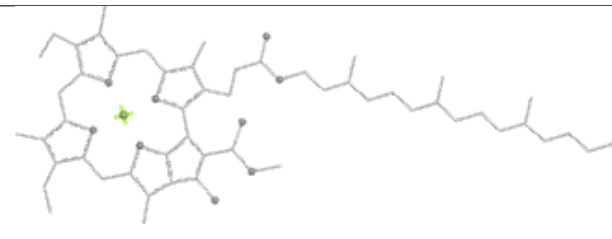


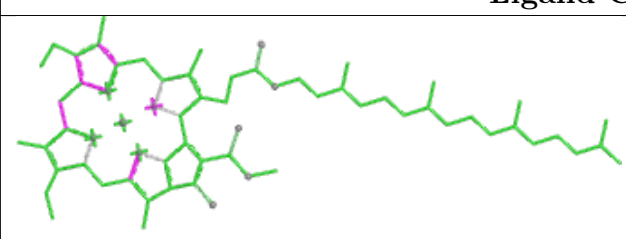
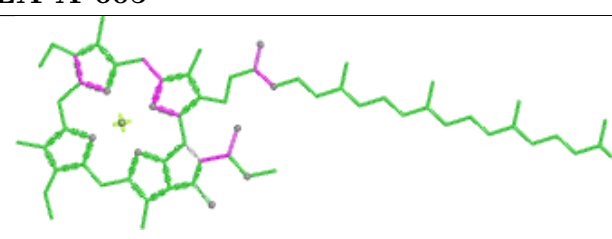
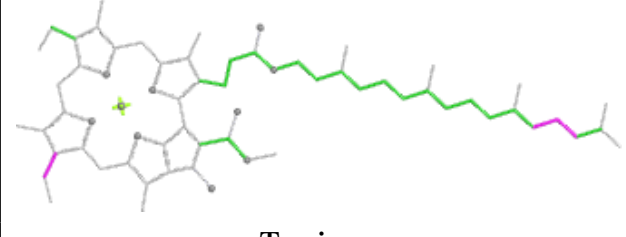
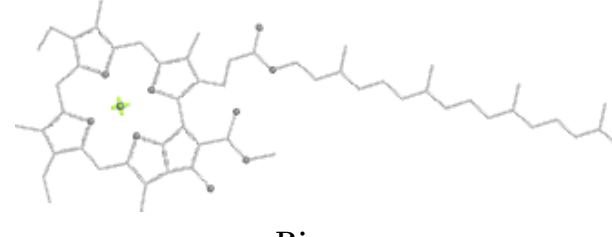






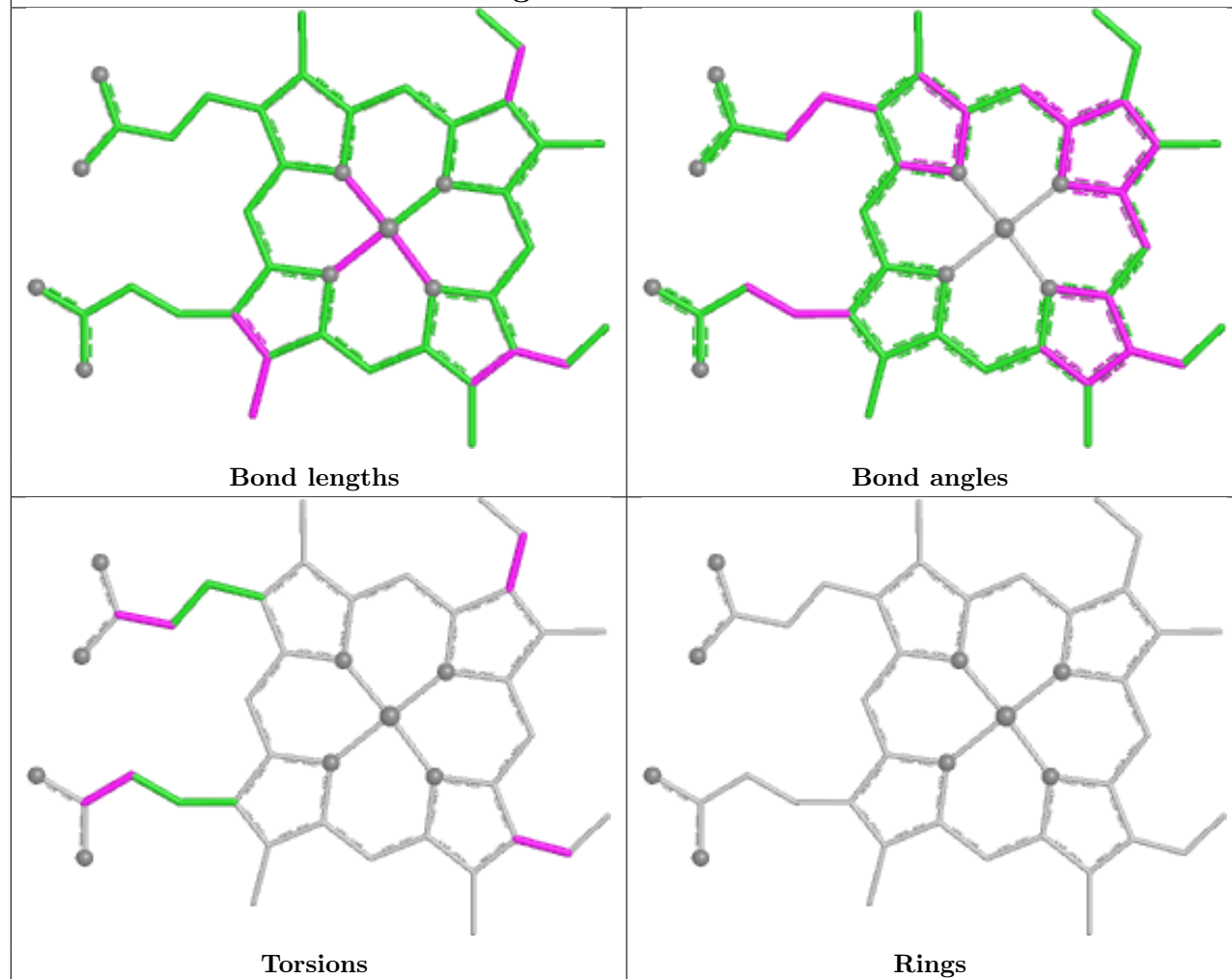


Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

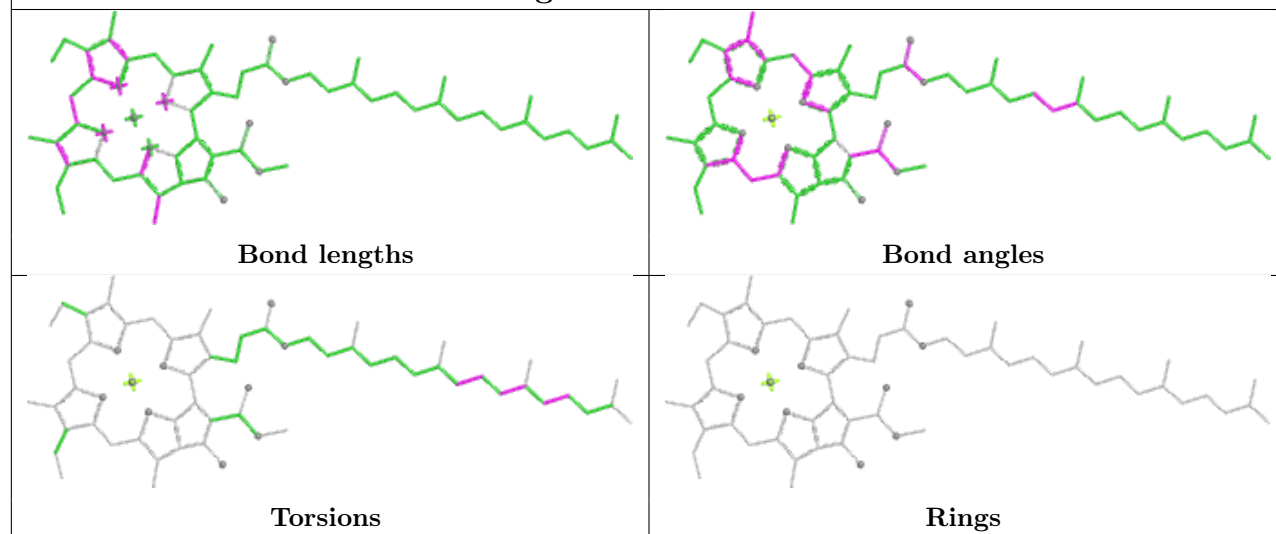
Ligand CLA A 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

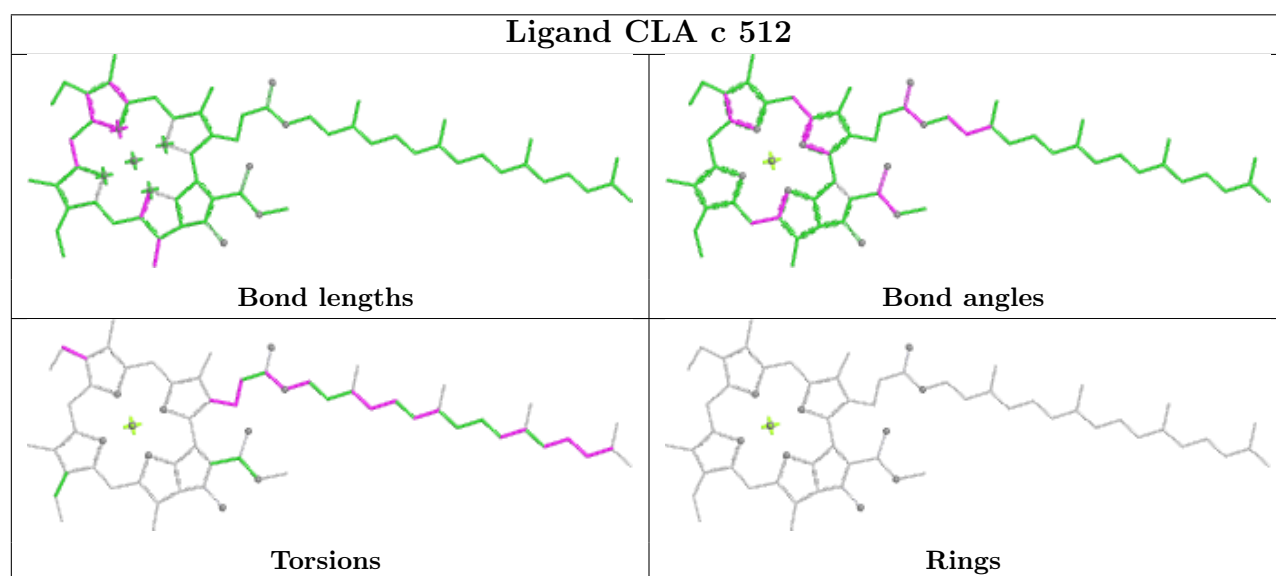
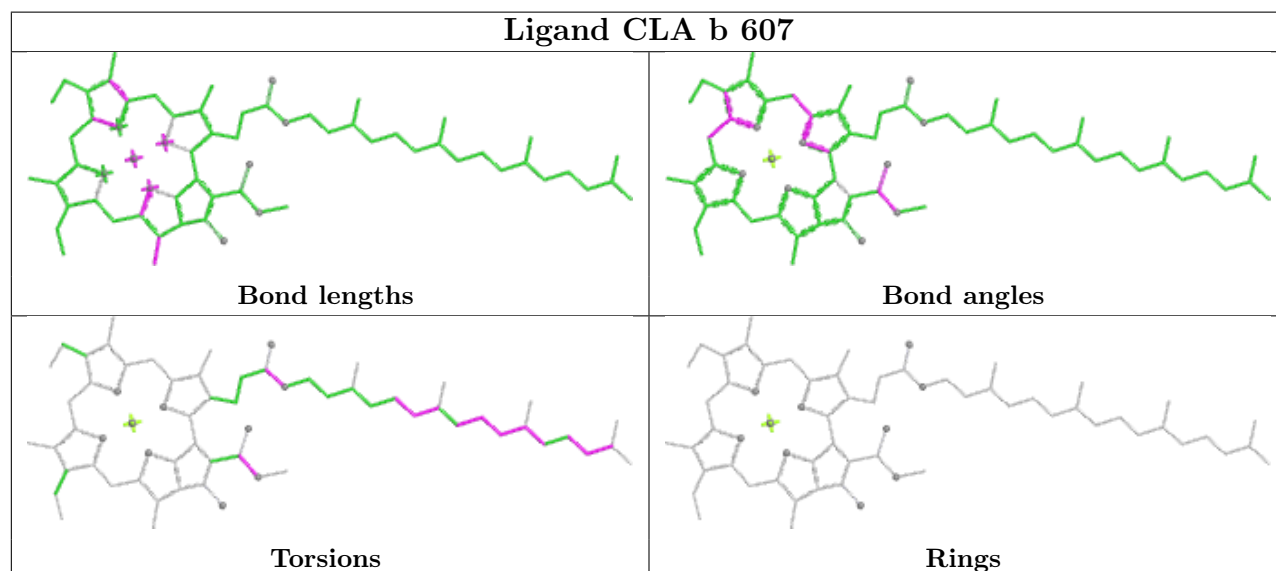
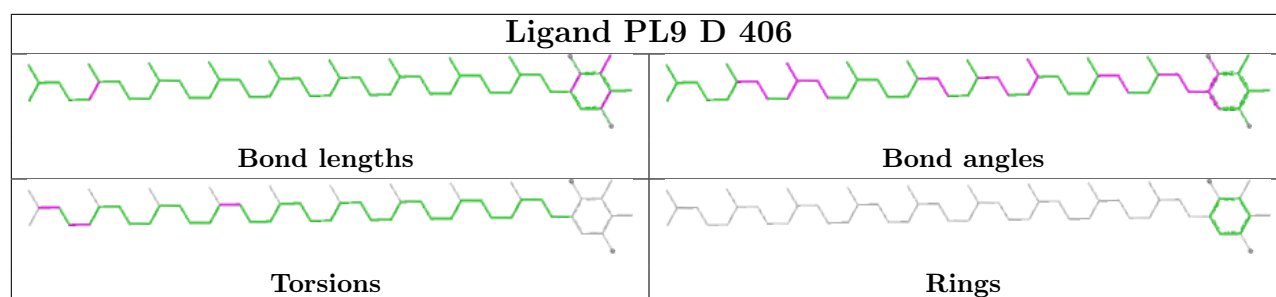
Ligand STE Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HEM e 102

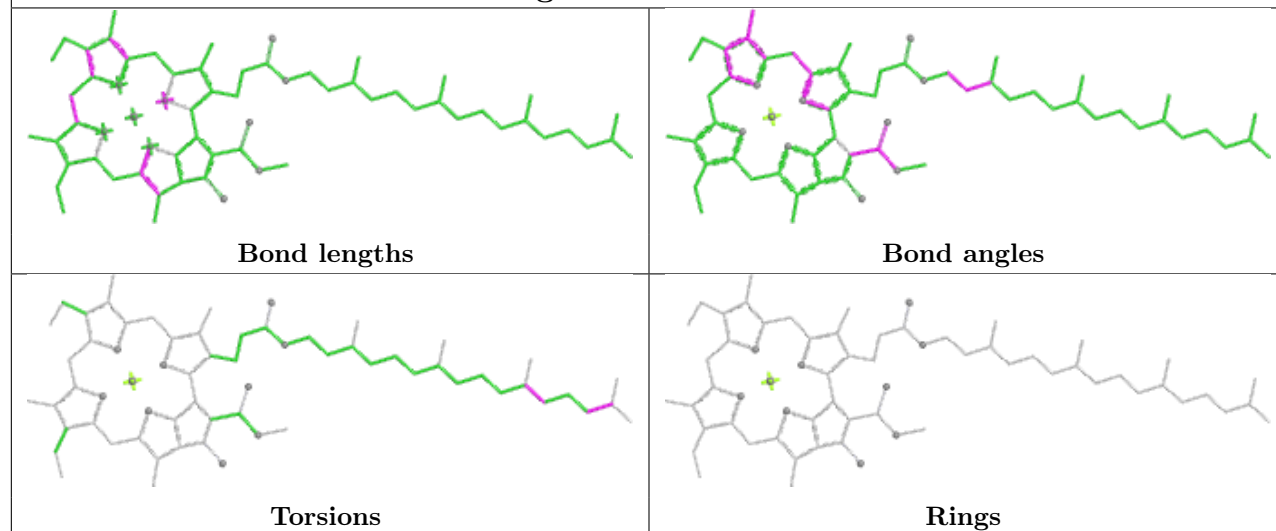


Ligand CLA b 608

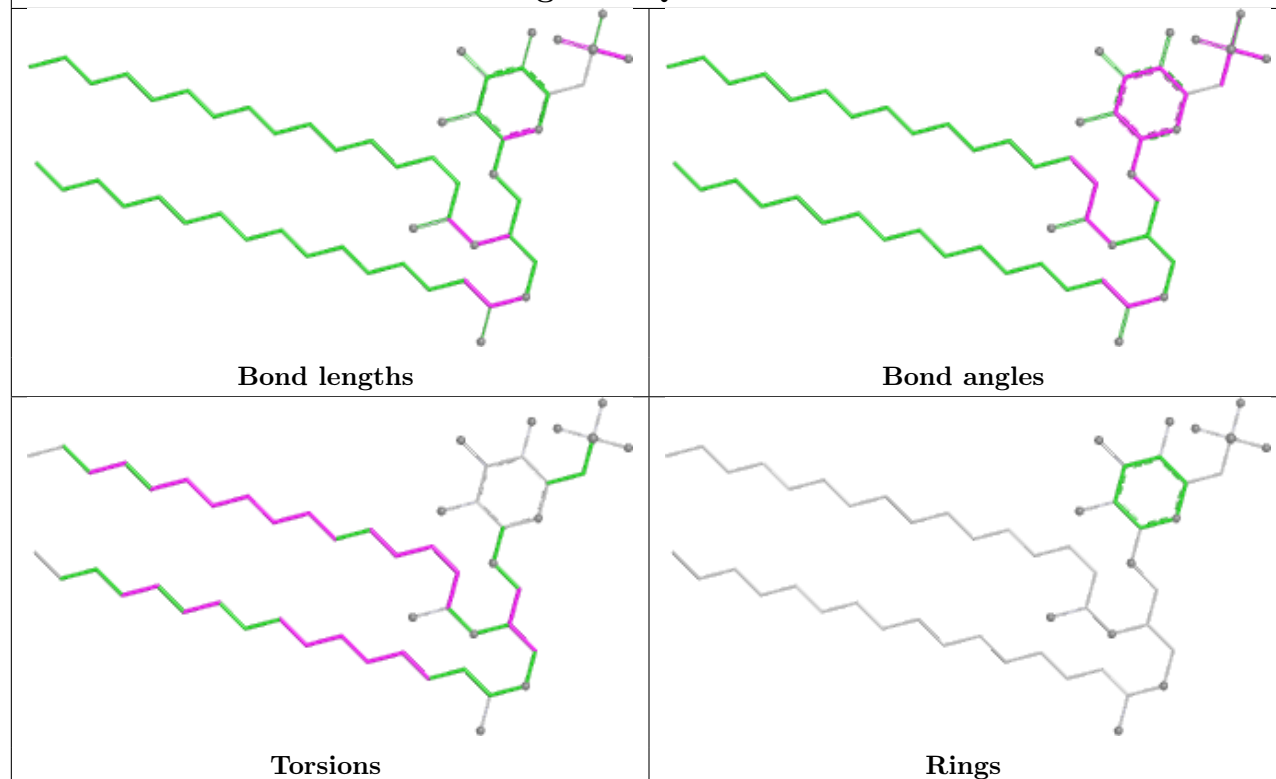


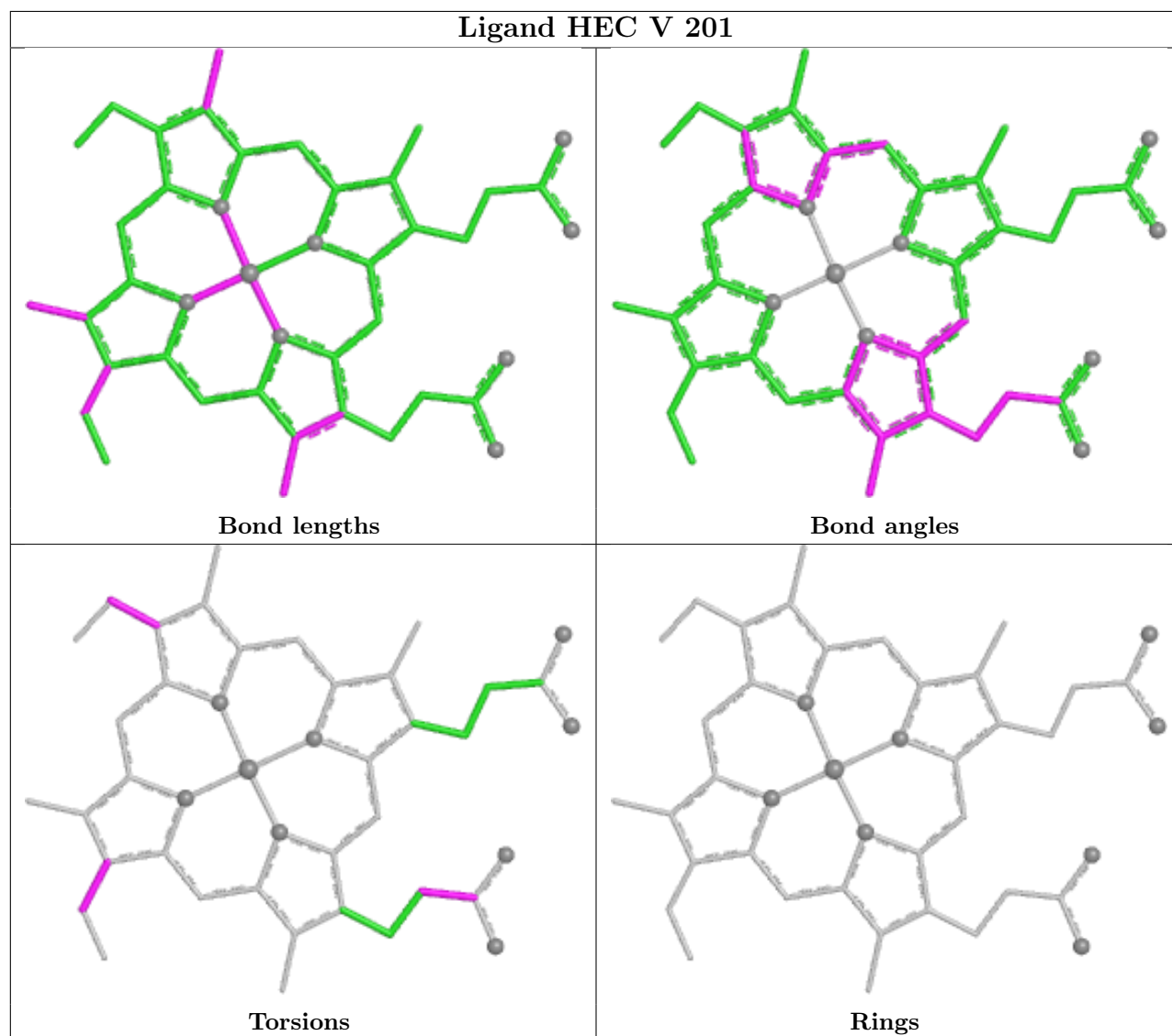
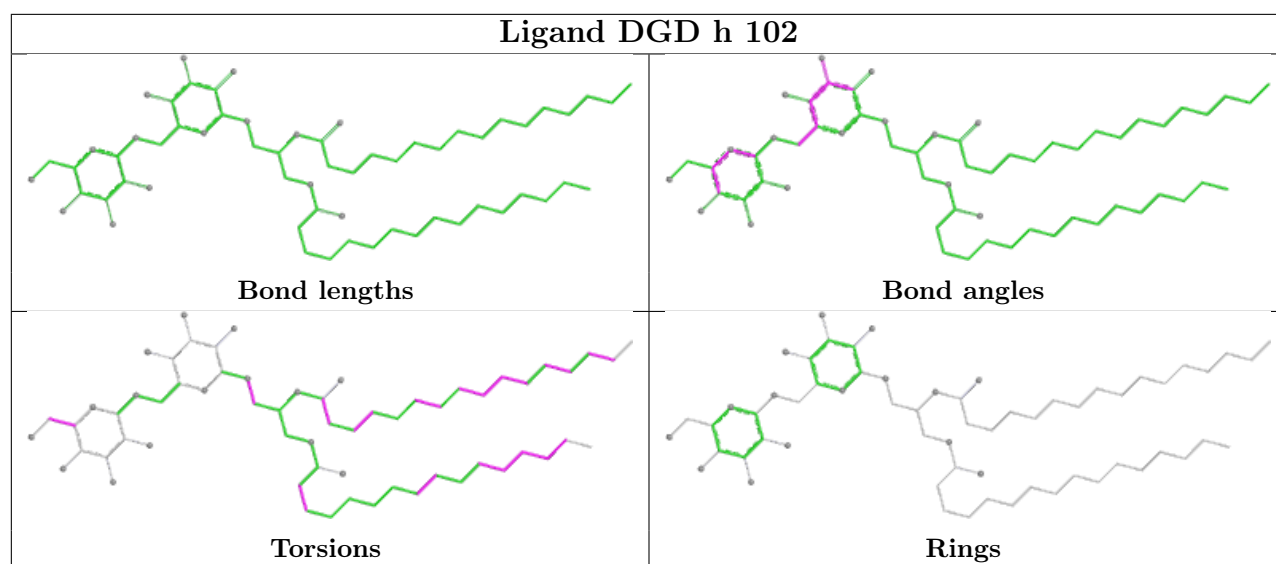


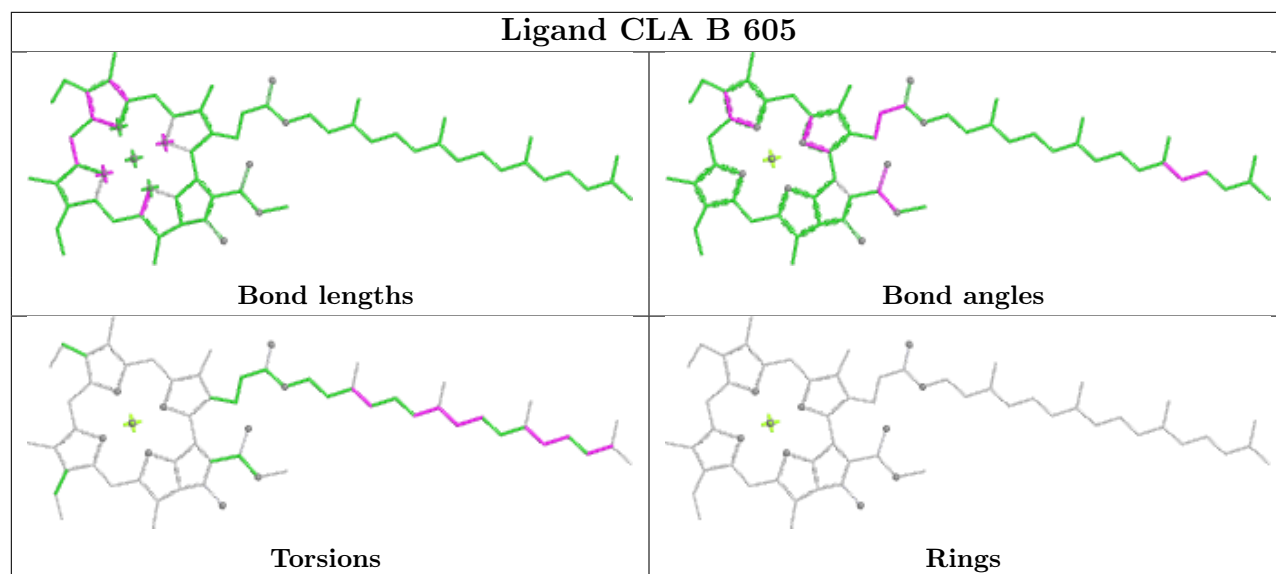
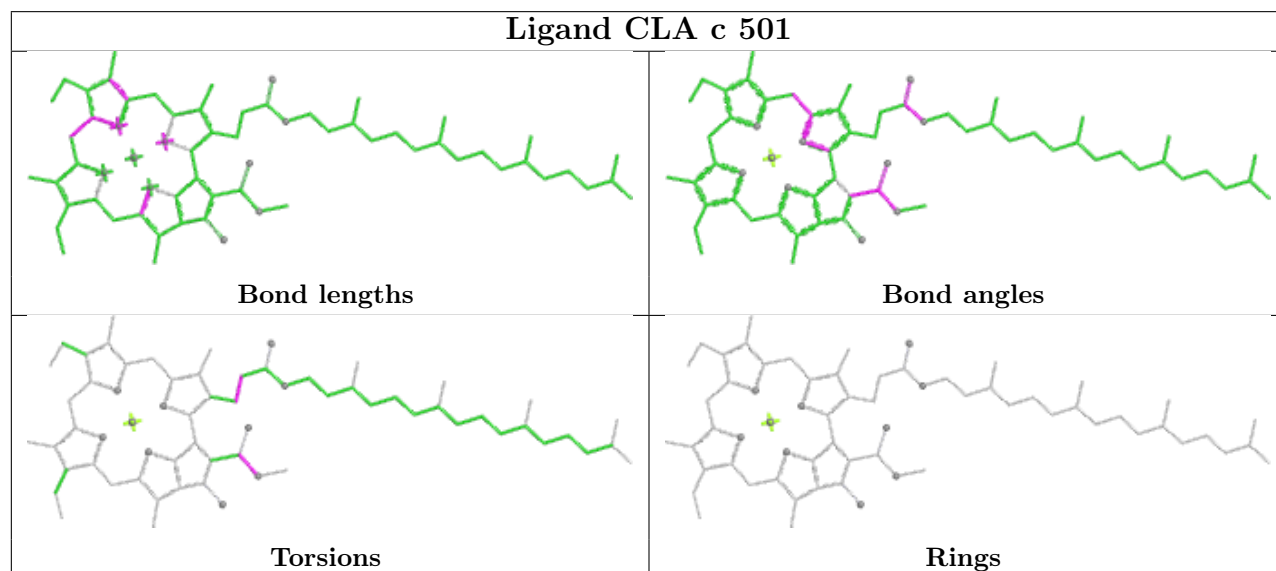
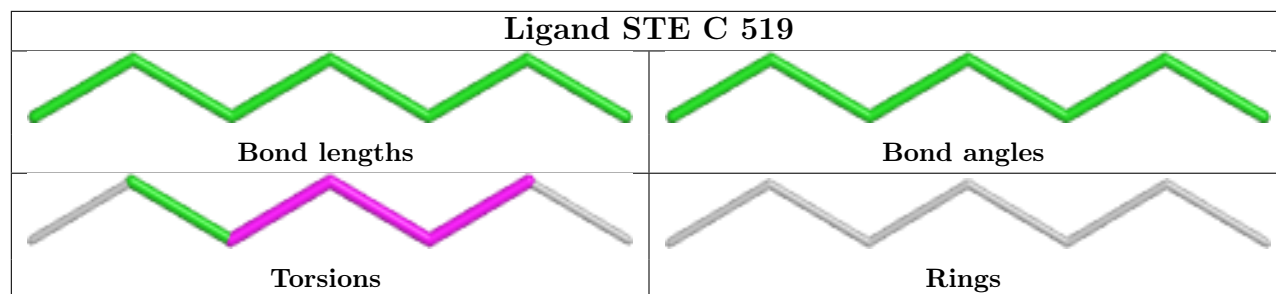
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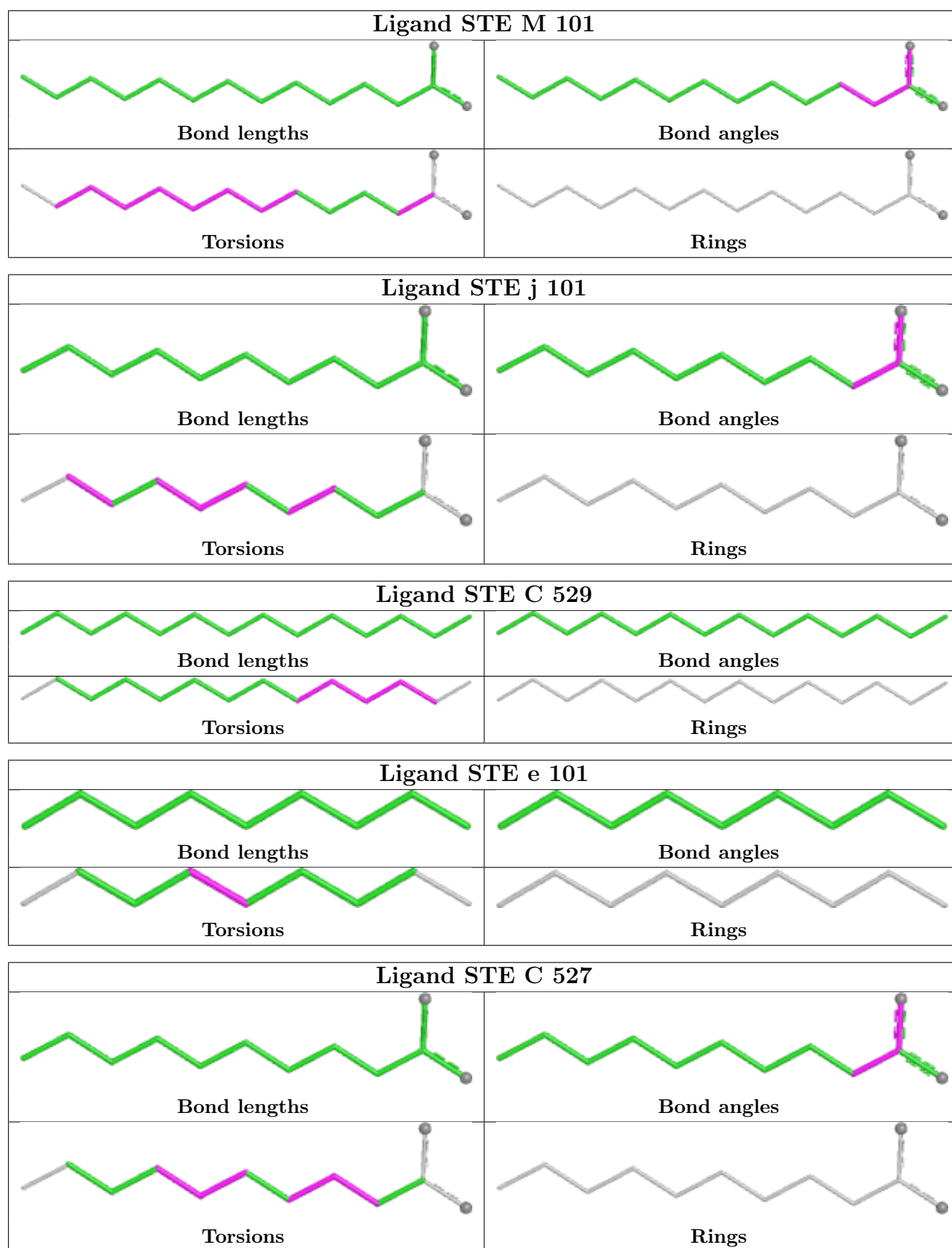


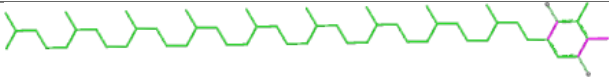
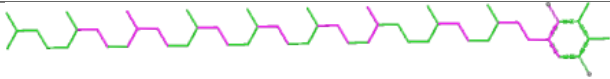
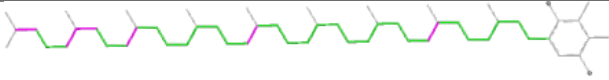
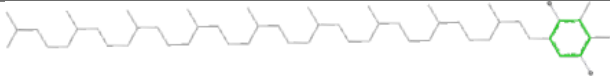
Ligand SQD a 613

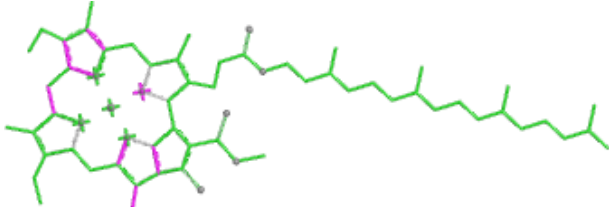
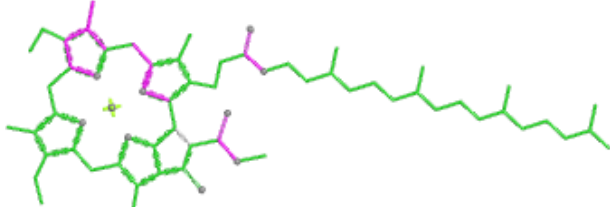
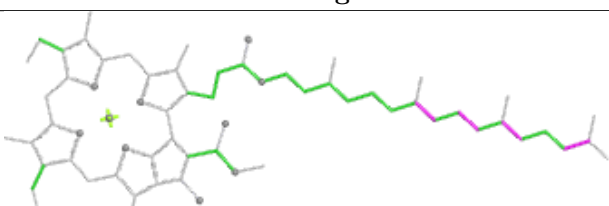
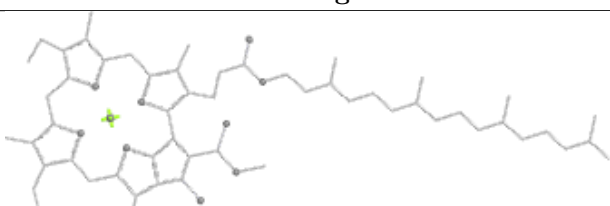


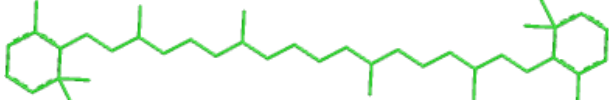
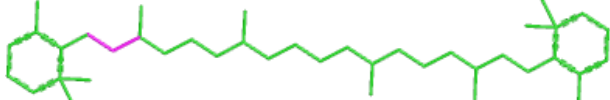
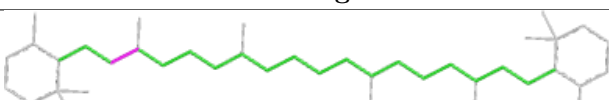
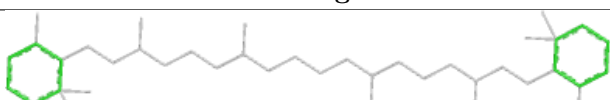




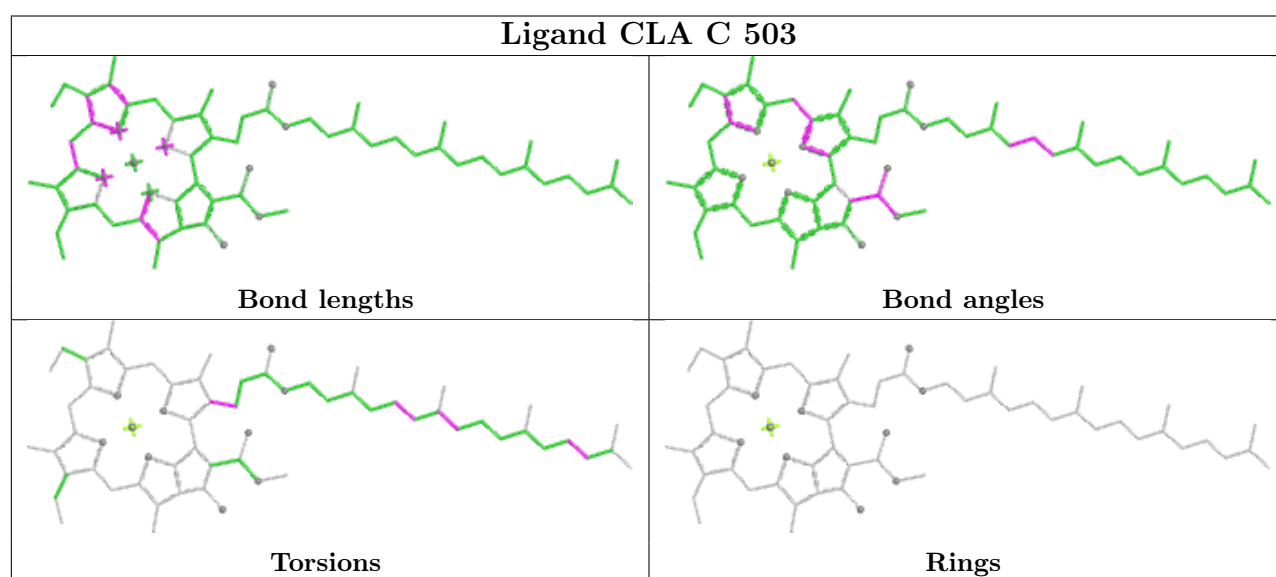
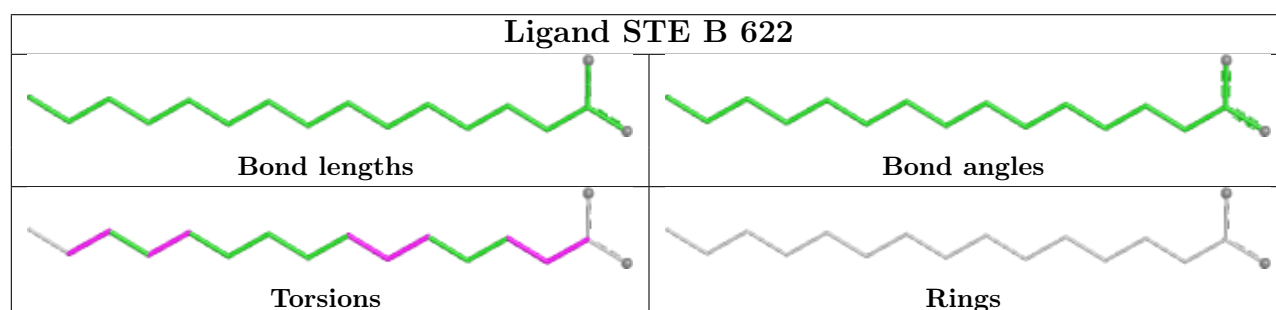
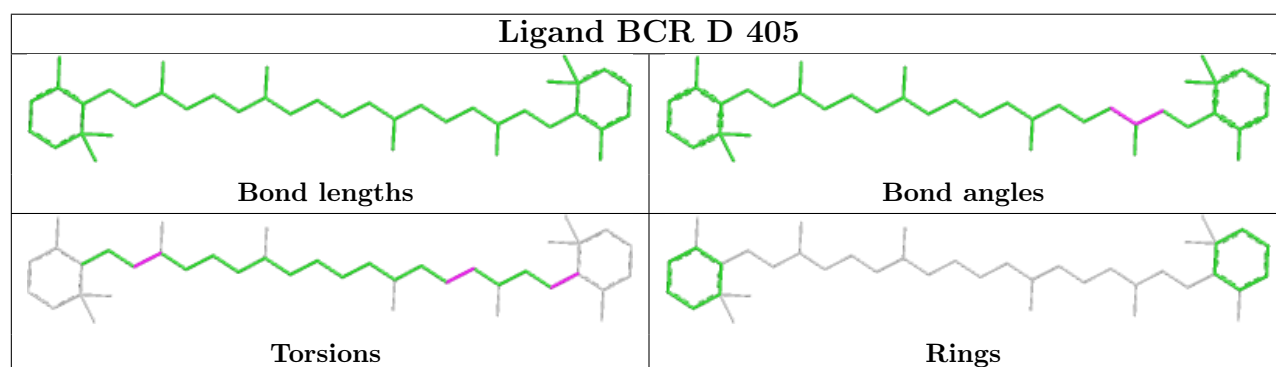
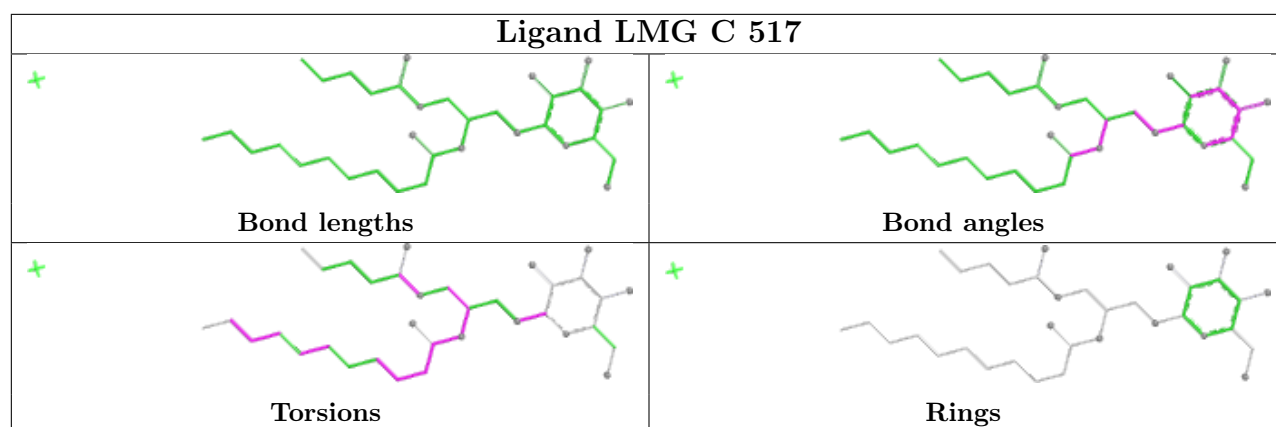


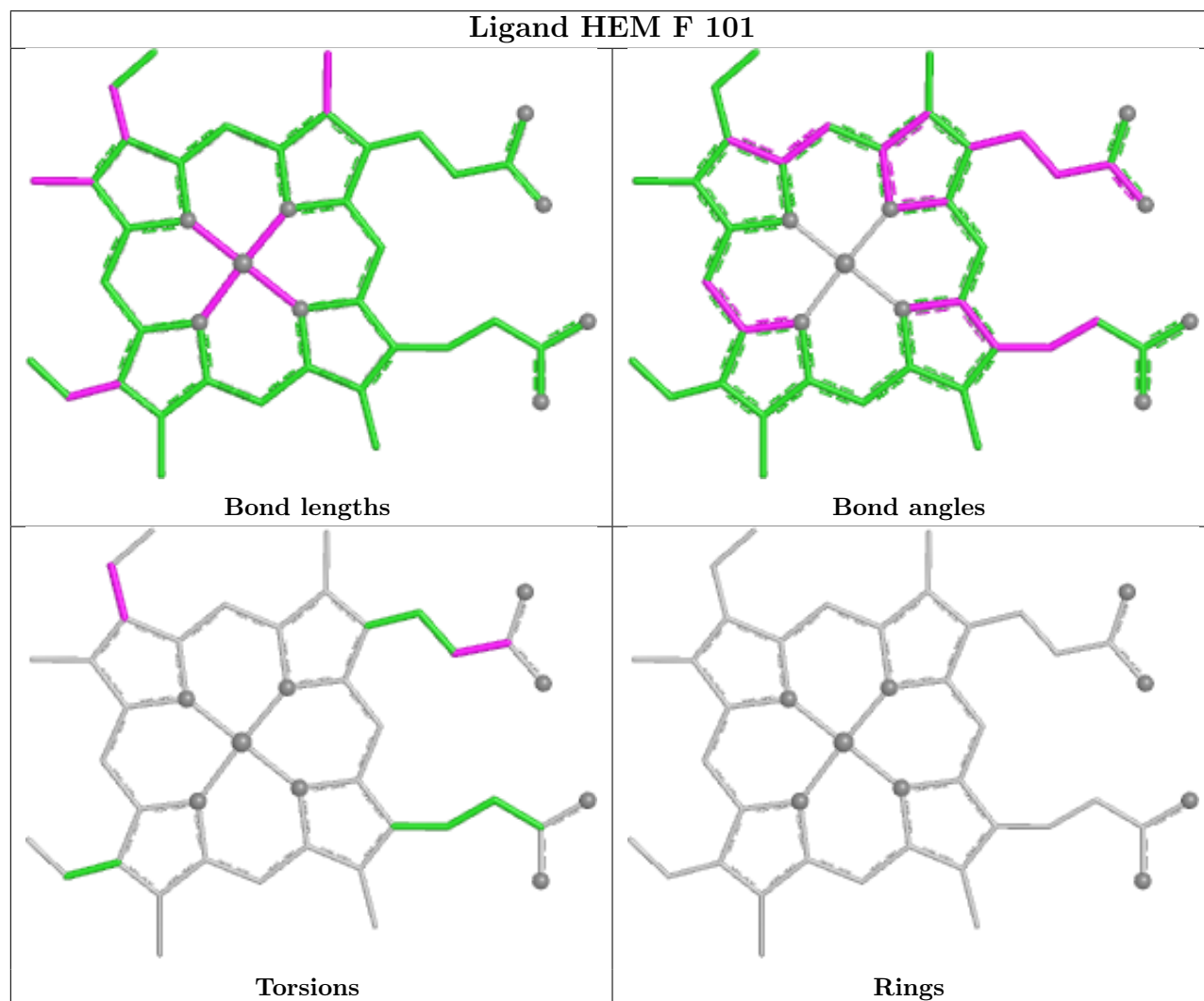
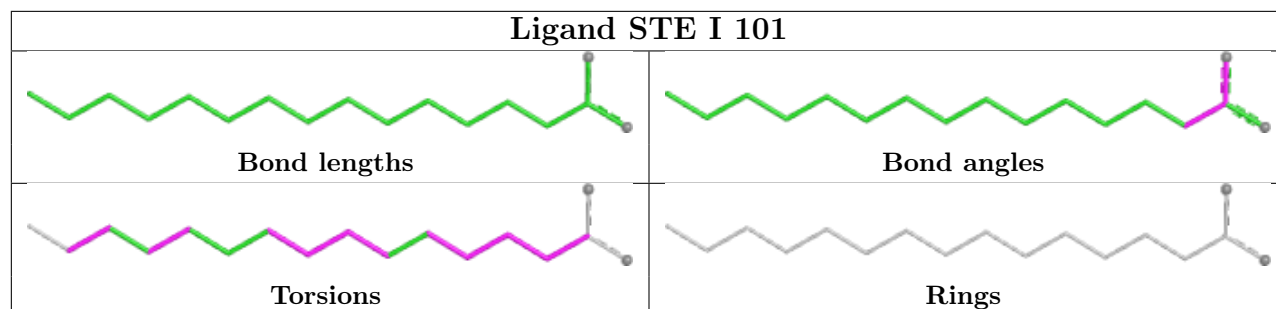
Ligand PL9 d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

