



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 02:54 PM EDT

PDB ID : 9Z36 / pdb_00009z36
Title : RT XFEL structure of dark-stable state of Photosystem II (0F, S1 rich) at 2.16 Angstrom obtained from anomalous data at 7 keV
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Minnetian, N.; Zhang, M.
Deposited on : 2025-11-05
Resolution : 2.16 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

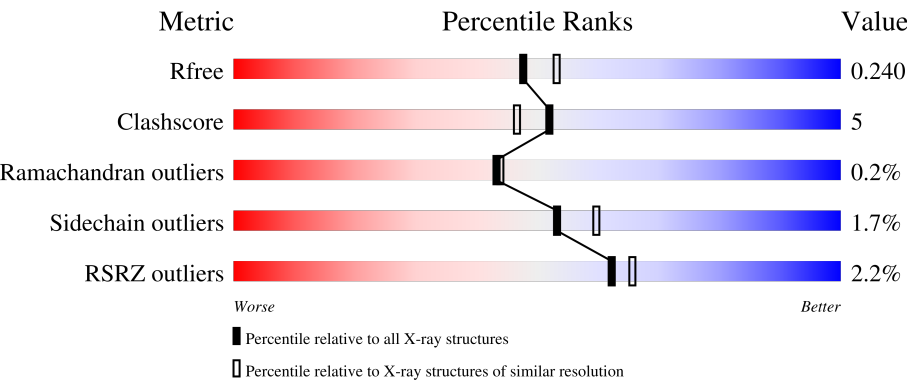
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.16 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.



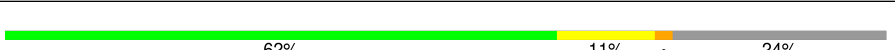
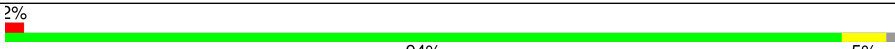
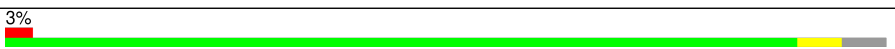
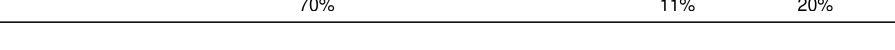
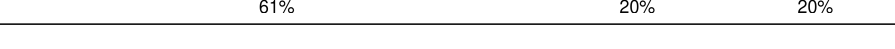
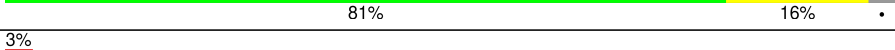
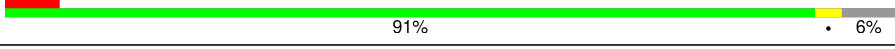
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	% 91%6%
1	a	344	% 89%8%
2	B	510	% 88%11%
2	b	510	2% 92%7%

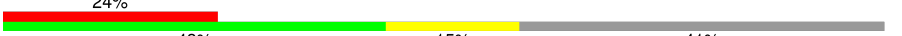
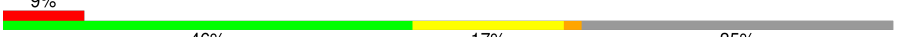
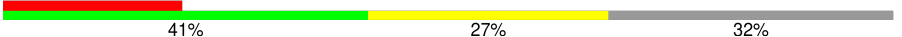
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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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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 52923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

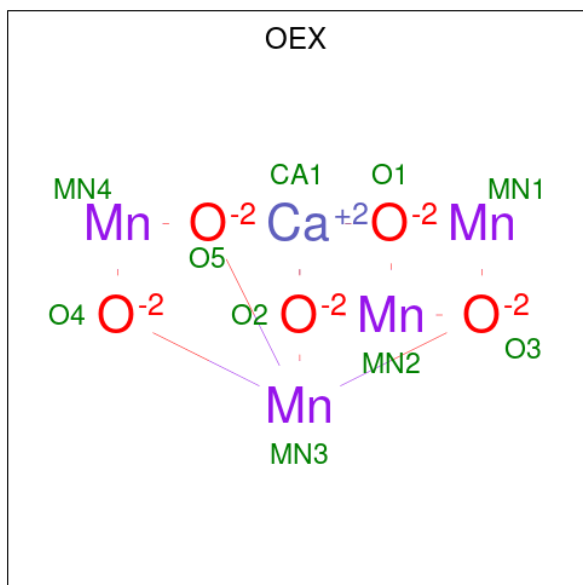
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	28	Total	C	N	O	0	0	0
			221	151	38	32			

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

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



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

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

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

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

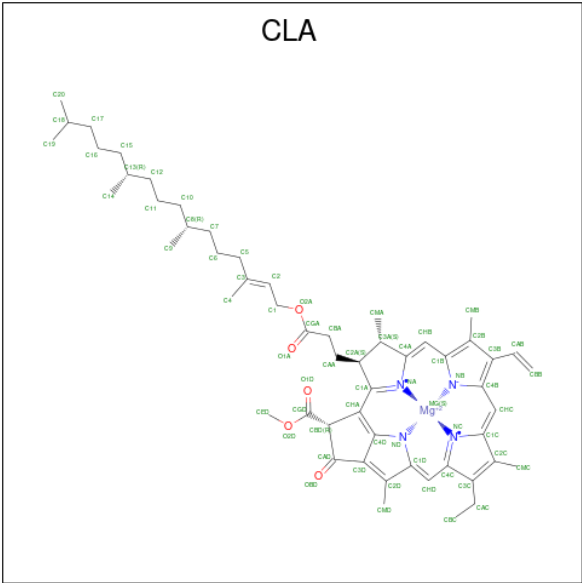
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		

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

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



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

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

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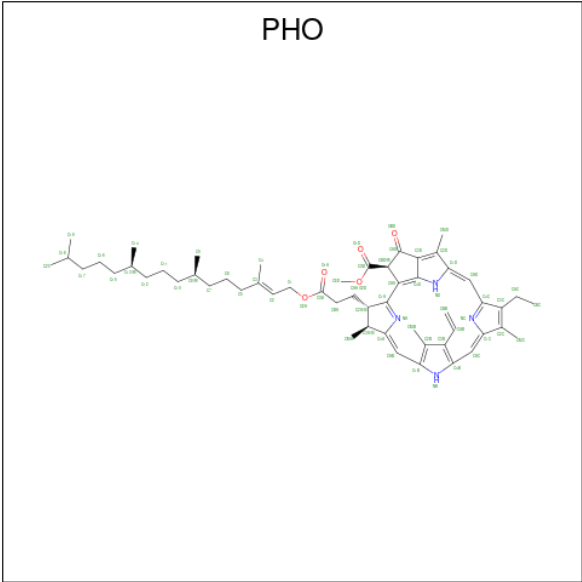
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total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

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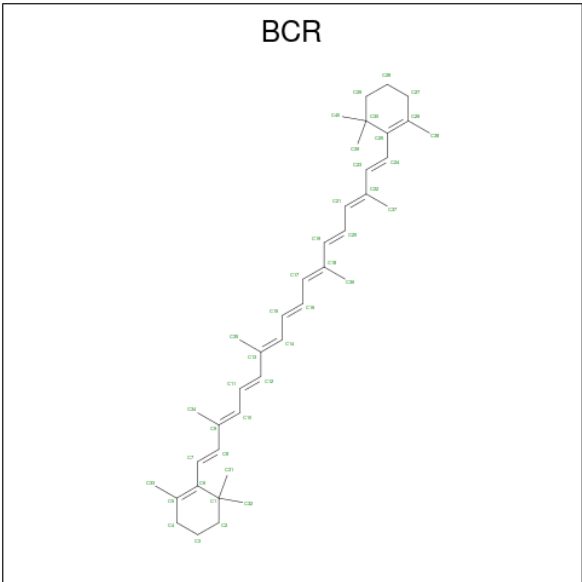
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5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

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



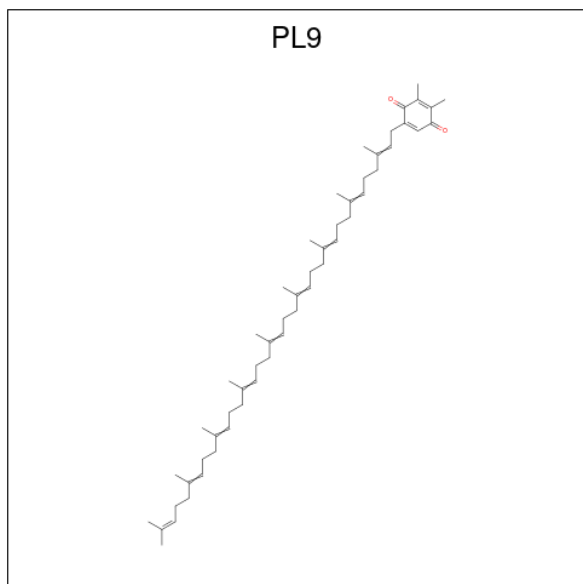
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



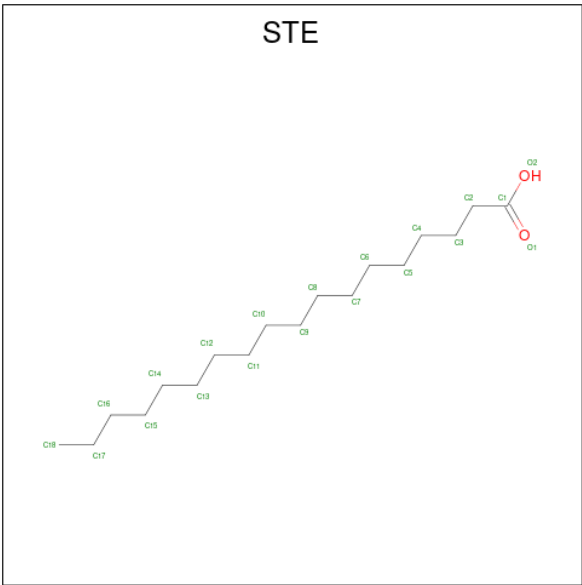
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	J	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

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



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

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



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

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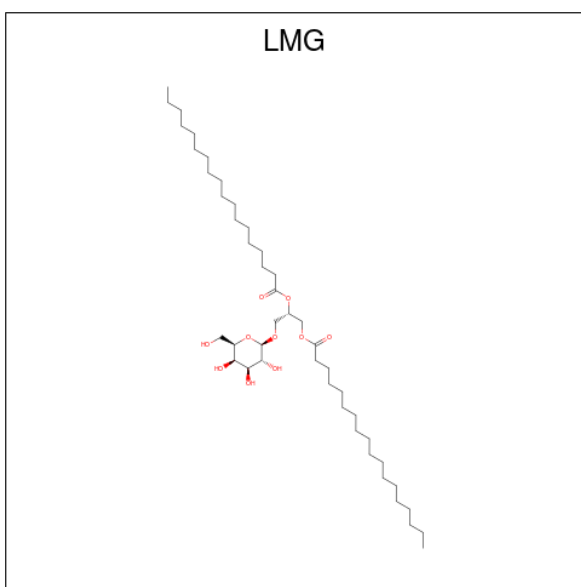
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C 16 16	0	0
28	C	1	Total C 14 14	0	0
28	C	1	Total C 14 14	0	0
28	E	1	Total C O 12 10 2	0	0
28	E	1	Total C 12 12	0	0
28	E	1	Total C O 20 18 2	0	0
28	H	1	Total C 18 18	0	0
28	H	1	Total C 9 9	0	0
28	I	1	Total C O 17 15 2	0	0
28	I	1	Total C O 15 13 2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

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



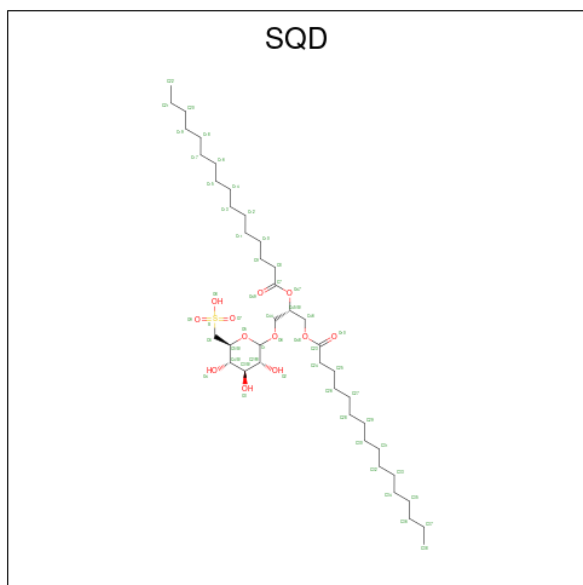
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			45	35	10		
29	B	1	Total	C	O	0	0
			55	45	10		
29	C	1	Total	C	O	0	0
			36	26	10		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			50	40	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	M	1	Total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

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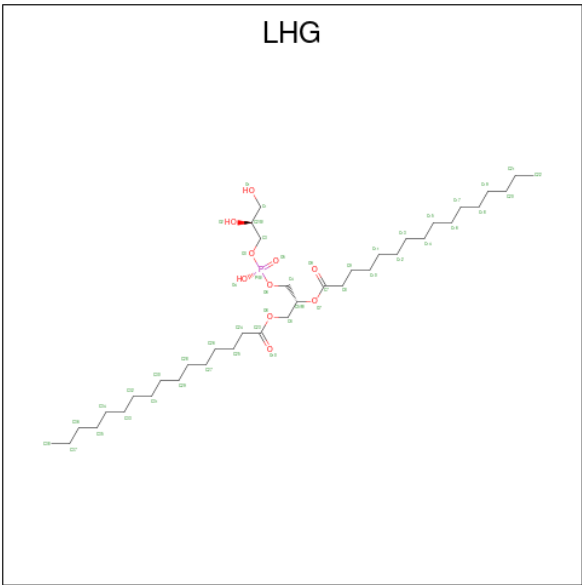
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			51	41	10		

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



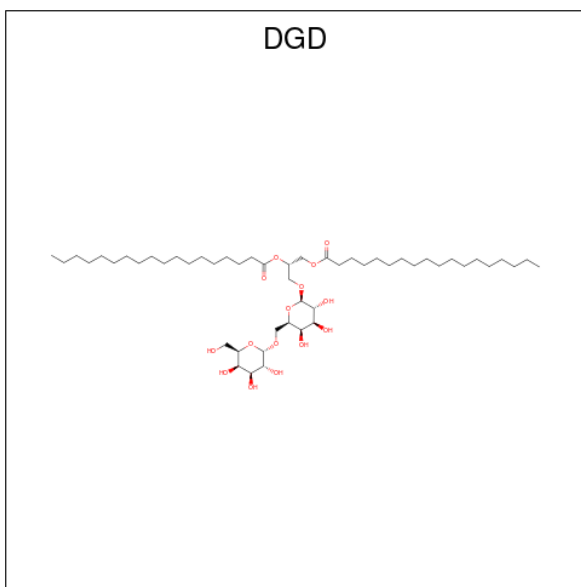
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	b	1	Total	C	O	S	0	0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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



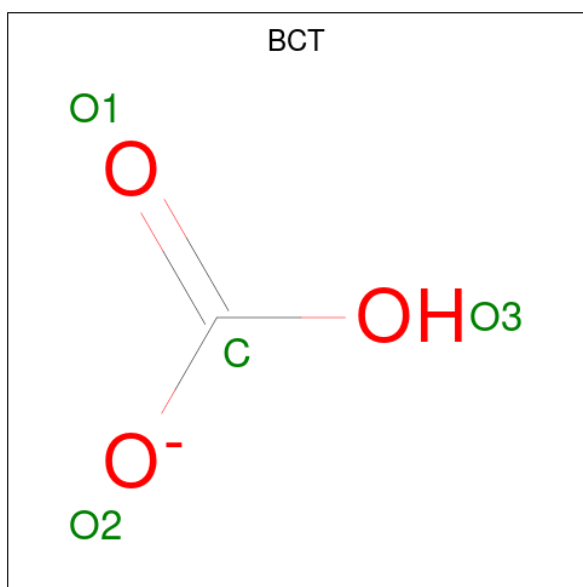
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	B	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			47	36	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



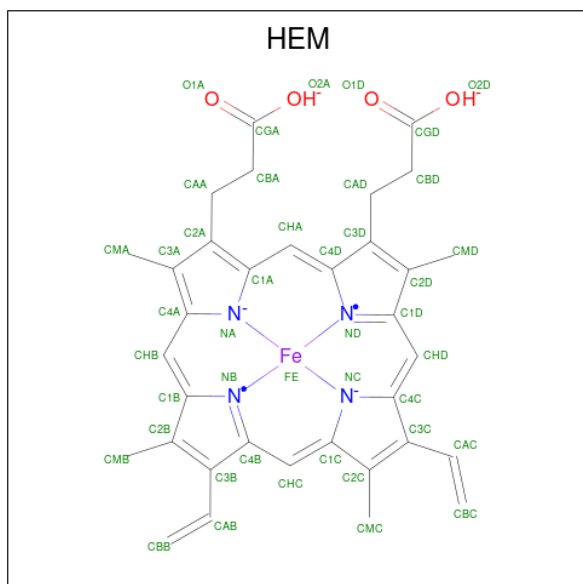
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			66	51	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	H	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total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

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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



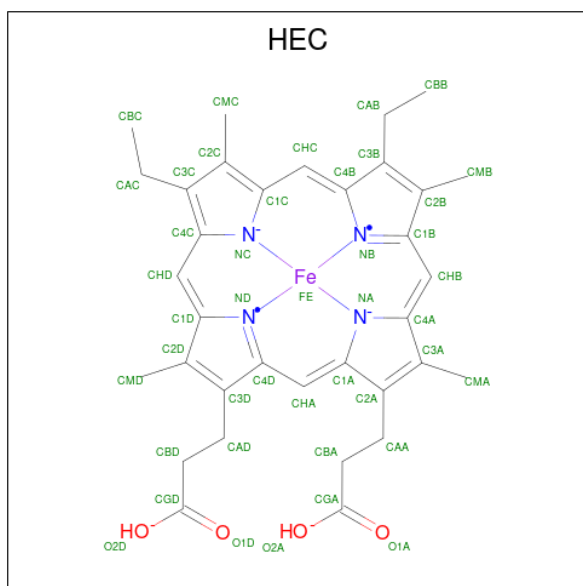
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	165	Total	O	0	0
			165	165		
36	B	266	Total	O	0	0
			266	266		
36	C	223	Total	O	0	0
			223	223		
36	D	137	Total	O	0	0
			137	137		
36	E	39	Total	O	0	0
			39	39		
36	F	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	H	33	Total O 33 33	0	0
36	I	20	Total O 20 20	0	0
36	J	19	Total O 19 19	0	0
36	K	7	Total O 7 7	0	0
36	L	8	Total O 8 8	0	0
36	M	13	Total O 13 13	0	0
36	O	124	Total O 124 124	0	0
36	T	10	Total O 10 10	0	0
36	U	46	Total O 46 46	0	0
36	V	87	Total O 87 87	0	0
36	Y	3	Total O 3 3	0	0
36	X	18	Total O 18 18	0	0
36	Z	5	Total O 5 5	0	0
36	a	137	Total O 137 137	0	0
36	b	247	Total O 247 247	0	0
36	c	181	Total O 181 181	0	0
36	d	145	Total O 145 145	0	0
36	e	22	Total O 22 22	0	0
36	f	11	Total O 11 11	0	0
36	h	24	Total O 24 24	0	0
36	i	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	j	8	Total 8	O 8	0	0
36	k	4	Total 4	O 4	0	0
36	l	20	Total 20	O 20	0	0
36	m	18	Total 18	O 18	0	0
36	o	137	Total 137	O 137	0	0
36	t	8	Total 8	O 8	0	0
36	u	74	Total 74	O 74	0	0
36	v	75	Total 75	O 75	0	0
36	y	3	Total 3	O 3	0	0
36	x	14	Total 14	O 14	0	0
36	z	8	Total 8	O 8	0	0
36	r	6	Total 6	O 6	0	0

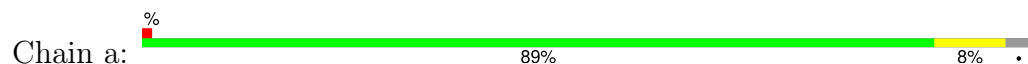
3 Residue-property plots [i](#)

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

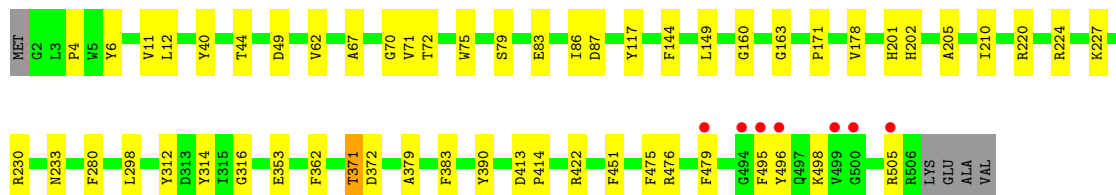
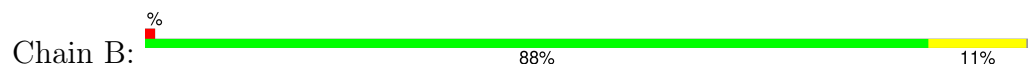
- Molecule 1: Photosystem II protein D1 1



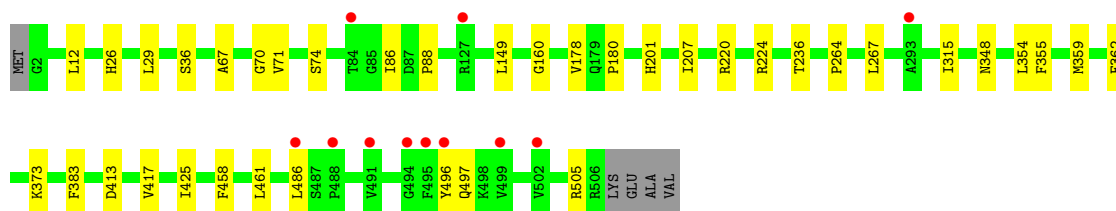
- Molecule 1: Photosystem II protein D1 1



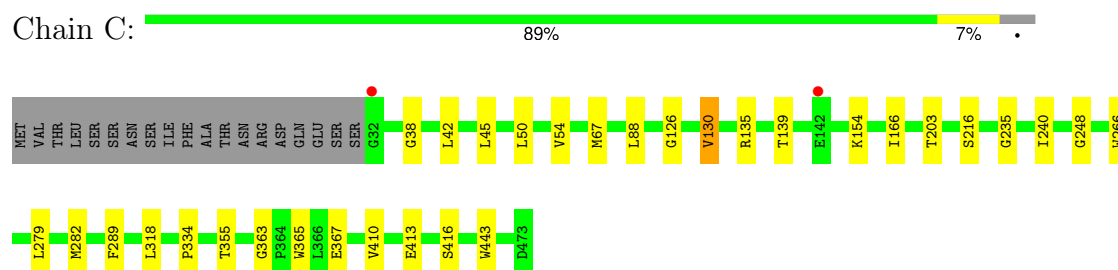
- Molecule 2: Photosystem II CP47 reaction center protein



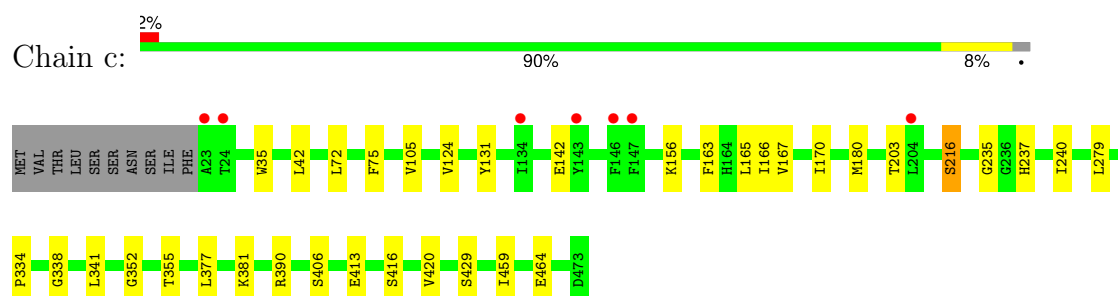
- Molecule 2: Photosystem II CP47 reaction center protein



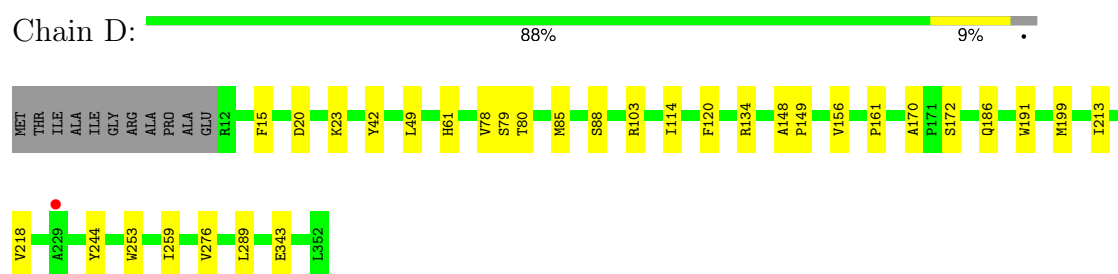
- Molecule 3: Photosystem II CP43 reaction center protein



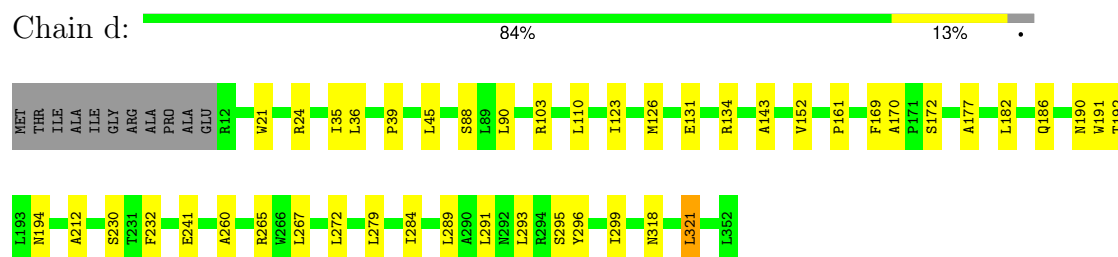
- Molecule 3: Photosystem II CP43 reaction center protein



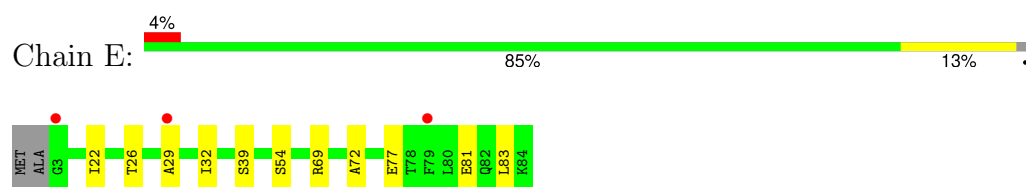
- Molecule 4: Photosystem II D2 protein



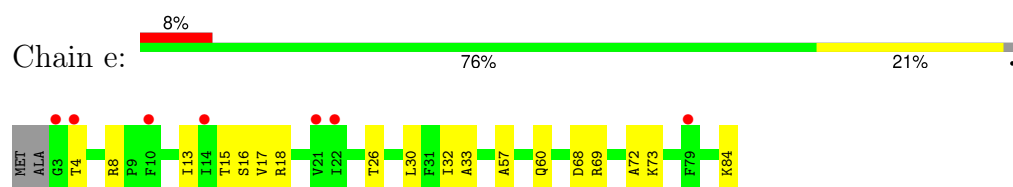
- Molecule 4: Photosystem II D2 protein



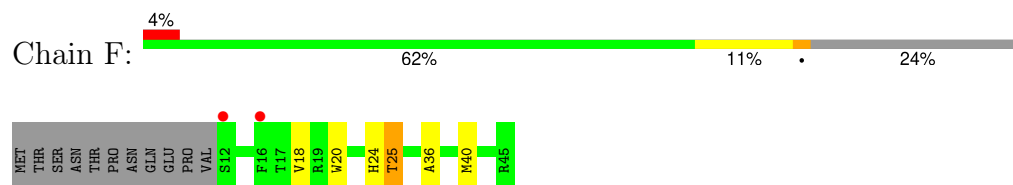
- Molecule 5: Cytochrome b559 subunit alpha



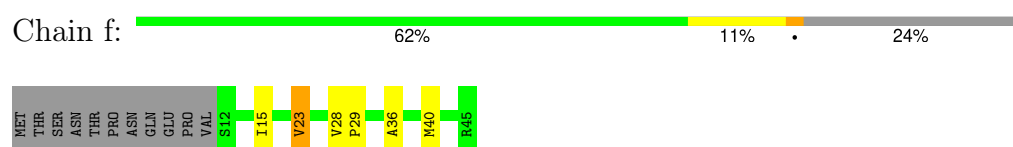
- Molecule 5: Cytochrome b559 subunit alpha



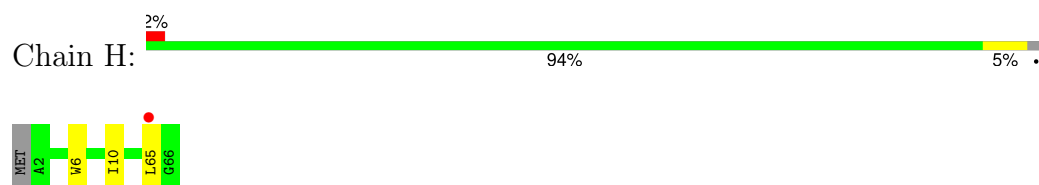
- Molecule 6: Cytochrome b559 subunit beta



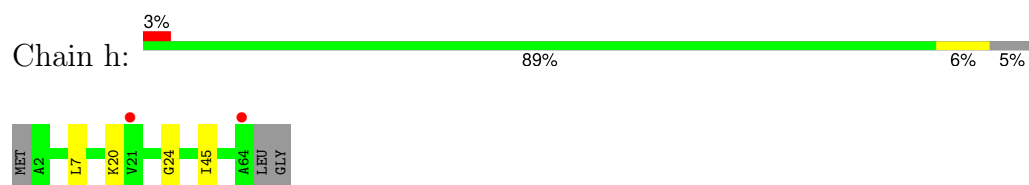
- Molecule 6: Cytochrome b559 subunit beta



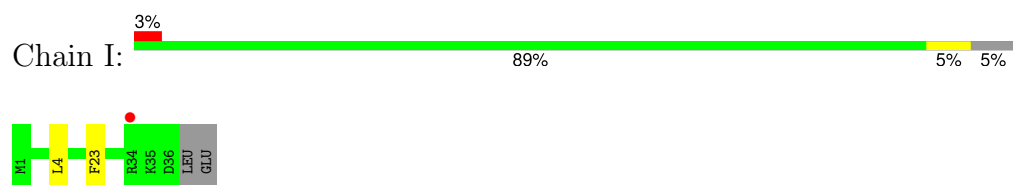
- Molecule 7: Photosystem II reaction center protein H



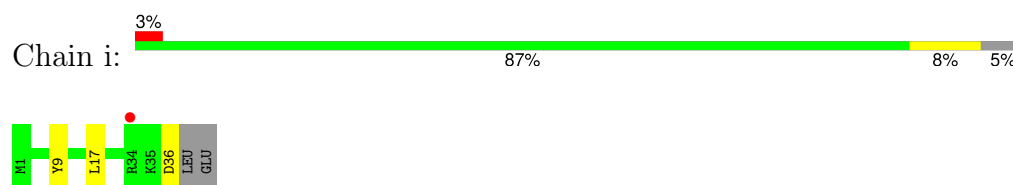
- Molecule 7: Photosystem II reaction center protein H



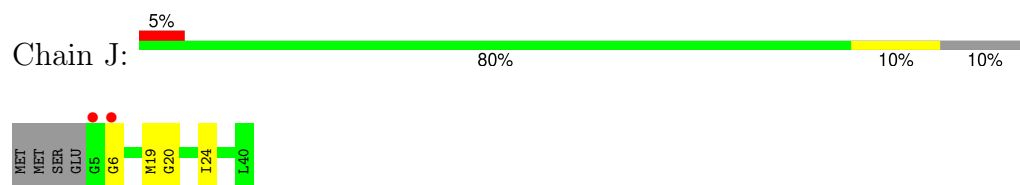
- Molecule 8: Photosystem II reaction center protein I



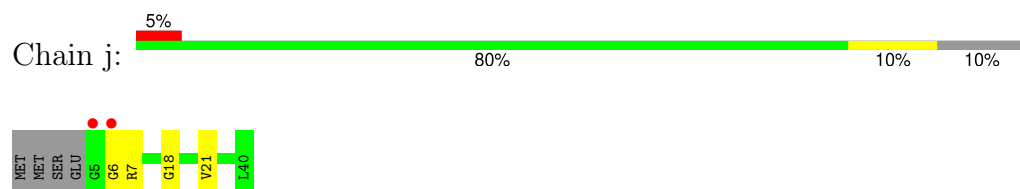
- Molecule 8: Photosystem II reaction center protein I



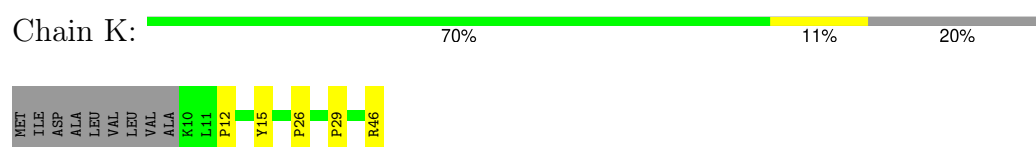
- Molecule 9: Photosystem II reaction center protein J



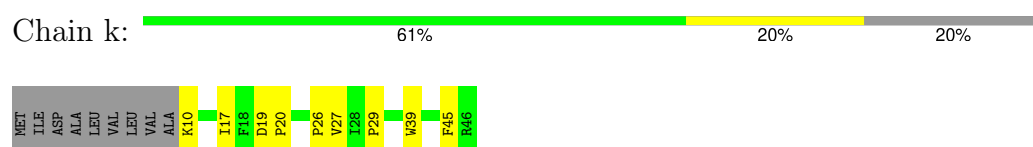
- Molecule 9: Photosystem II reaction center protein J



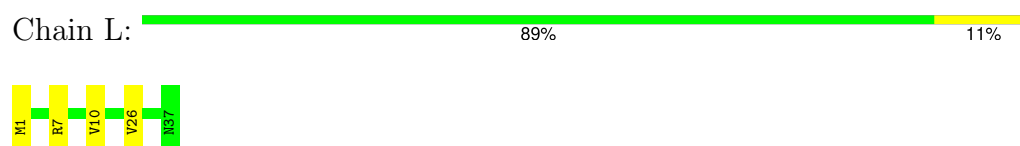
- Molecule 10: Photosystem II reaction center protein K



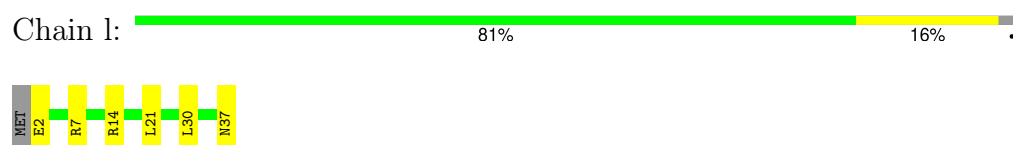
- Molecule 10: Photosystem II reaction center protein K



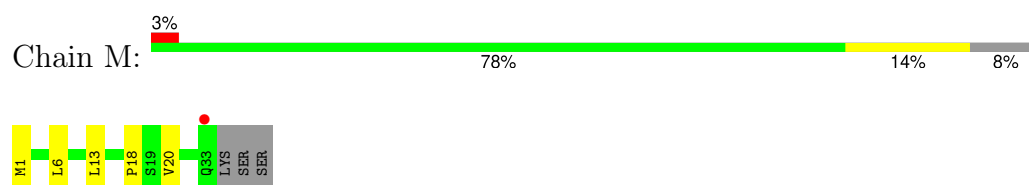
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

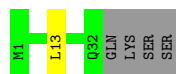


- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

Chain m:  86% • 11%



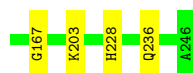
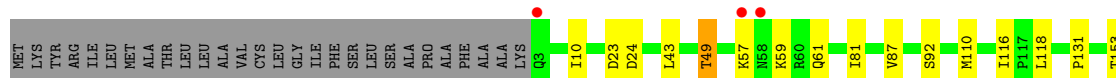
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  80% 9% • 10%



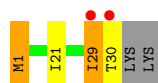
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  82% 7% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 6% 6% 6%



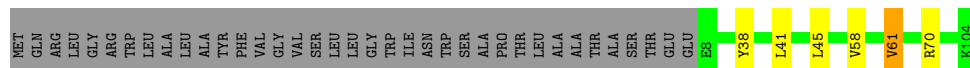
- Molecule 14: Photosystem II reaction center protein T

Chain t:  91% • 6%



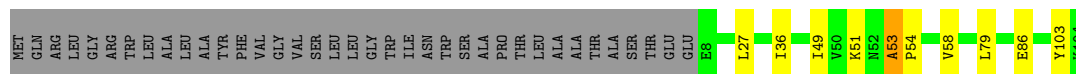
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  68% 28%



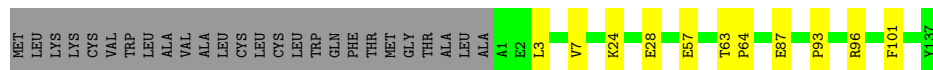
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 



- Molecule 16: Cytochrome c-550

Chain V: 

