



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 02:03 PM EDT

PDB ID : 9Z34 / pdb_00009z34
Title : RT XFEL structure of one-flash state of Photosystem II (1F, S2 rich) at 1.98 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 : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

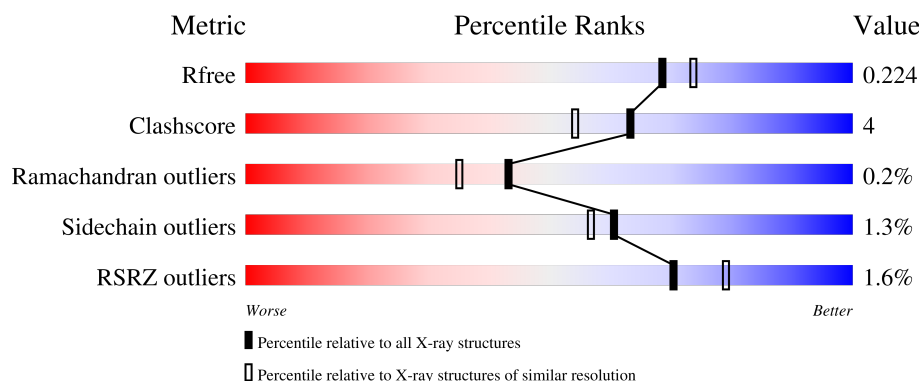
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

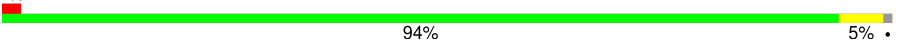
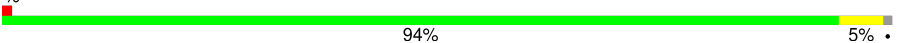
The reported resolution of this entry is 1.98 Å.

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.



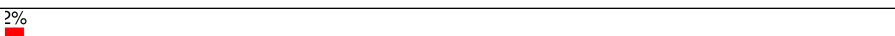
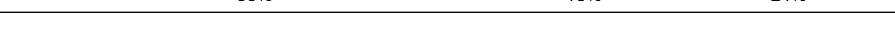
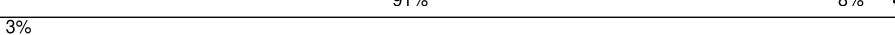
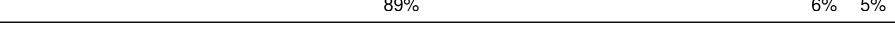
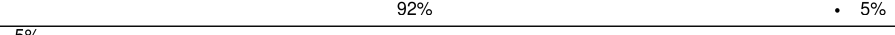
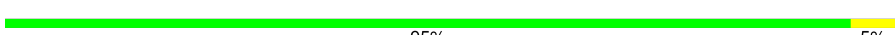
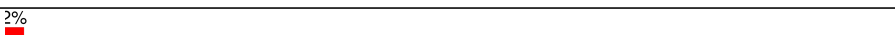
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	 92% 6% .
1	a	344	 90% 7% . .
2	B	510	 94% 5% .
2	b	510	 94% 5% .

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

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Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 52680 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.

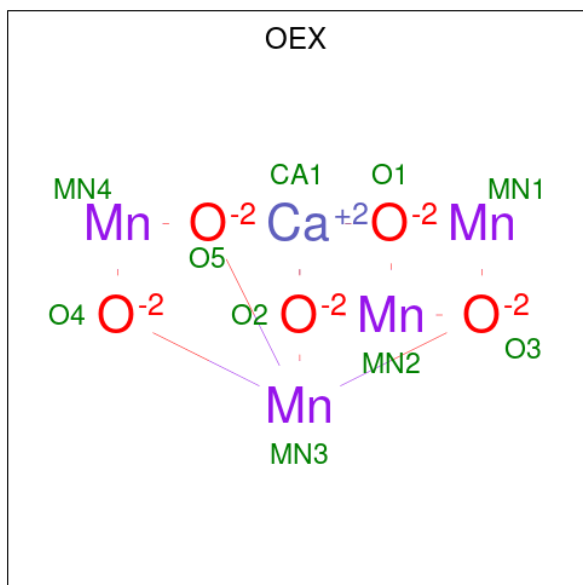
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	28	Total	C	N	O	0	0	0
			221	151	38	32			

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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).

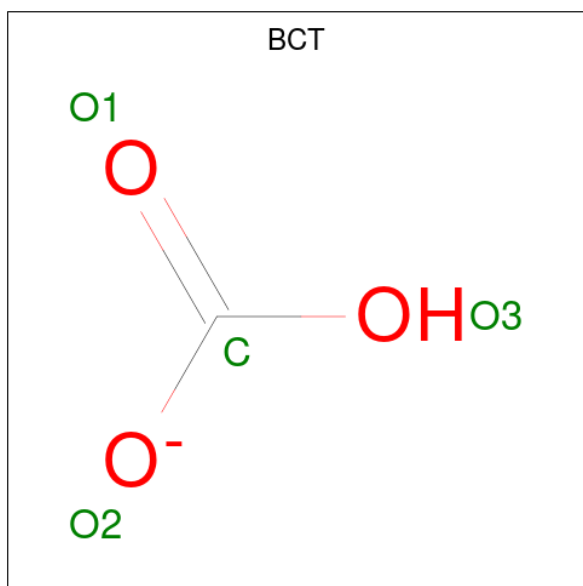
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		

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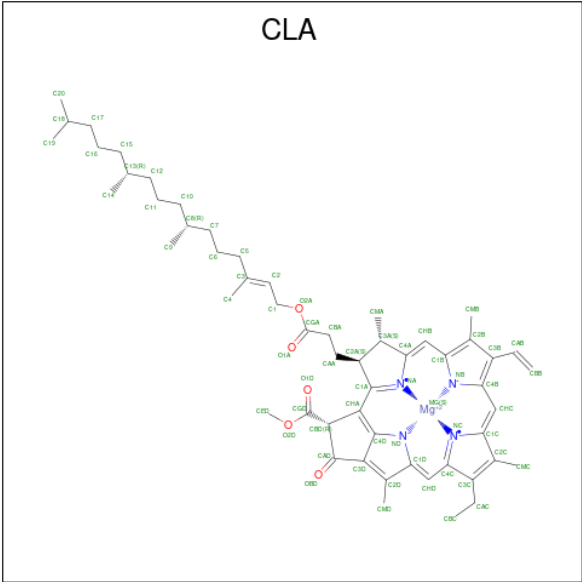
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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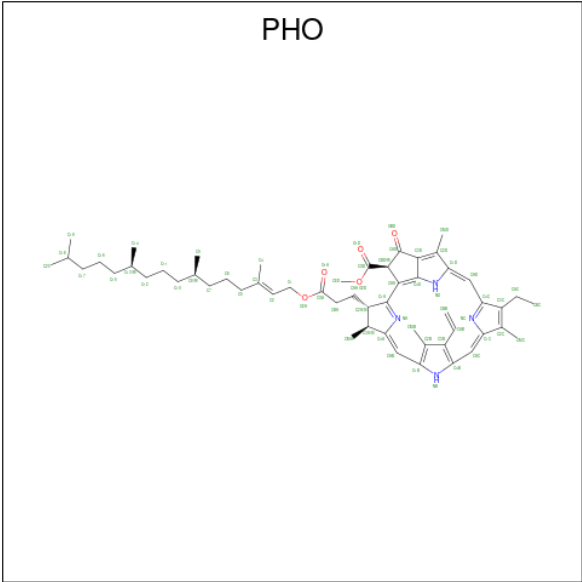
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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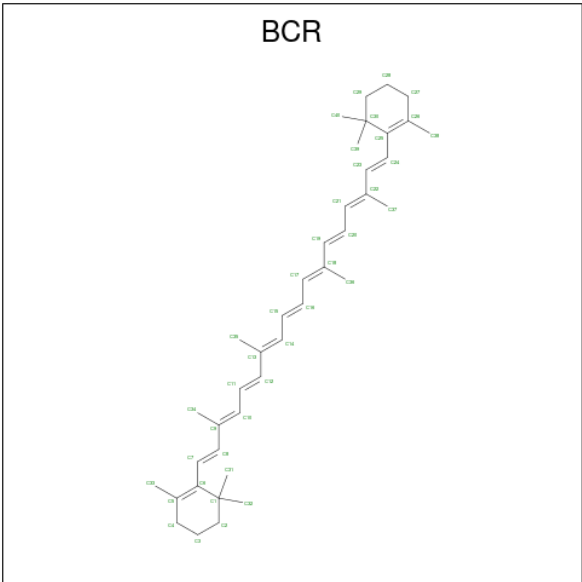
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



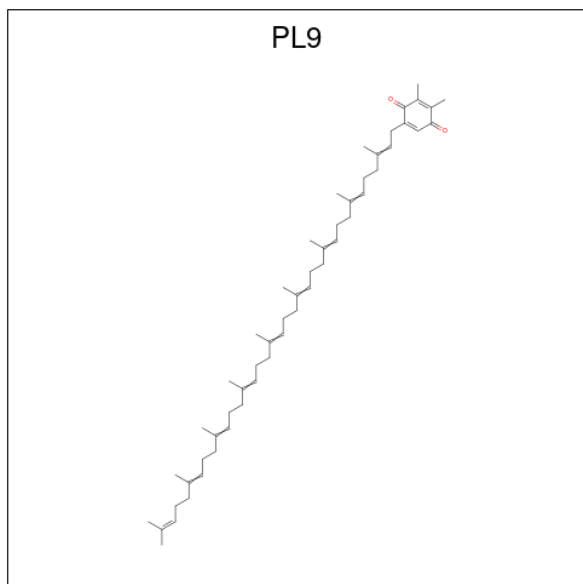
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



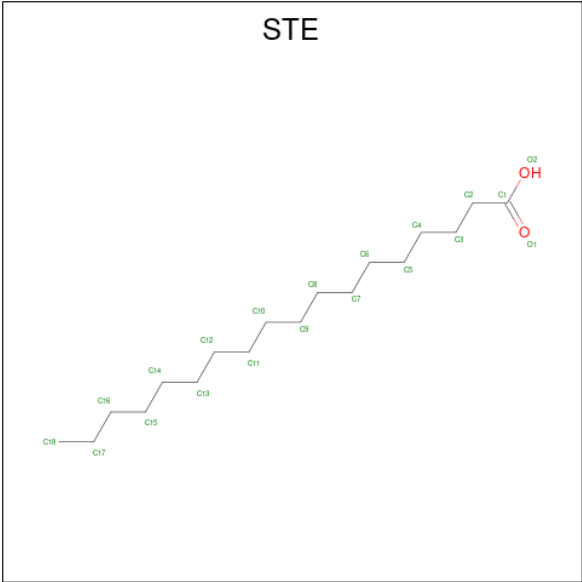
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 29 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



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

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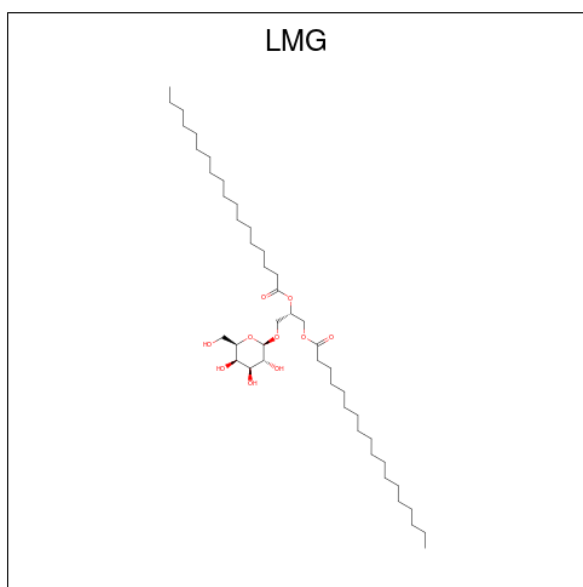
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	1	Total C 14 14	0	0
29	D	1	Total C 9 9	0	0
29	E	1	Total C O 12 10 2	0	0
29	E	1	Total C 12 12	0	0
29	E	1	Total C O 20 18 2	0	0
29	H	1	Total C 18 18	0	0
29	I	1	Total C O 17 15 2	0	0
29	I	1	Total C O 15 13 2	0	0
29	J	1	Total C O 12 10 2	0	0
29	K	1	Total C 14 14	0	0
29	M	1	Total C O 15 13 2	0	0
29	M	1	Total C 10 10	0	0
29	M	1	Total C 15 15	0	0
29	T	1	Total C 16 16	0	0
29	X	1	Total C O 20 18 2	0	0
29	Z	1	Total C 17 17	0	0
29	a	1	Total C O 12 10 2	0	0
29	b	1	Total C O 20 18 2	0	0
29	b	1	Total C O 16 14 2	0	0
29	b	1	Total C 10 10	0	0
29	b	1	Total C 11 11	0	0

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

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



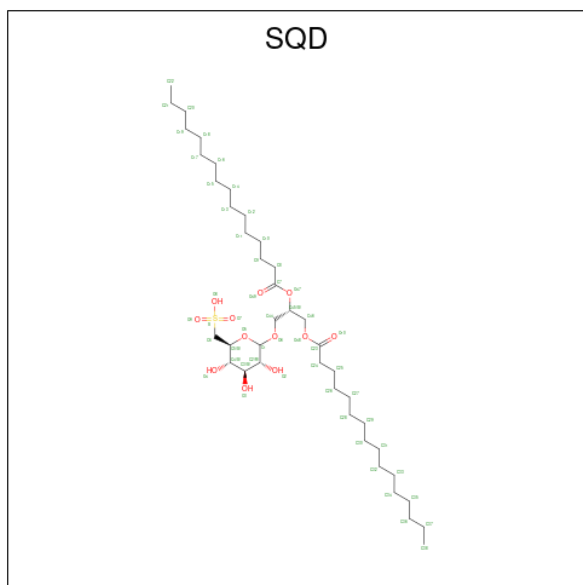
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			48	38	10		
30	B	1	Total	C	O	0	0
			45	35	10		
30	C	1	Total	C	O	0	0
			36	26	10		
30	C	1	Total	C	O	0	0
			48	38	10		
30	D	1	Total	C	O	0	0
			50	40	10		
30	D	1	Total	C	O	0	0
			51	41	10		
30	M	1	Total	C	O	0	0
			51	41	10		
30	a	1	Total	C	O	0	0
			55	45	10		
30	b	1	Total	C	O	0	0
			55	45	10		
30	c	1	Total	C	O	0	0
			30	25	5		
30	c	1	Total	C	O	0	0
			46	36	10		
30	c	1	Total	C	O	0	0
			48	38	10		
30	c	1	Total	C	O	0	0
			49	39	10		
30	d	1	Total	C	O	0	0
			44	34	10		

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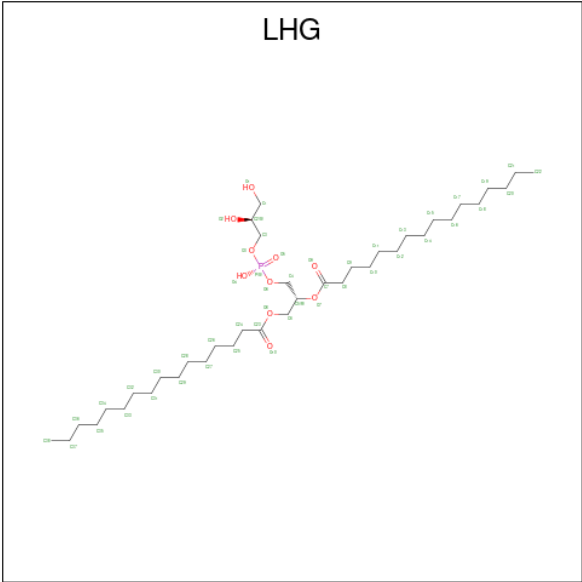
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



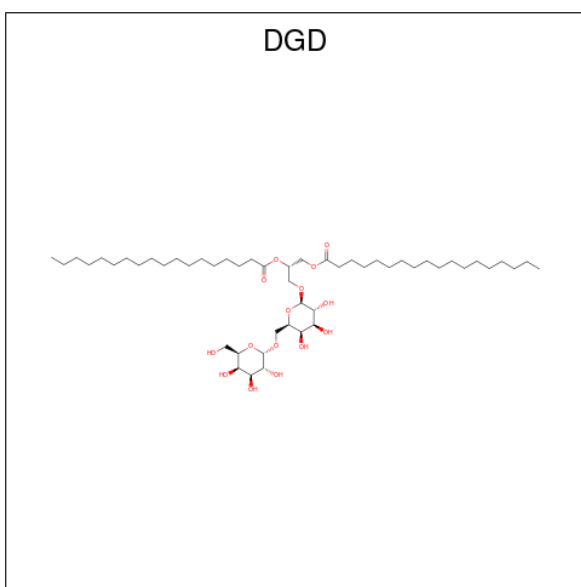
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	S	0	0
			52	39	12	1		
31	A	1	Total	C	O	S	0	0
			43	30	12	1		
31	B	1	Total	C	O	S	0	0
			54	41	12	1		
31	D	1	Total	C	O	S	0	0
			36	25	10	1		
31	a	1	Total	C	O	S	0	0
			54	41	12	1		
31	a	1	Total	C	O	S	0	0
			54	41	12	1		
31	b	1	Total	C	O	S	0	0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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



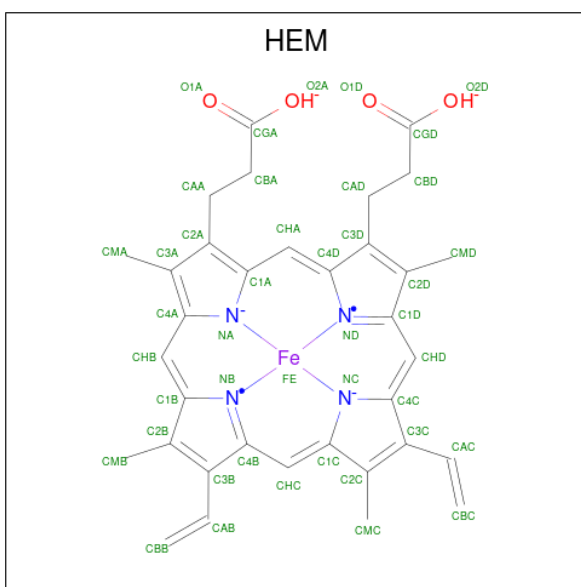
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			47	36	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	a	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0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

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



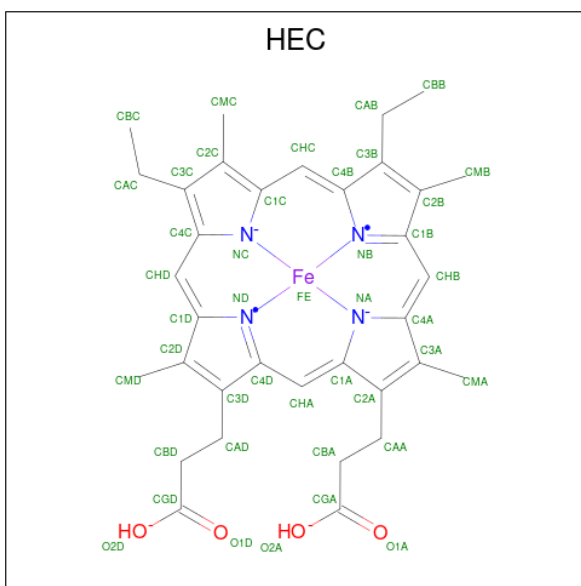
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			66	51	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total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

- Molecule 34 is 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	f	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	146	Total O 146 146	0	0
36	B	231	Total O 231 231	0	0
36	C	197	Total O 197 197	0	0
36	D	142	Total O 142 142	0	0
36	E	28	Total O 28 28	0	0
36	F	11	Total O 11 11	0	0
36	H	26	Total O 26 26	0	0
36	I	15	Total O 15 15	0	0
36	J	11	Total O 11 11	0	0
36	K	8	Total O 8 8	0	0
36	L	8	Total O 8 8	0	0
36	M	9	Total O 9 9	0	0
36	O	122	Total O 122 122	0	0
36	T	10	Total O 10 10	0	0
36	U	57	Total O 57 57	0	0
36	V	74	Total O 74 74	0	0
36	Y	4	Total O 4 4	0	0
36	X	11	Total O 11 11	0	0
36	Z	2	Total O 2 2	0	0
36	R	2	Total O 2 2	0	0
36	a	132	Total O 132 132	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	b	211	Total 211	O 211	0	0
36	c	183	Total 183	O 183	0	0
36	d	128	Total 128	O 128	0	0
36	e	21	Total 21	O 21	0	0
36	f	8	Total 8	O 8	0	0
36	h	17	Total 17	O 17	0	0
36	i	11	Total 11	O 11	0	0
36	j	7	Total 7	O 7	0	0
36	k	9	Total 9	O 9	0	0
36	l	14	Total 14	O 14	0	0
36	m	13	Total 13	O 13	0	0
36	o	125	Total 125	O 125	0	0
36	t	11	Total 11	O 11	0	0
36	u	59	Total 59	O 59	0	0
36	v	64	Total 64	O 64	0	0
36	y	3	Total 3	O 3	0	0
36	x	8	Total 8	O 8	0	0
36	z	2	Total 2	O 2	0	0
36	r	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

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

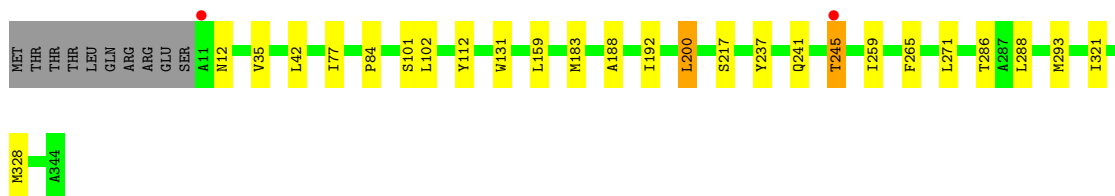
- Molecule 1: Photosystem II protein D1 1

Chain A: 

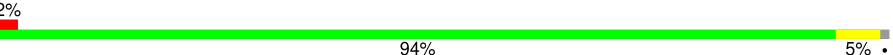


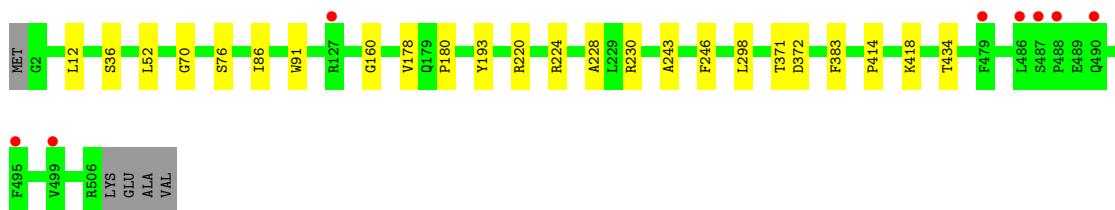
- Molecule 1: Photosystem II protein D1 1

Chain a: 

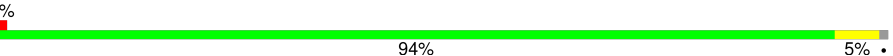


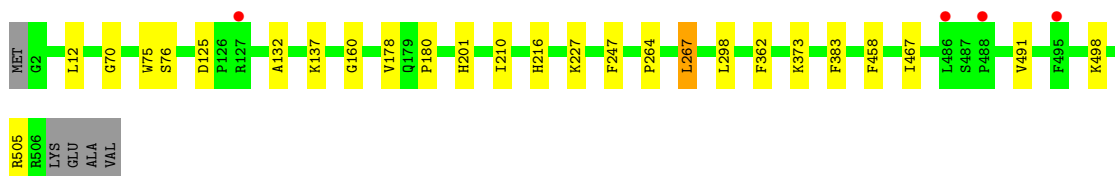
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

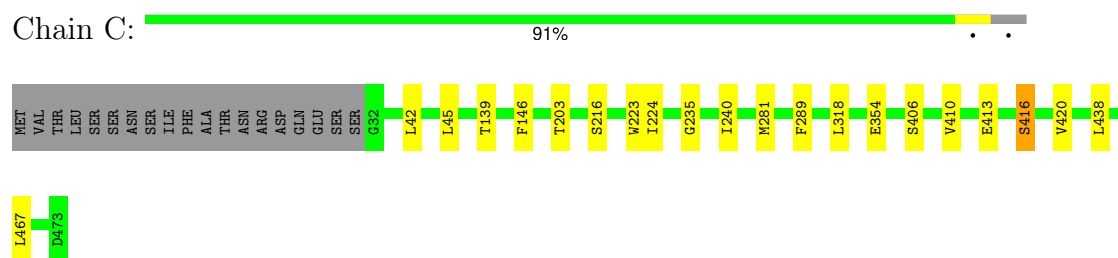


- Molecule 2: Photosystem II CP47 reaction center protein

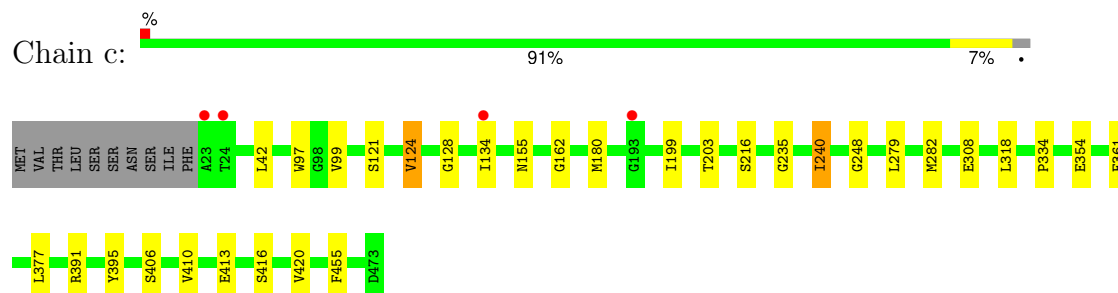
Chain b: 



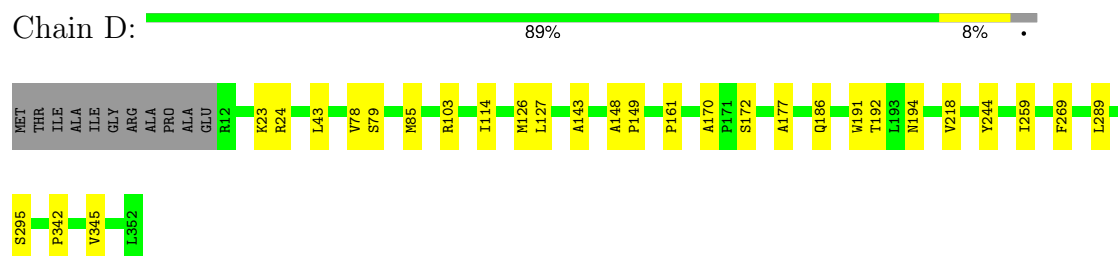
- Molecule 3: Photosystem II CP43 reaction center protein



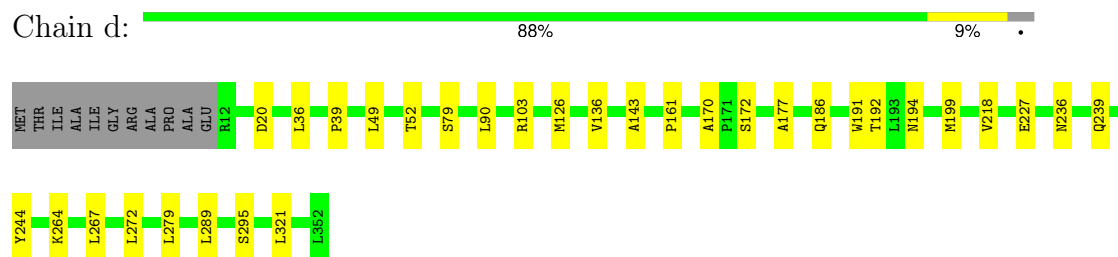
- Molecule 3: Photosystem II CP43 reaction center protein



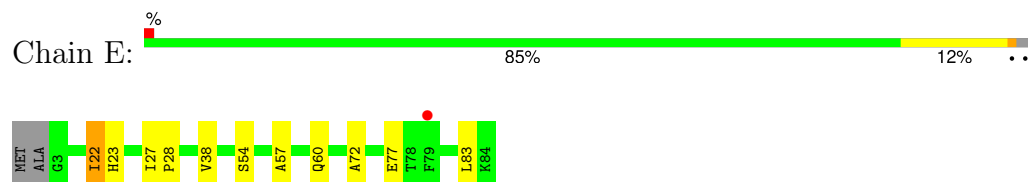
- Molecule 4: Photosystem II D2 protein



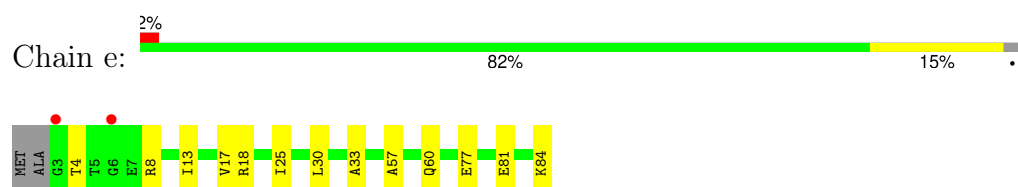
- Molecule 4: Photosystem II D2 protein



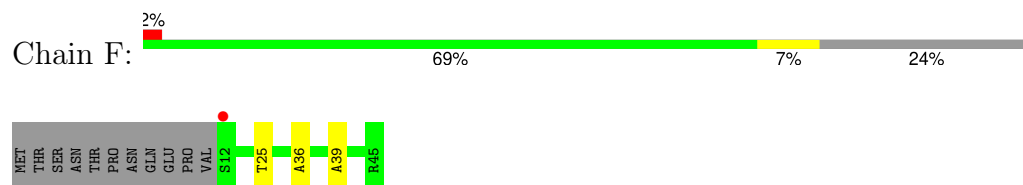
- Molecule 5: Cytochrome b559 subunit alpha



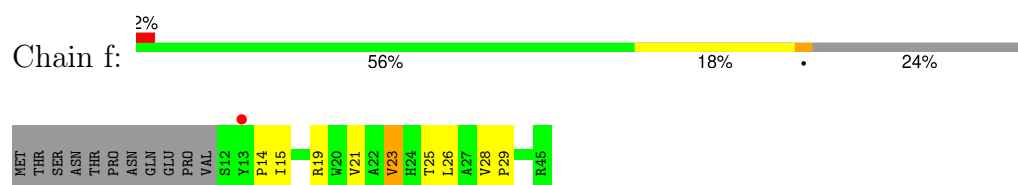
- Molecule 5: Cytochrome b559 subunit alpha



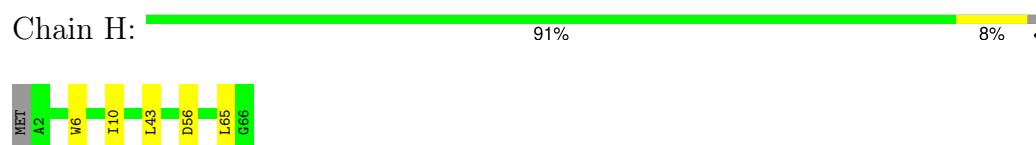
- Molecule 6: Cytochrome b559 subunit beta



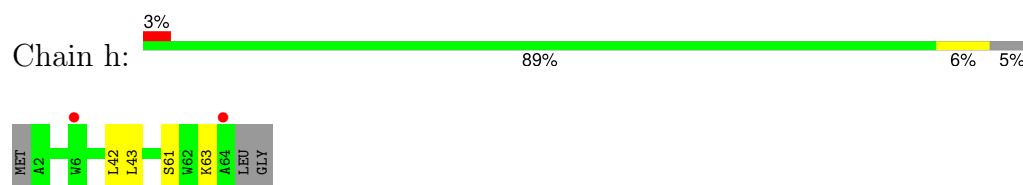
- Molecule 6: Cytochrome b559 subunit beta



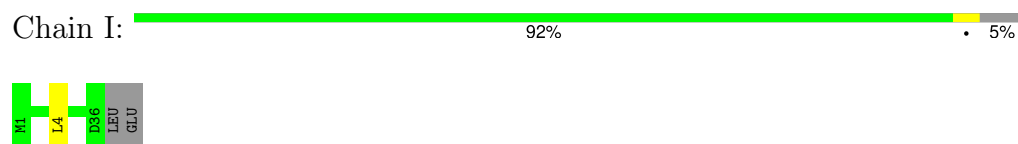
- Molecule 7: Photosystem II reaction center protein H



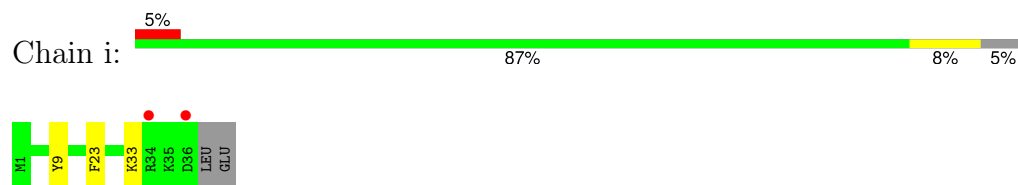
- Molecule 7: Photosystem II reaction center protein H



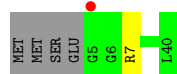
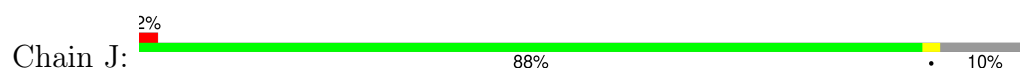
- Molecule 8: Photosystem II reaction center protein I



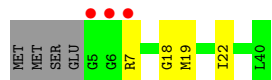
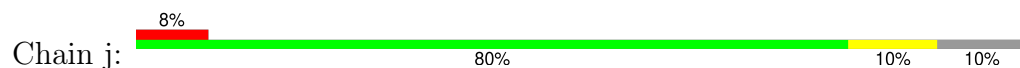
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



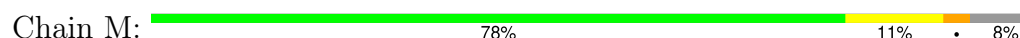
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



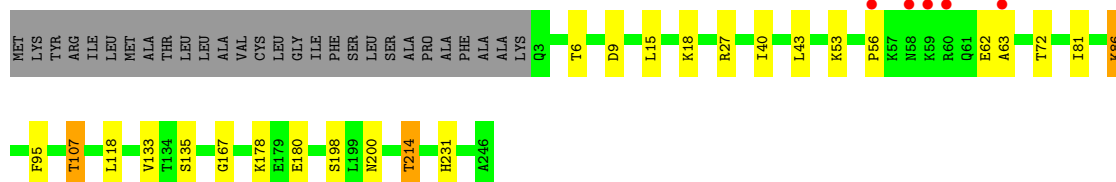
- Molecule 12: Photosystem II reaction center protein M

Chain m: 



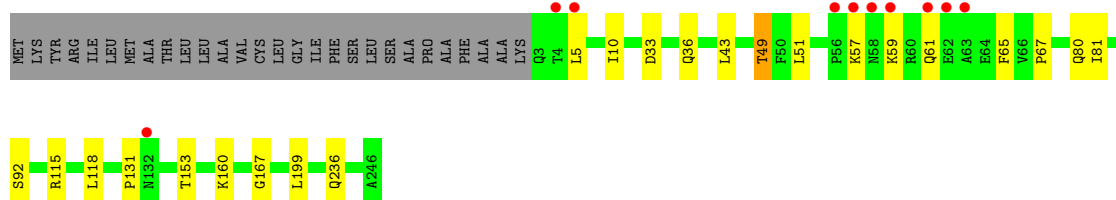
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 



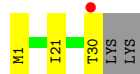
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 



- Molecule 14: Photosystem II reaction center protein T

Chain T: 



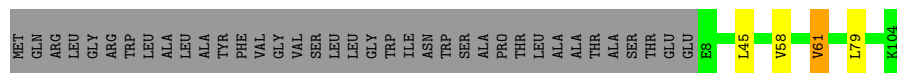
- Molecule 14: Photosystem II reaction center protein T

Chain t: 

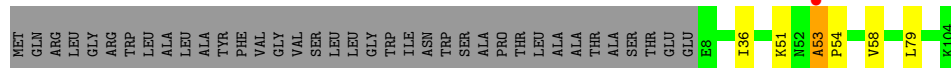


- Molecule 15: Photosystem II 12 kDa extrinsic protein

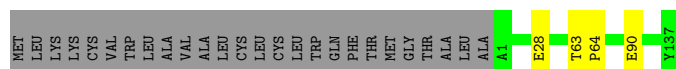
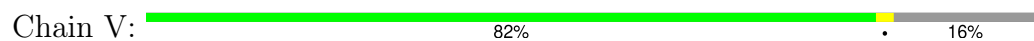
Chain U: 



- Molecule 15: Photosystem II 12 kDa extrinsic protein



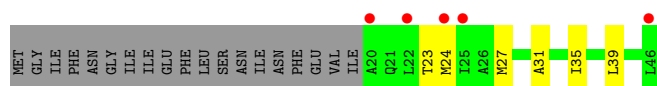
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



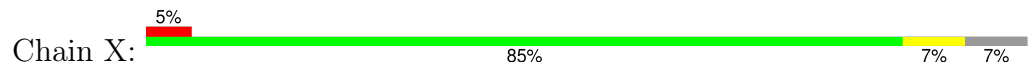
- Molecule 17: Photosystem II reaction center protein Ycf12



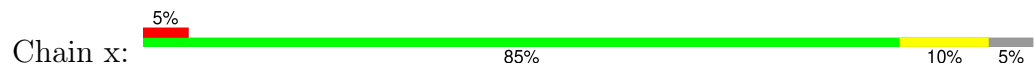
- Molecule 17: Photosystem II reaction center protein Ycf12



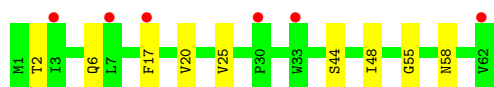
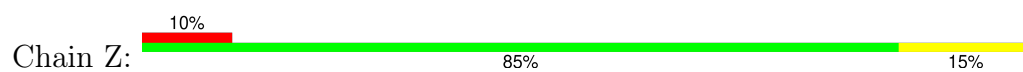
- Molecule 18: Photosystem II reaction center X protein



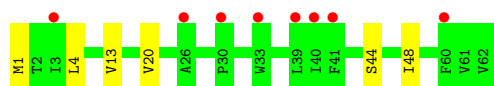
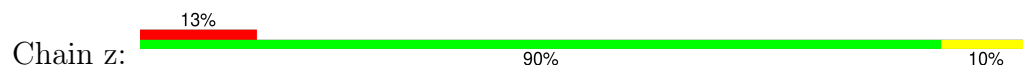
- Molecule 18: Photosystem II reaction center X protein



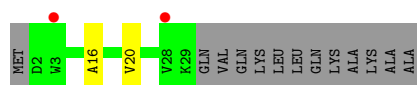
- Molecule 19: Photosystem II reaction center protein Z



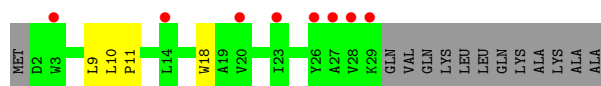
- Molecule 19: Photosystem II reaction center protein Z



- 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	117.55Å 222.83Å 309.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.44 – 1.98 37.44 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.44-1.98) 83.2 (37.44-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.32 (at 1.98Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.188 , 0.224 0.188 , 0.224	Depositor DCC
R_{free} test set	4966 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52680	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: FE2, HEM, CL, LHG, HEC, DGD, SQD, CLA, BCR, OEX, FME, BCT, LMG, STE, PHO, 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	0.34	0/2707	0.50	0/3692
1	a	0.33	0/2704	0.50	0/3688
2	B	0.31	0/4166	0.45	0/5675
2	b	0.29	0/4127	0.45	0/5623
3	C	0.29	0/3539	0.45	0/4819
3	c	0.28	0/3619	0.43	0/4926
4	D	0.33	0/2812	0.48	0/3832
4	d	0.31	0/2821	0.46	0/3844
5	E	0.25	0/688	0.45	0/940
5	e	0.23	0/683	0.44	0/932
6	F	0.25	0/284	0.38	0/387
6	f	0.25	0/284	0.48	0/387
7	H	0.27	0/517	0.44	0/705
7	h	0.25	0/505	0.43	0/689
8	I	0.29	0/293	0.45	0/396
8	i	0.30	0/293	0.43	0/396
9	J	0.25	0/263	0.37	0/356
9	j	0.21	0/263	0.36	0/356
10	K	0.26	0/303	0.42	0/416
10	k	0.26	0/303	0.43	0/416
11	L	0.32	0/311	0.43	0/422
11	l	0.32	0/303	0.42	0/412
12	M	0.30	0/249	0.50	0/341
12	m	0.31	0/244	0.49	0/334
13	O	0.29	0/1904	0.49	0/2585
13	o	0.29	0/1905	0.47	0/2583
14	T	0.32	0/257	0.47	0/349
14	t	0.28	0/255	0.38	0/346
15	U	0.27	0/785	0.43	0/1064
15	u	0.27	0/785	0.46	0/1064
16	V	0.28	0/1085	0.47	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	0.19	0/197	0.31	0/264
17	y	0.18	0/219	0.34	0/294
18	X	0.25	0/284	0.39	0/384
18	x	0.20	0/289	0.31	0/391
19	Z	0.19	0/490	0.41	0/669
19	z	0.19	0/488	0.30	0/666
20	R	0.19	0/227	0.31	0/313
20	r	0.20	0/227	0.36	0/313
All	All	0.29	0/42763	0.45	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	10	0
1	a	2619	0	2510	17	0
2	B	4016	0	3883	19	0
2	b	3984	0	3842	20	0
3	C	3426	0	3353	12	0
3	c	3500	0	3426	22	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	249	0	264	4	0
25	B	1035	0	1139	19	0
25	C	839	0	922	15	0
25	D	130	0	144	3	0
25	a	260	0	288	9	0
25	b	1035	0	1139	21	0
25	c	839	0	919	15	0
25	d	130	0	144	5	0
26	A	128	0	148	1	0
26	a	64	0	74	1	0
26	d	64	0	74	2	0
27	A	40	0	56	1	0
27	B	120	0	168	2	0
27	C	80	0	112	3	0
27	D	40	0	56	1	0
27	H	40	0	56	1	0
27	J	40	0	56	2	0
27	K	40	0	56	0	0
27	T	40	0	56	3	0
27	a	40	0	56	1	0
27	b	120	0	168	2	0
27	c	80	0	112	2	0
27	d	40	0	56	1	0
27	h	40	0	56	4	0
27	k	80	0	112	4	0
27	t	40	0	56	4	0
28	A	55	0	80	3	0
28	D	55	0	80	2	0
28	a	55	0	80	3	0
28	d	55	0	80	2	0
29	A	45	0	83	1	0
29	B	62	0	96	3	0
29	C	78	0	126	1	0
29	D	9	0	17	0	0
29	E	44	0	74	0	0
29	H	18	0	35	1	0
29	I	32	0	48	0	0
29	J	12	0	16	0	0
29	K	14	0	27	1	0
29	M	40	0	67	3	0
29	T	16	0	31	4	0
29	X	20	0	35	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Z	17	0	33	0	0
29	a	12	0	16	0	0
29	b	57	0	96	3	0
29	c	31	0	57	1	0
29	d	60	0	105	6	0
29	e	31	0	52	0	0
29	f	8	0	15	0	0
29	h	10	0	19	0	0
29	i	18	0	24	1	0
29	j	28	0	47	0	0
29	k	14	0	20	0	0
29	m	30	0	51	1	0
29	t	24	0	36	0	0
29	z	9	0	14	0	0
30	A	48	0	66	2	0
30	B	45	0	60	4	0
30	C	84	0	106	3	0
30	D	101	0	142	6	0
30	M	51	0	72	2	0
30	a	55	0	86	3	0
30	b	55	0	86	1	0
30	c	173	0	240	3	0
30	d	44	0	58	0	0
30	m	51	0	72	3	0
31	A	95	0	124	2	0
31	B	54	0	78	4	0
31	D	36	0	46	0	0
31	a	108	0	156	3	0
31	b	49	0	65	3	0
31	f	41	0	49	3	0
32	A	49	0	74	1	0
32	D	145	0	215	14	0
32	L	49	0	74	2	0
32	a	49	0	74	3	0
32	d	88	0	125	0	0
32	e	42	0	57	1	0
32	l	49	0	74	2	0
33	A	66	0	96	2	0
33	C	186	0	246	1	0
33	H	62	0	82	1	0
33	c	186	0	246	4	0
33	h	62	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	F	43	0	30	2	0
34	f	43	0	30	5	0
35	V	43	0	30	0	0
35	v	43	0	30	1	0
36	A	146	0	0	2	0
36	B	231	0	0	2	0
36	C	197	0	0	1	0
36	D	142	0	0	0	0
36	E	28	0	0	0	0
36	F	11	0	0	2	0
36	H	26	0	0	0	0
36	I	15	0	0	0	0
36	J	11	0	0	0	0
36	K	8	0	0	0	0
36	L	8	0	0	0	0
36	M	9	0	0	0	0
36	O	122	0	0	3	0
36	R	2	0	0	0	0
36	T	10	0	0	0	0
36	U	57	0	0	0	0
36	V	74	0	0	2	0
36	X	11	0	0	0	0
36	Y	4	0	0	0	0
36	Z	2	0	0	0	0
36	a	132	0	0	3	0
36	b	211	0	0	2	0
36	c	183	0	0	2	0
36	d	128	0	0	3	0
36	e	21	0	0	0	0
36	f	8	0	0	1	0
36	h	17	0	0	0	0
36	i	11	0	0	0	0
36	j	7	0	0	0	0
36	k	9	0	0	2	0
36	l	14	0	0	0	0
36	m	13	0	0	1	0
36	o	125	0	0	0	0
36	r	2	0	0	0	0
36	t	11	0	0	0	0
36	u	59	0	0	0	0
36	v	64	0	0	2	0
36	x	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	y	3	0	0	0	0
36	z	2	0	0	0	0
All	All	52680	0	52200	412	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 4.

All (412) 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)
32:D:410:LHG:H152	32:L:101:LHG:H281	1.59	0.84
28:A:612:PL9:H361	6:F:25:THR:HG21	1.61	0.81
1:a:101:SER:HB2	30:a:616:LMG:H132	1.63	0.81
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.66	0.78
1:a:102:LEU:H	30:a:616:LMG:H121	1.50	0.76
10:k:18:PHE:HE2	19:z:13:VAL:HG21	1.51	0.76
29:B:623:STE:H22	30:M:101:LMG:HC5	1.69	0.74
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.70	0.73
34:f:101:HEM:HHD	34:f:101:HEM:HBC2	1.71	0.73
25:B:604:CLA:H43	25:B:605:CLA:H2	1.70	0.73
30:B:620:LMG:HC92	30:D:405:LMG:H172	1.71	0.72
32:a:613:LHG:H223	25:b:613:CLA:H192	1.71	0.72
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.71	0.72
3:c:180:MET:HE1	30:c:523:LMG:HC72	1.73	0.71
4:d:103:ARG:HH21	5:e:77:GLU:HG3	1.57	0.69
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.75	0.69
4:d:236:ASN:H	4:d:239:GLN:HE21	1.42	0.68
25:C:502:CLA:H61	25:C:512:CLA:H42	1.74	0.67
27:t:101:BCR:HC8	27:t:101:BCR:H311	1.75	0.67
32:D:409:LHG:H142	32:D:409:LHG:H322	1.76	0.66
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.79	0.65
16:v:101:PHE:HB2	36:v:301:HOH:O	1.97	0.64
27:J:101:BCR:H321	27:J:101:BCR:HC8	1.80	0.64
4:D:23:LYS:HZ1	30:D:405:LMG:H151	1.62	0.64
5:E:38:VAL:HB	36:F:211:HOH:O	1.97	0.63
25:B:605:CLA:HHC	25:B:605:CLA:HBB1	1.80	0.62
18:X:16:SER:HB3	29:X:101:STE:H102	1.82	0.62
19:z:1:MET:HB2	19:z:4:LEU:HB3	1.81	0.62
2:b:264:PRO:HG2	2:b:267:LEU:HD22	1.81	0.62
2:B:434:THR:HG23	36:B:701:HOH:O	1.99	0.61
4:d:236:ASN:H	4:d:239:GLN:NE2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:90:GLU:HG2	36:V:342:HOH:O	2.02	0.60
13:o:5:LEU:HD13	13:o:10:ILE:HD11	1.82	0.60
25:B:614:CLA:H171	30:M:101:LMG:H412	1.83	0.60
10:k:15:TYR:HB2	36:k:203:HOH:O	2.01	0.60
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.83	0.60
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.83	0.60
25:a:609:CLA:H52	25:a:609:CLA:H111	1.84	0.59
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.82	0.59
27:J:101:BCR:H322	19:Z:17:PHE:CE2	2.37	0.59
15:U:58:VAL:O	15:U:61:VAL:HG22	2.03	0.58
30:C:524:LMG:H191	10:K:27:VAL:HG11	1.86	0.58
2:B:228:ALA:HB2	30:D:405:LMG:H322	1.86	0.58
13:O:107:THR:HG22	36:O:333:HOH:O	2.03	0.58
28:a:611:PL9:H48	4:d:39:PRO:HG3	1.86	0.57
19:z:1:MET:HG3	19:z:4:LEU:HD23	1.85	0.57
25:C:506:CLA:H8	27:C:515:BCR:H12C	1.86	0.57
29:b:625:STE:H171	29:d:409:STE:H61	1.87	0.57
25:B:607:CLA:H203	32:D:410:LHG:H162	1.85	0.57
25:B:615:CLA:H2	25:B:616:CLA:HBB2	1.85	0.57
30:C:517:LMG:HC3	36:C:697:HOH:O	2.04	0.57
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.87	0.57
6:F:36:ALA:HB1	36:F:211:HOH:O	2.06	0.56
10:k:11:LEU:HB3	36:k:203:HOH:O	2.05	0.56
33:c:520:DGD:HA81	33:c:521:DGD:HB72	1.87	0.56
25:B:614:CLA:H201	29:B:623:STE:H122	1.88	0.56
5:e:30:LEU:HD11	34:f:101:HEM:HBB2	1.86	0.56
10:k:27:VAL:O	10:k:30:VAL:HG12	2.06	0.56
6:f:21:VAL:HG21	31:f:102:SQD:H261	1.88	0.55
27:c:515:BCR:HC32	8:i:23:PHE:HB3	1.88	0.55
3:C:42:LEU:HD21	25:C:511:CLA:H2A	1.89	0.55
31:A:618:SQD:H5	36:A:837:HOH:O	2.07	0.55
1:a:200:LEU:HD13	33:c:521:DGD:HAT2	1.87	0.55
4:d:49:LEU:C	36:d:501:HOH:O	2.50	0.55
9:j:19:MET:HA	9:j:22:ILE:HD12	1.87	0.55
25:C:507:CLA:H192	29:C:527:STE:H82	1.89	0.54
4:D:186:GLN:HB2	25:D:401:CLA:HBC1	1.89	0.54
36:A:743:HOH:O	13:O:107:THR:HG21	2.07	0.54
25:b:615:CLA:H2	25:b:616:CLA:CBB	2.38	0.54
16:v:77:LYS:HG2	16:v:95:LEU:HD12	1.90	0.54
4:d:126:MET:HE3	4:d:143:ALA:O	2.07	0.54
29:b:625:STE:H162	29:d:409:STE:H71	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:MET:HE3	4:D:143:ALA:O	2.08	0.54
17:Y:23:THR:HB	17:Y:24:MET:HE2	1.90	0.54
13:o:33:ASP:HB3	13:o:36:GLN:HB2	1.89	0.54
1:A:84:PRO:HA	1:A:112:TYR:CG	2.44	0.53
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.39	0.53
4:d:199:MET:HG2	28:d:405:PL9:H321	1.91	0.53
27:t:101:BCR:H23C	27:t:101:BCR:H382	1.91	0.53
2:B:230:ARG:HH12	30:B:620:LMG:HC1	1.74	0.52
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.91	0.52
4:d:279:LEU:HD22	26:d:401:PHO:HBC3	1.92	0.52
3:c:279:LEU:HD23	3:c:282:MET:HE3	1.92	0.52
32:a:613:LHG:H351	32:a:613:LHG:H102	1.91	0.51
28:A:612:PL9:H271	32:A:617:LHG:H202	1.93	0.51
3:C:406:SER:HA	3:C:420:VAL:HG23	1.92	0.51
25:C:511:CLA:H143	19:Z:20:VAL:HG13	1.92	0.51
4:D:194:ASN:HA	4:D:295:SER:OG	2.10	0.51
25:B:614:CLA:HBA1	31:B:622:SQD:H91	1.92	0.51
5:e:30:LEU:HD11	34:f:101:HEM:CBB	2.41	0.51
1:A:227:THR:HB	1:A:231:GLU:HG3	1.92	0.51
2:b:125:ASP:HB2	2:b:132:ALA:HB3	1.93	0.51
13:O:200:ASN:HD22	13:O:214:THR:HG22	1.76	0.50
17:y:31:ALA:O	17:y:35:ILE:HG13	2.11	0.50
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.11	0.50
19:Z:55:GLY:HA2	19:Z:58:ASN:HB3	1.94	0.50
33:A:619:DGD:HE4	2:b:76:SER:HB3	1.93	0.50
27:T:101:BCR:H382	27:T:101:BCR:H23C	1.92	0.50
19:z:44:SER:O	19:z:48:ILE:HG13	2.12	0.50
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.94	0.50
5:e:25:ILE:HD12	20:r:18:TRP:CE2	2.47	0.50
16:V:28:GLU:HG2	36:V:347:HOH:O	2.11	0.49
1:a:321:ILE:HG22	36:a:750:HOH:O	2.11	0.49
2:b:247:PHE:CE2	25:b:602:CLA:H102	2.47	0.49
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.48	0.49
31:A:618:SQD:H142	27:T:101:BCR:HC41	1.95	0.49
3:c:155:ASN:C	36:c:602:HOH:O	2.54	0.49
25:c:511:CLA:H192	19:z:20:VAL:HA	1.93	0.49
25:b:614:CLA:H43	31:b:620:SQD:H101	1.95	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.49
5:e:17:VAL:HG23	9:j:7:ARG:HB2	1.94	0.49
27:d:404:BCR:H392	27:d:404:BCR:H23C	1.94	0.49
30:m:101:LMG:H341	30:m:101:LMG:H371	1.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:THR:HG23	2:B:372:ASP:O	2.13	0.49
19:Z:2:THR:HG22	19:Z:6:GLN:NE2	2.28	0.49
5:E:54:SER:HB2	5:E:83:LEU:HD13	1.94	0.49
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.95	0.49
2:B:230:ARG:NH2	30:B:620:LMG:HC5	2.29	0.48
30:D:406:LMG:H161	30:D:406:LMG:H191	1.70	0.48
7:H:56:ASP:OD2	18:X:2:THR:HA	2.13	0.48
33:c:519:DGD:HB51	33:c:519:DGD:HA31	1.94	0.48
27:H:101:BCR:HC8	27:H:101:BCR:H331	1.94	0.48
3:c:406:SER:HA	3:c:420:VAL:HG23	1.94	0.48
19:Z:44:SER:O	19:Z:48:ILE:HG13	2.14	0.48
3:c:391[A]:ARG:HD2	3:c:395:TYR:CZ	2.48	0.48
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.49	0.48
34:F:101:HEM:HBB2	34:F:101:HEM:HMB1	1.95	0.48
29:T:102:STE:H62	29:T:102:STE:H92	1.51	0.48
25:b:610:CLA:HBB1	27:h:101:BCR:HC22	1.95	0.48
4:d:52:THR:N	36:d:501:HOH:O	2.46	0.48
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.96	0.48
1:a:84:PRO:HA	1:a:112:TYR:CG	2.49	0.48
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.95	0.48
5:E:57:ALA:HB3	5:E:60:GLN:HB2	1.95	0.48
2:B:91:TRP:HE1	29:B:621:STE:H32	1.79	0.47
2:b:12:LEU:HB2	25:b:612:CLA:HMC2	1.97	0.47
31:f:102:SQD:H312	18:x:27:VAL:HG11	1.96	0.47
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.95	0.47
1:A:243:GLU:H	1:A:243:GLU:CD	2.22	0.47
25:B:613:CLA:H71	25:B:613:CLA:H112	1.68	0.47
13:O:27:ARG:O	13:O:27:ARG:HG2	2.15	0.47
25:b:603:CLA:H202	7:h:42:LEU:HD12	1.95	0.47
25:c:504:CLA:H13	25:c:508:CLA:H143	1.97	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
16:v:90:GLU:HB2	36:v:338:HOH:O	2.14	0.47
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.49	0.47
3:c:318:LEU:C	3:c:318:LEU:HD23	2.40	0.47
30:c:523:LMG:H332	30:c:523:LMG:H361	1.57	0.47
4:d:186:GLN:HB2	25:d:402:CLA:HBC1	1.97	0.47
5:e:18:ARG:HH12	6:f:15:ILE:HD11	1.79	0.47
5:e:57:ALA:H	5:e:60:GLN:HG2	1.79	0.47
6:f:14:PRO:HB2	36:f:202:HOH:O	2.13	0.47
17:y:17:GLU:HG2	17:y:18:VAL:H	1.80	0.47
30:A:615:LMG:HC72	3:C:216:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:7:ARG:H	9:j:7:ARG:HD3	1.79	0.47
33:A:619:DGD:HD5	2:b:75:TRP:HB3	1.97	0.47
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.97	0.47
20:R:16:ALA:O	20:R:20:VAL:HG23	2.15	0.47
32:D:409:LHG:H141	32:D:409:LHG:H341	1.97	0.46
27:b:618:BCR:H20C	27:b:618:BCR:H361	1.80	0.46
4:d:264:LYS:HG2	36:d:515:HOH:O	2.15	0.46
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.97	0.46
25:b:614:CLA:H142	25:b:614:CLA:H91	1.96	0.46
25:B:613:CLA:H51	32:D:410:LHG:H351	1.96	0.46
3:C:438:LEU:HD23	33:C:521:DGD:HBF1	1.98	0.46
25:C:511:CLA:HMB1	25:C:511:CLA:HBB1	1.98	0.46
6:f:26:LEU:O	6:f:29:PRO:HD2	2.16	0.46
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.97	0.46
2:B:224:ARG:NH1	30:D:405:LMG:H112	2.30	0.46
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.81	0.46
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.46
14:T:1:FME:HCN	29:T:102:STE:H102	1.97	0.46
1:a:265:PHE:CD2	1:a:271:LEU:HD23	2.51	0.46
1:A:201:GLY:HA3	1:A:286:THR:HB	1.97	0.46
25:A:614:CLA:H141	25:A:614:CLA:H161	1.64	0.46
12:M:27:VAL:HG13	29:m:103:STE:H62	1.97	0.46
31:a:615:SQD:H302	31:a:615:SQD:H331	1.58	0.46
25:b:608:CLA:HBC2	25:b:609:CLA:H111	1.97	0.46
3:c:410:VAL:HA	36:c:613:HOH:O	2.16	0.46
2:B:52:LEU:HD12	13:o:59:LYS:HE2	1.98	0.46
5:e:57:ALA:N	5:e:60:GLN:HG2	2.31	0.46
29:K:102:STE:H62	29:K:102:STE:H91	1.59	0.46
13:O:178:LYS:HA	13:O:178:LYS:HD3	1.68	0.46
4:D:23:LYS:NZ	30:D:405:LMG:H151	2.30	0.45
3:c:203:THR:O	3:c:235:GLY:HA3	2.16	0.45
4:d:36:LEU:HB2	29:d:406:STE:H162	1.96	0.45
4:d:79:SER:HA	4:d:172:SER:HB3	1.97	0.45
5:e:81:GLU:O	5:e:84:LYS:HE2	2.16	0.45
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.98	0.45
14:T:1:FME:H	29:T:102:STE:C3	2.30	0.45
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.98	0.45
31:b:620:SQD:H122	31:b:620:SQD:H152	1.52	0.45
1:A:183:MET:HA	25:A:606:CLA:HMD1	1.99	0.45
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.50	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:455:PHE:HD2	8:i:33:LYS:HG3	1.81	0.45
5:e:18:ARG:HD2	34:f:101:HEM:O1A	2.16	0.45
13:o:59:LYS:H	13:o:59:LYS:HG3	1.53	0.45
30:B:620:LMG:H172	4:D:127:LEU:HD13	1.98	0.45
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.99	0.45
31:f:102:SQD:H282	31:f:102:SQD:H252	1.49	0.45
12:m:4:ASN:HD21	30:m:101:LMG:H292	1.81	0.45
25:A:606:CLA:HBD	25:A:614:CLA:HAC2	1.99	0.45
6:f:19:ARG:O	6:f:23:VAL:HG13	2.17	0.45
27:C:514:BCR:H361	27:C:514:BCR:H20C	1.85	0.45
32:D:408:LHG:H321	14:T:21:ILE:HD11	1.98	0.45
16:v:12:LEU:HD23	16:v:17:LYS:HD3	1.97	0.45
32:D:409:LHG:H242	32:D:409:LHG:H272	1.71	0.45
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.52	0.45
25:b:601:CLA:H141	25:b:601:CLA:H162	1.63	0.45
16:v:77:LYS:O	16:v:96:ARG:HB2	2.17	0.45
25:a:606:CLA:HMB3	25:a:606:CLA:HBB1	1.99	0.44
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.99	0.44
1:a:217:SER:HA	4:d:272:LEU:HD12	1.99	0.44
25:a:606:CLA:H122	26:a:608:PHO:H3A	1.99	0.44
10:k:16:ALA:O	10:k:19:ASP:HB2	2.17	0.44
10:k:17:ILE:HG13	10:k:18:PHE:HD1	1.82	0.44
2:B:12:LEU:HB2	25:B:612:CLA:HMC2	1.99	0.44
13:O:133:VAL:C	13:O:135:SER:H	2.24	0.44
4:d:192:THR:HG23	25:d:402:CLA:HBC2	1.98	0.44
6:f:21:VAL:O	6:f:25:THR:HG23	2.16	0.44
29:M:104:STE:H91	29:T:102:STE:H71	2.00	0.44
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.99	0.44
16:v:41:HIS:HA	16:v:45:ILE:O	2.18	0.44
1:A:234:ASN:HD21	32:D:410:LHG:HC11	1.83	0.44
14:t:18:PHE:HB2	27:t:101:BCR:HC8	2.00	0.44
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.53	0.44
36:B:701:HOH:O	13:O:178:LYS:HE3	2.16	0.44
4:D:24:ARG:HD3	18:X:37:VAL:HG12	2.00	0.44
25:c:509:CLA:H142	25:c:509:CLA:H111	1.73	0.44
2:b:137:LYS:HE2	36:b:738:HOH:O	2.18	0.44
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.89	0.44
1:a:271:LEU:HD21	28:a:611:PL9:HC71	1.99	0.44
2:b:498:LYS:HE3	4:d:20:ASP:HA	1.99	0.44
3:c:97:TRP:HE1	30:c:518:LMG:HC91	1.82	0.43
27:D:403:BCR:H23C	27:D:403:BCR:H392	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:491:VAL:HG12	4:d:136:VAL:HG13	2.00	0.43
3:c:134:ILE:HD12	25:c:511:CLA:H43	1.99	0.43
25:B:614:CLA:H62	25:B:614:CLA:H92	1.72	0.43
10:K:26:PRO:O	10:K:29:PRO:HD2	2.18	0.43
31:b:620:SQD:H141	31:b:620:SQD:H172	1.55	0.43
25:c:503:CLA:H62	25:c:503:CLA:H102	1.62	0.43
29:d:409:STE:H61	29:d:409:STE:H31	1.92	0.43
10:k:18:PHE:CE2	19:z:13:VAL:HG21	2.42	0.43
17:y:20:ALA:O	17:y:24:MET:HG2	2.17	0.43
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.53	0.43
1:a:183:MET:HA	25:a:606:CLA:HMD1	2.00	0.43
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.00	0.43
25:c:511:CLA:HBA1	27:k:102:BCR:H271	2.00	0.43
5:E:38:VAL:HG11	6:F:39:ALA:HB3	2.01	0.43
29:M:104:STE:H81	29:M:104:STE:H111	1.83	0.43
16:v:87:GLU:CD	16:v:96:ARG:HH12	2.26	0.43
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.84	0.43
2:b:458:PHE:HB3	25:b:604:CLA:HBC2	2.01	0.43
25:b:615:CLA:H92	25:b:615:CLA:H61	1.83	0.43
28:D:404:PL9:H412	11:L:29:LEU:HD23	2.01	0.43
32:D:409:LHG:H161	32:D:409:LHG:H111	2.00	0.43
31:a:615:SQD:H1	36:a:802:HOH:O	2.18	0.43
2:b:160:GLY:HA3	2:b:180:PRO:HB3	2.00	0.43
2:b:373:LYS:HG3	36:b:716:HOH:O	2.18	0.43
25:b:609:CLA:C2B	27:h:101:BCR:H323	2.49	0.43
1:A:85:SER:HA	1:A:109:GLY:HA3	2.01	0.43
4:D:269:PHE:CG	32:D:410:LHG:HC12	2.53	0.43
25:c:513:CLA:H92	29:c:516:STE:H62	2.00	0.43
25:B:611:CLA:H72	25:B:611:CLA:H112	1.82	0.43
31:B:622:SQD:H382	31:B:622:SQD:H352	1.80	0.43
31:B:622:SQD:O9	11:L:7:ARG:HD3	2.19	0.43
25:b:603:CLA:H2	25:b:605:CLA:H91	2.01	0.43
25:c:509:CLA:HMB1	25:c:509:CLA:HBB1	2.00	0.43
12:m:29:THR:HA	36:m:202:HOH:O	2.17	0.43
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.43
3:C:467:LEU:HD23	3:C:467:LEU:HA	1.77	0.43
17:Y:31:ALA:O	17:Y:35:ILE:HG13	2.18	0.43
3:c:121:SER:O	3:c:124:VAL:HG13	2.18	0.43
15:u:51:LYS:HE2	15:u:51:LYS:HB2	1.70	0.43
16:v:126:LEU:HB3	16:v:129:LYS:HB2	2.01	0.43
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:180:GLU:CD	13:O:180:GLU:H	2.27	0.42
27:b:617:BCR:H313	30:m:101:LMG:H112	2.02	0.42
25:c:503:CLA:H203	25:c:510:CLA:HAB	2.00	0.42
3:C:146:PHE:HZ	25:C:512:CLA:HBB2	1.82	0.42
7:H:6:TRP:CZ2	7:H:10:ILE:HD11	2.55	0.42
25:a:607:CLA:H203	25:a:607:CLA:H161	1.81	0.42
4:d:194:ASN:HA	4:d:295:SER:OG	2.19	0.42
27:k:102:BCR:H20C	27:k:102:BCR:H361	1.91	0.42
17:y:38:LEU:HD13	17:y:38:LEU:HA	1.92	0.42
25:B:615:CLA:H93	25:B:615:CLA:H62	1.79	0.42
25:C:506:CLA:H91	25:C:506:CLA:H111	1.80	0.42
3:c:180:MET:HG2	3:c:199:ILE:O	2.19	0.42
12:m:17:VAL:HB	12:m:18:PRO:HD3	2.02	0.42
2:B:36:SER:OG	27:B:618:BCR:H362	2.18	0.42
25:C:509:CLA:H92	25:C:509:CLA:H62	1.81	0.42
13:O:15:LEU:HD23	13:O:18:LYS:HD2	2.02	0.42
25:b:608:CLA:H172	25:b:609:CLA:H192	2.02	0.42
4:d:90:LEU:HD23	4:d:90:LEU:HA	1.90	0.42
25:B:613:CLA:H62	25:B:613:CLA:H41	1.89	0.42
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.01	0.42
29:H:103:STE:H82	29:H:103:STE:H112	1.85	0.42
13:O:231:HIS:HE1	36:O:313:HOH:O	2.02	0.42
27:T:101:BCR:H311	27:T:101:BCR:HC8	2.01	0.42
30:a:616:LMG:H332	30:a:616:LMG:H202	2.00	0.42
2:b:201:HIS:HB2	25:b:602:CLA:CHB	2.50	0.42
4:d:267:LEU:C	4:d:267:LEU:HD23	2.44	0.42
25:d:403:CLA:H92	18:x:18:ALA:HB2	2.01	0.42
3:C:45:LEU:HA	3:C:139:THR:HG22	2.01	0.42
31:a:614:SQD:H282	31:a:614:SQD:H251	1.44	0.42
32:l:101:LHG:H271	12:m:22:LEU:HD21	2.02	0.42
17:y:22:LEU:HA	17:y:25:ILE:HG22	2.01	0.42
32:D:409:LHG:H121	32:D:409:LHG:H151	1.87	0.42
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.35	0.42
19:Z:2:THR:HG22	19:Z:6:GLN:HE22	1.85	0.42
2:b:467:ILE:HD13	2:b:467:ILE:HA	1.87	0.42
3:c:377:LEU:H	13:o:80:GLN:HE22	1.66	0.42
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.01	0.42
4:D:269:PHE:CD2	32:D:410:LHG:HC12	2.54	0.42
33:H:102:DGD:HB21	33:H:102:DGD:HB51	1.80	0.42
25:a:609:CLA:H172	8:i:9:TYR:HB3	2.02	0.42
2:b:298:LEU:HD23	2:b:298:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:604:CLA:H62	25:b:604:CLA:H41	1.73	0.42
13:o:57:LYS:HB3	13:o:59:LYS:HE3	2.02	0.42
25:B:614:CLA:H62	25:B:614:CLA:H41	1.66	0.42
25:C:505:CLA:HBC2	27:C:515:BCR:H341	2.02	0.42
25:a:606:CLA:CBD	25:a:612:CLA:HAC2	2.50	0.42
9:j:18:GLY:HA3	27:k:101:BCR:H371	2.02	0.42
15:u:36:ILE:HD13	16:v:52:LEU:HD13	2.02	0.42
16:v:76:MET:HE3	35:v:201:HEC:HBB3	2.02	0.42
25:A:610:CLA:H61	25:A:610:CLA:H41	1.86	0.41
30:A:615:LMG:H391	3:C:281:MET:HG3	2.02	0.41
25:C:513:CLA:HBB1	25:C:513:CLA:HMB3	2.02	0.41
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.00	0.41
1:a:77:ILE:HD11	14:t:6:TYR:HB3	2.02	0.41
25:d:403:CLA:H93	25:d:403:CLA:H61	1.66	0.41
5:e:8:ARG:HG2	5:e:13:ILE:HG13	2.02	0.41
28:D:404:PL9:H43	32:D:408:LHG:H222	2.02	0.41
13:O:53:LYS:HD3	13:O:63:ALA:HB3	2.02	0.41
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.41
13:o:92:SER:HB3	13:o:131:PRO:HA	2.01	0.41
28:A:612:PL9:H171	28:A:612:PL9:H151	1.78	0.41
25:B:615:CLA:H2	25:B:616:CLA:CBB	2.50	0.41
25:C:508:CLA:H172	30:C:524:LMG:H371	2.02	0.41
12:M:8:LEU:HD11	29:M:104:STE:H162	2.02	0.41
1:a:12:ASN:HB2	36:a:805:HOH:O	2.21	0.41
4:d:236:ASN:O	4:d:239:GLN:HG2	2.19	0.41
29:i:101:STE:H91	29:i:101:STE:H61	1.65	0.41
13:o:59:LYS:HB2	13:o:61:GLN:HG2	2.02	0.41
2:B:193:TYR:O	7:H:65:LEU:HD23	2.21	0.41
2:B:220:ARG:HD2	2:B:220:ARG:HA	1.87	0.41
13:O:27:ARG:HG3	36:O:303:HOH:O	2.21	0.41
26:d:401:PHO:CHB	25:d:402:CLA:H101	2.51	0.41
25:b:610:CLA:HBB1	27:h:101:BCR:C2	2.50	0.41
3:c:391[A]:ARG:HD2	3:c:395:TYR:CE2	2.55	0.41
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.02	0.41
29:A:622:STE:H152	29:A:622:STE:H121	1.79	0.41
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.51	0.41
27:k:102:BCR:H311	27:k:102:BCR:HC7	1.75	0.41
27:t:101:BCR:H20C	27:t:101:BCR:H361	1.92	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
2:b:216:HIS:HE1	25:b:609:CLA:C1A	2.33	0.41
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:512:CLA:H142	25:c:512:CLA:H112	1.72	0.41
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.86	0.41
2:B:414:PRO:O	2:B:418:LYS:HG3	2.21	0.41
27:B:618:BCR:H20C	27:B:618:BCR:H361	1.89	0.41
4:D:85:MET:HE1	5:E:72:ALA:HB2	2.02	0.41
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.55	0.41
25:b:602:CLA:H111	25:b:602:CLA:H152	1.72	0.41
3:c:128:GLY:HA3	25:c:513:CLA:C3C	2.51	0.41
3:c:155:ASN:CG	3:c:155:ASN:O	2.63	0.41
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.85	0.41
33:c:521:DGD:HBH2	33:c:521:DGD:HBT2	1.73	0.41
28:d:405:PL9:H311	32:l:101:LHG:H201	2.03	0.41
25:B:603:CLA:H141	25:B:603:CLA:H162	1.81	0.41
25:B:613:CLA:HMB1	25:B:613:CLA:HBB1	2.02	0.41
3:C:203:THR:O	3:C:235:GLY:HA3	2.21	0.41
3:C:223:TRP:CG	3:C:224:ILE:H	2.38	0.41
3:C:410:VAL:HG22	3:C:413[B]:GLU:HG2	2.03	0.41
4:D:192:THR:HG23	25:D:401:CLA:HBC2	2.03	0.41
13:O:72:THR:HG21	13:O:107:THR:HG23	2.03	0.41
13:O:86:LYS:HB2	13:O:86:LYS:HE3	1.74	0.41
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.86	0.41
25:a:606:CLA:HBD	25:a:612:CLA:HAC2	2.03	0.41
32:a:613:LHG:H132	32:a:613:LHG:H101	1.74	0.41
2:b:210:ILE:HG21	30:b:622:LMG:H231	2.03	0.41
29:b:621:STE:H152	29:b:621:STE:H122	1.71	0.41
29:d:409:STE:H82	29:d:409:STE:H52	1.44	0.41
27:h:101:BCR:H361	27:h:101:BCR:H20C	1.79	0.41
13:o:160:LYS:HD2	13:o:160:LYS:HA	1.93	0.41
17:y:23:THR:O	17:y:27:MET:HG3	2.21	0.41
25:C:512:CLA:H93	25:C:512:CLA:H111	1.93	0.41
4:D:79:SER:HA	4:D:172:SER:HB3	2.02	0.41
4:D:342:PRO:O	4:D:345:VAL:HG22	2.21	0.41
5:e:33:ALA:HB2	20:r:11:PRO:HG2	2.02	0.41
27:A:611:BCR:H24C	27:A:611:BCR:H371	1.94	0.40
32:D:410:LHG:H112	32:D:410:LHG:H141	1.85	0.40
32:L:101:LHG:H311	12:M:21:PHE:CD2	2.55	0.40
32:e:102:LHG:H301	32:e:102:LHG:H271	1.83	0.40
31:B:622:SQD:H442	14:t:23:PHE:HB3	2.04	0.40
3:C:318:LEU:C	3:C:318:LEU:HD23	2.46	0.40
1:a:42:LEU:HD13	27:a:610:BCR:H353	2.03	0.40
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:609:CLA:H141	8:i:9:TYR:HD2	1.86	0.40
25:C:505:CLA:HBB1	25:C:505:CLA:HMB3	2.03	0.40
25:D:402:CLA:H42	7:H:43:LEU:HD11	2.03	0.40
29:d:411:STE:H32	18:x:12:ILE:HG21	2.02	0.40
26:A:609:PHO:HBC2	26:A:609:PHO:HHD	2.03	0.40
25:B:609:CLA:H91	25:B:609:CLA:H112	1.84	0.40
25:C:502:CLA:H161	25:C:502:CLA:H141	1.77	0.40
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.56	0.40
13:O:56:PRO:HD3	13:O:63:ALA:HB2	2.03	0.40
28:a:611:PL9:H151	28:a:611:PL9:H172	1.79	0.40
13:o:51:LEU:HD23	13:o:67:PRO:HA	2.03	0.40
16:v:95:LEU:HD11	16:v:112:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	36	27
1	a	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	27
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	504/510 (99%)	495 (98%)	8 (2%)	1 (0%)	43	35
3	C	441/461 (96%)	432 (98%)	8 (2%)	1 (0%)	43	35
3	c	451/461 (98%)	442 (98%)	8 (2%)	1 (0%)	43	35
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	58 (95%)	2 (3%)	1 (2%)	7	2
8	I	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	0
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	30 (100%)	0	0	100	100
13	O	243/272 (89%)	231 (95%)	11 (4%)	1 (0%)	30	20
13	o	242/272 (89%)	235 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	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%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	26 (100%)	0	0	100	100
All	All	5231/5700 (92%)	5114 (98%)	107 (2%)	10 (0%)	43	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
15	u	53	ALA
2	b	505	ARG
7	h	63	LYS
9	J	7	ARG
13	O	62	GLU
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	268 (99%)	2 (1%)	76	73
1	a	269/280 (96%)	263 (98%)	6 (2%)	45	38
2	B	408/407 (100%)	406 (100%)	2 (0%)	81	79
2	b	403/407 (99%)	401 (100%)	2 (0%)	81	79
3	C	345/362 (95%)	341 (99%)	4 (1%)	63	58
3	c	354/362 (98%)	347 (98%)	7 (2%)	48	42
4	D	276/283 (98%)	274 (99%)	2 (1%)	76	73
4	d	277/283 (98%)	274 (99%)	3 (1%)	65	61
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	29
5	e	71/73 (97%)	70 (99%)	1 (1%)	59	54
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	31	20
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	19
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	26

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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%)	27 (90%)	3 (10%)	7	1
10	k	30/37 (81%)	28 (93%)	2 (7%)	15	5
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%)	203 (98%)	4 (2%)	50	44
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%)	82 (98%)	2 (2%)	43	35
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
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%)	22 (100%)	0	100	100
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%)	52 (100%)	0	100	100
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	20 (91%)	2 (9%)	9	2
All	All	4321/4654 (93%)	4260 (99%)	61 (1%)	61	54

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	205	VAL
2	B	76	SER

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Mol	Chain	Res	Type
2	B	86	ILE
3	C	240	ILE
3	C	289	PHE
3	C	354	GLU
3	C	416	SER
4	D	43	LEU
4	D	259	ILE
5	E	22[A]	ILE
5	E	22[B]	ILE
8	I	4	LEU
10	K	13	GLU
10	K	17	ILE
10	K	19	ASP
12	M	20	VAL
12	M	25	LEU
13	O	86	LYS
13	O	107	THR
13	O	118	LEU
13	O	198	SER
13	O	214	THR
14	T	30	THR
15	U	45	LEU
15	U	61	VAL
1	a	35	VAL
1	a	159	LEU
1	a	200	LEU
1	a	245	THR
1	a	286	THR
1	a	288	LEU
2	b	267	LEU
2	b	362	PHE
3	c	99	VAL
3	c	124	VAL
3	c	216	SER
3	c	240	ILE
3	c	354	GLU
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	321	LEU
5	e	4	THR

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Mol	Chain	Res	Type
6	f	23	VAL
7	h	43	LEU
7	h	61	SER
10	k	19	ASP
10	k	27	VAL
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	49	THR
13	o	115	ARG
13	o	118	LEU
13	o	199	LEU
16	v	52	LEU
18	x	2	THR
20	r	9	LEU
20	r	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	234	ASN
1	A	338	ASN
2	B	331	ASN
2	B	409	GLN
3	C	155	ASN
3	C	201	ASN
3	C	327	ASN
3	C	385	GLN
3	C	415	ASN
5	E	82	GLN
11	L	8	GLN
13	O	36	GLN
13	O	124	ASN
13	O	147	ASN
13	O	155	ASN
13	O	200	ASN
13	O	231	HIS
19	Z	6	GLN
20	R	22	ASN
1	a	165	GLN
1	a	181	ASN

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Mol	Chain	Res	Type
1	a	296	ASN
2	b	14	ASN
2	b	331	ASN
2	b	338	GLN
2	b	394	GLN
2	b	409	GLN
2	b	497	GLN
3	c	322	GLN
3	c	378	ASN
3	c	415	ASN
4	d	61	HIS
4	d	186	GLN
4	d	239	GLN
4	d	338	ASN
5	e	82	GLN
7	h	59	ASN
12	m	5	GLN
12	m	32	GLN
13	o	61	GLN
13	o	80	GLN
13	o	88	ASN
13	o	132	ASN
13	o	155	ASN
13	o	196	GLN
18	x	33	GLN
18	x	38	GLN
19	z	6	GLN
19	z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.47	0	8,9,11	0.76	0
14	FME	t	1	14	8,9,10	0.51	0	8,9,11	0.92	0
12	FME	M	1	12	8,9,10	0.44	0	8,9,11	0.95	0
14	FME	T	1	14	8,9,10	0.44	0	8,9,11	0.88	0
12	FME	m	1	12	8,9,10	0.43	0	8,9,11	0.60	0
8	FME	i	1	8	8,9,10	0.49	0	8,9,11	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	2/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
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	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	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	$\# Z > 2$
29	STE	h	103	-	9,9,19	0.39	0	8,8,19	0.69	0
30	LMG	d	410	-	44,44,55	0.51	0	52,52,63	0.66	0
29	STE	C	520	-	9,9,19	0.35	0	8,8,19	0.80	0
35	HEC	v	201	16	50,50,50	1.67	8 (16%)	68,82,82	1.32	6 (8%)
25	CLA	A	614	36	69,73,73	1.34	8 (11%)	82,113,113	1.22	6 (7%)
21	OEX	A	601	3,1,36	0,14,14	-	-	-	-	-
27	BCR	B	617	-	41,41,41	0.42	0	56,56,56	0.72	1 (1%)
29	STE	E	103	-	19,19,19	0.63	0	19,19,19	1.02	1 (5%)
29	STE	C	518	-	4,4,19	0.39	0	3,3,19	0.46	0
33	DGD	c	520	-	63,63,67	0.52	0	77,77,81	0.78	2 (2%)
25	CLA	c	507	36	69,73,73	1.12	4 (5%)	82,113,113	1.34	7 (8%)
25	CLA	c	503	3	69,73,73	1.30	8 (11%)	82,113,113	1.45	8 (9%)
31	SQD	A	616	-	50,52,54	1.55	7 (14%)	60,63,65	1.94	11 (18%)
30	LMG	c	522	-	46,46,55	0.53	0	54,54,63	0.69	0
29	STE	e	104	-	12,12,19	0.68	0	12,12,19	1.24	2 (16%)
25	CLA	b	605	2	69,73,73	1.12	7 (10%)	82,113,113	1.25	7 (8%)
29	STE	M	104	-	14,14,19	0.33	0	13,13,19	0.88	0
29	STE	d	409	-	19,19,19	0.56	0	19,19,19	1.08	1 (5%)
25	CLA	B	606	2	69,73,73	1.39	8 (11%)	82,113,113	1.39	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	STE	B	623	-	17,17,19	0.61	0	17,17,19	1.20	2 (11%)
25	CLA	B	616	2	64,68,73	1.31	7 (10%)	76,107,113	1.45	9 (11%)
25	CLA	c	506	3	69,73,73	1.26	7 (10%)	82,113,113	1.15	5 (6%)
30	LMG	B	620	-	45,45,55	0.52	0	53,53,63	0.97	2 (3%)
31	SQD	f	102	-	39,41,54	1.66	7 (17%)	49,52,65	1.76	10 (20%)
28	PL9	a	611	-	55,55,55	0.81	1 (1%)	68,69,69	1.51	11 (16%)
29	STE	E	102	-	11,11,19	0.34	0	10,10,19	0.73	0
25	CLA	C	513	3	69,73,73	1.33	6 (8%)	82,113,113	1.35	8 (9%)
29	STE	J	102	-	11,11,19	0.70	0	11,11,19	1.23	0
29	STE	c	516	-	12,12,19	0.36	0	11,11,19	0.76	0
29	STE	C	516	-	13,13,19	0.78	0	13,13,19	0.91	0
27	BCR	T	101	-	41,41,41	0.46	0	56,56,56	0.97	2 (3%)
26	PHO	a	608	-	58,69,69	2.08	9 (15%)	55,99,99	1.60	9 (16%)
27	BCR	h	101	-	41,41,41	0.44	0	56,56,56	0.89	2 (3%)
29	STE	f	103	-	7,7,19	0.37	0	6,6,19	0.68	0
25	CLA	C	504	36	63,67,73	1.30	8 (12%)	74,105,113	1.20	7 (9%)
29	STE	I	102	-	14,14,19	0.70	0	14,14,19	1.05	0
25	CLA	c	511	3	69,73,73	1.50	7 (10%)	82,113,113	1.45	5 (6%)
29	STE	B	624	-	11,11,19	0.67	0	11,11,19	1.31	2 (18%)
27	BCR	A	611	-	41,41,41	0.40	0	56,56,56	0.87	3 (5%)
29	STE	b	624	-	9,9,19	0.33	0	8,8,19	0.78	0
29	STE	e	103	-	8,8,19	0.37	0	7,7,19	0.70	0
32	LHG	D	408	-	48,48,48	0.60	1 (2%)	51,54,54	0.65	2 (3%)
33	DGD	A	619	-	67,67,67	0.55	0	81,81,81	0.96	6 (7%)
25	CLA	C	501	3	69,73,73	1.33	7 (10%)	82,113,113	1.44	6 (7%)
29	STE	b	621	-	19,19,19	0.61	0	19,19,19	1.05	0
25	CLA	c	501	3	69,73,73	1.08	5 (7%)	82,113,113	1.26	6 (7%)
25	CLA	B	603	2	69,73,73	1.32	5 (7%)	82,113,113	1.29	8 (9%)
25	CLA	B	608	2	69,73,73	1.15	8 (11%)	82,113,113	1.37	10 (12%)
29	STE	z	101	-	8,8,19	0.38	0	7,7,19	0.63	0
25	CLA	b	616	2	64,68,73	1.22	6 (9%)	76,107,113	1.42	8 (10%)
32	LHG	D	410	-	48,48,48	0.58	1 (2%)	51,54,54	0.79	2 (3%)
32	LHG	e	102	-	41,41,48	0.57	0	44,47,54	0.57	0
29	STE	B	625	-	14,14,19	0.35	0	13,13,19	0.85	0
27	BCR	k	101	-	41,41,41	0.35	0	56,56,56	0.85	2 (3%)
25	CLA	d	403	4	69,73,73	1.27	9 (13%)	82,113,113	1.22	9 (10%)
27	BCR	D	403	-	41,41,41	0.41	0	56,56,56	0.84	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	L	101	-	48,48,48	0.49	0	51,54,54	0.73	0
25	CLA	b	609	2	69,73,73	1.19	6 (8%)	82,113,113	1.38	10 (12%)
31	SQD	D	407	-	34,36,54	1.46	4 (11%)	42,45,65	1.70	9 (21%)
29	STE	M	103	-	9,9,19	0.33	0	8,8,19	0.78	0
25	CLA	D	402	4	69,73,73	1.21	6 (8%)	82,113,113	1.30	7 (8%)
29	STE	j	102	-	15,15,19	0.38	0	14,14,19	0.73	0
25	CLA	B	604	2	69,73,73	1.41	7 (10%)	82,113,113	1.58	8 (9%)
31	SQD	a	614	-	52,54,54	1.48	6 (11%)	62,65,65	1.97	12 (19%)
25	CLA	C	510	3	69,73,73	1.29	8 (11%)	82,113,113	1.38	8 (9%)
30	LMG	A	615	-	48,48,55	0.48	0	56,56,63	0.65	1 (1%)
32	LHG	a	613	-	48,48,48	0.55	0	51,54,54	0.61	0
29	STE	b	623	-	15,15,19	0.68	0	15,15,19	1.19	1 (6%)
29	STE	k	103	-	13,13,19	0.69	0	13,13,19	1.09	0
25	CLA	b	603	2	69,73,73	1.24	8 (11%)	82,113,113	1.37	8 (9%)
31	SQD	B	622	-	52,54,54	1.57	8 (15%)	62,65,65	1.82	14 (22%)
33	DGD	H	102	-	63,63,67	0.53	0	77,77,81	0.92	3 (3%)
30	LMG	c	518	-	29,29,55	0.43	0	31,31,63	0.61	0
25	CLA	b	610	36	69,73,73	1.21	7 (10%)	82,113,113	1.32	8 (9%)
31	SQD	b	620	-	47,49,54	1.60	9 (19%)	57,60,65	1.85	13 (22%)
29	STE	m	102	-	11,11,19	0.66	0	11,11,19	1.41	2 (18%)
29	STE	A	622	-	10,10,19	0.33	0	9,9,19	0.83	0
25	CLA	a	607	36	69,73,73	1.20	6 (8%)	82,113,113	1.23	7 (8%)
25	CLA	a	612	36	69,73,73	1.27	8 (11%)	82,113,113	1.32	11 (13%)
25	CLA	b	615	2	69,73,73	1.47	10 (14%)	82,113,113	1.31	6 (7%)
27	BCR	K	101	-	41,41,41	0.37	0	56,56,56	0.91	0
25	CLA	B	613	2	69,73,73	1.37	9 (13%)	82,113,113	1.43	8 (9%)
25	CLA	B	611	2	69,73,73	1.15	7 (10%)	82,113,113	1.32	6 (7%)
34	HEM	F	101	6,5	50,50,50	1.42	8 (16%)	67,82,82	1.15	3 (4%)
30	LMG	b	622	-	55,55,55	0.50	0	63,63,63	0.88	4 (6%)
25	CLA	C	505	3	69,73,73	1.24	7 (10%)	82,113,113	1.41	9 (10%)
27	BCR	b	618	-	41,41,41	0.42	0	56,56,56	0.93	3 (5%)
29	STE	C	526	-	15,15,19	0.33	0	14,14,19	0.84	0
29	STE	K	102	-	13,13,19	0.37	0	12,12,19	0.66	0
25	CLA	B	601	36	69,73,73	1.35	7 (10%)	82,113,113	1.35	4 (4%)
24	BCT	a	605	22	3,3,3	0.79	0	2,3,3	2.06	1 (50%)
27	BCR	c	515	-	41,41,41	0.39	0	56,56,56	0.99	2 (3%)
27	BCR	H	101	-	41,41,41	0.45	0	56,56,56	1.15	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	601	36	69,73,73	1.27	7 (10%)	82,113,113	1.32	5 (6%)
30	LMG	a	616	-	55,55,55	0.48	0	63,63,63	1.29	7 (11%)
25	CLA	b	606	2	69,73,73	1.40	6 (8%)	82,113,113	1.42	5 (6%)
29	STE	A	613	-	8,8,19	0.37	0	7,7,19	0.74	0
30	LMG	M	101	-	51,51,55	0.45	0	59,59,63	0.85	2 (3%)
28	PL9	A	612	-	55,55,55	0.67	0	68,69,69	1.48	7 (10%)
27	BCR	c	514	-	41,41,41	0.32	0	56,56,56	0.57	0
29	STE	C	527	-	13,13,19	0.35	0	12,12,19	0.78	0
32	LHG	l	101	-	48,48,48	0.46	0	51,54,54	0.62	0
30	LMG	C	517	-	35,35,55	0.51	0	43,43,63	1.45	6 (13%)
25	CLA	c	505	3	69,73,73	1.17	6 (8%)	82,113,113	1.34	8 (9%)
29	STE	C	519	-	6,6,19	0.38	0	5,5,19	0.64	0
33	DGD	h	102	-	63,63,67	0.54	0	77,77,81	0.95	6 (7%)
30	LMG	D	406	-	51,51,55	0.48	0	59,59,63	0.64	1 (1%)
25	CLA	c	504	36	64,68,73	1.16	6 (9%)	76,107,113	1.34	8 (10%)
29	STE	E	101	-	11,11,19	0.74	0	11,11,19	1.20	1 (9%)
27	BCR	a	610	-	41,41,41	0.42	0	56,56,56	0.74	0
28	PL9	D	404	-	55,55,55	1.04	3 (5%)	68,69,69	1.57	12 (17%)
25	CLA	B	602	2	69,73,73	1.21	7 (10%)	82,113,113	1.32	8 (9%)
26	PHO	A	609	-	58,69,69	2.08	9 (15%)	55,99,99	1.71	11 (20%)
25	CLA	A	607	36	69,73,73	1.16	6 (8%)	82,113,113	1.36	7 (8%)
25	CLA	B	609	2	69,73,73	1.22	5 (7%)	82,113,113	1.32	7 (8%)
25	CLA	B	607	36	69,73,73	1.29	8 (11%)	82,113,113	1.29	7 (8%)
25	CLA	b	608	2	69,73,73	1.16	7 (10%)	82,113,113	1.35	8 (9%)
29	STE	I	101	-	16,16,19	0.75	0	16,16,19	0.95	1 (6%)
29	STE	m	103	-	17,17,19	0.35	0	16,16,19	0.82	0
25	CLA	D	401	4	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)
33	DGD	C	521	-	63,63,67	0.57	0	77,77,81	0.85	3 (3%)
25	CLA	B	614	2	69,73,73	1.37	7 (10%)	82,113,113	1.37	11 (13%)
27	BCR	k	102	-	41,41,41	0.39	0	56,56,56	0.90	2 (3%)
26	PHO	d	401	-	58,69,69	2.19	10 (17%)	55,99,99	1.69	11 (20%)
24	BCT	A	605	22	3,3,3	0.81	0	2,3,3	1.96	1 (50%)
29	STE	t	102	-	13,13,19	0.65	0	13,13,19	1.27	2 (15%)
33	DGD	C	522	-	63,63,67	0.60	0	77,77,81	0.77	2 (2%)
27	BCR	C	514	-	41,41,41	0.34	0	56,56,56	0.58	0
25	CLA	C	511	3	69,73,73	1.35	7 (10%)	82,113,113	1.39	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	615	2	69,73,73	1.62	10 (14%)	82,113,113	1.45	5 (6%)
25	CLA	b	613	2	69,73,73	1.21	6 (8%)	82,113,113	1.31	7 (8%)
29	STE	c	517	-	17,17,19	0.39	0	16,16,19	0.68	0
32	LHG	D	409	-	46,46,48	0.56	0	49,52,54	0.59	0
25	CLA	B	610	36	69,73,73	1.29	7 (10%)	82,113,113	1.45	10 (12%)
25	CLA	b	604	2	69,73,73	1.22	8 (11%)	82,113,113	1.55	14 (17%)
27	BCR	t	101	-	41,41,41	0.54	0	56,56,56	1.19	6 (10%)
29	STE	a	617	-	11,11,19	0.75	0	11,11,19	1.09	1 (9%)
25	CLA	B	612	2	69,73,73	1.14	6 (8%)	82,113,113	1.36	8 (9%)
27	BCR	B	618	-	41,41,41	0.43	0	56,56,56	0.76	1 (1%)
27	BCR	J	101	-	41,41,41	0.35	0	56,56,56	0.86	1 (1%)
25	CLA	A	610	1	58,62,73	1.24	6 (10%)	68,99,113	1.33	6 (8%)
25	CLA	c	510	3	69,73,73	1.29	8 (11%)	82,113,113	1.26	7 (8%)
29	STE	D	411	-	8,8,19	0.34	0	7,7,19	0.73	0
31	SQD	A	618	-	41,43,54	1.77	8 (19%)	51,54,65	1.51	9 (17%)
25	CLA	b	602	2	69,73,73	1.15	7 (10%)	82,113,113	1.33	7 (8%)
25	CLA	C	512	3	69,73,73	1.40	10 (14%)	82,113,113	1.36	8 (9%)
29	STE	d	406	-	19,19,19	0.67	0	19,19,19	0.97	1 (5%)
32	LHG	d	407	-	48,48,48	0.53	0	51,54,54	0.71	2 (3%)
29	STE	H	103	-	17,17,19	0.39	0	16,16,19	0.77	0
28	PL9	d	405	-	55,55,55	0.96	2 (3%)	68,69,69	1.57	14 (20%)
29	STE	Z	101	-	16,16,19	0.36	0	15,15,19	0.74	0
35	HEC	V	201	16	50,50,50	1.66	7 (14%)	68,82,82	1.43	9 (13%)
30	LMG	c	524	-	49,49,55	0.51	0	57,57,63	0.84	4 (7%)
21	OEX	a	601	3,1,36	0,14,14	-	-	-	-	-
29	STE	T	102	-	15,15,19	0.37	0	14,14,19	0.76	0
25	CLA	d	402	4	69,73,73	1.19	7 (10%)	82,113,113	1.29	6 (7%)
29	STE	X	101	-	19,19,19	0.61	0	19,19,19	1.15	0
27	BCR	B	619	-	41,41,41	0.38	0	56,56,56	0.79	1 (1%)
25	CLA	C	507	36	69,73,73	1.11	6 (8%)	82,113,113	1.43	7 (8%)
27	BCR	d	404	-	41,41,41	0.45	0	56,56,56	0.91	2 (3%)
25	CLA	C	506	3	69,73,73	1.13	7 (10%)	82,113,113	1.23	5 (6%)
25	CLA	c	509	3	69,73,73	1.12	5 (7%)	82,113,113	1.34	7 (8%)
25	CLA	C	509	3	69,73,73	1.11	6 (8%)	82,113,113	1.24	5 (6%)
32	LHG	d	408	-	38,38,48	0.56	0	41,44,54	0.67	0
25	CLA	c	512	3	69,73,73	1.17	8 (11%)	82,113,113	1.21	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	503	3	69,73,73	1.33	8 (11%)	82,113,113	1.48	10 (12%)
25	CLA	c	508	3	68,72,73	1.33	9 (13%)	80,111,113	1.41	9 (11%)
25	CLA	c	513	3	69,73,73	1.25	7 (10%)	82,113,113	1.19	6 (7%)
29	STE	d	411	-	19,19,19	0.57	0	19,19,19	1.04	0
25	CLA	C	508	3	69,73,73	1.25	8 (11%)	82,113,113	1.31	5 (6%)
29	STE	A	620	-	7,7,19	0.32	0	6,6,19	0.80	0
27	BCR	C	515	-	41,41,41	0.34	0	56,56,56	0.59	0
29	STE	M	102	-	14,14,19	0.66	0	14,14,19	1.11	1 (7%)
25	CLA	b	612	2	69,73,73	1.22	9 (13%)	82,113,113	1.22	8 (9%)
32	LHG	A	617	-	48,48,48	0.53	0	51,54,54	0.54	0
30	LMG	m	101	-	51,51,55	0.49	0	59,59,63	0.76	1 (1%)
29	STE	i	102	-	5,5,19	0.35	0	4,4,19	0.56	0
29	STE	C	525	-	11,11,19	0.75	0	11,11,19	1.30	2 (18%)
31	SQD	a	615	-	52,54,54	1.64	8 (15%)	62,65,65	1.45	8 (12%)
26	PHO	A	608	-	58,69,69	1.93	7 (12%)	55,99,99	1.59	7 (12%)
33	DGD	c	519	-	63,63,67	0.62	0	77,77,81	0.83	3 (3%)
34	HEM	f	101	6,5	50,50,50	1.51	9 (18%)	67,82,82	1.40	7 (10%)
25	CLA	A	606	1	69,73,73	1.22	6 (8%)	82,113,113	1.19	5 (6%)
29	STE	A	621	-	16,16,19	0.35	0	15,15,19	0.81	0
29	STE	i	101	-	11,11,19	0.75	0	11,11,19	1.12	0
29	STE	B	621	-	16,16,19	0.62	0	16,16,19	1.19	0
30	LMG	D	405	-	50,50,55	0.43	0	58,58,63	1.12	3 (5%)
29	STE	j	101	-	11,11,19	0.74	0	11,11,19	1.34	1 (9%)
30	LMG	C	524	-	48,48,55	0.50	0	56,56,63	0.65	1 (1%)
30	LMG	c	523	-	48,48,55	0.47	0	56,56,63	0.67	0
25	CLA	a	609	1	69,73,73	1.17	6 (8%)	82,113,113	1.19	7 (8%)
25	CLA	c	502	3	69,73,73	1.14	5 (7%)	82,113,113	1.40	9 (10%)
29	STE	b	625	-	10,10,19	0.36	0	9,9,19	0.73	0
25	CLA	C	502	3	69,73,73	1.22	8 (11%)	82,113,113	1.23	5 (6%)
27	BCR	b	619	-	41,41,41	0.37	0	56,56,56	0.77	0
25	CLA	b	611	2	69,73,73	1.22	6 (8%)	82,113,113	1.22	7 (8%)
25	CLA	B	605	2	69,73,73	1.21	7 (10%)	82,113,113	1.26	7 (8%)
25	CLA	a	606	1	69,73,73	1.30	9 (13%)	82,113,113	1.32	8 (9%)
27	BCR	b	617	-	41,41,41	0.41	0	56,56,56	0.76	2 (3%)
25	CLA	b	607	36	69,73,73	1.23	6 (8%)	82,113,113	1.24	7 (8%)
29	STE	t	103	-	9,9,19	0.39	0	8,8,19	0.70	0
25	CLA	b	614	2	69,73,73	1.30	8 (11%)	82,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	DGD	C	523	-	63,63,67	0.60	1 (1%)	77,77,81	0.76	1 (1%)
33	DGD	c	521	-	63,63,67	0.51	0	77,77,81	0.68	2 (2%)
29	STE	e	101	-	8,8,19	0.40	0	7,7,19	0.59	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
29	STE	h	103	-	-	4/7/7/17	-
30	LMG	d	410	-	-	9/39/59/70	0/1/1/1
29	STE	C	520	-	-	4/7/7/17	-
35	HEC	v	201	16	1/1/3/7	4/14/54/54	-
25	CLA	A	614	36	-	3/39/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
29	STE	E	103	-	-	12/17/17/17	-
29	STE	C	518	-	-	0/2/2/17	-
33	DGD	c	520	-	-	17/51/91/95	0/2/2/2
25	CLA	c	507	36	-	8/39/115/115	-
25	CLA	c	503	3	-	10/39/115/115	-
31	SQD	A	616	-	-	19/47/67/69	0/1/1/1
30	LMG	c	522	-	-	15/41/61/70	0/1/1/1
29	STE	e	104	-	-	3/10/10/17	-
25	CLA	b	605	2	-	10/39/115/115	-
29	STE	M	104	-	-	9/12/12/17	-
29	STE	d	409	-	-	11/17/17/17	-
25	CLA	B	606	2	-	12/39/115/115	-
29	STE	B	623	-	-	9/15/15/17	-
25	CLA	B	616	2	-	10/33/109/115	-
25	CLA	c	506	3	-	15/39/115/115	-
30	LMG	B	620	-	-	14/40/60/70	0/1/1/1
31	SQD	f	102	-	-	17/36/56/69	0/1/1/1
28	PL9	a	611	-	-	13/53/73/73	0/1/1/1
29	STE	E	102	-	-	3/9/9/17	-
25	CLA	C	513	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	STE	J	102	-	-	8/9/9/17	-
29	STE	c	516	-	-	5/10/10/17	-
29	STE	C	516	-	-	6/11/11/17	-
27	BCR	T	101	-	-	7/29/63/63	0/2/2/2
26	PHO	a	608	-	-	4/37/103/103	0/5/6/6
27	BCR	h	101	-	-	1/29/63/63	0/2/2/2
29	STE	f	103	-	-	3/5/5/17	-
25	CLA	C	504	36	-	7/32/108/115	-
29	STE	I	102	-	-	3/12/12/17	-
25	CLA	c	511	3	-	4/39/115/115	-
29	STE	B	624	-	-	2/9/9/17	-
27	BCR	A	611	-	-	0/29/63/63	0/2/2/2
29	STE	b	624	-	-	4/7/7/17	-
29	STE	e	103	-	-	3/6/6/17	-
32	LHG	D	408	-	-	19/53/53/53	-
33	DGD	A	619	-	-	24/55/95/95	0/2/2/2
25	CLA	C	501	3	-	5/39/115/115	-
29	STE	b	621	-	-	7/17/17/17	-
25	CLA	c	501	3	-	1/39/115/115	-
25	CLA	B	603	2	-	4/39/115/115	-
25	CLA	B	608	2	-	1/39/115/115	-
29	STE	z	101	-	-	3/6/6/17	-
25	CLA	b	616	2	-	9/33/109/115	-
32	LHG	D	410	-	-	19/53/53/53	-
32	LHG	e	102	-	-	19/46/46/53	-
29	STE	B	625	-	-	4/12/12/17	-
27	BCR	k	101	-	-	7/29/63/63	0/2/2/2
25	CLA	d	403	4	-	10/39/115/115	-
27	BCR	D	403	-	-	2/29/63/63	0/2/2/2
32	LHG	L	101	-	-	14/53/53/53	-
25	CLA	b	609	2	-	6/39/115/115	-
31	SQD	D	407	-	-	15/28/48/69	0/1/1/1
29	STE	M	103	-	-	4/7/7/17	-
25	CLA	D	402	4	-	9/39/115/115	-
29	STE	j	102	-	-	6/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	604	2	-	7/39/115/115	-
31	SQD	a	614	-	-	27/49/69/69	0/1/1/1
25	CLA	C	510	3	-	7/39/115/115	-
30	LMG	A	615	-	-	20/43/63/70	0/1/1/1
32	LHG	a	613	-	-	24/53/53/53	-
29	STE	b	623	-	-	7/13/13/17	-
29	STE	k	103	-	-	5/11/11/17	-
25	CLA	b	603	2	-	6/39/115/115	-
31	SQD	B	622	-	-	24/49/69/69	0/1/1/1
33	DGD	H	102	-	-	17/51/91/95	0/2/2/2
30	LMG	c	518	-	-	8/31/31/70	-
25	CLA	b	610	36	-	6/39/115/115	-
31	SQD	b	620	-	-	20/44/64/69	0/1/1/1
29	STE	m	102	-	-	4/9/9/17	-
29	STE	A	622	-	-	6/8/8/17	-
25	CLA	a	607	36	-	5/39/115/115	-
25	CLA	a	612	36	-	2/39/115/115	-
25	CLA	b	615	2	-	3/39/115/115	-
27	BCR	K	101	-	-	2/29/63/63	0/2/2/2
25	CLA	B	613	2	-	11/39/115/115	-
25	CLA	B	611	2	-	4/39/115/115	-
34	HEM	F	101	6,5	-	3/14/54/54	-
30	LMG	b	622	-	-	20/50/70/70	0/1/1/1
25	CLA	C	505	3	-	8/39/115/115	-
27	BCR	b	618	-	-	0/29/63/63	0/2/2/2
29	STE	C	526	-	-	4/13/13/17	-
29	STE	K	102	-	-	8/11/11/17	-
25	CLA	B	601	36	-	14/39/115/115	-
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
27	BCR	H	101	-	-	3/29/63/63	0/2/2/2
25	CLA	b	601	36	-	15/39/115/115	-
30	LMG	a	616	-	-	26/50/70/70	0/1/1/1
25	CLA	b	606	2	-	7/39/115/115	-
29	STE	A	613	-	-	2/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	M	101	-	-	17/46/66/70	0/1/1/1
28	PL9	A	612	-	-	21/53/73/73	0/1/1/1
27	BCR	c	514	-	-	1/29/63/63	0/2/2/2
29	STE	C	527	-	-	6/11/11/17	-
32	LHG	l	101	-	-	17/53/53/53	-
30	LMG	C	517	-	-	12/30/50/70	0/1/1/1
25	CLA	c	505	3	-	7/39/115/115	-
29	STE	C	519	-	-	3/4/4/17	-
33	DGD	h	102	-	-	17/51/91/95	0/2/2/2
30	LMG	D	406	-	-	12/46/66/70	0/1/1/1
25	CLA	c	504	36	-	9/33/109/115	-
29	STE	E	101	-	-	1/9/9/17	-
27	BCR	a	610	-	-	0/29/63/63	0/2/2/2
28	PL9	D	404	-	-	6/53/73/73	0/1/1/1
25	CLA	B	602	2	-	6/39/115/115	-
26	PHO	A	609	-	-	2/37/103/103	0/5/6/6
25	CLA	A	607	36	-	6/39/115/115	-
25	CLA	B	609	2	-	2/39/115/115	-
25	CLA	B	607	36	-	3/39/115/115	-
25	CLA	b	608	2	-	7/39/115/115	-
29	STE	I	101	-	-	6/14/14/17	-
29	STE	m	103	-	-	11/15/15/17	-
25	CLA	D	401	4	-	2/39/115/115	-
33	DGD	C	521	-	-	17/51/91/95	0/2/2/2
25	CLA	B	614	2	-	12/39/115/115	-
27	BCR	k	102	-	-	3/29/63/63	0/2/2/2
26	PHO	d	401	-	-	1/37/103/103	0/5/6/6
29	STE	t	102	-	-	6/11/11/17	-
33	DGD	C	522	-	-	20/51/91/95	0/2/2/2
27	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	CLA	C	511	3	-	6/39/115/115	-
25	CLA	B	615	2	-	14/39/115/115	-
25	CLA	b	613	2	-	4/39/115/115	-
29	STE	c	517	-	-	10/15/15/17	-
32	LHG	D	409	-	-	14/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	610	36	-	6/39/115/115	-
25	CLA	b	604	2	-	9/39/115/115	-
27	BCR	t	101	-	-	5/29/63/63	0/2/2/2
29	STE	a	617	-	-	4/9/9/17	-
25	CLA	B	612	2	-	8/39/115/115	-
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	J	101	-	-	4/29/63/63	0/2/2/2
25	CLA	A	610	1	-	2/26/102/115	-
25	CLA	c	510	3	-	7/39/115/115	-
29	STE	D	411	-	-	3/6/6/17	-
31	SQD	A	618	-	-	12/38/58/69	0/1/1/1
25	CLA	b	602	2	-	7/39/115/115	-
25	CLA	C	512	3	-	13/39/115/115	-
29	STE	d	406	-	-	7/17/17/17	-
32	LHG	d	407	-	-	17/53/53/53	-
29	STE	H	103	-	-	7/15/15/17	-
28	PL9	d	405	-	-	10/53/73/73	0/1/1/1
29	STE	Z	101	-	-	9/14/14/17	-
35	HEC	V	201	16	1/1/3/7	6/14/54/54	-
30	LMG	c	524	-	-	16/44/64/70	0/1/1/1
29	STE	X	101	-	-	10/17/17/17	-
29	STE	T	102	-	-	9/13/13/17	-
25	CLA	d	402	4	-	7/39/115/115	-
27	BCR	B	619	-	-	2/29/63/63	0/2/2/2
25	CLA	C	507	36	-	9/39/115/115	-
27	BCR	d	404	-	-	4/29/63/63	0/2/2/2
25	CLA	C	506	3	-	11/39/115/115	-
25	CLA	c	509	3	-	16/39/115/115	-
25	CLA	C	509	3	-	11/39/115/115	-
32	LHG	d	408	-	-	9/43/43/53	-
25	CLA	c	512	3	-	15/39/115/115	-
25	CLA	C	503	3	-	2/39/115/115	-
25	CLA	c	508	3	-	6/38/114/115	-
25	CLA	c	513	3	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	STE	d	411	-	-	9/17/17/17	-
25	CLA	C	508	3	-	3/39/115/115	-
29	STE	A	620	-	-	3/5/5/17	-
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
29	STE	M	102	-	-	5/12/12/17	-
25	CLA	b	612	2	-	2/39/115/115	-
32	LHG	A	617	-	-	23/53/53/53	-
30	LMG	m	101	-	-	18/46/66/70	0/1/1/1
29	STE	i	102	-	-	2/3/3/17	-
29	STE	C	525	-	-	3/9/9/17	-
31	SQD	a	615	-	-	15/49/69/69	0/1/1/1
26	PHO	A	608	-	-	1/37/103/103	0/5/6/6
33	DGD	c	519	-	-	22/51/91/95	0/2/2/2
34	HEM	f	101	6,5	-	4/14/54/54	-
25	CLA	A	606	1	-	6/39/115/115	-
29	STE	A	621	-	-	9/14/14/17	-
29	STE	i	101	-	-	6/9/9/17	-
29	STE	B	621	-	-	6/14/14/17	-
30	LMG	D	405	-	-	15/45/65/70	0/1/1/1
29	STE	j	101	-	-	3/9/9/17	-
30	LMG	C	524	-	-	12/43/63/70	0/1/1/1
30	LMG	c	523	-	-	17/43/63/70	0/1/1/1
25	CLA	a	609	1	-	11/39/115/115	-
25	CLA	c	502	3	-	6/39/115/115	-
29	STE	b	625	-	-	6/8/8/17	-
25	CLA	C	502	3	-	6/39/115/115	-
27	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	CLA	b	611	2	-	4/39/115/115	-
25	CLA	B	605	2	-	10/39/115/115	-
25	CLA	a	606	1	-	3/39/115/115	-
27	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	CLA	b	607	36	-	11/39/115/115	-
29	STE	t	103	-	-	4/7/7/17	-
25	CLA	b	614	2	-	13/39/115/115	-
33	DGD	C	523	-	-	13/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	c	521	-	-	15/51/91/95	0/2/2/2
29	STE	e	101	-	-	3/6/6/17	-