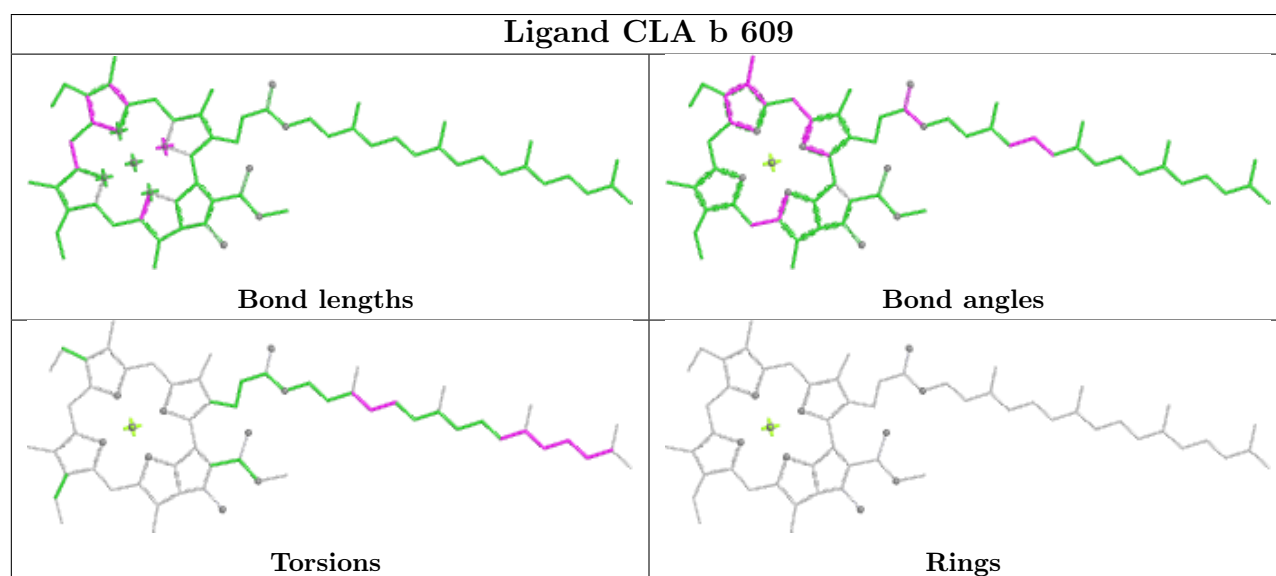
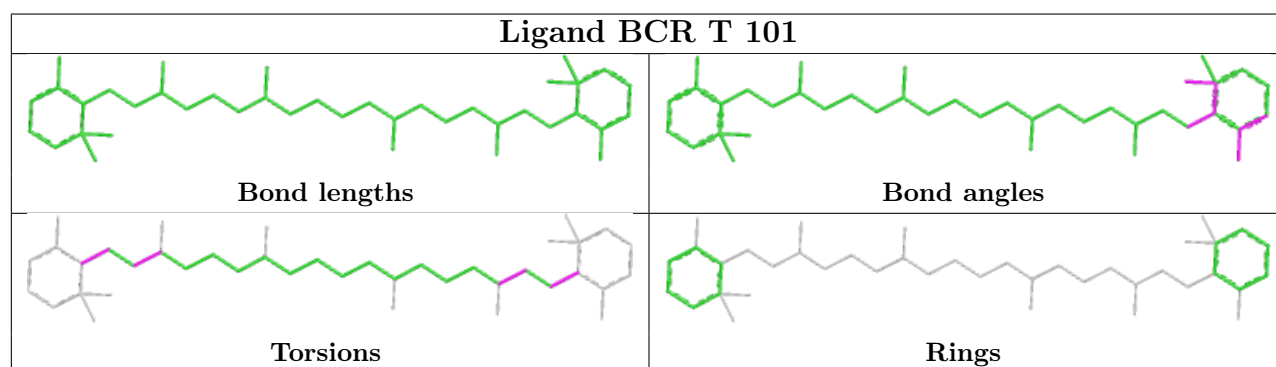
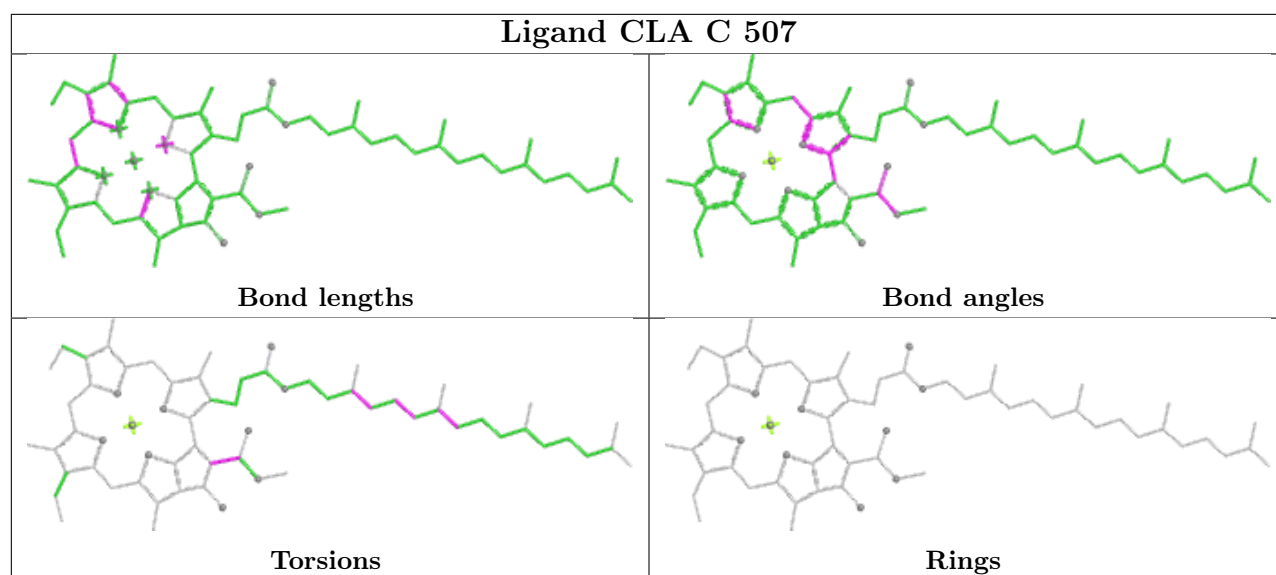
Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

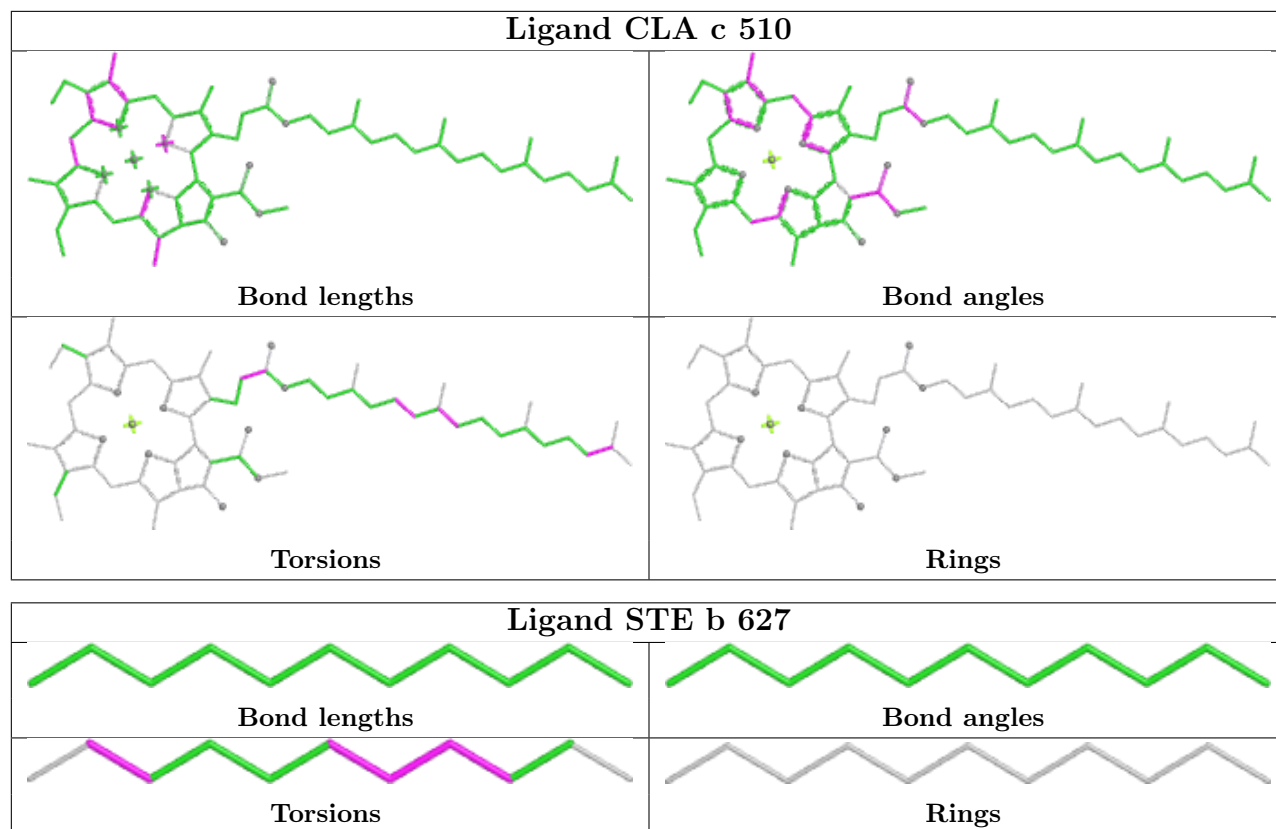
Ligand BCR k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

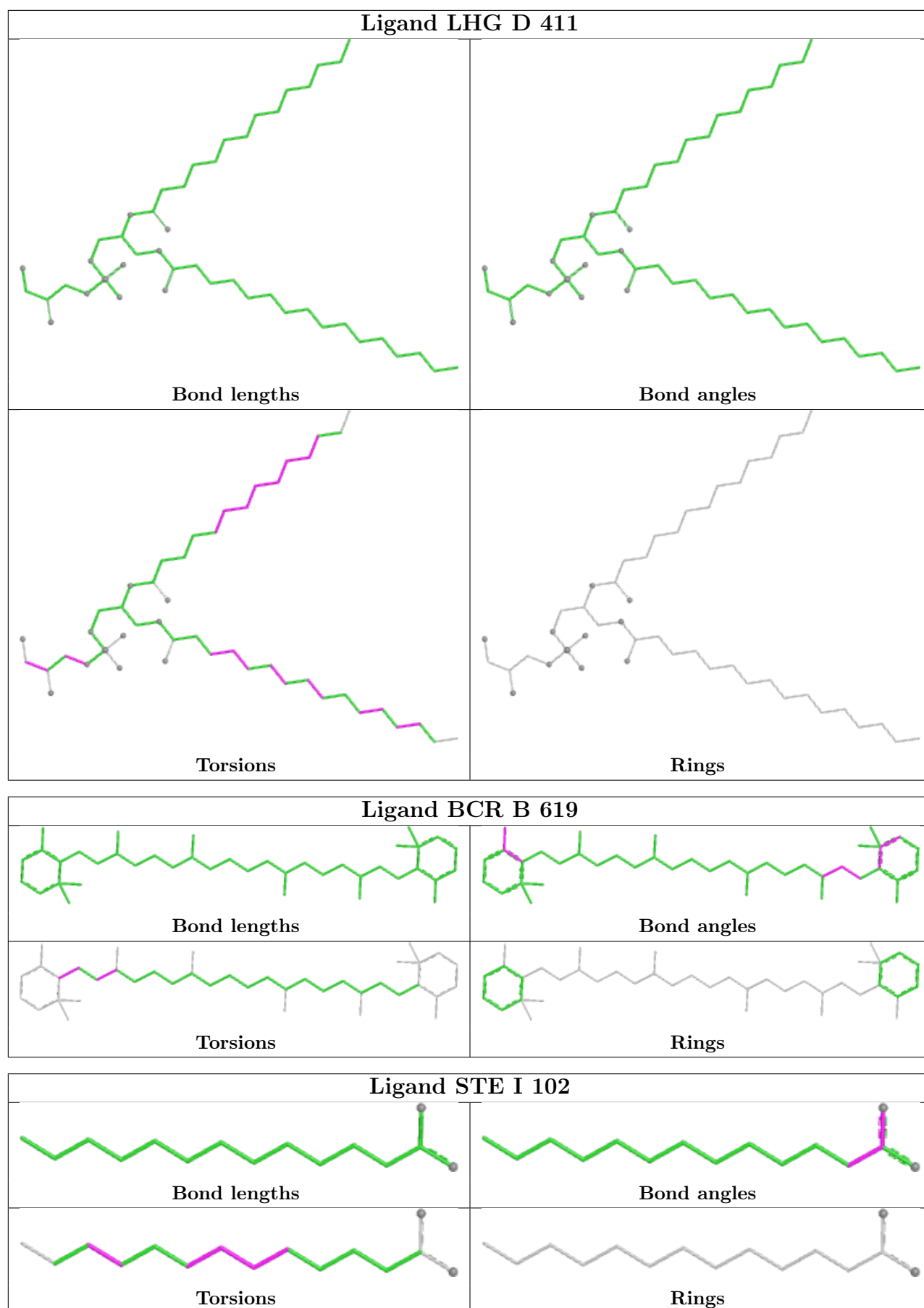
Ligand STE A 617	
 Bond lengths	 Bond angles
 Torsions	 Rings



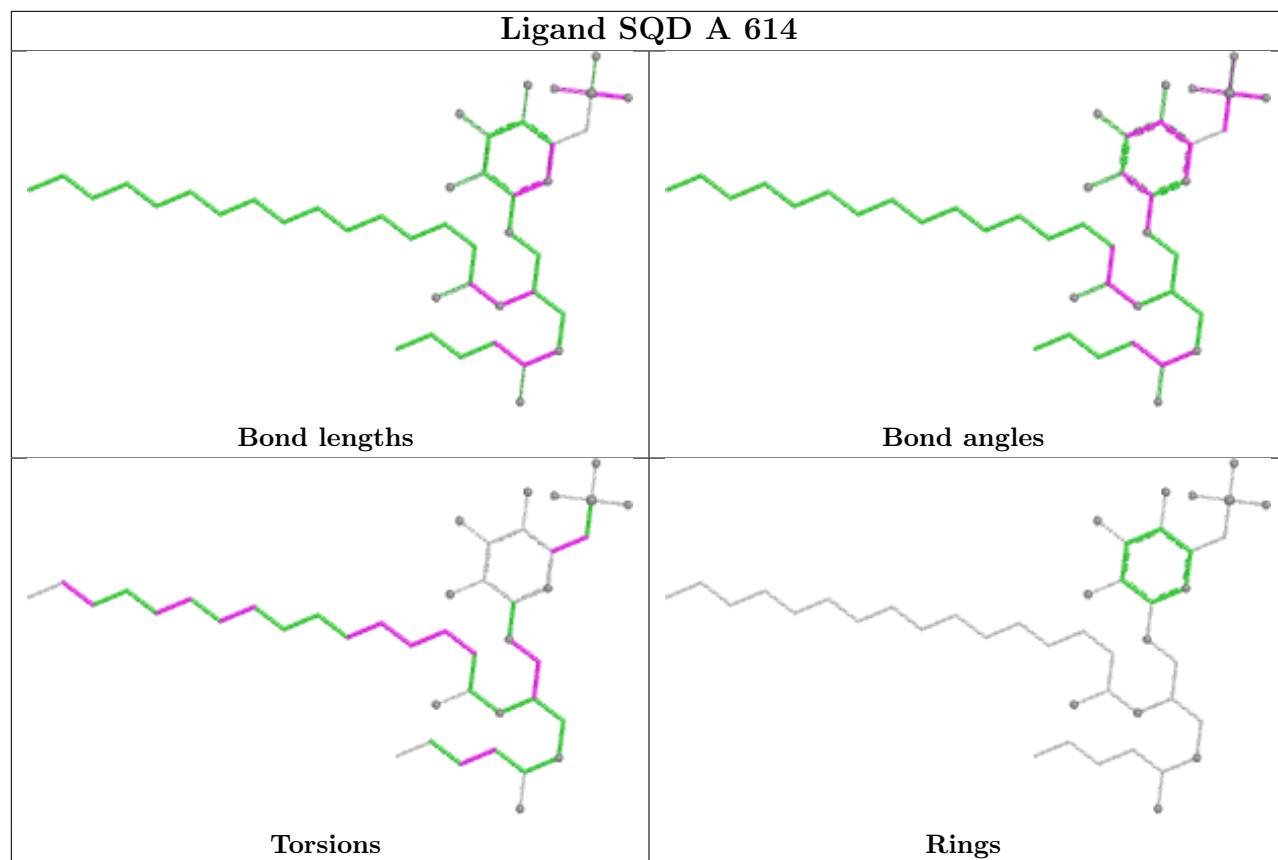




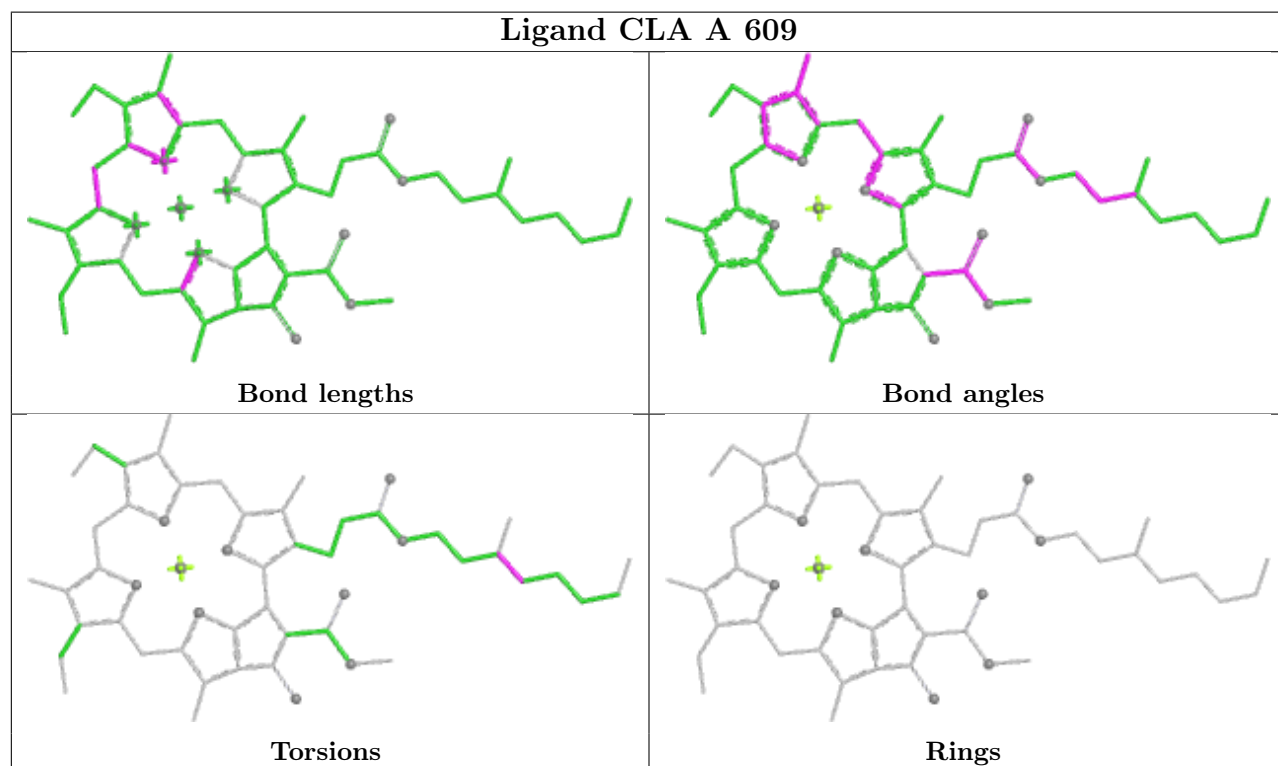




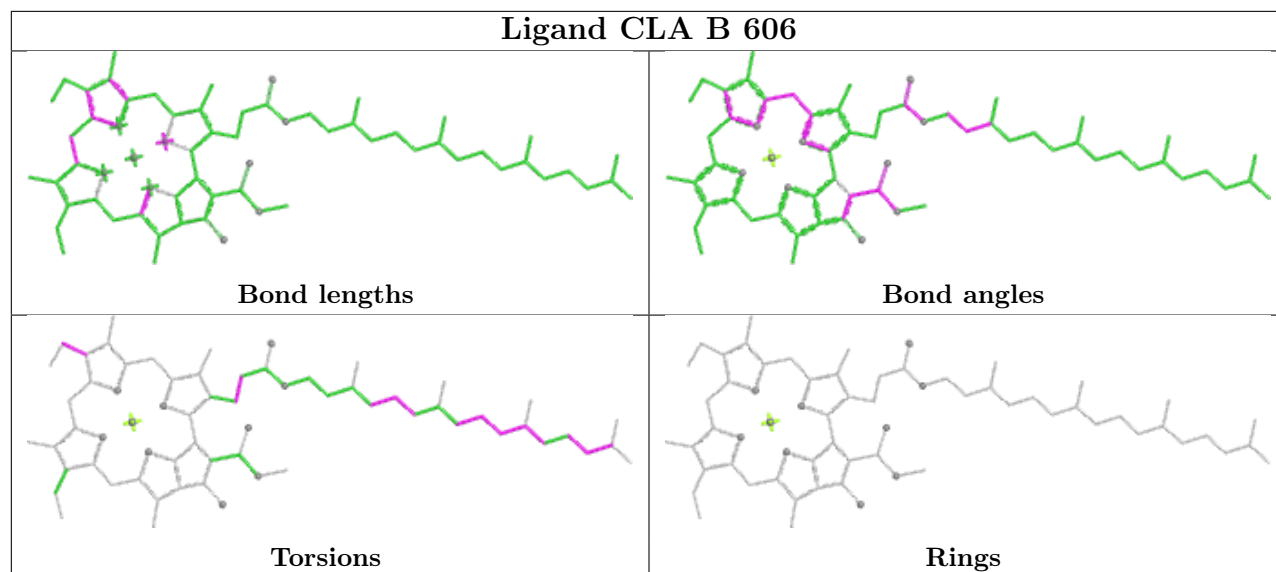
Ligand SQD A 614



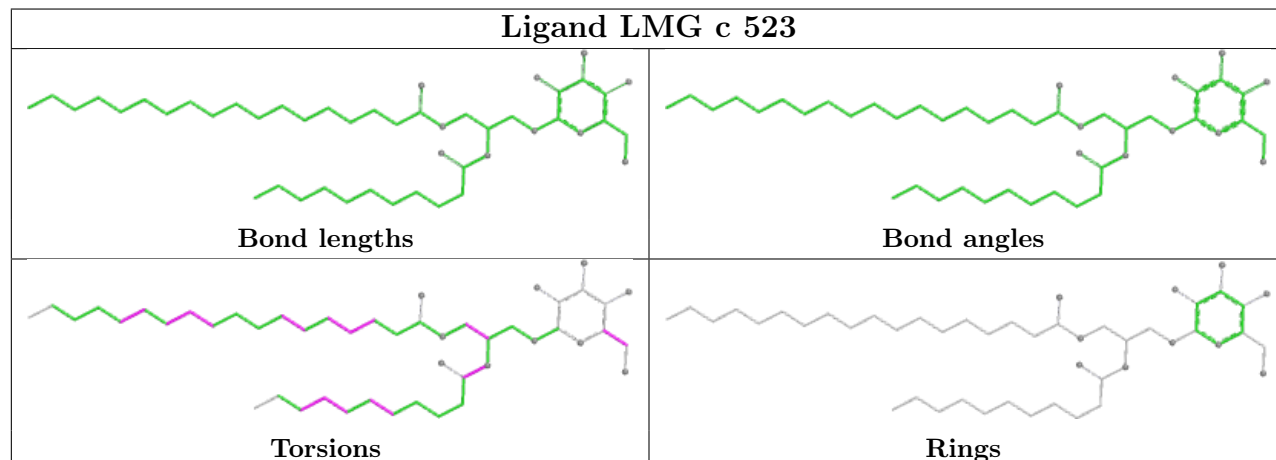
Ligand CLA A 609



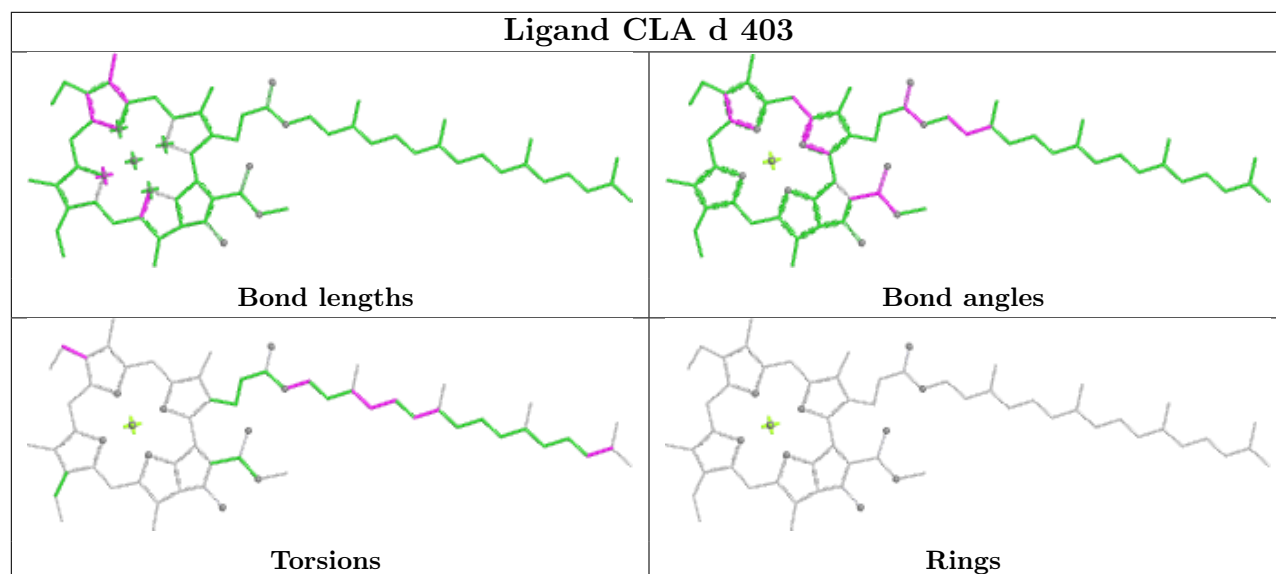
Ligand CLA B 606

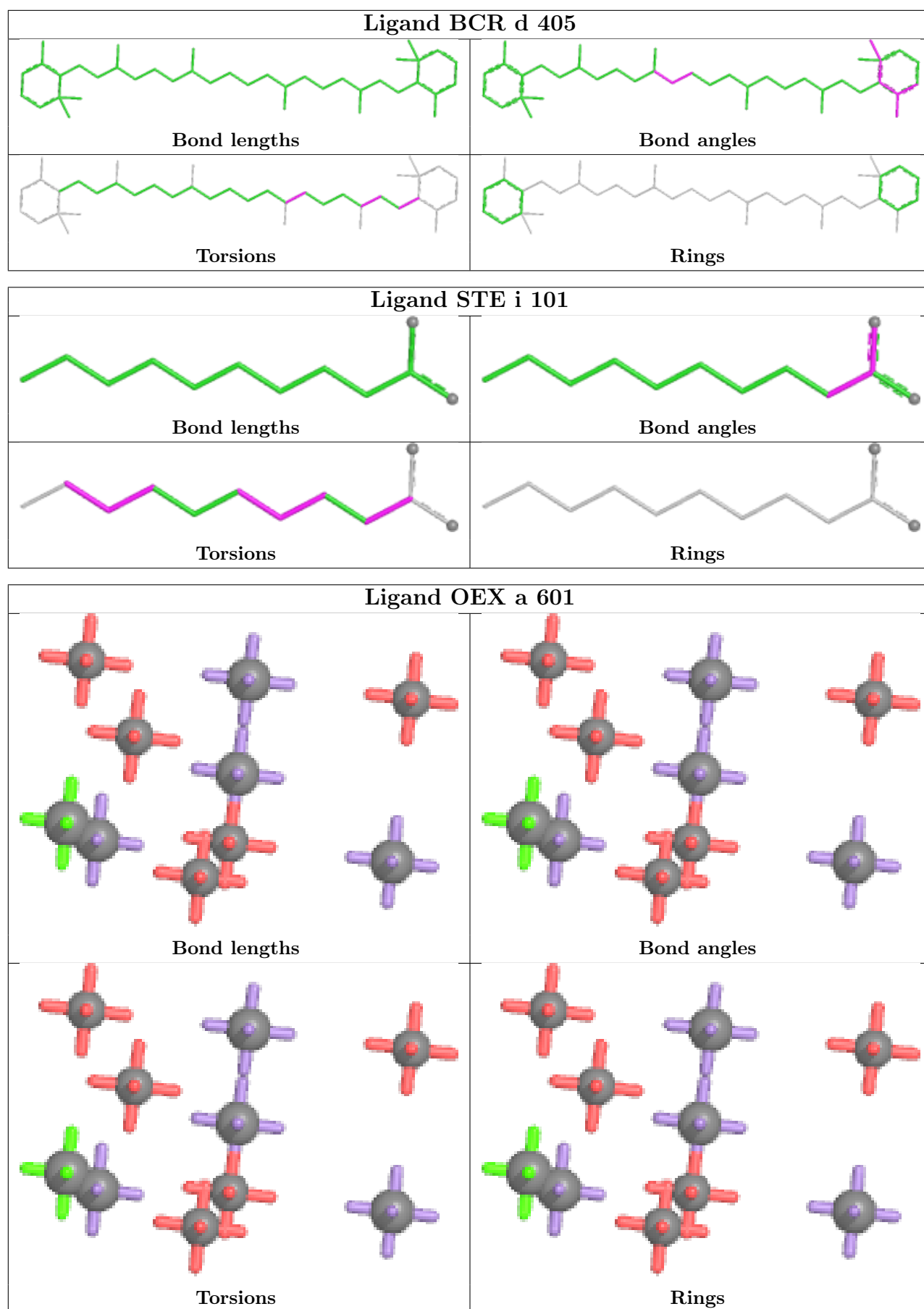


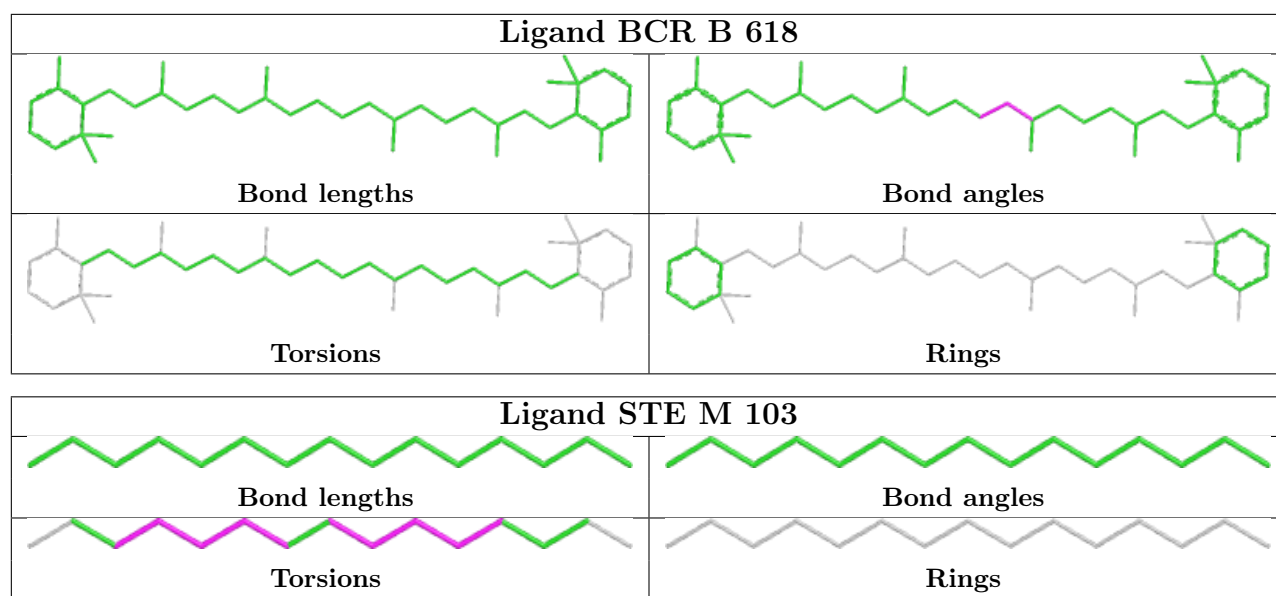
Ligand LMG c 523



Ligand CLA d 403







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.30	3 (0%) 81 86	23, 28, 47, 72	0
1	a	334/344 (97%)	-0.20	4 (1%) 76 83	23, 30, 57, 75	0
2	B	505/510 (99%)	-0.15	5 (0%) 79 86	18, 32, 61, 89	5 (0%)
2	b	505/510 (99%)	0.01	9 (1%) 67 76	26, 36, 69, 108	1 (0%)
3	C	442/461 (95%)	-0.06	1 (0%) 91 94	16, 35, 51, 73	1 (0%)
3	c	451/461 (97%)	0.09	5 (1%) 78 84	22, 40, 60, 90	2 (0%)
4	D	341/352 (96%)	-0.30	0 100 100	22, 30, 47, 77	0
4	d	341/352 (96%)	-0.12	3 (0%) 81 86	23, 34, 60, 78	1 (0%)
5	E	82/84 (97%)	0.62	4 (4%) 35 44	34, 52, 69, 85	1 (1%)
5	e	82/84 (97%)	0.76	3 (3%) 45 55	38, 60, 79, 87	0
6	F	34/45 (75%)	0.32	1 (2%) 53 63	37, 44, 62, 83	0
6	f	34/45 (75%)	0.59	0 100 100	43, 54, 77, 91	0
7	H	65/66 (98%)	0.22	1 (1%) 72 80	34, 40, 57, 73	0
7	h	63/66 (95%)	0.52	2 (3%) 50 60	42, 51, 61, 64	0
8	I	35/38 (92%)	-0.11	1 (2%) 53 63	32, 38, 60, 76	0
8	i	35/38 (92%)	0.19	1 (2%) 53 63	31, 39, 67, 87	0
9	J	36/40 (90%)	0.56	1 (2%) 55 65	36, 50, 80, 93	0
9	j	36/40 (90%)	0.58	0 100 100	41, 56, 85, 89	0
10	K	37/46 (80%)	0.48	0 100 100	42, 51, 67, 74	0
10	k	37/46 (80%)	0.61	0 100 100	49, 57, 70, 83	0
11	L	37/37 (100%)	-0.29	0 100 100	26, 28, 57, 64	0
11	l	36/37 (97%)	-0.33	0 100 100	27, 30, 63, 76	0
12	M	32/36 (88%)	-0.16	0 100 100	27, 32, 54, 73	0
12	m	31/36 (86%)	-0.26	0 100 100	29, 33, 49, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.05	1 (0%) 88 92	25, 41, 75, 120	1 (0%)
13	o	244/272 (89%)	0.14	4 (1%) 70 79	25, 40, 74, 116	0
14	T	29/32 (90%)	-0.32	1 (3%) 48 58	27, 31, 53, 71	0
14	t	29/32 (90%)	-0.22	2 (6%) 23 30	27, 31, 64, 82	0
15	U	97/134 (72%)	0.07	0 100 100	32, 42, 65, 85	0
15	u	97/134 (72%)	-0.03	1 (1%) 79 86	30, 40, 56, 82	0
16	V	137/163 (84%)	-0.04	0 100 100	28, 39, 54, 65	0
16	v	137/163 (84%)	0.25	1 (0%) 84 89	35, 48, 66, 79	0
17	Y	27/46 (58%)	1.50	8 (29%) 1 1	52, 68, 92, 97	0
17	y	30/46 (65%)	1.04	2 (6%) 24 31	61, 72, 82, 96	0
18	X	38/41 (92%)	0.38	3 (7%) 18 25	41, 52, 70, 76	0
18	x	39/41 (95%)	0.61	2 (5%) 33 43	50, 60, 79, 94	0
19	Z	62/62 (100%)	1.05	6 (9%) 13 19	54, 66, 106, 113	0
19	z	62/62 (100%)	1.16	7 (11%) 10 13	61, 74, 110, 124	0
20	R	28/41 (68%)	1.22	4 (14%) 6 8	61, 69, 85, 88	0
20	r	28/41 (68%)	1.95	14 (50%) 0 0	74, 90, 110, 118	0
All	All	5293/5700 (92%)	0.05	100 (1%) 66 75	16, 37, 72, 124	12 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.5
3	c	24	THR	4.3
20	r	28	VAL	4.2
19	z	33	TRP	3.5
7	h	64	ALA	3.5
5	E	79	PHE	3.5
17	Y	25	ILE	3.4
18	x	37	VAL	3.4
1	A	265	PHE	3.4
9	J	5	GLY	3.2
19	Z	33	TRP	3.2
2	B	491	VAL	3.2
3	c	23	ALA	3.1
2	b	495	PHE	3.1
13	o	56	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
14	t	30	THR	3.1
17	Y	22	LEU	3.0
20	r	29	LYS	3.0
7	H	65	LEU	3.0
18	X	2	THR	3.0
1	a	248	ILE	3.0
20	r	14	LEU	2.9
2	B	479[A]	PHE	2.9
13	O	56	PRO	2.9
20	r	3	TRP	2.9
2	b	488	PRO	2.8
17	Y	41	VAL	2.8
3	c	134	ILE	2.8
19	Z	62	VAL	2.7
20	r	8	VAL	2.7
2	b	496	TYR	2.7
17	Y	20	ALA	2.7
19	Z	30	PRO	2.7
2	B	499	VAL	2.7
13	o	63	ALA	2.7
20	r	10	LEU	2.7
2	b	499	VAL	2.7
20	r	12	VAL	2.7
20	r	27	ALA	2.6
2	B	488	PRO	2.6
1	a	11	ALA	2.6
20	R	28	VAL	2.6
18	X	3	ILE	2.6
19	z	29	SER	2.6
20	r	23	ILE	2.5
19	Z	41	PHE	2.5
19	z	40	ILE	2.5
2	b	127	ARG	2.5
5	E	29	ALA	2.5
8	i	36	ASP	2.5
2	b	486	LEU	2.5
20	r	24	LEU	2.5
17	Y	40	ALA	2.5
5	e	79	PHE	2.4
20	R	7	VAL	2.4
3	c	147	PHE	2.4
15	u	53	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
4	d	28	VAL	2.4
19	z	30	PRO	2.3
16	v	21	LEU	2.3
20	R	6	LEU	2.3
19	Z	27	TYR	2.3
2	b	494	GLY	2.3
4	d	55	VAL	2.3
1	A	266	ASN	2.3
1	a	265	PHE	2.3
4	d	97	ALA	2.3
19	z	3	ILE	2.3
20	r	5	VAL	2.3
20	R	3	TRP	2.2
5	E	3	GLY	2.2
19	Z	3	ILE	2.2
18	X	37	VAL	2.2
5	e	4	THR	2.2
17	Y	46	LEU	2.2
3	C	44	ASN	2.2
17	y	22	LEU	2.2
19	z	26	ALA	2.2
20	r	19	ALA	2.2
19	z	39	LEU	2.2
14	t	29	ILE	2.1
14	T	30	THR	2.1
8	I	34	ARG	2.1
20	r	15	ALA	2.1
20	r	18	TRP	2.1
3	c	112	PHE	2.1
5	e	22	ILE	2.1
6	F	13	TYR	2.1
1	a	264	SER	2.1
2	b	491	VAL	2.1
17	Y	21	GLN	2.1
2	b	293	ALA	2.1
2	B	489	GLU	2.0
17	Y	24	MET	2.0
17	y	34	MET	2.0
18	x	2	THR	2.0
7	h	6	TRP	2.0
13	o	98	GLU	2.0
1	A	248	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
5	E	22[A]	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.92	0.11	38,43,54,65	0
14	FME	T	1	10/11	0.92	0.09	29,35,52,63	0
8	FME	I	1	10/11	0.94	0.08	36,42,51,53	0
14	FME	t	1	10/11	0.94	0.07	29,32,49,54	0
8	FME	i	1	10/11	0.96	0.09	39,44,49,49	0
12	FME	m	1	10/11	0.97	0.06	30,42,54,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
28	STE	C	520	10/20	0.59	0.19	54,61,68,74	0
28	STE	i	101	12/20	0.66	0.14	62,79,95,95	0
28	STE	C	529	14/20	0.67	0.20	61,69,80,83	0
28	STE	A	618	11/20	0.67	0.20	53,64,75,76	0
28	STE	i	102	6/20	0.67	0.19	50,62,74,76	0
28	STE	j	102	16/20	0.68	0.20	59,70,88,88	0
28	STE	C	518	5/20	0.69	0.21	50,57,60,62	0
28	STE	E	104	20/20	0.71	0.17	48,67,76,76	0
28	STE	E	103	12/20	0.71	0.19	64,74,95,98	0
31	LMG	D	407	50/55	0.71	0.16	39,64,91,91	0
28	STE	I	101	17/20	0.72	0.16	57,66,78,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	c	517	18/20	0.72	0.19	60,72,83,84	0
27	PL9	a	610	55/55	0.72	0.21	47,66,78,84	0
28	STE	A	617	17/20	0.73	0.14	55,61,68,72	0
28	STE	e	101	9/20	0.73	0.21	67,73,80,81	0
31	LMG	c	518	30/55	0.73	0.17	48,75,82,84	0
33	LHG	E	101	49/49	0.73	0.17	45,75,98,105	0
28	STE	C	516	14/20	0.74	0.18	52,61,67,68	0
27	PL9	A	611	55/55	0.75	0.19	43,62,75,78	0
28	STE	b	625	16/20	0.75	0.21	57,60,83,83	0
31	LMG	C	517	36/55	0.75	0.16	50,58,68,75	0
28	STE	B	626	12/20	0.75	0.16	48,55,72,75	0
28	STE	H	103	18/20	0.75	0.18	57,66,72,73	0
28	STE	H	104	9/20	0.75	0.19	52,61,65,67	0
28	STE	d	413	10/20	0.76	0.18	63,69,75,76	0
31	LMG	a	615	55/55	0.76	0.15	39,55,70,76	0
33	LHG	e	103	42/49	0.76	0.16	51,79,97,102	0
28	STE	A	612	9/20	0.77	0.15	57,58,68,70	0
28	STE	d	414	14/20	0.77	0.16	62,69,81,84	0
28	STE	K	102	14/20	0.77	0.14	52,59,70,75	0
28	STE	B	627	15/20	0.78	0.22	45,59,76,77	0
28	STE	E	102	12/20	0.78	0.17	64,74,79,80	0
30	DGD	A	615	66/66	0.78	0.15	46,58,78,85	0
28	STE	b	621	16/20	0.79	0.19	40,49,76,79	0
31	LMG	B	620	45/55	0.79	0.15	39,51,80,87	0
31	LMG	c	523	48/55	0.79	0.15	51,66,77,81	0
28	STE	C	527	12/20	0.79	0.17	40,48,55,59	0
28	STE	e	105	9/20	0.79	0.19	64,68,74,78	0
28	STE	C	519	7/20	0.80	0.18	51,59,62,64	0
28	STE	e	106	13/20	0.80	0.17	70,76,84,89	0
28	STE	a	617	12/20	0.81	0.13	55,63,73,75	0
31	LMG	b	624	55/55	0.81	0.15	50,62,73,82	0
28	STE	t	102	10/20	0.82	0.14	44,51,57,61	0
28	STE	c	516	13/20	0.83	0.16	62,68,72,74	0
28	STE	e	104	8/20	0.83	0.18	59,60,67,69	0
28	STE	Z	101	17/20	0.83	0.19	46,67,82,84	0
28	STE	d	407	20/20	0.83	0.14	47,53,76,79	0
28	STE	d	410	20/20	0.83	0.14	52,63,83,84	0
28	STE	d	412	20/20	0.83	0.13	40,56,65,71	0
28	STE	B	625	18/20	0.83	0.13	41,49,73,75	0
28	STE	b	627	11/20	0.83	0.20	58,63,67,67	0
28	STE	z	101	9/20	0.83	0.22	59,68,68,70	0
29	SQD	a	614	54/54	0.83	0.13	43,55,83,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	J	101	12/20	0.84	0.13	51,54,65,65	0
28	STE	B	622	17/20	0.84	0.14	35,48,65,67	0
28	STE	b	623	20/20	0.85	0.13	41,52,64,66	0
29	SQD	f	101	41/54	0.85	0.14	59,74,85,89	0
28	STE	I	102	15/20	0.85	0.14	42,48,61,63	0
28	STE	b	626	10/20	0.85	0.14	46,53,60,72	0
24	CLA	b	601	65/65	0.85	0.12	47,64,87,93	0
29	SQD	A	614	43/54	0.85	0.11	38,50,80,85	0
28	STE	j	101	12/20	0.86	0.12	51,57,61,63	0
28	STE	D	413	20/20	0.86	0.13	36,46,73,80	0
28	STE	M	103	15/20	0.86	0.14	44,51,72,72	0
31	LMG	B	621	51/55	0.86	0.12	29,48,58,62	0
28	STE	C	528	16/20	0.87	0.13	40,48,55,61	0
29	SQD	b	620	49/54	0.87	0.11	41,57,72,76	0
28	STE	M	101	15/20	0.87	0.12	37,44,55,67	0
31	LMG	c	522	46/55	0.87	0.12	44,65,74,75	0
31	LMG	C	522	48/55	0.87	0.12	37,55,63,67	0
31	LMG	C	526	48/55	0.87	0.14	47,63,78,83	0
29	SQD	B	623	54/54	0.87	0.11	41,52,66,70	0
28	STE	m	101	12/20	0.88	0.12	45,48,62,67	0
28	STE	A	616	8/20	0.88	0.13	52,55,58,59	0
31	LMG	a	616	49/55	0.89	0.12	38,54,63,71	0
31	LMG	b	622	51/55	0.89	0.10	36,48,58,68	0
28	STE	B	624	14/20	0.89	0.11	41,48,56,62	0
26	BCR	k	101	40/40	0.89	0.11	48,58,65,66	0
28	STE	M	102	10/20	0.89	0.14	44,47,53,59	0
24	CLA	C	513	65/65	0.89	0.11	45,55,78,82	0
24	CLA	B	601	65/65	0.89	0.12	37,50,75,80	0
26	BCR	C	521	40/40	0.89	0.10	40,50,61,62	0
26	BCR	h	101	40/40	0.90	0.11	42,54,62,63	0
26	BCR	C	514	40/40	0.90	0.11	44,53,57,63	0
26	BCR	H	101	40/40	0.90	0.10	33,44,53,55	0
26	BCR	c	514	40/40	0.90	0.12	53,58,63,65	0
29	SQD	a	613	54/54	0.90	0.11	37,58,73,77	0
28	STE	m	102	18/20	0.90	0.12	34,41,65,65	0
30	DGD	h	102	62/66	0.91	0.10	34,46,54,56	0
24	CLA	c	513	65/65	0.91	0.11	50,63,80,86	0
24	CLA	C	512	65/65	0.91	0.10	43,47,73,79	0
26	BCR	d	405	40/40	0.91	0.10	40,49,74,76	0
24	CLA	c	512	65/65	0.91	0.11	48,53,76,77	0
29	SQD	D	409	36/54	0.91	0.13	49,69,77,80	0
30	DGD	C	524	62/66	0.91	0.10	32,46,86,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DGD	H	102	62/66	0.91	0.10	31,42,51,54	0
29	SQD	A	613	52/54	0.92	0.10	29,50,70,80	0
26	BCR	D	405	40/40	0.92	0.11	34,45,79,83	0
24	CLA	c	503	65/65	0.92	0.09	35,43,47,54	0
30	DGD	c	520	62/66	0.92	0.09	37,47,74,76	0
26	BCR	k	102	40/40	0.92	0.12	44,51,61,68	0
26	BCR	C	515	40/40	0.93	0.10	27,36,45,48	0
24	CLA	b	606	65/65	0.93	0.09	27,35,60,67	0
24	CLA	C	511	65/65	0.93	0.10	35,46,57,61	0
24	CLA	c	511	65/65	0.93	0.11	40,52,63,67	0
31	LMG	D	408	51/55	0.93	0.12	31,49,68,71	0
26	BCR	K	101	40/40	0.93	0.10	41,47,58,62	0
26	BCR	b	619	40/40	0.93	0.09	32,39,55,56	0
24	CLA	C	503	65/65	0.93	0.08	32,39,44,50	0
26	BCR	c	515	40/40	0.93	0.10	32,43,51,53	0
24	CLA	C	508	65/65	0.93	0.09	31,36,82,92	0
30	DGD	c	521	62/66	0.93	0.09	31,49,67,74	0
26	BCR	B	618	40/40	0.93	0.07	25,33,40,46	0
31	LMG	d	411	44/55	0.93	0.10	38,49,73,81	0
32	BCT	d	401	4/4	0.93	0.08	34,38,44,45	0
26	BCR	B	619	40/40	0.93	0.08	27,38,48,52	0
33	LHG	d	408	49/49	0.93	0.11	34,46,58,60	0
24	CLA	C	510	65/65	0.93	0.08	32,38,50,58	0
24	CLA	c	504	60/65	0.94	0.08	28,42,65,69	0
25	PHO	d	402	64/64	0.94	0.07	30,38,42,48	0
26	BCR	A	610	40/40	0.94	0.07	26,33,38,38	0
27	PL9	d	406	55/55	0.94	0.07	27,32,39,39	0
30	DGD	C	525	62/66	0.94	0.09	31,40,63,77	0
26	BCR	T	101	40/40	0.94	0.07	28,34,44,45	0
26	BCR	b	617	40/40	0.94	0.07	28,36,41,46	0
26	BCR	b	618	40/40	0.94	0.07	25,35,43,47	0
26	BCR	B	617	40/40	0.94	0.07	27,35,40,42	0
24	CLA	c	507	65/65	0.94	0.08	33,40,51,54	0
32	BCT	D	401	4/4	0.94	0.10	28,35,35,38	0
24	CLA	c	508	64/65	0.94	0.09	34,42,77,86	0
33	LHG	D	411	47/49	0.94	0.10	29,40,66,70	0
33	LHG	D	412	49/49	0.94	0.10	27,39,55,58	0
24	CLA	c	509	65/65	0.94	0.10	35,45,55,57	0
33	LHG	a	612	39/49	0.94	0.10	34,42,61,68	0
24	CLA	C	502	65/65	0.94	0.08	29,35,49,52	0
24	CLA	B	606	65/65	0.94	0.08	22,31,55,64	0
24	CLA	b	608	65/65	0.95	0.07	32,38,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	b	609	65/65	0.95	0.08	35,41,55,64	0
24	CLA	b	610	65/65	0.95	0.08	27,34,41,45	0
25	PHO	A	607	64/64	0.95	0.06	21,27,31,34	0
25	PHO	A	608	64/64	0.95	0.07	24,31,35,40	0
25	PHO	a	607	64/64	0.95	0.06	23,28,33,36	0
24	CLA	b	614	65/65	0.95	0.08	26,33,65,69	0
24	CLA	b	615	65/65	0.95	0.08	26,36,53,60	0
24	CLA	b	616	60/65	0.95	0.09	31,37,80,85	0
26	BCR	t	101	40/40	0.95	0.07	27,33,44,46	0
24	CLA	c	502	65/65	0.95	0.07	33,39,53,59	0
27	PL9	D	406	55/55	0.95	0.07	20,29,37,39	0
24	CLA	a	605	65/65	0.95	0.07	21,27,37,48	0
24	CLA	a	606	65/65	0.95	0.09	29,36,84,89	0
24	CLA	c	505	65/65	0.95	0.08	29,37,53,61	0
30	DGD	C	523	62/66	0.95	0.08	25,36,62,66	0
24	CLA	c	506	65/65	0.95	0.09	34,41,73,75	0
24	CLA	a	608	65/65	0.95	0.09	21,27,64,72	0
24	CLA	C	506	65/65	0.95	0.09	31,39,69,73	0
30	DGD	c	519	62/66	0.95	0.09	25,37,60,68	0
24	CLA	C	504	59/65	0.95	0.08	32,38,73,77	0
24	CLA	c	510	65/65	0.95	0.08	35,44,55,61	0
26	BCR	a	609	40/40	0.95	0.06	23,30,39,41	0
33	LHG	l	101	49/49	0.95	0.08	31,41,47,56	0
24	CLA	A	606	65/65	0.96	0.09	21,31,77,85	0
24	CLA	B	607	65/65	0.96	0.07	20,26,47,53	0
24	CLA	B	608	65/65	0.96	0.06	24,30,48,53	0
24	CLA	B	609	65/65	0.96	0.07	25,35,48,56	0
24	CLA	D	402	65/65	0.96	0.06	21,26,40,49	0
24	CLA	D	403	65/65	0.96	0.06	21,26,44,52	0
24	CLA	D	404	65/65	0.96	0.08	27,33,102,109	0
24	CLA	B	610	65/65	0.96	0.07	22,28,35,39	0
24	CLA	d	403	65/65	0.96	0.07	23,28,49,56	0
24	CLA	d	404	65/65	0.96	0.08	30,38,72,75	0
24	CLA	B	611	65/65	0.96	0.06	20,26,42,48	0
24	CLA	B	612	65/65	0.96	0.07	21,27,39,45	0
24	CLA	a	611	65/65	0.96	0.06	20,28,40,46	0
24	CLA	B	614	65/65	0.96	0.07	24,30,59,65	0
24	CLA	b	602	65/65	0.96	0.08	29,36,53,55	0
24	CLA	b	603	65/65	0.96	0.08	24,31,56,65	0
24	CLA	b	604	65/65	0.96	0.08	24,31,58,71	0
24	CLA	b	605	65/65	0.96	0.07	22,31,43,44	0
24	CLA	B	615	65/65	0.96	0.07	24,30,47,51	0