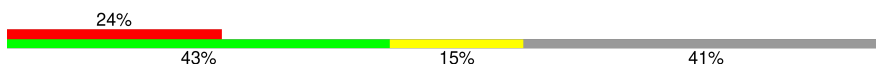


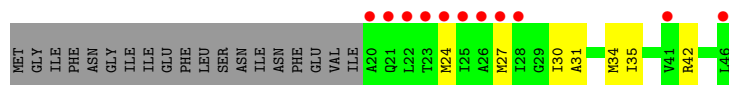
- Molecule 16: Cytochrome c-550

Chain v: 



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 



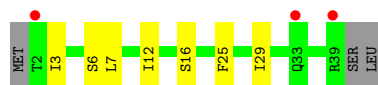
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 



- Molecule 18: Photosystem II reaction center X protein

Chain X: 

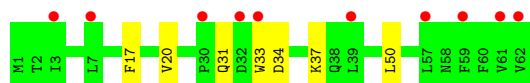
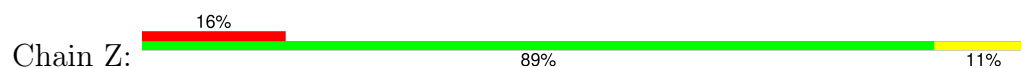


- Molecule 18: Photosystem II reaction center X protein

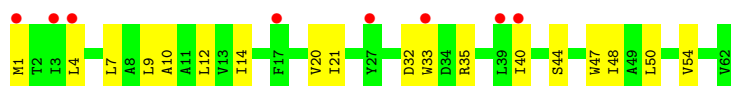
Chain x: 



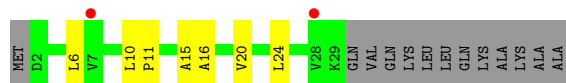
- Molecule 19: Photosystem II reaction center protein Z



- 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	117.57Å 222.87Å 309.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.99 – 2.16 37.99 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.99-2.16) 82.8 (37.99-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.40 (at 2.16Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.198 , 0.240 0.198 , 0.240	Depositor DCC
R_{free} test set	3841 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	52923	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: FME, STE, PL9, CL, BCT, DGD, HEM, SQD, PHO, OEX, FE2, CLA, LHG, LMG, BCR, HEC

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	0.36	0/2707	0.53	0/3692
1	a	0.34	0/2704	0.53	0/3688
2	B	0.32	0/4166	0.48	0/5675
2	b	0.31	0/4127	0.47	0/5623
3	C	0.32	0/3539	0.48	0/4819
3	c	0.30	0/3619	0.47	0/4926
4	D	0.35	0/2812	0.53	0/3832
4	d	0.33	0/2821	0.50	0/3844
5	E	0.25	0/688	0.42	0/940
5	e	0.25	0/683	0.42	0/932
6	F	0.27	0/284	0.40	0/387
6	f	0.24	0/284	0.47	0/387
7	H	0.28	0/517	0.43	0/705
7	h	0.28	0/505	0.47	0/689
8	I	0.32	0/293	0.49	0/396
8	i	0.29	0/293	0.42	0/396
9	J	0.29	0/263	0.51	0/356
9	j	0.27	0/263	0.42	0/356
10	K	0.28	0/303	0.46	0/416
10	k	0.25	0/303	0.46	0/416
11	L	0.35	0/311	0.46	0/422
11	l	0.33	0/303	0.46	0/412
12	M	0.31	0/249	0.54	0/341
12	m	0.33	0/244	0.52	0/334
13	O	0.31	0/1904	0.51	0/2585
13	o	0.31	0/1905	0.48	0/2583
14	T	0.34	0/257	0.55	0/349
14	t	0.29	0/255	0.44	0/346
15	U	0.30	0/785	0.47	0/1064
15	u	0.31	0/785	0.48	0/1064
16	V	0.32	0/1085	0.55	0/1473
16	v	0.27	0/1085	0.44	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.27	0/197	0.48	0/264
17	y	0.18	0/219	0.31	0/294
18	X	0.27	0/284	0.42	0/384
18	x	0.24	0/289	0.37	0/391
19	Z	0.20	0/490	0.41	0/669
19	z	0.20	0/488	0.34	0/666
20	R	0.21	0/227	0.37	0/313
20	r	0.21	0/227	0.36	0/313
All	All	0.31	0/42763	0.48	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	15	0
1	a	2619	0	2510	20	0
2	B	4016	0	3883	39	0
2	b	3984	0	3842	26	0
3	C	3426	0	3353	19	0
3	c	3500	0	3426	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2717	0	2621	24	0
4	d	2723	0	2627	33	0
5	E	666	0	651	11	0
5	e	664	0	648	16	0
6	F	275	0	282	5	0
6	f	275	0	282	4	0
7	H	505	0	528	2	0
7	h	493	0	514	3	0
8	I	296	0	311	1	0
8	i	296	0	311	3	0
9	J	257	0	268	2	0
9	j	257	0	268	7	0
10	K	293	0	305	2	0
10	k	293	0	305	4	0
11	L	304	0	316	3	0
11	l	296	0	304	5	0
12	M	256	0	269	4	0
12	m	251	0	267	0	0
13	O	1870	0	1830	15	0
13	o	1874	0	1846	12	0
14	T	258	0	261	3	0
14	t	256	0	256	1	0
15	U	774	0	773	4	0
15	u	774	0	773	8	0
16	V	1064	0	1073	4	0
16	v	1064	0	1073	10	0
17	Y	196	0	217	7	0
17	y	218	0	241	6	0
18	X	281	0	312	5	0
18	x	286	0	314	4	0
19	Z	479	0	516	7	0
19	z	477	0	509	14	0
20	R	221	0	238	5	0
20	r	221	0	238	6	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	184	0	192	8	0
24	B	1035	0	1139	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	839	0	922	15	0
24	D	195	0	216	5	0
24	a	195	0	216	7	0
24	b	1035	0	1139	32	0
24	c	839	0	919	26	0
24	d	195	0	216	5	0
25	A	64	0	74	1	0
25	D	64	0	74	0	0
25	a	128	0	148	2	0
26	A	40	0	56	2	0
26	B	120	0	168	7	0
26	C	80	0	112	5	0
26	D	40	0	56	3	0
26	H	40	0	56	3	0
26	J	40	0	56	4	0
26	K	40	0	56	0	0
26	T	40	0	56	2	0
26	a	40	0	56	1	0
26	b	120	0	168	2	0
26	c	120	0	168	2	0
26	d	40	0	56	1	0
26	k	40	0	56	0	0
26	t	40	0	56	7	0
26	x	40	0	56	3	0
27	A	55	0	80	9	0
27	D	55	0	80	1	0
27	a	55	0	80	8	0
27	d	55	0	80	1	0
28	A	45	0	83	3	0
28	B	76	0	116	4	0
28	C	92	0	153	3	0
28	E	44	0	74	2	0
28	H	27	0	52	2	0
28	I	32	0	48	2	0
28	J	12	0	16	0	0
28	M	25	0	38	1	0
28	T	16	0	31	2	0
28	X	20	0	35	3	0
28	Z	17	0	33	0	0
28	a	12	0	16	0	0
28	b	61	0	104	0	0
28	d	74	0	125	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	e	31	0	52	1	0
28	f	24	0	46	0	0
28	h	21	0	40	2	0
28	i	18	0	24	1	0
28	j	12	0	16	1	0
28	l	18	0	35	1	0
28	m	12	0	16	0	0
28	t	10	0	16	0	0
28	z	40	0	71	2	0
29	A	48	0	66	1	0
29	B	100	0	146	7	0
29	C	84	0	106	1	0
29	D	101	0	142	12	0
29	M	51	0	72	4	0
29	a	49	0	68	2	0
29	b	55	0	86	1	0
29	c	124	0	172	3	0
29	d	44	0	58	0	0
29	m	51	0	72	1	0
30	A	95	0	124	3	0
30	B	54	0	78	3	0
30	D	36	0	46	1	0
30	a	108	0	156	5	0
30	b	49	0	65	2	0
30	f	41	0	49	1	0
31	A	49	0	74	2	0
31	B	49	0	74	4	0
31	D	96	0	141	5	0
31	L	49	0	74	3	0
31	a	49	0	74	3	0
31	d	88	0	125	0	0
31	e	42	0	57	1	0
31	l	49	0	74	2	0
32	A	66	0	96	3	0
32	C	186	0	246	4	0
32	H	62	0	82	2	0
32	c	186	0	246	3	0
32	h	62	0	82	3	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	2	0
34	e	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	V	43	0	30	0	0
35	v	43	0	30	0	0
36	A	165	0	0	6	0
36	B	266	0	0	5	0
36	C	223	0	0	2	0
36	D	137	0	0	3	0
36	E	39	0	0	2	0
36	F	9	0	0	0	0
36	H	33	0	0	0	0
36	I	20	0	0	0	0
36	J	19	0	0	2	0
36	K	7	0	0	1	0
36	L	8	0	0	0	0
36	M	13	0	0	1	0
36	O	124	0	0	4	0
36	T	10	0	0	0	0
36	U	46	0	0	0	0
36	V	87	0	0	1	0
36	X	18	0	0	0	0
36	Y	3	0	0	2	0
36	Z	5	0	0	0	0
36	a	137	0	0	4	0
36	b	247	0	0	6	0
36	c	181	0	0	4	0
36	d	145	0	0	3	0
36	e	22	0	0	0	0
36	f	11	0	0	0	0
36	h	24	0	0	0	0
36	i	11	0	0	0	0
36	j	8	0	0	0	0
36	k	4	0	0	0	0
36	l	20	0	0	1	0
36	m	18	0	0	0	0
36	o	137	0	0	2	0
36	r	6	0	0	0	0
36	t	8	0	0	0	0
36	u	74	0	0	1	0
36	v	75	0	0	0	0
36	x	14	0	0	1	0
36	y	3	0	0	0	0
36	z	8	0	0	0	0
All	All	52923	0	52200	522	0

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

All (522) 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)
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.40	0.87
31:D:412:LHG:H142	31:D:412:LHG:H341	1.61	0.83
24:A:606:CLA:H193	27:A:610:PL9:H23	1.64	0.78
24:b:604:CLA:H42	24:b:605:CLA:H2	1.66	0.78
34:e:102:HEM:HHD	34:e:102:HEM:HBC2	1.67	0.76
2:B:495:PHE:HD2	2:B:505:ARG:HH12	1.33	0.74
4:D:23:LYS:HZ2	29:D:408:LMG:HC5	1.54	0.73
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.71	0.73
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.68	0.73
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.70	0.72
24:b:615:CLA:H2	24:b:616:CLA:HBB2	1.72	0.71
30:B:623:SQD:H383	30:B:623:SQD:H192	1.72	0.70
34:e:102:HEM:HHC	34:e:102:HEM:HBB2	1.73	0.70
19:z:32:ASP:HA	19:z:35:ARG:HD3	1.74	0.70
18:X:16:SER:HB3	28:X:101:STE:H102	1.73	0.69
24:b:602:CLA:H43	7:h:45:ILE:HG22	1.74	0.68
28:d:412:STE:H41	18:x:12:ILE:HG21	1.74	0.68
30:A:613:SQD:H302	24:C:508:CLA:H71	1.76	0.68
24:B:608:CLA:H142	28:X:101:STE:H183	1.74	0.68
24:A:606:CLA:H172	27:A:610:PL9:H261	1.77	0.67
4:d:134:ARG:HG2	28:d:407:STE:H41	1.78	0.66
27:a:611:PL9:H28	31:e:103:LHG:H223	1.77	0.66
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.77	0.66
26:t:101:BCR:HC8	26:t:101:BCR:H311	1.78	0.65
24:B:604:CLA:H43	24:B:605:CLA:H2	1.78	0.65
24:a:609:CLA:H52	24:a:609:CLA:H111	1.79	0.65
31:B:622:LHG:H222	12:M:18:PRO:HG3	1.78	0.65
24:c:501:CLA:H192	24:c:507:CLA:HBB1	1.78	0.64
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.78	0.64
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.79	0.64
24:B:608:CLA:H152	24:B:609:CLA:H193	1.79	0.64
15:u:86:GLU:H	15:u:86:GLU:CD	2.05	0.64
1:a:227:THR:HB	1:a:231:GLU:HG3	1.78	0.63
26:T:101:BCR:H311	26:T:101:BCR:HC8	1.81	0.63
27:A:610:PL9:H361	6:F:25:THR:HG21	1.81	0.63
1:a:245:THR:HB	4:d:265:ARG:HE	1.64	0.63
31:B:622:LHG:H161	31:L:101:LHG:H281	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:610:PL9:H271	31:A:614:LHG:H191	1.82	0.62
3:c:180:MET:HE1	29:c:522:LMG:HC72	1.82	0.62
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.81	0.61
2:B:202:HIS:C	36:B:701:HOH:O	2.44	0.61
27:A:610:PL9:H33	4:D:42:TYR:HB2	1.81	0.61
29:D:408:LMG:HC1	29:D:408:LMG:H131	1.83	0.61
2:b:355:PHE:HE1	2:b:373:LYS:HG2	1.66	0.61
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.83	0.60
5:e:17:VAL:HG23	9:j:7:ARG:HD3	1.82	0.60
29:B:620:LMG:HC8	36:B:754:HOH:O	2.00	0.60
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.82	0.60
4:d:123:ILE:HD11	32:h:101:DGD:HAW2	1.84	0.60
26:T:101:BCR:H382	26:T:101:BCR:H23C	1.83	0.60
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.84	0.60
2:B:205:ALA:N	36:B:701:HOH:O	2.34	0.60
24:c:503:CLA:H203	24:c:510:CLA:HAB	1.83	0.59
15:U:70:ARG:HH11	15:U:70:ARG:HB3	1.66	0.59
4:d:241:GLU:CD	4:d:241:GLU:H	2.09	0.59
29:B:620:LMG:HC92	29:D:408:LMG:H161	1.84	0.59
17:y:34:MET:HE2	19:z:21:ILE:HD13	1.84	0.59
1:A:234:ASN:HD21	31:B:622:LHG:HC11	1.68	0.58
3:c:237:HIS:C	36:c:602:HOH:O	2.45	0.58
24:b:602:CLA:H192	32:h:101:DGD:HBT1	1.85	0.58
1:A:234:ASN:ND2	31:B:622:LHG:HC11	2.18	0.58
24:c:501:CLA:C3D	24:c:503:CLA:H2	2.33	0.58
24:A:606:CLA:H91	29:D:409:LMG:H241	1.84	0.58
2:B:371:THR:HG23	2:B:372:ASP:O	2.04	0.58
30:b:620:SQD:H223	36:b:909:HOH:O	2.04	0.58
30:A:613:SQD:H271	31:D:412:LHG:H151	1.86	0.57
4:D:186:GLN:HB2	24:D:404:CLA:HBC1	1.85	0.57
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.87	0.57
4:D:15:PHE:HE1	29:D:408:LMG:H121	1.70	0.56
26:J:101:BCR:H322	19:Z:17:PHE:CE2	2.40	0.56
3:c:170:ILE:HD11	29:c:522:LMG:H381	1.85	0.56
5:e:68:ASP:O	5:e:72:ALA:HB2	2.04	0.56
26:b:618:BCR:H17C	36:b:909:HOH:O	2.04	0.56
30:B:623:SQD:H361	26:t:101:BCR:H362	1.87	0.56
27:A:610:PL9:H512	24:D:405:CLA:HBC1	1.87	0.56
1:a:214:MET:HE1	1:a:255:PHE:CE1	2.41	0.56
3:c:459:ILE:HG21	3:c:464:GLU:HG3	1.88	0.56
2:b:264:PRO:HG2	2:b:267:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:615:CLA:H2	24:B:616:CLA:HBB2	1.87	0.56
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.88	0.56
5:E:39:SER:HB3	28:E:103:STE:H162	1.87	0.56
1:a:84:PRO:HA	1:a:112:TYR:CG	2.41	0.56
1:a:217:SER:HA	4:d:272:LEU:HD12	1.88	0.55
24:A:606:CLA:H192	31:A:614:LHG:H171	1.88	0.55
9:J:19:MET:HG3	36:J:216:HOH:O	2.06	0.55
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.87	0.55
24:c:506:CLA:H142	24:c:506:CLA:H61	1.88	0.55
2:b:29:LEU:HA	36:b:909:HOH:O	2.06	0.55
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.42	0.55
24:b:615:CLA:H52	24:b:616:CLA:HBB1	1.88	0.55
13:o:92:SER:HB3	13:o:131:PRO:HA	1.89	0.55
3:c:142:GLU:CD	3:c:142:GLU:H	2.15	0.55
28:d:410:STE:H71	28:h:103:STE:H171	1.89	0.55
26:t:101:BCR:H23C	26:t:101:BCR:H382	1.88	0.55
11:l:7:ARG:HH12	28:l:102:STE:H21	1.70	0.55
1:A:189:GLU:HG2	36:A:854:HOH:O	2.06	0.54
29:B:625:LMG:H341	29:B:625:LMG:H292	1.89	0.54
9:J:20:GLY:O	9:J:24:ILE:HG13	2.07	0.54
11:L:26:VAL:HG11	31:L:101:LHG:H211	1.90	0.54
14:T:29:ILE:HG22	14:T:30:THR:HG23	1.89	0.54
19:Z:34:ASP:HA	19:Z:37:LYS:HE3	1.89	0.54
19:z:4:LEU:HA	19:z:7:LEU:HB2	1.90	0.54
19:z:1:MET:HB3	19:z:4:LEU:HD21	1.90	0.54
15:U:58:VAL:O	15:U:61:VAL:HG22	2.08	0.53
34:e:102:HEM:HBD2	6:f:23:VAL:HG21	1.91	0.53
30:a:613:SQD:H132	30:a:613:SQD:H242	1.89	0.53
3:c:240:ILE:N	36:c:602:HOH:O	2.40	0.53
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.90	0.53
5:e:18:ARG:H	9:j:7:ARG:NH1	2.07	0.53
28:B:626:STE:H22	29:M:101:LMG:HC5	1.91	0.53
31:a:612:LHG:H212	24:b:613:CLA:H172	1.89	0.53
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.91	0.53
11:l:2:GLU:HB2	36:l:215:HOH:O	2.09	0.53
17:y:20:ALA:O	17:y:24:MET:HG2	2.08	0.53
26:C:514:BCR:H352	28:C:519:STE:H32	1.91	0.52
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.90	0.52
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.92	0.52
30:B:623:SQD:H172	30:B:623:SQD:H341	1.91	0.52
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD11	27:A:610:PL9:HC71	1.92	0.52
4:d:126:MET:HE3	4:d:143:ALA:O	2.09	0.52
17:Y:42:ARG:HH11	19:Z:31:GLN:HE22	1.58	0.52
24:b:601:CLA:CHA	24:b:601:CLA:HBA2	2.39	0.52
30:a:613:SQD:H462	4:d:232:PHE:CE2	2.45	0.52
5:e:33:ALA:HB2	20:r:11:PRO:HG2	1.91	0.52
27:a:611:PL9:H48	4:d:39:PRO:HG3	1.90	0.52
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.92	0.52
17:y:17:GLU:HB3	17:y:19:ILE:HG23	1.91	0.52
24:a:609:CLA:H172	8:i:9:TYR:HB3	1.92	0.52
26:H:101:BCR:H353	28:H:103:STE:H111	1.91	0.52
4:d:260:ALA:HB3	36:d:509:HOH:O	2.09	0.52
17:y:39:LEU:HB3	17:y:46:LEU:HD21	1.92	0.52
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.93	0.51
19:z:33:TRP:H	19:z:35:ARG:HH11	1.56	0.51
27:d:406:PL9:H322	31:l:101:LHG:H222	1.92	0.51
28:d:410:STE:H52	28:h:103:STE:H183	1.92	0.51
5:e:16:SER:HA	9:j:7:ARG:HD2	1.93	0.51
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.92	0.51
24:B:613:CLA:H143	29:M:101:LMG:H221	1.93	0.51
26:J:101:BCR:H20C	36:J:216:HOH:O	2.10	0.51
24:b:613:CLA:H13	29:m:101:LMG:H241	1.93	0.51
4:D:61:HIS:HD2	36:D:627:HOH:O	1.94	0.51
24:b:615:CLA:H2	24:b:616:CLA:CBB	2.38	0.51
24:C:513:CLA:H193	28:C:526:STE:H171	1.91	0.51
12:M:13:LEU:HB3	29:M:101:LMG:H401	1.92	0.51
3:C:334:PRO:HA	13:O:153:THR:OG1	2.10	0.51
3:c:166:ILE:HG21	24:c:512:CLA:H202	1.93	0.51
4:d:186:GLN:HB2	24:d:403:CLA:HBC1	1.93	0.51
29:D:408:LMG:H132	29:D:408:LMG:H341	1.93	0.50
32:A:616:DGD:HB21	36:A:845:HOH:O	2.09	0.50
19:z:10:ALA:O	19:z:14:ILE:HG12	2.11	0.50
1:A:286:THR:HG23	24:A:605:CLA:HED3	1.94	0.50
2:B:12:LEU:HB2	24:B:612:CLA:HMC2	1.93	0.50
20:R:16:ALA:O	20:R:20:VAL:HG23	2.11	0.50
15:u:36:ILE:HD13	16:v:52:LEU:HD13	1.93	0.50
18:X:12:ILE:HG21	28:X:101:STE:H31	1.92	0.50
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.50
2:B:495:PHE:HD2	2:B:505:ARG:NH1	2.06	0.50
1:A:329:GLU:HG3	36:A:848:HOH:O	2.12	0.50
24:B:612:CLA:HBB1	24:B:612:CLA:HMB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.42	0.50
26:J:101:BCR:H321	26:J:101:BCR:HC8	1.94	0.50
13:O:107:THR:HG22	36:O:323:HOH:O	2.12	0.50
2:B:160:GLY:HA2	2:B:163:GLY:O	2.12	0.49
5:E:29:ALA:HA	36:E:230:HOH:O	2.11	0.49
32:A:616:DGD:HB62	32:A:616:DGD:HBE2	1.94	0.49
5:E:26:THR:HA	20:R:15:ALA:HB1	1.93	0.49
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.12	0.49
29:a:615:LMG:HC8	3:c:216:SER:HB2	1.94	0.49
2:b:86:ILE:HD12	2:b:88:PRO:HD3	1.94	0.49
19:z:47:TRP:CD2	28:z:703:STE:H72	2.47	0.49
31:D:411:LHG:H321	14:T:21:ILE:HD11	1.94	0.49
1:A:227:THR:HB	1:A:231:GLU:HG3	1.94	0.49
26:B:618:BCR:H383	26:t:101:BCR:H352	1.95	0.49
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.48	0.49
24:b:614:CLA:H43	30:b:620:SQD:H122	1.94	0.49
2:B:496:TYR:HD1	2:B:505:ARG:HA	1.77	0.49
26:d:405:BCR:H403	26:d:405:BCR:H23C	1.93	0.49
2:B:227:LYS:HG2	29:D:408:LMG:H302	1.94	0.49
5:E:39:SER:HA	28:E:103:STE:H183	1.95	0.49
28:I:102:STE:H22	24:b:606:CLA:H192	1.93	0.49
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.93	0.49
18:X:25:PHE:O	18:X:29:ILE:HG12	2.13	0.49
24:c:511:CLA:H171	19:z:20:VAL:HA	1.94	0.49
29:A:612:LMG:HC72	3:C:216:SER:HB2	1.94	0.48
4:D:61:HIS:HE1	4:D:80:THR:O	1.96	0.48
13:O:133:VAL:C	13:O:135:SER:H	2.21	0.48
27:a:611:PL9:H172	27:a:611:PL9:H151	1.57	0.48
3:c:167:VAL:HG13	24:c:512:CLA:H102	1.95	0.48
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.95	0.48
1:a:214:MET:HE3	27:a:611:PL9:HC8	1.95	0.48
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.48	0.48
16:v:41:HIS:HA	16:v:45:ILE:O	2.13	0.48
18:X:3:ILE:HD12	18:X:7:LEU:HD23	1.95	0.48
2:b:36:SER:OG	26:b:618:BCR:H362	2.13	0.48
3:c:406:SER:HA	3:c:420:VAL:HG23	1.96	0.48
15:U:70:ARG:HB3	15:U:70:ARG:NH1	2.29	0.48
2:b:12:LEU:HB2	24:b:612:CLA:HMC2	1.96	0.48
2:B:230:ARG:NH2	29:B:620:LMG:HC5	2.28	0.48
6:f:36:ALA:O	6:f:40:MET:HG3	2.13	0.48
1:a:117:PHE:HB3	29:a:615:LMG:H152	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:ARG:HD2	36:O:379:HOH:O	2.14	0.47
24:B:606:CLA:H72	26:B:619:BCR:H311	1.95	0.47
5:e:84:LYS:HB2	5:e:84:LYS:HE3	1.67	0.47
24:C:502:CLA:H61	24:C:512:CLA:H42	1.97	0.47
4:d:194:ASN:HA	4:d:295:SER:OG	2.15	0.47
18:x:18:ALA:HA	36:x:211:HOH:O	2.15	0.47
19:Z:33:TRP:O	19:Z:37:LYS:HG3	2.14	0.47
24:a:609:CLA:H11	8:i:9:TYR:CE1	2.50	0.47
2:b:373:LYS:HG3	36:b:707:HOH:O	2.15	0.47
24:b:610:CLA:HBB1	26:x:101:BCR:C2	2.44	0.47
24:c:508:CLA:HMB3	24:c:508:CLA:HBB1	1.95	0.47
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.96	0.47
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.96	0.47
32:c:519:DGD:HA51	28:j:101:STE:H92	1.96	0.47
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.96	0.46
2:b:496:TYR:CE1	2:b:505:ARG:HG2	2.50	0.46
17:Y:30:ILE:HG22	36:Y:101:HOH:O	2.14	0.46
4:d:36:LEU:HB2	28:d:407:STE:H171	1.97	0.46
28:d:410:STE:H31	28:d:410:STE:H61	1.37	0.46
19:z:33:TRP:N	19:z:35:ARG:HH11	2.13	0.46
24:C:509:CLA:H93	24:C:509:CLA:H112	1.82	0.46
24:C:513:CLA:HBB1	24:C:513:CLA:HMB3	1.97	0.46
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.75	0.46
4:D:199:MET:HG2	27:D:407:PL9:H312	1.96	0.46
26:J:101:BCR:H322	19:Z:17:PHE:CZ	2.51	0.46
27:a:611:PL9:HC2	36:a:786:HOH:O	2.15	0.46
30:a:614:SQD:H1	36:a:778:HOH:O	2.15	0.46
3:c:352:GLY:O	3:c:355:THR:HG22	2.16	0.46
2:B:62:VAL:HB	24:B:605:CLA:HED3	1.98	0.46
2:B:233:ASN:HD21	2:B:476:ARG:CZ	2.29	0.46
16:V:28:GLU:HG2	36:V:359:HOH:O	2.15	0.46
27:A:610:PL9:C36	6:F:25:THR:HG21	2.45	0.46
32:C:523:DGD:HAH1	29:D:409:LMG:H212	1.98	0.46
5:E:54:SER:HB2	5:E:83:LEU:HD13	1.97	0.46
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.97	0.46
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.51	0.46
2:b:486:LEU:HD11	36:b:813:HOH:O	2.15	0.46
26:c:514:BCR:H24C	26:c:514:BCR:H371	1.79	0.46
5:e:15:THR:OG1	9:j:6:GLY:HA2	2.16	0.46
3:C:38:GLY:HA3	24:C:511:CLA:HMD2	1.97	0.46
17:Y:34:MET:HA	17:Y:34:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:614:SQD:H302	30:a:614:SQD:H331	1.54	0.46
2:b:224:ARG:HG2	7:h:24:GLY:O	2.16	0.46
36:c:613:HOH:O	10:k:39:TRP:HZ2	1.98	0.46
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.51	0.46
24:b:604:CLA:H61	24:b:604:CLA:H41	1.85	0.45
2:B:40:TYR:O	2:B:44:THR:HG23	2.16	0.45
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.50	0.45
10:K:26:PRO:O	10:K:29:PRO:HD2	2.16	0.45
24:c:508:CLA:H141	24:c:508:CLA:H162	1.72	0.45
30:A:615:SQD:H223	24:D:403:CLA:H201	1.98	0.45
3:C:126:GLY:O	3:C:130:VAL:HG13	2.16	0.45
1:a:245:THR:HG22	36:a:739:HOH:O	2.15	0.45
3:c:203:THR:O	3:c:235:GLY:HA3	2.17	0.45
3:C:135:ARG:O	3:C:135:ARG:HD3	2.16	0.45
13:O:6:THR:HG23	13:O:8:ASP:H	1.82	0.45
4:d:169:PHE:HB3	36:d:502:HOH:O	2.17	0.45
5:e:17:VAL:H	9:j:7:ARG:HD2	1.82	0.45
1:A:179:THR:O	1:A:183:MET:HG3	2.17	0.45
24:B:614:CLA:H62	24:B:614:CLA:H41	1.81	0.45
13:O:110:MET:HB3	13:O:110:MET:HE2	1.71	0.45
24:D:403:CLA:H161	24:D:403:CLA:H141	1.64	0.45
3:C:45:LEU:HA	3:C:139:THR:HG22	1.99	0.45
4:D:23:LYS:NZ	29:D:408:LMG:HC5	2.27	0.45
6:F:36:ALA:O	6:F:40:MET:HG3	2.16	0.45
2:B:475:PHE:O	2:B:479[B]:PHE:HD1	2.00	0.45
24:a:609:CLA:H141	24:a:609:CLA:H203	1.98	0.45
2:b:149:LEU:HD23	2:b:149:LEU:HA	1.83	0.45
24:c:509:CLA:H143	24:c:509:CLA:H111	1.76	0.45
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.98	0.45
28:i:101:STE:O2	28:i:101:STE:H61	2.17	0.45
2:B:149[B]:LEU:HD11	24:B:604:CLA:H161	1.97	0.45
24:C:503:CLA:HBB1	24:C:503:CLA:HMB3	1.98	0.45
16:V:87:GLU:CD	16:V:96:ARG:HH12	2.25	0.45
4:d:21:TRP:HA	4:d:24:ARG:HG2	1.99	0.45
27:A:610:PL9:H422	27:A:610:PL9:H401	1.76	0.45
28:A:618:STE:H171	28:A:619:STE:H111	1.98	0.45
28:C:527:STE:H121	28:C:527:STE:H92	1.73	0.45
36:b:899:HOH:O	11:l:7:ARG:HD2	2.17	0.45
36:A:734:HOH:O	13:O:107:THR:HG21	2.16	0.44
26:B:617:BCR:H333	12:M:13:LEU:HD12	2.00	0.44
24:c:512:CLA:H112	24:c:513:CLA:H142	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:TRP:HD1	36:C:618:HOH:O	1.98	0.44
1:a:279:PRO:HG2	4:d:212:ALA:HB2	2.00	0.44
24:b:614:CLA:H203	24:b:614:CLA:H161	1.68	0.44
24:c:511:CLA:H141	24:c:511:CLA:H162	1.69	0.44
4:d:192:THR:HG23	24:d:403:CLA:HBC2	1.99	0.44
13:o:23:ASP:HB2	36:o:364:HOH:O	2.18	0.44
24:C:507:CLA:H62	24:C:507:CLA:H41	1.82	0.44
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.99	0.44
2:b:497:GLN:HE22	18:x:38:GLN:H	1.63	0.44
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.67	0.44
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.52	0.44
36:D:617:HOH:O	18:X:6:SER:HA	2.15	0.44
29:M:101:LMG:HC61	36:M:207:HOH:O	2.16	0.44
13:O:27:ARG:HG3	36:O:303:HOH:O	2.17	0.44
28:T:102:STE:H122	28:T:102:STE:H91	1.74	0.44
24:c:510:CLA:H142	24:c:510:CLA:H111	1.83	0.44
3:C:67:MET:HB3	3:C:88:LEU:HD12	1.99	0.44
17:Y:31:ALA:N	36:Y:101:HOH:O	2.50	0.44
24:b:614:CLA:H62	24:b:614:CLA:H41	1.47	0.44
15:u:51:LYS:HB2	15:u:51:LYS:HE2	1.72	0.44
17:y:34:MET:HG2	17:y:38:LEU:HD11	2.00	0.44
24:C:511:CLA:H143	19:Z:20:VAL:HG13	1.99	0.44
5:e:8:ARG:HG2	5:e:13:ILE:HG13	2.00	0.44
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.98	0.44
24:B:603:CLA:H142	24:B:603:CLA:H112	1.80	0.44
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.99	0.44
2:B:201:HIS:HB2	24:B:602:CLA:CHB	2.48	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
4:D:49:LEU:HD13	26:D:406:BCR:C15	2.48	0.44
24:b:611:CLA:H72	24:b:611:CLA:H112	1.84	0.44
4:d:267:LEU:C	4:d:267:LEU:HD23	2.42	0.44
13:o:228:HIS:HD2	36:o:301:HOH:O	2.01	0.44
3:C:410:VAL:HG22	3:C:413[B]:GLU:HG2	2.00	0.43
24:C:505:CLA:HBC2	26:C:515:BCR:H341	2.00	0.43
6:f:15:ILE:HG12	20:r:23:ILE:HD11	2.00	0.43
15:u:53:ALA:HB1	15:u:54:PRO:CD	2.47	0.43
2:B:117:TYR:HA	11:L:1:MET:HE1	1.99	0.43
30:f:101:SQD:H281	30:f:101:SQD:H252	1.41	0.43
36:K:207:HOH:O	17:Y:24:MET:HE3	2.18	0.43
24:c:511:CLA:HBA1	26:c:517:BCR:H271	2.00	0.43
2:B:86:ILE:HG12	2:B:87:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:606:CLA:H112	24:B:606:CLA:H93	1.72	0.43
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.99	0.43
19:z:35:ARG:H	19:z:35:ARG:HD2	1.83	0.43
29:B:625:LMG:H341	36:B:715:HOH:O	2.18	0.43
24:a:606:CLA:H192	24:a:606:CLA:H161	1.77	0.43
2:b:160:GLY:HA3	2:b:180:PRO:HB3	2.00	0.43
3:c:131:TYR:OH	24:c:513:CLA:HED2	2.18	0.43
28:A:619:STE:H141	36:A:850:HOH:O	2.19	0.43
28:B:626:STE:H21	12:M:6:LEU:HD11	2.00	0.43
31:a:612:LHG:H151	31:l:101:LHG:H282	2.01	0.43
4:d:318:ASN:HA	4:d:321:LEU:HD22	2.00	0.43
2:B:4:PRO:HB2	2:B:6:TYR:CE1	2.53	0.43
32:C:522:DGD:HAE2	32:C:522:DGD:HA62	2.00	0.43
5:E:77:GLU:O	5:E:81:GLU:HG2	2.19	0.43
34:F:101:HEM:HBB2	34:F:101:HEM:HMB1	2.01	0.43
20:R:20:VAL:O	20:R:24:LEU:HB2	2.19	0.43
3:c:163:PHE:CG	24:c:512:CLA:HAB	2.52	0.43
5:e:30:LEU:HD23	20:r:12:VAL:HG12	2.01	0.43
31:D:412:LHG:H322	31:D:412:LHG:H161	2.01	0.43
4:d:230:SER:HB2	36:d:587:HOH:O	2.18	0.43
28:z:702:STE:H172	28:z:702:STE:H141	1.80	0.43
32:A:616:DGD:HA72	28:I:102:STE:O2	2.19	0.43
24:B:609:CLA:C2B	26:H:101:BCR:H323	2.48	0.43
1:a:214:MET:CE	27:a:611:PL9:HC8	2.49	0.43
27:a:611:PL9:H302	4:d:45:LEU:HD22	2.00	0.43
4:d:131:GLU:HA	28:d:407:STE:H61	2.01	0.43
32:C:522:DGD:HB32	32:C:522:DGD:HB61	1.86	0.43
4:D:156:VAL:HG23	36:D:501:HOH:O	2.17	0.43
3:c:42:LEU:HD21	24:c:511:CLA:H2A	2.01	0.43
8:i:17:LEU:HD23	8:i:17:LEU:HA	1.80	0.43
26:t:101:BCR:H23C	26:t:101:BCR:C38	2.49	0.43
16:v:34:GLN:HA	16:v:38:ALA:HB2	2.01	0.43
26:x:101:BCR:H20C	26:x:101:BCR:H361	1.85	0.43
19:z:44:SER:O	19:z:48:ILE:HG13	2.19	0.43
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.54	0.42
3:C:135:ARG:HD2	36:C:747:HOH:O	2.17	0.42
30:D:410:SQD:O8	6:F:18:VAL:HG23	2.19	0.42
24:b:615:CLA:H61	24:b:615:CLA:H92	1.77	0.42
3:c:334:PRO:HA	13:o:153:THR:OG1	2.19	0.42
4:d:35:ILE:HG22	28:d:407:STE:H183	2.01	0.42
4:d:299:ILE:HD12	11:l:37:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:407:STE:H31	28:d:410:STE:H51	2.00	0.42
5:E:32:ILE:HG12	36:E:236:HOH:O	2.19	0.42
13:O:34:SER:HB3	13:O:87:VAL:HG11	2.01	0.42
1:a:202:VAL:HG11	24:a:606:CLA:C3D	2.49	0.42
25:a:608:PHO:CHB	24:d:403:CLA:H101	2.49	0.42
24:c:512:CLA:H92	24:c:512:CLA:H61	1.80	0.42
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.54	0.42
13:O:56:PRO:HD2	36:O:412:HOH:O	2.17	0.42
24:b:609:CLA:C2B	26:x:101:BCR:H323	2.50	0.42
24:b:612:CLA:H122	24:b:612:CLA:H162	1.87	0.42
24:b:613:CLA:H143	24:b:613:CLA:H111	1.72	0.42
29:c:522:LMG:H362	29:c:522:LMG:H331	1.78	0.42
24:A:608:CLA:H41	24:A:608:CLA:H62	1.67	0.42
26:B:619:BCR:H20C	26:B:619:BCR:H361	1.81	0.42
24:C:505:CLA:H193	24:C:505:CLA:H162	1.76	0.42
5:E:26:THR:HG22	20:R:15:ALA:HB1	2.00	0.42
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.55	0.42
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.49	0.42
2:B:72:THR:O	2:B:79:SER:HB2	2.20	0.42
1:a:214:MET:HE3	1:a:214:MET:HB3	1.58	0.42
1:a:271:LEU:HD21	27:a:611:PL9:HC71	2.01	0.42
15:u:27:LEU:HD22	15:u:49:ILE:HG21	2.01	0.42
2:B:67:ALA:HA	2:B:71:VAL:O	2.19	0.42
2:b:201:HIS:HB2	24:b:602:CLA:CHB	2.49	0.42
24:b:616:CLA:H91	24:b:616:CLA:H112	1.65	0.42
3:c:390:ARG:CZ	16:v:100:ILE:HD12	2.49	0.42
28:A:619:STE:H132	28:A:619:STE:H162	1.91	0.42
2:B:171:PRO:HA	7:H:65:LEU:HD12	2.02	0.42
24:a:606:CLA:H143	24:a:606:CLA:H112	1.85	0.42
3:c:429:SER:HB3	32:c:519:DGD:HBT2	2.02	0.42
4:d:152:VAL:HG21	4:d:279:LEU:HG	2.02	0.42
15:u:103:TYR:HB3	36:u:237:HOH:O	2.18	0.42
24:A:605:CLA:H203	24:D:403:CLA:H203	2.02	0.42
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.55	0.42
24:B:608:CLA:H151	4:D:120:PHE:CZ	2.55	0.42
29:B:620:LMG:HC71	4:D:134:ARG:HG2	2.01	0.42
17:Y:24:MET:SD	17:Y:27:MET:HB2	2.60	0.42
24:c:502:CLA:H202	24:c:502:CLA:H161	1.87	0.42
5:e:57:ALA:H	5:e:60:GLN:HG2	1.84	0.42
10:k:26:PRO:O	10:k:29:PRO:HD2	2.19	0.42
24:C:506:CLA:H111	24:C:506:CLA:H91	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:SER:HA	4:D:172:SER:HB3	2.01	0.42
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.02	0.42
26:D:406:BCR:H24C	26:D:406:BCR:H371	1.84	0.42
13:O:92:SER:C	13:O:93:LEU:HD23	2.44	0.42
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.54	0.42
31:a:612:LHG:H212	24:b:613:CLA:H192	2.02	0.42
3:c:279:LEU:HD23	3:c:279:LEU:HA	1.88	0.42
32:c:518:DGD:HAT1	32:c:518:DGD:HA72	1.80	0.42
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.84	0.42
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.01	0.42
28:B:628:STE:H41	28:B:628:STE:H71	1.90	0.42
14:T:1:FME:H	28:T:102:STE:C3	2.32	0.42
25:a:608:PHO:HHD	25:a:608:PHO:HBC2	2.02	0.42
5:e:26:THR:HA	20:r:15:ALA:HB1	2.02	0.42
13:o:24:ASP:HA	13:o:203:LYS:HE2	2.01	0.42
2:B:451:PHE:CD1	2:B:451:PHE:C	2.97	0.41
24:B:610:CLA:H8	24:B:610:CLA:H51	1.90	0.41
3:C:318:LEU:C	3:C:318:LEU:HD23	2.45	0.41
24:C:504:CLA:H42	32:C:522:DGD:HB31	2.02	0.41
2:b:355:PHE:CE1	2:b:373:LYS:HG2	2.51	0.41
19:z:12:LEU:HD13	19:z:50:LEU:HB2	2.00	0.41
2:B:75:TRP:HB3	29:B:625:LMG:HC91	2.02	0.41
29:C:524:LMG:H181	29:C:524:LMG:H151	1.90	0.41
26:D:406:BCR:H382	29:D:409:LMG:H151	2.01	0.41
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.55	0.41
19:Z:50:LEU:HD23	19:Z:50:LEU:HA	1.85	0.41
30:a:614:SQD:H222	26:t:101:BCR:H322	2.02	0.41
24:c:501:CLA:C19	24:c:507:CLA:HBB1	2.46	0.41
24:c:506:CLA:H62	24:c:506:CLA:H41	1.77	0.41
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.92	0.41
24:B:613:CLA:H62	24:B:613:CLA:H41	1.69	0.41
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.08	0.41
24:b:601:CLA:H161	24:b:601:CLA:H202	1.82	0.41
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.01	0.41
13:o:110:MET:HE2	13:o:116:ILE:HD11	2.03	0.41
20:r:20:VAL:O	20:r:24:LEU:HB2	2.20	0.41
24:B:611:CLA:H112	24:B:611:CLA:H72	1.76	0.41
3:C:166:ILE:HG13	3:C:248:GLY:HA3	2.02	0.41
26:C:515:BCR:H20C	26:C:515:BCR:H361	1.94	0.41
26:C:515:BCR:H371	26:C:515:BCR:H24C	1.84	0.41
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:607:CLA:H93	24:b:607:CLA:H111	1.94	0.41
24:d:402:CLA:H43	24:d:402:CLA:O1A	2.20	0.41
5:e:17:VAL:H	9:j:7:ARG:CD	2.32	0.41
16:v:3:LEU:HA	16:v:3:LEU:HD12	1.85	0.41
2:B:11:VAL:HG11	24:B:614:CLA:HED2	2.01	0.41
26:B:618:BCR:H363	26:t:101:BCR:H19C	2.03	0.41
26:C:515:BCR:HC32	8:I:23:PHE:HB3	2.01	0.41
2:b:67:ALA:HA	2:b:71:VAL:O	2.20	0.41
2:b:359:MET:HB2	2:b:425:ILE:HD12	2.02	0.41
24:b:601:CLA:H141	24:b:601:CLA:H162	1.90	0.41
24:b:605:CLA:HMA1	24:b:606:CLA:H3A	2.03	0.41
3:c:338:GLY:HA3	3:c:341:LEU:O	2.20	0.41
24:c:504:CLA:H62	24:c:504:CLA:H41	1.91	0.41
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.55	0.41
9:j:18:GLY:O	9:j:21:VAL:HG22	2.21	0.41
20:r:18:TRP:O	20:r:22:ASN:HB2	2.21	0.41
24:A:605:CLA:H122	24:A:605:CLA:H162	1.82	0.41
2:B:220:ARG:HA	2:B:220:ARG:HD2	1.88	0.41
2:B:224:ARG:HD2	29:D:408:LMG:H312	2.01	0.41
24:B:605:CLA:H8	24:B:612:CLA:H203	2.02	0.41
24:B:610:CLA:H193	24:B:610:CLA:H162	1.89	0.41
3:C:50:LEU:O	3:C:54:VAL:HG23	2.20	0.41
31:D:412:LHG:H151	31:D:412:LHG:H121	1.74	0.41
17:Y:31:ALA:O	17:Y:35:ILE:HG13	2.20	0.41
32:H:102:DGD:HB71	32:H:102:DGD:HBT1	1.88	0.41
28:H:103:STE:H141	28:H:103:STE:H172	1.79	0.41
2:b:207:ILE:HD11	29:b:622:LMG:H321	2.02	0.41
24:c:507:CLA:H61	24:c:507:CLA:H41	1.66	0.41
26:A:609:BCR:H24C	26:A:609:BCR:H371	1.94	0.41
2:B:83:GLU:N	36:B:702:HOH:O	2.44	0.41
24:b:615:CLA:H111	24:b:615:CLA:H142	1.73	0.41
24:c:503:CLA:H62	24:c:503:CLA:H102	1.84	0.41
5:e:32:ILE:HG12	28:e:104:STE:H152	2.03	0.41
1:A:95:PRO:HD2	1:A:98:GLU:HG3	2.02	0.41
1:A:201:GLY:HA3	1:A:286:THR:HB	2.03	0.41
1:A:334:ARG:HD3	36:A:820:HOH:O	2.20	0.41
2:B:49:ASP:OD2	13:o:57:LYS:HG2	2.21	0.41
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.92	0.41
24:B:614:CLA:HMD2	28:M:102:STE:H41	2.02	0.41
26:B:617:BCR:H24C	26:B:617:BCR:H371	1.92	0.41
24:b:602:CLA:H61	32:h:101:DGD:HB62	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:163:PHE:O	3:c:167:VAL:HG23	2.21	0.41
24:c:507:CLA:H61	24:c:507:CLA:H92	1.81	0.41
4:d:103:ARG:HD2	5:e:73:LYS:HG3	2.03	0.41
24:B:604:CLA:H12	24:B:605:CLA:ND	2.36	0.41
1:a:310:LYS:HD2	16:v:1:ALA:HB1	2.02	0.41
3:c:35:TRP:CD1	10:k:45:PHE:HB3	2.55	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.56	0.40
32:H:102:DGD:HAW1	32:H:102:DGD:HAN2	1.93	0.40
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.87	0.40
16:V:57:GLU:H	16:V:57:GLU:CD	2.28	0.40
11:l:14:ARG:HB3	14:t:25:GLU:HG2	2.03	0.40
1:a:16:ARG:HE	1:a:16:ARG:HB3	1.57	0.40
10:k:20:PRO:HB3	17:y:21:GLN:HG3	2.03	0.40
19:z:35:ARG:H	19:z:35:ARG:CD	2.34	0.40
2:B:280:PHE:CD2	2:B:312:TYR:HB3	2.56	0.40
2:b:413:ASP:O	2:b:417:VAL:HG23	2.20	0.40
2:b:458:PHE:HB3	24:b:604:CLA:HBC2	2.04	0.40
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.98	0.40
28:B:628:STE:H111	36:a:832:HOH:O	2.22	0.40
3:C:363:GLY:O	3:C:367:GLU:HG2	2.21	0.40
11:L:7:ARG:CZ	11:L:7:ARG:HB3	2.51	0.40
1:a:112:TYR:O	1:a:116:ILE:HG12	2.22	0.40
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.84	0.40
1:A:43:ALA:HB1	26:A:609:BCR:H362	2.03	0.40
25:A:607:PHO:HBC2	25:A:607:PHO:HHD	2.03	0.40
2:B:224:ARG:HH12	29:D:408:LMG:H112	1.85	0.40
3:C:443:TRP:CE2	24:C:508:CLA:HMD2	2.57	0.40
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.91	0.40
31:L:101:LHG:H172	31:L:101:LHG:H142	1.78	0.40
26:a:610:BCR:H11C	26:a:610:BCR:H341	1.95	0.40
2:b:26:HIS:CE1	24:b:612:CLA:HMA2	2.56	0.40
24:c:508:CLA:H111	24:c:508:CLA:H91	1.62	0.40
36:c:610:HOH:O	13:o:10:ILE:HD13	2.20	0.40
24:d:404:CLA:H62	18:x:14:LEU:HD23	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%)	328 (99%)	4 (1%)	0	100	100
1	a	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	34
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
2	b	504/510 (99%)	497 (99%)	7 (1%)	0	100	100
3	C	441/461 (96%)	430 (98%)	10 (2%)	1 (0%)	43	44
3	c	451/461 (98%)	441 (98%)	9 (2%)	1 (0%)	43	44
4	D	339/352 (96%)	327 (96%)	11 (3%)	1 (0%)	36	34
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	30 (100%)	0	0	100	100
13	O	243/272 (89%)	233 (96%)	8 (3%)	2 (1%)	16	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	7
16	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	18	13
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
All	All	5231/5700 (92%)	5102 (98%)	120 (2%)	9 (0%)	43	44