All (627) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	401	PHO	C1B-C2B	9.69	1.50	1.39
26	d	401	PHO	C3B-C4B	9.45	1.51	1.41
26	a	608	PHO	C1B-C2B	9.18	1.49	1.39
26	A	609	PHO	C1B-C2B	9.11	1.49	1.39
26	A	609	PHO	C3B-C4B	8.59	1.50	1.41
26	a	608	PHO	C3B-C4B	8.03	1.49	1.41
26	A	608	PHO	C1B-C2B	7.81	1.48	1.39
25	b	606	CLA	MG-NA	7.67	2.24	2.06
35	v	201	HEC	C3D-C2D	7.53	1.53	1.36
26	A	608	PHO	C3B-C4B	7.38	1.49	1.41
25	c	511	CLA	MG-NA	7.30	2.23	2.06
35	V	201	HEC	C3D-C2D	7.11	1.52	1.36
25	B	606	CLA	MG-NA	6.87	2.22	2.06
25	B	603	CLA	MG-NA	6.50	2.21	2.06
25	C	511	CLA	MG-NA	6.01	2.20	2.06
25	B	615	CLA	MG-NA	5.94	2.20	2.06
25	B	615	CLA	MG-NB	5.60	2.16	2.05
25	b	615	CLA	MG-NA	5.51	2.19	2.06
25	B	613	CLA	MG-NC	5.48	2.19	2.06
25	b	611	CLA	MG-NA	5.37	2.19	2.06
25	b	615	CLA	MG-NB	5.37	2.16	2.05
25	B	604	CLA	MG-NA	5.28	2.18	2.06
35	V	201	HEC	FE-ND	5.26	2.11	1.94
25	B	601	CLA	MG-NA	5.17	2.18	2.06
25	c	510	CLA	MG-NA	5.16	2.18	2.06
25	b	603	CLA	MG-NA	4.99	2.18	2.06
25	C	513	CLA	MG-NA	4.94	2.18	2.06
25	a	612	CLA	MG-NA	4.90	2.17	2.06
25	C	501	CLA	MG-NA	4.84	2.17	2.06
31	D	407	SQD	O48-C23	4.84	1.47	1.33
31	a	615	SQD	O48-C23	4.76	1.47	1.33
31	f	102	SQD	O48-C23	4.74	1.47	1.33
31	B	622	SQD	O48-C23	4.68	1.47	1.33
25	c	503	CLA	MG-NA	4.65	2.17	2.06
31	A	618	SQD	O48-C23	4.61	1.46	1.33
26	A	609	PHO	C1D-C2D	4.59	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	FE-NA	4.59	2.10	1.95
26	A	608	PHO	C1D-C2D	4.59	1.44	1.39
25	b	604	CLA	MG-NA	4.54	2.17	2.06
31	A	616	SQD	O48-C23	4.54	1.46	1.33
25	A	614	CLA	MG-NB	4.52	2.14	2.05
25	b	610	CLA	MG-NB	-4.46	1.96	2.05
25	C	501	CLA	C1D-ND	4.46	1.43	1.37
26	a	608	PHO	C1D-C2D	4.45	1.44	1.39
25	B	614	CLA	C1D-ND	4.40	1.43	1.37
25	B	609	CLA	MG-NA	4.34	2.16	2.06
25	C	504	CLA	MG-NA	4.28	2.16	2.06
25	B	614	CLA	MG-NA	4.27	2.16	2.06
25	A	606	CLA	MG-NB	4.22	2.14	2.05
25	C	503	CLA	MG-NA	4.22	2.16	2.06
25	D	402	CLA	C1D-ND	4.21	1.43	1.37
25	b	607	CLA	MG-NA	4.20	2.16	2.06
31	a	614	SQD	O48-C23	4.19	1.45	1.33
25	B	604	CLA	C1D-ND	4.17	1.43	1.37
25	b	609	CLA	MG-NA	4.15	2.16	2.06
25	B	607	CLA	C1D-ND	4.14	1.43	1.37
31	b	620	SQD	O48-C23	4.12	1.45	1.33
25	c	505	CLA	MG-NA	4.11	2.16	2.06
34	F	101	HEM	FE-NC	4.07	2.08	1.95
25	A	607	CLA	MG-NA	4.06	2.15	2.06
31	a	614	SQD	O47-C45	-4.04	1.37	1.46
25	c	511	CLA	C1D-ND	4.04	1.43	1.37
25	d	403	CLA	MG-ND	-4.01	1.97	2.05
25	B	604	CLA	MG-NC	3.99	2.15	2.06
25	C	505	CLA	C1D-ND	3.97	1.43	1.37
25	B	610	CLA	C1D-ND	3.96	1.43	1.37
25	a	606	CLA	C1D-ND	3.96	1.43	1.37
25	B	607	CLA	MG-NA	3.95	2.15	2.06
25	b	613	CLA	C1D-ND	3.95	1.43	1.37
25	A	614	CLA	C1D-ND	3.94	1.43	1.37
25	C	512	CLA	MG-NB	3.93	2.13	2.05
31	A	616	SQD	O47-C45	-3.92	1.37	1.46
25	B	616	CLA	C1D-ND	3.92	1.43	1.37
25	B	610	CLA	MG-NA	3.90	2.15	2.06
25	B	616	CLA	MG-NC	3.90	2.15	2.06
25	D	402	CLA	MG-NC	3.90	2.15	2.06
25	C	505	CLA	MG-NA	3.87	2.15	2.06
25	b	612	CLA	C1D-ND	3.86	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	611	CLA	MG-NA	3.84	2.15	2.06
26	d	401	PHO	C1D-C2D	3.83	1.43	1.39
25	a	606	CLA	MG-NB	3.81	2.13	2.05
31	a	615	SQD	O5-C1	3.81	1.51	1.41
25	B	615	CLA	C1D-ND	3.80	1.42	1.37
25	C	503	CLA	MG-NC	3.80	2.15	2.06
25	C	512	CLA	MG-NA	3.78	2.15	2.06
25	B	602	CLA	C1D-ND	3.78	1.42	1.37
35	v	201	HEC	FE-ND	3.76	2.06	1.94
25	b	614	CLA	C1D-ND	3.76	1.42	1.37
34	f	101	HEM	FE-NB	3.76	2.06	1.94
25	B	613	CLA	C1D-ND	3.74	1.42	1.37
31	f	102	SQD	O47-C7	3.74	1.44	1.34
25	b	614	CLA	C4B-NB	3.74	1.42	1.37
25	b	616	CLA	C1D-ND	3.73	1.42	1.37
25	c	502	CLA	C1D-ND	3.73	1.42	1.37
25	C	502	CLA	MG-NA	3.73	2.15	2.06
25	B	601	CLA	C1D-ND	3.71	1.42	1.37
25	a	607	CLA	C4B-NB	3.70	1.42	1.37
25	b	601	CLA	C1D-ND	3.70	1.42	1.37
31	a	615	SQD	O47-C45	-3.68	1.37	1.46
25	B	612	CLA	MG-NA	3.66	2.15	2.06
25	B	615	CLA	MG-NC	3.66	2.15	2.06
31	A	618	SQD	O47-C45	-3.65	1.38	1.46
26	a	608	PHO	C4D-CHA	3.65	1.45	1.39
25	a	609	CLA	C1D-ND	3.65	1.42	1.37
31	b	620	SQD	O47-C7	3.64	1.44	1.34
25	B	609	CLA	C1D-ND	3.64	1.42	1.37
25	C	510	CLA	C1D-ND	3.60	1.42	1.37
25	d	403	CLA	C1D-ND	3.59	1.42	1.37
25	b	607	CLA	C1D-ND	3.58	1.42	1.37
25	c	508	CLA	C1D-ND	3.58	1.42	1.37
25	C	510	CLA	MG-NB	3.57	2.12	2.05
25	C	512	CLA	C1D-ND	3.55	1.42	1.37
25	B	606	CLA	C1D-ND	3.55	1.42	1.37
25	A	606	CLA	C1D-ND	3.53	1.42	1.37
25	c	513	CLA	C1D-ND	3.53	1.42	1.37
25	b	602	CLA	C1D-ND	3.52	1.42	1.37
31	B	622	SQD	O47-C7	3.52	1.44	1.34
25	B	610	CLA	C4B-NB	3.50	1.42	1.37
25	B	614	CLA	C4B-NB	3.49	1.42	1.37
25	b	601	CLA	MG-NA	3.48	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C1D-ND	3.47	1.42	1.37
25	C	509	CLA	C1D-ND	3.46	1.42	1.37
25	c	510	CLA	C1D-ND	3.44	1.42	1.37
25	B	605	CLA	MG-NA	3.41	2.14	2.06
25	c	501	CLA	C1D-ND	3.41	1.42	1.37
31	A	618	SQD	O5-C1	3.40	1.50	1.41
25	C	508	CLA	MG-NA	3.39	2.14	2.06
25	B	612	CLA	C1D-ND	3.39	1.42	1.37
25	B	613	CLA	C4B-NB	3.38	1.42	1.37
25	a	606	CLA	MG-NC	3.38	2.14	2.06
25	C	513	CLA	C1D-ND	3.37	1.42	1.37
25	B	601	CLA	C4B-NB	3.36	1.42	1.37
25	C	503	CLA	C1D-ND	3.36	1.42	1.37
25	c	506	CLA	MG-NC	3.35	2.14	2.06
25	b	614	CLA	MG-NC	3.35	2.14	2.06
25	B	615	CLA	C4B-NB	3.35	1.42	1.37
25	C	508	CLA	MG-NC	3.35	2.14	2.06
25	B	605	CLA	C1D-ND	3.34	1.42	1.37
26	d	401	PHO	C4D-CHA	3.32	1.44	1.39
25	C	502	CLA	C1D-ND	3.32	1.42	1.37
25	C	504	CLA	C4B-NB	3.30	1.42	1.37
25	b	602	CLA	C4B-NB	3.30	1.42	1.37
25	C	508	CLA	C1D-ND	3.30	1.42	1.37
25	b	615	CLA	C1D-ND	3.30	1.42	1.37
25	B	615	CLA	C1B-C2B	3.29	1.50	1.43
25	b	601	CLA	C4B-NB	3.29	1.42	1.37
25	C	512	CLA	C4B-NB	3.28	1.42	1.37
35	v	201	HEC	FE-NA	3.28	2.06	1.95
31	a	615	SQD	O47-C7	3.28	1.43	1.34
25	c	504	CLA	C4B-NB	3.28	1.42	1.37
31	A	618	SQD	O47-C7	3.27	1.43	1.34
25	d	403	CLA	C4B-NB	3.27	1.42	1.37
31	B	622	SQD	O47-C45	-3.26	1.38	1.46
25	C	504	CLA	C1D-ND	3.26	1.42	1.37
31	D	407	SQD	C24-C23	3.26	1.60	1.50
25	A	607	CLA	C1B-C2B	3.25	1.50	1.43
25	A	614	CLA	C4B-NB	3.24	1.42	1.37
25	c	512	CLA	C1D-ND	3.24	1.42	1.37
25	c	506	CLA	C4B-NB	3.24	1.42	1.37
25	c	508	CLA	MG-NB	3.23	2.12	2.05
25	c	513	CLA	MG-NA	3.23	2.13	2.06
25	b	603	CLA	C1D-ND	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	MG-ND	-3.23	1.99	2.05
31	A	618	SQD	C24-C23	3.22	1.60	1.50
25	c	509	CLA	C1D-ND	3.21	1.42	1.37
25	b	613	CLA	C4B-NB	3.20	1.42	1.37
31	f	102	SQD	O47-C45	-3.19	1.39	1.46
25	C	513	CLA	MG-ND	3.19	2.12	2.05
25	b	612	CLA	C4B-NB	3.19	1.42	1.37
25	C	501	CLA	C4B-NB	3.18	1.42	1.37
25	a	607	CLA	C1D-ND	3.18	1.42	1.37
31	b	620	SQD	O5-C1	3.17	1.50	1.41
25	C	511	CLA	C1D-ND	3.16	1.42	1.37
25	B	607	CLA	MG-ND	-3.16	1.99	2.05
25	C	508	CLA	C1B-C2B	3.15	1.50	1.43
25	b	610	CLA	C1D-ND	3.15	1.42	1.37
25	c	503	CLA	C1D-ND	3.15	1.42	1.37
25	B	605	CLA	C4B-NB	3.14	1.42	1.37
25	c	509	CLA	C1B-C2B	3.14	1.50	1.43
25	b	603	CLA	C4B-NB	3.14	1.42	1.37
34	F	101	HEM	FE-NA	3.14	2.05	1.95
25	C	510	CLA	C1B-C2B	3.13	1.50	1.43
28	d	405	PL9	C3-C4	-3.13	1.44	1.49
25	c	507	CLA	C1D-ND	3.13	1.42	1.37
25	d	402	CLA	C1B-C2B	3.12	1.50	1.43
25	d	403	CLA	MG-NA	3.12	2.13	2.06
31	A	616	SQD	C24-C23	3.11	1.59	1.50
25	b	604	CLA	C1D-ND	3.11	1.41	1.37
25	B	601	CLA	MG-NB	-3.10	1.99	2.05
25	B	614	CLA	MG-NC	3.10	2.13	2.06
31	b	620	SQD	C24-C23	3.10	1.59	1.50
25	a	607	CLA	MG-NC	3.09	2.13	2.06
25	c	508	CLA	MG-NC	3.08	2.13	2.06
31	B	622	SQD	C24-C23	3.08	1.59	1.50
25	c	512	CLA	C1B-C2B	3.07	1.50	1.43
25	d	402	CLA	C4B-NB	3.06	1.41	1.37
25	a	607	CLA	CHC-C1C	3.06	1.44	1.38
25	A	610	CLA	C1D-ND	3.06	1.41	1.37
25	b	611	CLA	C1D-ND	3.06	1.41	1.37
31	a	615	SQD	C24-C23	3.05	1.59	1.50
25	C	506	CLA	C1D-ND	3.05	1.41	1.37
25	b	609	CLA	C1D-ND	3.05	1.41	1.37
26	A	608	PHO	C4D-CHA	3.04	1.44	1.39
25	A	606	CLA	C1B-C2B	3.04	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	CLA	MG-NA	3.04	2.13	2.06
25	c	502	CLA	C4B-NB	3.04	1.41	1.37
25	d	402	CLA	C1D-ND	3.04	1.41	1.37
25	B	616	CLA	MG-ND	3.03	2.11	2.05
31	A	616	SQD	O47-C7	3.03	1.42	1.34
25	c	510	CLA	C4B-NB	3.02	1.41	1.37
25	D	401	CLA	C1B-C2B	3.01	1.50	1.43
25	a	609	CLA	C4B-NB	3.01	1.41	1.37
25	b	601	CLA	C1B-C2B	3.01	1.50	1.43
25	b	606	CLA	C1B-C2B	3.00	1.50	1.43
25	A	614	CLA	C3B-C4B	3.00	1.51	1.42
25	B	602	CLA	C4B-NB	3.00	1.41	1.37
25	a	612	CLA	C1D-ND	3.00	1.41	1.37
25	c	511	CLA	C4B-NB	3.00	1.41	1.37
26	A	608	PHO	C3D-C4D	3.00	1.45	1.41
25	a	609	CLA	MG-NB	-3.00	1.99	2.05
25	B	614	CLA	MG-ND	-2.99	1.99	2.05
25	B	603	CLA	C1B-C2B	2.99	1.50	1.43
25	A	610	CLA	MG-ND	-2.99	1.99	2.05
25	B	611	CLA	C1B-C2B	2.98	1.50	1.43
25	B	608	CLA	C1D-ND	2.98	1.41	1.37
25	c	513	CLA	C4B-NB	2.98	1.41	1.37
25	c	503	CLA	MG-NB	2.98	2.11	2.05
25	C	507	CLA	C1B-C2B	2.98	1.50	1.43
25	b	616	CLA	C1B-C2B	2.98	1.50	1.43
25	B	612	CLA	C4B-NB	2.98	1.41	1.37
25	A	614	CLA	CHC-C1C	2.98	1.44	1.38
25	c	513	CLA	MG-NC	2.98	2.13	2.06
25	C	511	CLA	C1B-C2B	2.98	1.50	1.43
25	c	502	CLA	C1B-C2B	2.96	1.50	1.43
25	d	403	CLA	C1B-C2B	2.96	1.50	1.43
25	B	605	CLA	CHC-C1C	2.96	1.44	1.38
25	C	503	CLA	C4B-NB	2.96	1.41	1.37
25	C	507	CLA	C1D-ND	2.95	1.41	1.37
25	b	605	CLA	C1B-C2B	2.95	1.50	1.43
25	b	616	CLA	MG-NC	2.95	2.13	2.06
25	b	602	CLA	C1B-C2B	2.94	1.50	1.43
25	c	507	CLA	C1B-C2B	2.94	1.50	1.43
25	c	513	CLA	C1B-C2B	2.94	1.50	1.43
25	b	606	CLA	C1D-ND	2.94	1.41	1.37
25	B	610	CLA	C1B-C2B	2.94	1.50	1.43
25	C	510	CLA	CHC-C1C	2.94	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	MG-NB	-2.93	2.00	2.05
31	A	616	SQD	O5-C1	2.93	1.49	1.41
31	f	102	SQD	C24-C23	2.93	1.59	1.50
25	C	509	CLA	C1B-C2B	2.93	1.50	1.43
25	C	513	CLA	C1B-C2B	2.92	1.50	1.43
31	a	614	SQD	O47-C7	2.92	1.42	1.34
25	c	505	CLA	C4B-NB	2.92	1.41	1.37
35	V	201	HEC	FE-NB	2.91	2.03	1.94
31	a	614	SQD	C24-C23	2.91	1.59	1.50
25	b	612	CLA	MG-NB	-2.90	2.00	2.05
25	b	610	CLA	C4B-NB	2.90	1.41	1.37
25	B	606	CLA	C1B-C2B	2.90	1.49	1.43
25	c	503	CLA	C1B-C2B	2.90	1.49	1.43
28	D	404	PL9	C6-C1	-2.90	1.43	1.48
34	F	101	HEM	CAB-C3B	2.90	1.55	1.47
25	b	614	CLA	MG-NA	2.90	2.13	2.06
25	b	608	CLA	C4B-NB	2.90	1.41	1.37
25	B	605	CLA	C3B-C4B	2.89	1.51	1.42
25	B	603	CLA	MG-ND	2.89	2.11	2.05
31	b	620	SQD	O47-C45	-2.89	1.39	1.46
25	B	611	CLA	C1D-ND	2.89	1.41	1.37
25	a	606	CLA	C1B-C2B	2.89	1.49	1.43
25	C	511	CLA	C4B-NB	2.89	1.41	1.37
34	F	101	HEM	CAC-C3C	2.88	1.55	1.47
25	b	612	CLA	C1B-C2B	2.88	1.49	1.43
25	C	502	CLA	C1B-C2B	2.87	1.49	1.43
25	C	503	CLA	C1B-C2B	2.86	1.49	1.43
25	c	508	CLA	C4B-NB	2.86	1.41	1.37
28	a	611	PL9	C53-C6	-2.86	1.44	1.50
25	c	508	CLA	CHC-C1C	2.86	1.44	1.38
25	C	505	CLA	C1B-C2B	2.86	1.49	1.43
31	f	102	SQD	O5-C1	2.86	1.49	1.41
25	b	615	CLA	C3B-C4B	2.86	1.51	1.42
34	f	101	HEM	CAC-C3C	2.85	1.55	1.47
25	c	510	CLA	C1B-C2B	2.85	1.49	1.43
25	a	609	CLA	C1B-C2B	2.85	1.49	1.43
31	B	622	SQD	O5-C1	2.85	1.49	1.41
25	c	511	CLA	C1B-C2B	2.84	1.49	1.43
25	b	613	CLA	C1B-C2B	2.84	1.49	1.43
34	F	101	HEM	FE-NB	2.84	2.03	1.94
25	b	610	CLA	C1B-C2B	2.84	1.49	1.43
25	B	612	CLA	C1B-C2B	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C1D-ND	2.83	1.41	1.37
25	C	502	CLA	C4B-NB	2.83	1.41	1.37
25	B	607	CLA	C4B-NB	2.83	1.41	1.37
25	b	613	CLA	MG-NA	2.83	2.13	2.06
31	a	614	SQD	O5-C1	2.82	1.49	1.41
25	B	608	CLA	C4B-NB	2.82	1.41	1.37
25	b	608	CLA	C1B-C2B	2.82	1.49	1.43
25	B	602	CLA	MG-NC	2.82	2.13	2.06
25	B	608	CLA	MG-NA	2.82	2.13	2.06
25	B	601	CLA	C1B-C2B	2.81	1.49	1.43
25	B	613	CLA	C1B-C2B	2.81	1.49	1.43
25	c	503	CLA	C4B-NB	2.80	1.41	1.37
25	C	510	CLA	C4B-NB	2.80	1.41	1.37
25	B	605	CLA	C1B-C2B	2.79	1.49	1.43
25	D	401	CLA	C4B-NB	2.79	1.41	1.37
25	C	507	CLA	C4B-NB	2.79	1.41	1.37
25	C	513	CLA	C4B-NB	2.78	1.41	1.37
25	b	608	CLA	C1D-ND	2.78	1.41	1.37
25	A	607	CLA	C1D-ND	2.78	1.41	1.37
25	a	612	CLA	C1B-C2B	2.78	1.49	1.43
25	b	608	CLA	C3B-C4B	2.77	1.50	1.42
25	C	501	CLA	CHC-C1C	2.76	1.44	1.38
25	b	604	CLA	C1B-C2B	2.75	1.49	1.43
25	B	606	CLA	C4B-NB	2.75	1.41	1.37
26	a	608	PHO	CMB-C2B	-2.75	1.46	1.51
25	B	607	CLA	C1B-C2B	2.75	1.49	1.43
25	c	512	CLA	C4B-NB	2.74	1.41	1.37
26	A	609	PHO	C4D-CHA	2.74	1.43	1.39
25	B	615	CLA	MG-ND	-2.74	2.00	2.05
25	b	605	CLA	C4B-NB	2.73	1.41	1.37
25	A	610	CLA	C1B-C2B	2.73	1.49	1.43
25	C	512	CLA	MG-NC	2.73	2.12	2.06
25	A	610	CLA	C4B-NB	2.73	1.41	1.37
25	a	607	CLA	C1B-C2B	2.73	1.49	1.43
25	c	508	CLA	C1B-C2B	2.72	1.49	1.43
25	a	607	CLA	C3B-C4B	2.72	1.50	1.42
25	c	505	CLA	C1D-ND	2.72	1.41	1.37
25	B	604	CLA	C1B-C2B	2.72	1.49	1.43
25	b	605	CLA	MG-NA	2.71	2.12	2.06
25	B	602	CLA	C1B-C2B	2.71	1.49	1.43
25	c	508	CLA	MG-NA	2.71	2.12	2.06
25	B	613	CLA	MG-ND	-2.71	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	C1B-C2B	2.70	1.49	1.43
25	B	616	CLA	MG-NB	-2.70	2.00	2.05
25	b	609	CLA	C1B-C2B	2.70	1.49	1.43
25	b	614	CLA	CHC-C1C	2.69	1.43	1.38
25	B	609	CLA	C4B-NB	2.69	1.41	1.37
25	b	615	CLA	C4B-NB	2.68	1.41	1.37
25	C	501	CLA	C3B-C4B	2.68	1.50	1.42
25	b	616	CLA	C4B-NB	2.68	1.41	1.37
34	f	101	HEM	FE-NC	2.68	2.04	1.95
25	C	504	CLA	C3B-C4B	2.67	1.50	1.42
25	C	511	CLA	C3B-C4B	2.67	1.50	1.42
25	b	615	CLA	C1B-C2B	2.67	1.49	1.43
25	C	508	CLA	C3B-C4B	2.66	1.50	1.42
25	C	508	CLA	C4B-NB	2.66	1.41	1.37
25	a	612	CLA	C4B-NB	2.65	1.41	1.37
25	C	505	CLA	MG-NC	2.65	2.12	2.06
25	c	505	CLA	C1B-C2B	2.64	1.49	1.43
25	b	614	CLA	C3B-C4B	2.64	1.50	1.42
25	C	512	CLA	C3B-C4B	2.64	1.50	1.42
25	c	508	CLA	C3B-C4B	2.63	1.50	1.42
26	a	608	PHO	C3D-C4D	2.63	1.44	1.41
25	A	614	CLA	C1B-C2B	2.63	1.49	1.43
25	b	611	CLA	C1B-C2B	2.63	1.49	1.43
25	b	612	CLA	CHC-C1C	2.63	1.43	1.38
25	B	616	CLA	C1B-C2B	2.62	1.49	1.43
25	c	501	CLA	C1B-C2B	2.62	1.49	1.43
25	C	505	CLA	C4B-NB	2.62	1.41	1.37
25	C	510	CLA	C3B-C4B	2.62	1.50	1.42
25	b	607	CLA	C1B-C2B	2.62	1.49	1.43
25	C	504	CLA	C1B-C2B	2.61	1.49	1.43
25	C	512	CLA	C1B-C2B	2.61	1.49	1.43
25	b	615	CLA	CHC-C1C	2.61	1.43	1.38
25	B	611	CLA	C4B-NB	2.61	1.41	1.37
26	d	401	PHO	CMD-C2D	-2.61	1.46	1.51
25	c	504	CLA	C1D-ND	2.60	1.41	1.37
31	D	407	SQD	O5-C1	2.60	1.48	1.41
25	C	512	CLA	CHC-C1C	2.60	1.43	1.38
25	B	609	CLA	C1B-C2B	2.60	1.49	1.43
25	A	607	CLA	C4B-NB	2.59	1.41	1.37
25	d	402	CLA	C3B-C4B	2.59	1.50	1.42
25	b	614	CLA	C1B-C2B	2.58	1.49	1.43
25	b	607	CLA	C4B-NB	2.58	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	601	CLA	CHC-C1C	2.58	1.43	1.38
25	c	506	CLA	CHC-C1C	2.58	1.43	1.38
25	B	604	CLA	CHC-C1C	2.56	1.43	1.38
26	A	609	PHO	CMD-C2D	-2.56	1.46	1.51
31	a	615	SQD	O5-C5	2.56	1.50	1.44
34	f	101	HEM	CAB-C3B	2.56	1.54	1.47
25	B	602	CLA	MG-NA	2.55	2.12	2.06
25	c	504	CLA	MG-ND	-2.55	2.00	2.05
25	b	605	CLA	C3B-C4B	2.55	1.50	1.42
25	c	504	CLA	C1B-C2B	2.55	1.49	1.43
25	D	402	CLA	C1B-C2B	2.55	1.49	1.43
25	a	612	CLA	MG-ND	-2.55	2.00	2.05
25	C	506	CLA	C1B-C2B	2.54	1.49	1.43
25	a	606	CLA	CHC-C1C	2.54	1.43	1.38
31	A	618	SQD	O9-S	2.54	1.52	1.45
25	b	608	CLA	CHC-C1C	2.54	1.43	1.38
25	C	512	CLA	MG-ND	-2.53	2.00	2.05
25	b	606	CLA	C4B-NB	2.53	1.41	1.37
25	c	507	CLA	C4B-NB	2.52	1.41	1.37
25	c	511	CLA	CHC-C1C	2.52	1.43	1.38
25	B	608	CLA	C1B-C2B	2.52	1.49	1.43
25	B	614	CLA	CHC-C1C	2.52	1.43	1.38
25	B	613	CLA	CHC-C1C	2.51	1.43	1.38
25	b	612	CLA	MG-NC	2.51	2.12	2.06
25	b	601	CLA	C3B-C4B	2.51	1.50	1.42
25	B	615	CLA	CHC-C1C	2.51	1.43	1.38
25	b	604	CLA	C4B-NB	2.51	1.41	1.37
25	b	602	CLA	MG-NC	2.51	2.12	2.06
25	b	605	CLA	C1D-ND	2.50	1.41	1.37
25	b	609	CLA	C4B-NB	2.50	1.41	1.37
25	c	505	CLA	CHC-C1C	2.49	1.43	1.38
35	V	201	HEC	CMB-C2B	2.48	1.55	1.50
25	c	506	CLA	C1B-C2B	2.48	1.49	1.43
25	B	610	CLA	C3B-C4B	2.48	1.50	1.42
25	c	513	CLA	C3B-C4B	2.47	1.49	1.42
31	a	615	SQD	O7-S	2.47	1.52	1.45
26	d	401	PHO	C4D-ND	-2.46	1.34	1.38
26	d	401	PHO	CMC-C2C	-2.46	1.46	1.50
25	C	506	CLA	C4B-NB	2.46	1.41	1.37
25	C	509	CLA	C3B-C4B	2.46	1.49	1.42
25	c	513	CLA	CHC-C1C	2.45	1.43	1.38
25	B	604	CLA	C3B-C4B	2.45	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	f	102	SQD	O9-S	2.44	1.52	1.45
25	A	606	CLA	C3B-C4B	2.44	1.49	1.42
25	B	604	CLA	MG-NB	2.44	2.10	2.05
31	B	622	SQD	O9-S	2.44	1.52	1.45
25	c	505	CLA	C3B-C4B	2.43	1.49	1.42
25	C	513	CLA	C3B-C4B	2.42	1.49	1.42
31	A	618	SQD	O7-S	2.42	1.51	1.45
31	a	615	SQD	O9-S	2.42	1.51	1.45
25	b	612	CLA	MG-NA	2.41	2.12	2.06
26	a	608	PHO	CMC-C2C	-2.41	1.46	1.50
25	C	508	CLA	CHC-C1C	2.41	1.43	1.38
25	C	502	CLA	MG-NB	-2.40	2.01	2.05
25	C	506	CLA	MG-NA	2.40	2.12	2.06
25	C	501	CLA	C1B-C2B	2.40	1.48	1.43
25	a	609	CLA	MG-NA	2.40	2.12	2.06
25	c	503	CLA	CHC-C1C	2.39	1.43	1.38
25	A	607	CLA	CHC-C1C	2.39	1.43	1.38
25	D	401	CLA	C3B-C4B	2.39	1.49	1.42
25	B	608	CLA	C3B-C4B	2.39	1.49	1.42
25	B	614	CLA	C1B-C2B	2.39	1.48	1.43
25	C	502	CLA	C3B-C4B	2.38	1.49	1.42
28	D	404	PL9	C3-C4	-2.38	1.45	1.49
26	A	608	PHO	CMD-C2D	-2.38	1.46	1.51
25	c	511	CLA	MG-NB	2.38	2.10	2.05
25	C	510	CLA	CMD-C2D	-2.37	1.45	1.50
25	a	606	CLA	C3B-C4B	2.37	1.49	1.42
25	b	615	CLA	CMD-C2D	-2.37	1.45	1.50
25	A	606	CLA	C4B-NB	2.37	1.41	1.37
25	B	606	CLA	MG-NC	2.37	2.11	2.06
31	b	620	SQD	O9-S	2.36	1.51	1.45
25	C	503	CLA	CHC-C1C	2.36	1.43	1.38
25	D	401	CLA	CMD-C2D	-2.35	1.45	1.50
25	c	512	CLA	CHC-C1C	2.35	1.43	1.38
25	D	402	CLA	C4B-NB	2.35	1.40	1.37
31	b	620	SQD	O7-S	2.35	1.51	1.45
25	B	611	CLA	CHC-C1C	2.35	1.43	1.38
25	B	601	CLA	C3B-C4B	2.34	1.49	1.42
25	D	401	CLA	CHC-C1C	2.34	1.43	1.38
35	v	201	HEC	FE-NB	2.34	2.02	1.94
25	C	505	CLA	CHC-C1C	2.34	1.43	1.38
25	b	609	CLA	CHC-C1C	2.34	1.43	1.38
25	C	504	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	C3B-C4B	2.33	1.49	1.42
25	b	608	CLA	MG-NB	2.33	2.10	2.05
25	d	402	CLA	CMB-C2B	-2.33	1.46	1.50
25	D	401	CLA	MG-NB	2.32	2.10	2.05
25	b	611	CLA	CHC-C1C	2.32	1.43	1.38
25	b	612	CLA	C3B-C4B	2.32	1.49	1.42
25	C	503	CLA	C3B-C4B	2.32	1.49	1.42
26	d	401	PHO	O2D-CGD	2.31	1.38	1.33
25	d	403	CLA	C3B-C4B	2.31	1.49	1.42
25	b	604	CLA	C3B-C4B	2.31	1.49	1.42
25	b	607	CLA	C3B-C4B	2.31	1.49	1.42
25	C	509	CLA	C4B-NB	2.30	1.40	1.37
25	c	512	CLA	C3B-C4B	2.30	1.49	1.42
25	b	613	CLA	CHC-C1C	2.30	1.43	1.38
25	b	606	CLA	C3B-C4B	2.30	1.49	1.42
34	f	101	HEM	C3B-C2B	-2.30	1.32	1.37
26	A	608	PHO	CMC-C2C	-2.30	1.47	1.50
34	F	101	HEM	CMD-C2D	2.29	1.55	1.50
25	a	612	CLA	CHC-C1C	2.29	1.43	1.38
25	c	508	CLA	MG-ND	2.29	2.10	2.05
25	B	602	CLA	CHC-C1C	2.29	1.43	1.38
26	d	401	PHO	C3D-C4D	2.29	1.44	1.41
25	B	612	CLA	CHC-C1C	2.29	1.43	1.38
25	B	613	CLA	MG-NA	2.28	2.11	2.06
26	A	609	PHO	C4D-ND	-2.28	1.35	1.38
25	C	510	CLA	MG-NC	2.28	2.11	2.06
26	A	609	PHO	CMC-C2C	-2.28	1.47	1.50
25	b	613	CLA	C3B-C4B	2.27	1.49	1.42
25	B	608	CLA	CHC-C1C	2.27	1.43	1.38
25	a	606	CLA	C4B-NB	2.27	1.40	1.37
25	C	506	CLA	CHC-C1C	2.26	1.43	1.38
25	C	511	CLA	CHC-C1C	2.26	1.43	1.38
25	B	611	CLA	C3B-C4B	2.26	1.49	1.42
25	B	601	CLA	CHC-C1C	2.25	1.43	1.38
25	B	608	CLA	MG-NC	2.25	2.11	2.06
35	V	201	HEC	FE-NA	2.25	2.02	1.95
25	C	506	CLA	C3B-C4B	2.25	1.49	1.42
25	b	610	CLA	CMD-C2D	-2.25	1.46	1.50
25	B	612	CLA	C3B-C4B	2.24	1.49	1.42
25	c	509	CLA	C4B-NB	2.24	1.40	1.37
25	c	509	CLA	C3B-C4B	2.24	1.49	1.42
34	f	101	HEM	CMC-C2C	2.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	C3B-C4B	2.23	1.49	1.42
25	d	403	CLA	CMD-C2D	-2.23	1.46	1.50
31	A	618	SQD	O5-C5	2.22	1.49	1.44
25	a	609	CLA	C3B-C4B	2.22	1.49	1.42
25	b	616	CLA	CHC-C1C	2.22	1.42	1.38
32	D	408	LHG	O7-C5	-2.22	1.41	1.46
25	b	604	CLA	CHC-C1C	2.22	1.42	1.38
25	c	504	CLA	C3B-C4B	2.22	1.49	1.42
25	B	607	CLA	CHC-C1C	2.21	1.42	1.38
35	v	201	HEC	CMA-C3A	2.21	1.55	1.50
25	B	606	CLA	CHC-C1C	2.21	1.42	1.38
25	b	611	CLA	C4B-NB	2.20	1.40	1.37
25	c	512	CLA	CMD-C2D	-2.20	1.46	1.50
25	D	401	CLA	C1D-ND	2.20	1.40	1.37
25	c	510	CLA	CHC-C1C	2.20	1.42	1.38
25	b	609	CLA	C3B-C4B	2.19	1.49	1.42
25	B	606	CLA	CMB-C2B	-2.19	1.46	1.50
25	C	512	CLA	CMB-C2B	-2.19	1.46	1.50
25	b	603	CLA	CMC-C2C	-2.19	1.46	1.50
25	c	503	CLA	C3B-C4B	2.18	1.49	1.42
25	c	506	CLA	C3B-C4B	2.18	1.49	1.42
31	f	102	SQD	O7-S	2.18	1.51	1.45
31	a	614	SQD	O7-S	2.18	1.51	1.45
25	C	502	CLA	CMB-C2B	-2.18	1.46	1.50
25	c	503	CLA	MG-NC	2.18	2.11	2.06
34	f	101	HEM	CMA-C3A	2.18	1.55	1.50
25	B	603	CLA	C3B-C4B	2.17	1.49	1.42
25	c	507	CLA	CMC-C2C	-2.17	1.46	1.50
25	C	507	CLA	MG-NA	2.17	2.11	2.06
25	b	603	CLA	CMD-C2D	-2.16	1.46	1.50
35	V	201	HEC	CAC-C3C	2.16	1.56	1.51
31	D	407	SQD	O9-S	2.16	1.51	1.45
25	B	605	CLA	MG-NB	2.16	2.10	2.05
25	B	602	CLA	C3B-C4B	2.16	1.49	1.42
26	A	609	PHO	CMB-C2B	-2.16	1.47	1.51
33	C	523	DGD	O2G-C2G	-2.16	1.41	1.46
25	a	612	CLA	MG-NC	2.16	2.11	2.06
25	B	610	CLA	CHC-C1C	2.15	1.42	1.38
25	B	606	CLA	C3B-C4B	2.15	1.49	1.42
26	A	609	PHO	C3D-C4D	2.14	1.44	1.41
25	b	612	CLA	CMC-C2C	-2.14	1.46	1.50
25	d	403	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	405	PL9	C46-C44	-2.14	1.46	1.51
25	b	602	CLA	CHC-C1C	2.14	1.42	1.38
25	A	607	CLA	C3B-C4B	2.14	1.49	1.42
25	B	615	CLA	CMB-C2B	-2.14	1.46	1.50
25	c	501	CLA	C4B-NB	2.14	1.40	1.37
25	D	402	CLA	CMC-C2C	-2.13	1.46	1.50
25	d	402	CLA	CHC-C1C	2.13	1.42	1.38
25	C	503	CLA	C1D-C2D	2.13	1.49	1.45
25	c	504	CLA	CHC-C1C	2.12	1.42	1.38
25	A	610	CLA	CHC-C1C	2.12	1.42	1.38
25	b	603	CLA	C3B-C4B	2.12	1.48	1.42
26	d	401	PHO	C4C-NC	2.12	1.44	1.37
25	B	607	CLA	C3B-C4B	2.12	1.48	1.42
25	B	616	CLA	C3B-C4B	2.12	1.48	1.42
25	c	502	CLA	MG-NC	2.12	2.11	2.06
35	V	201	HEC	FE-NC	2.12	2.02	1.95
25	A	614	CLA	MG-NC	2.12	2.11	2.06
25	b	602	CLA	C3B-C4B	2.11	1.48	1.42
25	b	614	CLA	MG-NB	-2.11	2.01	2.05
31	b	620	SQD	C8-C7	2.11	1.56	1.50
31	A	616	SQD	O9-S	2.11	1.51	1.45
31	b	620	SQD	O5-C5	2.11	1.49	1.44
34	F	101	HEM	C2A-C3A	-2.11	1.33	1.38
25	B	613	CLA	CMD-C2D	-2.11	1.46	1.50
25	c	509	CLA	CHC-C1C	2.11	1.42	1.38
32	D	410	LHG	O7-C5	-2.11	1.41	1.46
25	b	605	CLA	CHC-C1C	2.10	1.42	1.38
25	d	403	CLA	CHC-C1C	2.10	1.42	1.38
25	B	616	CLA	C4B-NB	2.10	1.40	1.37
28	D	404	PL9	C52-C5	-2.10	1.46	1.50
25	C	507	CLA	C1B-NB	-2.10	1.35	1.37
25	A	614	CLA	CMD-C2D	-2.10	1.46	1.50
25	A	606	CLA	CHC-C1C	2.10	1.42	1.38
25	b	611	CLA	CMD-C2D	-2.09	1.46	1.50
31	B	622	SQD	O7-S	2.09	1.51	1.45
31	B	622	SQD	C8-C7	2.09	1.56	1.50
35	v	201	HEC	FE-NC	2.09	2.02	1.95
25	C	507	CLA	CHC-C1C	2.08	1.42	1.38
25	c	510	CLA	CMD-C2D	-2.08	1.46	1.50
34	f	101	HEM	C2A-C3A	-2.08	1.33	1.38
25	C	502	CLA	CHC-C1C	2.08	1.42	1.38
25	C	511	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	509	CLA	O2D-CGD	2.08	1.38	1.33
25	B	615	CLA	C3B-C4B	2.08	1.48	1.42
25	C	504	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	603	CLA	CHC-C1C	2.07	1.42	1.38
25	B	607	CLA	CMB-C2B	-2.07	1.46	1.50
25	b	606	CLA	CHC-C1C	2.07	1.42	1.38
25	C	501	CLA	MG-NC	2.07	2.11	2.06
25	c	510	CLA	C3B-C4B	2.07	1.48	1.42
25	B	613	CLA	C3B-C4B	2.06	1.48	1.42
25	b	605	CLA	MG-NB	2.06	2.09	2.05
25	c	501	CLA	C3B-C4B	2.06	1.48	1.42
25	c	510	CLA	CMB-C2B	-2.06	1.46	1.50
31	A	616	SQD	C8-C7	2.05	1.56	1.50
26	a	608	PHO	C4D-ND	-2.05	1.35	1.38
25	c	512	CLA	CMB-C2B	-2.05	1.46	1.50
25	b	607	CLA	MG-NB	-2.05	2.01	2.05
25	c	501	CLA	CHC-C1C	2.05	1.42	1.38
25	B	608	CLA	C1D-C2D	2.05	1.49	1.45
26	a	608	PHO	CAC-C3C	-2.05	1.48	1.51
35	v	201	HEC	CMD-C2D	2.04	1.55	1.50
25	a	606	CLA	MG-NA	2.04	2.11	2.06
34	F	101	HEM	CMA-C3A	2.04	1.55	1.50
25	c	502	CLA	CMD-C2D	-2.04	1.46	1.50
25	b	604	CLA	CMD-C2D	-2.04	1.46	1.50
25	D	402	CLA	C3B-C4B	2.03	1.48	1.42
25	b	604	CLA	MG-NB	2.03	2.09	2.05
25	B	611	CLA	CMD-C2D	-2.03	1.46	1.50
25	a	606	CLA	C3D-C4D	2.03	1.48	1.44
25	b	615	CLA	MG-ND	-2.03	2.01	2.05
25	b	601	CLA	CMD-C2D	-2.03	1.46	1.50
25	c	512	CLA	CMC-C2C	-2.03	1.46	1.50
25	C	506	CLA	CMC-C2C	-2.03	1.46	1.50
35	v	201	HEC	CMB-C2B	2.02	1.54	1.50
25	A	610	CLA	MG-NB	2.02	2.09	2.05
25	b	610	CLA	CMB-C2B	-2.01	1.46	1.50
25	C	504	CLA	CMB-C2B	-2.01	1.46	1.50
25	C	508	CLA	C1D-C2D	2.01	1.49	1.45
25	b	610	CLA	C3B-C4B	2.01	1.48	1.42
25	b	602	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	509	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	616	CLA	C3B-C4B	2.01	1.48	1.42
25	B	609	CLA	CHC-C1C	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	612	CLA	C3B-C4B	2.00	1.48	1.42
25	b	615	CLA	CMB-C2B	-2.00	1.46	1.50
25	b	608	CLA	C3C-C2C	2.00	1.41	1.36

All (827) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	615	CLA	C4A-NA-C1A	9.29	110.92	106.68
25	B	604	CLA	C4A-NA-C1A	9.15	110.85	106.68
25	c	511	CLA	C4A-NA-C1A	8.25	110.44	106.68
25	c	503	CLA	C4A-NA-C1A	8.03	110.34	106.68
25	C	511	CLA	C4A-NA-C1A	7.94	110.30	106.68
25	C	507	CLA	C4A-NA-C1A	7.93	110.30	106.68
25	C	503	CLA	C4A-NA-C1A	7.90	110.28	106.68
25	B	601	CLA	C4A-NA-C1A	7.82	110.25	106.68
25	C	510	CLA	C4A-NA-C1A	7.82	110.25	106.68
25	c	502	CLA	C4A-NA-C1A	7.66	110.17	106.68
25	b	601	CLA	C4A-NA-C1A	7.44	110.07	106.68
25	b	606	CLA	C4A-NA-C1A	7.38	110.05	106.68
25	B	606	CLA	C4A-NA-C1A	7.32	110.02	106.68
25	C	501	CLA	C4A-NA-C1A	7.30	110.01	106.68
31	a	614	SQD	O6-C1-C2	7.17	119.16	108.27
25	b	613	CLA	C4A-NA-C1A	7.03	109.89	106.68
25	B	613	CLA	C4A-NA-C1A	6.95	109.85	106.68
25	c	507	CLA	C4A-NA-C1A	6.83	109.80	106.68
25	B	610	CLA	C4A-NA-C1A	6.74	109.76	106.68
31	a	614	SQD	C1-O5-C5	-6.72	100.60	113.72
25	c	509	CLA	C4A-NA-C1A	6.71	109.74	106.68
25	a	606	CLA	C4A-NA-C1A	6.61	109.69	106.68
25	B	607	CLA	C4A-NA-C1A	6.51	109.65	106.68
25	d	402	CLA	C4A-NA-C1A	6.50	109.65	106.68
25	C	505	CLA	C4A-NA-C1A	6.46	109.62	106.68
25	B	609	CLA	C4A-NA-C1A	6.44	109.62	106.68
25	B	612	CLA	C4A-NA-C1A	6.42	109.61	106.68
25	b	616	CLA	C4A-NA-C1A	6.38	109.59	106.68
25	C	513	CLA	C4A-NA-C1A	6.36	109.58	106.68
25	b	615	CLA	C4A-NA-C1A	6.35	109.57	106.68
25	B	614	CLA	C4A-NA-C1A	6.32	109.56	106.68
25	c	513	CLA	C4A-NA-C1A	6.32	109.56	106.68
25	B	616	CLA	C4A-NA-C1A	6.28	109.55	106.68
25	C	508	CLA	C4A-NA-C1A	6.28	109.54	106.68
26	d	401	PHO	C4D-CHA-CBD	-6.28	105.44	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	616	SQD	O6-C1-C2	6.27	117.80	108.27
28	A	612	PL9	C7-C3-C4	6.24	122.05	116.91
25	c	505	CLA	C4A-NA-C1A	6.19	109.50	106.68
25	c	508	CLA	C4A-NA-C1A	6.16	109.49	106.68
25	B	608	CLA	C4A-NA-C1A	6.04	109.44	106.68
25	b	604	CLA	C4A-NA-C1A	5.97	109.40	106.68
26	A	608	PHO	C4D-CHA-CBD	-5.91	105.62	108.45
26	a	608	PHO	C4D-CHA-CBD	-5.86	105.64	108.45
31	b	620	SQD	O6-C1-C2	5.82	117.12	108.27
31	B	622	SQD	O6-C1-C2	5.78	117.04	108.27
30	a	616	LMG	O1-C1-C2	5.77	117.04	108.27
25	b	614	CLA	C4A-NA-C1A	5.72	109.29	106.68
31	A	616	SQD	C1-O5-C5	-5.70	102.58	113.72
25	c	501	CLA	C4A-NA-C1A	5.64	109.25	106.68
25	c	510	CLA	C4A-NA-C1A	5.60	109.23	106.68
25	b	609	CLA	C4A-NA-C1A	5.60	109.23	106.68
25	c	512	CLA	C4A-NA-C1A	5.60	109.23	106.68
31	D	407	SQD	O6-C1-C2	5.57	116.73	108.27
25	b	603	CLA	C4A-NA-C1A	5.56	109.22	106.68
31	A	616	SQD	C1-C2-C3	-5.56	98.32	110.01
25	A	610	CLA	C4A-NA-C1A	5.51	109.19	106.68
25	b	607	CLA	C4A-NA-C1A	5.46	109.17	106.68
25	C	502	CLA	C4A-NA-C1A	5.44	109.16	106.68
25	C	512	CLA	C4A-NA-C1A	5.42	109.15	106.68
28	a	611	PL9	C7-C3-C4	5.42	121.37	116.91
25	C	509	CLA	C4A-NA-C1A	5.41	109.15	106.68
35	V	201	HEC	C1D-ND-C4D	5.41	111.61	105.21
25	c	504	CLA	C4A-NA-C1A	5.34	109.11	106.68
25	a	607	CLA	C4A-NA-C1A	5.32	109.11	106.68
25	B	603	CLA	C4A-NA-C1A	5.31	109.10	106.68
25	B	602	CLA	C4A-NA-C1A	5.30	109.10	106.68
25	b	602	CLA	C4A-NA-C1A	5.27	109.08	106.68
25	D	402	CLA	C4A-NA-C1A	5.26	109.08	106.68
25	B	611	CLA	C4A-NA-C1A	5.22	109.06	106.68
30	C	517	LMG	C4-C3-C2	5.14	119.85	110.83
25	C	506	CLA	C4A-NA-C1A	5.07	108.99	106.68
35	v	201	HEC	C1D-ND-C4D	5.04	111.18	105.21
25	b	608	CLA	C4A-NA-C1A	5.00	108.96	106.68
25	A	606	CLA	C4A-NA-C1A	4.96	108.94	106.68
25	b	610	CLA	C4A-NA-C1A	4.87	108.90	106.68
28	d	405	PL9	C7-C3-C4	4.79	120.86	116.91
25	B	613	CLA	C1-C2-C3	-4.77	118.39	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	622	SQD	O47-C7-C8	4.72	121.69	111.48
25	A	607	CLA	C4A-NA-C1A	4.70	108.82	106.68
25	b	615	CLA	C3B-C4B-NB	-4.67	106.36	110.53
26	A	608	PHO	CMA-C3A-C4A	-4.66	104.58	114.61
25	d	403	CLA	C4A-NA-C1A	4.63	108.79	106.68
25	C	504	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	c	506	CLA	C4A-NA-C1A	4.62	108.79	106.68
31	B	622	SQD	C1-O5-C5	-4.61	104.71	113.72
25	B	605	CLA	C4A-NA-C1A	4.60	108.78	106.68
25	b	611	CLA	C4A-NA-C1A	4.55	108.76	106.68
25	A	607	CLA	O2D-CGD-O1D	-4.54	115.01	123.85
31	f	102	SQD	O9-S-O7	-4.52	99.11	113.82
25	C	501	CLA	O2D-CGD-O1D	-4.45	115.19	123.85
25	b	603	CLA	O2D-CGD-O1D	-4.45	115.19	123.85
26	a	608	PHO	CMA-C3A-C4A	-4.41	105.12	114.61
26	A	609	PHO	CBC-CAC-C3C	4.39	119.16	112.87
25	B	610	CLA	O2D-CGD-O1D	-4.37	115.33	123.85
31	b	620	SQD	O47-C7-C8	4.37	120.94	111.48
25	A	614	CLA	C4A-NA-C1A	4.36	108.67	106.68
28	D	404	PL9	C7-C3-C4	4.32	120.47	116.91
30	D	405	LMG	O6-C5-C4	4.31	117.46	109.70
31	f	102	SQD	O6-C1-C2	4.31	114.81	108.27
25	b	605	CLA	C4A-NA-C1A	4.28	108.63	106.68
26	A	609	PHO	O1D-CGD-CBD	4.27	131.21	124.72
31	a	615	SQD	O7-S-C6	4.25	113.10	106.76
25	b	606	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
26	A	609	PHO	O2D-CGD-O1D	-4.18	115.71	123.85
25	A	607	CLA	O2D-CGD-CBD	4.18	118.53	111.23
25	b	604	CLA	C1-C2-C3	-4.17	119.36	126.20
25	A	614	CLA	C3B-C4B-NB	-4.14	106.84	110.53
28	a	611	PL9	C7-C3-C2	-4.10	118.55	123.39
31	A	618	SQD	O47-C7-C8	4.10	120.36	111.48
25	B	616	CLA	C1-C2-C3	-4.10	119.48	126.20
31	A	616	SQD	O47-C7-C8	4.04	120.23	111.48
25	C	513	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
28	A	612	PL9	C7-C3-C2	-4.04	118.63	123.39
25	a	612	CLA	C4A-NA-C1A	3.98	108.49	106.68
25	C	501	CLA	C3B-C4B-NB	-3.97	106.99	110.53
31	f	102	SQD	O9-S-C6	3.96	112.67	106.76
25	b	616	CLA	O2D-CGD-O1D	-3.95	116.16	123.85
25	b	612	CLA	C4A-NA-C1A	3.92	108.47	106.68
27	c	515	BCR	C2-C1-C6	3.92	116.13	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	618	SQD	O5-C5-C4	3.90	116.72	109.70
30	a	616	LMG	C1-C2-C3	-3.89	101.82	110.01
25	B	602	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
25	c	501	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
26	d	401	PHO	CMA-C3A-C4A	-3.81	106.39	114.61
25	b	602	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
25	c	502	CLA	O2D-CGD-O1D	-3.81	116.44	123.85
25	C	505	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
25	c	509	CLA	O2A-CGA-O1A	-3.79	114.14	123.63
34	f	101	HEM	CBD-CAD-C3D	-3.79	102.06	112.53
28	d	405	PL9	C40-C39-C41	3.79	121.80	115.23
25	B	606	CLA	O2D-CGD-O1D	-3.77	116.52	123.85
26	d	401	PHO	C1-C2-C3	-3.76	120.04	126.20
31	a	614	SQD	O47-C7-C8	3.74	119.57	111.48
25	B	611	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
26	A	608	PHO	CMB-C2B-C3B	3.73	132.14	124.68
25	B	608	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
31	a	615	SQD	O9-S-O7	-3.73	101.70	113.82
25	c	508	CLA	C3B-C4B-NB	-3.72	107.21	110.53
25	B	605	CLA	C3B-C4B-NB	-3.71	107.21	110.53
27	H	101	BCR	C2-C1-C6	3.71	115.83	110.44
25	C	507	CLA	O2D-CGD-O1D	-3.71	116.63	123.85
26	A	609	PHO	CMA-C3A-C4A	-3.70	106.64	114.61
26	A	609	PHO	C4D-CHA-CBD	-3.67	106.70	108.45
31	b	620	SQD	O9-S-O7	-3.64	101.99	113.82
25	c	509	CLA	CHB-C4A-NA	3.63	129.63	124.40
25	b	603	CLA	O2D-CGD-CBD	3.62	117.56	111.23
31	A	616	SQD	O9-S-O7	-3.61	102.08	113.82
31	B	622	SQD	O48-C23-C24	3.60	122.81	111.83
30	C	517	LMG	C8-O7-C10	3.60	126.41	117.80
31	a	615	SQD	O47-C7-C8	3.60	119.26	111.48
25	C	502	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
31	D	407	SQD	O8-S-C6	3.56	112.85	105.97
25	D	402	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
31	a	614	SQD	C1-C2-C3	-3.56	102.53	110.01
31	B	622	SQD	O9-S-O7	-3.55	102.27	113.82
25	d	403	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
25	C	512	CLA	C3B-C4B-NB	-3.55	107.36	110.53
31	b	620	SQD	O7-S-C6	3.55	112.05	106.76
28	D	404	PL9	C27-C28-C29	-3.54	119.52	127.62
31	a	614	SQD	C44-O6-C1	-3.53	106.22	113.80
25	b	606	CLA	O2D-CGD-CBD	3.51	117.37	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	610	CLA	CHB-C4A-NA	3.51	129.46	124.40
25	d	402	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
25	a	609	CLA	C4A-NA-C1A	3.49	108.27	106.68
25	A	606	CLA	CHB-C4A-NA	3.48	129.43	124.40
31	b	620	SQD	O9-S-C6	3.48	111.95	106.76
25	B	605	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
34	F	101	HEM	CBD-CAD-C3D	-3.47	102.94	112.53
25	b	602	CLA	O2D-CGD-CBD	3.46	117.28	111.23
25	C	501	CLA	O2D-CGD-CBD	3.46	117.28	111.23
25	b	608	CLA	C3B-C4B-NB	-3.46	107.44	110.53
25	B	603	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
31	f	102	SQD	C1-O5-C5	-3.44	107.00	113.72
25	b	614	CLA	C1-C2-C3	-3.44	120.56	126.20
25	b	601	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
30	C	517	LMG	O6-C5-C4	3.44	115.89	109.70
33	A	619	DGD	C3G-O3G-C1D	3.43	121.15	113.80
25	B	614	CLA	C3B-C4B-NB	-3.43	107.47	110.53
25	b	614	CLA	C3B-C4B-NB	-3.42	107.47	110.53
34	f	101	HEM	CBA-CAA-C2A	-3.42	103.07	112.53
25	c	512	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
25	b	608	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
27	k	102	BCR	C7-C8-C9	-3.41	121.19	126.23
25	D	401	CLA	C4A-NA-C1A	3.41	108.23	106.68
31	b	620	SQD	O5-C5-C4	3.41	115.84	109.70
25	a	607	CLA	C3B-C4B-NB	-3.40	107.50	110.53
28	d	405	PL9	C7-C3-C2	-3.39	119.39	123.39
25	c	504	CLA	C1-C2-C3	-3.39	120.65	126.20
31	A	616	SQD	O7-S-C6	3.38	111.80	106.76
25	a	609	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
27	H	101	BCR	C16-C17-C18	-3.37	122.55	127.28
25	c	505	CLA	C3B-C4B-NB	-3.37	107.52	110.53
27	b	618	BCR	C2-C1-C6	3.37	115.33	110.44
25	b	605	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
31	f	102	SQD	O7-S-C6	3.35	111.77	106.76
25	C	508	CLA	C3B-C4B-NB	-3.35	107.54	110.53
25	C	506	CLA	C3B-C4B-NB	-3.35	107.54	110.53
25	c	505	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
31	A	618	SQD	O9-S-O7	-3.34	102.95	113.82
31	a	615	SQD	C3-C4-C5	3.34	116.29	110.23
25	b	612	CLA	C3B-C4B-NB	-3.33	107.56	110.53
25	b	611	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
35	V	201	HEC	CBD-CAD-C3D	-3.32	103.35	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	612	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
25	a	612	CLA	O2D-CGD-CBD	3.31	117.02	111.23
26	a	608	PHO	C2B-C1B-NB	-3.31	107.04	109.43
26	A	609	PHO	C1-C2-C3	-3.30	120.79	126.20
30	a	616	LMG	C8-O7-C10	3.30	125.69	117.80
25	C	512	CLA	C1-C2-C3	-3.30	120.80	126.20
25	B	604	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
25	b	610	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	C	508	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
25	b	608	CLA	CHB-C4A-NA	3.26	129.11	124.40
25	B	601	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	b	604	CLA	C6-C7-C8	-3.25	105.15	115.97
33	A	619	DGD	O5D-C1E-C2E	3.24	113.20	108.27
28	D	404	PL9	C7-C8-C9	-3.24	121.25	126.83
25	C	510	CLA	C3B-C4B-NB	-3.22	107.65	110.53
26	d	401	PHO	CBC-CAC-C3C	3.21	117.47	112.87
25	B	614	CLA	C1-C2-C3	-3.21	120.94	126.20
25	A	614	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
25	c	510	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
25	c	506	CLA	C3B-C4B-NB	-3.20	107.67	110.53
25	B	612	CLA	O2A-CGA-O1A	-3.20	115.63	123.63
25	b	605	CLA	C1-C2-C3	-3.19	120.98	126.20
25	a	606	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	C	512	CLA	CHB-C4A-NA	3.17	128.98	124.40
31	a	614	SQD	O9-S-O7	-3.16	103.54	113.82
25	C	513	CLA	O2D-CGD-CBD	3.16	116.76	111.23
25	a	612	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
25	A	614	CLA	O2D-CGD-CBD	3.15	116.74	111.23
31	b	620	SQD	C1-C2-C3	-3.15	103.38	110.01
25	c	507	CLA	CHB-C4A-NA	3.15	128.94	124.40
28	D	404	PL9	C22-C23-C24	-3.14	120.44	127.62
25	B	604	CLA	C3B-C4B-NB	-3.14	107.73	110.53
25	C	503	CLA	C7-C6-C5	-3.14	104.91	113.26
25	B	602	CLA	O2D-CGD-CBD	3.13	116.70	111.23
31	B	622	SQD	O7-S-C6	3.13	111.43	106.76
25	C	507	CLA	CHB-C4A-NA	3.13	128.91	124.40
25	C	504	CLA	C3B-C4B-NB	-3.12	107.75	110.53
25	B	614	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
27	A	611	BCR	C2-C1-C6	3.11	114.96	110.44
25	b	613	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
25	b	609	CLA	C7-C6-C5	-3.10	104.99	113.26
25	b	608	CLA	O2D-CGD-CBD	3.09	116.63	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	404	PL9	C37-C38-C39	-3.09	120.56	127.62
25	B	608	CLA	CMB-C2B-C1B	-3.08	120.72	125.42
25	B	609	CLA	C3B-C4B-NB	-3.08	107.78	110.53
25	c	508	CLA	C1-C2-C3	-3.08	121.15	126.20
25	b	601	CLA	C3B-C4B-NB	-3.07	107.78	110.53
25	c	511	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
25	c	507	CLA	C3B-C4B-NB	-3.06	107.80	110.53
30	D	405	LMG	C1-C2-C3	-3.06	103.58	110.01
25	c	504	CLA	CMB-C2B-C1B	-3.06	120.76	125.42
25	B	611	CLA	O2D-CGD-CBD	3.05	116.57	111.23
26	A	609	PHO	CMB-C2B-C3B	3.04	130.76	124.68
26	d	401	PHO	C2B-C1B-NB	-3.04	107.23	109.43
25	c	513	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	B	605	CLA	O1D-CGD-CBD	3.03	130.50	124.52
31	a	614	SQD	O48-C23-C24	3.03	121.06	111.83
28	d	405	PL9	C37-C38-C39	-3.03	120.70	127.62
25	B	608	CLA	O2D-CGD-CBD	3.03	116.52	111.23
25	B	608	CLA	C3B-C4B-NB	-3.02	107.83	110.53
25	b	611	CLA	C3B-C4B-NB	-3.02	107.83	110.53
25	B	601	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
31	A	618	SQD	O48-C23-C24	3.01	121.02	111.83
25	B	606	CLA	C3B-C4B-NB	-3.01	107.84	110.53
28	D	404	PL9	C12-C13-C14	-3.01	120.73	127.62
28	D	404	PL9	C7-C3-C2	-3.01	119.84	123.39
25	B	606	CLA	O2A-CGA-O1A	-3.00	116.12	123.63
31	D	407	SQD	O9-S-C6	2.99	111.22	106.76
25	C	509	CLA	CHB-C4A-NA	2.99	128.71	124.40
25	B	610	CLA	C3B-C4B-NB	-2.98	107.87	110.53
28	d	405	PL9	C22-C23-C24	-2.98	120.80	127.62
25	a	607	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	D	401	CLA	O2A-CGA-O1A	-2.98	116.19	123.63
30	M	101	LMG	C8-O7-C10	2.97	124.90	117.80
28	a	611	PL9	C37-C38-C39	-2.97	120.83	127.62
31	b	620	SQD	O5-C1-C2	-2.96	104.29	110.37
25	A	610	CLA	O2D-CGD-CBD	2.96	116.40	111.23
25	a	607	CLA	CHB-C4A-NA	2.95	128.66	124.40
27	A	611	BCR	C4-C5-C6	-2.95	118.71	122.70
25	B	604	CLA	CHB-C4A-NA	2.95	128.66	124.40
28	d	405	PL9	C32-C33-C34	-2.95	120.88	127.62
25	b	602	CLA	C1-C2-C3	-2.94	121.37	126.20
31	f	102	SQD	O5-C5-C4	2.94	115.00	109.70
25	B	610	CLA	O2A-CGA-O1A	-2.94	116.29	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	612	PL9	C40-C39-C41	2.93	120.32	115.23
25	a	607	CLA	O2D-CGD-CBD	2.93	116.35	111.23
25	B	603	CLA	C3B-C4B-NB	-2.92	107.92	110.53
25	b	616	CLA	O2D-CGD-CBD	2.92	116.34	111.23
25	c	511	CLA	C3B-C4B-NB	-2.92	107.92	110.53
25	B	611	CLA	C1-C2-C3	-2.91	121.42	126.20
26	a	608	PHO	CMB-C2B-C3B	2.91	130.50	124.68
25	B	615	CLA	C3B-C4B-NB	-2.91	107.94	110.53
25	A	610	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
26	d	401	PHO	O1D-CGD-CBD	2.90	129.13	124.72
28	D	404	PL9	C42-C43-C44	-2.90	121.00	127.62
31	A	618	SQD	O6-C1-C2	2.90	112.67	108.27
31	A	618	SQD	O7-S-C6	2.89	111.08	106.76
25	C	505	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	b	610	CLA	CAA-CBA-CGA	-2.89	105.00	113.21
25	A	607	CLA	CHB-C4A-NA	2.89	128.57	124.40
25	b	602	CLA	CHB-C4A-NA	2.89	128.57	124.40
34	F	101	HEM	CBA-CAA-C2A	-2.89	104.55	112.53
30	M	101	LMG	O1-C7-C8	-2.88	103.81	110.82
25	b	604	CLA	CHB-C4A-NA	2.88	128.55	124.40
25	D	401	CLA	C3B-C4B-NB	-2.88	107.96	110.53
25	B	602	CLA	C3B-C4B-NB	-2.87	107.96	110.53
25	a	612	CLA	C3B-C4B-NB	-2.87	107.97	110.53
25	C	503	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
29	j	101	STE	O2-C1-C2	2.86	123.05	114.00
25	d	402	CLA	CHB-C4A-NA	2.86	128.53	124.40
25	B	612	CLA	CHB-C4A-NA	2.86	128.53	124.40
25	B	603	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
31	D	407	SQD	O5-C1-C2	-2.85	104.51	110.37
25	B	611	CLA	CHB-C4A-NA	2.85	128.51	124.40
25	b	610	CLA	C1-C2-C3	-2.84	121.54	126.20
27	h	101	BCR	C29-C30-C25	2.84	114.57	110.44
31	D	407	SQD	O48-C23-C24	2.84	120.50	111.83
25	B	604	CLA	O2D-CGD-CBD	2.84	116.19	111.23
25	C	512	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
25	c	503	CLA	C3B-C4B-NB	-2.84	108.00	110.53
25	c	505	CLA	C1-C2-C3	-2.83	121.56	126.20
25	b	610	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
25	c	508	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	B	610	CLA	O2D-CGD-CBD	2.83	116.17	111.23
25	a	609	CLA	C1-C2-C3	-2.83	121.57	126.20
25	C	512	CLA	O2D-CGD-O1D	-2.83	118.35	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	401	PHO	CMB-C2B-C3B	2.83	130.33	124.68
25	d	403	CLA	O2A-CGA-O1A	-2.82	116.57	123.63
25	B	612	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
25	a	609	CLA	O2D-CGD-CBD	2.81	116.14	111.23
26	a	608	PHO	C1-C2-C3	-2.81	121.60	126.20
25	B	603	CLA	O2D-CGD-CBD	2.79	116.11	111.23
30	C	517	LMG	C7-O1-C1	2.79	119.78	113.80
25	B	616	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
27	B	617	BCR	C29-C30-C25	2.78	114.48	110.44
26	a	608	PHO	OBD-CAD-CBD	-2.78	121.75	125.82
28	d	405	PL9	C27-C28-C29	-2.77	121.28	127.62
27	H	101	BCR	C33-C5-C6	2.77	127.51	124.48
25	b	612	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
25	b	607	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	C	503	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	c	506	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
25	C	501	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
31	a	615	SQD	O5-C5-C4	2.76	114.68	109.70
25	c	507	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
25	b	611	CLA	O2D-CGD-CBD	2.76	116.06	111.23
25	c	512	CLA	C3B-C4B-NB	-2.76	108.07	110.53
28	a	611	PL9	C40-C39-C41	2.76	120.01	115.23
31	a	615	SQD	O6-C1-C2	2.76	112.46	108.27
25	c	510	CLA	C3B-C4B-NB	-2.75	108.07	110.53
33	C	521	DGD	C3D-C4D-C5D	-2.75	105.25	110.23
31	B	622	SQD	O5-C5-C4	2.74	114.64	109.70
25	D	401	CLA	CHB-C4A-NA	2.74	128.35	124.40
25	a	606	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
25	b	601	CLA	CHB-C4A-NA	2.73	128.34	124.40
27	t	101	BCR	C31-C1-C6	2.73	114.53	110.24
27	h	101	BCR	C33-C5-C6	2.73	127.46	124.48
25	b	604	CLA	C3B-C4B-NB	-2.73	108.09	110.53
31	f	102	SQD	O48-C23-C24	2.73	120.15	111.83
25	C	513	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
25	C	512	CLA	C6-C5-C3	-2.73	106.83	113.47
25	b	616	CLA	C1-C2-C3	-2.72	121.73	126.20
25	C	502	CLA	C3B-C4B-NB	-2.72	108.10	110.53
25	c	505	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
34	f	101	HEM	C3B-C4B-NB	-2.72	107.51	109.47
25	c	508	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
25	b	609	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
31	b	620	SQD	O48-C23-C24	2.71	120.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	C3B-C4B-NB	-2.71	108.11	110.53
25	B	616	CLA	CHC-C4B-NB	2.70	128.10	124.05
25	b	603	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
25	b	612	CLA	C1-C2-C3	-2.70	121.77	126.20
33	H	102	DGD	C3G-O3G-C1D	2.70	119.58	113.80
29	m	102	STE	C3-C2-C1	-2.70	107.47	114.51
31	B	622	SQD	C3-C4-C5	2.69	115.11	110.23
34	f	101	HEM	CHB-C1B-NB	2.69	127.70	124.37
25	b	616	CLA	CHB-C4A-NA	2.69	128.29	124.40
25	C	509	CLA	C1-C2-C3	-2.69	121.79	126.20
25	B	604	CLA	O2A-CGA-O1A	-2.68	116.91	123.63
25	a	606	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
25	B	609	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
25	B	605	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
30	m	101	LMG	O1-C7-C8	-2.68	104.31	110.82
25	c	513	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	B	615	CLA	CHB-C4A-NA	2.67	128.26	124.40
25	B	608	CLA	CMB-C2B-C3B	2.67	132.83	126.55
25	B	602	CLA	CHB-C4A-NA	2.67	128.25	124.40
25	b	613	CLA	CHB-C4A-NA	2.66	128.25	124.40
25	B	602	CLA	CMB-C2B-C1B	-2.66	121.36	125.42
25	A	610	CLA	CHB-C4A-NA	2.66	128.24	124.40
32	D	410	LHG	O7-C5-C4	-2.66	98.80	108.34
31	A	616	SQD	C45-O47-C7	-2.66	111.44	117.80
25	b	602	CLA	C3B-C4B-NB	-2.66	108.16	110.53
28	a	611	PL9	C27-C28-C29	-2.65	121.55	127.62
31	f	102	SQD	O5-C1-C2	-2.65	104.92	110.37
25	b	605	CLA	C3B-C4B-NB	-2.65	108.16	110.53
25	C	510	CLA	CHB-C4A-NA	2.65	128.22	124.40
25	D	401	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
25	A	610	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
25	c	512	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	b	603	CLA	C3B-C4B-NB	-2.64	108.18	110.53
30	b	622	LMG	C1-O6-C5	-2.64	108.57	113.72
27	k	101	BCR	C23-C22-C21	-2.63	114.87	119.01
25	A	606	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
25	B	610	CLA	C1-C2-C3	-2.63	121.89	126.20
25	b	616	CLA	C3B-C4B-NB	-2.63	108.18	110.53
32	D	410	LHG	C6-C5-C4	2.62	117.90	111.78
31	A	616	SQD	O8-S-C6	2.62	111.04	105.97
25	c	504	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
25	b	607	CLA	O2D-CGD-O1D	-2.62	118.75	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	606	CLA	CHB-C4A-NA	2.62	128.18	124.40
25	B	613	CLA	O2A-CGA-O1A	-2.62	117.08	123.63
33	c	521	DGD	C3G-O3G-C1D	2.62	119.41	113.80
25	C	507	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	d	402	CLA	O2D-CGD-CBD	2.61	115.79	111.23
34	f	101	HEM	CAB-C3B-C2B	-2.61	119.95	128.43
28	A	612	PL9	O2-C1-C2	-2.61	115.89	121.83
25	b	606	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	B	616	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
25	c	505	CLA	O2D-CGD-CBD	2.60	115.77	111.23
25	b	609	CLA	C3B-C4B-NB	-2.60	108.21	110.53
25	B	611	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	a	615	SQD	O48-C23-C24	2.59	119.74	111.83
25	b	609	CLA	C1-C2-C3	-2.59	121.95	126.20
25	c	504	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
25	b	614	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
25	B	608	CLA	CHB-C4A-NA	2.59	128.13	124.40
34	f	101	HEM	C3B-C2B-C1B	2.58	108.35	106.41
26	A	608	PHO	CMA-C3A-C2A	-2.58	104.16	114.13
28	a	611	PL9	C32-C33-C34	-2.58	121.72	127.62
25	b	610	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	D	407	SQD	O9-S-O7	-2.58	105.44	113.82
25	d	402	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
25	A	606	CLA	C3B-C4B-NB	-2.57	108.23	110.53
25	A	614	CLA	CHB-C4A-NA	2.57	128.11	124.40
25	c	503	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
25	B	601	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
26	A	609	PHO	C2B-C1B-NB	-2.57	107.57	109.43
31	B	622	SQD	O9-S-C6	2.57	110.59	106.76
31	a	614	SQD	C3-C4-C5	2.57	114.89	110.23
25	b	615	CLA	CHB-C4A-NA	2.57	128.10	124.40
30	b	622	LMG	C8-O7-C10	2.56	123.93	117.80
25	b	604	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
25	B	609	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
25	B	612	CLA	C1-C2-C3	-2.55	122.01	126.20
31	b	620	SQD	C3-C4-C5	2.55	114.86	110.23
25	B	614	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
25	b	604	CLA	CAC-C3C-C4C	2.55	128.10	124.79
25	c	504	CLA	CHB-C4A-NA	2.54	128.07	124.40
25	C	505	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
27	T	101	BCR	C38-C26-C25	2.54	127.26	124.48
25	C	508	CLA	O2D-CGD-CBD	2.54	115.67	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	616	SQD	O48-C23-C24	2.54	119.58	111.83
33	C	521	DGD	C3G-O3G-C1D	2.53	119.23	113.80
28	a	611	PL9	C22-C23-C24	-2.53	121.83	127.62
25	B	609	CLA	CHC-C4B-NB	2.53	127.84	124.05
28	A	612	PL9	O2-C1-C6	2.53	124.50	120.48
25	C	505	CLA	O2D-CGD-CBD	2.53	115.65	111.23
31	f	102	SQD	O47-C7-C8	2.52	120.20	110.93
25	c	503	CLA	C7-C6-C5	-2.52	106.54	113.26
24	A	605	BCT	O2-C-O1	2.52	126.13	119.68
25	B	616	CLA	C3B-C4B-NB	-2.52	108.28	110.53
31	B	622	SQD	O5-C1-C2	-2.52	105.19	110.37
28	D	404	PL9	C40-C39-C41	2.52	119.60	115.23
31	a	614	SQD	O8-S-C6	2.51	110.83	105.97
28	d	405	PL9	C7-C8-C9	-2.51	122.50	126.83
25	C	506	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
25	C	503	CLA	CHB-C4A-NA	2.51	128.02	124.40
33	c	519	DGD	C3D-C4D-C5D	-2.51	105.69	110.23
25	D	402	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
33	c	519	DGD	C3G-O3G-C1D	2.51	119.17	113.80
24	a	605	BCT	O2-C-O1	2.51	126.08	119.68
25	B	607	CLA	CHB-C4A-NA	2.50	128.01	124.40
28	d	405	PL9	C42-C43-C44	-2.50	121.91	127.62
33	H	102	DGD	C3E-C4E-C5E	-2.50	105.71	110.23
30	C	517	LMG	O4-C4-C5	2.50	115.47	109.32
28	A	612	PL9	C22-C23-C24	-2.49	121.92	127.62
33	h	102	DGD	C3D-C4D-C5D	-2.49	105.71	110.23
33	h	102	DGD	C1E-O6E-C5E	2.49	118.58	113.72
25	C	511	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
25	C	511	CLA	CHB-C4A-NA	2.49	127.99	124.40
35	V	201	HEC	CHA-C4D-ND	2.48	127.10	124.42
35	v	201	HEC	CHA-C4D-ND	2.48	127.10	124.42
25	C	509	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
30	C	524	LMG	O1-C7-C8	-2.48	104.78	110.82
25	b	609	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
25	b	614	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
25	C	506	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
35	v	201	HEC	CBD-CAD-C3D	-2.48	105.69	112.53
30	B	620	LMG	O3-C3-C2	-2.47	104.55	110.38
25	B	608	CLA	C6-C7-C8	-2.47	107.74	115.97
25	B	612	CLA	O1D-CGD-CBD	2.47	129.39	124.52
25	C	505	CLA	C1-C2-C3	-2.47	122.15	126.20
25	a	606	CLA	O1D-CGD-CBD	2.47	129.39	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	510	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
25	c	508	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	B	612	CLA	C3B-C4B-NB	-2.46	108.34	110.53
25	a	612	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
26	A	609	PHO	CMA-C3A-C2A	-2.45	104.65	114.13
25	b	604	CLA	O2D-CGD-CBD	2.45	115.52	111.23
28	a	611	PL9	O2-C1-C2	-2.45	116.25	121.83
25	a	609	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
25	c	504	CLA	CMB-C2B-C3B	2.45	132.31	126.55
25	b	609	CLA	C6-C5-C3	2.45	119.43	113.47
30	a	616	LMG	O8-C9-C8	2.45	115.45	108.40
25	c	510	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
25	C	510	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
28	d	405	PL9	C20-C19-C21	2.44	119.47	115.23
25	D	402	CLA	CHB-C4A-NA	2.44	127.92	124.40
33	h	102	DGD	C6D-C5D-C4D	2.44	117.18	112.07
25	c	501	CLA	CHB-C4A-NA	2.44	127.92	124.40
30	c	524	LMG	C3-C4-C5	-2.44	105.82	110.23
31	A	616	SQD	O47-C7-O49	-2.43	118.01	123.70
25	a	612	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
25	c	508	CLA	C7-C6-C5	-2.41	106.83	113.26
25	b	615	CLA	C1-C2-C3	-2.41	122.25	126.20
25	b	605	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
33	C	522	DGD	C3E-C4E-C5E	-2.41	105.87	110.23
26	d	401	PHO	O2D-CGD-O1D	-2.41	119.17	123.85
26	d	401	PHO	O2A-CGA-O1A	-2.40	117.61	123.63
25	A	607	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
25	C	511	CLA	C3B-C4B-NB	-2.40	108.39	110.53
28	D	404	PL9	C20-C19-C21	2.40	119.39	115.23
29	d	409	STE	C3-C2-C1	-2.40	108.25	114.51
29	b	623	STE	O2-C1-C2	2.39	121.56	114.00
33	h	102	DGD	O6E-C5E-C4E	2.39	114.01	109.70
25	b	616	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
33	A	619	DGD	C4E-C3E-C2E	-2.39	106.64	110.83
33	c	519	DGD	C6D-O5D-C1E	2.39	118.91	113.80
25	c	509	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
25	a	612	CLA	CHC-C4B-NB	2.38	127.62	124.05
25	C	506	CLA	CHB-C4A-NA	2.38	127.84	124.40
25	d	403	CLA	C3B-C4B-NB	-2.38	108.40	110.53
27	d	404	BCR	C30-C25-C26	-2.38	119.38	122.64
35	V	201	HEC	CMD-C2D-C1D	2.38	128.75	125.03
25	b	609	CLA	O1D-CGD-CBD	2.38	129.21	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	b	610	CLA	CHB-C4A-NA	2.38	127.83	124.40
30	D	406	LMG	O3-C3-C2	-2.37	104.78	110.38
31	b	620	SQD	O2-C2-C1	2.37	115.73	110.08
25	C	504	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
25	a	606	CLA	CMB-C2B-C3B	2.37	132.12	126.55
25	C	503	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
25	B	605	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	f	102	SQD	C3-C4-C5	2.36	114.52	110.23
25	B	604	CLA	C2D-C1D-ND	-2.36	107.79	110.13
25	c	511	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
25	b	604	CLA	C1D-ND-C4D	2.35	107.96	106.31
32	D	408	LHG	C5-O7-C7	2.35	123.42	117.80
25	A	607	CLA	C1D-ND-C4D	2.35	107.96	106.31
25	c	501	CLA	C3B-C4B-NB	-2.35	108.43	110.53
35	V	201	HEC	CAD-CBD-CGD	-2.35	107.44	113.67
25	c	509	CLA	O2A-CGA-CBA	2.35	118.99	111.83
29	t	102	STE	O2-C1-C2	2.35	121.41	114.00
28	D	404	PL9	C36-C34-C33	-2.35	115.90	121.17
25	c	510	CLA	C7-C6-C5	-2.35	107.01	113.26
30	b	622	LMG	O5-C6-C5	-2.34	103.35	111.33
25	B	613	CLA	C3B-C4B-NB	-2.34	108.44	110.53
28	A	612	PL9	C27-C28-C29	-2.34	122.26	127.62
25	D	402	CLA	O2D-CGD-CBD	2.34	115.32	111.23
31	A	616	SQD	O5-C1-C2	-2.34	105.56	110.37
33	A	619	DGD	O2E-C2E-C3E	2.34	115.89	110.38
28	a	611	PL9	O2-C1-C6	2.34	124.20	120.48
35	V	201	HEC	C1D-C2D-C3D	-2.33	104.53	106.98
25	b	608	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
25	C	513	CLA	CHB-C4A-NA	2.33	127.76	124.40
27	T	101	BCR	C38-C26-C27	-2.33	108.63	113.60
31	b	620	SQD	O48-C23-O10	-2.33	117.80	123.63
25	c	507	CLA	O2D-CGD-CBD	2.33	115.30	111.23
25	B	607	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
25	c	502	CLA	C1-C2-C3	-2.33	122.38	126.20
25	d	403	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	b	604	CLA	C11-C12-C13	-2.33	108.23	115.97
25	c	502	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	b	604	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
29	C	525	STE	C3-C2-C1	-2.32	108.45	114.51
25	b	612	CLA	C11-C12-C13	-2.32	108.25	115.97
35	v	201	HEC	CAD-CBD-CGD	-2.32	107.51	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
35	V	201	HEC	C4B-NB-C1B	2.32	107.95	105.21
25	b	609	CLA	CMB-C2B-C3B	2.32	132.00	126.55
28	a	611	PL9	O1-C4-C3	-2.32	118.29	120.73
25	A	614	CLA	C1-C2-C3	-2.32	122.40	126.20
25	B	607	CLA	C3B-C4B-NB	-2.31	108.47	110.53
25	c	508	CLA	C1D-ND-C4D	2.31	107.93	106.31
25	b	611	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	B	614	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
25	C	504	CLA	CHB-C4A-NA	2.31	127.73	124.40
31	D	407	SQD	C1-O5-C5	-2.30	109.22	113.72
25	B	616	CLA	CAC-C3C-C4C	2.30	127.79	124.79
33	c	521	DGD	C6D-O5D-C1E	2.30	118.73	113.80
25	a	607	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
26	d	401	PHO	CMA-C3A-C2A	-2.30	105.25	114.13
25	b	616	CLA	CHC-C4B-NB	2.29	127.49	124.05
25	c	501	CLA	O2D-CGD-CBD	2.29	115.24	111.23
25	B	603	CLA	CHC-C4B-NB	2.29	127.48	124.05
25	c	507	CLA	CHC-C4B-NB	2.29	127.48	124.05
25	C	510	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
29	C	525	STE	O2-C1-C2	2.29	121.22	114.00
25	C	505	CLA	CHB-C4A-NA	2.28	127.70	124.40
25	c	502	CLA	CHB-C4A-NA	2.28	127.70	124.40
25	C	501	CLA	CHB-C1B-NB	2.28	127.47	124.05
31	a	614	SQD	O48-C23-O10	-2.28	117.92	123.63
25	c	510	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	c	503	CLA	CHB-C4A-NA	2.28	127.68	124.40
25	B	614	CLA	CHB-C1B-NB	2.27	127.46	124.05
26	a	608	PHO	OBD-CAD-C3D	2.27	131.44	127.89
25	B	604	CLA	C11-C12-C13	-2.27	108.42	115.97
28	a	611	PL9	C7-C8-C9	-2.27	122.92	126.83
25	c	513	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
25	b	602	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
25	B	615	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
25	D	401	CLA	C4-C3-C5	2.26	119.15	115.23
25	D	402	CLA	C3B-C4B-NB	-2.26	108.52	110.53
25	c	507	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
25	a	612	CLA	C1-C2-C3	-2.25	122.50	126.20
27	b	617	BCR	C11-C10-C9	-2.25	124.12	127.28
29	B	624	STE	O2-C1-C2	2.25	121.11	114.00
25	B	602	CLA	CMB-C2B-C3B	2.25	131.84	126.55
28	d	405	PL9	O2-C1-C6	2.25	124.06	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	606	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
25	B	606	CLA	O2D-CGD-CBD	2.25	115.16	111.23
31	B	622	SQD	O48-C23-O10	-2.25	118.01	123.63
25	C	513	CLA	C3B-C4B-NB	-2.25	108.53	110.53
35	V	201	HEC	C3D-C4D-ND	-2.25	108.18	110.35
26	a	608	PHO	CMA-C3A-C2A	-2.24	105.47	114.13
25	c	512	CLA	C1-C2-C3	-2.24	122.52	126.20
25	b	601	CLA	O1D-CGD-CBD	2.24	128.94	124.52
25	B	606	CLA	CHB-C4A-NA	2.24	127.63	124.40
25	d	403	CLA	CMB-C2B-C3B	2.24	131.82	126.55
25	a	612	CLA	CMB-C2B-C3B	2.24	131.82	126.55
31	a	614	SQD	O7-S-C6	2.24	110.10	106.76
25	d	403	CLA	O2D-CGD-CBD	2.23	115.14	111.23
25	B	614	CLA	CHB-C4A-NA	2.23	127.62	124.40
25	c	505	CLA	CMB-C2B-C3B	2.23	131.80	126.55
35	v	201	HEC	CBA-CAA-C2A	-2.23	106.36	112.53
25	C	505	CLA	C11-C10-C8	-2.23	108.55	115.97
25	C	507	CLA	O2D-CGD-CBD	2.23	115.13	111.23
29	B	624	STE	C3-C2-C1	-2.23	108.69	114.51
30	a	616	LMG	O7-C8-C9	2.23	116.34	108.34
25	b	613	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	C	510	CLA	C1-C2-C3	-2.23	122.55	126.20
25	A	606	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
25	d	403	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
32	d	407	LHG	C5-O7-C7	2.22	123.11	117.80
26	A	609	PHO	CAA-C2A-C3A	-2.22	107.00	113.00
25	c	502	CLA	CHC-C4B-NB	2.22	127.38	124.05
25	C	503	CLA	O1D-CGD-CBD	2.22	128.89	124.52
25	C	507	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
26	A	608	PHO	C3D-C4D-ND	2.21	110.54	107.71
25	C	508	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
25	B	603	CLA	CHB-C4A-NA	2.21	127.59	124.40
29	d	406	STE	O2-C1-C2	2.21	120.98	114.00
31	D	407	SQD	O5-C5-C4	2.20	113.67	109.70
29	E	103	STE	O2-C1-C2	2.20	120.96	114.00
25	b	610	CLA	CHC-C4B-NB	2.20	127.35	124.05
25	a	612	CLA	CHB-C4A-NA	2.20	127.58	124.40
31	A	618	SQD	O8-S-C6	2.20	110.22	105.97
25	b	606	CLA	CHB-C4A-NA	2.20	127.57	124.40
33	C	521	DGD	O2E-C2E-C3E	2.20	115.55	110.38
30	B	620	LMG	O1-C7-C8	-2.19	105.48	110.82
25	B	614	CLA	CED-O2D-CGD	2.19	120.89	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C2D-C1D-ND	-2.19	107.96	110.13
25	C	503	CLA	CMB-C2B-C3B	2.19	131.69	126.55
25	B	603	CLA	CHD-C1D-ND	-2.19	121.73	124.80
25	C	503	CLA	C1-O2A-CGA	2.18	121.94	116.65
25	A	607	CLA	C3B-C4B-NB	-2.18	108.58	110.53
25	C	513	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
25	c	506	CLA	O1D-CGD-CBD	2.18	128.82	124.52
33	c	520	DGD	C3D-C4D-C5D	-2.18	106.28	110.23
25	d	403	CLA	C1-C2-C3	-2.18	122.63	126.20
25	D	401	CLA	CHD-C1D-ND	-2.18	121.74	124.80
30	c	524	LMG	O1-C1-C2	2.18	111.58	108.27
35	v	201	HEC	C2A-C1A-NA	-2.17	108.22	110.32
26	d	401	PHO	C3B-C4B-NB	-2.17	106.05	107.46
25	d	402	CLA	C3B-C4B-NB	-2.17	108.59	110.53
28	d	405	PL9	C12-C13-C14	-2.17	122.66	127.62
25	C	510	CLA	CMB-C2B-C3B	2.17	131.66	126.55
25	c	502	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	b	612	CLA	CHC-C4B-NB	2.17	127.30	124.05
25	b	604	CLA	C11-C10-C8	-2.17	108.76	115.97
25	D	402	CLA	CMB-C2B-C3B	2.17	131.65	126.55
32	d	407	LHG	O4-P-O5	2.16	122.51	112.44
27	t	101	BCR	C12-C13-C14	-2.16	115.61	119.01
25	B	614	CLA	CMB-C2B-C3B	2.16	131.63	126.55
25	b	607	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
25	C	512	CLA	CHA-C1A-NA	-2.16	121.51	126.39
25	C	502	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
31	B	622	SQD	C9-C8-C7	-2.16	105.80	113.69
31	A	618	SQD	C3-C4-C5	2.16	114.14	110.23
25	b	603	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
27	b	618	BCR	C15-C14-C13	-2.15	124.26	127.28
25	c	505	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
33	A	619	DGD	O4E-C4E-C5E	2.15	114.61	109.32
25	B	607	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
25	B	615	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
25	c	513	CLA	CHB-C4A-NA	2.14	127.49	124.40
27	B	619	BCR	C29-C30-C25	2.14	113.55	110.44
25	c	512	CLA	O2D-CGD-CBD	2.14	114.97	111.23
25	a	609	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	c	502	CLA	O1D-CGD-CBD	2.14	128.74	124.52
25	b	603	CLA	CHD-C1D-ND	-2.14	121.79	124.80
25	c	513	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
33	C	523	DGD	O3E-C3E-C2E	-2.14	105.34	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	E	101	STE	C3-C2-C1	-2.14	108.94	114.51
25	C	504	CLA	CED-O2D-CGD	2.13	120.76	115.92
25	B	610	CLA	C2A-C1A-CHA	2.13	127.57	123.87
25	b	613	CLA	O2D-CGD-CBD	2.13	114.96	111.23
29	e	104	STE	O2-C1-C2	2.13	120.73	114.00
33	H	102	DGD	O3D-C3D-C2D	-2.13	105.36	110.38
25	c	509	CLA	C1-O2A-CGA	-2.13	111.50	116.65
33	A	619	DGD	O4E-C4E-C3E	-2.13	105.37	110.38
25	b	613	CLA	CED-O2D-CGD	2.12	120.73	115.92
28	d	405	PL9	O1-C4-C3	-2.12	118.49	120.73
25	B	613	CLA	CHB-C4A-NA	2.12	127.46	124.40
25	b	611	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
29	a	617	STE	O2-C1-C2	2.12	120.69	114.00
29	B	623	STE	C3-C2-C1	-2.12	108.98	114.51
25	c	503	CLA	C11-C12-C13	-2.12	108.93	115.97
27	B	618	BCR	C2-C1-C6	2.11	113.51	110.44
25	B	613	CLA	CHA-C1A-NA	-2.11	121.61	126.39
26	a	608	PHO	O2A-CGA-O1A	-2.11	118.35	123.63
27	b	618	BCR	C33-C5-C6	2.11	126.79	124.48
33	C	522	DGD	C3G-O3G-C1D	2.11	118.32	113.80
31	A	618	SQD	O48-C23-O10	-2.11	118.35	123.63
29	m	102	STE	O2-C1-C2	2.11	120.66	114.00
31	a	615	SQD	C9-C8-C7	-2.11	105.98	113.69
25	B	613	CLA	CHC-C4B-NB	2.11	127.21	124.05
29	e	104	STE	C3-C2-C1	-2.11	109.02	114.51
27	D	403	BCR	C32-C1-C6	2.10	113.54	110.24
27	c	515	BCR	C11-C10-C9	-2.10	124.33	127.28
34	F	101	HEM	O2D-CGD-CBD	2.10	120.64	114.00
25	c	503	CLA	O1D-CGD-CBD	2.10	128.66	124.52
30	a	616	LMG	O3-C3-C4	2.10	115.33	110.38
33	h	102	DGD	O3D-C3D-C2D	-2.10	105.43	110.38
25	C	513	CLA	CHD-C1D-ND	-2.10	121.85	124.80
25	b	607	CLA	CHB-C4A-NA	2.10	127.43	124.40
25	C	509	CLA	C3B-C4B-NB	-2.10	108.66	110.53
27	t	101	BCR	C15-C16-C17	-2.10	119.23	123.52
25	C	504	CLA	CHD-C4C-NC	2.10	127.48	124.23
25	b	611	CLA	CHB-C4A-NA	2.10	127.43	124.40
25	b	603	CLA	CHC-C4B-NB	2.10	127.19	124.05
31	a	614	SQD	O9-S-C6	2.09	109.88	106.76
25	b	613	CLA	C1-C2-C3	-2.09	122.77	126.20
25	c	509	CLA	C3B-C4B-NB	-2.09	108.66	110.53
25	b	608	CLA	C6-C7-C8	-2.09	109.02	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	C1-O2A-CGA	2.08	121.69	116.65
25	B	616	CLA	O2D-CGD-CBD	2.08	114.87	111.23
25	a	609	CLA	C3B-C4B-NB	-2.08	108.67	110.53
27	d	404	BCR	C40-C30-C25	2.08	113.50	110.24
25	b	607	CLA	CMB-C2B-C3B	2.08	131.44	126.55
25	B	609	CLA	CHB-C4A-NA	2.08	127.39	124.40
28	d	405	PL9	O2-C1-C2	-2.07	117.11	121.83
25	c	508	CLA	O2D-CGD-CBD	2.07	114.85	111.23
28	D	404	PL9	C50-C49-C48	-2.07	116.44	122.66
25	b	612	CLA	CHB-C4A-NA	2.07	127.39	124.40
25	B	616	CLA	CHB-C4A-NA	2.07	127.39	124.40
25	a	612	CLA	CHA-C1A-NA	-2.07	121.70	126.39
30	D	405	LMG	O6-C1-C2	-2.07	106.12	110.37
25	b	607	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
27	t	101	BCR	C38-C26-C25	2.07	126.74	124.48
25	b	605	CLA	O2D-CGD-CBD	2.07	114.84	111.23
27	J	101	BCR	C2-C1-C6	2.07	113.44	110.44
30	b	622	LMG	C3-C4-C5	-2.06	106.49	110.23
27	t	101	BCR	C11-C10-C9	-2.06	124.38	127.28
31	B	622	SQD	C1-C2-C3	-2.06	105.67	110.01
25	B	606	CLA	CHA-C4D-ND	2.06	136.80	132.55
25	b	614	CLA	CHB-C4A-NA	2.06	127.38	124.40
25	C	503	CLA	O2A-C1-C2	-2.06	100.17	108.11
27	k	102	BCR	C7-C6-C5	2.06	126.30	121.56
25	B	608	CLA	C1-C2-C3	-2.06	122.82	126.20
26	A	608	PHO	OBD-CAD-C3D	2.06	131.10	127.89
25	B	609	CLA	O1D-CGD-CBD	2.06	128.57	124.52
25	B	607	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
25	B	607	CLA	C4-C3-C5	2.05	118.79	115.23
25	C	504	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
25	B	612	CLA	CAC-C3C-C4C	2.05	127.46	124.79
30	A	615	LMG	C8-O7-C10	2.05	122.70	117.80
29	I	101	STE	O2-C1-C2	2.05	120.47	114.00
25	C	502	CLA	O2D-CGD-CBD	2.05	114.81	111.23
25	B	614	CLA	CHA-C4D-ND	2.04	136.77	132.55
25	b	605	CLA	CHD-C1D-ND	-2.04	121.93	124.80
30	C	517	LMG	C3-C4-C5	2.04	113.94	110.23
29	t	102	STE	C3-C2-C1	-2.04	109.18	114.51
30	c	524	LMG	O1-C7-C8	-2.04	105.86	110.82
25	c	501	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
25	c	503	CLA	C1-C2-C3	-2.03	122.87	126.20
31	D	407	SQD	C1-C2-C3	-2.03	105.73	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	b	614	CLA	CHB-C1B-NB	2.03	127.10	124.05
35	V	201	HEC	C2A-C1A-NA	-2.03	108.36	110.32
25	c	502	CLA	O2D-CGD-CBD	2.03	114.78	111.23
25	c	510	CLA	O1D-CGD-CBD	2.03	128.52	124.52
25	B	610	CLA	CHA-C1A-NA	-2.03	121.79	126.39
25	a	607	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	b	604	CLA	C4-C3-C5	2.03	118.75	115.23
27	H	101	BCR	C29-C30-C25	2.03	113.39	110.44
25	b	615	CLA	CHA-C4D-ND	2.03	136.73	132.55
33	h	102	DGD	C6E-C5E-C4E	-2.03	108.04	113.02
26	A	609	PHO	O2A-CGA-O1A	-2.03	118.56	123.63
25	B	605	CLA	C7-C6-C5	-2.02	107.87	113.26
25	A	610	CLA	C3B-C4B-NB	-2.02	108.72	110.53
26	A	608	PHO	C2B-C1B-NB	-2.02	107.97	109.43
27	A	611	BCR	C20-C21-C22	-2.02	124.44	127.28
30	c	524	LMG	O3-C3-C4	2.02	115.14	110.38
34	f	101	HEM	C4C-NC-C1C	2.02	109.12	105.82
25	C	505	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
25	c	511	CLA	CHB-C4A-NA	2.02	127.31	124.40
30	a	616	LMG	O2-C2-C1	2.02	114.89	110.08
25	B	610	CLA	O1D-CGD-CBD	2.02	128.49	124.52
29	M	102	STE	O2-C1-C2	2.02	120.37	114.00
27	b	617	BCR	C29-C30-C25	2.01	113.36	110.44
29	B	623	STE	O2-C1-C2	2.01	120.36	114.00
27	k	101	BCR	C20-C21-C22	2.01	130.10	127.28
31	B	622	SQD	O8-S-C6	2.01	109.86	105.97
25	C	507	CLA	CHC-C4B-NB	2.01	127.06	124.05
33	c	520	DGD	O4E-C4E-C5E	2.01	114.27	109.32
31	b	620	SQD	O8-S-C6	2.01	109.85	105.97
25	B	613	CLA	C2A-C1A-CHA	2.01	127.35	123.87
25	B	606	CLA	CHB-C1B-NB	2.01	127.06	124.05
32	D	408	LHG	O4-P-O5	2.01	121.78	112.44
25	B	608	CLA	CHB-C1B-NB	2.00	127.05	124.05
27	t	101	BCR	C2-C1-C6	2.00	113.35	110.44
25	b	608	CLA	CAC-C3C-C2C	2.00	131.23	127.56

All (2) chirality outliers are listed below:

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

All (1663) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	601	CLA	CBA-CGA-O2A-C1
25	B	601	CLA	O1A-CGA-O2A-C1
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C11-C10-C8-C9
25	D	402	CLA	C4-C3-C5-C6
25	D	402	CLA	C11-C12-C13-C14
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C3A-C2A-CAA-CBA
25	c	512	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
25	c	513	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	C11-C12-C13-C14
27	D	403	BCR	C23-C24-C25-C26
27	D	403	BCR	C23-C24-C25-C30
27	J	101	BCR	C1-C6-C7-C8
27	J	101	BCR	C5-C6-C7-C8
27	J	101	BCR	C21-C22-C23-C24
27	K	101	BCR	C7-C8-C9-C10
27	T	101	BCR	C23-C24-C25-C26
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C17-C18-C19-C20
27	k	102	BCR	C7-C8-C9-C10
27	k	102	BCR	C7-C8-C9-C34
28	A	612	PL9	C27-C28-C29-C30
28	A	612	PL9	C27-C28-C29-C31
28	D	404	PL9	C32-C33-C34-C36
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C24-C26-C27-C28
30	A	615	LMG	O6-C1-O1-C7
30	A	615	LMG	O9-C10-O7-C8
30	A	615	LMG	C11-C10-O7-C8
30	C	517	LMG	C2-C1-O1-C7
30	D	405	LMG	O6-C1-O1-C7
30	a	616	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
30	c	518	LMG	O1-C7-C8-O7
30	c	524	LMG	C2-C1-O1-C7
30	c	524	LMG	O6-C1-O1-C7
31	A	618	SQD	O5-C5-C6-S
31	B	622	SQD	C2-C1-O6-C44
31	B	622	SQD	O5-C1-O6-C44
31	B	622	SQD	O49-C7-O47-C45
31	D	407	SQD	C45-C44-O6-C1
31	D	407	SQD	C2-C1-O6-C44
31	D	407	SQD	O5-C1-O6-C44
31	a	615	SQD	O5-C5-C6-S
31	b	620	SQD	C8-C7-O47-C45
31	f	102	SQD	O5-C1-O6-C44
32	A	617	LHG	C3-O3-P-O4
32	A	617	LHG	C3-O3-P-O5
32	A	617	LHG	C3-O3-P-O6
32	D	408	LHG	O2-C2-C3-O3
32	D	408	LHG	C3-O3-P-O4
32	D	408	LHG	C3-O3-P-O5
32	D	408	LHG	C3-O3-P-O6
32	D	410	LHG	O1-C1-C2-C3
32	D	410	LHG	C3-O3-P-O4
32	D	410	LHG	C3-O3-P-O6
32	L	101	LHG	C4-O6-P-O4
32	a	613	LHG	O1-C1-C2-C3
32	a	613	LHG	C1-C2-C3-O3
32	d	407	LHG	C3-O3-P-O5
32	e	102	LHG	C3-O3-P-O5
32	e	102	LHG	C3-O3-P-O6
32	l	101	LHG	C4-O6-P-O3
32	l	101	LHG	C4-O6-P-O4
30	b	622	LMG	O10-C28-O8-C9
31	f	102	SQD	O10-C23-O48-C46
28	a	611	PL9	C47-C48-C49-C50
28	a	611	PL9	C47-C48-C49-C51
30	b	622	LMG	C29-C28-O8-C9
31	B	622	SQD	C24-C23-O48-C46
31	f	102	SQD	C24-C23-O48-C46
30	B	620	LMG	O10-C28-O8-C9
31	B	622	SQD	O10-C23-O48-C46
25	c	513	CLA	O1D-CGD-O2D-CED
25	C	512	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C3-C5-C6-C7
30	B	620	LMG	C29-C28-O8-C9
33	A	619	DGD	C2A-C1A-O1G-C1G
25	C	513	CLA	CBD-CGD-O2D-CED
31	B	622	SQD	C8-C7-O47-C45
25	A	610	CLA	C4-C3-C5-C6
25	B	603	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	a	609	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
28	A	612	PL9	C35-C34-C36-C37
28	A	612	PL9	C40-C39-C41-C42
28	d	405	PL9	C40-C39-C41-C42
25	A	610	CLA	C2-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	D	402	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
28	A	612	PL9	C13-C14-C16-C17
28	d	405	PL9	C38-C39-C41-C42
28	D	404	PL9	C47-C48-C49-C51
25	B	604	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
25	B	616	CLA	CBA-CGA-O2A-C1
31	D	407	SQD	C24-C23-O48-C46
28	A	612	PL9	C32-C33-C34-C36
25	B	616	CLA	O1A-CGA-O2A-C1
31	D	407	SQD	O10-C23-O48-C46
33	A	619	DGD	O1A-C1A-O1G-C1G
31	b	620	SQD	O49-C7-O47-C45
28	A	612	PL9	C47-C48-C49-C51
28	D	404	PL9	C47-C48-C49-C50
25	B	615	CLA	C3-C5-C6-C7
25	C	506	CLA	C3-C5-C6-C7
32	D	410	LHG	O2-C2-C3-O3
30	C	517	LMG	C29-C28-O8-C9
30	c	523	LMG	C11-C10-O7-C8
33	C	521	DGD	O6E-C5E-C6E-O5E
32	l	101	LHG	C7-C8-C9-C10
25	b	614	CLA	C4-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	A	612	PL9	C33-C34-C36-C37
28	A	612	PL9	C38-C39-C41-C42
28	a	611	PL9	C44-C46-C47-C48
33	A	619	DGD	O6E-C5E-C6E-O5E
31	b	620	SQD	C11-C10-C9-C8
30	C	517	LMG	O10-C28-O8-C9
31	b	620	SQD	C24-C23-O48-C46
30	D	406	LMG	C16-C17-C18-C19
32	a	613	LHG	C10-C11-C12-C13
32	D	410	LHG	C1-C2-C3-O3
32	d	407	LHG	C1-C2-C3-O3
30	c	523	LMG	C33-C34-C35-C36
33	c	520	DGD	C3B-C4B-C5B-C6B
29	d	409	STE	C5-C6-C7-C8
32	D	409	LHG	C24-C25-C26-C27
33	C	521	DGD	C2A-C3A-C4A-C5A
25	B	605	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	B	603	CLA	C2-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	a	609	CLA	C2-C3-C5-C6
28	A	612	PL9	C28-C29-C31-C32
25	B	616	CLA	C3-C5-C6-C7
25	B	605	CLA	C6-C7-C8-C9
25	B	613	CLA	C11-C12-C13-C14
25	B	615	CLA	C6-C7-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C10-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	b	607	CLA	C11-C10-C8-C9
25	b	610	CLA	C14-C13-C15-C16
25	c	504	CLA	C6-C7-C8-C9
25	c	512	CLA	C6-C7-C8-C9
30	D	405	LMG	C2-C1-O1-C7
31	f	102	SQD	C2-C1-O6-C44
31	b	620	SQD	C14-C15-C16-C17
32	a	613	LHG	O2-C2-C3-O3
27	J	101	BCR	C37-C22-C23-C24
27	K	101	BCR	C7-C8-C9-C34
27	T	101	BCR	C7-C8-C9-C34
27	k	101	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	K	102	STE	C11-C10-C9-C8
30	a	616	LMG	O7-C8-C9-O8
31	A	618	SQD	O6-C44-C45-O47
25	B	614	CLA	C13-C15-C16-C17
25	C	503	CLA	C5-C6-C7-C8
25	c	508	CLA	C8-C10-C11-C12
29	B	623	STE	C1-C2-C3-C4
25	C	513	CLA	O1D-CGD-O2D-CED
35	V	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C2C-C3C-CAC-CBC
25	b	616	CLA	CBD-CGD-O2D-CED
28	A	612	PL9	C32-C33-C34-C35
28	a	611	PL9	C32-C33-C34-C35
29	b	621	STE	C12-C13-C14-C15
25	B	613	CLA	C8-C10-C11-C12
25	b	601	CLA	CBD-CGD-O2D-CED
29	i	101	STE	C6-C7-C8-C9
25	B	611	CLA	C12-C13-C15-C16
25	B	613	CLA	C11-C10-C8-C7
25	b	602	CLA	C11-C12-C13-C15
25	b	606	CLA	C6-C7-C8-C10
30	a	616	LMG	C29-C28-O8-C9
28	a	611	PL9	C15-C14-C16-C17
31	a	614	SQD	C12-C13-C14-C15
25	B	615	CLA	C5-C6-C7-C8
30	c	523	LMG	O9-C10-O7-C8
30	c	522	LMG	O6-C5-C6-O5
28	A	612	PL9	C19-C21-C22-C23
28	A	612	PL9	C39-C41-C42-C43
29	K	102	STE	C6-C7-C8-C9
31	f	102	SQD	C25-C26-C27-C28
31	B	622	SQD	C45-C46-O48-C23
30	b	622	LMG	O6-C5-C6-O5
32	e	102	LHG	C27-C28-C29-C30
30	D	405	LMG	C28-C29-C30-C31
30	c	522	LMG	C28-C29-C30-C31
31	D	407	SQD	C23-C24-C25-C26
32	A	617	LHG	C7-C8-C9-C10
25	A	614	CLA	C13-C15-C16-C17
25	B	606	CLA	C13-C15-C16-C17
25	B	611	CLA	C8-C10-C11-C12
25	b	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	c	512	CLA	C2A-CAA-CBA-CGA
25	a	606	CLA	C15-C16-C17-C18
25	a	609	CLA	C5-C6-C7-C8
25	b	601	CLA	C13-C15-C16-C17
25	b	607	CLA	C5-C6-C7-C8
25	b	611	CLA	C8-C10-C11-C12
25	b	614	CLA	C10-C11-C12-C13
25	c	506	CLA	C13-C15-C16-C17
29	E	103	STE	C1-C2-C3-C4
30	m	101	LMG	C28-C29-C30-C31
31	A	616	SQD	C7-C8-C9-C10
32	a	613	LHG	C7-C8-C9-C10
33	c	521	DGD	C1A-C2A-C3A-C4A
32	D	409	LHG	C12-C13-C14-C15
25	A	614	CLA	C15-C16-C17-C18
25	B	605	CLA	C13-C15-C16-C17
25	b	605	CLA	C5-C6-C7-C8
25	b	605	CLA	C10-C11-C12-C13
25	b	606	CLA	C15-C16-C17-C18
25	b	607	CLA	C10-C11-C12-C13
25	b	614	CLA	C13-C15-C16-C17
25	c	505	CLA	C8-C10-C11-C12
30	D	405	LMG	C16-C17-C18-C19
31	a	615	SQD	C30-C31-C32-C33
33	C	523	DGD	CAB-CBB-CCB-CDB
32	d	407	LHG	O2-C2-C3-O3
25	c	510	CLA	CBD-CGD-O2D-CED
31	b	620	SQD	O10-C23-O48-C46
32	e	102	LHG	C7-C8-C9-C10
25	C	510	CLA	C10-C11-C12-C13
29	c	517	STE	C14-C15-C16-C17
30	m	101	LMG	C34-C35-C36-C37
31	b	620	SQD	C12-C13-C14-C15
25	c	513	CLA	C3-C5-C6-C7
25	B	601	CLA	C8-C10-C11-C12
25	C	501	CLA	CBD-CGD-O2D-CED
30	D	405	LMG	C10-C11-C12-C13
33	A	619	DGD	C1A-C2A-C3A-C4A
25	C	506	CLA	C8-C10-C11-C12
25	C	506	CLA	C13-C15-C16-C17
25	b	601	CLA	C8-C10-C11-C12
25	C	513	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	C	521	DGD	C4E-C5E-C6E-O5E
26	A	609	PHO	C2C-C3C-CAC-CBC
32	A	617	LHG	C8-C7-O7-C5
29	C	525	STE	C2-C3-C4-C5
33	C	523	DGD	C8A-C9A-CAA-CBA
30	a	616	LMG	O10-C28-O8-C9
25	c	512	CLA	C15-C16-C17-C18
29	d	409	STE	C7-C8-C9-C10
33	c	521	DGD	CAB-CBB-CCB-CDB
29	H	103	STE	C11-C10-C9-C8
32	L	101	LHG	C7-C8-C9-C10
32	A	617	LHG	O9-C7-O7-C5
32	D	408	LHG	C1-C2-C3-O3
25	B	606	CLA	C2A-CAA-CBA-CGA
25	c	506	CLA	CBA-CGA-O2A-C1
25	A	607	CLA	C13-C15-C16-C17
25	C	509	CLA	C13-C15-C16-C17
25	a	612	CLA	C15-C16-C17-C18
25	b	615	CLA	C5-C6-C7-C8
32	e	102	LHG	C25-C26-C27-C28
35	v	201	HEC	C4C-C3C-CAC-CBC
25	C	512	CLA	C10-C11-C12-C13
25	a	609	CLA	C13-C15-C16-C17
25	b	607	CLA	C8-C10-C11-C12
25	b	615	CLA	C13-C15-C16-C17
25	c	513	CLA	C13-C15-C16-C17
25	d	403	CLA	C15-C16-C17-C18
25	B	601	CLA	C5-C6-C7-C8
25	b	611	CLA	C13-C15-C16-C17
29	C	516	STE	C1-C2-C3-C4
30	a	616	LMG	C10-C11-C12-C13
25	C	504	CLA	C4-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
25	B	613	CLA	C10-C11-C12-C13
32	e	102	LHG	C8-C7-O7-C5
32	e	102	LHG	O9-C7-O7-C5
29	m	102	STE	C1-C2-C3-C4
28	a	611	PL9	C39-C41-C42-C43
25	A	606	CLA	C16-C17-C18-C20
25	c	511	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C19
25	b	608	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	C8-C10-C11-C12
27	B	619	BCR	C7-C8-C9-C34
27	H	101	BCR	C7-C8-C9-C34
35	V	201	HEC	C4C-C3C-CAC-CBC
32	A	617	LHG	O1-C1-C2-C3
32	d	408	LHG	C23-C24-C25-C26
31	b	620	SQD	C46-C45-O47-C7
25	B	614	CLA	C16-C17-C18-C20
25	C	510	CLA	C16-C17-C18-C19
31	a	615	SQD	C27-C28-C29-C30
25	c	506	CLA	O1A-CGA-O2A-C1
31	b	620	SQD	O5-C1-O6-C44
25	c	503	CLA	C10-C11-C12-C13
25	c	507	CLA	C2-C3-C5-C6
31	a	615	SQD	O6-C44-C45-O47
30	C	517	LMG	C28-C29-C30-C31
29	H	103	STE	C14-C15-C16-C17
25	b	614	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C20
25	C	513	CLA	O1A-CGA-O2A-C1
25	C	509	CLA	C10-C11-C12-C13
29	A	613	STE	C4-C5-C6-C7
29	m	103	STE	C6-C7-C8-C9
33	C	522	DGD	C5A-C6A-C7A-C8A
33	c	519	DGD	C3B-C4B-C5B-C6B
29	B	623	STE	C2-C3-C4-C5
29	H	103	STE	C6-C7-C8-C9
29	c	517	STE	C11-C10-C9-C8
29	c	517	STE	C9-C10-C11-C12
29	h	103	STE	C10-C11-C12-C13
29	j	102	STE	C10-C11-C12-C13
30	m	101	LMG	C35-C36-C37-C38
31	b	620	SQD	C11-C12-C13-C14
33	A	619	DGD	CEB-CFB-CGB-CHB
25	C	505	CLA	C15-C16-C17-C18
30	D	406	LMG	C12-C13-C14-C15
30	D	406	LMG	C13-C14-C15-C16
30	b	622	LMG	C29-C30-C31-C32
30	c	524	LMG	C17-C18-C19-C20
31	a	614	SQD	C31-C32-C33-C34
33	C	522	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
29	B	623	STE	C5-C6-C7-C8
29	E	103	STE	C3-C4-C5-C6
29	E	103	STE	C7-C8-C9-C10
29	E	103	STE	C11-C10-C9-C8
29	d	409	STE	C4-C5-C6-C7
29	e	101	STE	C11-C12-C13-C14
31	B	622	SQD	C33-C34-C35-C36
32	D	409	LHG	C29-C30-C31-C32
33	A	619	DGD	C8A-C9A-CAA-CBA
33	c	520	DGD	CBA-CCA-CDA-CEA
33	c	520	DGD	C7B-C8B-C9B-CAB
32	A	617	LHG	O1-C1-C2-O2
32	a	613	LHG	O1-C1-C2-O2
29	J	102	STE	C2-C3-C4-C5
30	A	615	LMG	C32-C33-C34-C35
30	D	405	LMG	C33-C34-C35-C36
32	D	409	LHG	C25-C26-C27-C28
33	c	519	DGD	C5B-C6B-C7B-C8B
25	b	602	CLA	C13-C15-C16-C17
30	M	101	LMG	C10-C11-C12-C13
31	a	614	SQD	C7-C8-C9-C10
29	A	622	STE	C10-C11-C12-C13
29	i	102	STE	C11-C10-C9-C8
29	m	103	STE	C3-C4-C5-C6
30	B	620	LMG	C33-C34-C35-C36
30	c	523	LMG	C30-C31-C32-C33
31	A	616	SQD	C29-C30-C31-C32
32	a	613	LHG	C17-C18-C19-C20
33	C	523	DGD	C5A-C6A-C7A-C8A
25	B	601	CLA	C16-C17-C18-C19
25	B	601	CLA	C16-C17-C18-C20
25	B	605	CLA	C16-C17-C18-C20
25	B	612	CLA	C16-C17-C18-C19
25	C	513	CLA	C16-C17-C18-C19
25	b	601	CLA	C16-C17-C18-C19
31	a	614	SQD	C25-C26-C27-C28
32	d	407	LHG	C13-C14-C15-C16
33	A	619	DGD	C2B-C1B-O2G-C2G
30	c	523	LMG	C31-C32-C33-C34
33	c	521	DGD	C4B-C5B-C6B-C7B
25	B	606	CLA	C6-C7-C8-C10
30	A	615	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	A	615	LMG	C35-C36-C37-C38
30	M	101	LMG	C13-C14-C15-C16
30	c	523	LMG	C34-C35-C36-C37
31	b	620	SQD	C15-C16-C17-C18
32	D	409	LHG	C13-C14-C15-C16
32	l	101	LHG	C34-C35-C36-C37
30	d	410	LMG	C28-C29-C30-C31
29	B	621	STE	C6-C7-C8-C9
29	k	103	STE	C7-C8-C9-C10
30	a	616	LMG	C36-C37-C38-C39
31	A	618	SQD	C10-C11-C12-C13
31	f	102	SQD	C28-C29-C30-C31
32	A	617	LHG	C28-C29-C30-C31
33	C	523	DGD	CBA-CCA-CDA-CEA
33	H	102	DGD	CCB-CDB-CEB-CFB
33	c	520	DGD	CBB-CCB-CDB-CEB
33	h	102	DGD	C2B-C3B-C4B-C5B
29	B	624	STE	C2-C3-C4-C5
29	M	104	STE	C9-C10-C11-C12
31	B	622	SQD	C16-C17-C18-C19
32	D	408	LHG	C11-C10-C9-C8
33	C	522	DGD	C9B-CAB-CBB-CCB
33	c	519	DGD	C3A-C4A-C5A-C6A
30	c	522	LMG	C36-C37-C38-C39
25	B	601	CLA	C13-C15-C16-C17
25	c	503	CLA	C15-C16-C17-C18
32	D	410	LHG	C13-C14-C15-C16
25	B	616	CLA	C11-C12-C13-C14
25	C	513	CLA	C16-C17-C18-C20
25	b	608	CLA	C16-C17-C18-C20
31	f	102	SQD	C27-C28-C29-C30
32	A	617	LHG	C32-C33-C34-C35
29	M	102	STE	C5-C6-C7-C8
29	c	516	STE	C7-C8-C9-C10
31	A	618	SQD	C16-C17-C18-C19
28	A	612	PL9	C24-C26-C27-C28
29	B	621	STE	C10-C11-C12-C13
30	c	522	LMG	C38-C39-C40-C41
33	c	521	DGD	C5A-C6A-C7A-C8A
29	C	526	STE	C4-C5-C6-C7
29	K	102	STE	C9-C10-C11-C12
29	m	103	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	c	523	LMG	C35-C36-C37-C38
30	m	101	LMG	C38-C39-C40-C41
32	a	613	LHG	C16-C17-C18-C19
33	C	521	DGD	C8B-C9B-CAB-CBB
33	H	102	DGD	C4B-C5B-C6B-C7B
33	A	619	DGD	C2B-C3B-C4B-C5B
33	C	522	DGD	CBA-CCA-CDA-CEA
29	D	411	STE	C12-C13-C14-C15
29	H	103	STE	C4-C5-C6-C7
30	c	523	LMG	C15-C16-C17-C18
31	A	616	SQD	C15-C16-C17-C18
29	J	102	STE	C5-C6-C7-C8
29	b	621	STE	C3-C4-C5-C6
29	b	621	STE	C14-C15-C16-C17
30	B	620	LMG	C32-C33-C34-C35
30	M	101	LMG	C38-C39-C40-C41
30	d	410	LMG	C39-C40-C41-C42
30	m	101	LMG	C12-C13-C14-C15
31	A	616	SQD	C30-C31-C32-C33
32	d	407	LHG	C18-C19-C20-C21
25	B	614	CLA	C16-C17-C18-C19
25	a	609	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
25	c	509	CLA	C16-C17-C18-C20
27	B	617	BCR	C1-C6-C7-C8
27	B	617	BCR	C5-C6-C7-C8
27	H	101	BCR	C5-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C23-C24-C25-C26
29	B	623	STE	C10-C11-C12-C13
29	e	104	STE	C3-C4-C5-C6
32	D	408	LHG	C14-C15-C16-C17
33	c	519	DGD	C7B-C8B-C9B-CAB
33	c	521	DGD	C4A-C5A-C6A-C7A
32	D	410	LHG	C17-C18-C19-C20
33	C	522	DGD	CCB-CDB-CEB-CFB
29	B	623	STE	C9-C10-C11-C12
29	C	527	STE	C14-C15-C16-C17
30	b	622	LMG	C21-C22-C23-C24
32	D	410	LHG	C29-C30-C31-C32
32	D	410	LHG	C31-C32-C33-C34
33	c	519	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
29	c	517	STE	C7-C8-C9-C10
31	a	615	SQD	C9-C10-C11-C12
31	f	102	SQD	C29-C30-C31-C32
32	d	407	LHG	C11-C10-C9-C8
33	h	102	DGD	CAA-CBA-CCA-CDA
33	h	102	DGD	C6B-C7B-C8B-C9B
33	A	619	DGD	O1B-C1B-O2G-C2G
32	D	410	LHG	C11-C12-C13-C14
33	C	523	DGD	C3B-C4B-C5B-C6B
25	C	506	CLA	C15-C16-C17-C18
25	c	507	CLA	C5-C6-C7-C8
25	B	612	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C19
29	B	623	STE	C4-C5-C6-C7
29	B	625	STE	C11-C10-C9-C8
29	c	517	STE	C12-C13-C14-C15
29	m	102	STE	C2-C3-C4-C5
32	l	101	LHG	C10-C11-C12-C13
33	h	102	DGD	CCA-CDA-CEA-CFA
33	h	102	DGD	C5B-C6B-C7B-C8B
25	B	606	CLA	C11-C12-C13-C14
25	B	606	CLA	C14-C13-C15-C16
25	C	502	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C12-C13-C14
29	C	520	STE	C5-C6-C7-C8
29	X	101	STE	C4-C5-C6-C7
29	d	411	STE	C2-C3-C4-C5
30	A	615	LMG	C33-C34-C35-C36
30	D	406	LMG	C30-C31-C32-C33
31	A	616	SQD	C16-C17-C18-C19
31	D	407	SQD	C25-C26-C27-C28
32	d	408	LHG	C24-C25-C26-C27
29	C	516	STE	C11-C10-C9-C8
29	M	102	STE	C2-C3-C4-C5
30	c	524	LMG	C32-C33-C34-C35
31	A	618	SQD	C11-C12-C13-C14
31	D	407	SQD	C31-C32-C33-C34
33	C	521	DGD	CCA-CDA-CEA-CFA
29	B	621	STE	C3-C4-C5-C6
30	B	620	LMG	C31-C32-C33-C34
32	D	410	LHG	C25-C26-C27-C28
32	l	101	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	B	614	CLA	C8-C10-C11-C12
25	c	503	CLA	C8-C10-C11-C12
29	j	101	STE	C4-C5-C6-C7
31	a	615	SQD	C31-C32-C33-C34
30	M	101	LMG	C12-C13-C14-C15
32	l	101	LHG	C11-C12-C13-C14
33	C	522	DGD	C6B-C7B-C8B-C9B
29	A	613	STE	C3-C4-C5-C6
29	X	101	STE	C7-C8-C9-C10
30	D	405	LMG	C30-C31-C32-C33
33	C	521	DGD	C4B-C5B-C6B-C7B
31	f	102	SQD	C8-C7-O47-C45
30	c	524	LMG	C10-C11-C12-C13
30	a	616	LMG	C29-C30-C31-C32
30	c	524	LMG	C36-C37-C38-C39
30	A	615	LMG	C40-C41-C42-C43
30	D	406	LMG	C22-C23-C24-C25
29	A	620	STE	C12-C13-C14-C15
31	A	616	SQD	C33-C34-C35-C36
31	B	622	SQD	C13-C14-C15-C16
32	A	617	LHG	C13-C14-C15-C16
33	H	102	DGD	C7A-C8A-C9A-CAA
33	C	522	DGD	CDB-CEB-CFB-CGB
25	A	607	CLA	C15-C16-C17-C18
25	c	509	CLA	C10-C11-C12-C13
33	H	102	DGD	C3B-C4B-C5B-C6B
29	c	517	STE	C10-C11-C12-C13
32	D	409	LHG	C15-C16-C17-C18
25	d	403	CLA	C3-C5-C6-C7
30	a	616	LMG	C8-C7-O1-C1
33	C	522	DGD	C2G-C3G-O3G-C1D
33	C	522	DGD	C5D-C6D-O5D-C1E
29	M	104	STE	C10-C11-C12-C13
29	j	101	STE	C5-C6-C7-C8
32	D	408	LHG	C11-C12-C13-C14
32	a	613	LHG	C14-C15-C16-C17
25	B	610	CLA	C16-C17-C18-C20
25	B	616	CLA	C11-C12-C13-C15
25	a	609	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C19
29	C	520	STE	C6-C7-C8-C9
29	M	102	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	c	516	STE	C2-C3-C4-C5
29	c	516	STE	C5-C6-C7-C8
30	a	616	LMG	C12-C13-C14-C15
31	A	616	SQD	C26-C27-C28-C29
31	B	622	SQD	C11-C10-C9-C8
33	C	523	DGD	C4B-C5B-C6B-C7B
33	c	519	DGD	C6A-C7A-C8A-C9A
29	I	101	STE	C11-C10-C9-C8
29	J	102	STE	C6-C7-C8-C9
29	M	103	STE	C6-C7-C8-C9
29	m	103	STE	C11-C10-C9-C8
25	C	512	CLA	C8-C10-C11-C12
29	T	102	STE	C4-C5-C6-C7
30	c	523	LMG	C32-C33-C34-C35
32	d	408	LHG	C30-C31-C32-C33
29	k	103	STE	C5-C6-C7-C8
32	l	101	LHG	C16-C17-C18-C19
33	c	520	DGD	CAA-CBA-CCA-CDA
25	B	609	CLA	C13-C15-C16-C17
25	c	512	CLA	C13-C15-C16-C17
30	M	101	LMG	C37-C38-C39-C40
33	A	619	DGD	C4E-C5E-C6E-O5E
29	A	621	STE	C11-C12-C13-C14
33	C	521	DGD	C5B-C6B-C7B-C8B
32	e	102	LHG	O6-C4-C5-O7
31	A	616	SQD	C11-C12-C13-C14
31	f	102	SQD	C30-C31-C32-C33
32	e	102	LHG	C11-C12-C13-C14
33	c	519	DGD	C2A-C3A-C4A-C5A
33	h	102	DGD	C7A-C8A-C9A-CAA
28	A	612	PL9	C34-C36-C37-C38
25	D	402	CLA	C5-C6-C7-C8
25	A	606	CLA	C16-C17-C18-C19
25	B	605	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C20
30	B	620	LMG	C29-C30-C31-C32
32	d	407	LHG	C33-C34-C35-C36
33	c	521	DGD	C8B-C9B-CAB-CBB
29	b	621	STE	C1-C2-C3-C4
31	A	616	SQD	C23-C24-C25-C26
33	C	522	DGD	C1B-C2B-C3B-C4B
29	b	625	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	c	517	STE	C3-C4-C5-C6
30	c	524	LMG	C39-C40-C41-C42
32	a	613	LHG	C18-C19-C20-C21
33	c	520	DGD	C9B-CAB-CBB-CCB
31	B	622	SQD	O6-C44-C45-O47
33	A	619	DGD	O2G-C2G-C3G-O3G
29	A	622	STE	C13-C14-C15-C16
29	E	103	STE	C13-C14-C15-C16
32	d	408	LHG	C25-C26-C27-C28
30	C	524	LMG	C30-C31-C32-C33
30	M	101	LMG	C17-C18-C19-C20
30	c	523	LMG	C13-C14-C15-C16
31	a	614	SQD	C27-C28-C29-C30
32	D	410	LHG	C28-C29-C30-C31
32	a	613	LHG	C12-C13-C14-C15
32	a	613	LHG	C30-C31-C32-C33
33	c	521	DGD	C3A-C4A-C5A-C6A
25	a	607	CLA	C15-C16-C17-C18
33	c	519	DGD	C8A-C9A-CAA-CBA
29	i	101	STE	C3-C4-C5-C6
30	A	615	LMG	C12-C13-C14-C15
32	L	101	LHG	C17-C18-C19-C20
32	l	101	LHG	C27-C28-C29-C30
33	C	522	DGD	C7B-C8B-C9B-CAB
33	c	519	DGD	C7A-C8A-C9A-CAA
30	d	410	LMG	O6-C5-C6-O5
33	h	102	DGD	CDB-CEB-CFB-CGB
28	A	612	PL9	C47-C48-C49-C50
29	A	621	STE	C10-C11-C12-C13
31	B	622	SQD	C25-C26-C27-C28
32	a	613	LHG	C29-C30-C31-C32
29	b	624	STE	C4-C5-C6-C7
29	d	409	STE	C14-C15-C16-C17
31	A	616	SQD	C11-C10-C9-C8
32	l	101	LHG	C15-C16-C17-C18
29	D	411	STE	C14-C15-C16-C17
29	Z	101	STE	C11-C12-C13-C14
32	A	617	LHG	C17-C18-C19-C20
33	C	521	DGD	CBA-CCA-CDA-CEA
25	C	504	CLA	C11-C12-C13-C14
25	B	612	CLA	C10-C11-C12-C13
25	C	512	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	T	102	STE	C11-C12-C13-C14
29	d	406	STE	C7-C8-C9-C10
30	d	410	LMG	C38-C39-C40-C41
32	d	407	LHG	C10-C11-C12-C13
32	l	101	LHG	C29-C30-C31-C32
33	c	520	DGD	CAB-CBB-CCB-CDB
30	m	101	LMG	C31-C32-C33-C34
25	c	513	CLA	C1A-C2A-CAA-CBA
25	c	510	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	C8-C10-C11-C12
25	D	401	CLA	C15-C16-C17-C18
31	B	622	SQD	C24-C25-C26-C27
25	b	616	CLA	O1D-CGD-O2D-CED
29	I	102	STE	C6-C7-C8-C9
29	M	104	STE	C11-C12-C13-C14
29	C	527	STE	C12-C13-C14-C15
29	Z	101	STE	C5-C6-C7-C8
29	d	411	STE	C5-C6-C7-C8
30	B	620	LMG	C14-C15-C16-C17
32	A	617	LHG	C29-C30-C31-C32
25	c	509	CLA	C13-C15-C16-C17
25	B	604	CLA	C6-C7-C8-C10
25	B	612	CLA	C12-C13-C15-C16
25	B	614	CLA	C12-C13-C15-C16
25	C	505	CLA	C12-C13-C15-C16
25	C	507	CLA	C11-C12-C13-C15
25	C	508	CLA	C11-C10-C8-C7
25	a	609	CLA	C6-C7-C8-C10
25	b	601	CLA	C11-C12-C13-C15
25	b	605	CLA	C11-C10-C8-C7
25	b	607	CLA	C6-C7-C8-C10
25	c	503	CLA	C6-C7-C8-C10
25	c	504	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	510	CLA	C11-C10-C8-C7
25	c	513	CLA	C12-C13-C15-C16
33	c	519	DGD	C8B-C9B-CAB-CBB
33	c	520	DGD	C8A-C9A-CAA-CBA
25	B	615	CLA	C16-C17-C18-C20
29	d	406	STE	C4-C5-C6-C7
31	a	614	SQD	C18-C19-C20-C21
33	C	521	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C8-C10-C11-C12
25	C	513	CLA	C13-C15-C16-C17
29	b	625	STE	C13-C14-C15-C16
32	l	101	LHG	C17-C18-C19-C20
28	d	405	PL9	C28-C29-C31-C32
32	l	101	LHG	C11-C10-C9-C8
25	B	602	CLA	C13-C15-C16-C17
25	c	505	CLA	C10-C11-C12-C13
25	B	604	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	C	508	CLA	C11-C10-C8-C9
25	C	511	CLA	C6-C7-C8-C9
25	b	604	CLA	C14-C13-C15-C16
25	b	607	CLA	C6-C7-C8-C9
25	b	614	CLA	C11-C12-C13-C14
25	c	504	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C10-C8-C9
25	c	510	CLA	C11-C10-C8-C9
25	c	513	CLA	C14-C13-C15-C16
29	C	520	STE	C7-C8-C9-C10
29	T	102	STE	C9-C10-C11-C12
31	a	614	SQD	C33-C34-C35-C36
33	C	523	DGD	C3A-C4A-C5A-C6A
29	T	102	STE	C5-C6-C7-C8
29	f	103	STE	C15-C16-C17-C18
33	c	519	DGD	C4A-C5A-C6A-C7A
29	m	102	STE	C6-C7-C8-C9
30	a	616	LMG	C22-C23-C24-C25
30	B	620	LMG	O6-C5-C6-O5
30	a	616	LMG	C7-C8-C9-O8
31	A	618	SQD	O6-C44-C45-C46
31	a	614	SQD	C44-C45-C46-O48
31	a	615	SQD	O6-C44-C45-C46
33	A	619	DGD	C1G-C2G-C3G-O3G
29	K	102	STE	C7-C8-C9-C10
33	A	619	DGD	CAA-CBA-CCA-CDA
29	C	526	STE	C5-C6-C7-C8
29	d	411	STE	C3-C4-C5-C6
33	c	519	DGD	C9A-CAA-CBA-CCA
25	A	606	CLA	C15-C16-C17-C18
25	a	609	CLA	C10-C11-C12-C13
25	d	403	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	t	102	STE	C3-C4-C5-C6
31	b	620	SQD	C17-C18-C19-C20
32	d	408	LHG	C32-C33-C34-C35
30	D	406	LMG	O6-C5-C6-O5
33	c	519	DGD	O6E-C5E-C6E-O5E
25	C	510	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C19
25	b	607	CLA	C16-C17-C18-C20
29	a	617	STE	C5-C6-C7-C8
29	b	621	STE	C11-C12-C13-C14
29	b	623	STE	C11-C10-C9-C8
30	M	101	LMG	C30-C31-C32-C33
29	E	103	STE	C14-C15-C16-C17
32	D	410	LHG	C24-C25-C26-C27
33	C	521	DGD	C5A-C6A-C7A-C8A
33	C	522	DGD	C8B-C9B-CAB-CBB
25	C	507	CLA	C5-C6-C7-C8
25	c	503	CLA	C5-C6-C7-C8
29	t	102	STE	C11-C10-C9-C8
30	M	101	LMG	C18-C19-C20-C21
31	f	102	SQD	C26-C27-C28-C29
33	H	102	DGD	C5B-C6B-C7B-C8B
29	C	526	STE	C7-C8-C9-C10
30	m	101	LMG	C14-C15-C16-C17
28	d	405	PL9	C13-C14-C16-C17
31	a	615	SQD	C34-C35-C36-C37
29	h	103	STE	C11-C12-C13-C14
30	c	523	LMG	O6-C5-C6-O5
25	c	513	CLA	C8-C10-C11-C12
29	b	625	STE	C11-C12-C13-C14
31	b	620	SQD	C18-C19-C20-C21
33	C	521	DGD	C4D-C5D-C6D-O5D
32	D	410	LHG	C7-C8-C9-C10
29	C	527	STE	C9-C10-C11-C12
29	I	102	STE	C5-C6-C7-C8
29	M	104	STE	C13-C14-C15-C16
30	b	622	LMG	C39-C40-C41-C42
33	c	521	DGD	C6B-C7B-C8B-C9B
29	T	102	STE	C6-C7-C8-C9
29	d	406	STE	C5-C6-C7-C8
29	i	101	STE	C4-C5-C6-C7
31	B	622	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	A	621	STE	C13-C14-C15-C16
29	c	516	STE	C9-C10-C11-C12
29	c	517	STE	C13-C14-C15-C16
30	A	615	LMG	C31-C32-C33-C34
31	A	618	SQD	C11-C10-C9-C8
31	a	614	SQD	C11-C12-C13-C14
32	a	613	LHG	C25-C26-C27-C28
32	d	407	LHG	C9-C10-C11-C12
27	t	101	BCR	C13-C14-C15-C16
30	B	620	LMG	C34-C35-C36-C37
31	D	407	SQD	C33-C34-C35-C36
29	d	411	STE	C7-C8-C9-C10
29	A	622	STE	C15-C16-C17-C18
29	J	102	STE	C4-C5-C6-C7
25	b	608	CLA	C4C-C3C-CAC-CBC
25	C	510	CLA	C2-C3-C5-C6
28	a	611	PL9	C43-C44-C46-C47
31	A	618	SQD	C9-C10-C11-C12
31	A	618	SQD	C14-C15-C16-C17
25	b	601	CLA	C16-C17-C18-C20
29	b	621	STE	C11-C10-C9-C8
30	a	616	LMG	C35-C36-C37-C38
30	c	524	LMG	C12-C13-C14-C15
32	D	408	LHG	C28-C29-C30-C31
33	A	619	DGD	C2A-C3A-C4A-C5A
29	e	101	STE	C15-C16-C17-C18
30	M	101	LMG	C40-C41-C42-C43
30	c	524	LMG	C28-C29-C30-C31
29	B	623	STE	C6-C7-C8-C9
29	d	409	STE	C9-C10-C11-C12
29	k	103	STE	C6-C7-C8-C9
31	D	407	SQD	C27-C28-C29-C30
30	D	405	LMG	O7-C8-C9-O8
31	a	614	SQD	O47-C45-C46-O48
33	A	619	DGD	CFB-CGB-CHB-CIB
30	c	522	LMG	C29-C30-C31-C32
29	j	102	STE	C3-C4-C5-C6
33	c	519	DGD	CDA-CEA-CFA-CGA
30	C	524	LMG	C15-C16-C17-C18
30	c	523	LMG	C36-C37-C38-C39
33	H	102	DGD	CDA-CEA-CFA-CGA
30	m	101	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
32	d	407	LHG	C14-C15-C16-C17
32	d	407	LHG	C17-C18-C19-C20
25	C	509	CLA	C3-C5-C6-C7
31	f	102	SQD	C32-C33-C34-C35
32	D	409	LHG	C35-C36-C37-C38
32	a	613	LHG	C19-C20-C21-C22
31	f	102	SQD	O49-C7-O47-C45
29	c	516	STE	C6-C7-C8-C9
29	A	620	STE	C11-C12-C13-C14
29	B	625	STE	C9-C10-C11-C12
25	C	512	CLA	C15-C16-C17-C18
31	A	616	SQD	C24-C25-C26-C27
33	c	521	DGD	C6A-C7A-C8A-C9A
33	H	102	DGD	O2G-C1B-C2B-C3B
30	D	405	LMG	C13-C14-C15-C16
33	h	102	DGD	C7B-C8B-C9B-CAB
25	c	509	CLA	C3-C5-C6-C7
29	b	621	STE	C7-C8-C9-C10
31	a	614	SQD	C24-C25-C26-C27
29	T	102	STE	C3-C4-C5-C6
29	b	623	STE	C1-C2-C3-C4
25	C	513	CLA	C8-C10-C11-C12
25	b	614	CLA	C8-C10-C11-C12
25	b	609	CLA	C16-C17-C18-C20
29	Z	101	STE	C11-C10-C9-C8
25	C	510	CLA	C4-C3-C5-C6
29	X	101	STE	C9-C10-C11-C12
32	A	617	LHG	C14-C15-C16-C17
29	t	103	STE	C7-C8-C9-C10
29	A	622	STE	C14-C15-C16-C17
29	I	101	STE	C2-C3-C4-C5
30	D	405	LMG	C32-C33-C34-C35
30	d	410	LMG	C34-C35-C36-C37
30	m	101	LMG	C37-C38-C39-C40
25	B	611	CLA	C11-C12-C13-C14
25	B	612	CLA	C14-C13-C15-C16
25	B	614	CLA	C14-C13-C15-C16
25	C	505	CLA	C14-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C9
25	a	609	CLA	C14-C13-C15-C16
25	b	601	CLA	C11-C12-C13-C14
25	b	607	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C11-C12-C13-C14
29	M	104	STE	C5-C6-C7-C8
32	e	102	LHG	C26-C27-C28-C29
33	C	522	DGD	C8A-C9A-CAA-CBA
25	C	509	CLA	C8-C10-C11-C12
25	b	610	CLA	C15-C16-C17-C18
25	b	616	CLA	C10-C11-C12-C13
25	c	506	CLA	C15-C16-C17-C18
25	B	615	CLA	C4B-C3B-CAB-CBB
25	C	502	CLA	C4B-C3B-CAB-CBB
25	d	402	CLA	C4B-C3B-CAB-CBB
31	b	620	SQD	C29-C30-C31-C32
32	d	408	LHG	C27-C28-C29-C30
25	b	601	CLA	O1D-CGD-O2D-CED
31	a	614	SQD	C26-C27-C28-C29
25	b	609	CLA	C13-C15-C16-C17
29	J	102	STE	C7-C8-C9-C10
30	b	622	LMG	C19-C20-C21-C22
28	A	612	PL9	C42-C43-C44-C46
29	D	411	STE	C13-C14-C15-C16
29	z	101	STE	C2-C3-C4-C5
30	M	101	LMG	C15-C16-C17-C18
32	a	613	LHG	C13-C14-C15-C16
33	C	523	DGD	C6A-C7A-C8A-C9A
33	C	523	DGD	C6B-C7B-C8B-C9B
29	M	104	STE	C12-C13-C14-C15
29	b	624	STE	C5-C6-C7-C8
31	D	407	SQD	C24-C25-C26-C27
32	L	101	LHG	C35-C36-C37-C38
32	e	102	LHG	O6-C4-C5-C6
29	B	621	STE	C11-C10-C9-C8
29	b	623	STE	C11-C12-C13-C14
30	m	101	LMG	C22-C23-C24-C25
25	B	615	CLA	C6-C7-C8-C10
25	C	506	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C7
25	C	511	CLA	C6-C7-C8-C10
25	C	512	CLA	C11-C10-C8-C7
25	D	402	CLA	C11-C12-C13-C15
25	a	607	CLA	C12-C13-C15-C16
25	a	609	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C12-C13-C15-C16
25	b	606	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C15
25	b	614	CLA	C11-C12-C13-C15
25	c	506	CLA	C11-C10-C8-C7
33	h	102	DGD	C9B-CAB-CBB-CCB
25	B	604	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	CBD-CGD-O2D-CED
29	B	623	STE	C13-C14-C15-C16
29	e	104	STE	C11-C10-C9-C8
30	c	518	LMG	C11-C12-C13-C14
25	B	601	CLA	C3A-C2A-CAA-CBA
28	a	611	PL9	C45-C44-C46-C47
25	b	611	CLA	C15-C16-C17-C18
33	c	519	DGD	O6D-C5D-C6D-O5D
32	d	407	LHG	C11-C12-C13-C14
29	I	102	STE	C9-C10-C11-C12
29	C	519	STE	C4-C5-C6-C7
29	E	102	STE	C11-C10-C9-C8
29	z	101	STE	C4-C5-C6-C7
25	d	402	CLA	C16-C17-C18-C20
32	D	408	LHG	C12-C13-C14-C15
29	A	621	STE	C3-C4-C5-C6
33	H	102	DGD	C6B-C7B-C8B-C9B
29	E	103	STE	C12-C13-C14-C15
30	m	101	LMG	C36-C37-C38-C39
29	A	621	STE	C9-C10-C11-C12
32	D	408	LHG	C34-C35-C36-C37
32	L	101	LHG	C26-C27-C28-C29
30	C	517	LMG	C7-C8-C9-O8
30	b	622	LMG	C7-C8-C9-O8
31	B	622	SQD	O6-C44-C45-C46
31	b	620	SQD	C44-C45-C46-O48
32	D	409	LHG	C17-C18-C19-C20
30	a	616	LMG	C40-C41-C42-C43
29	H	103	STE	C15-C16-C17-C18
29	f	103	STE	C11-C12-C13-C14
29	j	101	STE	C2-C3-C4-C5
31	f	102	SQD	C34-C35-C36-C37
30	c	518	LMG	O1-C7-C8-C9
33	c	521	DGD	CDA-CEA-CFA-CGA
30	A	615	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	c	524	LMG	C19-C20-C21-C22
33	h	102	DGD	C8B-C9B-CAB-CBB
25	B	607	CLA	C3-C5-C6-C7
25	B	610	CLA	C15-C16-C17-C18
25	d	402	CLA	C16-C17-C18-C19
29	B	625	STE	C12-C13-C14-C15
30	c	522	LMG	C40-C41-C42-C43
29	I	101	STE	C7-C8-C9-C10
29	M	102	STE	C3-C4-C5-C6
29	b	624	STE	C3-C4-C5-C6
30	C	524	LMG	C32-C33-C34-C35
25	C	501	CLA	O1D-CGD-O2D-CED
27	T	101	BCR	C5-C6-C7-C8
29	j	102	STE	C11-C10-C9-C8
30	C	524	LMG	C39-C40-C41-C42
30	m	101	LMG	C15-C16-C17-C18
31	A	616	SQD	C25-C26-C27-C28
32	D	409	LHG	C30-C31-C32-C33
29	A	621	STE	C2-C3-C4-C5
30	c	522	LMG	C12-C13-C14-C15
31	A	616	SQD	C13-C14-C15-C16
29	C	516	STE	C5-C6-C7-C8
29	d	409	STE	C11-C12-C13-C14
32	e	102	LHG	C12-C13-C14-C15
29	h	103	STE	C12-C13-C14-C15
31	D	407	SQD	C34-C35-C36-C37
32	D	409	LHG	C33-C34-C35-C36
25	B	615	CLA	C16-C17-C18-C19
32	D	410	LHG	C23-C24-C25-C26
25	B	615	CLA	C10-C11-C12-C13
31	b	620	SQD	O47-C45-C46-O48
32	e	102	LHG	O7-C5-C6-O8
28	A	612	PL9	C4-C3-C7-C8
28	a	611	PL9	C4-C3-C7-C8
29	X	101	STE	C10-C11-C12-C13
32	D	409	LHG	C27-C28-C29-C30
30	D	406	LMG	C10-C11-C12-C13
33	c	519	DGD	CDB-CEB-CFB-CGB
28	d	405	PL9	C30-C29-C31-C32
29	A	620	STE	C13-C14-C15-C16
29	B	625	STE	C7-C8-C9-C10
32	D	408	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
32	L	101	LHG	C11-C10-C9-C8
29	e	101	STE	C14-C15-C16-C17
31	a	614	SQD	C9-C10-C11-C12
25	c	509	CLA	C16-C17-C18-C19
29	T	102	STE	C10-C11-C12-C13
29	h	103	STE	C14-C15-C16-C17
30	A	615	LMG	C14-C15-C16-C17
30	a	616	LMG	C39-C40-C41-C42
33	c	521	DGD	C2A-C3A-C4A-C5A
25	A	614	CLA	C14-C13-C15-C16
25	B	604	CLA	C11-C10-C8-C9
25	B	606	CLA	C11-C10-C8-C9
25	D	402	CLA	C14-C13-C15-C16
25	a	607	CLA	C14-C13-C15-C16
25	a	609	CLA	C6-C7-C8-C9
25	b	608	CLA	C11-C12-C13-C14
25	b	616	CLA	C11-C10-C8-C9
25	c	512	CLA	C11-C12-C13-C14
29	z	101	STE	C3-C4-C5-C6
33	A	619	DGD	C6A-C7A-C8A-C9A
25	B	610	CLA	C16-C17-C18-C19
31	a	615	SQD	C10-C11-C12-C13
31	A	618	SQD	C17-C18-C19-C20
29	Z	101	STE	C9-C10-C11-C12
30	c	524	LMG	C40-C41-C42-C43
32	D	408	LHG	C18-C19-C20-C21
25	c	504	CLA	C11-C12-C13-C15
30	a	616	LMG	C11-C10-O7-C8
30	b	622	LMG	C11-C10-O7-C8
25	C	505	CLA	C10-C11-C12-C13
29	J	102	STE	C1-C2-C3-C4
29	C	519	STE	C2-C3-C4-C5
29	K	102	STE	C10-C11-C12-C13
30	D	406	LMG	C17-C18-C19-C20
33	C	522	DGD	CAB-CBB-CCB-CDB
33	h	102	DGD	O2G-C1B-C2B-C3B
25	B	606	CLA	C8-C10-C11-C12
29	K	102	STE	C5-C6-C7-C8
25	b	608	CLA	C16-C17-C18-C19
29	c	517	STE	C6-C7-C8-C9
30	B	620	LMG	C15-C16-C17-C18
25	b	605	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	b	620	SQD	C16-C17-C18-C19
25	A	607	CLA	C11-C10-C8-C7
25	B	602	CLA	C11-C12-C13-C15
25	B	613	CLA	C11-C12-C13-C15
25	B	615	CLA	C11-C12-C13-C15
25	C	507	CLA	C11-C10-C8-C7
25	C	513	CLA	C11-C10-C8-C7
25	D	402	CLA	C12-C13-C15-C16
25	b	603	CLA	C6-C7-C8-C10
25	b	603	CLA	C11-C10-C8-C7
25	b	608	CLA	C11-C12-C13-C15
25	b	614	CLA	C11-C10-C8-C7
25	b	616	CLA	C11-C10-C8-C7
25	c	507	CLA	C11-C12-C13-C15
31	A	616	SQD	C9-C10-C11-C12
31	a	615	SQD	C11-C10-C9-C8
33	c	521	DGD	C5B-C6B-C7B-C8B
29	m	102	STE	C7-C8-C9-C10
29	d	411	STE	C6-C7-C8-C9
31	D	407	SQD	C29-C30-C31-C32
32	l	101	LHG	C26-C27-C28-C29
29	B	621	STE	C12-C13-C14-C15
27	B	619	BCR	C7-C8-C9-C10
27	H	101	BCR	C7-C8-C9-C10
27	T	101	BCR	C7-C8-C9-C10
27	k	101	BCR	C21-C22-C23-C24
30	M	101	LMG	C29-C28-O8-C9
30	c	522	LMG	C29-C28-O8-C9
30	c	522	LMG	C39-C40-C41-C42
33	H	102	DGD	C2B-C3B-C4B-C5B
33	c	520	DGD	C2G-C3G-O3G-C1D
33	c	520	DGD	C5D-C6D-O5D-C1E
31	A	618	SQD	C7-C8-C9-C10
33	c	520	DGD	C1A-C2A-C3A-C4A
25	b	602	CLA	C16-C17-C18-C20
30	b	622	LMG	O9-C10-O7-C8
30	a	616	LMG	C15-C16-C17-C18
30	c	518	LMG	C30-C31-C32-C33
28	d	405	PL9	C45-C44-C46-C47
25	B	616	CLA	C5-C6-C7-C8
25	b	601	CLA	C10-C11-C12-C13
31	A	616	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	h	102	DGD	C1A-C2A-C3A-C4A
29	K	102	STE	C11-C12-C13-C14
30	a	616	LMG	C9-C8-O7-C10
25	b	609	CLA	C16-C17-C18-C19
29	A	622	STE	C11-C10-C9-C8
29	m	103	STE	C14-C15-C16-C17
31	A	616	SQD	C34-C35-C36-C37
31	D	407	SQD	C32-C33-C34-C35
30	B	620	LMG	C17-C18-C19-C20
32	A	617	LHG	C12-C13-C14-C15
33	C	521	DGD	O6E-C1E-O5D-C6D
33	C	522	DGD	O6E-C1E-O5D-C6D
32	e	102	LHG	C4-C5-C6-O8
30	b	622	LMG	C10-C11-C12-C13
25	C	502	CLA	C13-C15-C16-C17
34	F	101	HEM	C4C-C3C-CAC-CBC
34	f	101	HEM	C4B-C3B-CAB-CBB
34	f	101	HEM	C4C-C3C-CAC-CBC
29	E	101	STE	C3-C4-C5-C6
28	d	405	PL9	C15-C14-C16-C17
33	C	522	DGD	CDA-CEA-CFA-CGA
32	a	613	LHG	C23-C24-C25-C26
35	V	201	HEC	C2B-C3B-CAB-CBB
25	B	602	CLA	C8-C10-C11-C12
25	B	612	CLA	C8-C10-C11-C12
25	d	403	CLA	C10-C11-C12-C13
29	i	101	STE	C5-C6-C7-C8
30	m	101	LMG	C30-C31-C32-C33
30	b	622	LMG	O7-C8-C9-O8
31	A	616	SQD	O6-C44-C45-O47
25	B	610	CLA	C14-C13-C15-C16
25	C	513	CLA	C11-C10-C8-C9
25	a	607	CLA	C11-C12-C13-C14
25	b	601	CLA	C14-C13-C15-C16
25	b	603	CLA	C6-C7-C8-C9
25	b	614	CLA	C11-C10-C8-C9
25	c	507	CLA	C14-C13-C15-C16
25	c	508	CLA	C14-C13-C15-C16
25	c	511	CLA	C14-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C9
29	M	104	STE	C14-C15-C16-C17
30	A	615	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
30	D	406	LMG	C11-C12-C13-C14
30	D	406	LMG	C21-C22-C23-C24
32	d	408	LHG	C31-C32-C33-C34
29	E	102	STE	C7-C8-C9-C10
30	d	410	LMG	C30-C31-C32-C33
33	A	619	DGD	CBA-CCA-CDA-CEA
25	C	508	CLA	C15-C16-C17-C18
31	a	614	SQD	C8-C7-O47-C45
33	C	522	DGD	C2E-C1E-O5D-C6D
25	C	506	CLA	C16-C17-C18-C20
30	M	101	LMG	C36-C37-C38-C39
30	C	524	LMG	C28-C29-C30-C31
33	C	521	DGD	C2B-C3B-C4B-C5B
32	A	617	LHG	C27-C28-C29-C30
32	L	101	LHG	C16-C17-C18-C19
30	M	101	LMG	C14-C15-C16-C17
29	C	520	STE	C9-C10-C11-C12
33	C	522	DGD	C2A-C3A-C4A-C5A
30	M	101	LMG	O10-C28-O8-C9
33	c	519	DGD	CBA-CCA-CDA-CEA
29	b	623	STE	C9-C10-C11-C12
31	B	622	SQD	C28-C29-C30-C31
32	D	410	LHG	O1-C1-C2-O2
33	c	519	DGD	C4D-C5D-C6D-O5D
30	c	522	LMG	C4-C5-C6-O5
25	B	601	CLA	C4B-C3B-CAB-CBB
25	C	504	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C4B-C3B-CAB-CBB
25	b	605	CLA	C4B-C3B-CAB-CBB
25	c	508	CLA	C1A-C2A-CAA-CBA
33	A	619	DGD	CDA-CEA-CFA-CGA
30	c	518	LMG	C28-C29-C30-C31
25	c	504	CLA	C4-C3-C5-C6
25	c	509	CLA	C4-C3-C5-C6
27	t	101	BCR	C11-C12-C13-C14
25	b	602	CLA	C16-C17-C18-C19
29	i	102	STE	C9-C10-C11-C12
30	D	405	LMG	C35-C36-C37-C38
30	a	616	LMG	O9-C10-O7-C8
31	a	614	SQD	O49-C7-O47-C45
33	H	102	DGD	C8A-C9A-CAA-CBA
25	B	605	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B	615	CLA	C12-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C10
25	C	505	CLA	C6-C7-C8-C10
25	C	509	CLA	C11-C12-C13-C15
25	c	505	CLA	C6-C7-C8-C10
25	c	506	CLA	C6-C7-C8-C10
25	d	402	CLA	C11-C12-C13-C15
26	a	608	PHO	C6-C7-C8-C10
29	d	409	STE	C15-C16-C17-C18
31	a	615	SQD	C11-C12-C13-C14
25	C	501	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C20
25	C	509	CLA	C5-C6-C7-C8
29	C	526	STE	C12-C13-C14-C15
29	C	527	STE	C11-C10-C9-C8
29	C	516	STE	C9-C10-C11-C12
29	E	102	STE	C9-C10-C11-C12
32	D	409	LHG	C2-C3-O3-P
32	d	408	LHG	C2-C3-O3-P
25	b	610	CLA	C2A-CAA-CBA-CGA
25	c	509	CLA	C2A-CAA-CBA-CGA
25	A	607	CLA	C11-C10-C8-C9
25	B	602	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C12-C13-C14
25	b	603	CLA	C11-C10-C8-C9
25	c	507	CLA	C11-C12-C13-C14
29	X	101	STE	C5-C6-C7-C8
29	m	103	STE	C9-C10-C11-C12
31	B	622	SQD	C14-C15-C16-C17
25	b	608	CLA	C13-C15-C16-C17
25	b	609	CLA	C15-C16-C17-C18
29	E	103	STE	C4-C5-C6-C7
30	c	524	LMG	C33-C34-C35-C36
30	a	616	LMG	C31-C32-C33-C34
30	c	522	LMG	O10-C28-O8-C9
30	C	517	LMG	O7-C8-C9-O8
33	c	520	DGD	C2E-C1E-O5D-C6D
29	C	525	STE	C1-C2-C3-C4
30	c	522	LMG	C34-C35-C36-C37
31	A	616	SQD	O6-C44-C45-C46
31	a	614	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C4-C3-C5-C6
33	A	619	DGD	C9A-CAA-CBA-CCA
25	B	601	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
31	a	614	SQD	C19-C20-C21-C22
30	d	410	LMG	C13-C14-C15-C16
32	d	407	LHG	C26-C27-C28-C29
25	B	615	CLA	C13-C15-C16-C17
32	D	410	LHG	C26-C27-C28-C29
33	H	102	DGD	C9B-CAB-CBB-CCB
29	E	103	STE	C11-C12-C13-C14
29	t	102	STE	C6-C7-C8-C9
30	c	523	LMG	C29-C30-C31-C32
25	B	601	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O2D
27	h	101	BCR	C9-C10-C11-C12
32	D	410	LHG	C3-O3-P-O5
32	L	101	LHG	C4-O6-P-O3
32	L	101	LHG	C4-O6-P-O5
32	e	102	LHG	C3-O3-P-O4
32	l	101	LHG	C4-O6-P-O5
28	d	405	PL9	C42-C43-C44-C45
25	c	506	CLA	C16-C17-C18-C20
32	A	617	LHG	C24-C25-C26-C27
25	C	504	CLA	C2B-C3B-CAB-CBB
27	T	101	BCR	C1-C6-C7-C8
27	b	617	BCR	C1-C6-C7-C8
33	h	102	DGD	CBA-CCA-CDA-CEA
28	d	405	PL9	C43-C44-C46-C47
29	C	527	STE	C7-C8-C9-C10
27	k	101	BCR	C37-C22-C23-C24
27	t	101	BCR	C11-C12-C13-C35
29	A	621	STE	C14-C15-C16-C17
32	d	407	LHG	C19-C20-C21-C22
33	c	520	DGD	C5A-C6A-C7A-C8A
31	B	622	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
30	D	406	LMG	C39-C40-C41-C42
29	m	103	STE	C10-C11-C12-C13
25	b	612	CLA	C3-C5-C6-C7
29	b	623	STE	C7-C8-C9-C10
30	c	524	LMG	C38-C39-C40-C41
28	d	405	PL9	C4-C3-C7-C8
29	b	623	STE	C5-C6-C7-C8
29	C	525	STE	C3-C4-C5-C6
33	H	102	DGD	C7B-C8B-C9B-CAB
30	c	524	LMG	C31-C32-C33-C34
32	a	613	LHG	C11-C10-C9-C8
30	C	517	LMG	C7-C8-O7-C10
31	B	622	SQD	C46-C45-O47-C7
29	Z	101	STE	C3-C4-C5-C6
32	d	407	LHG	C29-C30-C31-C32
30	b	622	LMG	C36-C37-C38-C39
25	B	610	CLA	C8-C10-C11-C12
29	T	102	STE	C12-C13-C14-C15
25	B	602	CLA	C6-C7-C8-C9
25	B	613	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C12-C13-C14
25	C	512	CLA	C11-C12-C13-C14
25	b	604	CLA	C11-C12-C13-C14
29	m	103	STE	C1-C2-C3-C4
25	C	504	CLA	C11-C10-C8-C7
25	c	512	CLA	C6-C7-C8-C10
25	B	614	CLA	C15-C16-C17-C18
29	a	617	STE	C1-C2-C3-C4
31	a	614	SQD	C15-C16-C17-C18
32	a	613	LHG	C32-C33-C34-C35
33	A	619	DGD	C7B-C8B-C9B-CAB
25	c	502	CLA	C16-C17-C18-C19
25	b	604	CLA	C13-C15-C16-C17
32	e	102	LHG	C13-C14-C15-C16
33	C	521	DGD	C6A-C7A-C8A-C9A
25	c	509	CLA	CAA-CBA-CGA-O2A
30	C	524	LMG	O10-C28-O8-C9
30	a	616	LMG	C41-C42-C43-C44
25	B	607	CLA	C13-C15-C16-C17
30	C	524	LMG	C29-C28-O8-C9
28	a	611	PL9	C21-C22-C23-C24
31	B	622	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	d	411	STE	C4-C5-C6-C7
31	a	614	SQD	O6-C44-C45-O47
31	D	407	SQD	O48-C23-C24-C25
25	a	606	CLA	C2C-C3C-CAC-CBC
30	b	622	LMG	C16-C17-C18-C19
30	b	622	LMG	C17-C18-C19-C20
30	B	620	LMG	C28-C29-C30-C31
31	a	615	SQD	C23-C24-C25-C26
29	d	406	STE	C2-C3-C4-C5
29	H	103	STE	C13-C14-C15-C16
31	a	614	SQD	C14-C15-C16-C17
30	C	517	LMG	C16-C17-C18-C19
33	C	523	DGD	O6D-C5D-C6D-O5D
27	T	101	BCR	C37-C22-C23-C24
29	d	409	STE	C10-C11-C12-C13
31	b	620	SQD	C27-C28-C29-C30
30	m	101	LMG	C29-C28-O8-C9
29	t	103	STE	C2-C3-C4-C5
30	M	101	LMG	C33-C34-C35-C36
31	a	614	SQD	C13-C14-C15-C16
31	a	615	SQD	C24-C25-C26-C27
25	c	501	CLA	C2A-CAA-CBA-CGA
33	c	519	DGD	CAA-CBA-CCA-CDA
35	V	201	HEC	C4B-C3B-CAB-CBB
29	c	517	STE	C4-C5-C6-C7
32	A	617	LHG	C1-C2-C3-O3
29	d	409	STE	C3-C4-C5-C6
29	e	104	STE	C4-C5-C6-C7
30	c	523	LMG	C37-C38-C39-C40
25	B	605	CLA	C11-C10-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	C	506	CLA	C14-C13-C15-C16
26	a	608	PHO	C6-C7-C8-C9
26	a	608	PHO	C11-C10-C8-C9
29	j	102	STE	C4-C5-C6-C7
33	c	521	DGD	C2A-C1A-O1G-C1G
25	B	606	CLA	C4B-C3B-CAB-CBB
25	C	512	CLA	C4B-C3B-CAB-CBB
30	m	101	LMG	C32-C33-C34-C35
33	H	102	DGD	C8B-C9B-CAB-CBB
25	B	608	CLA	C15-C16-C17-C18
30	c	518	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
30	m	101	LMG	O10-C28-O8-C9
30	c	518	LMG	O8-C28-C29-C30
30	c	518	LMG	O10-C28-O8-C9
25	C	506	CLA	C16-C17-C18-C19
32	a	613	LHG	C26-C27-C28-C29
31	a	615	SQD	C17-C18-C19-C20
25	D	402	CLA	C11-C10-C8-C7
29	b	625	STE	C9-C10-C11-C12
29	Z	101	STE	C4-C5-C6-C7
25	c	502	CLA	O1A-CGA-O2A-C1
33	c	521	DGD	O1A-C1A-O1G-C1G
29	Z	101	STE	C2-C3-C4-C5
33	A	619	DGD	O1G-C1G-C2G-O2G
29	d	411	STE	C10-C11-C12-C13
25	c	509	CLA	C2-C3-C5-C6
30	a	616	LMG	C17-C18-C19-C20
29	A	621	STE	C4-C5-C6-C7
30	d	410	LMG	C35-C36-C37-C38
30	m	101	LMG	C29-C30-C31-C32
25	c	509	CLA	O1D-CGD-O2D-CED
27	k	101	BCR	C19-C20-C21-C22
32	D	408	LHG	C29-C30-C31-C32
33	C	522	DGD	C3B-C4B-C5B-C6B
29	X	101	STE	C3-C4-C5-C6
32	L	101	LHG	C31-C32-C33-C34
29	E	103	STE	O1-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O1D
25	C	506	CLA	C2-C3-C5-C6
25	B	606	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C20
29	T	102	STE	C13-C14-C15-C16
32	a	613	LHG	C27-C28-C29-C30
30	D	405	LMG	C20-C21-C22-C23
28	D	404	PL9	C44-C46-C47-C48
25	C	511	CLA	C3-C5-C6-C7
25	C	513	CLA	C10-C11-C12-C13
25	B	613	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	507	CLA	C14-C13-C15-C16
25	C	511	CLA	C14-C13-C15-C16
25	D	402	CLA	C11-C10-C8-C9
25	b	609	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	611	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C9
25	c	511	CLA	C11-C10-C8-C9
25	d	402	CLA	C11-C12-C13-C14
31	B	622	SQD	C29-C30-C31-C32
29	e	103	STE	C10-C11-C12-C13
25	c	502	CLA	CBA-CGA-O2A-C1
30	a	616	LMG	C34-C35-C36-C37
29	d	409	STE	O1-C1-C2-C3
30	A	615	LMG	C9-C8-O7-C10
32	A	617	LHG	C4-C5-O7-C7
32	A	617	LHG	C6-C5-O7-C7
29	C	516	STE	C6-C7-C8-C9
29	d	406	STE	C14-C15-C16-C17
29	a	617	STE	O2-C1-C2-C3
33	H	102	DGD	C3A-C4A-C5A-C6A
25	B	610	CLA	C2A-CAA-CBA-CGA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C1A-C2A-CAA-CBA
29	E	103	STE	O2-C1-C2-C3
29	Z	101	STE	C13-C14-C15-C16
32	a	613	LHG	C33-C34-C35-C36
25	B	601	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C2B-C3B-CAB-CBB
25	b	601	CLA	C2B-C3B-CAB-CBB
27	b	617	BCR	C5-C6-C7-C8
27	k	102	BCR	C5-C6-C7-C8
32	D	408	LHG	C23-C24-C25-C26
32	D	408	LHG	C33-C34-C35-C36
32	e	102	LHG	C2-C3-O3-P
30	a	616	LMG	C32-C33-C34-C35
25	c	509	CLA	CBD-CGD-O2D-CED
29	a	617	STE	O1-C1-C2-C3
29	d	409	STE	O2-C1-C2-C3
29	t	102	STE	C4-C5-C6-C7
30	b	622	LMG	C37-C38-C39-C40
25	C	501	CLA	C11-C12-C13-C15
25	C	509	CLA	C12-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C15
25	b	603	CLA	C11-C12-C13-C15
25	b	610	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	d	403	CLA	C12-C13-C15-C16
25	b	612	CLA	C10-C11-C12-C13
31	f	102	SQD	O6-C44-C45-O47
30	C	524	LMG	C17-C18-C19-C20
33	H	102	DGD	C5A-C6A-C7A-C8A
32	D	410	LHG	C18-C19-C20-C21
35	v	201	HEC	CAD-CBD-CGD-O2D
29	Z	101	STE	C12-C13-C14-C15
31	b	620	SQD	C28-C29-C30-C31
33	h	102	DGD	C4E-C5E-C6E-O5E
31	a	615	SQD	C19-C20-C21-C22
29	t	102	STE	C5-C6-C7-C8
25	C	511	CLA	C8-C10-C11-C12
27	d	404	BCR	C7-C8-C9-C34
25	b	606	CLA	C4-C3-C5-C6
28	A	612	PL9	C17-C18-C19-C21
33	C	521	DGD	C7B-C8B-C9B-CAB
31	f	102	SQD	C23-C24-C25-C26
29	C	527	STE	C13-C14-C15-C16
25	B	611	CLA	C14-C13-C15-C16
29	M	103	STE	C4-C5-C6-C7
29	X	101	STE	C11-C10-C9-C8
29	J	102	STE	O2-C1-C2-C3
28	A	612	PL9	C22-C23-C24-C25
25	B	601	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
25	c	513	CLA	C4-C3-C5-C6
25	c	504	CLA	C2-C3-C5-C6
25	c	512	CLA	C2-C3-C5-C6
25	B	613	CLA	C5-C6-C7-C8
25	A	606	CLA	C2C-C3C-CAC-CBC
25	B	606	CLA	C16-C17-C18-C19
33	C	521	DGD	C2E-C1E-O5D-C6D
29	M	103	STE	C7-C8-C9-C10
30	D	405	LMG	C7-C8-C9-O8
34	F	101	HEM	CAD-CBD-CGD-O1D
25	B	604	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	C2A-CAA-CBA-CGA
34	f	101	HEM	CAD-CBD-CGD-O1D
35	V	201	HEC	CAD-CBD-CGD-O2D
29	A	621	STE	C5-C6-C7-C8
31	B	622	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
32	D	408	LHG	O1-C1-C2-O2
32	d	407	LHG	O1-C1-C2-O2
32	a	613	LHG	C34-C35-C36-C37
29	E	103	STE	C2-C3-C4-C5
33	H	102	DGD	O1B-C1B-C2B-C3B
30	d	410	LMG	C12-C13-C14-C15
32	A	617	LHG	C9-C10-C11-C12
30	a	616	LMG	C28-C29-C30-C31
29	I	101	STE	C11-C12-C13-C14
25	B	616	CLA	C10-C11-C12-C13
29	M	103	STE	C1-C2-C3-C4
29	m	103	STE	C15-C16-C17-C18
30	A	615	LMG	O1-C7-C8-O7
33	H	102	DGD	C1A-C2A-C3A-C4A
33	c	520	DGD	C9A-CAA-CBA-CCA
33	c	520	DGD	O6E-C1E-O5D-C6D
29	t	103	STE	C1-C2-C3-C4
25	B	613	CLA	C12-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C10
29	d	411	STE	C1-C2-C3-C4
29	d	406	STE	O1-C1-C2-C3
29	j	102	STE	C11-C12-C13-C14
29	B	621	STE	C11-C12-C13-C14
29	t	103	STE	C4-C5-C6-C7
29	d	406	STE	O2-C1-C2-C3
25	C	513	CLA	C11-C12-C13-C14
25	b	605	CLA	C11-C12-C13-C14
25	c	505	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C10-C8-C9
25	c	510	CLA	C6-C7-C8-C9
25	d	403	CLA	C11-C12-C13-C14
25	a	606	CLA	C4C-C3C-CAC-CBC
33	h	102	DGD	C9A-CAA-CBA-CCA
31	a	614	SQD	C5-C6-S-O8
25	B	613	CLA	C2-C1-O2A-CGA
25	C	512	CLA	C2-C1-O2A-CGA
25	D	401	CLA	C2-C1-O2A-CGA
25	d	402	CLA	C2-C1-O2A-CGA
25	A	607	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C19
29	J	102	STE	O1-C1-C2-C3
29	m	103	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	C	523	DGD	C9A-CAA-CBA-CCA
33	c	519	DGD	CCB-CDB-CEB-CFB
30	A	615	LMG	C7-C8-O7-C10
30	D	405	LMG	C11-C12-C13-C14
33	A	619	DGD	C6B-C7B-C8B-C9B
33	C	523	DGD	CBB-CCB-CDB-CEB
26	a	608	PHO	C10-C11-C12-C13
29	b	625	STE	C10-C11-C12-C13
31	B	622	SQD	C34-C35-C36-C37
30	A	615	LMG	C37-C38-C39-C40
29	C	516	STE	C3-C4-C5-C6
30	A	615	LMG	C7-C8-C9-O8
25	B	602	CLA	C15-C16-C17-C18
25	c	508	CLA	C10-C11-C12-C13
29	B	624	STE	C7-C8-C9-C10
29	C	519	STE	C3-C4-C5-C6
30	b	622	LMG	C40-C41-C42-C43
29	H	103	STE	C7-C8-C9-C10
30	A	615	LMG	O7-C8-C9-O8
35	V	201	HEC	CAD-CBD-CGD-O1D
25	C	505	CLA	C6-C7-C8-C9
25	C	511	CLA	C11-C10-C8-C9
25	b	613	CLA	C14-C13-C15-C16
25	c	506	CLA	C6-C7-C8-C9
26	A	608	PHO	C14-C13-C15-C16
26	A	609	PHO	C6-C7-C8-C9
30	c	522	LMG	C35-C36-C37-C38
25	B	612	CLA	CAA-CBA-CGA-O2A
30	M	101	LMG	O8-C28-C29-C30
30	C	524	LMG	C13-C14-C15-C16
29	X	101	STE	C15-C16-C17-C18
29	m	103	STE	C4-C5-C6-C7
30	c	522	LMG	O7-C10-C11-C12
30	c	524	LMG	O8-C28-C29-C30
34	F	101	HEM	CAD-CBD-CGD-O2D
25	C	501	CLA	C2A-CAA-CBA-CGA
25	B	603	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C10-C8-C7
25	b	605	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C12-C13-C15
25	c	506	CLA	C12-C13-C15-C16
25	c	508	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	d	403	CLA	C11-C12-C13-C15
30	B	620	LMG	C20-C21-C22-C23
25	A	606	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	615	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
25	b	609	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C2B-C3B-CAB-CBB
25	c	513	CLA	C2B-C3B-CAB-CBB
25	d	402	CLA	C2B-C3B-CAB-CBB
27	c	514	BCR	C23-C24-C25-C26
27	d	404	BCR	C23-C24-C25-C26
27	d	404	BCR	C23-C24-C25-C30
32	A	617	LHG	C10-C11-C12-C13
30	C	517	LMG	C29-C30-C31-C32
30	c	523	LMG	O8-C28-C29-C30
25	c	506	CLA	C2-C1-O2A-CGA
31	A	616	SQD	C31-C32-C33-C34
25	b	613	CLA	C13-C15-C16-C17
29	f	103	STE	C12-C13-C14-C15
29	b	625	STE	C15-C16-C17-C18
29	e	103	STE	C12-C13-C14-C15
25	b	601	CLA	C2A-CAA-CBA-CGA
29	b	623	STE	C4-C5-C6-C7
31	a	614	SQD	C29-C30-C31-C32
25	c	505	CLA	C5-C6-C7-C8
32	L	101	LHG	C5-C6-O8-C23
29	k	103	STE	C9-C10-C11-C12
34	f	101	HEM	CAD-CBD-CGD-O2D
29	d	411	STE	C11-C12-C13-C14
30	C	524	LMG	C19-C20-C21-C22
29	t	102	STE	C1-C2-C3-C4
29	i	101	STE	O2-C1-C2-C3
30	D	406	LMG	C38-C39-C40-C41
30	C	524	LMG	C10-C11-C12-C13
25	b	606	CLA	C2-C3-C5-C6
26	d	401	PHO	C2C-C3C-CAC-CBC
30	b	622	LMG	C32-C33-C34-C35
32	D	408	LHG	C15-C16-C17-C18
25	A	607	CLA	C11-C12-C13-C14
25	C	506	CLA	C11-C10-C8-C9
25	d	403	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
32	l	101	LHG	O7-C7-C8-C9
33	A	619	DGD	O1G-C1G-C2G-C3G
25	C	512	CLA	C1A-C2A-CAA-CBA
25	a	607	CLA	C4B-C3B-CAB-CBB
25	b	616	CLA	C4-C3-C5-C6
30	C	524	LMG	C36-C37-C38-C39
30	C	517	LMG	O7-C10-C11-C12
30	a	616	LMG	O7-C10-C11-C12
32	L	101	LHG	O7-C7-C8-C9
27	d	404	BCR	C7-C8-C9-C10
25	c	512	CLA	C8-C10-C11-C12
33	c	519	DGD	O2G-C1B-C2B-C3B
32	e	102	LHG	O10-C23-O8-C6
29	e	103	STE	C14-C15-C16-C17
29	k	103	STE	C3-C4-C5-C6
31	a	614	SQD	C5-C6-S-O7
30	c	523	LMG	C16-C17-C18-C19
33	h	102	DGD	O1B-C1B-C2B-C3B
25	B	605	CLA	C6-C7-C8-C10
25	B	606	CLA	C12-C13-C15-C16
25	B	607	CLA	C12-C13-C15-C16
25	b	602	CLA	C12-C13-C15-C16
25	c	513	CLA	C11-C10-C8-C7
25	c	513	CLA	C11-C12-C13-C15
29	K	102	STE	C12-C13-C14-C15
32	D	408	LHG	C30-C31-C32-C33
29	I	101	STE	O1-C1-C2-C3
25	b	603	CLA	C16-C17-C18-C20
25	c	503	CLA	O1A-CGA-O2A-C1
25	C	505	CLA	C8-C10-C11-C12
25	c	506	CLA	C8-C10-C11-C12
29	B	623	STE	C11-C10-C9-C8
31	a	614	SQD	C16-C17-C18-C19
29	M	104	STE	C15-C16-C17-C18
30	c	522	LMG	O9-C10-C11-C12
31	a	614	SQD	C32-C33-C34-C35
29	M	102	STE	O1-C1-C2-C3
25	c	510	CLA	CAA-CBA-CGA-O2A
30	c	523	LMG	O10-C28-C29-C30
28	A	612	PL9	C20-C19-C21-C22
33	C	521	DGD	O2G-C1B-C2B-C3B
28	D	404	PL9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
29	X	101	STE	O2-C1-C2-C3
32	D	409	LHG	C26-C27-C28-C29
30	C	517	LMG	C11-C12-C13-C14
32	D	409	LHG	C16-C17-C18-C19
32	e	102	LHG	C24-C23-O8-C6
33	C	523	DGD	CAA-CBA-CCA-CDA
29	i	101	STE	O1-C1-C2-C3
28	D	404	PL9	C46-C47-C48-C49
25	a	612	CLA	C13-C15-C16-C17
25	b	616	CLA	C8-C10-C11-C12
25	c	503	CLA	CBA-CGA-O2A-C1
25	B	603	CLA	C11-C10-C8-C9
25	C	504	CLA	C11-C10-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	b	602	CLA	C14-C13-C15-C16
25	c	505	CLA	C11-C12-C13-C14
29	b	624	STE	C2-C3-C4-C5
33	c	521	DGD	CBB-CCB-CDB-CEB
30	b	622	LMG	C18-C19-C20-C21
30	b	622	LMG	C20-C21-C22-C23
31	a	614	SQD	C30-C31-C32-C33
25	c	506	CLA	C16-C17-C18-C19
30	c	524	LMG	O10-C28-C29-C30
25	b	607	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	CAA-CBA-CGA-O2A
29	I	101	STE	O2-C1-C2-C3
33	C	522	DGD	CCA-CDA-CEA-CFA
32	a	613	LHG	C24-C25-C26-C27
29	M	104	STE	C6-C7-C8-C9
25	b	613	CLA	CAA-CBA-CGA-O2A
27	T	101	BCR	C21-C22-C23-C24
30	M	101	LMG	O10-C28-C29-C30
33	c	519	DGD	O1B-C1B-C2B-C3B
25	B	604	CLA	C8-C10-C11-C12
30	m	101	LMG	C8-C7-O1-C1
31	b	620	SQD	C45-C44-O6-C1
33	h	102	DGD	C2G-C3G-O3G-C1D
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	602	CLA	C2A-CAA-CBA-CGA
29	A	622	STE	C12-C13-C14-C15
25	C	507	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	A	615	LMG	O1-C7-C8-C9
31	f	102	SQD	O6-C44-C45-C46
32	d	408	LHG	C4-C5-C6-O8
32	l	101	LHG	O9-C7-C8-C9
25	B	609	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
32	A	617	LHG	C31-C32-C33-C34
30	a	616	LMG	O9-C10-C11-C12
32	L	101	LHG	O9-C7-C8-C9
32	d	407	LHG	C30-C31-C32-C33
25	A	606	CLA	C4C-C3C-CAC-CBC
32	L	101	LHG	C19-C20-C21-C22
31	A	618	SQD	O48-C23-C24-C25
30	B	620	LMG	C16-C17-C18-C19
25	b	616	CLA	C3-C5-C6-C7
29	X	101	STE	O1-C1-C2-C3
33	c	520	DGD	C2A-C3A-C4A-C5A
25	b	613	CLA	CAA-CBA-CGA-O1A
30	D	405	LMG	O8-C28-C29-C30
30	C	517	LMG	O9-C10-C11-C12
33	c	520	DGD	C3A-C4A-C5A-C6A
33	A	619	DGD	C3A-C4A-C5A-C6A
25	b	610	CLA	C4C-C3C-CAC-CBC
29	j	102	STE	C13-C14-C15-C16

There are no ring outliers.

132 monomers are involved in 215 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	v	201	HEC	1	0
25	A	614	CLA	2	0
33	c	520	DGD	1	0
25	c	507	CLA	1	0
25	c	503	CLA	3	0
25	b	605	CLA	1	0
29	M	104	STE	3	0
29	d	409	STE	4	0
29	B	623	STE	2	0
25	B	616	CLA	2	0
30	B	620	LMG	4	0
31	f	102	SQD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	611	PL9	3	0
25	C	513	CLA	1	0
29	c	516	STE	1	0
27	T	101	BCR	3	0
26	a	608	PHO	1	0
27	h	101	BCR	4	0
25	c	511	CLA	4	0
27	A	611	BCR	1	0
32	D	408	LHG	2	0
33	A	619	DGD	2	0
29	b	621	STE	1	0
25	c	501	CLA	2	0
25	B	603	CLA	1	0
25	b	616	CLA	2	0
32	D	410	LHG	7	0
32	e	102	LHG	1	0
27	k	101	BCR	1	0
25	d	403	CLA	2	0
27	D	403	BCR	1	0
32	L	101	LHG	2	0
25	b	609	CLA	4	0
25	D	402	CLA	1	0
25	B	604	CLA	1	0
31	a	614	SQD	1	0
30	A	615	LMG	2	0
32	a	613	LHG	3	0
25	b	603	CLA	2	0
31	B	622	SQD	4	0
33	H	102	DGD	1	0
30	c	518	LMG	1	0
25	b	610	CLA	2	0
31	b	620	SQD	3	0
29	A	622	STE	1	0
25	a	607	CLA	1	0
25	a	612	CLA	2	0
25	b	615	CLA	3	0
25	B	613	CLA	4	0
25	B	611	CLA	1	0
34	F	101	HEM	2	0
30	b	622	LMG	1	0
25	C	505	CLA	2	0
27	b	618	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	K	102	STE	1	0
27	c	515	BCR	1	0
27	H	101	BCR	1	0
25	b	601	CLA	1	0
30	a	616	LMG	3	0
30	M	101	LMG	2	0
28	A	612	PL9	3	0
27	c	514	BCR	1	0
29	C	527	STE	1	0
32	l	101	LHG	2	0
30	C	517	LMG	1	0
25	c	505	CLA	1	0
30	D	406	LMG	1	0
25	c	504	CLA	1	0
27	a	610	BCR	1	0
28	D	404	PL9	2	0
26	A	609	PHO	1	0
25	B	609	CLA	1	0
25	B	607	CLA	1	0
25	b	608	CLA	2	0
29	m	103	STE	1	0
25	D	401	CLA	2	0
33	C	521	DGD	1	0
25	B	614	CLA	5	0
27	k	102	BCR	3	0
26	d	401	PHO	2	0
27	C	514	BCR	1	0
25	C	511	CLA	3	0
25	B	615	CLA	3	0
25	b	613	CLA	1	0
32	D	409	LHG	5	0
25	b	604	CLA	2	0
27	t	101	BCR	4	0
25	B	612	CLA	1	0
27	B	618	BCR	2	0
27	J	101	BCR	2	0
25	A	610	CLA	1	0
25	c	510	CLA	1	0
31	A	618	SQD	2	0
25	b	602	CLA	3	0
25	C	512	CLA	3	0
29	d	406	STE	1	0

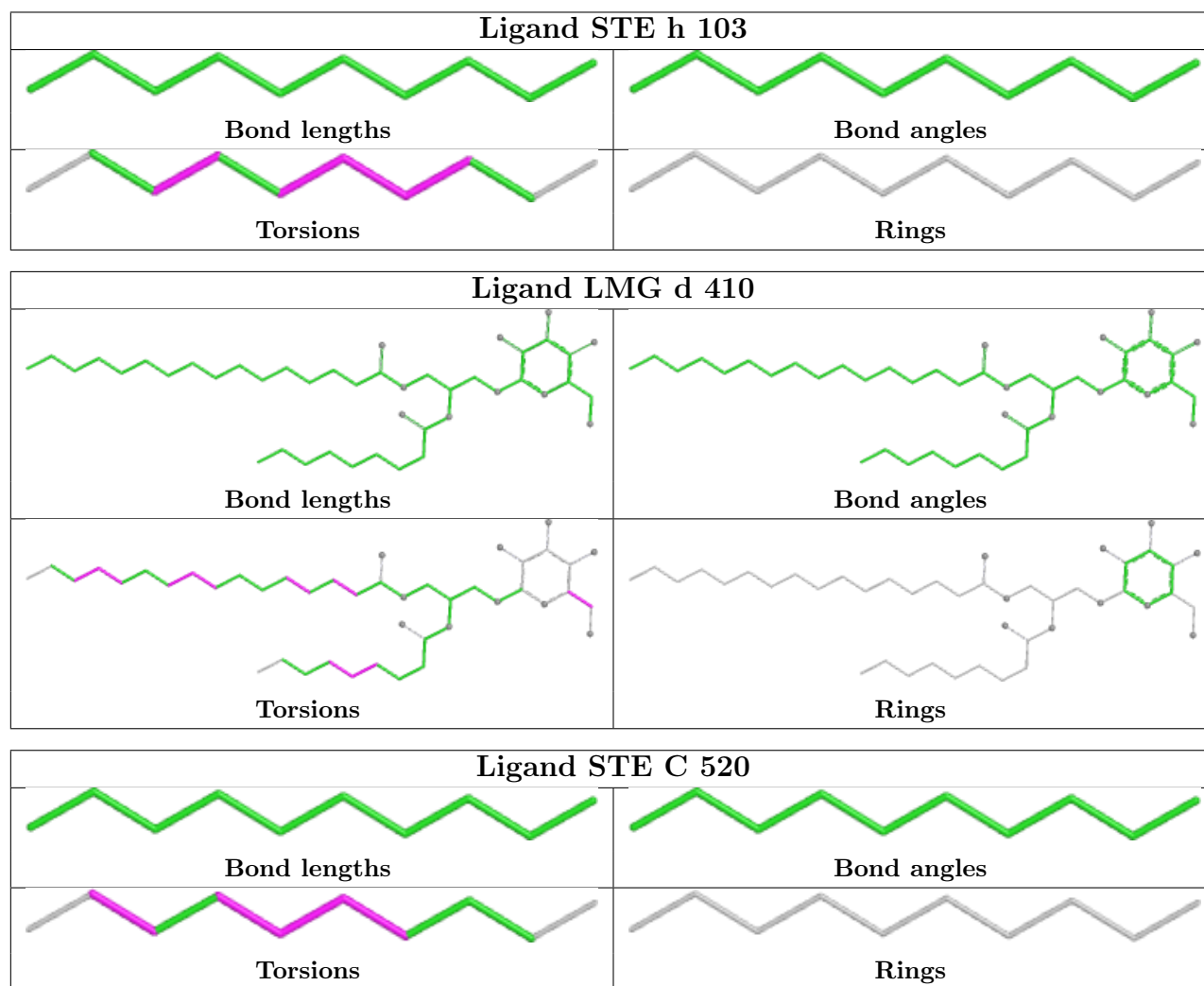
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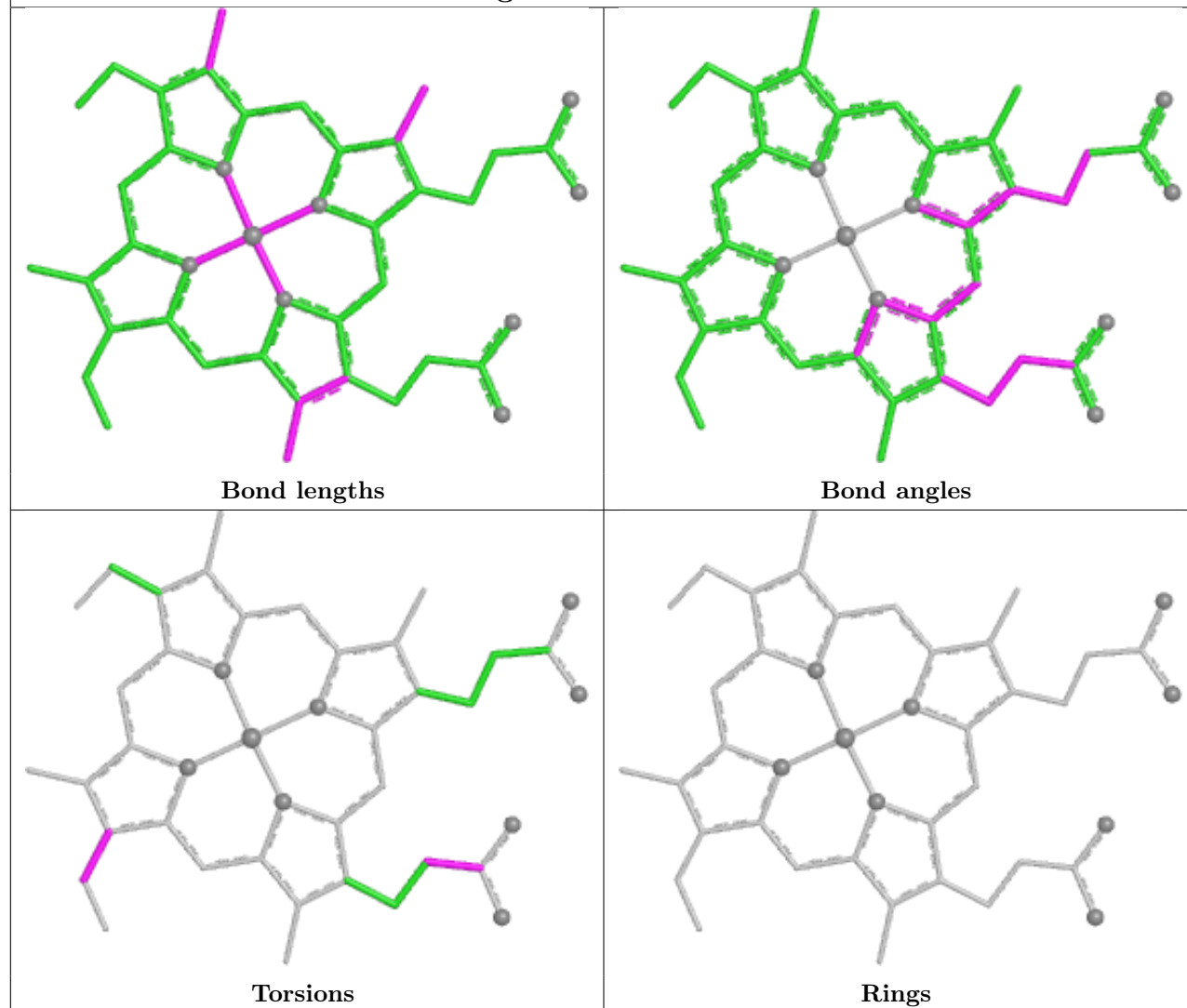
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	H	103	STE	1	0
28	d	405	PL9	2	0
29	T	102	STE	4	0
25	d	402	CLA	3	0
29	X	101	STE	1	0
25	C	507	CLA	1	0
27	d	404	BCR	1	0
25	C	506	CLA	2	0
25	c	509	CLA	2	0
25	C	509	CLA	1	0
25	c	512	CLA	1	0
25	c	508	CLA	1	0
25	c	513	CLA	2	0
29	d	411	STE	1	0
25	C	508	CLA	1	0
27	C	515	BCR	2	0
25	b	612	CLA	1	0
32	A	617	LHG	1	0
30	m	101	LMG	3	0
31	a	615	SQD	2	0
33	c	519	DGD	1	0
34	f	101	HEM	5	0
25	A	606	CLA	2	0
29	i	101	STE	1	0
29	B	621	STE	1	0
30	D	405	LMG	5	0
30	C	524	LMG	2	0
30	c	523	LMG	2	0
25	a	609	CLA	3	0
29	b	625	STE	2	0
25	C	502	CLA	2	0
25	B	605	CLA	2	0
25	a	606	CLA	5	0
27	b	617	BCR	1	0
25	b	614	CLA	2	0
33	c	521	DGD	3	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

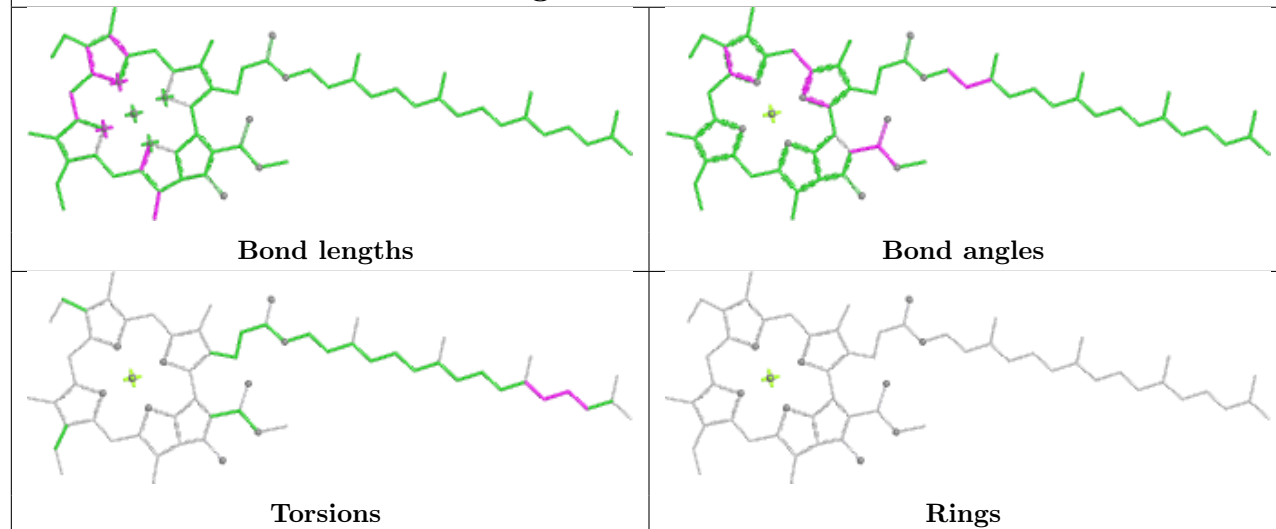
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

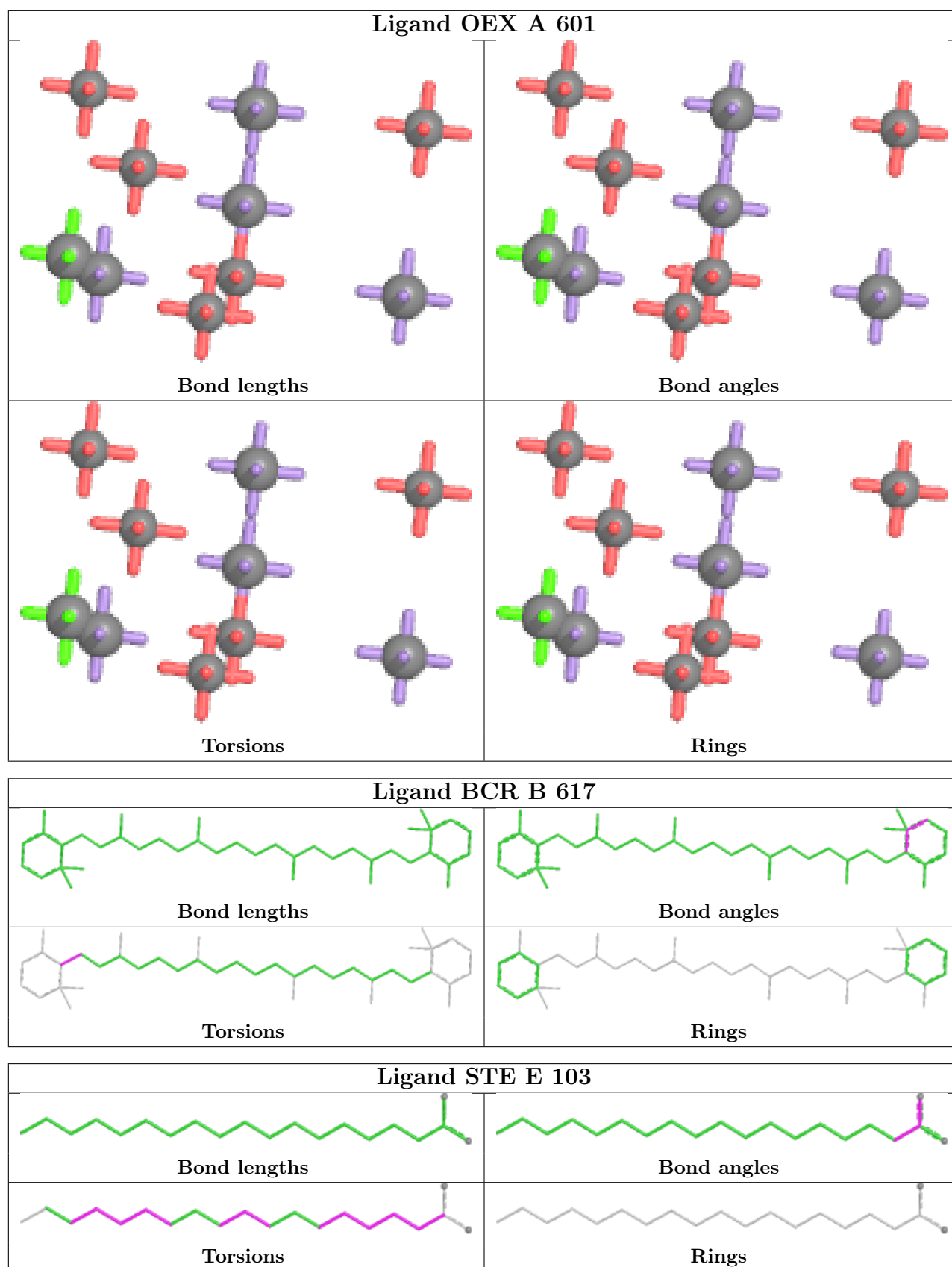


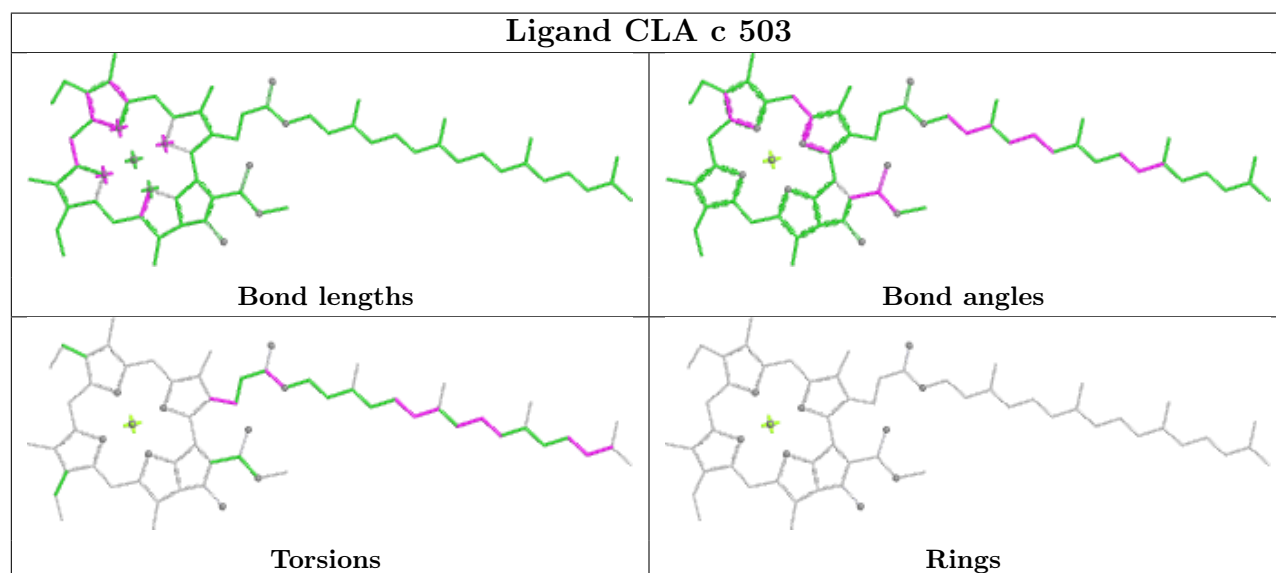
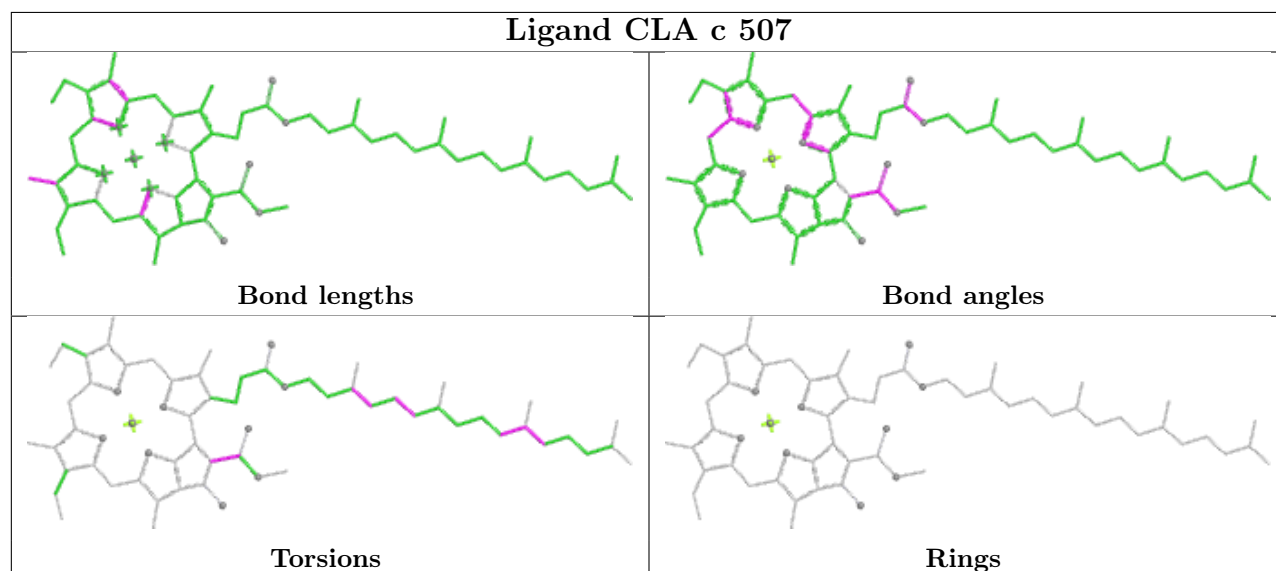
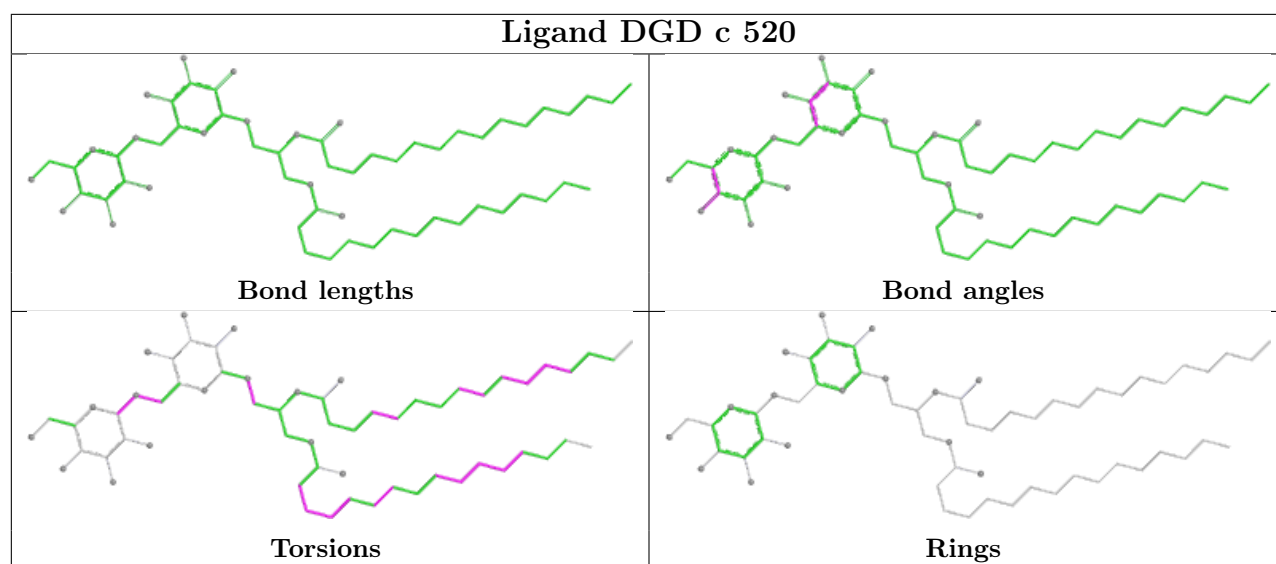
Ligand HEC v 201



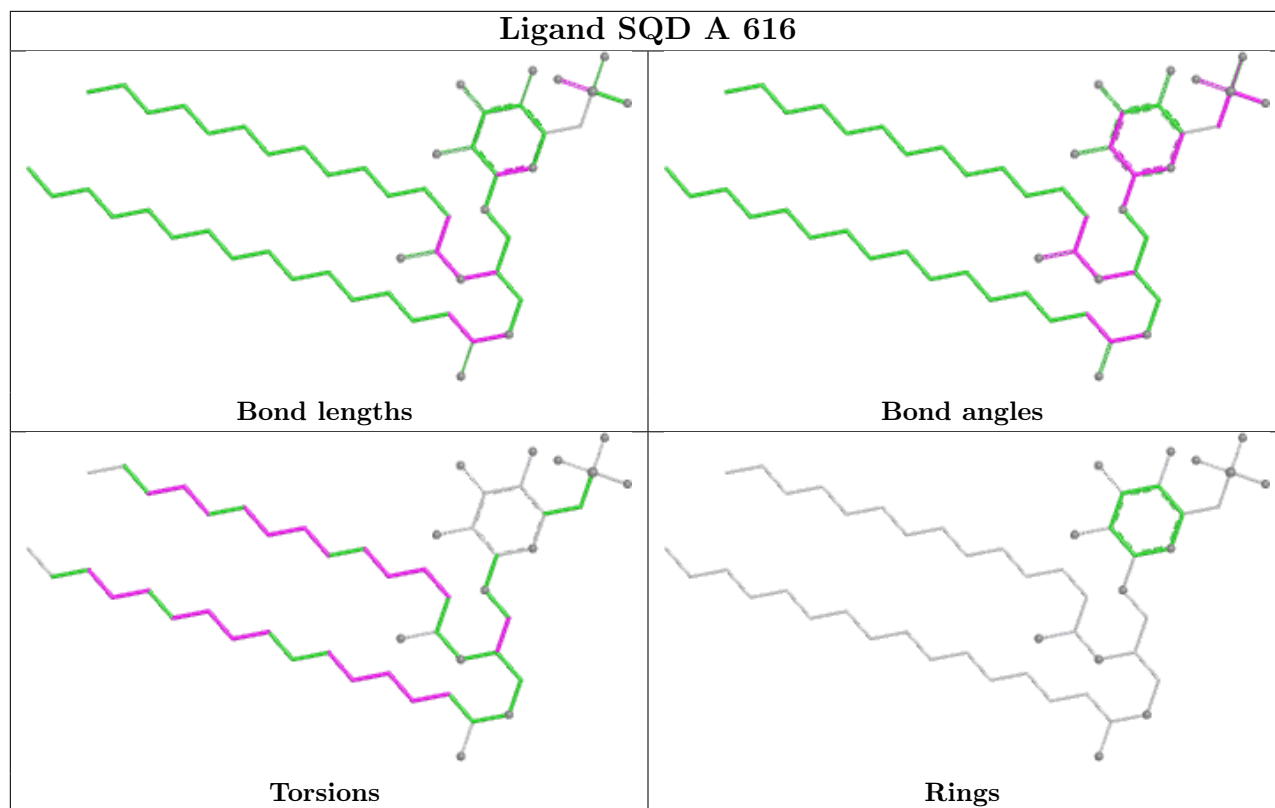
Ligand CLA A 614



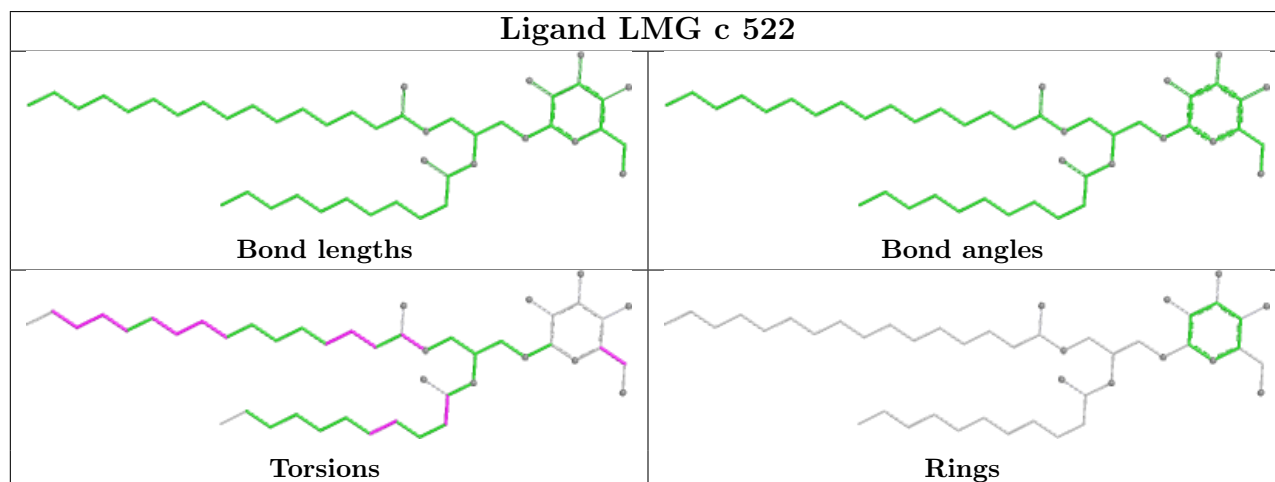




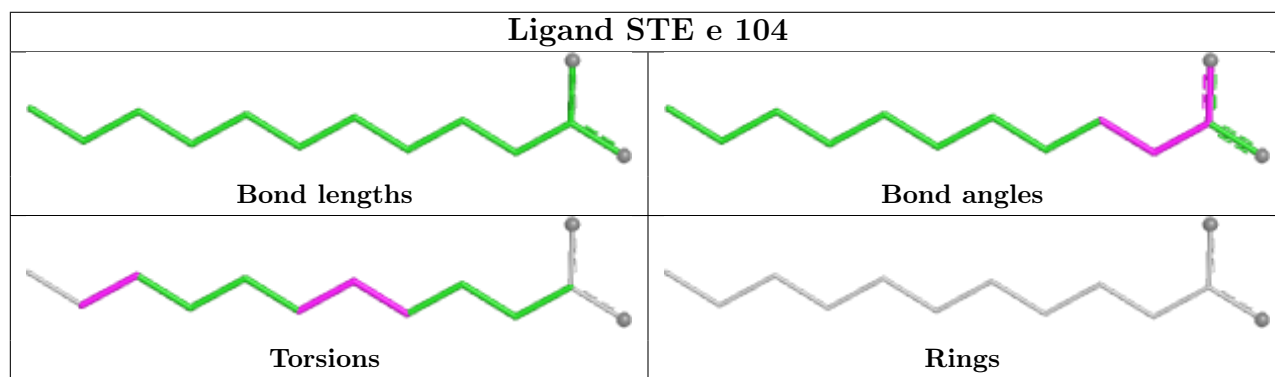
Ligand SQD A 616

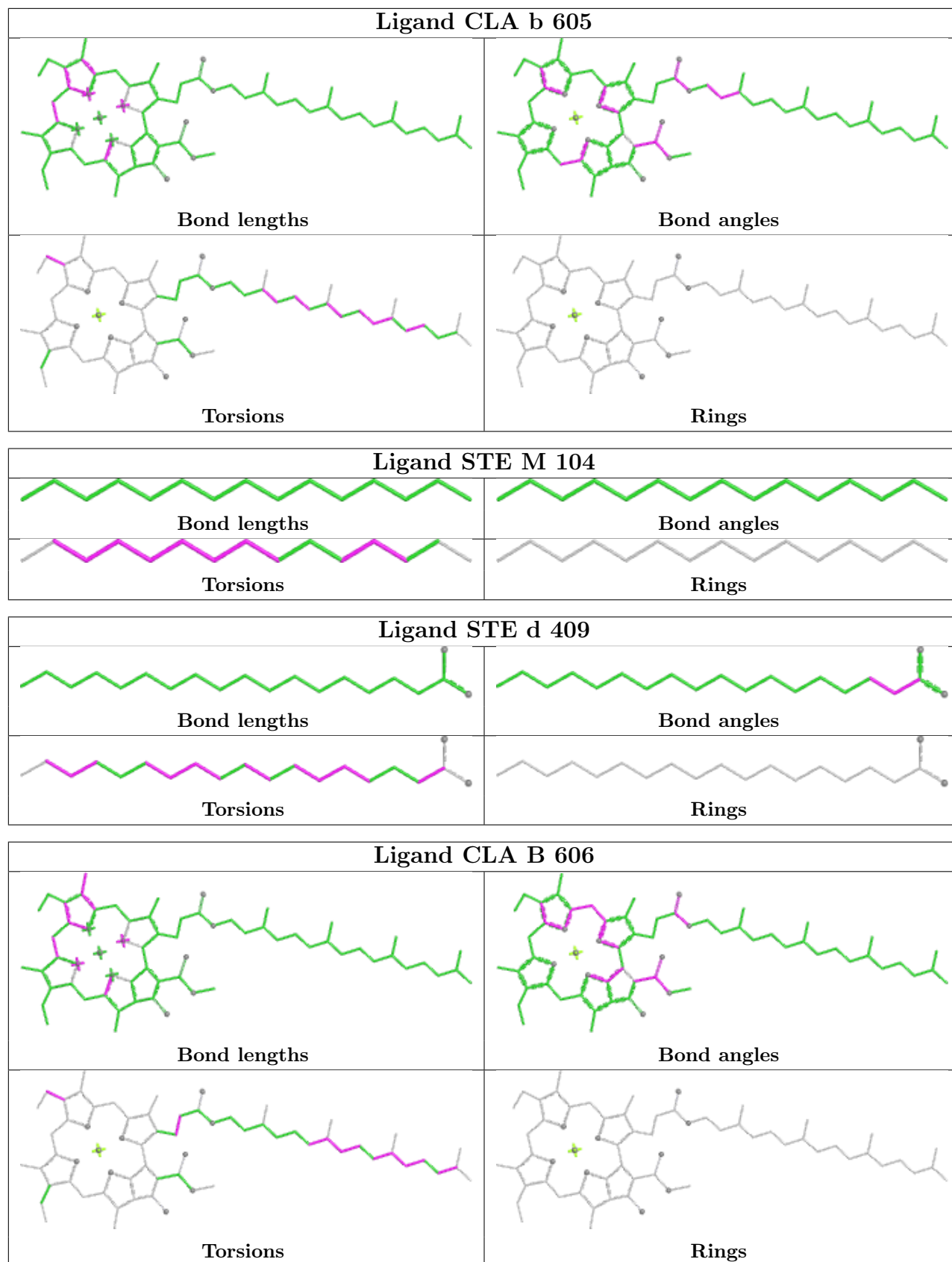


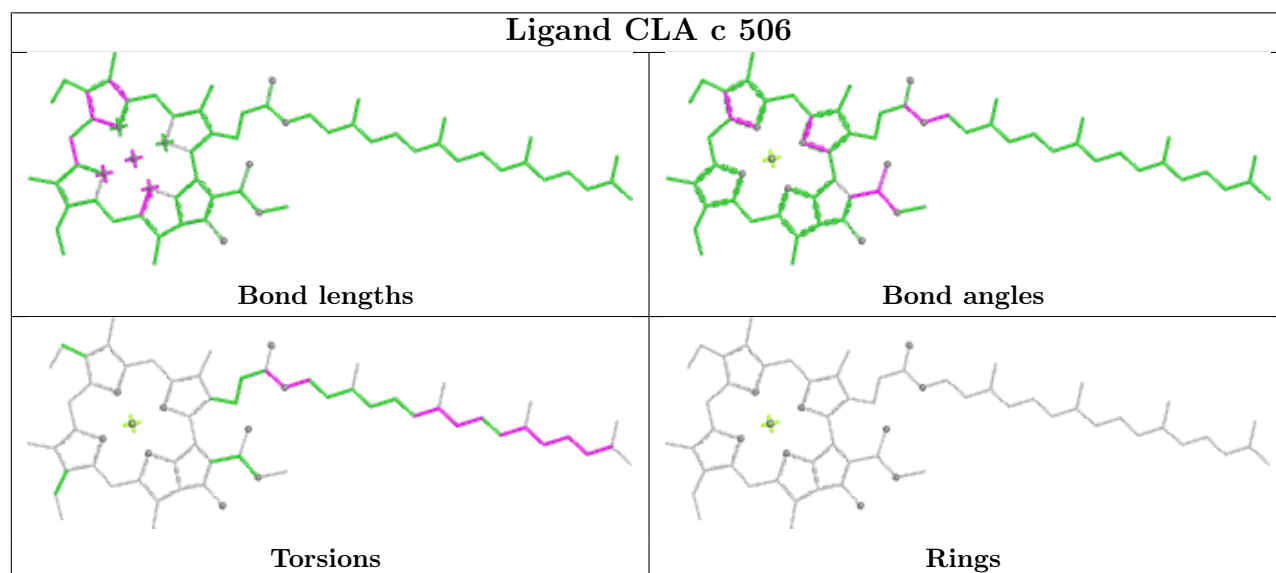
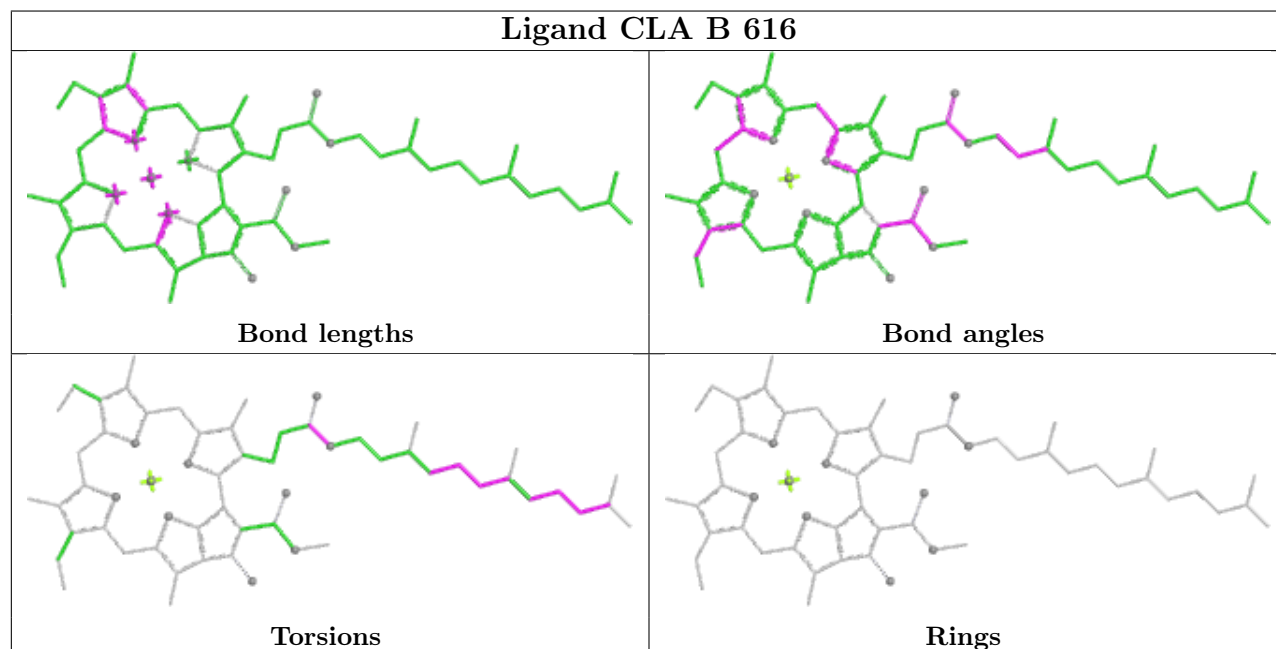
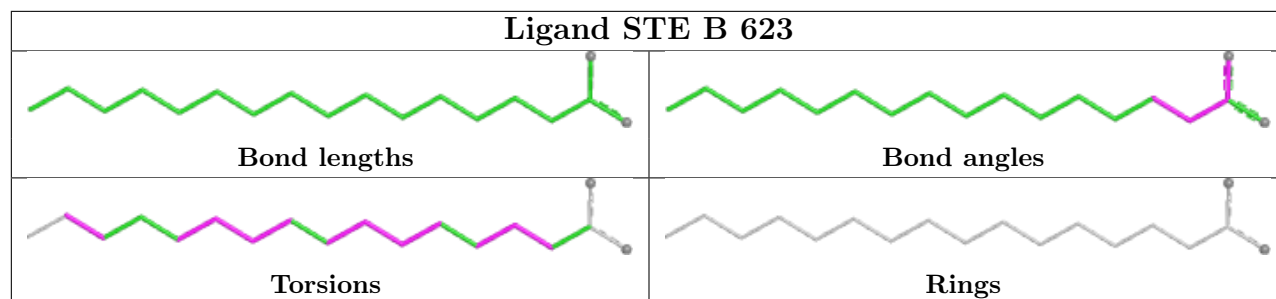
Ligand LMG c 522

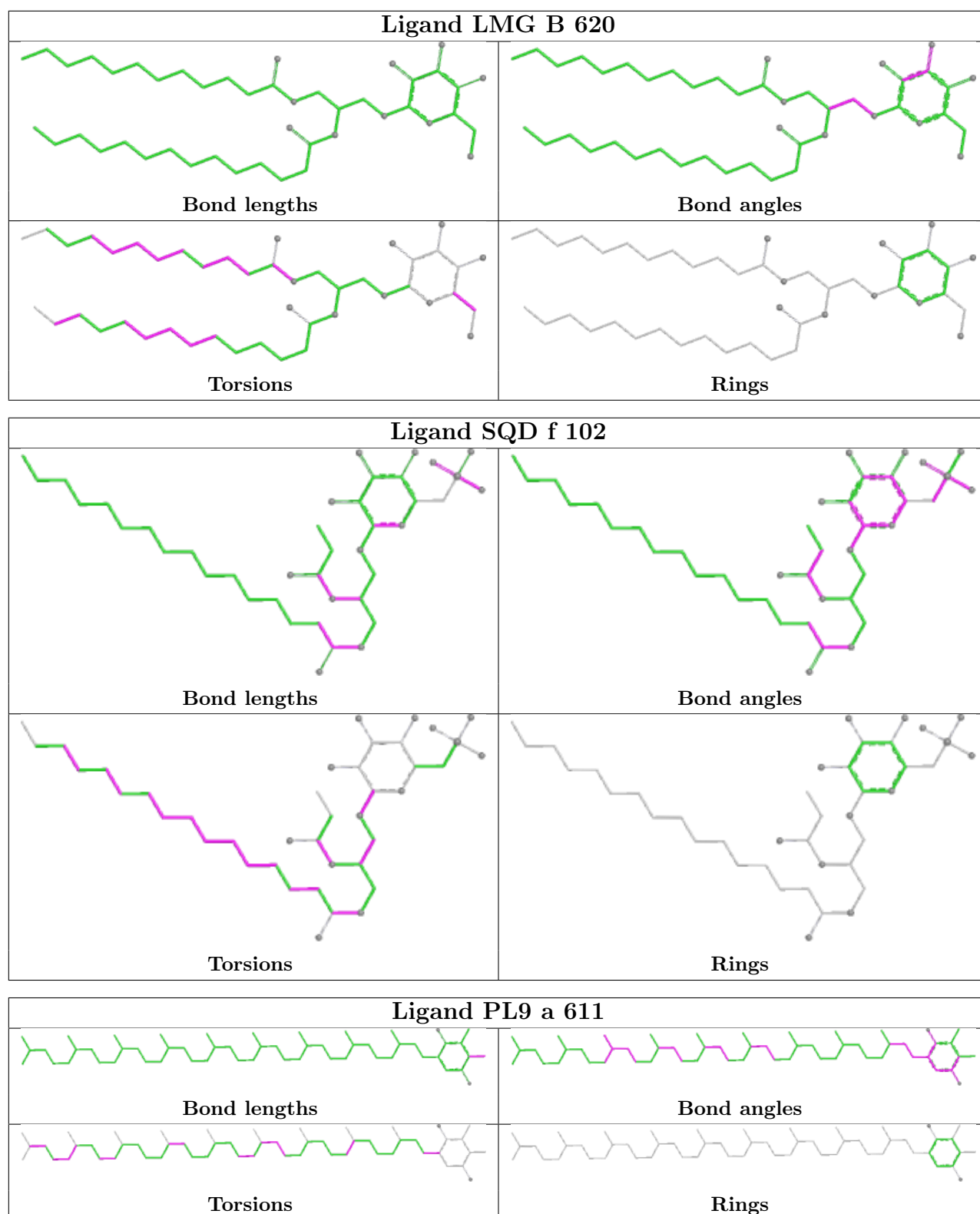


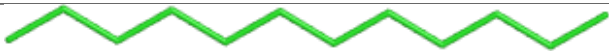
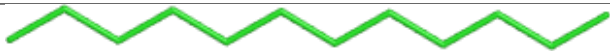
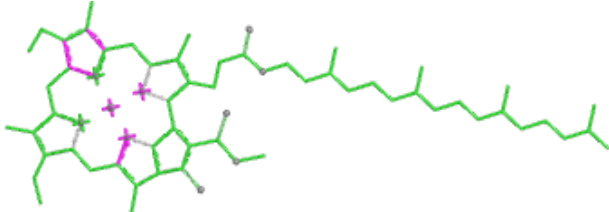
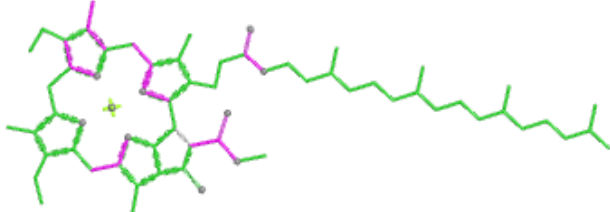
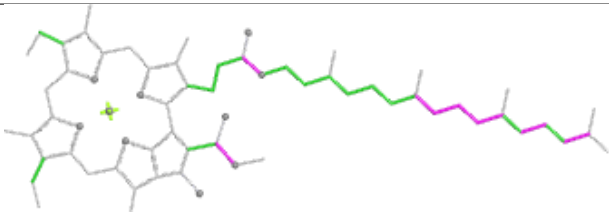
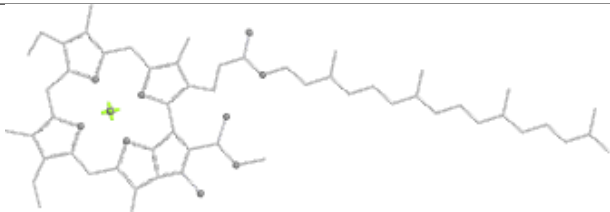
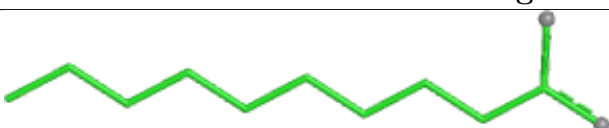
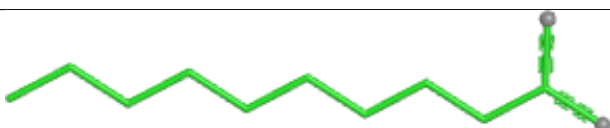
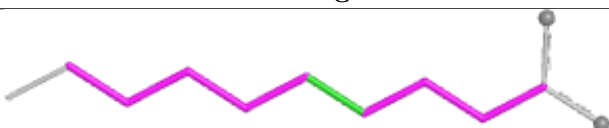
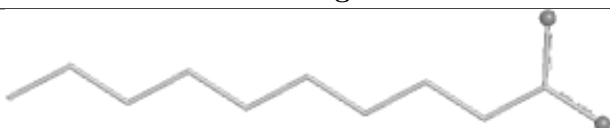
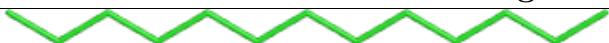
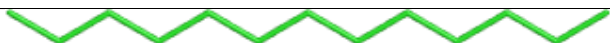
Ligand STE e 104

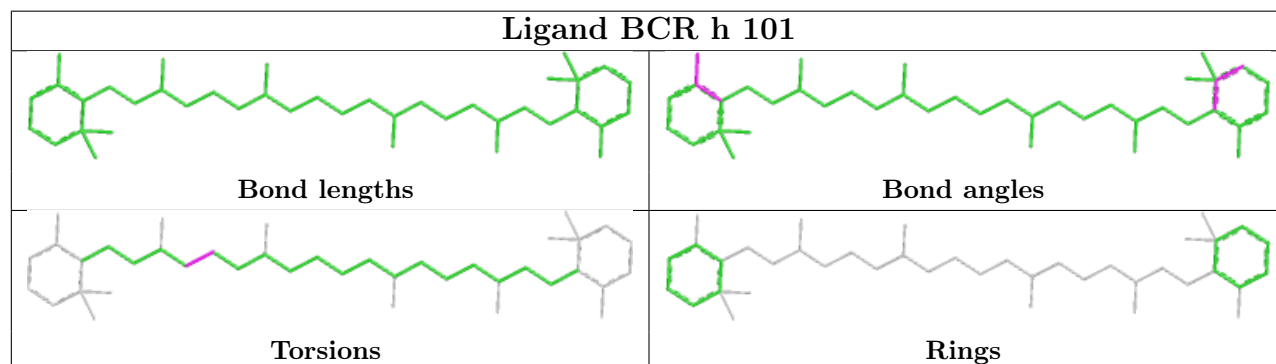
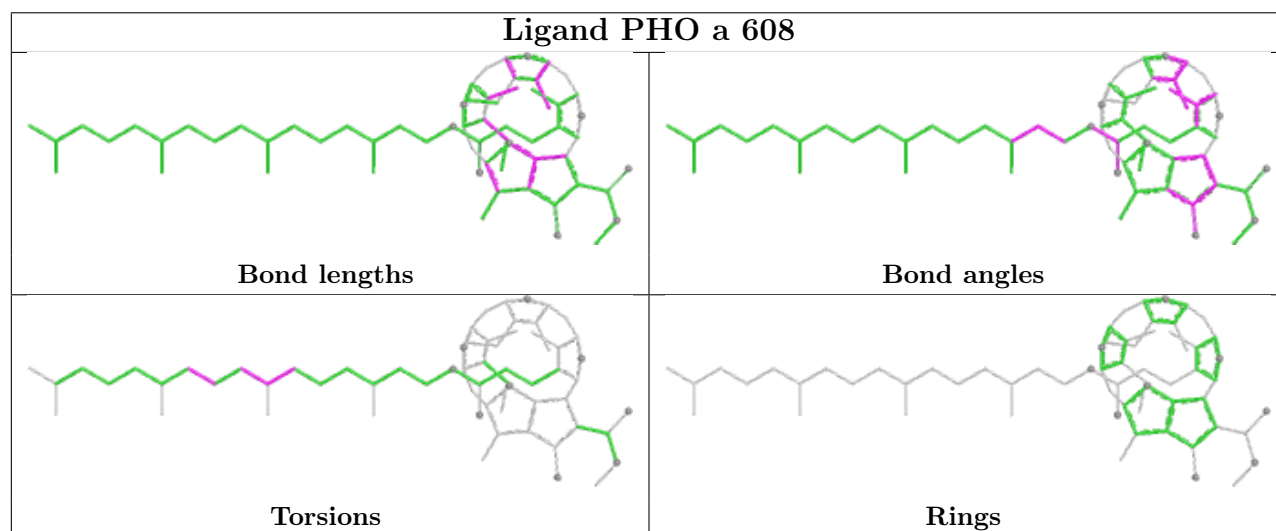
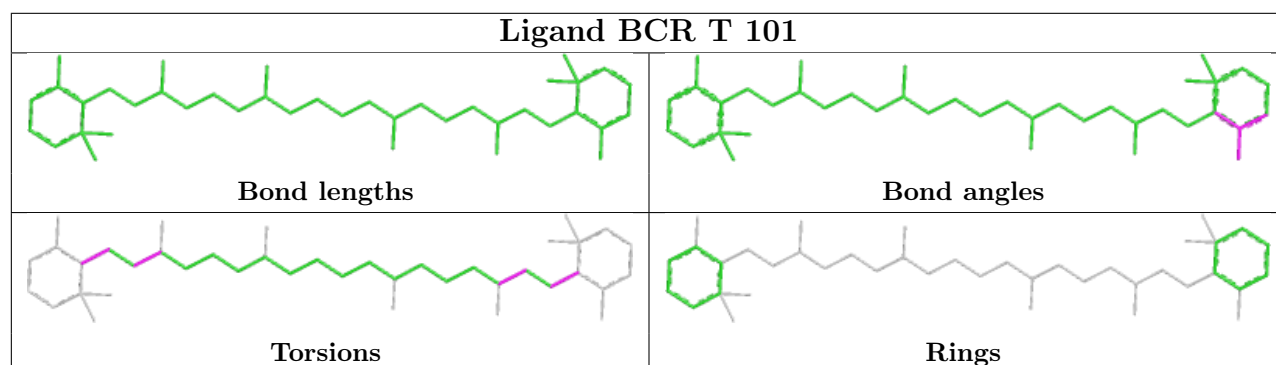
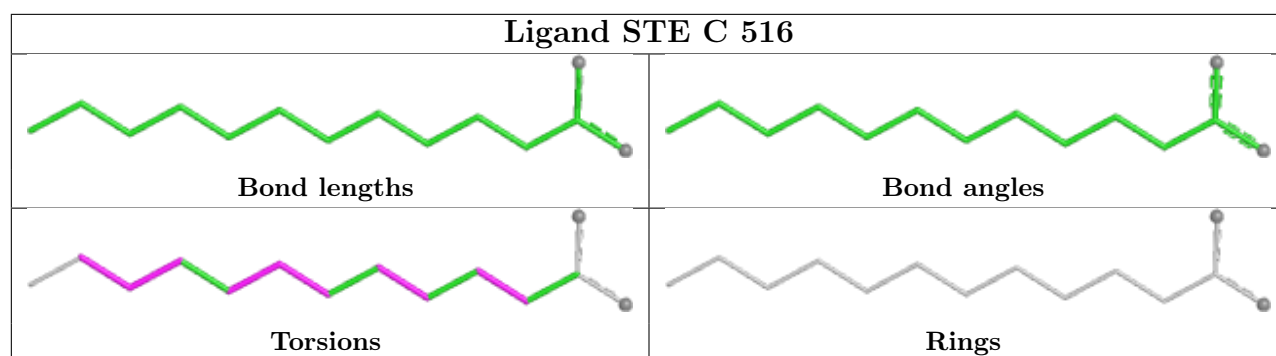


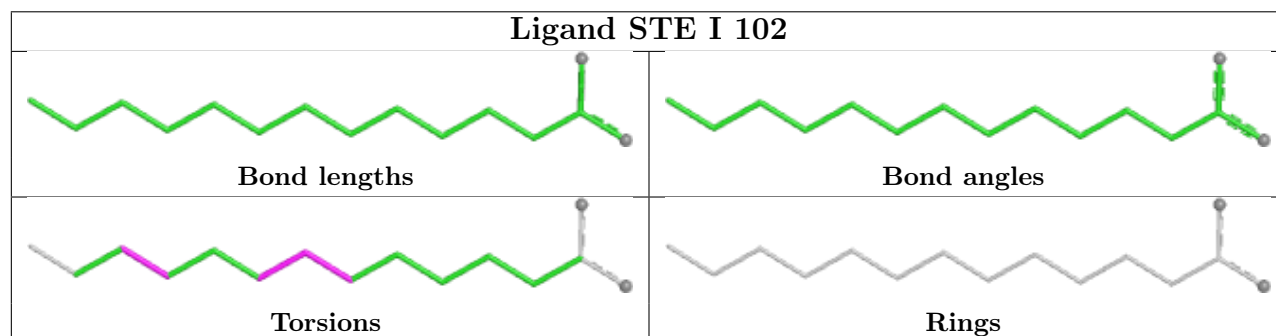
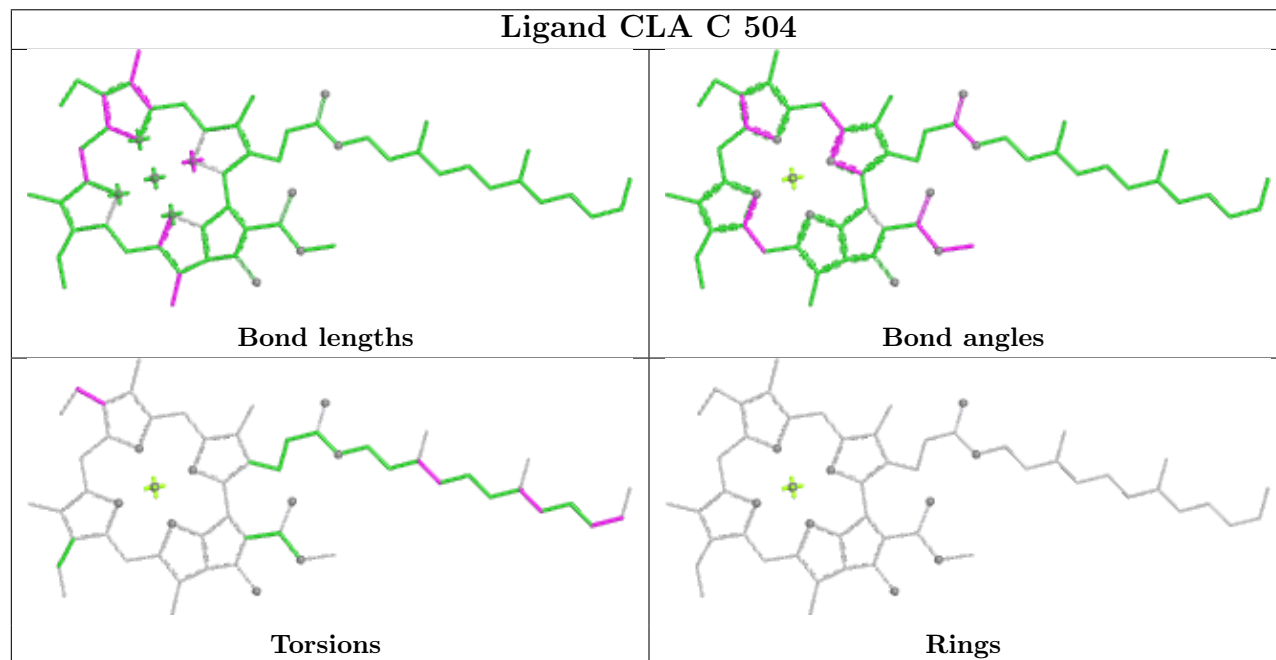
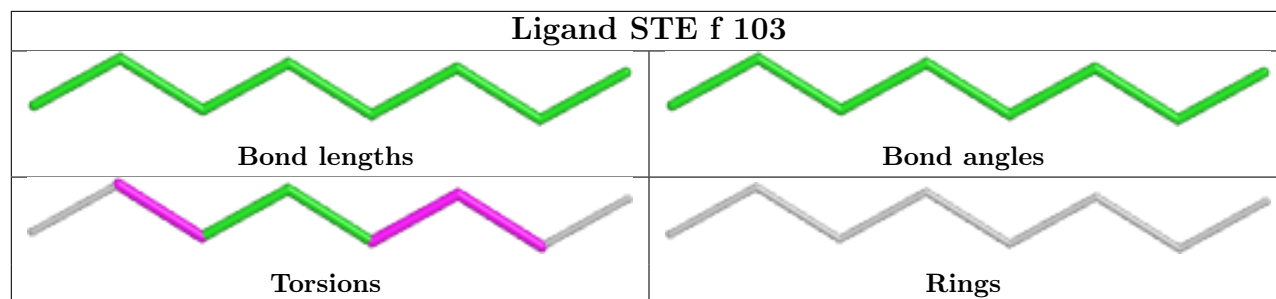


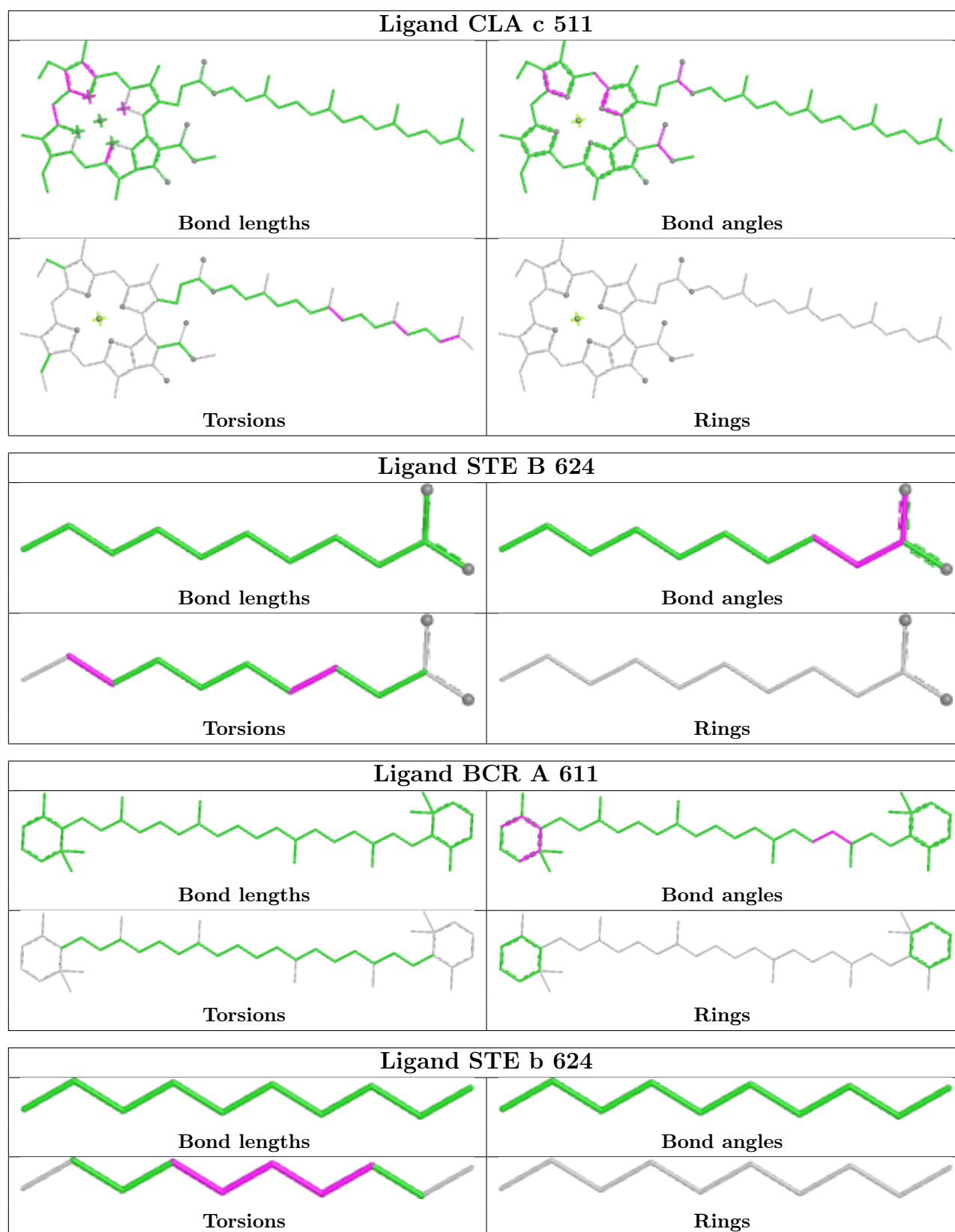


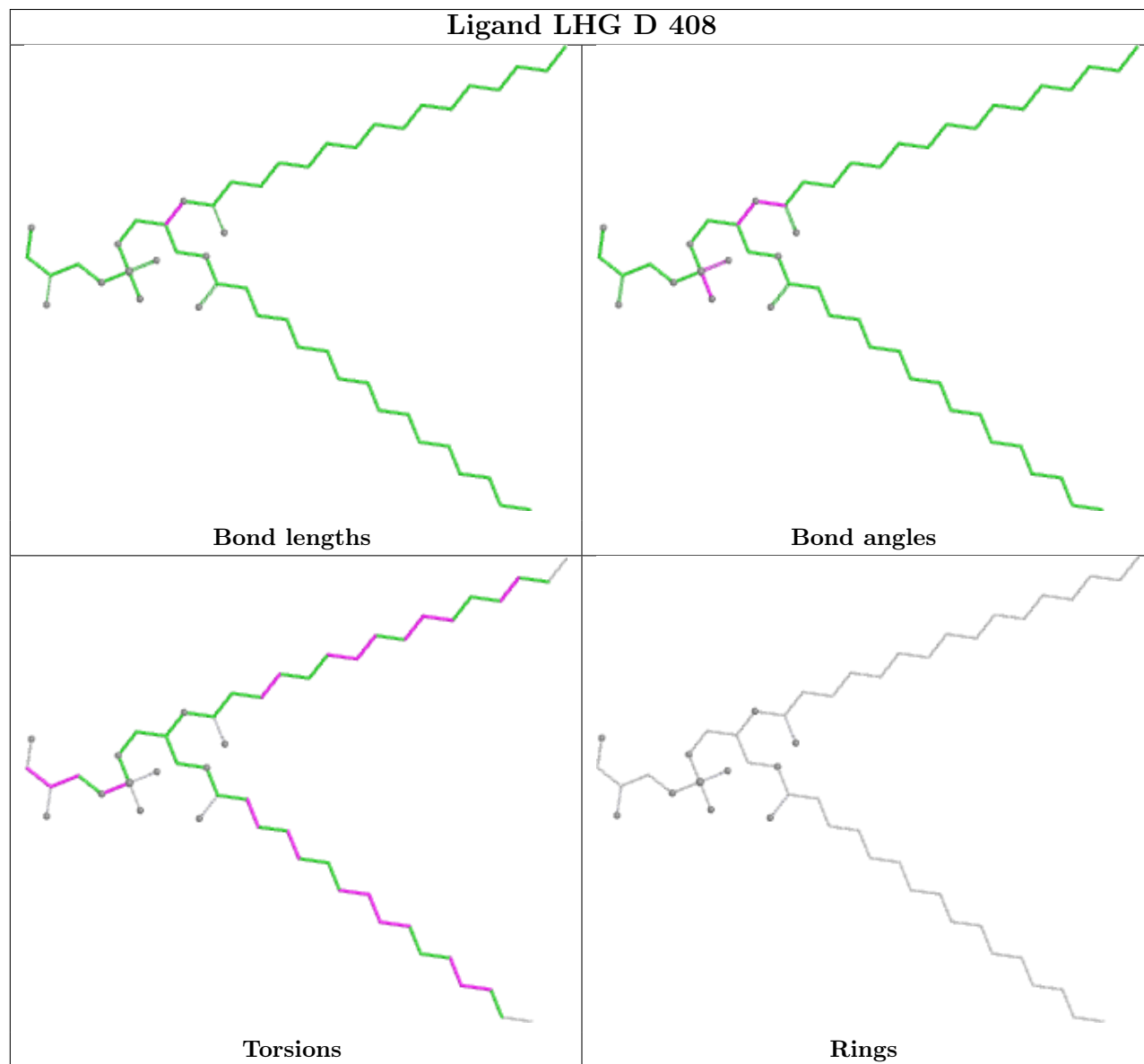
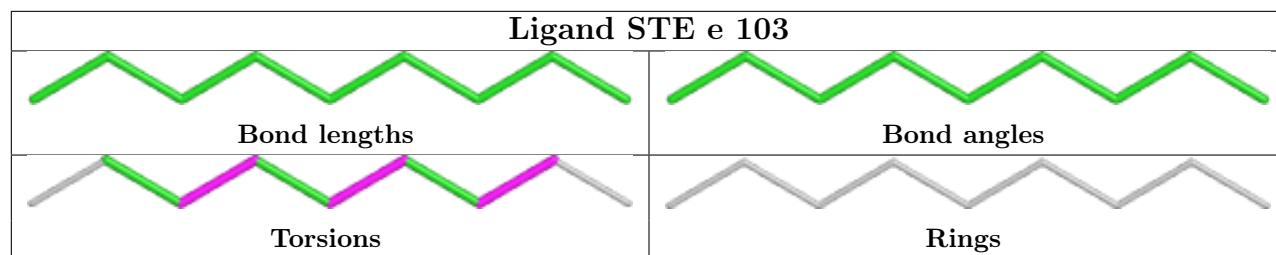