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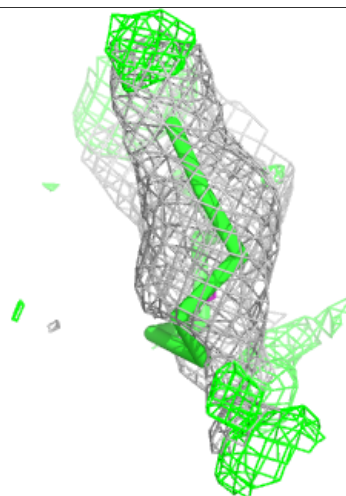
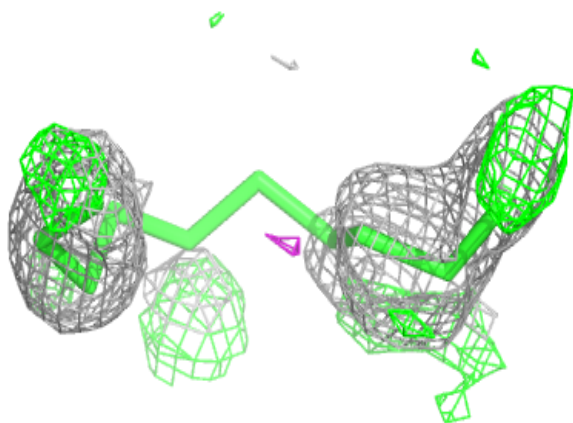
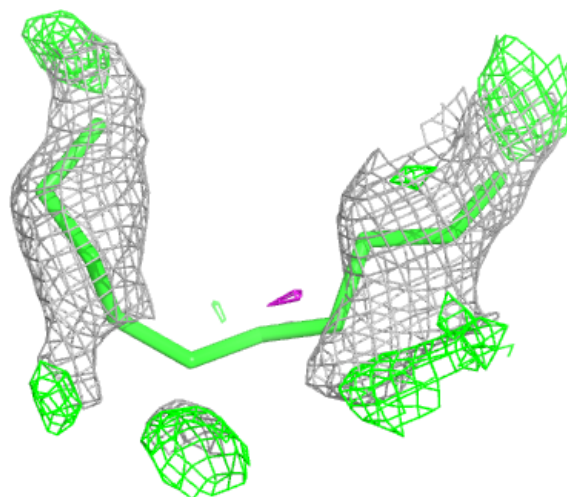
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	b	607	65/65	0.96	0.08	22,30,50,58	0
24	CLA	B	616	60/65	0.96	0.08	24,32,71,75	0
24	CLA	C	501	65/65	0.96	0.07	26,31,45,48	0
24	CLA	A	605	65/65	0.96	0.06	19,25,39,43	0
24	CLA	b	611	65/65	0.96	0.06	25,31,44,49	0
24	CLA	b	612	65/65	0.96	0.07	23,31,39,44	0
24	CLA	b	613	65/65	0.96	0.08	21,28,61,66	0
24	CLA	B	602	65/65	0.96	0.07	25,31,50,55	0
24	CLA	B	603	65/65	0.96	0.07	22,27,53,56	0
24	CLA	C	505	65/65	0.96	0.08	25,33,56,62	0
24	CLA	c	501	65/65	0.96	0.07	29,36,44,49	0
33	LHG	L	101	49/49	0.96	0.07	30,37,46,59	0
24	CLA	B	604	65/65	0.96	0.08	20,27,58,61	0
24	CLA	C	507	65/65	0.96	0.07	26,35,54,58	0
33	LHG	d	409	49/49	0.96	0.08	28,37,47,54	0
24	CLA	B	605	65/65	0.96	0.06	21,27,39,40	0
24	CLA	C	509	65/65	0.96	0.08	30,38,55,58	0
34	HEM	F	101	43/43	0.96	0.09	40,47,54,64	0
24	CLA	A	609	54/65	0.97	0.06	20,26,51,56	0
33	LHG	D	410	49/49	0.97	0.07	25,36,45,48	0
24	CLA	B	613	65/65	0.97	0.06	21,26,54,59	0
34	HEM	e	102	43/43	0.97	0.09	54,59,71,78	0
23	CL	A	603	1/1	0.98	0.04	27,27,27,27	0
35	HEC	V	201	43/43	0.98	0.06	25,29,35,43	0
35	HEC	v	201	43/43	0.98	0.06	31,35,42,46	0
21	OEX	a	601	10/10	0.99	0.02	27,28,32,34	0
22	FE2	A	602	1/1	0.99	0.04	32,32,32,32	0
22	FE2	a	602	1/1	0.99	0.02	37,37,37,37	0
21	OEX	A	601	10/10	0.99	0.03	24,28,31,32	0
23	CL	A	604	1/1	0.99	0.05	27,27,27,27	0
23	CL	a	603	1/1	0.99	0.05	29,29,29,29	0
23	CL	a	604	1/1	0.99	0.08	29,29,29,29	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.

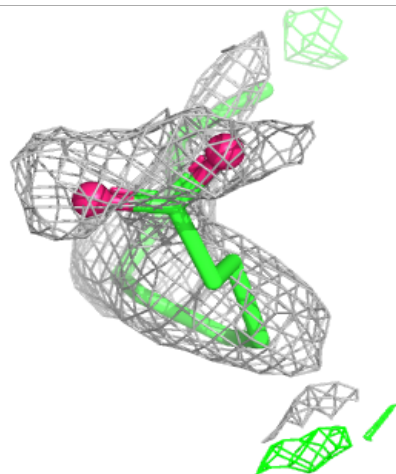
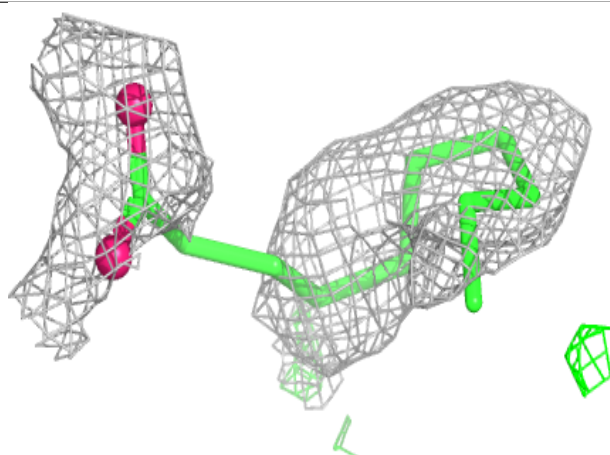
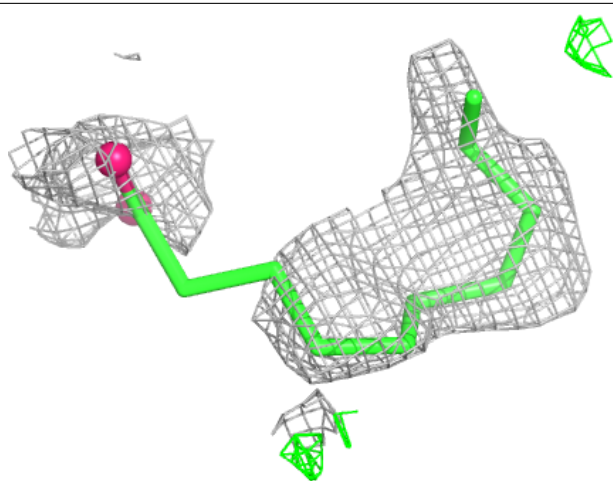
Electron density around STE C 520:

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



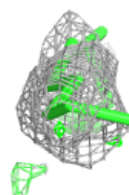
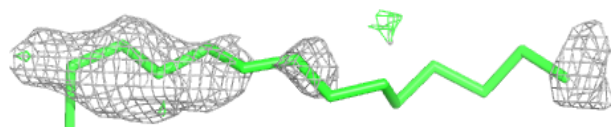
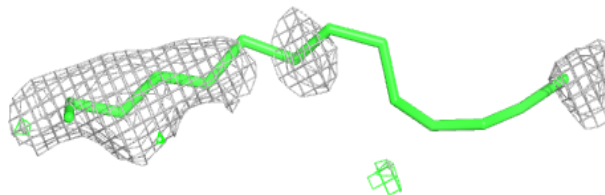
Electron density around STE i 101:

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

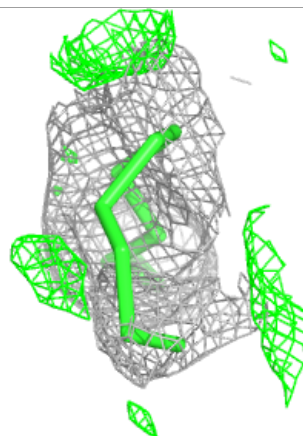
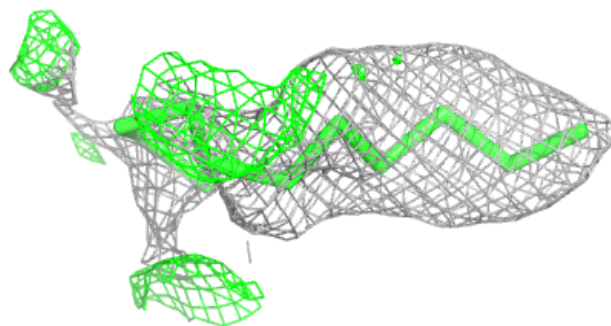
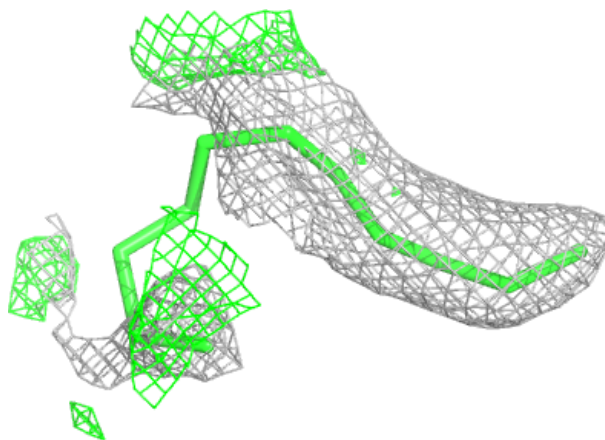


Electron density around STE C 529:

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

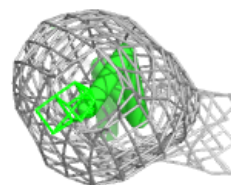
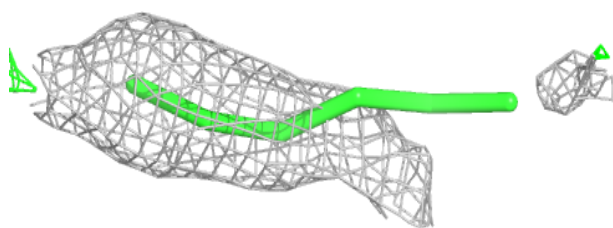
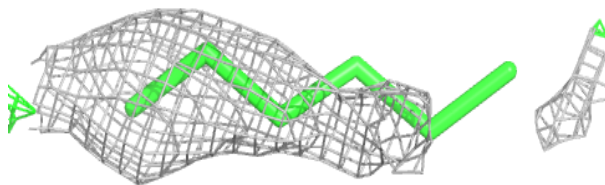
**Electron density around STE A 618:**

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

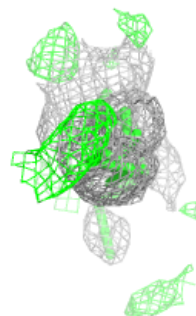
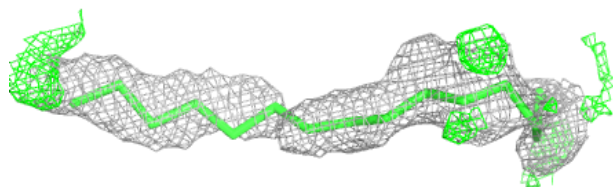
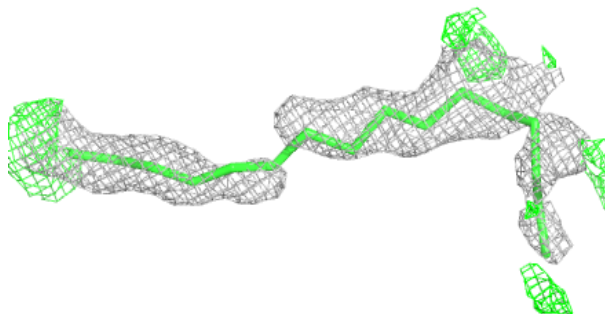


Electron density around STE i 102:

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

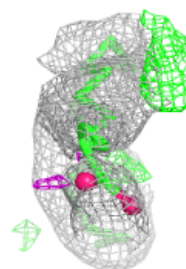
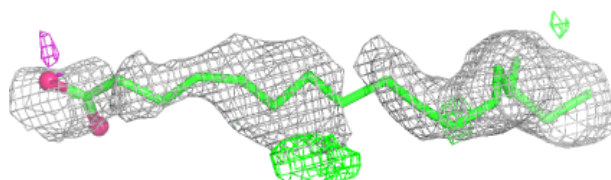
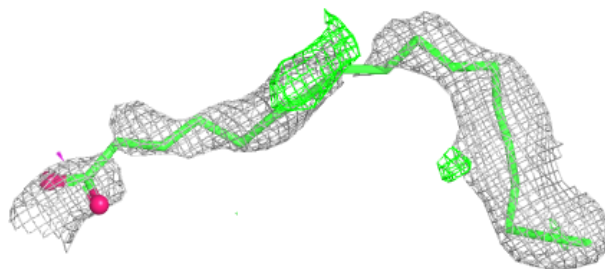
**Electron density around STE j 102:**

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

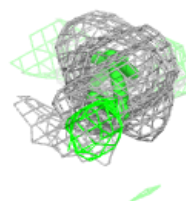
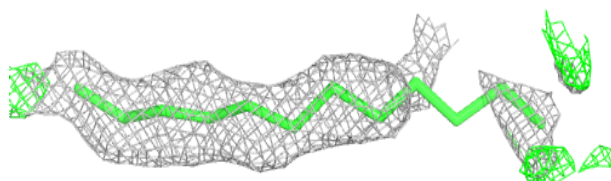
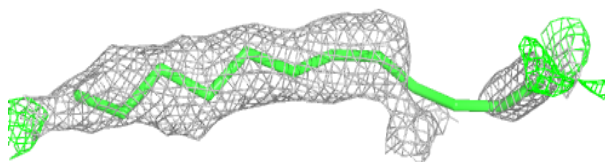


Electron density around STE E 104:

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

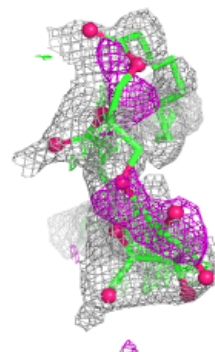
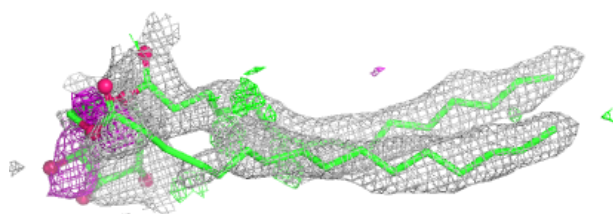
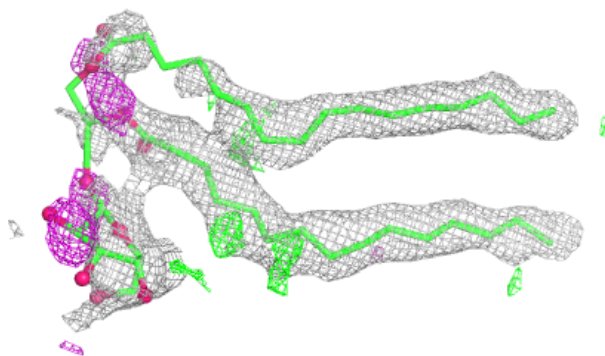
**Electron density around STE E 103:**

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

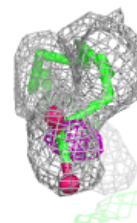
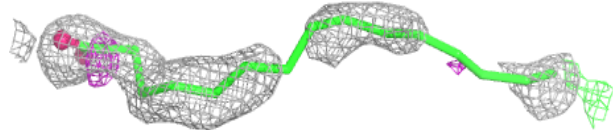
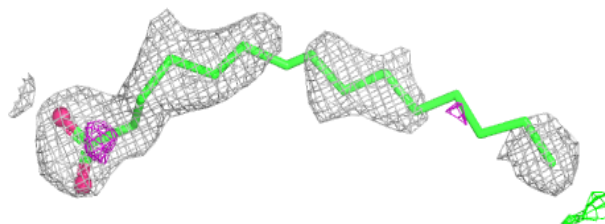


Electron density around LMG D 407:

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

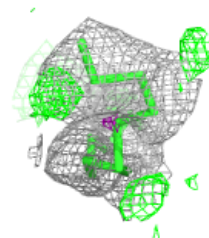
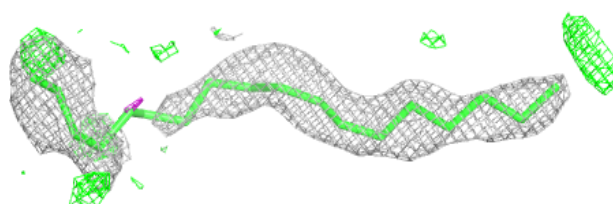
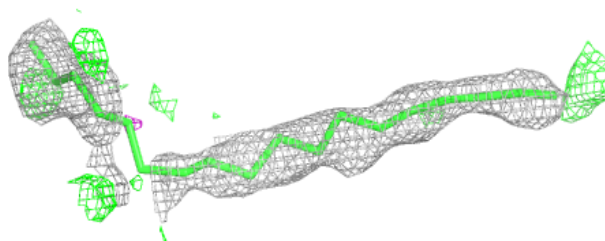
**Electron density around STE I 101:**

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

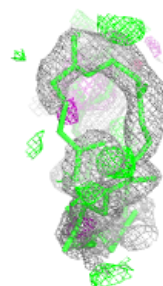
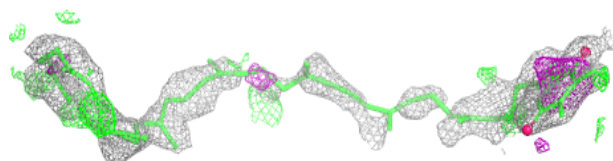
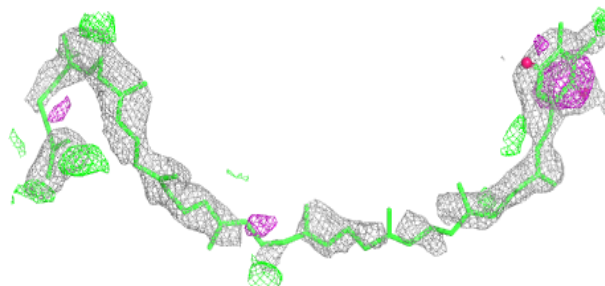


Electron density around STE c 517:

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and green (positive)

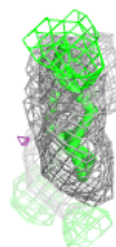
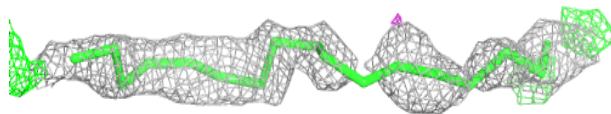
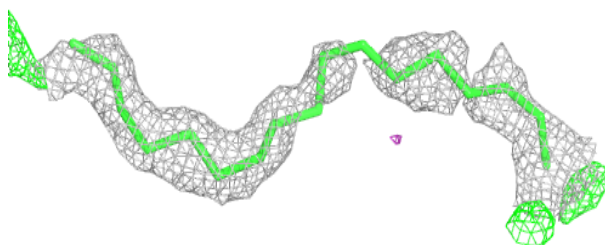
**Electron density around PL9 a 610:**

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

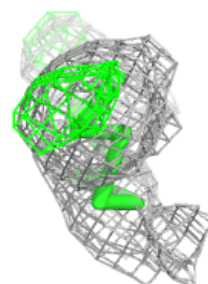
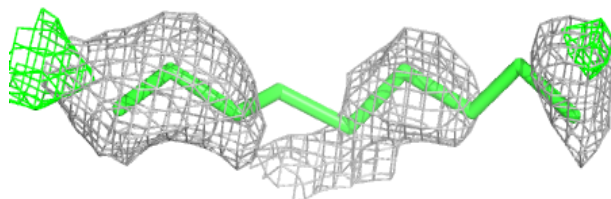
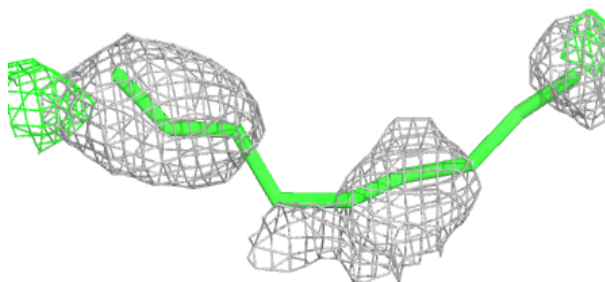


Electron density around STE A 617:

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and green (positive)

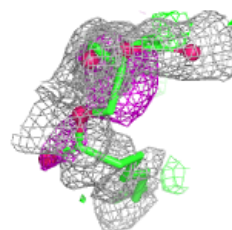
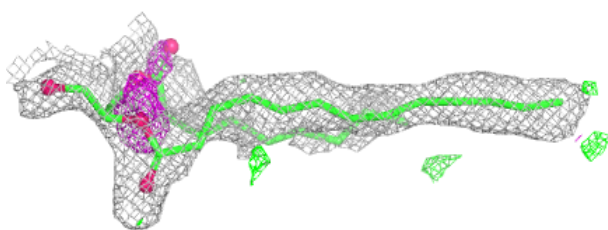
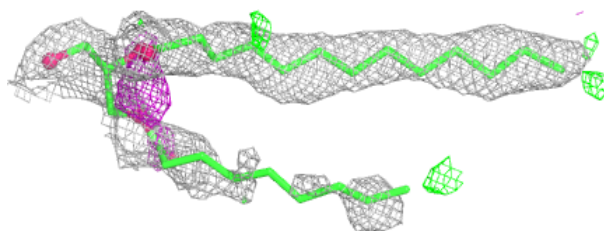
**Electron density around STE e 101:**

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

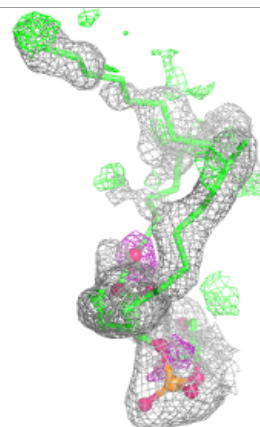
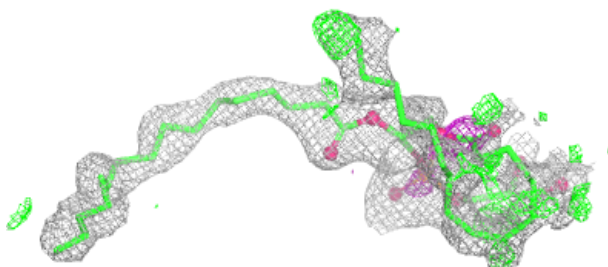
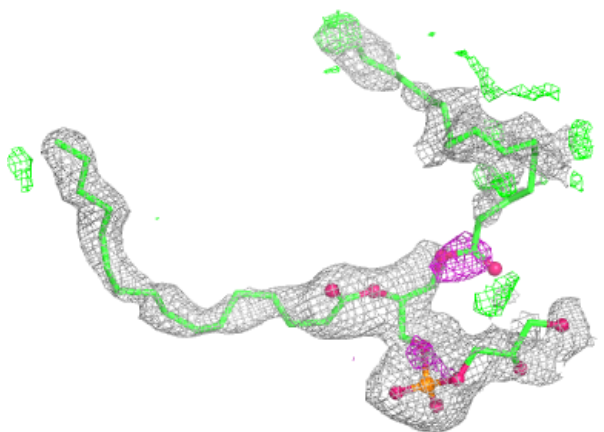


Electron density around LMG c 518:

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

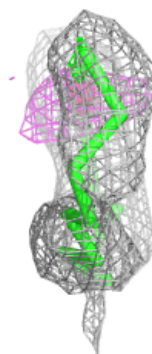
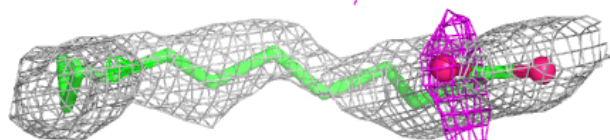
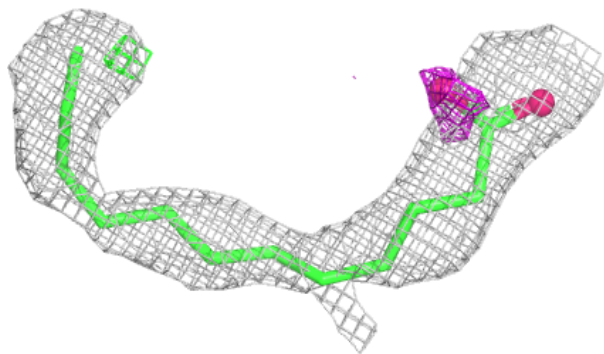
**Electron density around LHG E 101:**

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

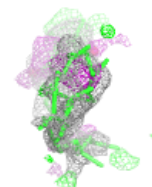
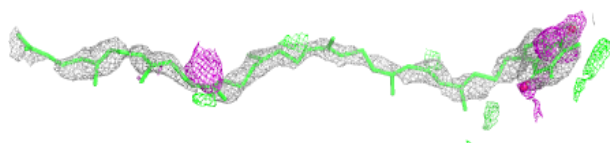
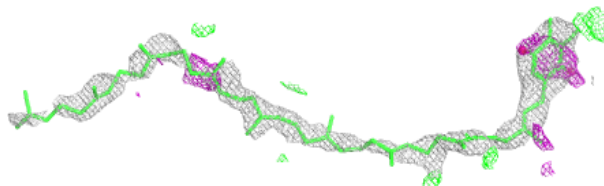


Electron density around STE C 516:

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

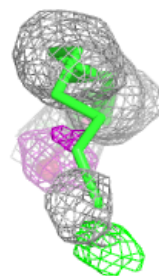
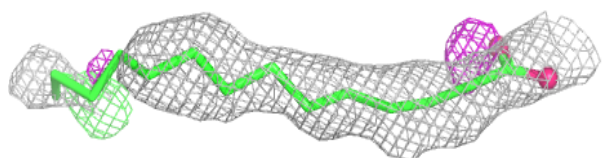
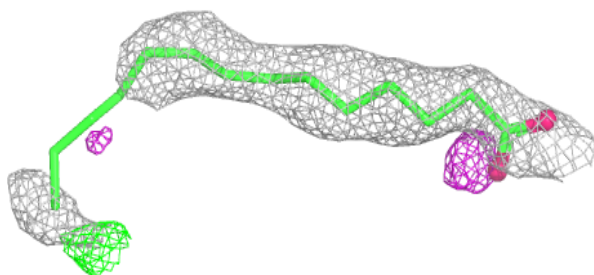
**Electron density around PL9 A 611:**

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

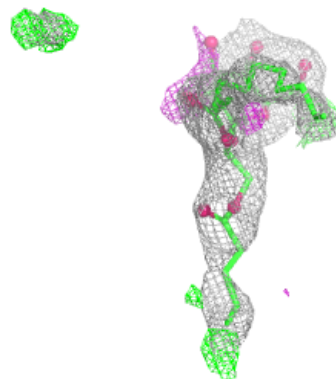
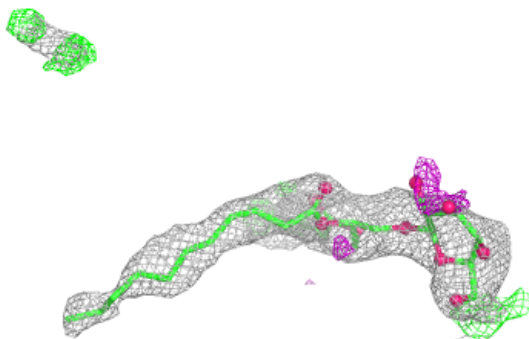
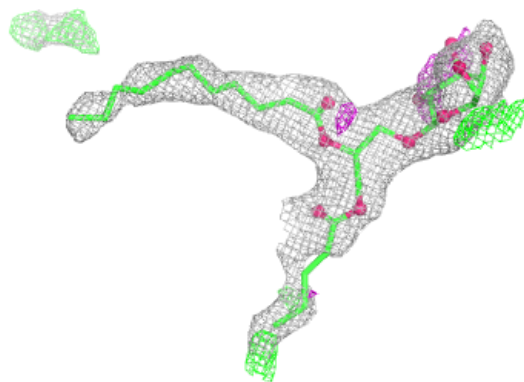


Electron density around STE b 625:

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

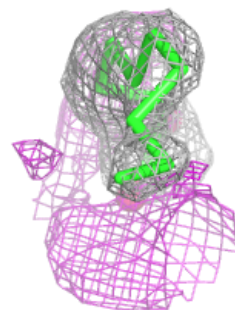
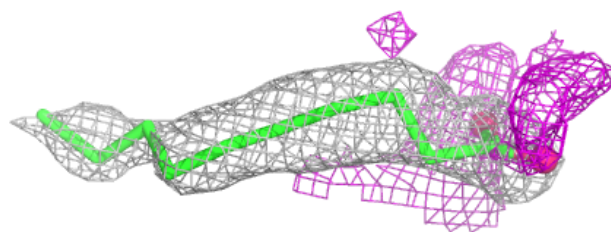
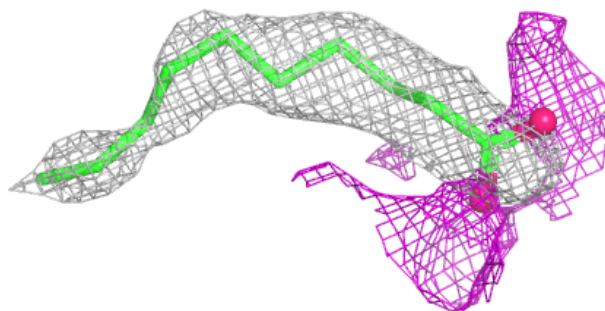
**Electron density around LMG C 517:**

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

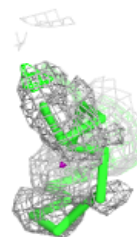
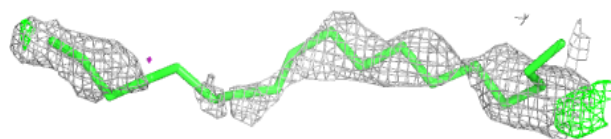
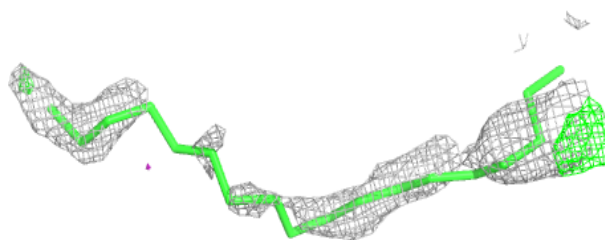


Electron density around STE B 626:

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

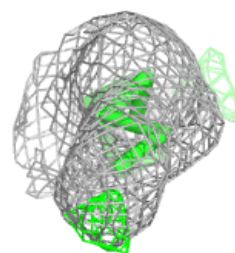
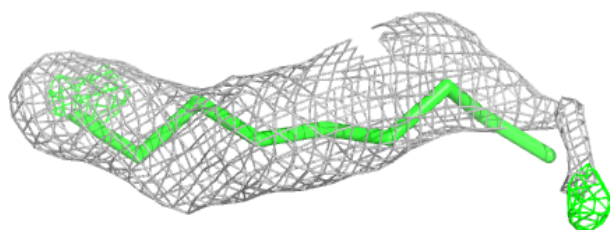
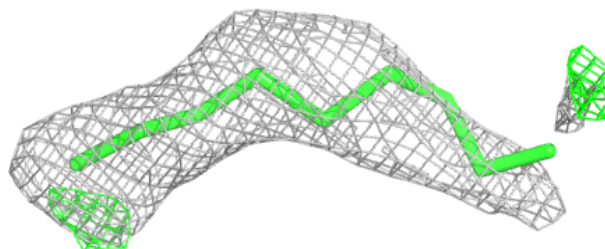
**Electron density around STE H 103:**

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

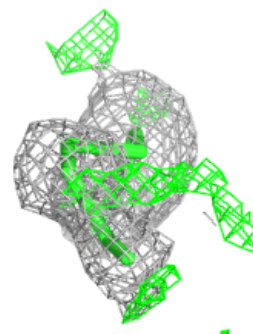
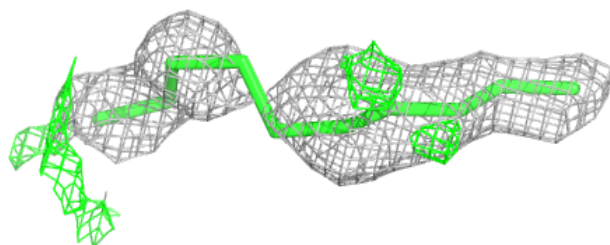
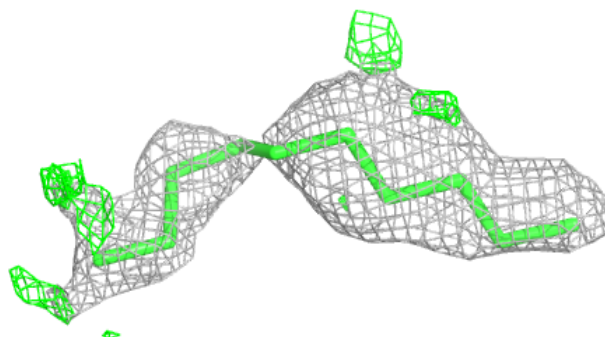


Electron density around STE H 104:

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

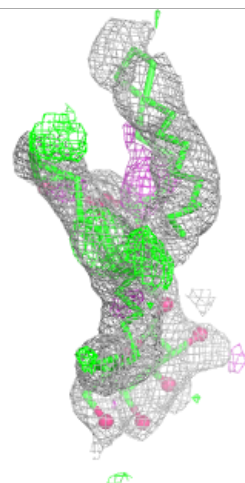
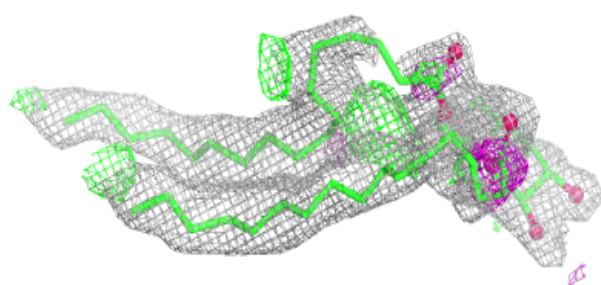
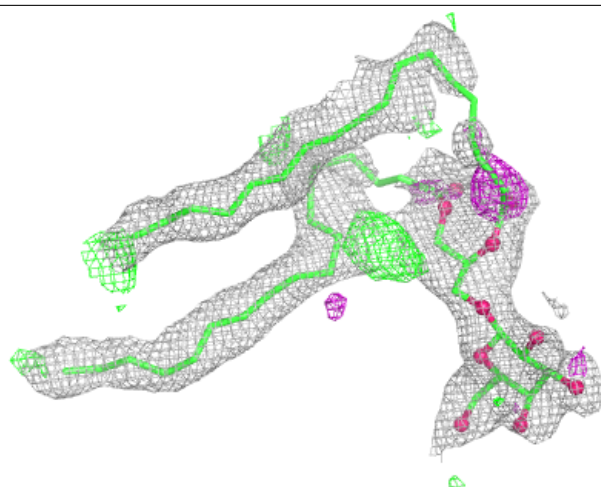
**Electron density around STE d 413:**

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



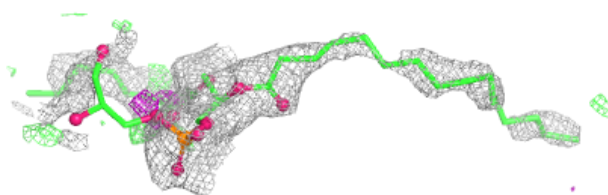
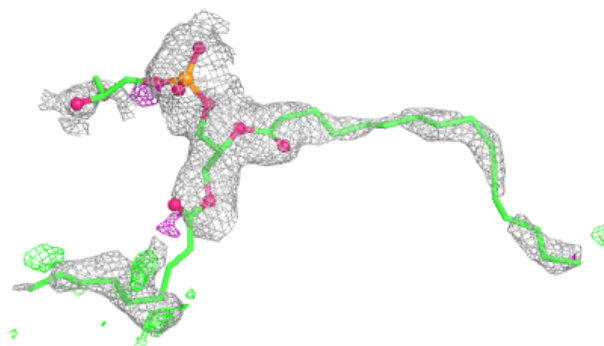
Electron density around LMG a 615:

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

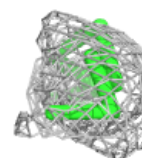
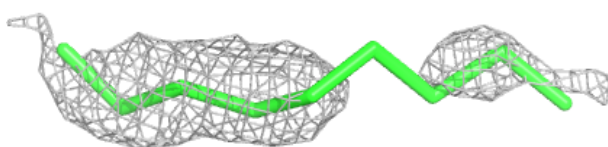
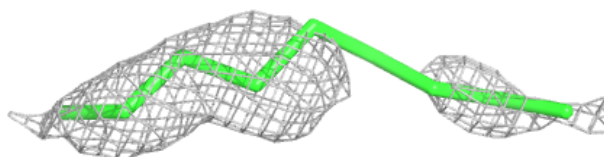


Electron density around LHG e 103:

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

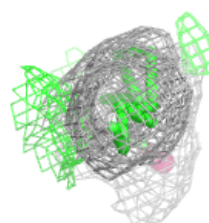
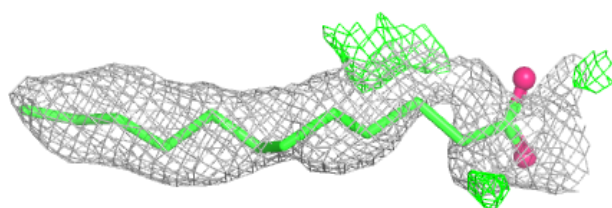
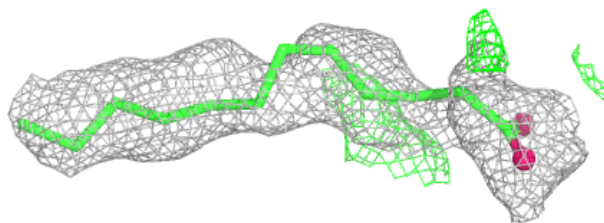
**Electron density around STE A 612:**

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

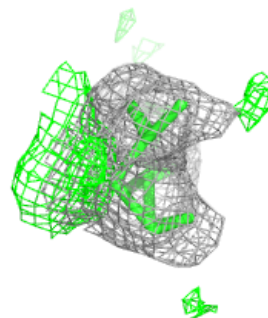
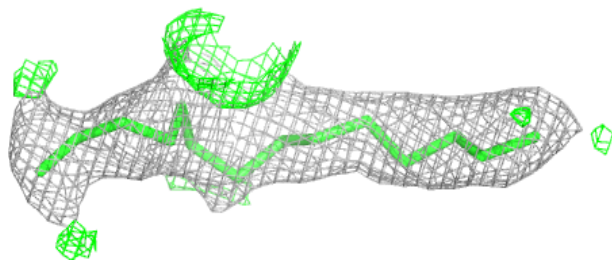
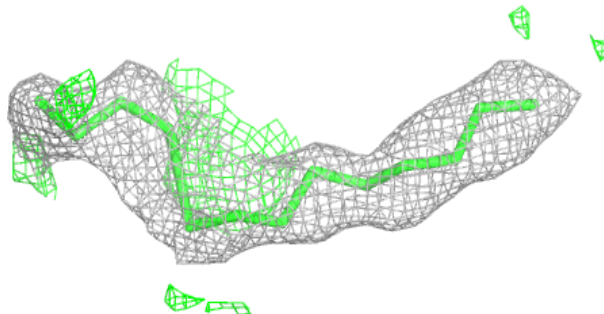


Electron density around STE d 414:

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

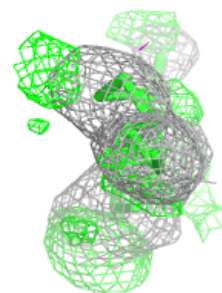
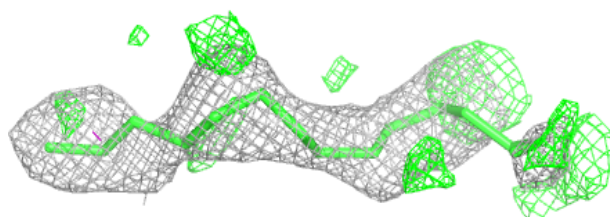
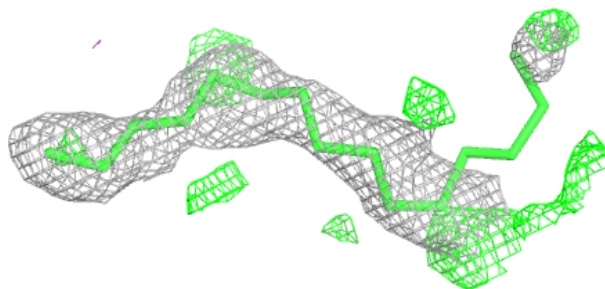
**Electron density around STE K 102:**