All (9) 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
9	J	6	GLY
13	O	57	LYS
4	D	343	GLU
13	O	134	THR
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	82
1	a	269/280 (96%)	263 (98%)	6 (2%)	45	51
2	B	408/407 (100%)	404 (99%)	4 (1%)	68	75
2	b	403/407 (99%)	399 (99%)	4 (1%)	68	75
3	C	345/362 (95%)	341 (99%)	4 (1%)	63	70
3	c	354/362 (98%)	347 (98%)	7 (2%)	48	54
4	D	276/283 (98%)	275 (100%)	1 (0%)	84	89
4	d	277/283 (98%)	273 (99%)	4 (1%)	59	66
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	40
5	e	71/73 (97%)	70 (99%)	1 (1%)	59	66
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	31
6	f	28/39 (72%)	27 (96%)	1 (4%)	31	31
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	56
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	37
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%)	29 (97%)	1 (3%)	33	34
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	39
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	13
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	31
13	O	206/228 (90%)	200 (97%)	6 (3%)	37	39
13	o	207/228 (91%)	204 (99%)	3 (1%)	59	66
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	29
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	82 (98%)	2 (2%)	43	47
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	114 (97%)	3 (3%)	40	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/138 (85%)	115 (98%)	2 (2%)	53	60
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	22
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	36
19	Z	52/52 (100%)	52 (100%)	0	100	100
19	z	51/52 (98%)	50 (98%)	1 (2%)	48	54
20	R	22/33 (67%)	21 (96%)	1 (4%)	24	22
20	r	22/33 (67%)	19 (86%)	3 (14%)	3	1
All	All	4321/4654 (93%)	4247 (98%)	74 (2%)	53	60

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	205	VAL
2	B	298	LEU
2	B	353	GLU
2	B	362	PHE
2	B	371	THR
3	C	130	VAL
3	C	240	ILE
3	C	289	PHE
3	C	355	THR
4	D	259	ILE
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
8	I	4	LEU
10	K	46	ARG
11	L	10	VAL
12	M	20	VAL
13	O	18	LYS
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	214	THR
14	T	29	ILE

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Mol	Chain	Res	Type
15	U	45	LEU
15	U	61	VAL
16	V	3	LEU
16	V	7	VAL
16	V	24	LYS
20	R	6	LEU
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	245	THR
1	a	286	THR
1	a	288	LEU
2	b	74	SER
2	b	236	THR
2	b	315	ILE
2	b	362	PHE
3	c	72	LEU
3	c	124	VAL
3	c	156	LYS
3	c	165	LEU
3	c	216	SER
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	182	LEU
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
5	e	4	THR
6	f	23	VAL
7	h	7	LEU
8	i	36	ASP
10	k	10	LYS
10	k	17	ILE
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	87	VAL
13	o	118	LEU
16	v	52	LEU

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Mol	Chain	Res	Type
16	v	107	LEU
17	y	19	ILE
18	x	2	THR
19	z	40	ILE
20	r	10	LEU
20	r	14	LEU
20	r	28	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	181	ASN
1	A	234	ASN
1	A	261	GLN
1	A	338	ASN
2	B	14	ASN
2	B	285	ASN
2	B	289	GLN
3	C	201	ASN
4	D	334	GLN
5	E	82	GLN
13	O	88	ASN
13	O	231	HIS
15	U	37	GLN
15	U	81	HIS
16	V	86	GLN
1	a	165	GLN
1	a	181	ASN
1	a	234	ASN
2	b	179	GLN
2	b	289	GLN
2	b	409	GLN
2	b	497	GLN
3	c	28	GLN
3	c	322	GLN
3	c	373	ASN
3	c	378	ASN
3	c	382	ASN
3	c	415	ASN
4	d	61	HIS
4	d	250	ASN

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Mol	Chain	Res	Type
5	e	82	GLN
11	l	8	GLN
13	o	3	GLN
13	o	132	ASN
13	o	155	ASN
16	v	34	GLN
17	y	45	ASN
18	x	33	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.32	0	8,9,11	1.70	2 (25%)
8	FME	i	1	8	8,9,10	0.47	0	8,9,11	0.66	0
14	FME	t	1	14	8,9,10	0.49	0	8,9,11	0.92	0
12	FME	M	1	12	8,9,10	0.50	0	8,9,11	1.11	1 (12%)
8	FME	I	1	8	8,9,10	0.49	0	8,9,11	1.00	0
12	FME	m	1	12	8,9,10	0.45	0	8,9,11	0.64	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	3.71	128.52	122.82
12	M	1	FME	CA-N-CN	-2.59	118.84	122.82
14	T	1	FME	CG-CB-CA	2.07	119.21	112.87

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C-CA-CB-CG
8	I	1	FME	CA-CB-CG-SD
14	T	1	FME	C-CA-CB-CG
14	T	1	FME	N-CA-CB-CG
8	I	1	FME	C-CA-CB-CG
8	i	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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$
24	CLA	c	507	36	69,73,73	1.40	8 (11%)	82,113,113	1.34	6 (7%)
24	CLA	b	607	36	69,73,73	1.11	8 (11%)	82,113,113	1.22	8 (9%)
26	BCR	J	101	-	41,41,41	0.38	0	56,56,56	0.99	2 (3%)
32	DGD	A	616	-	67,67,67	0.49	0	81,81,81	1.04	6 (7%)
28	STE	z	703	-	8,8,19	0.40	0	7,7,19	0.58	0
24	CLA	b	603	2	69,73,73	1.14	9 (13%)	82,113,113	1.28	6 (7%)
29	LMG	D	409	-	51,51,55	0.45	0	59,59,63	0.68	2 (3%)
24	CLA	B	602	2	69,73,73	1.24	8 (11%)	82,113,113	1.41	9 (10%)
28	STE	e	105	-	12,12,19	0.68	0	12,12,19	1.33	2 (16%)
24	CLA	b	613	2	69,73,73	1.24	9 (13%)	82,113,113	1.31	10 (12%)
24	CLA	b	605	2	69,73,73	1.18	6 (8%)	82,113,113	1.52	9 (10%)
24	CLA	c	513	3	69,73,73	1.29	10 (14%)	82,113,113	1.17	7 (8%)
28	STE	j	101	-	11,11,19	0.78	0	11,11,19	1.05	0
24	CLA	c	511	3	69,73,73	1.40	7 (10%)	82,113,113	1.44	5 (6%)
28	STE	J	102	-	11,11,19	0.75	0	11,11,19	1.10	0
26	BCR	H	101	-	41,41,41	0.44	0	56,56,56	0.94	4 (7%)
24	CLA	c	509	3	69,73,73	1.25	7 (10%)	82,113,113	1.32	7 (8%)
26	BCR	C	514	-	41,41,41	0.33	0	56,56,56	0.77	0
28	STE	C	519	-	6,6,19	0.43	0	5,5,19	0.52	0
28	STE	z	702	-	17,17,19	0.42	0	16,16,19	0.67	0
24	CLA	B	610	36	69,73,73	1.39	11 (15%)	82,113,113	1.39	11 (13%)
24	CLA	b	611	2	69,73,73	1.33	7 (10%)	82,113,113	1.33	9 (10%)
28	STE	I	102	-	14,14,19	0.69	0	14,14,19	1.16	1 (7%)
28	STE	X	101	-	19,19,19	0.59	0	19,19,19	1.16	2 (10%)
24	CLA	b	609	2	69,73,73	1.31	8 (11%)	82,113,113	1.27	9 (10%)
26	BCR	C	515	-	41,41,41	0.33	0	56,56,56	0.72	0
28	STE	d	413	-	13,13,19	0.74	0	13,13,19	1.07	0
28	STE	A	611	-	8,8,19	0.39	0	7,7,19	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	B	617	-	41,41,41	0.41	0	56,56,56	0.75	1 (1%)
28	STE	e	101	-	8,8,19	0.38	0	7,7,19	0.68	0
32	DGD	H	102	-	63,63,67	0.54	0	77,77,81	0.97	4 (5%)
24	CLA	B	613	2	69,73,73	1.27	7 (10%)	82,113,113	1.37	5 (6%)
24	CLA	C	505	3	69,73,73	1.43	7 (10%)	82,113,113	1.43	6 (7%)
24	CLA	C	508	3	69,73,73	1.31	8 (11%)	82,113,113	1.43	8 (9%)
28	STE	C	527	-	13,13,19	0.34	0	12,12,19	0.86	0
29	LMG	a	615	-	49,49,55	0.48	0	57,57,63	0.96	3 (5%)
28	STE	i	102	-	5,5,19	0.41	0	4,4,19	0.46	0
28	STE	f	103	-	15,15,19	0.36	0	14,14,19	0.78	0
26	BCR	b	617	-	41,41,41	0.38	0	56,56,56	0.72	0
26	BCR	B	619	-	41,41,41	0.41	0	56,56,56	0.93	3 (5%)
29	LMG	C	517	-	35,35,55	0.50	0	43,43,63	1.43	6 (13%)
24	CLA	D	403	36	69,73,73	1.42	8 (11%)	82,113,113	1.35	8 (9%)
24	CLA	B	615	2	69,73,73	1.42	8 (11%)	82,113,113	1.37	5 (6%)
32	DGD	h	101	-	63,63,67	0.56	0	77,77,81	0.94	7 (9%)
28	STE	A	618	-	16,16,19	0.42	0	15,15,19	0.64	0
34	HEM	F	101	5,6	50,50,50	1.46	8 (16%)	67,82,82	1.23	3 (4%)
24	CLA	B	606	2	69,73,73	1.30	8 (11%)	82,113,113	1.35	7 (8%)
24	CLA	C	507	36	69,73,73	1.28	7 (10%)	82,113,113	1.48	8 (9%)
28	STE	e	104	-	8,8,19	0.38	0	7,7,19	0.72	0
32	DGD	c	518	-	63,63,67	0.62	0	77,77,81	0.89	3 (3%)
24	CLA	B	614	2	69,73,73	1.24	7 (10%)	82,113,113	1.46	8 (9%)
31	LHG	d	409	-	38,38,48	0.59	0	41,44,54	0.68	0
21	OEX	a	601	36,1,3	0,14,14	-	-	-	-	-
24	CLA	b	608	2	69,73,73	1.17	7 (10%)	82,113,113	1.34	10 (12%)
24	CLA	C	504	36	63,67,73	1.32	8 (12%)	74,105,113	1.29	7 (9%)
25	PHO	a	608	-	58,69,69	2.15	8 (13%)	55,99,99	1.76	13 (23%)
24	CLA	b	615	2	69,73,73	1.38	9 (13%)	82,113,113	1.40	5 (6%)
31	LHG	e	103	-	41,41,48	0.57	0	44,47,54	0.58	0
34	HEM	e	102	5,6	50,50,50	1.58	8 (16%)	67,82,82	1.35	9 (13%)
31	LHG	D	412	-	46,46,48	0.54	0	49,52,54	0.64	1 (2%)
24	CLA	C	502	3	69,73,73	1.45	9 (13%)	82,113,113	1.22	4 (4%)
28	STE	B	621	-	16,16,19	0.65	0	16,16,19	1.16	0
28	STE	B	624	-	13,13,19	0.67	0	13,13,19	1.26	2 (15%)
28	STE	C	528	-	13,13,19	0.31	0	12,12,19	0.83	0
21	OEX	A	601	36,1,3	0,14,14	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	B	620	-	45,45,55	0.59	0	53,53,63	1.23	6 (11%)
28	STE	b	621	-	19,19,19	0.62	0	19,19,19	1.13	0
26	BCR	K	101	-	41,41,41	0.38	0	56,56,56	0.85	0
24	CLA	b	604	2	69,73,73	1.36	6 (8%)	82,113,113	1.58	11 (13%)
28	STE	M	102	-	14,14,19	0.62	0	14,14,19	1.25	1 (7%)
24	CLA	A	608	1	58,62,73	1.17	5 (8%)	68,99,113	1.36	10 (14%)
28	STE	t	102	-	9,9,19	0.39	0	8,8,19	0.69	0
24	CLA	b	614	2	69,73,73	1.26	8 (11%)	82,113,113	1.38	9 (10%)
24	CLA	C	512	3	69,73,73	1.32	10 (14%)	82,113,113	1.32	7 (8%)
27	PL9	d	406	-	55,55,55	1.10	4 (7%)	68,69,69	1.54	15 (22%)
28	STE	H	104	-	8,8,19	0.37	0	7,7,19	0.71	0
24	CLA	C	510	3	69,73,73	1.40	10 (14%)	82,113,113	1.34	5 (6%)
31	LHG	D	411	-	48,48,48	0.55	0	51,54,54	0.67	1 (1%)
28	STE	C	525	-	11,11,19	0.83	0	11,11,19	1.21	1 (9%)
28	STE	d	412	-	19,19,19	0.64	0	19,19,19	0.90	0
24	CLA	a	609	1	69,73,73	1.16	7 (10%)	82,113,113	1.23	9 (10%)
24	CLA	b	606	2	69,73,73	1.50	9 (13%)	82,113,113	1.43	7 (8%)
30	SQD	a	613	-	52,54,54	1.50	7 (13%)	62,65,65	1.70	13 (20%)
28	STE	C	526	-	15,15,19	0.32	0	14,14,19	0.84	0
28	STE	l	102	-	17,17,19	0.31	0	16,16,19	0.91	0
24	CLA	b	601	36	69,73,73	1.25	8 (11%)	82,113,113	1.32	8 (9%)
27	PL9	A	610	-	55,55,55	0.81	2 (3%)	68,69,69	1.61	10 (14%)
28	STE	E	102	-	11,11,19	0.35	0	10,10,19	0.77	0
28	STE	C	516	-	13,13,19	0.78	0	13,13,19	1.11	1 (7%)
28	STE	b	625	-	9,9,19	0.36	0	8,8,19	0.67	0
28	STE	d	410	-	19,19,19	0.60	0	19,19,19	1.10	1 (5%)
29	LMG	A	612	-	48,48,55	0.47	0	56,56,63	0.77	0
28	STE	C	518	-	4,4,19	0.41	0	3,3,19	0.41	0
29	LMG	C	524	-	48,48,55	0.47	0	56,56,63	0.67	0
31	LHG	a	612	-	48,48,48	0.58	0	51,54,54	0.55	0
35	HEC	V	201	16	50,50,50	1.75	6 (12%)	68,82,82	1.48	7 (10%)
28	STE	H	103	-	17,17,19	0.41	0	16,16,19	0.75	0
24	CLA	c	501	3	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
24	CLA	b	610	36	69,73,73	1.33	8 (11%)	82,113,113	1.23	9 (10%)
24	CLA	B	609	2	69,73,73	1.33	6 (8%)	82,113,113	1.29	6 (7%)
26	BCR	a	610	-	41,41,41	0.38	0	56,56,56	0.75	1 (1%)
28	STE	E	101	-	11,11,19	0.74	0	11,11,19	1.16	1 (9%)
28	STE	a	616	-	11,11,19	0.76	0	11,11,19	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	404	4	69,73,73	1.28	11 (15%)	82,113,113	1.20	9 (10%)
26	BCR	c	515	-	41,41,41	0.37	0	56,56,56	0.81	1 (1%)
27	PL9	a	611	-	55,55,55	0.67	0	68,69,69	1.61	10 (14%)
24	CLA	c	505	3	69,73,73	1.22	9 (13%)	82,113,113	1.36	10 (12%)
28	STE	h	103	-	10,10,19	0.34	0	9,9,19	0.71	0
30	SQD	D	410	-	34,36,54	1.50	4 (11%)	42,45,65	1.91	9 (21%)
28	STE	Z	101	-	16,16,19	0.40	0	15,15,19	0.70	0
28	STE	E	103	-	19,19,19	0.62	0	19,19,19	1.15	2 (10%)
29	LMG	B	625	-	55,55,55	0.49	0	63,63,63	1.25	4 (6%)
30	SQD	a	614	-	52,54,54	1.59	8 (15%)	62,65,65	1.70	11 (17%)
28	STE	d	407	-	19,19,19	0.67	0	19,19,19	0.92	1 (5%)
24	CLA	A	605	1	69,73,73	1.44	9 (13%)	82,113,113	1.35	8 (9%)
24	CLA	B	604	2	69,73,73	1.36	7 (10%)	82,113,113	1.39	7 (8%)
24	CLA	c	506	3	69,73,73	1.23	8 (11%)	82,113,113	1.17	7 (8%)
25	PHO	a	607	-	58,69,69	2.03	11 (18%)	55,99,99	1.60	11 (20%)
24	CLA	c	512	3	69,73,73	1.31	8 (11%)	82,113,113	1.34	6 (7%)
28	STE	m	102	-	11,11,19	0.68	0	11,11,19	1.38	2 (18%)
24	CLA	c	510	3	69,73,73	1.30	9 (13%)	82,113,113	1.28	6 (7%)
30	SQD	A	613	-	50,52,54	1.57	7 (14%)	60,63,65	1.98	12 (20%)
29	LMG	D	408	-	50,50,55	0.42	0	58,58,63	1.18	7 (12%)
28	STE	A	617	-	7,7,19	0.34	0	6,6,19	0.70	0
24	CLA	c	504	36	64,68,73	1.24	8 (12%)	76,107,113	1.37	10 (13%)
24	CLA	C	513	3	69,73,73	1.48	10 (14%)	82,113,113	1.33	10 (12%)
24	CLA	B	608	2	69,73,73	1.20	6 (8%)	82,113,113	1.19	7 (8%)
24	CLA	A	606	36	69,73,73	1.36	8 (11%)	82,113,113	1.31	10 (12%)
24	CLA	C	501	3	69,73,73	1.43	8 (11%)	82,113,113	1.32	6 (7%)
28	STE	B	627	-	11,11,19	0.73	0	11,11,19	1.11	1 (9%)
28	STE	i	101	-	11,11,19	0.75	0	11,11,19	1.18	1 (9%)
29	LMG	c	516	-	29,29,55	0.40	0	31,31,63	0.63	1 (3%)
32	DGD	C	522	-	63,63,67	0.60	0	77,77,81	0.81	1 (1%)
28	STE	z	701	-	12,12,19	0.36	0	11,11,19	0.73	0
28	STE	b	624	-	14,14,19	0.32	0	13,13,19	0.89	0
30	SQD	b	620	-	47,49,54	1.61	8 (17%)	57,60,65	1.92	13 (22%)
26	BCR	c	514	-	41,41,41	0.33	0	56,56,56	0.50	0
31	LHG	B	622	-	48,48,48	0.60	1 (2%)	51,54,54	0.92	2 (3%)
26	BCR	k	101	-	41,41,41	0.38	0	56,56,56	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	612	2	69,73,73	1.17	8 (11%)	82,113,113	1.57	11 (13%)
28	STE	f	102	-	7,7,19	0.38	0	6,6,19	0.66	0
32	DGD	C	521	-	63,63,67	0.58	0	77,77,81	0.89	2 (2%)
24	CLA	b	612	2	69,73,73	1.29	8 (11%)	82,113,113	1.42	12 (14%)
33	BCT	d	401	22	3,3,3	0.81	0	2,3,3	2.02	1 (50%)
28	STE	I	101	-	16,16,19	0.72	0	16,16,19	1.02	1 (6%)
24	CLA	c	503	3	69,73,73	1.39	9 (13%)	82,113,113	1.39	8 (9%)
28	STE	b	623	-	15,15,19	0.74	0	15,15,19	1.14	2 (13%)
24	CLA	D	404	4	69,73,73	1.24	8 (11%)	82,113,113	1.26	9 (10%)
24	CLA	C	503	3	69,73,73	1.40	8 (11%)	82,113,113	1.59	11 (13%)
25	PHO	A	607	-	58,69,69	2.03	9 (15%)	55,99,99	1.84	10 (18%)
28	STE	B	628	-	14,14,19	0.40	0	13,13,19	0.78	0
28	STE	h	102	-	9,9,19	0.38	0	8,8,19	0.66	0
26	BCR	T	101	-	41,41,41	0.52	0	56,56,56	1.00	2 (3%)
27	PL9	D	407	-	55,55,55	0.98	2 (3%)	68,69,69	1.47	14 (20%)
30	SQD	A	615	-	41,43,54	1.79	9 (21%)	51,54,65	1.57	8 (15%)
31	LHG	L	101	-	48,48,48	0.49	0	51,54,54	0.72	1 (1%)
29	LMG	c	522	-	48,48,55	0.49	0	56,56,63	0.84	3 (5%)
24	CLA	C	509	3	69,73,73	1.17	6 (8%)	82,113,113	1.31	8 (9%)
24	CLA	D	405	4	69,73,73	1.20	9 (13%)	82,113,113	1.26	7 (8%)
29	LMG	c	521	-	46,46,55	0.51	0	54,54,63	0.65	0
35	HEC	v	201	16	50,50,50	1.77	9 (18%)	68,82,82	1.39	9 (13%)
28	STE	B	626	-	17,17,19	0.58	0	17,17,19	1.26	2 (11%)
28	STE	M	103	-	9,9,19	0.39	0	8,8,19	0.75	0
30	SQD	B	623	-	52,54,54	1.56	8 (15%)	62,65,65	1.81	14 (22%)
24	CLA	a	605	1	69,73,73	1.48	11 (15%)	82,113,113	1.36	7 (8%)
24	CLA	d	402	36	69,73,73	1.42	7 (10%)	82,113,113	1.35	7 (8%)
32	DGD	c	519	-	63,63,67	0.60	0	77,77,81	0.87	5 (6%)
32	DGD	c	520	-	63,63,67	0.56	0	77,77,81	0.79	2 (2%)
26	BCR	B	618	-	41,41,41	0.40	0	56,56,56	0.84	1 (1%)
28	STE	T	102	-	15,15,19	0.41	0	14,14,19	0.74	0
24	CLA	B	603	2	69,73,73	1.23	5 (7%)	82,113,113	1.16	5 (6%)
31	LHG	d	408	-	48,48,48	0.50	0	51,54,54	0.72	1 (1%)
28	STE	C	520	-	9,9,19	0.39	0	8,8,19	0.67	0
24	CLA	a	606	36	69,73,73	1.17	5 (7%)	82,113,113	1.32	6 (7%)
31	LHG	A	614	-	48,48,48	0.55	0	51,54,54	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	403	4	69,73,73	1.35	10 (14%)	82,113,113	1.34	6 (7%)
26	BCR	d	405	-	41,41,41	0.43	0	56,56,56	1.03	2 (3%)
24	CLA	C	506	3	69,73,73	1.21	8 (11%)	82,113,113	1.31	7 (8%)
24	CLA	b	602	2	69,73,73	1.36	8 (11%)	82,113,113	1.43	7 (8%)
28	STE	A	619	-	10,10,19	0.39	0	9,9,19	0.67	0
29	LMG	d	411	-	44,44,55	0.52	0	52,52,63	0.69	2 (3%)
26	BCR	x	101	-	41,41,41	0.40	0	56,56,56	0.79	1 (1%)
33	BCT	D	401	22	3,3,3	0.83	0	2,3,3	1.58	1 (50%)
26	BCR	b	618	-	41,41,41	0.46	0	56,56,56	1.00	4 (7%)
26	BCR	b	619	-	41,41,41	0.39	0	56,56,56	0.67	1 (1%)
26	BCR	c	517	-	41,41,41	0.40	0	56,56,56	0.84	1 (1%)
29	LMG	m	101	-	51,51,55	0.49	0	59,59,63	0.98	3 (5%)
24	CLA	C	511	3	69,73,73	1.36	9 (13%)	82,113,113	1.33	6 (7%)
24	CLA	B	616	2	64,68,73	1.36	10 (15%)	76,107,113	1.50	11 (14%)
29	LMG	M	101	-	51,51,55	0.47	0	59,59,63	0.80	1 (1%)
24	CLA	B	601	36	69,73,73	1.39	7 (10%)	82,113,113	1.40	7 (8%)
24	CLA	B	607	36	69,73,73	1.24	5 (7%)	82,113,113	1.30	8 (9%)
30	SQD	f	101	-	39,41,54	1.67	7 (17%)	49,52,65	1.84	10 (20%)
24	CLA	c	502	3	69,73,73	1.25	8 (11%)	82,113,113	1.39	8 (9%)
31	LHG	l	101	-	48,48,48	0.50	0	51,54,54	0.52	0
29	LMG	b	622	-	55,55,55	0.47	0	63,63,63	1.00	4 (6%)
24	CLA	c	508	3	68,72,73	1.26	9 (13%)	80,111,113	1.36	10 (12%)
26	BCR	D	406	-	41,41,41	0.42	0	56,56,56	0.93	1 (1%)
26	BCR	A	609	-	41,41,41	0.46	0	56,56,56	0.84	1 (1%)
24	CLA	b	616	2	64,68,73	1.33	7 (10%)	76,107,113	1.51	10 (13%)
24	CLA	B	605	2	69,73,73	1.15	5 (7%)	82,113,113	1.24	6 (7%)
26	BCR	t	101	-	41,41,41	0.49	0	56,56,56	1.11	4 (7%)
32	DGD	C	523	-	63,63,67	0.60	0	77,77,81	0.86	2 (2%)
25	PHO	D	402	-	58,69,69	2.05	13 (22%)	55,99,99	1.56	8 (14%)
24	CLA	B	611	2	69,73,73	1.22	9 (13%)	82,113,113	1.46	9 (10%)