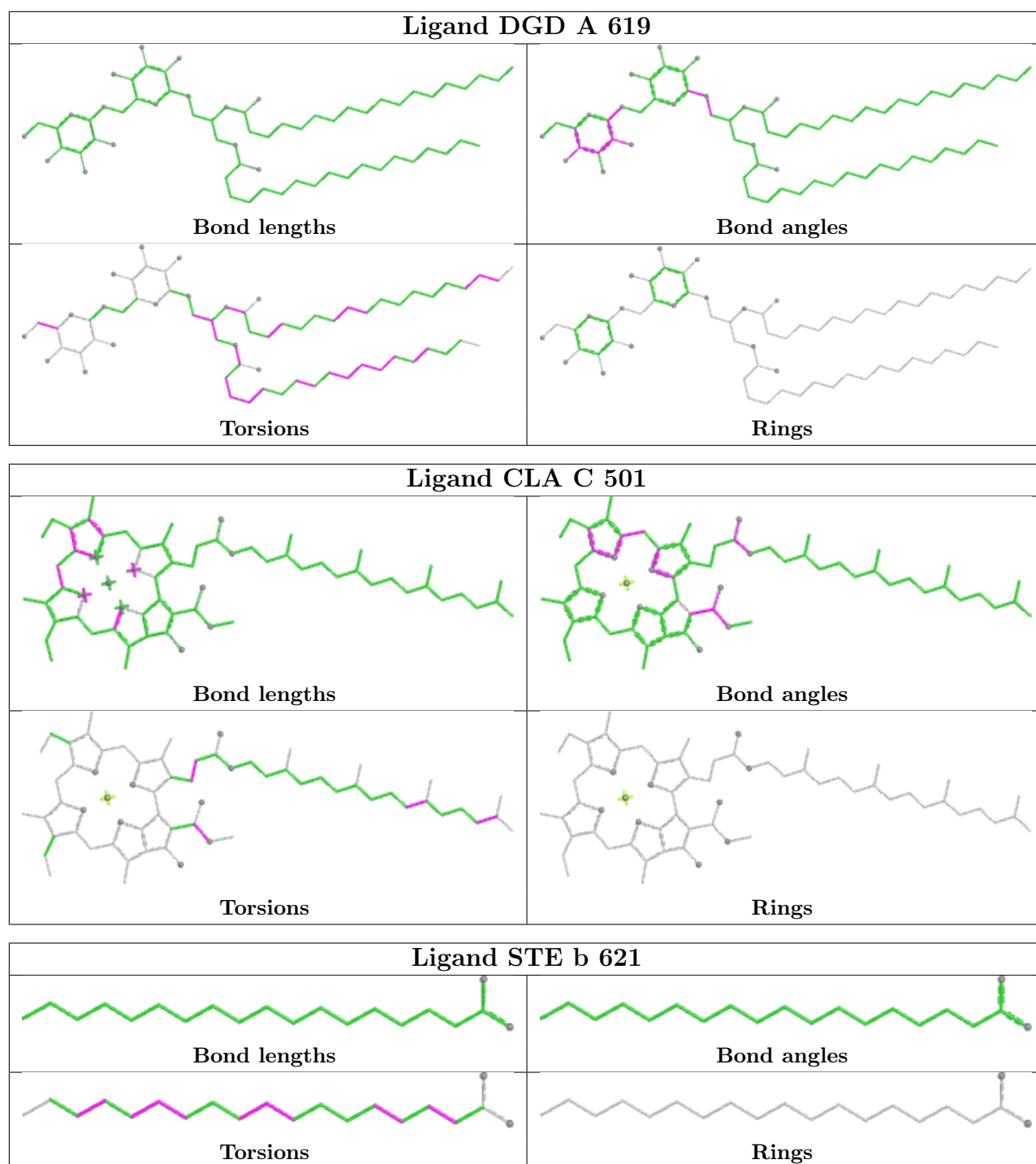
Ligand STE E 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE c 516	
 Bond lengths	 Bond angles
 Torsions	 Rings



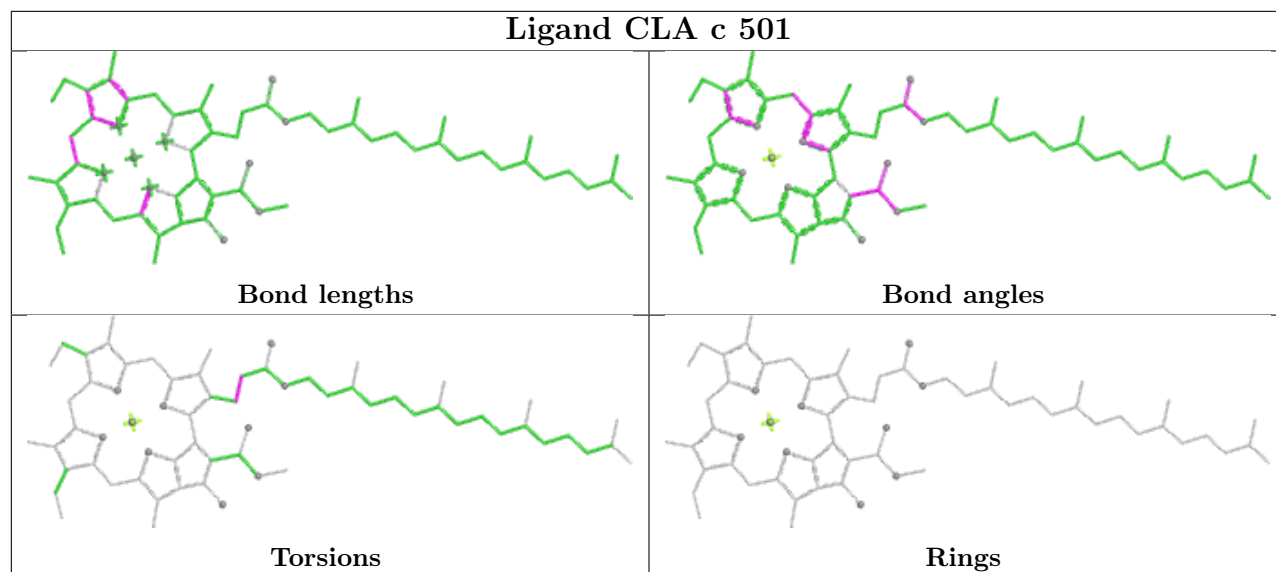




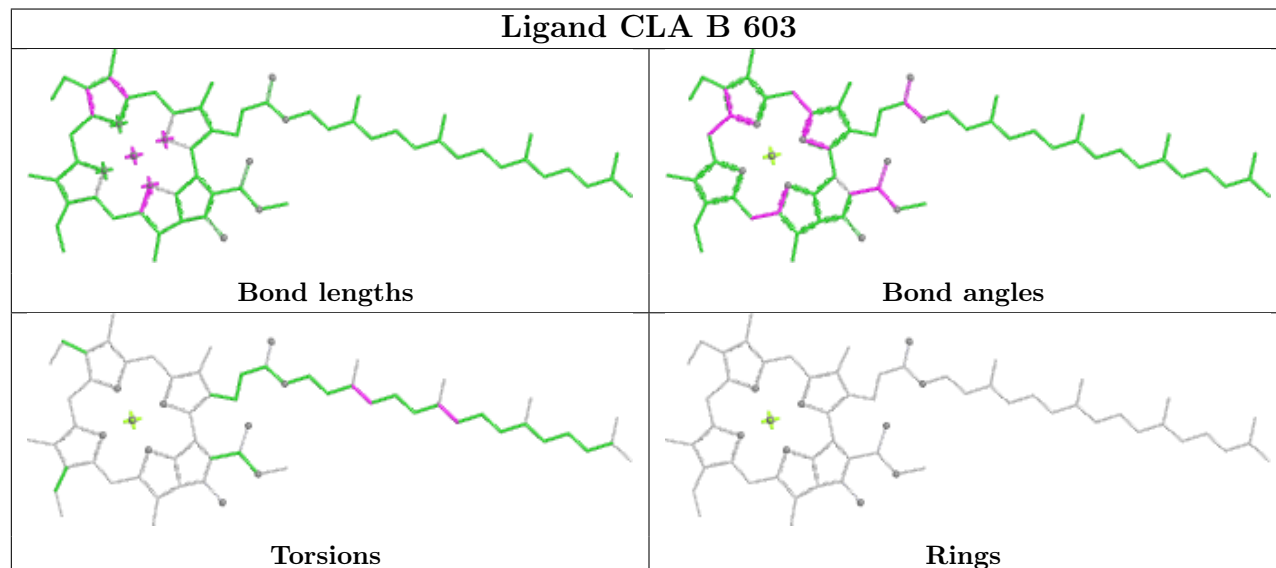




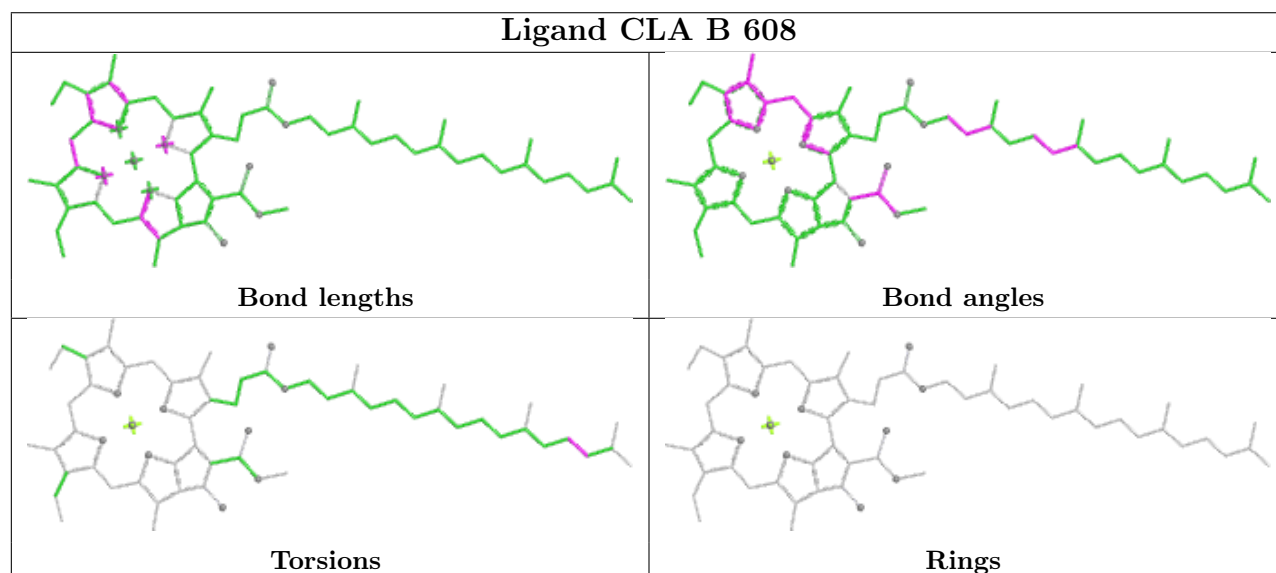
Ligand CLA c 501

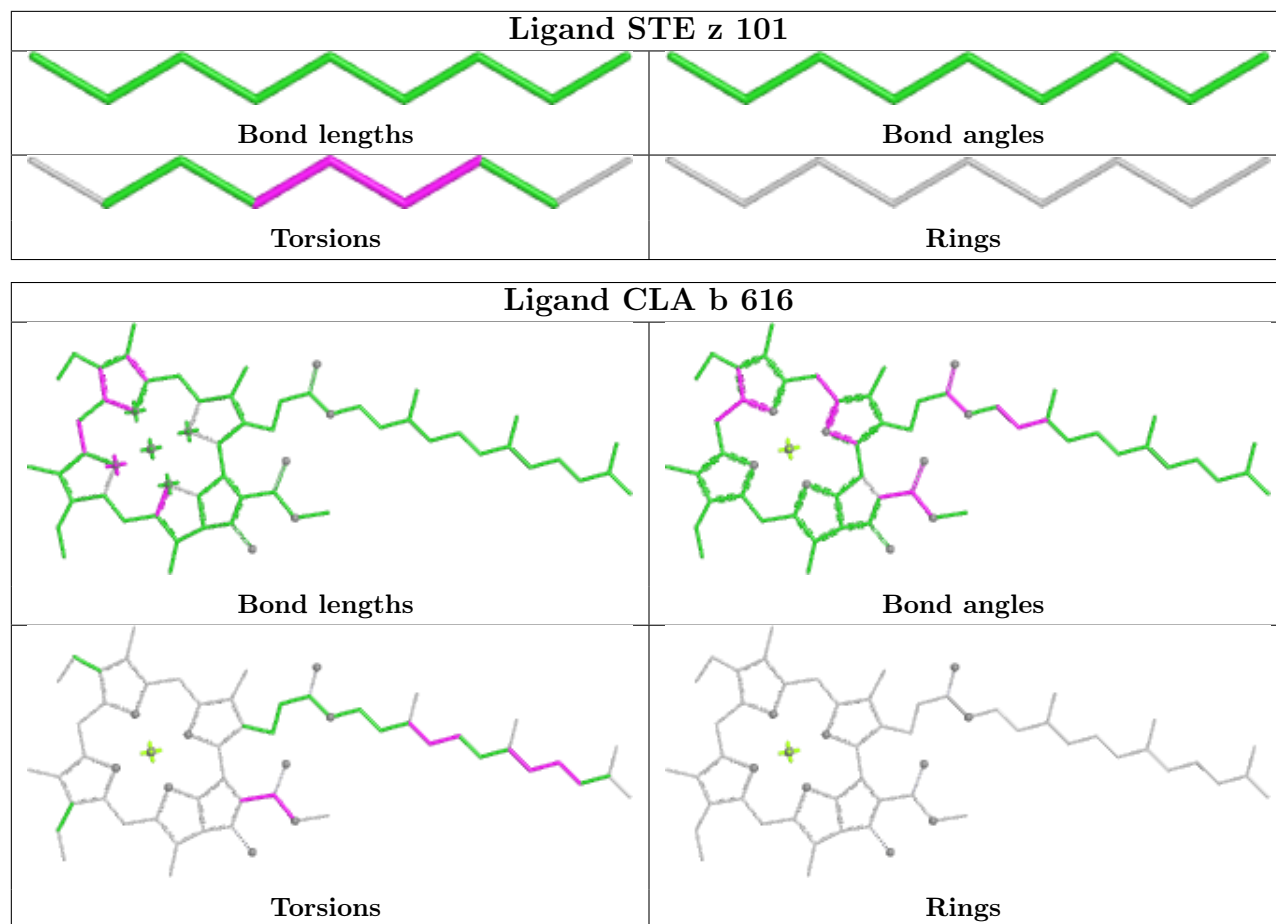


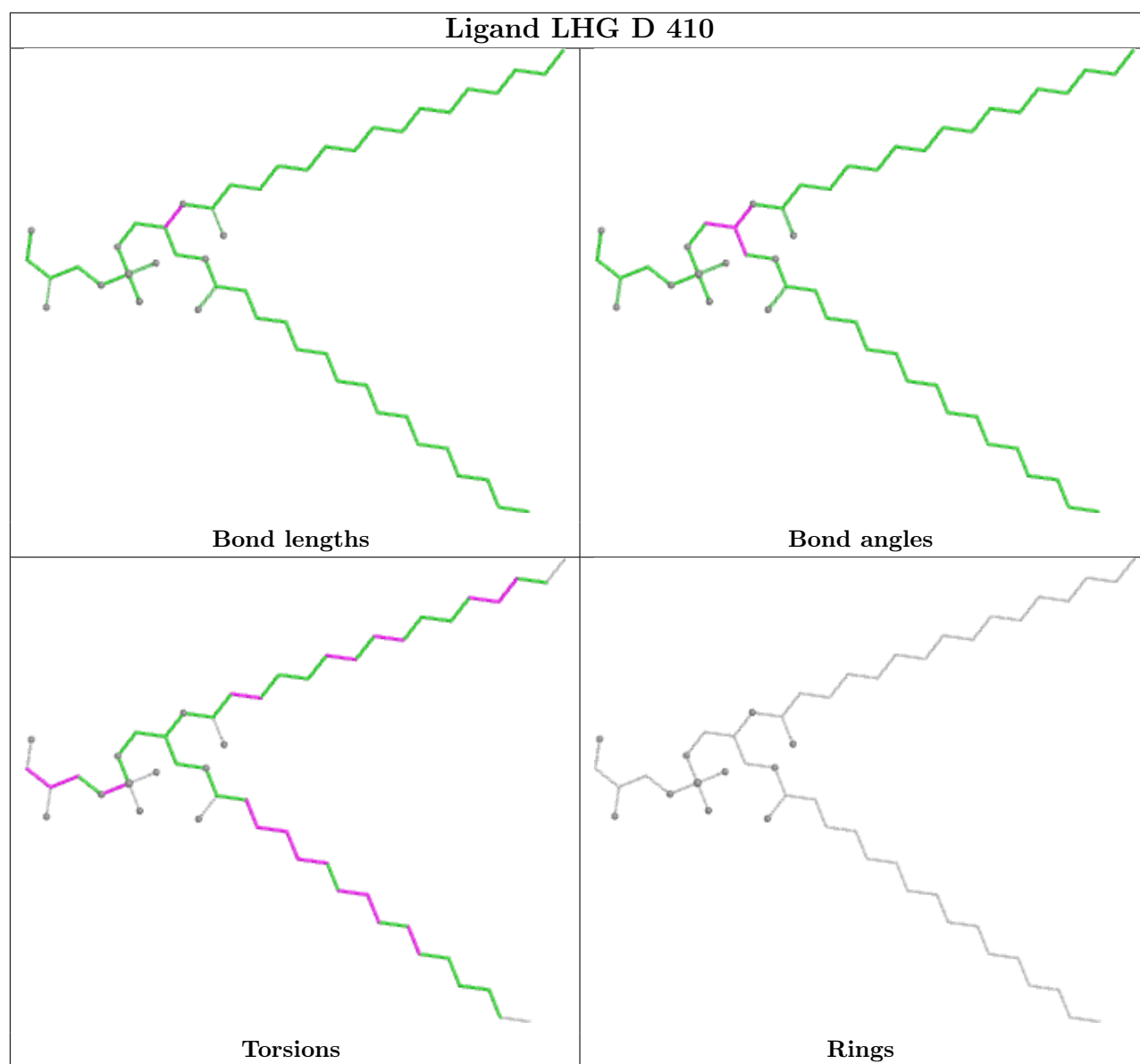
Ligand CLA B 603

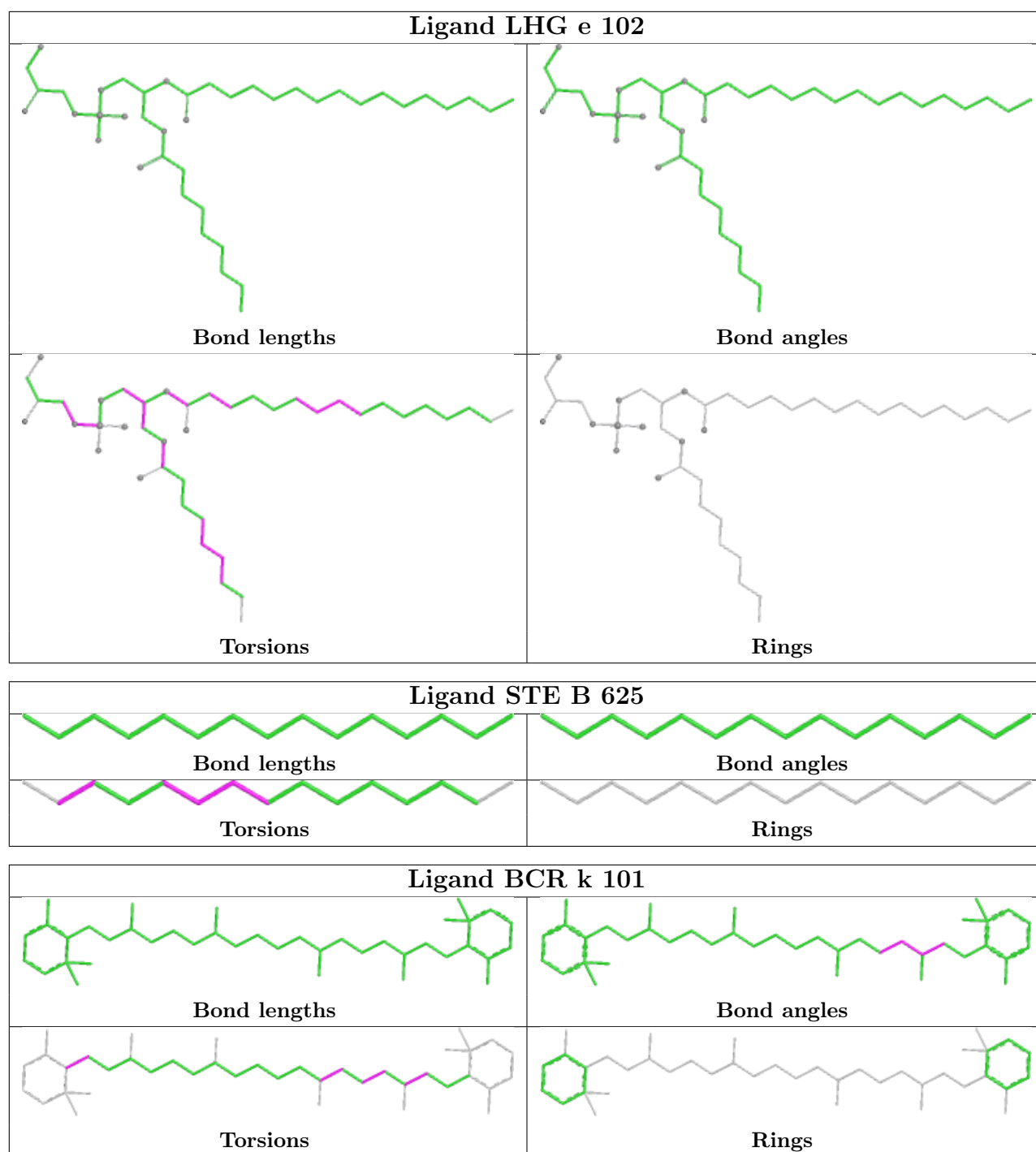


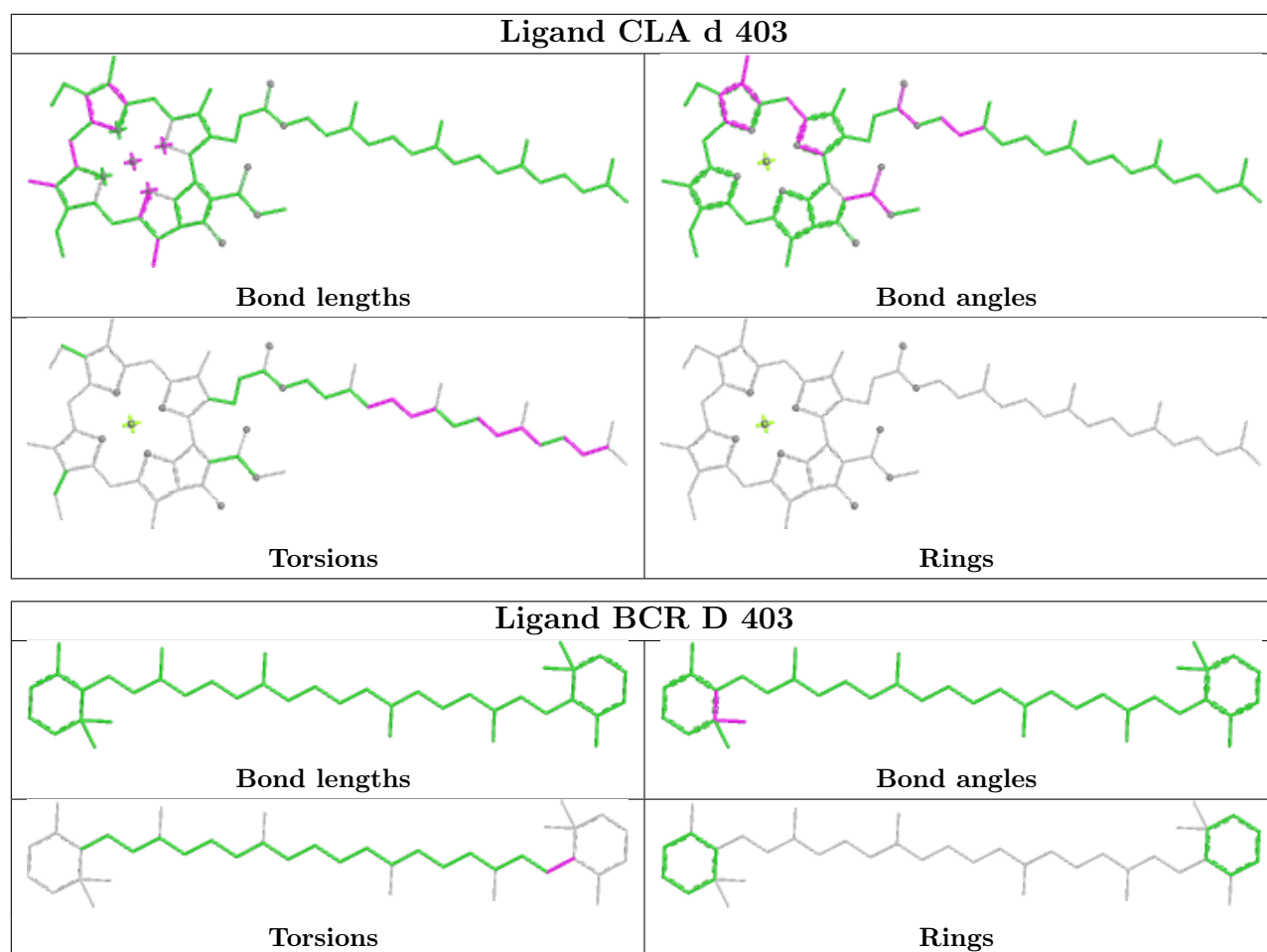
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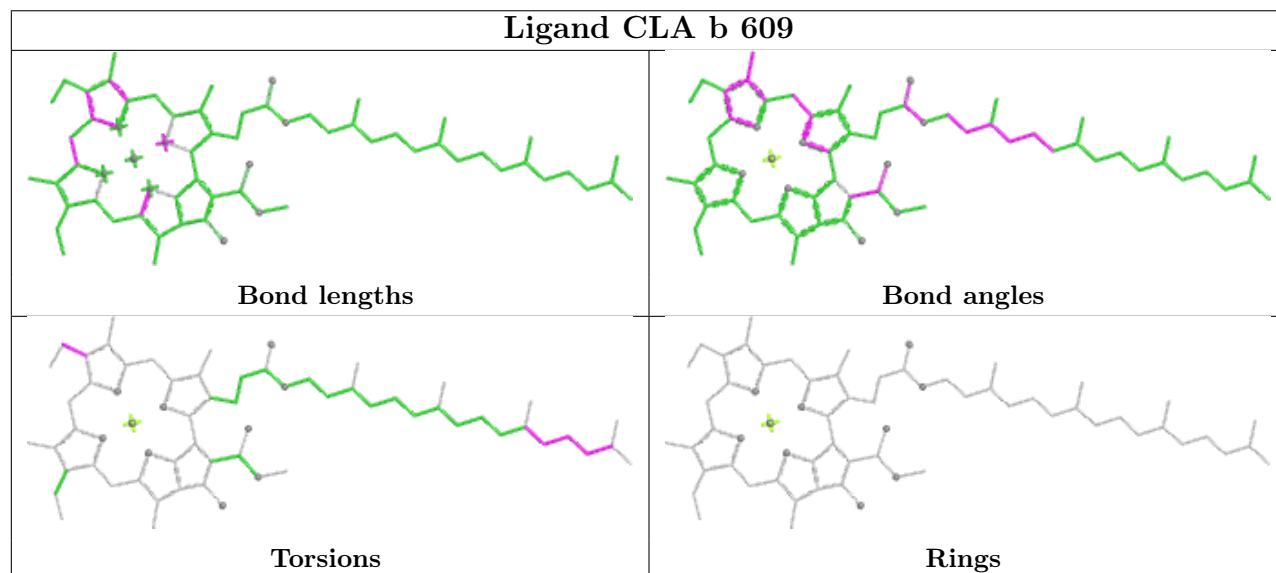
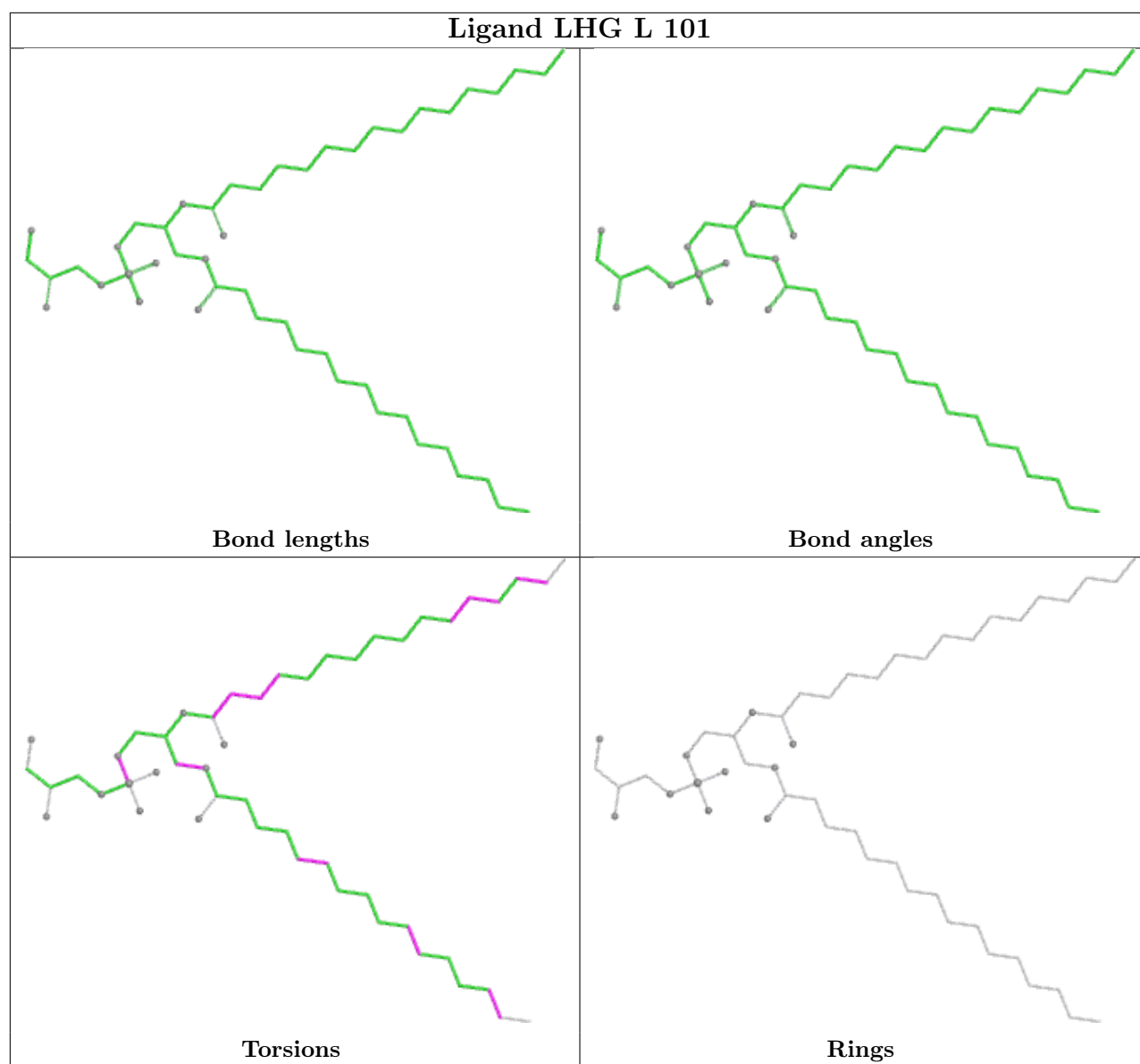


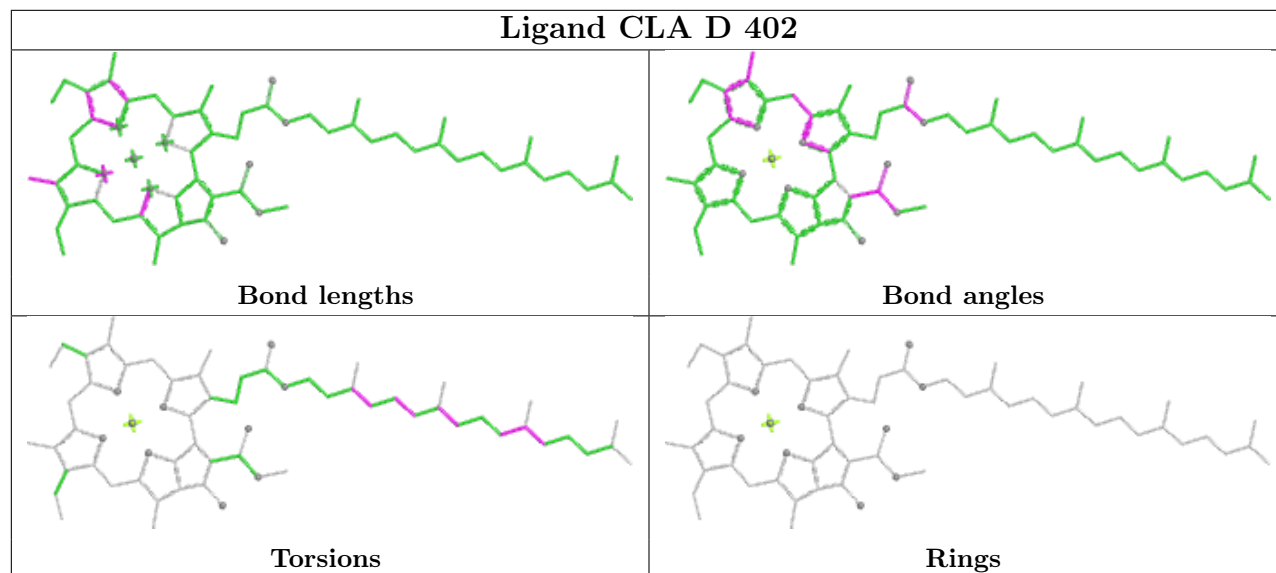
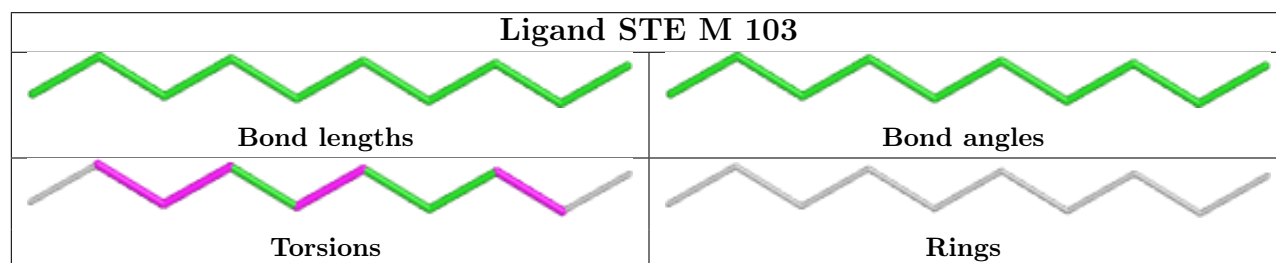
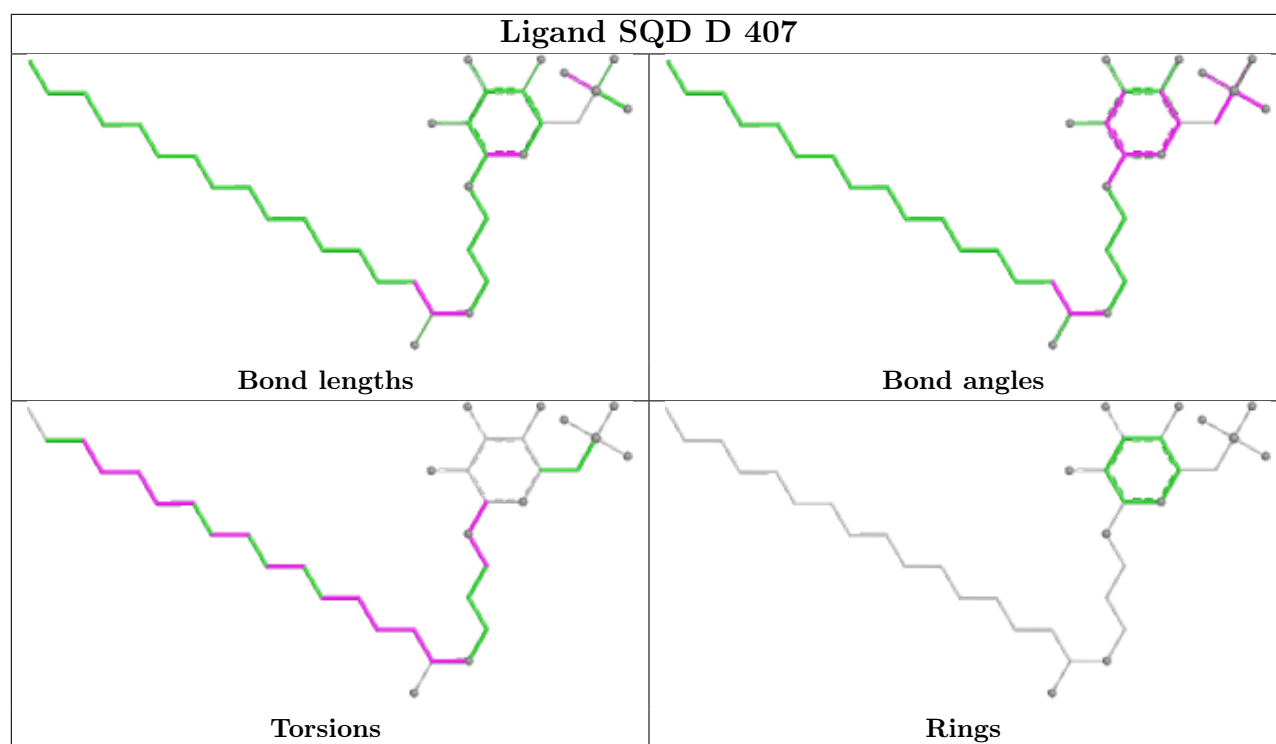


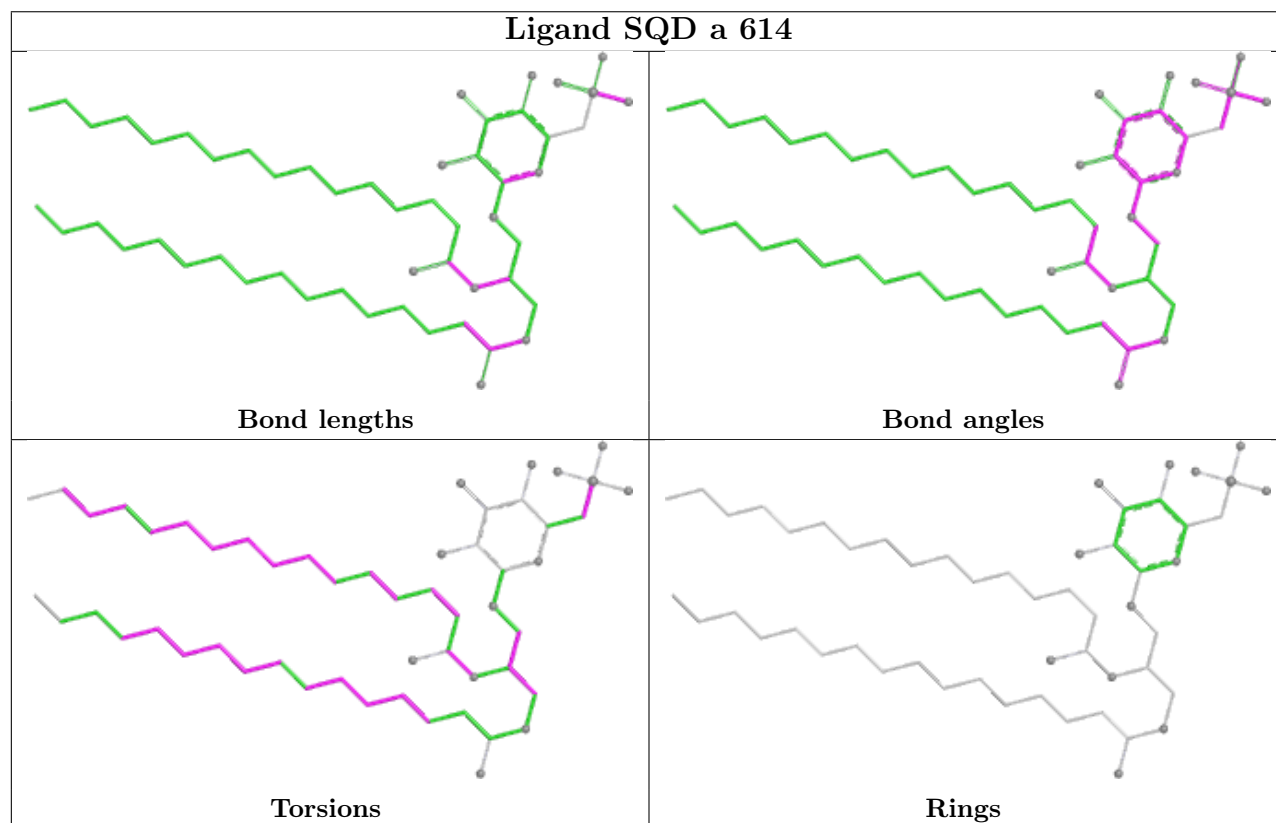
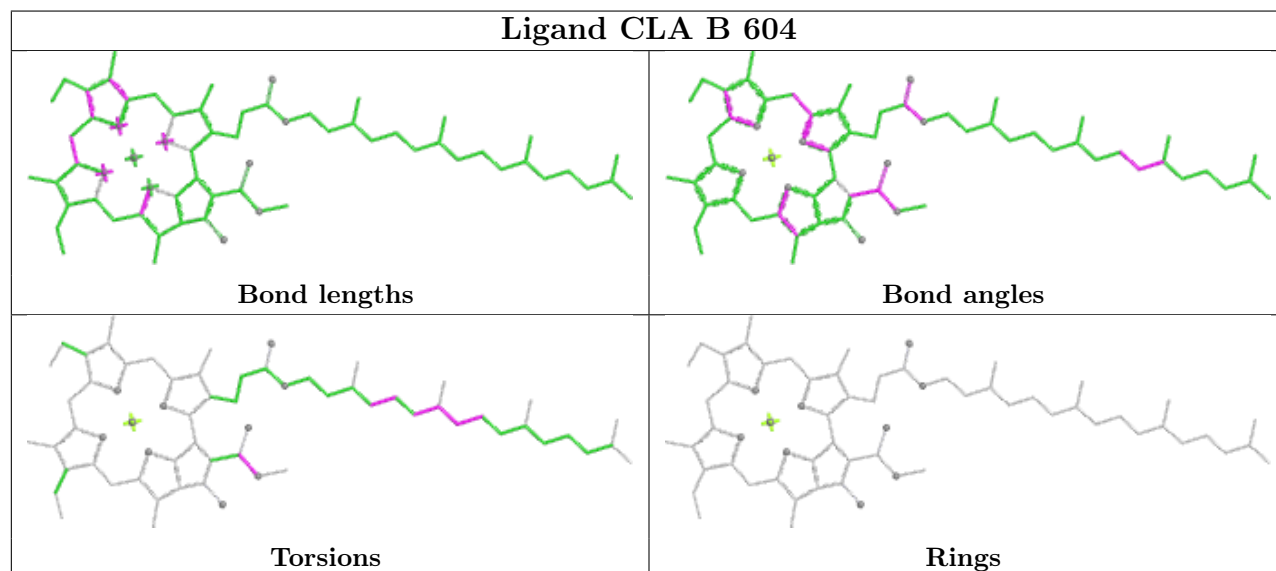
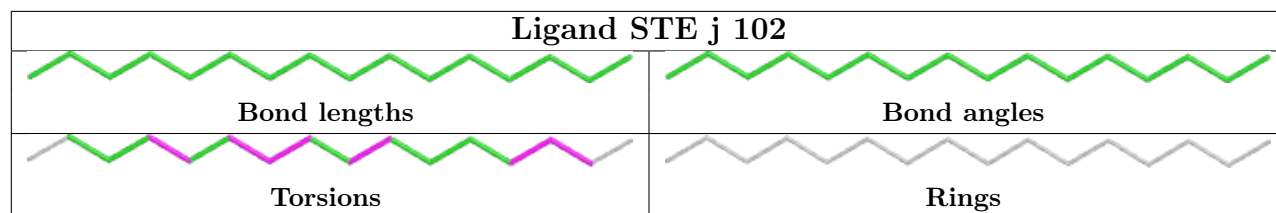


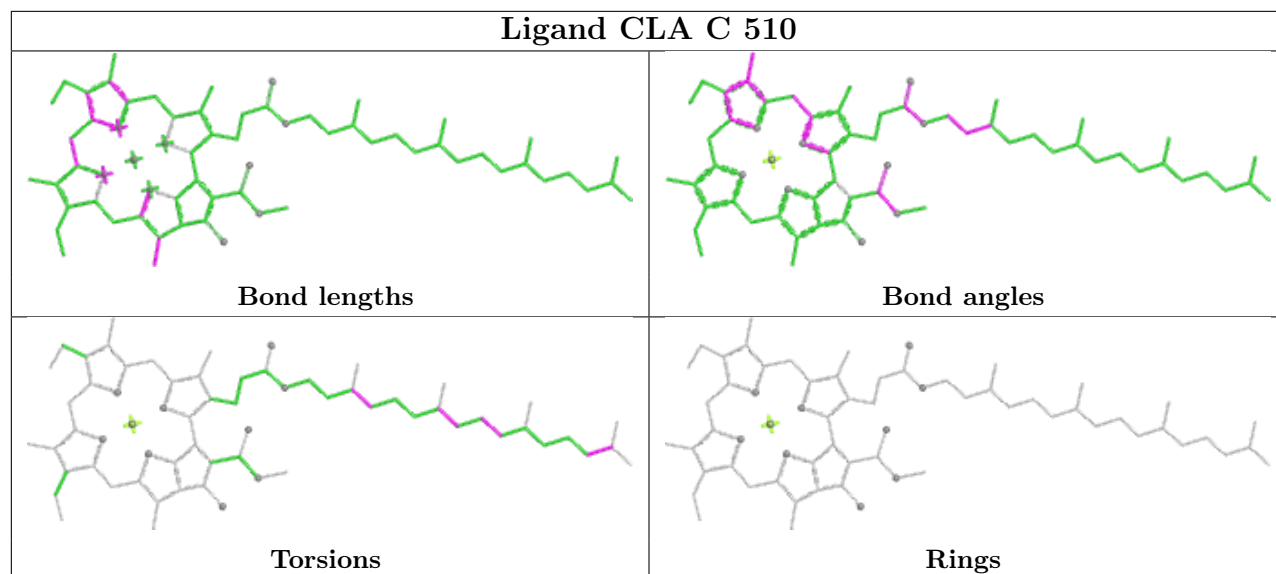
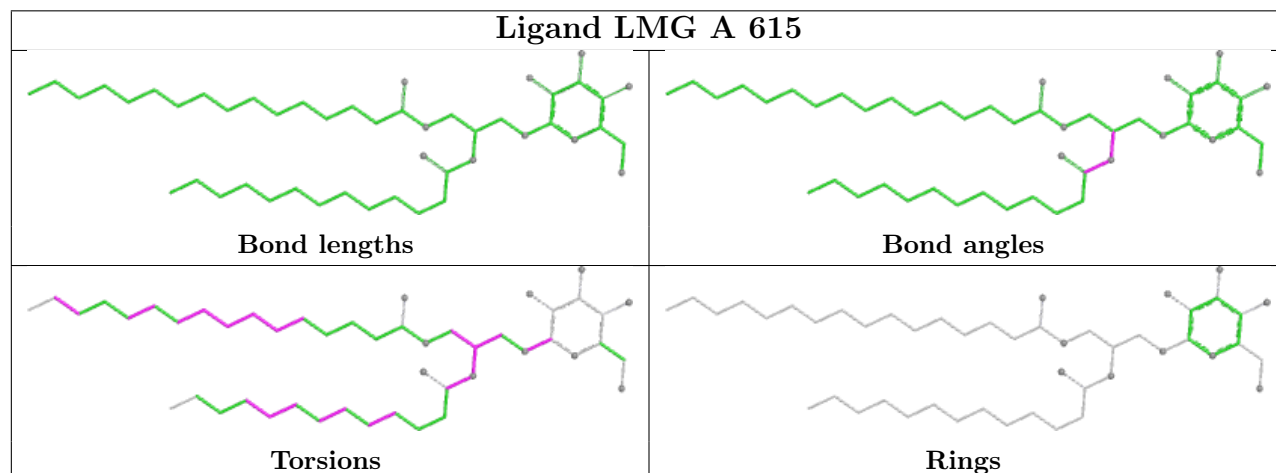




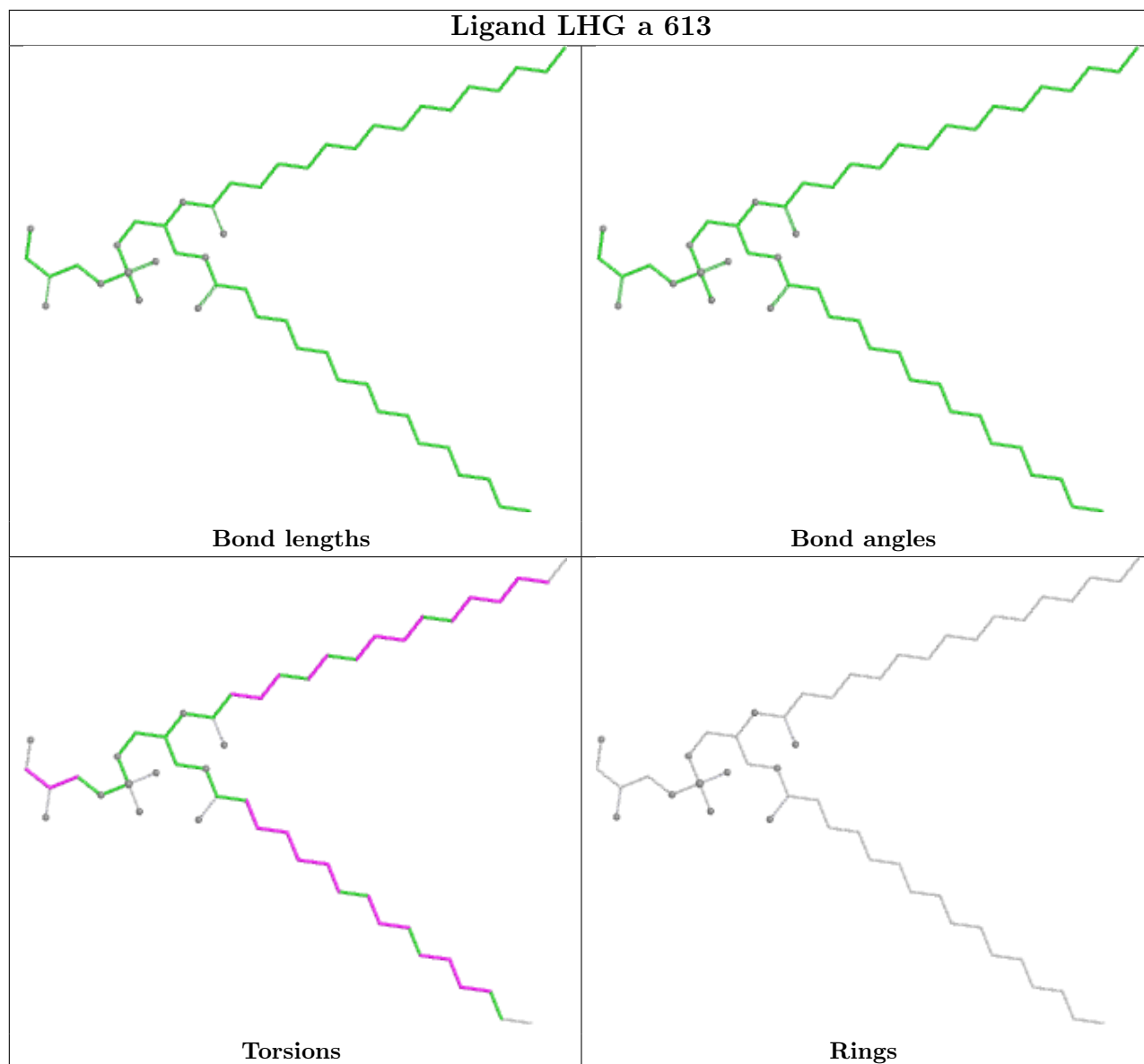




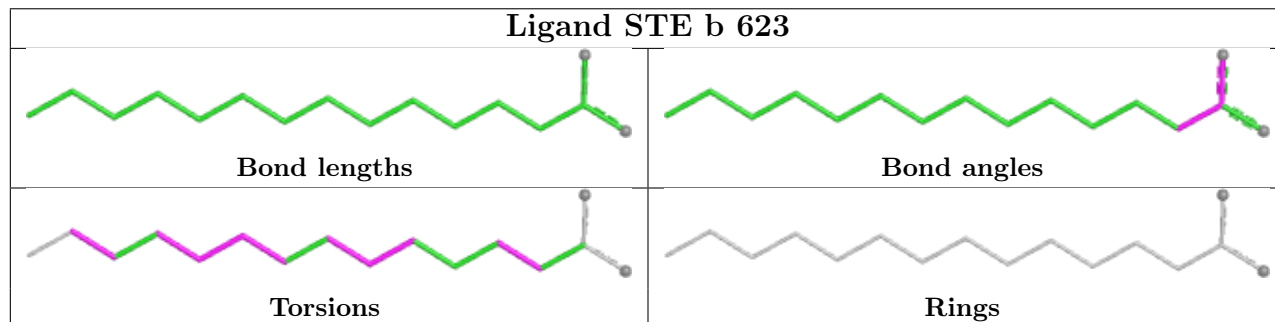


Ligand CLA C 510**Ligand LMG A 615**

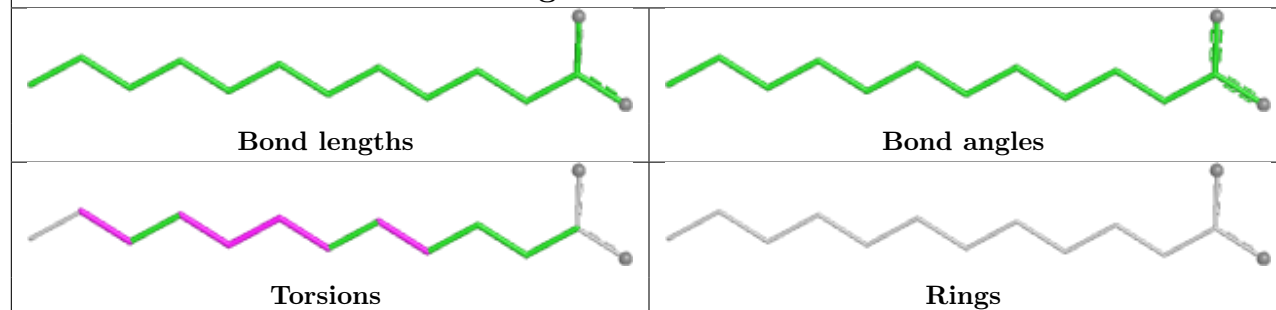
Ligand LHG a 613



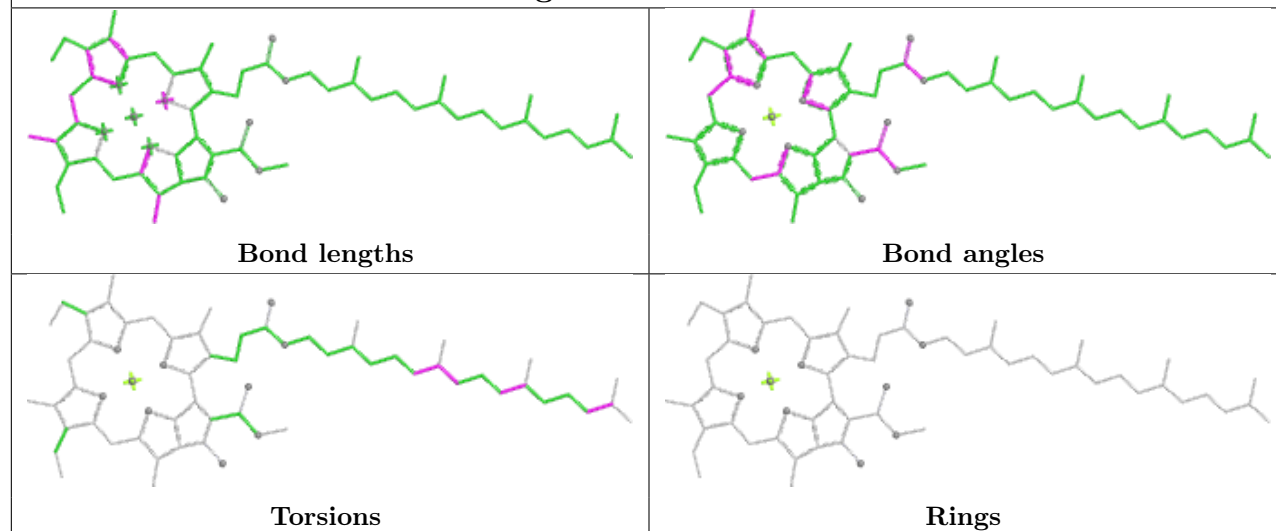
Ligand STE b 623



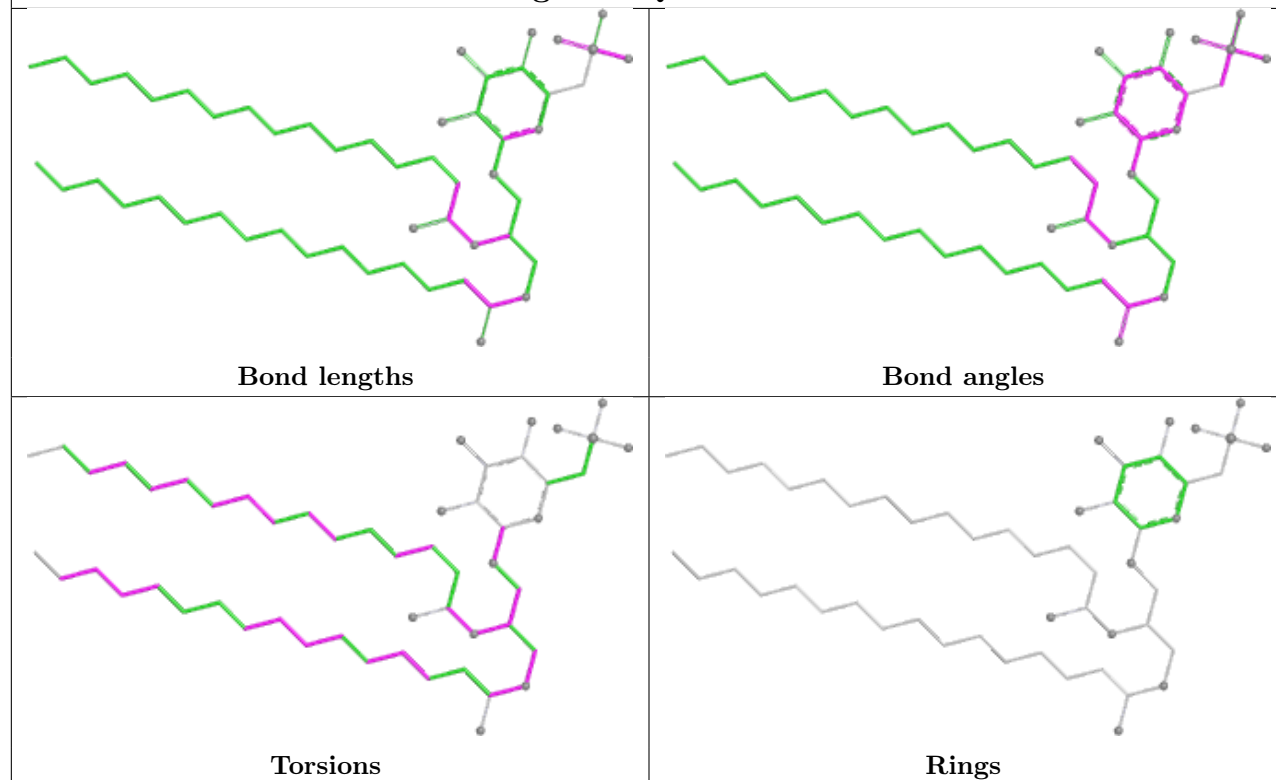
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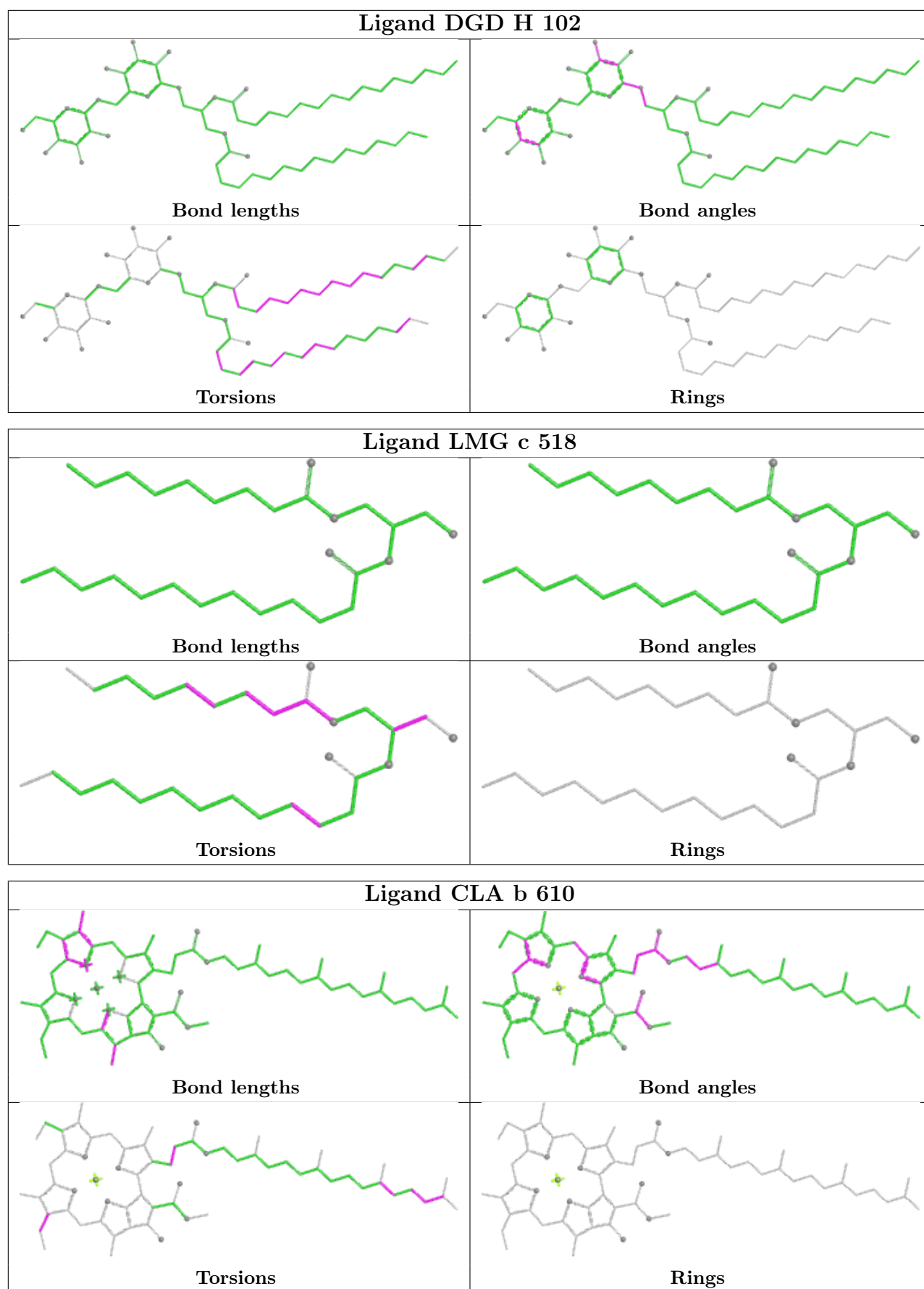


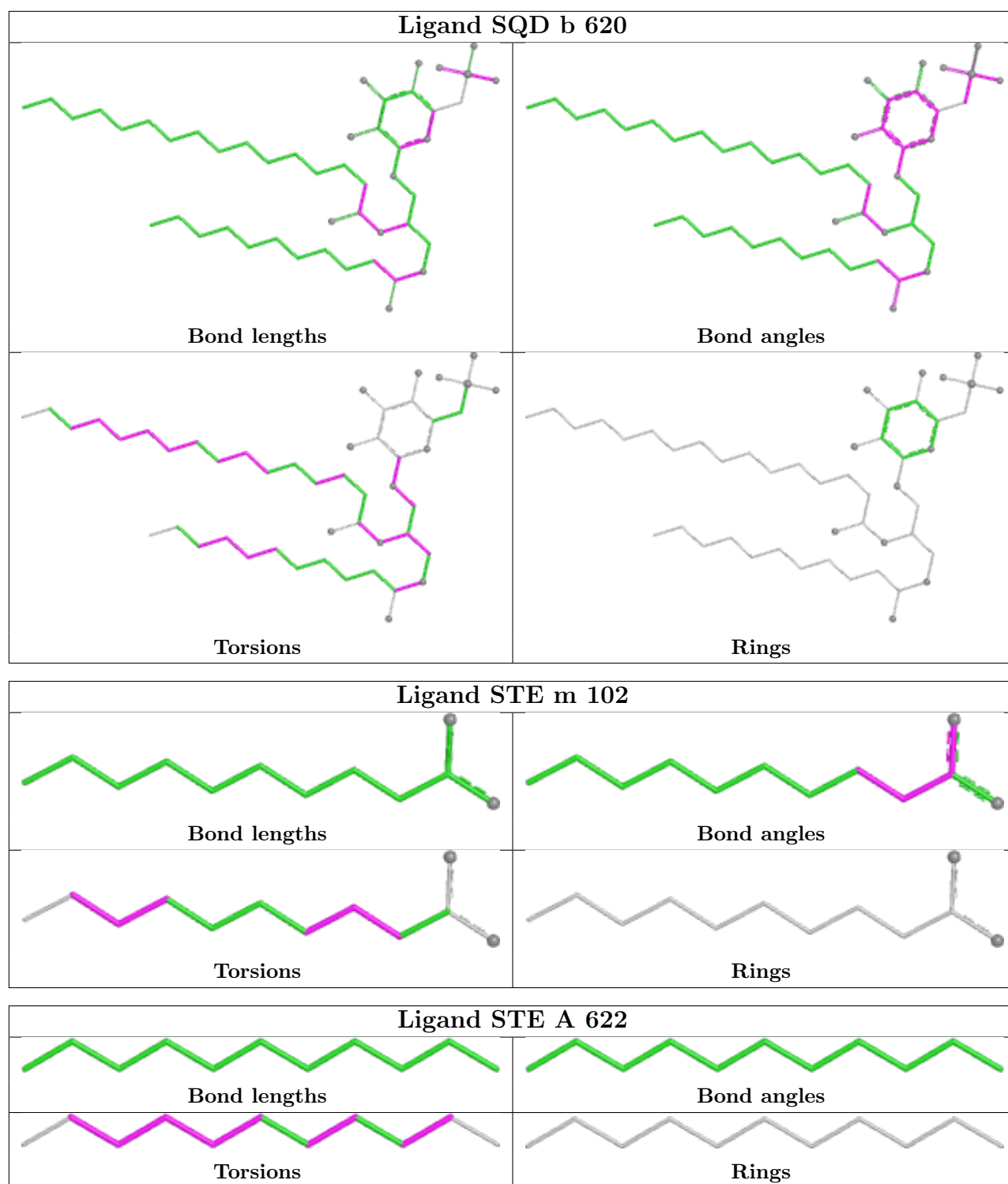
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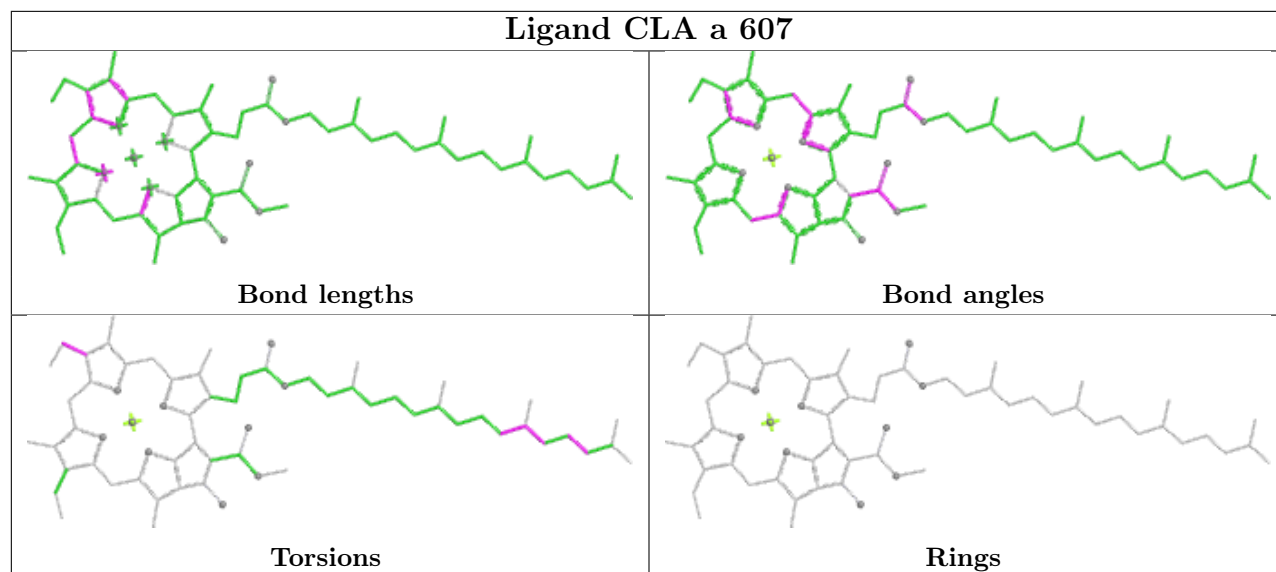
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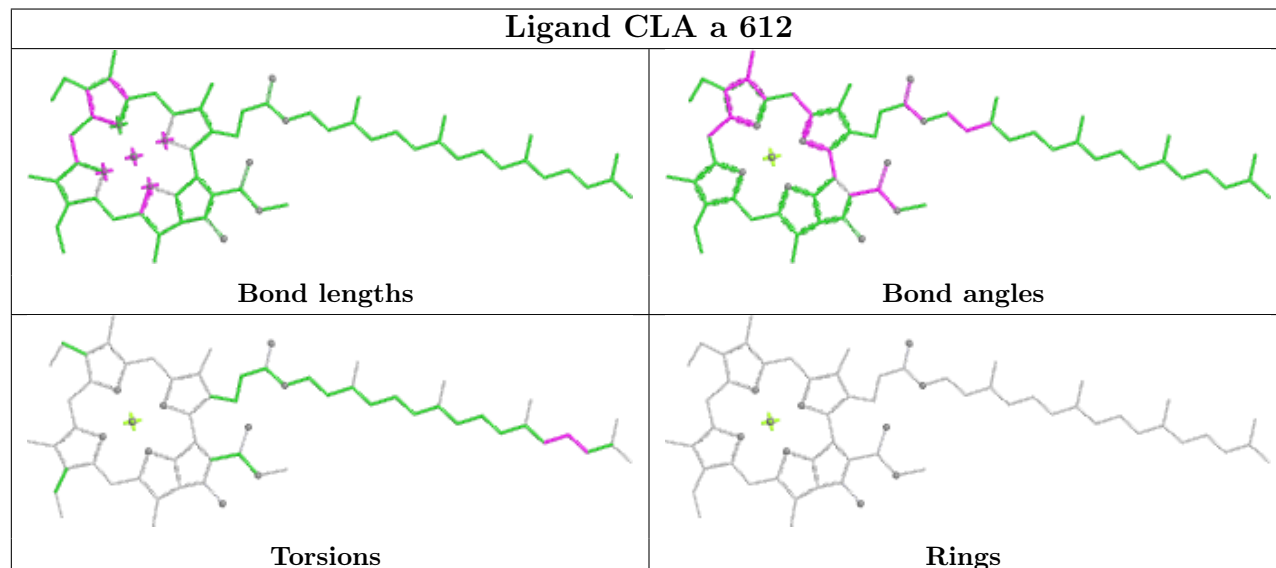




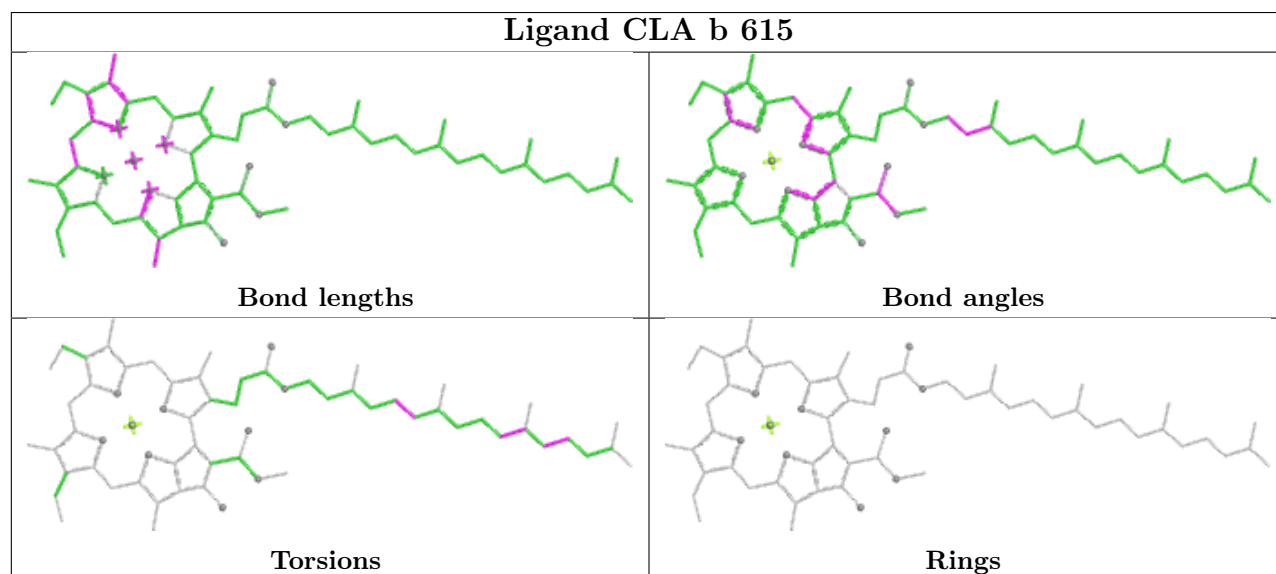
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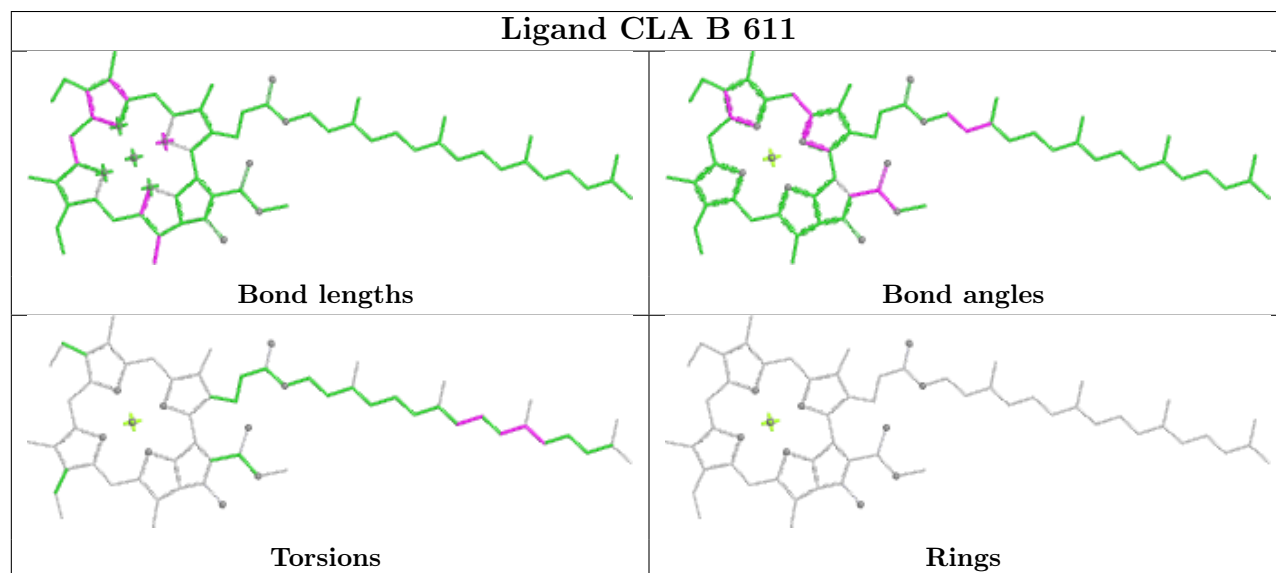
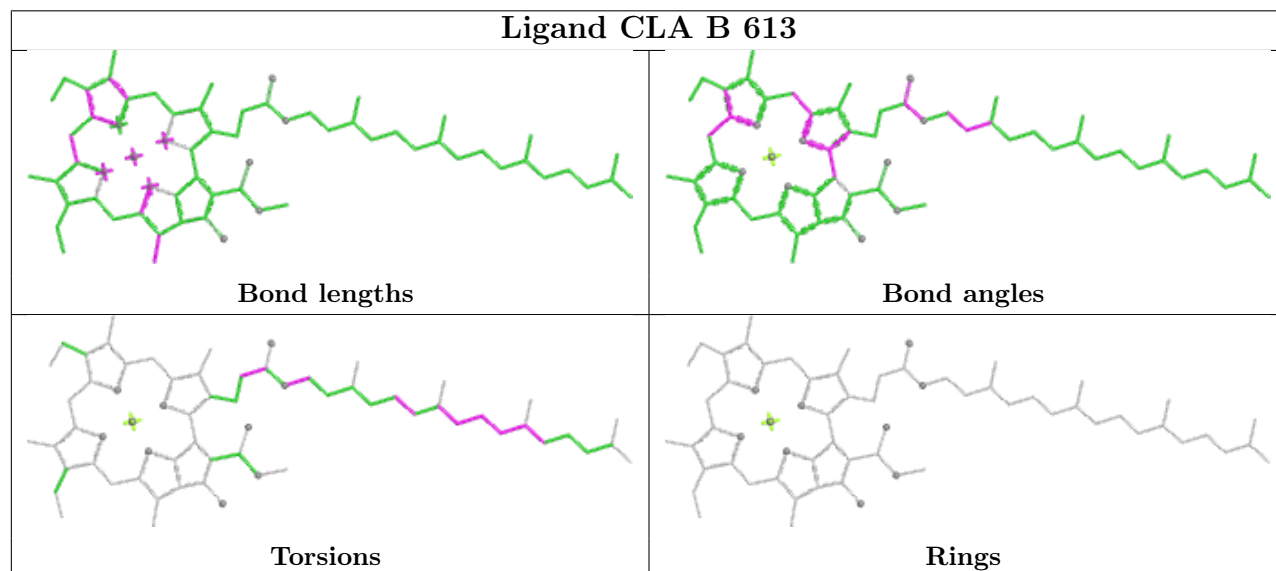
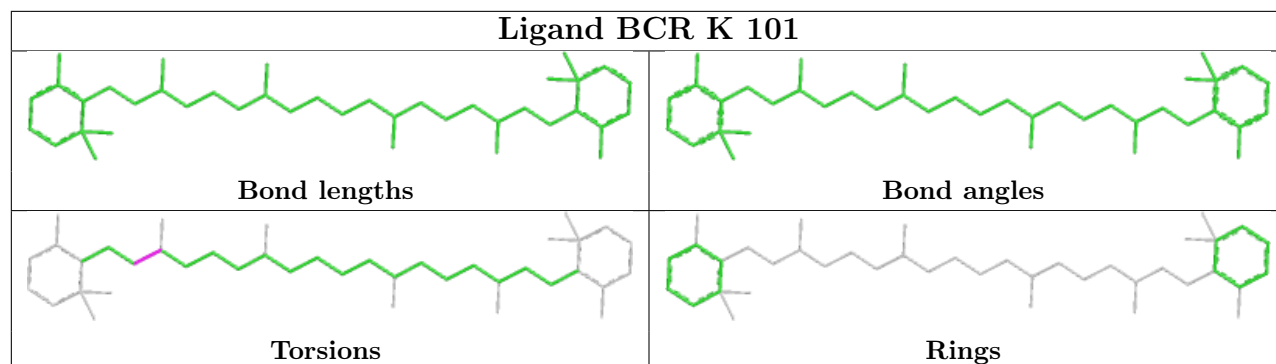


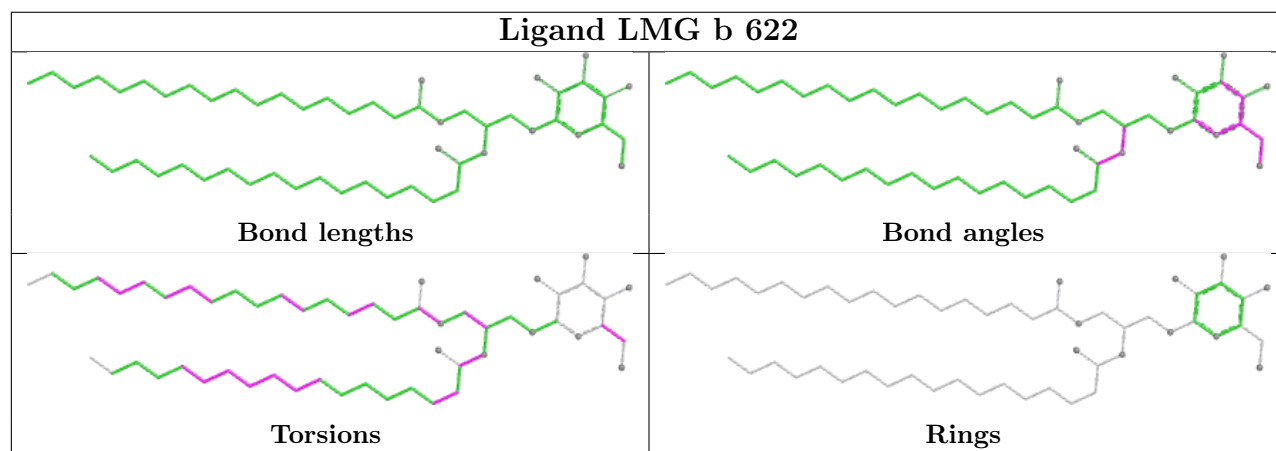
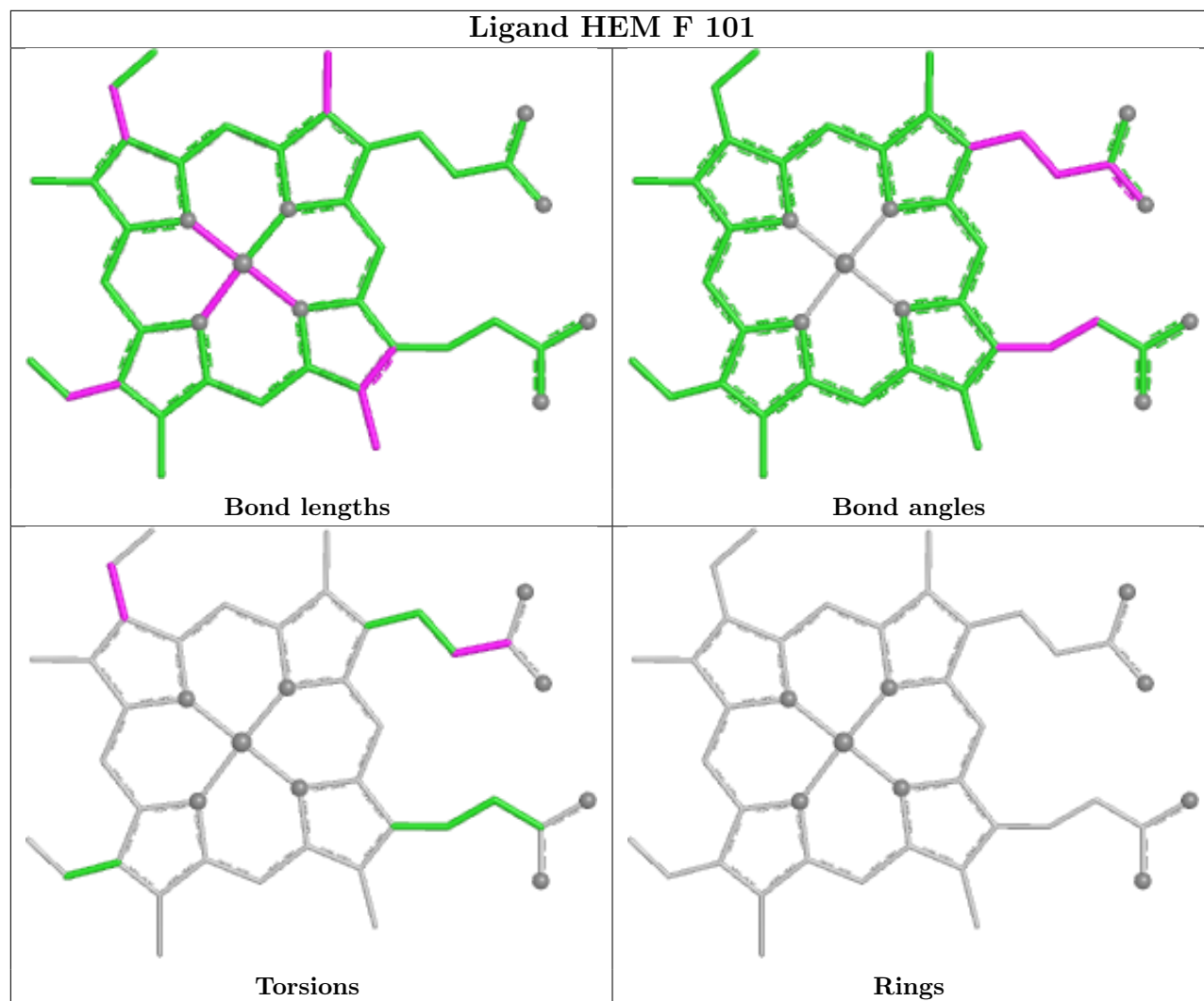
Ligand CLA a 612

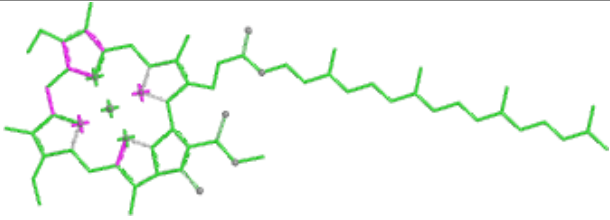
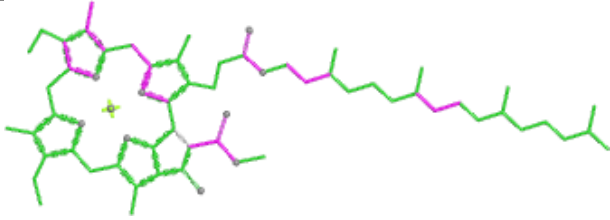
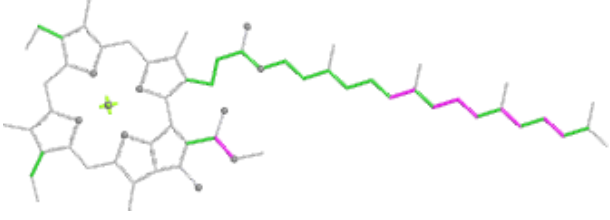
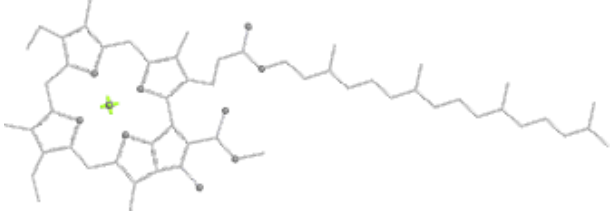
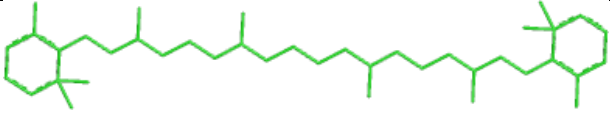
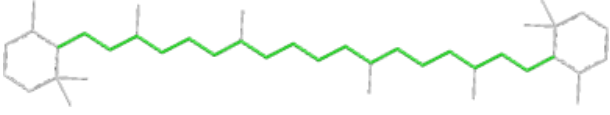
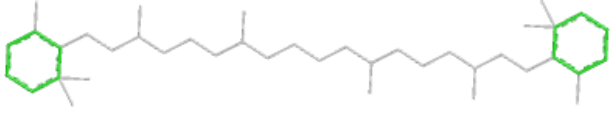
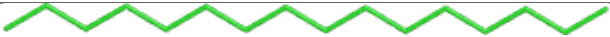
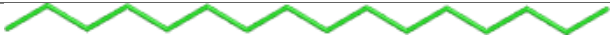


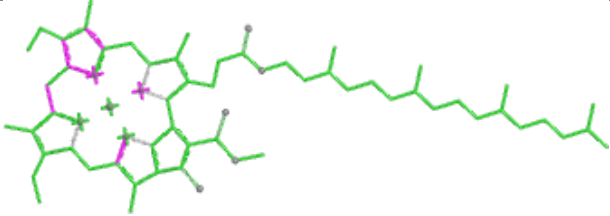
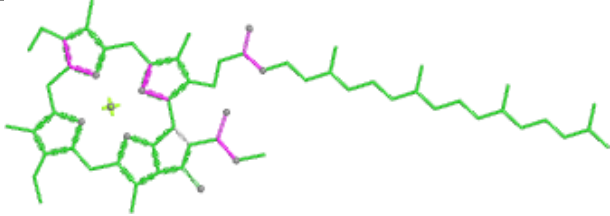
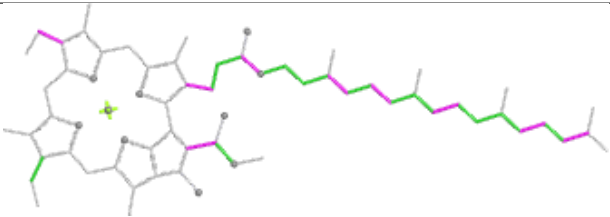
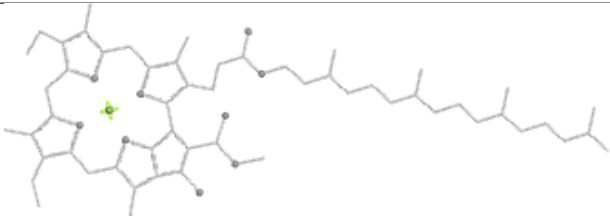
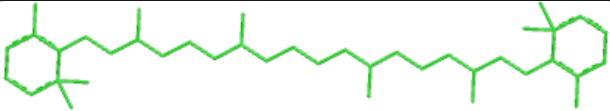
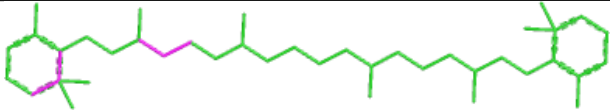
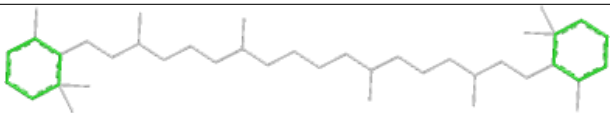
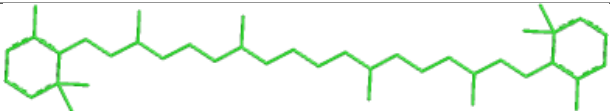
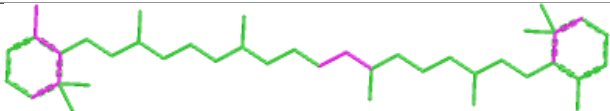
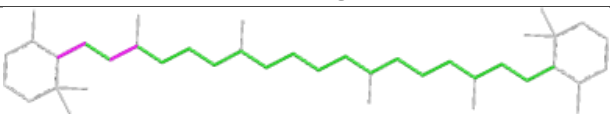
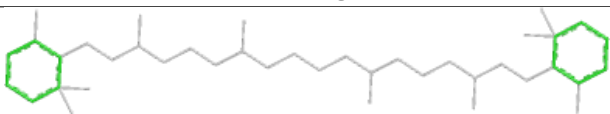
Ligand CLA b 615



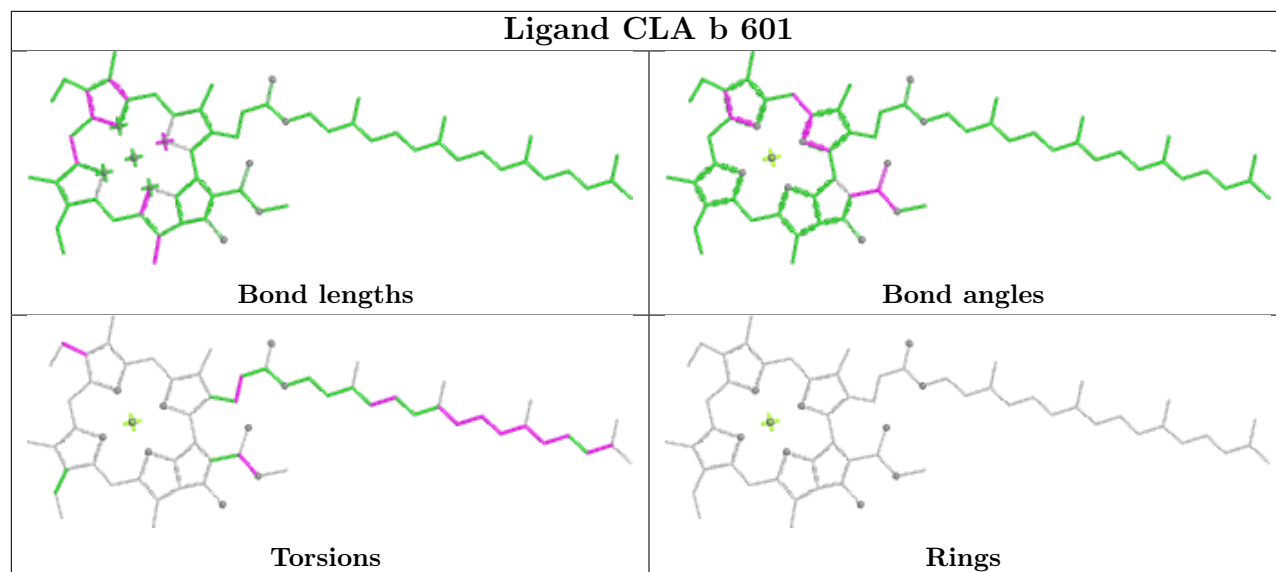




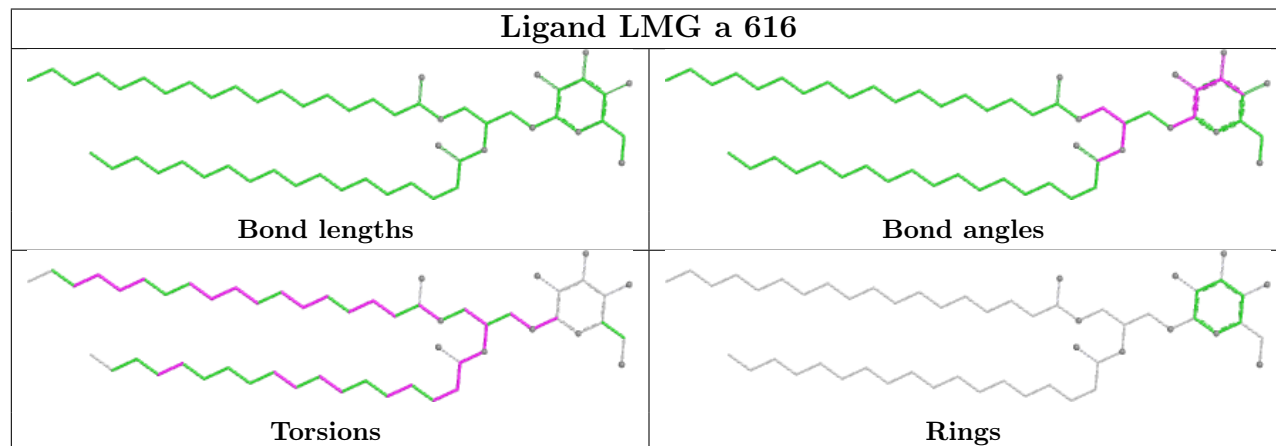
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE C 526	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

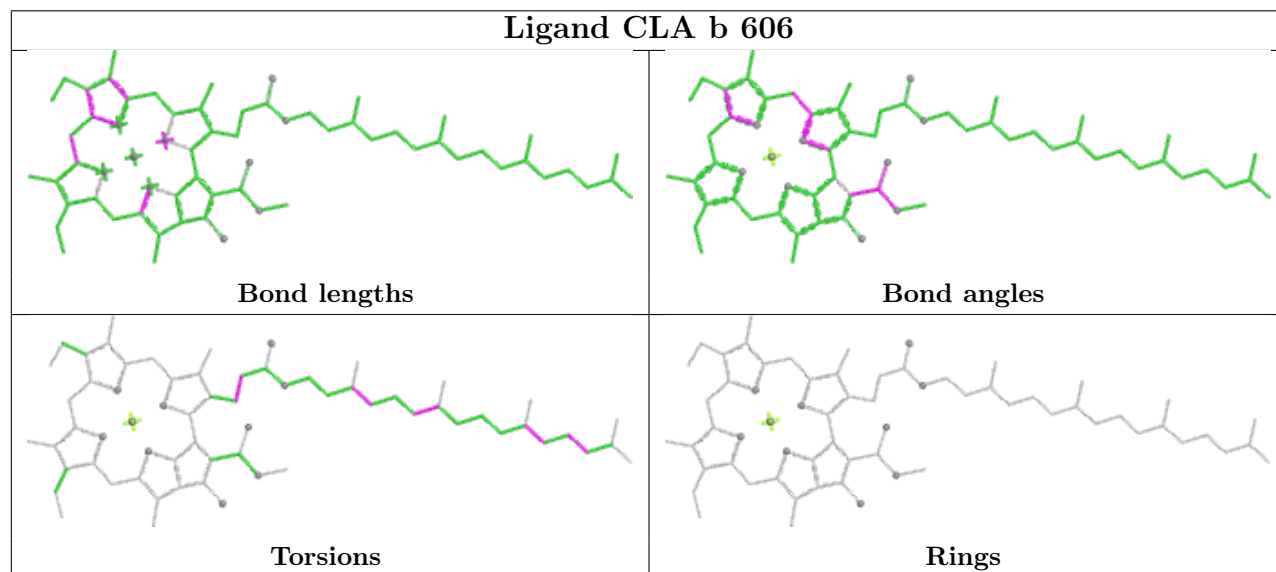
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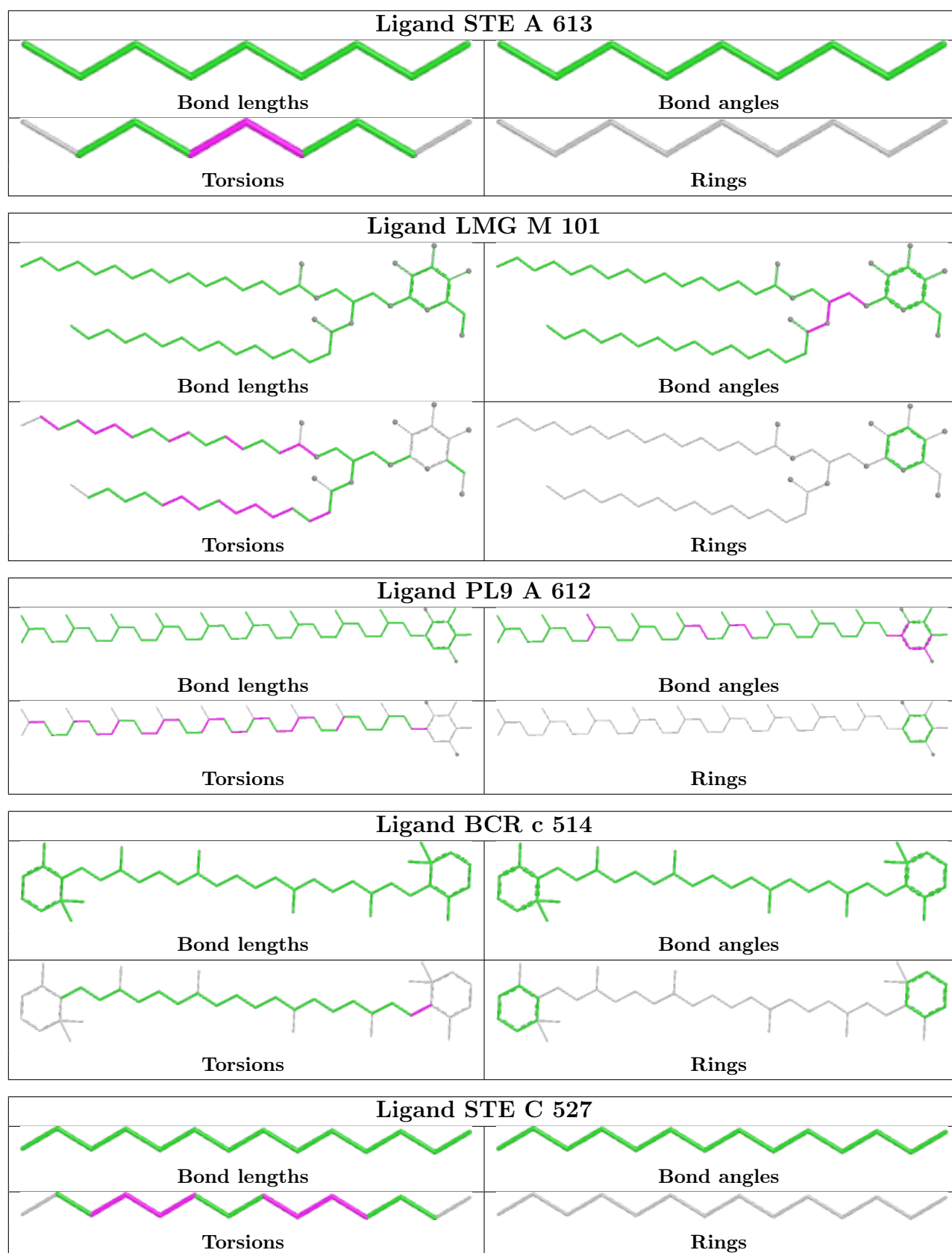


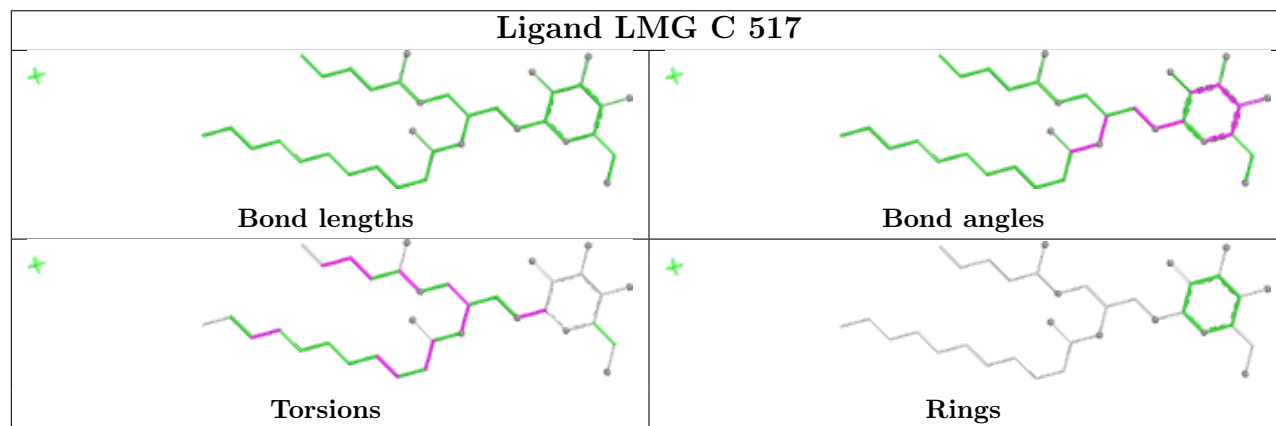
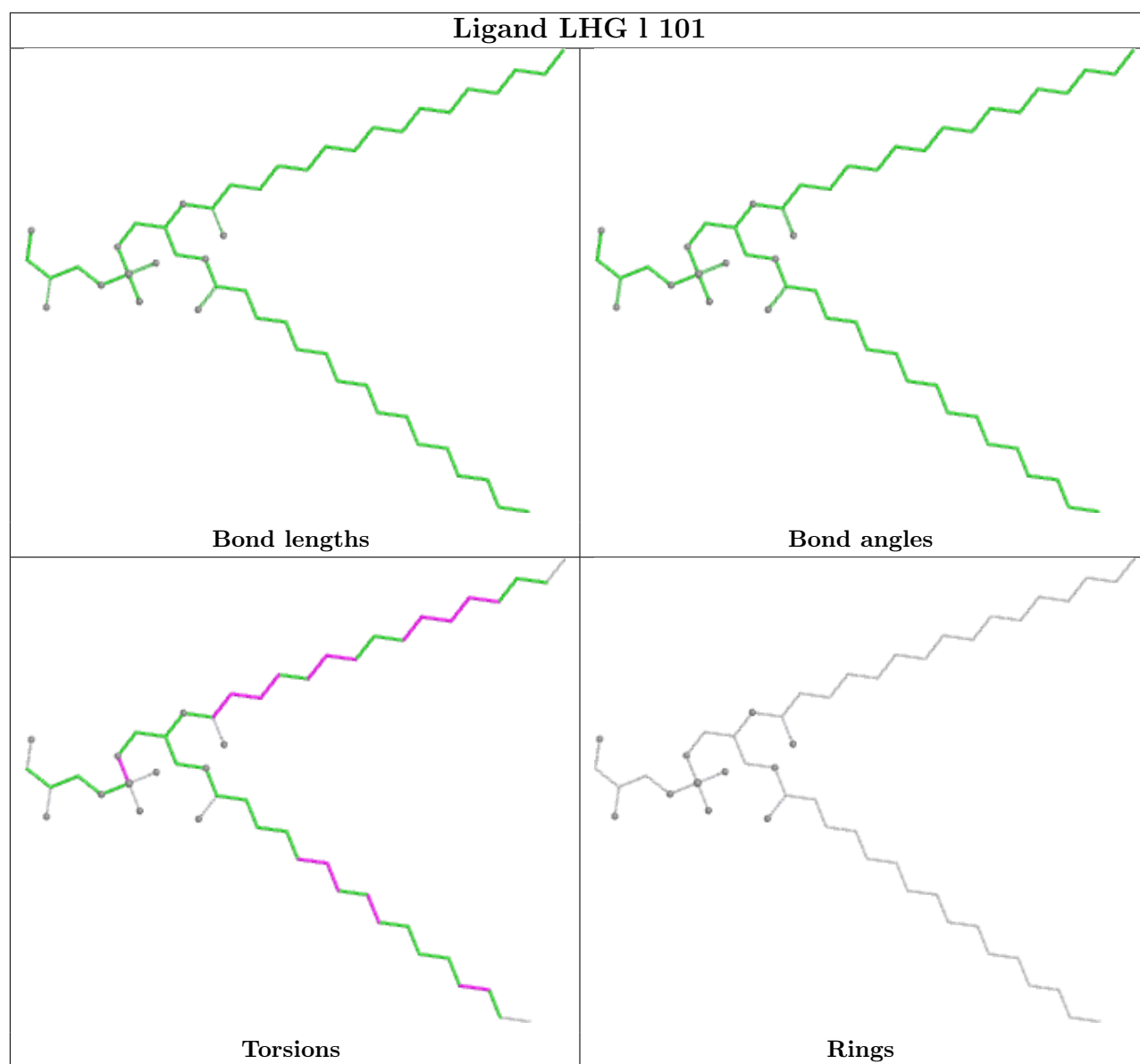
Ligand LMG a 616



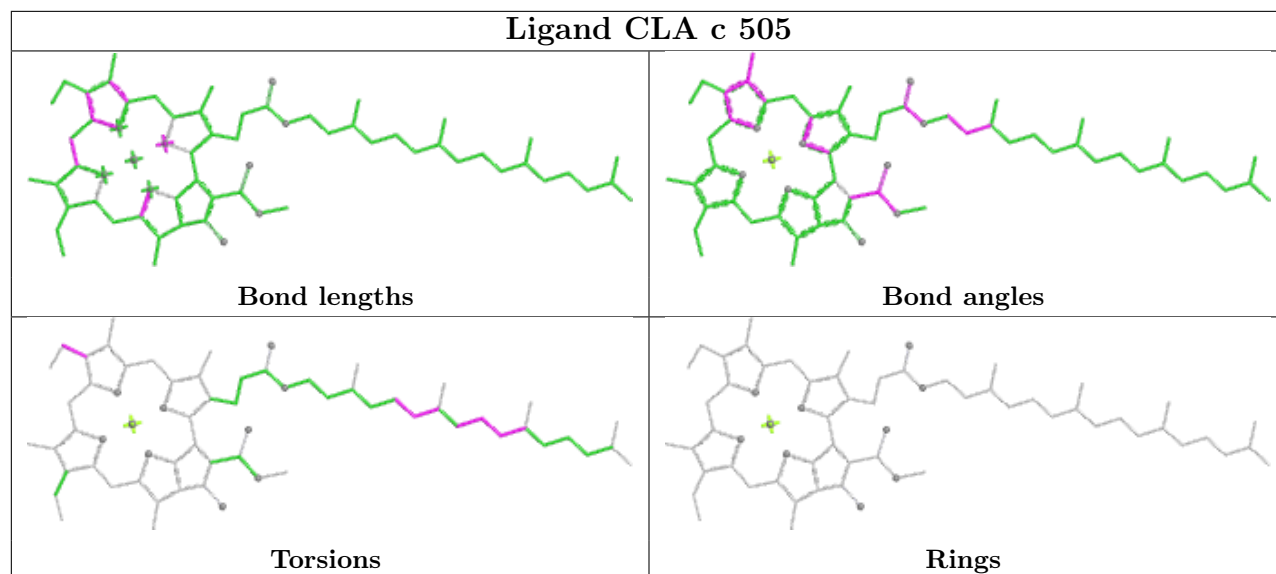
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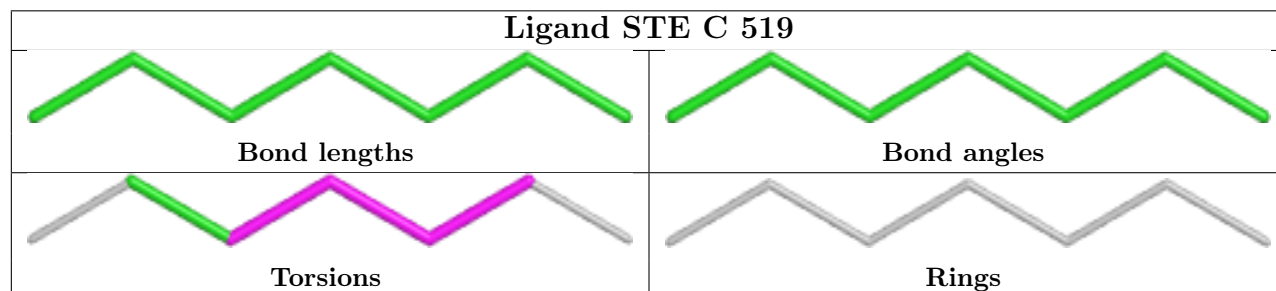




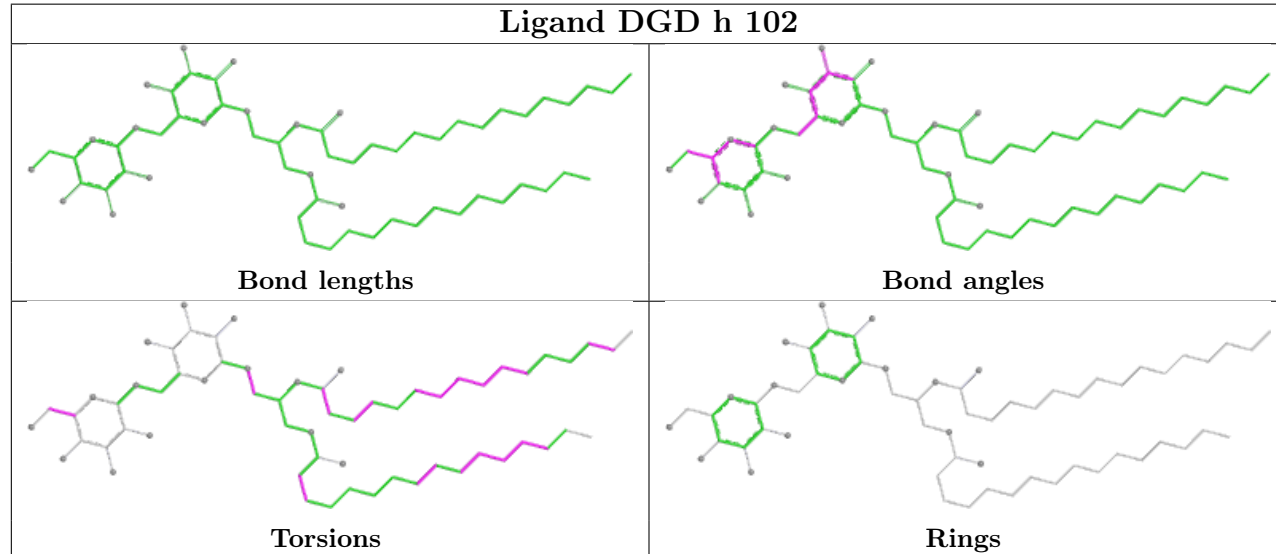
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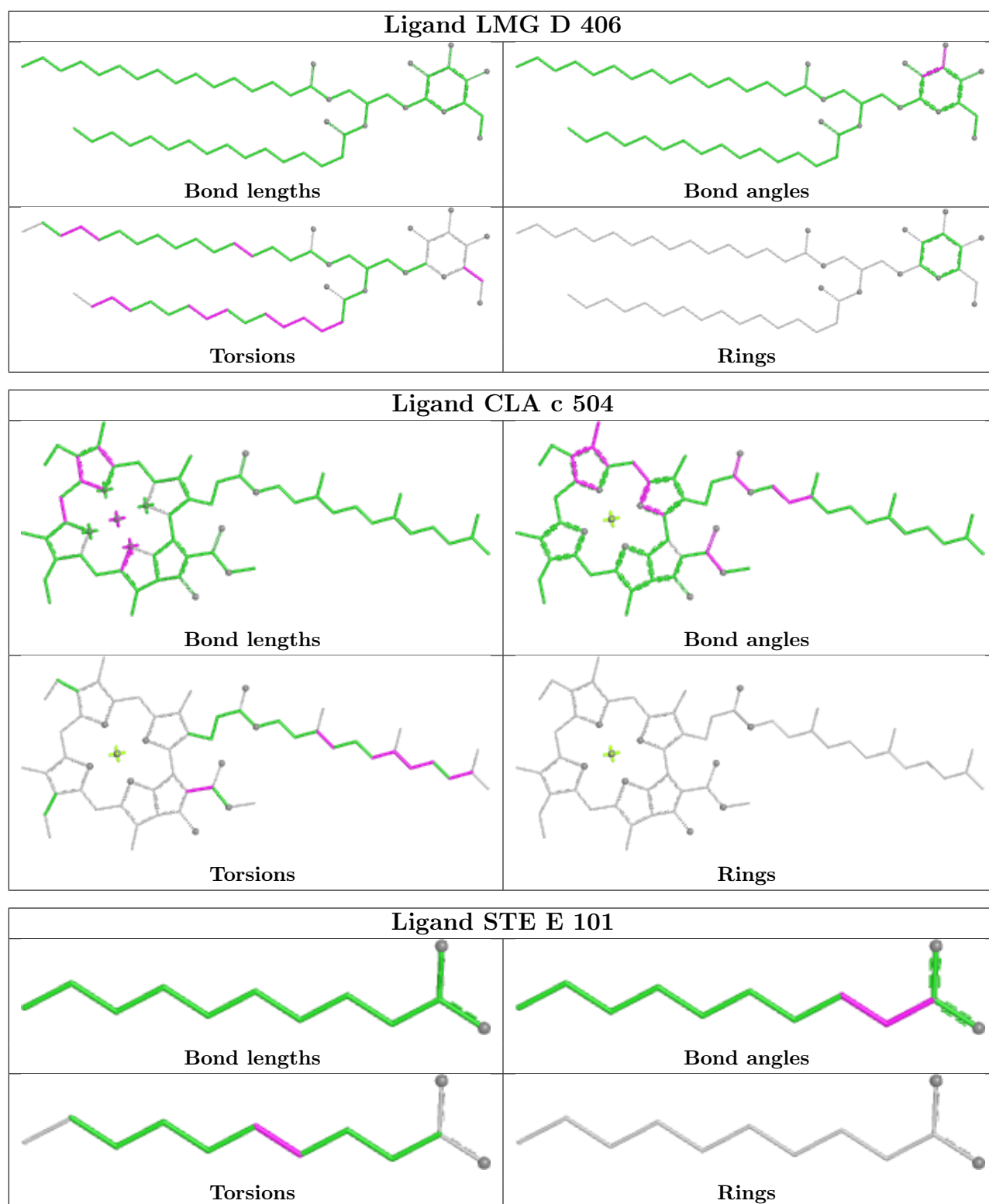