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

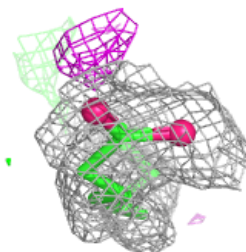
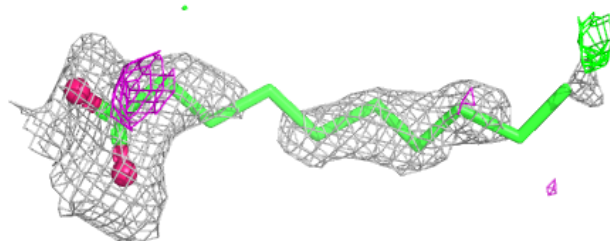
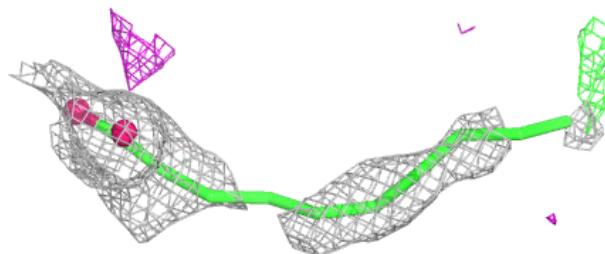


Electron density around STE B 627:

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

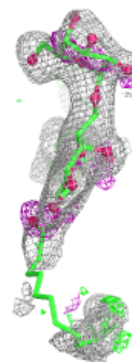
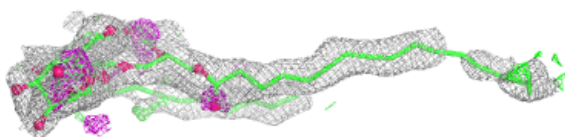
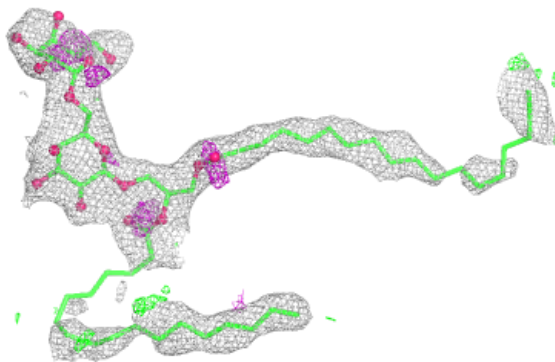
**Electron density around STE E 102:**

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

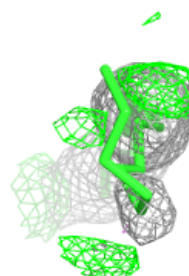
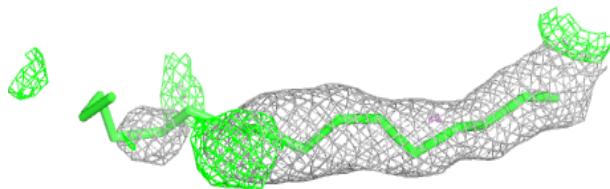
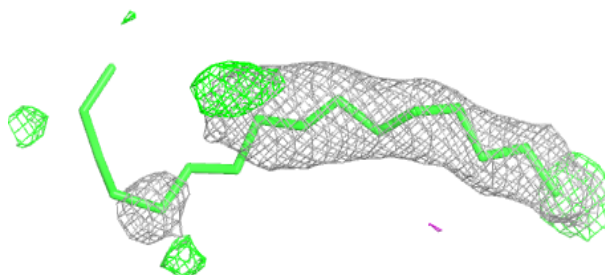


Electron density around DGD A 615:

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

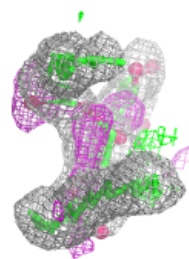
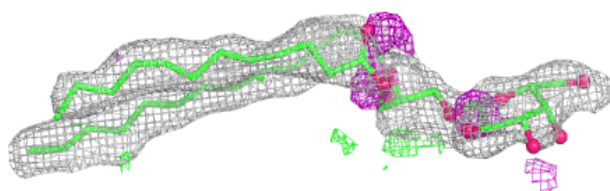
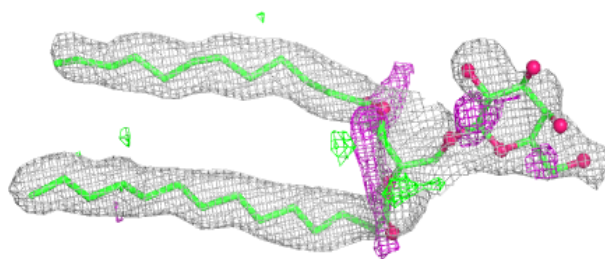
**Electron density around STE b 621:**

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

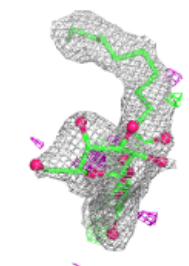
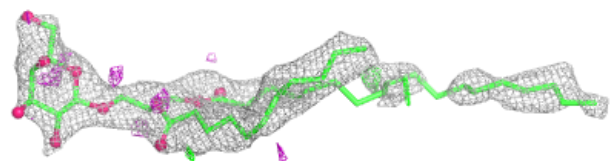
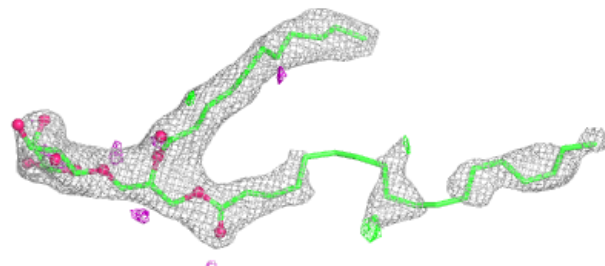


Electron density around LMG B 620:

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

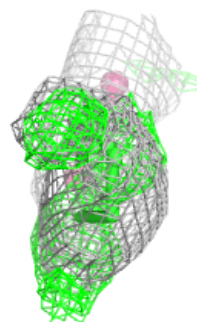
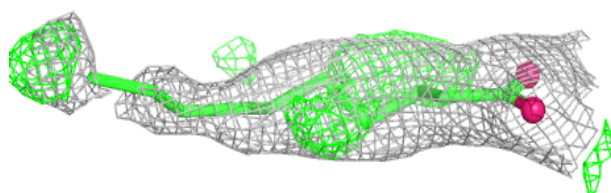
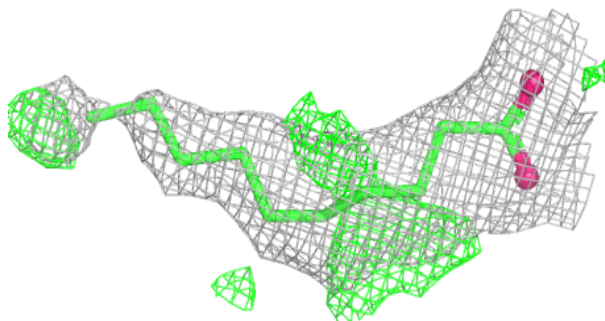
**Electron density around LMG c 523:**

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

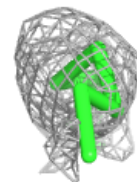
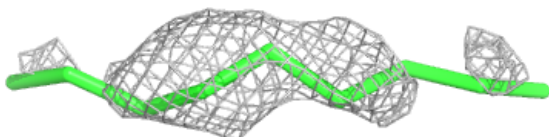
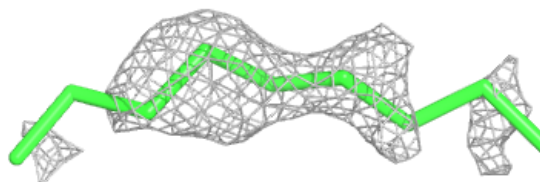


Electron density around STE C 527:

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

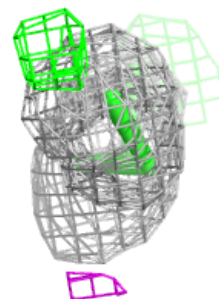
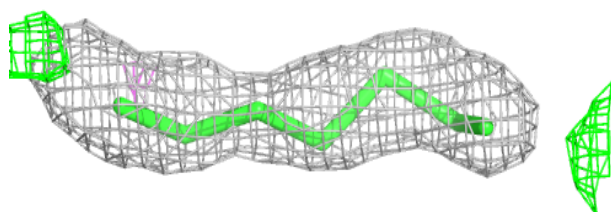
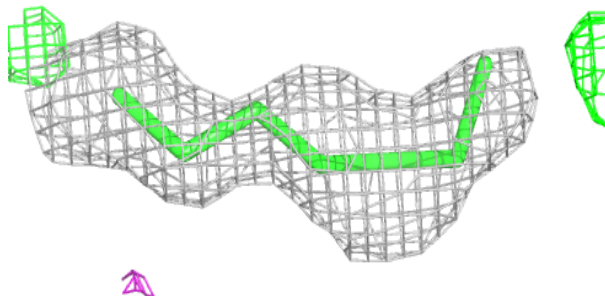
**Electron density around STE e 105:**

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

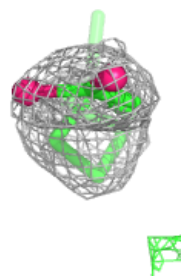
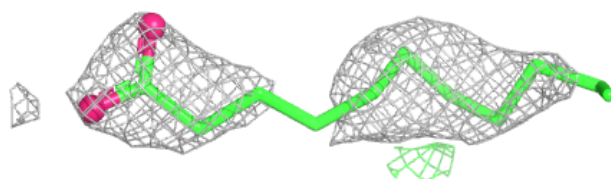
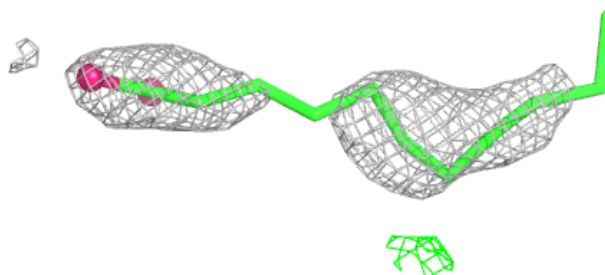


Electron density around STE C 519:

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

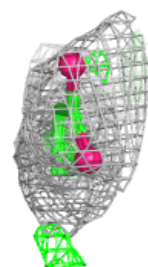
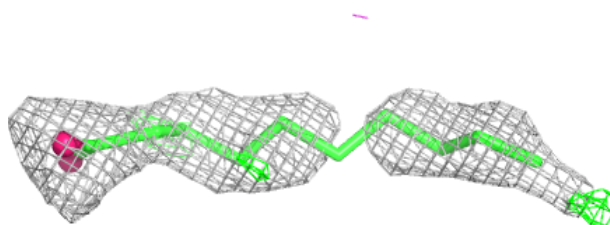
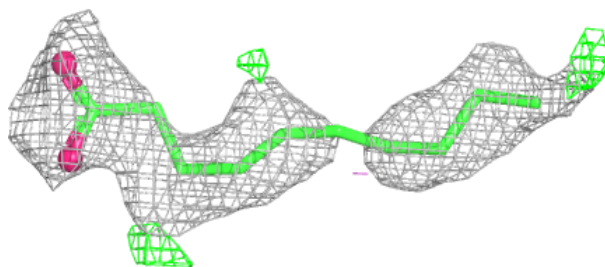
**Electron density around STE e 106:**

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

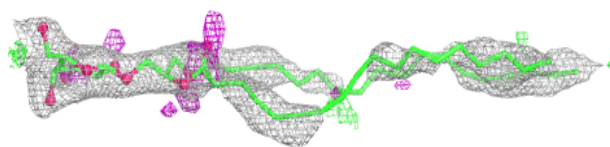
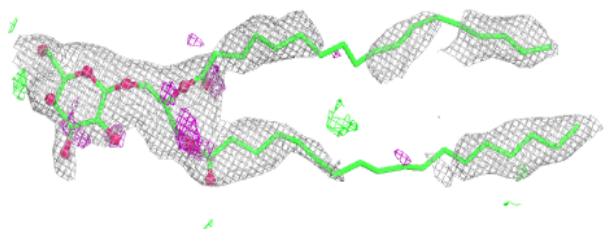


Electron density around STE a 617:

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

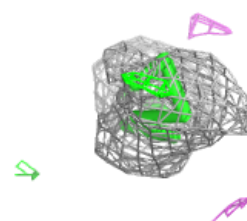
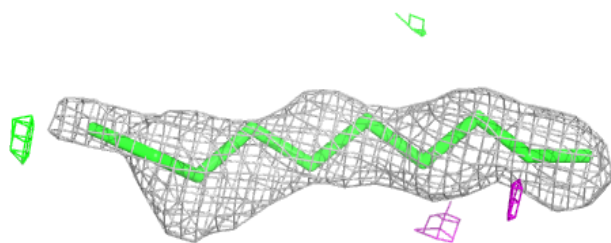
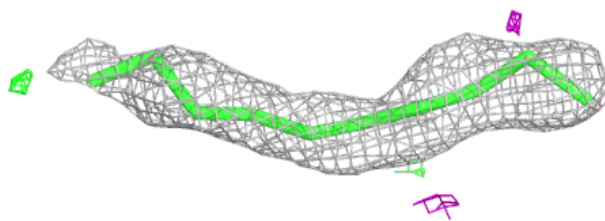
**Electron density around LMG b 624:**

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

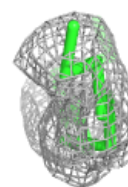
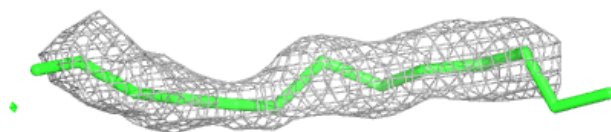
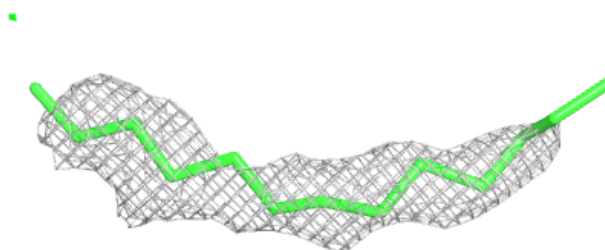


Electron density around STE t 102:

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

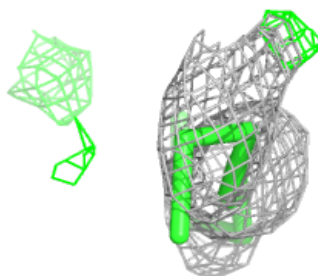
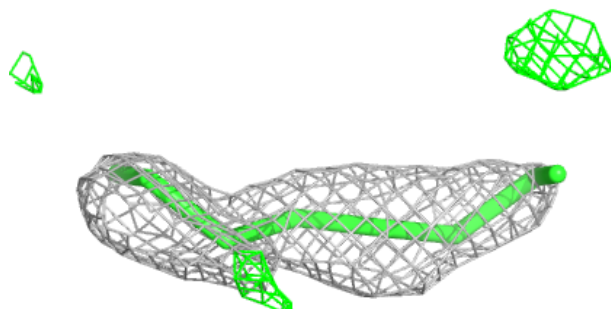
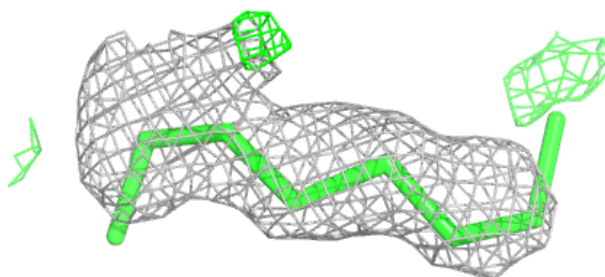
**Electron density around STE c 516:**

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

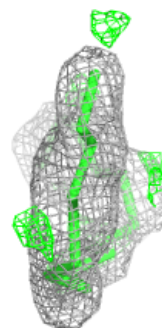
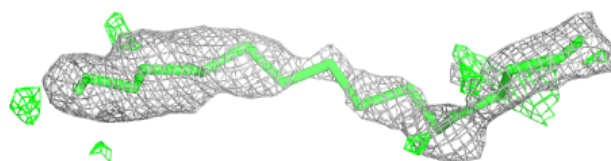
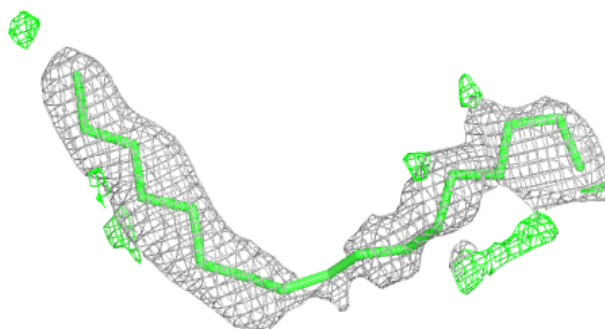


Electron density around STE e 104:

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

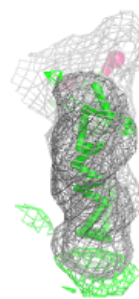
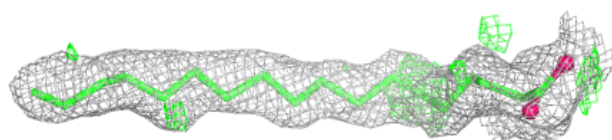
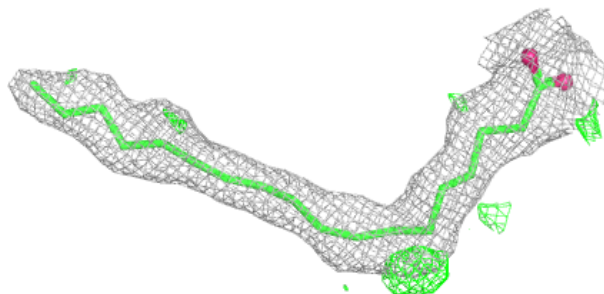
**Electron density around STE Z 101:**

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

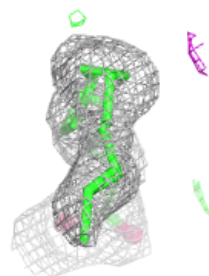
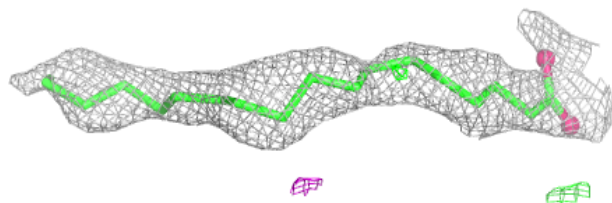
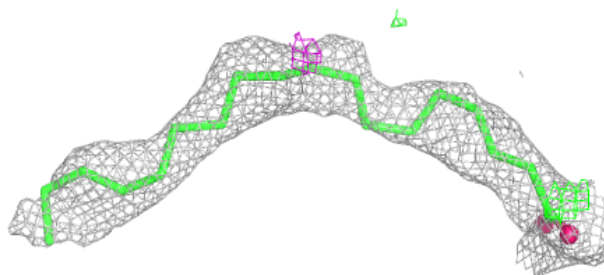


Electron density around STE d 407:

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

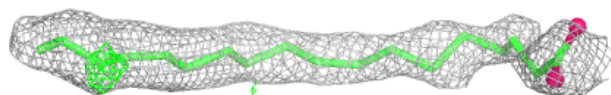
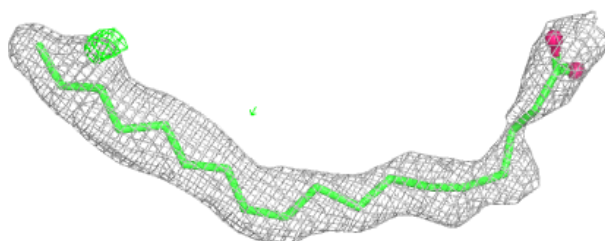
**Electron density around STE d 410:**

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

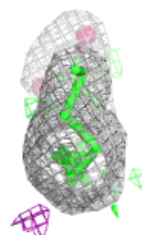
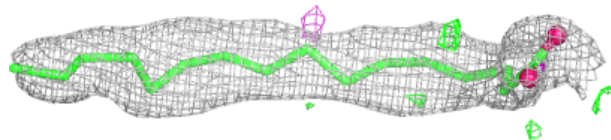
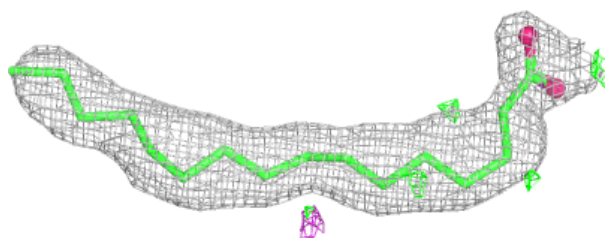


Electron density around STE d 412:

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

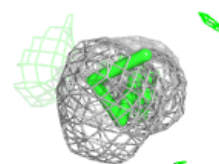
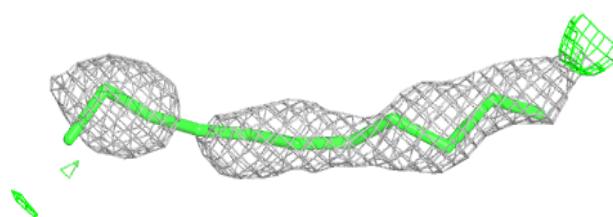
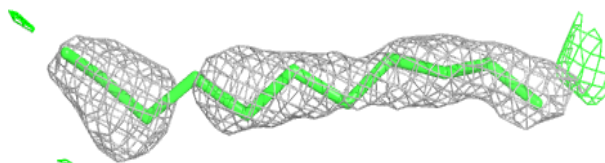
**Electron density around STE B 625:**

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

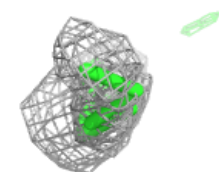
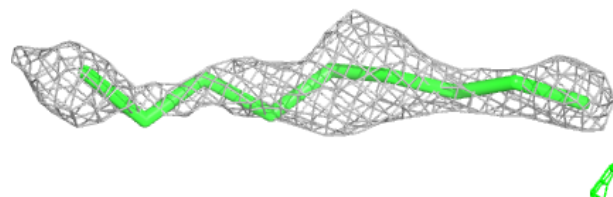
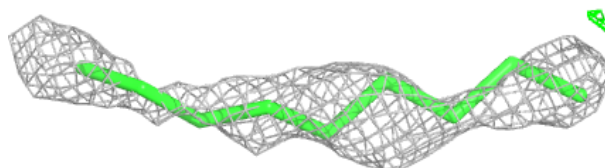


Electron density around STE b 627:

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

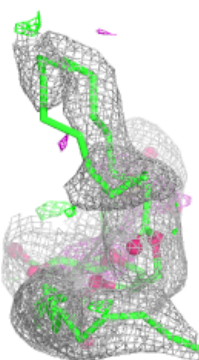
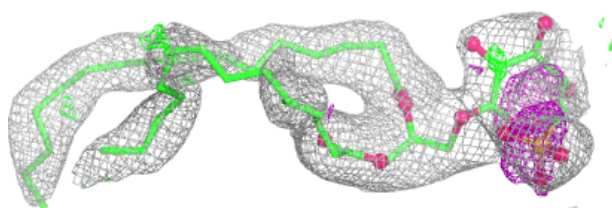
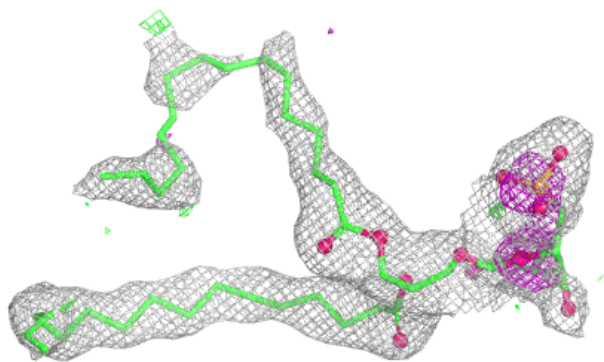
**Electron density around STE z 101:**

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

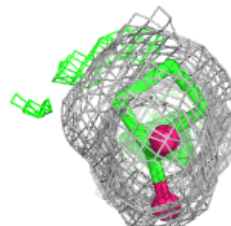
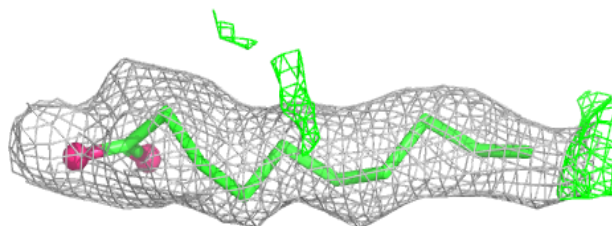
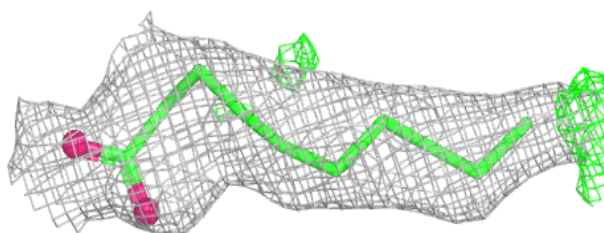


Electron density around SQD a 614:

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

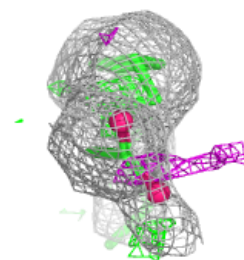
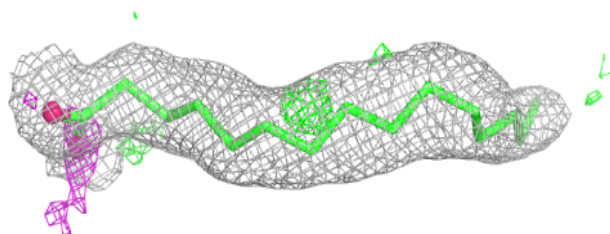
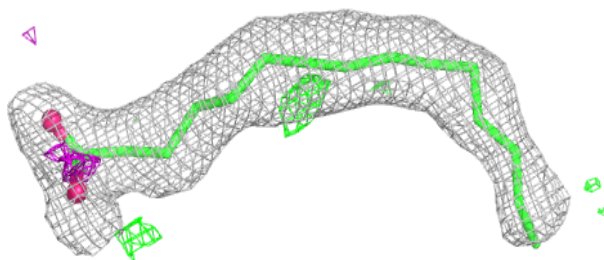
**Electron density around STE J 101:**

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

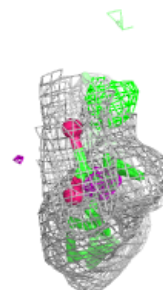
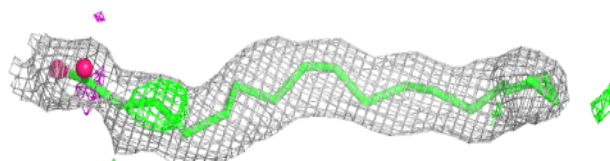
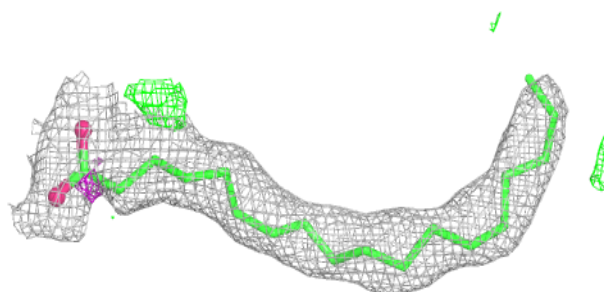


Electron density around STE B 622:

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

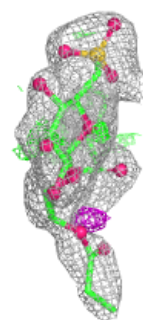
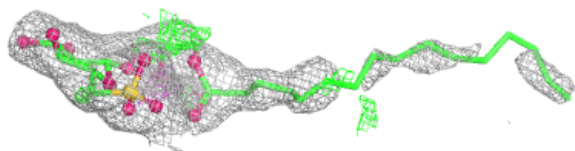
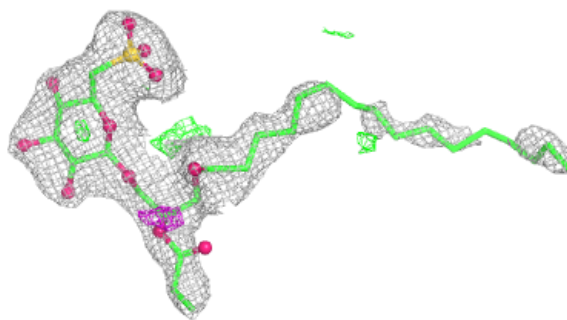
**Electron density around STE b 623:**

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

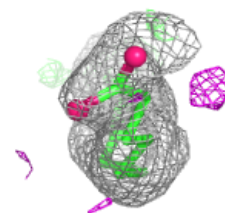
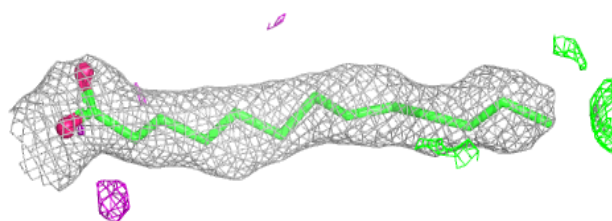
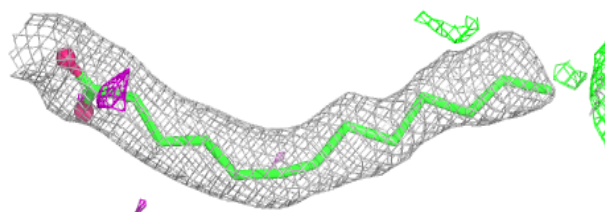


Electron density around SQD f 101:

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

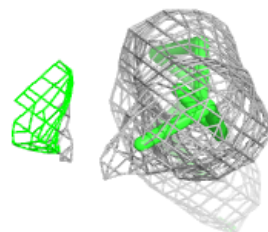
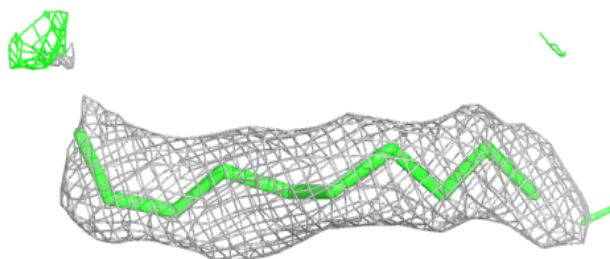
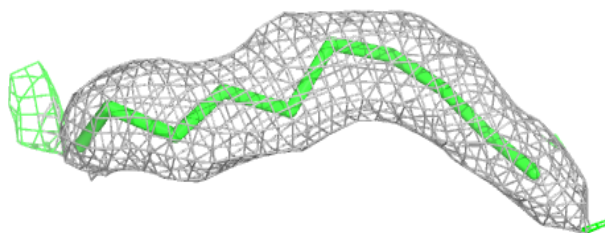
**Electron density around STE I 102:**

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

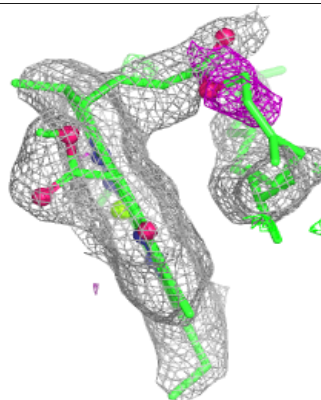
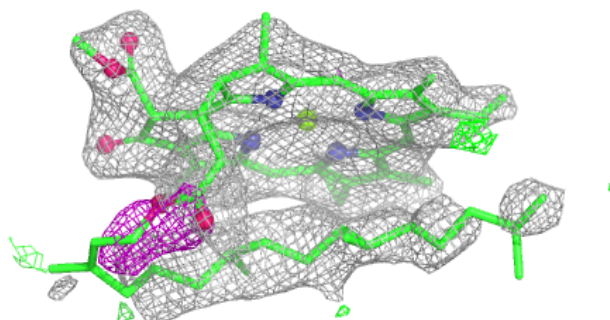
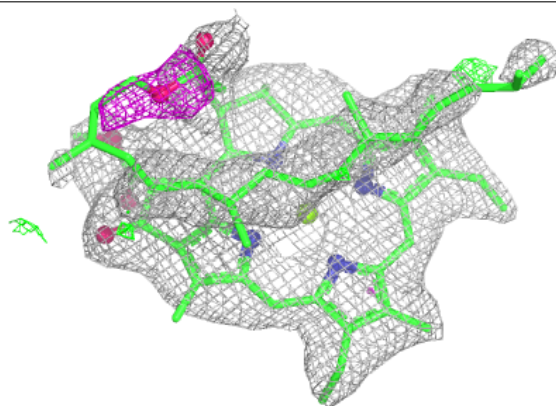


Electron density around STE b 626:

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

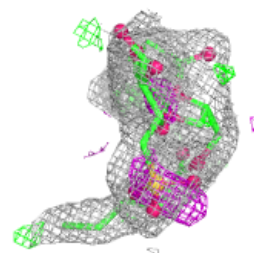
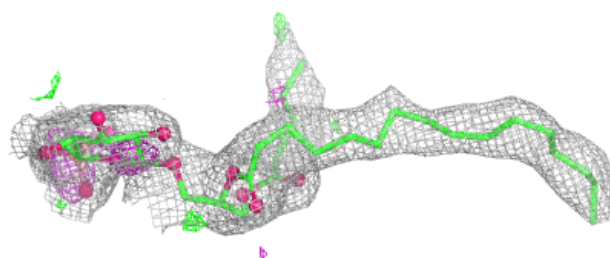
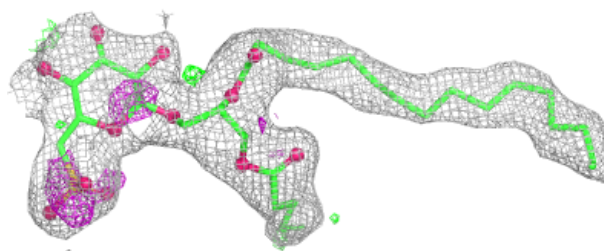
**Electron density around CLA b 601:**

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

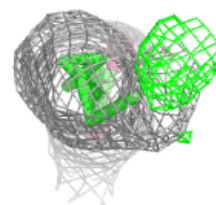
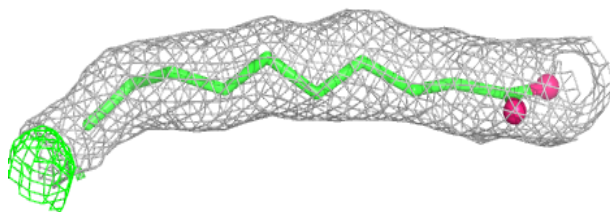
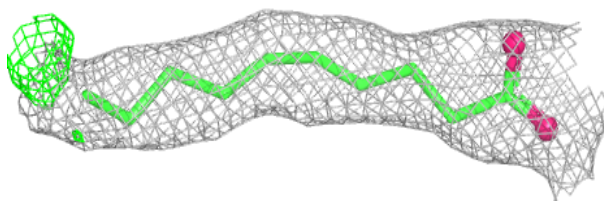


Electron density around SQD A 614:

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

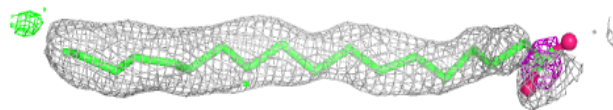
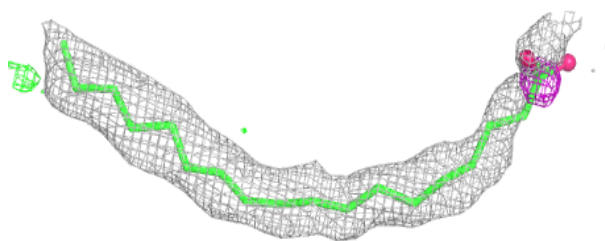
**Electron density around STE j 101:**

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

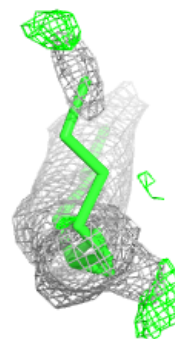
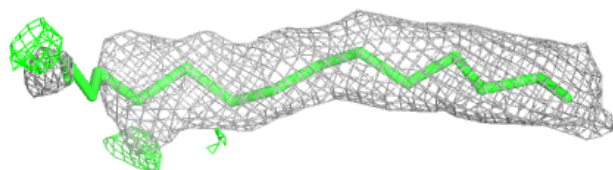
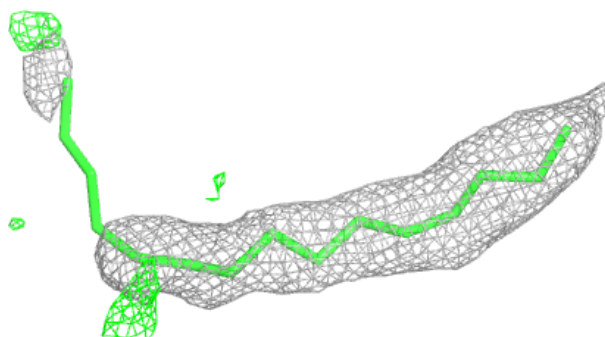


Electron density around STE D 413:

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

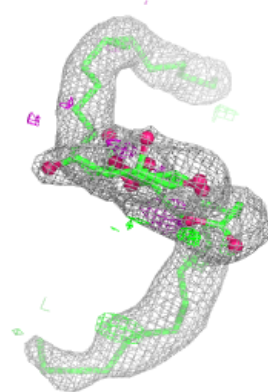
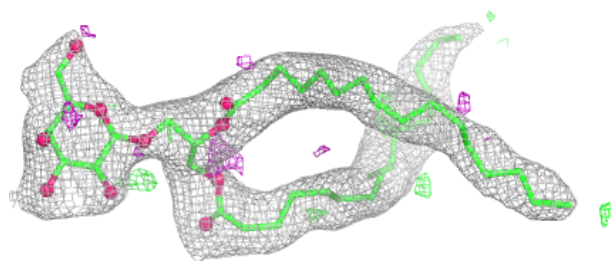
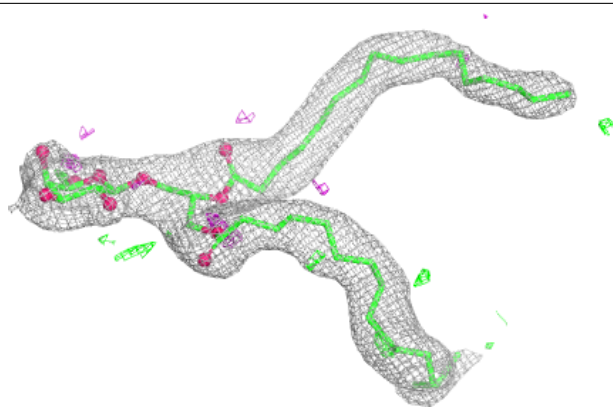
**Electron density around STE M 103:**

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

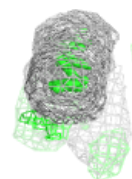
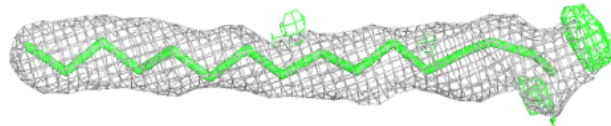
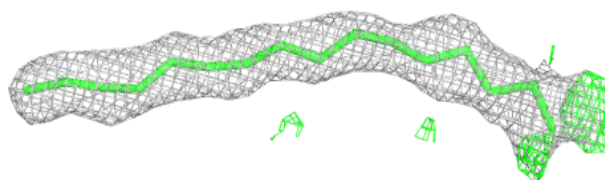


Electron density around LMG B 621:

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

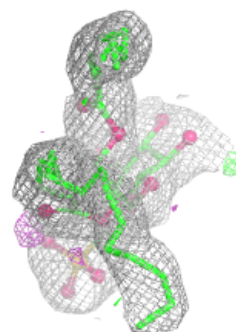
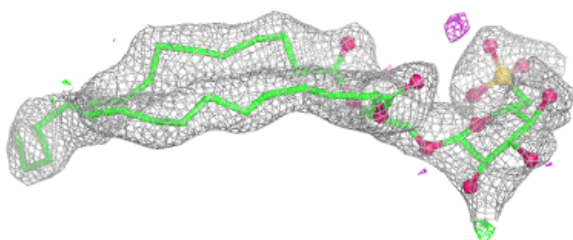
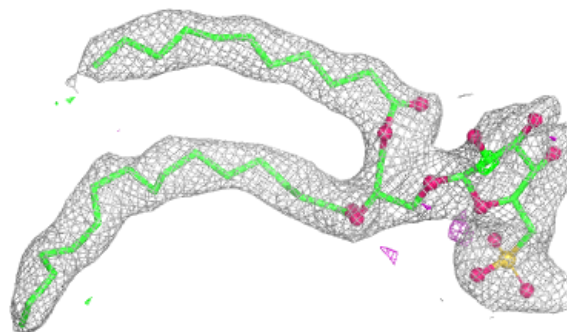
**Electron density around STE C 528:**

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

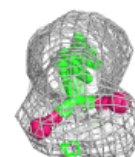
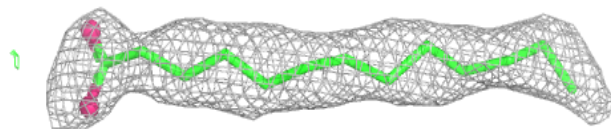
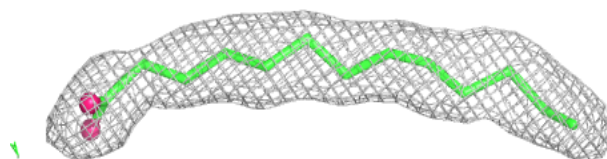


Electron density around SQD b 620:

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

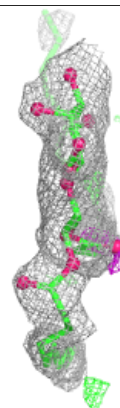
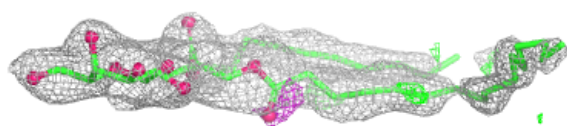
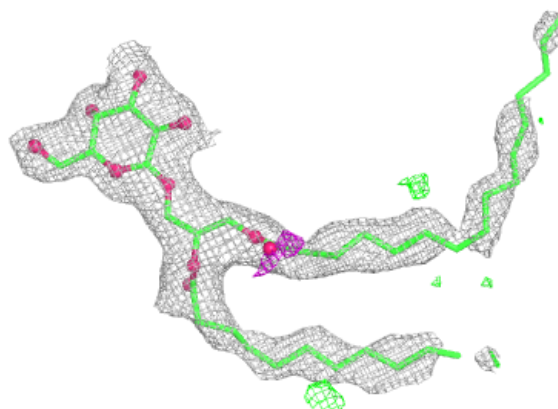
**Electron density around STE M 101:**

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

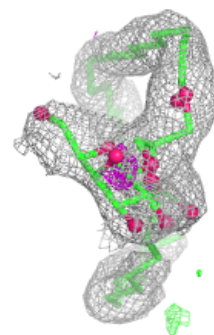
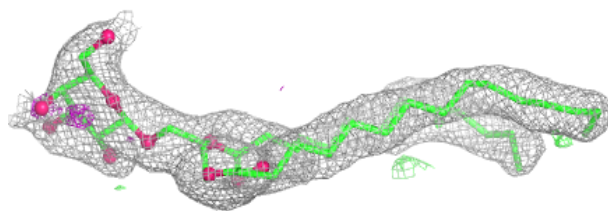
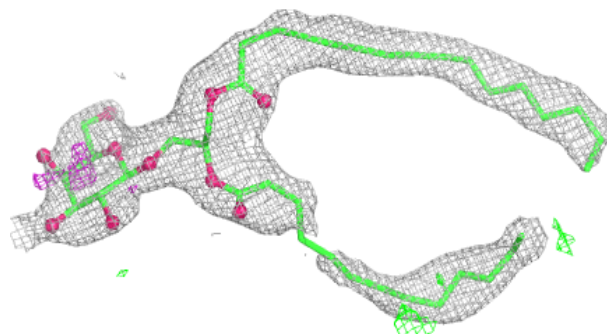


Electron density around LMG c 522:

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

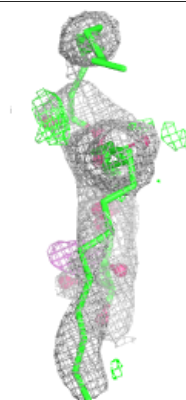
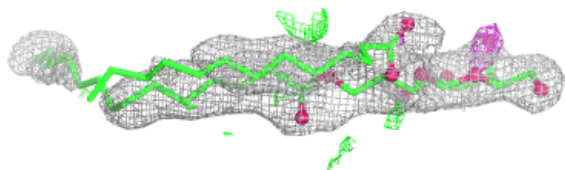
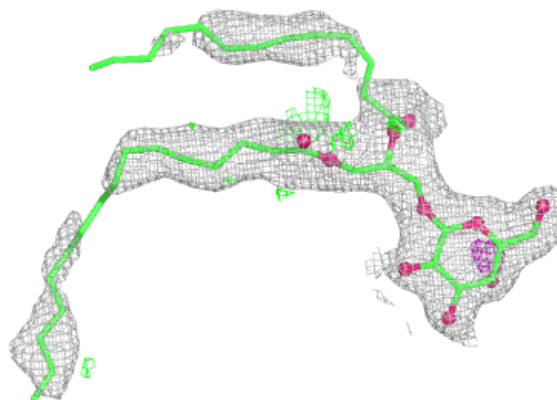
**Electron density around LMG C 522:**

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

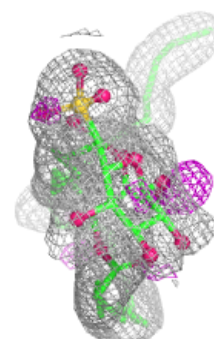
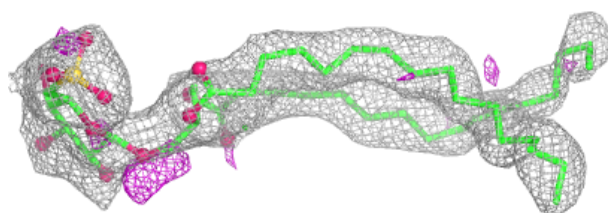
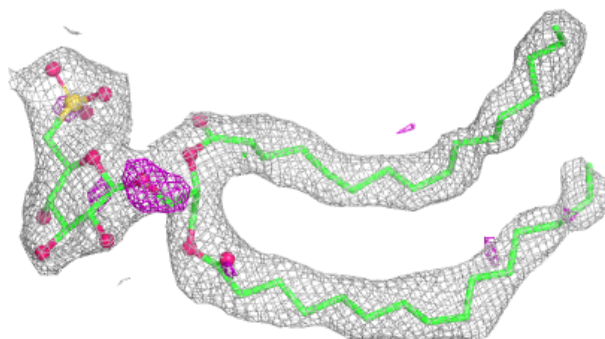


Electron density around LMG C 526:

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

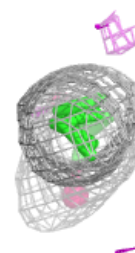
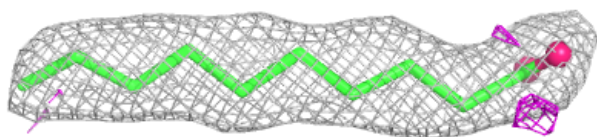
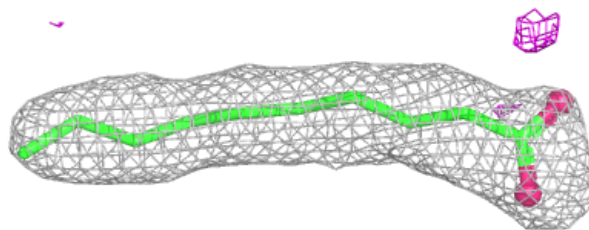
**Electron density around SQD B 623:**

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

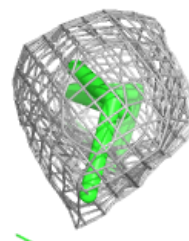
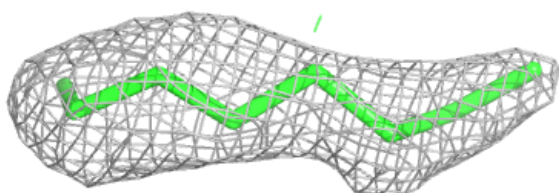
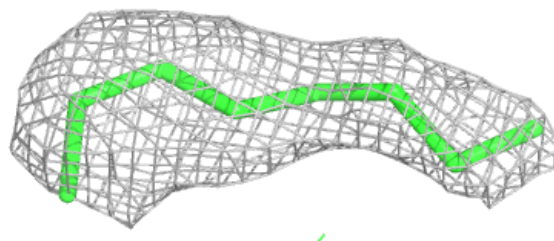


Electron density around STE m 101:

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

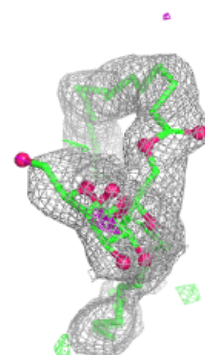
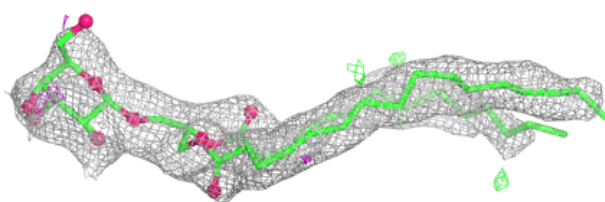
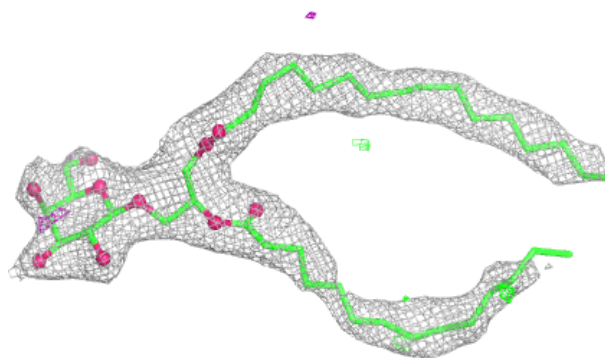
**Electron density around STE A 616:**

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

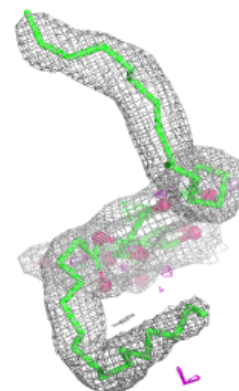
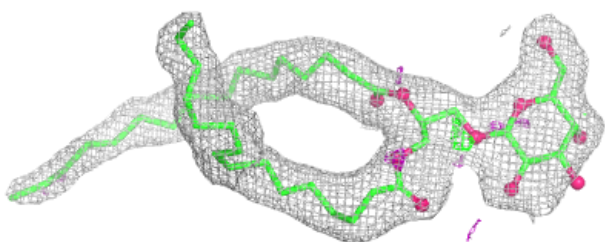
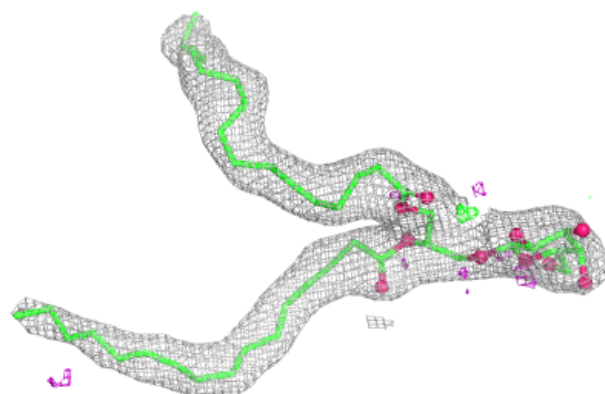


Electron density around LMG a 616:

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

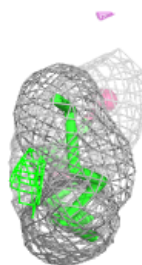
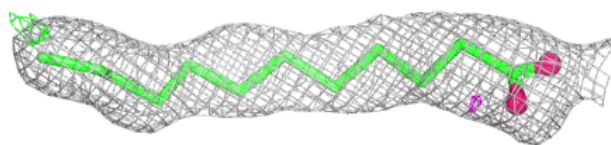
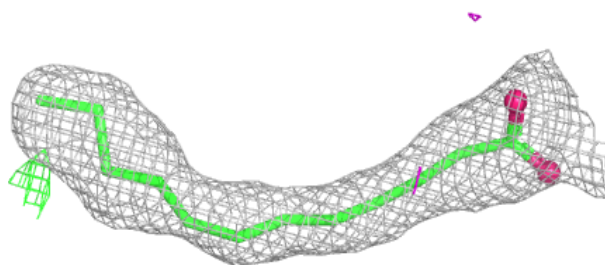
**Electron density around LMG b 622:**

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

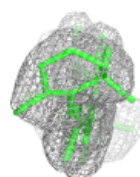
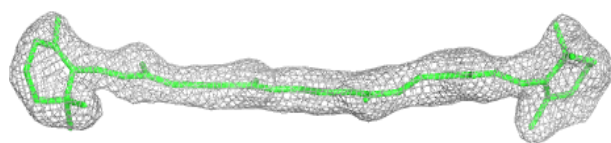
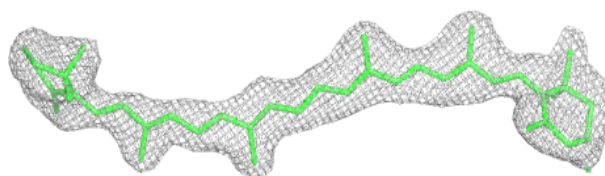


Electron density around STE B 624:

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

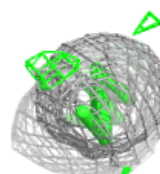
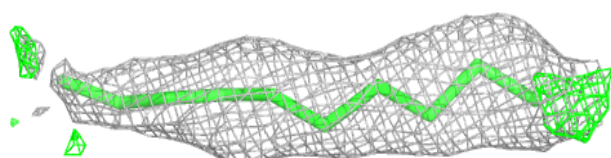
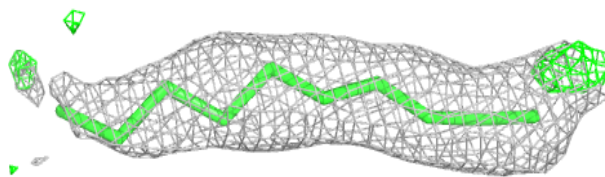
**Electron density around BCR k 101:**

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

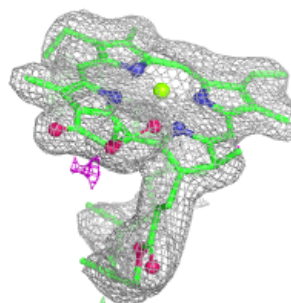
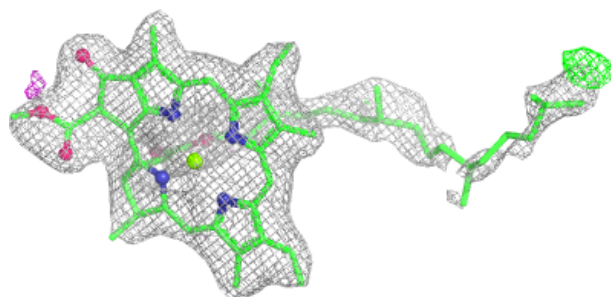
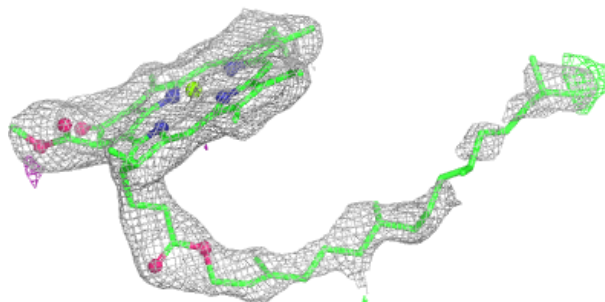


Electron density around STE M 102:

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

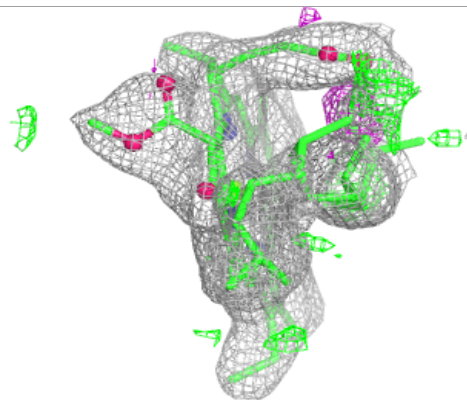
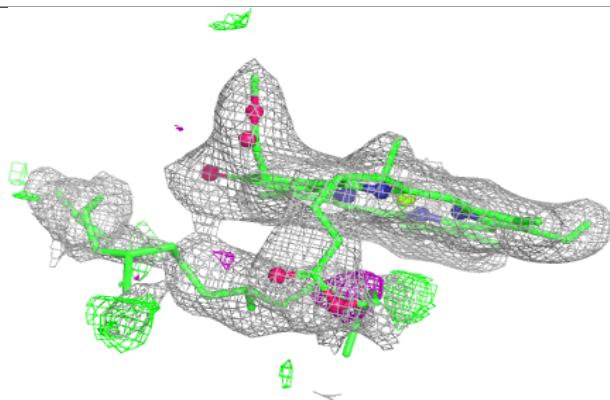
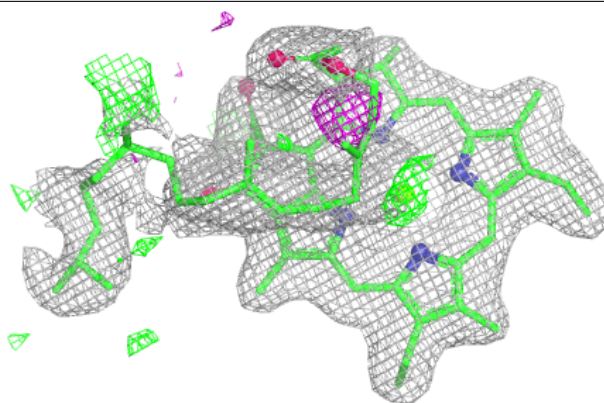
**Electron density around CLA C 513:**

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

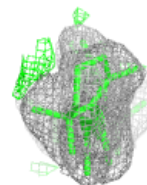
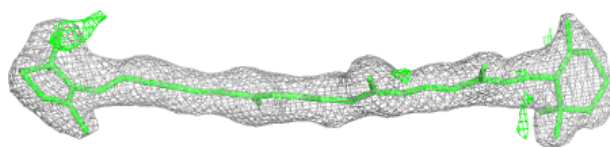
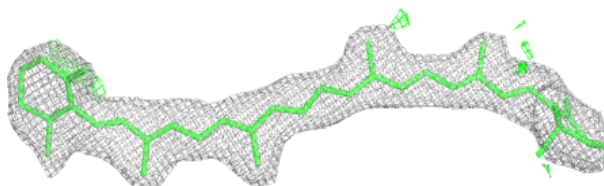


Electron density around CLA B 601:

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

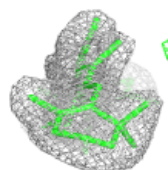
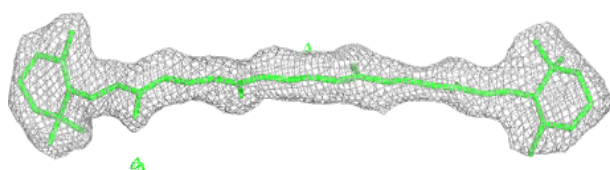
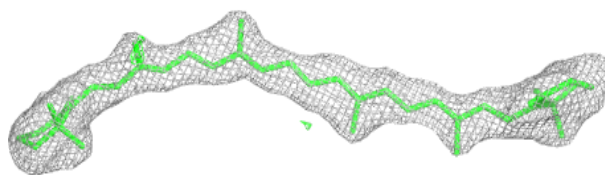
**Electron density around BCR C 521:**

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

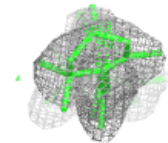
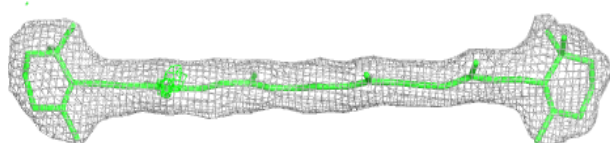
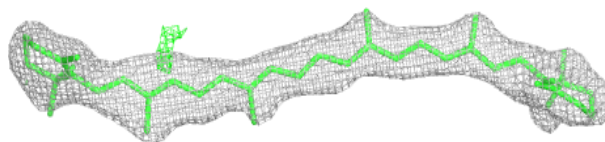


Electron density around BCR h 101:

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

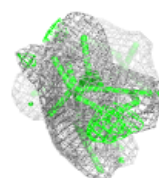
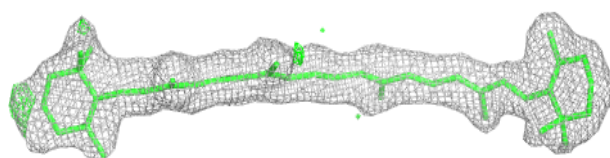
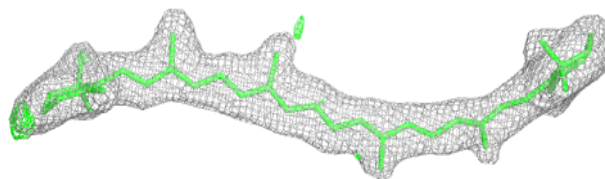
**Electron density around BCR C 514:**

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



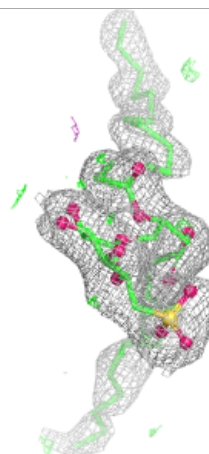
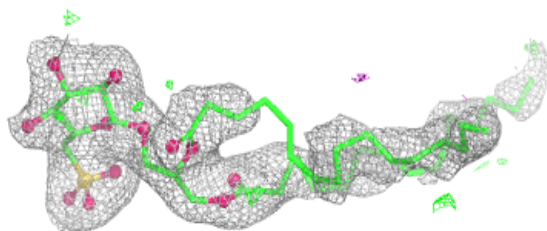
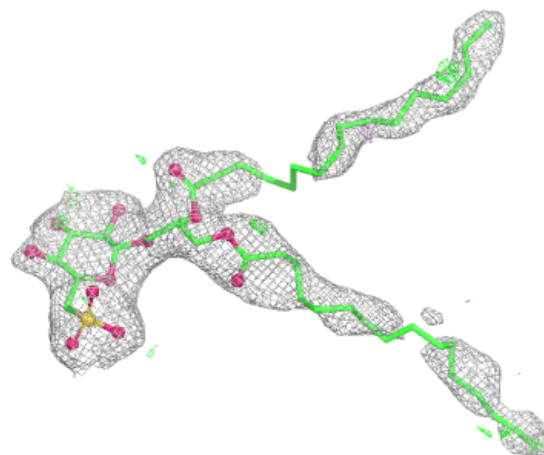
Electron density around BCR H 101:

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



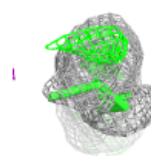
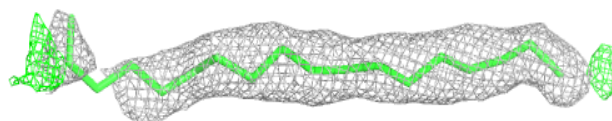
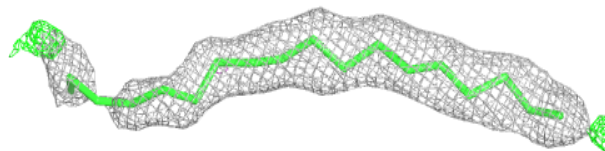
Electron density around SQD a 613:

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

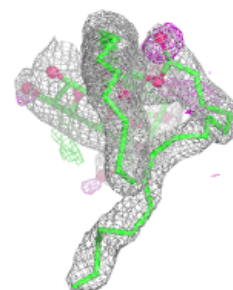
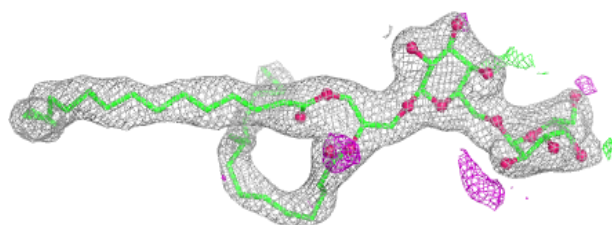
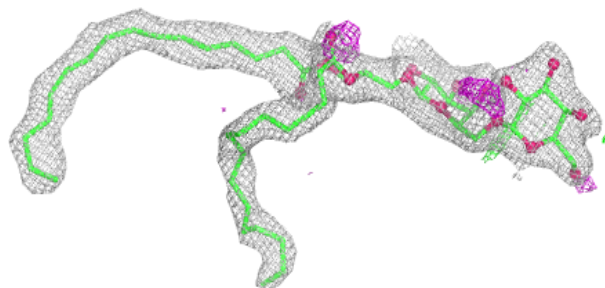


Electron density around STE m 102:

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

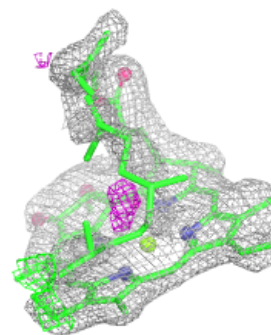
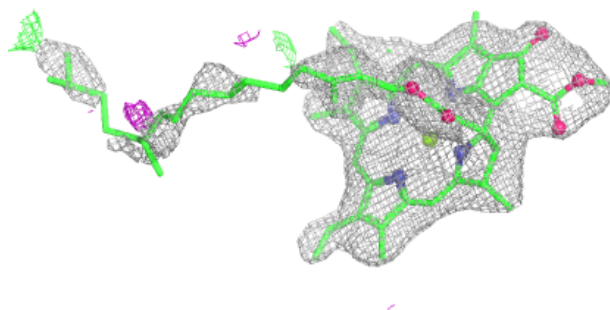
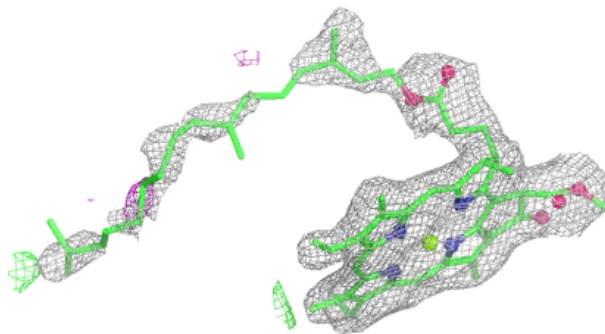
**Electron density around DGD h 102:**

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



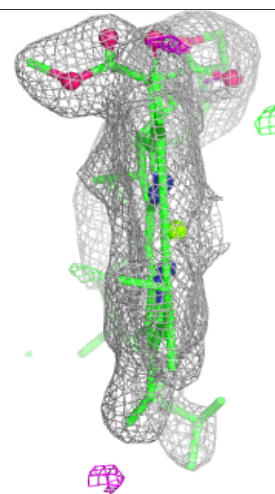
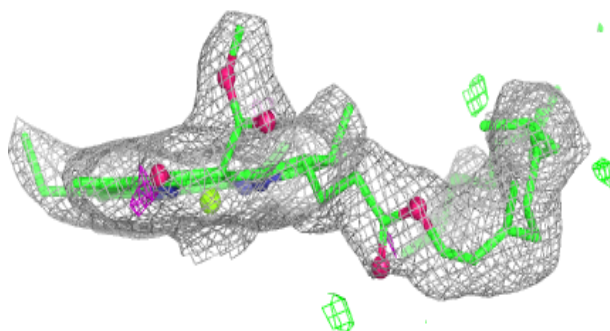
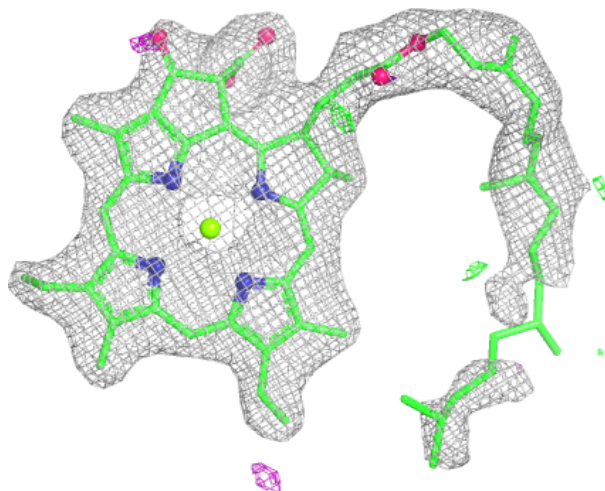
Electron density around CLA c 513:

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



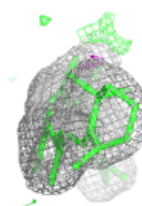
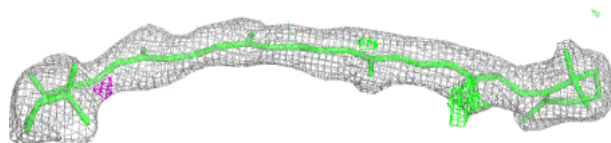
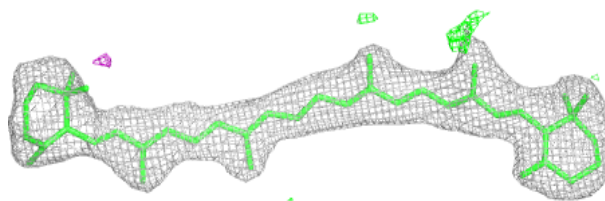
Electron density around CLA C 512:

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



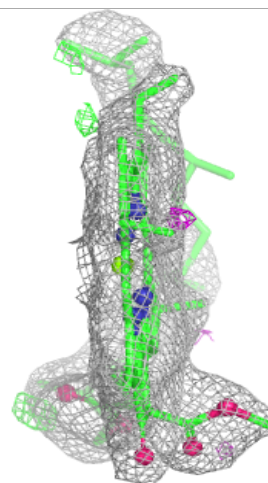
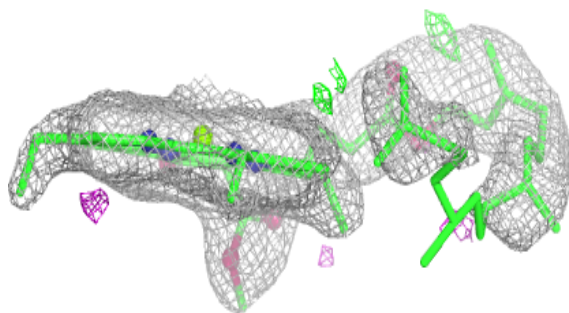
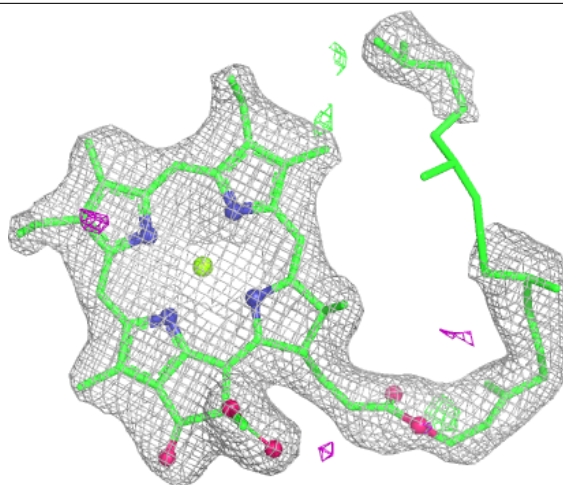
Electron density around BCR d 405:

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



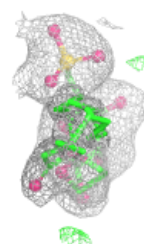
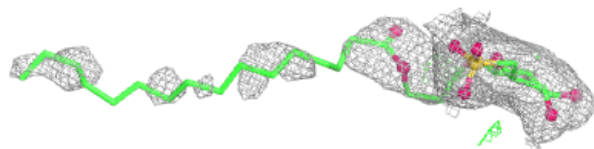
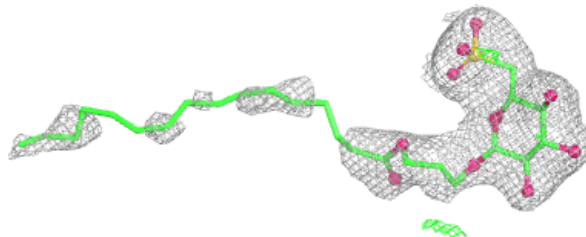
Electron density around CLA c 512:

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



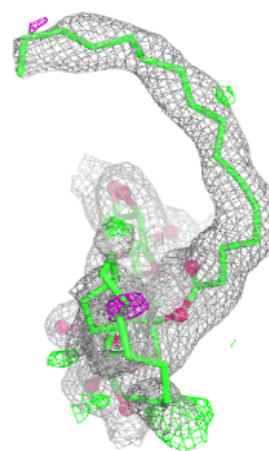
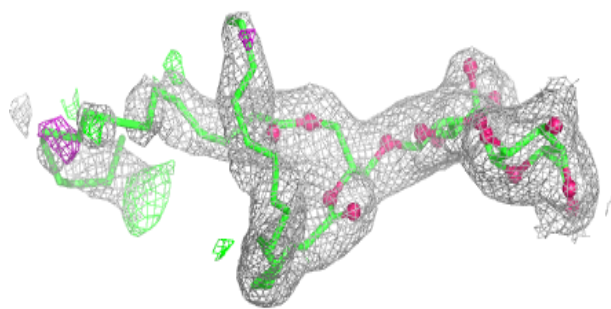
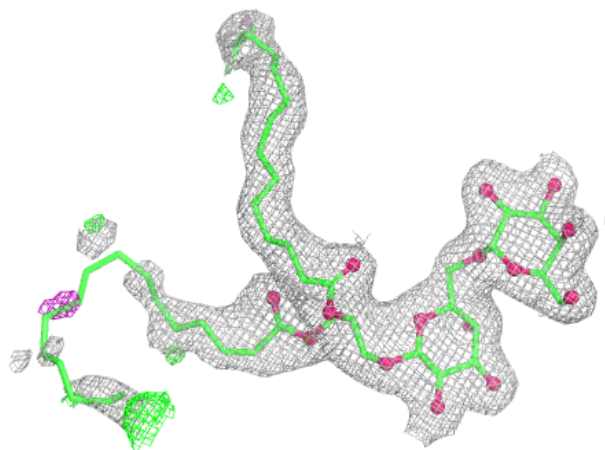
Electron density around SQD D 409:

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



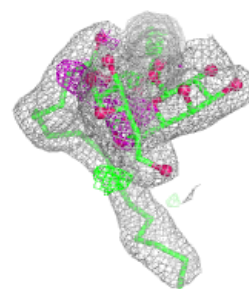
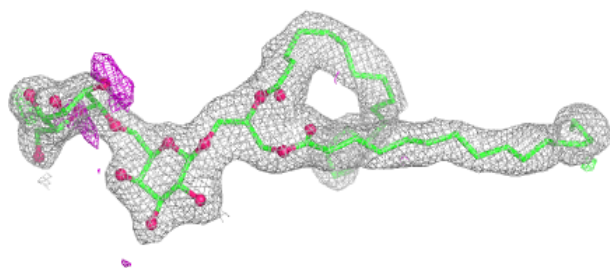
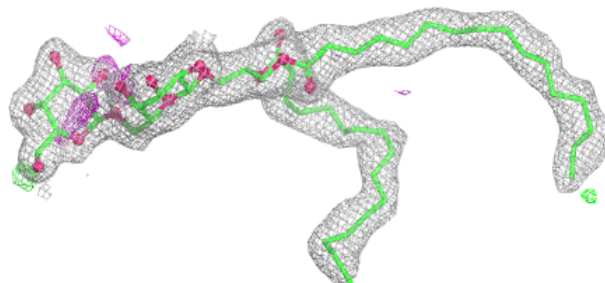
Electron density around DGD C 524:

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

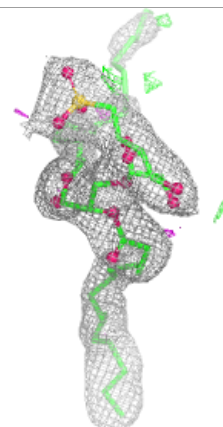
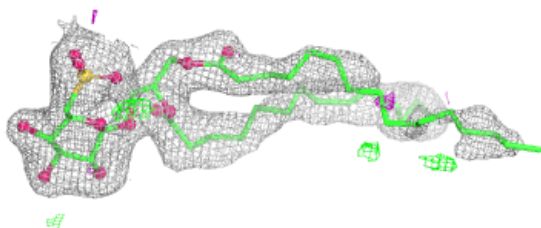


Electron density around DGD H 102:

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

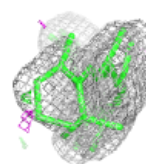
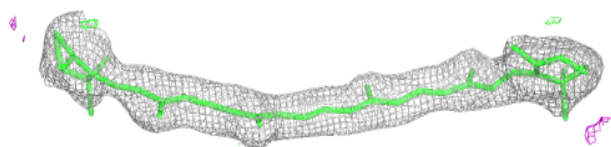
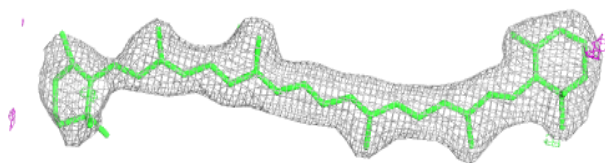
**Electron density around SQD A 613:**

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



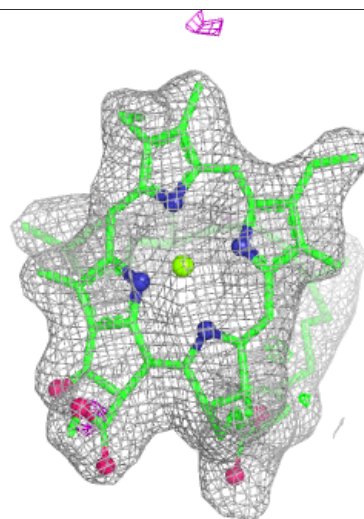
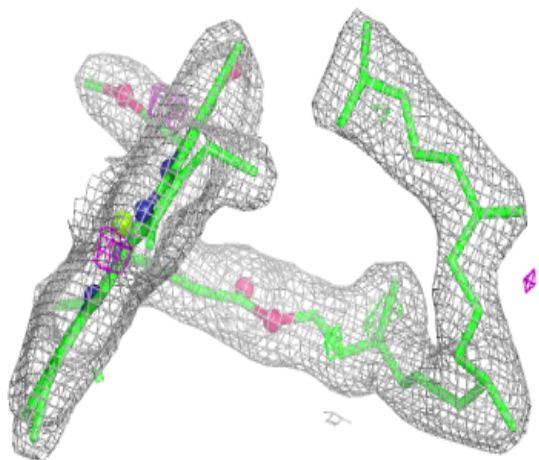
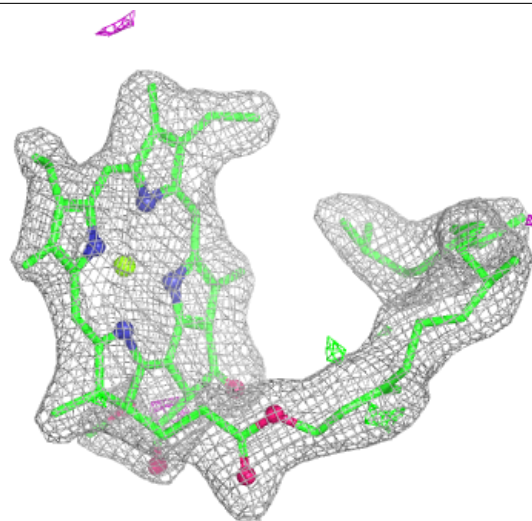
Electron density around BCR D 405:

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



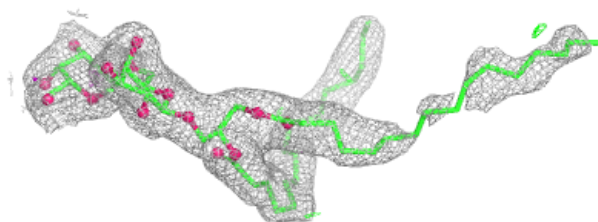
Electron density around CLA c 503:

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

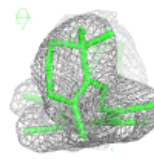
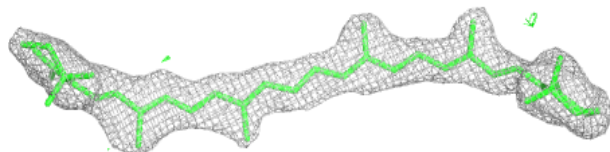
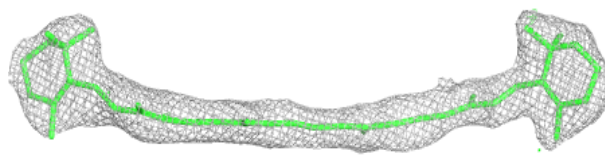


Electron density around DGD c 520:

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

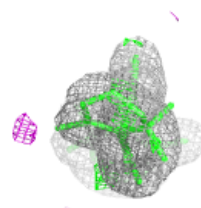
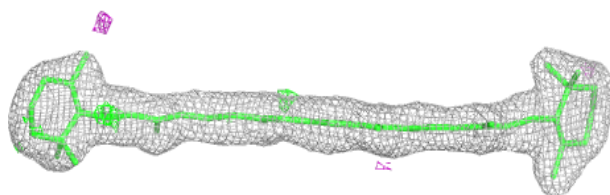
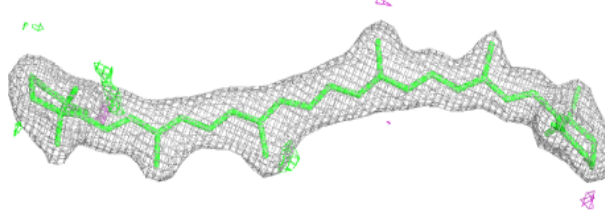
**Electron density around BCR k 102:**

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

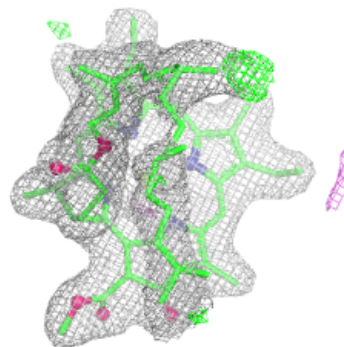
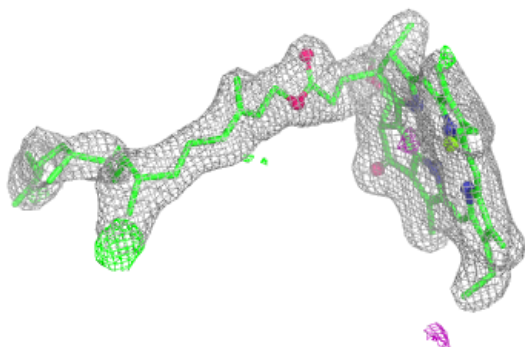
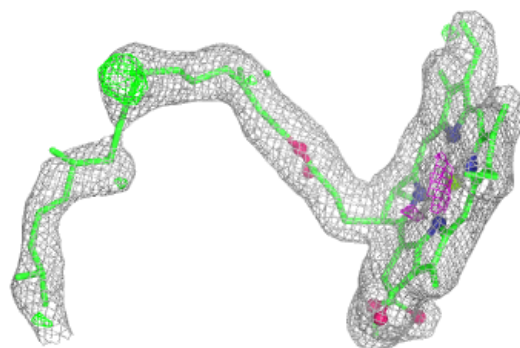


Electron density around BCR C 515:

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

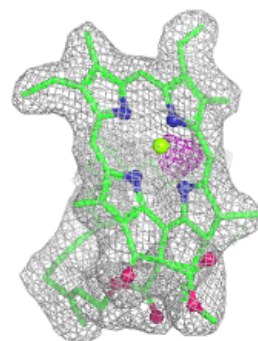
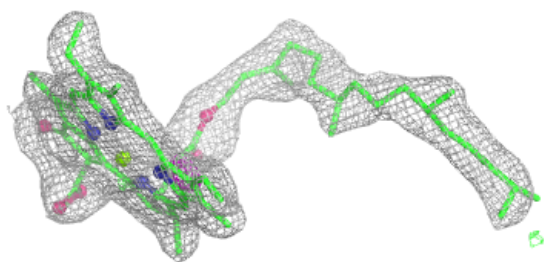
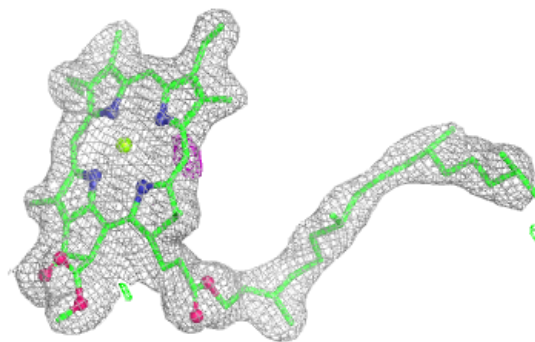
**Electron density around CLA b 606:**

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

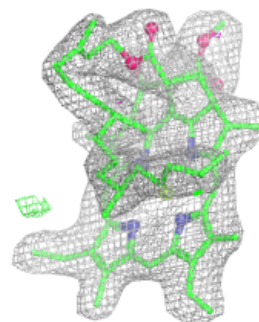
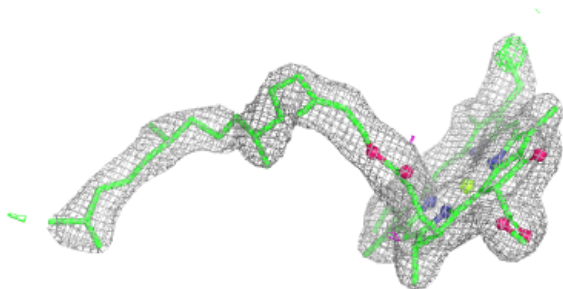
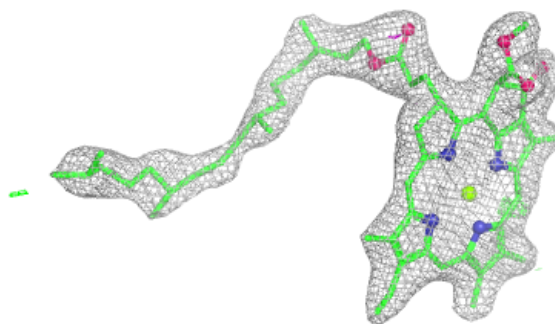


Electron density around CLA C 511:

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

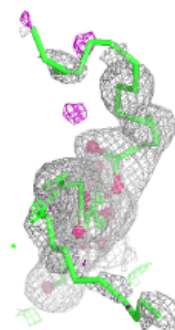
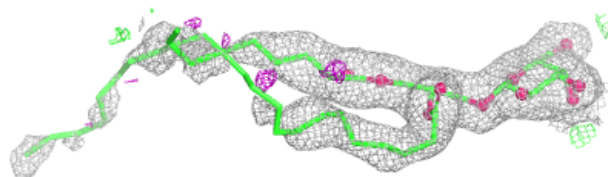
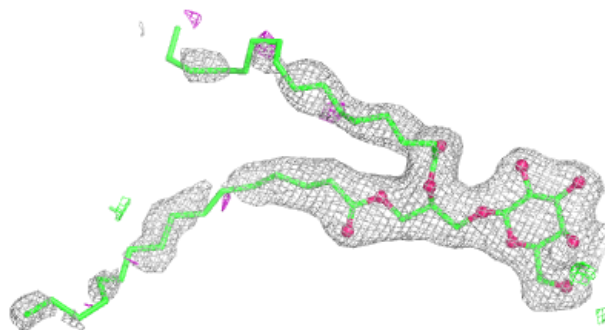
**Electron density around CLA c 511:**

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

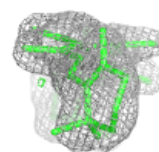
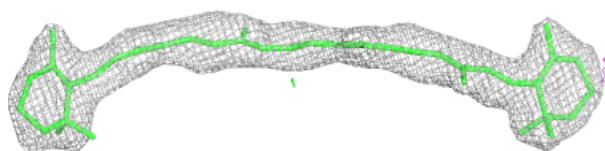


Electron density around LMG D 408:

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

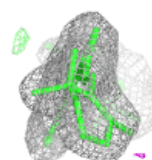
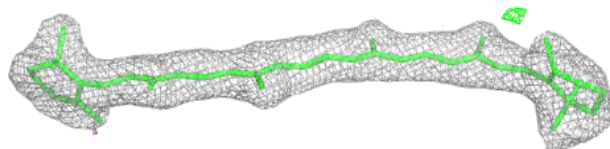
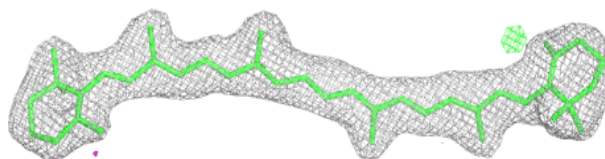
**Electron density around BCR K 101:**

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



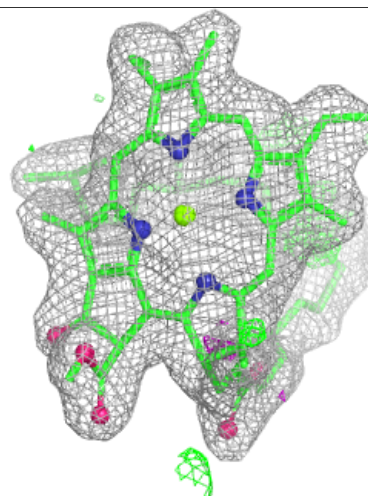
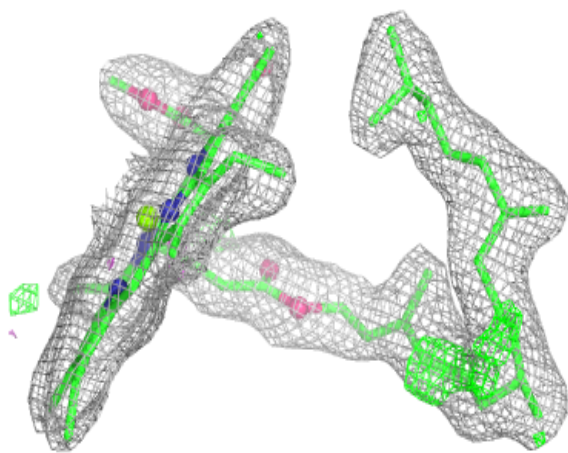
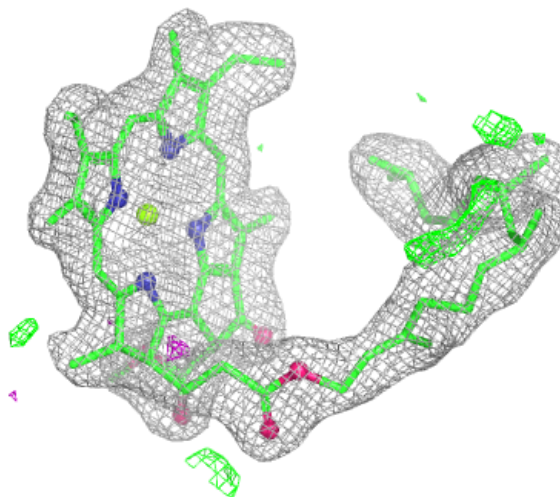
Electron density around BCR b 619:

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



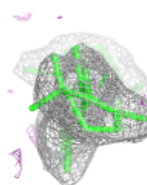
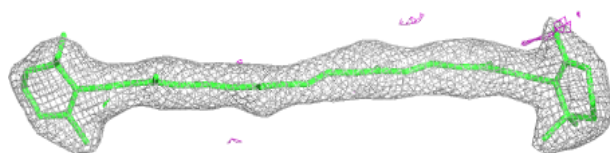
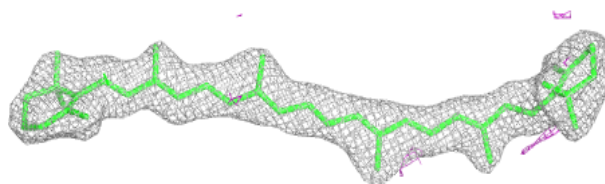
Electron density around CLA C 503:

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

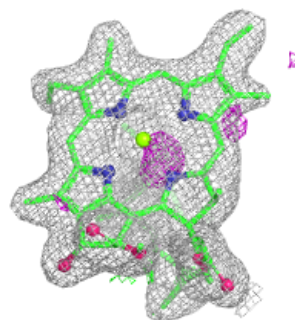
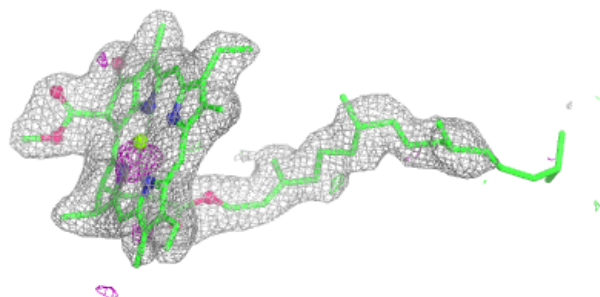
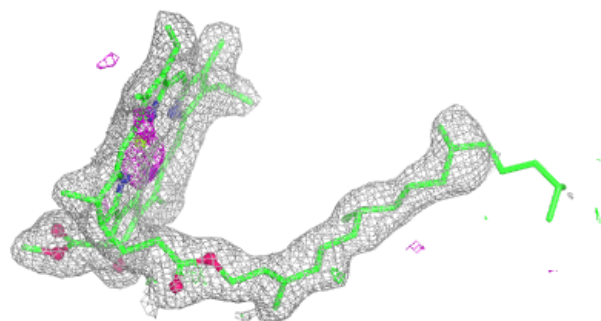


Electron density around BCR c 515:

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

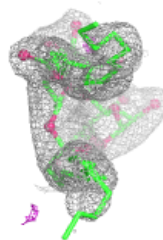
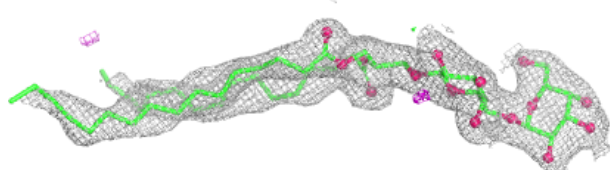
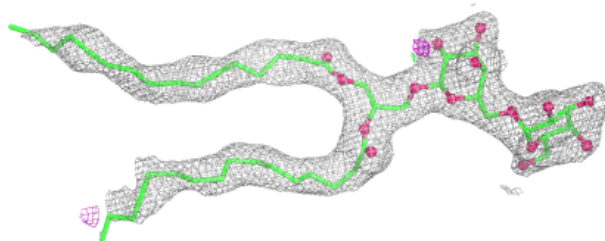
**Electron density around CLA C 508:**

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

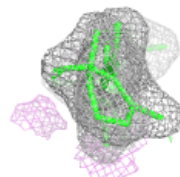
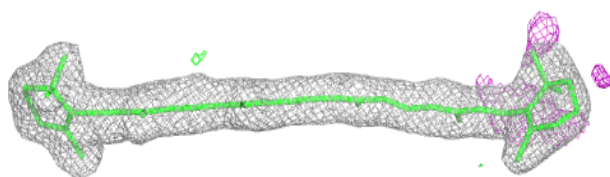
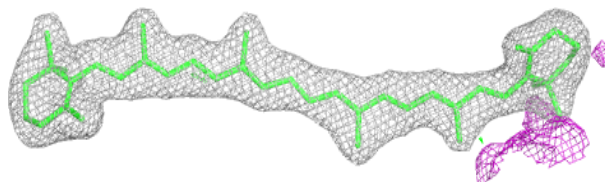


Electron density around DGD c 521:

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

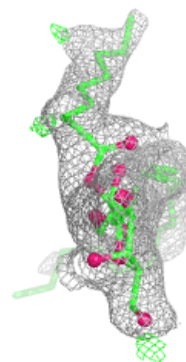
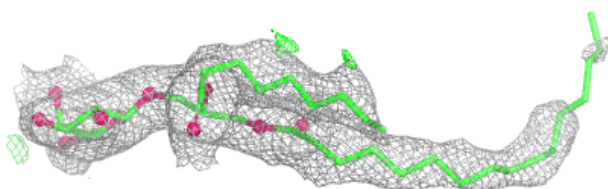
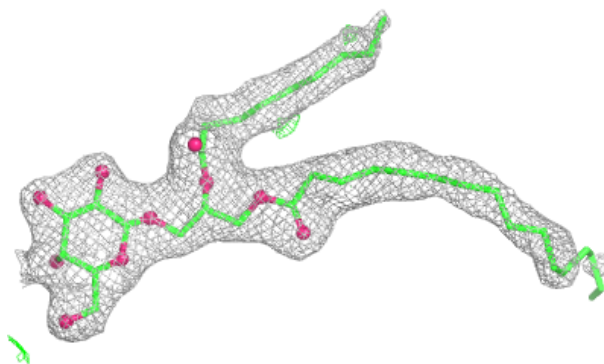
**Electron density around BCR B 618:**