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
24	CLA	c	507	36	-	13/39/115/115	-
24	CLA	b	607	36	-	16/39/115/115	-
26	BCR	J	101	-	-	4/29/63/63	0/2/2/2
32	DGD	A	616	-	-	18/55/95/95	0/2/2/2
28	STE	z	703	-	-	4/6/6/17	-
24	CLA	b	603	2	-	8/39/115/115	-
29	LMG	D	409	-	-	10/46/66/70	0/1/1/1
24	CLA	B	602	2	-	5/39/115/115	-
28	STE	e	105	-	-	2/10/10/17	-
24	CLA	b	613	2	-	8/39/115/115	-
24	CLA	b	605	2	-	13/39/115/115	-
24	CLA	c	513	3	-	12/39/115/115	-
28	STE	j	101	-	-	3/9/9/17	-
24	CLA	c	511	3	-	4/39/115/115	-
28	STE	J	102	-	-	7/9/9/17	-
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
24	CLA	c	509	3	-	14/39/115/115	-
26	BCR	C	514	-	-	5/29/63/63	0/2/2/2
28	STE	C	519	-	-	3/4/4/17	-
28	STE	z	702	-	-	7/15/15/17	-
24	CLA	B	610	36	-	10/39/115/115	-
24	CLA	b	611	2	-	6/39/115/115	-
28	STE	I	102	-	-	6/12/12/17	-
28	STE	X	101	-	-	9/17/17/17	-
24	CLA	b	609	2	-	4/39/115/115	-
26	BCR	C	515	-	-	1/29/63/63	0/2/2/2
28	STE	d	413	-	-	4/11/11/17	-
28	STE	A	611	-	-	5/6/6/17	-
26	BCR	B	617	-	-	3/29/63/63	0/2/2/2
28	STE	e	101	-	-	2/6/6/17	-
32	DGD	H	102	-	-	15/51/91/95	0/2/2/2
24	CLA	B	613	2	-	16/39/115/115	-
24	CLA	C	505	3	-	9/39/115/115	-
24	CLA	C	508	3	-	5/39/115/115	-
28	STE	C	527	-	-	9/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	a	615	-	-	18/44/64/70	0/1/1/1
28	STE	i	102	-	-	2/3/3/17	-
28	STE	f	103	-	-	5/13/13/17	-
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMG	C	517	-	-	11/30/50/70	0/1/1/1
24	CLA	D	403	36	-	3/39/115/115	-
24	CLA	B	615	2	-	14/39/115/115	-
32	DGD	h	101	-	-	12/51/91/95	0/2/2/2
28	STE	A	618	-	-	11/14/14/17	-
34	HEM	F	101	5,6	-	2/14/54/54	-
24	CLA	B	606	2	-	12/39/115/115	-
24	CLA	C	507	36	-	12/39/115/115	-
28	STE	e	104	-	-	3/6/6/17	-
32	DGD	c	518	-	-	21/51/91/95	0/2/2/2
24	CLA	B	614	2	-	13/39/115/115	-
31	LHG	d	409	-	-	15/43/43/53	-
24	CLA	b	608	2	-	2/39/115/115	-
24	CLA	C	504	36	-	3/32/108/115	-
25	PHO	a	608	-	-	1/37/103/103	0/5/6/6
24	CLA	b	615	2	-	6/39/115/115	-
31	LHG	e	103	-	-	21/46/46/53	-
34	HEM	e	102	5,6	-	4/14/54/54	-
31	LHG	D	412	-	-	12/51/51/53	-
24	CLA	C	502	3	-	12/39/115/115	-
28	STE	B	621	-	-	9/14/14/17	-
28	STE	B	624	-	-	2/11/11/17	-
28	STE	C	528	-	-	7/11/11/17	-
29	LMG	B	620	-	-	13/40/60/70	0/1/1/1
28	STE	b	621	-	-	11/17/17/17	-
26	BCR	K	101	-	-	4/29/63/63	0/2/2/2
24	CLA	b	604	2	-	9/39/115/115	-
28	STE	M	102	-	-	10/12/12/17	-
24	CLA	A	608	1	-	3/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	t	102	-	-	2/7/7/17	-
24	CLA	b	614	2	-	17/39/115/115	-
24	CLA	C	512	3	-	14/39/115/115	-
27	PL9	d	406	-	-	13/53/73/73	0/1/1/1
28	STE	H	104	-	-	4/6/6/17	-
24	CLA	C	510	3	-	7/39/115/115	-
31	LHG	D	411	-	-	19/53/53/53	-
28	STE	C	525	-	-	3/9/9/17	-
28	STE	d	412	-	-	10/17/17/17	-
24	CLA	a	609	1	-	14/39/115/115	-
24	CLA	b	606	2	-	6/39/115/115	-
30	SQD	a	613	-	-	20/49/69/69	0/1/1/1
28	STE	C	526	-	-	8/13/13/17	-
28	STE	l	102	-	-	4/15/15/17	-
24	CLA	b	601	36	-	19/39/115/115	-
27	PL9	A	610	-	-	18/53/73/73	0/1/1/1
28	STE	E	102	-	-	5/9/9/17	-
28	STE	C	516	-	-	8/11/11/17	-
28	STE	b	625	-	-	6/7/7/17	-
28	STE	d	410	-	-	7/17/17/17	-
29	LMG	A	612	-	-	19/43/63/70	0/1/1/1
28	STE	C	518	-	-	0/2/2/17	-
29	LMG	C	524	-	-	21/43/63/70	0/1/1/1
31	LHG	a	612	-	-	18/53/53/53	-
35	HEC	V	201	16	1/1/3/7	5/14/54/54	-
28	STE	H	103	-	-	7/15/15/17	-
24	CLA	c	501	3	-	4/39/115/115	-
24	CLA	b	610	36	-	5/39/115/115	-
24	CLA	B	609	2	-	5/39/115/115	-
26	BCR	a	610	-	-	0/29/63/63	0/2/2/2
28	STE	E	101	-	-	4/9/9/17	-
28	STE	a	616	-	-	3/9/9/17	-
24	CLA	d	404	4	-	10/39/115/115	-
26	BCR	c	515	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	a	611	-	-	26/53/73/73	0/1/1/1
24	CLA	c	505	3	-	10/39/115/115	-
28	STE	h	103	-	-	7/8/8/17	-
30	SQD	D	410	-	-	16/28/48/69	0/1/1/1
28	STE	Z	101	-	-	8/14/14/17	-
28	STE	E	103	-	-	6/17/17/17	-
29	LMG	B	625	-	-	26/50/70/70	0/1/1/1
30	SQD	a	614	-	-	24/49/69/69	0/1/1/1
28	STE	d	407	-	-	10/17/17/17	-
24	CLA	A	605	1	-	11/39/115/115	-
24	CLA	B	604	2	-	10/39/115/115	-
24	CLA	c	506	3	-	17/39/115/115	-
25	PHO	a	607	-	-	6/37/103/103	0/5/6/6
24	CLA	c	512	3	-	17/39/115/115	-
28	STE	m	102	-	-	3/9/9/17	-
24	CLA	c	510	3	-	6/39/115/115	-
30	SQD	A	613	-	-	19/47/67/69	0/1/1/1
29	LMG	D	408	-	-	19/45/65/70	0/1/1/1
28	STE	A	617	-	-	4/5/5/17	-
24	CLA	c	504	36	-	5/33/109/115	-
24	CLA	C	513	3	-	14/39/115/115	-
24	CLA	B	608	2	-	10/39/115/115	-
24	CLA	A	606	36	-	9/39/115/115	-
24	CLA	C	501	3	-	4/39/115/115	-
28	STE	B	627	-	-	6/9/9/17	-
28	STE	i	101	-	-	6/9/9/17	-
29	LMG	c	516	-	-	8/31/31/70	-
32	DGD	C	522	-	-	19/51/91/95	0/2/2/2
28	STE	z	701	-	-	6/10/10/17	-
28	STE	b	624	-	-	9/12/12/17	-
30	SQD	b	620	-	-	19/44/64/69	0/1/1/1
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
31	LHG	B	622	-	-	18/53/53/53	-
26	BCR	k	101	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	612	2	-	10/39/115/115	-
28	STE	f	102	-	-	4/5/5/17	-
32	DGD	C	521	-	-	24/51/91/95	0/2/2/2
24	CLA	b	612	2	-	3/39/115/115	-
28	STE	I	101	-	-	8/14/14/17	-
24	CLA	c	503	3	-	8/39/115/115	-
28	STE	b	623	-	-	6/13/13/17	-
24	CLA	D	404	4	-	7/39/115/115	-
24	CLA	C	503	3	-	3/39/115/115	-
25	PHO	A	607	-	-	1/37/103/103	0/5/6/6
28	STE	B	628	-	-	7/12/12/17	-
28	STE	h	102	-	-	4/7/7/17	-
26	BCR	T	101	-	-	9/29/63/63	0/2/2/2
27	PL9	D	407	-	-	6/53/73/73	0/1/1/1
30	SQD	A	615	-	-	13/38/58/69	0/1/1/1
31	LHG	L	101	-	-	18/53/53/53	-
29	LMG	c	522	-	-	19/43/63/70	0/1/1/1
24	CLA	C	509	3	-	9/39/115/115	-
35	HEC	v	201	16	1/1/3/7	6/14/54/54	-
24	CLA	D	405	4	-	4/39/115/115	-
29	LMG	c	521	-	-	15/41/61/70	0/1/1/1
28	STE	B	626	-	-	8/15/15/17	-
28	STE	M	103	-	-	1/7/7/17	-
30	SQD	B	623	-	-	20/49/69/69	0/1/1/1
24	CLA	a	605	1	-	5/39/115/115	-
24	CLA	d	402	36	-	5/39/115/115	-
32	DGD	c	519	-	-	12/51/91/95	0/2/2/2
32	DGD	c	520	-	-	16/51/91/95	0/2/2/2
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
28	STE	T	102	-	-	7/13/13/17	-
24	CLA	B	603	2	-	7/39/115/115	-
31	LHG	d	408	-	-	20/53/53/53	-
28	STE	C	520	-	-	5/7/7/17	-
24	CLA	a	606	36	-	11/39/115/115	-
31	LHG	A	614	-	-	20/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	403	4	-	8/39/115/115	-
26	BCR	d	405	-	-	4/29/63/63	0/2/2/2
24	CLA	C	506	3	-	8/39/115/115	-
24	CLA	b	602	2	-	6/39/115/115	-
28	STE	A	619	-	-	4/8/8/17	-
29	LMG	d	411	-	-	8/39/59/70	0/1/1/1
26	BCR	x	101	-	-	1/29/63/63	0/2/2/2
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
26	BCR	c	517	-	-	3/29/63/63	0/2/2/2
29	LMG	m	101	-	-	21/46/66/70	0/1/1/1
24	CLA	C	511	3	-	8/39/115/115	-
24	CLA	B	616	2	-	13/33/109/115	-
29	LMG	M	101	-	-	21/46/66/70	0/1/1/1
24	CLA	B	601	36	-	27/39/115/115	-
24	CLA	B	607	36	-	7/39/115/115	-
30	SQD	f	101	-	-	16/36/56/69	0/1/1/1
24	CLA	c	502	3	-	11/39/115/115	-
31	LHG	l	101	-	-	17/53/53/53	-
29	LMG	b	622	-	-	23/50/70/70	0/1/1/1
24	CLA	c	508	3	-	6/38/114/115	-
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
26	BCR	A	609	-	-	3/29/63/63	0/2/2/2
24	CLA	b	616	2	-	9/33/109/115	-
24	CLA	B	605	2	-	10/39/115/115	-
26	BCR	t	101	-	-	11/29/63/63	0/2/2/2
32	DGD	C	523	-	-	15/51/91/95	0/2/2/2
25	PHO	D	402	-	-	1/37/103/103	0/5/6/6
24	CLA	B	611	2	-	9/39/115/115	-

All (694) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	608	PHO	C3B-C4B	9.29	1.50	1.41
25	a	608	PHO	C1B-C2B	9.21	1.49	1.39
25	A	607	PHO	C3B-C4B	8.53	1.50	1.41
25	D	402	PHO	C3B-C4B	8.51	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	607	PHO	C1B-C2B	8.26	1.48	1.39
25	a	607	PHO	C1B-C2B	8.24	1.48	1.39
25	D	402	PHO	C1B-C2B	8.00	1.48	1.39
25	a	607	PHO	C3B-C4B	7.81	1.49	1.41
24	C	505	CLA	MG-NA	7.61	2.24	2.06
35	v	201	HEC	C3D-C2D	7.41	1.52	1.36
35	V	201	HEC	C3D-C2D	7.27	1.52	1.36
24	d	402	CLA	MG-NA	7.09	2.23	2.06
24	b	606	CLA	MG-NA	6.93	2.22	2.06
24	C	501	CLA	MG-NA	6.54	2.21	2.06
35	V	201	HEC	FE-ND	6.38	2.14	1.94
24	B	609	CLA	MG-NA	6.26	2.21	2.06
24	b	611	CLA	MG-NA	6.23	2.21	2.06
24	c	511	CLA	MG-NA	6.18	2.21	2.06
24	B	615	CLA	MG-NA	5.89	2.20	2.06
24	B	604	CLA	MG-NA	5.83	2.20	2.06
24	C	513	CLA	MG-ND	5.77	2.17	2.05
24	B	601	CLA	MG-NA	5.65	2.19	2.06
34	e	102	HEM	FE-NB	5.55	2.12	1.94
24	c	503	CLA	MG-NB	5.46	2.16	2.05
24	A	605	CLA	MG-ND	-5.42	1.95	2.05
25	a	607	PHO	C1D-C2D	5.41	1.45	1.39
24	C	503	CLA	MG-NA	5.35	2.19	2.06
24	C	502	CLA	MG-NA	5.28	2.18	2.06
24	a	605	CLA	MG-NB	5.28	2.16	2.05
24	A	606	CLA	MG-NB	-5.25	1.95	2.05
24	D	403	CLA	MG-NB	5.25	2.16	2.05
24	C	511	CLA	MG-NA	5.22	2.18	2.06
24	B	603	CLA	MG-NA	5.16	2.18	2.06
24	B	610	CLA	MG-NA	5.04	2.18	2.06
24	b	610	CLA	MG-NB	-4.91	1.96	2.05
24	b	602	CLA	MG-ND	-4.91	1.96	2.05
24	C	502	CLA	MG-NB	-4.88	1.96	2.05
24	B	606	CLA	MG-NA	4.88	2.17	2.06
30	D	410	SQD	O48-C23	4.86	1.47	1.33
30	a	614	SQD	O48-C23	4.84	1.47	1.33
24	C	504	CLA	MG-NA	4.80	2.17	2.06
35	v	201	HEC	FE-NA	4.74	2.10	1.95
30	B	623	SQD	O48-C23	4.73	1.47	1.33
30	A	615	SQD	O48-C23	4.73	1.47	1.33
30	f	101	SQD	O48-C23	4.73	1.47	1.33
30	A	613	SQD	O48-C23	4.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	MG-NA	4.72	2.17	2.06
24	C	512	CLA	MG-NB	4.70	2.15	2.05
34	e	102	HEM	FE-NA	4.62	2.10	1.95
30	b	620	SQD	O48-C23	4.59	1.46	1.33
24	C	507	CLA	MG-NA	4.58	2.17	2.06
25	A	607	PHO	C1D-C2D	4.56	1.44	1.39
24	b	616	CLA	MG-NA	4.54	2.17	2.06
35	v	201	HEC	FE-NB	4.52	2.08	1.94
24	b	606	CLA	MG-NB	4.52	2.14	2.05
24	b	609	CLA	MG-NC	4.50	2.17	2.06
27	d	406	PL9	C3-C4	-4.46	1.42	1.49
24	c	507	CLA	MG-NB	-4.43	1.97	2.05
24	D	404	CLA	MG-NC	4.37	2.16	2.06
24	c	510	CLA	MG-NA	4.36	2.16	2.06
25	a	608	PHO	C1D-C2D	4.36	1.44	1.39
24	d	403	CLA	MG-NB	-4.33	1.97	2.05
24	c	505	CLA	MG-NA	4.28	2.16	2.06
30	a	613	SQD	O48-C23	4.27	1.45	1.33
34	F	101	HEM	FE-NC	4.15	2.08	1.95
24	B	607	CLA	MG-NA	4.15	2.16	2.06
24	A	605	CLA	MG-NB	4.14	2.14	2.05
24	b	615	CLA	MG-NA	4.14	2.16	2.06
24	B	613	CLA	MG-NC	4.09	2.16	2.06
24	B	604	CLA	C1D-ND	4.01	1.43	1.37
24	c	509	CLA	MG-NB	-3.97	1.97	2.05
24	D	405	CLA	C1D-ND	3.97	1.43	1.37
24	b	605	CLA	MG-NA	3.90	2.15	2.06
24	C	501	CLA	C1D-ND	3.89	1.43	1.37
24	B	613	CLA	C1D-ND	3.88	1.43	1.37
24	B	602	CLA	MG-NC	3.86	2.15	2.06
30	a	613	SQD	O47-C45	-3.85	1.37	1.46
24	a	609	CLA	C1D-ND	3.84	1.42	1.37
24	c	503	CLA	MG-NA	3.83	2.15	2.06
24	c	504	CLA	C4B-NB	3.83	1.42	1.37
24	b	604	CLA	C1D-ND	3.83	1.42	1.37
24	C	513	CLA	MG-NB	-3.82	1.98	2.05
24	C	510	CLA	C1D-ND	3.82	1.42	1.37
24	b	609	CLA	C1D-ND	3.82	1.42	1.37
24	d	403	CLA	MG-NA	3.82	2.15	2.06
24	b	614	CLA	MG-NA	3.80	2.15	2.06
24	C	513	CLA	MG-NA	3.78	2.15	2.06
24	b	610	CLA	C1D-ND	3.78	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	C1D-ND	3.75	1.42	1.37
24	b	612	CLA	MG-NC	3.75	2.15	2.06
24	c	509	CLA	C1D-ND	3.75	1.42	1.37
24	B	615	CLA	C1D-ND	3.75	1.42	1.37
24	a	605	CLA	C1D-ND	3.74	1.42	1.37
24	c	507	CLA	C1D-ND	3.74	1.42	1.37
30	A	615	SQD	O5-C1	3.72	1.51	1.41
24	b	602	CLA	C1D-ND	3.71	1.42	1.37
24	c	512	CLA	C1D-ND	3.71	1.42	1.37
24	b	615	CLA	C1D-ND	3.68	1.42	1.37
24	A	605	CLA	C1D-ND	3.67	1.42	1.37
30	A	613	SQD	O47-C45	-3.66	1.38	1.46
30	a	614	SQD	O5-C1	3.65	1.51	1.41
24	C	503	CLA	MG-ND	3.64	2.13	2.05
24	B	610	CLA	C4B-NB	3.64	1.42	1.37
24	b	606	CLA	C1D-ND	3.64	1.42	1.37
24	b	604	CLA	C4B-NB	3.64	1.42	1.37
24	c	510	CLA	C1D-ND	3.63	1.42	1.37
24	C	510	CLA	C4B-NB	3.63	1.42	1.37
24	D	403	CLA	C1D-ND	3.63	1.42	1.37
25	D	402	PHO	C1D-C2D	3.63	1.43	1.39
24	B	601	CLA	C4B-NB	3.62	1.42	1.37
24	B	608	CLA	MG-NA	3.61	2.14	2.06
30	f	101	SQD	O47-C45	-3.61	1.38	1.46
24	b	614	CLA	C4B-NB	3.60	1.42	1.37
24	B	607	CLA	C1D-ND	3.60	1.42	1.37
30	b	620	SQD	O47-C7	3.60	1.44	1.34
24	b	601	CLA	C1D-ND	3.58	1.42	1.37
24	B	616	CLA	C1D-ND	3.58	1.42	1.37
24	b	613	CLA	C4B-NB	3.58	1.42	1.37
24	c	513	CLA	C1D-ND	3.58	1.42	1.37
24	d	402	CLA	C1D-ND	3.58	1.42	1.37
24	C	508	CLA	MG-NA	3.58	2.14	2.06
24	C	508	CLA	C1D-ND	3.57	1.42	1.37
24	c	511	CLA	C1D-ND	3.57	1.42	1.37
24	C	509	CLA	C1D-ND	3.57	1.42	1.37
25	a	607	PHO	C4D-CHA	3.56	1.44	1.39
24	c	508	CLA	C1D-ND	3.56	1.42	1.37
24	B	602	CLA	C1D-ND	3.56	1.42	1.37
24	b	612	CLA	C1D-ND	3.56	1.42	1.37
24	A	608	CLA	C1D-ND	3.56	1.42	1.37
34	F	101	HEM	FE-NA	3.55	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	615	SQD	O47-C7	3.55	1.44	1.34
24	B	608	CLA	C1D-ND	3.54	1.42	1.37
24	B	614	CLA	C1D-ND	3.54	1.42	1.37
25	a	608	PHO	C4D-CHA	3.50	1.44	1.39
24	c	506	CLA	MG-ND	-3.50	1.98	2.05
24	b	616	CLA	C1D-ND	3.50	1.42	1.37
30	B	623	SQD	O47-C45	-3.50	1.38	1.46
30	a	614	SQD	O47-C7	3.49	1.44	1.34
24	b	604	CLA	C1B-C2B	3.48	1.51	1.43
24	C	502	CLA	C1D-ND	3.47	1.42	1.37
24	d	404	CLA	C4B-NB	3.47	1.42	1.37
24	B	606	CLA	C1D-ND	3.47	1.42	1.37
24	c	502	CLA	C1D-ND	3.45	1.42	1.37
24	C	506	CLA	C1D-ND	3.43	1.42	1.37
24	a	605	CLA	MG-NA	3.42	2.14	2.06
24	c	513	CLA	MG-NA	3.41	2.14	2.06
24	B	609	CLA	C1D-ND	3.40	1.42	1.37
24	C	507	CLA	MG-ND	-3.39	1.99	2.05
24	C	513	CLA	C1D-ND	3.39	1.42	1.37
24	C	504	CLA	C4B-NB	3.38	1.42	1.37
24	D	403	CLA	CHC-C1C	3.37	1.45	1.38
30	f	101	SQD	O47-C7	3.37	1.43	1.34
24	B	602	CLA	C4B-NB	3.37	1.42	1.37
24	c	506	CLA	C1D-ND	3.35	1.42	1.37
24	c	507	CLA	C1B-C2B	3.35	1.51	1.43
24	B	601	CLA	C1D-ND	3.35	1.42	1.37
24	b	614	CLA	C1D-ND	3.34	1.42	1.37
24	C	503	CLA	C1D-ND	3.34	1.42	1.37
24	c	507	CLA	C4B-NB	3.33	1.42	1.37
30	A	613	SQD	O47-C7	3.33	1.43	1.34
30	A	615	SQD	C24-C23	3.33	1.60	1.50
24	b	615	CLA	MG-ND	-3.32	1.99	2.05
24	B	615	CLA	C4B-NB	3.31	1.42	1.37
24	b	612	CLA	C4B-NB	3.31	1.42	1.37
24	c	512	CLA	C4B-NB	3.31	1.42	1.37
24	A	606	CLA	MG-ND	3.31	2.12	2.05
24	C	507	CLA	C1D-ND	3.31	1.42	1.37
24	C	501	CLA	C4B-NB	3.30	1.42	1.37
24	C	505	CLA	C1D-ND	3.29	1.42	1.37
24	d	404	CLA	C1D-ND	3.29	1.42	1.37
24	b	613	CLA	C1D-ND	3.28	1.42	1.37
24	c	503	CLA	C1D-ND	3.28	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C1B-C2B	3.28	1.50	1.43
24	c	511	CLA	C4B-NB	3.28	1.42	1.37
24	B	616	CLA	MG-NA	3.28	2.14	2.06
24	B	605	CLA	C1B-C2B	3.28	1.50	1.43
24	c	501	CLA	C1D-ND	3.27	1.42	1.37
30	B	623	SQD	O47-C7	3.26	1.43	1.34
24	b	605	CLA	C1B-C2B	3.26	1.50	1.43
24	B	614	CLA	C4B-NB	3.25	1.42	1.37
24	A	605	CLA	C1B-C2B	3.25	1.50	1.43
24	b	612	CLA	MG-ND	-3.25	1.99	2.05
24	c	507	CLA	MG-NA	3.25	2.14	2.06
24	a	606	CLA	C4B-NB	3.25	1.42	1.37
24	a	605	CLA	C1B-C2B	3.24	1.50	1.43
24	a	606	CLA	CHC-C1C	3.24	1.45	1.38
24	B	611	CLA	C1D-ND	3.24	1.42	1.37
24	B	616	CLA	C4B-NB	3.23	1.42	1.37
24	B	610	CLA	C1D-ND	3.23	1.42	1.37
24	D	404	CLA	C1B-C2B	3.23	1.50	1.43
24	c	512	CLA	C1B-C2B	3.23	1.50	1.43
24	B	616	CLA	MG-NC	3.22	2.13	2.06
24	b	615	CLA	C4B-NB	3.22	1.42	1.37
24	C	510	CLA	MG-NA	3.22	2.13	2.06
30	A	615	SQD	O47-C45	-3.21	1.39	1.46
24	C	511	CLA	C1B-C2B	3.20	1.50	1.43
24	a	609	CLA	C4B-NB	3.20	1.42	1.37
24	c	512	CLA	MG-NC	3.19	2.13	2.06
24	b	608	CLA	C4B-NB	3.19	1.42	1.37
24	D	403	CLA	C4B-NB	3.19	1.42	1.37
24	b	602	CLA	MG-NA	3.18	2.13	2.06
24	C	510	CLA	MG-NB	-3.18	1.99	2.05
24	b	604	CLA	MG-NC	3.17	2.13	2.06
30	f	101	SQD	C24-C23	3.17	1.59	1.50
25	D	402	PHO	C3D-C4D	3.17	1.45	1.41
24	b	601	CLA	C1B-C2B	3.17	1.50	1.43
25	D	402	PHO	CMC-C2C	-3.16	1.45	1.50
24	b	610	CLA	MG-NC	3.16	2.13	2.06
24	b	613	CLA	MG-NA	3.14	2.13	2.06
24	c	512	CLA	MG-NB	3.14	2.12	2.05
24	c	510	CLA	C1B-C2B	3.14	1.50	1.43
24	B	607	CLA	C4B-NB	3.13	1.42	1.37
24	C	511	CLA	C4B-NB	3.13	1.42	1.37
24	b	601	CLA	C4B-NB	3.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C1D-ND	3.12	1.42	1.37
30	b	620	SQD	O5-C1	3.12	1.49	1.41
24	C	508	CLA	C4B-NB	3.12	1.42	1.37
24	d	402	CLA	C1B-C2B	3.12	1.50	1.43
24	C	506	CLA	C4B-NB	3.12	1.42	1.37
24	B	610	CLA	MG-NB	-3.12	1.99	2.05
24	C	512	CLA	C1D-ND	3.11	1.42	1.37
24	B	611	CLA	C1B-C2B	3.11	1.50	1.43
30	D	410	SQD	C24-C23	3.11	1.59	1.50
24	b	601	CLA	MG-NA	3.11	2.13	2.06
24	b	608	CLA	C1D-ND	3.10	1.41	1.37
24	B	603	CLA	C1D-ND	3.10	1.41	1.37
30	a	614	SQD	C24-C23	3.10	1.59	1.50
24	B	615	CLA	C1B-C2B	3.09	1.50	1.43
24	C	502	CLA	C4B-NB	3.09	1.41	1.37
24	B	613	CLA	C1B-C2B	3.09	1.50	1.43
24	a	605	CLA	C4B-NB	3.09	1.41	1.37
24	c	513	CLA	C4B-NB	3.08	1.41	1.37
24	B	603	CLA	C1B-C2B	3.08	1.50	1.43
24	b	615	CLA	C1B-C2B	3.08	1.50	1.43
24	B	614	CLA	MG-NC	3.07	2.13	2.06
30	a	614	SQD	O47-C45	-3.07	1.39	1.46
24	B	606	CLA	C4B-NB	3.07	1.41	1.37
24	B	614	CLA	MG-NA	3.06	2.13	2.06
24	c	508	CLA	C4B-NB	3.05	1.41	1.37
24	c	502	CLA	MG-NB	-3.04	1.99	2.05
24	C	511	CLA	C1D-ND	3.04	1.41	1.37
24	D	403	CLA	C3B-C4B	3.04	1.51	1.42
25	A	607	PHO	C4D-CHA	3.03	1.44	1.39
24	c	502	CLA	MG-NA	3.03	2.13	2.06
24	D	404	CLA	C1D-ND	3.02	1.41	1.37
30	a	613	SQD	O47-C7	3.02	1.42	1.34
24	d	404	CLA	MG-NB	-3.00	1.99	2.05
24	b	616	CLA	MG-ND	3.00	2.11	2.05
24	C	508	CLA	C1B-C2B	3.00	1.50	1.43
30	b	620	SQD	O47-C45	-3.00	1.39	1.46
24	b	603	CLA	C1D-ND	3.00	1.41	1.37
24	C	504	CLA	C1D-ND	3.00	1.41	1.37
24	B	616	CLA	MG-ND	2.99	2.11	2.05
24	b	606	CLA	C1B-C2B	2.99	1.50	1.43
35	v	201	HEC	FE-ND	2.98	2.04	1.94
30	b	620	SQD	C24-C23	2.97	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	MG-NC	2.97	2.13	2.06
30	A	613	SQD	C24-C23	2.96	1.59	1.50
24	a	606	CLA	C1D-ND	2.96	1.41	1.37
24	C	505	CLA	C1B-C2B	2.96	1.50	1.43
24	C	503	CLA	C1B-C2B	2.96	1.50	1.43
24	B	612	CLA	C4B-NB	2.96	1.41	1.37
30	D	410	SQD	O5-C1	2.96	1.49	1.41
24	A	606	CLA	C4B-NB	2.95	1.41	1.37
24	c	513	CLA	MG-ND	-2.95	1.99	2.05
24	B	614	CLA	MG-ND	-2.95	1.99	2.05
24	b	602	CLA	MG-NB	2.95	2.11	2.05
24	b	609	CLA	C4B-NB	2.95	1.41	1.37
24	C	502	CLA	C1B-C2B	2.94	1.50	1.43
30	a	613	SQD	O5-C1	2.94	1.49	1.41
24	c	508	CLA	MG-ND	2.93	2.11	2.05
24	c	511	CLA	C1B-C2B	2.93	1.50	1.43
25	D	402	PHO	C4D-CHA	2.93	1.43	1.39
35	V	201	HEC	FE-NA	2.92	2.04	1.95
24	c	509	CLA	C1B-C2B	2.92	1.50	1.43
24	B	616	CLA	C1B-C2B	2.92	1.50	1.43
30	B	623	SQD	O5-C1	2.91	1.49	1.41
24	b	602	CLA	C1B-C2B	2.91	1.49	1.43
24	C	513	CLA	C4B-NB	2.91	1.41	1.37
24	C	506	CLA	MG-NA	2.90	2.13	2.06
24	b	611	CLA	C1D-ND	2.90	1.41	1.37
24	d	404	CLA	MG-NA	2.90	2.13	2.06
24	B	601	CLA	MG-NB	-2.90	2.00	2.05
24	B	609	CLA	C1B-C2B	2.90	1.49	1.43
24	B	604	CLA	C1B-C2B	2.90	1.49	1.43
24	C	505	CLA	C4B-NB	2.90	1.41	1.37
24	b	605	CLA	C4B-NB	2.90	1.41	1.37
24	c	504	CLA	MG-ND	-2.89	2.00	2.05
24	b	608	CLA	C3B-C4B	2.89	1.51	1.42
24	b	607	CLA	MG-NA	2.89	2.13	2.06
24	c	506	CLA	C4B-NB	2.89	1.41	1.37
24	b	612	CLA	C1B-C2B	2.89	1.49	1.43
24	A	605	CLA	MG-NA	2.88	2.13	2.06
30	a	613	SQD	C24-C23	2.87	1.59	1.50
24	c	501	CLA	C4B-NB	2.86	1.41	1.37
24	c	502	CLA	C1B-C2B	2.86	1.49	1.43
24	b	608	CLA	CHC-C1C	2.85	1.44	1.38
24	c	513	CLA	C1B-C2B	2.85	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	MG-NB	2.85	2.11	2.05
24	C	503	CLA	C4B-NB	2.85	1.41	1.37
24	B	609	CLA	C4B-NB	2.84	1.41	1.37
24	B	612	CLA	CHC-C1C	2.84	1.44	1.38
30	B	623	SQD	C24-C23	2.84	1.58	1.50
34	F	101	HEM	CAB-C3B	2.83	1.54	1.47
24	d	404	CLA	C1B-C2B	2.83	1.49	1.43
24	b	615	CLA	MG-NB	2.83	2.11	2.05
24	B	613	CLA	MG-NA	2.83	2.13	2.06
24	B	608	CLA	C1B-C2B	2.82	1.49	1.43
24	C	507	CLA	C4B-NB	2.82	1.41	1.37
34	F	101	HEM	FE-ND	2.82	2.03	1.94
24	D	405	CLA	C1B-C2B	2.81	1.49	1.43
24	C	501	CLA	CHC-C1C	2.81	1.44	1.38
24	B	610	CLA	C1B-C2B	2.80	1.49	1.43
24	c	508	CLA	C1B-C2B	2.80	1.49	1.43
27	D	407	PL9	C6-C1	-2.80	1.43	1.48
24	c	503	CLA	C1B-C2B	2.80	1.49	1.43
24	b	610	CLA	C1B-C2B	2.79	1.49	1.43
24	b	602	CLA	C4B-NB	2.79	1.41	1.37
24	B	601	CLA	C1B-C2B	2.79	1.49	1.43
25	a	608	PHO	CMD-C2D	-2.79	1.46	1.51
24	A	605	CLA	C4B-NB	2.79	1.41	1.37
24	b	607	CLA	C1D-ND	2.78	1.41	1.37
34	F	101	HEM	CAC-C3C	2.78	1.54	1.47
24	C	513	CLA	C1B-C2B	2.78	1.49	1.43
30	A	613	SQD	O5-C1	2.77	1.49	1.41
24	B	608	CLA	C4B-NB	2.77	1.41	1.37
24	b	616	CLA	C1B-C2B	2.77	1.49	1.43
24	b	611	CLA	C4B-NB	2.77	1.41	1.37
24	b	613	CLA	C1B-C2B	2.77	1.49	1.43
30	f	101	SQD	O5-C1	2.77	1.49	1.41
24	c	502	CLA	C4B-NB	2.76	1.41	1.37
34	F	101	HEM	FE-NB	2.76	2.03	1.94
24	a	605	CLA	CHC-C1C	2.76	1.44	1.38
24	c	506	CLA	C1B-C2B	2.76	1.49	1.43
24	A	605	CLA	CHC-C1C	2.75	1.44	1.38
25	a	607	PHO	C3D-C4D	2.75	1.45	1.41
24	B	605	CLA	C1D-ND	2.74	1.41	1.37
24	c	505	CLA	C1D-ND	2.74	1.41	1.37
24	c	501	CLA	C1B-C2B	2.74	1.49	1.43
34	e	102	HEM	CAC-C3C	2.74	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C1B-C2B	2.74	1.49	1.43
24	d	403	CLA	MG-ND	2.73	2.11	2.05
24	B	606	CLA	C1B-C2B	2.73	1.49	1.43
24	B	610	CLA	C3B-C4B	2.73	1.50	1.42
24	c	501	CLA	MG-NC	2.73	2.12	2.06
24	B	610	CLA	CHC-C1C	2.73	1.44	1.38
24	C	504	CLA	C1B-C2B	2.73	1.49	1.43
24	B	602	CLA	C1B-C2B	2.72	1.49	1.43
24	C	508	CLA	C3B-C4B	2.72	1.50	1.42
24	A	606	CLA	C1D-ND	2.72	1.41	1.37
24	b	613	CLA	MG-NC	2.71	2.12	2.06
24	C	506	CLA	C1B-C2B	2.71	1.49	1.43
24	b	614	CLA	CHC-C1C	2.71	1.43	1.38
24	C	510	CLA	MG-NC	2.71	2.12	2.06
24	D	404	CLA	C4B-NB	2.70	1.41	1.37
24	c	512	CLA	CHC-C1C	2.69	1.43	1.38
24	C	512	CLA	C4B-NB	2.69	1.41	1.37
24	C	503	CLA	MG-NC	2.69	2.12	2.06
24	a	609	CLA	C1B-C2B	2.69	1.49	1.43
25	D	402	PHO	C3B-C2B	-2.68	1.36	1.40
24	c	509	CLA	C4B-NB	2.68	1.41	1.37
24	b	611	CLA	C1B-C2B	2.68	1.49	1.43
24	b	607	CLA	C4B-NB	2.67	1.41	1.37
25	A	607	PHO	CMB-C2B	-2.67	1.46	1.51
24	D	403	CLA	C1B-C2B	2.67	1.49	1.43
24	d	403	CLA	C1B-C2B	2.66	1.49	1.43
24	c	508	CLA	CHC-C1C	2.65	1.43	1.38
24	b	614	CLA	C1B-C2B	2.65	1.49	1.43
27	d	406	PL9	C6-C1	-2.65	1.44	1.48
24	C	512	CLA	MG-NC	2.64	2.12	2.06
24	C	504	CLA	C3B-C4B	2.64	1.50	1.42
24	c	504	CLA	C1D-ND	2.64	1.41	1.37
24	a	605	CLA	MG-NC	2.64	2.12	2.06
24	c	510	CLA	C4B-NB	2.63	1.41	1.37
24	d	402	CLA	C4B-NB	2.62	1.41	1.37
35	V	201	HEC	FE-NB	2.62	2.03	1.94
24	d	403	CLA	C4B-NB	2.61	1.41	1.37
24	c	503	CLA	C4B-NB	2.61	1.41	1.37
24	b	605	CLA	C1D-ND	2.61	1.41	1.37
24	C	512	CLA	C1B-C2B	2.61	1.49	1.43
24	B	616	CLA	CHC-C1C	2.61	1.43	1.38
24	c	513	CLA	C3B-C4B	2.60	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	CHC-C1C	2.60	1.43	1.38
25	D	402	PHO	CMD-C2D	-2.60	1.46	1.51
30	A	615	SQD	O9-S	2.60	1.52	1.45
24	b	609	CLA	MG-NA	2.60	2.12	2.06
24	C	511	CLA	C3B-C4B	2.59	1.50	1.42
24	B	614	CLA	CHC-C1C	2.59	1.43	1.38
24	c	504	CLA	C1B-C2B	2.59	1.49	1.43
24	b	610	CLA	CMD-C2D	-2.59	1.45	1.50
24	C	501	CLA	C1B-C2B	2.58	1.49	1.43
24	C	510	CLA	CHC-C1C	2.58	1.43	1.38
25	D	402	PHO	C4D-ND	-2.58	1.34	1.38
24	A	606	CLA	C3B-C4B	2.58	1.50	1.42
24	D	404	CLA	MG-ND	2.58	2.10	2.05
24	b	608	CLA	MG-NA	2.58	2.12	2.06
24	c	511	CLA	CHC-C1C	2.58	1.43	1.38
24	c	505	CLA	C4B-NB	2.57	1.41	1.37
24	B	612	CLA	MG-ND	2.57	2.10	2.05
24	b	603	CLA	C4B-NB	2.57	1.41	1.37
24	B	605	CLA	C3B-C4B	2.57	1.50	1.42
24	C	501	CLA	C3B-C4B	2.57	1.50	1.42
24	B	611	CLA	MG-ND	2.56	2.10	2.05
24	B	611	CLA	MG-NC	2.56	2.12	2.06
24	B	607	CLA	C1B-C2B	2.56	1.49	1.43
25	a	608	PHO	CMC-C2C	-2.56	1.46	1.50
24	B	615	CLA	CHC-C1C	2.55	1.43	1.38
24	C	512	CLA	C3B-C4B	2.55	1.50	1.42
24	C	510	CLA	MG-ND	2.55	2.10	2.05
24	c	508	CLA	C3B-C4B	2.55	1.50	1.42
24	c	510	CLA	MG-ND	-2.54	2.00	2.05
25	a	607	PHO	CMB-C2B	-2.54	1.46	1.51
24	C	512	CLA	CHC-C1C	2.54	1.43	1.38
24	b	603	CLA	CMD-C2D	-2.53	1.45	1.50
24	C	509	CLA	MG-NB	-2.52	2.00	2.05
24	b	616	CLA	C4B-NB	2.52	1.41	1.37
24	b	612	CLA	C3B-C4B	2.52	1.50	1.42
24	B	605	CLA	MG-ND	2.52	2.10	2.05
30	a	614	SQD	O7-S	2.50	1.52	1.45
24	B	613	CLA	C4B-NB	2.50	1.41	1.37
30	A	615	SQD	O7-S	2.50	1.52	1.45
24	B	601	CLA	C3B-C4B	2.50	1.50	1.42
24	A	606	CLA	C1B-C2B	2.49	1.49	1.43
24	d	402	CLA	CHC-C1C	2.49	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	608	CLA	C4B-NB	2.49	1.41	1.37
24	B	606	CLA	MG-NC	2.49	2.12	2.06
24	C	511	CLA	MG-NB	-2.48	2.00	2.05
24	b	615	CLA	C3B-C4B	2.48	1.50	1.42
30	A	613	SQD	O9-S	2.48	1.52	1.45
24	b	610	CLA	C4B-NB	2.48	1.41	1.37
24	D	405	CLA	C4B-NB	2.47	1.41	1.37
24	b	607	CLA	C1B-C2B	2.47	1.48	1.43
24	C	509	CLA	C1B-C2B	2.47	1.48	1.43
24	A	606	CLA	MG-NA	2.47	2.12	2.06
24	B	612	CLA	C1B-C2B	2.47	1.48	1.43
24	C	509	CLA	C3B-C4B	2.46	1.49	1.42
34	e	102	HEM	CAB-C3B	2.46	1.54	1.47
24	B	601	CLA	CHC-C1C	2.46	1.43	1.38
30	b	620	SQD	O9-S	2.46	1.52	1.45
24	B	612	CLA	C3B-C4B	2.46	1.49	1.42
24	C	510	CLA	C3B-C4B	2.46	1.49	1.42
25	D	402	PHO	C1D-ND	2.46	1.42	1.38
24	b	615	CLA	CMB-C2B	-2.45	1.45	1.50
24	b	603	CLA	C1B-C2B	2.45	1.48	1.43
24	c	506	CLA	MG-NC	2.45	2.12	2.06
24	c	513	CLA	CHC-C1C	2.44	1.43	1.38
25	a	607	PHO	C4D-ND	-2.44	1.34	1.38
24	c	512	CLA	C3B-C4B	2.44	1.49	1.42
24	C	502	CLA	C3B-C4B	2.44	1.49	1.42
24	C	513	CLA	C3B-C4B	2.44	1.49	1.42
30	a	614	SQD	O9-S	2.43	1.52	1.45
27	D	407	PL9	C3-C4	-2.43	1.45	1.49
25	A	607	PHO	CMD-C2D	-2.43	1.46	1.51
24	a	606	CLA	C1B-C2B	2.43	1.48	1.43
24	c	506	CLA	CHC-C1C	2.43	1.43	1.38
24	B	616	CLA	CMC-C2C	-2.42	1.45	1.50
24	b	607	CLA	CHC-C1C	2.42	1.43	1.38
24	b	606	CLA	C3B-C4B	2.42	1.49	1.42
24	c	505	CLA	CHC-C1C	2.42	1.43	1.38
24	D	405	CLA	MG-NC	2.42	2.12	2.06
24	a	606	CLA	C3B-C4B	2.41	1.49	1.42
24	c	505	CLA	CMB-C2B	-2.41	1.45	1.50
24	B	612	CLA	MG-NA	2.41	2.12	2.06
24	B	611	CLA	C4B-NB	2.41	1.41	1.37
24	A	606	CLA	CHC-C1C	2.41	1.43	1.38
24	c	510	CLA	C3B-C4B	2.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	f	101	SQD	O9-S	2.40	1.51	1.45
24	c	504	CLA	CHC-C1C	2.40	1.43	1.38
24	B	604	CLA	C4B-NB	2.39	1.41	1.37
24	C	512	CLA	MG-ND	-2.39	2.01	2.05
24	A	605	CLA	C3B-C4B	2.39	1.49	1.42
24	d	403	CLA	C3B-C4B	2.38	1.49	1.42
24	c	507	CLA	MG-NC	2.38	2.11	2.06
24	c	507	CLA	CMC-C2C	-2.38	1.45	1.50
24	b	605	CLA	CHC-C1C	2.38	1.43	1.38
24	B	608	CLA	CHC-C1C	2.37	1.43	1.38
24	B	605	CLA	C4B-NB	2.37	1.41	1.37
25	A	607	PHO	C4D-ND	-2.36	1.35	1.38
24	b	609	CLA	C3B-C4B	2.36	1.49	1.42
24	b	611	CLA	CHC-C1C	2.36	1.43	1.38
24	C	508	CLA	CHC-C1C	2.36	1.43	1.38
24	a	605	CLA	CMB-C2B	-2.36	1.45	1.50
24	b	608	CLA	C1B-C2B	2.36	1.48	1.43
24	C	503	CLA	C3B-C4B	2.36	1.49	1.42
30	A	615	SQD	O5-C5	2.36	1.50	1.44
24	B	603	CLA	C3B-C4B	2.36	1.49	1.42
24	A	608	CLA	C1B-C2B	2.35	1.48	1.43
24	c	503	CLA	CHC-C1C	2.35	1.43	1.38
24	C	506	CLA	C3B-C4B	2.35	1.49	1.42
24	b	601	CLA	CHC-C1C	2.35	1.43	1.38
24	d	404	CLA	C3B-C4B	2.35	1.49	1.42
24	a	605	CLA	C3B-C4B	2.35	1.49	1.42
24	b	606	CLA	C4B-NB	2.35	1.40	1.37
24	c	513	CLA	MG-NB	2.35	2.10	2.05
24	b	612	CLA	CHC-C1C	2.34	1.43	1.38
24	b	601	CLA	C3B-C4B	2.34	1.49	1.42
24	b	609	CLA	C1B-C2B	2.34	1.48	1.43
24	b	603	CLA	CMC-C2C	-2.34	1.46	1.50
24	B	606	CLA	CHC-C1C	2.34	1.43	1.38
24	c	508	CLA	MG-NC	2.34	2.11	2.06
24	b	613	CLA	CMD-C2D	-2.34	1.46	1.50
24	b	603	CLA	CMB-C2B	-2.34	1.46	1.50
24	B	611	CLA	C3B-C4B	2.34	1.49	1.42
24	d	403	CLA	CHC-C1C	2.33	1.43	1.38
30	B	623	SQD	O9-S	2.33	1.51	1.45
24	b	602	CLA	C3B-C4B	2.31	1.49	1.42
24	B	602	CLA	C3B-C4B	2.31	1.49	1.42
34	e	102	HEM	C3B-C2B	-2.30	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	CMD-C2D	-2.30	1.46	1.50
24	c	510	CLA	CMB-C2B	-2.30	1.46	1.50
24	c	510	CLA	CMD-C2D	-2.29	1.46	1.50
30	a	614	SQD	O5-C5	2.29	1.50	1.44
24	C	505	CLA	CHC-C1C	2.29	1.43	1.38
24	D	404	CLA	C3B-C4B	2.29	1.49	1.42
24	C	502	CLA	CMB-C2B	-2.29	1.46	1.50
30	D	410	SQD	O9-S	2.29	1.51	1.45
24	c	509	CLA	C3B-C4B	2.29	1.49	1.42
24	C	509	CLA	C4B-NB	2.28	1.40	1.37
31	B	622	LHG	O7-C5	-2.28	1.41	1.46
24	a	609	CLA	MG-NC	2.28	2.11	2.06
24	b	614	CLA	CMC-C2C	-2.28	1.46	1.50
24	C	511	CLA	CHC-C1C	2.27	1.43	1.38
27	d	406	PL9	C31-C29	-2.27	1.46	1.51
24	D	405	CLA	C3B-C4B	2.27	1.49	1.42
24	B	610	CLA	MG-ND	2.27	2.10	2.05
25	A	607	PHO	CMC-C2C	-2.27	1.47	1.50
24	c	504	CLA	CMB-C2B	-2.27	1.46	1.50
24	C	509	CLA	CMD-C2D	-2.27	1.46	1.50
24	D	403	CLA	MG-NA	2.27	2.11	2.06
24	c	505	CLA	C3B-C4B	2.27	1.49	1.42
24	d	404	CLA	CMD-C2D	-2.26	1.46	1.50
24	B	615	CLA	CMB-C2B	-2.26	1.46	1.50
24	C	513	CLA	CHC-C1C	2.26	1.43	1.38
24	B	603	CLA	CMD-C2D	-2.26	1.46	1.50
24	B	606	CLA	CMD-C2D	-2.26	1.46	1.50
24	c	509	CLA	CHC-C1C	2.25	1.43	1.38
24	b	607	CLA	CMC-C2C	-2.25	1.46	1.50
24	B	614	CLA	C1B-C2B	2.25	1.48	1.43
24	b	611	CLA	C3B-C4B	2.24	1.49	1.42
24	c	504	CLA	C3B-C4B	2.24	1.49	1.42
24	a	609	CLA	C3B-C4B	2.24	1.49	1.42
25	A	607	PHO	C3D-C4D	2.23	1.44	1.41
24	b	611	CLA	CMD-C2D	-2.23	1.46	1.50
24	b	605	CLA	C3B-C4B	2.23	1.49	1.42
34	e	102	HEM	CMC-C2C	2.23	1.55	1.50
27	A	610	PL9	C53-C6	-2.23	1.46	1.50
24	c	511	CLA	C3B-C4B	2.23	1.49	1.42
24	b	609	CLA	CHC-C1C	2.23	1.43	1.38
24	c	503	CLA	C3B-C4B	2.22	1.49	1.42
34	e	102	HEM	FE-NC	2.22	2.02	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	CHC-C1C	2.22	1.42	1.38
24	B	606	CLA	C3B-C4B	2.22	1.49	1.42
24	b	606	CLA	CMD-C2D	-2.22	1.46	1.50
25	a	608	PHO	C4D-ND	-2.22	1.35	1.38
27	d	406	PL9	C26-C24	-2.22	1.46	1.51
24	C	502	CLA	CHC-C1C	2.22	1.42	1.38
24	C	501	CLA	CMD-C2D	-2.21	1.46	1.50
24	C	504	CLA	CHC-C1C	2.21	1.42	1.38
24	b	609	CLA	MG-ND	-2.21	2.01	2.05
24	B	602	CLA	MG-ND	-2.21	2.01	2.05
24	D	405	CLA	CMD-C2D	-2.21	1.46	1.50
24	c	502	CLA	C3B-C4B	2.20	1.49	1.42
24	B	616	CLA	C3B-C4B	2.20	1.49	1.42
24	B	611	CLA	C1D-C2D	2.20	1.49	1.45
24	C	503	CLA	CHC-C1C	2.20	1.42	1.38
24	b	614	CLA	C3B-C4B	2.20	1.49	1.42
24	C	512	CLA	CMD-C2D	-2.20	1.46	1.50
24	d	404	CLA	CHC-C1C	2.20	1.42	1.38
24	b	607	CLA	C3B-C4B	2.20	1.49	1.42
24	b	601	CLA	O2A-CGA	2.19	1.39	1.33
24	C	510	CLA	CMD-C2D	-2.19	1.46	1.50
24	B	610	CLA	CMB-C2B	-2.19	1.46	1.50
35	V	201	HEC	FE-NC	2.19	2.02	1.95
30	b	620	SQD	O7-S	2.19	1.51	1.45
24	B	604	CLA	C3B-C4B	2.18	1.49	1.42
24	c	505	CLA	MG-ND	2.18	2.10	2.05
24	B	613	CLA	CHC-C1C	2.18	1.42	1.38
24	D	405	CLA	CMB-C2B	-2.18	1.46	1.50
24	D	404	CLA	CMD-C2D	-2.17	1.46	1.50
24	c	502	CLA	CHC-C1C	2.17	1.42	1.38
24	B	610	CLA	C1D-C2D	2.17	1.49	1.45
24	a	605	CLA	MG-ND	-2.17	2.01	2.05
24	c	501	CLA	MG-NB	-2.17	2.01	2.05
24	B	608	CLA	CMD-C2D	-2.17	1.46	1.50
30	b	620	SQD	O5-C5	2.17	1.49	1.44
24	d	404	CLA	CMC-C2C	-2.17	1.46	1.50
24	B	602	CLA	CHC-C1C	2.17	1.42	1.38
24	B	604	CLA	CHC-C1C	2.17	1.42	1.38
24	b	603	CLA	MG-NA	2.17	2.11	2.06
24	B	613	CLA	C3B-C4B	2.16	1.49	1.42
24	b	613	CLA	CMB-C2B	-2.16	1.46	1.50
24	c	507	CLA	C3D-C4D	2.16	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	CHC-C1C	2.16	1.42	1.38
24	C	505	CLA	C3B-C4B	2.16	1.49	1.42
24	c	502	CLA	MG-ND	2.16	2.10	2.05
24	b	615	CLA	CMD-C2D	-2.16	1.46	1.50
24	C	502	CLA	CMC-C2C	-2.16	1.46	1.50
24	c	505	CLA	C1B-C2B	2.16	1.48	1.43
24	c	509	CLA	MG-ND	2.15	2.10	2.05
24	b	616	CLA	CHC-C1C	2.15	1.42	1.38
24	b	610	CLA	CMB-C2B	-2.15	1.46	1.50
34	F	101	HEM	CMA-C3A	2.15	1.55	1.50
34	F	101	HEM	CMD-C2D	2.15	1.55	1.50
24	C	504	CLA	CMD-C2D	-2.15	1.46	1.50
24	c	513	CLA	CMB-C2B	-2.15	1.46	1.50
24	d	403	CLA	CMC-C2C	-2.15	1.46	1.50
25	a	607	PHO	O2D-CGD	2.15	1.38	1.33
35	V	201	HEC	CMB-C2B	2.15	1.55	1.50
35	v	201	HEC	FE-NC	2.14	2.02	1.95
24	b	604	CLA	C3B-C4B	2.14	1.49	1.42
25	D	402	PHO	CMB-C2B	-2.14	1.47	1.51
24	C	508	CLA	MG-ND	2.13	2.10	2.05
24	b	610	CLA	C3B-C4B	2.13	1.49	1.42
30	f	101	SQD	O7-S	2.13	1.51	1.45
24	D	403	CLA	C1D-C2D	2.12	1.49	1.45
24	c	506	CLA	CMD-C2D	-2.12	1.46	1.50
24	B	607	CLA	CMC-C2C	-2.11	1.46	1.50
24	b	603	CLA	C3B-C4B	2.11	1.48	1.42
24	C	504	CLA	O2D-CGD	2.11	1.38	1.33
24	C	511	CLA	CMB-C2B	-2.11	1.46	1.50
30	a	613	SQD	O9-S	2.10	1.51	1.45
24	c	511	CLA	CMD-C2D	-2.10	1.46	1.50
24	a	605	CLA	CMD-C2D	-2.10	1.46	1.50
25	a	607	PHO	CBD-CGD	-2.10	1.49	1.52
24	C	506	CLA	MG-ND	-2.10	2.01	2.05
24	c	505	CLA	MG-NB	-2.10	2.01	2.05
27	A	610	PL9	C25-C24	-2.10	1.45	1.50
24	c	508	CLA	MG-NA	2.10	2.11	2.06
24	c	513	CLA	CMD-C2D	-2.09	1.46	1.50
24	D	405	CLA	MG-NB	-2.09	2.01	2.05
35	v	201	HEC	CMD-C2D	2.09	1.55	1.50
24	B	612	CLA	MG-NC	2.09	2.11	2.06
24	b	606	CLA	CHC-C1C	2.09	1.42	1.38
35	v	201	HEC	CMC-C2C	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	402	PHO	O2D-CGD	2.08	1.38	1.33
24	B	609	CLA	CMC-C2C	-2.08	1.46	1.50
24	B	609	CLA	CMD-C2D	-2.08	1.46	1.50
24	c	501	CLA	CMC-C2C	-2.08	1.46	1.50
24	A	605	CLA	CMC-C2C	-2.08	1.46	1.50
25	a	607	PHO	CMD-C2D	-2.08	1.47	1.51
24	C	501	CLA	MG-NC	-2.07	2.01	2.06
24	d	403	CLA	CMB-C2B	-2.07	1.46	1.50
24	C	505	CLA	C3C-C2C	2.07	1.41	1.36
30	B	623	SQD	O7-S	2.07	1.51	1.45
24	b	612	CLA	MG-NA	2.07	2.11	2.06
24	b	607	CLA	CMD-C2D	-2.07	1.46	1.50
24	A	608	CLA	CHC-C1C	2.07	1.42	1.38
24	B	611	CLA	MG-NA	2.07	2.11	2.06
24	b	606	CLA	C3D-C4D	2.06	1.48	1.44
24	a	609	CLA	MG-NB	-2.06	2.01	2.05
24	b	608	CLA	CMB-C2B	-2.06	1.46	1.50
24	c	506	CLA	C3B-C4B	2.06	1.48	1.42
24	b	601	CLA	CMD-C2D	-2.06	1.46	1.50
24	d	402	CLA	CMB-C2B	-2.06	1.46	1.50
24	b	602	CLA	C1D-C2D	2.05	1.49	1.45
24	C	511	CLA	CMD-C2D	-2.05	1.46	1.50
24	C	513	CLA	C1D-C2D	2.05	1.49	1.45
24	a	609	CLA	CMD-C2D	-2.05	1.46	1.50
24	B	604	CLA	C3C-C2C	2.05	1.41	1.36
24	c	508	CLA	CMC-C2C	-2.05	1.46	1.50
24	d	402	CLA	C3B-C4B	2.04	1.48	1.42
24	B	602	CLA	CMD-C2D	-2.04	1.46	1.50
24	C	513	CLA	MG-NC	2.04	2.11	2.06
24	c	503	CLA	CMC-C2C	-2.04	1.46	1.50
35	v	201	HEC	CMA-C3A	2.04	1.55	1.50
24	b	613	CLA	C3B-C4B	2.04	1.48	1.42
24	b	614	CLA	CMB-C2B	-2.04	1.46	1.50
24	A	608	CLA	CMD-C2D	-2.03	1.46	1.50
24	c	503	CLA	CMD-C2D	-2.03	1.46	1.50
35	v	201	HEC	CMB-C2B	2.03	1.54	1.50
24	b	616	CLA	C3D-C4D	2.03	1.48	1.44
24	C	507	CLA	C3C-C2C	2.03	1.41	1.36
30	A	613	SQD	C8-C7	2.03	1.56	1.50
24	B	615	CLA	CMC-C2C	-2.03	1.46	1.50
24	D	405	CLA	CMC-C2C	-2.03	1.46	1.50
24	C	512	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	CMC-C2C	-2.03	1.46	1.50
25	D	402	PHO	CAC-C3C	-2.03	1.48	1.51
24	B	616	CLA	C1D-C2D	2.02	1.49	1.45
30	B	623	SQD	O5-C5	2.02	1.49	1.44
25	a	607	PHO	C4C-NC	2.02	1.43	1.37
24	B	610	CLA	C3D-C4D	2.02	1.48	1.44
34	e	102	HEM	CMA-C3A	2.02	1.54	1.50
30	a	613	SQD	O7-S	2.02	1.50	1.45
24	b	613	CLA	CHC-C1C	2.02	1.42	1.38
30	A	615	SQD	C46-C45	2.02	1.57	1.50
25	a	608	PHO	CMB-C2B	-2.01	1.47	1.51
24	b	603	CLA	CHC-C1C	2.01	1.42	1.38
24	D	404	CLA	CMB-C2B	-2.01	1.46	1.50
24	d	404	CLA	MG-NC	2.01	2.11	2.06
24	d	404	CLA	CMB-C2B	-2.00	1.46	1.50
24	c	510	CLA	CHC-C1C	2.00	1.42	1.38
24	c	501	CLA	C3B-C4B	2.00	1.48	1.42
24	C	506	CLA	CMC-C2C	-2.00	1.46	1.50