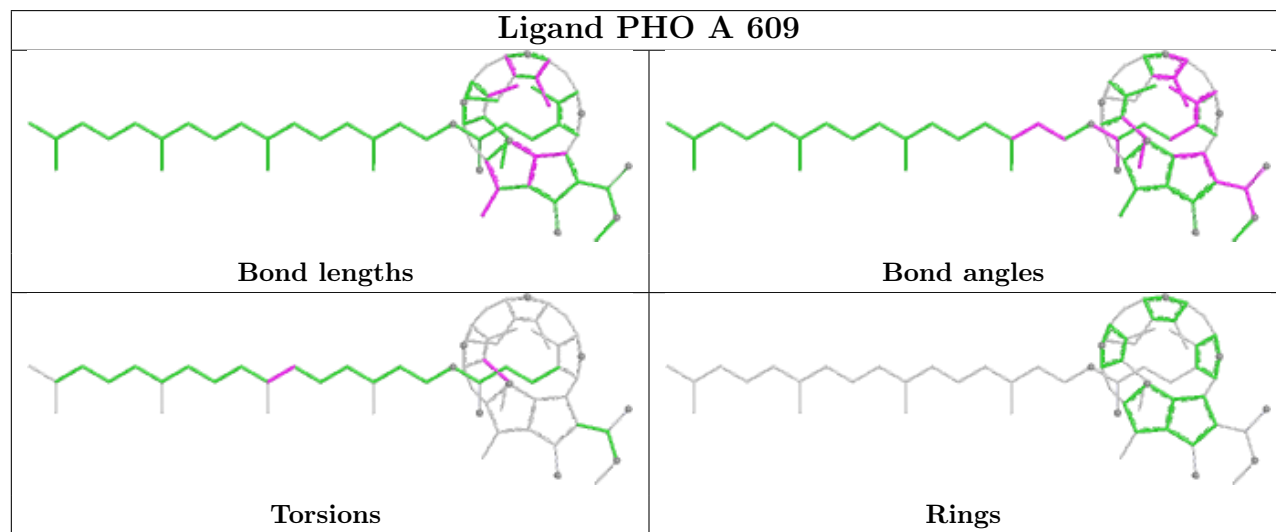
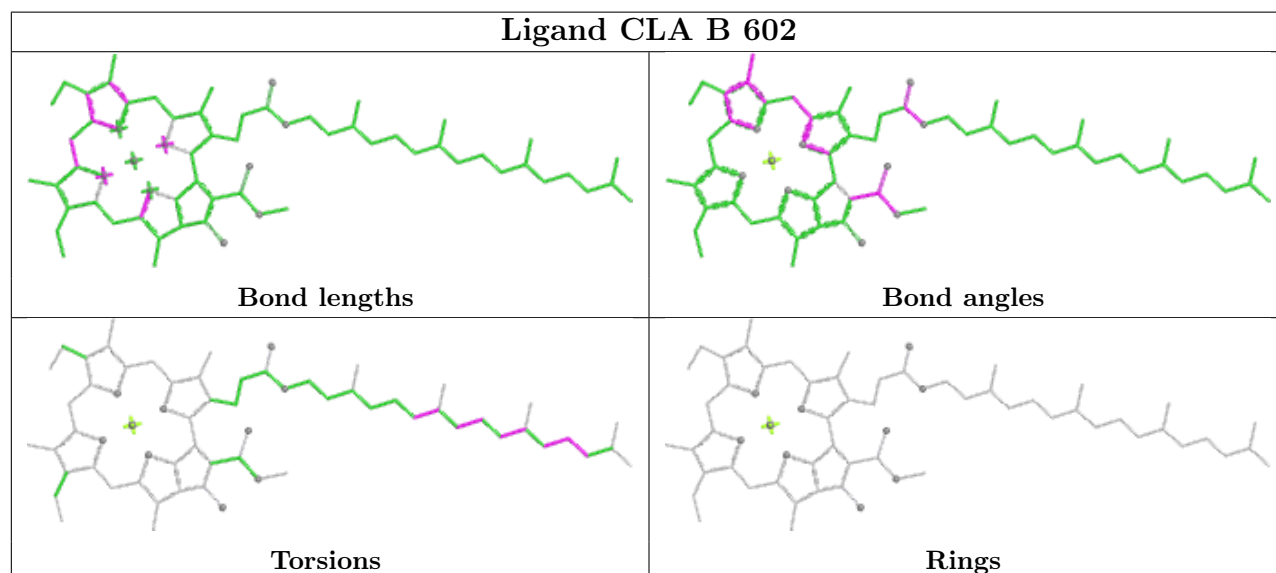
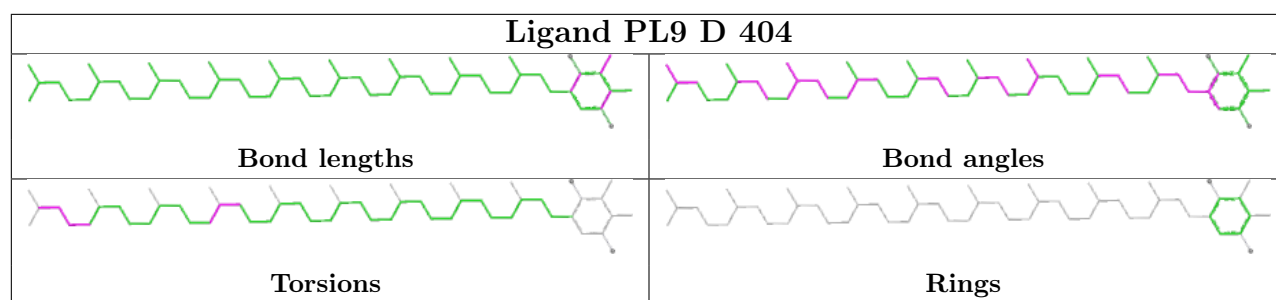
Ligand STE C 519



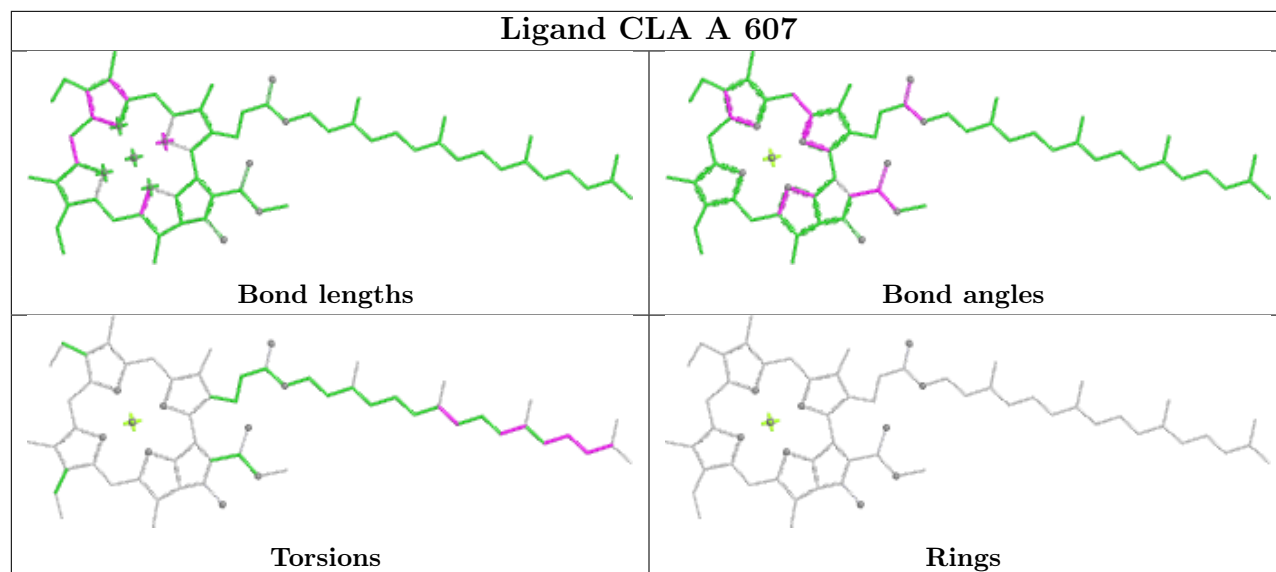
Ligand DGD h 102



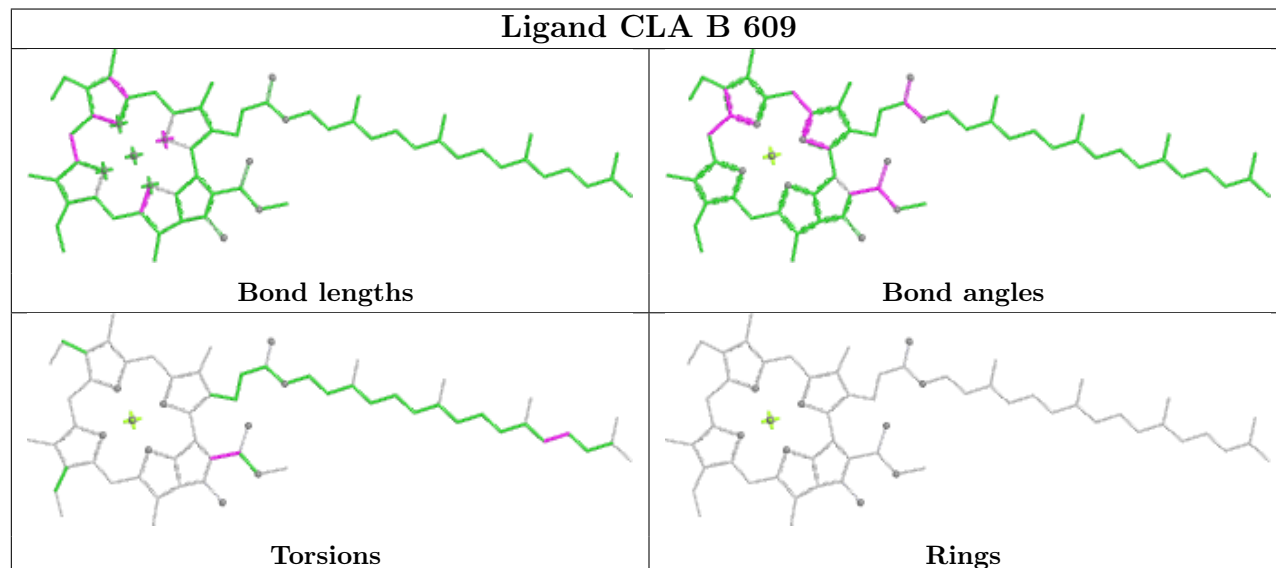




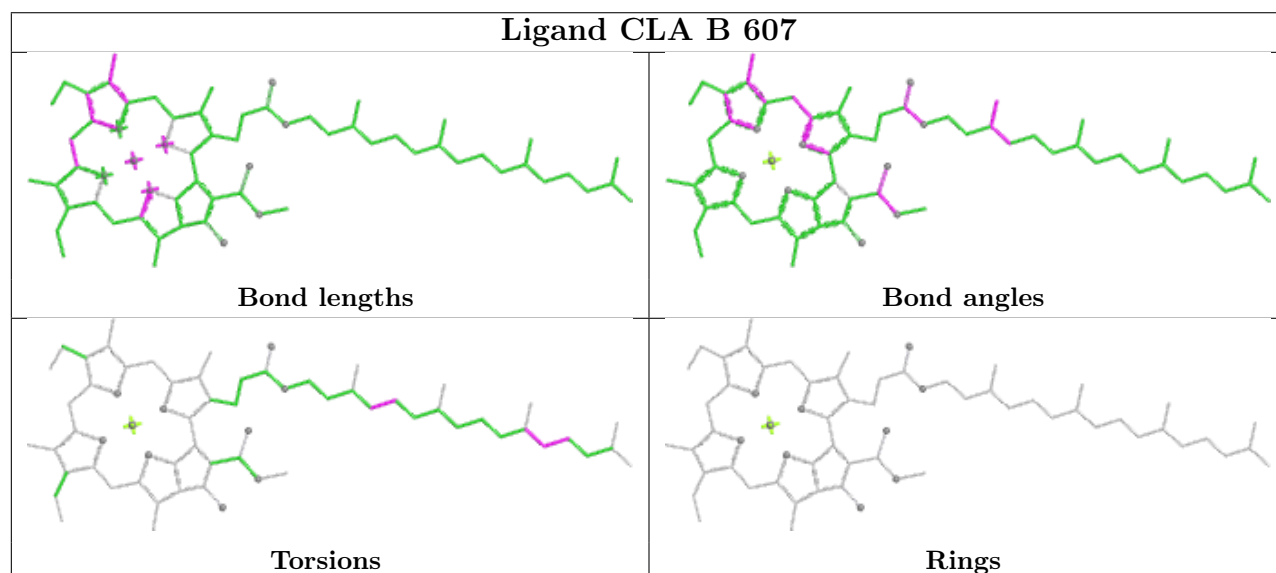
Ligand CLA A 607

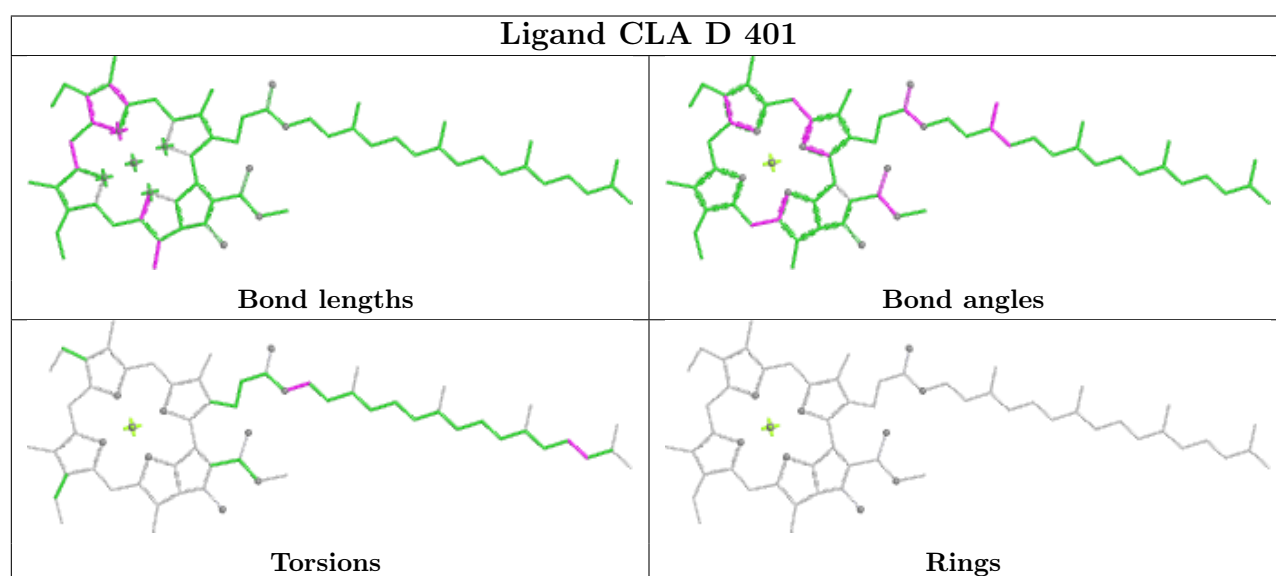
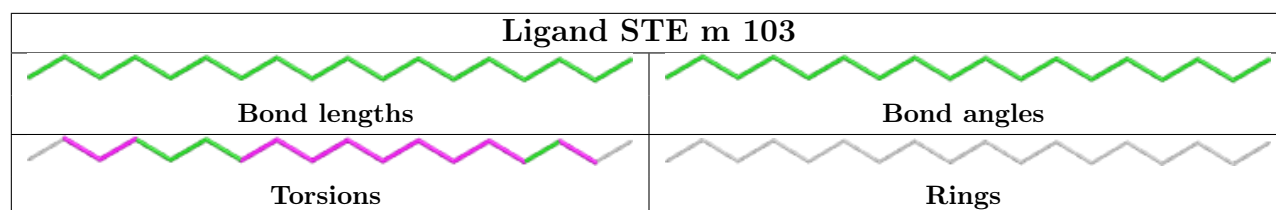
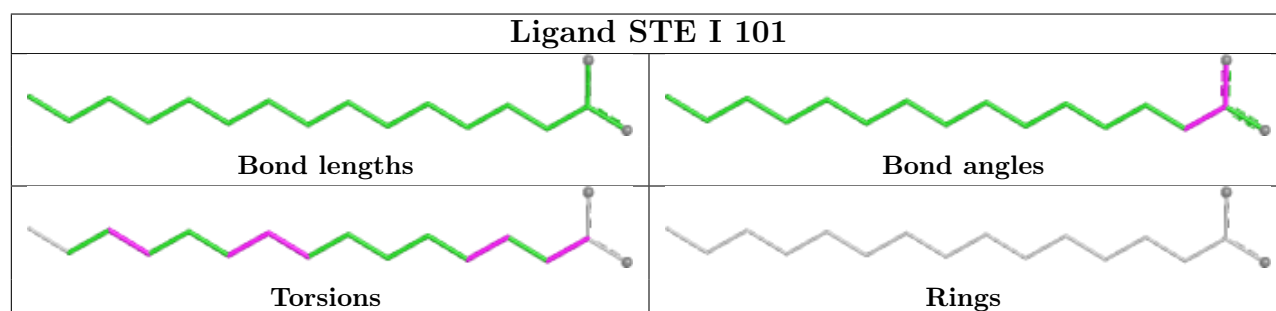
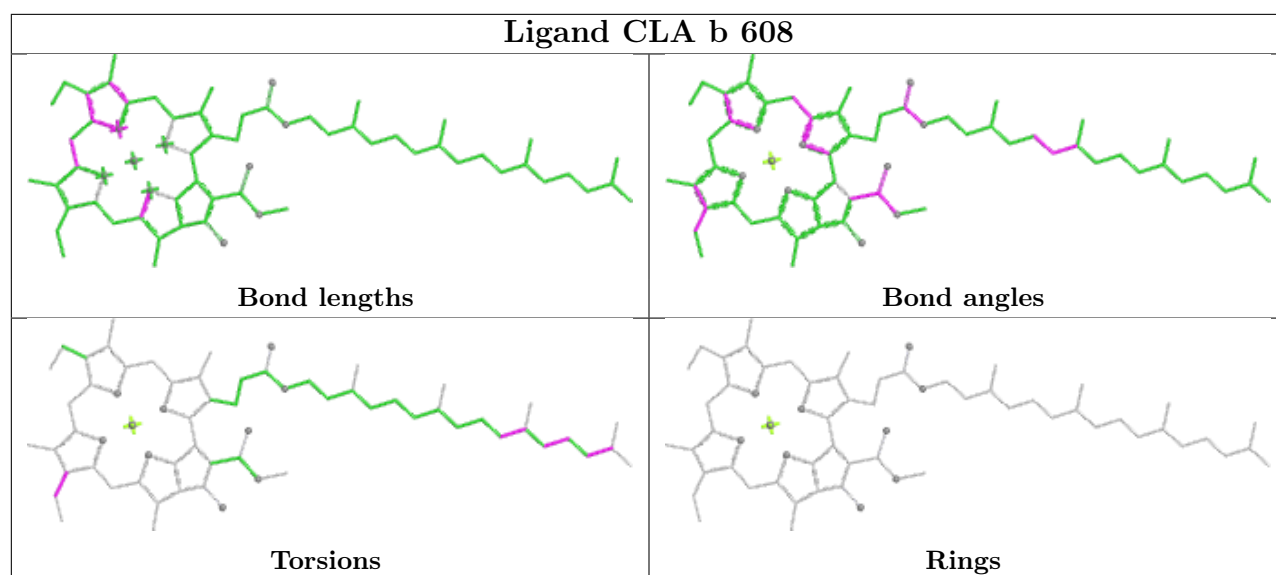


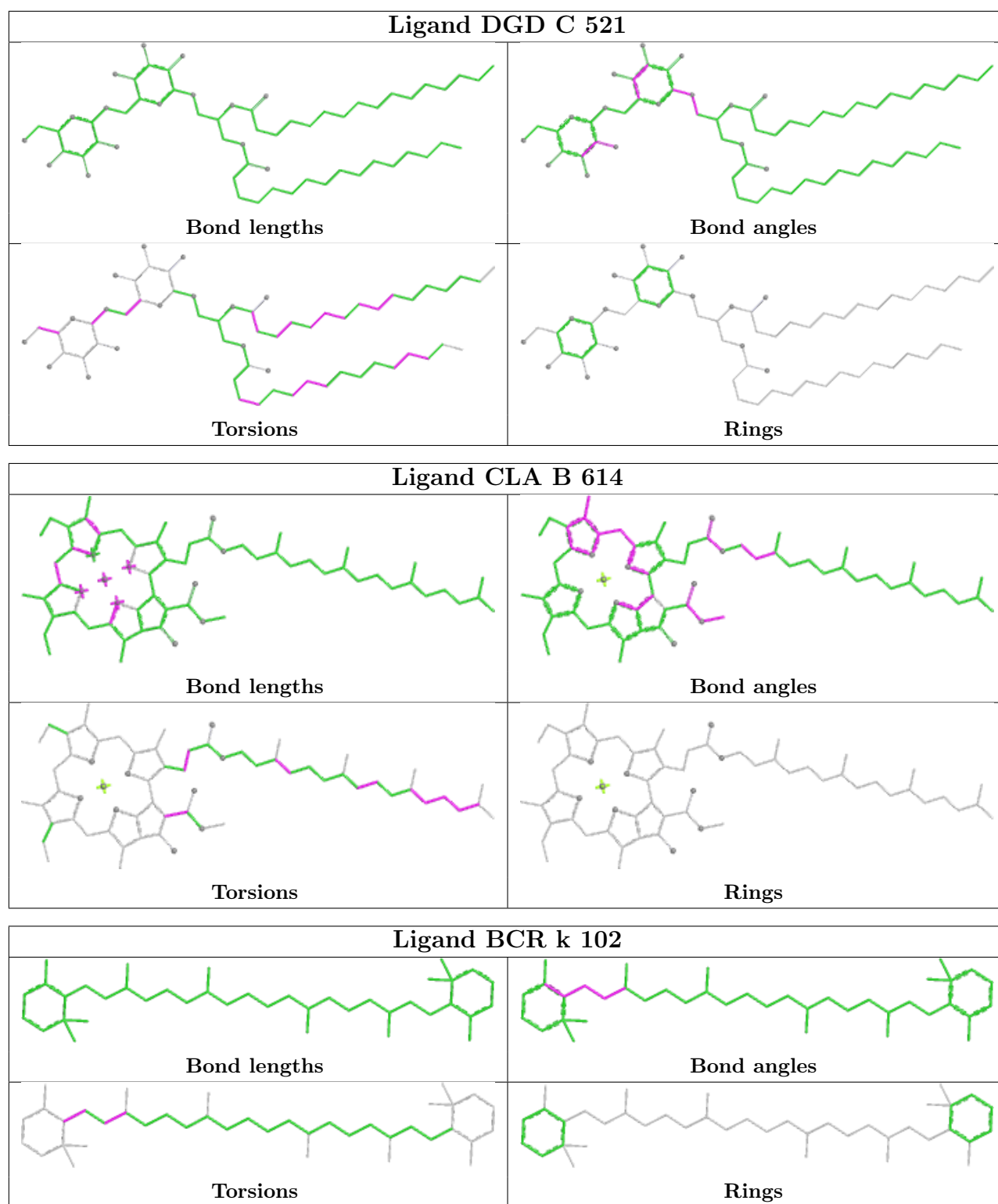
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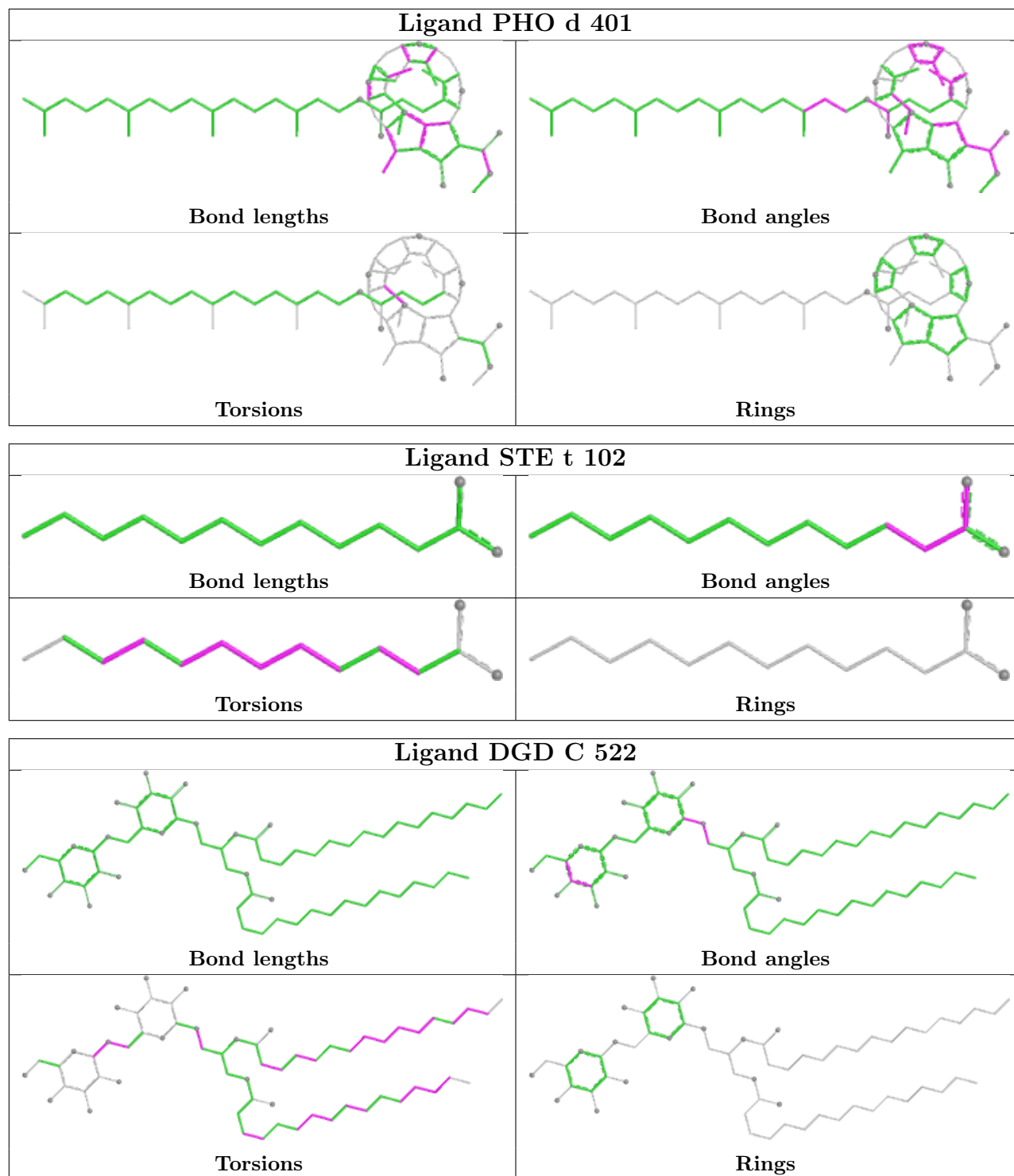


Ligand CLA B 607

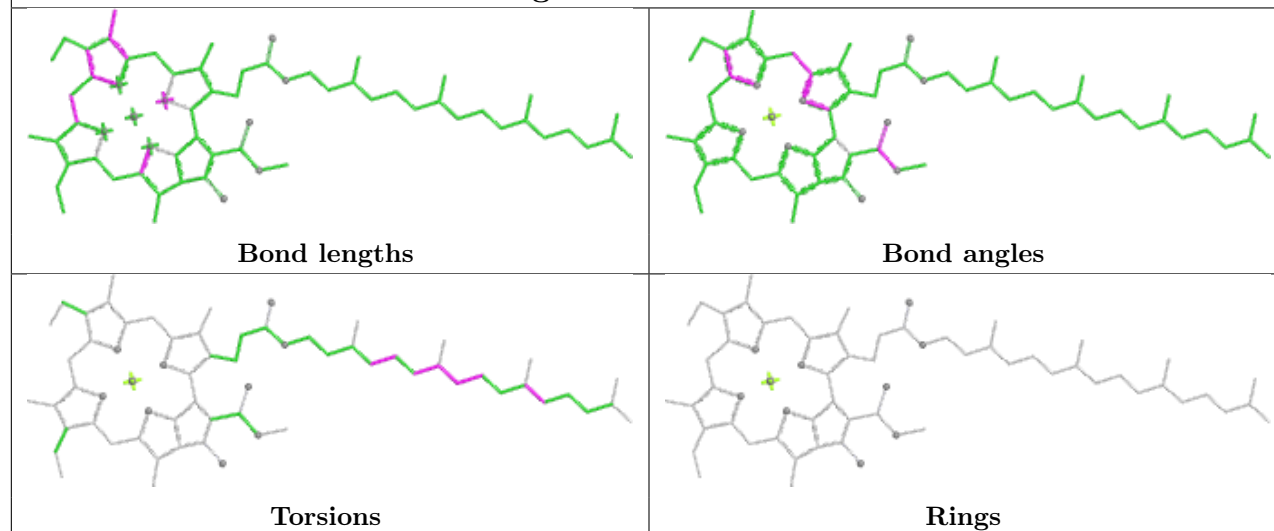




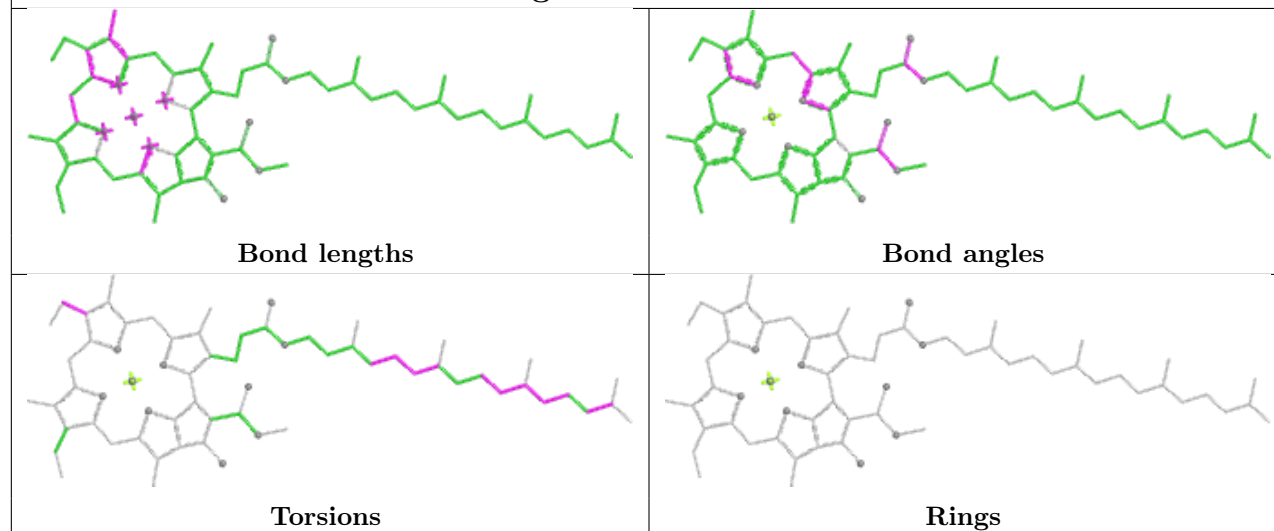




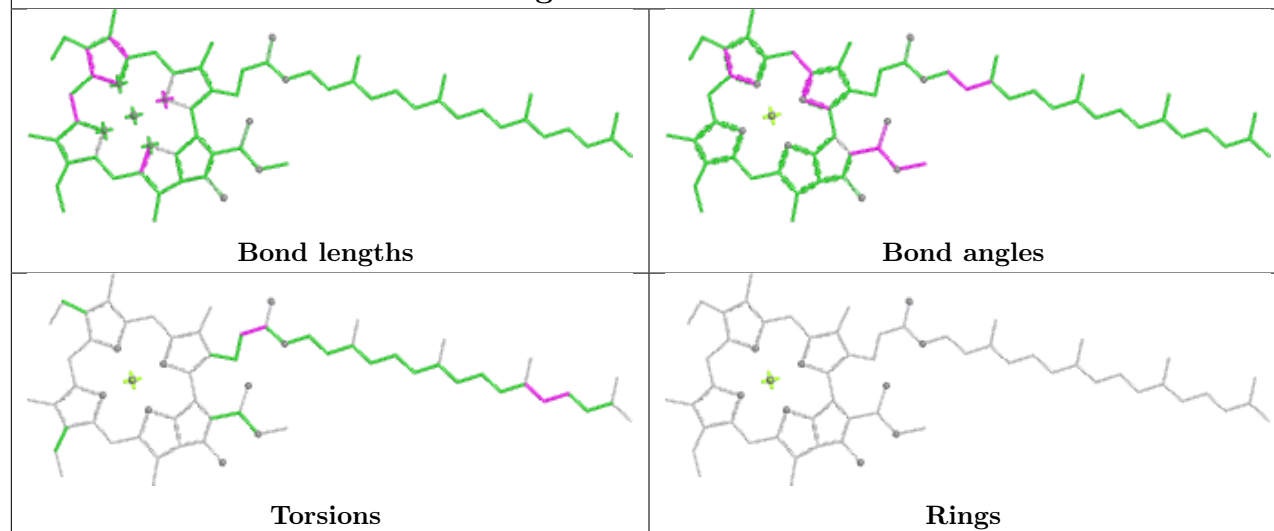
Ligand CLA C 511

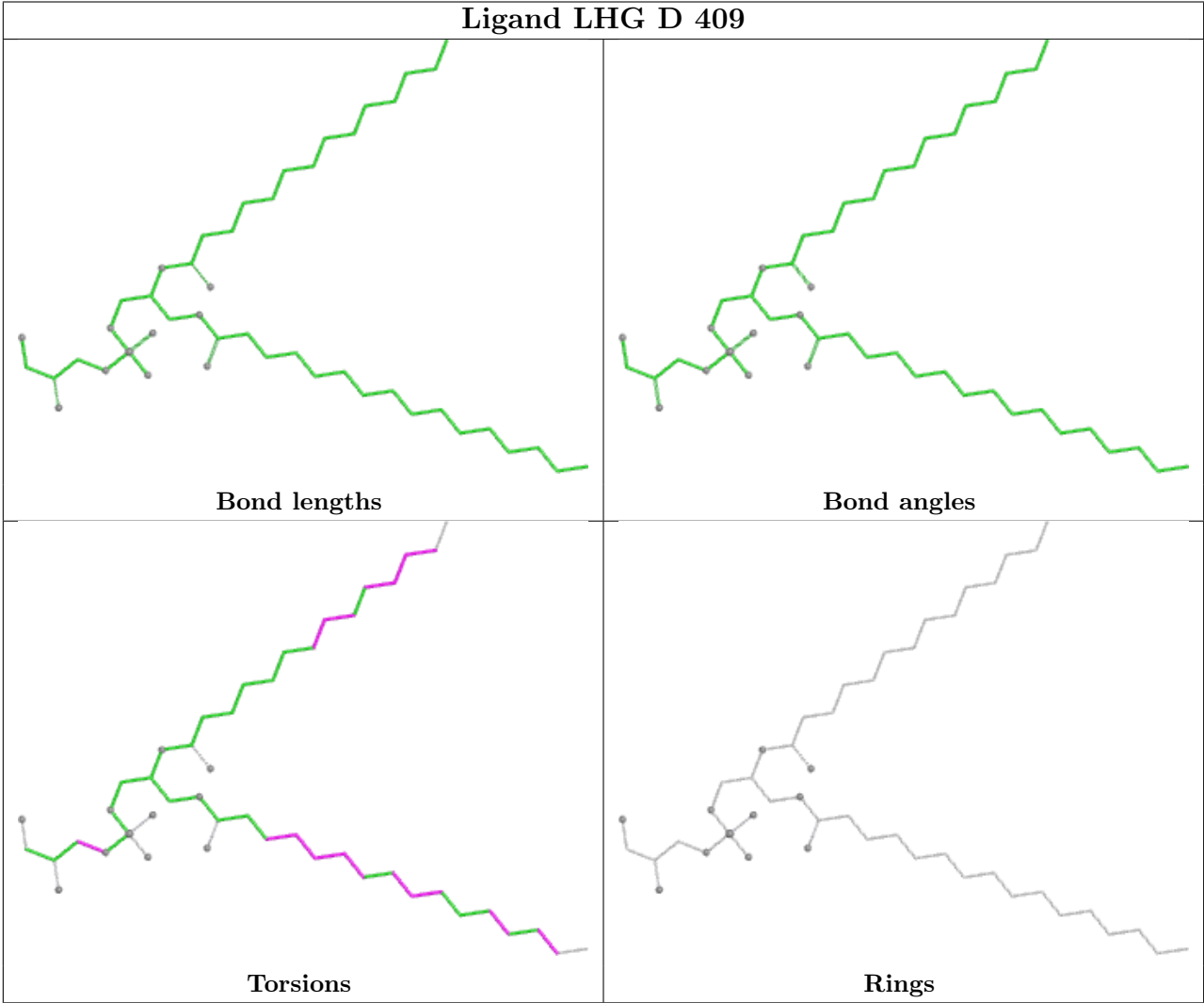
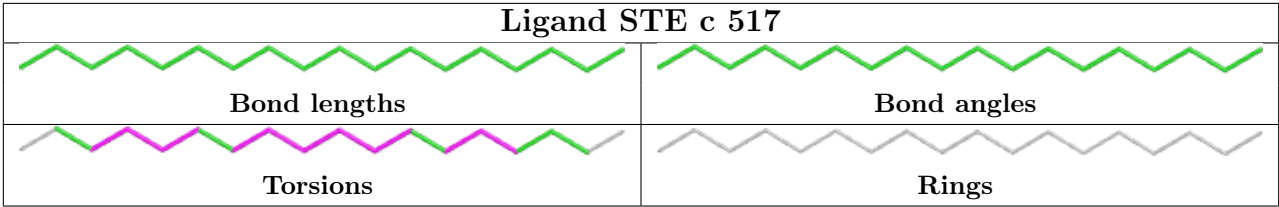


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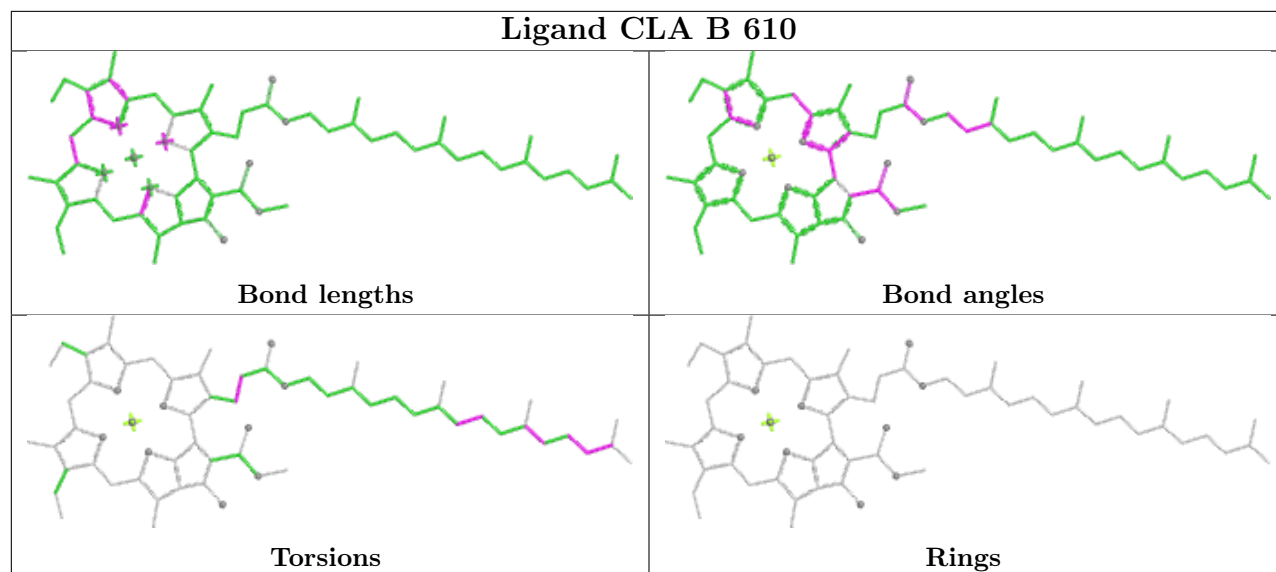


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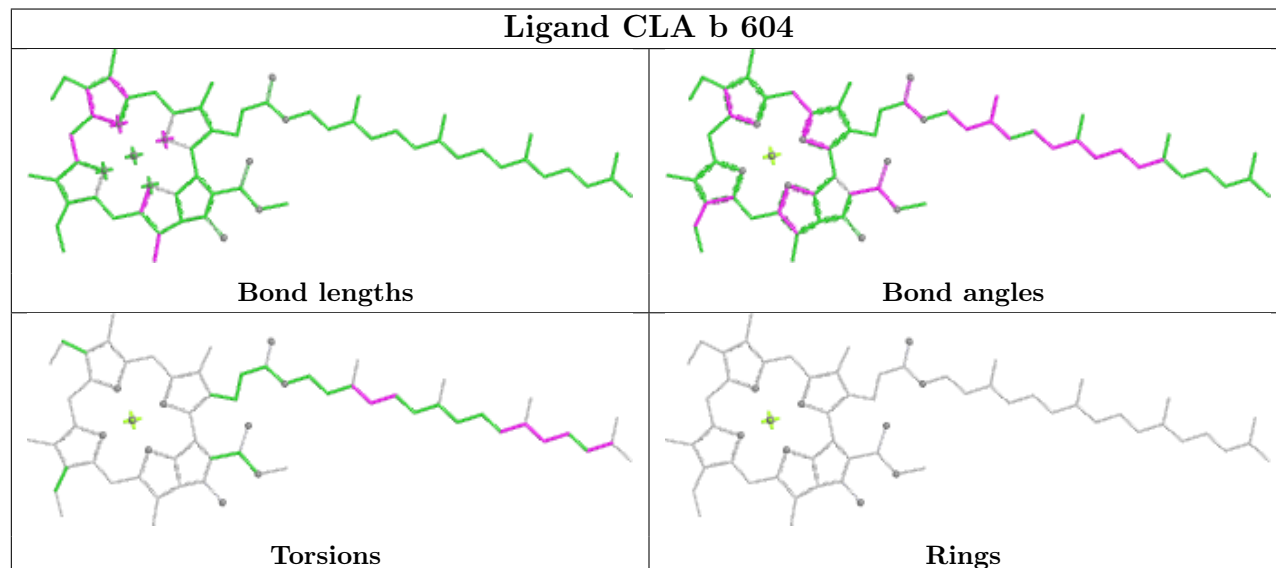




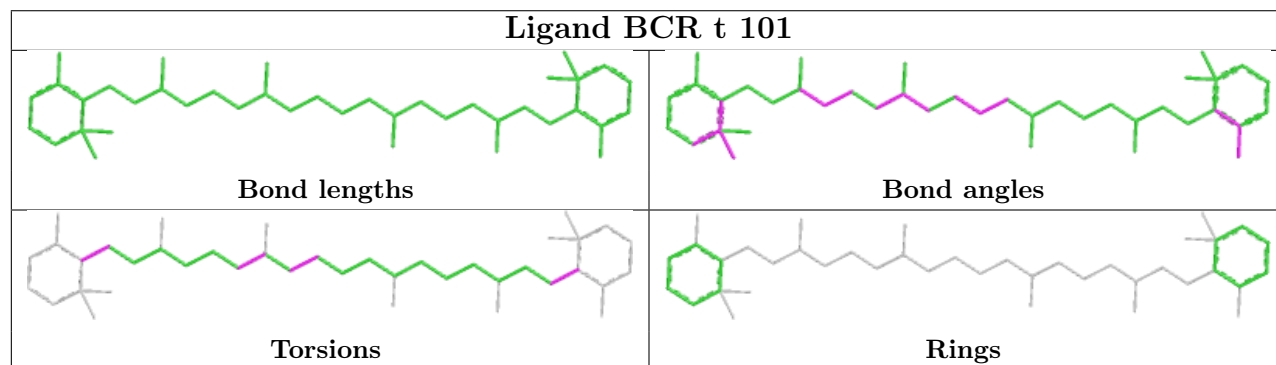
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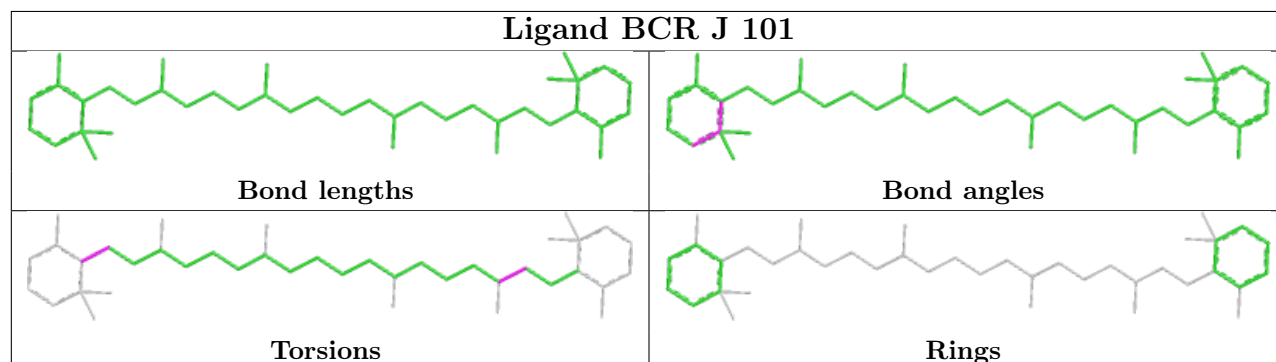
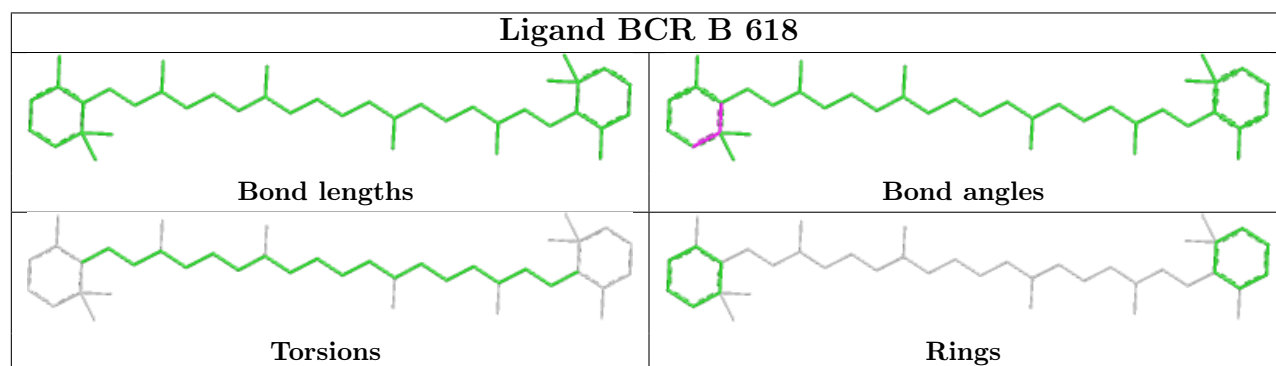
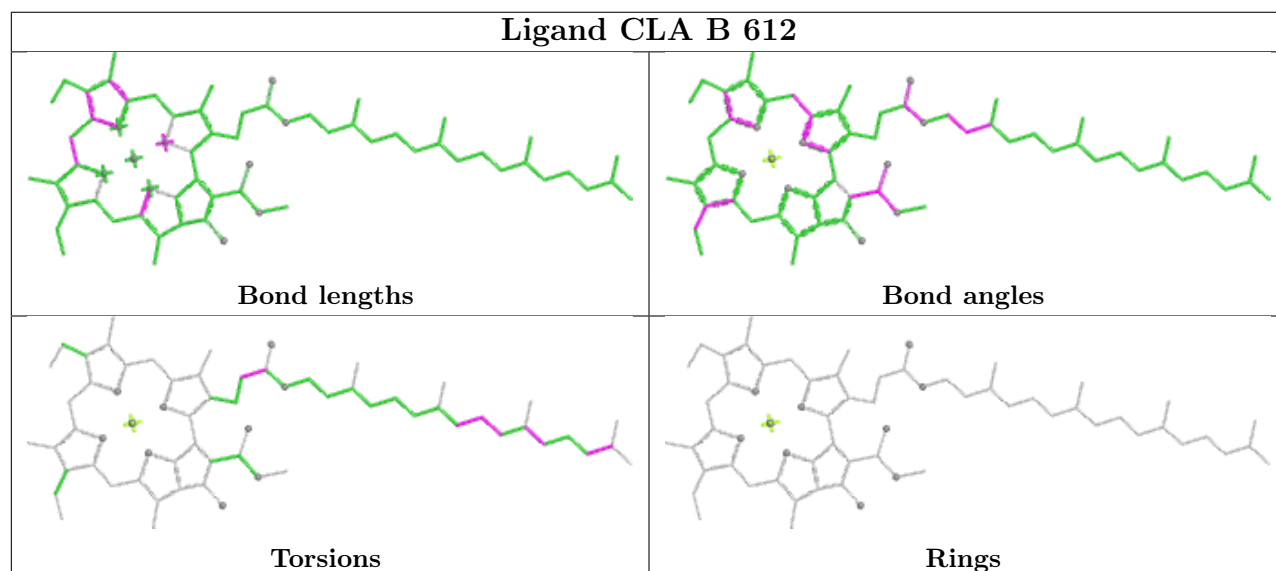
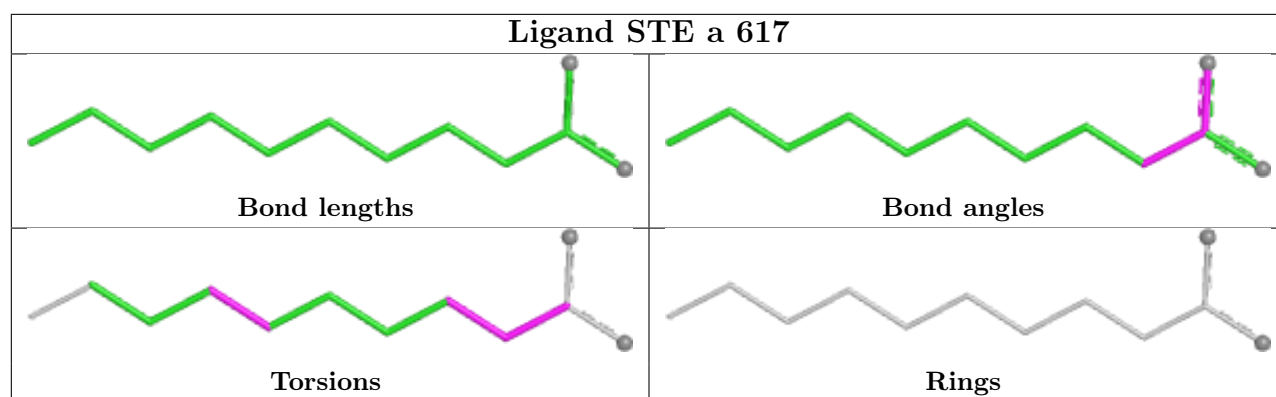


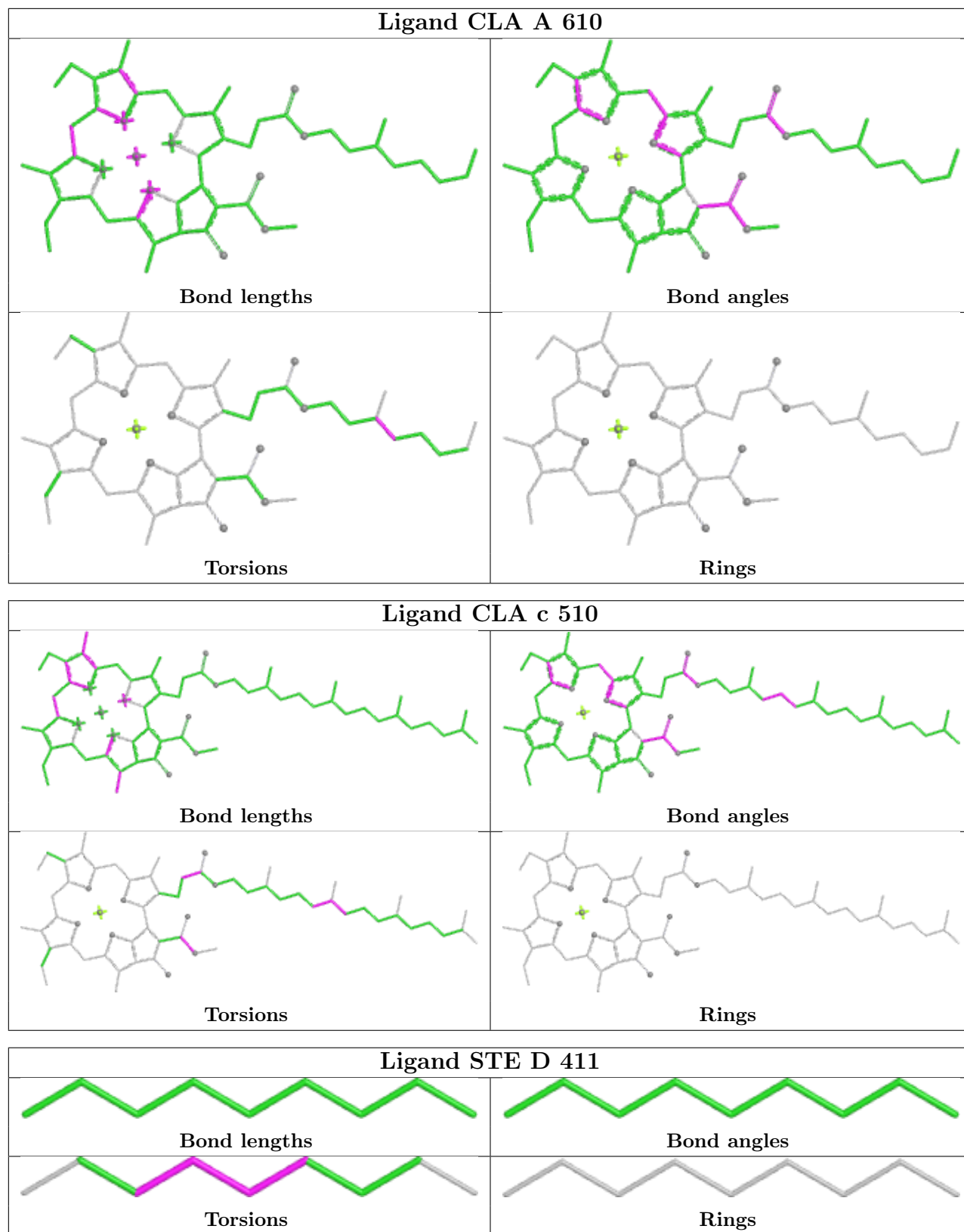
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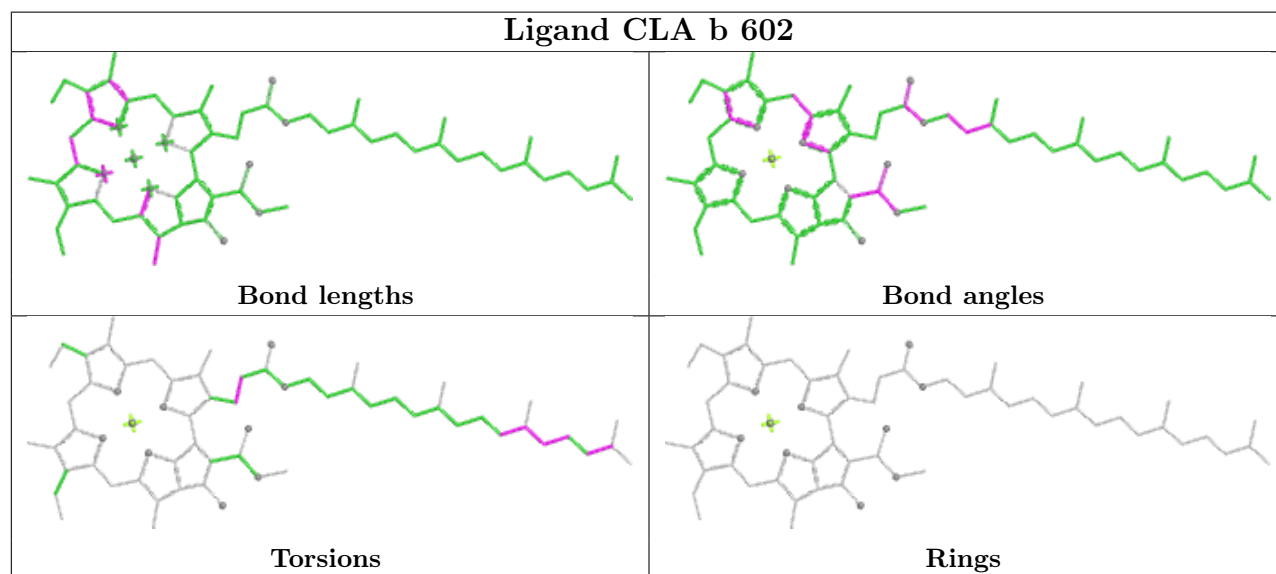
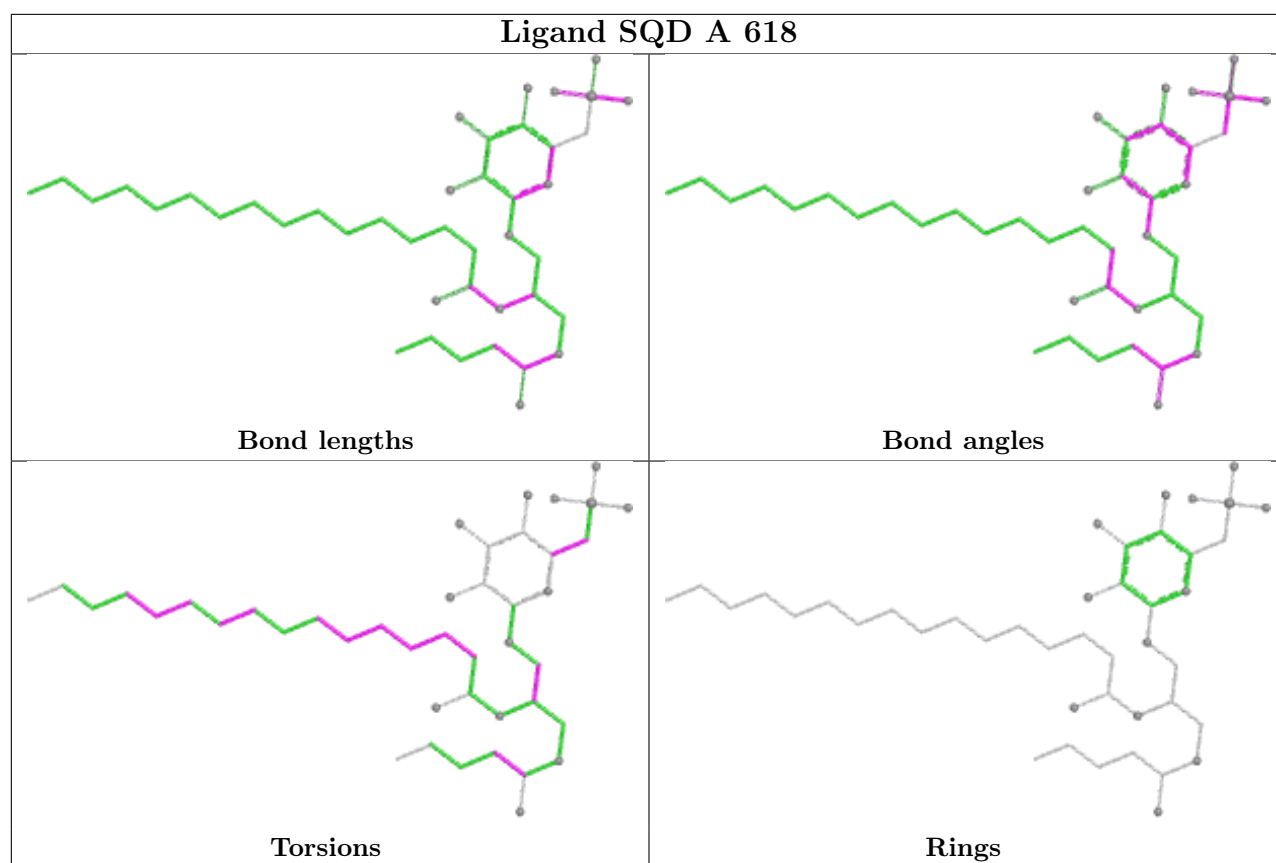


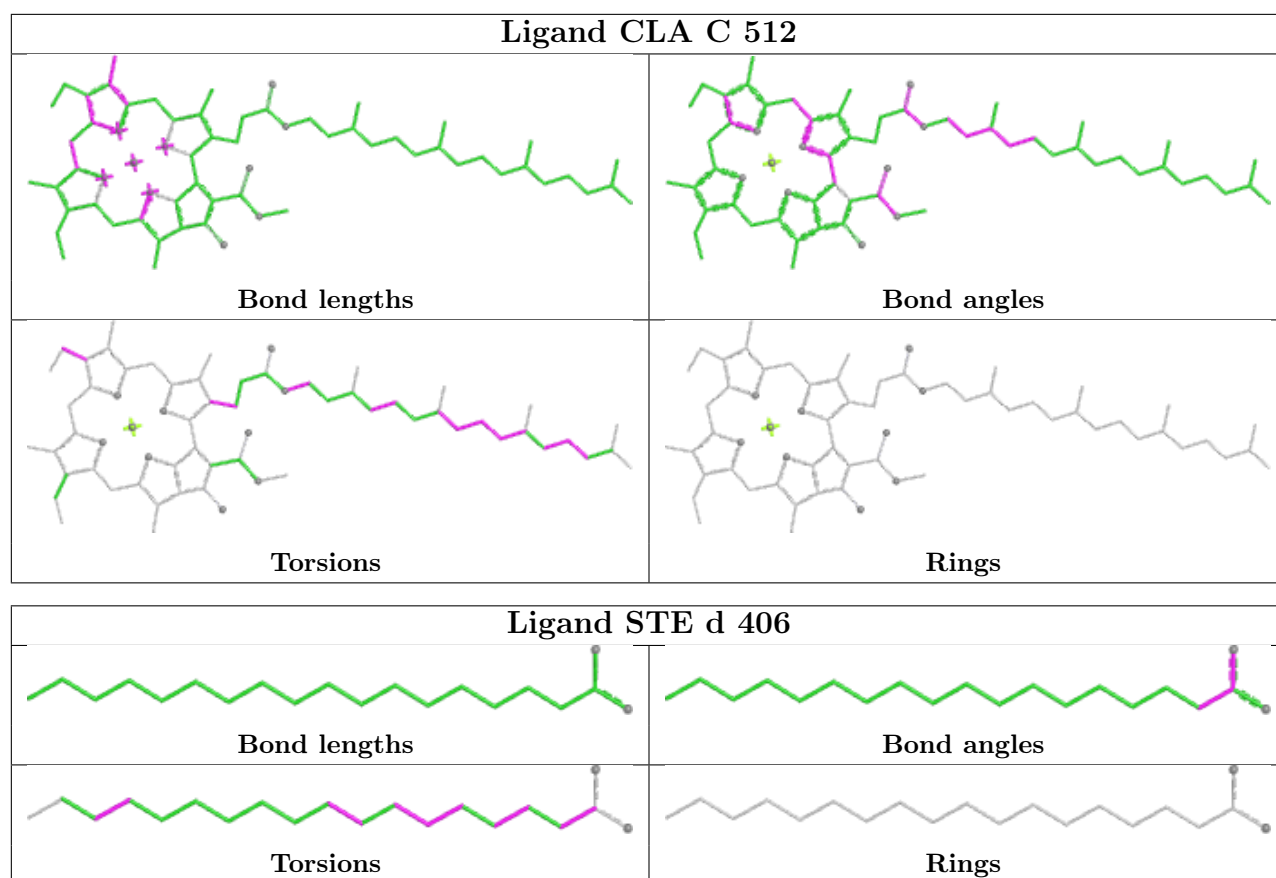
Ligand BCR t 101

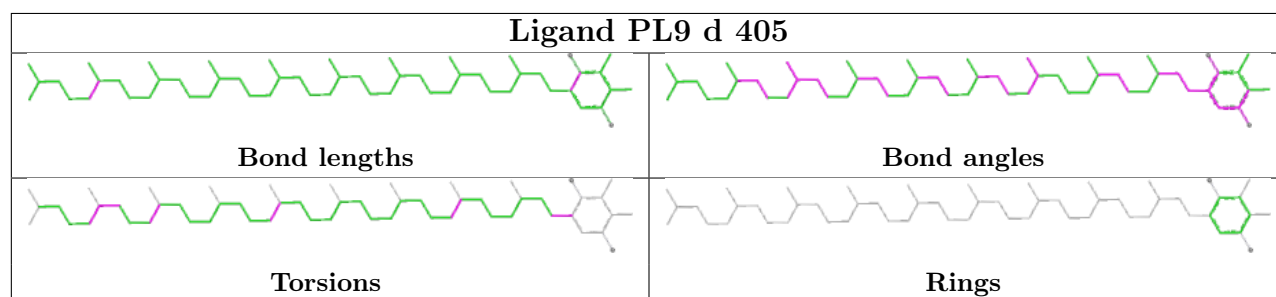
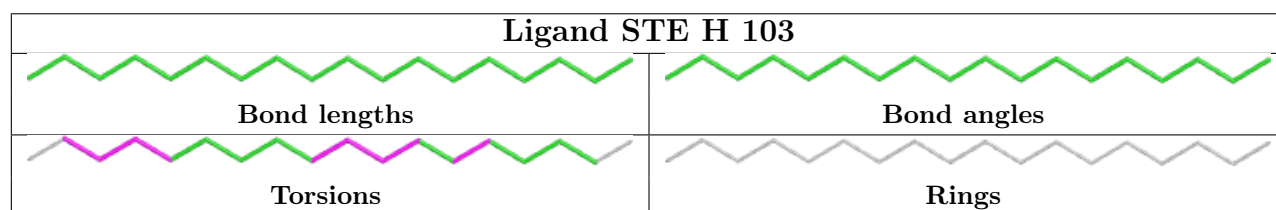
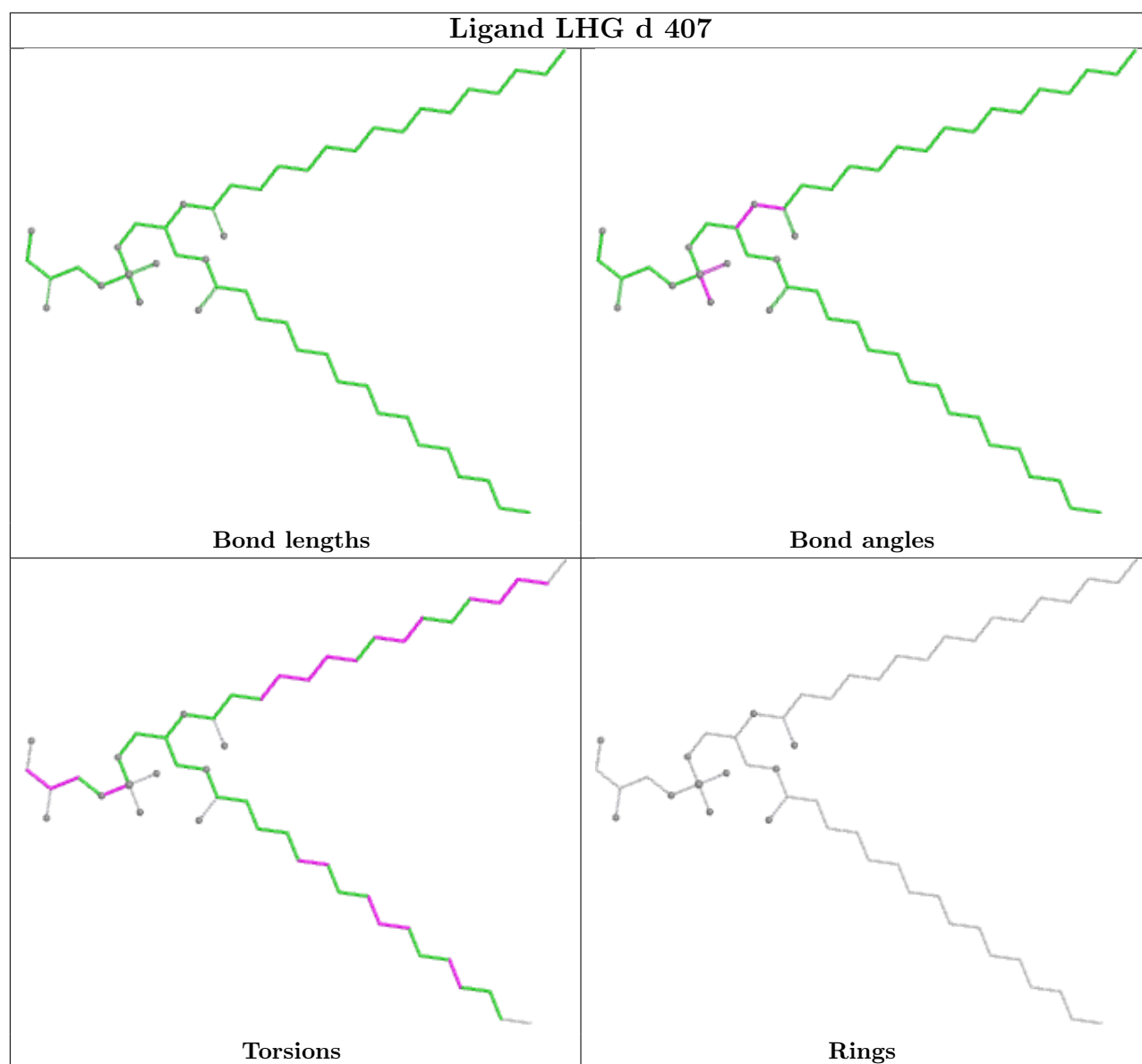


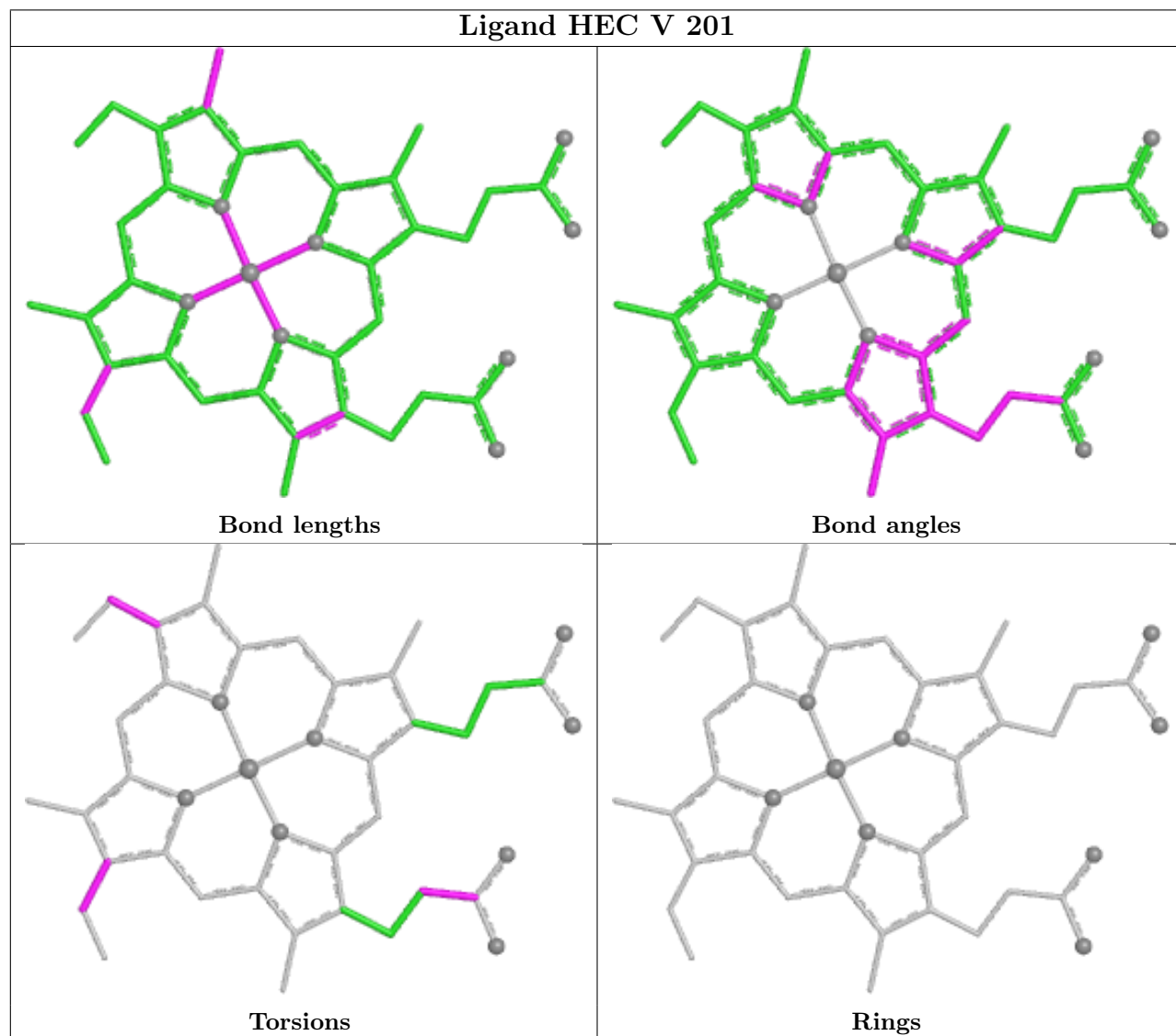
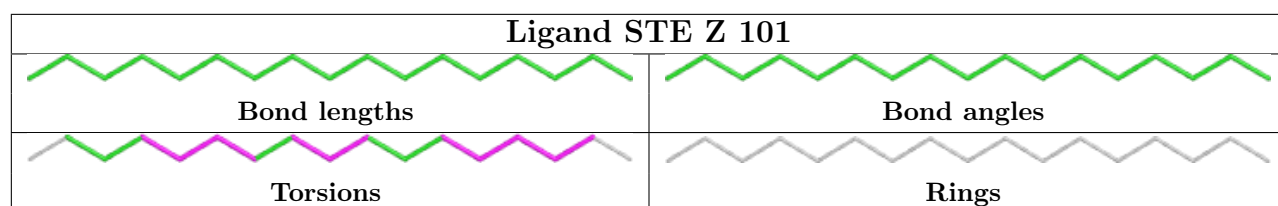


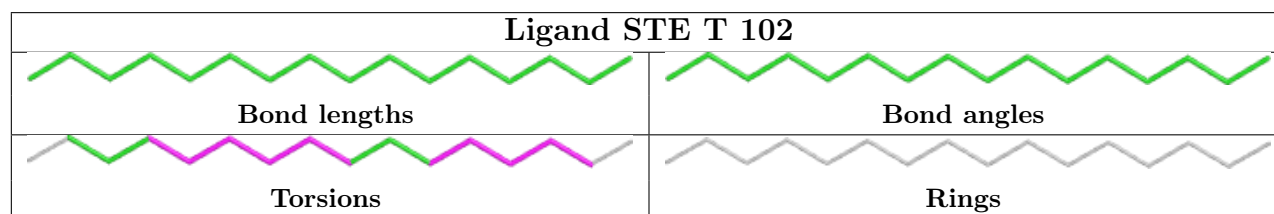
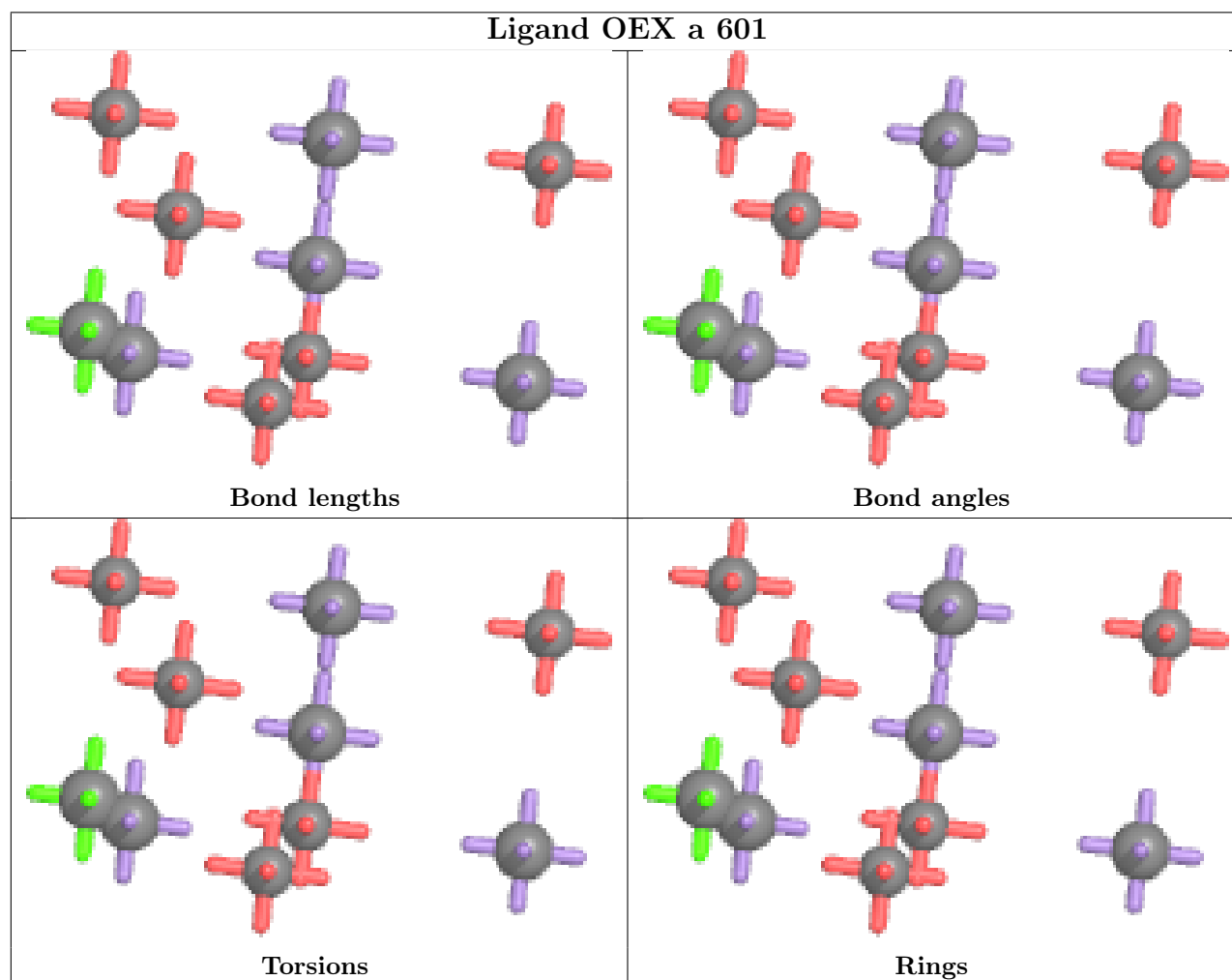
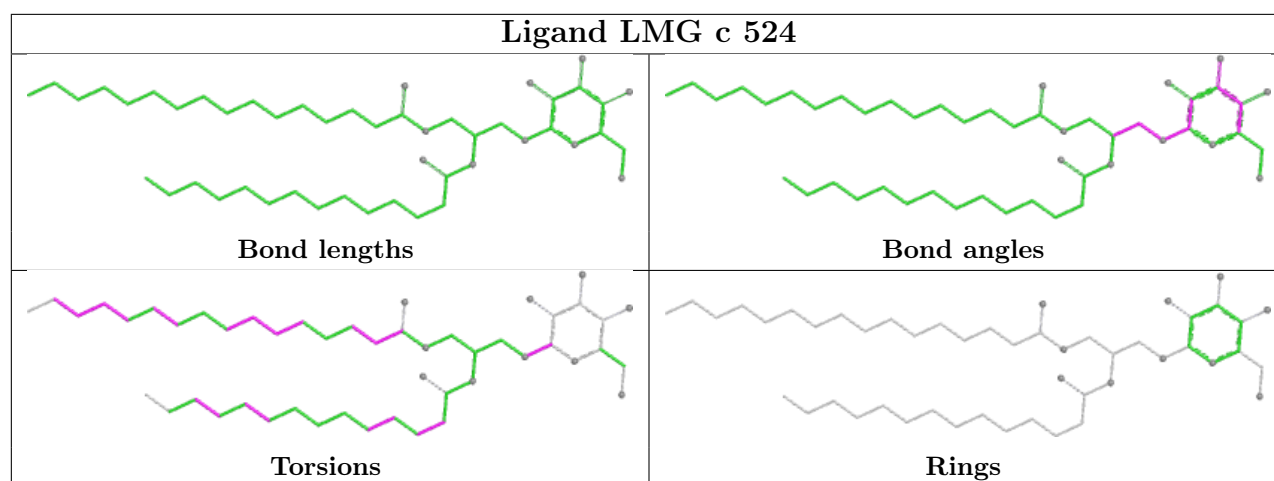


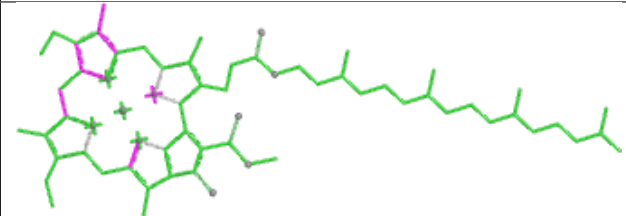
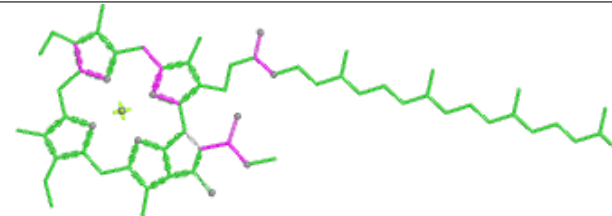
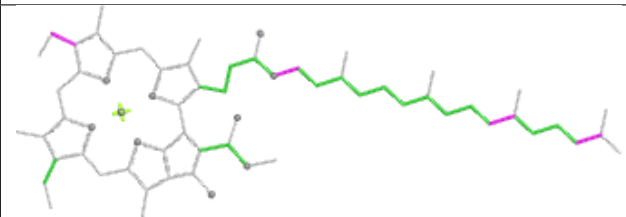
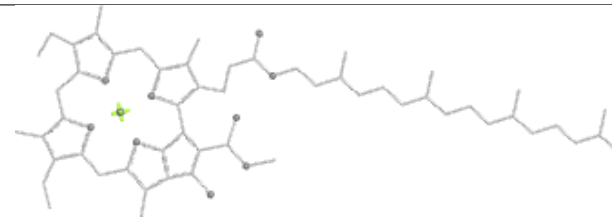




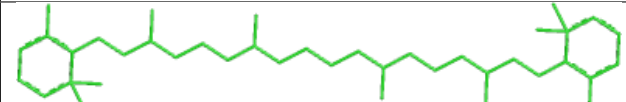
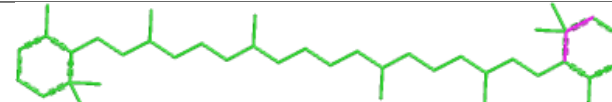
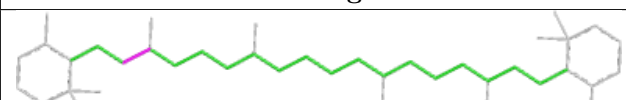
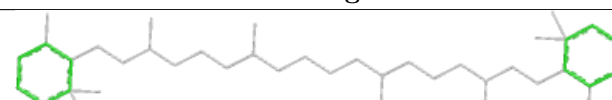


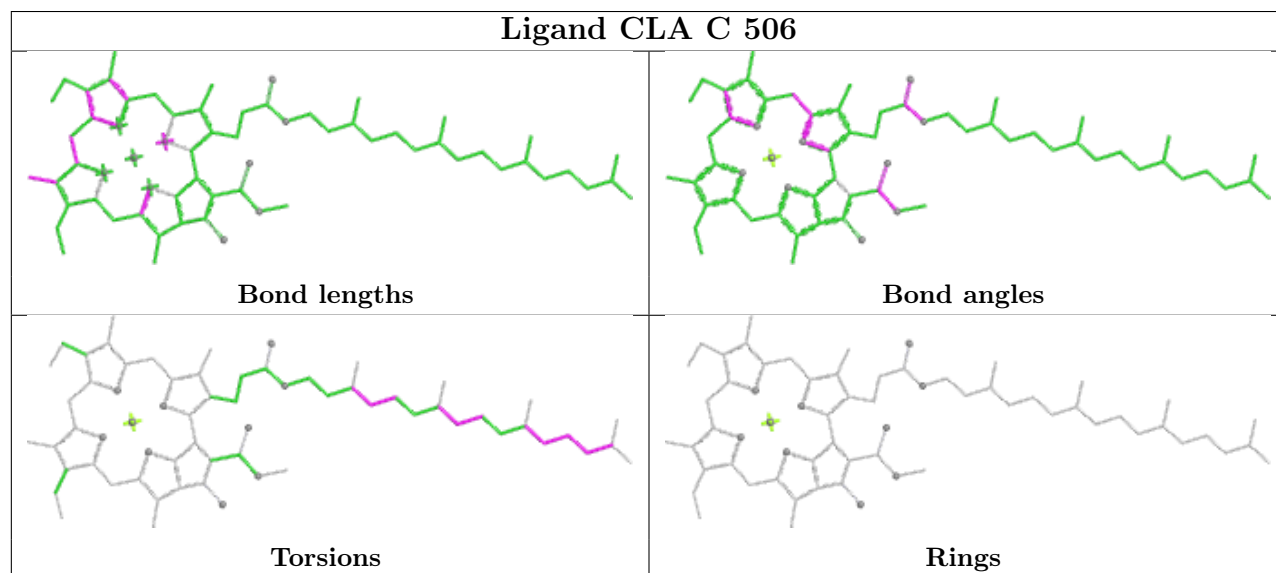
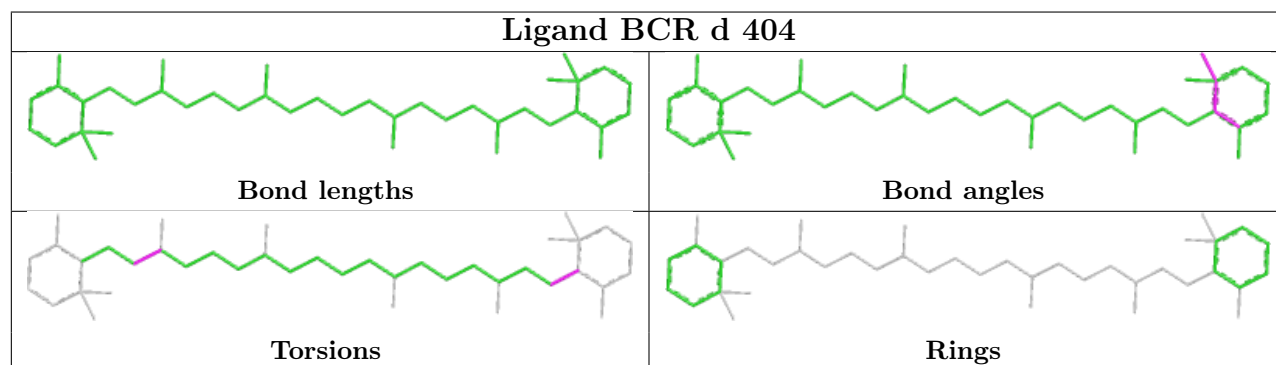
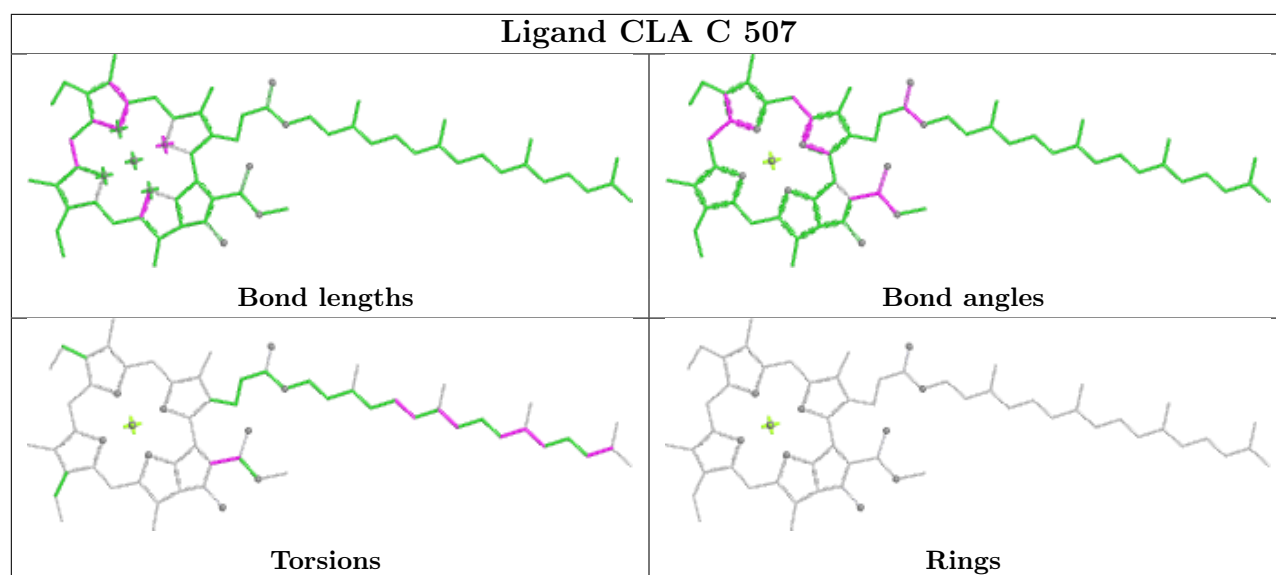




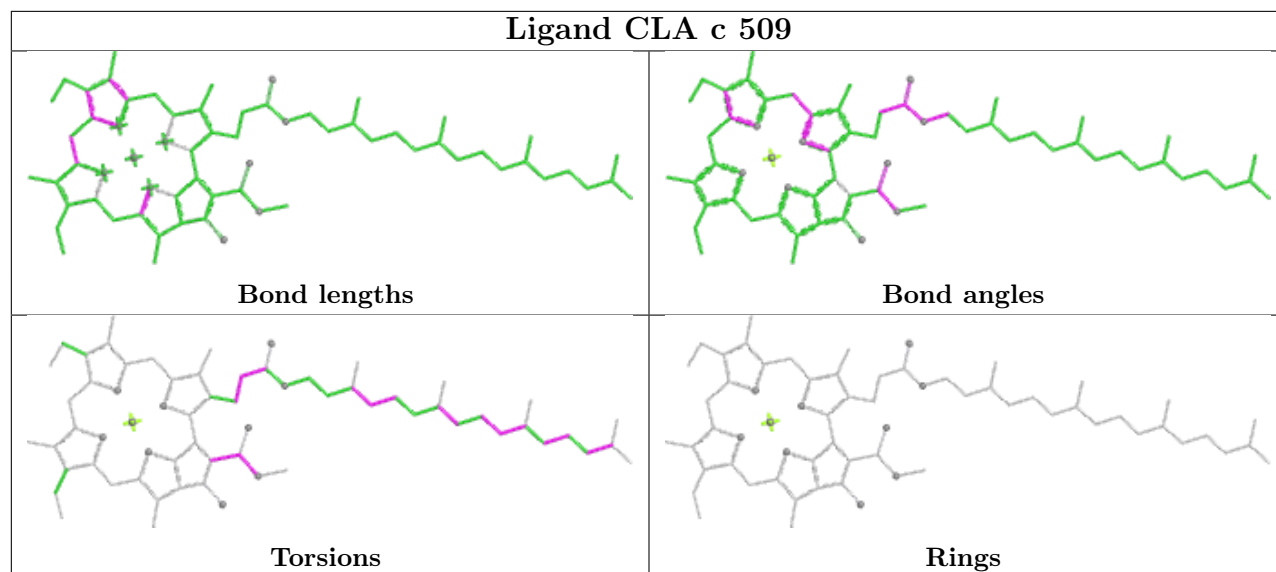
Ligand CLA d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE X 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

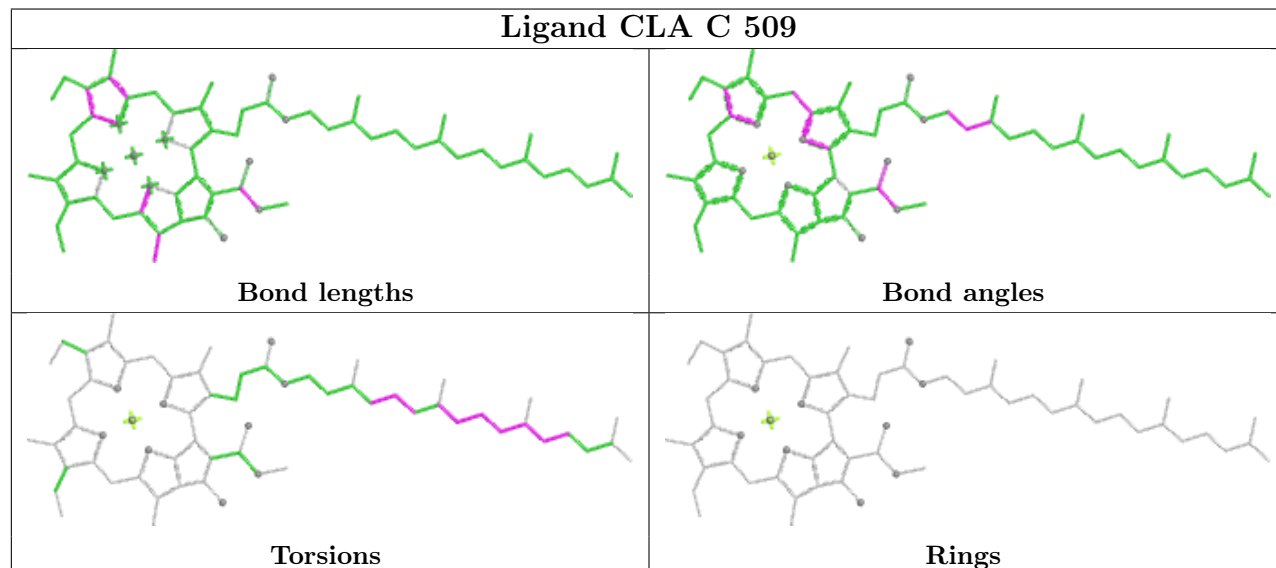
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

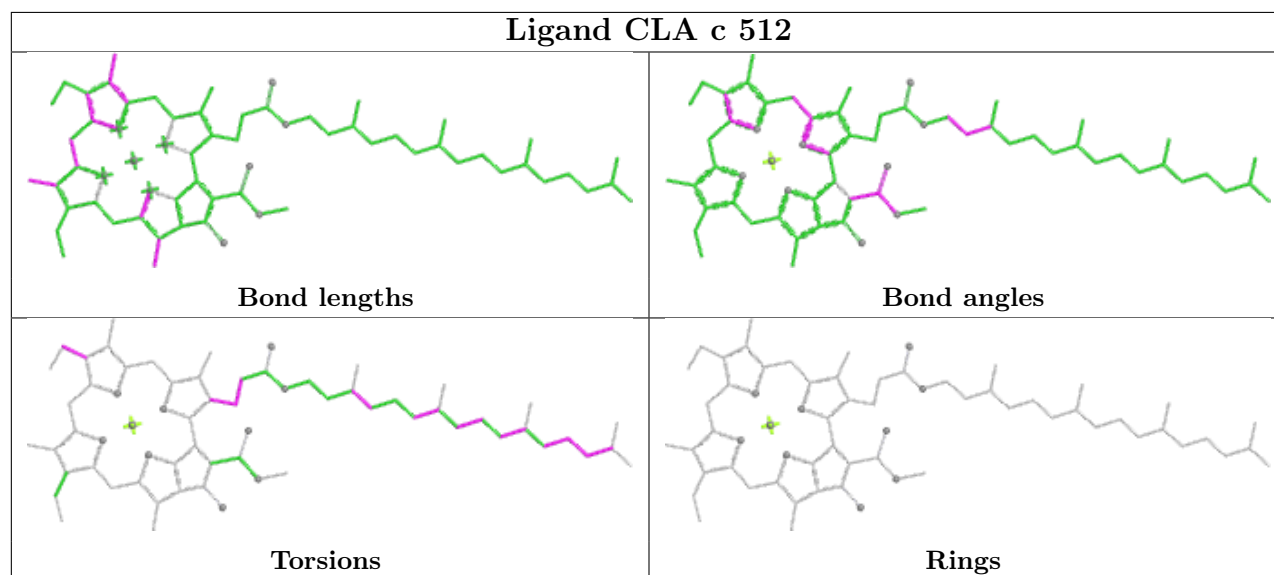
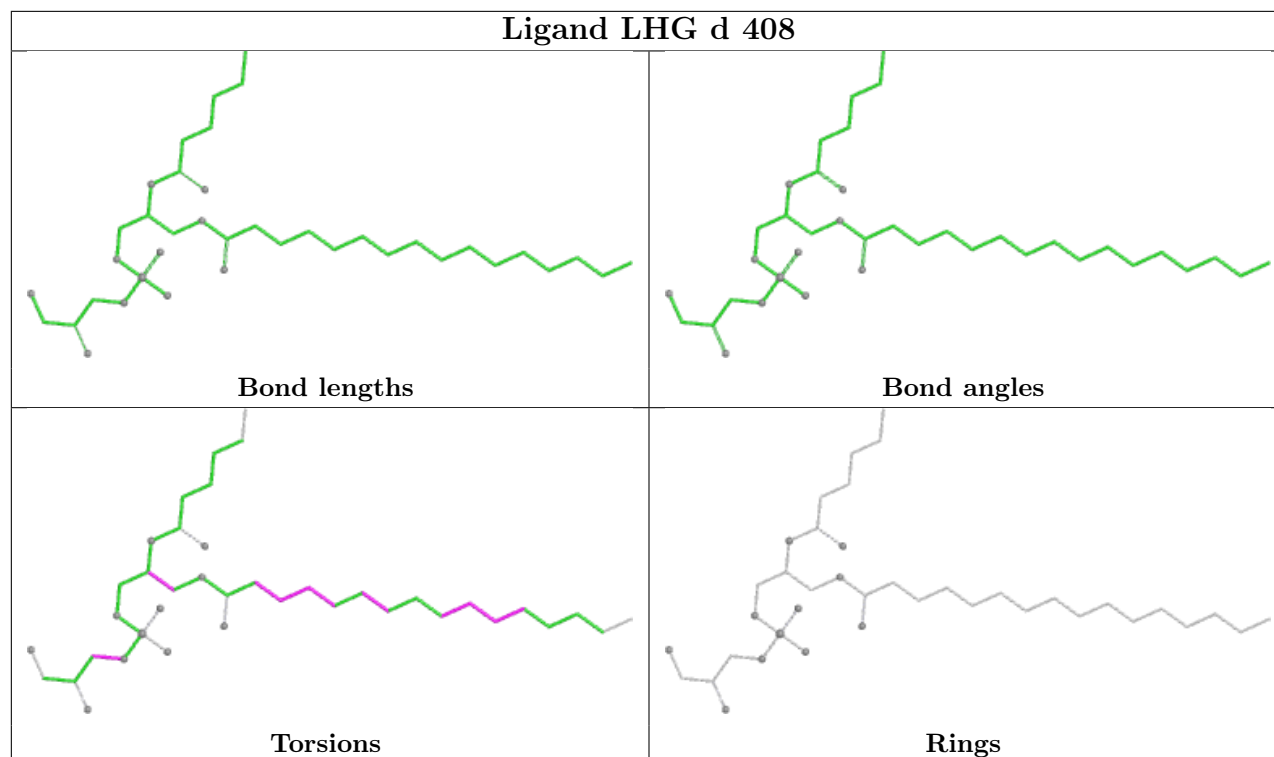


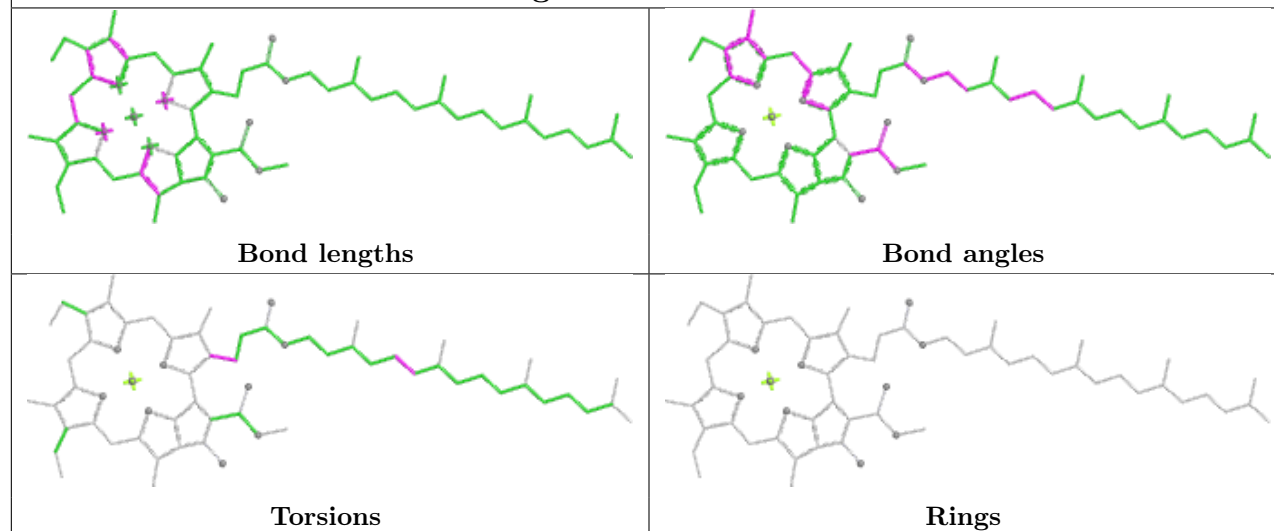
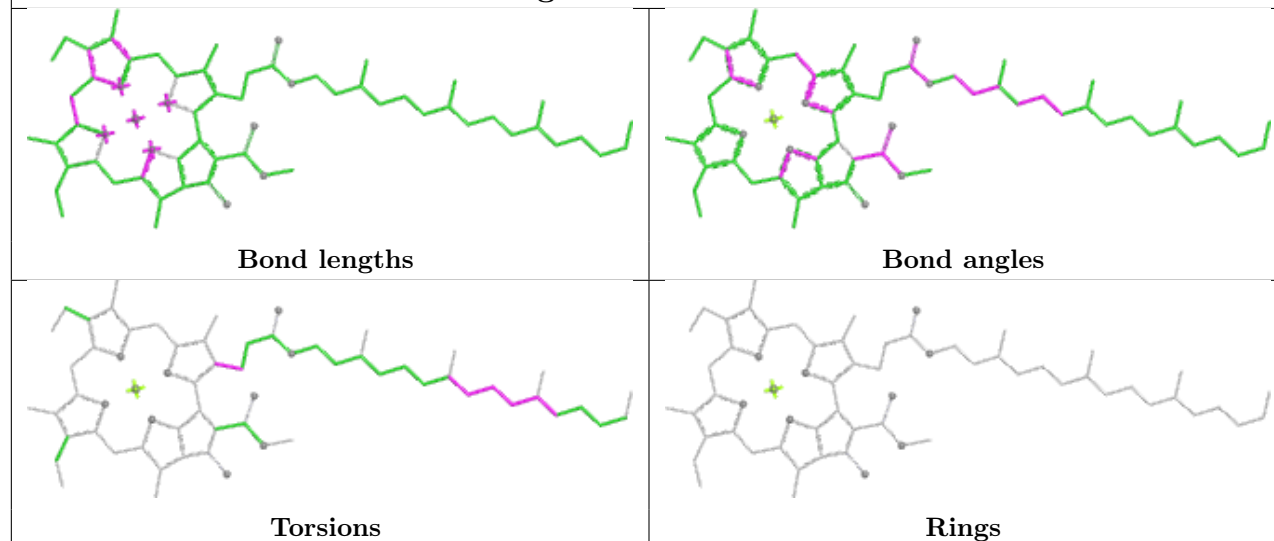
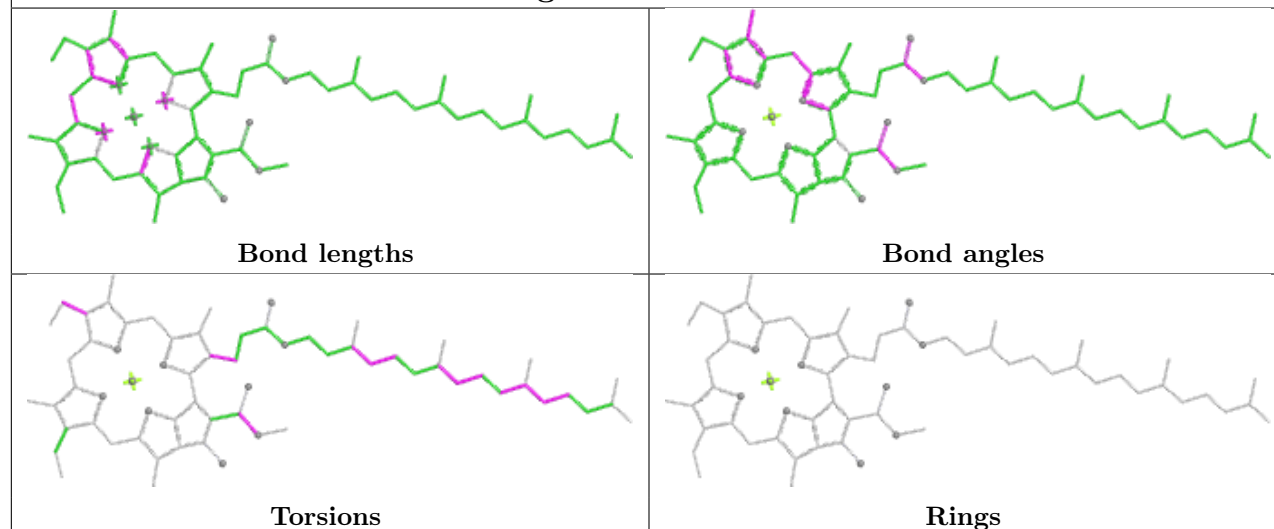
Ligand CLA c 509

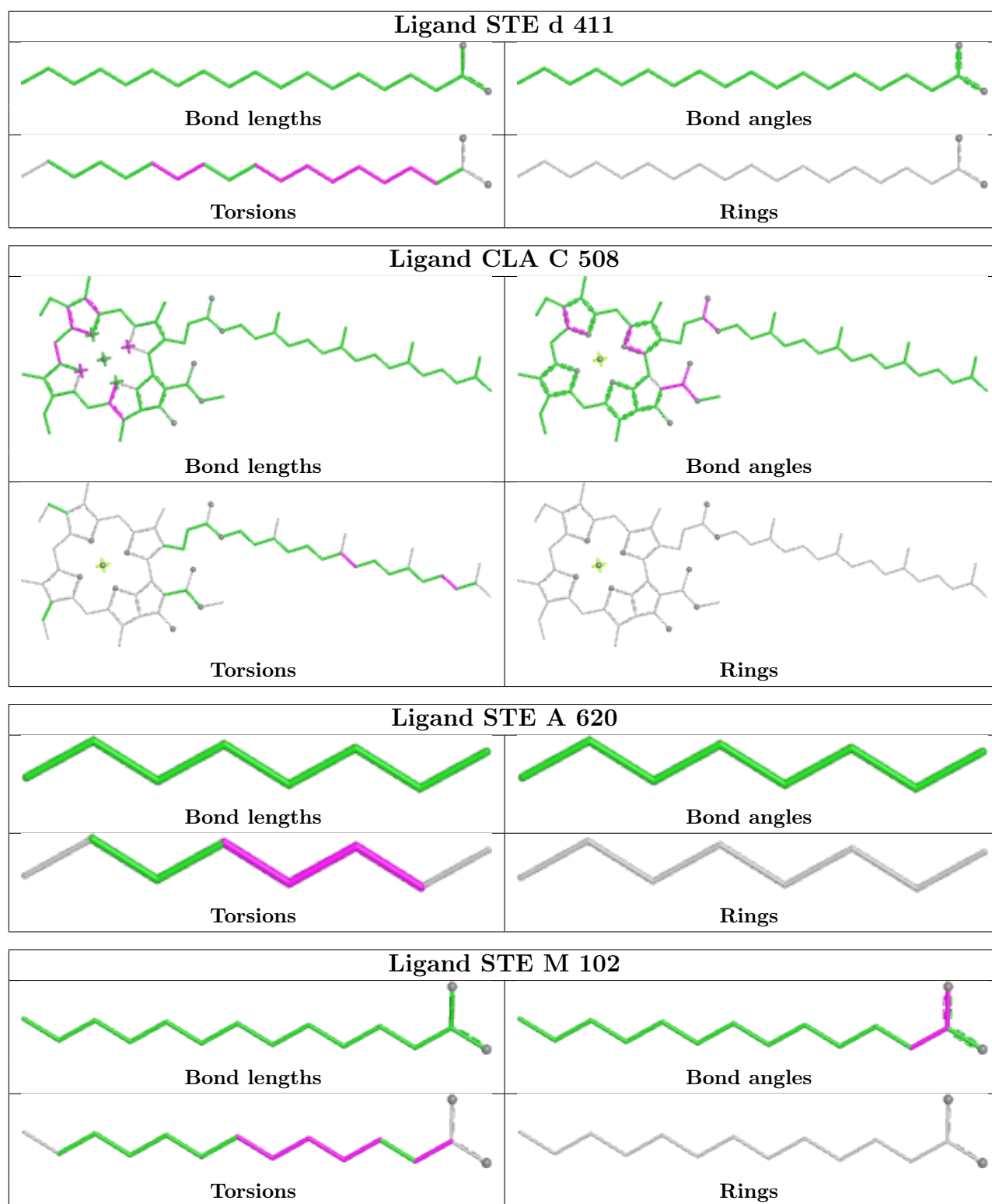


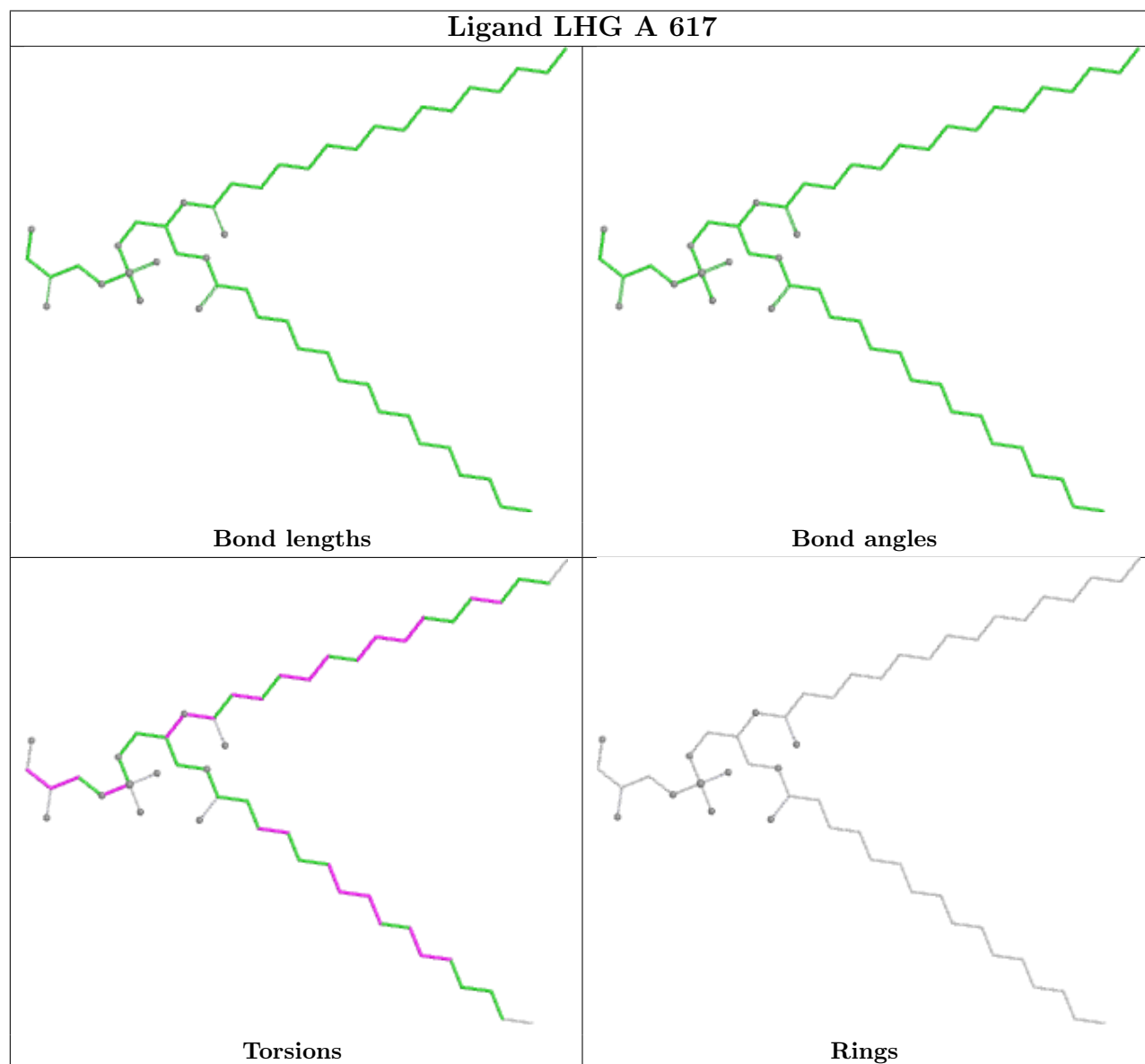
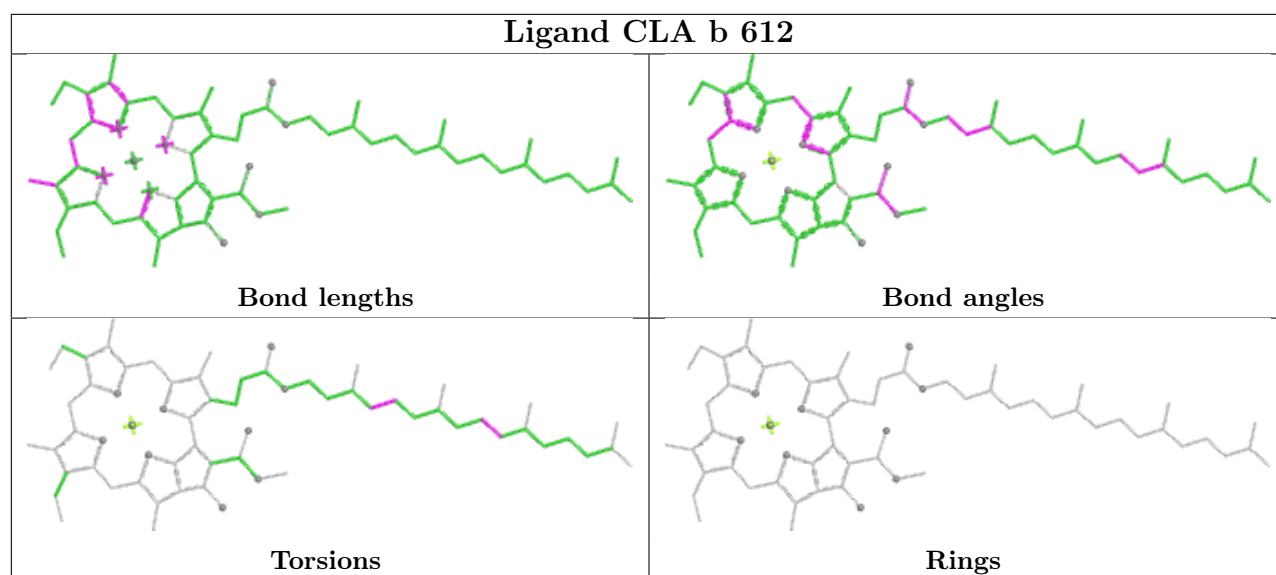
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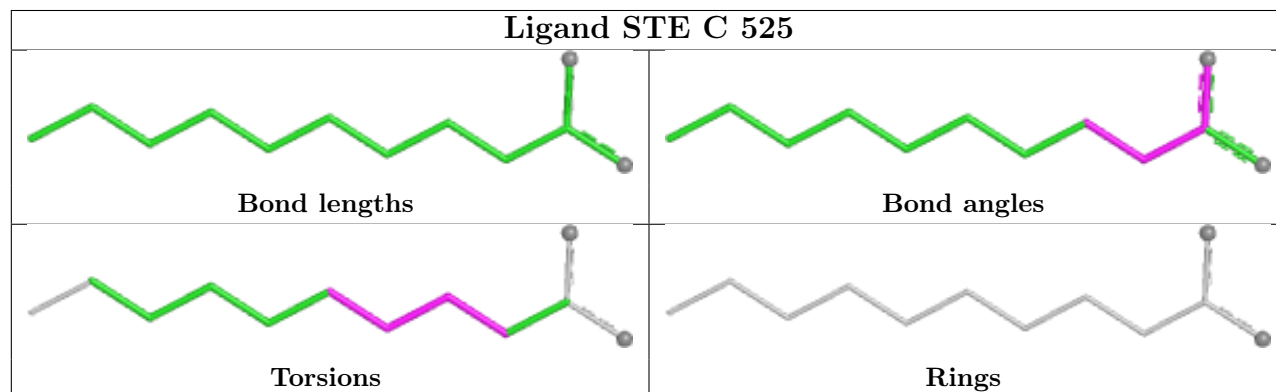
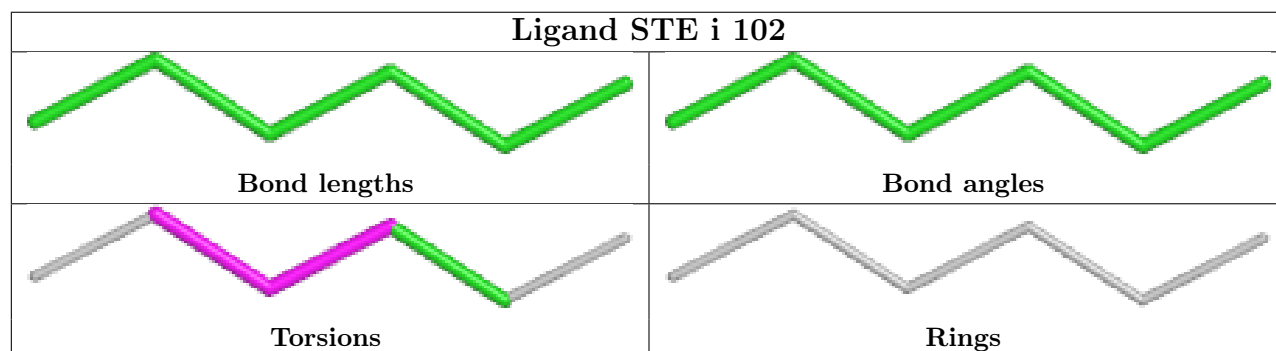
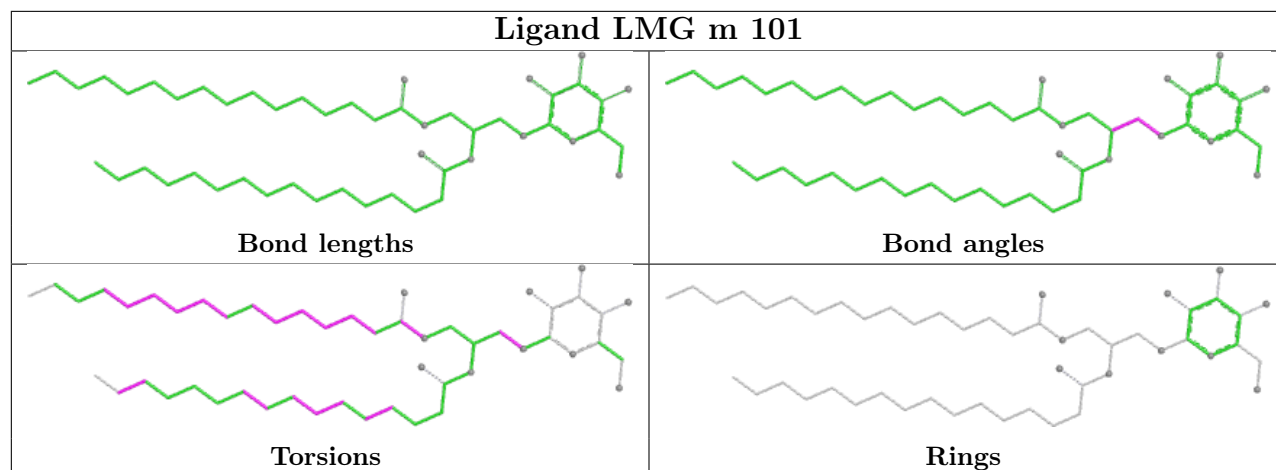