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

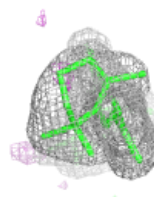
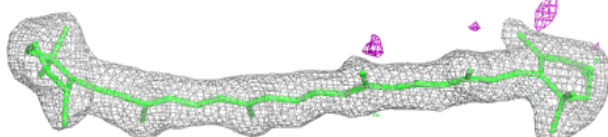
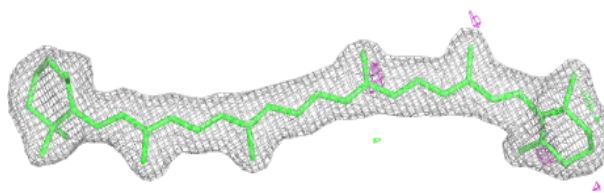


Electron density around LMG d 411:

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

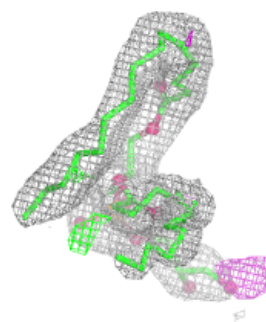
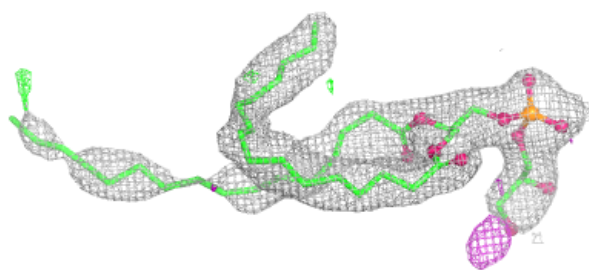
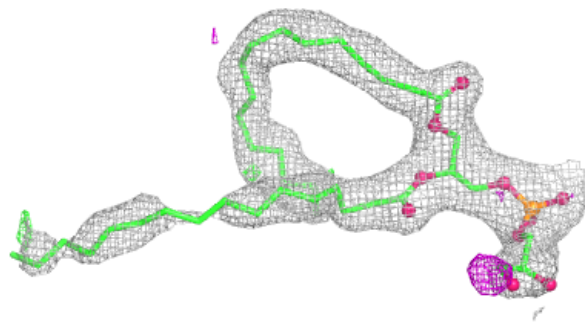
**Electron density around BCR B 619:**

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



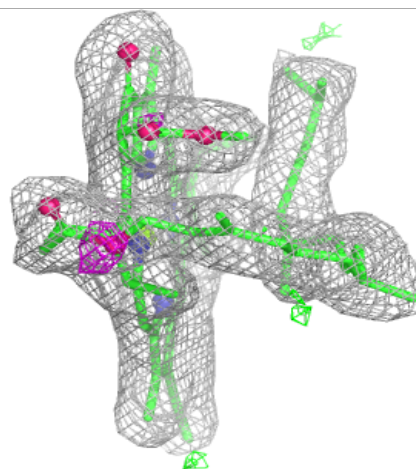
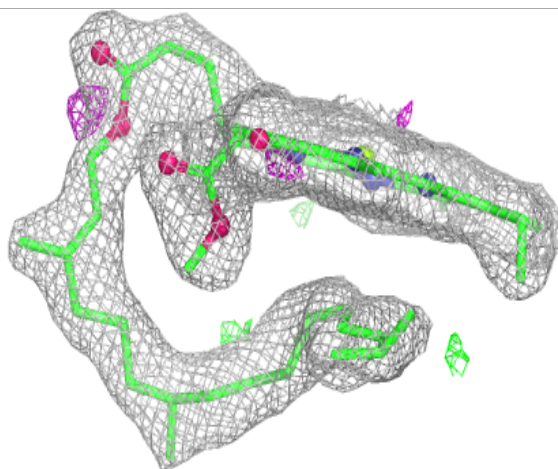
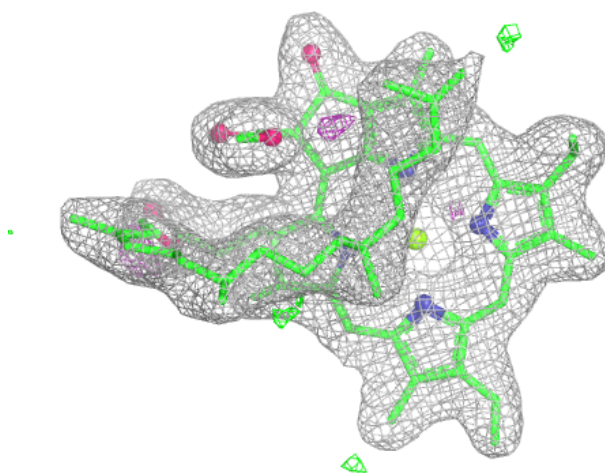
Electron density around LHG d 408:

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



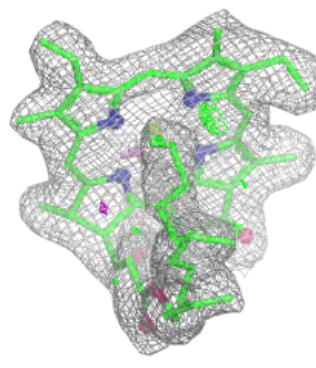
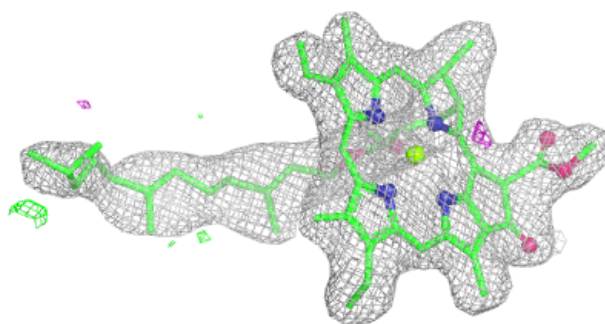
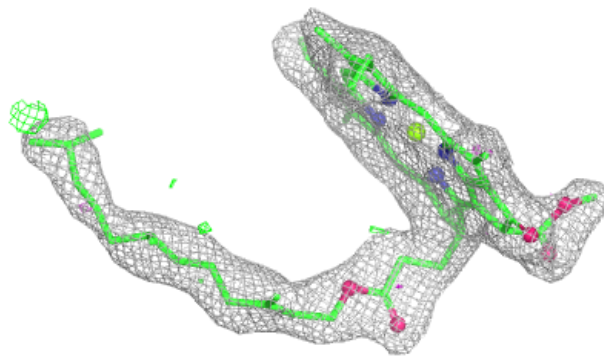
Electron density around CLA C 510:

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



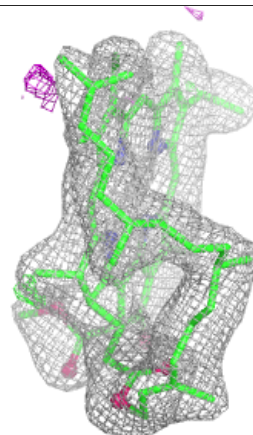
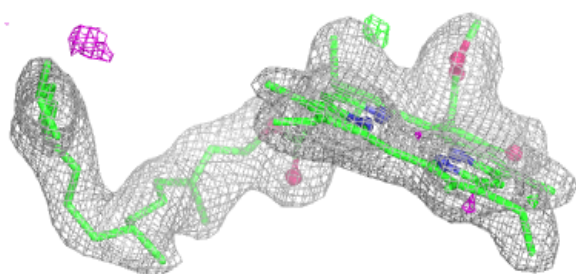
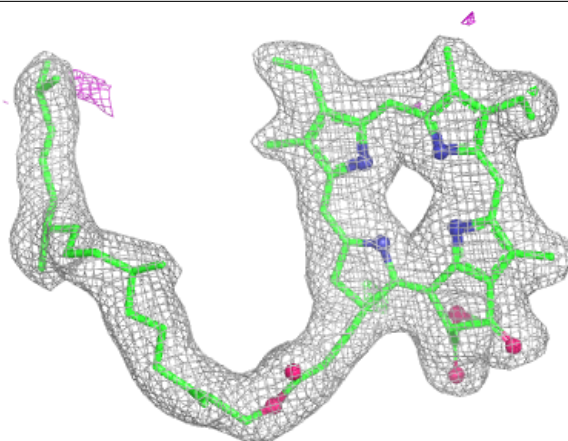
Electron density around CLA c 504:

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

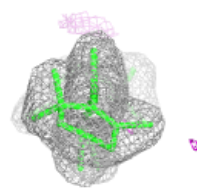
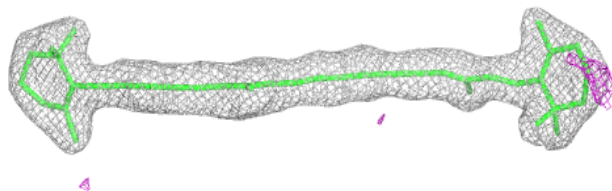
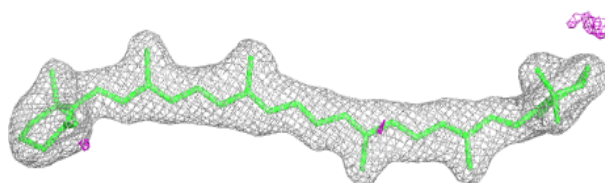


Electron density around PHO d 402:

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

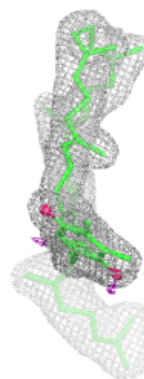
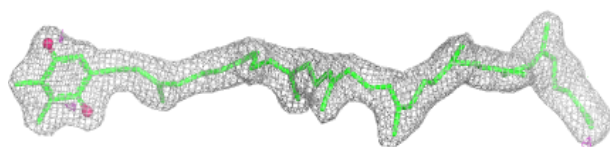
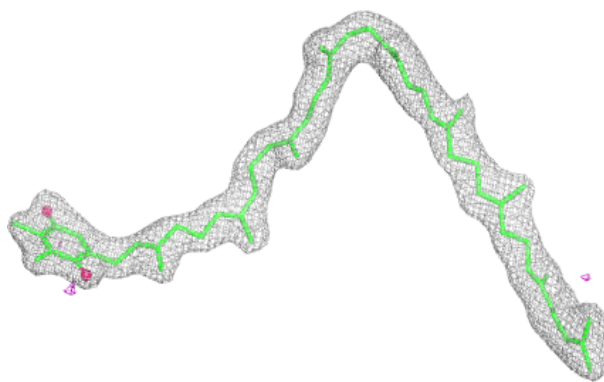
**Electron density around BCR A 610:**

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

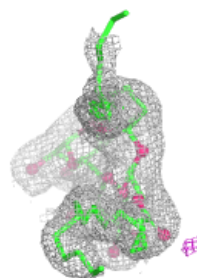
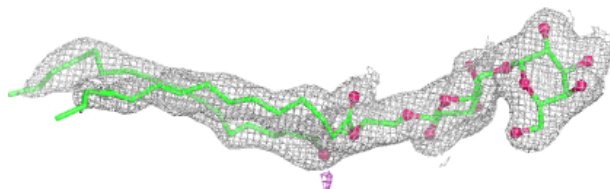
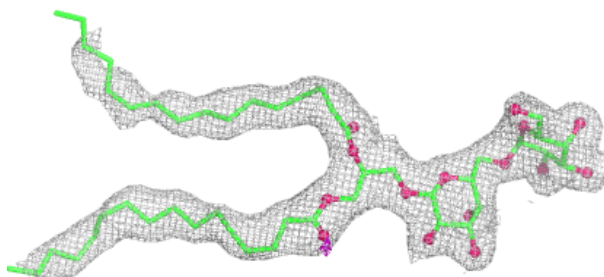


Electron density around PL9 d 406:

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

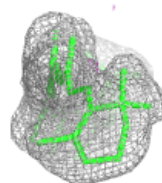
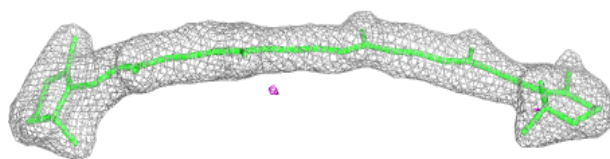
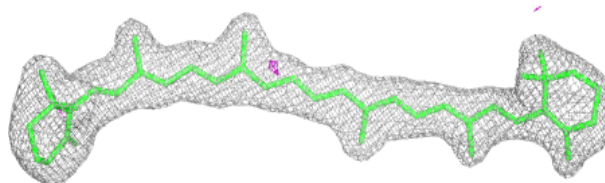
**Electron density around DGD C 525:**

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

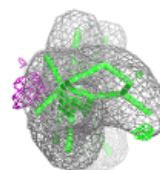
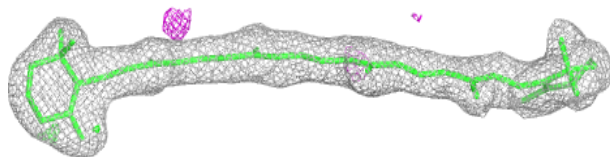
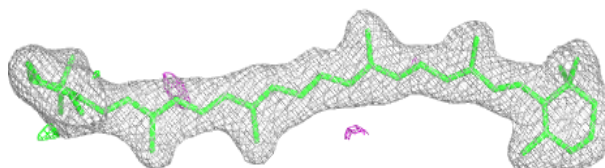


Electron density around BCR T 101:

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

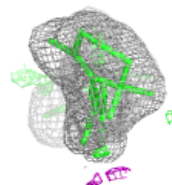
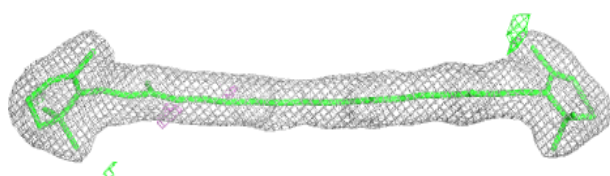
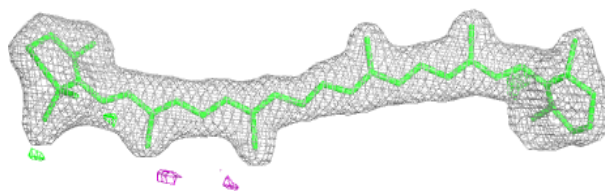
**Electron density around BCR b 617:**

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

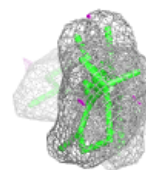
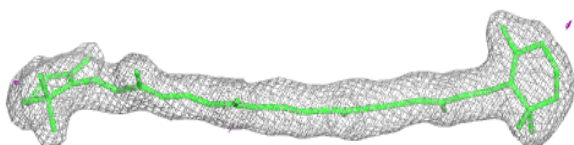
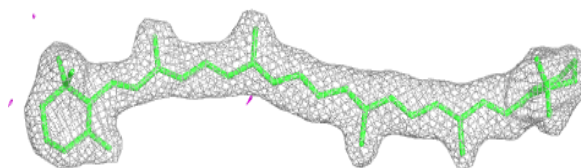


Electron density around BCR b 618:

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

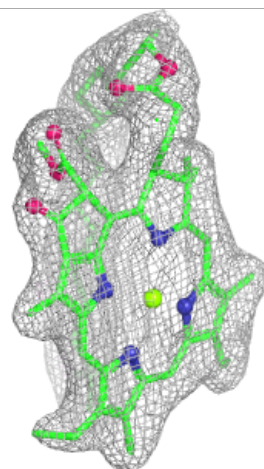
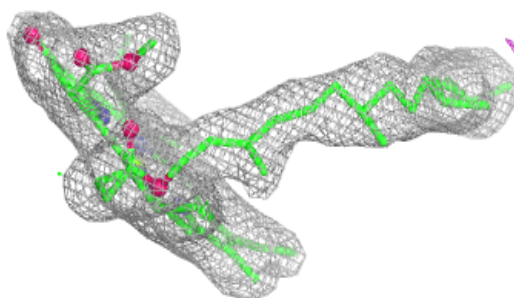
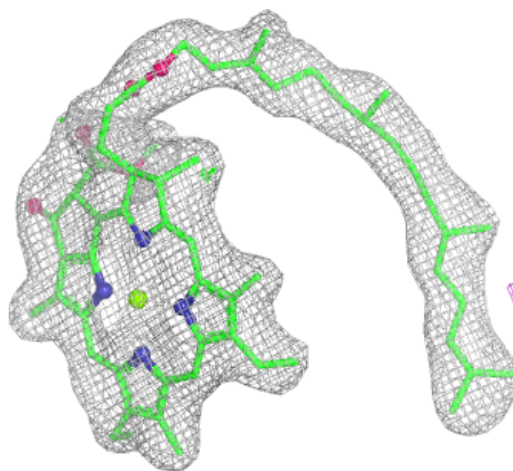
**Electron density around BCR B 617:**

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



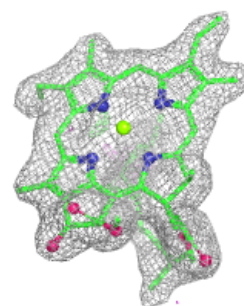
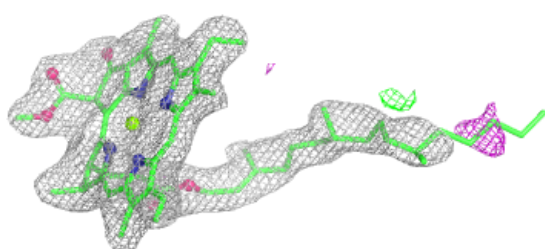
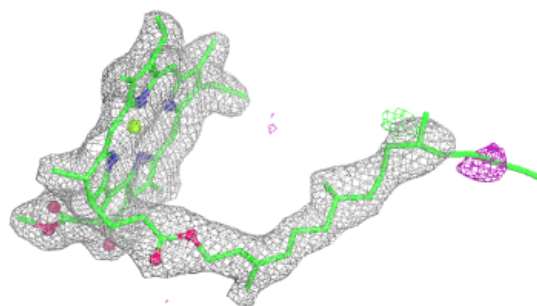
Electron density around CLA c 507:

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

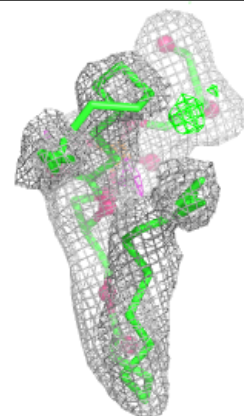
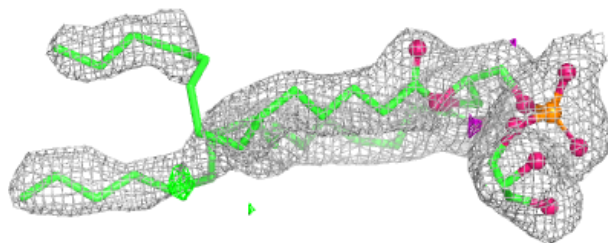
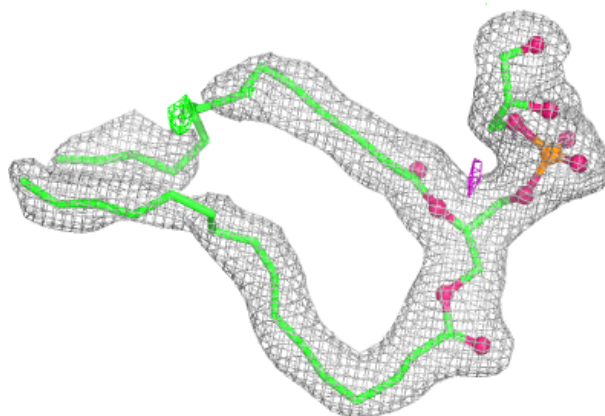


Electron density around CLA c 508:

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

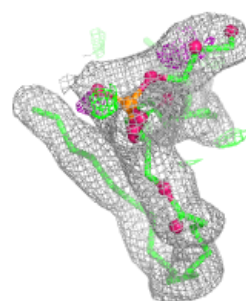
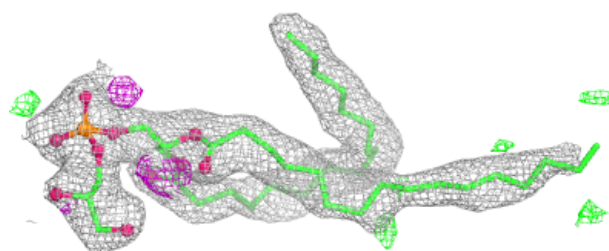
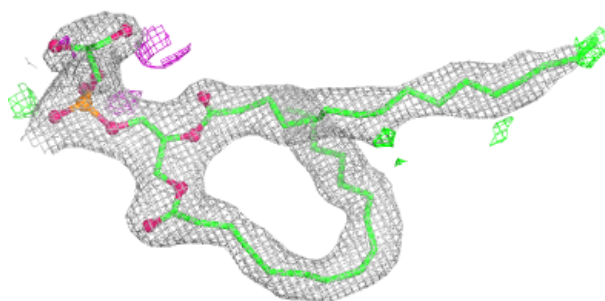
**Electron density around LHG D 411:**

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



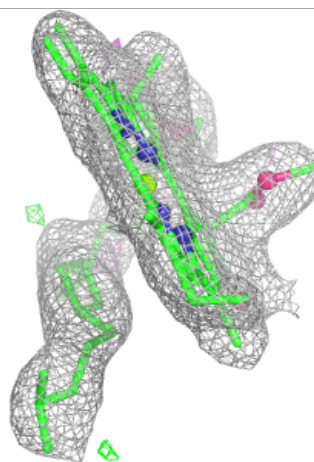
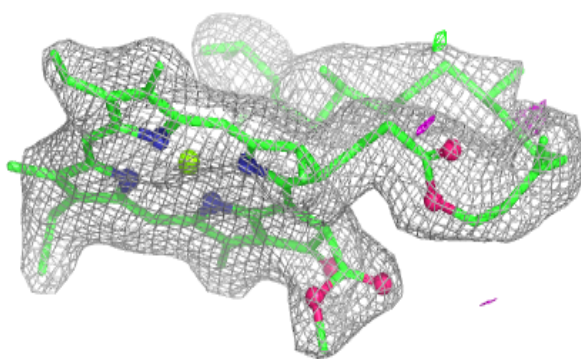
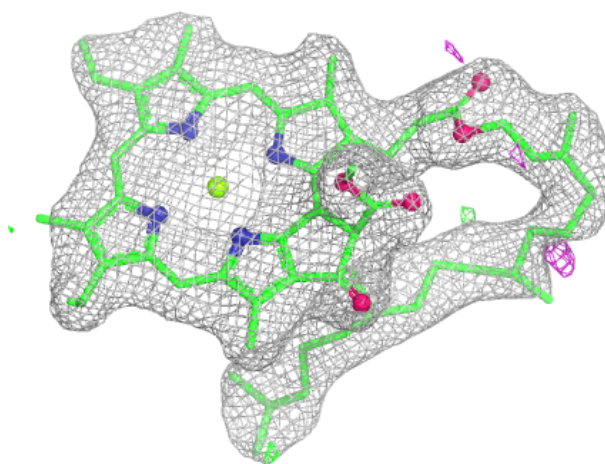
Electron density around LHG D 412:

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



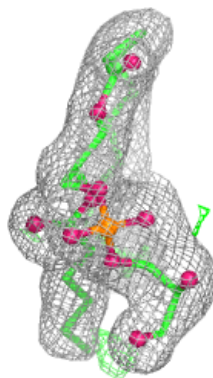
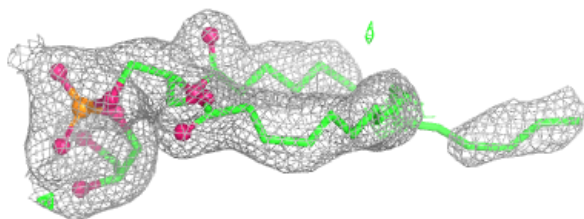
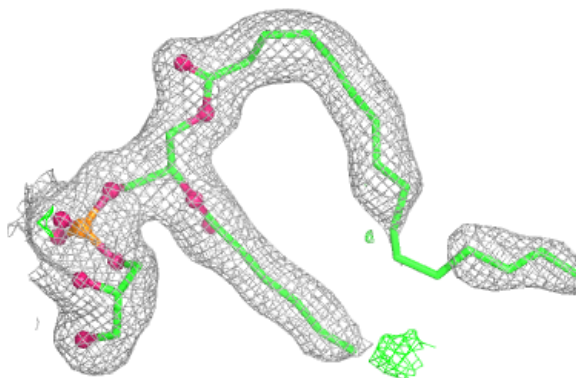
Electron density around CLA c 509:

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

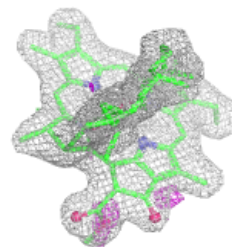
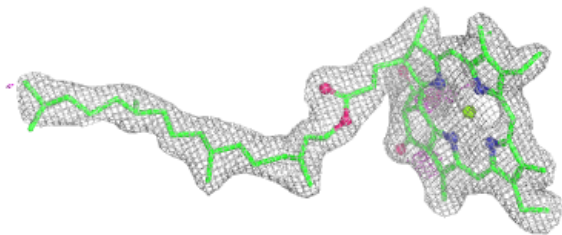
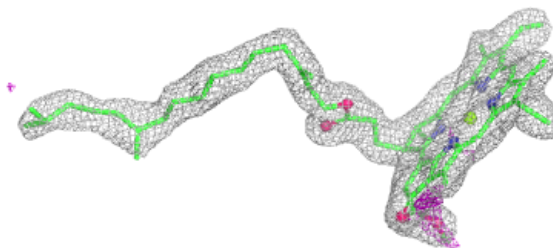


Electron density around LHG a 612:

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

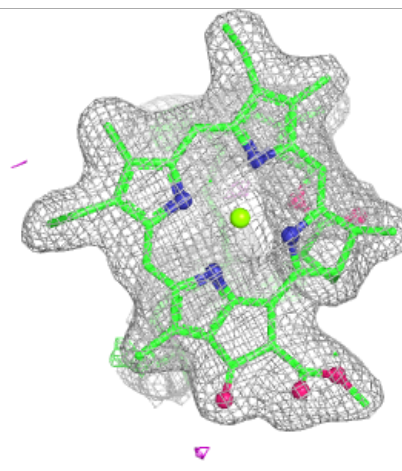
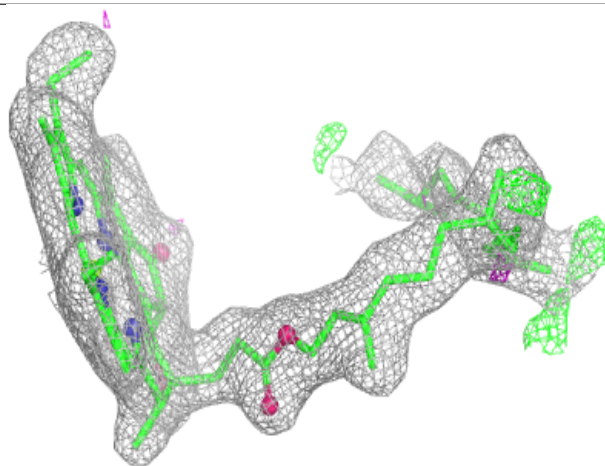
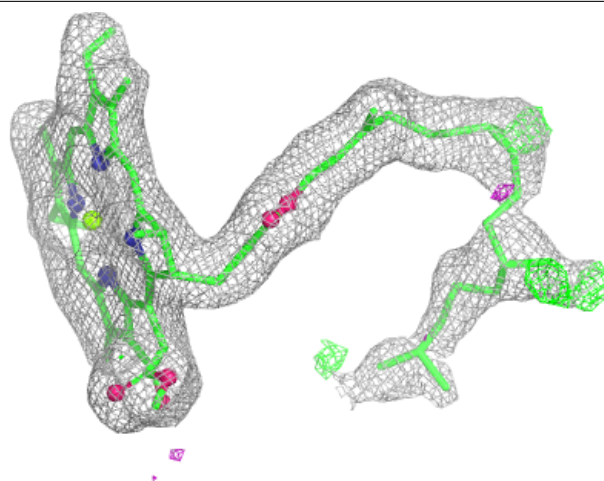
**Electron density around CLA C 502:**

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



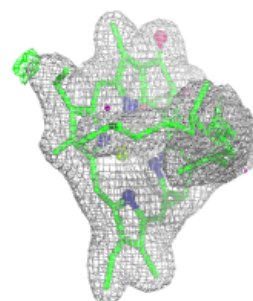
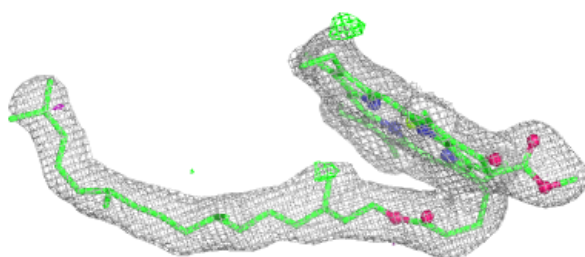
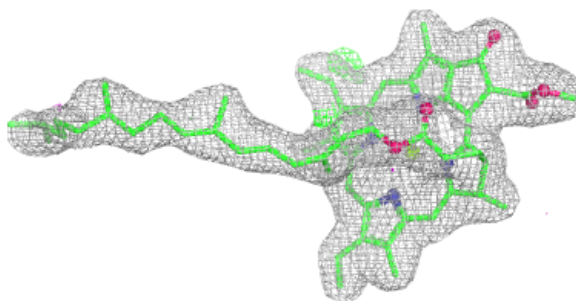
Electron density around CLA B 606:

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

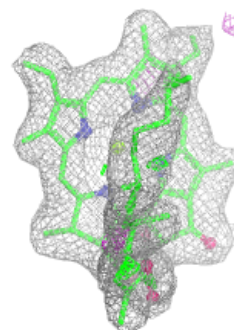
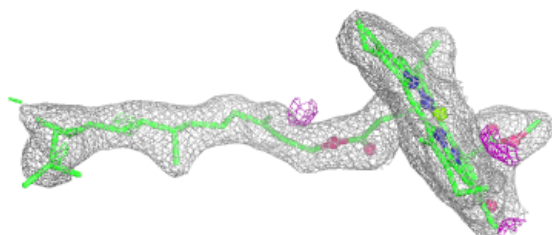
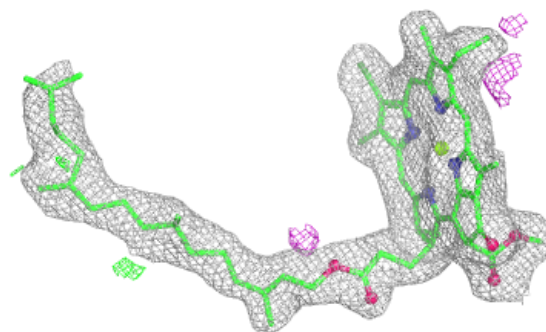


Electron density around CLA b 608:

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

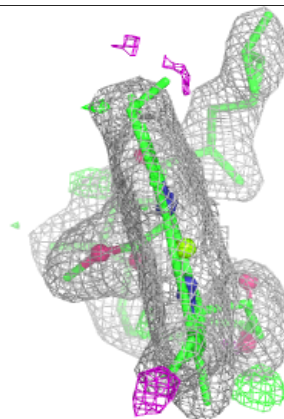
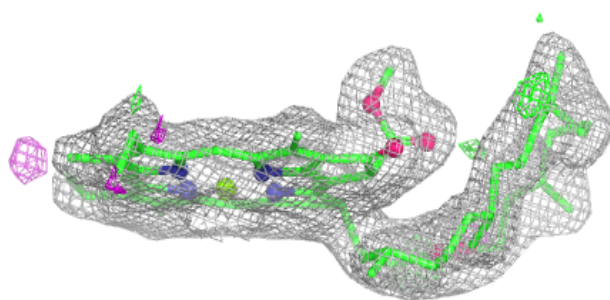
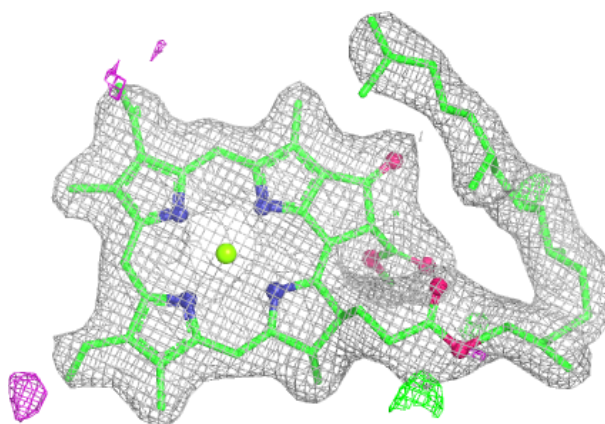
**Electron density around CLA b 609:**

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



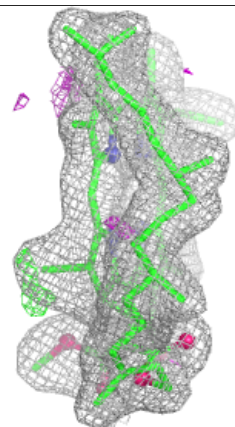
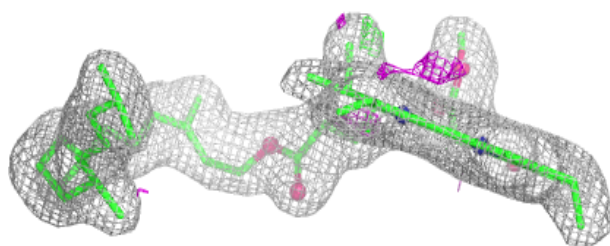
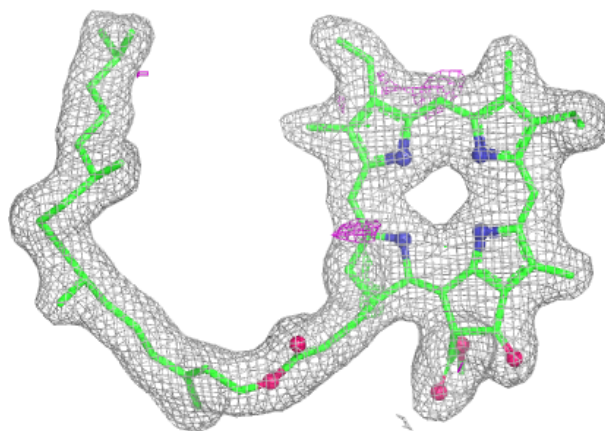
Electron density around CLA b 610:

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



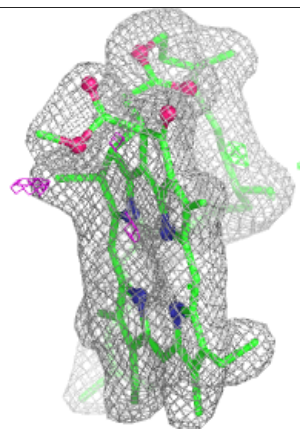
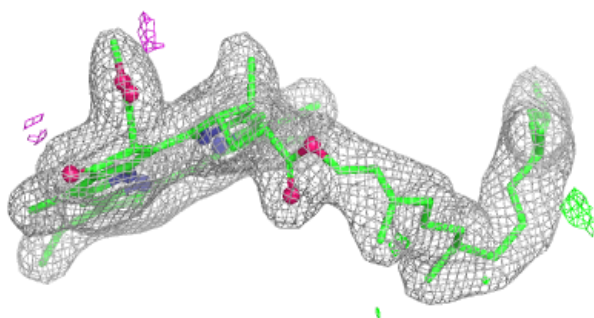
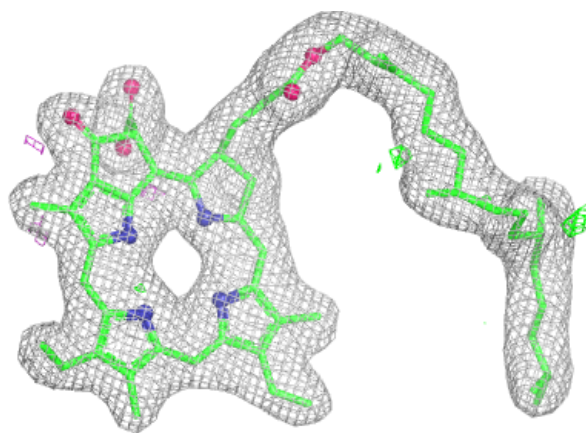
Electron density around PHO A 607:

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



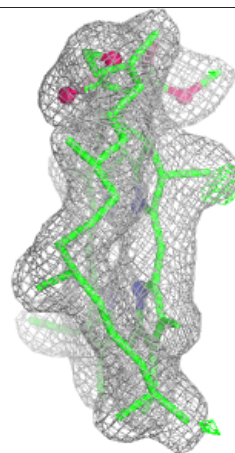
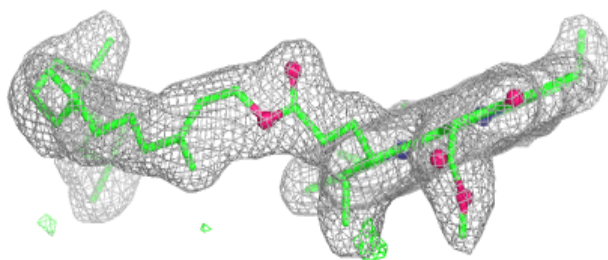
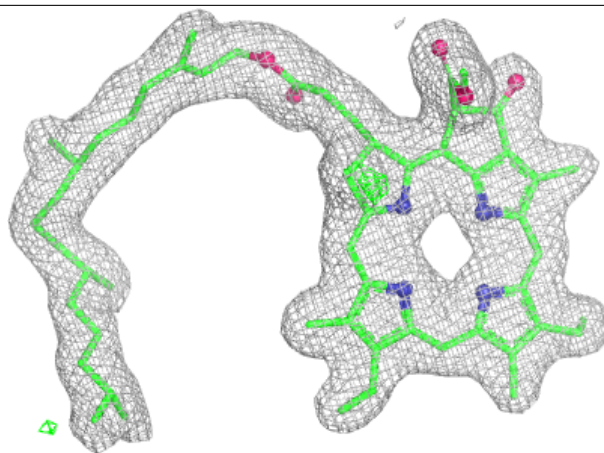
Electron density around PHO A 608:

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



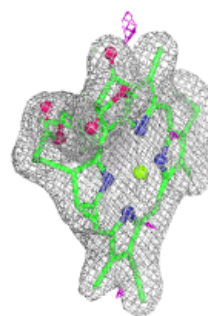
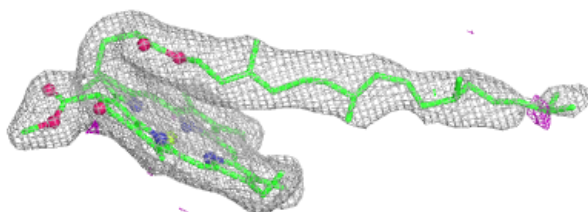
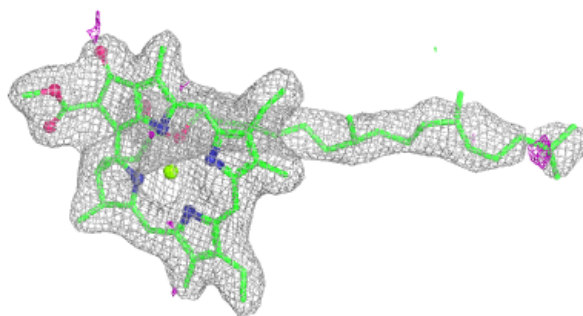
Electron density around PHO a 607:

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



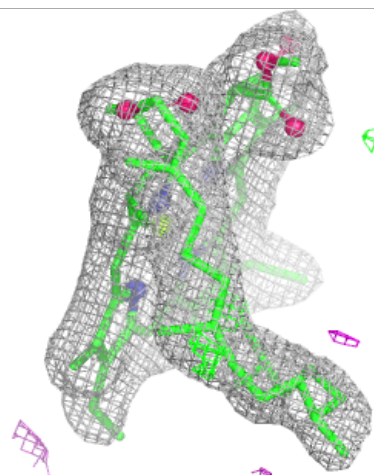
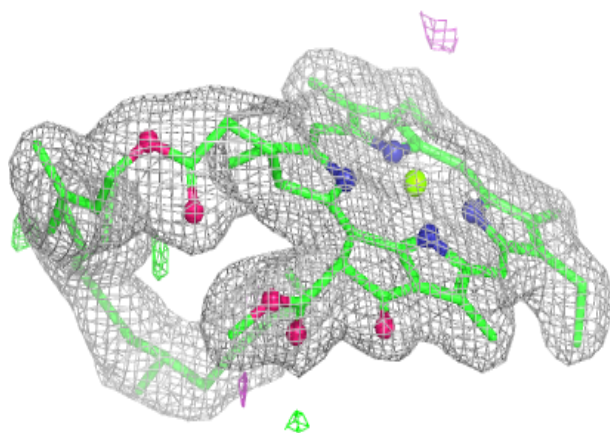
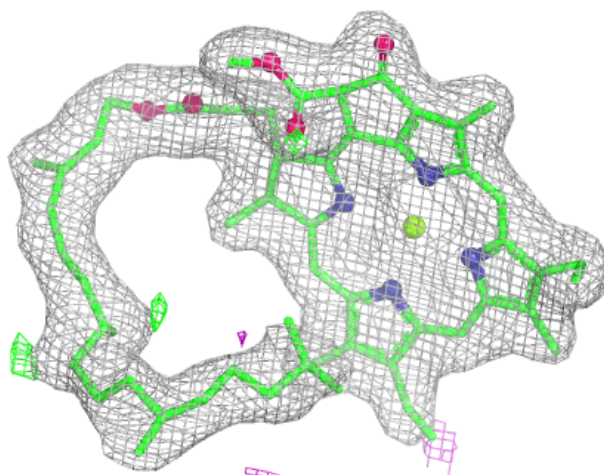
Electron density around CLA b 614:

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



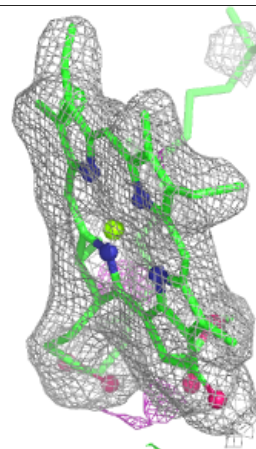
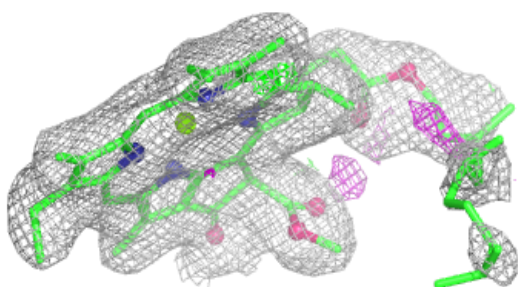
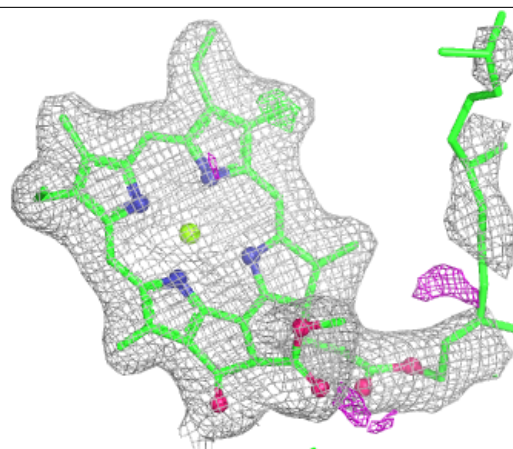
Electron density around CLA b 615:

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

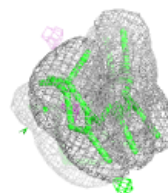
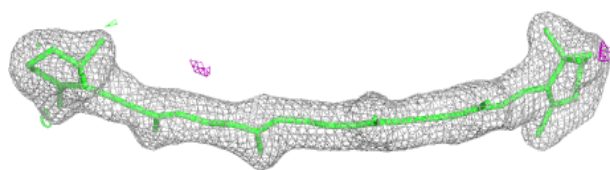
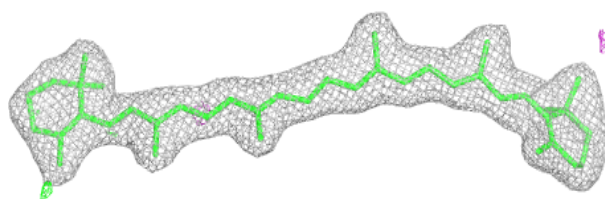


Electron density around CLA b 616:

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

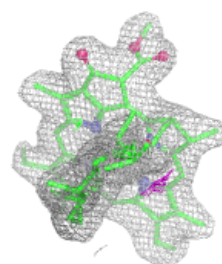
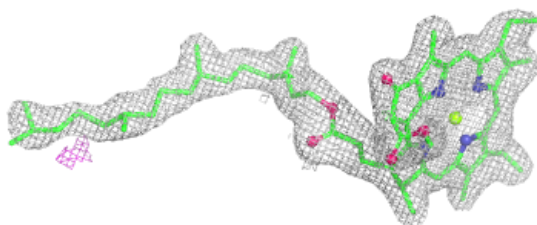
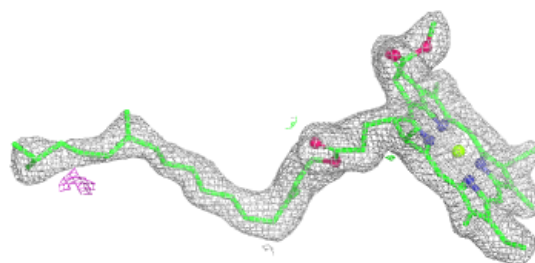
**Electron density around BCR t 101:**

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

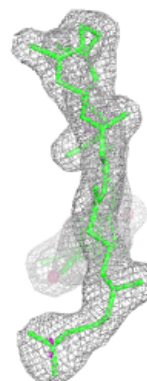
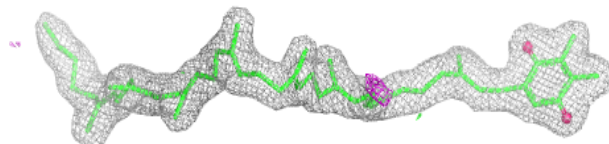
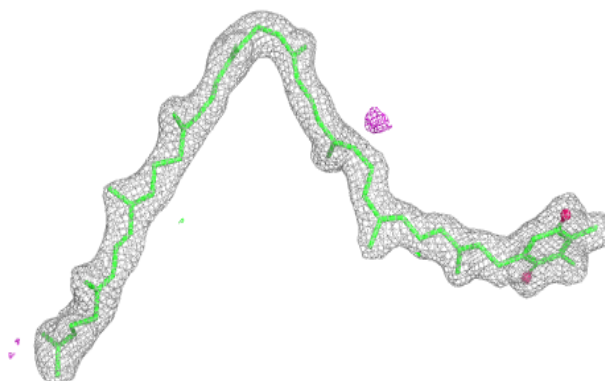


Electron density around CLA c 502:

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

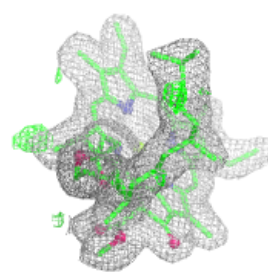
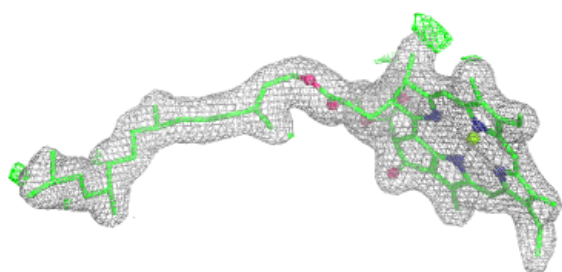
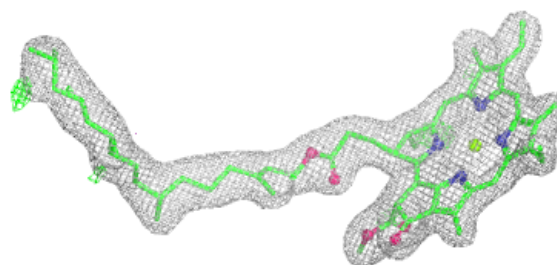
**Electron density around PL9 D 406:**