All (891) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	C4A-NA-C1A	9.08	110.82	106.68
24	C	507	CLA	C4A-NA-C1A	8.57	110.59	106.68
24	c	511	CLA	C4A-NA-C1A	8.57	110.59	106.68
24	C	503	CLA	C4A-NA-C1A	8.47	110.54	106.68
24	b	615	CLA	C4A-NA-C1A	8.25	110.44	106.68
24	b	606	CLA	C4A-NA-C1A	8.24	110.44	106.68
24	B	612	CLA	C4A-NA-C1A	8.18	110.41	106.68
24	b	605	CLA	C4A-NA-C1A	8.16	110.40	106.68
24	C	511	CLA	C4A-NA-C1A	8.12	110.39	106.68
24	B	601	CLA	C4A-NA-C1A	8.04	110.35	106.68
24	C	505	CLA	C4A-NA-C1A	7.65	110.17	106.68
24	c	507	CLA	C4A-NA-C1A	7.56	110.13	106.68
24	B	615	CLA	C4A-NA-C1A	7.51	110.11	106.68
24	C	508	CLA	C4A-NA-C1A	7.22	109.97	106.68
30	A	613	SQD	O6-C1-C2	7.20	119.20	108.27
30	D	410	SQD	O6-C1-C2	7.15	119.13	108.27
24	B	606	CLA	C4A-NA-C1A	7.14	109.94	106.68
24	B	616	CLA	C4A-NA-C1A	7.07	109.91	106.68
24	B	611	CLA	C4A-NA-C1A	7.05	109.90	106.68
24	b	616	CLA	C4A-NA-C1A	6.96	109.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C4A-NA-C1A	6.95	109.85	106.68
24	c	503	CLA	C4A-NA-C1A	6.86	109.81	106.68
27	A	610	PL9	C7-C3-C4	6.80	122.51	116.91
29	B	625	LMG	O1-C1-C2	6.74	118.51	108.27
24	B	604	CLA	C4A-NA-C1A	6.73	109.75	106.68
24	c	502	CLA	C4A-NA-C1A	6.72	109.75	106.68
30	b	620	SQD	O6-C1-C2	6.71	118.47	108.27
24	B	613	CLA	C4A-NA-C1A	6.66	109.72	106.68
24	C	510	CLA	C4A-NA-C1A	6.61	109.69	106.68
24	B	614	CLA	C4A-NA-C1A	6.59	109.69	106.68
24	c	509	CLA	C4A-NA-C1A	6.59	109.69	106.68
24	b	601	CLA	C4A-NA-C1A	6.56	109.67	106.68
24	a	605	CLA	C4A-NA-C1A	6.38	109.59	106.68
24	C	506	CLA	C4A-NA-C1A	6.29	109.55	106.68
27	a	611	PL9	C7-C3-C4	6.26	122.07	116.91
24	B	607	CLA	C4A-NA-C1A	6.26	109.53	106.68
24	A	605	CLA	C4A-NA-C1A	6.23	109.52	106.68
24	d	403	CLA	C4A-NA-C1A	6.20	109.51	106.68
24	c	501	CLA	C4A-NA-C1A	6.19	109.50	106.68
24	C	509	CLA	C4A-NA-C1A	6.18	109.50	106.68
24	B	602	CLA	C4A-NA-C1A	6.17	109.49	106.68
24	b	602	CLA	C4A-NA-C1A	6.13	109.48	106.68
24	d	402	CLA	C4A-NA-C1A	6.10	109.46	106.68
24	b	611	CLA	C4A-NA-C1A	6.00	109.42	106.68
24	C	513	CLA	C4A-NA-C1A	5.96	109.40	106.68
24	C	501	CLA	C4A-NA-C1A	5.92	109.38	106.68
24	C	502	CLA	C4A-NA-C1A	5.84	109.34	106.68
24	b	613	CLA	C4A-NA-C1A	5.80	109.33	106.68
24	c	510	CLA	C4A-NA-C1A	5.73	109.29	106.68
24	c	505	CLA	C4A-NA-C1A	5.68	109.27	106.68
24	B	609	CLA	C4A-NA-C1A	5.67	109.27	106.68
24	b	614	CLA	C4A-NA-C1A	5.66	109.26	106.68
35	v	201	HEC	C1D-ND-C4D	5.59	111.82	105.21
25	a	607	PHO	C4D-CHA-CBD	-5.57	105.78	108.45
24	D	403	CLA	C4A-NA-C1A	5.47	109.18	106.68
24	D	404	CLA	C4A-NA-C1A	5.44	109.16	106.68
25	D	402	PHO	C4D-CHA-CBD	-5.43	105.85	108.45
24	b	612	CLA	C4A-NA-C1A	5.42	109.15	106.68
24	c	508	CLA	C4A-NA-C1A	5.41	109.15	106.68
24	B	605	CLA	C4A-NA-C1A	5.37	109.13	106.68
24	c	504	CLA	C4A-NA-C1A	5.34	109.11	106.68
24	b	609	CLA	C4A-NA-C1A	5.30	109.09	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	606	CLA	C4A-NA-C1A	5.28	109.09	106.68
24	C	512	CLA	C4A-NA-C1A	5.21	109.06	106.68
35	V	201	HEC	C1D-ND-C4D	5.18	111.34	105.21
24	c	506	CLA	C4A-NA-C1A	5.13	109.02	106.68
24	D	403	CLA	C3B-C4B-NB	-5.00	106.06	110.53
29	B	620	LMG	O3-C3-C2	-5.00	98.60	110.38
30	a	614	SQD	O47-C7-C8	4.97	122.23	111.48
24	C	504	CLA	C4A-NA-C1A	4.95	108.94	106.68
25	A	607	PHO	C1-C2-C3	-4.93	118.12	126.20
30	A	613	SQD	C1-O5-C5	-4.90	104.15	113.72
24	b	607	CLA	C4A-NA-C1A	4.87	108.90	106.68
30	B	623	SQD	C1-O5-C5	-4.85	104.24	113.72
30	A	613	SQD	C1-C2-C3	-4.85	99.82	110.01
25	a	608	PHO	O1D-CGD-CBD	4.82	132.03	124.72
30	a	614	SQD	O7-S-C6	4.79	113.91	106.76
30	B	623	SQD	O47-C7-C8	4.79	121.84	111.48
25	A	607	PHO	O1D-CGD-CBD	4.78	131.97	124.72
30	a	613	SQD	O6-C1-C2	4.77	115.52	108.27
24	B	608	CLA	C4A-NA-C1A	4.77	108.85	106.68
24	c	513	CLA	C4A-NA-C1A	4.76	108.85	106.68
29	b	622	LMG	C8-O7-C10	4.73	129.11	117.80
30	a	613	SQD	C1-O5-C5	-4.73	104.49	113.72
24	d	404	CLA	C4A-NA-C1A	4.71	108.83	106.68
24	b	608	CLA	C4A-NA-C1A	4.70	108.83	106.68
24	B	610	CLA	C4A-NA-C1A	4.70	108.82	106.68
29	C	517	LMG	C8-O7-C10	4.70	129.04	117.80
30	B	623	SQD	O6-C1-C2	4.67	115.37	108.27
27	A	610	PL9	C7-C3-C2	-4.61	117.95	123.39
24	B	613	CLA	C1-C2-C3	-4.56	118.72	126.20
24	B	603	CLA	C4A-NA-C1A	4.56	108.76	106.68
24	D	405	CLA	C4A-NA-C1A	4.54	108.75	106.68
24	B	614	CLA	O2D-CGD-O1D	-4.53	115.04	123.85
30	f	101	SQD	O9-S-O7	-4.52	99.11	113.82
30	A	613	SQD	O9-S-O7	-4.52	99.14	113.82
25	a	608	PHO	C1-C2-C3	-4.50	118.83	126.20
30	f	101	SQD	O7-S-C6	4.50	113.47	106.76
25	A	607	PHO	O2D-CGD-O1D	-4.48	115.13	123.85
24	A	608	CLA	C4A-NA-C1A	4.44	108.70	106.68
24	b	608	CLA	C3B-C4B-NB	-4.43	106.58	110.53
27	a	611	PL9	C7-C3-C2	-4.40	118.20	123.39
24	b	612	CLA	C1-C2-C3	-4.39	119.00	126.20
24	b	603	CLA	O2D-CGD-O1D	-4.36	115.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	O2D-CGD-O1D	-4.33	115.42	123.85
24	b	603	CLA	C4A-NA-C1A	4.31	108.64	106.68
24	b	610	CLA	C4A-NA-C1A	4.28	108.63	106.68
25	a	608	PHO	C4D-CHA-CBD	-4.27	106.41	108.45
30	f	101	SQD	O9-S-C6	4.27	113.13	106.76
24	b	616	CLA	O2D-CGD-O1D	-4.26	115.55	123.85
24	C	513	CLA	O2D-CGD-O1D	-4.25	115.58	123.85
24	c	501	CLA	O2D-CGD-O1D	-4.23	115.61	123.85
24	A	606	CLA	C4A-NA-C1A	4.21	108.60	106.68
25	D	402	PHO	CMA-C3A-C4A	-4.16	105.64	114.61
30	A	613	SQD	O47-C7-C8	4.13	120.42	111.48
25	A	607	PHO	C4D-CHA-CBD	-4.13	106.47	108.45
24	B	602	CLA	O2D-CGD-CBD	4.11	118.42	111.23
30	a	613	SQD	O9-S-O7	-4.01	100.77	113.82
27	d	406	PL9	C22-C23-C24	-4.00	118.48	127.62
24	d	403	CLA	O2D-CGD-O1D	-3.97	116.13	123.85
24	a	606	CLA	C3B-C4B-NB	-3.96	106.99	110.53
25	A	607	PHO	CMA-C3A-C4A	-3.95	106.09	114.61
24	B	614	CLA	O2D-CGD-CBD	3.95	118.14	111.23
30	a	614	SQD	O9-S-O7	-3.95	100.98	113.82
24	B	612	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
25	A	607	PHO	CBC-CAC-C3C	3.91	118.47	112.87
24	C	512	CLA	C3B-C4B-NB	-3.90	107.05	110.53
25	a	607	PHO	CMA-C3A-C4A	-3.90	106.21	114.61
30	b	620	SQD	O7-S-C6	3.89	112.57	106.76
25	a	608	PHO	CBC-CAC-C3C	3.89	118.44	112.87
34	F	101	HEM	CBD-CAD-C3D	-3.88	101.80	112.53
24	C	505	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
30	f	101	SQD	C3-C4-C5	3.84	117.20	110.23
29	C	517	LMG	C7-O1-C1	3.84	122.02	113.80
27	D	407	PL9	C7-C3-C4	3.83	120.07	116.91
24	B	614	CLA	C3B-C4B-NB	-3.83	107.11	110.53
24	B	611	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
24	C	501	CLA	C3B-C4B-NB	-3.79	107.14	110.53
29	B	625	LMG	C1-C2-C3	-3.79	102.03	110.01
29	D	408	LMG	C3-C4-C5	-3.79	103.36	110.23
30	b	620	SQD	C1-C2-C3	-3.77	102.07	110.01
30	A	613	SQD	O7-S-C6	3.76	112.38	106.76
29	D	408	LMG	C1-O6-C5	3.74	121.03	113.72
24	B	601	CLA	C3B-C4B-NB	-3.73	107.20	110.53
24	B	610	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
24	b	604	CLA	C1-C2-C3	-3.70	120.14	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
30	b	620	SQD	O9-S-C6	3.69	112.26	106.76
30	D	410	SQD	O5-C1-C2	-3.66	102.84	110.37
30	b	620	SQD	O47-C7-C8	3.66	119.41	111.48
32	A	616	DGD	C3G-O3G-C1D	3.66	121.64	113.80
30	b	620	SQD	O9-S-O7	-3.66	101.92	113.82
30	B	623	SQD	O48-C23-C24	3.65	122.97	111.83
24	B	615	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
24	A	606	CLA	C3B-C4B-NB	-3.63	107.29	110.53
24	C	501	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
24	a	606	CLA	CHB-C4A-NA	3.61	129.60	124.40
24	c	511	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
24	b	608	CLA	CHB-C4A-NA	3.57	129.56	124.40
30	A	615	SQD	O47-C7-C8	3.56	119.19	111.48
30	B	623	SQD	O5-C5-C4	3.56	116.11	109.70
24	b	614	CLA	C1-C2-C3	-3.55	120.38	126.20
29	a	615	LMG	C3-C4-C5	-3.54	103.81	110.23
24	c	509	CLA	O2A-CGA-O1A	-3.53	114.80	123.63
24	b	602	CLA	CHB-C4A-NA	3.52	129.48	124.40
30	f	101	SQD	C1-O5-C5	-3.51	106.86	113.72
30	A	615	SQD	O48-C23-C24	3.51	122.55	111.83
24	c	508	CLA	C1-C2-C3	-3.51	120.44	126.20
30	A	615	SQD	O5-C5-C4	3.50	116.01	109.70
24	B	612	CLA	C3B-C4B-NB	-3.50	107.41	110.53
24	b	609	CLA	C3B-C4B-NB	-3.50	107.41	110.53
25	a	608	PHO	O2D-CGD-O1D	-3.49	117.05	123.85
24	b	602	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
24	b	601	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
24	C	512	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
24	D	405	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
24	b	606	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
30	D	410	SQD	O9-S-C6	3.44	111.89	106.76
24	b	615	CLA	C3B-C4B-NB	-3.43	107.47	110.53
24	C	512	CLA	CHB-C4A-NA	3.43	129.35	124.40
24	B	606	CLA	C3B-C4B-NB	-3.41	107.49	110.53
30	A	615	SQD	O9-S-O7	-3.40	102.78	113.82
24	b	614	CLA	C3B-C4B-NB	-3.39	107.50	110.53
25	a	608	PHO	CMA-C3A-C4A	-3.38	107.32	114.61
24	C	510	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
24	A	608	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
24	B	605	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
34	e	102	HEM	CBD-CAD-C3D	-3.37	103.22	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	C1-C2-C3	-3.36	120.69	126.20
24	c	505	CLA	C3B-C4B-NB	-3.36	107.53	110.53
24	B	614	CLA	C1-C2-C3	-3.36	120.69	126.20
30	f	101	SQD	O6-C1-C2	3.36	113.38	108.27
27	d	406	PL9	C40-C39-C41	3.35	121.05	115.23
24	B	609	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
24	b	614	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
32	A	616	DGD	O5D-C1E-C2E	3.34	113.35	108.27
32	A	616	DGD	C4E-C3E-C2E	-3.34	104.97	110.83
30	A	615	SQD	O7-S-C6	3.34	111.74	106.76
24	b	603	CLA	O2D-CGD-CBD	3.33	117.06	111.23
27	a	611	PL9	C22-C23-C24	-3.32	120.01	127.62
30	f	101	SQD	O5-C5-C4	3.32	115.68	109.70
24	d	402	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
24	c	510	CLA	C1-C2-C3	-3.32	120.76	126.20
29	C	517	LMG	C4-C3-C2	3.32	116.65	110.83
24	c	508	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
25	a	607	PHO	C2B-C1B-NB	-3.30	107.04	109.43
24	c	512	CLA	CHB-C4A-NA	3.30	129.16	124.40
24	A	605	CLA	CHB-C4A-NA	3.29	129.15	124.40
24	b	604	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
26	b	618	BCR	C2-C1-C6	3.29	115.22	110.44
24	B	604	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
24	B	616	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
30	a	613	SQD	O47-C7-C8	3.28	118.58	111.48
25	A	607	PHO	C2B-C1B-NB	-3.27	107.06	109.43
24	a	609	CLA	C4A-NA-C1A	3.27	108.17	106.68
24	d	402	CLA	O2D-CGD-CBD	3.26	116.92	111.23
26	d	405	BCR	C30-C25-C26	-3.25	118.20	122.64
24	a	609	CLA	C1-C2-C3	-3.25	120.88	126.20
24	a	606	CLA	O2D-CGD-CBD	3.25	116.91	111.23
24	A	606	CLA	C1-C2-C3	-3.25	120.88	126.20
24	C	512	CLA	C1-C2-C3	-3.24	120.88	126.20
24	B	610	CLA	C3B-C4B-NB	-3.24	107.64	110.53
24	c	512	CLA	C3B-C4B-NB	-3.23	107.65	110.53
24	c	503	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
29	a	615	LMG	O1-C1-C2	3.23	113.17	108.27
25	a	607	PHO	CMB-C2B-C3B	3.21	131.11	124.68
27	d	406	PL9	O1-C4-C3	-3.21	117.34	120.73
25	a	608	PHO	CMB-C2B-C3B	3.21	131.09	124.68
24	c	505	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
24	B	602	CLA	CMB-C2B-C1B	-3.20	120.54	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	C1-C2-C3	-3.20	120.96	126.20
30	b	620	SQD	O5-C5-C4	3.19	115.45	109.70
24	B	602	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
24	C	503	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
30	B	623	SQD	C3-C4-C5	3.18	115.99	110.23
24	b	602	CLA	C1-C2-C3	-3.18	121.00	126.20
24	b	602	CLA	O2D-CGD-CBD	3.17	116.78	111.23
24	c	512	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
30	a	613	SQD	O48-C23-C24	3.17	121.50	111.83
24	B	611	CLA	C3B-C4B-NB	-3.16	107.71	110.53
30	A	613	SQD	O5-C1-C2	-3.16	103.88	110.37
24	c	508	CLA	C3B-C4B-NB	-3.16	107.71	110.53
26	b	618	BCR	C33-C5-C6	3.16	127.93	124.48
24	C	513	CLA	O2D-CGD-CBD	3.15	116.75	111.23
30	a	614	SQD	O48-C23-C24	3.15	121.45	111.83
24	b	606	CLA	O2D-CGD-CBD	3.15	116.74	111.23
27	D	407	PL9	C37-C38-C39	-3.15	120.41	127.62
25	A	607	PHO	CMB-C2B-C3B	3.15	130.97	124.68
24	b	608	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
24	c	506	CLA	C3B-C4B-NB	-3.15	107.72	110.53
35	V	201	HEC	C4B-NB-C1B	3.14	108.93	105.21
24	a	609	CLA	O2D-CGD-CBD	3.14	116.72	111.23
26	c	517	BCR	C7-C8-C9	-3.13	121.60	126.23
30	D	410	SQD	O9-S-O7	-3.13	103.64	113.82
24	c	502	CLA	C1-C2-C3	-3.13	121.07	126.20
24	c	504	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
24	B	601	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
27	d	406	PL9	C27-C28-C29	-3.11	120.50	127.62
24	B	615	CLA	CHB-C4A-NA	3.11	128.89	124.40
24	b	610	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
24	a	606	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
29	C	517	LMG	O6-C5-C4	3.10	115.29	109.70
24	B	612	CLA	CHB-C4A-NA	3.10	128.88	124.40
25	D	402	PHO	CMB-C2B-C3B	3.10	130.88	124.68
24	d	403	CLA	C3B-C4B-NB	-3.10	107.77	110.53
24	B	610	CLA	CHB-C4A-NA	3.10	128.87	124.40
24	c	503	CLA	CHB-C4A-NA	3.09	128.86	124.40
24	b	605	CLA	O2A-CGA-O1A	-3.09	115.91	123.63
24	c	513	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
27	A	610	PL9	O2-C1-C2	-3.08	114.82	121.83
24	C	506	CLA	C3B-C4B-NB	-3.08	107.78	110.53
28	M	102	STE	C3-C2-C1	-3.08	106.48	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	O2D-CGD-CBD	3.08	116.61	111.23
27	D	407	PL9	C27-C28-C29	-3.06	120.62	127.62
24	b	616	CLA	C1-C2-C3	-3.06	121.18	126.20
29	D	408	LMG	C7-O1-C1	3.05	120.34	113.80
24	c	511	CLA	C3B-C4B-NB	-3.05	107.81	110.53
32	H	102	DGD	C3E-C4E-C5E	-3.04	104.72	110.23
24	b	610	CLA	CHB-C4A-NA	3.04	128.79	124.40
24	B	611	CLA	C1-C2-C3	-3.03	121.23	126.20
24	B	603	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
25	a	608	PHO	C2B-C1B-NB	-3.02	107.25	109.43
29	B	620	LMG	O1-C7-C8	-3.01	103.49	110.82
24	C	506	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
30	B	623	SQD	O9-S-O7	-3.00	104.05	113.82
29	M	101	LMG	C8-O7-C10	3.00	124.98	117.80
24	C	508	CLA	C3B-C4B-NB	-3.00	107.85	110.53
35	V	201	HEC	CAD-CBD-CGD	-2.99	105.72	113.67
24	a	605	CLA	CHB-C4A-NA	2.99	128.72	124.40
24	c	505	CLA	CMB-C2B-C1B	-2.99	120.87	125.42
32	h	101	DGD	C6D-C5D-C4D	2.99	118.34	112.07
32	C	522	DGD	C3E-C4E-C5E	-2.98	104.82	110.23
24	B	605	CLA	C3B-C4B-NB	-2.98	107.87	110.53
24	C	507	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
30	a	613	SQD	O9-S-C6	2.97	111.20	106.76
24	C	508	CLA	O2D-CGD-CBD	2.97	116.41	111.23
24	d	403	CLA	O2A-CGA-O1A	-2.96	116.23	123.63
32	C	523	DGD	C6D-O5D-C1E	2.95	120.13	113.80
24	a	606	CLA	O2A-CGA-O1A	-2.95	116.24	123.63
24	C	507	CLA	CHB-C4A-NA	2.95	128.66	124.40
25	a	607	PHO	C3B-C4B-NB	-2.95	105.54	107.46
24	c	506	CLA	C1-O2A-CGA	2.95	123.79	116.65
24	b	605	CLA	C1-C2-C3	-2.95	121.37	126.20
32	c	518	DGD	C3G-O3G-C1D	2.94	120.10	113.80
24	C	502	CLA	C3B-C4B-NB	-2.94	107.91	110.53
32	C	521	DGD	C3D-C4D-C5D	-2.94	104.90	110.23
24	D	405	CLA	O2A-CGA-O1A	-2.93	116.29	123.63
24	a	605	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
24	b	616	CLA	O2D-CGD-CBD	2.93	116.35	111.23
27	d	406	PL9	C7-C3-C4	2.92	119.32	116.91
24	c	502	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
24	b	601	CLA	C3B-C4B-NB	-2.92	107.92	110.53
24	C	509	CLA	CHB-C4A-NA	2.92	128.61	124.40
24	b	616	CLA	CHB-C4A-NA	2.92	128.61	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C3B-C4B-NB	-2.91	107.93	110.53
24	c	504	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
24	c	509	CLA	C3B-C4B-NB	-2.90	107.94	110.53
30	a	614	SQD	O5-C1-C2	2.89	116.31	110.37
26	x	101	BCR	C16-C17-C18	-2.89	123.23	127.28
27	d	406	PL9	C37-C38-C39	-2.89	121.02	127.62
24	c	503	CLA	C3B-C4B-NB	-2.88	107.96	110.53
24	C	507	CLA	C3B-C4B-NB	-2.88	107.96	110.53
24	C	503	CLA	C3B-C4B-NB	-2.88	107.96	110.53
30	D	410	SQD	O8-S-C6	2.88	111.53	105.97
29	m	101	LMG	C4-C3-C2	2.88	115.88	110.83
24	d	404	CLA	C3B-C4B-NB	-2.88	107.96	110.53
24	b	612	CLA	C11-C12-C13	-2.88	106.40	115.97
24	c	513	CLA	CHB-C4A-NA	2.88	128.55	124.40
29	B	620	LMG	C4-C3-C2	2.87	115.88	110.83
24	c	504	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
24	C	504	CLA	C3B-C4B-NB	-2.87	107.97	110.53
24	b	615	CLA	C1-C2-C3	-2.87	121.49	126.20
24	D	404	CLA	O2A-CGA-O1A	-2.86	116.46	123.63
24	c	510	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
24	C	512	CLA	O2D-CGD-CBD	2.86	116.23	111.23
30	A	613	SQD	O9-S-C6	2.86	111.03	106.76
24	D	404	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
24	b	605	CLA	C3B-C4B-NB	-2.85	107.98	110.53
30	a	614	SQD	C1-C2-C3	2.85	116.01	110.01
27	d	406	PL9	C7-C8-C9	-2.85	121.92	126.83
24	D	405	CLA	CHB-C4A-NA	2.84	128.50	124.40
32	h	101	DGD	O3E-C3E-C4E	2.84	117.07	110.38
24	a	609	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
24	B	612	CLA	O1D-CGD-CBD	2.84	130.12	124.52
24	B	608	CLA	O2D-CGD-CBD	2.83	116.19	111.23
24	b	613	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
24	B	612	CLA	O2A-CGA-O1A	-2.83	116.55	123.63
32	C	521	DGD	C6D-O5D-C1E	2.83	119.85	113.80
24	D	403	CLA	O2D-CGD-CBD	2.82	116.17	111.23
27	A	610	PL9	O2-C1-C6	2.82	124.97	120.48
24	B	612	CLA	C1-C2-C3	-2.82	121.58	126.20
27	a	611	PL9	C40-C39-C41	2.82	120.12	115.23
24	b	611	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
27	a	611	PL9	C37-C38-C39	-2.81	121.19	127.62
24	d	402	CLA	C1-C2-C3	-2.81	121.59	126.20
27	d	406	PL9	C8-C7-C3	2.81	119.29	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	520	DGD	C6D-O5D-C1E	2.81	119.81	113.80
27	d	406	PL9	C12-C13-C14	-2.80	121.21	127.62
24	B	602	CLA	CHB-C4A-NA	2.80	128.44	124.40
24	c	507	CLA	CHC-C4B-NB	2.80	128.25	124.05
24	b	601	CLA	CHB-C4A-NA	2.80	128.44	124.40
24	B	606	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
30	a	614	SQD	C9-C8-C7	-2.79	103.46	113.69
35	v	201	HEC	CHA-C4D-ND	2.79	127.43	124.42
29	C	517	LMG	O4-C4-C5	2.79	116.19	109.32
27	a	611	PL9	O2-C1-C2	-2.79	115.49	121.83
24	B	608	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	a	613	SQD	O7-S-C6	2.79	110.92	106.76
24	D	403	CLA	CHB-C4A-NA	2.79	128.42	124.40
30	b	620	SQD	O48-C23-C24	2.78	120.31	111.83
24	c	504	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	A	606	CLA	O2D-CGD-CBD	2.78	116.09	111.23
24	b	603	CLA	O2A-CGA-O1A	-2.78	116.68	123.63
24	c	505	CLA	O2D-CGD-CBD	2.77	116.08	111.23
24	A	608	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
35	V	201	HEC	C3B-C4B-NB	-2.77	107.13	110.17
25	a	607	PHO	O2A-CGA-O1A	-2.77	116.70	123.63
24	b	611	CLA	O2D-CGD-CBD	2.76	116.06	111.23
30	a	614	SQD	C4-C3-C2	2.76	115.68	110.83
24	B	602	CLA	C3B-C4B-NB	-2.76	108.06	110.53
24	B	610	CLA	CAC-C3C-C4C	2.76	128.38	124.79
30	B	623	SQD	O9-S-C6	2.76	110.88	106.76
27	A	610	PL9	C7-C8-C9	-2.76	122.08	126.83
24	b	603	CLA	C3B-C4B-NB	-2.76	108.07	110.53
30	B	623	SQD	O5-C1-C2	-2.76	104.71	110.37
30	a	613	SQD	O8-S-C6	2.76	111.29	105.97
24	b	605	CLA	O1D-CGD-CBD	2.75	129.95	124.52
24	B	611	CLA	O2D-CGD-CBD	2.75	116.03	111.23
24	a	605	CLA	C3B-C4B-NB	-2.74	108.08	110.53
30	b	620	SQD	O5-C1-C2	-2.74	104.73	110.37
24	b	611	CLA	C3B-C4B-NB	-2.74	108.08	110.53
24	B	611	CLA	CHB-C4A-NA	2.74	128.36	124.40
24	A	605	CLA	C1-C2-C3	-2.74	121.71	126.20
26	B	619	BCR	C2-C1-C6	2.74	114.42	110.44
29	m	101	LMG	O3-C3-C2	-2.74	103.92	110.38
30	b	620	SQD	C3-C4-C5	2.73	115.17	110.23
30	A	615	SQD	O6-C1-C2	2.72	112.41	108.27
24	B	610	CLA	O2A-CGA-O1A	-2.72	116.82	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	C3B-C4B-NB	-2.72	108.10	110.53
30	A	613	SQD	O8-S-C6	2.72	111.23	105.97
25	D	402	PHO	C1-C2-C3	-2.72	121.74	126.20
29	D	408	LMG	O6-C1-C2	2.72	115.95	110.37
24	C	507	CLA	C2A-C1A-CHA	2.71	128.57	123.87
35	V	201	HEC	CMD-C2D-C1D	2.71	129.26	125.03
27	D	407	PL9	C36-C34-C33	-2.70	115.10	121.17
26	B	617	BCR	C29-C30-C25	2.70	114.36	110.44
30	D	410	SQD	C1-C2-C3	-2.70	104.34	110.01
27	D	407	PL9	C22-C23-C24	-2.70	121.45	127.62
24	b	612	CLA	O2A-CGA-O1A	-2.69	116.89	123.63
24	B	602	CLA	CMB-C2B-C3B	2.69	132.88	126.55
24	C	510	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	c	507	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	A	608	CLA	CHB-C4A-NA	2.69	128.28	124.40
24	A	605	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
24	C	501	CLA	O2D-CGD-CBD	2.67	115.90	111.23
28	C	516	STE	C3-C2-C1	-2.67	107.55	114.51
24	B	608	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
24	C	505	CLA	C3B-C4B-NB	-2.66	108.15	110.53
29	D	408	LMG	O6-C1-O1	-2.66	103.76	110.04
29	B	625	LMG	C8-O7-C10	2.66	124.16	117.80
30	D	410	SQD	O2-C2-C1	2.66	116.41	110.08
32	A	616	DGD	C2G-O2G-C1B	2.66	124.16	117.80
32	c	519	DGD	C3D-C4D-C5D	-2.66	105.42	110.23
27	a	611	PL9	O2-C1-C6	2.66	124.70	120.48
24	C	512	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
32	A	616	DGD	O4D-C4D-C5D	2.65	115.86	109.32
28	d	410	STE	C3-C2-C1	-2.65	107.59	114.51
30	B	623	SQD	C25-C24-C23	-2.65	104.00	113.69
24	B	604	CLA	CHB-C4A-NA	2.64	128.22	124.40
24	b	613	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	B	603	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	c	508	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
24	C	504	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
24	B	613	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
29	m	101	LMG	O1-C7-C8	-2.63	104.42	110.82
24	C	502	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
32	c	520	DGD	C3G-O3G-C1D	2.63	119.43	113.80
24	B	610	CLA	C1-C2-C3	-2.63	121.90	126.20
26	H	101	BCR	C16-C15-C14	-2.62	118.15	123.52
24	B	610	CLA	O2D-CGD-CBD	2.62	115.81	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	D	404	CLA	C4-C3-C5	2.62	119.77	115.23
25	D	402	PHO	O2D-CGD-CBD	2.62	113.82	110.95
24	C	503	CLA	CHB-C4A-NA	2.61	128.17	124.40
24	A	605	CLA	C3B-C4B-NB	-2.61	108.20	110.53
35	v	201	HEC	C4B-NB-C1B	2.61	108.30	105.21
24	C	509	CLA	C3B-C4B-NB	-2.61	108.20	110.53
28	e	105	STE	C3-C2-C1	-2.61	107.70	114.51
24	D	405	CLA	C1-C2-C3	-2.60	121.93	126.20
24	A	606	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
25	D	402	PHO	O2A-CGA-O1A	-2.60	117.12	123.63