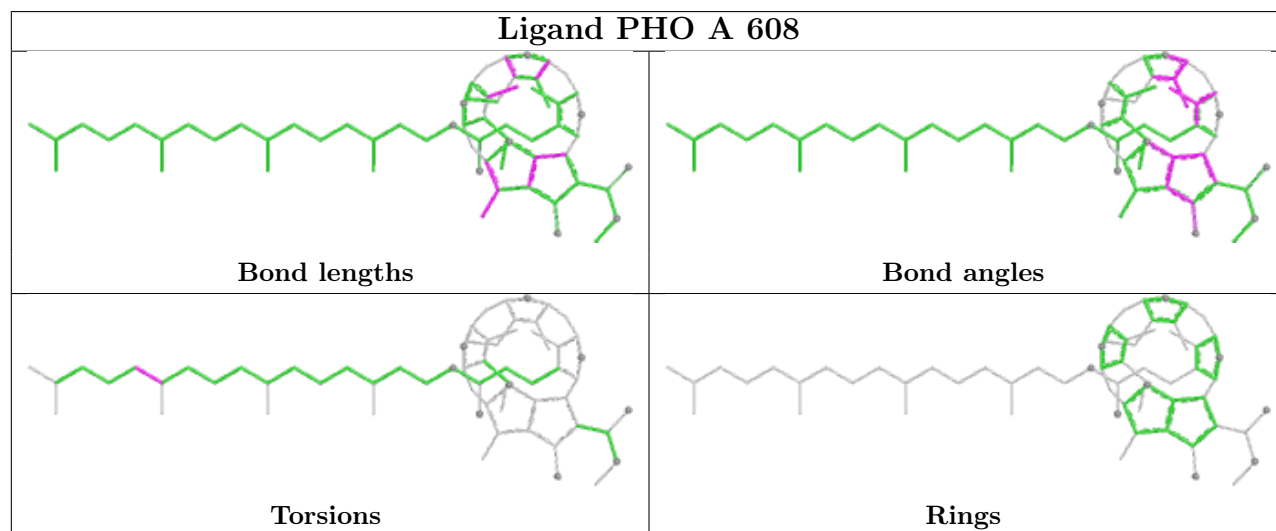
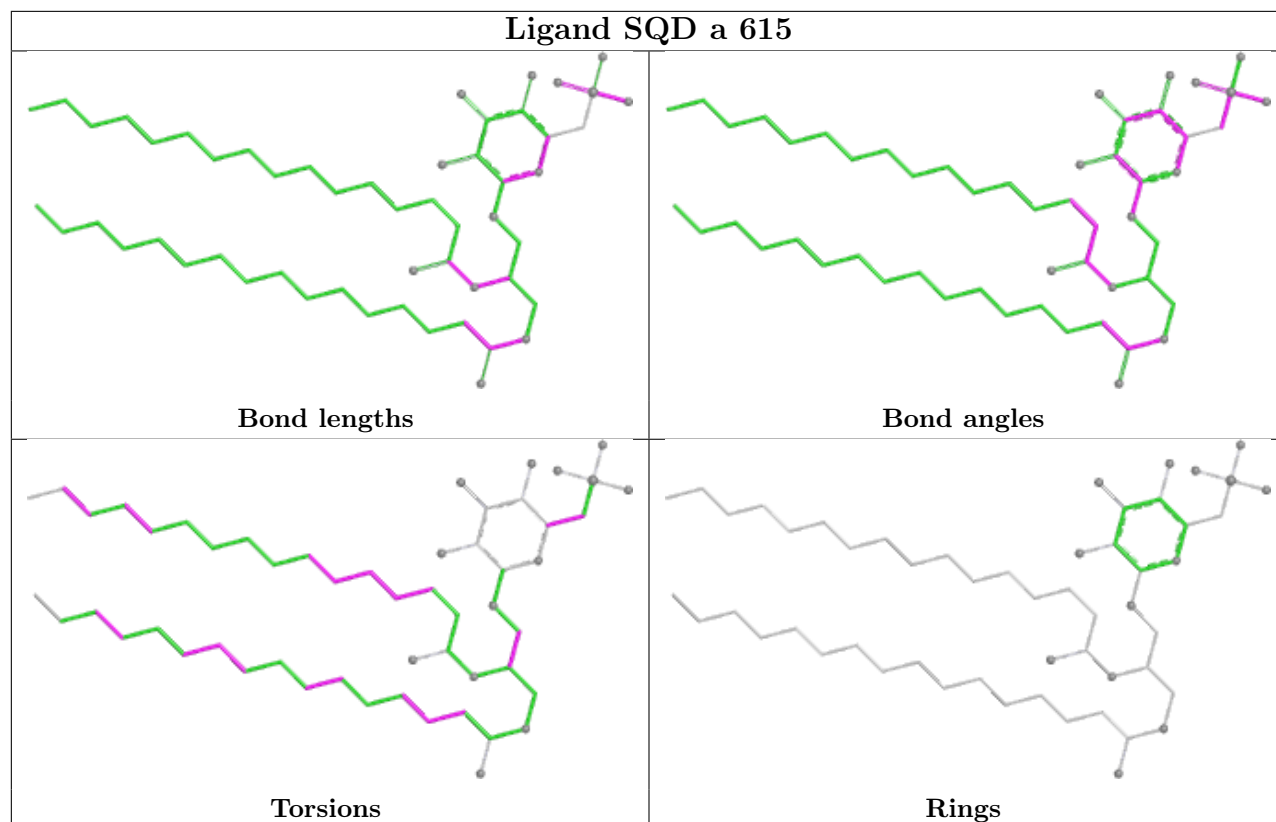


Ligand CLA C 503**Ligand CLA c 508****Ligand CLA c 513**

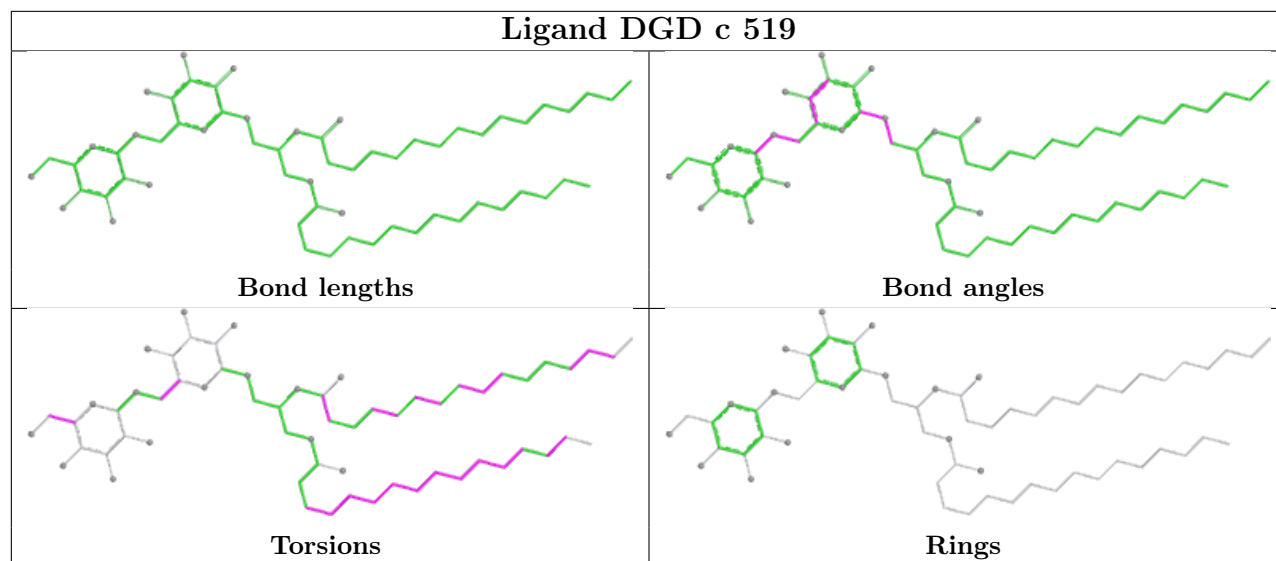




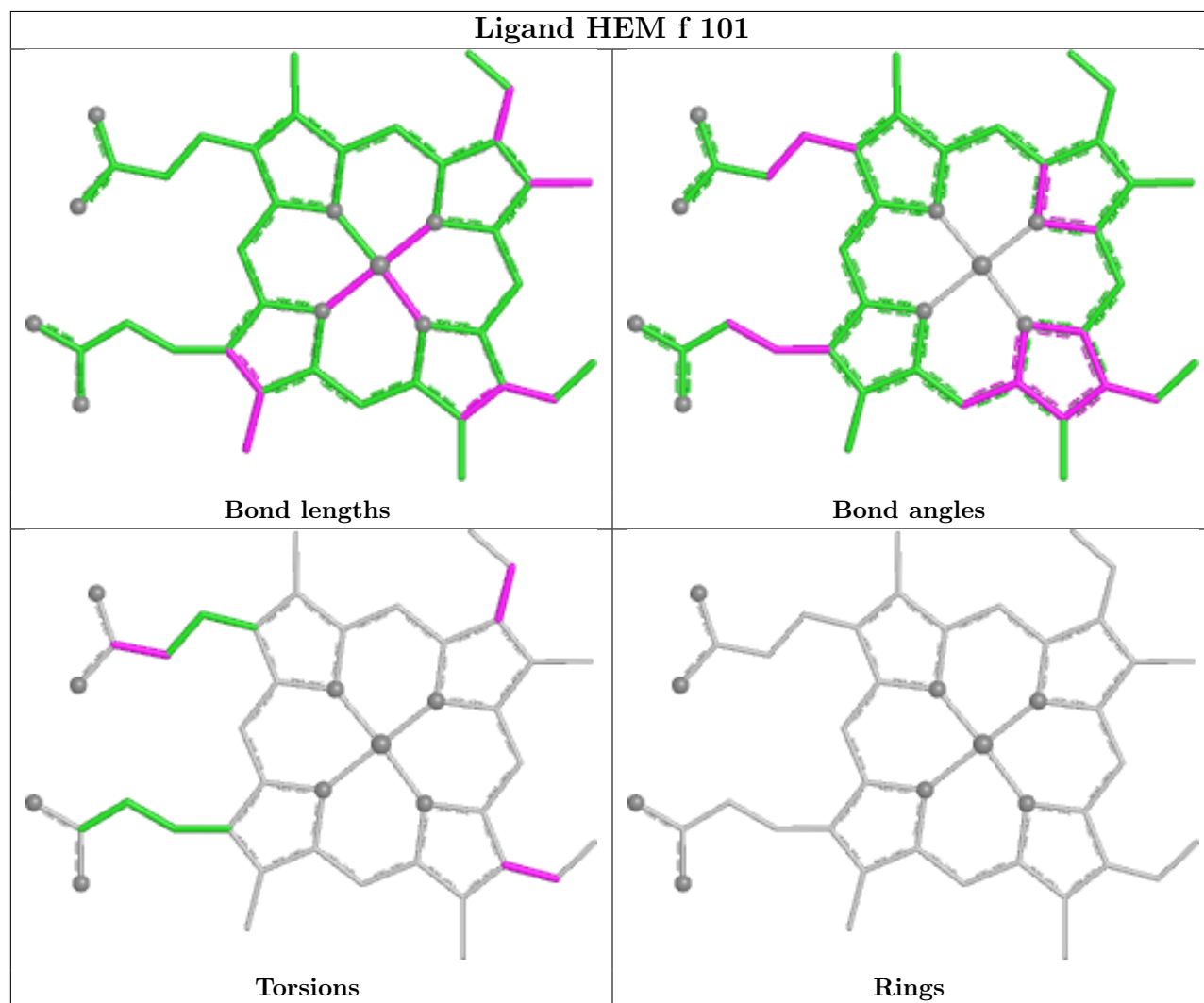


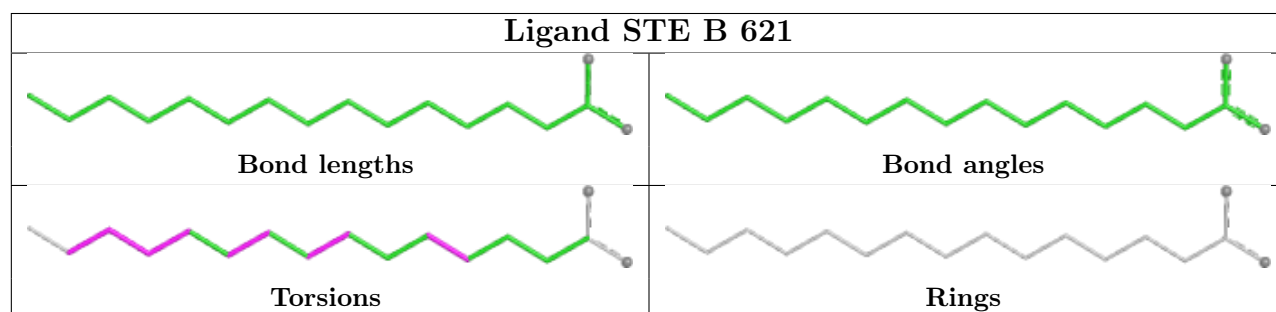
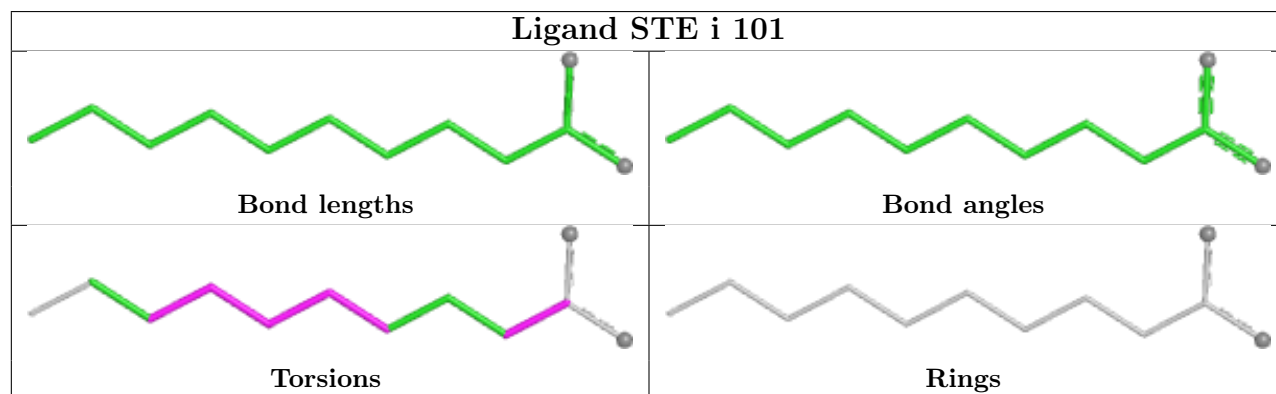
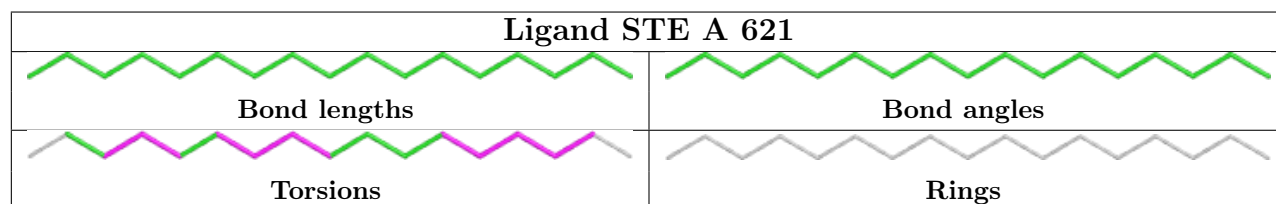
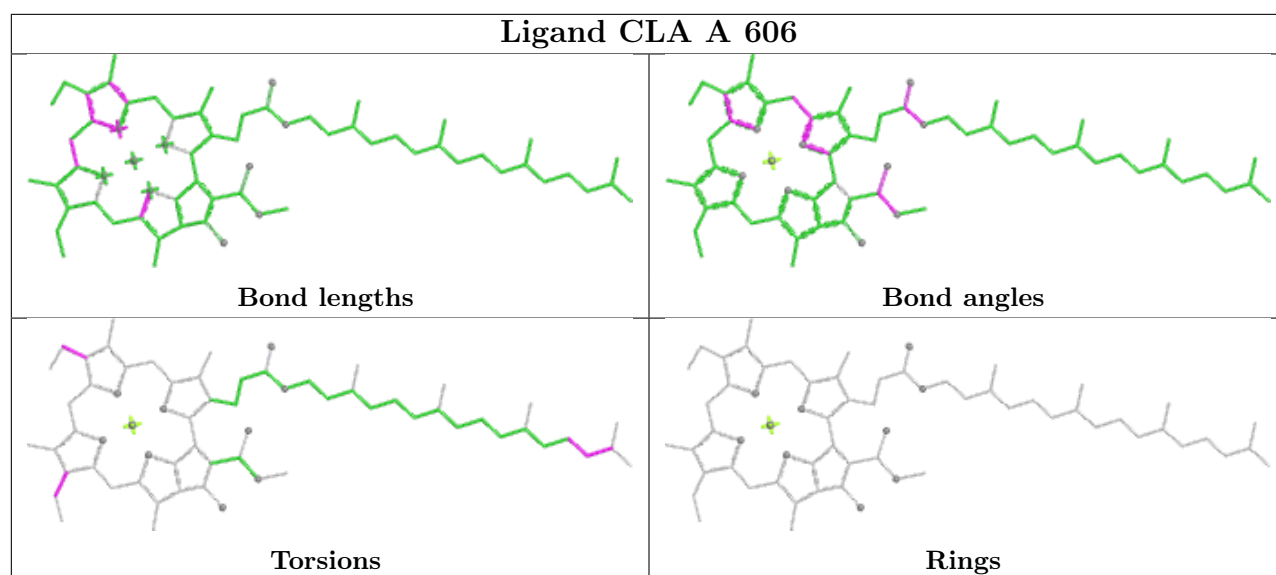


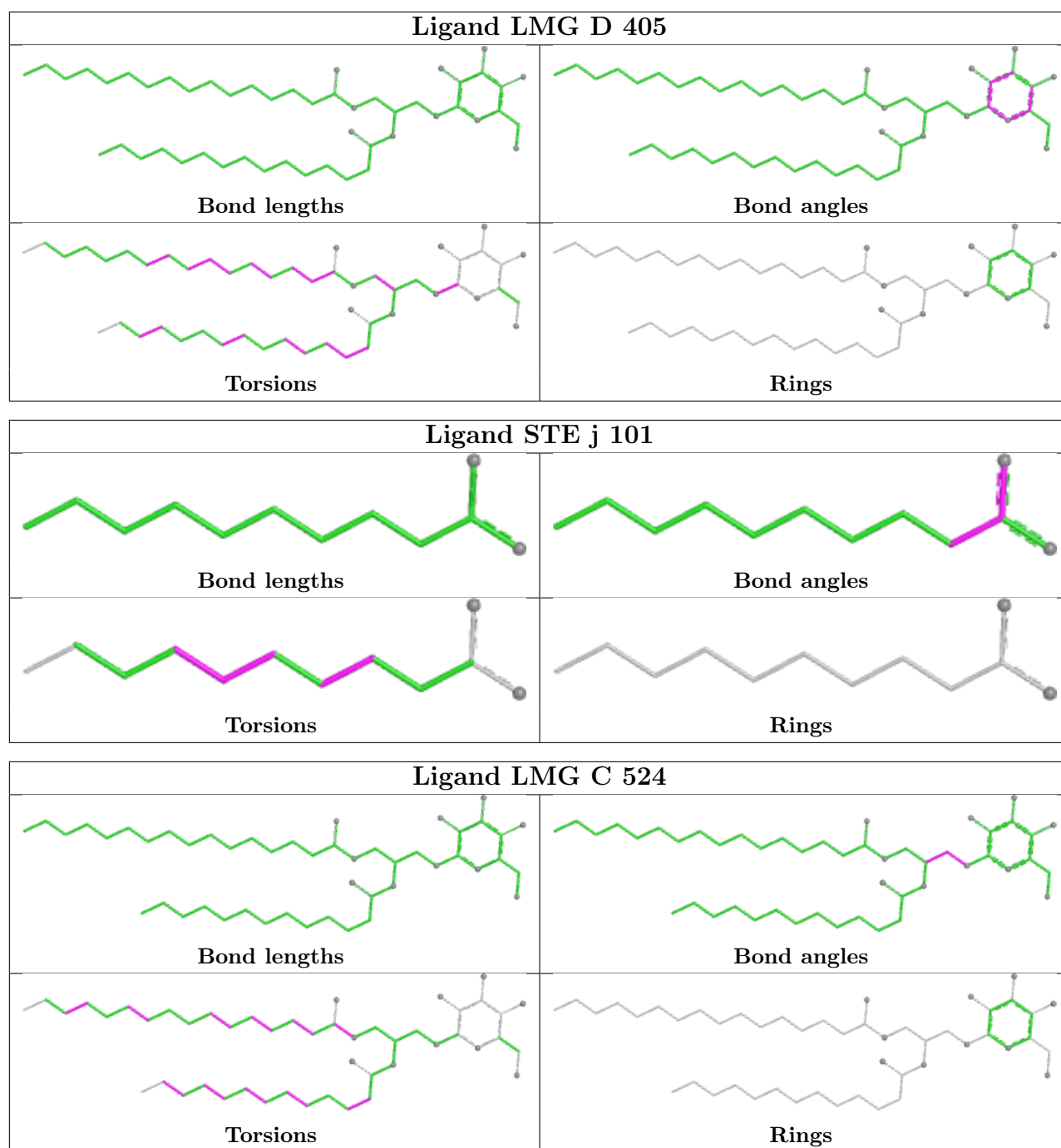
Ligand DGD c 519

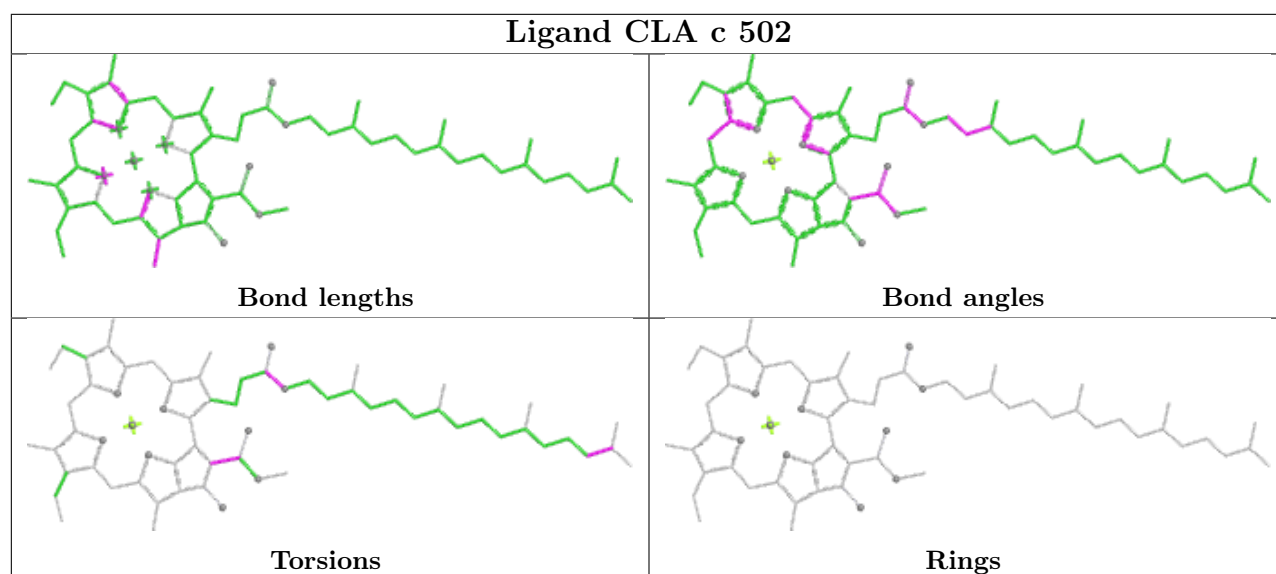
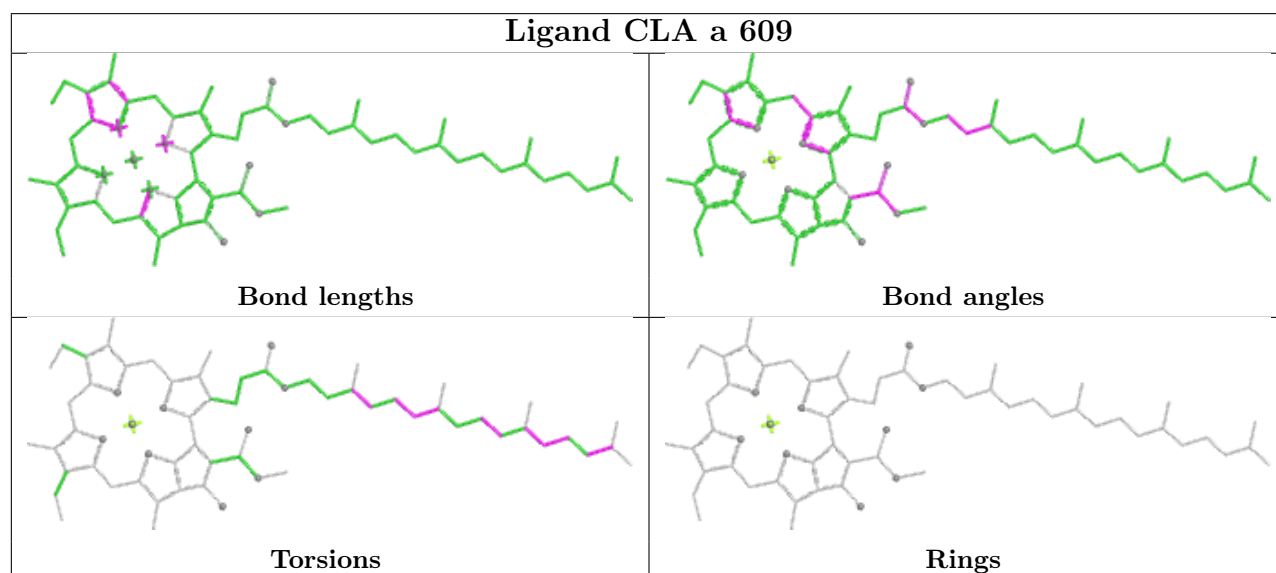
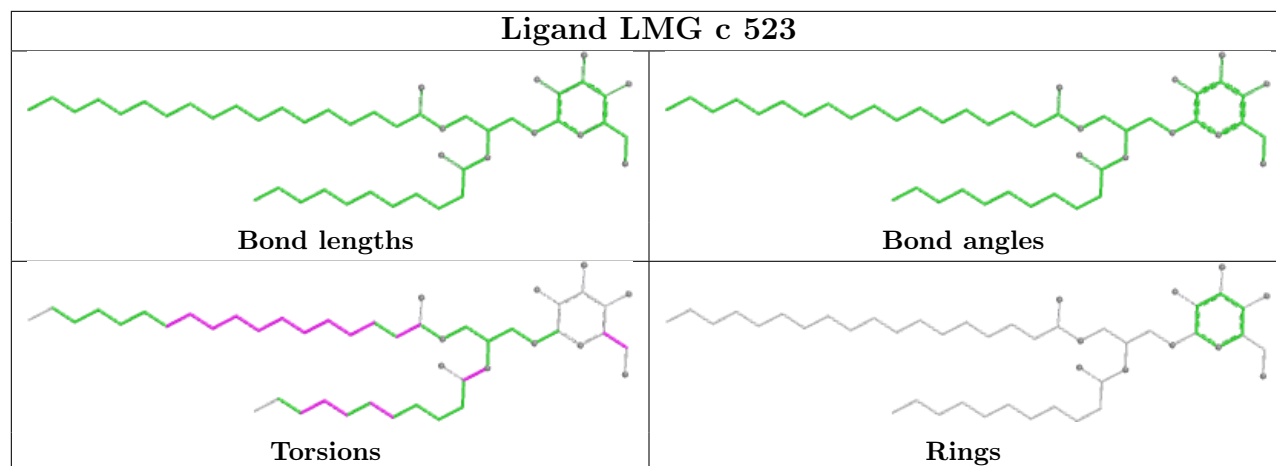


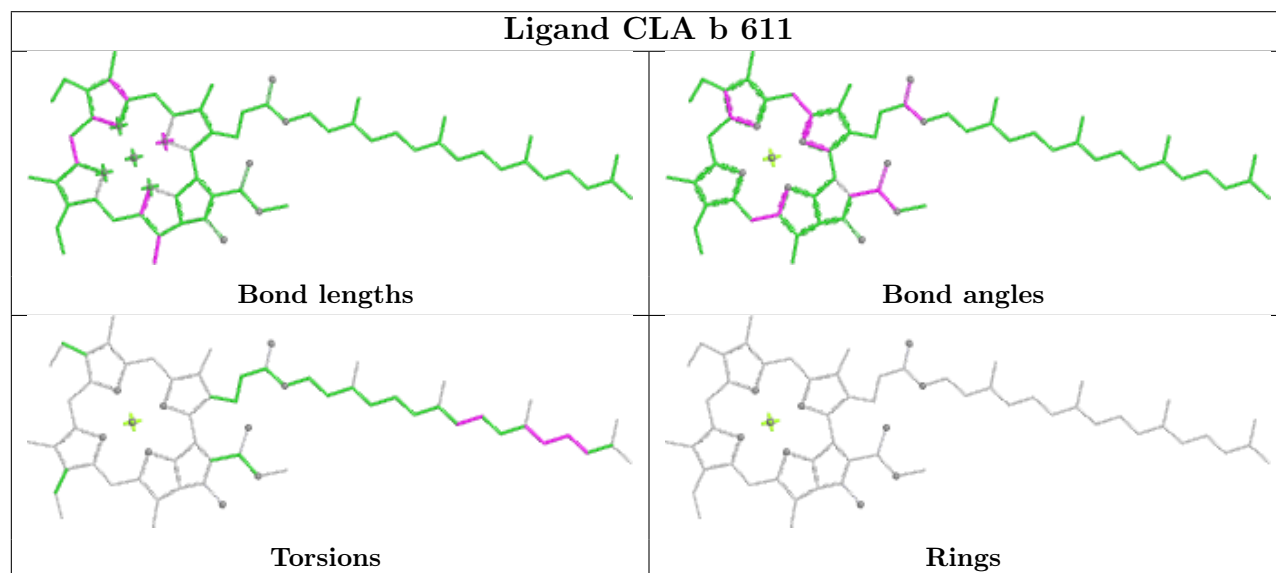
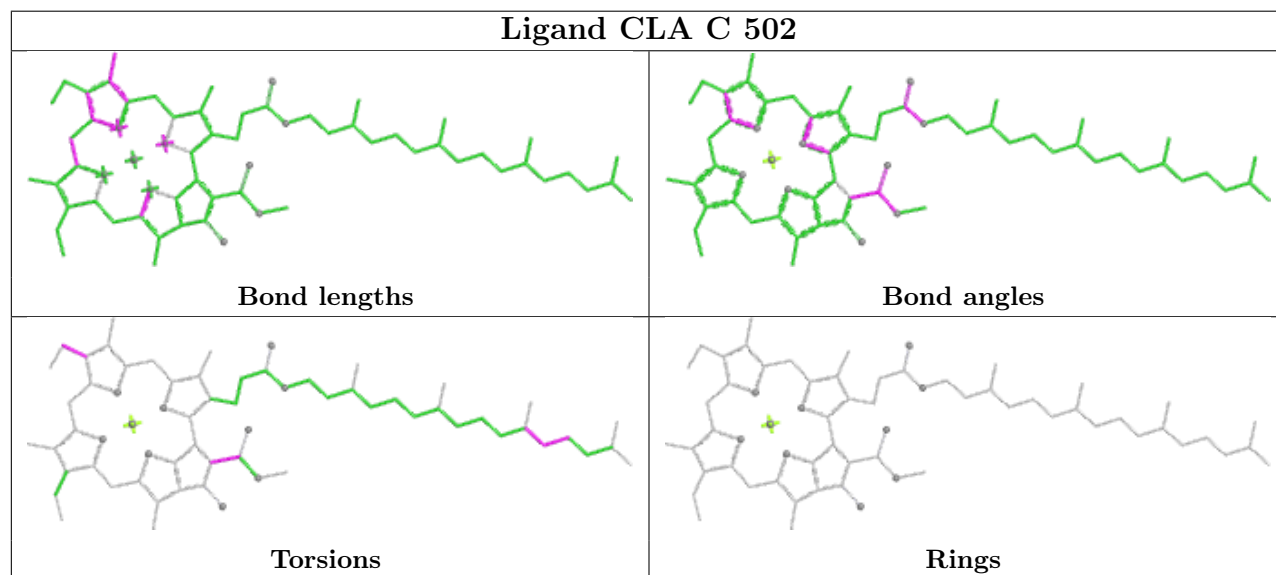
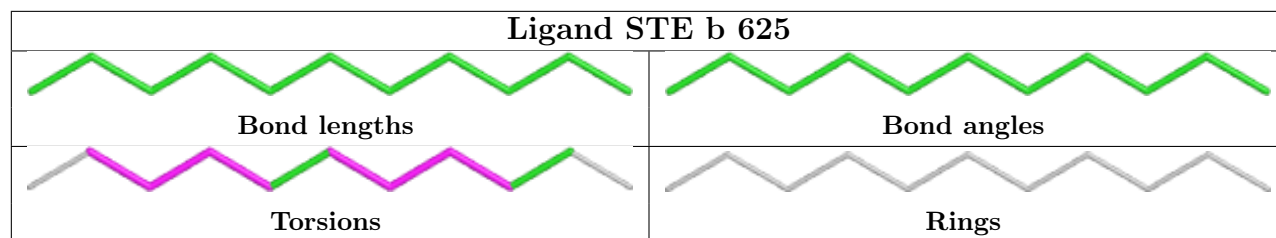
Ligand HEM f 101

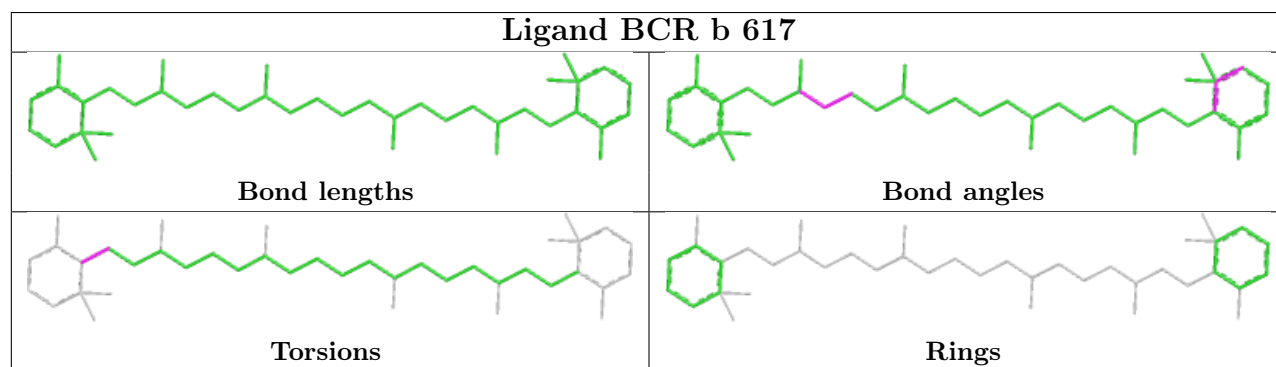
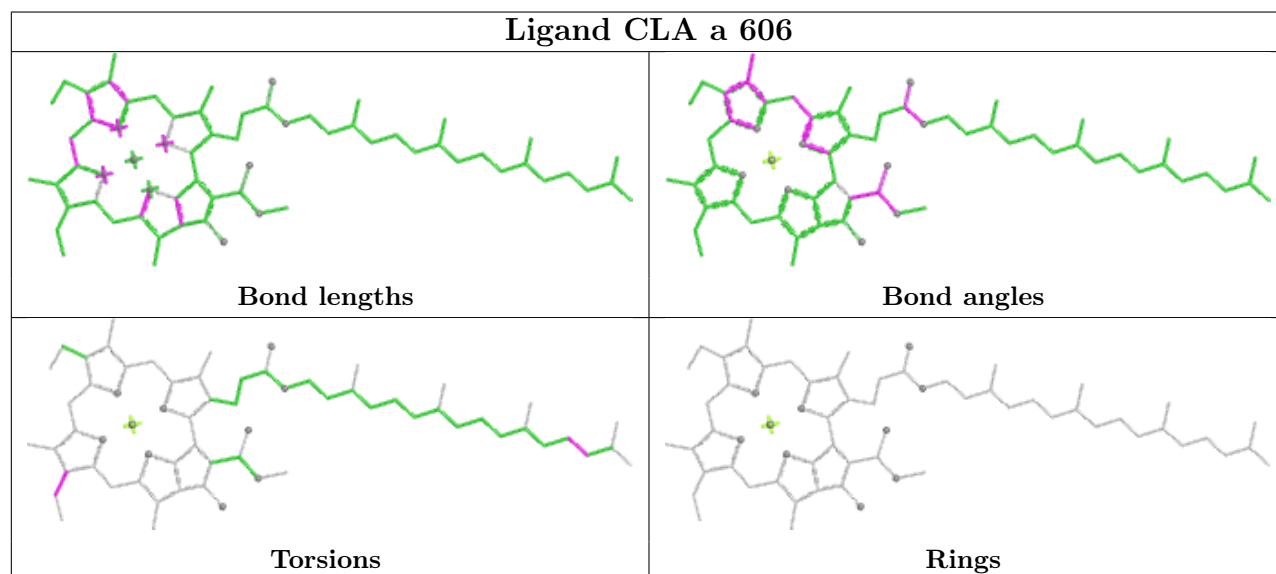
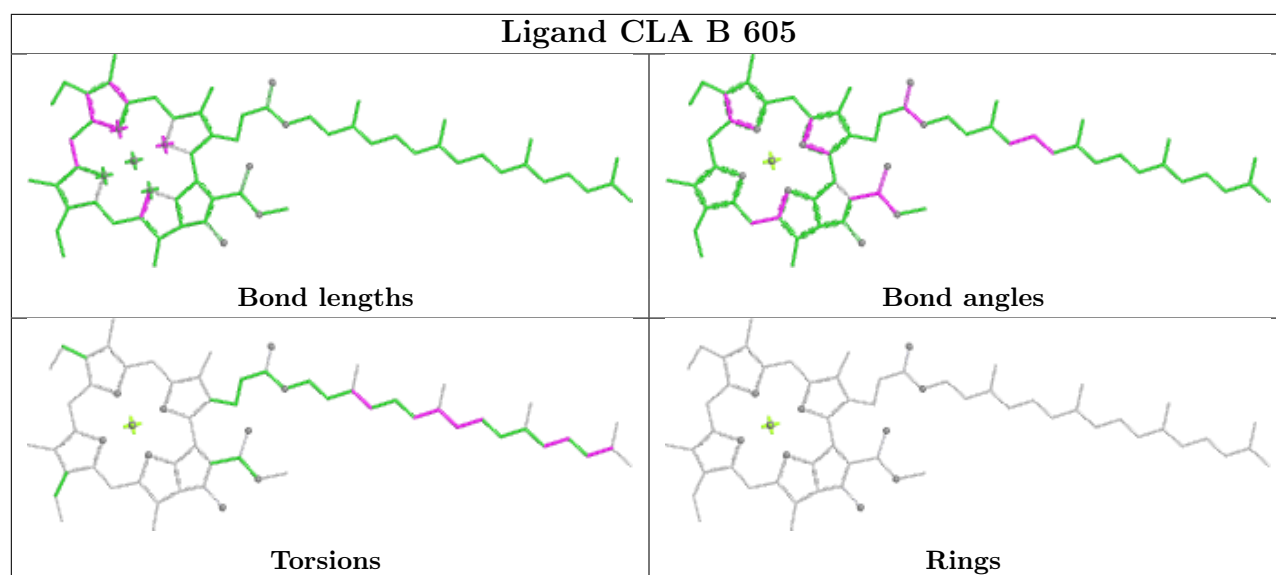


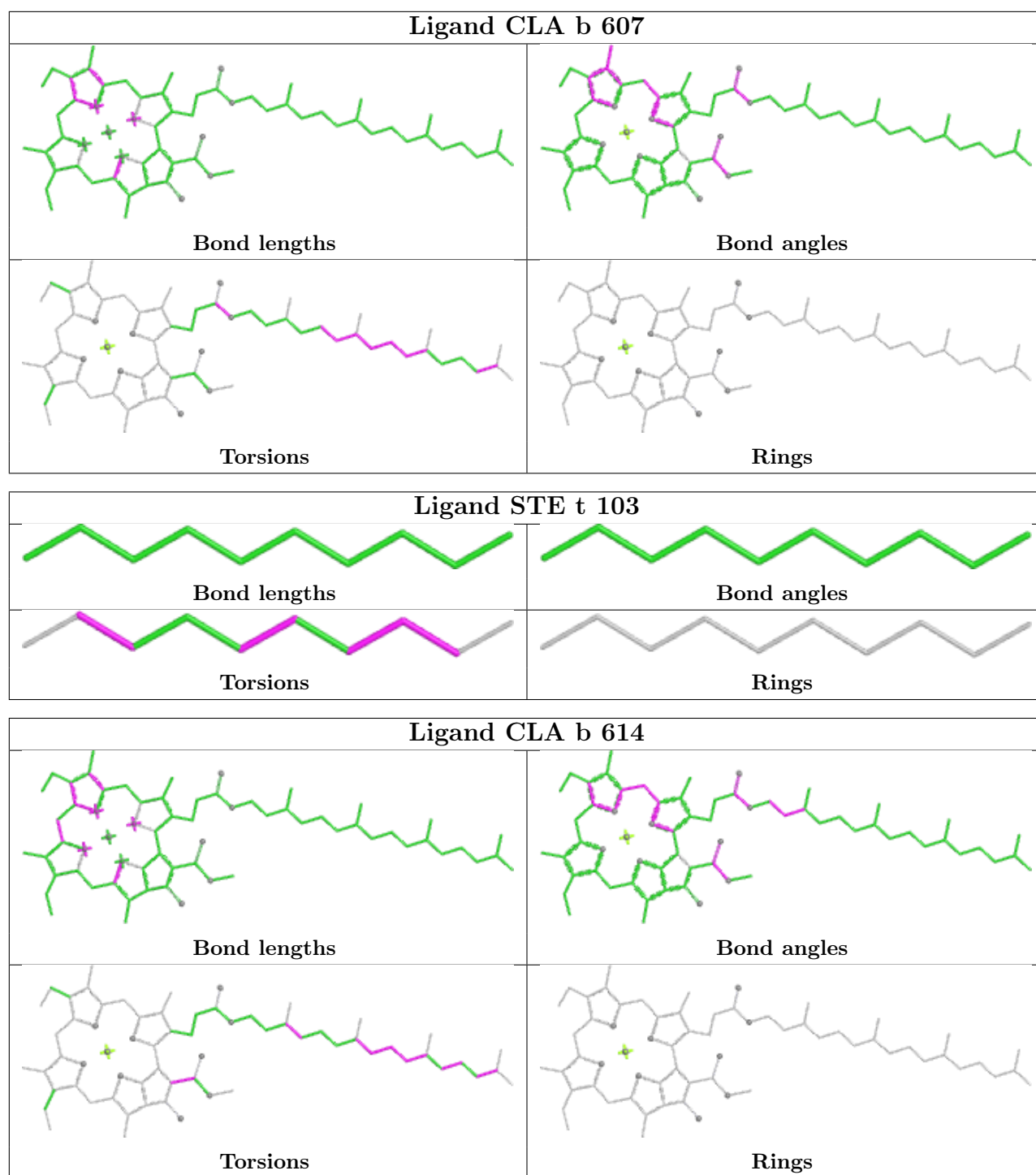


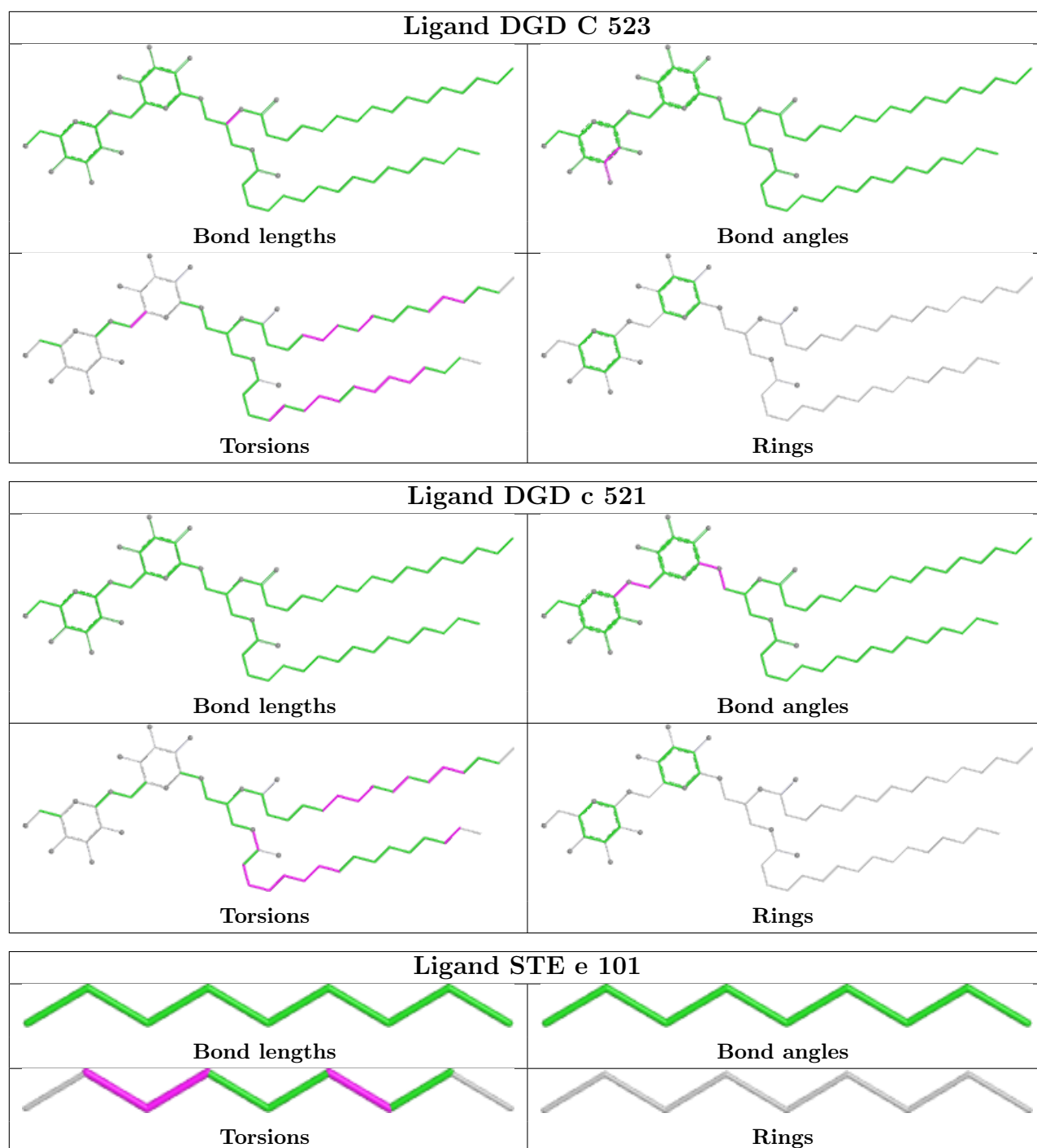












5.7 Other polymers [i](#)

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%)	-0.41	1 (0%) 90 93	22, 27, 43, 74	0
1	a	334/344 (97%)	-0.25	2 (0%) 85 90	22, 29, 52, 73	0
2	B	505/510 (99%)	-0.18	8 (1%) 70 79	17, 31, 55, 84	5 (0%)
2	b	505/510 (99%)	-0.05	4 (0%) 82 87	25, 34, 64, 94	1 (0%)
3	C	442/461 (95%)	-0.14	0 100 100	16, 34, 49, 69	1 (0%)
3	c	451/461 (97%)	0.04	4 (0%) 81 86	19, 38, 56, 91	2 (0%)
4	D	341/352 (96%)	-0.42	0 100 100	22, 28, 43, 68	0
4	d	341/352 (96%)	-0.21	0 100 100	23, 33, 52, 69	1 (0%)
5	E	82/84 (97%)	0.48	1 (1%) 76 83	30, 47, 62, 82	1 (1%)
5	e	82/84 (97%)	0.64	2 (2%) 59 69	38, 54, 72, 81	0
6	F	34/45 (75%)	0.21	1 (2%) 53 63	33, 40, 54, 78	0
6	f	34/45 (75%)	0.49	1 (2%) 53 63	40, 47, 67, 84	0
7	H	65/66 (98%)	0.10	0 100 100	28, 38, 50, 70	0
7	h	63/66 (95%)	0.37	2 (3%) 50 60	36, 46, 56, 61	0
8	I	35/38 (92%)	-0.01	0 100 100	31, 37, 57, 72	0
8	i	35/38 (92%)	0.22	2 (5%) 29 38	31, 39, 65, 86	0
9	J	36/40 (90%)	0.41	1 (2%) 55 65	30, 46, 72, 81	0
9	j	36/40 (90%)	0.60	3 (8%) 17 24	36, 52, 78, 84	0
10	K	37/46 (80%)	0.37	0 100 100	38, 46, 61, 72	0
10	k	37/46 (80%)	0.44	0 100 100	44, 50, 67, 75	0
11	L	37/37 (100%)	-0.31	0 100 100	24, 27, 56, 64	0
11	l	36/37 (97%)	-0.36	0 100 100	25, 29, 63, 77	0
12	M	32/36 (88%)	-0.04	0 100 100	27, 31, 52, 71	0
12	m	31/36 (86%)	-0.24	0 100 100	27, 32, 49, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.09	5 (2%) 65 74	24, 39, 72, 119	1 (0%)
13	o	244/272 (89%)	0.16	10 (4%) 41 51	25, 39, 74, 114	0
14	T	29/32 (90%)	-0.21	1 (3%) 48 58	25, 30, 48, 65	0
14	t	29/32 (90%)	-0.20	2 (6%) 23 30	25, 31, 61, 76	0
15	U	97/134 (72%)	0.07	0 100 100	30, 39, 62, 89	0
15	u	97/134 (72%)	0.02	1 (1%) 79 86	29, 38, 53, 81	0
16	V	137/163 (84%)	-0.07	0 100 100	28, 38, 52, 69	0
16	v	137/163 (84%)	0.23	0 100 100	32, 44, 61, 82	0
17	Y	27/46 (58%)	1.41	5 (18%) 3 4	50, 64, 88, 90	0
17	y	30/46 (65%)	0.92	0 100 100	55, 65, 74, 87	0
18	X	38/41 (92%)	0.38	2 (5%) 32 41	36, 46, 61, 71	0
18	x	39/41 (95%)	0.49	2 (5%) 33 43	43, 54, 73, 90	0
19	Z	62/62 (100%)	1.19	6 (9%) 13 19	49, 62, 97, 108	0
19	z	62/62 (100%)	1.18	8 (12%) 7 10	54, 66, 107, 122	0
20	R	28/41 (68%)	1.03	2 (7%) 22 29	53, 64, 74, 81	0
20	r	28/41 (68%)	1.63	8 (28%) 1 1	63, 77, 92, 97	0
All	All	5293/5700 (92%)	-0.00	84 (1%) 70 79	16, 36, 65, 122	12 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	6.0
19	z	33	TRP	5.0
3	c	23	ALA	4.9
19	Z	62	VAL	4.2
17	Y	25	ILE	4.0
19	Z	33	TRP	3.9
20	r	28	VAL	3.9
3	c	24	THR	3.8
13	O	56	PRO	3.7
1	a	11	ALA	3.5
17	Y	22	LEU	3.5
14	t	29	ILE	3.4
17	Y	20	ALA	3.4
20	r	3	TRP	3.4
2	b	488	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	79	PHE	3.2
13	o	59	LYS	3.2
18	X	2	THR	3.1
2	B	479[A]	PHE	3.1
9	j	5	GLY	3.1
14	t	30	THR	3.1
2	B	495	PHE	3.0
20	r	27	ALA	2.9
20	R	3	TRP	2.9
5	e	3	GLY	2.9
20	r	20	VAL	2.8
1	A	11	ALA	2.6
15	u	53	ALA	2.6
13	o	57	LYS	2.6
13	o	62	GLU	2.6
13	O	60	ARG	2.5
2	b	495	PHE	2.5
13	o	61	GLN	2.5
19	z	60	PHE	2.5
18	x	2	THR	2.5
13	o	56	PRO	2.5
8	i	34	ARG	2.4
9	j	6	GLY	2.4
17	Y	46	LEU	2.4
19	Z	17	PHE	2.4
6	F	12	SER	2.4
20	R	28	VAL	2.4
7	h	64	ALA	2.4
13	O	58	ASN	2.4
13	o	5	LEU	2.4
3	c	193	GLY	2.3
9	J	5	GLY	2.3
13	O	59	LYS	2.3
9	j	7	ARG	2.3
13	o	4	THR	2.3
14	T	30	THR	2.3
13	o	63	ALA	2.3
17	Y	24	MET	2.3
20	r	29	LYS	2.3
19	z	26	ALA	2.3
2	b	127	ARG	2.3
2	B	486	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
7	h	6	TRP	2.2
6	f	13	TYR	2.2
2	B	490	GLN	2.2
8	i	36	ASP	2.2
13	o	132	ASN	2.2
19	Z	30	PRO	2.2
19	z	30	PRO	2.2
3	c	134	ILE	2.2
19	z	39	LEU	2.2
19	z	41	PHE	2.1
19	z	3	ILE	2.1
20	r	23	ILE	2.1
2	B	499	VAL	2.1
18	X	3	ILE	2.1
19	Z	3	ILE	2.1
2	B	487	SER	2.1
1	a	245	THR	2.1
2	b	486	LEU	2.1
20	r	14	LEU	2.1
2	B	127	ARG	2.1
19	z	40	ILE	2.0
19	Z	7	LEU	2.0
13	O	63	ALA	2.0
5	e	6	GLY	2.0
20	r	26	TYR	2.0
2	B	488	PRO	2.0
18	x	37	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	31,36,52,60	0
14	FME	t	1	10/11	0.94	0.07	30,35,52,57	0
12	FME	M	1	10/11	0.95	0.09	33,42,54,58	0
12	FME	m	1	10/11	0.96	0.09	31,44,61,67	0
8	FME	I	1	10/11	0.96	0.08	37,44,51,52	0
8	FME	i	1	10/11	0.97	0.07	36,44,50,51	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
29	STE	I	101	17/20	0.62	0.17	50,60,66,66	0
29	STE	i	101	12/20	0.62	0.15	62,75,94,95	0
29	STE	C	520	10/20	0.63	0.21	51,70,79,80	0
29	STE	e	101	9/20	0.65	0.25	63,70,76,78	0
29	STE	j	102	16/20	0.67	0.22	57,63,90,91	0
29	STE	K	102	14/20	0.68	0.17	54,60,74,76	0
29	STE	C	527	14/20	0.69	0.19	57,69,77,82	0
29	STE	C	518	5/20	0.69	0.22	54,59,60,61	0
29	STE	A	621	17/20	0.71	0.15	52,60,68,69	0
30	LMG	c	518	30/55	0.71	0.18	42,75,94,96	0
30	LMG	D	405	50/55	0.72	0.17	35,62,93,96	0
29	STE	c	517	18/20	0.72	0.20	61,71,79,80	0
29	STE	E	103	20/20	0.73	0.18	43,60,70,72	0
29	STE	H	103	18/20	0.73	0.17	52,62,68,72	0
29	STE	E	102	12/20	0.75	0.19	61,67,86,87	0
29	STE	b	625	11/20	0.75	0.22	52,57,60,65	0
29	STE	C	516	14/20	0.76	0.18	51,58,64,64	0
30	LMG	C	517	36/55	0.76	0.15	43,54,63,66	0
29	STE	b	623	16/20	0.76	0.18	45,55,71,75	0
30	LMG	b	622	55/55	0.76	0.18	45,62,73,77	0
29	STE	i	102	6/20	0.76	0.16	48,59,67,70	0
30	LMG	c	523	48/55	0.76	0.16	49,66,77,86	0
32	LHG	e	102	42/49	0.76	0.17	52,77,88,100	0
29	STE	A	613	9/20	0.77	0.16	53,56,73,75	0
29	STE	e	103	9/20	0.77	0.17	51,62,70,71	0
32	LHG	A	617	49/49	0.77	0.16	45,66,89,90	0
29	STE	h	103	10/20	0.77	0.19	58,66,72,75	0
30	LMG	a	616	55/55	0.78	0.15	38,54,67,74	0
29	STE	T	102	16/20	0.78	0.19	40,49,73,76	0
29	STE	e	104	13/20	0.78	0.19	70,73,81,85	0
29	STE	I	102	15/20	0.79	0.18	46,51,64,71	0
29	STE	k	103	14/20	0.79	0.15	51,63,74,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	STE	Z	101	17/20	0.79	0.20	49,66,84,85	0
29	STE	a	617	12/20	0.79	0.14	57,61,74,77	0
29	STE	C	525	12/20	0.79	0.16	43,48,54,55	0
30	LMG	B	620	45/55	0.80	0.15	35,51,78,83	0
29	STE	A	622	11/20	0.80	0.15	54,58,66,67	0
28	PL9	a	611	55/55	0.80	0.17	36,59,72,73	0
29	STE	b	624	10/20	0.81	0.14	47,50,56,65	0
29	STE	C	519	7/20	0.81	0.16	53,55,58,58	0
29	STE	B	625	15/20	0.81	0.20	41,50,63,73	0
31	SQD	a	615	54/54	0.81	0.14	42,54,85,88	0
29	STE	j	101	12/20	0.81	0.15	48,52,56,64	0
29	STE	f	103	8/20	0.81	0.19	53,57,62,64	0
29	STE	d	409	20/20	0.82	0.15	44,56,80,80	0
29	STE	z	101	9/20	0.82	0.22	55,61,64,65	0
29	STE	B	624	12/20	0.82	0.13	48,55,63,67	0
33	DGD	A	619	66/66	0.82	0.14	44,54,76,80	0
29	STE	J	102	12/20	0.83	0.14	46,50,62,67	0
29	STE	E	101	12/20	0.83	0.15	59,65,75,76	0
29	STE	M	104	15/20	0.84	0.16	45,49,71,74	0
31	SQD	A	618	43/54	0.84	0.12	39,50,79,83	0
28	PL9	A	612	55/55	0.84	0.15	31,55,70,77	0
29	STE	d	406	20/20	0.85	0.13	38,47,71,77	0
29	STE	t	103	10/20	0.85	0.14	42,53,56,57	0
29	STE	B	623	18/20	0.85	0.13	43,51,81,84	0
29	STE	d	411	20/20	0.85	0.14	36,48,62,71	0
29	STE	D	411	9/20	0.85	0.15	51,56,66,68	0
29	STE	A	620	8/20	0.86	0.15	51,52,56,57	0
29	STE	C	526	16/20	0.86	0.13	37,43,58,63	0
29	STE	B	621	17/20	0.86	0.13	39,47,65,67	0
29	STE	c	516	13/20	0.86	0.15	59,62,68,69	0
25	CLA	b	601	65/65	0.86	0.12	44,59,79,85	0
30	LMG	A	615	48/55	0.86	0.12	39,52,64,68	0
30	LMG	m	101	51/55	0.87	0.12	37,48,57,64	0
29	STE	M	102	15/20	0.87	0.11	36,43,60,73	0
31	SQD	B	622	54/54	0.87	0.11	37,54,68,69	0
29	STE	X	101	20/20	0.87	0.13	34,43,64,73	0
31	SQD	b	620	49/54	0.87	0.11	38,53,66,72	0
29	STE	b	621	20/20	0.87	0.13	34,50,61,65	0
30	LMG	M	101	51/55	0.87	0.11	32,47,58,60	0
30	LMG	c	524	49/55	0.87	0.12	39,56,66,74	0
29	STE	m	102	12/20	0.88	0.12	44,47,66,67	0
29	STE	t	102	14/20	0.88	0.11	36,46,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	STE	m	103	18/20	0.89	0.14	36,42,62,63	0
30	LMG	C	524	48/55	0.89	0.13	42,60,72,75	0
31	SQD	f	102	41/54	0.89	0.13	48,68,79,82	0
25	CLA	c	513	65/65	0.90	0.12	43,56,75,78	0
27	BCR	C	514	40/40	0.90	0.11	43,48,54,59	0
30	LMG	c	522	46/55	0.90	0.12	37,61,67,68	0
27	BCR	J	101	40/40	0.90	0.10	37,45,57,58	0
25	CLA	C	513	65/65	0.90	0.11	41,53,78,82	0
25	CLA	B	601	65/65	0.90	0.11	30,45,74,79	0
29	STE	M	103	10/20	0.90	0.11	40,44,52,56	0
27	BCR	k	101	40/40	0.91	0.11	46,50,57,59	0
31	SQD	a	614	54/54	0.91	0.12	40,55,71,75	0
27	BCR	c	514	40/40	0.91	0.11	46,53,58,59	0
27	BCR	h	101	40/40	0.91	0.10	38,45,56,58	0
27	BCR	d	404	40/40	0.92	0.10	38,43,69,80	0
27	BCR	k	102	40/40	0.92	0.12	40,46,55,59	0
31	SQD	D	407	36/54	0.92	0.12	42,59,72,72	0
25	CLA	c	512	65/65	0.92	0.10	43,50,71,74	0
31	SQD	A	616	52/54	0.92	0.10	30,48,68,74	0
33	DGD	h	102	62/66	0.92	0.10	34,41,50,52	0
27	BCR	b	619	40/40	0.93	0.09	30,39,53,57	0
25	CLA	C	503	65/65	0.93	0.08	30,36,41,47	0
27	BCR	B	618	40/40	0.93	0.08	26,34,41,47	0
25	CLA	C	511	65/65	0.93	0.09	28,43,54,56	0
27	BCR	D	403	40/40	0.93	0.10	30,39,64,73	0
32	LHG	a	613	49/49	0.93	0.11	34,43,56,61	0
27	BCR	H	101	40/40	0.93	0.08	30,39,47,49	0
25	CLA	C	512	65/65	0.93	0.10	36,43,70,78	0
33	DGD	C	522	62/66	0.93	0.10	31,41,82,89	0
33	DGD	H	102	62/66	0.93	0.09	30,37,48,55	0
27	BCR	T	101	40/40	0.93	0.08	29,35,45,46	0
25	CLA	B	606	65/65	0.94	0.08	24,31,59,69	0
28	PL9	d	405	55/55	0.94	0.07	25,31,36,38	0
27	BCR	K	101	40/40	0.94	0.10	34,44,55,57	0
25	CLA	b	606	65/65	0.94	0.08	28,34,59,67	0
27	BCR	b	617	40/40	0.94	0.08	28,36,43,47	0
25	CLA	d	403	65/65	0.94	0.09	30,36,67,75	0
30	LMG	D	406	51/55	0.94	0.11	29,43,67,77	0
26	PHO	d	401	64/64	0.94	0.07	28,34,39,42	0
27	BCR	c	515	40/40	0.94	0.09	29,42,49,50	0
32	LHG	D	410	49/49	0.94	0.10	29,39,55,57	0
25	CLA	b	616	60/65	0.94	0.09	31,37,73,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	c	503	65/65	0.94	0.08	33,39,45,47	0
27	BCR	C	515	40/40	0.94	0.08	28,37,46,47	0
25	CLA	c	509	65/65	0.94	0.09	33,39,52,54	0
27	BCR	t	101	40/40	0.94	0.07	24,33,45,47	0
33	DGD	c	520	62/66	0.94	0.10	34,43,73,77	0
25	CLA	c	511	65/65	0.94	0.09	37,48,57,65	0
25	CLA	C	506	65/65	0.95	0.09	30,36,70,76	0
25	CLA	b	608	65/65	0.95	0.07	29,36,47,51	0
25	CLA	b	609	65/65	0.95	0.07	32,39,55,60	0
25	CLA	b	614	65/65	0.95	0.08	26,33,64,71	0
25	CLA	b	615	65/65	0.95	0.08	27,35,54,59	0
25	CLA	C	508	65/65	0.95	0.08	28,34,81,92	0
25	CLA	C	509	65/65	0.95	0.08	29,34,51,57	0
27	BCR	a	610	40/40	0.95	0.06	23,31,39,40	0
25	CLA	c	505	65/65	0.95	0.08	28,36,55,60	0
30	LMG	d	410	44/55	0.95	0.09	34,43,66,72	0
27	BCR	b	618	40/40	0.95	0.07	25,34,45,48	0
25	CLA	c	506	65/65	0.95	0.09	35,41,72,79	0
25	CLA	c	507	65/65	0.95	0.07	31,40,49,50	0
25	CLA	c	508	64/65	0.95	0.09	31,38,75,91	0
25	CLA	C	510	65/65	0.95	0.08	29,35,48,57	0
25	CLA	c	510	65/65	0.95	0.07	32,40,50,55	0
25	CLA	C	501	65/65	0.95	0.07	25,31,43,44	0
25	CLA	C	502	65/65	0.95	0.07	27,33,44,50	0
25	CLA	B	610	65/65	0.95	0.07	21,29,35,38	0
25	CLA	a	606	65/65	0.95	0.07	21,26,36,49	0
32	LHG	D	409	47/49	0.95	0.11	30,37,69,71	0
28	PL9	D	404	55/55	0.95	0.07	17,28,37,41	0
26	PHO	A	608	64/64	0.95	0.06	19,26,30,33	0
32	LHG	d	408	39/49	0.95	0.09	27,39,56,60	0
26	PHO	A	609	64/64	0.95	0.06	23,28,33,33	0
25	CLA	a	607	65/65	0.95	0.09	26,34,78,84	0
33	DGD	C	521	62/66	0.95	0.10	24,35,67,70	0
27	BCR	A	611	40/40	0.95	0.06	25,32,36,39	0
33	DGD	C	523	62/66	0.95	0.10	27,40,66,80	0
27	BCR	B	617	40/40	0.95	0.07	26,34,42,44	0
33	DGD	c	519	62/66	0.95	0.09	24,36,63,72	0
25	CLA	C	504	59/65	0.95	0.08	27,35,70,74	0
33	DGD	c	521	62/66	0.95	0.10	29,42,70,77	0
27	BCR	B	619	40/40	0.95	0.07	26,36,50,54	0
25	CLA	a	612	65/65	0.96	0.06	20,26,40,45	0
25	CLA	C	505	65/65	0.96	0.07	23,32,51,65	0

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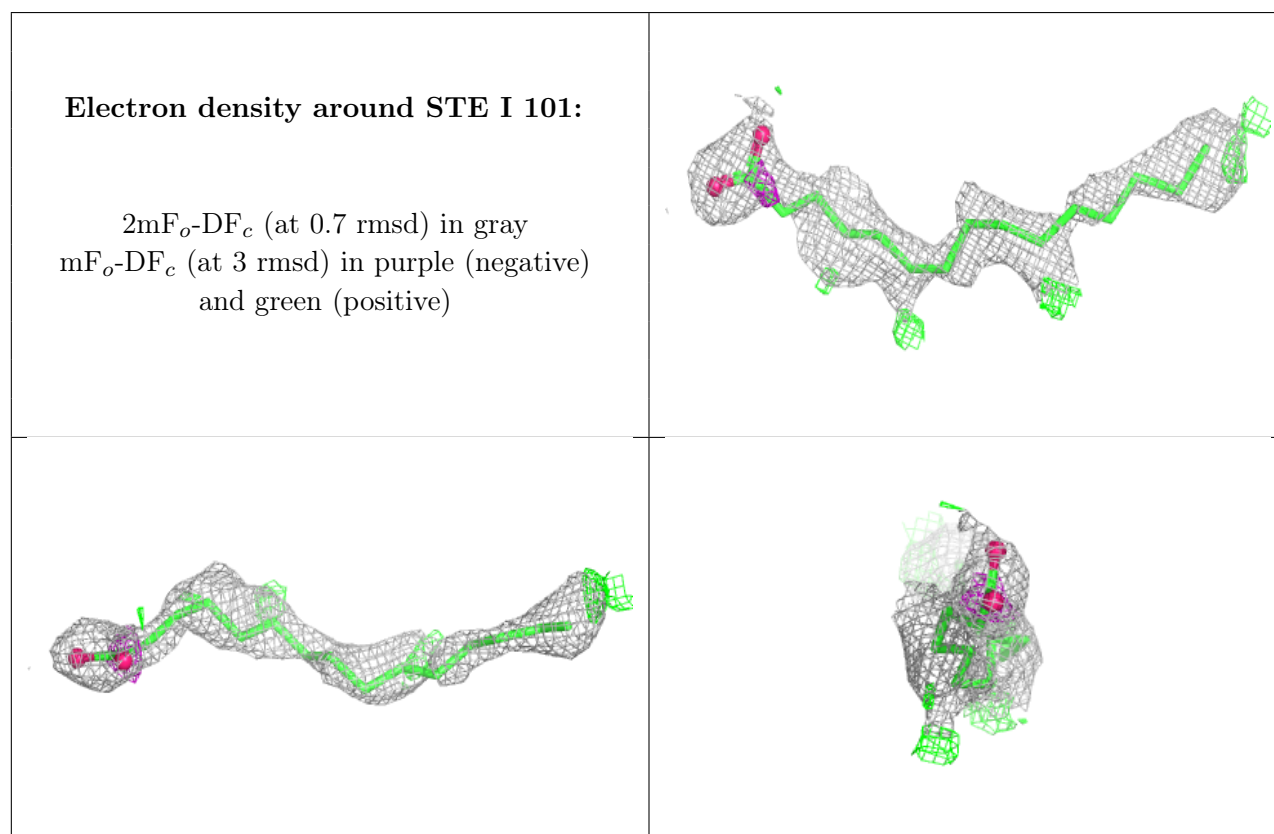
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	602	65/65	0.96	0.08	28,34,48,55	0
25	CLA	b	603	65/65	0.96	0.07	25,30,54,58	0
25	CLA	b	604	65/65	0.96	0.08	21,29,58,74	0
25	CLA	d	402	65/65	0.96	0.06	20,27,48,53	0
25	CLA	b	605	65/65	0.96	0.06	24,30,41,44	0
25	CLA	B	609	65/65	0.96	0.06	24,31,46,52	0
25	CLA	b	607	65/65	0.96	0.07	22,30,51,57	0
26	PHO	a	608	64/64	0.96	0.06	22,27,33,39	0
25	CLA	C	507	65/65	0.96	0.07	24,33,49,55	0
25	CLA	B	603	65/65	0.96	0.07	22,27,50,53	0
32	LHG	D	408	49/49	0.96	0.08	24,34,42,48	0
25	CLA	b	610	65/65	0.96	0.07	28,34,40,43	0
25	CLA	b	611	65/65	0.96	0.06	25,30,45,51	0
32	LHG	L	101	49/49	0.96	0.08	28,35,43,56	0
25	CLA	b	613	65/65	0.96	0.08	22,27,64,68	0
32	LHG	d	407	49/49	0.96	0.07	28,36,48,53	0
25	CLA	B	612	65/65	0.96	0.07	21,27,38,42	0
25	CLA	B	614	65/65	0.96	0.07	22,30,59,67	0
25	CLA	B	616	60/65	0.96	0.08	25,33,75,80	0
25	CLA	c	501	65/65	0.96	0.07	28,35,46,49	0
25	CLA	c	502	65/65	0.96	0.07	27,34,46,58	0
25	CLA	B	604	65/65	0.96	0.07	20,26,54,58	0
25	CLA	c	504	60/65	0.96	0.07	27,38,65,67	0
25	CLA	B	602	65/65	0.96	0.07	24,30,46,49	0
25	CLA	B	607	65/65	0.96	0.07	21,27,51,56	0
25	CLA	B	608	65/65	0.96	0.06	23,29,44,48	0
25	CLA	a	609	65/65	0.96	0.09	22,27,66,73	0
34	HEM	F	101	43/43	0.96	0.09	37,42,49,52	0
25	CLA	A	607	65/65	0.97	0.08	21,29,79,85	0
25	CLA	A	610	54/65	0.97	0.06	21,27,51,61	0
32	LHG	l	101	49/49	0.97	0.07	30,39,48,55	0
25	CLA	B	611	65/65	0.97	0.06	22,26,39,43	0
25	CLA	D	401	65/65	0.97	0.06	19,23,47,52	0
25	CLA	D	402	65/65	0.97	0.08	25,32,95,102	0
25	CLA	B	605	65/65	0.97	0.06	20,26,39,42	0
25	CLA	B	613	65/65	0.97	0.06	21,26,56,59	0
25	CLA	A	614	65/65	0.97	0.06	20,25,40,49	0
25	CLA	B	615	65/65	0.97	0.07	25,31,49,55	0
25	CLA	b	612	65/65	0.97	0.06	24,30,40,41	0
24	BCT	A	605	4/4	0.97	0.05	26,30,30,33	0
25	CLA	A	606	65/65	0.97	0.06	17,24,38,48	0
34	HEM	f	101	43/43	0.97	0.09	44,50,59,68	0

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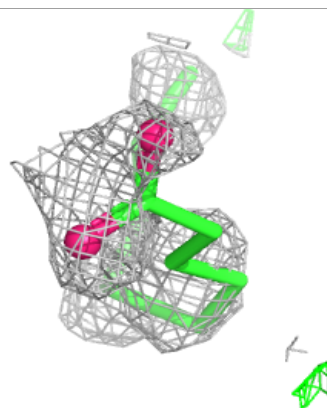
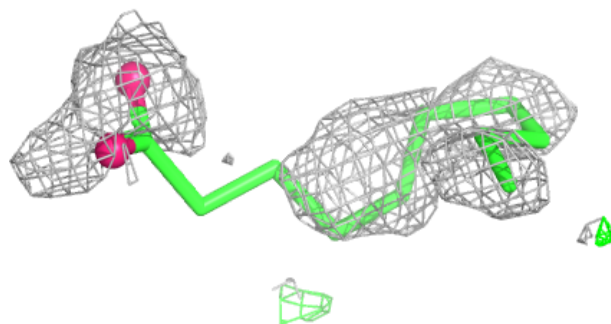
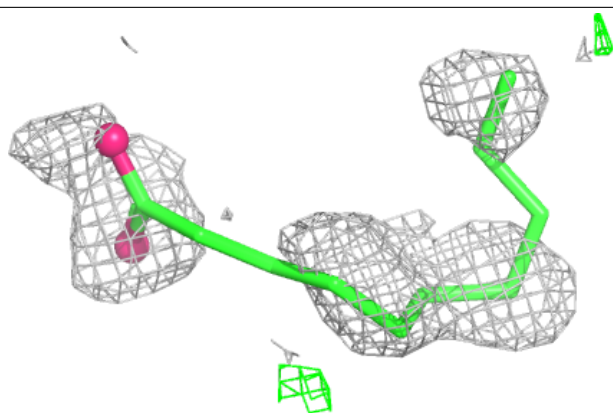
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCT	a	605	4/4	0.98	0.06	32,34,42,43	0
35	HEC	V	201	43/43	0.98	0.05	24,28,35,41	0
35	HEC	v	201	43/43	0.98	0.06	28,31,36,41	0
23	CL	a	603	1/1	0.99	0.05	27,27,27,27	0
23	CL	a	604	1/1	0.99	0.07	28,28,28,28	0
21	OEX	a	601	10/10	0.99	0.03	22,27,29,30	0
23	CL	A	603	1/1	0.99	0.05	26,26,26,26	0
23	CL	A	604	1/1	0.99	0.04	28,28,28,28	0
21	OEX	A	601	10/10	1.00	0.03	25,26,29,29	0
22	FE2	A	602	1/1	1.00	0.01	27,27,27,27	0
22	FE2	a	602	1/1	1.00	0.02	34,34,34,34	0

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



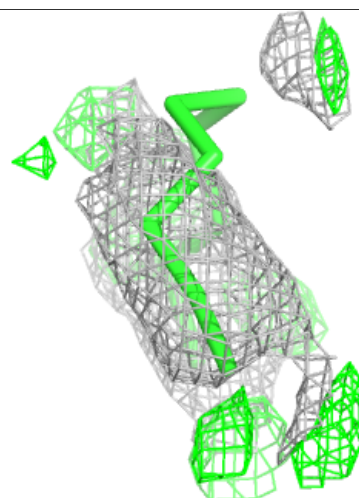
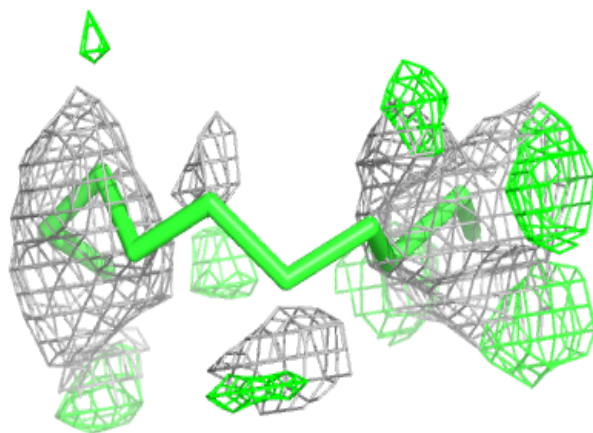
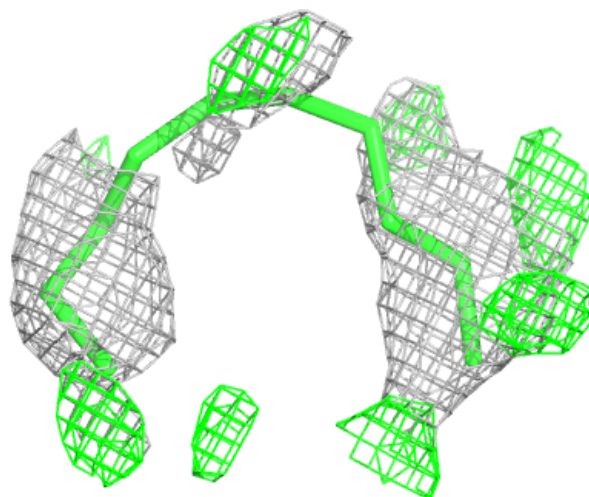
Electron density around STE i 101:

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



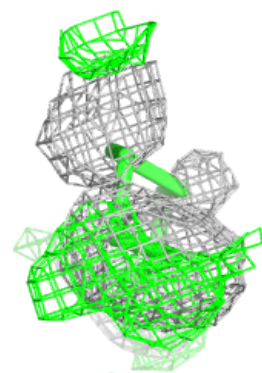
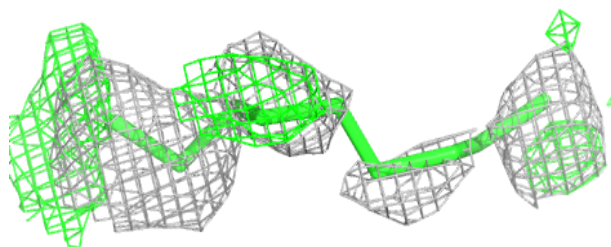
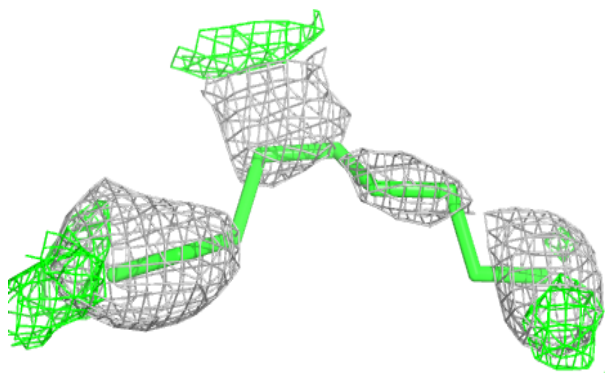
Electron density around STE C 520:

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

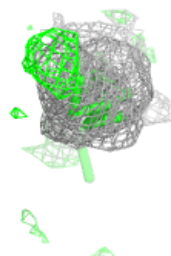
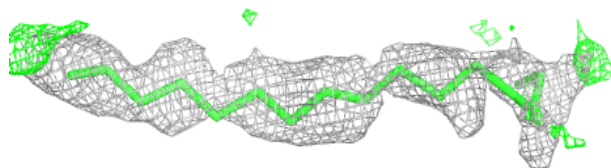
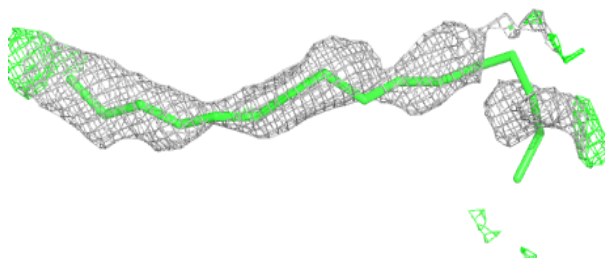


Electron density around STE e 101:

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

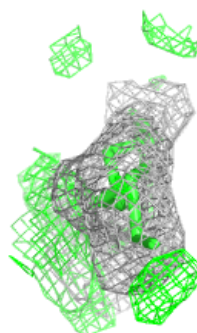
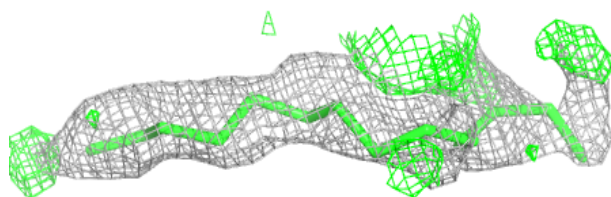
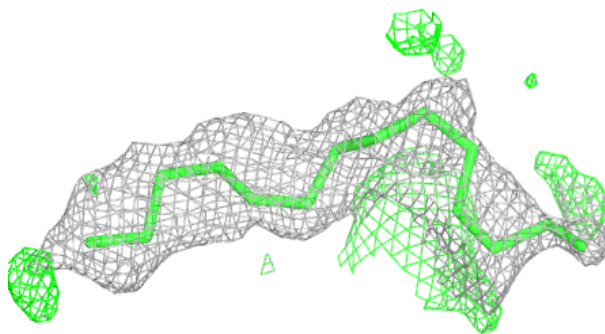
**Electron density around STE j 102:**

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

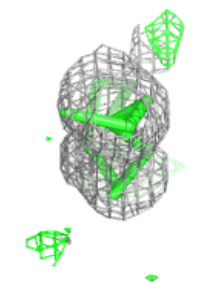
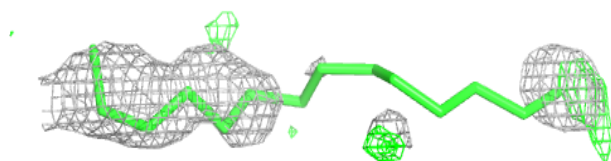
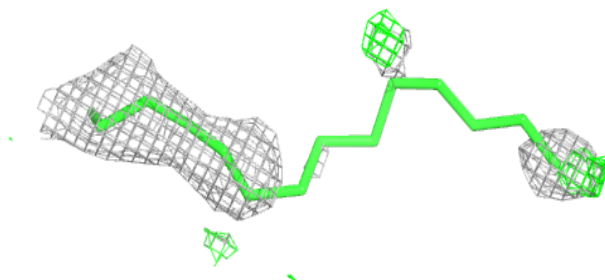


Electron density around STE K 102:

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

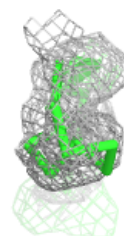
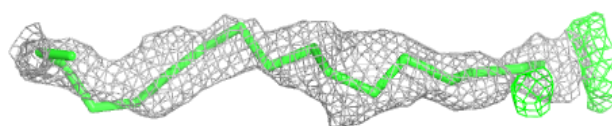
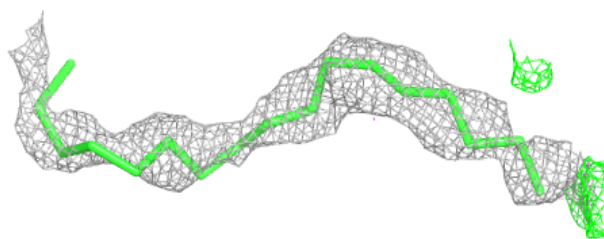
**Electron density around STE C 527:**

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

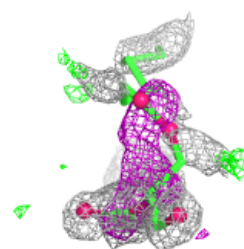
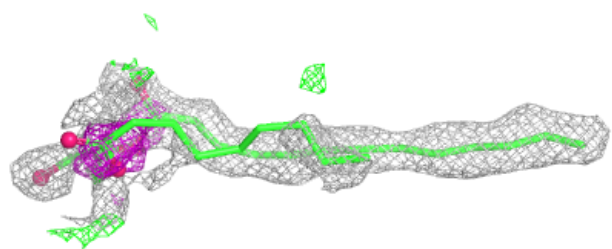
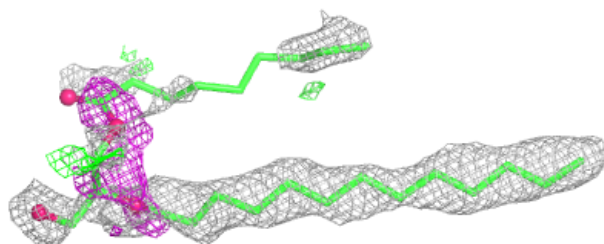


Electron density around STE A 621:

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

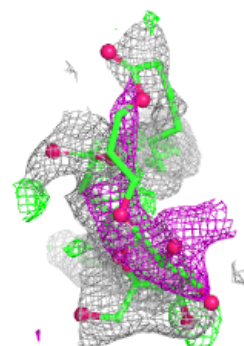
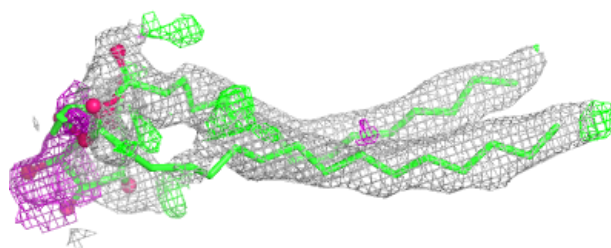
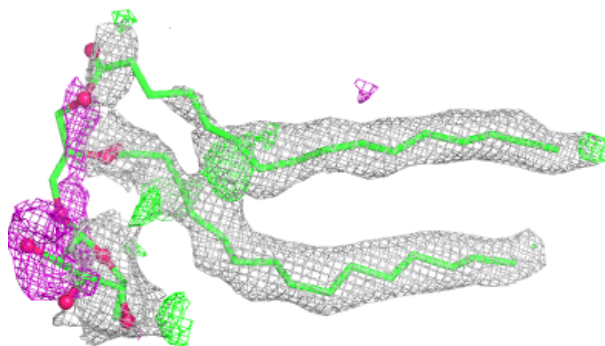
**Electron density around LMG c 518:**

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

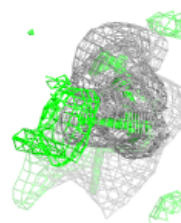
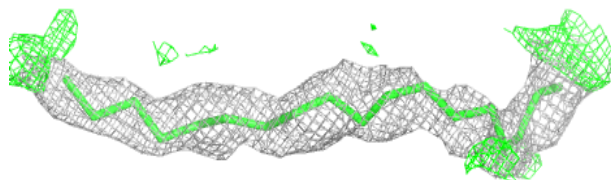
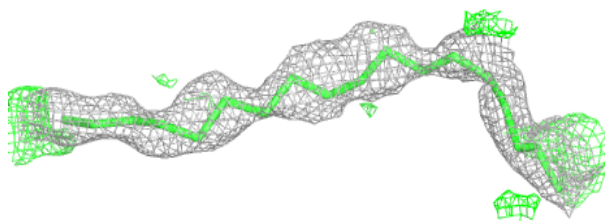


Electron density around LMG D 405:

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

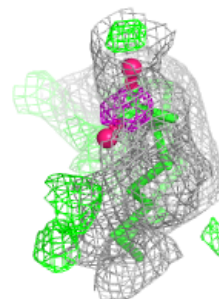
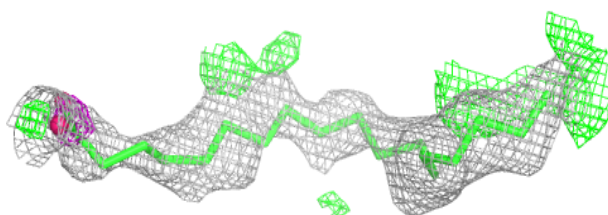
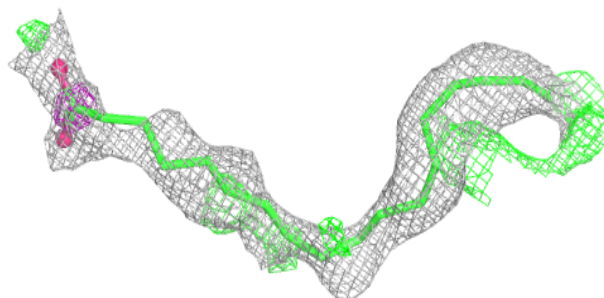
**Electron density around STE c 517:**

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

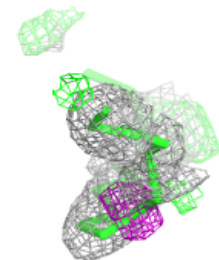
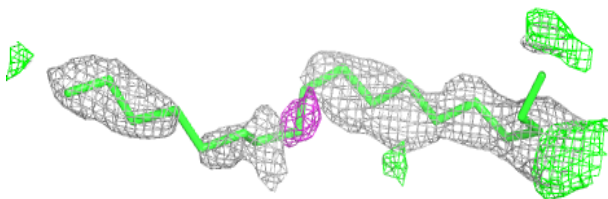
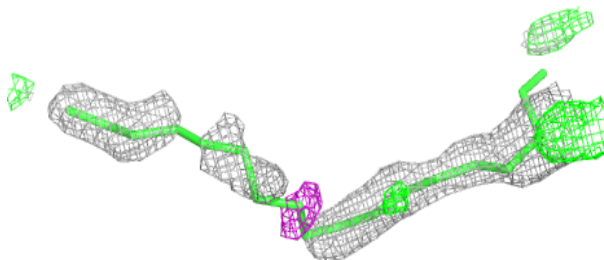


Electron density around STE E 103:

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

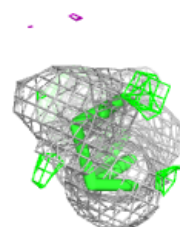
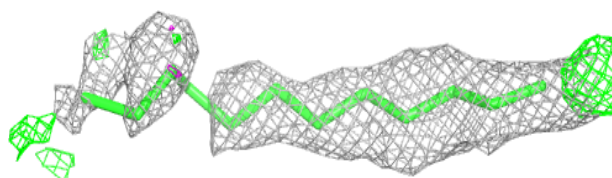
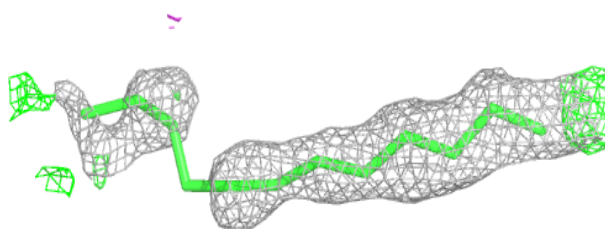
**Electron density around STE H 103:**

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

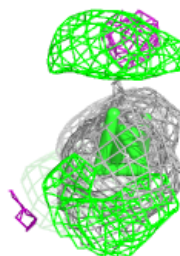
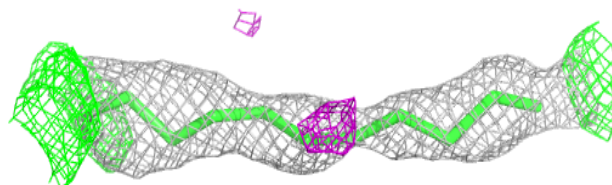
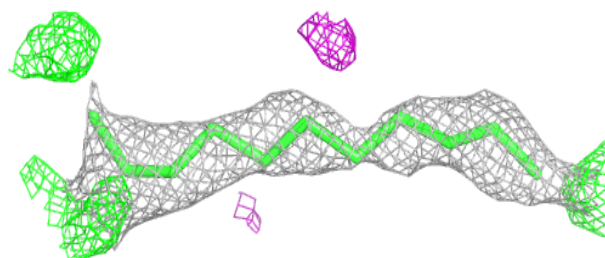


Electron density around STE E 102:

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

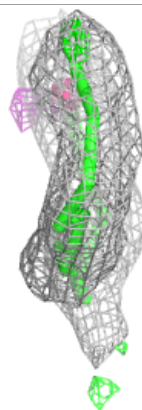
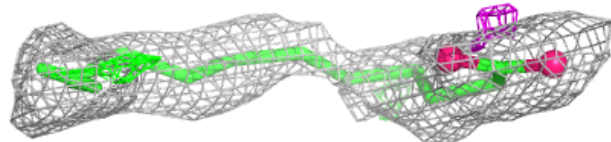
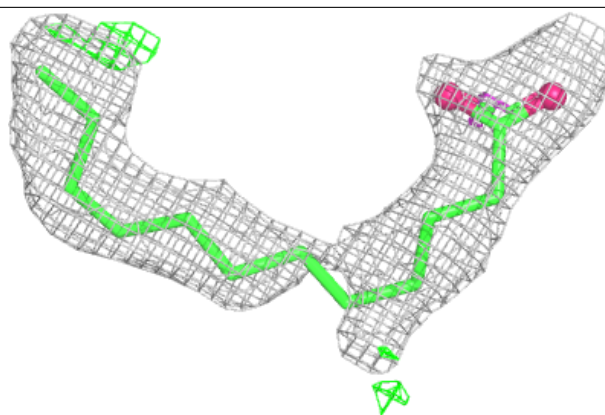
**Electron density around STE b 625:**

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

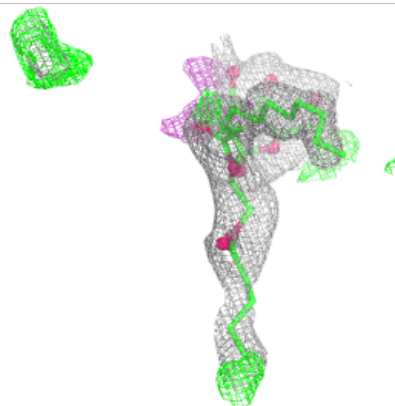
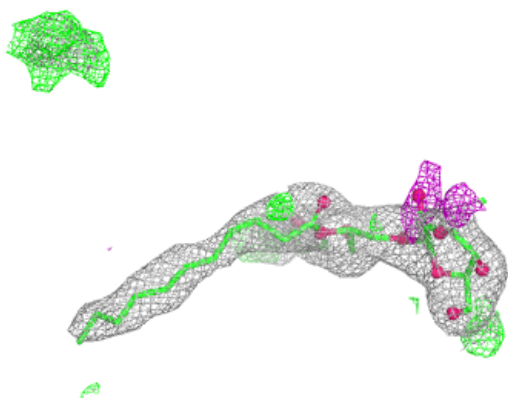
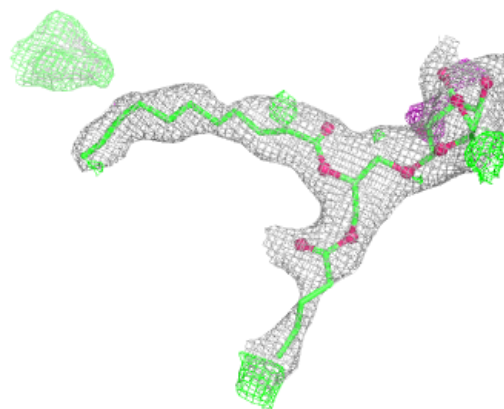


Electron density around STE C 516:

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

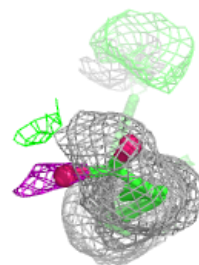
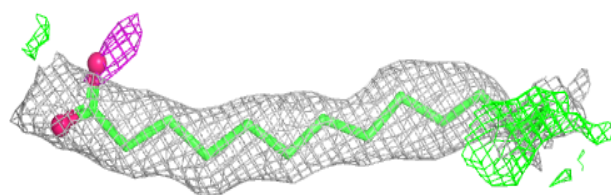
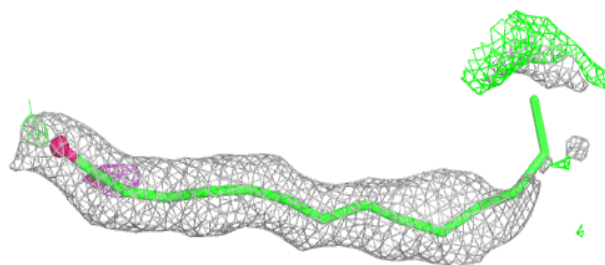
**Electron density around LMG C 517:**

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

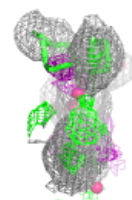
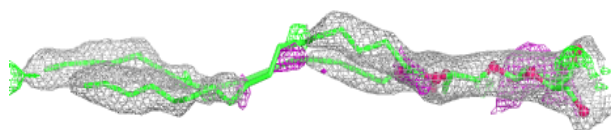
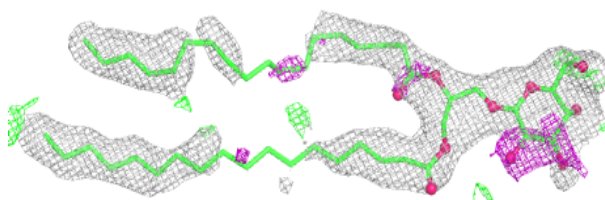


Electron density around STE b 623:

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

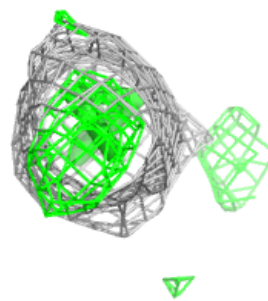
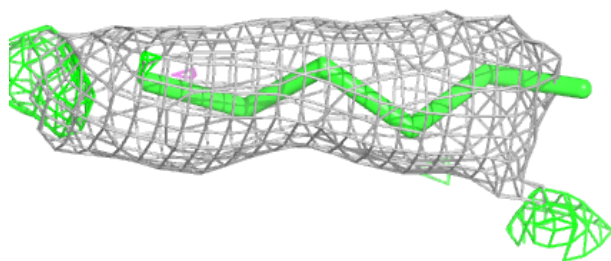
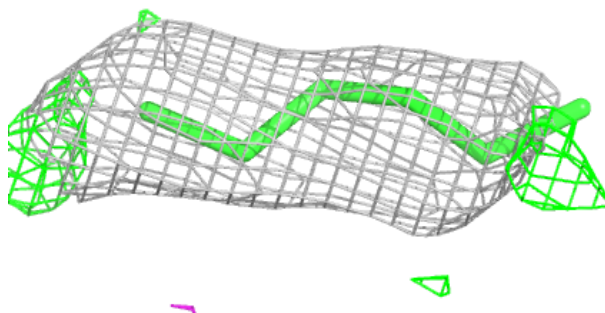
**Electron density around LMG b 622:**

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

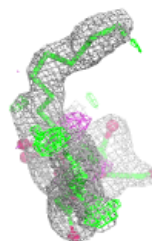
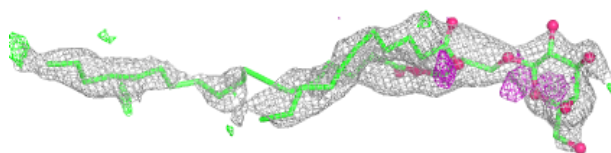
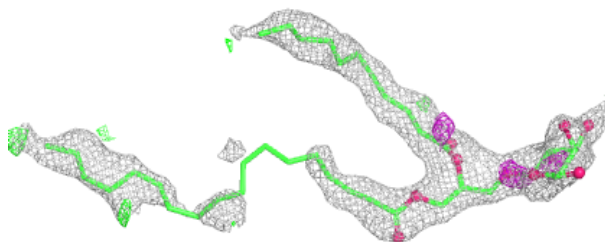


Electron density around STE i 102:

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

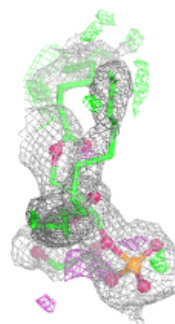
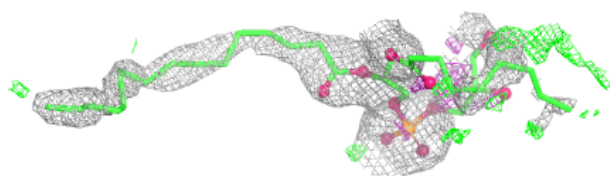
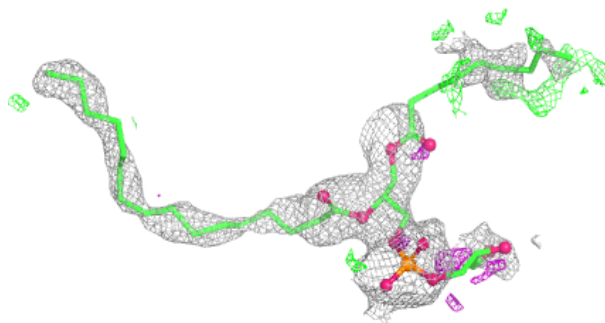
**Electron density around LMG c 523:**

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

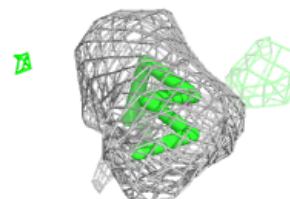
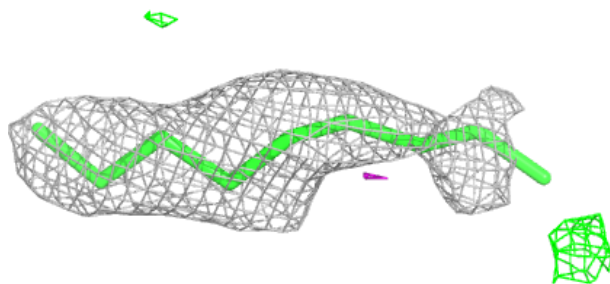
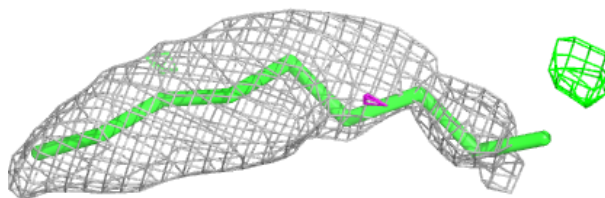


Electron density around LHG e 102:

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

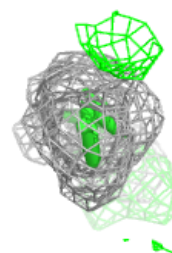
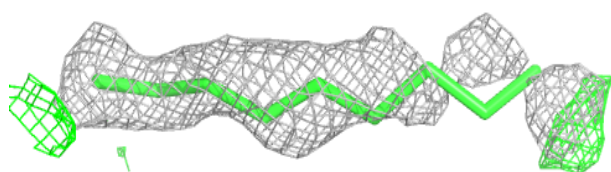
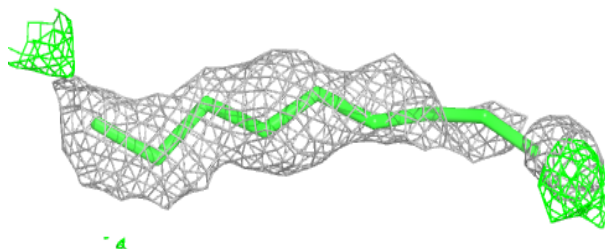
**Electron density around STE A 613:**

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

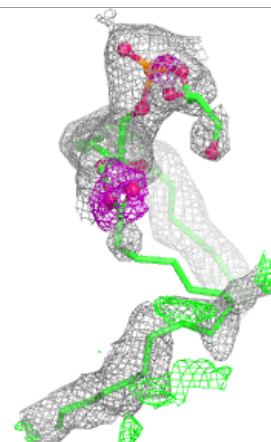
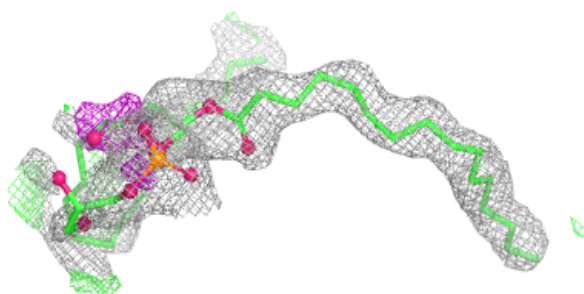
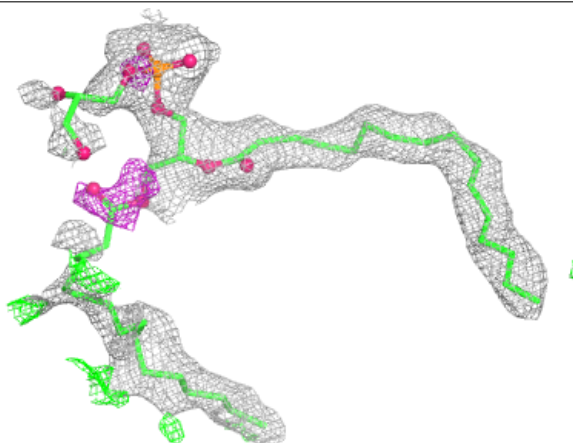


Electron density around STE e 103:

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

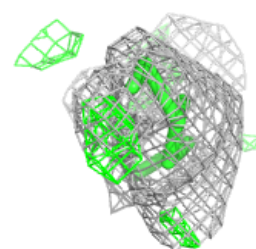
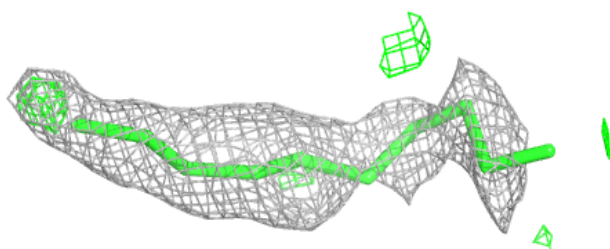
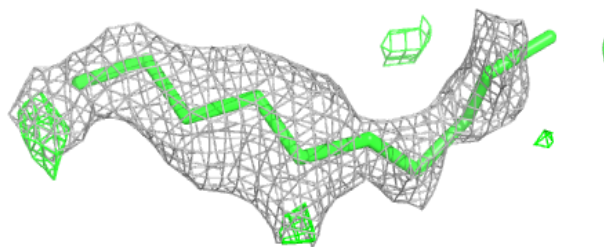
**Electron density around LHG A 617:**

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

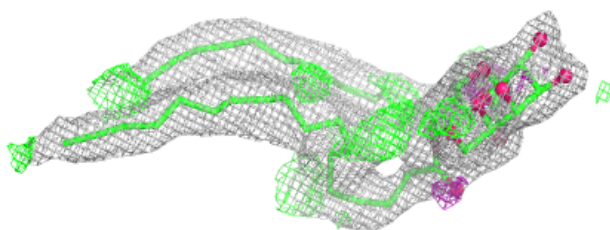
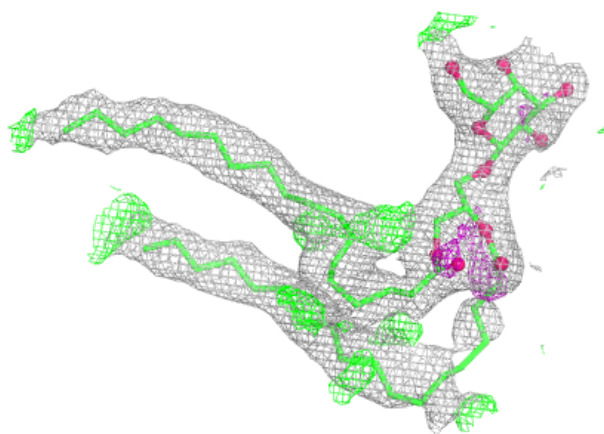


Electron density around STE h 103:

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

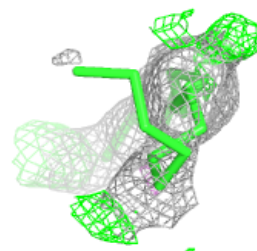
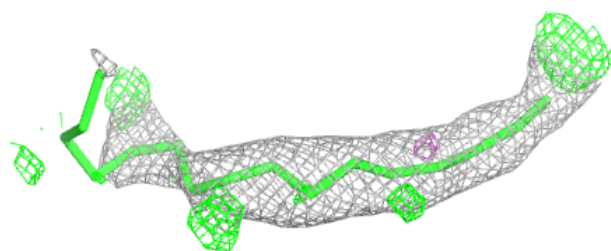
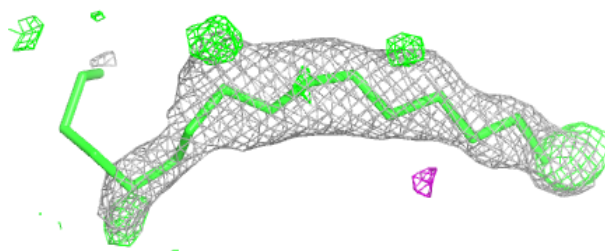
**Electron density around LMG a 616:**

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

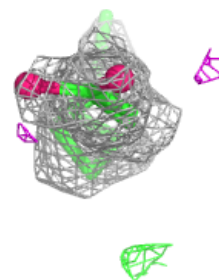
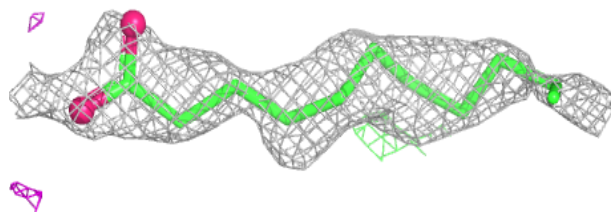
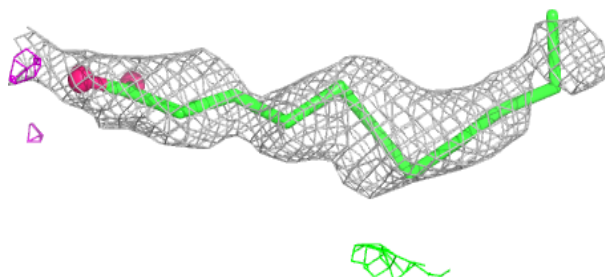


Electron density around STE T 102:

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

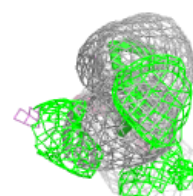
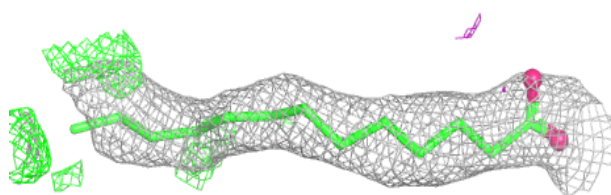
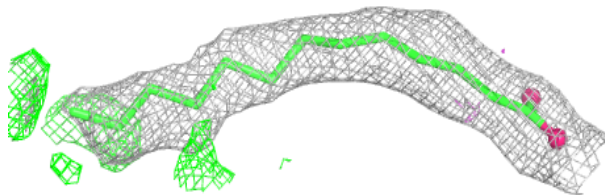
**Electron density around STE e 104:**

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

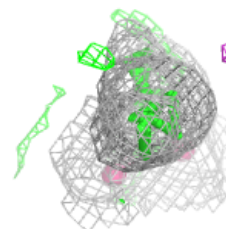
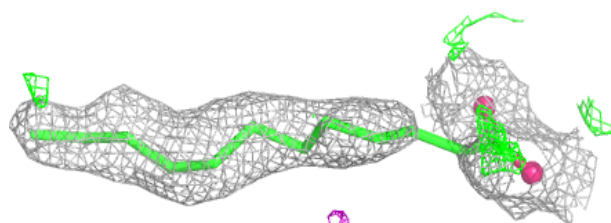
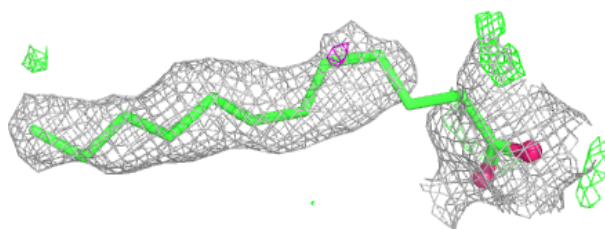


Electron density around STE I 102:

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

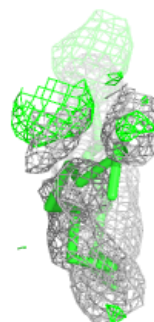
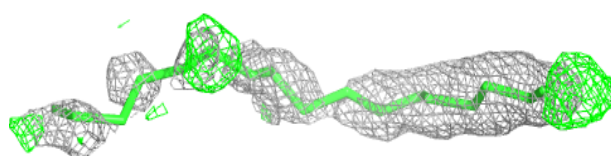
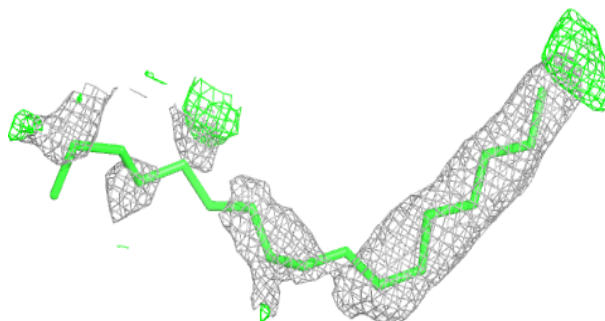
**Electron density around STE k 103:**

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

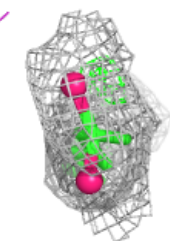
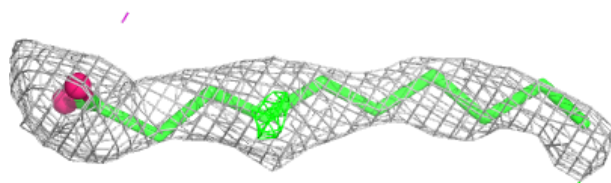
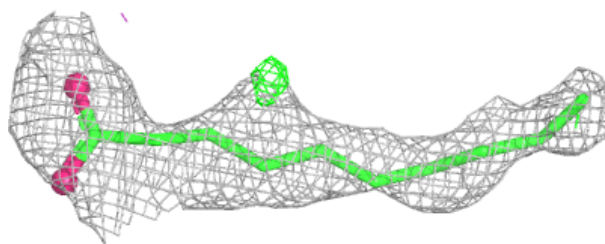


Electron density around STE Z 101:

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

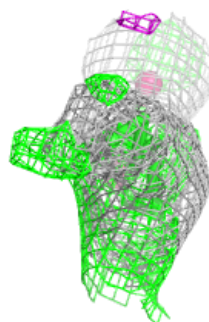
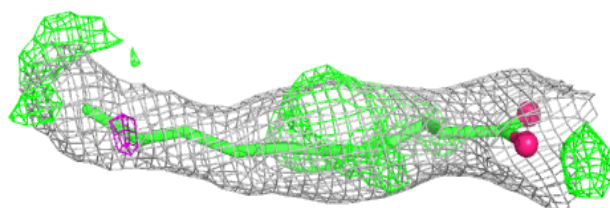
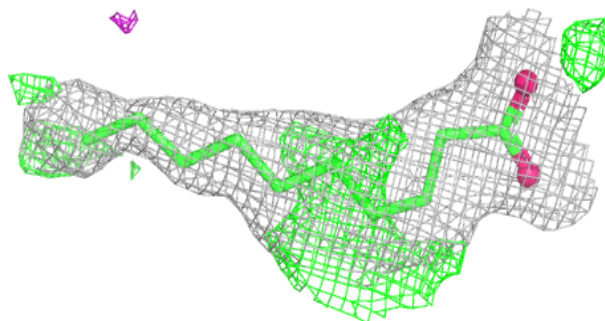
**Electron density around STE a 617:**