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

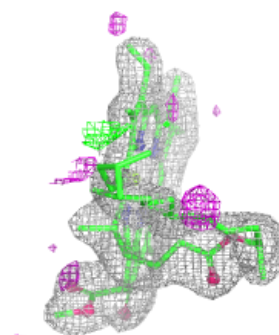
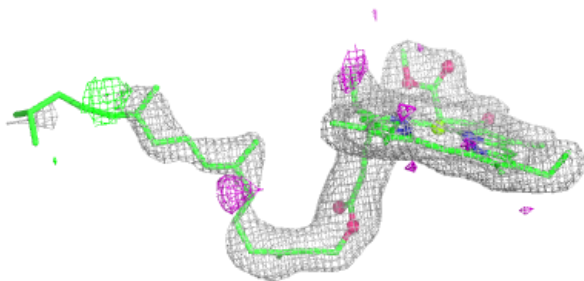
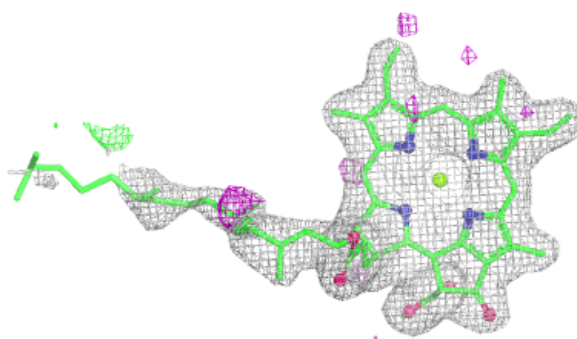


Electron density around CLA a 605:

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

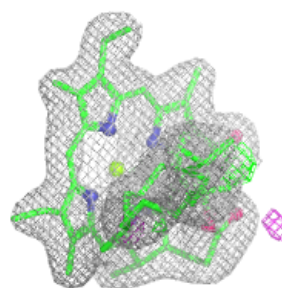
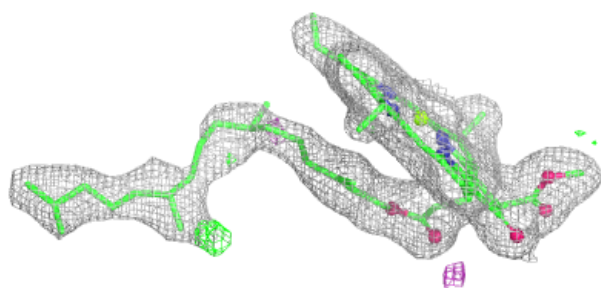
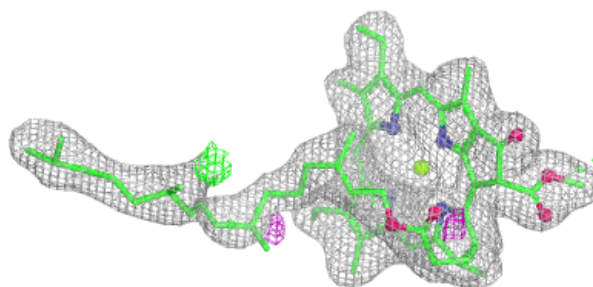
**Electron density around CLA a 606:**

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

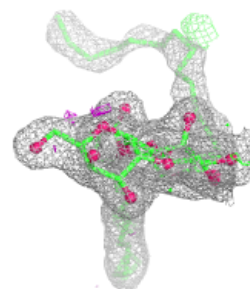
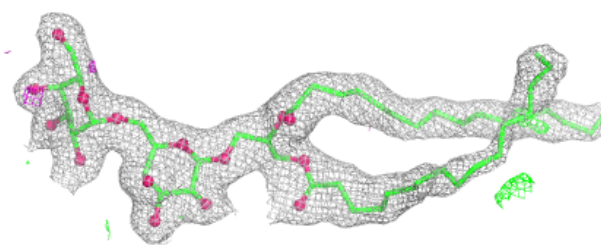
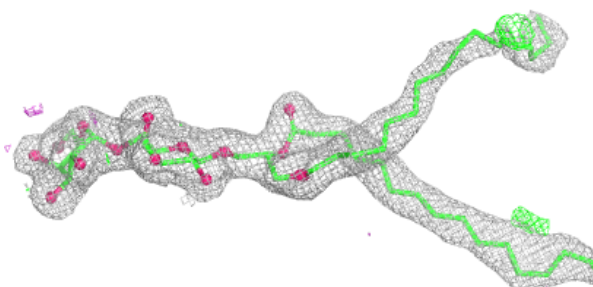


Electron density around CLA c 505:

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

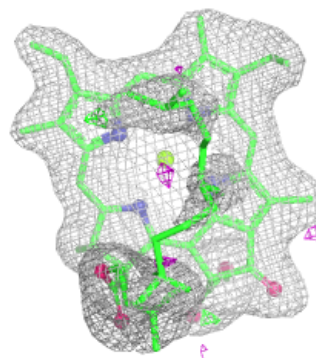
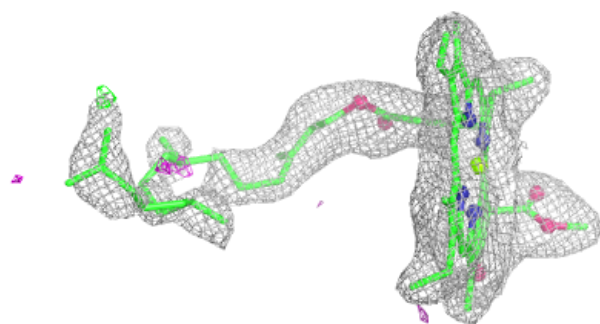
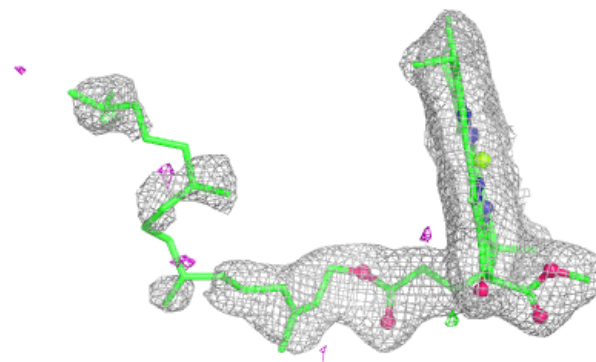
**Electron density around DGD C 523:**

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



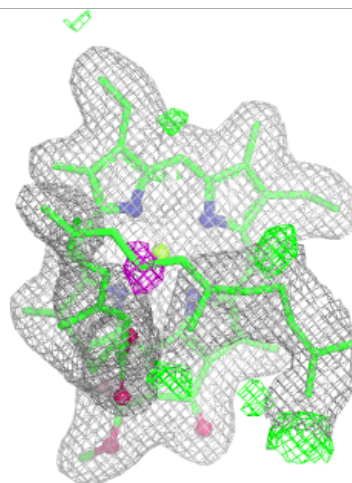
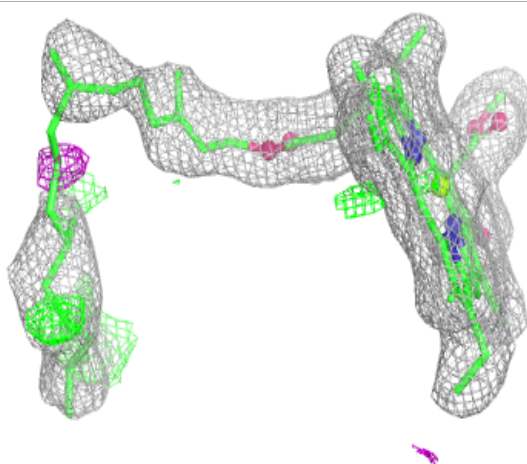
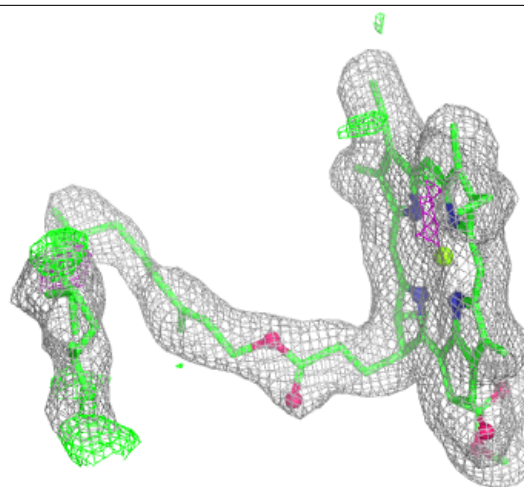
Electron density around CLA c 506:

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



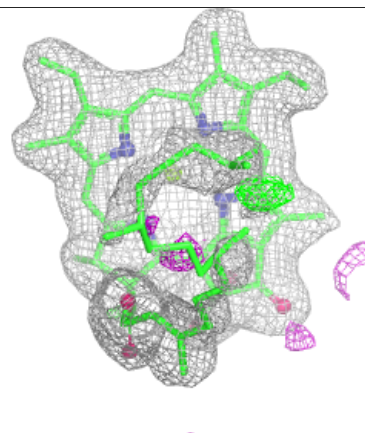
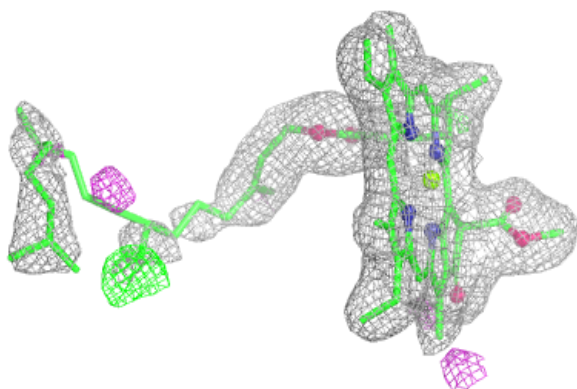
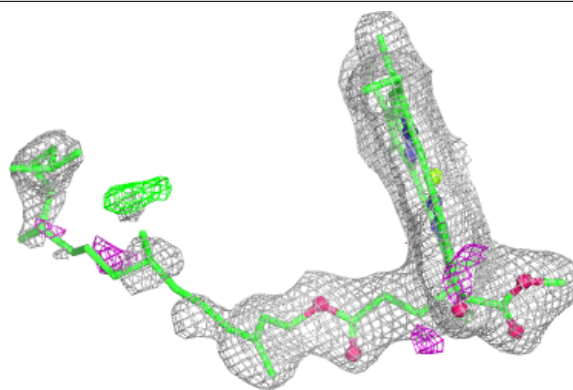
Electron density around CLA a 608:

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

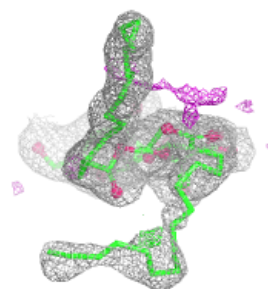
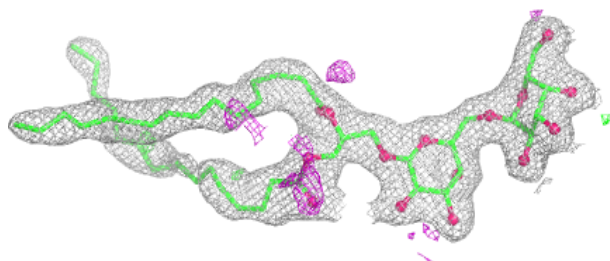
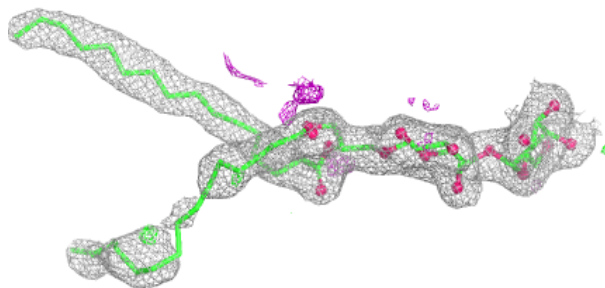


Electron density around CLA C 506:

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

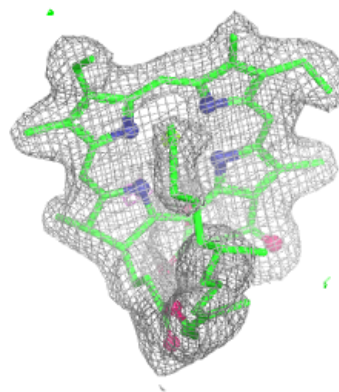
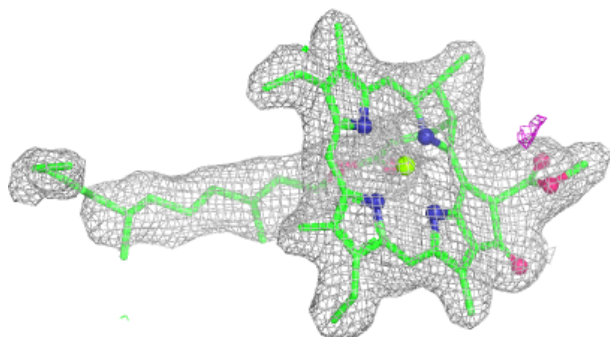
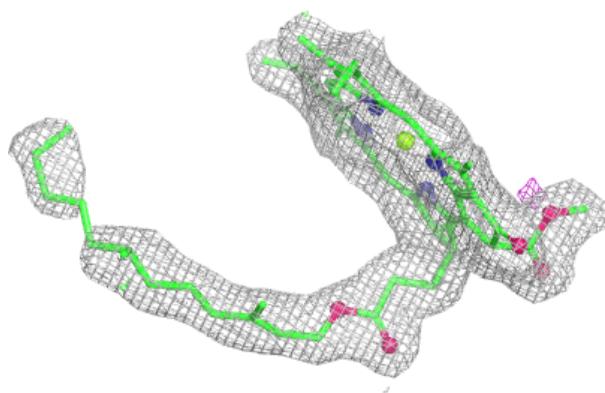
**Electron density around DGD c 519:**

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



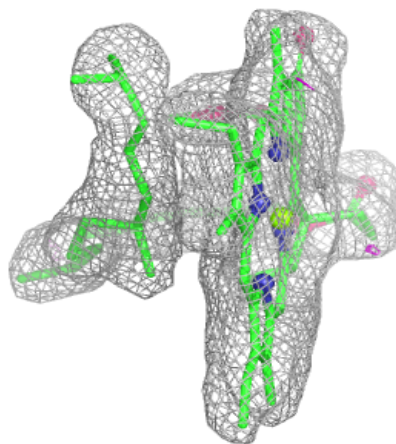
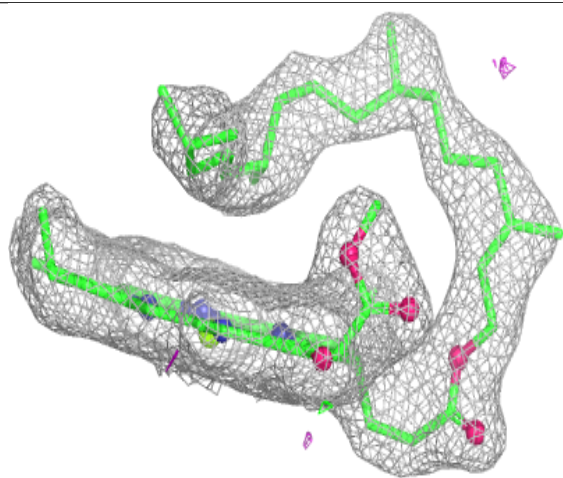
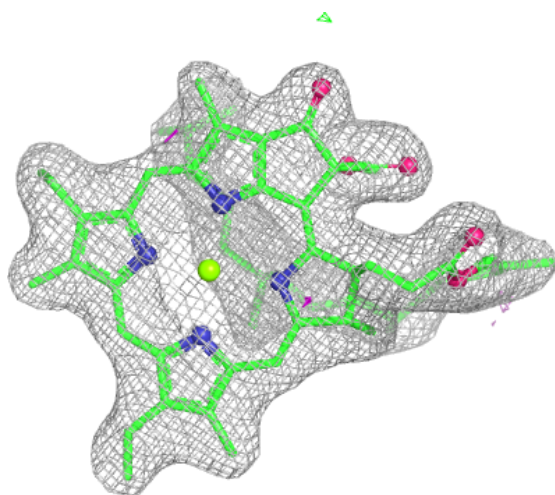
Electron density around CLA C 504:

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



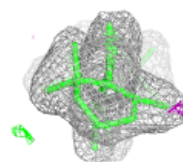
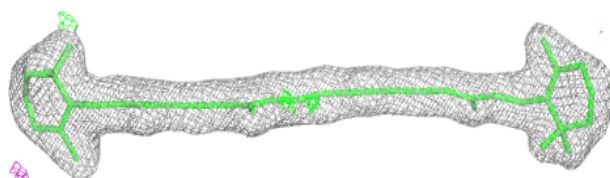
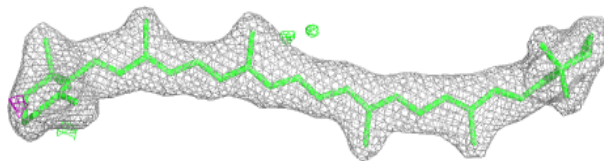
Electron density around CLA c 510:

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



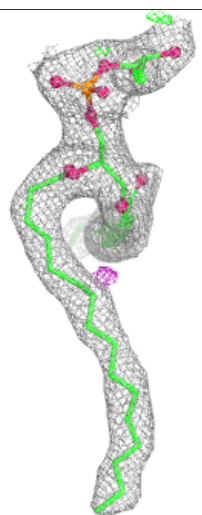
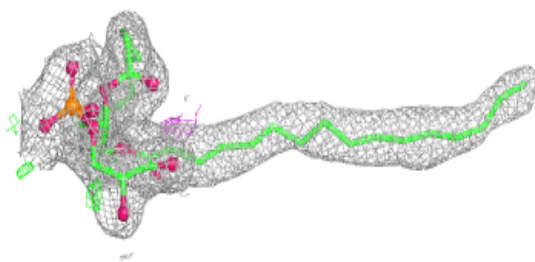
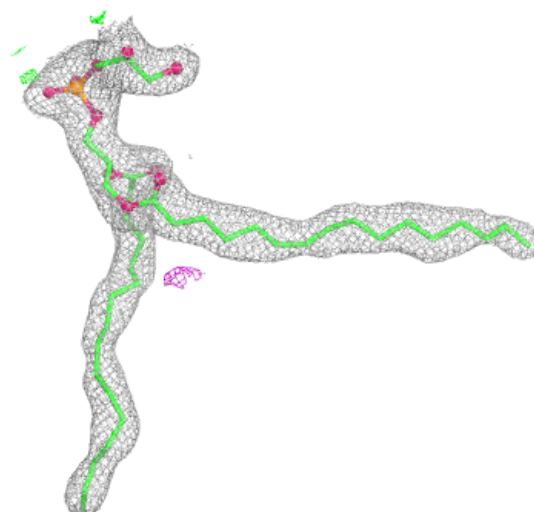
Electron density around BCR a 609:

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



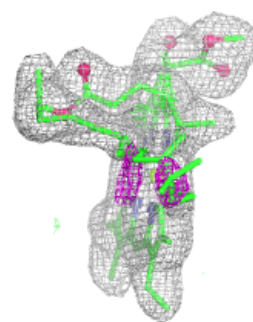
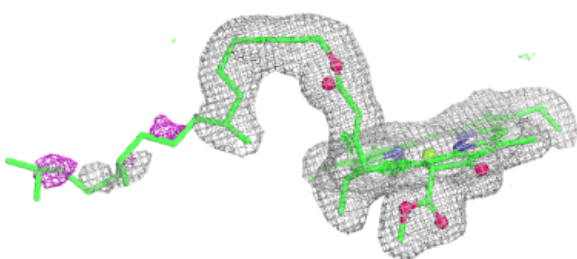
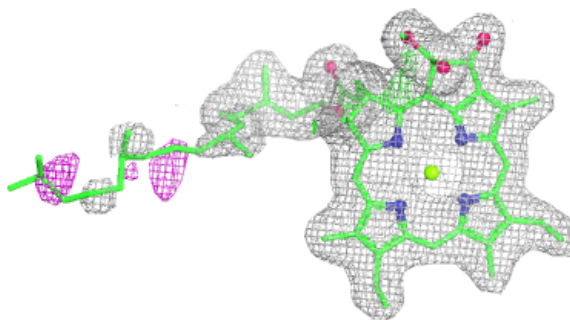
Electron density around LHG 1 101:

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

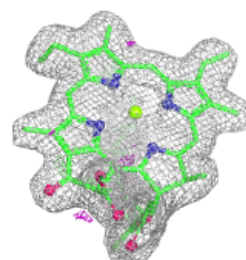
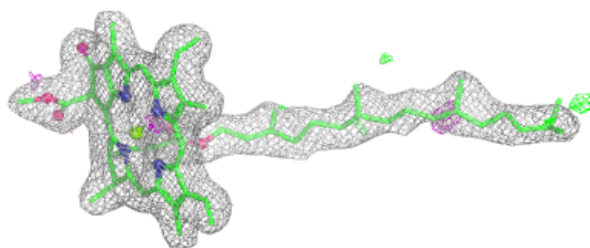
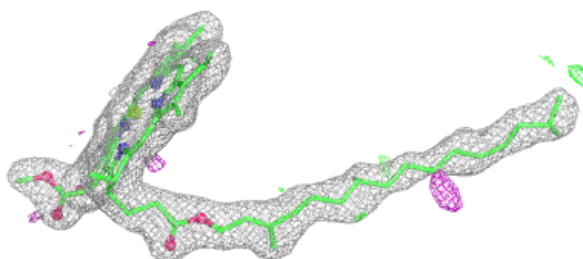


Electron density around CLA A 606:

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

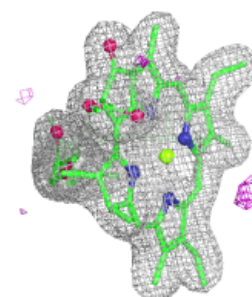
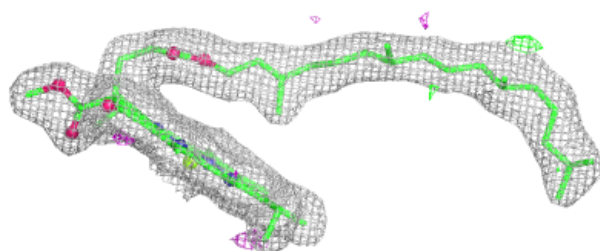
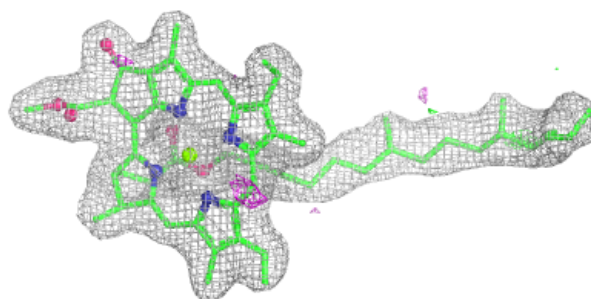
**Electron density around CLA B 607:**

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

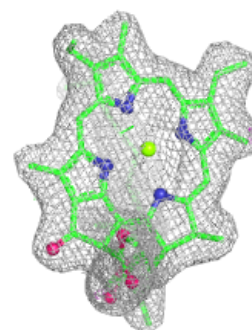
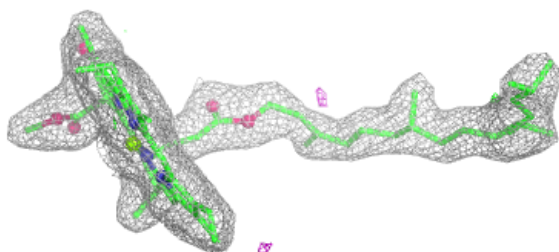
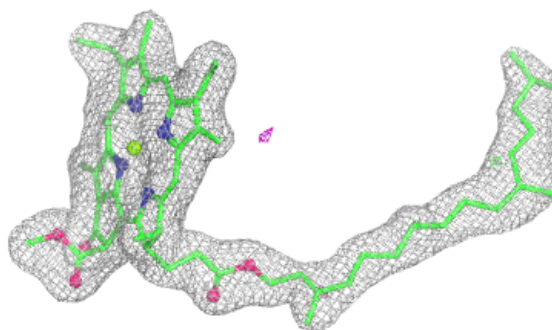


Electron density around CLA B 608:

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

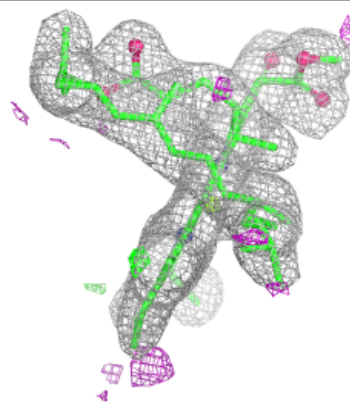
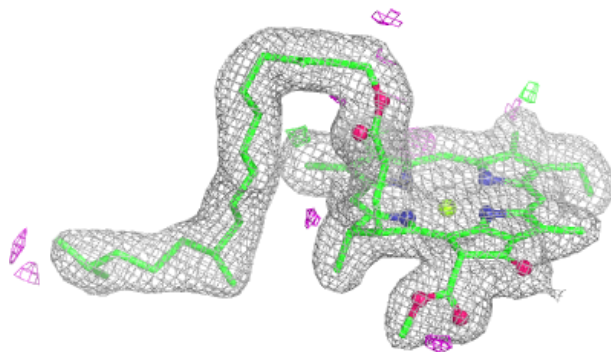
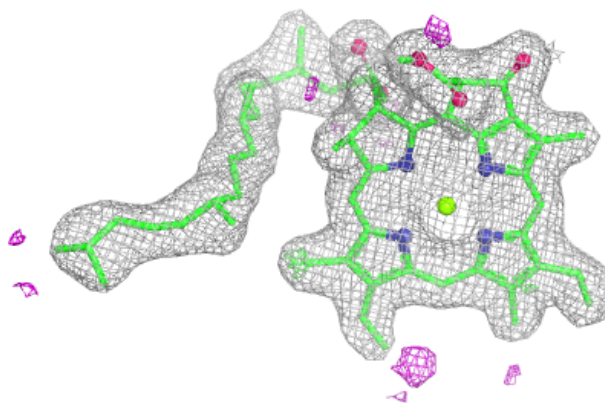
**Electron density around CLA B 609:**

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

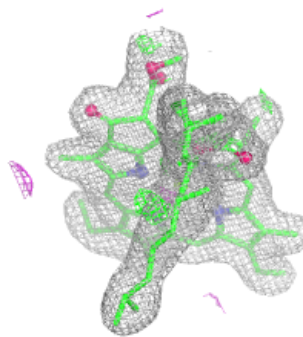
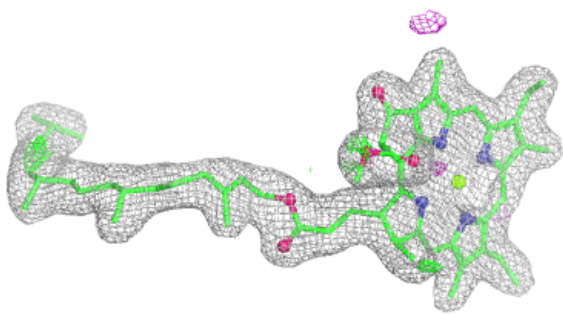
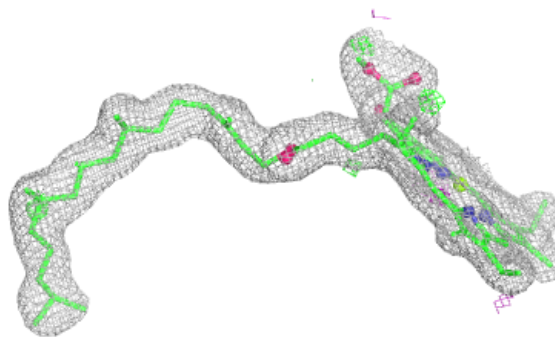


Electron density around CLA D 402:

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

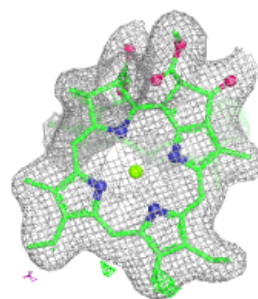
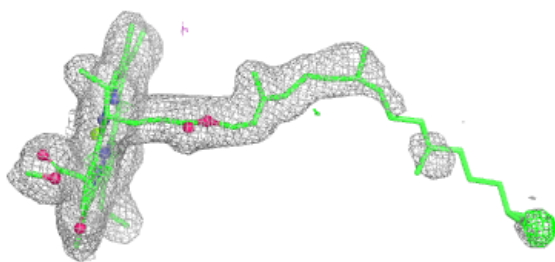
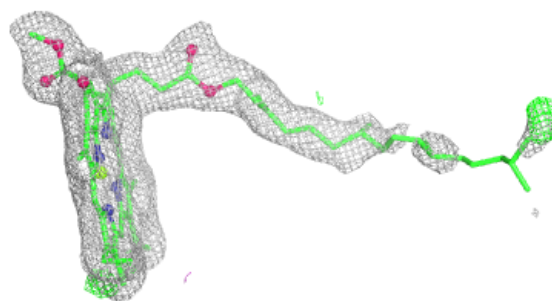
**Electron density around CLA D 403:**

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



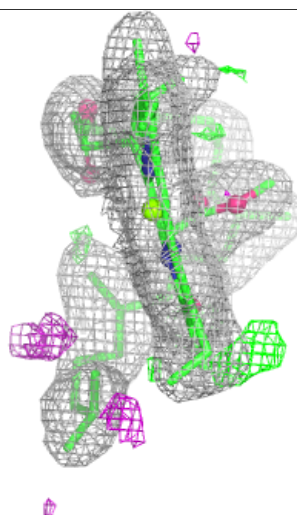
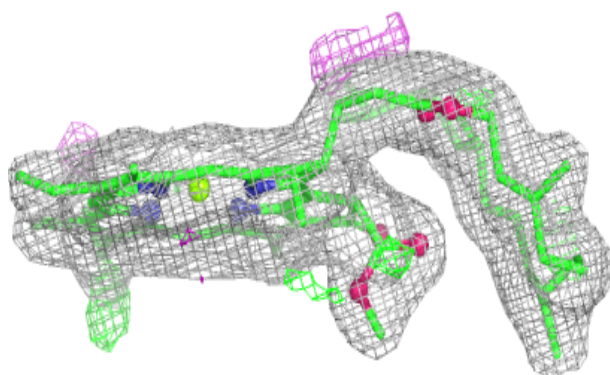
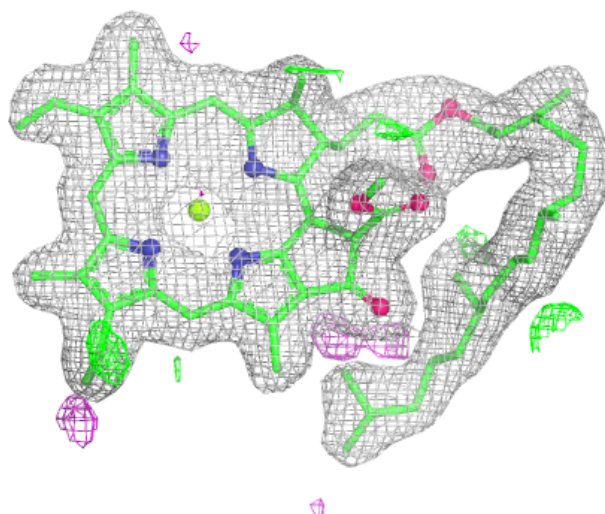
Electron density around CLA D 404:

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



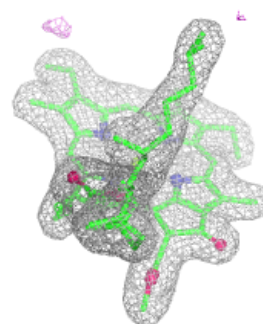
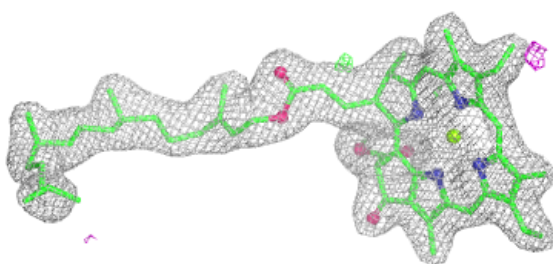
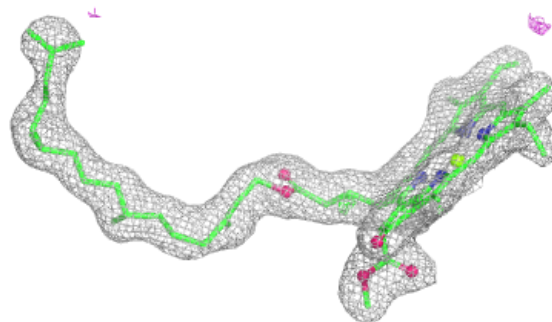
Electron density around CLA B 610:

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

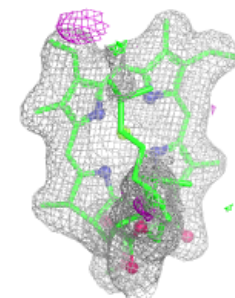
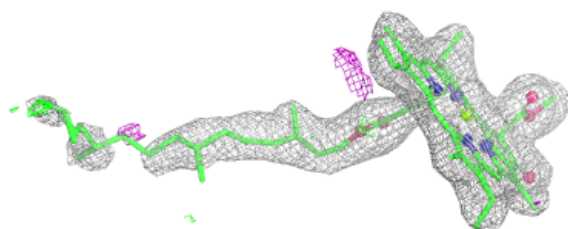
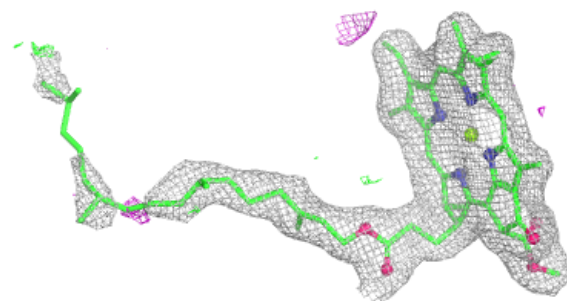


Electron density around CLA d 403:

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

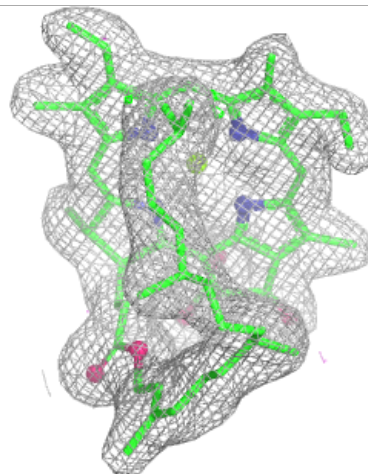
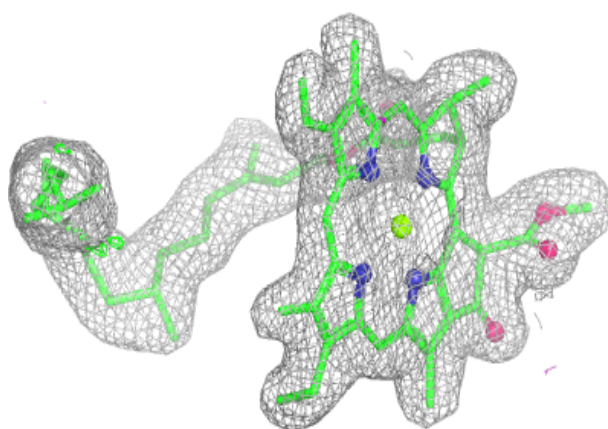
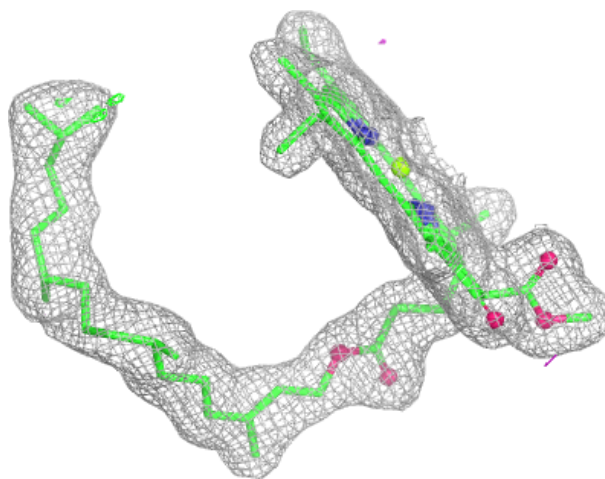
**Electron density around CLA d 404:**

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



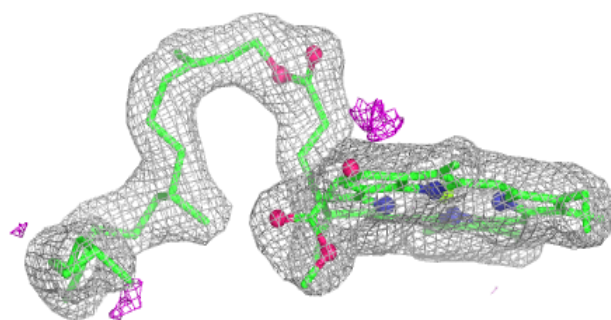
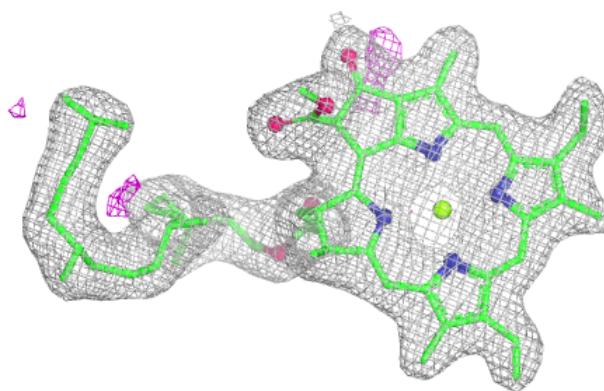
Electron density around CLA B 611:

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

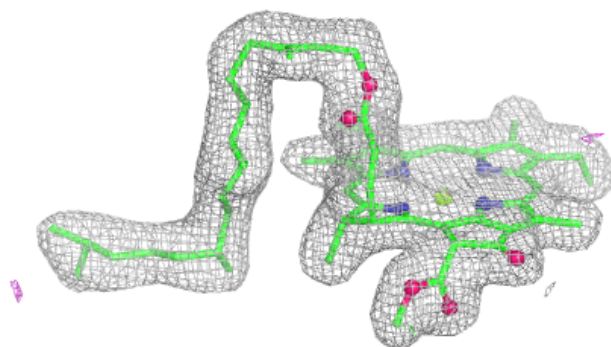
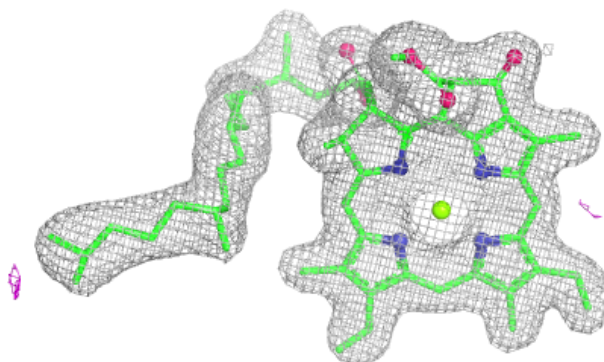


Electron density around CLA B 612:

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

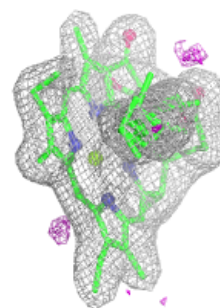
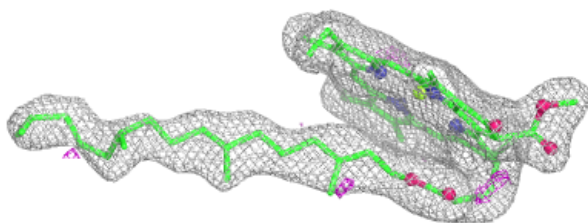
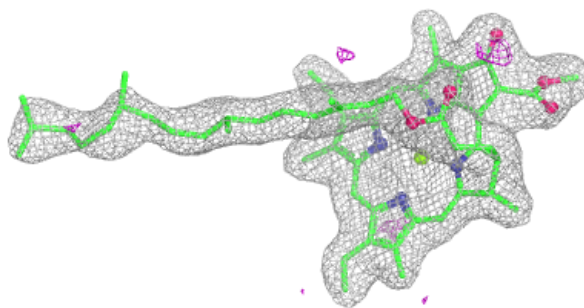
**Electron density around CLA a 611:**

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

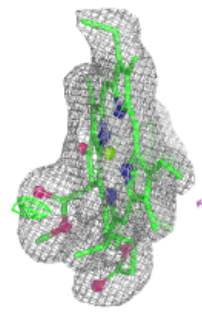
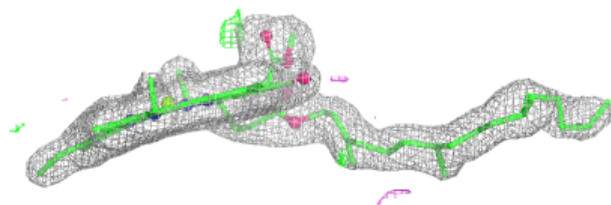
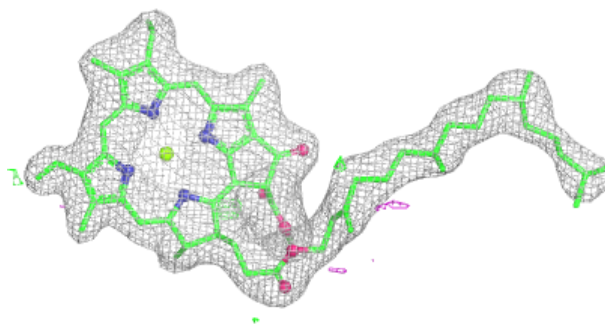


Electron density around CLA B 614:

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

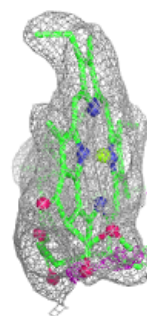
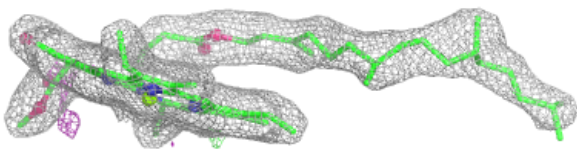
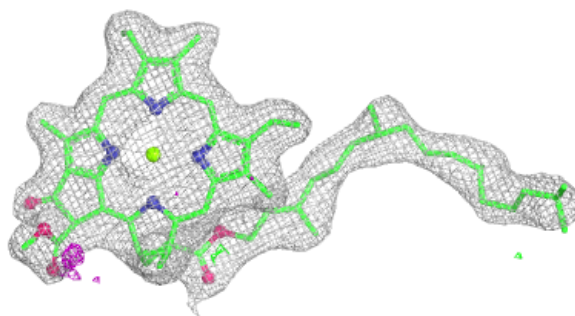
**Electron density around CLA b 602:**

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

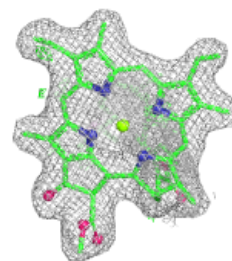
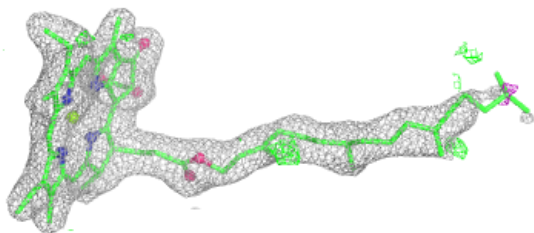
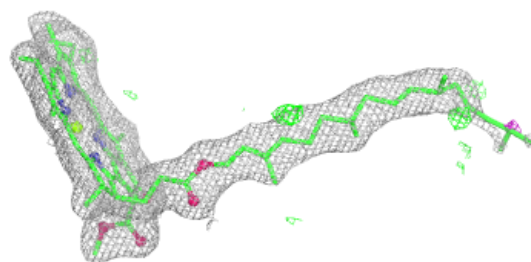


Electron density around CLA b 603:

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

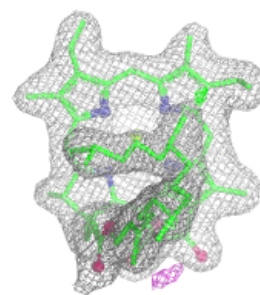
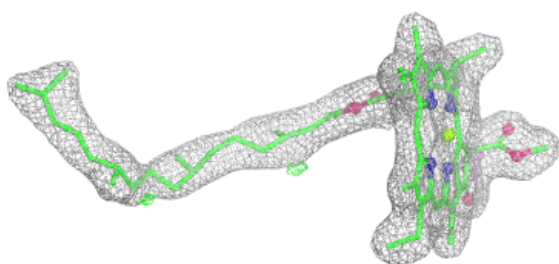
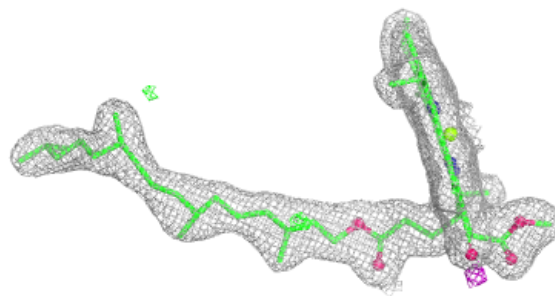
**Electron density around CLA b 604:**

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



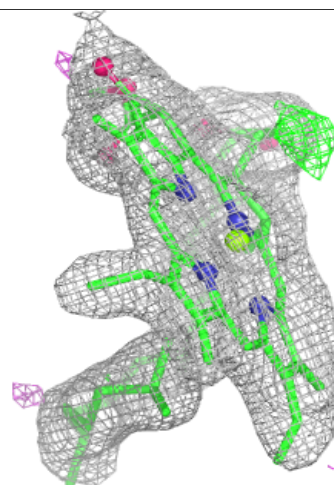
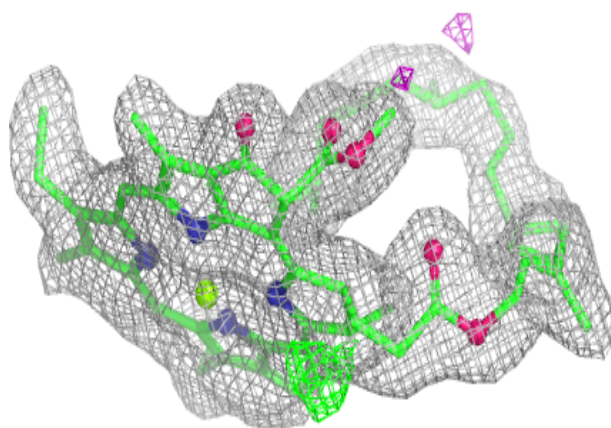
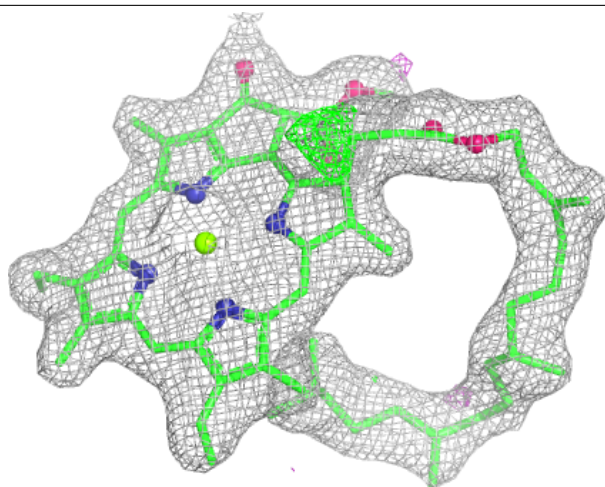
Electron density around CLA b 605:

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



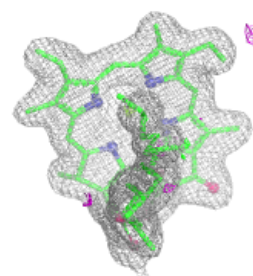
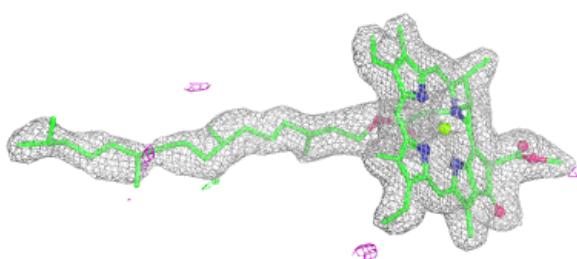
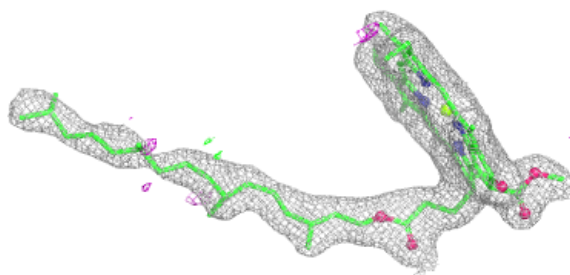
Electron density around CLA B 615:

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



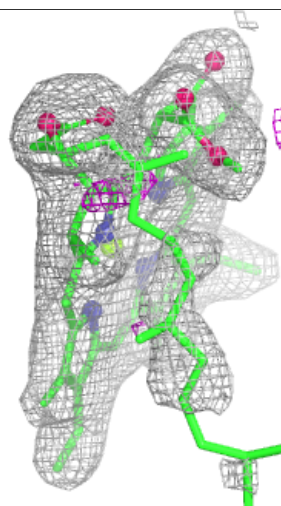
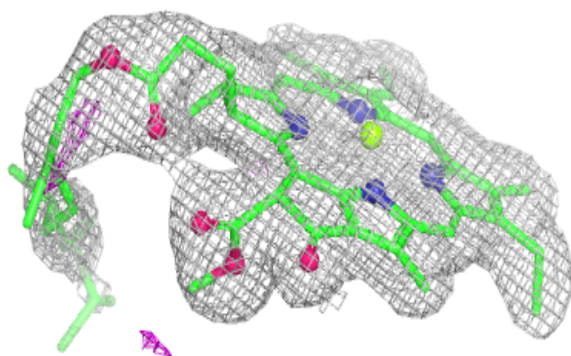
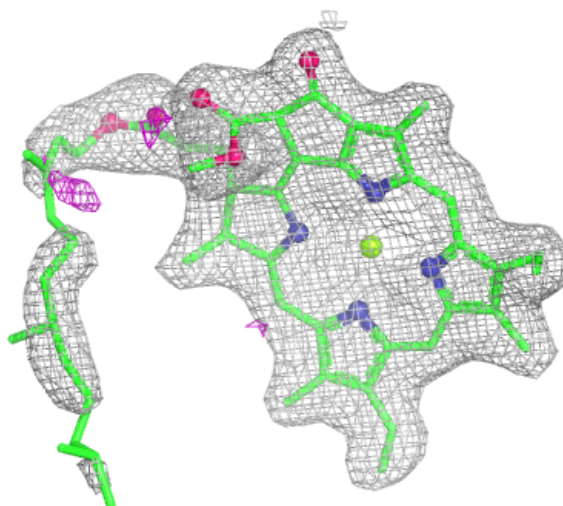
Electron density around CLA b 607:

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



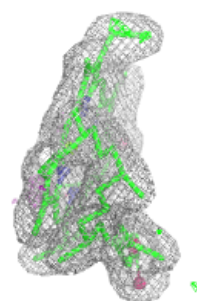
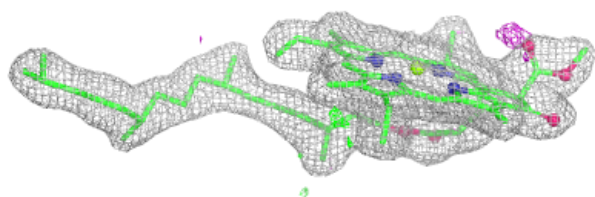
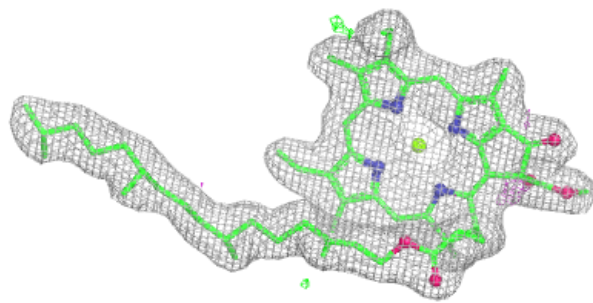
Electron density around CLA B 616:

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

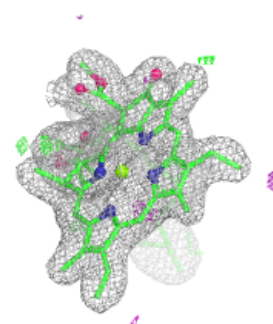
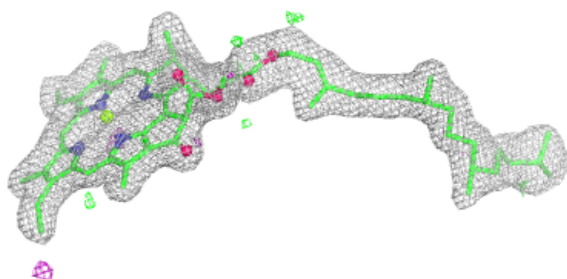
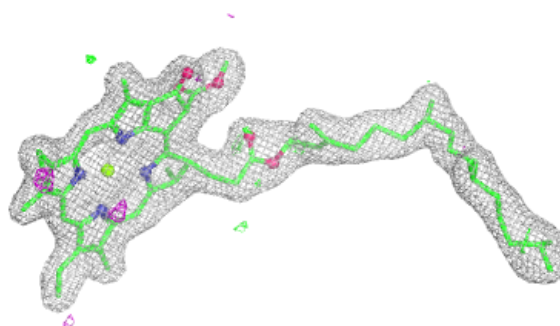


Electron density around CLA C 501:

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

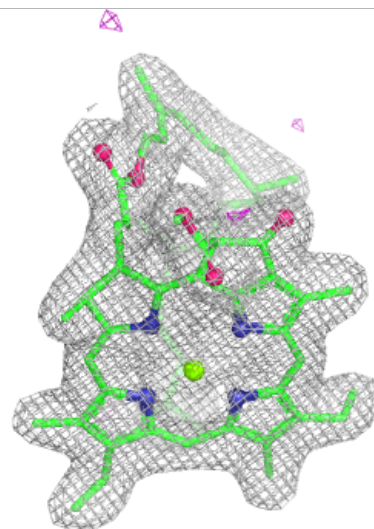
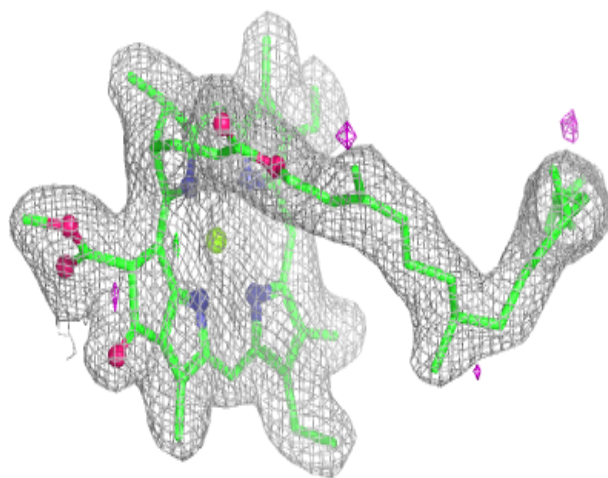
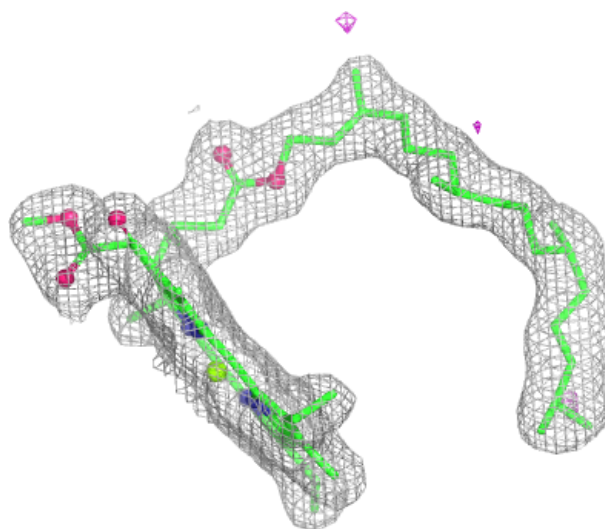
**Electron density around CLA A 605:**

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



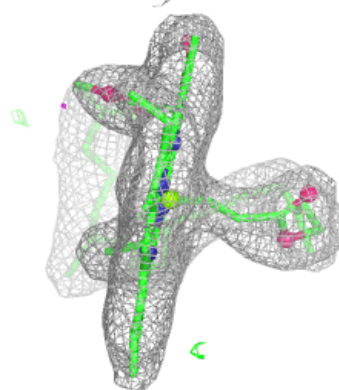
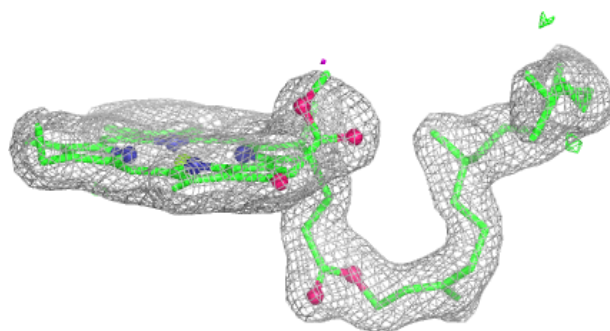
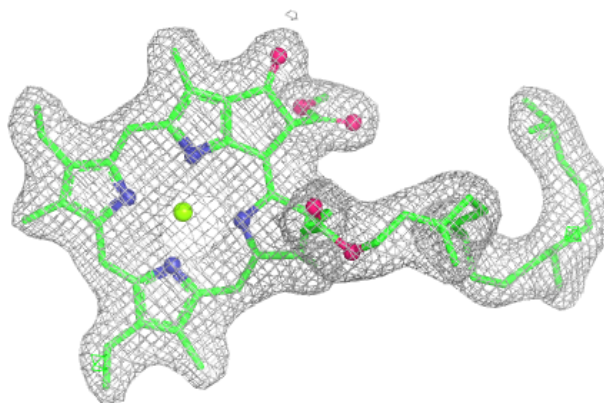
Electron density around CLA b 611:

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



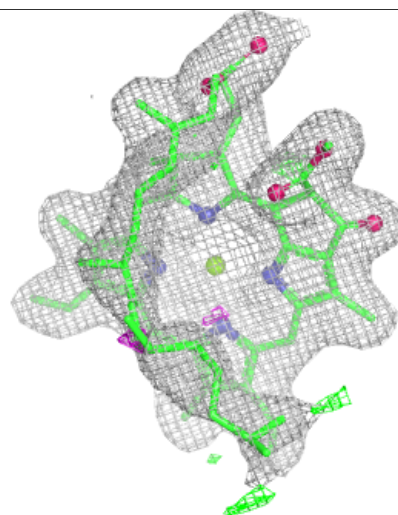
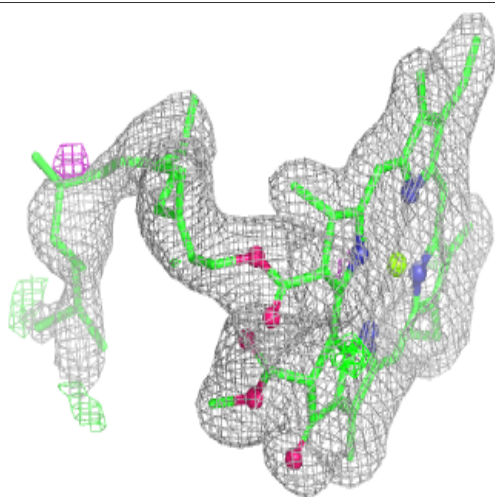
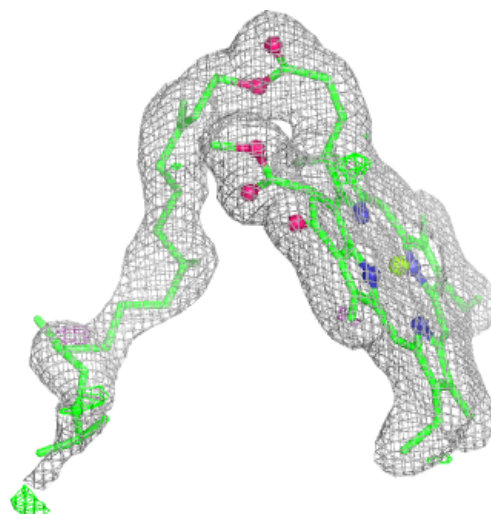
Electron density around CLA b 612:

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



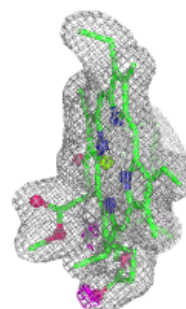
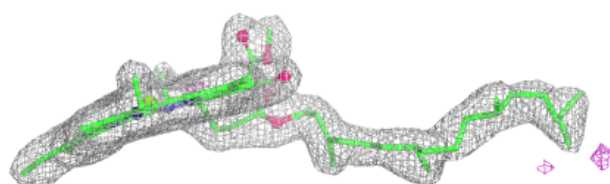
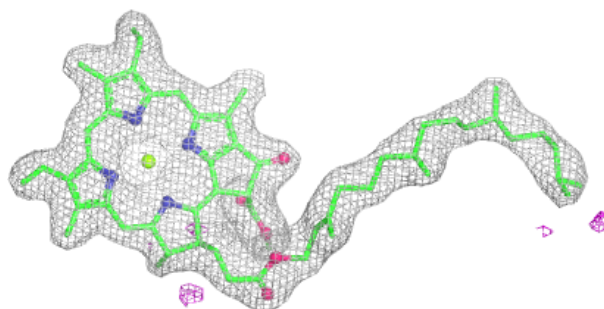
Electron density around CLA b 613:

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

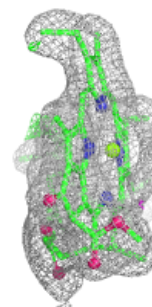
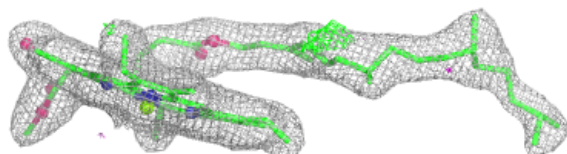
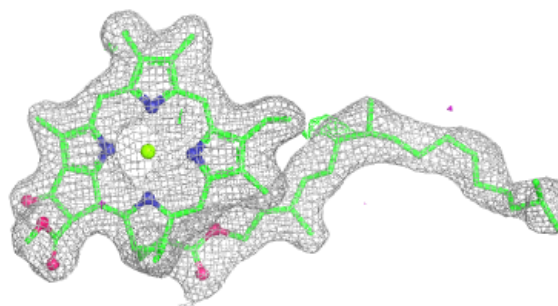


Electron density around CLA B 602:

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

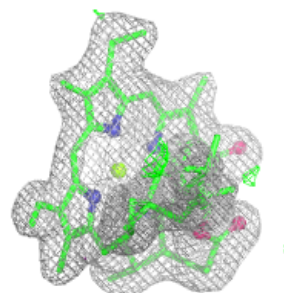
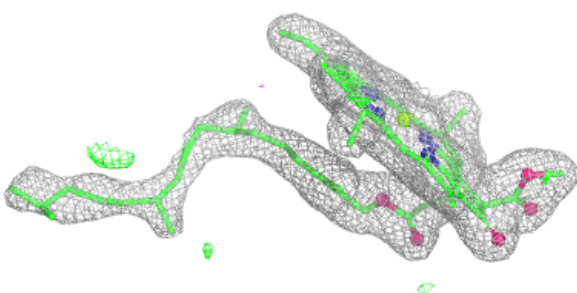
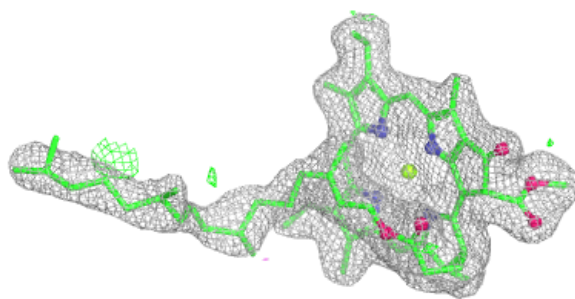
**Electron density around CLA B 603:**

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

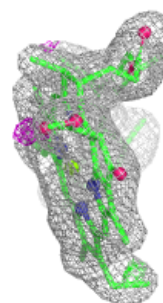
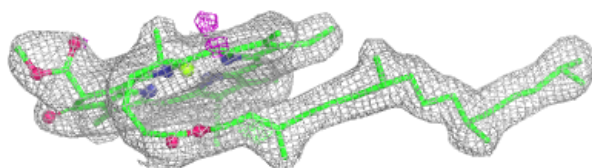
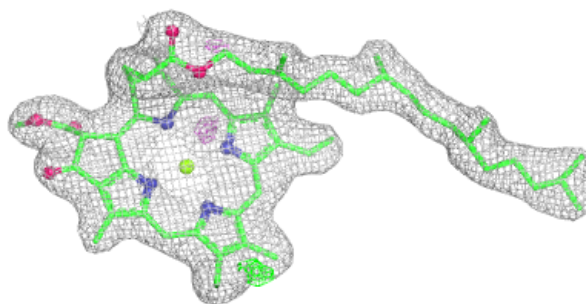


Electron density around CLA C 505:

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

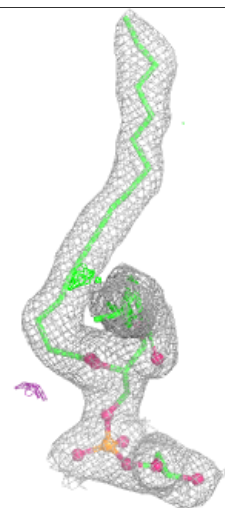
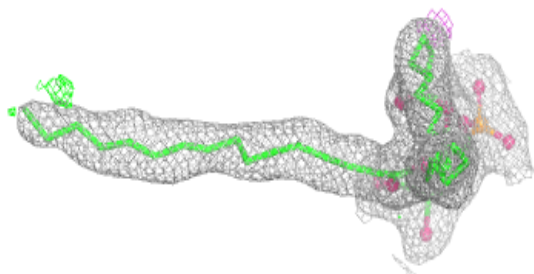
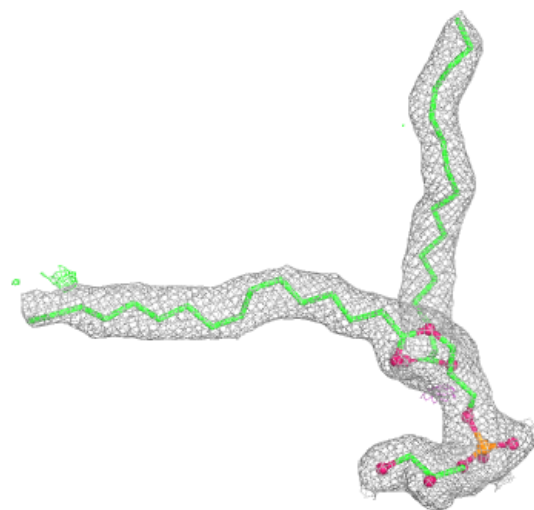
**Electron density around CLA c 501:**

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



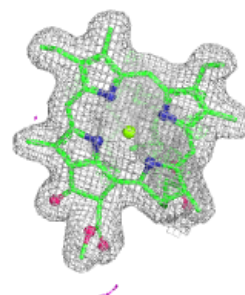
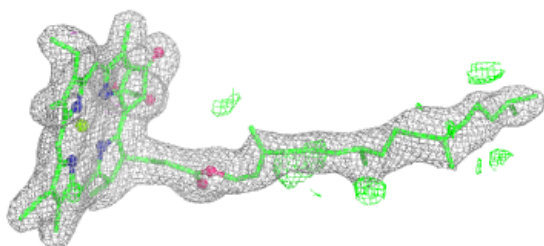
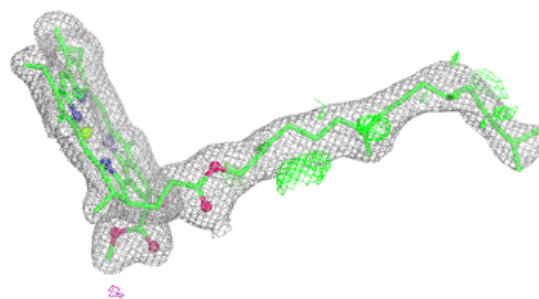
Electron density around LHG L 101:

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



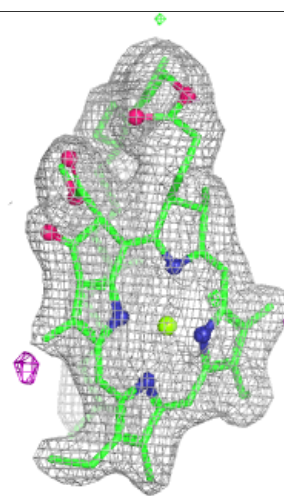
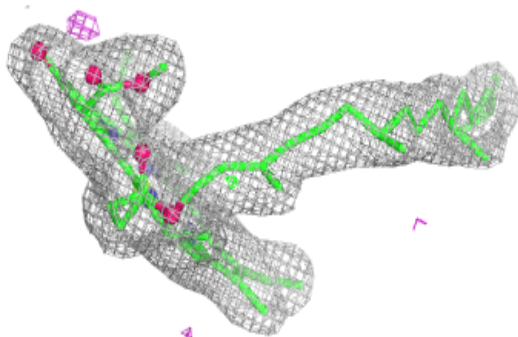
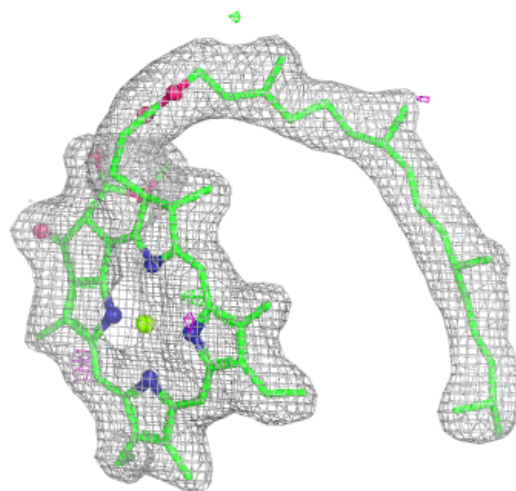
Electron density around CLA B 604:

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



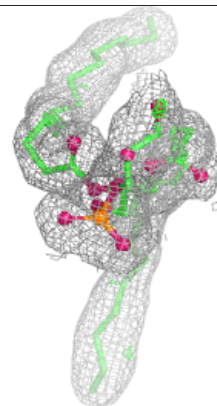
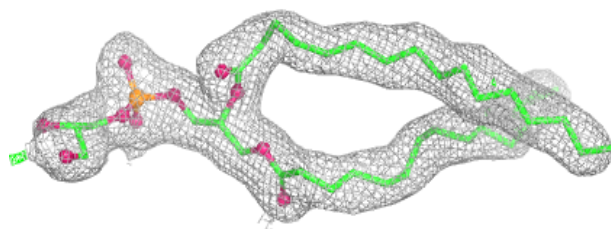
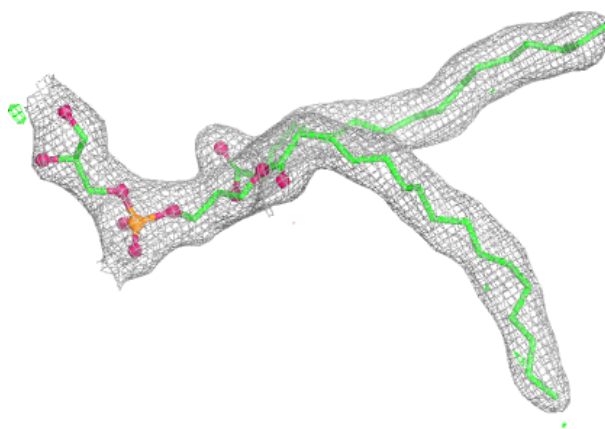
Electron density around CLA C 507:

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

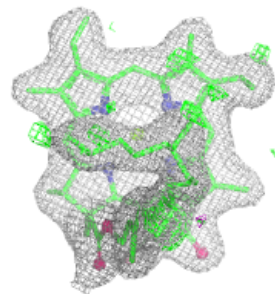
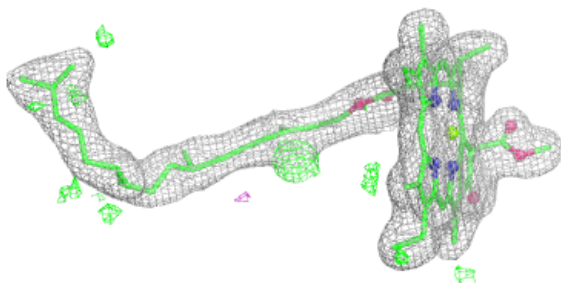
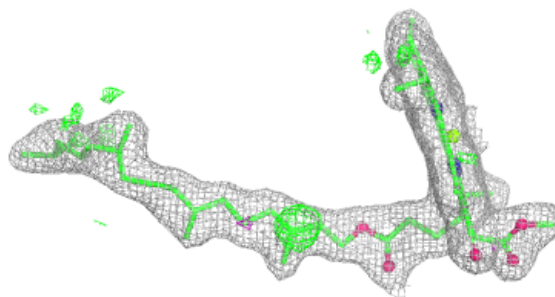


Electron density around LHG d 409:

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

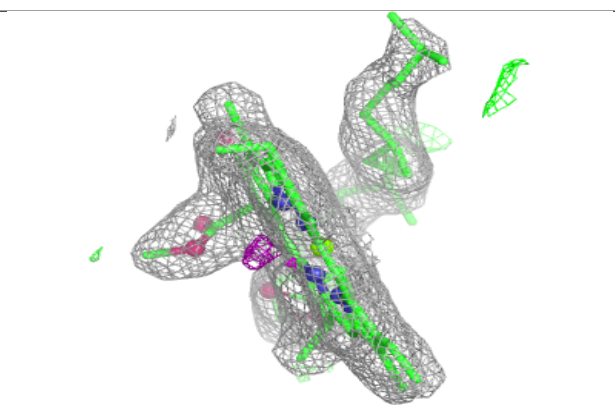
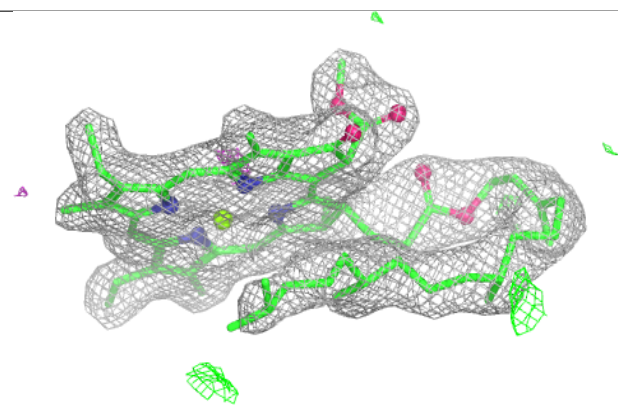
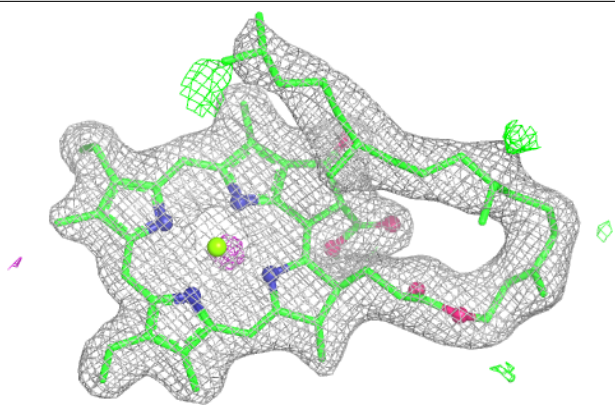
**Electron density around CLA B 605:**

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



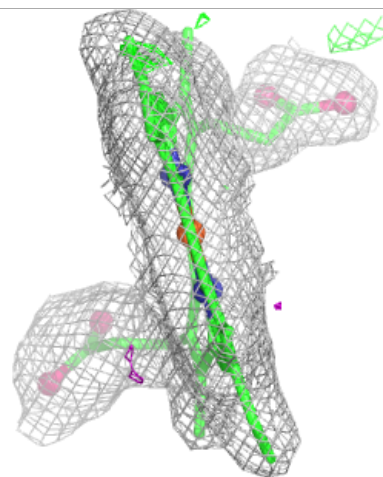
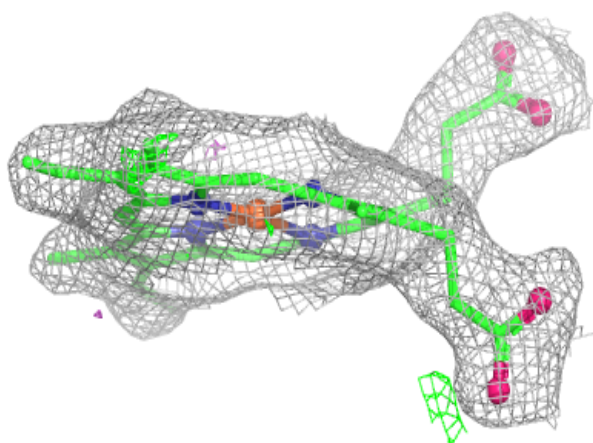
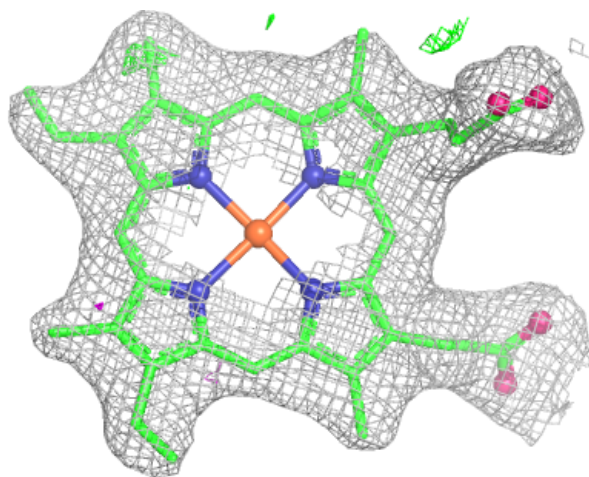
Electron density around CLA C 509:

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



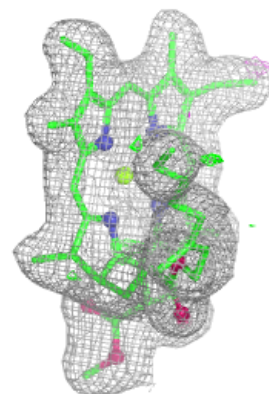
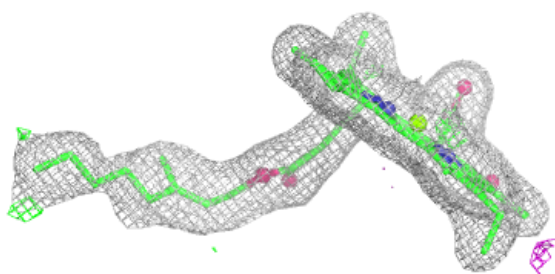
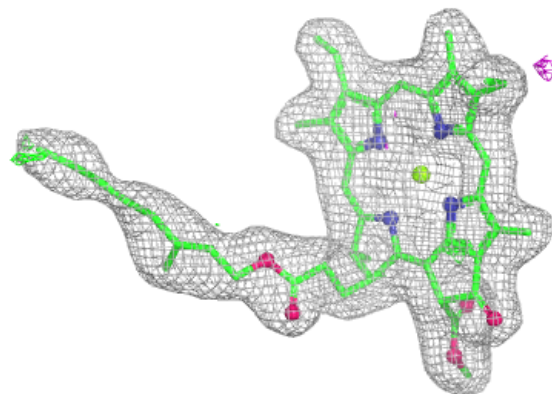
Electron density around HEM F 101:

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



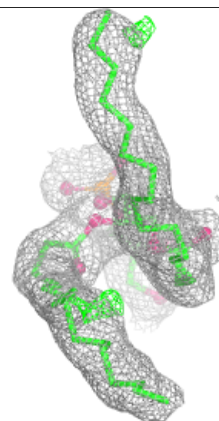
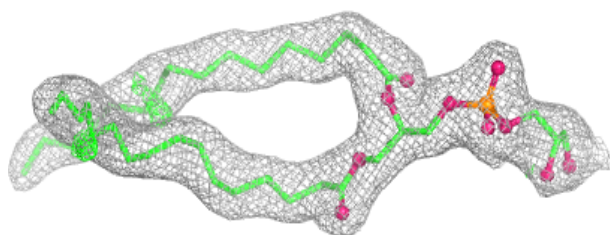
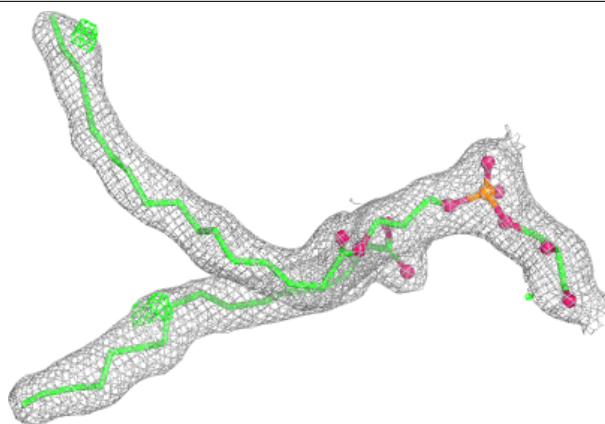
Electron density around CLA A 609:

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



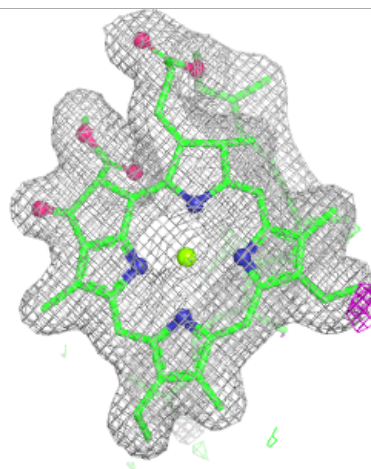
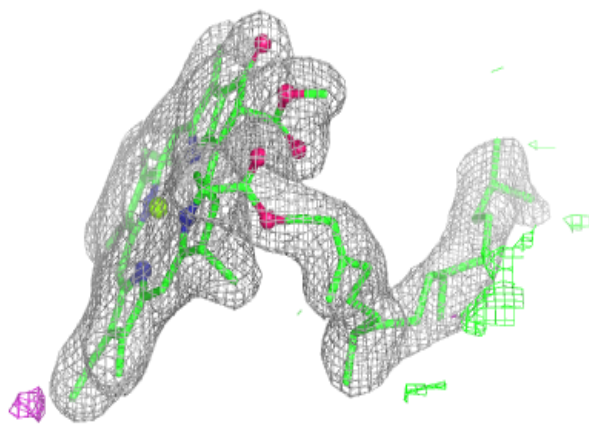
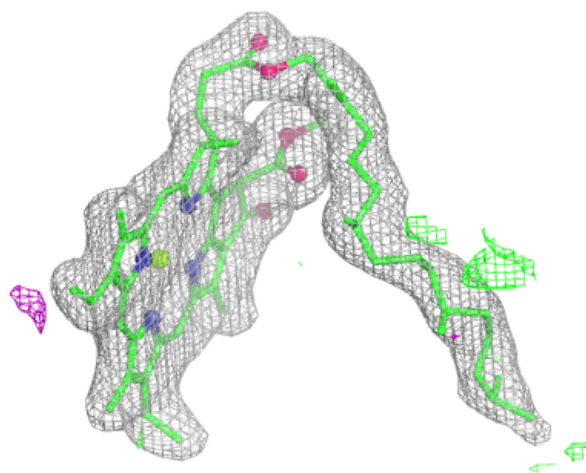
Electron density around LHG D 410:

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



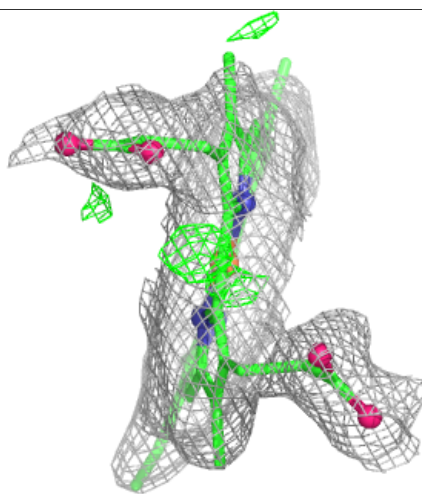
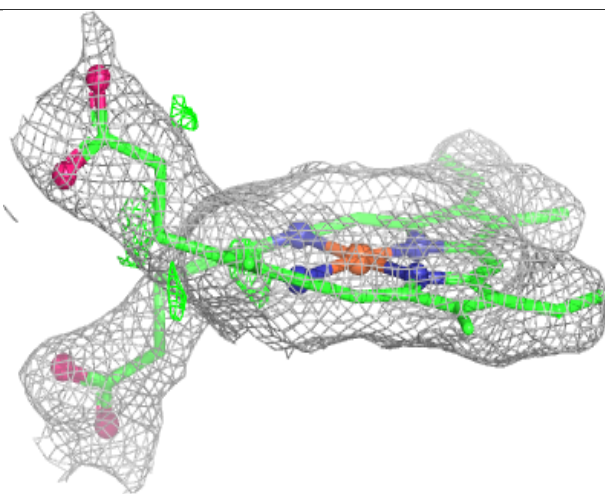
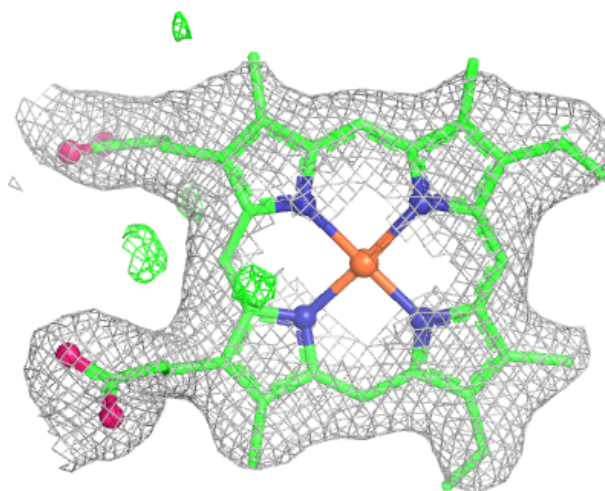
Electron density around CLA B 613:

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



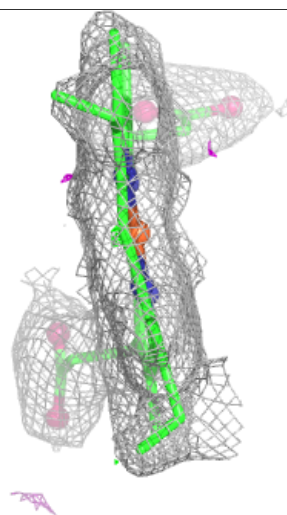
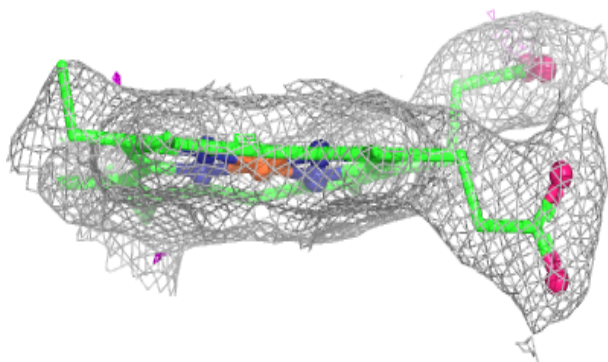
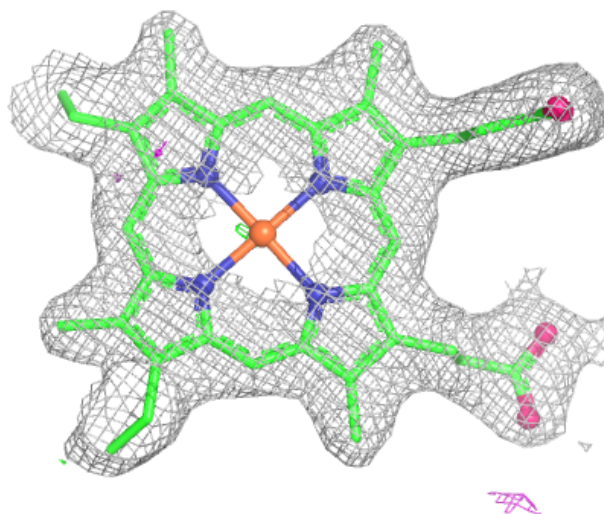
Electron density around HEM e 102:

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



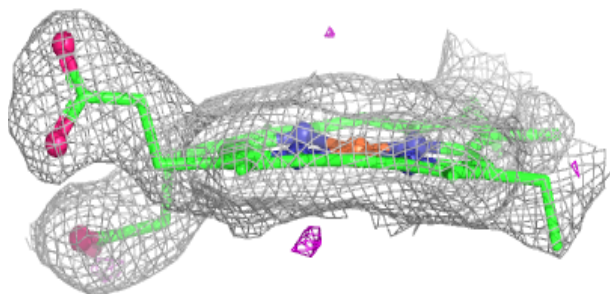
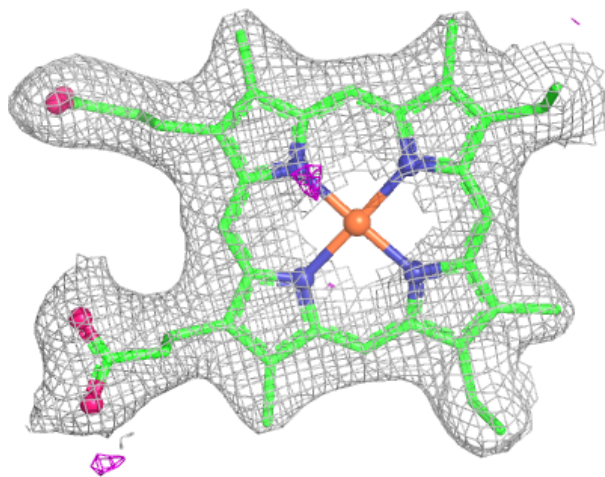
Electron density around HEC V 201:

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



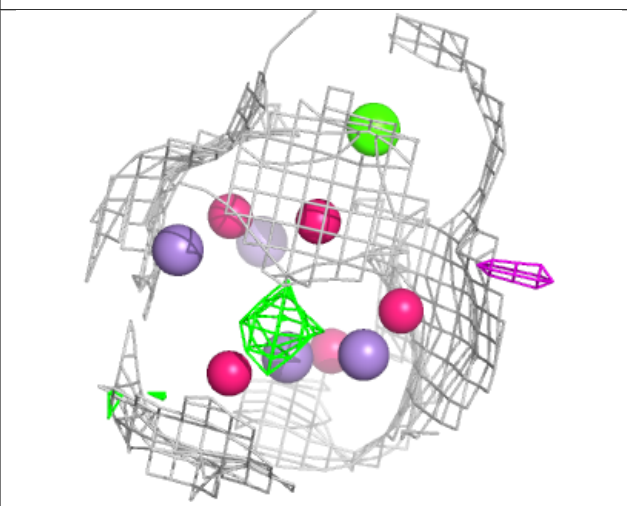
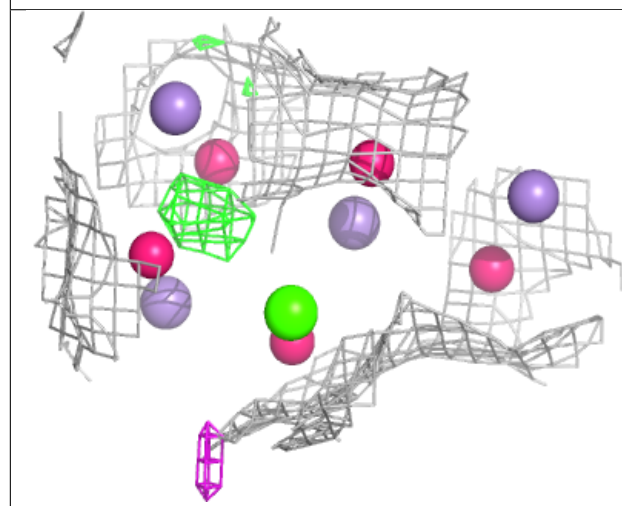
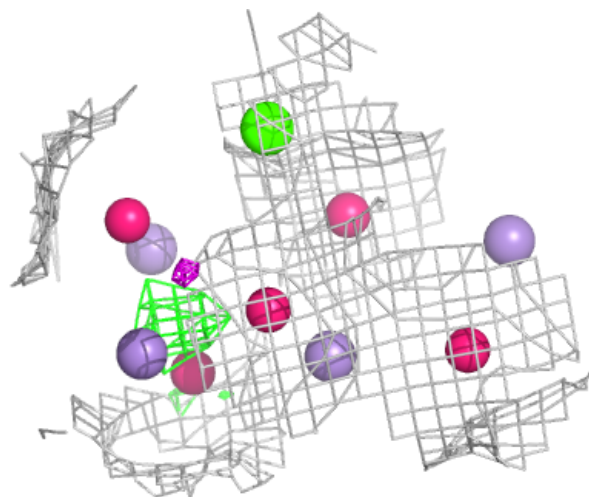
Electron density around HEC v 201:

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



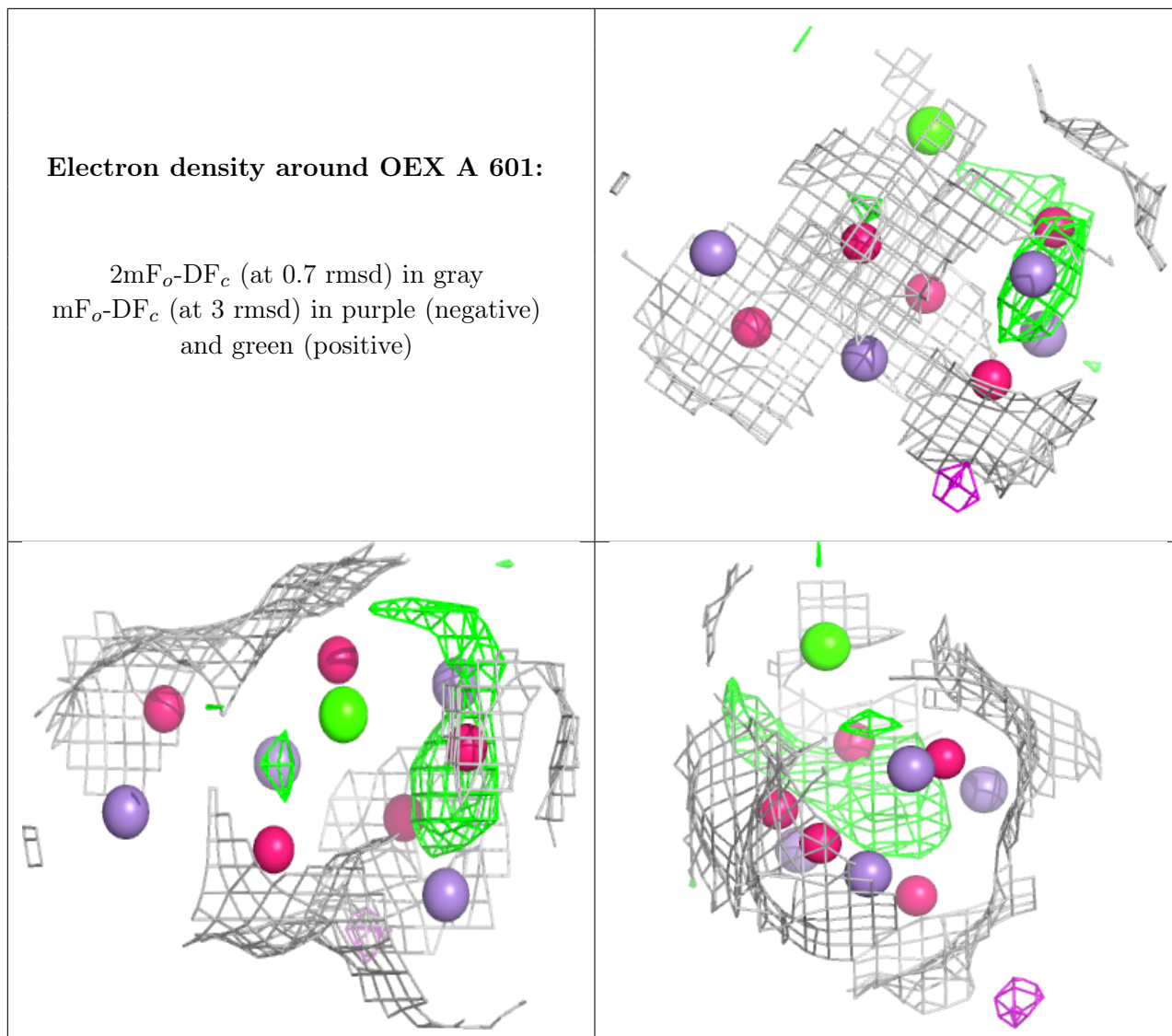
Electron density around OEX a 601:

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



Electron density around OEX A 601:

$2mF_o-DF_c$ (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.