24	b	616	CLA	C3B-C4B-NB	-2.60	108.21	110.53
34	e	102	HEM	C3B-C2B-C1B	2.60	108.36	106.41
24	c	502	CLA	C3B-C4B-NB	-2.60	108.21	110.53
30	A	613	SQD	O48-C23-C24	2.60	119.75	111.83
24	B	609	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
24	A	608	CLA	O2A-CGA-O1A	-2.60	117.14	123.63
30	A	615	SQD	O8-S-C6	2.60	110.98	105.97
24	B	607	CLA	C1-C2-C3	-2.59	121.95	126.20
24	D	404	CLA	C3B-C4B-NB	-2.59	108.22	110.53
32	c	518	DGD	C3D-C4D-C5D	-2.59	105.54	110.23
24	b	614	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
24	b	612	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
27	A	610	PL9	C40-C39-C41	2.59	119.72	115.23
27	D	407	PL9	C7-C8-C9	-2.58	122.38	126.83
24	C	513	CLA	CHD-C1D-ND	-2.58	121.17	124.80
24	D	403	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
26	c	515	BCR	C2-C1-C6	2.58	114.18	110.44
28	m	102	STE	C3-C2-C1	-2.57	107.79	114.51
24	c	513	CLA	C3B-C4B-NB	-2.57	108.23	110.53
25	a	607	PHO	C1-C2-C3	-2.57	121.98	126.20
24	c	506	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	B	616	CLA	C1-C2-C3	-2.56	122.00	126.20
24	B	614	CLA	CHC-C4B-NB	2.55	127.88	124.05
24	c	502	CLA	CHD-C1D-ND	-2.55	121.21	124.80
32	H	102	DGD	C6D-C5D-C4D	2.55	117.42	112.07
27	D	407	PL9	C20-C19-C21	2.54	119.64	115.23
24	d	402	CLA	C3B-C4B-NB	-2.54	108.27	110.53
27	D	407	PL9	C12-C13-C14	-2.53	121.83	127.62
24	C	513	CLA	C3B-C4B-NB	-2.53	108.27	110.53
30	a	613	SQD	C44-O6-C1	-2.53	108.38	113.80
24	B	614	CLA	O2A-CGA-O1A	-2.53	117.31	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	605	CLA	O1D-CGD-CBD	2.52	129.50	124.52
24	B	606	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	b	605	CLA	CHB-C4A-NA	2.52	128.04	124.40
34	e	102	HEM	CBA-CAA-C2A	-2.52	105.56	112.53
24	A	608	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	b	604	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	c	504	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	b	620	SQD	O2-C2-C1	2.52	116.08	110.08
24	c	510	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
24	C	510	CLA	C11-C10-C8	-2.52	107.60	115.97
24	B	616	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
30	A	615	SQD	O48-C23-O10	-2.52	117.33	123.63
25	D	402	PHO	CMA-C3A-C2A	-2.52	104.41	114.13
24	b	611	CLA	CHB-C4A-NA	2.51	128.03	124.40
24	A	608	CLA	O2D-CGD-CBD	2.51	115.62	111.23
24	b	612	CLA	C3B-C4B-NB	-2.51	108.29	110.53
32	H	102	DGD	C6D-O5D-C1E	2.51	119.18	113.80
24	d	404	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
26	T	101	BCR	C38-C26-C27	-2.51	108.25	113.60
24	B	612	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
24	b	613	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
24	c	508	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	c	509	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	b	612	CLA	O1D-CGD-CBD	2.50	129.46	124.52
30	f	101	SQD	O47-C7-C8	2.50	120.10	110.93
29	D	408	LMG	C8-O7-C10	2.49	123.76	117.80
24	B	608	CLA	CHB-C4A-NA	2.49	128.00	124.40
35	V	201	HEC	CAC-C3C-C2C	2.49	130.83	126.89
24	b	606	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	B	613	CLA	C3B-C4B-NB	-2.49	108.31	110.53
24	b	609	CLA	CHC-C4B-NB	2.49	127.78	124.05
30	D	410	SQD	C44-O6-C1	2.49	117.93	113.68
34	e	102	HEM	C4D-ND-C1D	2.49	108.15	105.21
24	b	602	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
24	c	508	CLA	CHD-C1D-ND	-2.48	121.31	124.80
24	b	604	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
24	B	608	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	b	614	CLA	CHD-C1D-ND	-2.48	121.32	124.80
24	C	502	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
33	d	401	BCT	O2-C-O1	2.48	126.01	119.68
24	C	506	CLA	C1-C2-C3	-2.47	122.14	126.20
26	H	101	BCR	C16-C17-C18	-2.47	123.81	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	605	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
27	A	610	PL9	C22-C23-C24	-2.47	121.96	127.62
24	A	608	CLA	CMB-C2B-C3B	2.47	132.37	126.55
25	a	608	PHO	O2A-CGA-O1A	-2.47	117.44	123.63
24	b	602	CLA	CAC-C3C-C4C	2.47	128.00	124.79
24	b	612	CLA	CAC-C3C-C4C	2.47	128.00	124.79
24	A	606	CLA	C1D-ND-C4D	2.47	108.04	106.31
24	B	601	CLA	O2D-CGD-CBD	2.46	115.54	111.23
24	c	501	CLA	CHB-C4A-NA	2.46	127.95	124.40
35	v	201	HEC	CHB-C1B-NB	2.46	127.07	124.42
24	B	607	CLA	CHC-C4B-NB	2.46	127.73	124.05
24	c	506	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
24	b	613	CLA	C1-C2-C3	-2.45	122.19	126.20
24	c	502	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	b	607	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
24	c	511	CLA	O2D-CGD-CBD	2.45	115.51	111.23
25	a	607	PHO	OBD-CAD-CBD	-2.44	122.24	125.82
24	b	607	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	C	506	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
30	f	101	SQD	O48-C23-C24	2.43	119.24	111.83
24	b	607	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
24	C	507	CLA	O2D-CGD-CBD	2.43	115.47	111.23
24	A	605	CLA	C11-C12-C13	-2.43	107.90	115.97
24	C	504	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
28	E	103	STE	C3-C2-C1	-2.43	108.18	114.51
24	a	609	CLA	CHB-C4A-NA	2.42	127.90	124.40
24	c	505	CLA	C1-C2-C3	-2.42	122.22	126.20
24	B	611	CLA	CHD-C1D-C2D	2.42	130.53	125.49
24	b	614	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	C	501	CLA	CHB-C1B-NB	2.42	127.67	124.05
24	b	615	CLA	CHB-C4A-NA	2.41	127.89	124.40
25	a	608	PHO	C3B-C4B-NB	-2.41	105.89	107.46
24	C	509	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
24	c	501	CLA	O2D-CGD-CBD	2.41	115.44	111.23
24	c	507	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
29	B	625	LMG	O6-C1-C2	-2.41	105.42	110.37
24	d	404	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
24	C	513	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
25	a	607	PHO	CMA-C3A-C2A	-2.40	104.85	114.13
27	A	610	PL9	C27-C28-C29	-2.40	122.12	127.62
24	d	404	CLA	CMB-C2B-C3B	2.40	132.19	126.55
24	B	601	CLA	CAA-CBA-CGA	-2.39	106.41	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	624	STE	O2-C1-C2	2.39	121.56	114.00
27	D	407	PL9	C42-C43-C44	-2.39	122.15	127.62
28	b	623	STE	O2-C1-C2	2.39	121.56	114.00
24	c	513	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
24	b	607	CLA	CHD-C1D-ND	-2.39	121.44	124.80
31	B	622	LHG	C5-O7-C7	2.38	123.50	117.80
24	B	603	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
26	J	101	BCR	C2-C1-C6	2.38	113.90	110.44
30	a	613	SQD	C1-C2-C3	-2.38	105.00	110.01
30	D	410	SQD	O48-C23-C24	2.38	119.09	111.83
27	d	406	PL9	C42-C43-C44	-2.38	122.17	127.62
24	C	506	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	C	504	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
24	a	609	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
24	B	607	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	c	503	CLA	C1-C2-C3	-2.37	122.32	126.20
24	B	607	CLA	C3B-C4B-NB	-2.37	108.42	110.53
30	a	614	SQD	C3-C4-C5	2.36	114.52	110.23
24	b	613	CLA	C16-C15-C13	-2.36	108.11	115.97
24	D	404	CLA	O2D-CGD-CBD	2.36	115.36	111.23
34	F	101	HEM	CHC-C1C-NC	2.36	127.02	124.45
24	B	612	CLA	C11-C12-C13	-2.36	108.13	115.97
24	D	403	CLA	CHD-C1D-ND	-2.36	121.49	124.80
27	A	610	PL9	C36-C34-C33	-2.36	115.88	121.17
28	C	525	STE	O2-C1-C2	2.35	121.44	114.00
24	b	604	CLA	CHC-C4B-NB	2.35	127.58	124.05
24	b	604	CLA	O2D-CGD-CBD	2.35	115.34	111.23
24	b	610	CLA	CAA-CBA-CGA	-2.35	106.54	113.21
29	a	615	LMG	O3-C3-C4	2.35	115.91	110.38
24	b	609	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
32	c	519	DGD	C1E-O6E-C5E	2.34	118.29	113.72
24	d	404	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	B	607	CLA	CHB-C1B-NB	2.34	127.56	124.05
24	C	509	CLA	C1-C2-C3	-2.34	122.37	126.20
24	B	607	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
24	B	602	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
35	v	201	HEC	CBD-CAD-C3D	-2.33	106.09	112.53
32	c	519	DGD	C3G-O3G-C1D	2.33	118.79	113.80
30	B	623	SQD	O7-S-C6	2.33	110.23	106.76
27	D	407	PL9	C7-C3-C2	-2.33	120.64	123.39
24	D	403	CLA	CHD-C1D-C2D	2.33	130.33	125.49
24	C	513	CLA	CHD-C1D-C2D	2.33	130.33	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	e	102	HEM	CAB-C3B-C2B	-2.33	120.87	128.43
35	v	201	HEC	C2A-C1A-NA	-2.32	108.08	110.32
29	c	522	LMG	C3-C4-C5	-2.32	106.02	110.23
24	c	502	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
35	v	201	HEC	C3C-C4C-NC	-2.32	107.58	110.15
24	b	601	CLA	O1D-CGD-CBD	2.32	129.09	124.52
24	B	611	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	B	602	CLA	C16-C15-C13	-2.32	108.26	115.97
24	B	610	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	B	610	CLA	CAA-CBA-CGA	-2.31	106.64	113.21
24	D	404	CLA	CHB-C4A-NA	2.31	127.74	124.40
24	B	606	CLA	CHB-C1B-NB	2.31	127.52	124.05
30	a	614	SQD	O9-S-C6	2.31	110.21	106.76
24	C	513	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
24	B	610	CLA	CHB-C1B-NB	2.31	127.51	124.05
24	C	505	CLA	O2D-CGD-CBD	2.30	115.26	111.23
24	c	505	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
24	b	607	CLA	CHB-C4A-NA	2.30	127.72	124.40
24	B	614	CLA	CHB-C4A-NA	2.30	127.72	124.40
24	B	605	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
24	b	610	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
24	B	604	CLA	C1-C2-C3	2.29	129.96	126.20
24	b	612	CLA	CHB-C4A-NA	2.29	127.71	124.40
24	C	509	CLA	CMB-C2B-C3B	2.29	131.94	126.55
34	e	102	HEM	C3B-C4B-NB	-2.29	107.82	109.47
24	A	605	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
24	c	513	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
24	C	503	CLA	C1-C2-C3	2.29	129.94	126.20
29	C	517	LMG	O3-C3-C2	-2.28	104.99	110.38
24	b	610	CLA	O1D-CGD-CBD	2.28	129.02	124.52
25	D	402	PHO	C2B-C1B-NB	-2.28	107.78	109.43
24	B	608	CLA	CMB-C2B-C3B	2.28	131.91	126.55
24	B	609	CLA	CHC-C4B-NB	2.28	127.47	124.05
24	B	604	CLA	C3B-C4B-NB	-2.27	108.50	110.53
32	c	518	DGD	O3D-C3D-C4D	2.27	115.73	110.38
24	b	608	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
24	b	611	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
24	c	509	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
24	b	607	CLA	CMB-C2B-C3B	2.26	131.88	126.55
24	c	501	CLA	C3B-C4B-NB	-2.26	108.51	110.53
24	C	511	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
24	c	503	CLA	CHD-C1D-ND	-2.26	121.62	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	O1D-CGD-CBD	2.26	128.98	124.52
28	E	103	STE	O2-C1-C2	2.25	121.12	114.00
34	F	101	HEM	CHC-C4B-NB	2.25	126.85	124.42
28	e	105	STE	O2-C1-C2	2.25	121.11	114.00
31	L	101	LHG	O7-C5-C4	-2.25	100.27	108.34
24	B	607	CLA	O2D-CGD-O1D	-2.25	119.48	123.85
24	c	504	CLA	CMB-C2B-C3B	2.24	131.83	126.55
24	c	501	CLA	O1D-CGD-CBD	2.24	128.94	124.52
24	b	609	CLA	CHA-C1A-NA	-2.24	121.31	126.39
24	C	511	CLA	C3B-C4B-NB	-2.24	108.53	110.53
24	A	606	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
26	t	101	BCR	C2-C1-C6	2.24	113.69	110.44
27	D	407	PL9	C8-C7-C3	2.24	117.82	112.03
24	C	509	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
29	c	516	LMG	C8-O7-C10	2.24	123.15	117.80
32	h	101	DGD	O3E-C3E-C2E	-2.24	105.10	110.38
29	B	620	LMG	O3-C3-C4	2.24	115.65	110.38
35	V	201	HEC	C2A-C1A-NA	-2.24	108.17	110.32
24	C	504	CLA	CHB-C4A-NA	2.24	127.63	124.40
24	c	509	CLA	CMB-C2B-C3B	2.24	131.81	126.55
27	d	406	PL9	O2-C1-C6	2.24	124.04	120.48
24	c	509	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
28	m	102	STE	O2-C1-C2	2.23	121.06	114.00
24	c	505	CLA	CHB-C1B-NB	2.23	127.40	124.05
24	b	614	CLA	O2D-CGD-CBD	2.23	115.13	111.23
24	c	505	CLA	CMB-C2B-C3B	2.23	131.79	126.55
24	B	601	CLA	CHB-C1B-NB	2.23	127.39	124.05
31	D	412	LHG	O4-P-O5	2.23	122.81	112.44
33	D	401	BCT	O2-C-O1	2.23	125.37	119.68
24	b	612	CLA	CHA-C1A-NA	-2.22	121.36	126.39
24	B	616	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
24	b	603	CLA	CHB-C4A-NA	2.22	127.60	124.40
32	h	101	DGD	C3E-C4E-C5E	-2.22	106.21	110.23
24	B	611	CLA	C2D-C1D-ND	-2.22	107.93	110.13
24	A	608	CLA	CHD-C1D-ND	-2.22	121.68	124.80
26	d	405	BCR	C38-C26-C25	-2.22	122.06	124.48
30	f	101	SQD	O5-C1-C2	-2.22	105.81	110.37
32	h	101	DGD	C3D-C4D-C5D	-2.21	106.22	110.23
27	a	611	PL9	C27-C28-C29	-2.21	122.56	127.62
24	a	609	CLA	C3B-C4B-NB	-2.21	108.56	110.53
28	B	626	STE	C3-C2-C1	-2.21	108.74	114.51
26	H	101	BCR	C2-C1-C6	2.21	113.65	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	616	DGD	O2E-C2E-C3E	2.21	115.58	110.38
24	b	608	CLA	O2D-CGD-CBD	2.21	115.09	111.23
25	a	608	PHO	C11-C12-C13	-2.21	108.63	115.97
24	D	404	CLA	C1-C2-C3	-2.21	122.58	126.20
26	H	101	BCR	C33-C5-C6	2.20	126.89	124.48
30	B	623	SQD	O8-S-C6	2.20	110.22	105.97
27	D	407	PL9	C32-C33-C34	-2.20	122.59	127.62
24	A	606	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	c	512	CLA	C1-C2-C3	-2.20	122.60	126.20
24	c	503	CLA	O1D-CGD-CBD	2.20	128.85	124.52
24	b	613	CLA	CHC-C4B-NB	2.20	127.34	124.05
24	B	606	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
24	b	615	CLA	CHC-C1C-NC	2.19	127.61	124.31
24	b	611	CLA	C7-C6-C5	-2.19	107.42	113.26
24	b	604	CLA	C3B-C4B-NB	-2.19	108.58	110.53
24	c	512	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
24	d	404	CLA	CGD-CBD-CAD	-2.19	103.77	110.85
35	v	201	HEC	CMD-C2D-C1D	2.19	128.45	125.03
29	c	522	LMG	C8-O7-C10	2.19	123.03	117.80
24	A	606	CLA	C2D-C1D-ND	-2.19	107.96	110.13
24	C	508	CLA	C11-C12-C13	-2.18	108.70	115.97
24	B	604	CLA	O2D-CGD-CBD	2.18	115.05	111.23
24	C	508	CLA	CHB-C4A-NA	2.18	127.55	124.40
24	b	616	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
25	a	607	PHO	OBD-CAD-C3D	2.18	131.29	127.89
32	h	101	DGD	O4E-C4E-C5E	2.18	114.69	109.32
24	c	508	CLA	CHD-C4C-NC	2.18	127.61	124.23
31	B	622	LHG	O7-C5-C4	-2.18	100.53	108.34
24	B	612	CLA	CMB-C2B-C3B	2.17	131.66	126.55
29	D	409	LMG	C1-O6-C5	2.17	117.96	113.72
28	X	101	STE	O2-C1-C2	2.17	120.86	114.00
27	d	406	PL9	C32-C33-C34	-2.17	122.65	127.62
29	d	411	LMG	O3-C3-C4	2.17	115.49	110.38
24	b	608	CLA	CHD-C4C-NC	2.17	127.60	124.23
26	B	618	BCR	C29-C30-C25	2.17	113.59	110.44
24	b	616	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
24	C	510	CLA	O2D-CGD-CBD	2.17	115.02	111.23
24	B	605	CLA	CHB-C4A-NA	2.16	127.52	124.40
30	a	613	SQD	O5-C1-C2	-2.16	105.93	110.37
27	a	611	PL9	C35-C34-C36	2.16	118.97	115.23
24	c	506	CLA	C1-C2-C3	-2.16	122.66	126.20
29	b	622	LMG	O2-C2-C1	-2.16	104.94	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	601	CLA	CHD-C1D-ND	-2.15	121.77	124.80
29	B	620	LMG	O6-C5-C4	2.15	113.57	109.70
24	b	606	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
24	b	613	CLA	CHB-C4A-NA	2.15	127.50	124.40
26	J	101	BCR	C23-C22-C21	-2.14	115.64	119.01
27	D	407	PL9	C35-C34-C36	2.14	118.95	115.23
24	b	609	CLA	C7-C6-C5	-2.14	107.55	113.26
28	B	626	STE	O2-C1-C2	2.14	120.77	114.00
24	A	606	CLA	CHB-C1B-NB	2.14	127.26	124.05
26	b	618	BCR	C4-C5-C6	-2.14	119.81	122.70
35	v	201	HEC	C3B-C4B-NB	-2.14	107.83	110.17
24	D	404	CLA	C6-C5-C3	2.14	118.67	113.47
26	A	609	BCR	C33-C5-C6	-2.14	122.15	124.48
26	t	101	BCR	C38-C26-C25	2.14	126.81	124.48
24	b	605	CLA	O1A-CGA-CBA	2.13	132.12	123.78
28	B	624	STE	C3-C2-C1	-2.13	108.95	114.51
34	e	102	HEM	C4C-C3C-C2C	2.13	108.66	106.81
24	C	504	CLA	CHB-C1B-NB	2.13	127.25	124.05
24	b	608	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
24	C	503	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
24	C	508	CLA	C11-C10-C8	-2.13	108.90	115.97
29	D	409	LMG	O3-C3-C4	2.13	115.39	110.38
28	d	407	STE	O2-C1-C2	2.13	120.72	114.00
24	c	502	CLA	CHD-C1D-C2D	2.13	129.91	125.49
24	c	507	CLA	CHB-C4A-NA	2.12	127.46	124.40
24	C	511	CLA	CHB-C4A-NA	2.12	127.46	124.40
24	a	609	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
26	a	610	BCR	C36-C18-C17	2.12	126.25	122.82
24	C	507	CLA	CHA-C1A-NA	-2.12	121.59	126.39
29	d	411	LMG	O3-C3-C2	-2.12	105.39	110.38
24	C	503	CLA	C1D-ND-C4D	2.12	107.80	106.31
24	B	616	CLA	CHD-C1D-C2D	2.11	129.88	125.49
30	A	613	SQD	C44-O6-C1	-2.11	109.27	113.80
26	T	101	BCR	C34-C9-C8	-2.11	114.86	118.09
24	c	506	CLA	O1D-CGD-CBD	2.11	128.68	124.52
26	b	618	BCR	C38-C26-C27	-2.11	109.09	113.60
24	C	508	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
24	b	604	CLA	C2A-C1A-CHA	2.11	127.53	123.87
24	B	603	CLA	CHC-C4B-NB	2.11	127.21	124.05
24	b	610	CLA	C3B-C4B-NB	-2.11	108.65	110.53
24	B	609	CLA	O2D-CGD-CBD	2.10	114.91	111.23
24	A	605	CLA	O2D-CGD-O1D	-2.10	119.75	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	407	PL9	O1-C4-C3	-2.10	118.51	120.73
24	c	510	CLA	O1D-CGD-CBD	2.10	128.66	124.52
24	b	609	CLA	CMB-C2B-C3B	2.10	131.50	126.55
32	C	523	DGD	O3G-C1D-C2D	-2.10	105.08	108.27
26	D	406	BCR	C40-C30-C25	2.10	113.54	110.24
29	D	408	LMG	O4-C4-C5	2.10	114.50	109.32
24	b	608	CLA	CHB-C1B-NB	2.10	127.20	124.05
31	d	408	LHG	O4-P-O5	2.10	122.20	112.44
24	c	507	CLA	O2D-CGD-CBD	2.10	114.89	111.23
24	C	511	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
24	c	510	CLA	CAC-C3C-C4C	2.10	127.52	124.79
24	C	511	CLA	O2D-CGD-O1D	-2.09	119.77	123.85
24	B	613	CLA	CED-O2D-CGD	2.09	120.66	115.92
25	a	607	PHO	C4A-C3A-C2A	2.09	104.83	102.84
28	B	627	STE	O2-C1-C2	2.09	120.61	114.00
24	b	612	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
24	b	614	CLA	CHD-C1D-C2D	2.09	129.83	125.49
30	b	620	SQD	C9-C8-C7	-2.09	106.04	113.69
26	t	101	BCR	C12-C13-C14	-2.09	115.73	119.01
28	I	101	STE	O2-C1-C2	2.09	120.59	114.00
32	h	101	DGD	C6D-O5D-C1E	2.08	118.27	113.80
30	a	613	SQD	O48-C23-O10	-2.08	118.42	123.63
24	C	513	CLA	CHB-C4A-NA	2.08	127.41	124.40
24	C	513	CLA	CMB-C2B-C3B	2.08	131.45	126.55
24	d	402	CLA	CHC-C4B-NB	2.08	127.17	124.05
24	b	616	CLA	CMB-C2B-C3B	2.08	131.44	126.55
24	D	405	CLA	O2D-CGD-CBD	2.08	114.87	111.23
27	a	611	PL9	C32-C33-C34	-2.08	122.86	127.62
28	i	101	STE	O2-C1-C2	2.08	120.56	114.00
24	B	616	CLA	CHD-C1D-ND	-2.08	121.88	124.80
26	b	619	BCR	C29-C30-C25	2.07	113.45	110.44
24	c	504	CLA	CHB-C1B-NB	2.07	127.16	124.05
24	b	601	CLA	CHD-C1D-C2D	2.07	129.80	125.49
24	C	505	CLA	C11-C10-C8	-2.07	109.07	115.97
24	C	503	CLA	CHD-C1D-ND	-2.07	121.89	124.80
24	b	613	CLA	CED-O2D-CGD	2.07	120.62	115.92
24	a	605	CLA	C2D-C1D-ND	-2.07	108.08	110.13
26	B	619	BCR	C27-C26-C25	-2.07	119.90	122.70
28	I	102	STE	C3-C2-C1	-2.07	109.11	114.51
24	b	601	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	A	607	PHO	OBD-CAD-CBD	-2.07	122.79	125.82
27	d	406	PL9	C50-C49-C48	-2.07	116.45	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	620	SQD	O4-C4-C3	-2.07	105.50	110.38
24	d	404	CLA	CHA-C1A-NA	-2.07	121.71	126.39
29	c	522	LMG	O4-C4-C5	2.06	114.41	109.32
24	c	504	CLA	O2D-CGD-CBD	2.06	114.84	111.23
31	D	411	LHG	O4-P-O5	2.06	122.04	112.44
24	C	503	CLA	C4D-CHA-C1A	2.06	123.70	121.24
24	C	503	CLA	CMB-C2B-C3B	2.06	131.40	126.55
29	B	620	LMG	O7-C8-C9	2.06	115.74	108.34
24	b	605	CLA	CHD-C4C-NC	2.06	127.43	124.23
24	C	509	CLA	CED-O2D-CGD	2.06	120.59	115.92
24	b	613	CLA	O2D-CGD-CBD	2.06	114.83	111.23
25	a	608	PHO	CAA-C2A-C3A	-2.05	107.46	113.00
24	b	607	CLA	CHC-C1C-NC	2.05	127.40	124.31
32	H	102	DGD	O3E-C3E-C4E	2.05	115.21	110.38
24	C	501	CLA	CHA-C4D-ND	2.05	136.78	132.55
24	B	616	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	b	604	CLA	C11-C10-C8	-2.05	109.16	115.97
30	B	623	SQD	C1-C2-C3	-2.05	105.70	110.01
30	A	613	SQD	O47-C7-O49	-2.05	118.92	123.70
24	b	612	CLA	C11-C10-C8	-2.05	109.16	115.97
28	E	101	STE	C3-C2-C1	-2.04	109.17	114.51
24	c	513	CLA	O2D-CGD-CBD	2.04	114.80	111.23
26	t	101	BCR	C30-C25-C24	-2.04	110.11	115.65
34	e	102	HEM	C2D-C1D-ND	-2.04	107.54	109.90
27	d	406	PL9	C36-C34-C33	-2.04	116.58	121.17
24	B	612	CLA	C16-C15-C13	-2.04	109.18	115.97
24	c	511	CLA	CHB-C4A-NA	2.04	127.34	124.40
30	B	623	SQD	C45-O47-C7	-2.04	112.92	117.80
30	a	614	SQD	O5-C5-C4	2.04	113.37	109.70
24	B	601	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
24	b	604	CLA	C4-C3-C5	2.04	118.76	115.23
27	d	406	PL9	C7-C3-C2	-2.03	120.99	123.39
24	B	615	CLA	O1D-CGD-CBD	2.03	128.53	124.52
25	a	608	PHO	CMA-C3A-C2A	-2.03	106.28	114.13
24	b	616	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
24	a	609	CLA	CMB-C2B-C3B	2.03	131.33	126.55
24	b	610	CLA	CHC-C4B-NB	2.03	127.10	124.05
24	c	505	CLA	CHD-C1D-ND	-2.03	121.94	124.80
34	e	102	HEM	CHB-C1B-NB	2.03	126.88	124.37
29	b	622	LMG	C9-C8-C7	2.03	116.52	111.78
28	X	101	STE	C3-C2-C1	-2.03	109.22	114.51
24	C	503	CLA	CHD-C1D-C2D	2.03	129.70	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
24	b	611	CLA	C1D-ND-C4D	2.02	107.73	106.31
24	d	403	CLA	CHA-C4D-ND	2.02	136.72	132.55
24	B	616	CLA	C1D-ND-C4D	2.02	107.73	106.31
24	d	404	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
24	C	506	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
25	A	607	PHO	C3B-C4B-NB	-2.02	106.15	107.46
24	B	609	CLA	C7-C6-C5	-2.02	107.89	113.26
26	B	619	BCR	C33-C5-C6	2.02	126.69	124.48
32	c	519	DGD	O4D-C4D-C5D	2.02	114.29	109.32
24	d	402	CLA	CHB-C4A-NA	2.02	127.31	124.40
24	B	616	CLA	CHC-C4B-NB	2.01	127.07	124.05
24	b	606	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
24	C	507	CLA	CHA-C4D-ND	2.01	136.70	132.55
28	b	623	STE	O2-C1-O1	-2.01	118.16	123.33
24	B	604	CLA	O2A-C1-C2	2.01	115.85	108.11
24	c	508	CLA	CHD-C1D-C2D	2.01	129.67	125.49
24	D	403	CLA	CHC-C1C-NC	2.01	127.34	124.31
24	B	606	CLA	C1-C2-C3	-2.01	122.91	126.20
24	c	503	CLA	C7-C6-C5	-2.01	107.91	113.26
24	b	608	CLA	CMB-C2B-C3B	2.01	131.27	126.55
24	c	508	CLA	O2D-CGD-CBD	2.01	114.74	111.23
27	A	610	PL9	C42-C43-C44	-2.01	123.03	127.62
30	a	613	SQD	C25-C24-C23	-2.01	106.35	113.69
24	D	405	CLA	C3B-C4B-NB	-2.00	108.74	110.53
24	b	611	CLA	CMB-C2B-C3B	2.00	131.26	126.55
29	b	622	LMG	O7-C8-C9	2.00	115.53	108.34
32	c	519	DGD	C6E-C5E-C4E	-2.00	108.10	113.02
24	b	609	CLA	C6-C5-C3	2.00	118.35	113.47
24	A	608	CLA	CHD-C4C-NC	2.00	127.33	124.23
24	C	505	CLA	CMB-C2B-C1B	-2.00	122.37	125.42