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

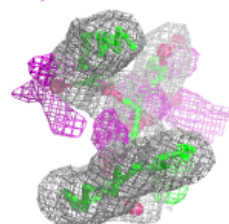
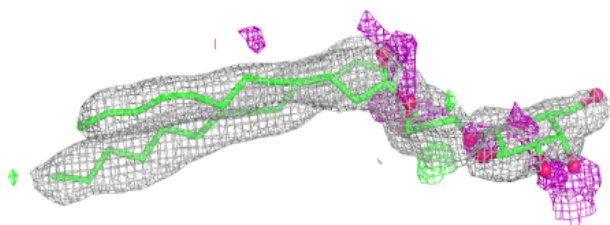
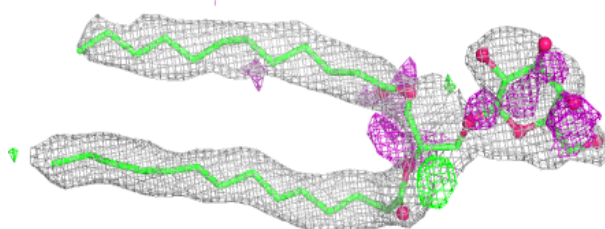


Electron density around STE C 525:

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

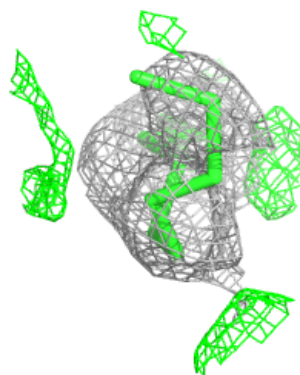
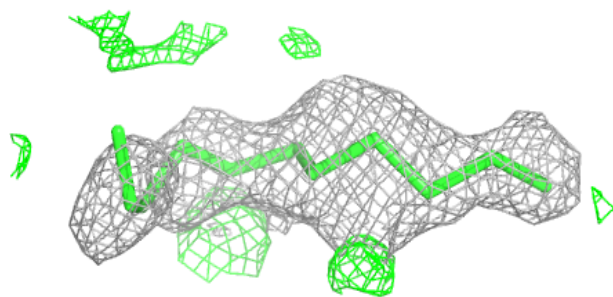
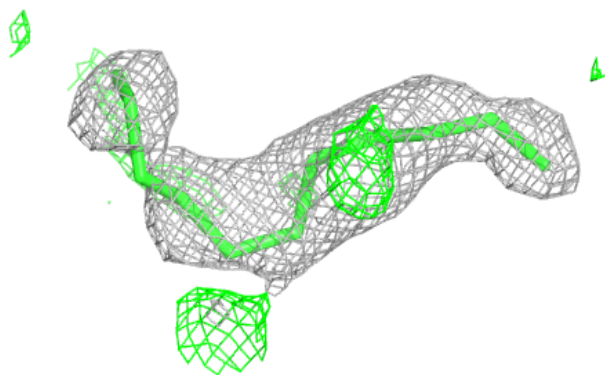
**Electron density around LMG B 620:**

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

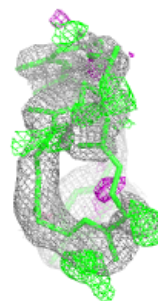
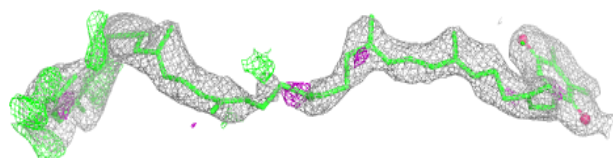
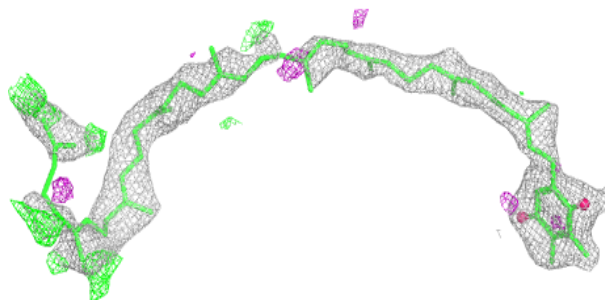


Electron density around STE A 622:

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

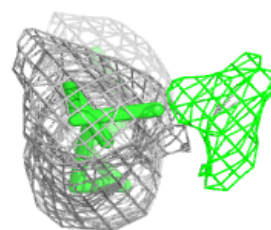
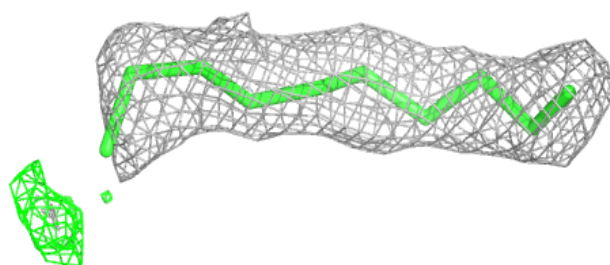
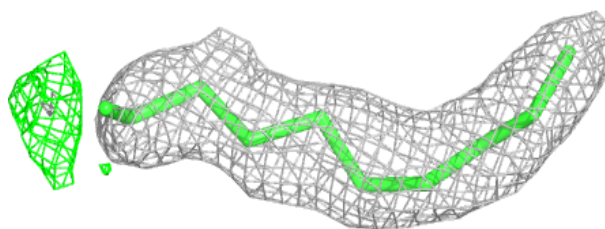
**Electron density around PL9 a 611:**

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

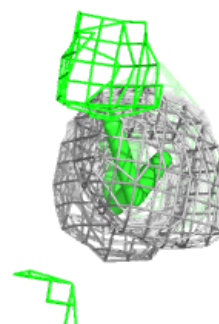
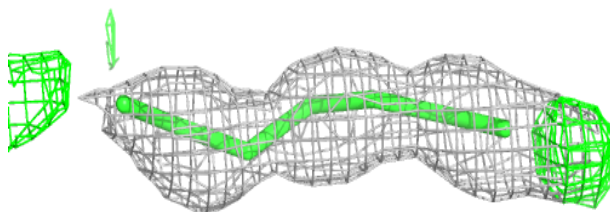
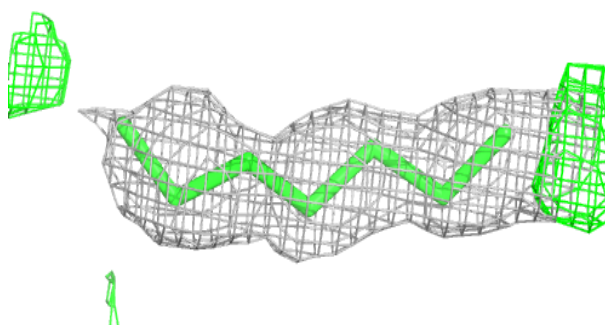


Electron density around STE b 624:

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

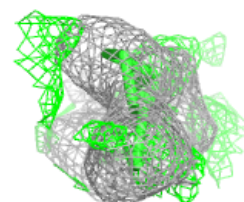
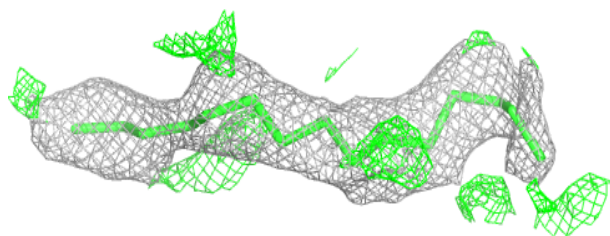
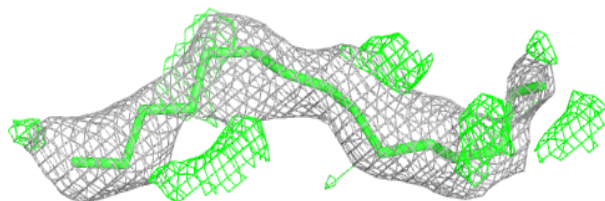
**Electron density around STE C 519:**

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

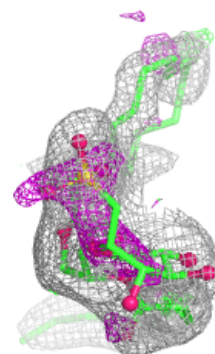
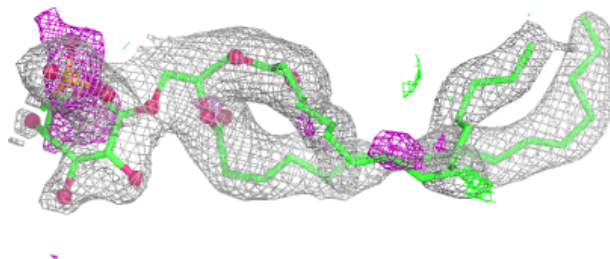
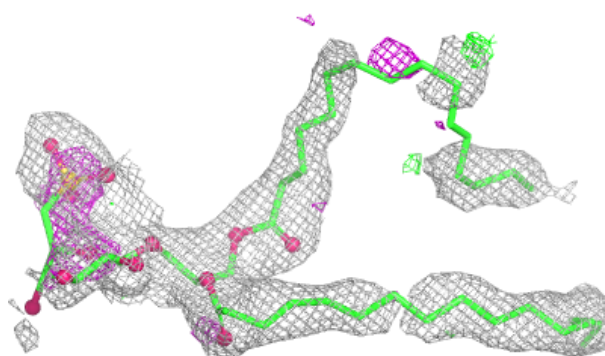


Electron density around STE B 625:

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

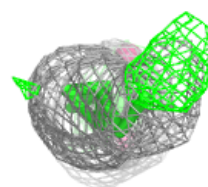
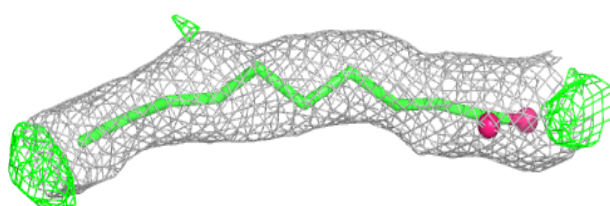
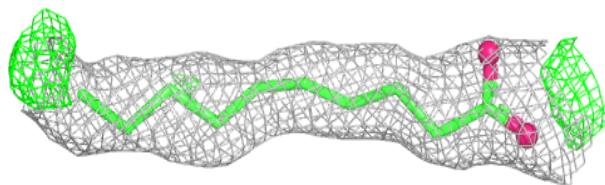
**Electron density around SQD a 615:**

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

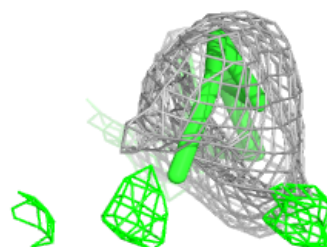
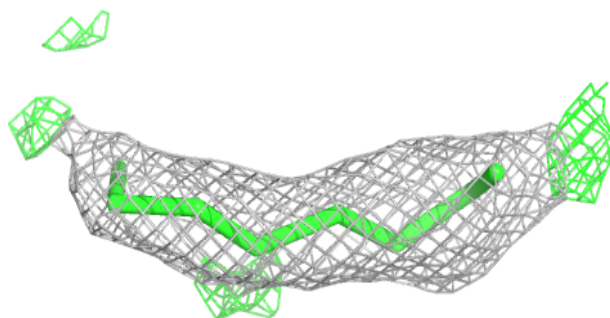
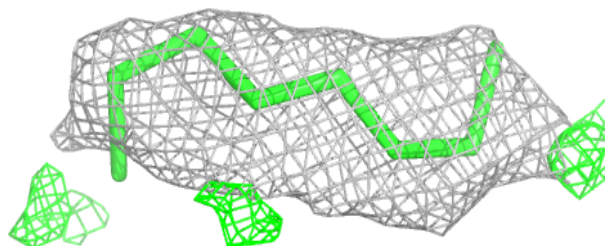


Electron density around STE j 101:

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

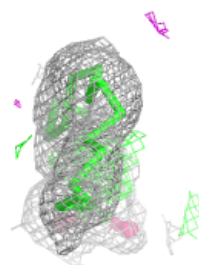
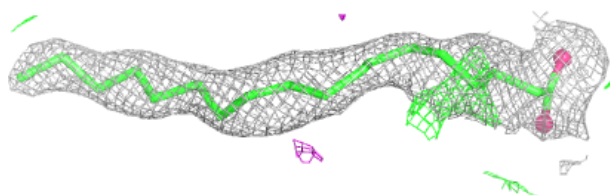
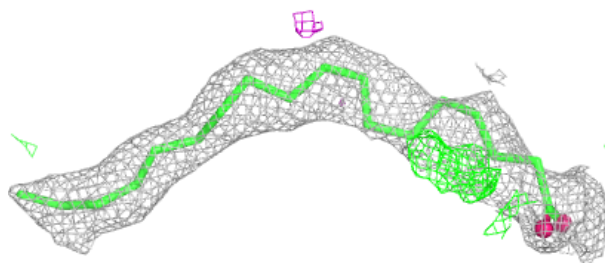
**Electron density around STE f 103:**

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

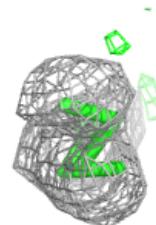
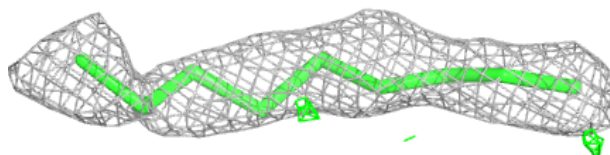
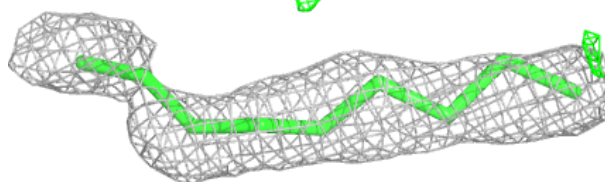


Electron density around STE d 409:

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

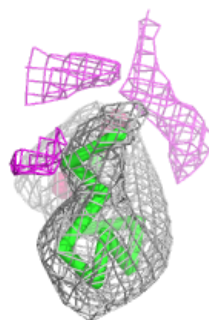
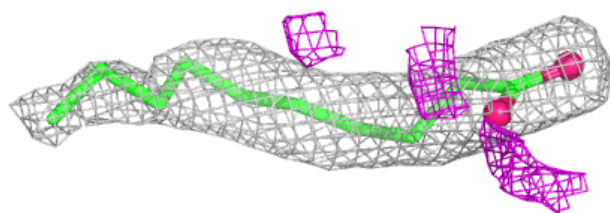
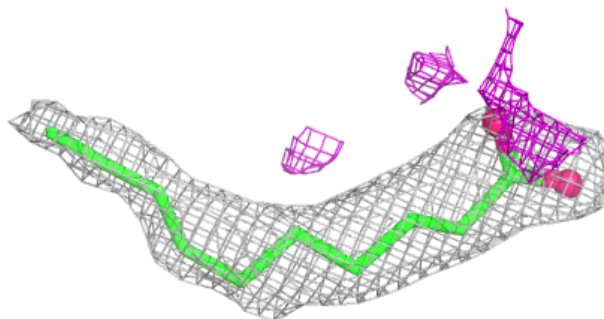
**Electron density around STE z 101:**

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

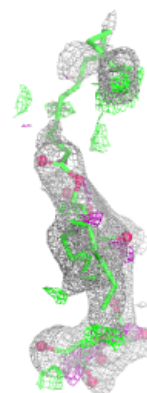
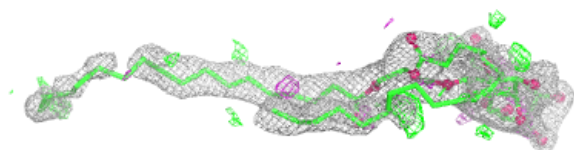
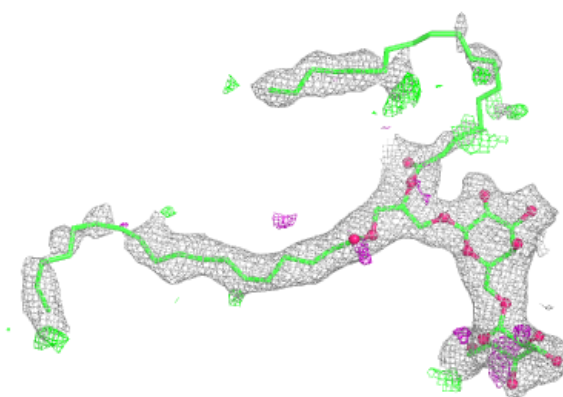


Electron density around STE B 624:

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

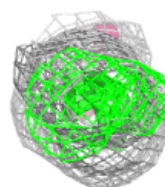
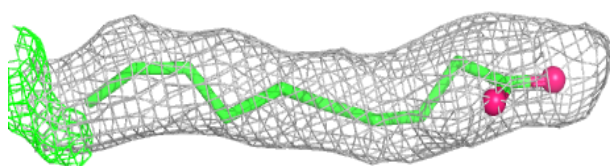
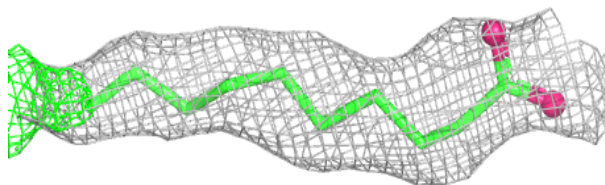
**Electron density around DGD A 619:**

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

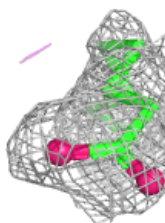
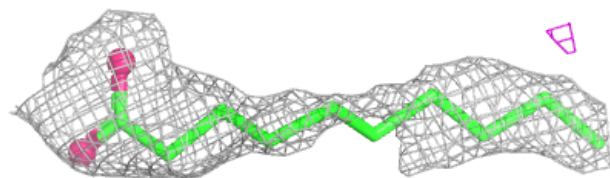
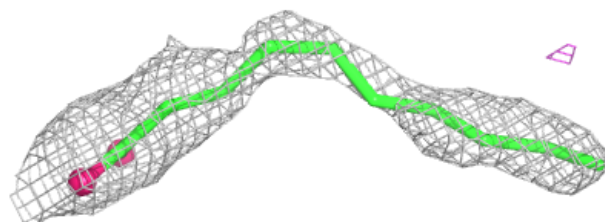


Electron density around STE J 102:

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

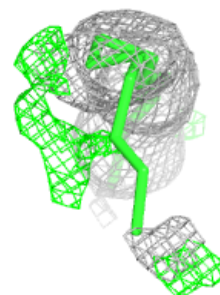
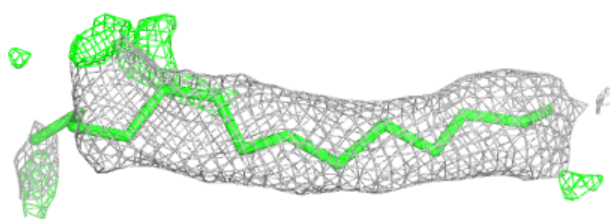
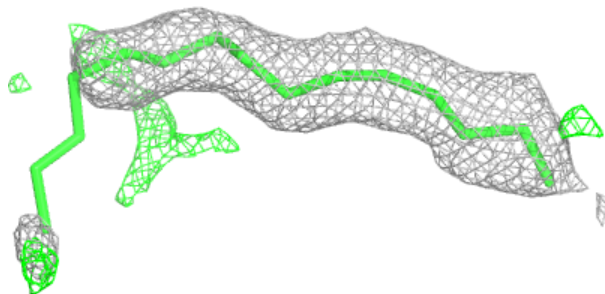
**Electron density around STE E 101:**

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

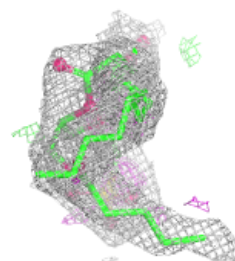
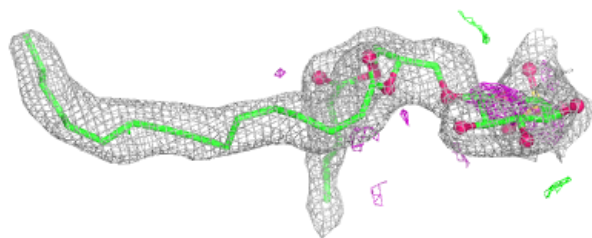
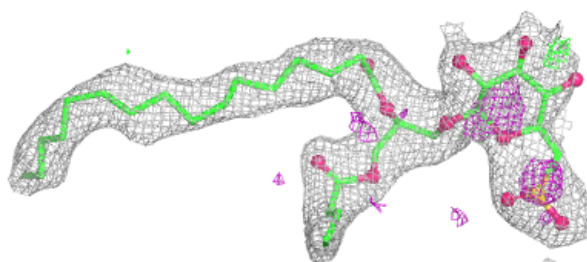


Electron density around STE M 104:

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

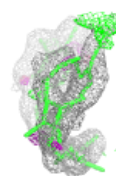
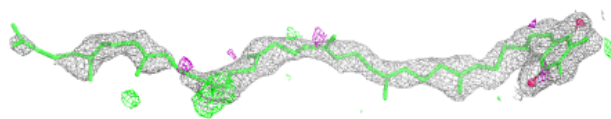
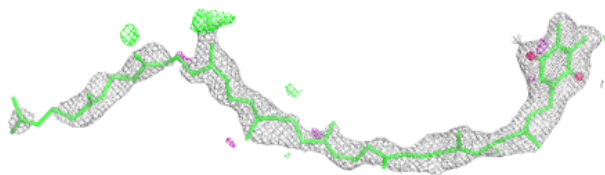
**Electron density around SQD A 618:**

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

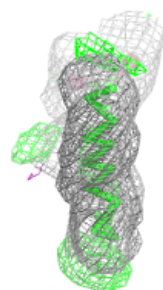
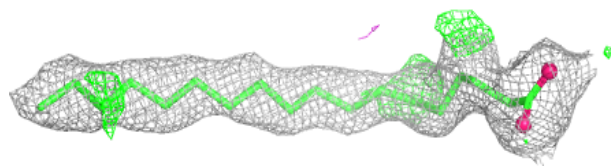
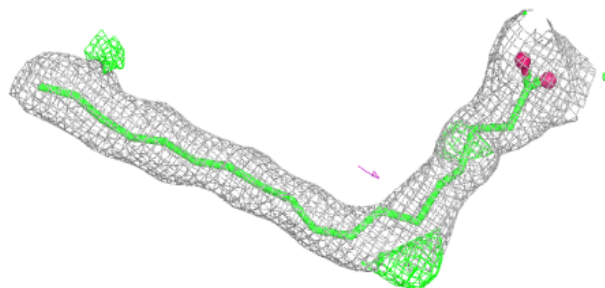


Electron density around PL9 A 612:

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

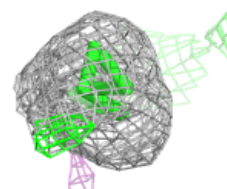
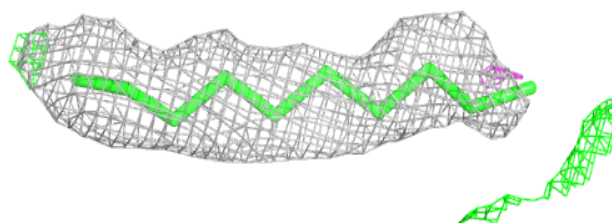
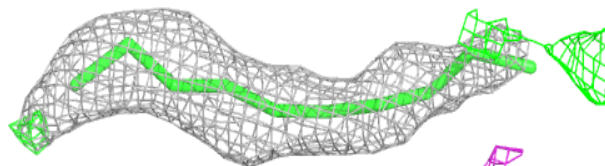
**Electron density around STE d 406:**

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

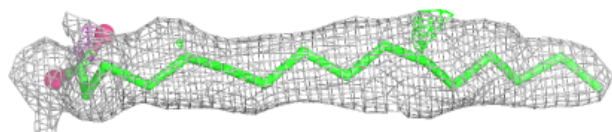
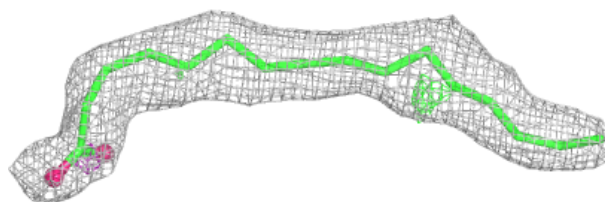


Electron density around STE t 103:

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

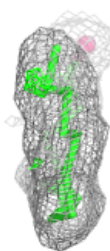
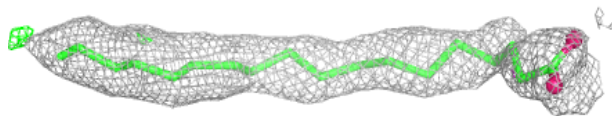
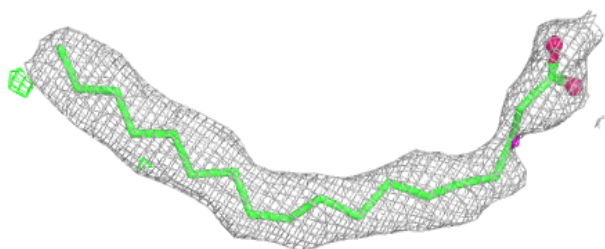
**Electron density around STE B 623:**

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

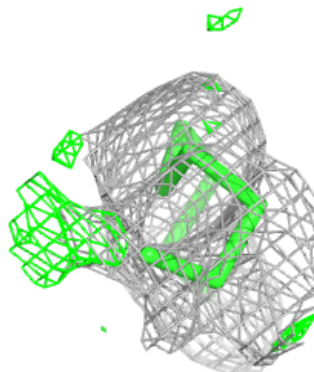
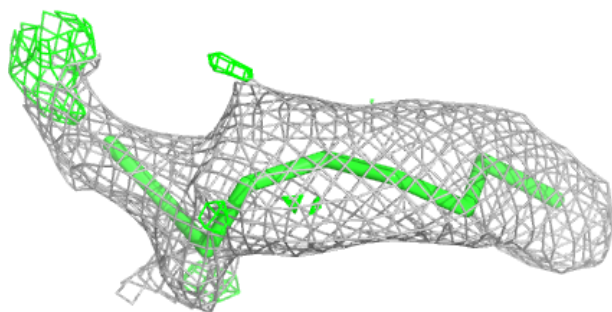
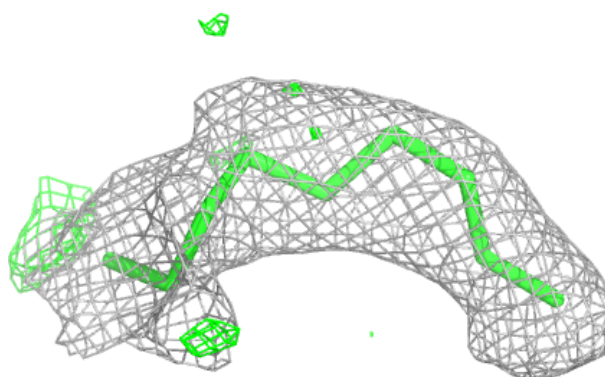


Electron density around STE d 411:

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

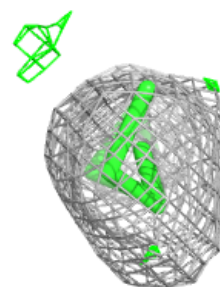
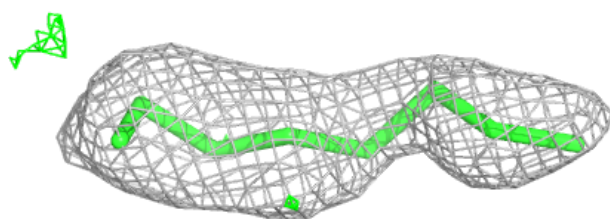
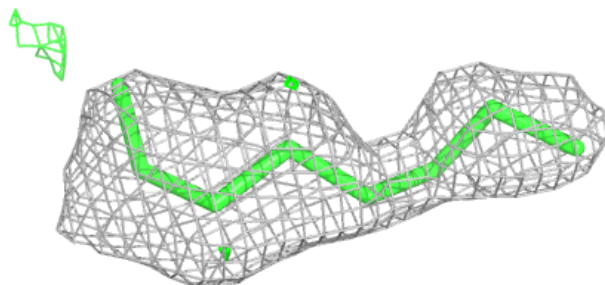
**Electron density around STE D 411:**

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

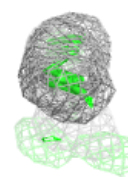
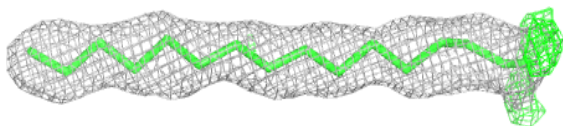
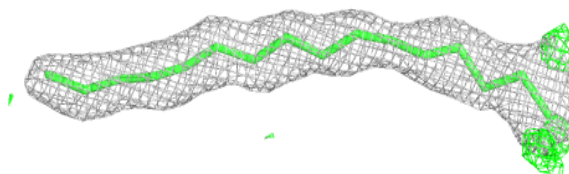


Electron density around STE A 620:

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

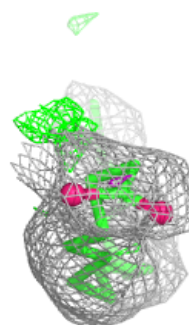
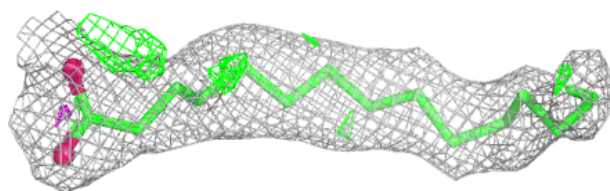
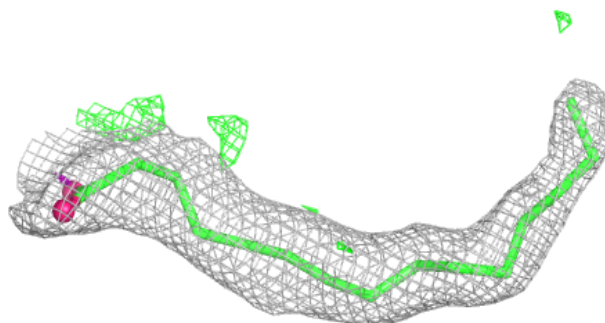
**Electron density around STE C 526:**

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

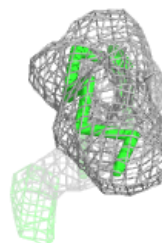
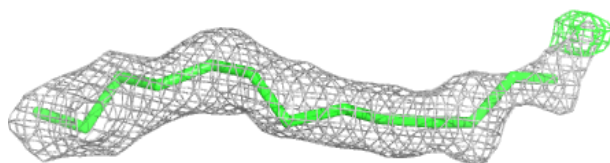
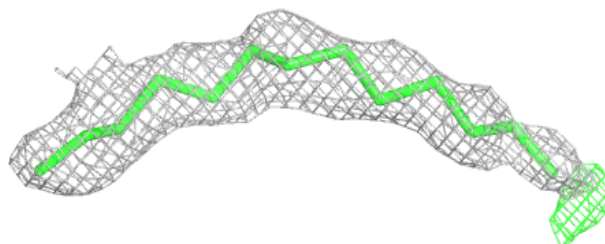


Electron density around STE B 621:

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

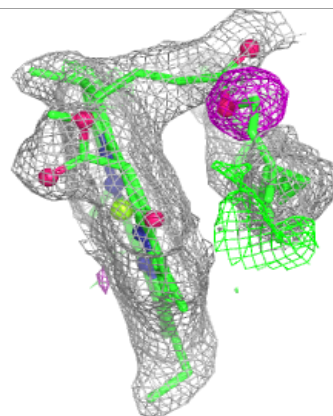
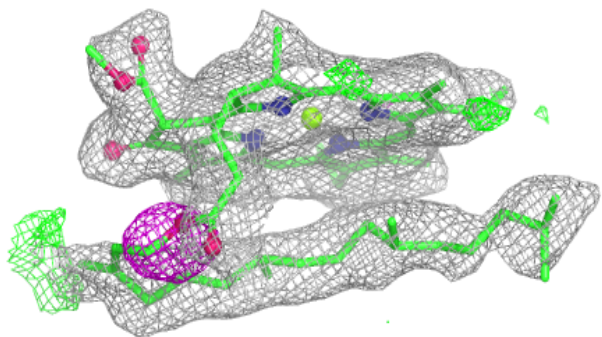
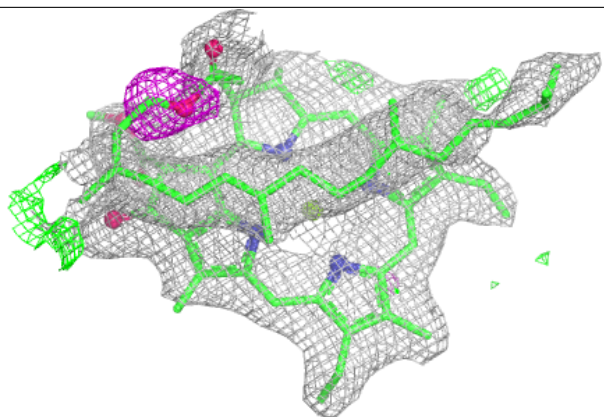
**Electron density around STE c 516:**

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

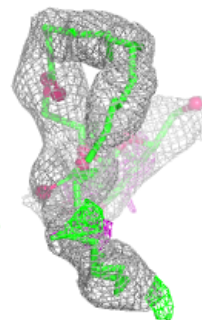
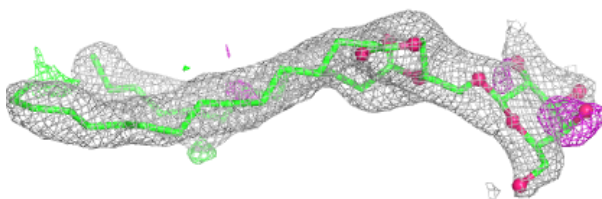
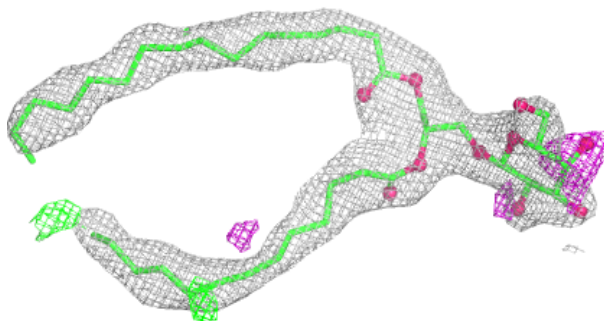


Electron density around CLA b 601:

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

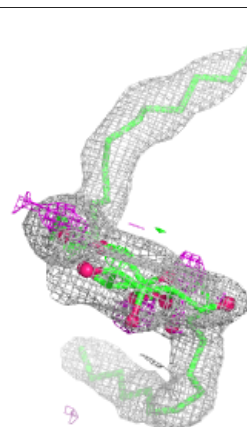
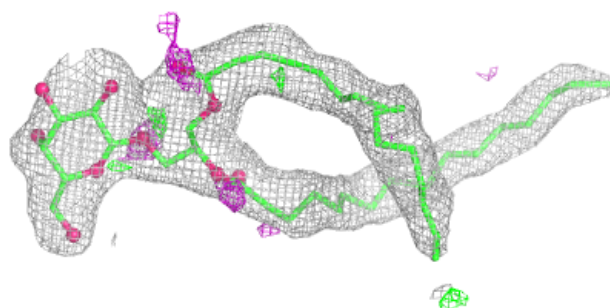
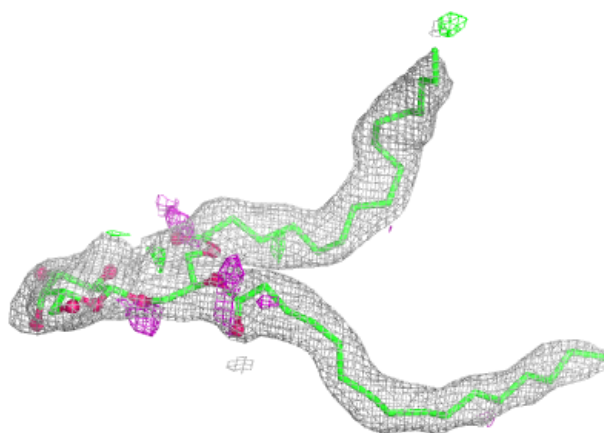
**Electron density around LMG A 615:**

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

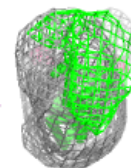
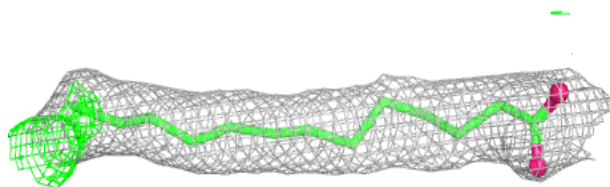
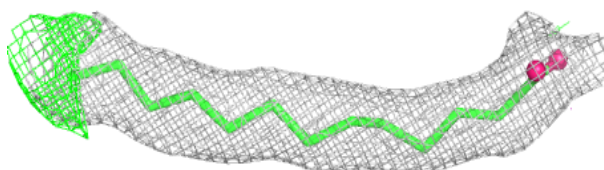


Electron density around LMG m 101:

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

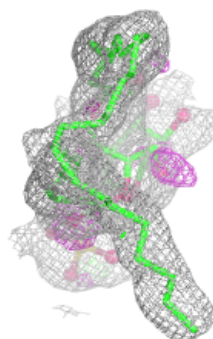
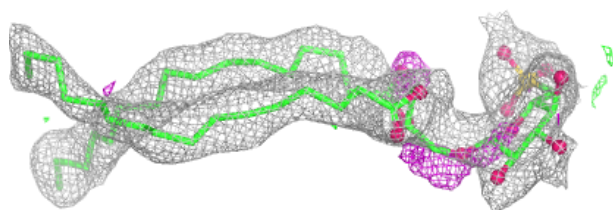
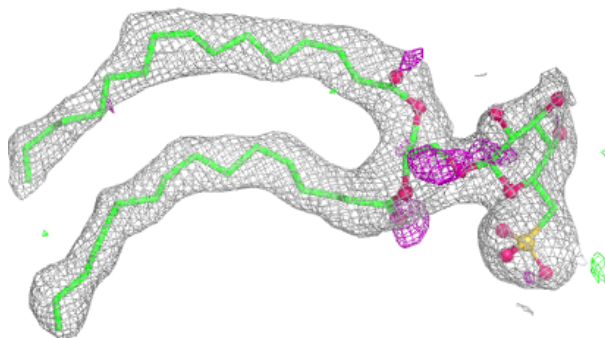
**Electron density around STE M 102:**

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

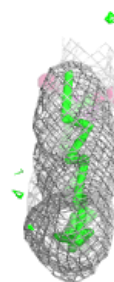
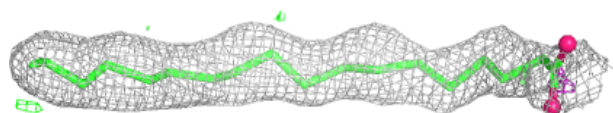
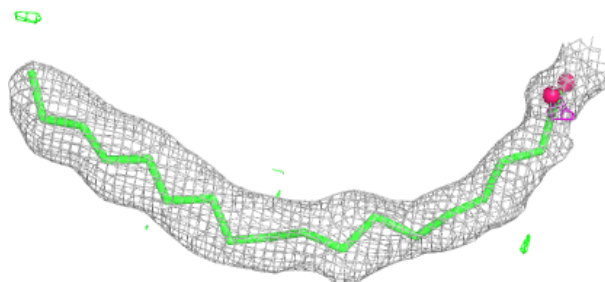


Electron density around SQD B 622:

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

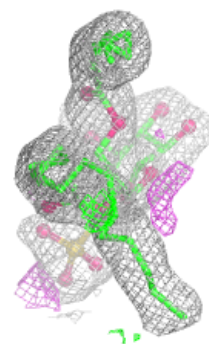
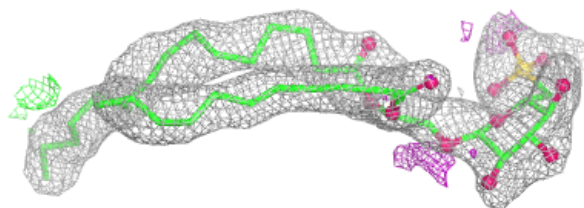
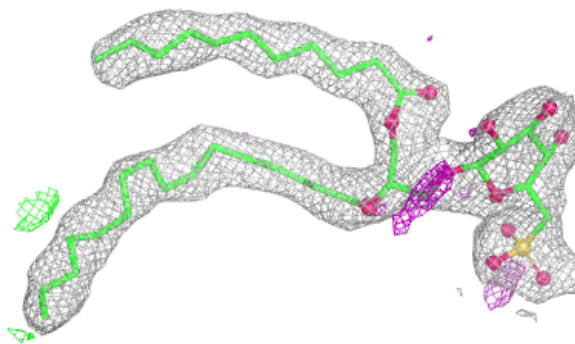
**Electron density around STE X 101:**

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

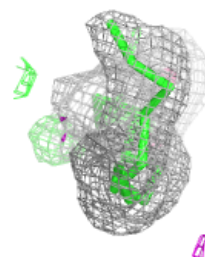
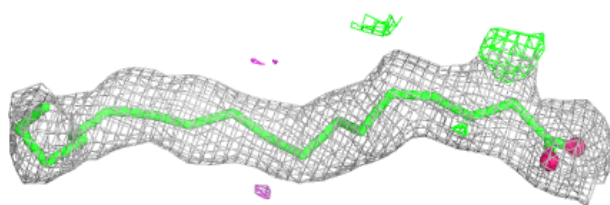
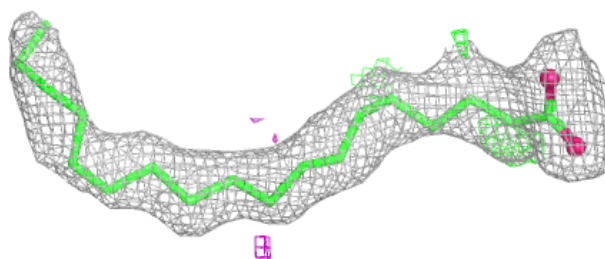


Electron density around SQD b 620:

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

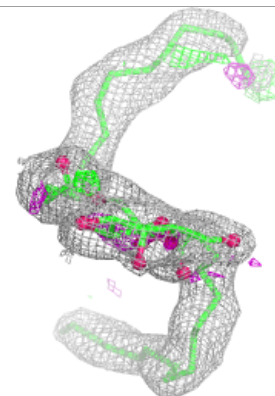
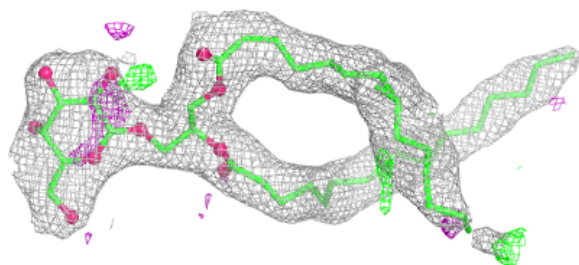
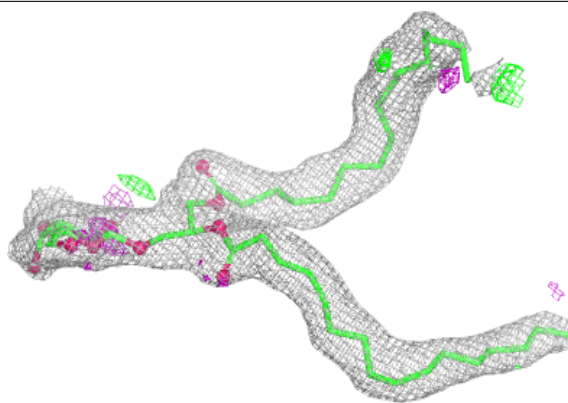
**Electron density around STE b 621:**

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

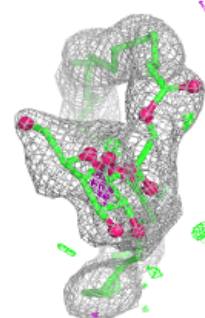
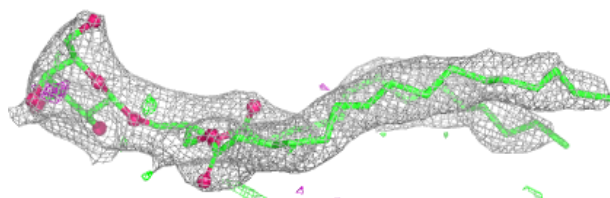
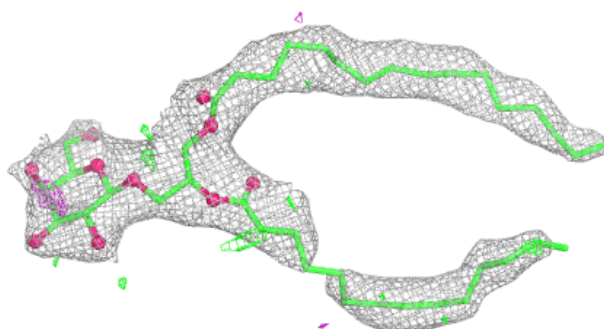


Electron density around LMG M 101:

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

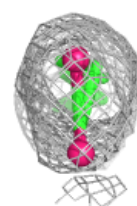
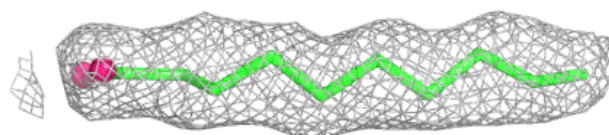
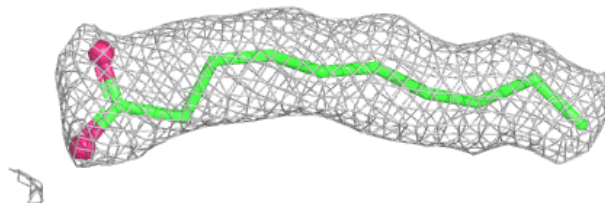
**Electron density around LMG c 524:**

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

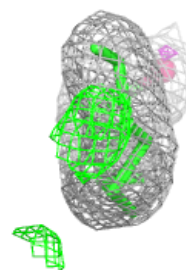
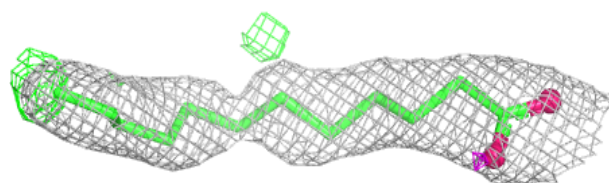
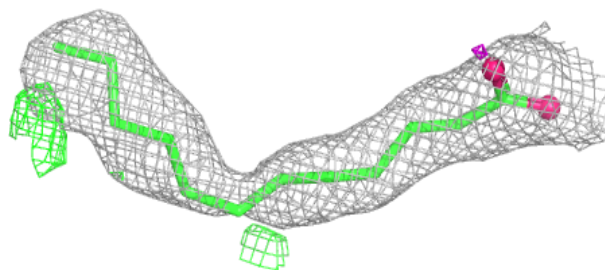


Electron density around STE m 102:

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

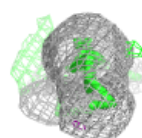
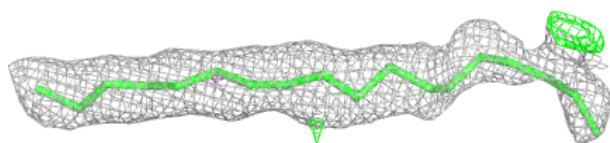
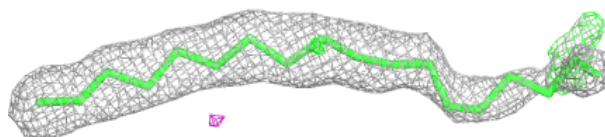
**Electron density around STE t 102:**

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

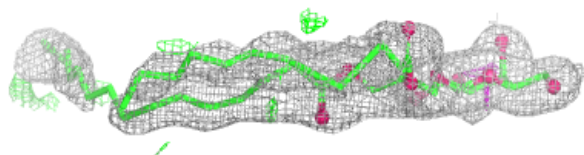
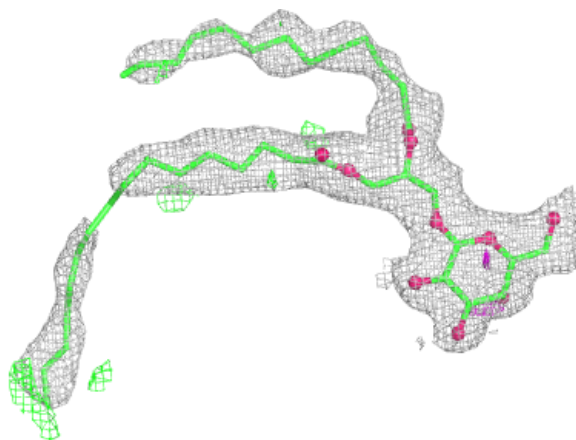


Electron density around STE m 103:

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

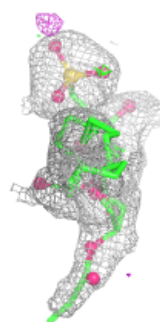
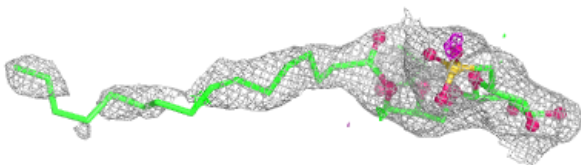
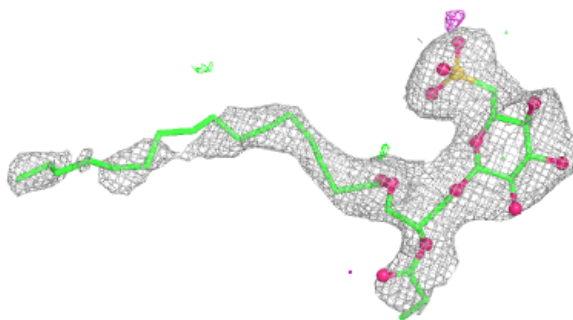
**Electron density around LMG C 524:**

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

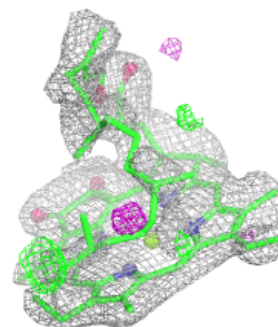
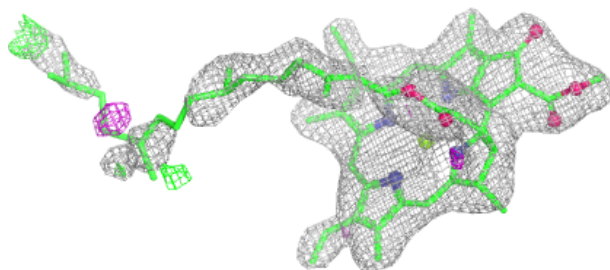
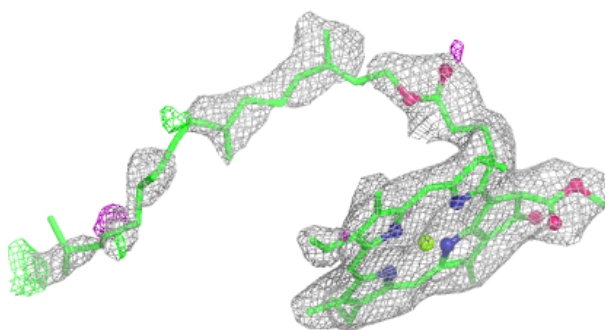


Electron density around SQD f 102:

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

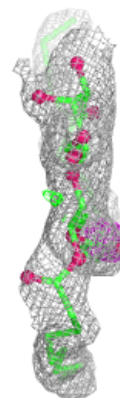
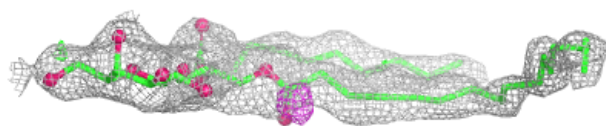
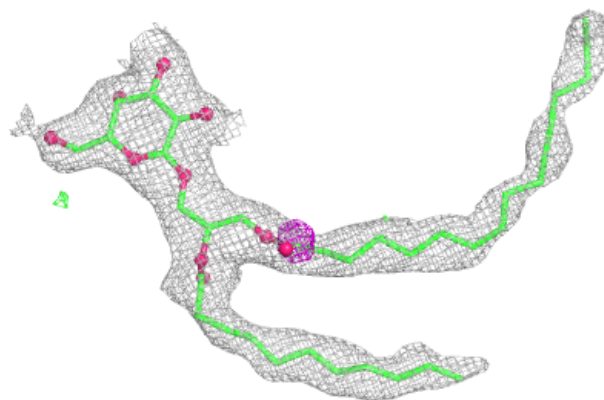
**Electron density around CLA c 513:**

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

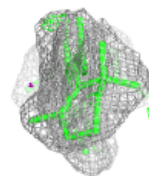
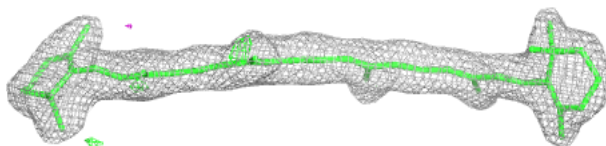
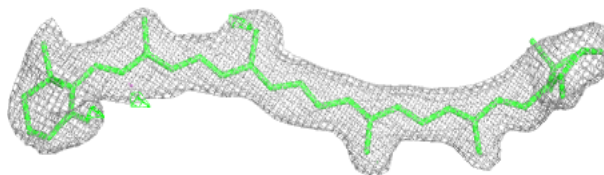


Electron density around LMG c 522:

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

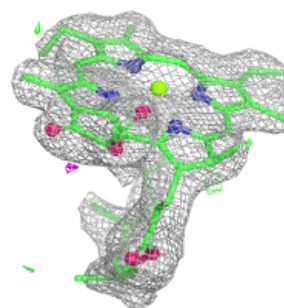
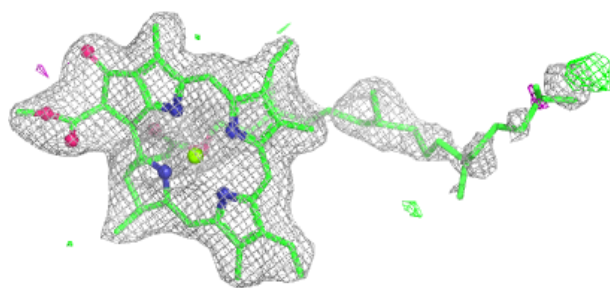
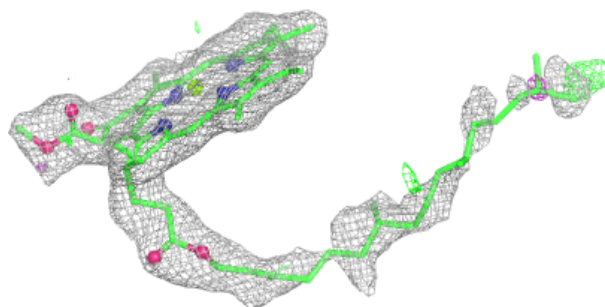
**Electron density around BCR J 101:**

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

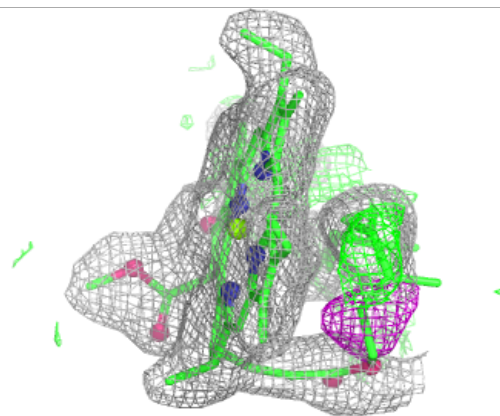
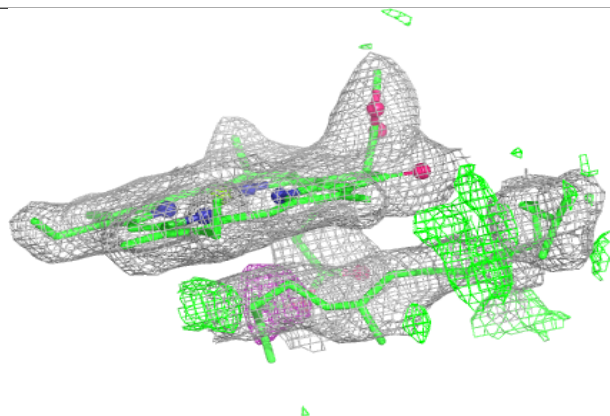
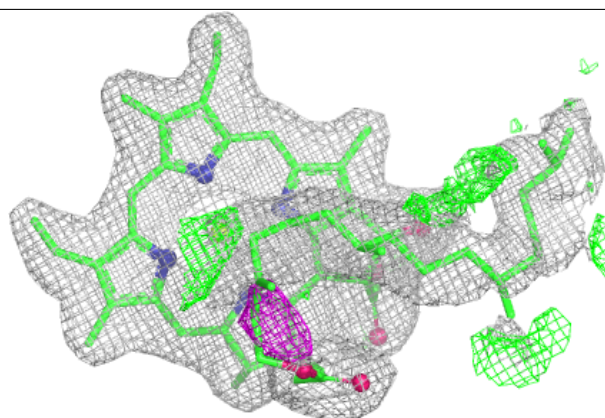


Electron density around CLA C 513:

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

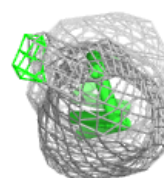
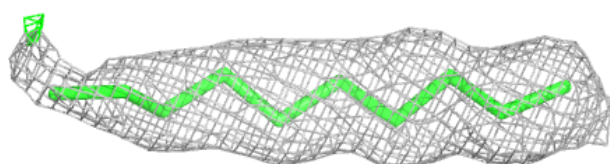
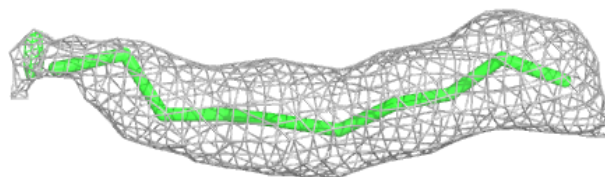
**Electron density around CLA B 601:**

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

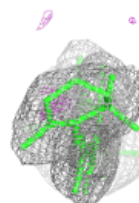
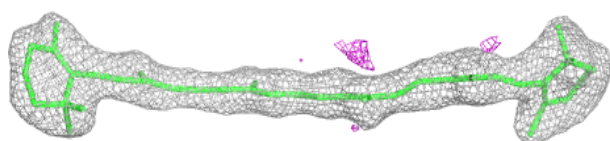
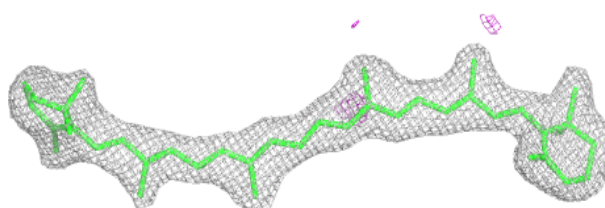


Electron density around STE M 103:

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

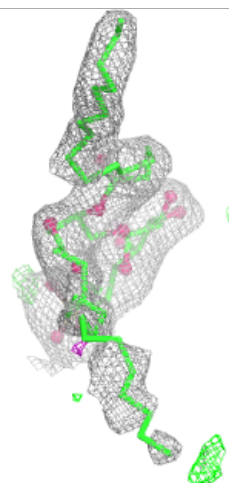
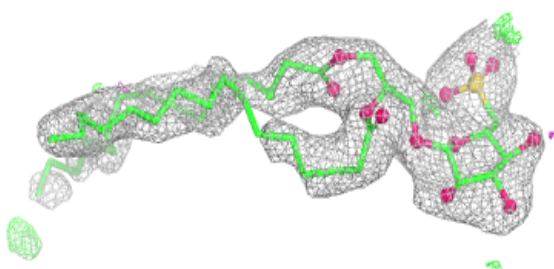
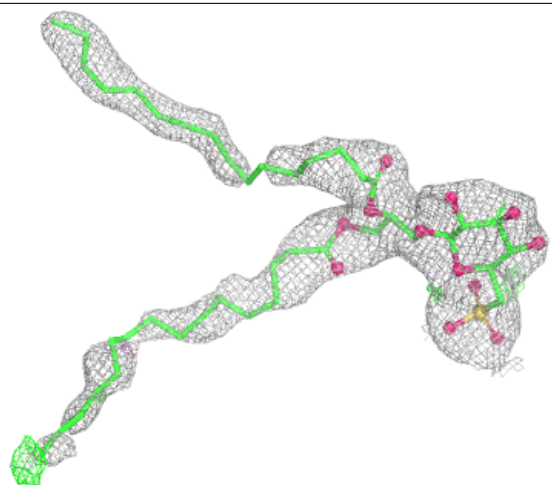
**Electron density around BCR k 101:**

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



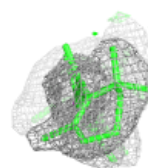
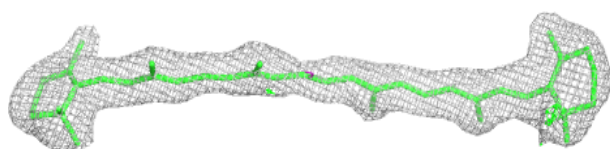
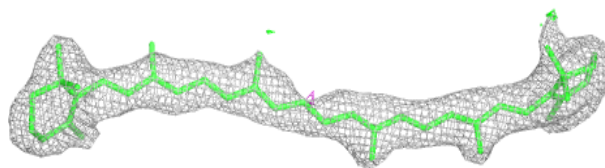
Electron density around SQD a 614:

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

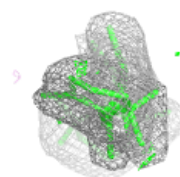
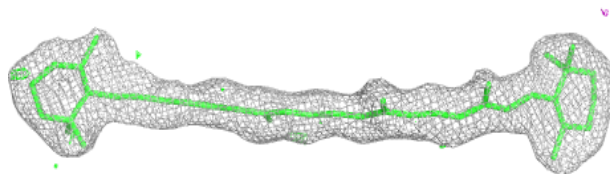
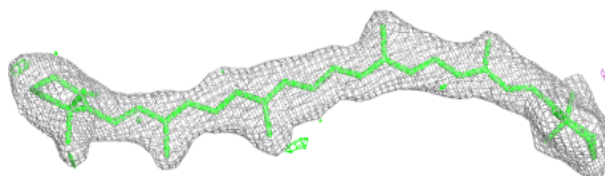


Electron density around BCR c 514:

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

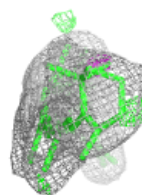
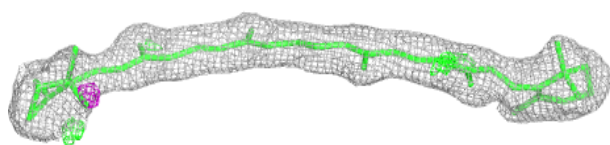
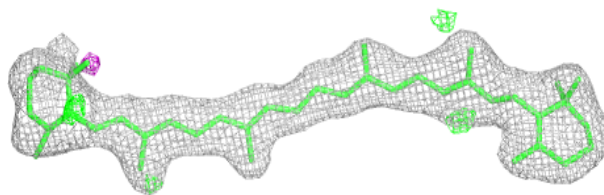
**Electron density around BCR h 101:**

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

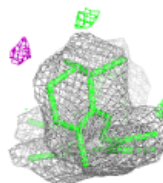
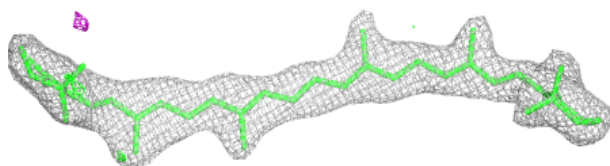
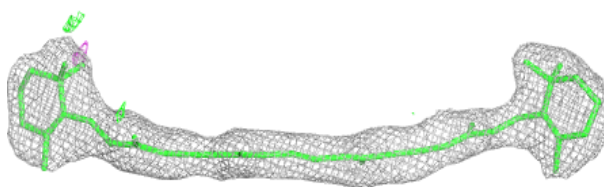


Electron density around BCR d 404:

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

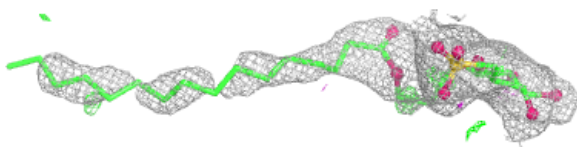
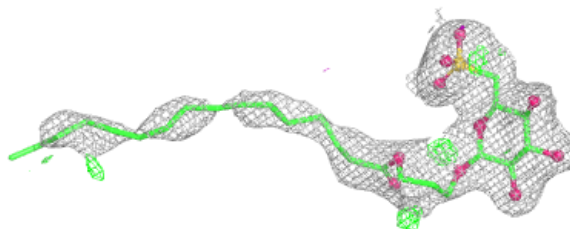
**Electron density around BCR k 102:**

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



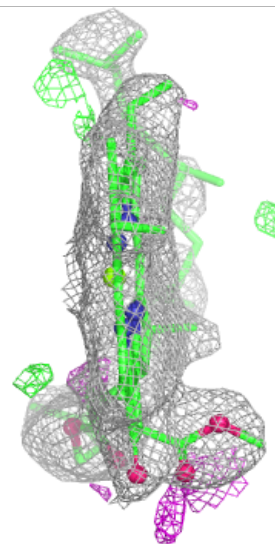
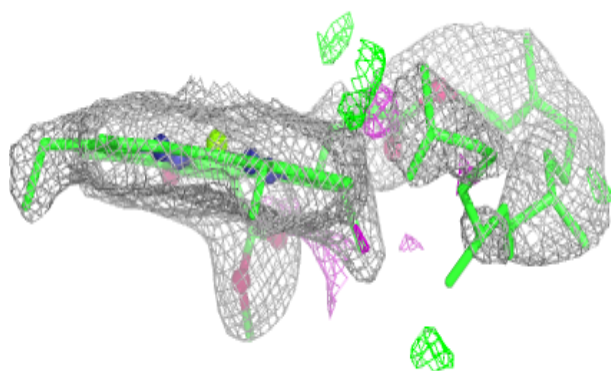
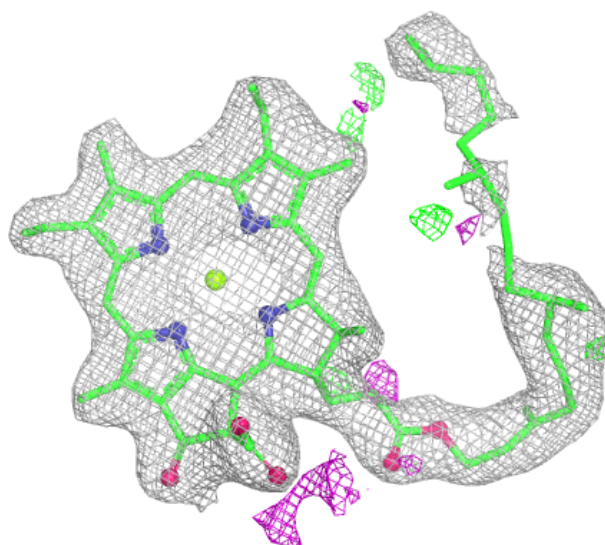
Electron density around SQD D 407:

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



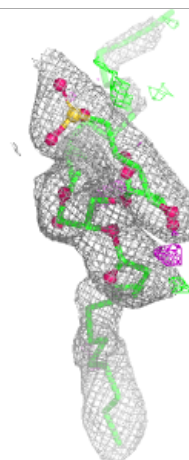
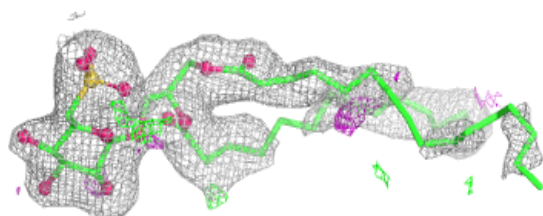
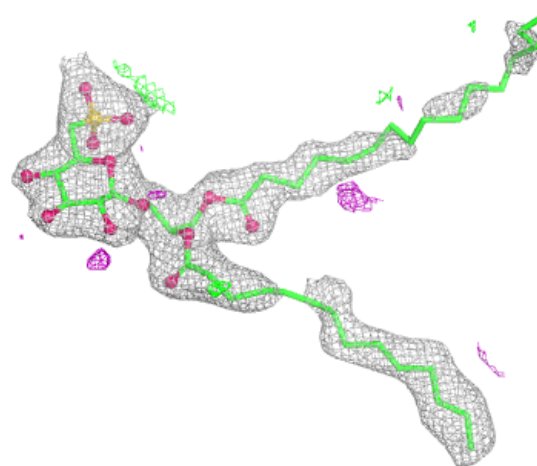
Electron density around CLA c 512:

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



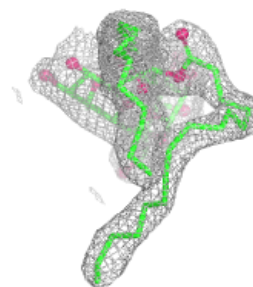
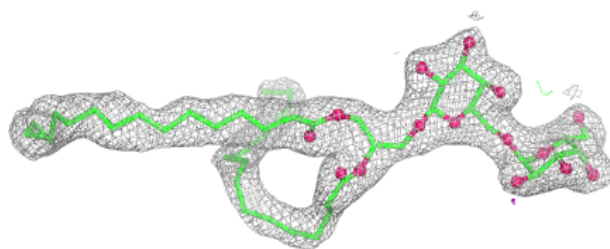
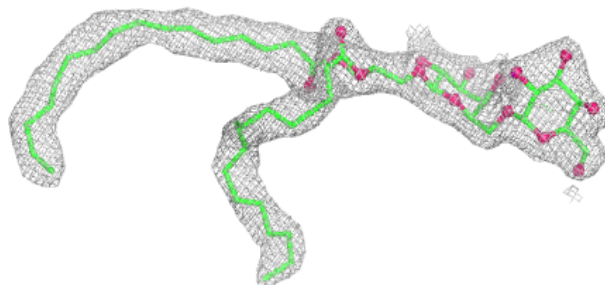
Electron density around SQD A 616:

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



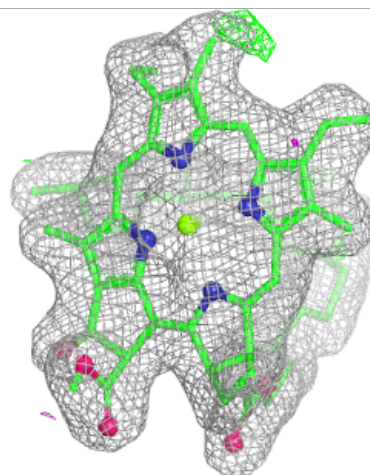
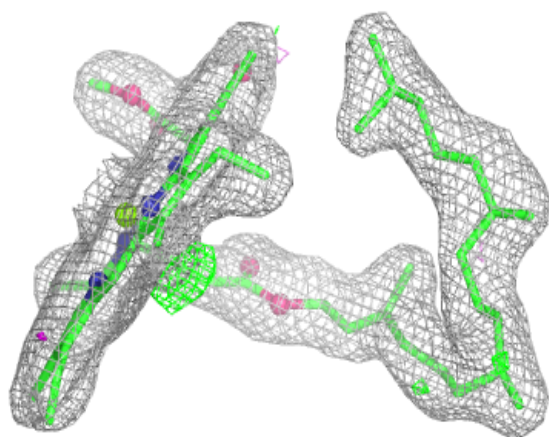
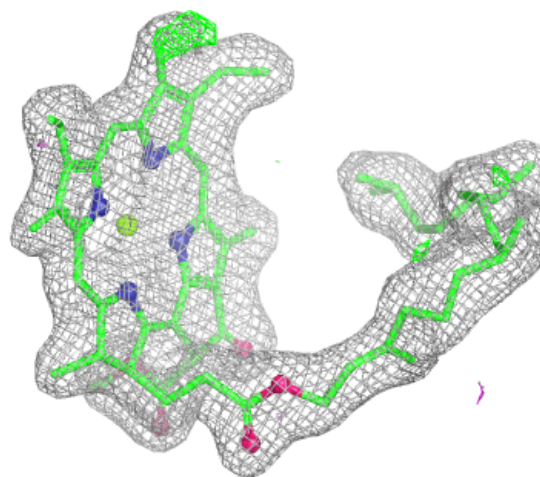
Electron density around DGD h 102:

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



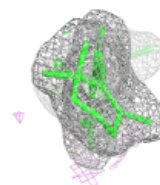
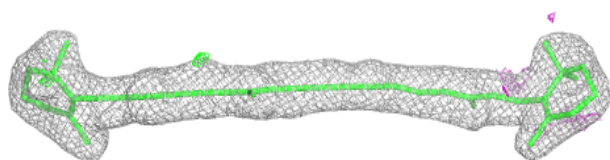
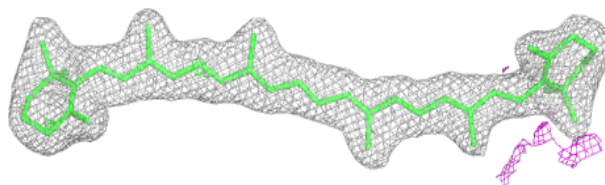
Electron density around CLA C 503:

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

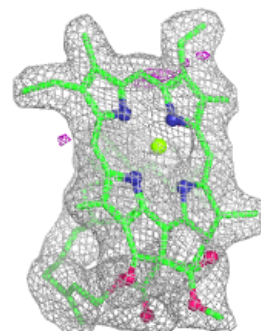
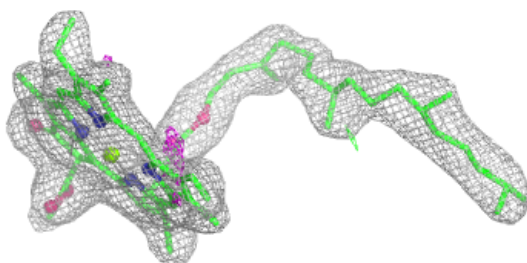
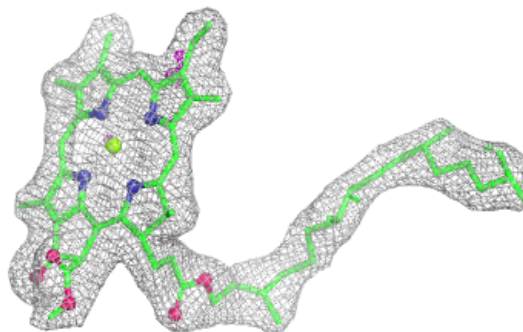


Electron density around BCR B 618:

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

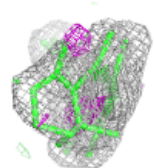
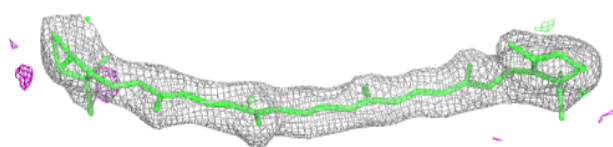
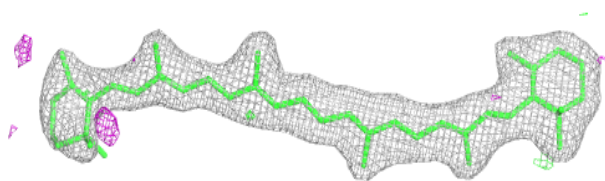
**Electron density around CLA C 511:**

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

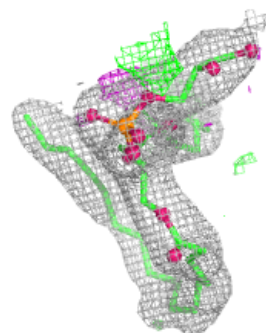
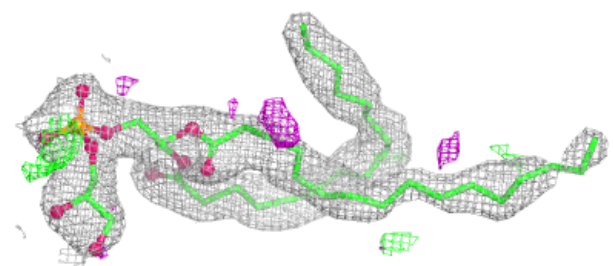
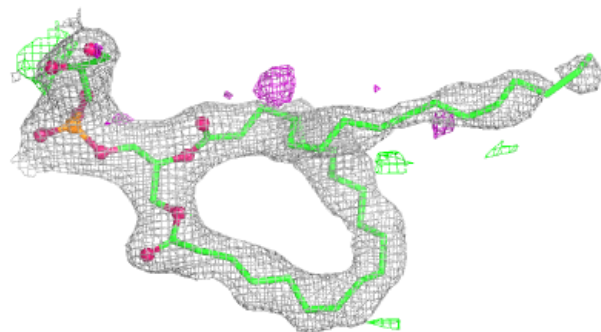


Electron density around BCR D 403:

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

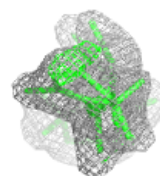
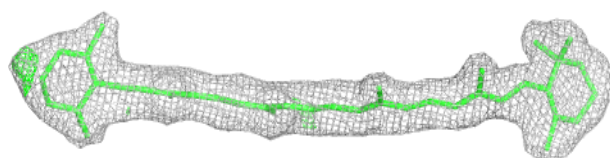
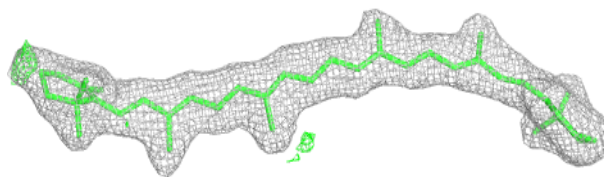
**Electron density around LHG a 613:**

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



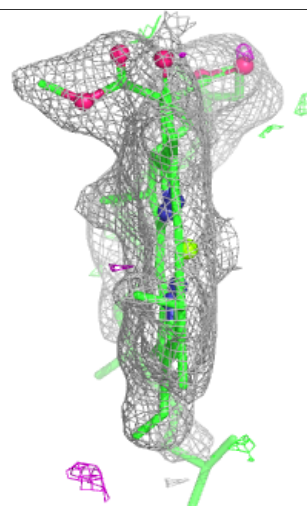
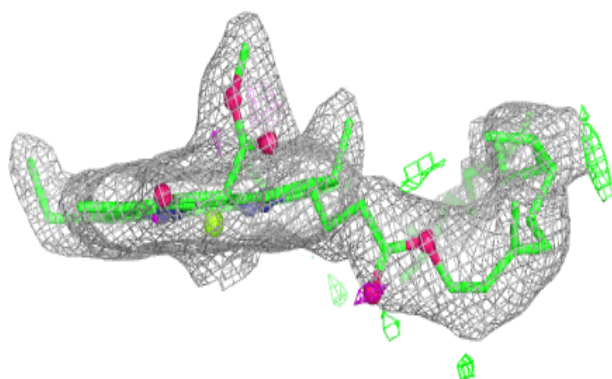
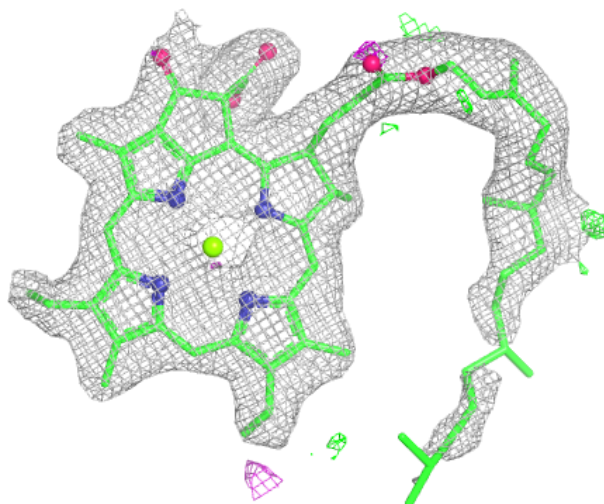
Electron density around BCR H 101:

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



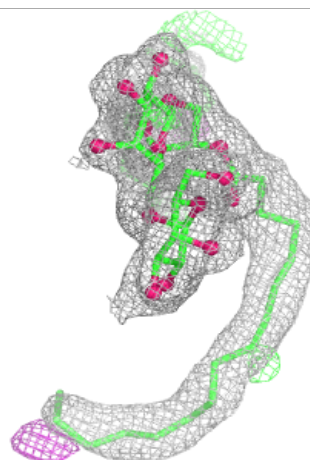
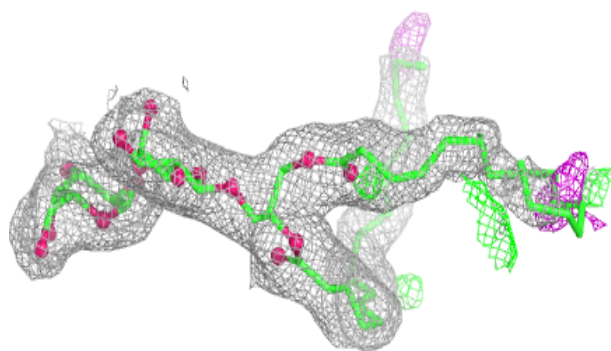
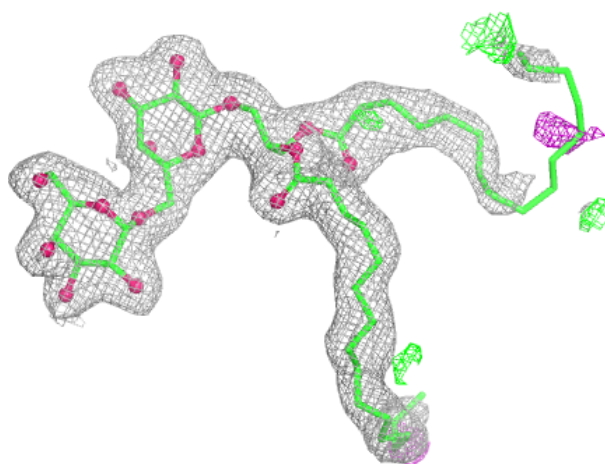
Electron density around CLA C 512:

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



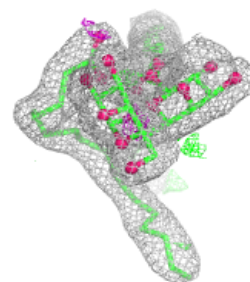
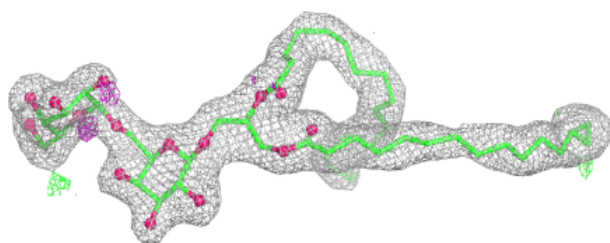
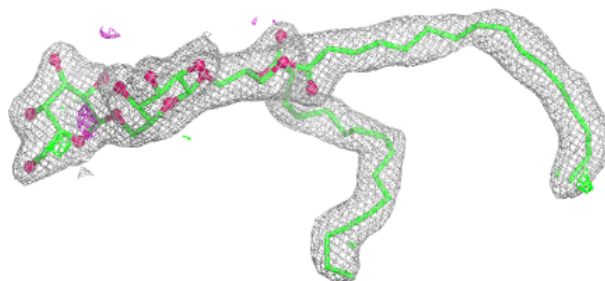
Electron density around DGD C 522:

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

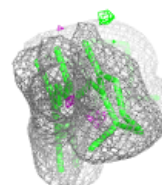
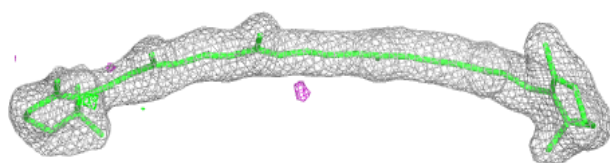
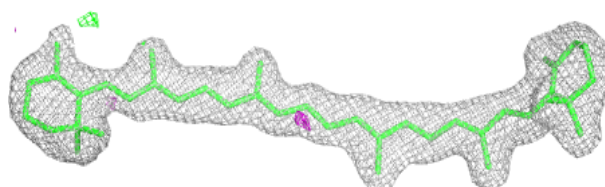


Electron density around DGD H 102:

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

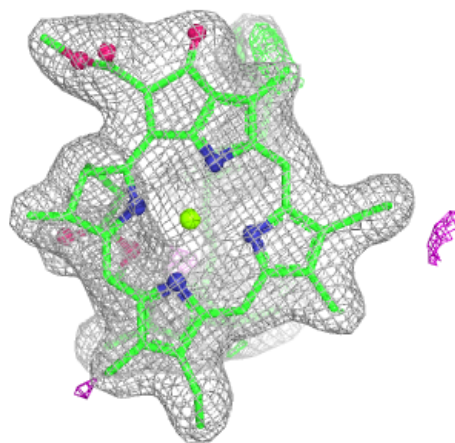
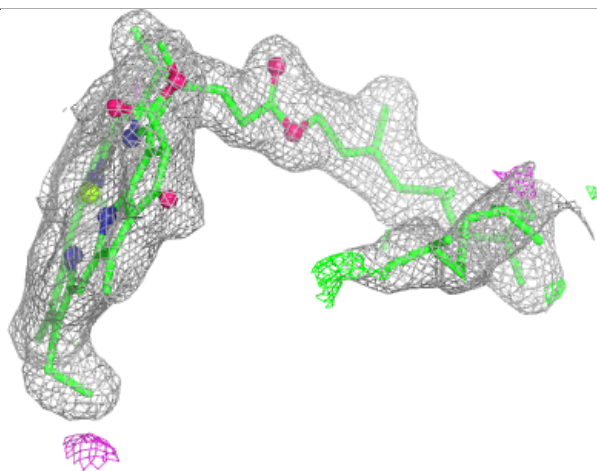
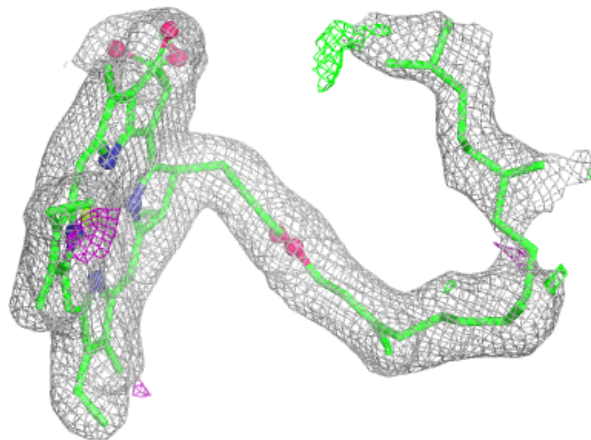
**Electron density around BCR T 101:**

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



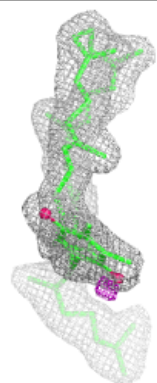
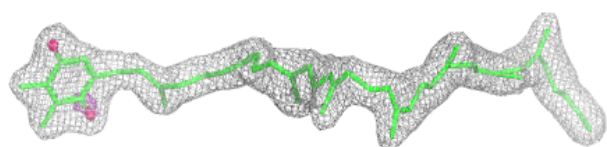
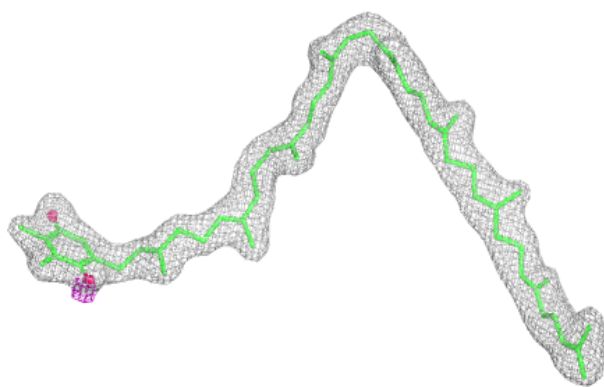
Electron density around CLA B 606:

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

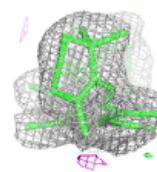
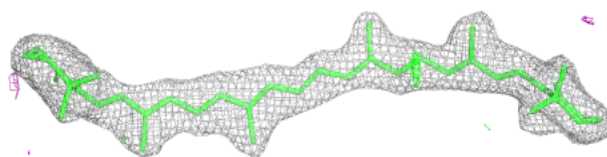
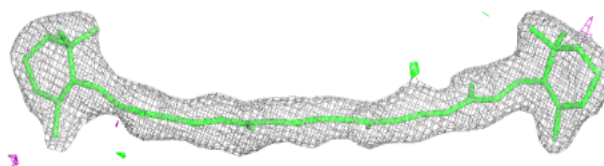


Electron density around PL9 d 405:

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

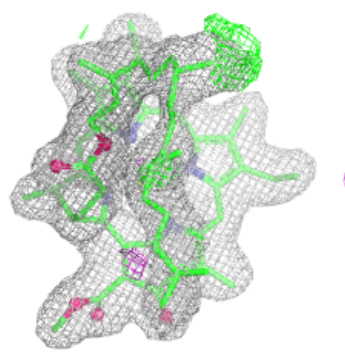
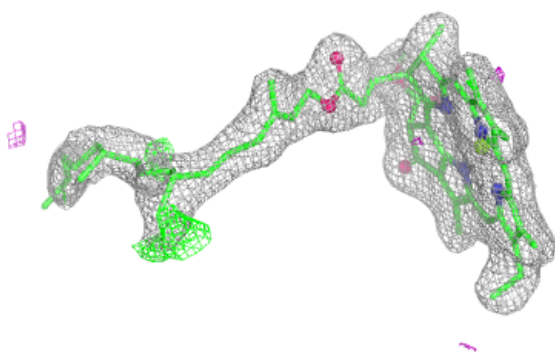
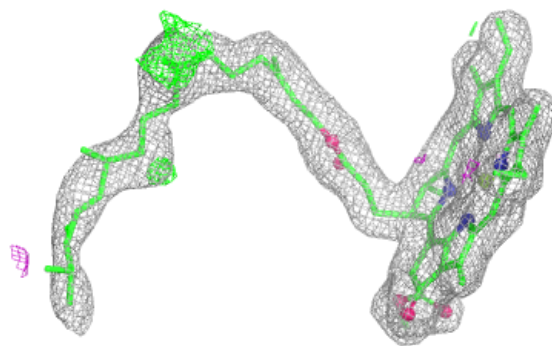
**Electron density around BCR K 101:**

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

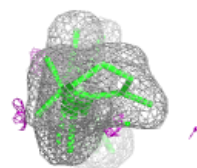
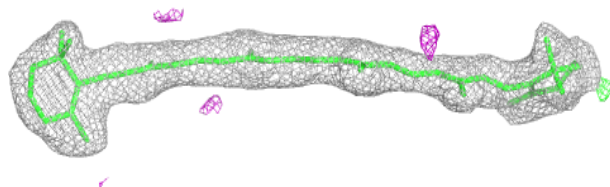
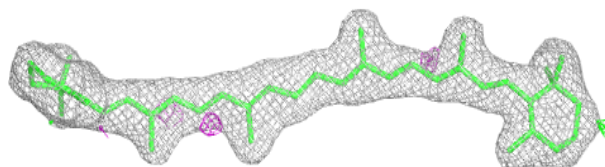


Electron density around CLA b 606:

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

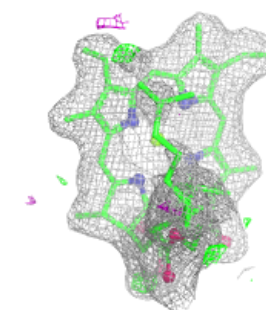
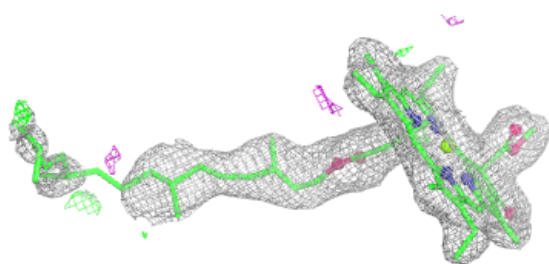
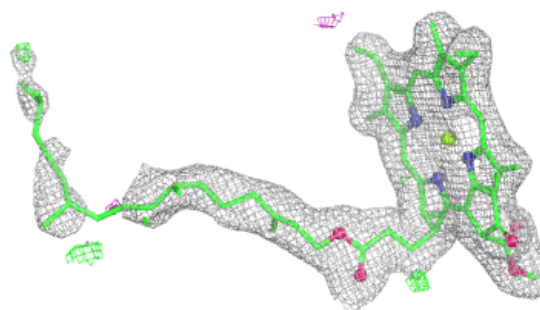
**Electron density around BCR b 617:**

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

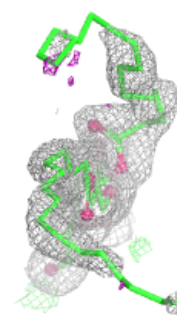
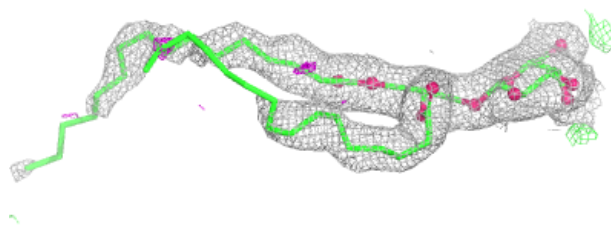
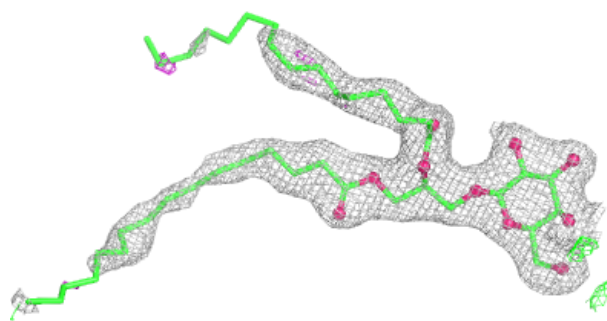


Electron density around CLA d 403:

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

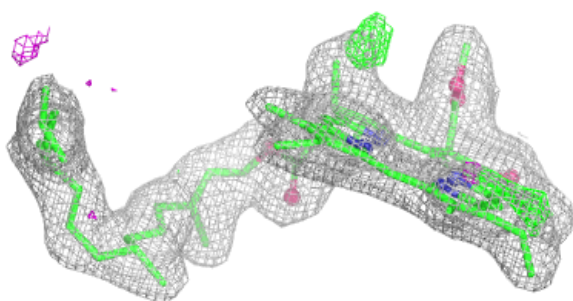
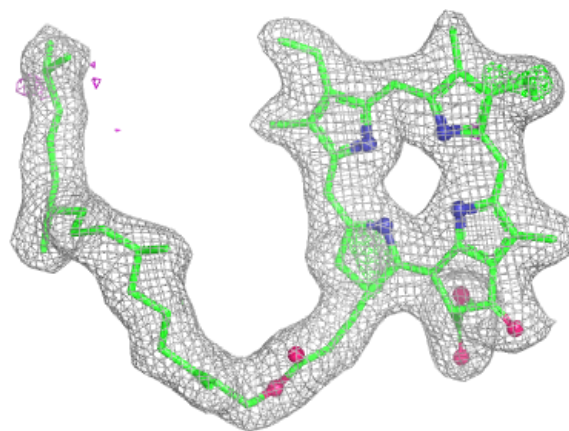
**Electron density around LMG D 406:**

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

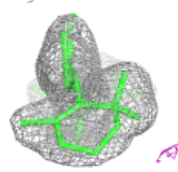
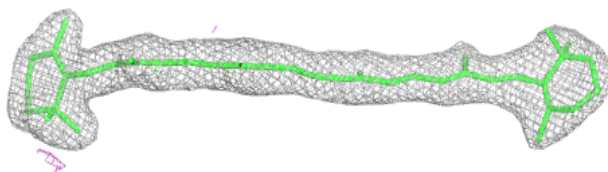
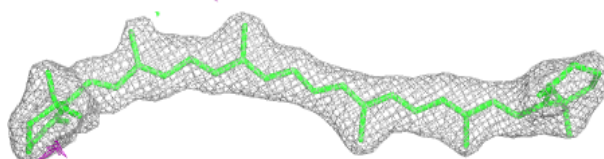


Electron density around PHO d 401:

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

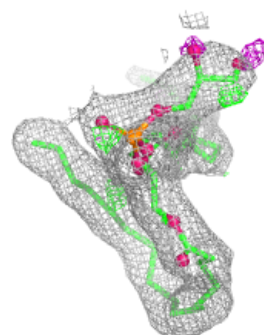
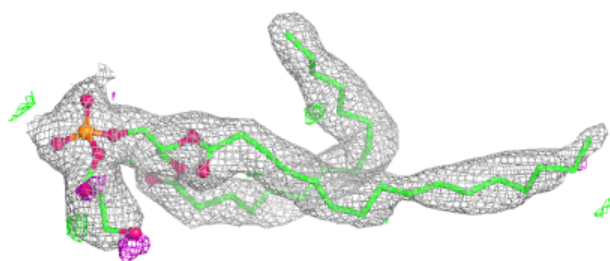
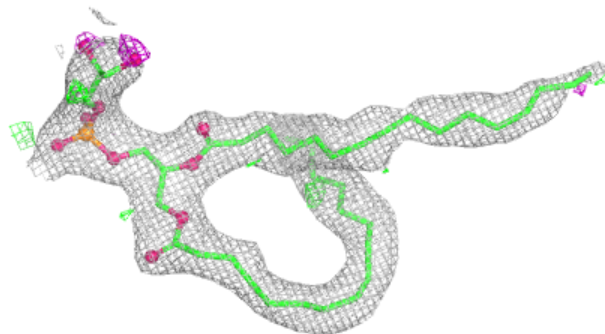
**Electron density around BCR c 515:**

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

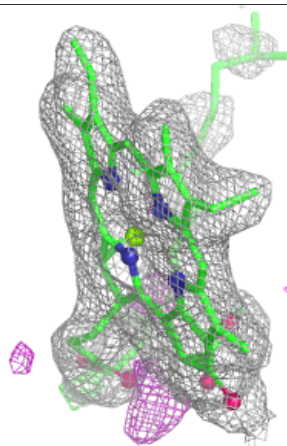
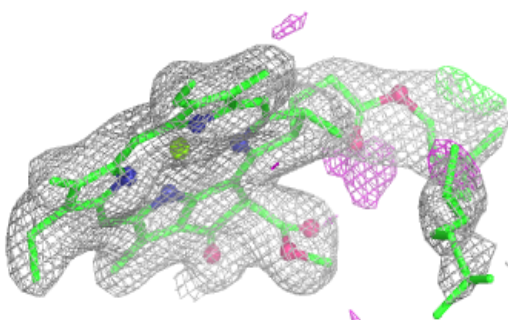
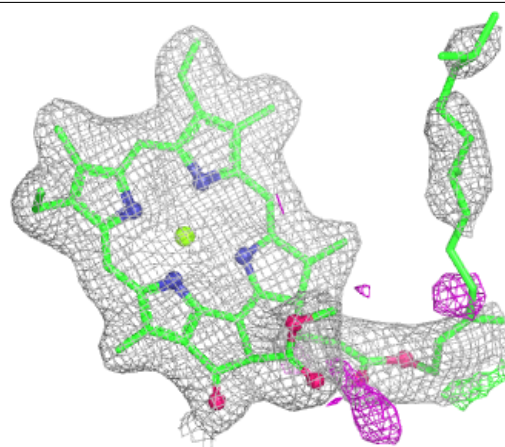


Electron density around LHG D 410:

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

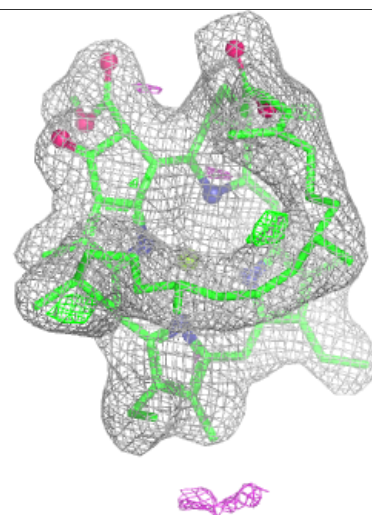
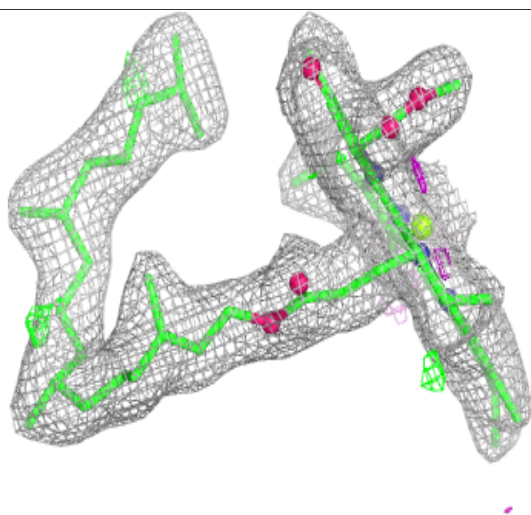
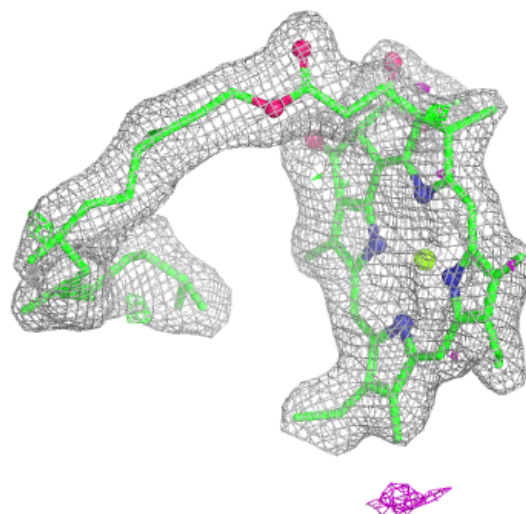
**Electron density around CLA b 616:**

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



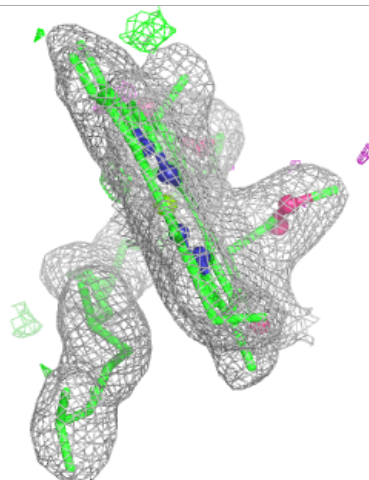
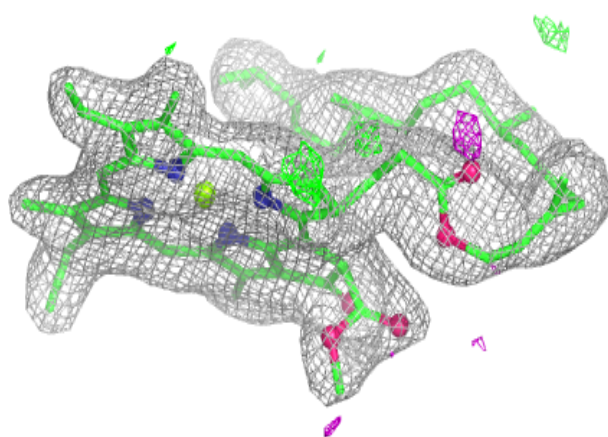
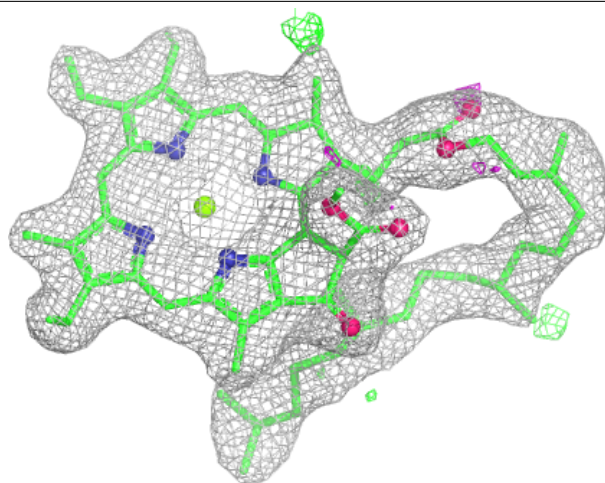
Electron density around CLA c 503:

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



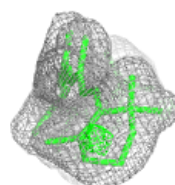
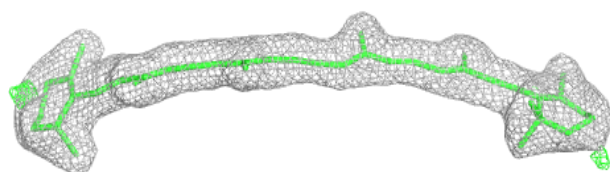
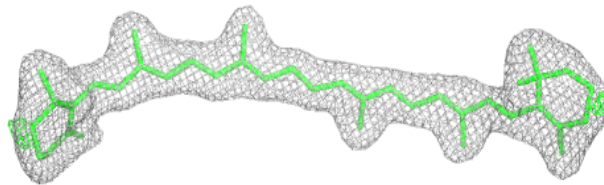
Electron density around CLA c 509:

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

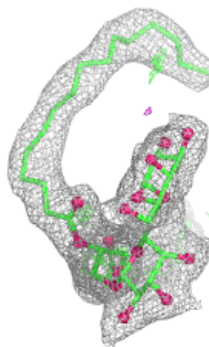
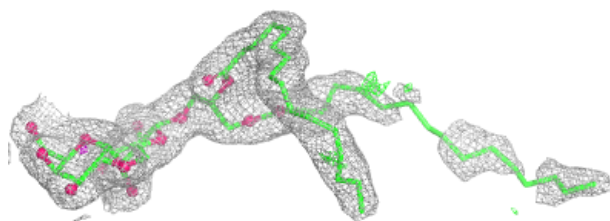
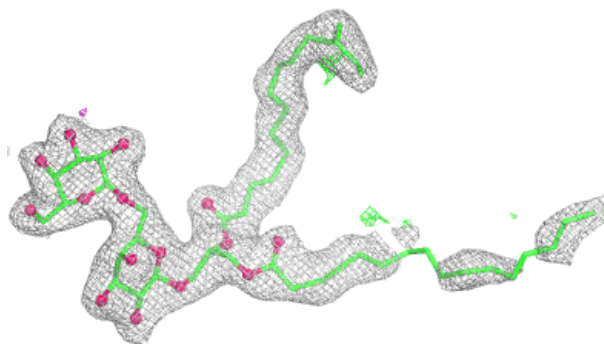


Electron density around BCR t 101:

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

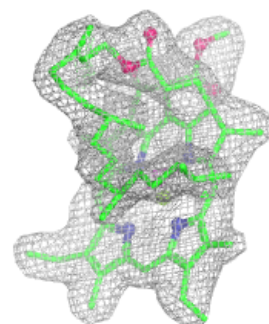
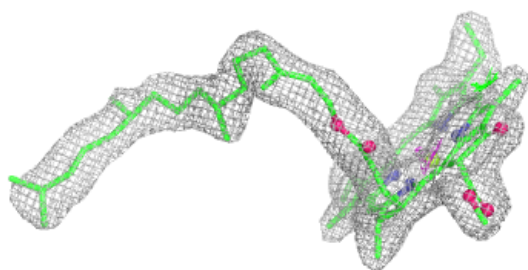
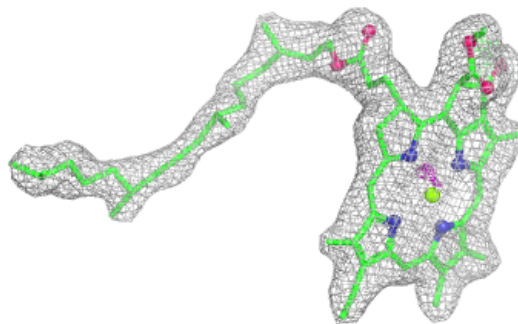
**Electron density around DGD c 520:**

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

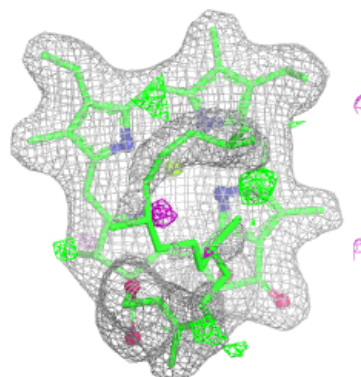
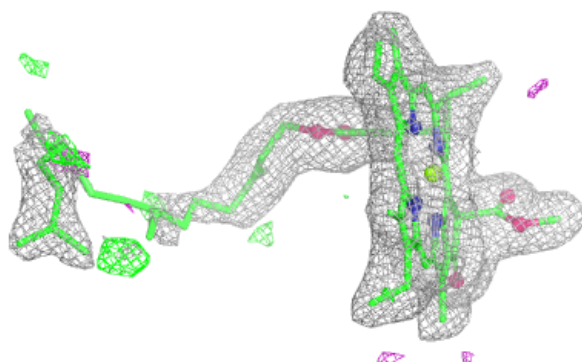
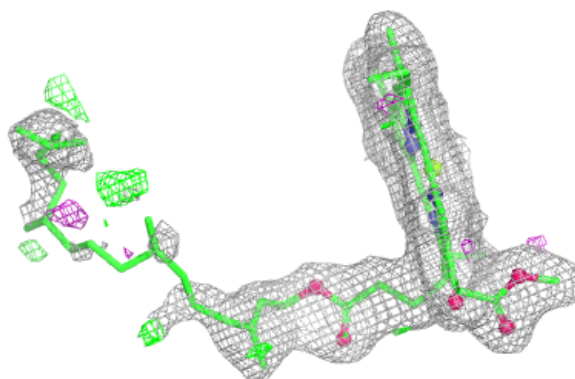


Electron density around CLA c 511:

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

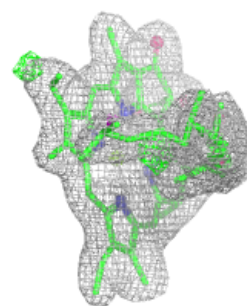
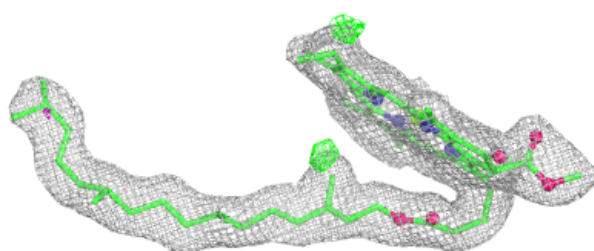
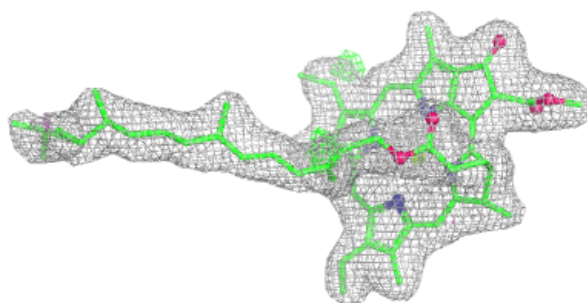
**Electron density around CLA C 506:**

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

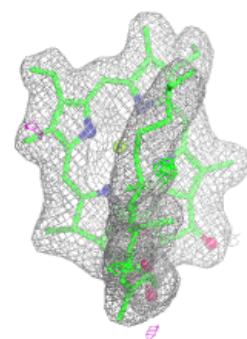
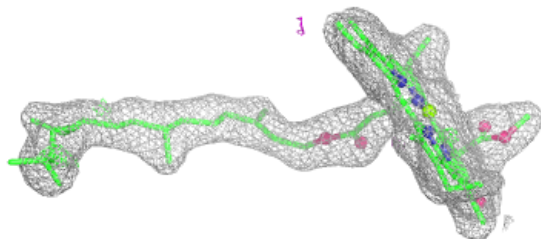
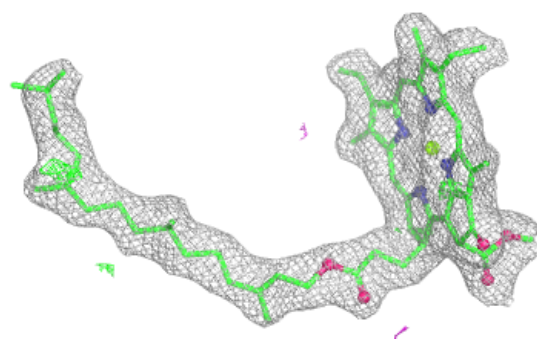


Electron density around CLA b 608:

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

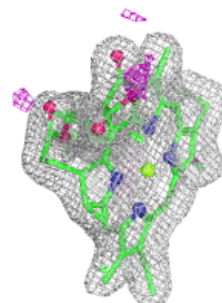
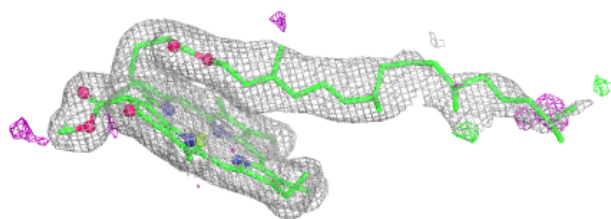
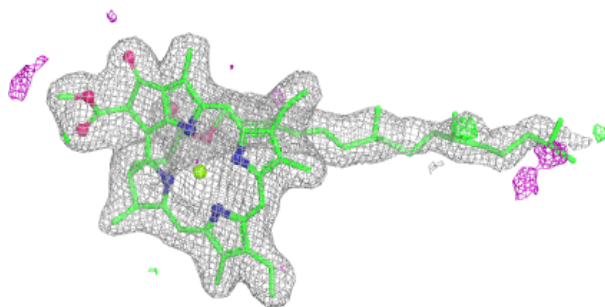
**Electron density around CLA b 609:**

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



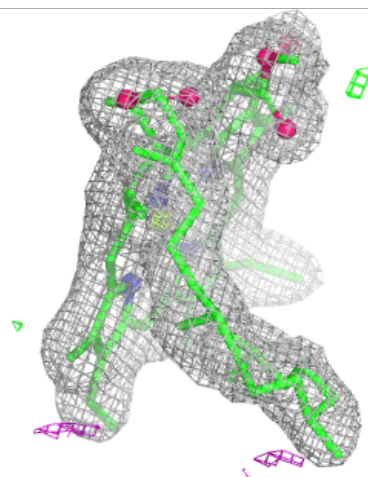
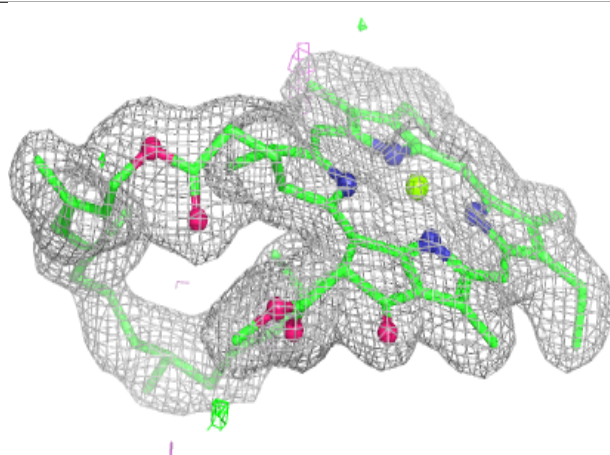
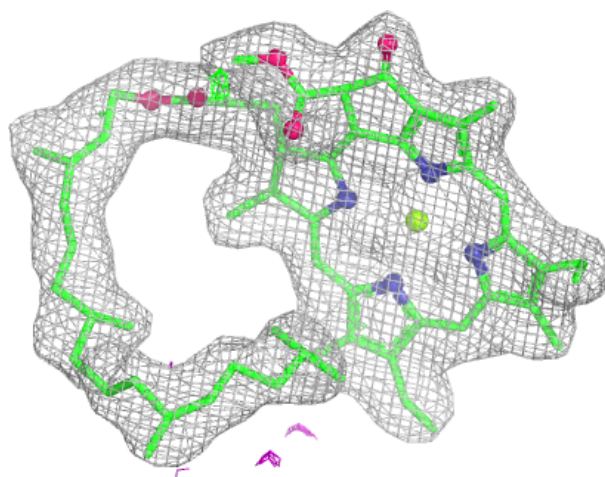
Electron density around CLA b 614:

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



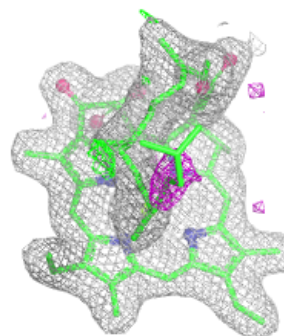
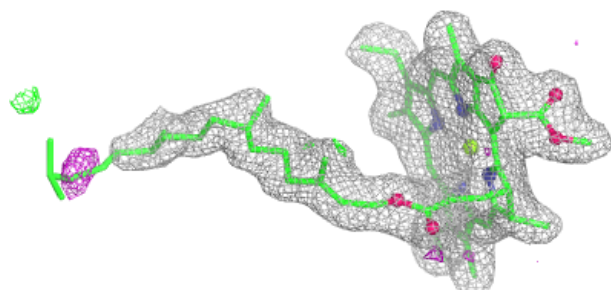
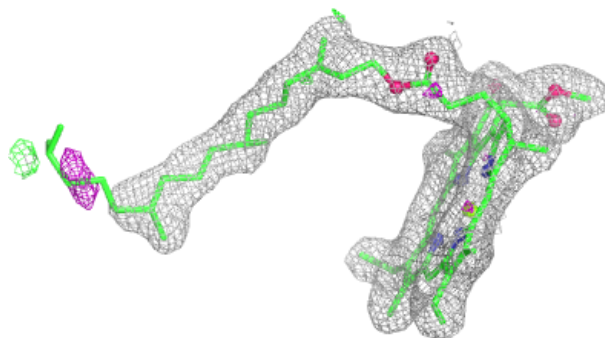
Electron density around CLA b 615:

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



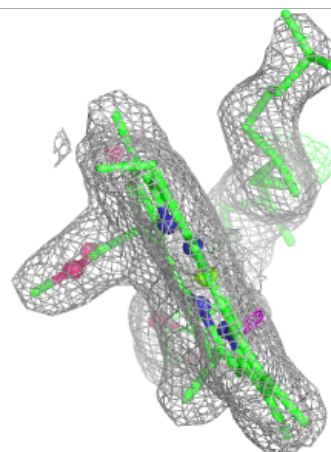
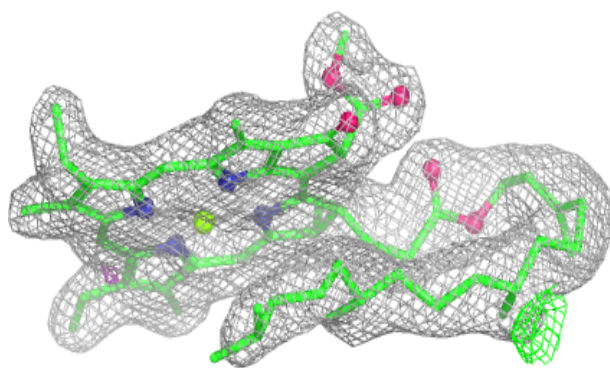
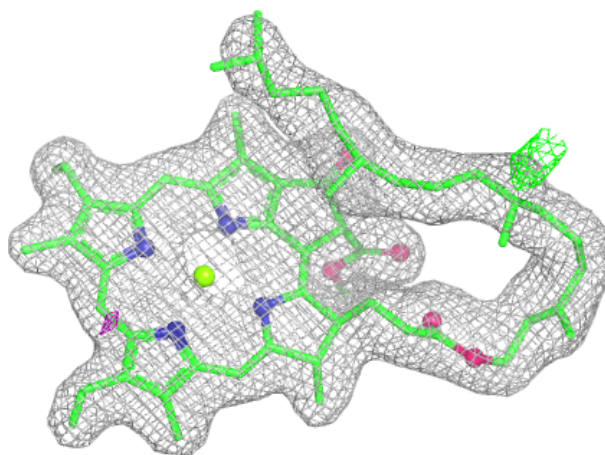
Electron density around CLA C 508:

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



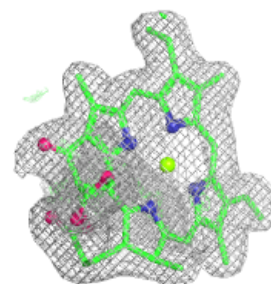
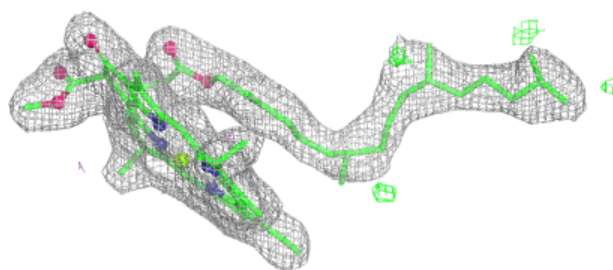
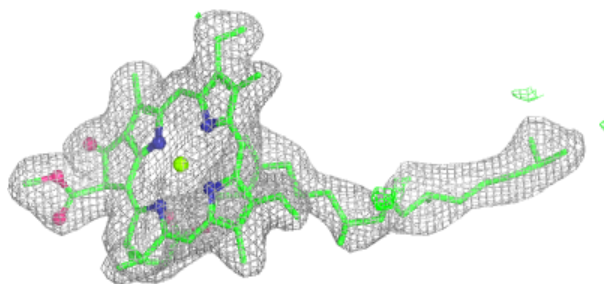
Electron density around CLA C 509:

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

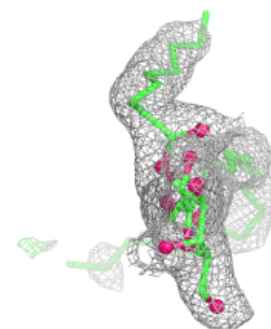
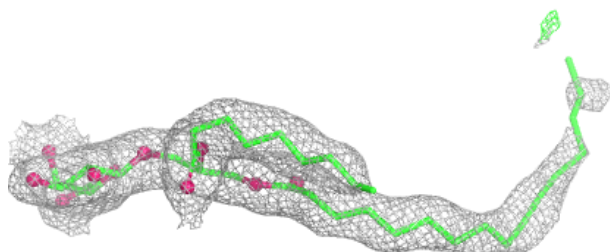
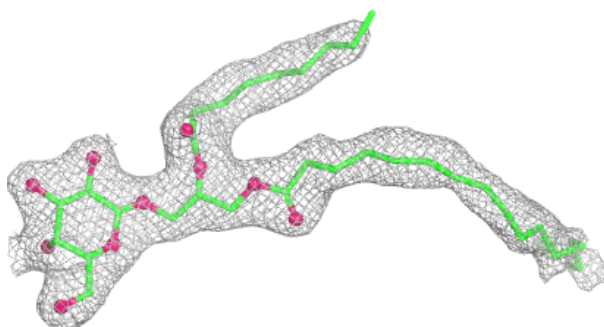


Electron density around CLA c 505:

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

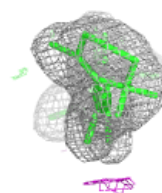
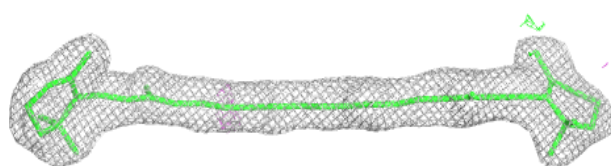
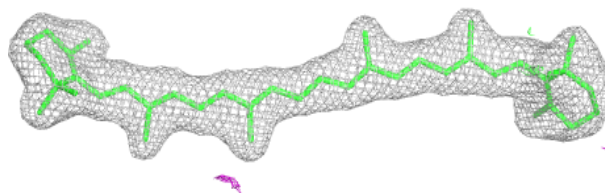
**Electron density around LMG d 410:**

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

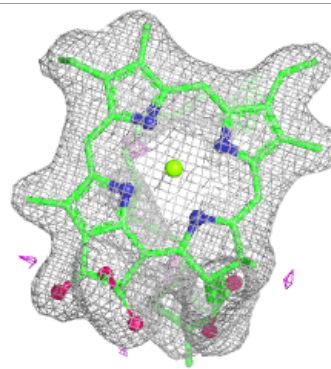
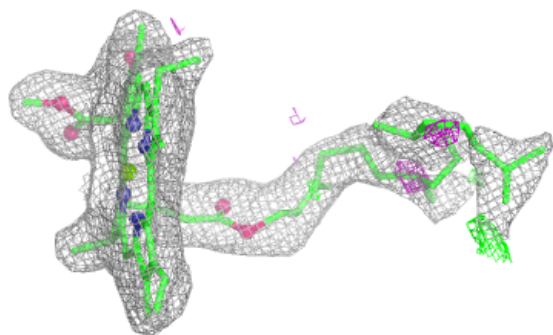
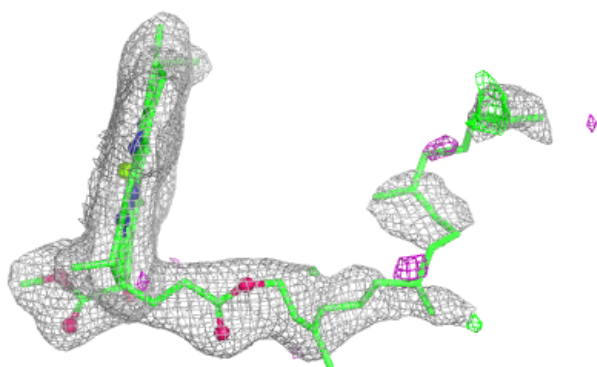


Electron density around BCR b 618:

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

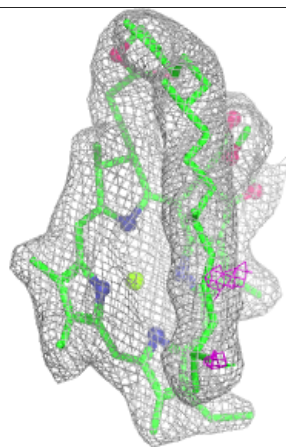
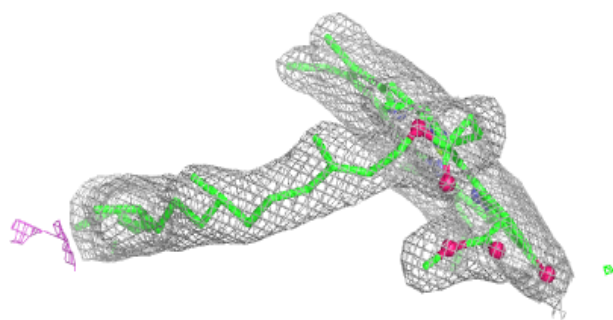
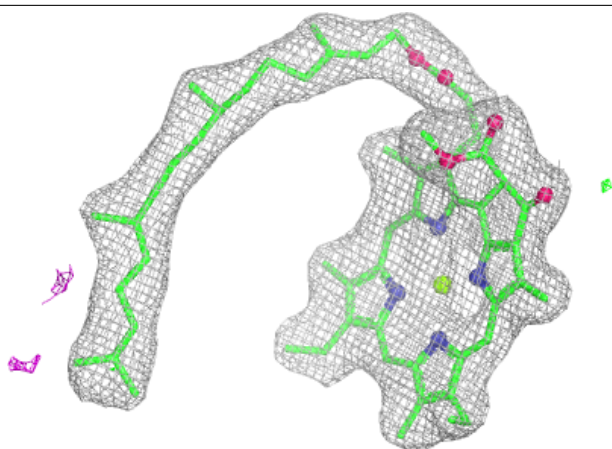
**Electron density around CLA c 506:**

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



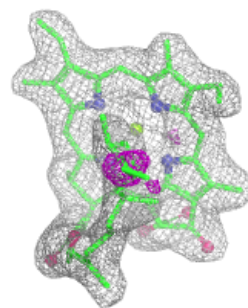
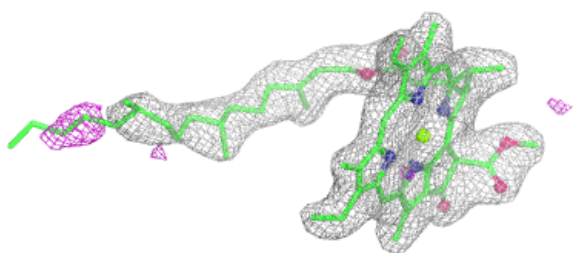
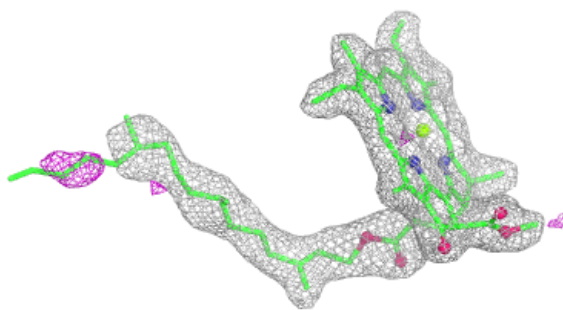
Electron density around CLA c 507:

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



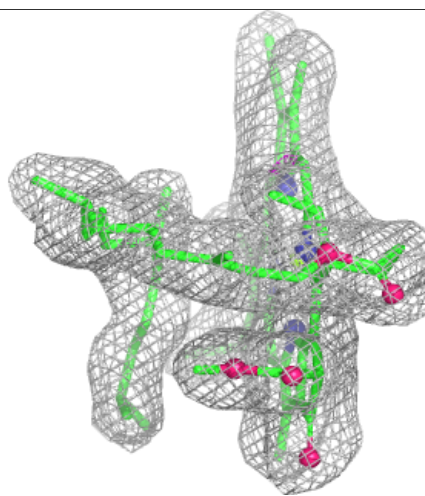
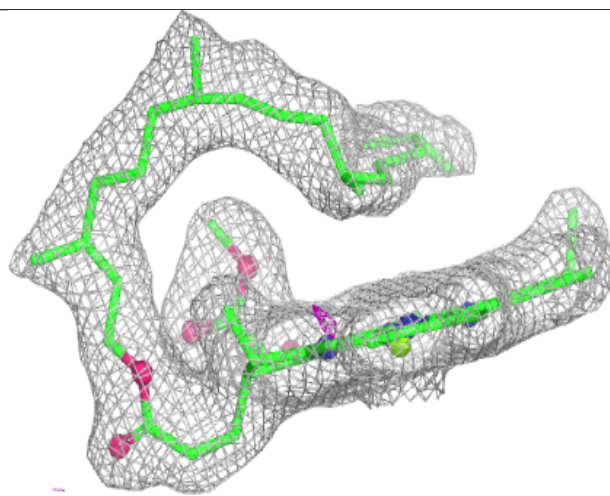
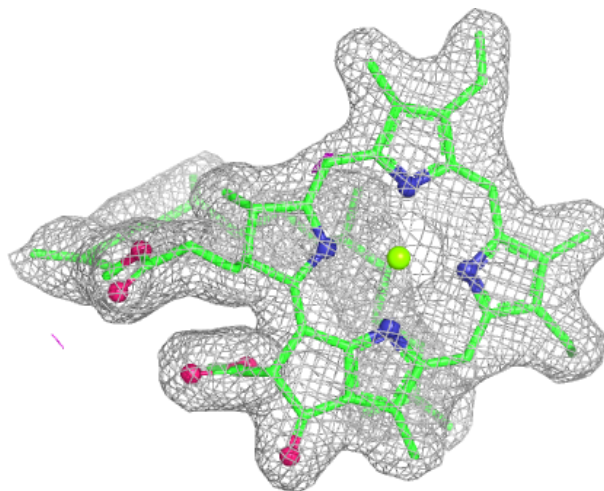
Electron density around CLA c 508:

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



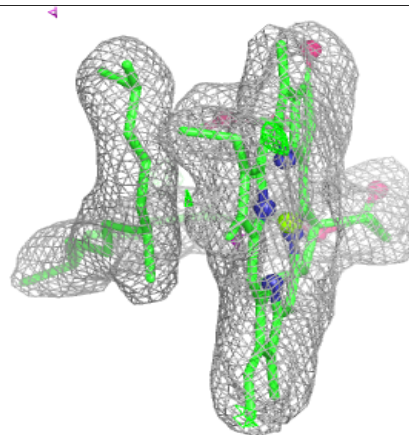
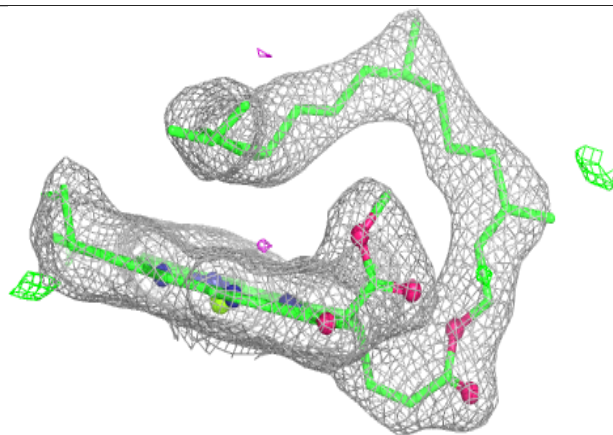
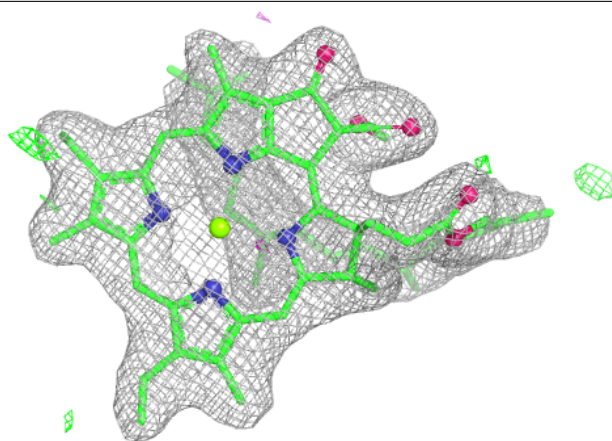
Electron density around CLA C 510:

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



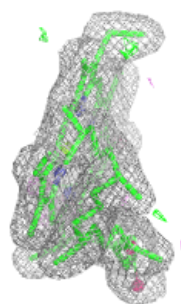
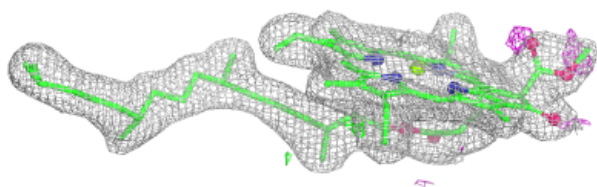
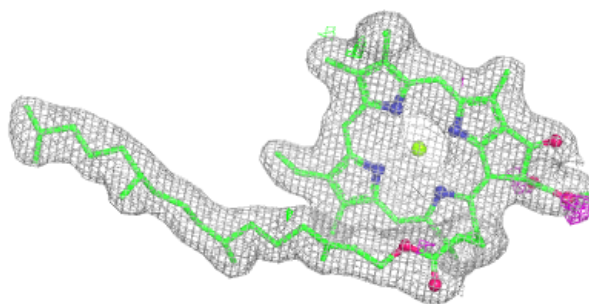
Electron density around CLA c 510:

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

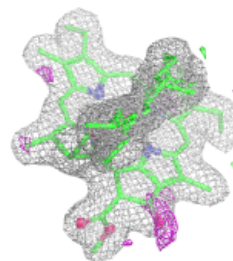
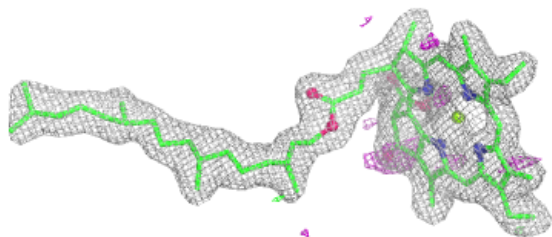
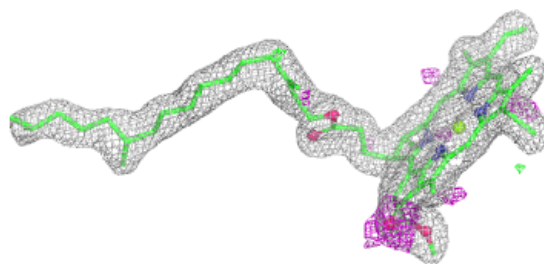


Electron density around CLA C 501:

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

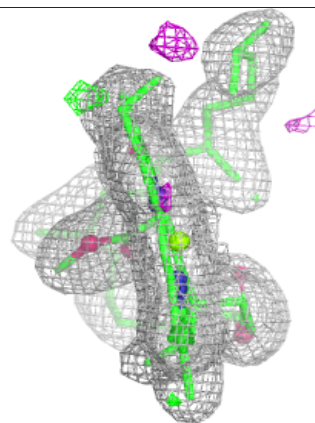
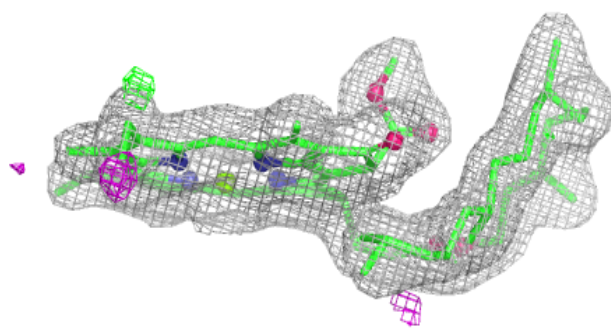
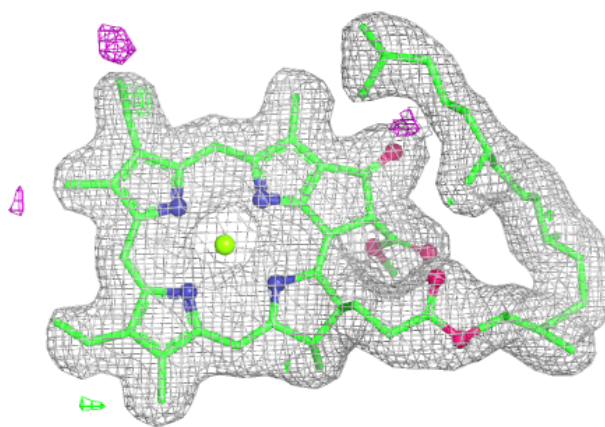
**Electron density around CLA C 502:**

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

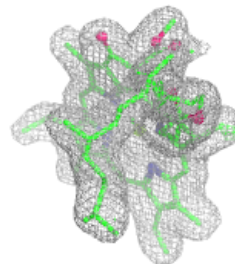
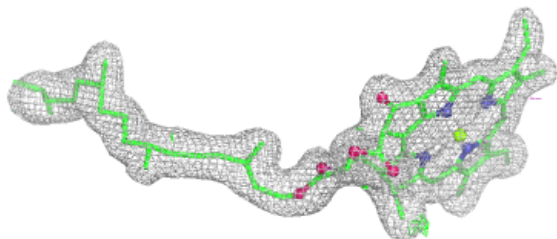
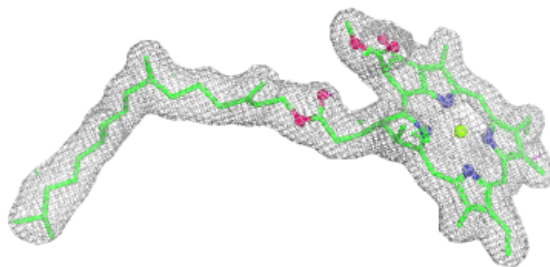


Electron density around CLA B 610:

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

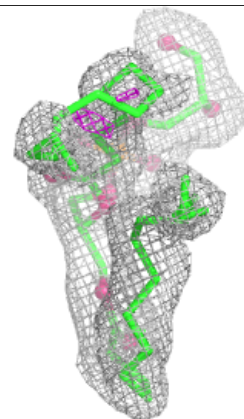
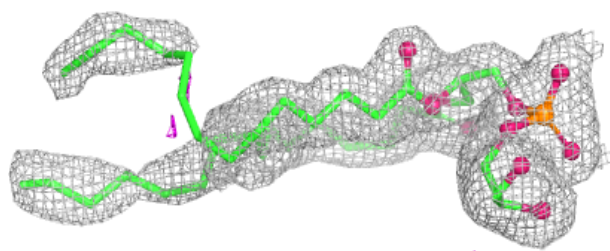
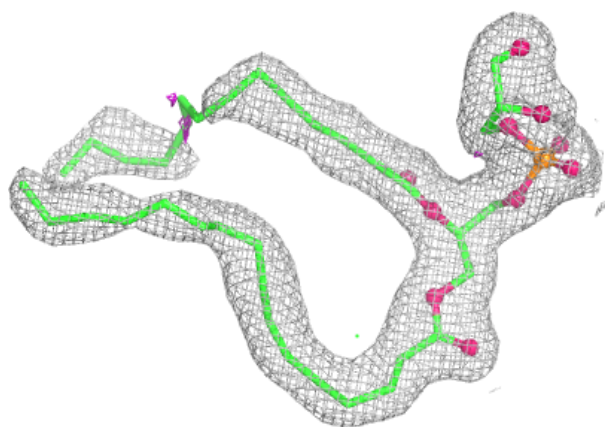
**Electron density around CLA a 606:**

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

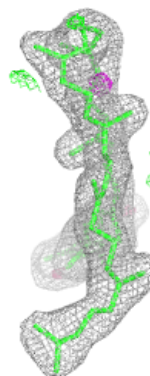
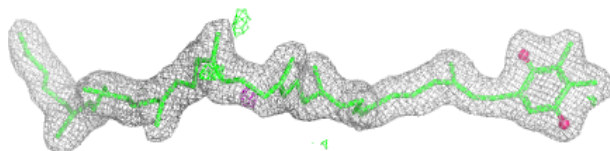
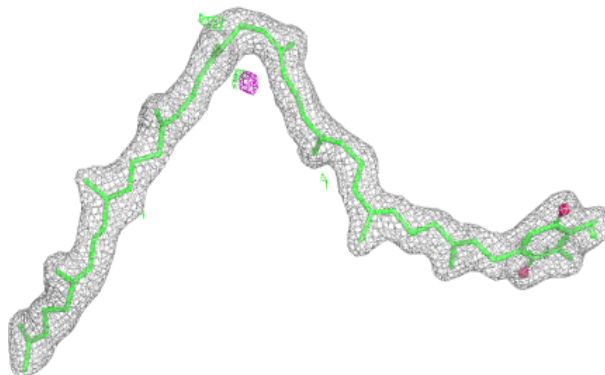


Electron density around LHG D 409:

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

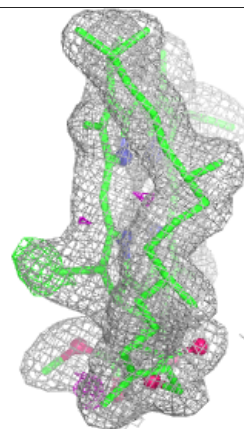
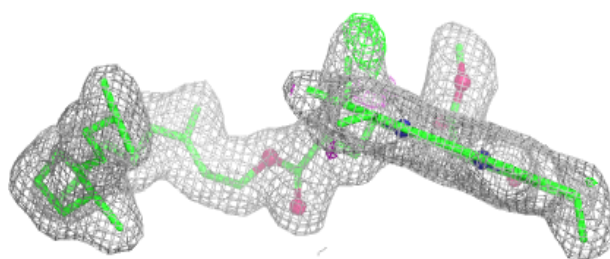
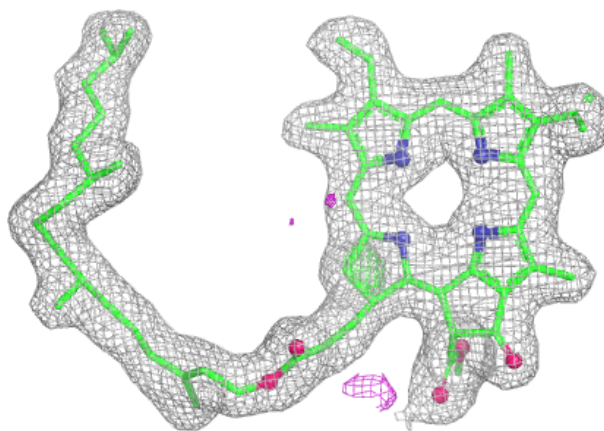
**Electron density around PL9 D 404:**

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

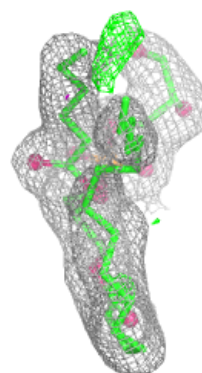
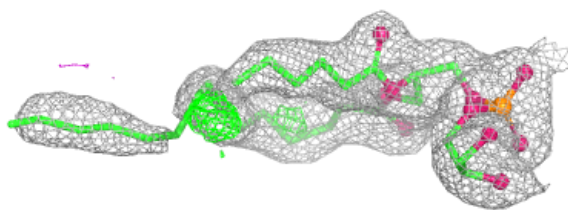
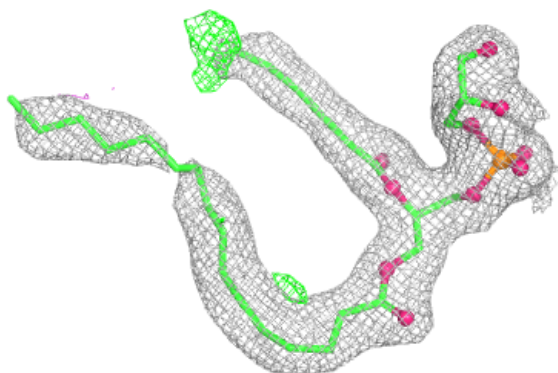


Electron density around PHO A 608:

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

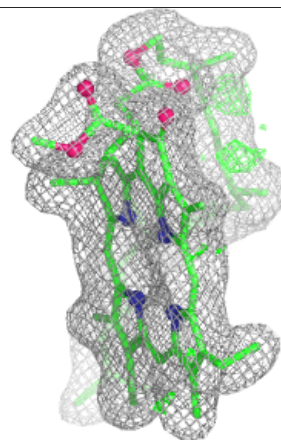
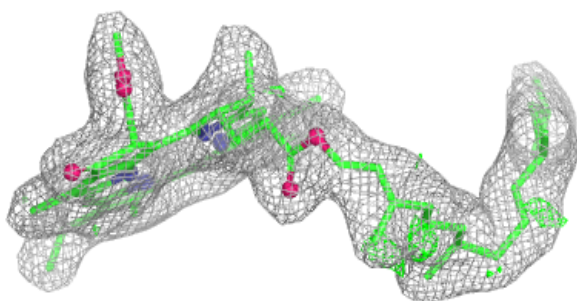
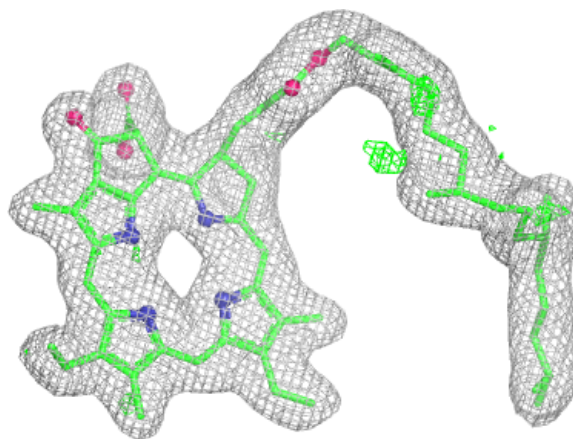
**Electron density around LHG d 408:**

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



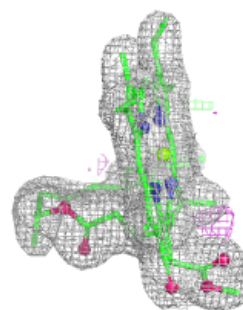
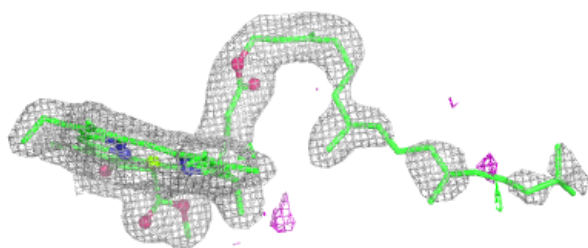
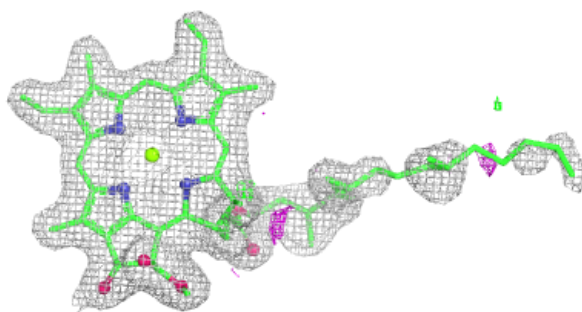
Electron density around PHO A 609:

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

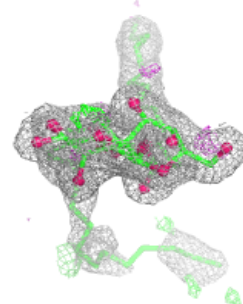
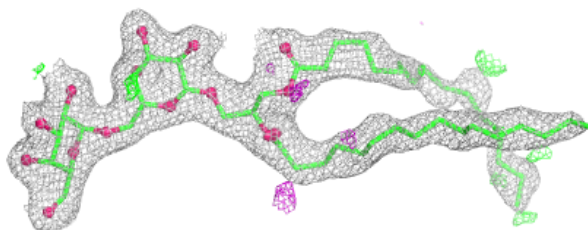
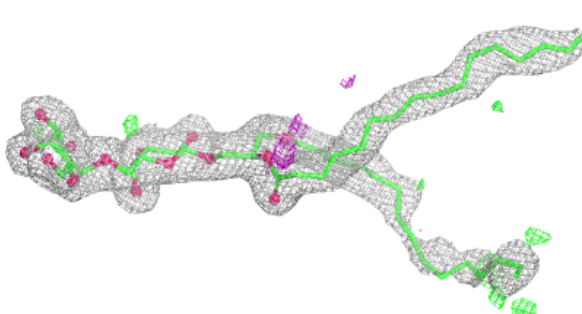


Electron density around CLA a 607:

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

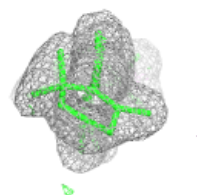
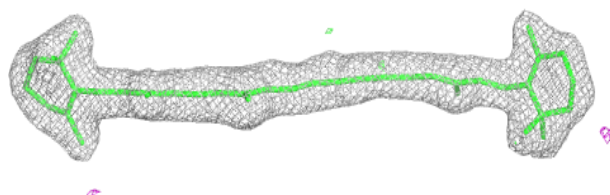
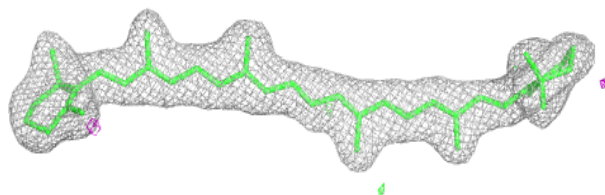
**Electron density around DGD C 521:**

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

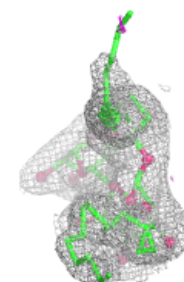
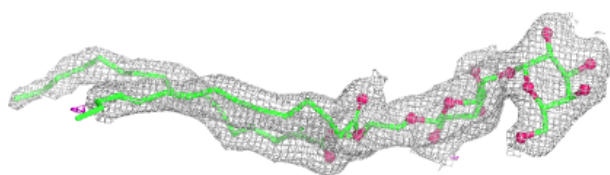
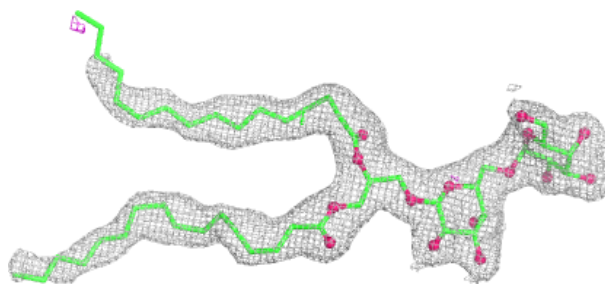


Electron density around BCR A 611:

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

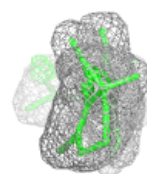
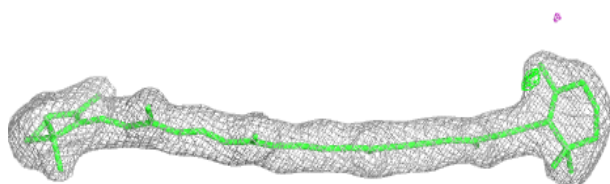
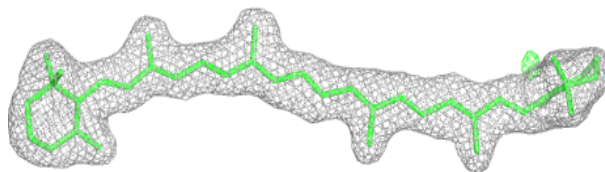
**Electron density around DGD C 523:**

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

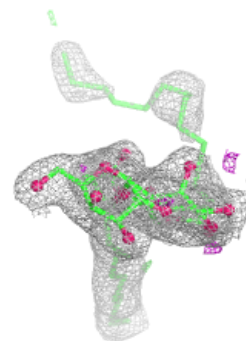
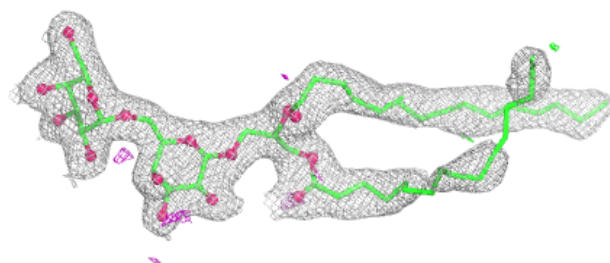
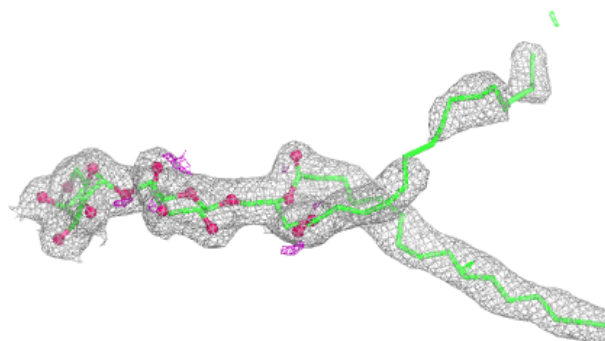


Electron density around BCR B 617:

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

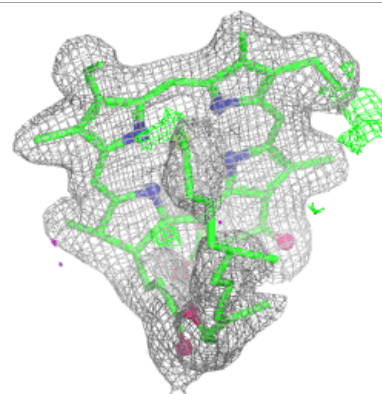
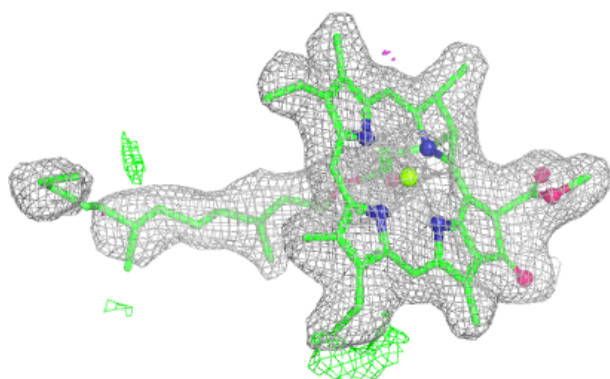
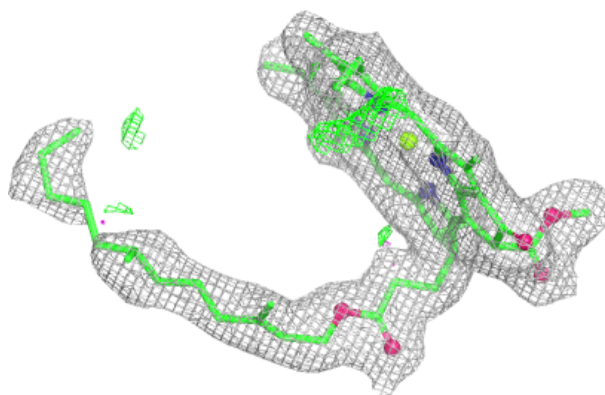
**Electron density around DGD c 519:**

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

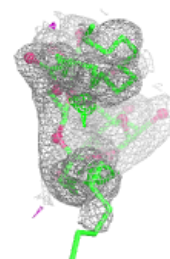
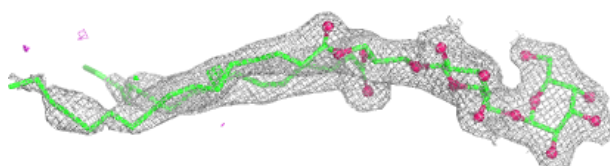
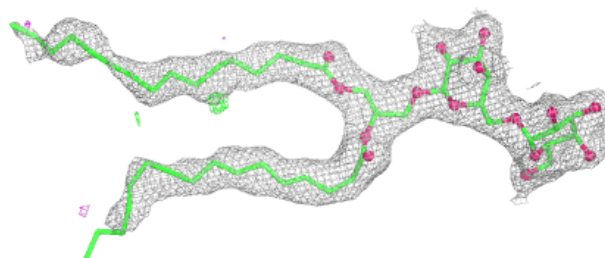


Electron density around CLA C 504:

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

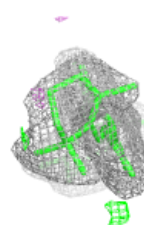
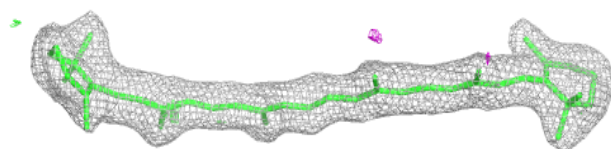
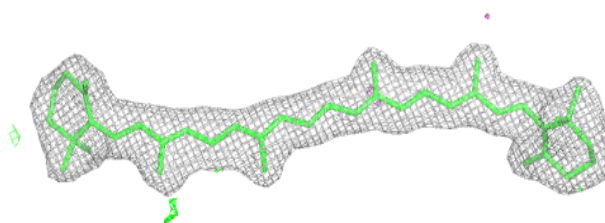
**Electron density around DGD c 521:**

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

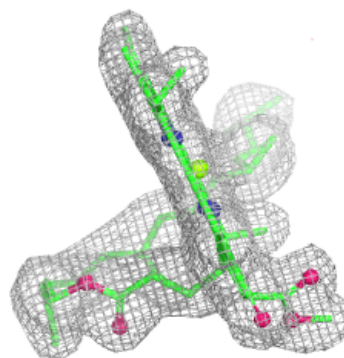
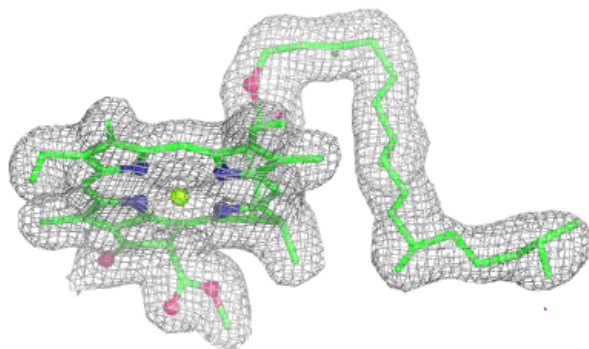
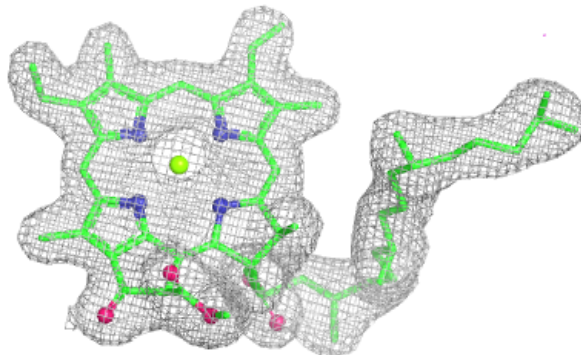


Electron density around BCR B 619:

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

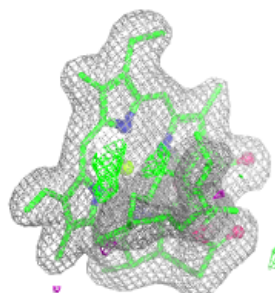
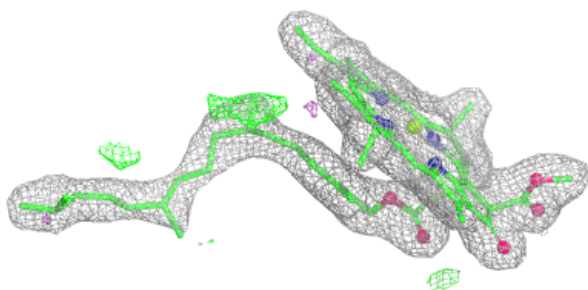
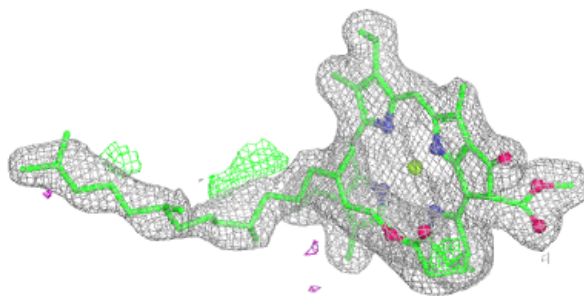
**Electron density around CLA a 612:**

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

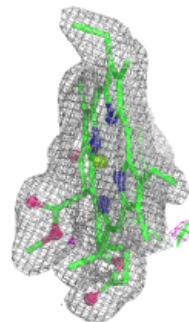
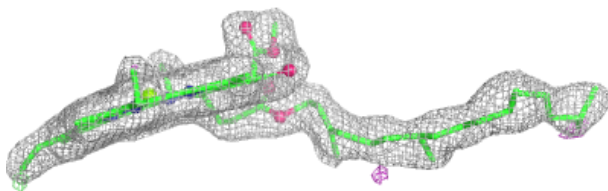
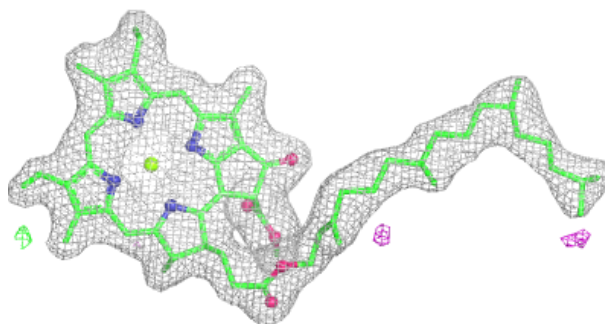


Electron density around CLA C 505:

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

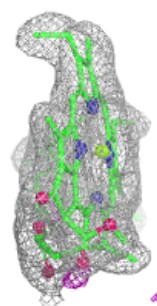
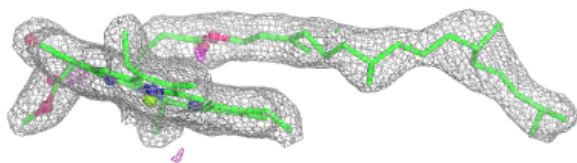
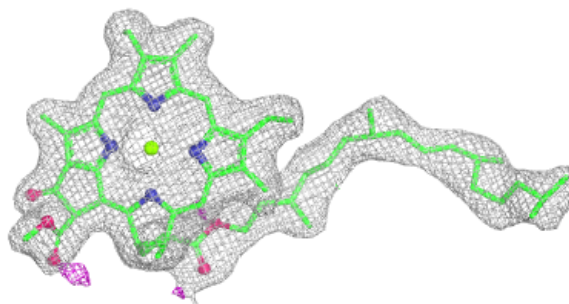
**Electron density around CLA b 602:**

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

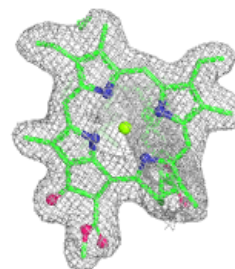
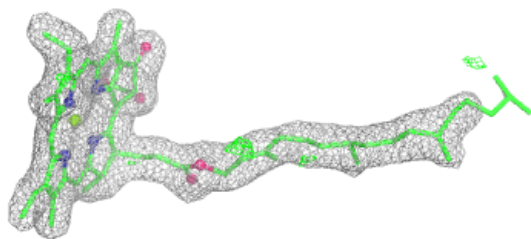
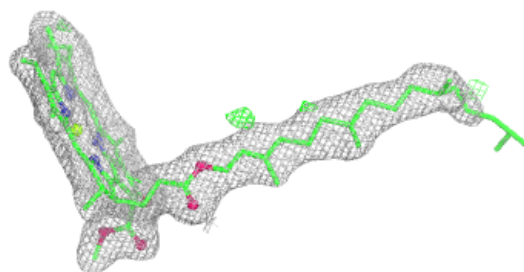


Electron density around CLA b 603:

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

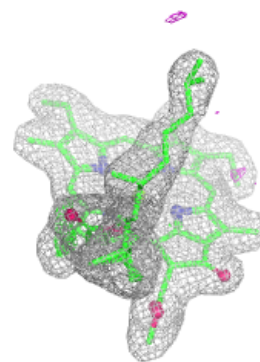
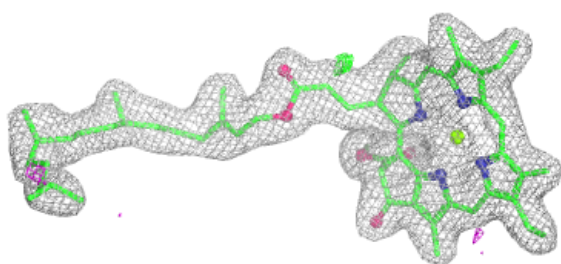
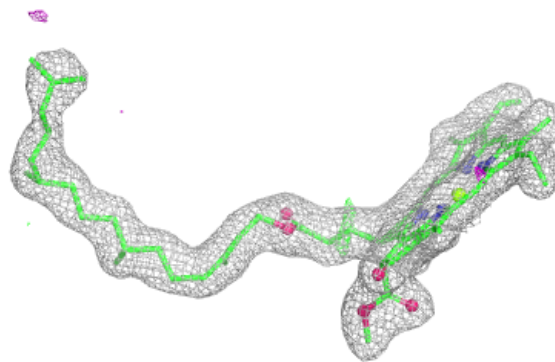
**Electron density around CLA b 604:**

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

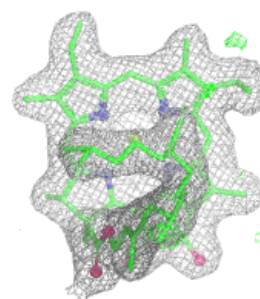
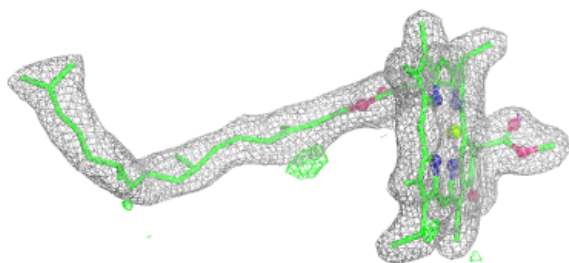
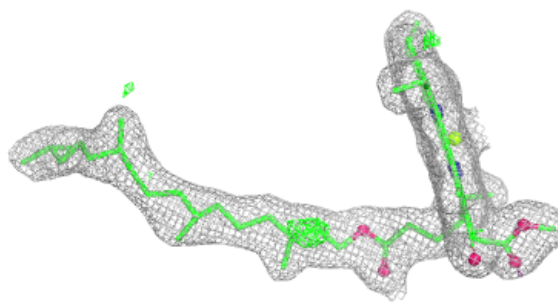


Electron density around CLA d 402:

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

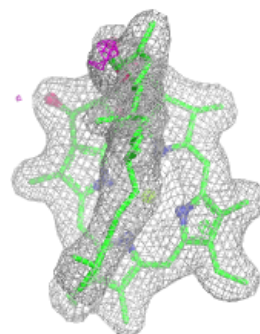
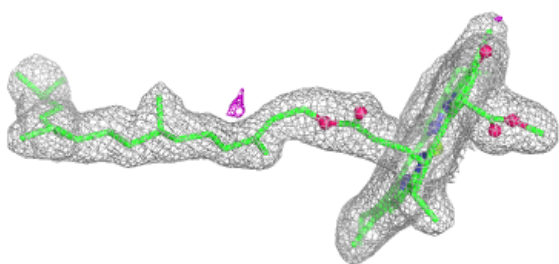
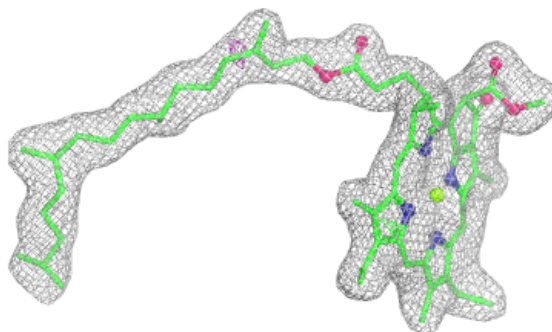
**Electron density around CLA b 605:**

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

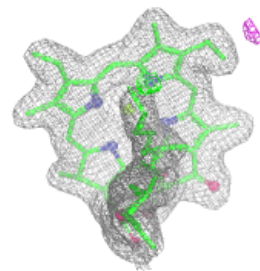
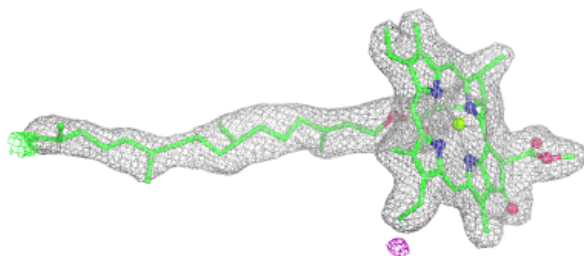
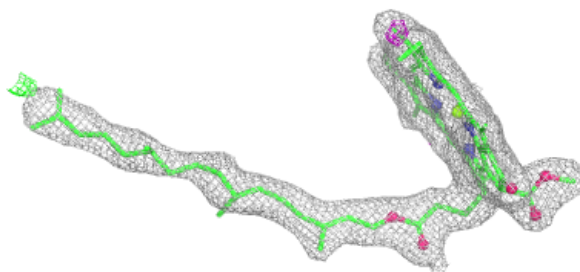


Electron density around CLA B 609:

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

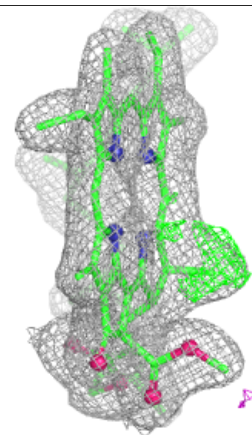
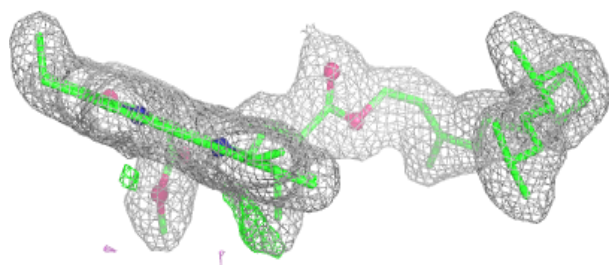
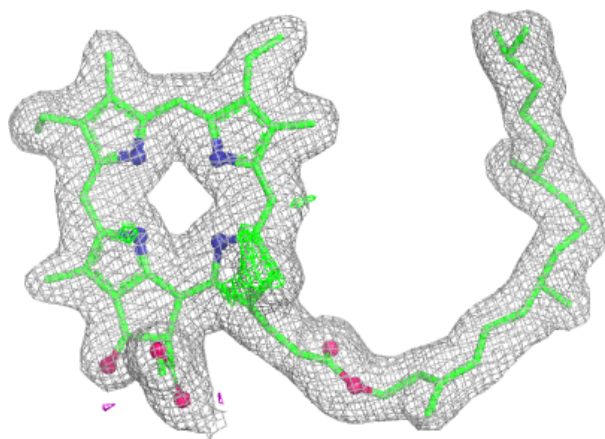
**Electron density around CLA b 607:**

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



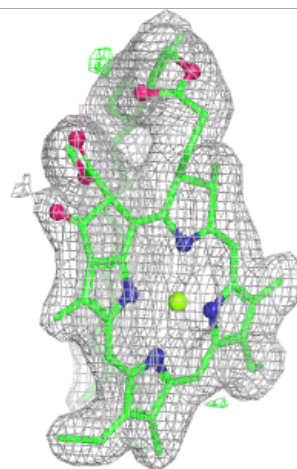
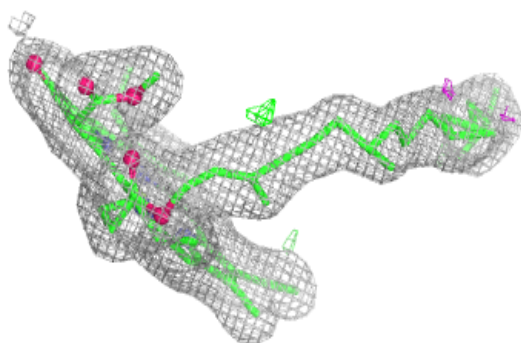
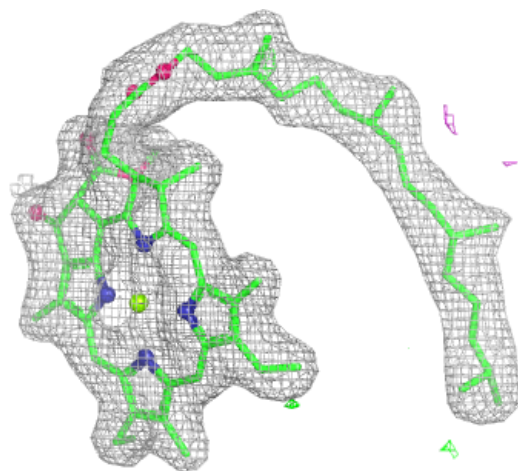
Electron density around PHO a 608:

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



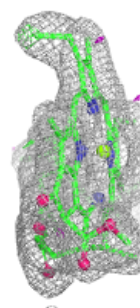
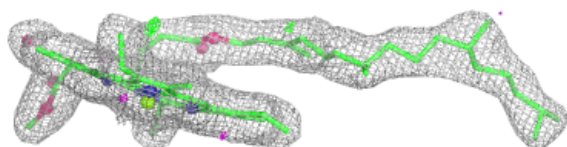
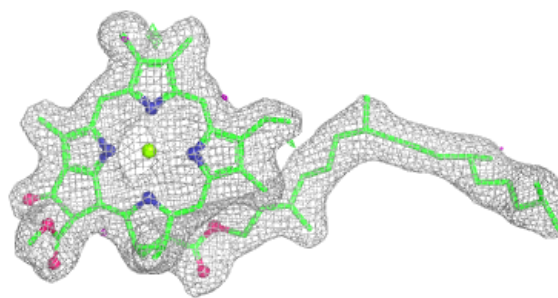
Electron density around CLA C 507:

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



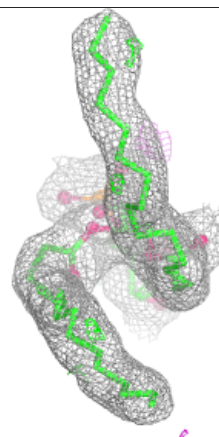
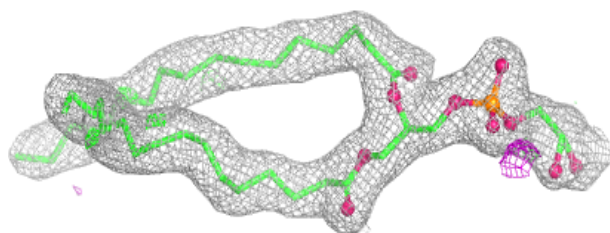
Electron density around CLA B 603:

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



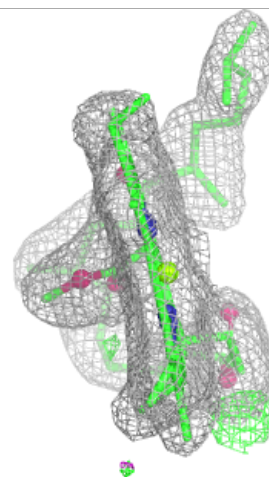
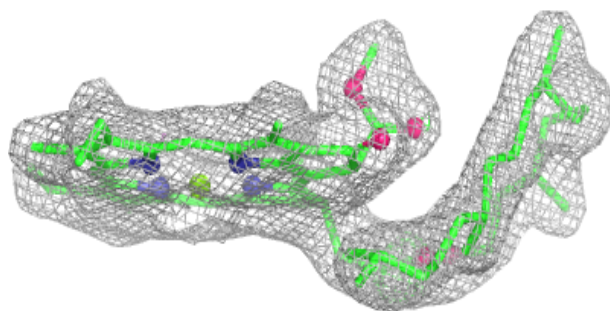
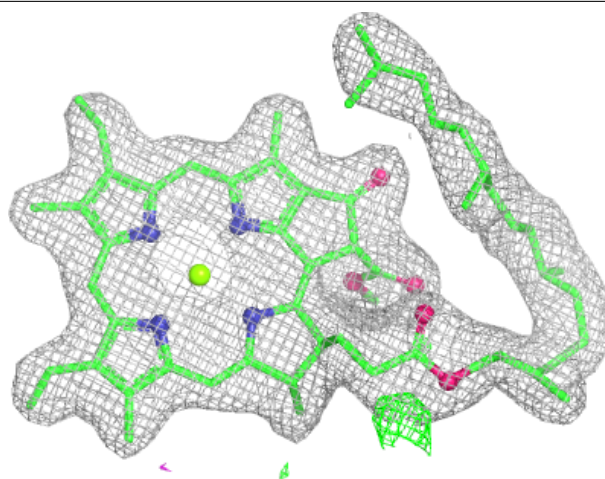
Electron density around LHG D 408:

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



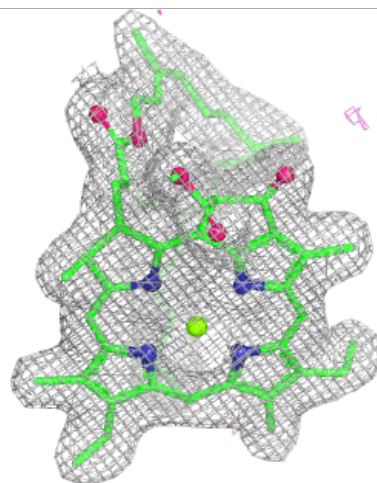
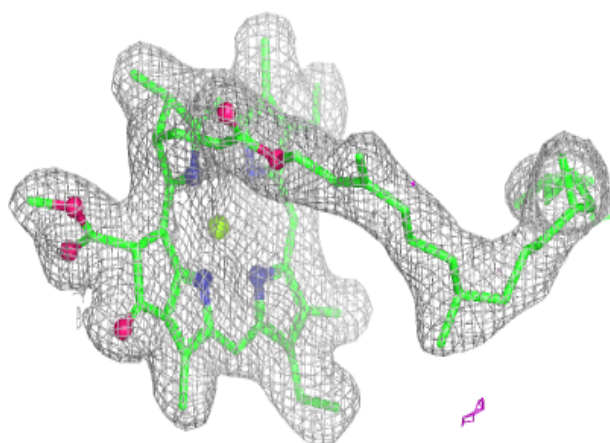
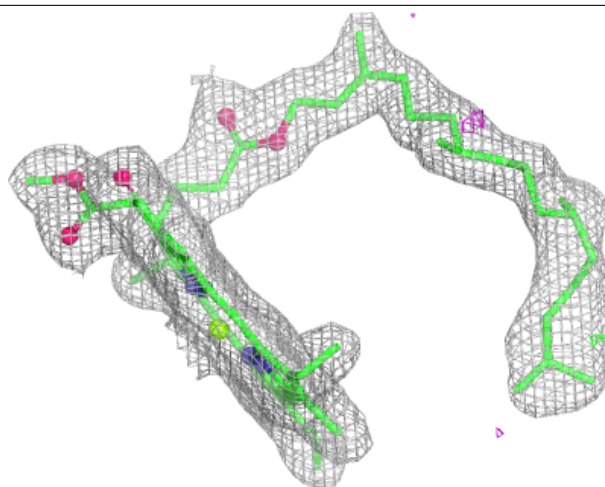
Electron density around CLA b 610:

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



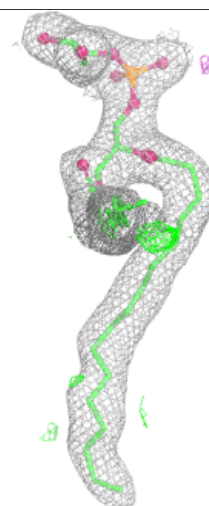
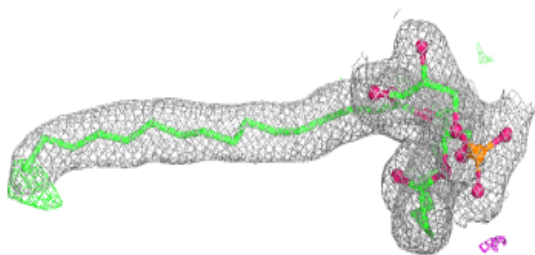
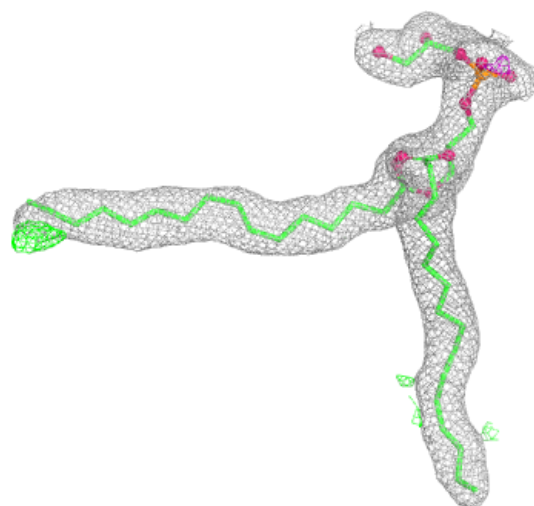
Electron density around CLA b 611:

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



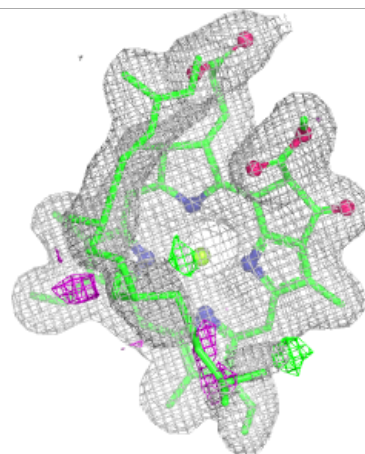
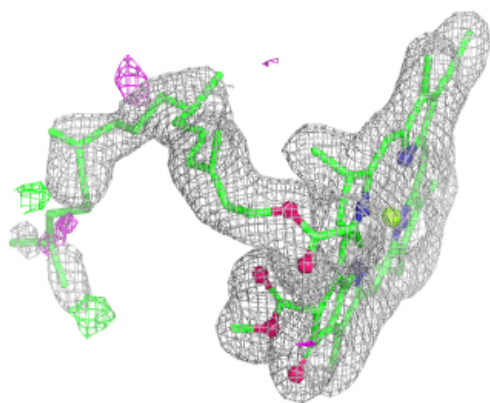
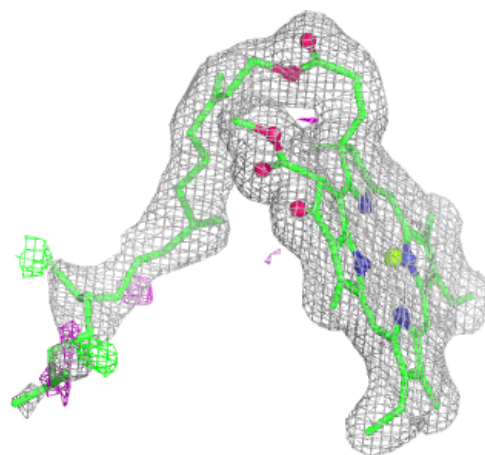
Electron density around LHG L 101:

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



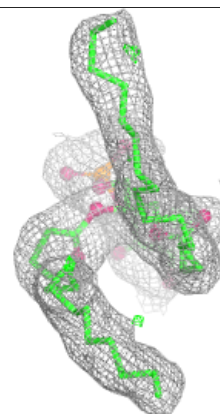
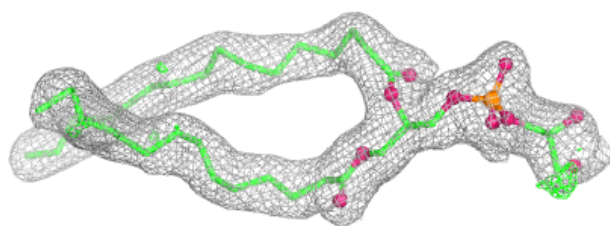
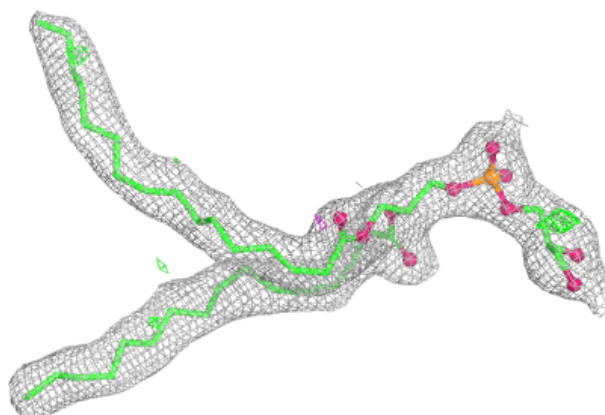
Electron density around CLA b 613:

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



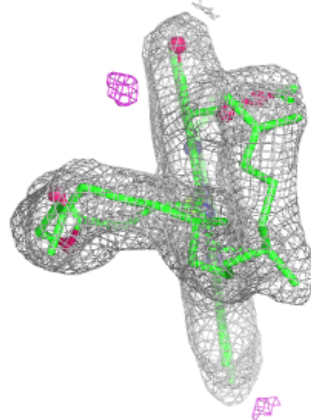
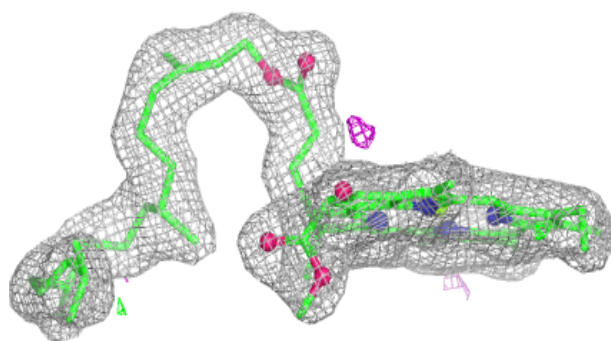
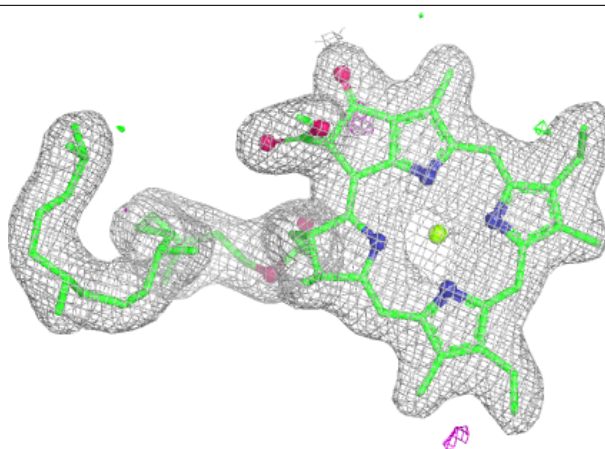
Electron density around LHG d 407:

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

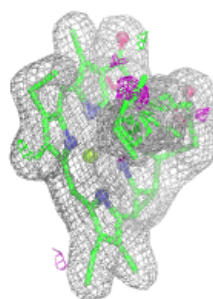
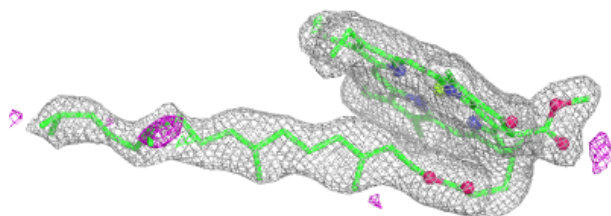
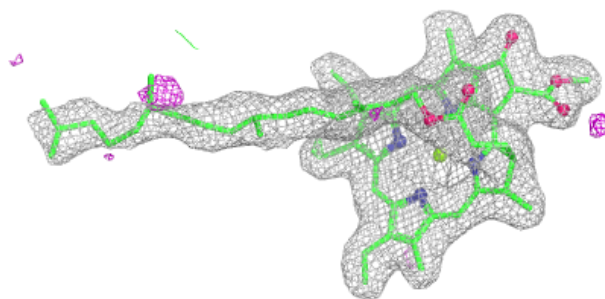


Electron density around CLA B 612:

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

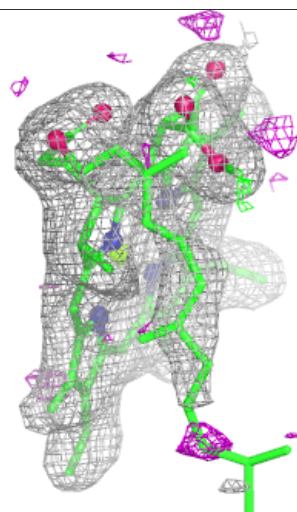
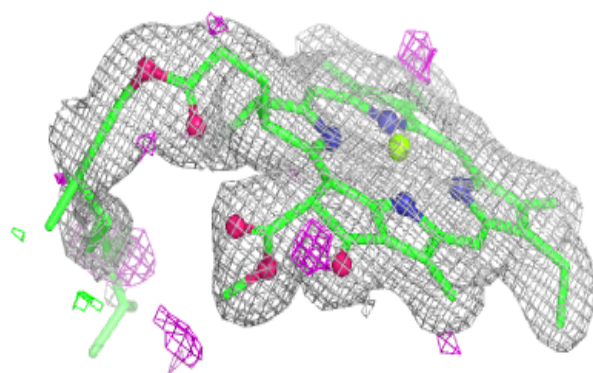
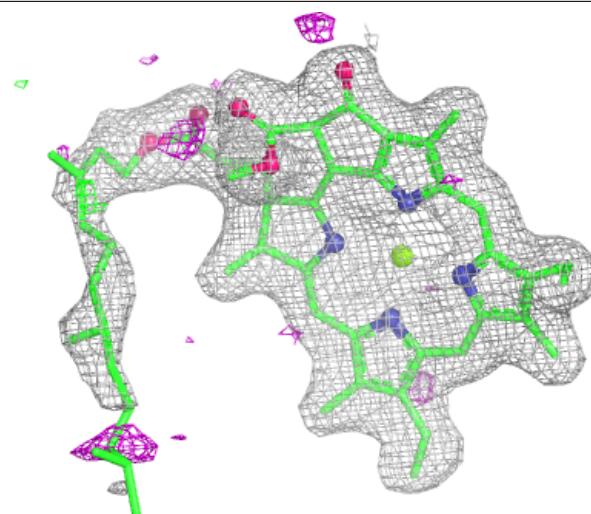
**Electron density around CLA B 614:**

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



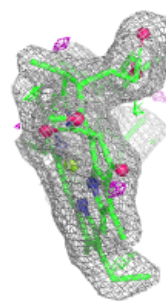
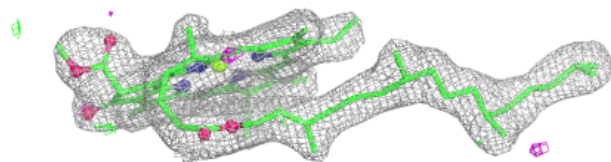
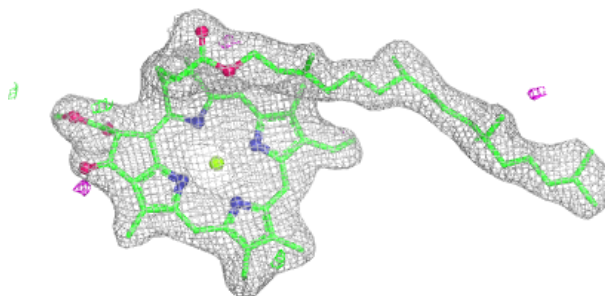
Electron density around CLA B 616:

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

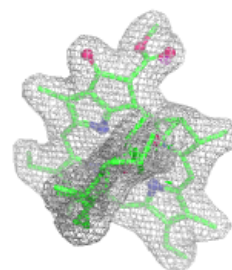
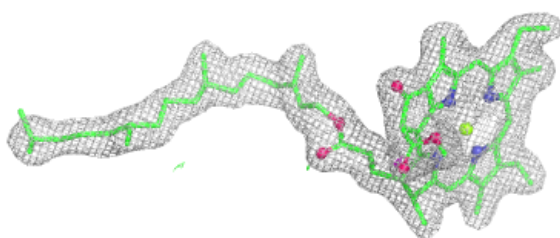
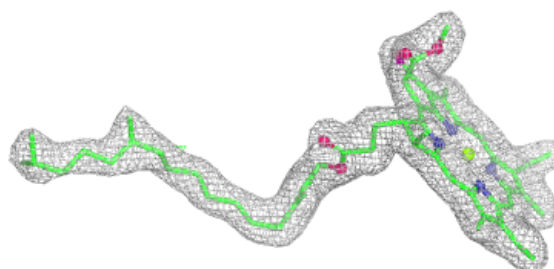


Electron density around CLA c 501:

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

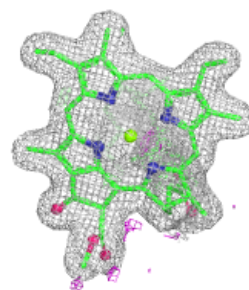
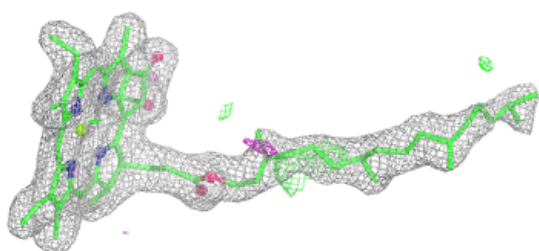
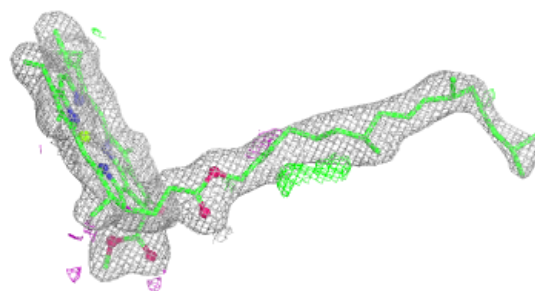
**Electron density around CLA c 502:**

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

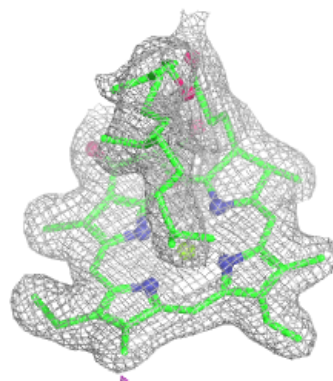
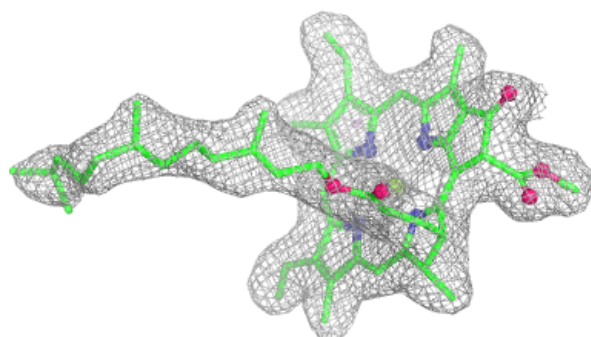
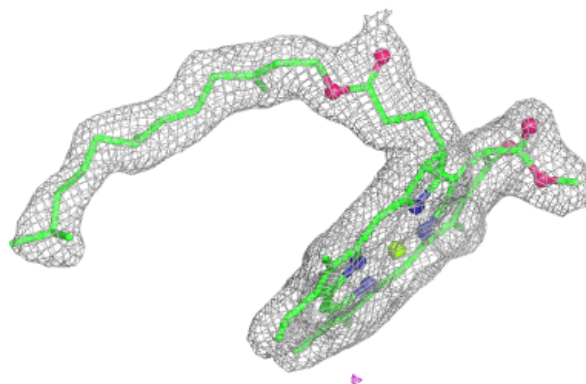


Electron density around CLA B 604:

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

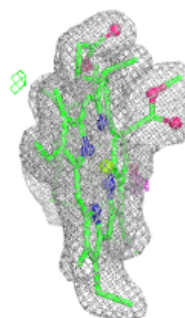
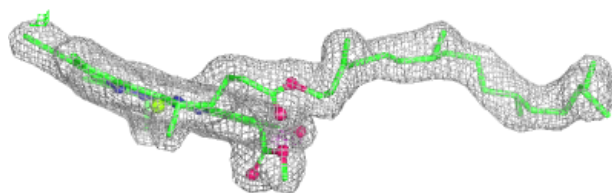
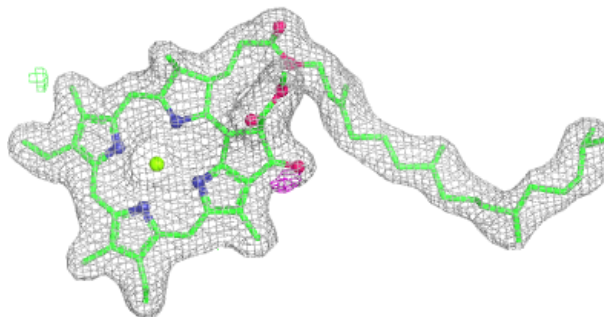
**Electron density around CLA c 504:**

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

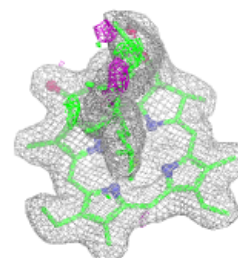
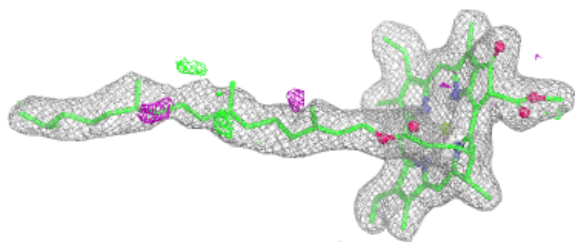
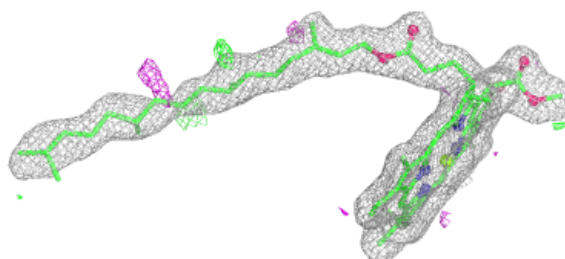


Electron density around CLA B 602:

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

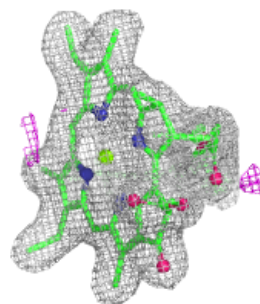
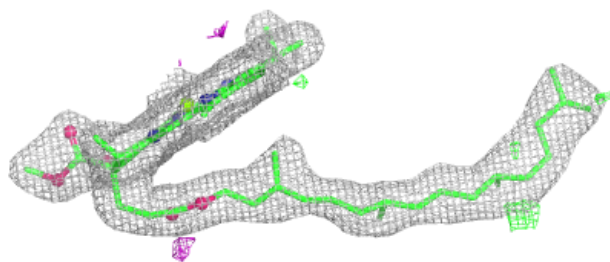
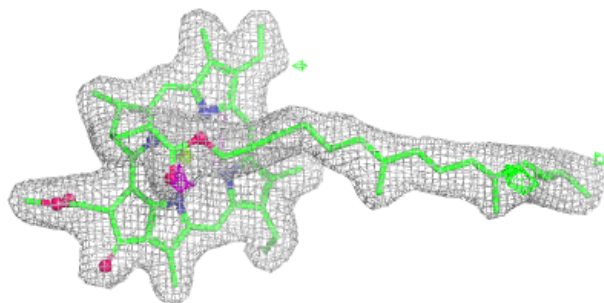
**Electron density around CLA B 607:**

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

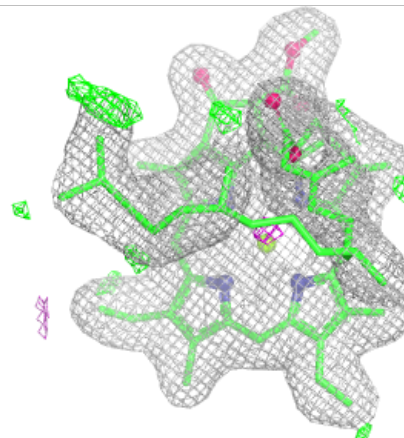
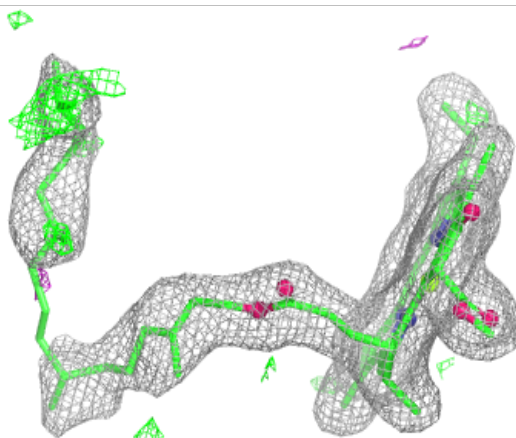
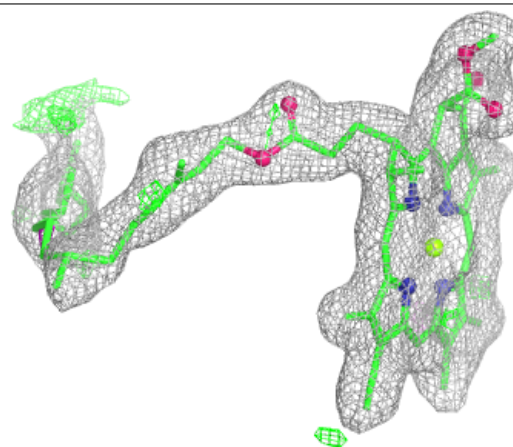


Electron density around CLA B 608:

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

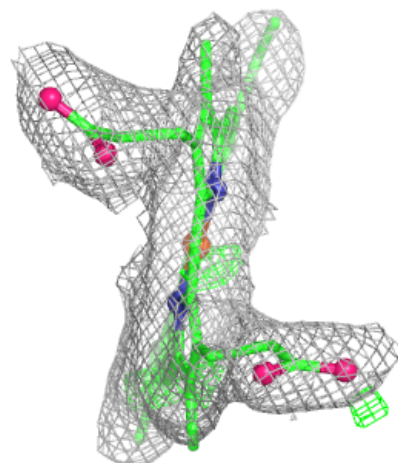
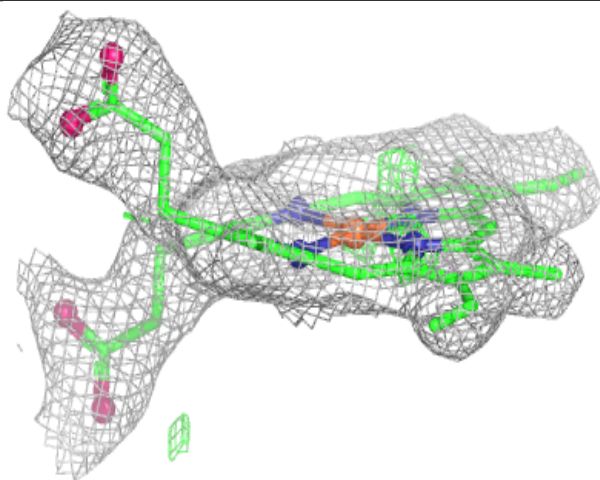
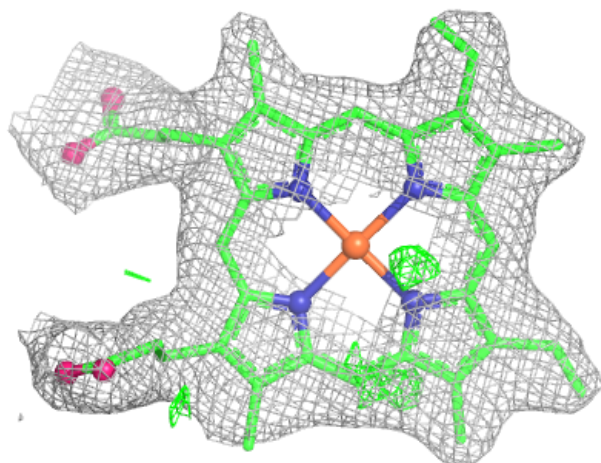
**Electron density around CLA a 609:**

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



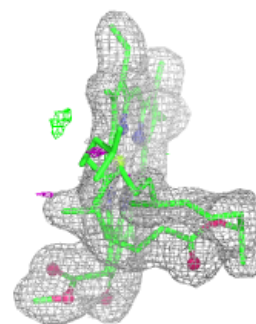
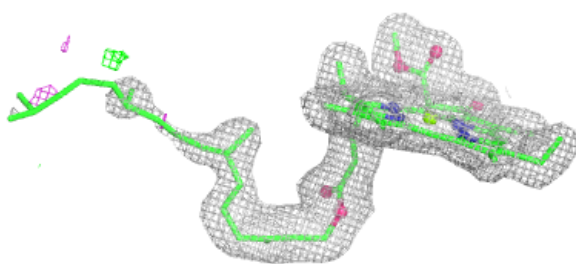
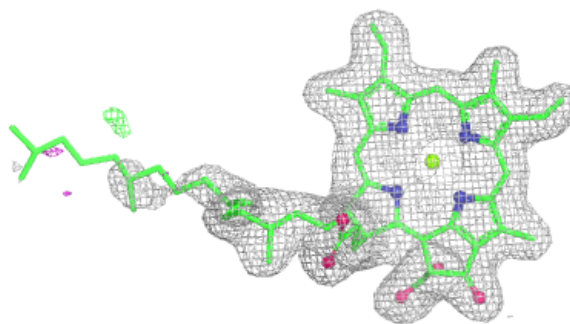
Electron density around HEM F 101:

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

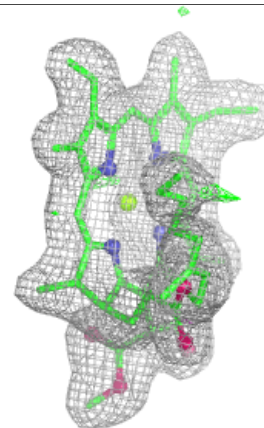
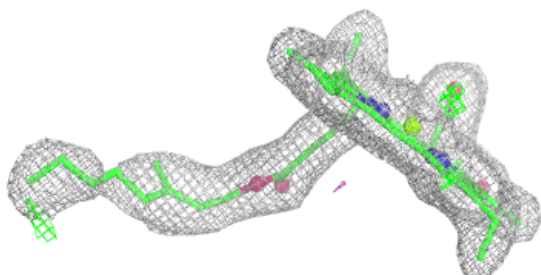
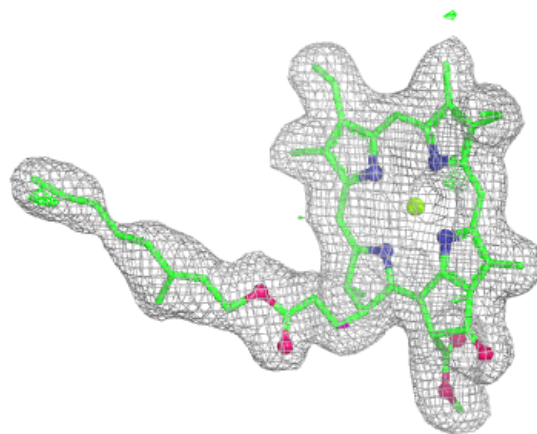


Electron density around CLA A 607:

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

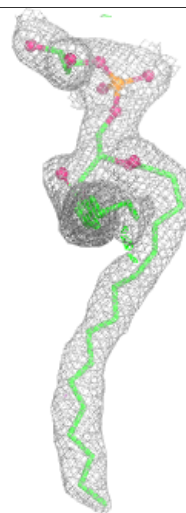
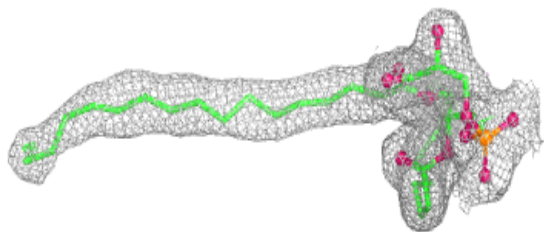
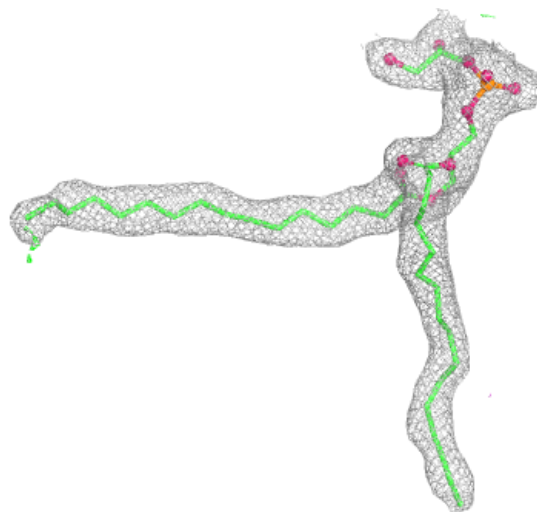
**Electron density around CLA A 610:**

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



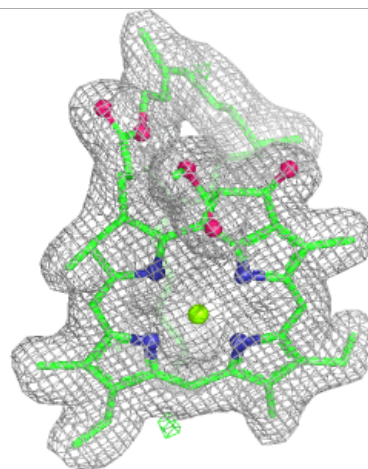
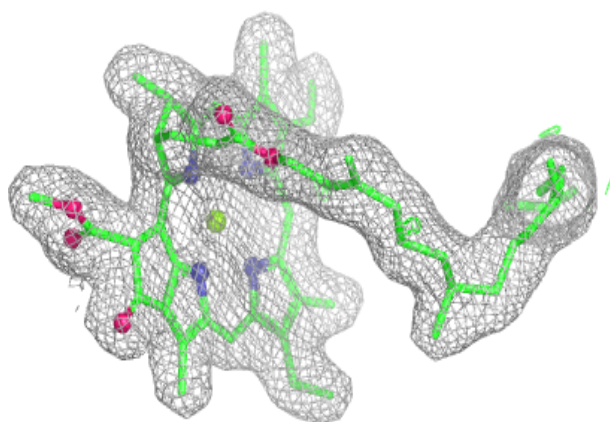
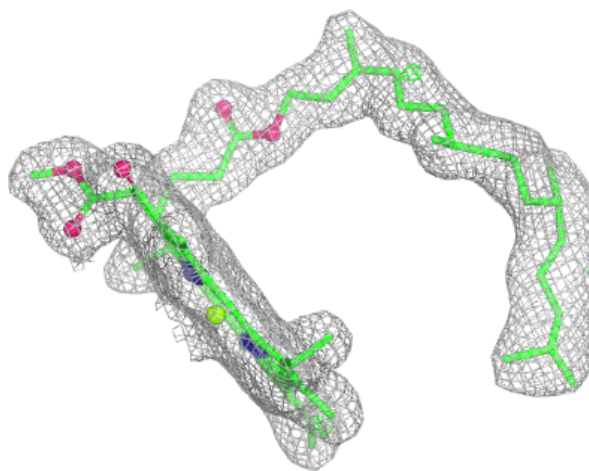
Electron density around LHG 1 101:

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



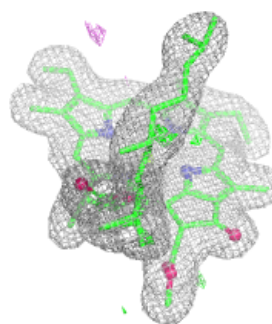
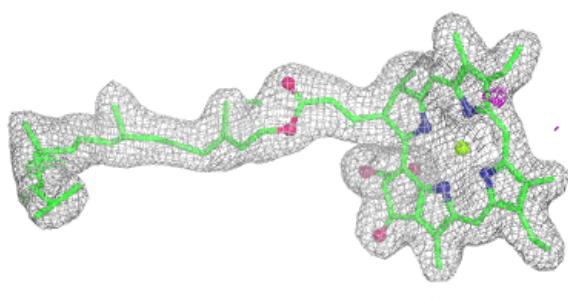
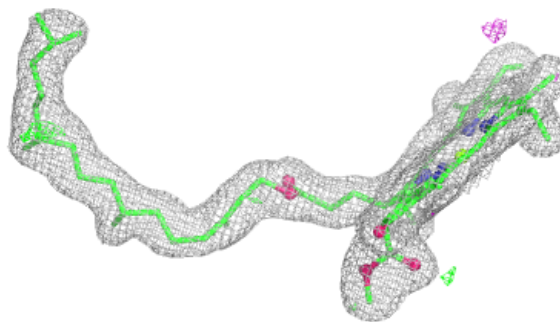
Electron density around CLA B 611:

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

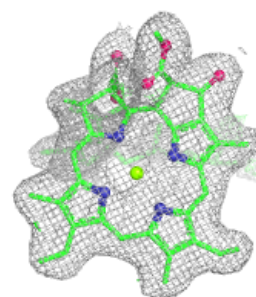
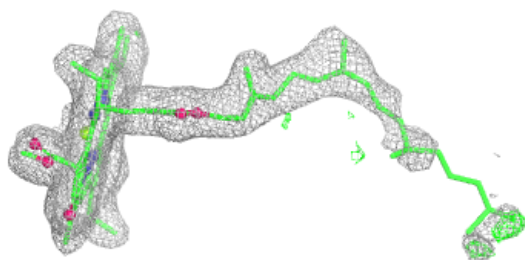
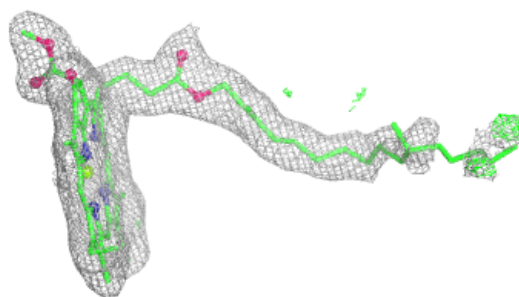


Electron density around CLA D 401:

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

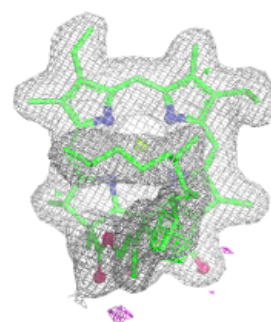
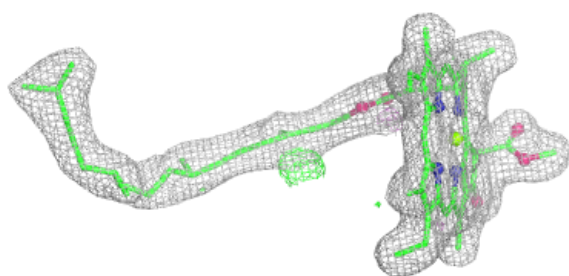
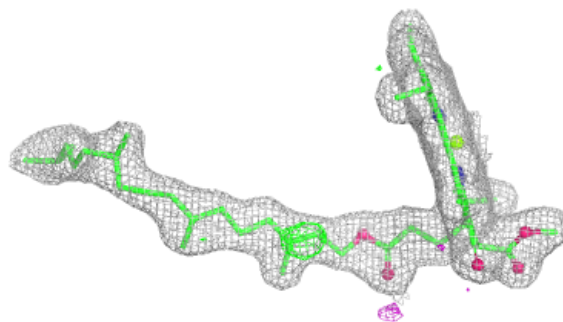
**Electron density around CLA D 402:**

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



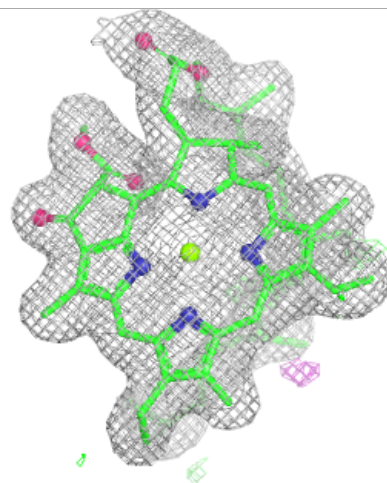
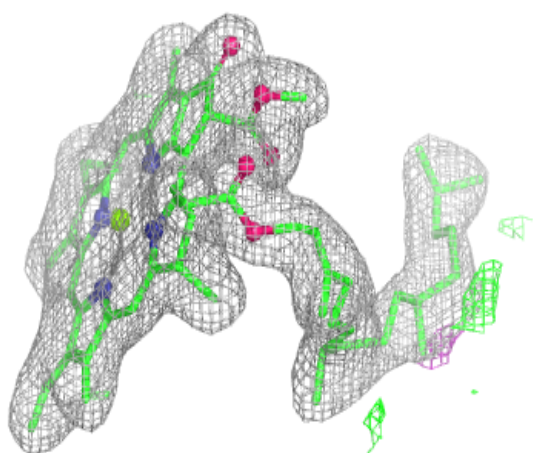
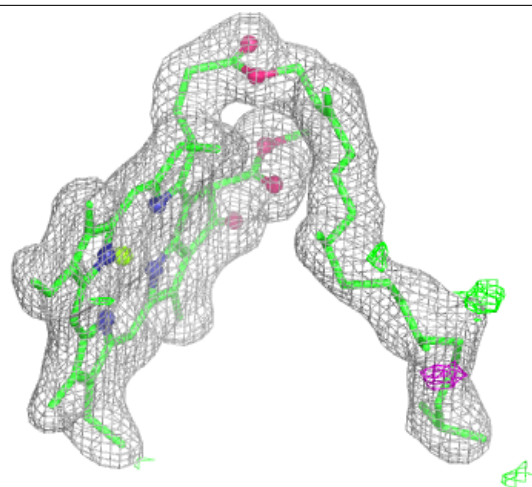
Electron density around CLA B 605:

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



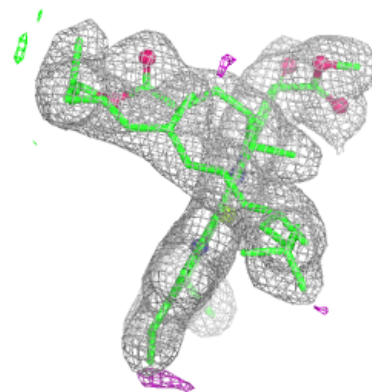
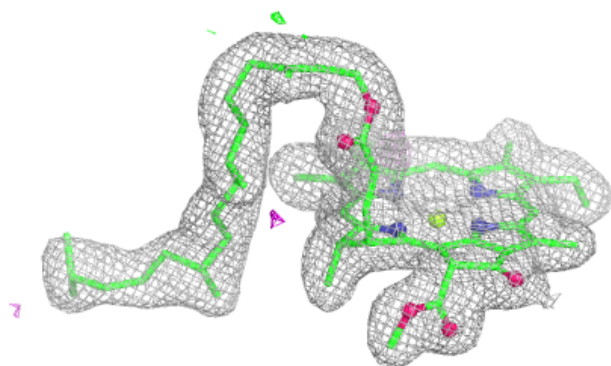
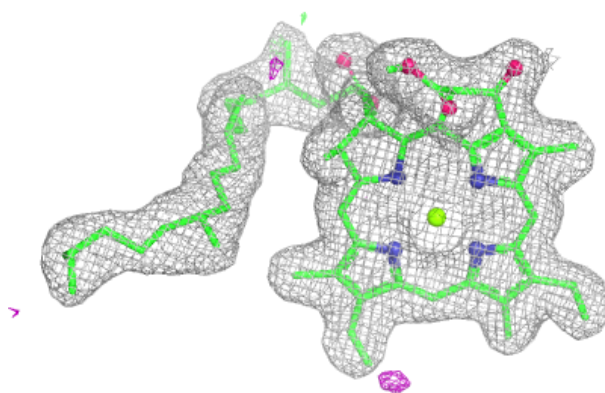
Electron density around CLA B 613:

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



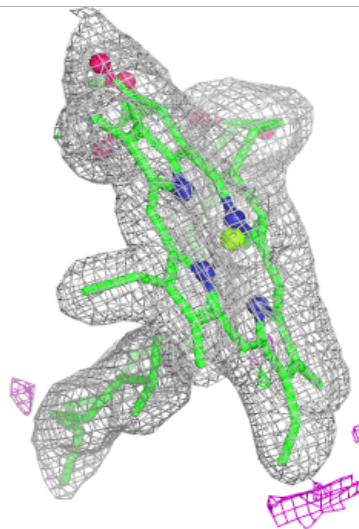
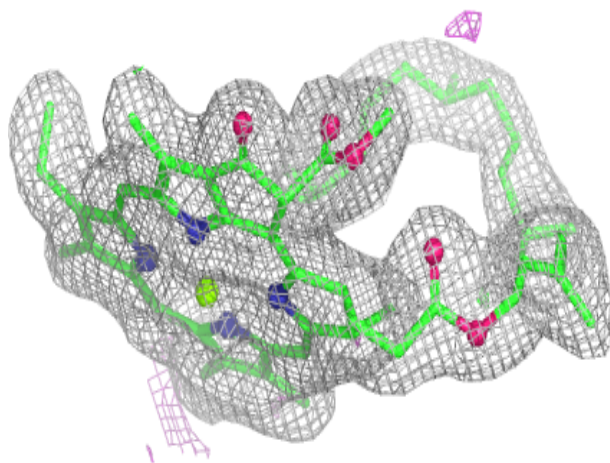
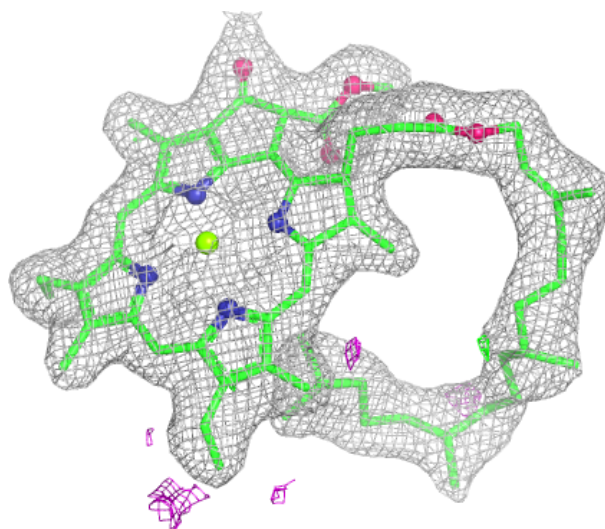
Electron density around CLA A 614:

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



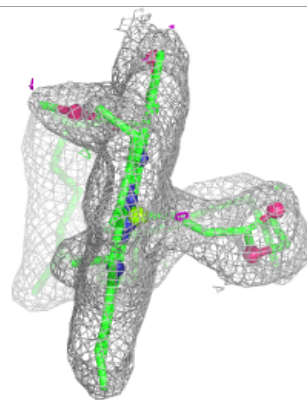
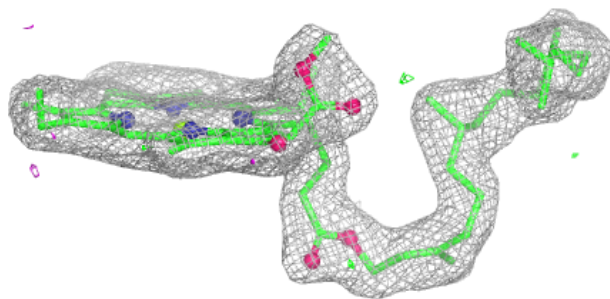
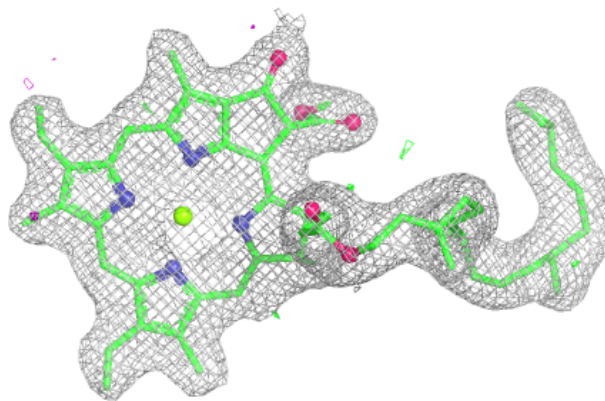
Electron density around CLA B 615:

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

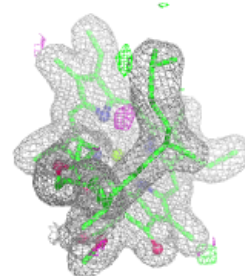
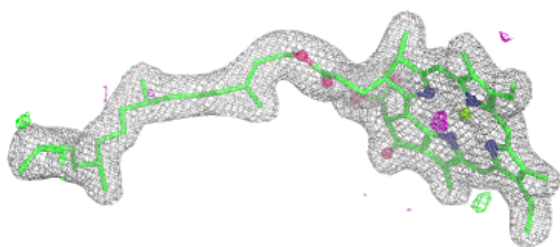
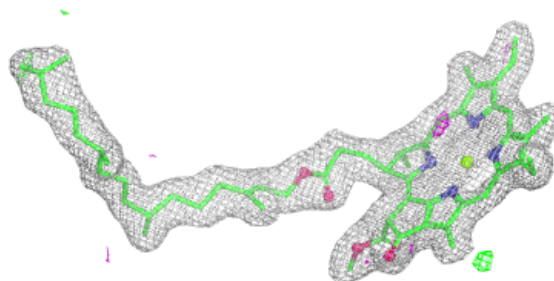


Electron density around CLA b 612:

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

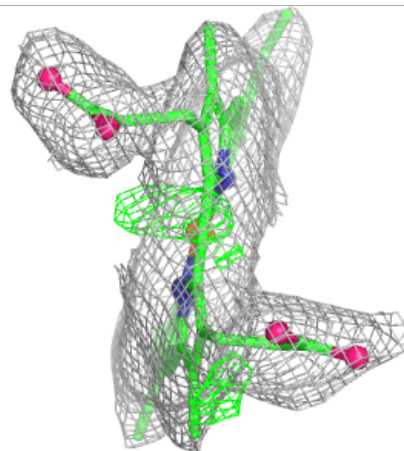
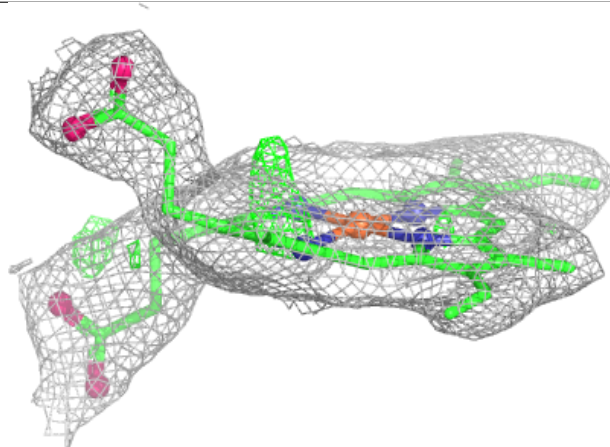
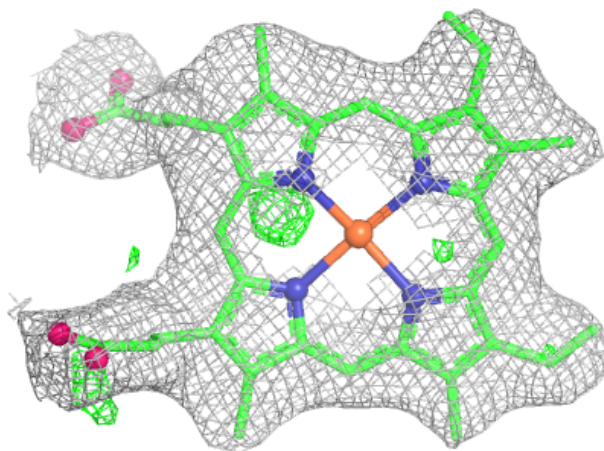
**Electron density around CLA A 606:**

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



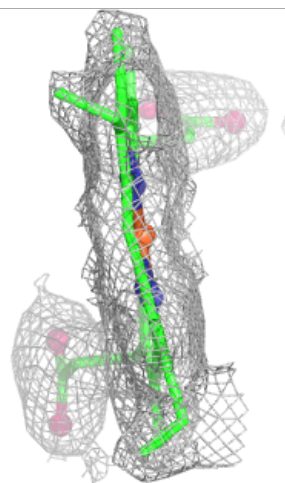
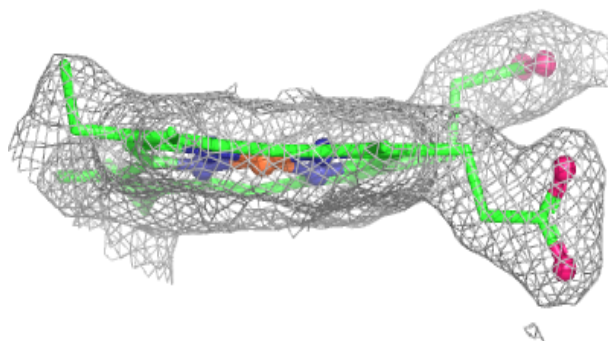
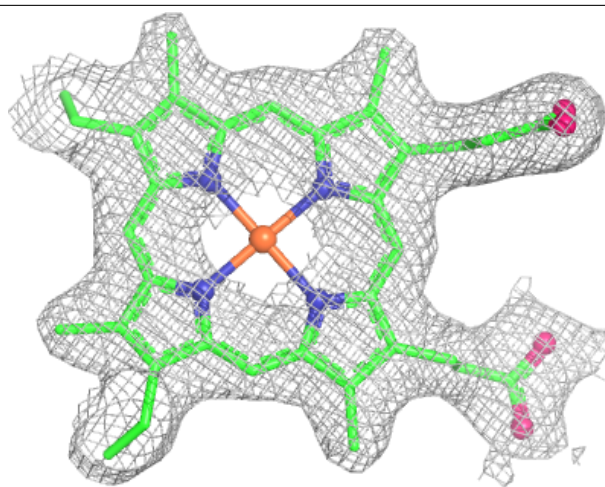
Electron density around HEM f 101:

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



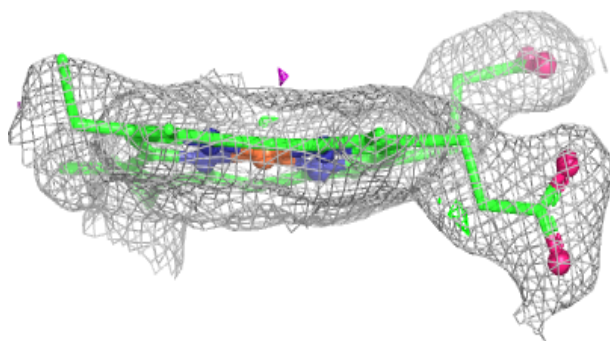
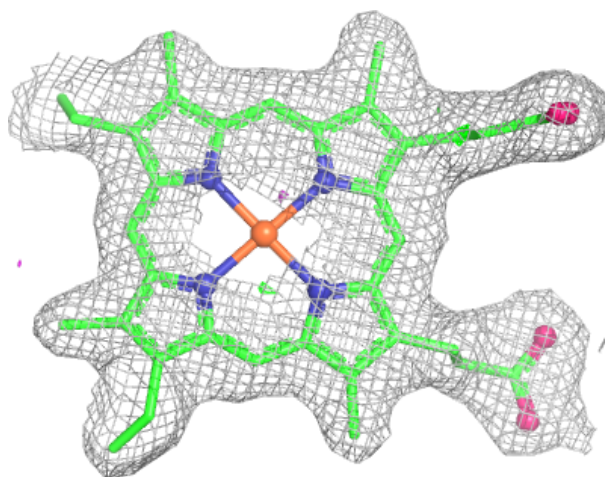
Electron density around HEC V 201:

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



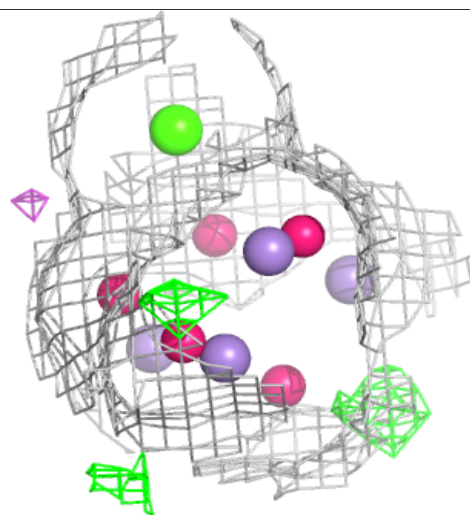
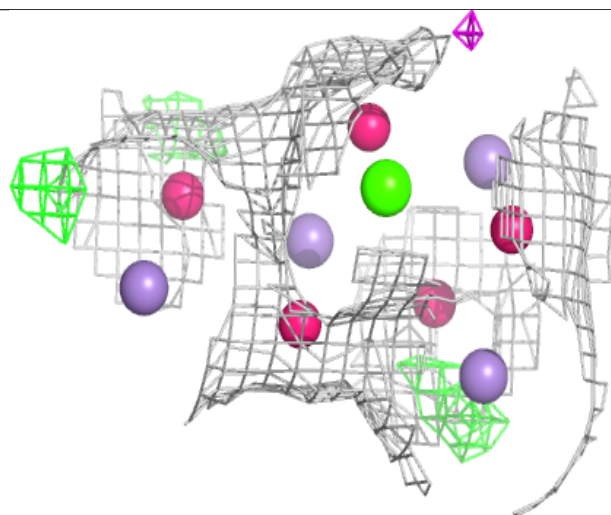
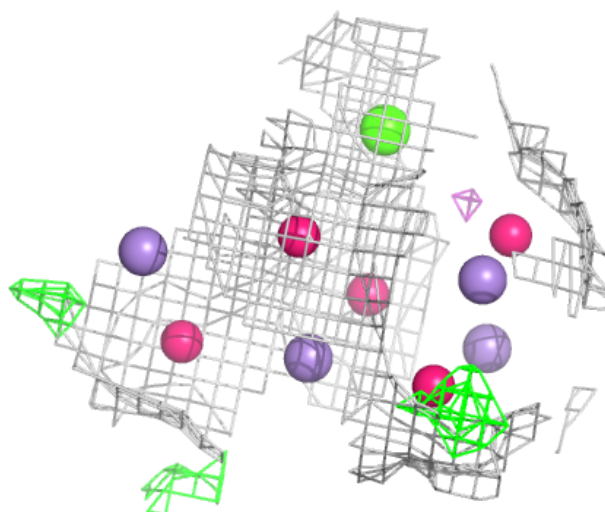
Electron density around HEC v 201:

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



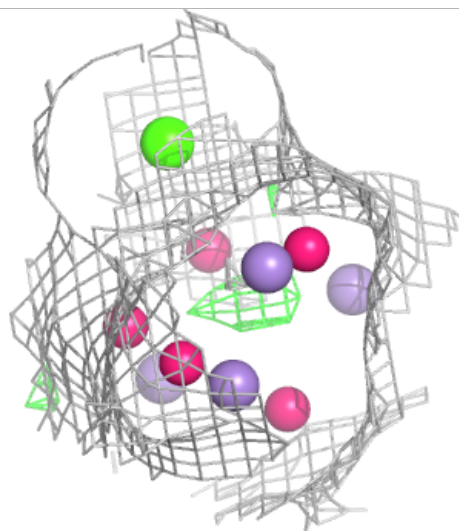
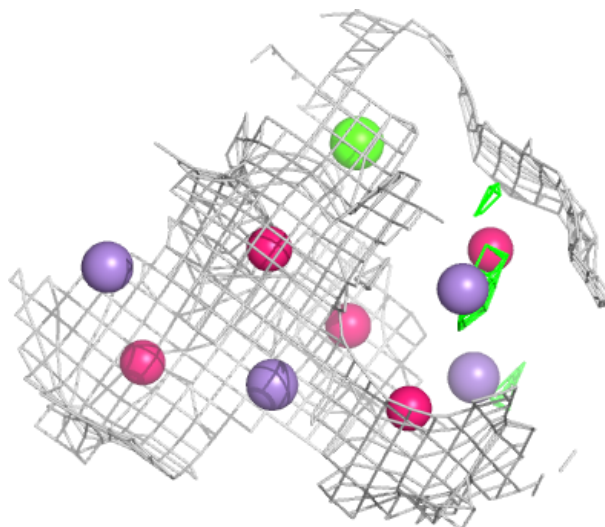
Electron density around OEX a 601:

$2mF_o-DF_c$ (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.