All (2) chirality outliers are listed below:

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

All (1829) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
24	C	503	CLA	C11-C10-C8-C9
24	C	504	CLA	C4-C3-C5-C6
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	C11-C10-C8-C9
24	D	404	CLA	C11-C10-C8-C9
24	b	601	CLA	C1A-C2A-CAA-CBA
24	b	601	CLA	C11-C10-C8-C9
24	b	605	CLA	C4B-C3B-CAB-CBB
24	b	605	CLA	C2-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
24	c	512	CLA	C11-C12-C13-C14
24	d	404	CLA	C6-C7-C8-C9
26	C	514	BCR	C21-C22-C23-C24
26	J	101	BCR	C21-C22-C23-C24
26	K	101	BCR	C7-C8-C9-C10
26	K	101	BCR	C17-C18-C19-C20
26	T	101	BCR	C21-C22-C23-C24
26	T	101	BCR	C37-C22-C23-C24
26	T	101	BCR	C23-C24-C25-C26
26	T	101	BCR	C23-C24-C25-C30
26	b	617	BCR	C5-C6-C7-C8
26	c	517	BCR	C7-C8-C9-C10
26	d	405	BCR	C21-C22-C23-C24
26	k	101	BCR	C1-C6-C7-C8
26	k	101	BCR	C5-C6-C7-C8
26	k	101	BCR	C17-C18-C19-C20
26	t	101	BCR	C11-C12-C13-C14
26	t	101	BCR	C21-C22-C23-C24
26	t	101	BCR	C37-C22-C23-C24
26	t	101	BCR	C23-C24-C25-C26
27	A	610	PL9	C22-C23-C24-C26
27	A	610	PL9	C27-C28-C29-C30
27	A	610	PL9	C37-C38-C39-C40
27	A	610	PL9	C37-C38-C39-C41
27	A	610	PL9	C38-C39-C41-C42
27	D	407	PL9	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	a	611	PL9	C12-C13-C14-C15
27	a	611	PL9	C12-C13-C14-C16
27	a	611	PL9	C17-C18-C19-C20
27	a	611	PL9	C17-C18-C19-C21
27	a	611	PL9	C22-C23-C24-C25
27	d	406	PL9	C32-C33-C34-C35
27	d	406	PL9	C32-C33-C34-C36
29	A	612	LMG	O9-C10-O7-C8
29	C	517	LMG	C2-C1-O1-C7
29	D	408	LMG	O6-C1-O1-C7
29	D	408	LMG	C11-C10-O7-C8
29	a	615	LMG	C2-C1-O1-C7
29	a	615	LMG	O6-C1-O1-C7
29	c	516	LMG	O1-C7-C8-C9
29	c	516	LMG	O1-C7-C8-O7
29	c	522	LMG	O9-C10-O7-C8
30	A	615	SQD	O6-C44-C45-O47
30	A	615	SQD	O5-C5-C6-S
30	B	623	SQD	C2-C1-O6-C44
30	B	623	SQD	O5-C1-O6-C44
30	B	623	SQD	O6-C44-C45-O47
30	B	623	SQD	O49-C7-O47-C45
30	B	623	SQD	C8-C7-O47-C45
30	D	410	SQD	O5-C1-O6-C44
30	a	614	SQD	C5-C6-S-O7
30	a	614	SQD	C5-C6-S-O8
30	a	614	SQD	C5-C6-S-O9
30	b	620	SQD	C46-C45-O47-C7
30	b	620	SQD	C8-C7-O47-C45
30	f	101	SQD	C2-C1-O6-C44
30	f	101	SQD	O5-C1-O6-C44
31	D	411	LHG	O1-C1-C2-C3
31	D	411	LHG	C3-O3-P-O4
31	D	411	LHG	C3-O3-P-O6
31	L	101	LHG	C3-O3-P-O4
31	L	101	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O4
31	a	612	LHG	O1-C1-C2-C3
31	a	612	LHG	C1-C2-C3-O3
31	a	612	LHG	C4-O6-P-O5
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
31	d	408	LHG	C4-O6-P-O4
31	e	103	LHG	C1-C2-C3-O3
31	e	103	LHG	C3-O3-P-O5
31	e	103	LHG	C4-O6-P-O5
31	e	103	LHG	O6-C4-C5-O7
31	l	101	LHG	C4-O6-P-O3
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
24	c	513	CLA	CBD-CGD-O2D-CED
24	B	601	CLA	O1A-CGA-O2A-C1
29	B	620	LMG	O10-C28-O8-C9
29	b	622	LMG	O10-C28-O8-C9
27	a	611	PL9	C47-C48-C49-C51
24	B	601	CLA	CBA-CGA-O2A-C1
29	M	101	LMG	O10-C28-O8-C9
30	f	101	SQD	O10-C23-O48-C46
29	D	408	LMG	O9-C10-O7-C8
30	b	620	SQD	O49-C7-O47-C45
24	b	601	CLA	C3-C5-C6-C7
24	b	614	CLA	C3-C5-C6-C7
29	B	620	LMG	C29-C28-O8-C9
29	b	622	LMG	C29-C28-O8-C9
30	f	101	SQD	C24-C23-O48-C46
24	B	614	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	CBD-CGD-O2D-CED
29	A	612	LMG	C11-C10-O7-C8
29	c	522	LMG	C11-C10-O7-C8
24	B	614	CLA	C4-C3-C5-C6
24	a	609	CLA	C4-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
24	c	507	CLA	C4-C3-C5-C6
27	a	611	PL9	C15-C14-C16-C17
27	d	406	PL9	C40-C39-C41-C42
24	B	614	CLA	C2-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	a	609	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
27	a	611	PL9	C33-C34-C36-C37
27	d	406	PL9	C38-C39-C41-C42
27	a	611	PL9	C47-C48-C49-C50
24	d	404	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	CBA-CGA-O2A-C1
29	M	101	LMG	C29-C28-O8-C9
30	b	620	SQD	C24-C23-O48-C46
27	A	610	PL9	C27-C28-C29-C31
27	D	407	PL9	C32-C33-C34-C36
27	a	611	PL9	C22-C23-C24-C26
24	B	615	CLA	C3-C5-C6-C7
24	B	616	CLA	C3-C5-C6-C7
24	b	607	CLA	CBD-CGD-O2D-CED
31	D	411	LHG	O2-C2-C3-O3
31	a	612	LHG	O2-C2-C3-O3
31	e	103	LHG	O2-C2-C3-O3
24	c	512	CLA	CBA-CGA-O2A-C1
24	B	616	CLA	O1A-CGA-O2A-C1
32	A	616	DGD	C2B-C1B-O2G-C2G
24	c	509	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	O1D-CGD-O2D-CED
24	A	608	CLA	C4-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	C	507	CLA	C4-C3-C5-C6
24	b	604	CLA	C4-C3-C5-C6
24	A	608	CLA	C2-C3-C5-C6
24	B	605	CLA	C2-C3-C5-C6
24	C	507	CLA	C2-C3-C5-C6
27	a	611	PL9	C13-C14-C16-C17
32	C	521	DGD	O6E-C5E-C6E-O5E
27	A	610	PL9	C9-C11-C12-C13
27	A	610	PL9	C19-C21-C22-C23
27	A	610	PL9	C24-C26-C27-C28
27	A	610	PL9	C34-C36-C37-C38
27	a	611	PL9	C9-C11-C12-C13
27	a	611	PL9	C14-C16-C17-C18
27	a	611	PL9	C24-C26-C27-C28
27	a	611	PL9	C44-C46-C47-C48
29	B	620	LMG	O6-C5-C6-O5
29	B	625	LMG	O6-C5-C6-O5
30	b	620	SQD	O10-C23-O48-C46
29	A	612	LMG	O6-C1-O1-C7
29	b	622	LMG	O6-C1-O1-C7
28	d	410	STE	C3-C4-C5-C6
24	C	501	CLA	CBD-CGD-O2D-CED
24	b	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	V	201	HEC	C2C-C3C-CAC-CBC
24	c	512	CLA	O1A-CGA-O2A-C1
31	L	101	LHG	C14-C15-C16-C17
29	a	615	LMG	C14-C15-C16-C17
24	B	616	CLA	CBD-CGD-O2D-CED
24	B	614	CLA	C13-C15-C16-C17
30	f	101	SQD	C25-C26-C27-C28
32	A	616	DGD	O1B-C1B-O2G-C2G
29	C	517	LMG	C29-C28-O8-C9
29	C	524	LMG	C29-C28-O8-C9
30	B	623	SQD	C24-C23-O48-C46
30	D	410	SQD	C24-C23-O48-C46
32	A	616	DGD	C2A-C1A-O1G-C1G
28	T	102	STE	C9-C10-C11-C12
30	B	623	SQD	C11-C10-C9-C8
27	a	611	PL9	C35-C34-C36-C37
24	c	507	CLA	C2-C3-C5-C6
24	A	606	CLA	C11-C12-C13-C14
24	B	608	CLA	C14-C13-C15-C16
24	B	610	CLA	C14-C13-C15-C16
24	B	615	CLA	C6-C7-C8-C9
24	C	512	CLA	C6-C7-C8-C9
24	C	513	CLA	C11-C12-C13-C14
24	a	606	CLA	C11-C12-C13-C14
24	b	605	CLA	C11-C10-C8-C9
24	b	606	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C10-C8-C9
24	b	609	CLA	C14-C13-C15-C16
24	b	610	CLA	C14-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C9
24	b	616	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C10-C8-C9
24	c	512	CLA	C6-C7-C8-C9
24	c	513	CLA	C11-C12-C13-C14
29	D	408	LMG	C2-C1-O1-C7
29	b	622	LMG	C2-C1-O1-C7
31	A	614	LHG	O2-C2-C3-O3
30	B	623	SQD	O10-C23-O48-C46
32	A	616	DGD	O1A-C1A-O1G-C1G
31	D	412	LHG	C12-C13-C14-C15
26	C	514	BCR	C37-C22-C23-C24
26	J	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	K	101	BCR	C7-C8-C9-C34
26	K	101	BCR	C36-C18-C19-C20
26	T	101	BCR	C7-C8-C9-C34
26	c	517	BCR	C7-C8-C9-C34
26	d	405	BCR	C37-C22-C23-C24
26	k	101	BCR	C36-C18-C19-C20
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C12-C13-C35
29	M	101	LMG	O6-C5-C6-O5
29	c	521	LMG	C28-C29-C30-C31
30	A	613	SQD	C23-C24-C25-C26
29	C	517	LMG	O10-C28-O8-C9
30	D	410	SQD	O10-C23-O48-C46
30	a	613	SQD	O47-C45-C46-O48
30	a	614	SQD	O6-C44-C45-O47
24	B	607	CLA	C5-C6-C7-C8
24	c	512	CLA	C13-C15-C16-C17
29	c	522	LMG	C10-C11-C12-C13
24	c	506	CLA	C2-C1-O2A-CGA
24	C	513	CLA	O1D-CGD-O2D-CED
27	a	611	PL9	C7-C8-C9-C10
32	c	519	DGD	C3B-C4B-C5B-C6B
24	B	603	CLA	C8-C10-C11-C12
24	B	613	CLA	C5-C6-C7-C8
24	C	505	CLA	C10-C11-C12-C13
24	D	403	CLA	C13-C15-C16-C17
29	A	612	LMG	C4-C5-C6-O5
29	c	522	LMG	O6-C5-C6-O5
24	A	605	CLA	C12-C13-C15-C16
24	B	601	CLA	C11-C12-C13-C15
24	B	602	CLA	C11-C12-C13-C15
24	b	606	CLA	C6-C7-C8-C10
35	V	201	HEC	C4C-C3C-CAC-CBC
29	c	522	LMG	C33-C34-C35-C36
32	C	523	DGD	C8A-C9A-CAA-CBA
24	B	606	CLA	C8-C10-C11-C12
24	C	503	CLA	C5-C6-C7-C8
24	c	509	CLA	C8-C10-C11-C12
28	d	412	STE	C1-C2-C3-C4
29	c	516	LMG	C28-C29-C30-C31
30	a	613	SQD	C7-C8-C9-C10
31	e	103	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	c	520	DGD	C1A-C2A-C3A-C4A
27	A	610	PL9	C29-C31-C32-C33
29	B	620	LMG	C4-C5-C6-O5
24	B	601	CLA	C5-C6-C7-C8
24	C	508	CLA	C13-C15-C16-C17
28	E	101	STE	C1-C2-C3-C4
30	b	620	SQD	C7-C8-C9-C10
24	B	614	CLA	O1D-CGD-O2D-CED
24	B	608	CLA	C15-C16-C17-C18
24	B	616	CLA	C5-C6-C7-C8
24	c	503	CLA	C8-C10-C11-C12
24	B	601	CLA	C2A-CAA-CBA-CGA
24	B	606	CLA	C2A-CAA-CBA-CGA
24	B	603	CLA	C13-C15-C16-C17
24	B	606	CLA	C13-C15-C16-C17
24	B	609	CLA	C13-C15-C16-C17
24	C	513	CLA	C13-C15-C16-C17
24	D	403	CLA	C15-C16-C17-C18
24	b	603	CLA	C5-C6-C7-C8
24	b	603	CLA	C8-C10-C11-C12
24	b	616	CLA	C8-C10-C11-C12
24	c	503	CLA	C5-C6-C7-C8
29	B	620	LMG	C28-C29-C30-C31
29	a	615	LMG	C10-C11-C12-C13
30	A	613	SQD	C7-C8-C9-C10
30	D	410	SQD	C23-C24-C25-C26
31	A	614	LHG	C23-C24-C25-C26
29	C	524	LMG	O10-C28-O8-C9
28	B	628	STE	C4-C5-C6-C7
29	A	612	LMG	C16-C17-C18-C19
31	e	103	LHG	C27-C28-C29-C30
32	c	518	DGD	C7A-C8A-C9A-CAA
24	B	605	CLA	C13-C15-C16-C17
24	C	506	CLA	C13-C15-C16-C17
24	b	601	CLA	C13-C15-C16-C17
24	b	611	CLA	C8-C10-C11-C12
24	b	611	CLA	C13-C15-C16-C17
24	b	615	CLA	C10-C11-C12-C13
24	c	502	CLA	C13-C15-C16-C17
24	c	506	CLA	C13-C15-C16-C17
24	c	513	CLA	C13-C15-C16-C17
24	d	404	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	A	607	PHO	C2C-C3C-CAC-CBC
25	a	608	PHO	C2C-C3C-CAC-CBC
30	a	614	SQD	C17-C18-C19-C20
32	C	522	DGD	C7A-C8A-C9A-CAA
31	d	408	LHG	O2-C2-C3-O3
24	b	601	CLA	CBD-CGD-O2D-CED
29	c	522	LMG	C28-C29-C30-C31
24	A	605	CLA	C15-C16-C17-C18
24	b	611	CLA	C15-C16-C17-C18
24	C	511	CLA	O1D-CGD-O2D-CED
24	B	615	CLA	C5-C6-C7-C8
24	a	609	CLA	C10-C11-C12-C13
24	c	502	CLA	C15-C16-C17-C18
24	c	505	CLA	C5-C6-C7-C8
28	C	525	STE	C1-C2-C3-C4
29	C	524	LMG	C28-C29-C30-C31
24	C	512	CLA	C10-C11-C12-C13
24	b	601	CLA	C8-C10-C11-C12
24	b	607	CLA	C10-C11-C12-C13
24	c	506	CLA	C15-C16-C17-C18
24	c	508	CLA	C13-C15-C16-C17
24	c	506	CLA	CBA-CGA-O2A-C1
28	B	626	STE	C1-C2-C3-C4
30	B	623	SQD	C23-C24-C25-C26
24	b	613	CLA	C13-C15-C16-C17
24	C	512	CLA	C3-C5-C6-C7
32	h	101	DGD	C9B-CAB-CBB-CCB
31	D	411	LHG	C1-C2-C3-O3
24	b	606	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	O1D-CGD-O2D-CED
24	B	602	CLA	C13-C15-C16-C17
24	B	610	CLA	C15-C16-C17-C18
24	C	506	CLA	C8-C10-C11-C12
24	C	512	CLA	C5-C6-C7-C8
24	b	607	CLA	C8-C10-C11-C12
29	c	521	LMG	C33-C34-C35-C36
24	B	608	CLA	C13-C15-C16-C17
24	B	611	CLA	C10-C11-C12-C13
24	C	509	CLA	C8-C10-C11-C12
28	C	528	STE	C11-C10-C9-C8
29	c	521	LMG	O6-C5-C6-O5
31	l	101	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	C13-C15-C16-C17
24	a	606	CLA	C13-C15-C16-C17
24	b	601	CLA	C15-C16-C17-C18
24	b	610	CLA	C15-C16-C17-C18
31	L	101	LHG	C7-C8-C9-C10
27	a	611	PL9	C23-C24-C26-C27
24	c	513	CLA	C8-C10-C11-C12
28	a	616	STE	C2-C3-C4-C5
32	c	519	DGD	C2E-C1E-O5D-C6D
24	b	601	CLA	C10-C11-C12-C13
31	d	409	LHG	C23-C24-C25-C26
24	b	612	CLA	C3-C5-C6-C7
31	d	409	LHG	C24-C25-C26-C27
24	C	505	CLA	C15-C16-C17-C18
29	A	612	LMG	O6-C5-C6-O5
26	T	101	BCR	C7-C8-C9-C10
26	t	101	BCR	C7-C8-C9-C10
29	C	524	LMG	C15-C16-C17-C18
31	d	409	LHG	O1-C1-C2-C3
29	C	524	LMG	C10-C11-C12-C13
24	c	509	CLA	O1D-CGD-O2D-CED
29	c	522	LMG	C35-C36-C37-C38
24	A	605	CLA	C16-C17-C18-C20
24	B	605	CLA	C16-C17-C18-C20
24	a	605	CLA	C16-C17-C18-C19
24	b	611	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C20
24	c	511	CLA	C16-C17-C18-C19
24	d	403	CLA	C16-C17-C18-C20
28	C	516	STE	C11-C10-C9-C8
24	c	506	CLA	O1A-CGA-O2A-C1
24	B	612	CLA	C10-C11-C12-C13
28	d	410	STE	C1-C2-C3-C4
24	b	604	CLA	C2-C3-C5-C6
29	B	625	LMG	C29-C28-O8-C9
24	B	612	CLA	C13-C15-C16-C17
24	B	610	CLA	CBD-CGD-O2D-CED
24	c	501	CLA	CBD-CGD-O2D-CED
29	B	620	LMG	C10-C11-C12-C13
31	a	612	LHG	C7-C8-C9-C10
24	B	601	CLA	C16-C17-C18-C20
24	B	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C16-C17-C18-C19
24	C	510	CLA	C16-C17-C18-C19
24	a	605	CLA	C16-C17-C18-C20
24	a	609	CLA	C16-C17-C18-C19
24	b	602	CLA	C16-C17-C18-C19
24	b	605	CLA	C16-C17-C18-C20
24	b	611	CLA	C16-C17-C18-C19
31	D	412	LHG	C16-C17-C18-C19
28	l	102	STE	C6-C7-C8-C9
29	A	612	LMG	C39-C40-C41-C42
30	a	613	SQD	C13-C14-C15-C16
30	a	613	SQD	C29-C30-C31-C32
31	B	622	LHG	C12-C13-C14-C15
31	a	612	LHG	C25-C26-C27-C28
28	A	618	STE	C12-C13-C14-C15
28	C	526	STE	C7-C8-C9-C10
28	T	102	STE	C4-C5-C6-C7
28	T	102	STE	C5-C6-C7-C8
28	b	625	STE	C4-C5-C6-C7
31	a	612	LHG	C28-C29-C30-C31
31	d	408	LHG	C33-C34-C35-C36
31	l	101	LHG	C29-C30-C31-C32
32	C	521	DGD	C4A-C5A-C6A-C7A
32	C	521	DGD	C7A-C8A-C9A-CAA
32	c	518	DGD	C5B-C6B-C7B-C8B
32	c	520	DGD	C2A-C3A-C4A-C5A
29	d	411	LMG	C28-C29-C30-C31
28	B	626	STE	C10-C11-C12-C13
29	B	620	LMG	C29-C30-C31-C32
29	m	101	LMG	C14-C15-C16-C17
31	d	409	LHG	C30-C31-C32-C33
32	A	616	DGD	C3B-C4B-C5B-C6B
28	E	103	STE	C14-C15-C16-C17
29	B	625	LMG	C13-C14-C15-C16
29	D	408	LMG	C32-C33-C34-C35
29	b	622	LMG	C12-C13-C14-C15
29	c	516	LMG	C13-C14-C15-C16
31	B	622	LHG	C31-C32-C33-C34
31	D	412	LHG	C14-C15-C16-C17
31	l	101	LHG	C15-C16-C17-C18
32	A	616	DGD	CDA-CEA-CFA-CGA
32	C	522	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
31	D	411	LHG	O1-C1-C2-O2
28	E	103	STE	C9-C10-C11-C12
28	d	413	STE	C4-C5-C6-C7
29	B	625	LMG	C41-C42-C43-C44
29	M	101	LMG	C15-C16-C17-C18
31	A	614	LHG	C28-C29-C30-C31
31	d	408	LHG	C12-C13-C14-C15
32	C	521	DGD	C4B-C5B-C6B-C7B
32	C	522	DGD	CBB-CCB-CDB-CEB
32	c	518	DGD	C8B-C9B-CAB-CBB
24	B	606	CLA	C4B-C3B-CAB-CBB
24	C	512	CLA	C4B-C3B-CAB-CBB
24	a	606	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C4B-C3B-CAB-CBB
29	D	408	LMG	C10-C11-C12-C13
32	C	521	DGD	CCA-CDA-CEA-CFA
24	A	605	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C20
24	c	511	CLA	C16-C17-C18-C20
24	d	403	CLA	C16-C17-C18-C19
24	b	601	CLA	C2A-CAA-CBA-CGA
30	A	613	SQD	C15-C16-C17-C18
24	A	606	CLA	C13-C15-C16-C17
24	B	616	CLA	C10-C11-C12-C13
24	b	607	CLA	C5-C6-C7-C8
24	b	609	CLA	C13-C15-C16-C17
30	f	101	SQD	C8-C7-O47-C45
31	A	614	LHG	C8-C7-O7-C5
30	A	615	SQD	C11-C12-C13-C14
32	C	523	DGD	CBA-CCA-CDA-CEA
29	B	625	LMG	C4-C5-C6-O5
24	B	611	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C12-C13-C15
28	b	621	STE	C13-C14-C15-C16
31	e	103	LHG	C24-C25-C26-C27
32	A	616	DGD	C9B-CAB-CBB-CCB
28	I	102	STE	C1-C2-C3-C4
29	M	101	LMG	C28-C29-C30-C31
28	A	611	STE	C4-C5-C6-C7
28	C	528	STE	C12-C13-C14-C15
28	b	621	STE	C11-C12-C13-C14
28	e	105	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
28	z	702	STE	C9-C10-C11-C12
29	B	625	LMG	C33-C34-C35-C36
29	D	409	LMG	C30-C31-C32-C33
29	b	622	LMG	C35-C36-C37-C38
31	D	411	LHG	C16-C17-C18-C19
31	D	411	LHG	C17-C18-C19-C20
31	d	408	LHG	C17-C18-C19-C20
32	C	521	DGD	C8A-C9A-CAA-CBA
32	C	522	DGD	C3B-C4B-C5B-C6B
32	H	102	DGD	C7A-C8A-C9A-CAA
24	b	601	CLA	C3A-C2A-CAA-CBA
28	C	520	STE	C7-C8-C9-C10
29	D	409	LMG	C17-C18-C19-C20
29	c	522	LMG	C11-C12-C13-C14
29	c	522	LMG	C36-C37-C38-C39
30	f	101	SQD	C24-C25-C26-C27
30	a	614	SQD	C9-C10-C11-C12
32	c	518	DGD	CAB-CBB-CCB-CDB
24	a	605	CLA	C15-C16-C17-C18
24	B	616	CLA	O1D-CGD-O2D-CED
32	H	102	DGD	C3B-C4B-C5B-C6B
32	c	520	DGD	C5B-C6B-C7B-C8B
24	B	604	CLA	C16-C17-C18-C19
24	a	609	CLA	C16-C17-C18-C20
28	f	103	STE	C11-C10-C9-C8
28	h	102	STE	C11-C12-C13-C14
30	a	613	SQD	C18-C19-C20-C21
32	A	616	DGD	C7A-C8A-C9A-CAA
28	B	628	STE	C5-C6-C7-C8
28	C	527	STE	C12-C13-C14-C15
28	T	102	STE	C7-C8-C9-C10
29	C	524	LMG	C29-C30-C31-C32
31	D	412	LHG	C11-C12-C13-C14
32	C	521	DGD	C4E-C5E-C6E-O5E
28	C	526	STE	C11-C10-C9-C8
29	D	409	LMG	C37-C38-C39-C40
29	b	622	LMG	C33-C34-C35-C36
24	b	615	CLA	C5-C6-C7-C8
24	c	508	CLA	C15-C16-C17-C18
28	E	103	STE	C11-C10-C9-C8
28	I	101	STE	C11-C10-C9-C8
28	d	410	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
28	l	102	STE	C4-C5-C6-C7
29	B	625	LMG	C39-C40-C41-C42
30	b	620	SQD	C29-C30-C31-C32
31	A	614	LHG	C9-C10-C11-C12
31	A	614	LHG	C34-C35-C36-C37
31	d	409	LHG	C25-C26-C27-C28
32	c	518	DGD	C7B-C8B-C9B-CAB
32	c	518	DGD	CCB-CDB-CEB-CFB
28	I	101	STE	C5-C6-C7-C8
28	M	102	STE	C4-C5-C6-C7
29	a	615	LMG	C38-C39-C40-C41
29	m	101	LMG	C17-C18-C19-C20
29	m	101	LMG	C31-C32-C33-C34
31	d	408	LHG	C11-C10-C9-C8
28	e	105	STE	C5-C6-C7-C8
30	f	101	SQD	C26-C27-C28-C29
32	c	519	DGD	CBA-CCA-CDA-CEA
29	D	408	LMG	C16-C17-C18-C19
29	d	411	LMG	C35-C36-C37-C38
30	A	613	SQD	C11-C10-C9-C8
31	d	409	LHG	C31-C32-C33-C34
31	l	101	LHG	C34-C35-C36-C37
32	A	616	DGD	C7B-C8B-C9B-CAB
32	C	522	DGD	CCA-CDA-CEA-CFA
24	B	601	CLA	C16-C17-C18-C19
24	b	607	CLA	C16-C17-C18-C20
24	A	606	CLA	C2B-C3B-CAB-CBB
24	C	512	CLA	C2B-C3B-CAB-CBB
24	b	605	CLA	C2B-C3B-CAB-CBB
26	J	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C1-C6-C7-C8
26	b	617	BCR	C1-C6-C7-C8
26	t	101	BCR	C23-C24-C25-C30
29	M	101	LMG	C31-C32-C33-C34
30	A	613	SQD	C30-C31-C32-C33
31	e	103	LHG	C8-C7-O7-C5
24	b	602	CLA	C10-C11-C12-C13
24	b	605	CLA	C5-C6-C7-C8
28	B	626	STE	C11-C10-C9-C8
30	b	620	SQD	C16-C17-C18-C19
32	A	616	DGD	C2A-C3A-C4A-C5A
28	b	625	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	B	620	LMG	C12-C13-C14-C15
30	A	615	SQD	C15-C16-C17-C18
24	b	613	CLA	C10-C11-C12-C13
29	c	516	LMG	C32-C33-C34-C35
31	B	622	LHG	C9-C10-C11-C12
32	C	522	DGD	C4B-C5B-C6B-C7B
32	H	102	DGD	C7B-C8B-C9B-CAB
32	h	101	DGD	C5B-C6B-C7B-C8B
29	B	625	LMG	O10-C28-O8-C9
27	a	611	PL9	C4-C3-C7-C8
27	d	406	PL9	C4-C3-C7-C8
29	A	612	LMG	C29-C30-C31-C32
30	f	101	SQD	O49-C7-O47-C45
31	A	614	LHG	O9-C7-O7-C5
24	b	613	CLA	O1D-CGD-O2D-CED
28	b	621	STE	C3-C4-C5-C6
31	L	101	LHG	C11-C10-C9-C8
24	C	502	CLA	C15-C16-C17-C18
24	a	606	CLA	C15-C16-C17-C18
24	b	614	CLA	C15-C16-C17-C18
24	c	508	CLA	C8-C10-C11-C12
24	c	503	CLA	C16-C17-C18-C20
28	C	520	STE	C11-C10-C9-C8
28	C	528	STE	C9-C10-C11-C12
28	b	621	STE	C4-C5-C6-C7
28	d	407	STE	C6-C7-C8-C9
29	C	524	LMG	C14-C15-C16-C17
29	b	622	LMG	C22-C23-C24-C25
32	C	523	DGD	C3A-C4A-C5A-C6A
32	c	520	DGD	C6B-C7B-C8B-C9B
29	b	622	LMG	C10-C11-C12-C13
24	c	509	CLA	C11-C12-C13-C14
28	z	701	STE	C7-C8-C9-C10
32	C	521	DGD	CBB-CCB-CDB-CEB
24	c	511	CLA	C15-C16-C17-C18
28	I	102	STE	C2-C3-C4-C5
29	A	612	LMG	C14-C15-C16-C17
31	A	614	LHG	C24-C25-C26-C27
32	C	522	DGD	CBA-CCA-CDA-CEA
28	B	621	STE	C3-C4-C5-C6
28	E	103	STE	C11-C12-C13-C14
28	J	102	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	b	623	STE	C11-C10-C9-C8
30	A	613	SQD	C9-C10-C11-C12
30	f	101	SQD	C33-C34-C35-C36
31	B	622	LHG	C26-C27-C28-C29
24	C	501	CLA	O1D-CGD-O2D-CED
30	D	410	SQD	C2-C1-O6-C44
24	B	616	CLA	C8-C10-C11-C12
28	H	103	STE	C9-C10-C11-C12
28	M	102	STE	C2-C3-C4-C5
30	B	623	SQD	C16-C17-C18-C19
31	B	622	LHG	C24-C25-C26-C27
27	A	610	PL9	C47-C48-C49-C51
28	B	626	STE	C2-C3-C4-C5
28	B	628	STE	C11-C10-C9-C8
28	Z	101	STE	C11-C12-C13-C14
28	e	104	STE	C13-C14-C15-C16
30	D	410	SQD	C25-C26-C27-C28
30	a	614	SQD	C14-C15-C16-C17
30	a	614	SQD	C24-C25-C26-C27
28	b	623	STE	C2-C3-C4-C5
28	h	103	STE	C13-C14-C15-C16
29	A	612	LMG	C35-C36-C37-C38
29	a	615	LMG	C17-C18-C19-C20
29	m	101	LMG	C29-C30-C31-C32
30	B	623	SQD	C33-C34-C35-C36
32	H	102	DGD	C8B-C9B-CAB-CBB
32	c	520	DGD	C5A-C6A-C7A-C8A
24	A	606	CLA	C16-C17-C18-C19
29	c	521	LMG	C11-C10-O7-C8
32	C	522	DGD	C1B-C2B-C3B-C4B
24	C	512	CLA	C15-C16-C17-C18
24	b	614	CLA	C13-C15-C16-C17
28	z	702	STE	C11-C12-C13-C14
29	b	622	LMG	C21-C22-C23-C24
31	A	614	LHG	C15-C16-C17-C18
29	M	101	LMG	C37-C38-C39-C40
29	d	411	LMG	C33-C34-C35-C36
32	C	522	DGD	C4A-C5A-C6A-C7A
32	c	519	DGD	C7A-C8A-C9A-CAA
32	c	520	DGD	CDA-CEA-CFA-CGA
24	B	601	CLA	C13-C15-C16-C17
24	c	512	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	z	701	STE	C9-C10-C11-C12
32	c	518	DGD	C9B-CAB-CBB-CCB
28	C	528	STE	C6-C7-C8-C9
29	M	101	LMG	C33-C34-C35-C36
32	C	521	DGD	CAA-CBA-CCA-CDA
32	C	523	DGD	C5A-C6A-C7A-C8A
28	b	621	STE	C5-C6-C7-C8
28	b	623	STE	C9-C10-C11-C12
29	A	612	LMG	C11-C12-C13-C14
31	d	409	LHG	C28-C29-C30-C31
24	B	605	CLA	C16-C17-C18-C19
24	b	607	CLA	C16-C17-C18-C19
28	B	628	STE	C9-C10-C11-C12
28	M	102	STE	C7-C8-C9-C10
28	d	412	STE	C2-C3-C4-C5
29	M	101	LMG	C38-C39-C40-C41
30	A	613	SQD	C33-C34-C35-C36
30	a	614	SQD	C30-C31-C32-C33
31	e	103	LHG	C12-C13-C14-C15
28	C	520	STE	C4-C5-C6-C7
28	t	102	STE	C4-C5-C6-C7
28	z	701	STE	C5-C6-C7-C8
29	A	612	LMG	C36-C37-C38-C39
31	l	101	LHG	C25-C26-C27-C28
24	a	609	CLA	C13-C15-C16-C17
24	c	503	CLA	C15-C16-C17-C18
30	f	101	SQD	C32-C33-C34-C35
28	i	101	STE	C6-C7-C8-C9
30	B	623	SQD	C11-C12-C13-C14
31	a	612	LHG	C14-C15-C16-C17
24	B	613	CLA	C8-C10-C11-C12
24	b	614	CLA	C5-C6-C7-C8
24	d	402	CLA	C13-C15-C16-C17
29	C	524	LMG	C12-C13-C14-C15
29	D	409	LMG	C21-C22-C23-C24
29	b	622	LMG	C30-C31-C32-C33
32	h	101	DGD	C7B-C8B-C9B-CAB
29	C	517	LMG	C28-C29-C30-C31
28	B	624	STE	C11-C10-C9-C8
29	D	408	LMG	C30-C31-C32-C33
31	d	408	LHG	C28-C29-C30-C31
32	A	616	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
32	c	519	DGD	CAA-CBA-CCA-CDA
29	c	521	LMG	O9-C10-O7-C8
28	B	628	STE	C7-C8-C9-C10
28	f	103	STE	C6-C7-C8-C9
30	a	613	SQD	C30-C31-C32-C33
31	A	614	LHG	C33-C34-C35-C36
31	D	412	LHG	C29-C30-C31-C32
31	L	101	LHG	C10-C11-C12-C13
32	A	616	DGD	CEB-CFB-CGB-CHB
27	D	407	PL9	C34-C36-C37-C38
24	c	507	CLA	C5-C6-C7-C8
34	e	102	HEM	C4B-C3B-CAB-CBB
28	d	407	STE	C4-C5-C6-C7
29	m	101	LMG	C32-C33-C34-C35
30	b	620	SQD	C10-C11-C12-C13
31	D	411	LHG	C12-C13-C14-C15
31	L	101	LHG	C31-C32-C33-C34
32	C	521	DGD	C3B-C4B-C5B-C6B
28	z	701	STE	C3-C4-C5-C6
32	c	518	DGD	C3B-C4B-C5B-C6B
28	B	621	STE	C1-C2-C3-C4
30	f	101	SQD	C23-C24-C25-C26
31	d	409	LHG	C7-C8-C9-C10
24	b	602	CLA	C15-C16-C17-C18
24	c	513	CLA	C15-C16-C17-C18
29	B	625	LMG	C11-C12-C13-C14
29	D	409	LMG	O6-C5-C6-O5
32	A	616	DGD	O2G-C2G-C3G-O3G
28	A	617	STE	C12-C13-C14-C15
28	h	102	STE	C12-C13-C14-C15
29	C	517	LMG	C11-C12-C13-C14
29	b	622	LMG	C32-C33-C34-C35
28	H	103	STE	C2-C3-C4-C5
28	z	701	STE	C6-C7-C8-C9
32	C	523	DGD	C4B-C5B-C6B-C7B
24	B	607	CLA	C8-C10-C11-C12
24	C	509	CLA	C10-C11-C12-C13
31	D	411	LHG	C18-C19-C20-C21
28	B	626	STE	C7-C8-C9-C10
29	c	522	LMG	C37-C38-C39-C40
30	A	613	SQD	C31-C32-C33-C34
32	C	523	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
27	d	406	PL9	C47-C48-C49-C51
28	E	102	STE	C14-C15-C16-C17
28	d	407	STE	C14-C15-C16-C17
29	B	620	LMG	C11-C12-C13-C14
29	C	517	LMG	C16-C17-C18-C19
24	B	613	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
27	D	407	PL9	C30-C29-C31-C32
31	A	614	LHG	C1-C2-C3-O3
28	A	611	STE	C2-C3-C4-C5
28	B	621	STE	C11-C10-C9-C8
28	h	103	STE	C14-C15-C16-C17
29	c	516	LMG	C15-C16-C17-C18
24	b	616	CLA	CBD-CGD-O2D-CED
29	D	409	LMG	C16-C17-C18-C19
30	A	613	SQD	C25-C26-C27-C28
31	A	614	LHG	C29-C30-C31-C32
31	B	622	LHG	C15-C16-C17-C18
32	C	522	DGD	C5B-C6B-C7B-C8B
30	D	410	SQD	C30-C31-C32-C33
32	H	102	DGD	C1A-C2A-C3A-C4A
28	z	702	STE	C2-C3-C4-C5
28	I	101	STE	C4-C5-C6-C7
29	D	409	LMG	C19-C20-C21-C22
29	b	622	LMG	C40-C41-C42-C43
31	d	409	LHG	C34-C35-C36-C37
31	a	612	LHG	O1-C1-C2-O2
28	b	625	STE	C3-C4-C5-C6
29	M	101	LMG	C4-C5-C6-O5
32	C	521	DGD	C6B-C7B-C8B-C9B
24	B	601	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
24	c	513	CLA	C1A-C2A-CAA-CBA
24	b	616	CLA	C5-C6-C7-C8
24	c	505	CLA	C13-C15-C16-C17
32	c	519	DGD	O6E-C1E-O5D-C6D
28	B	621	STE	C9-C10-C11-C12
29	c	521	LMG	C14-C15-C16-C17
30	a	614	SQD	C15-C16-C17-C18
32	h	101	DGD	C7A-C8A-C9A-CAA
28	E	101	STE	C3-C4-C5-C6
28	b	621	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	a	615	LMG	C33-C34-C35-C36
28	C	528	STE	C7-C8-C9-C10
28	J	102	STE	C2-C3-C4-C5
28	Z	101	STE	C9-C10-C11-C12
28	b	624	STE	C7-C8-C9-C10
28	z	702	STE	C7-C8-C9-C10
30	a	614	SQD	C29-C30-C31-C32
28	E	103	STE	C13-C14-C15-C16
29	A	612	LMG	C37-C38-C39-C40
29	m	101	LMG	C38-C39-C40-C41
24	B	604	CLA	C11-C10-C8-C7
24	B	606	CLA	C12-C13-C15-C16
24	B	608	CLA	C12-C13-C15-C16
24	B	614	CLA	C12-C13-C15-C16
24	C	502	CLA	C11-C12-C13-C15
24	D	405	CLA	C6-C7-C8-C10
24	b	607	CLA	C11-C12-C13-C15
24	b	613	CLA	C11-C10-C8-C7
24	b	614	CLA	C6-C7-C8-C10
24	c	513	CLA	C12-C13-C15-C16
24	d	403	CLA	C11-C12-C13-C15
24	d	404	CLA	C11-C12-C13-C15
30	D	410	SQD	C27-C28-C29-C30
24	b	602	CLA	C16-C17-C18-C20
24	B	612	CLA	C8-C10-C11-C12
24	B	601	CLA	C10-C11-C12-C13
24	B	614	CLA	C8-C10-C11-C12
32	A	616	DGD	C1B-C2B-C3B-C4B
28	T	102	STE	C6-C7-C8-C9
27	A	610	PL9	C47-C48-C49-C50
28	h	103	STE	C11-C12-C13-C14
32	A	616	DGD	O6E-C5E-C6E-O5E
32	C	522	DGD	C3A-C4A-C5A-C6A
24	B	604	CLA	C11-C10-C8-C9
24	B	614	CLA	C14-C13-C15-C16
24	D	403	CLA	C14-C13-C15-C16
24	a	609	CLA	C14-C13-C15-C16
24	b	602	CLA	C11-C10-C8-C9
24	b	604	CLA	C14-C13-C15-C16
24	b	615	CLA	C11-C10-C8-C9
24	c	505	CLA	C11-C12-C13-C14
28	A	619	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	b	624	STE	C14-C15-C16-C17
31	D	411	LHG	C34-C35-C36-C37
28	B	621	STE	C11-C12-C13-C14
28	H	103	STE	C14-C15-C16-C17
31	d	408	LHG	C11-C12-C13-C14
28	X	101	STE	C11-C10-C9-C8
31	e	103	LHG	O9-C7-O7-C5
24	a	609	CLA	C5-C6-C7-C8
28	M	102	STE	C3-C4-C5-C6
29	M	101	LMG	C7-C8-C9-O8
31	e	103	LHG	C4-C5-C6-O8
24	c	503	CLA	CBD-CGD-O2D-CED
28	E	102	STE	C11-C10-C9-C8
29	B	625	LMG	C29-C30-C31-C32
30	a	614	SQD	C34-C35-C36-C37
28	A	617	STE	C15-C16-C17-C18
28	b	624	STE	C11-C12-C13-C14
30	B	623	SQD	C13-C14-C15-C16
28	b	625	STE	C7-C8-C9-C10
29	b	622	LMG	O6-C5-C6-O5
32	c	518	DGD	O6E-C5E-C6E-O5E
28	A	618	STE	C10-C11-C12-C13
28	H	104	STE	C11-C12-C13-C14
31	A	614	LHG	C30-C31-C32-C33
32	C	523	DGD	C6A-C7A-C8A-C9A
28	i	101	STE	C2-C3-C4-C5
30	a	613	SQD	C26-C27-C28-C29
28	A	617	STE	C13-C14-C15-C16
30	B	623	SQD	C34-C35-C36-C37
28	I	101	STE	C3-C4-C5-C6
29	D	408	LMG	C28-C29-C30-C31
31	l	101	LHG	C7-C8-C9-C10
30	A	615	SQD	C9-C10-C11-C12
30	D	410	SQD	C34-C35-C36-C37
27	a	611	PL9	C45-C44-C46-C47
24	c	510	CLA	C2-C3-C5-C6
27	a	611	PL9	C43-C44-C46-C47
27	d	406	PL9	C28-C29-C31-C32
24	b	614	CLA	C8-C10-C11-C12
24	A	606	CLA	C16-C17-C18-C20
24	B	616	CLA	C11-C12-C13-C14
24	C	505	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
28	M	102	STE	C9-C10-C11-C12
28	j	101	STE	C4-C5-C6-C7
30	f	101	SQD	C31-C32-C33-C34
32	C	521	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	O6D-C5D-C6D-O5D
28	Z	101	STE	C6-C7-C8-C9
29	d	411	LMG	O6-C5-C6-O5
29	B	625	LMG	C16-C17-C18-C19
24	b	605	CLA	C10-C11-C12-C13
32	C	521	DGD	C8B-C9B-CAB-CBB
32	C	523	DGD	C7A-C8A-C9A-CAA
28	b	621	STE	C2-C3-C4-C5
29	a	615	LMG	C12-C13-C14-C15
24	B	604	CLA	O2A-C1-C2-C3
29	D	408	LMG	C7-C8-O7-C10
29	b	622	LMG	C9-C8-O7-C10
28	A	618	STE	C13-C14-C15-C16
28	C	527	STE	C7-C8-C9-C10
28	C	527	STE	C11-C10-C9-C8
29	B	625	LMG	C14-C15-C16-C17
29	C	524	LMG	C37-C38-C39-C40
29	m	101	LMG	C12-C13-C14-C15
29	m	101	LMG	C19-C20-C21-C22
30	b	620	SQD	C14-C15-C16-C17
31	a	612	LHG	C11-C10-C9-C8
32	C	521	DGD	C7B-C8B-C9B-CAB
24	C	510	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C19
28	E	102	STE	C7-C8-C9-C10
24	C	512	CLA	CBD-CGD-O2D-CED
24	A	605	CLA	C13-C15-C16-C17
31	B	622	LHG	C29-C30-C31-C32
29	C	524	LMG	C32-C33-C34-C35
31	D	411	LHG	C15-C16-C17-C18
28	H	103	STE	C1-C2-C3-C4
29	m	101	LMG	C34-C35-C36-C37
28	e	104	STE	C11-C12-C13-C14
31	d	409	LHG	C29-C30-C31-C32
24	c	504	CLA	C4-C3-C5-C6
28	C	526	STE	C12-C13-C14-C15
28	e	104	STE	C12-C13-C14-C15
30	A	615	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	A	614	LHG	C11-C12-C13-C14
28	X	101	STE	C9-C10-C11-C12
28	d	410	STE	C4-C5-C6-C7
28	d	412	STE	C6-C7-C8-C9
28	j	101	STE	C2-C3-C4-C5
29	B	625	LMG	C22-C23-C24-C25
29	c	521	LMG	C13-C14-C15-C16
31	B	622	LHG	C25-C26-C27-C28
31	d	408	LHG	C9-C10-C11-C12
32	H	102	DGD	C2B-C3B-C4B-C5B
28	h	103	STE	C15-C16-C17-C18
28	I	102	STE	C6-C7-C8-C9
30	A	613	SQD	O6-C44-C45-O47
31	A	614	LHG	O7-C5-C6-O8
28	A	618	STE	C2-C3-C4-C5
29	a	615	LMG	C34-C35-C36-C37
29	b	622	LMG	C11-C12-C13-C14
31	a	612	LHG	C9-C10-C11-C12
28	b	625	STE	C1-C2-C3-C4
29	m	101	LMG	C40-C41-C42-C43
30	a	613	SQD	C23-C24-C25-C26
28	b	624	STE	C9-C10-C11-C12
28	d	412	STE	C3-C4-C5-C6
29	c	521	LMG	C11-C12-C13-C14
29	M	101	LMG	C40-C41-C42-C43
28	B	626	STE	C12-C13-C14-C15
28	M	102	STE	C6-C7-C8-C9
24	c	503	CLA	C16-C17-C18-C19
30	a	613	SQD	C10-C11-C12-C13
29	D	408	LMG	C29-C28-O8-C9
30	a	613	SQD	C35-C36-C37-C38
31	D	411	LHG	C9-C10-C11-C12
29	d	411	LMG	C40-C41-C42-C43
28	C	526	STE	C10-C11-C12-C13
32	C	523	DGD	C3B-C4B-C5B-C6B
24	a	609	CLA	C15-C16-C17-C18
31	D	411	LHG	C32-C33-C34-C35
32	C	522	DGD	C7B-C8B-C9B-CAB
29	A	612	LMG	C19-C20-C21-C22
24	C	507	CLA	C5-C6-C7-C8
24	b	616	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	c	505	CLA	C4-C3-C5-C6
29	m	101	LMG	C29-C28-O8-C9
28	E	102	STE	C9-C10-C11-C12
31	a	612	LHG	C16-C17-C18-C19
28	d	407	STE	C2-C3-C4-C5
29	B	625	LMG	C19-C20-C21-C22
30	a	614	SQD	C11-C12-C13-C14
24	B	606	CLA	C14-C13-C15-C16
24	B	613	CLA	C11-C12-C13-C14
24	B	615	CLA	C11-C12-C13-C14
24	C	502	CLA	C11-C12-C13-C14
24	C	513	CLA	C11-C10-C8-C9
24	D	405	CLA	C6-C7-C8-C9
24	b	603	CLA	C11-C12-C13-C14
24	b	607	CLA	C6-C7-C8-C9
24	b	607	CLA	C11-C12-C13-C14
24	b	615	CLA	C11-C12-C13-C14
24	c	506	CLA	C11-C10-C8-C9
24	c	506	CLA	C11-C12-C13-C14
24	c	507	CLA	C14-C13-C15-C16
24	c	513	CLA	C14-C13-C15-C16
24	d	403	CLA	C11-C12-C13-C14
24	d	404	CLA	C11-C12-C13-C14
29	D	408	LMG	C33-C34-C35-C36
31	d	409	LHG	C2-C3-O3-P
24	b	601	CLA	C4B-C3B-CAB-CBB
24	c	502	CLA	C4B-C3B-CAB-CBB
31	B	622	LHG	C11-C10-C9-C8
28	A	619	STE	C10-C11-C12-C13
24	b	606	CLA	C15-C16-C17-C18
29	A	612	LMG	C40-C41-C42-C43
32	h	101	DGD	CDB-CEB-CFB-CGB
28	X	101	STE	C4-C5-C6-C7
28	d	412	STE	C5-C6-C7-C8
29	D	408	LMG	C13-C14-C15-C16
29	a	615	LMG	C31-C32-C33-C34
30	a	613	SQD	C31-C32-C33-C34
31	d	408	LHG	C14-C15-C16-C17
28	d	412	STE	C10-C11-C12-C13
30	f	101	SQD	C27-C28-C29-C30
31	B	622	LHG	C14-C15-C16-C17
32	A	616	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
32	c	519	DGD	C5A-C6A-C7A-C8A
31	e	103	LHG	O6-C4-C5-C6
29	B	625	LMG	C12-C13-C14-C15
29	D	409	LMG	C20-C21-C22-C23
30	D	410	SQD	C29-C30-C31-C32
31	B	622	LHG	C30-C31-C32-C33
31	d	409	LHG	C27-C28-C29-C30
28	B	628	STE	C12-C13-C14-C15
28	M	102	STE	C11-C10-C9-C8
24	B	601	CLA	C11-C10-C8-C7
24	B	603	CLA	C12-C13-C15-C16
24	B	613	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	C	503	CLA	C11-C10-C8-C7
24	C	505	CLA	C6-C7-C8-C10
24	C	506	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	C	512	CLA	C6-C7-C8-C10
24	C	513	CLA	C11-C10-C8-C7
24	a	606	CLA	C11-C12-C13-C15
24	a	609	CLA	C12-C13-C15-C16
24	b	601	CLA	C11-C10-C8-C7
24	b	602	CLA	C11-C10-C8-C7
24	b	603	CLA	C11-C12-C13-C15
24	b	604	CLA	C12-C13-C15-C16
24	b	605	CLA	C11-C10-C8-C7
24	b	606	CLA	C12-C13-C15-C16
24	b	607	CLA	C6-C7-C8-C10
24	b	615	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
24	c	512	CLA	C6-C7-C8-C10
28	C	527	STE	C15-C16-C17-C18
28	b	624	STE	C4-C5-C6-C7
24	b	601	CLA	O1D-CGD-O2D-CED
28	z	701	STE	C11-C10-C9-C8
29	m	101	LMG	C20-C21-C22-C23
30	A	615	SQD	C14-C15-C16-C17
29	c	516	LMG	C29-C30-C31-C32
32	h	101	DGD	CAA-CBA-CCA-CDA
28	e	101	STE	C15-C16-C17-C18
27	d	406	PL9	C15-C14-C16-C17
28	A	618	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	B	620	LMG	C30-C31-C32-C33
30	b	620	SQD	O5-C1-O6-C44
30	A	613	SQD	C14-C15-C16-C17
28	A	618	STE	C11-C10-C9-C8
28	e	101	STE	C13-C14-C15-C16
31	A	614	LHG	C13-C14-C15-C16
26	k	101	BCR	C19-C20-C21-C22
24	B	616	CLA	C11-C12-C13-C15
28	E	101	STE	C6-C7-C8-C9
28	f	103	STE	C9-C10-C11-C12
31	L	101	LHG	C16-C17-C18-C19
31	D	412	LHG	C33-C34-C35-C36
29	m	101	LMG	C22-C23-C24-C25
30	a	614	SQD	C26-C27-C28-C29
29	C	517	LMG	C7-C8-C9-O8
29	a	615	LMG	C7-C8-C9-O8
30	A	613	SQD	O6-C44-C45-C46
30	a	613	SQD	C44-C45-C46-O48
32	A	616	DGD	C1G-C2G-C3G-O3G
31	d	408	LHG	C35-C36-C37-C38
24	B	604	CLA	C3-C5-C6-C7
28	B	627	STE	C3-C4-C5-C6
28	I	101	STE	C7-C8-C9-C10
32	C	521	DGD	CDB-CEB-CFB-CGB
31	d	408	LHG	C18-C19-C20-C21
28	z	703	STE	C5-C6-C7-C8
24	C	513	CLA	C4-C3-C5-C6
27	d	406	PL9	C30-C29-C31-C32
24	C	506	CLA	C2-C3-C5-C6
24	B	610	CLA	O1D-CGD-O2D-CED
28	A	618	STE	C15-C16-C17-C18
28	d	412	STE	C7-C8-C9-C10
24	c	506	CLA	C16-C17-C18-C20
32	C	523	DGD	CAB-CBB-CCB-CDB
24	a	606	CLA	C2B-C3B-CAB-CBB
26	t	101	BCR	C5-C6-C7-C8
29	B	625	LMG	C34-C35-C36-C37
28	i	102	STE	C9-C10-C11-C12
28	d	407	STE	C13-C14-C15-C16
28	l	102	STE	C9-C10-C11-C12
32	c	520	DGD	CBB-CCB-CDB-CEB
28	C	527	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	b	622	LMG	C16-C17-C18-C19
29	c	522	LMG	C14-C15-C16-C17
31	d	409	LHG	C32-C33-C34-C35
32	c	520	DGD	C9B-CAB-CBB-CCB
24	b	605	CLA	C16-C17-C18-C19
29	B	625	LMG	O7-C8-C9-O8
29	b	622	LMG	O1-C7-C8-O7
31	D	412	LHG	C30-C31-C32-C33
30	b	620	SQD	C9-C10-C11-C12
32	H	102	DGD	C5B-C6B-C7B-C8B
32	h	101	DGD	C8A-C9A-CAA-CBA
31	e	103	LHG	C23-C24-C25-C26
28	B	628	STE	C6-C7-C8-C9
28	h	103	STE	C10-C11-C12-C13
29	c	521	LMG	C29-C30-C31-C32
31	l	101	LHG	C28-C29-C30-C31
24	C	513	CLA	C8-C10-C11-C12
24	c	505	CLA	C2-C3-C5-C6
29	C	524	LMG	C36-C37-C38-C39
30	a	614	SQD	C27-C28-C29-C30
31	D	412	LHG	C28-C29-C30-C31
24	B	613	CLA	C14-C13-C15-C16
24	b	607	CLA	C14-C13-C15-C16
28	C	527	STE	C11-C12-C13-C14
30	b	620	SQD	C11-C10-C9-C8
28	I	102	STE	C5-C6-C7-C8
28	J	102	STE	C6-C7-C8-C9
32	c	520	DGD	C7B-C8B-C9B-CAB
24	B	604	CLA	C16-C17-C18-C20
24	B	610	CLA	C16-C17-C18-C19
24	C	505	CLA	C16-C17-C18-C19
28	d	413	STE	C7-C8-C9-C10
28	b	624	STE	C6-C7-C8-C9
29	C	524	LMG	C30-C31-C32-C33
24	B	613	CLA	C15-C16-C17-C18
32	c	518	DGD	CDA-CEA-CFA-CGA
24	c	505	CLA	C15-C16-C17-C18
27	D	407	PL9	C28-C29-C31-C32
24	B	615	CLA	C16-C17-C18-C19
24	a	606	CLA	C16-C17-C18-C20
32	c	518	DGD	C3A-C4A-C5A-C6A
31	B	622	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	i	101	STE	C4-C5-C6-C7
31	l	101	LHG	C16-C17-C18-C19
32	h	101	DGD	C3B-C4B-C5B-C6B
30	a	614	SQD	C19-C20-C21-C22
28	X	101	STE	C10-C11-C12-C13
24	B	604	CLA	C10-C11-C12-C13
32	c	519	DGD	C9A-CAA-CBA-CCA
30	b	620	SQD	C27-C28-C29-C30
24	B	607	CLA	C10-C11-C12-C13
24	a	606	CLA	C8-C10-C11-C12
28	C	526	STE	C11-C12-C13-C14
28	b	621	STE	C11-C10-C9-C8
24	B	611	CLA	C11-C12-C13-C15
24	B	612	CLA	C12-C13-C15-C16
24	B	615	CLA	C6-C7-C8-C10
24	C	510	CLA	C11-C10-C8-C7
24	C	513	CLA	C12-C13-C15-C16
24	b	604	CLA	C11-C12-C13-C15
24	b	610	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C10-C8-C7
24	c	507	CLA	C11-C12-C13-C15
24	c	509	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C12-C13-C15
24	d	404	CLA	C6-C7-C8-C10
28	Z	101	STE	C10-C11-C12-C13
31	B	622	LHG	C27-C28-C29-C30
26	d	405	BCR	C17-C18-C19-C20
30	a	613	SQD	C14-C15-C16-C17
29	B	625	LMG	C8-C7-O1-C1
32	C	522	DGD	C2G-C3G-O3G-C1D
32	C	522	DGD	C5D-C6D-O5D-C1E
32	c	519	DGD	C2G-C3G-O3G-C1D
28	l	102	STE	C2-C3-C4-C5
29	m	101	LMG	C39-C40-C41-C42
24	c	503	CLA	O1D-CGD-O2D-CED
28	Z	101	STE	C14-C15-C16-C17
29	B	625	LMG	C31-C32-C33-C34
29	D	408	LMG	O10-C28-O8-C9
24	d	403	CLA	C3-C5-C6-C7
24	C	512	CLA	O1D-CGD-O2D-CED
32	C	521	DGD	C2A-C1A-O1G-C1G
29	m	101	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
29	d	411	LMG	C14-C15-C16-C17
24	C	502	CLA	C10-C11-C12-C13
24	C	513	CLA	C15-C16-C17-C18
24	c	509	CLA	C10-C11-C12-C13
28	H	103	STE	C7-C8-C9-C10
28	f	103	STE	C3-C4-C5-C6
29	m	101	LMG	C35-C36-C37-C38
28	b	621	STE	C15-C16-C17-C18
28	b	623	STE	C11-C12-C13-C14
28	b	624	STE	C15-C16-C17-C18
24	c	503	CLA	C10-C11-C12-C13
28	C	516	STE	C3-C4-C5-C6
28	m	102	STE	C5-C6-C7-C8
29	C	517	LMG	O6-C1-O1-C7
31	L	101	LHG	C18-C19-C20-C21
29	b	622	LMG	O1-C7-C8-C9
30	A	615	SQD	O6-C44-C45-C46
30	B	623	SQD	O6-C44-C45-C46
30	a	614	SQD	O6-C44-C45-C46
31	A	614	LHG	C4-C5-C6-O8
28	h	102	STE	C9-C10-C11-C12
34	e	102	HEM	C4C-C3C-CAC-CBC
28	A	617	STE	C11-C12-C13-C14
29	c	522	LMG	C32-C33-C34-C35
31	l	101	LHG	C12-C13-C14-C15
29	c	516	LMG	C33-C34-C35-C36
24	b	612	CLA	C8-C10-C11-C12
24	c	512	CLA	C4-C3-C5-C6
27	d	406	PL9	C45-C44-C46-C47
27	d	406	PL9	C43-C44-C46-C47
28	M	103	STE	C1-C2-C3-C4
29	c	521	LMG	C40-C41-C42-C43
24	a	605	CLA	C13-C15-C16-C17
29	B	625	LMG	C36-C37-C38-C39
30	A	613	SQD	C27-C28-C29-C30
32	c	518	DGD	C4D-C5D-C6D-O5D
24	B	611	CLA	C11-C12-C13-C14
24	B	612	CLA	C14-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C9
24	C	513	CLA	C14-C13-C15-C16
24	b	615	CLA	C6-C7-C8-C9
24	c	502	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	507	CLA	C11-C10-C8-C9
24	c	509	CLA	C11-C10-C8-C9
24	B	612	CLA	C16-C17-C18-C20
31	L	101	LHG	C26-C27-C28-C29
32	c	520	DGD	CAA-CBA-CCA-CDA
28	b	623	STE	C3-C4-C5-C6
29	M	101	LMG	C20-C21-C22-C23
28	d	412	STE	C11-C12-C13-C14
32	c	519	DGD	C8A-C9A-CAA-CBA
28	X	101	STE	C12-C13-C14-C15
24	B	601	CLA	C2-C1-O2A-CGA
24	c	501	CLA	O1D-CGD-O2D-CED
29	c	522	LMG	C29-C28-O8-C9
24	a	606	CLA	C16-C17-C18-C19
31	D	412	LHG	C2-C3-O3-P
29	C	524	LMG	C17-C18-C19-C20
24	A	605	CLA	C2C-C3C-CAC-CBC
28	M	102	STE	C1-C2-C3-C4
31	B	622	LHG	C23-C24-C25-C26
28	f	102	STE	C11-C12-C13-C14
24	B	612	CLA	C16-C17-C18-C19
24	B	615	CLA	C16-C17-C18-C20
24	b	616	CLA	C11-C12-C13-C14
32	C	523	DGD	C2A-C3A-C4A-C5A
28	A	611	STE	C5-C6-C7-C8
28	B	624	STE	C6-C7-C8-C9
28	B	627	STE	C4-C5-C6-C7
31	B	622	LHG	C18-C19-C20-C21
32	c	520	DGD	C4B-C5B-C6B-C7B
28	C	520	STE	C9-C10-C11-C12
28	C	516	STE	C6-C7-C8-C9
28	b	624	STE	C5-C6-C7-C8
28	i	101	STE	C3-C4-C5-C6
26	B	617	BCR	C36-C18-C19-C20
27	a	611	PL9	C34-C36-C37-C38
32	C	523	DGD	CCB-CDB-CEB-CFB
32	C	521	DGD	O1A-C1A-O1G-C1G
30	D	410	SQD	O48-C23-C24-C25
26	B	617	BCR	C17-C18-C19-C20
24	B	606	CLA	C16-C17-C18-C20
28	C	519	STE	C3-C4-C5-C6
29	a	615	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	m	101	LMG	C33-C34-C35-C36
30	b	620	SQD	C12-C13-C14-C15
29	D	409	LMG	C22-C23-C24-C25
28	d	407	STE	C5-C6-C7-C8
29	M	101	LMG	C13-C14-C15-C16
24	D	404	CLA	C10-C11-C12-C13
28	Z	101	STE	C12-C13-C14-C15
28	b	625	STE	C6-C7-C8-C9
31	A	614	LHG	C17-C18-C19-C20
24	A	606	CLA	C11-C12-C13-C15
24	B	605	CLA	C11-C10-C8-C7
24	B	608	CLA	C6-C7-C8-C10
24	B	610	CLA	C12-C13-C15-C16
24	B	612	CLA	C11-C12-C13-C15
24	B	613	CLA	C6-C7-C8-C10
24	B	616	CLA	C6-C7-C8-C10
24	C	502	CLA	C11-C10-C8-C7
24	C	507	CLA	C11-C10-C8-C7
24	C	509	CLA	C12-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C10
24	b	603	CLA	C6-C7-C8-C10
24	b	609	CLA	C12-C13-C15-C16
24	b	614	CLA	C12-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C10
24	d	404	CLA	C12-C13-C15-C16
24	B	607	CLA	C16-C17-C18-C20
24	b	604	CLA	C16-C17-C18-C19
28	C	527	STE	C13-C14-C15-C16
29	d	411	LMG	C36-C37-C38-C39
29	c	521	LMG	C34-C35-C36-C37
32	c	520	DGD	O6D-C5D-C6D-O5D
29	b	622	LMG	C36-C37-C38-C39
28	C	516	STE	C5-C6-C7-C8
28	C	526	STE	C13-C14-C15-C16
28	a	616	STE	C5-C6-C7-C8
31	d	408	LHG	C32-C33-C34-C35
32	C	522	DGD	C6B-C7B-C8B-C9B
32	c	520	DGD	C3A-C4A-C5A-C6A
32	h	101	DGD	C6B-C7B-C8B-C9B
29	B	620	LMG	C34-C35-C36-C37
32	H	102	DGD	CAB-CBB-CCB-CDB
31	e	103	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	C	516	STE	C9-C10-C11-C12
28	X	101	STE	C15-C16-C17-C18
24	B	603	CLA	C14-C13-C15-C16
24	C	505	CLA	C6-C7-C8-C9
24	C	510	CLA	C11-C10-C8-C9
24	b	604	CLA	C11-C12-C13-C14
30	a	613	SQD	C32-C33-C34-C35
30	b	620	SQD	C28-C29-C30-C31
28	m	102	STE	C6-C7-C8-C9
31	a	612	LHG	C18-C19-C20-C21
26	C	514	BCR	C19-C20-C21-C22
26	c	517	BCR	C9-C10-C11-C12
32	C	521	DGD	C4D-C5D-C6D-O5D
29	c	522	LMG	C30-C31-C32-C33
24	B	615	CLA	C13-C15-C16-C17
30	a	614	SQD	O5-C5-C6-S
28	B	621	STE	C5-C6-C7-C8
29	M	101	LMG	C12-C13-C14-C15
30	A	615	SQD	C11-C10-C9-C8
30	a	613	SQD	C27-C28-C29-C30
29	c	522	LMG	O10-C28-O8-C9
29	C	517	LMG	O7-C8-C9-O8
29	C	524	LMG	O1-C7-C8-O7
29	a	615	LMG	O7-C8-C9-O8
24	B	610	CLA	C8-C10-C11-C12
24	B	611	CLA	C8-C10-C11-C12
28	z	703	STE	C2-C3-C4-C5
29	D	408	LMG	O1-C7-C8-C9
28	E	102	STE	C13-C14-C15-C16
28	z	702	STE	C3-C4-C5-C6
30	A	613	SQD	C35-C36-C37-C38
29	b	622	LMG	C39-C40-C41-C42
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
30	a	613	SQD	C8-C7-O47-C45
28	C	527	STE	C5-C6-C7-C8
28	h	102	STE	C10-C11-C12-C13
30	a	614	SQD	C11-C10-C9-C8
29	a	615	LMG	C40-C41-C42-C43
28	t	102	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	b	623	STE	C4-C5-C6-C7
29	B	625	LMG	C15-C16-C17-C18
24	A	608	CLA	C6-C7-C8-C9
28	E	101	STE	C7-C8-C9-C10
29	D	408	LMG	C14-C15-C16-C17
30	a	613	SQD	O49-C7-O47-C45
32	c	519	DGD	C6B-C7B-C8B-C9B
32	c	518	DGD	C6A-C7A-C8A-C9A
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	607	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O5
31	a	612	LHG	C4-O6-P-O3
31	d	408	LHG	C4-O6-P-O3
32	C	522	DGD	CAA-CBA-CCA-CDA
28	B	627	STE	C7-C8-C9-C10
24	c	509	CLA	C4-C3-C5-C6
24	B	606	CLA	C2B-C3B-CAB-CBB
24	b	601	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
30	D	410	SQD	C32-C33-C34-C35
24	c	512	CLA	C2-C3-C5-C6
27	D	407	PL9	C33-C34-C36-C37
26	d	405	BCR	C36-C18-C19-C20
24	B	606	CLA	C5-C6-C7-C8
32	A	616	DGD	CFA-CGA-CHA-CIA
28	A	618	STE	C5-C6-C7-C8
28	d	410	STE	C11-C12-C13-C14
31	B	622	LHG	O1-C1-C2-O2
27	A	610	PL9	C4-C3-C7-C8
32	C	521	DGD	O6D-C5D-C6D-O5D
32	c	518	DGD	CCA-CDA-CEA-CFA
24	B	614	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	A	612	LMG	C9-C8-O7-C10
29	B	625	LMG	C9-C8-O7-C10
29	C	517	LMG	C7-C8-O7-C10
24	B	613	CLA	C2-C3-C5-C6
24	c	504	CLA	C2-C3-C5-C6
24	b	607	CLA	CBA-CGA-O2A-C1
28	i	101	STE	C7-C8-C9-C10
24	A	605	CLA	C11-C10-C8-C9
24	B	601	CLA	C11-C10-C8-C9
24	B	601	CLA	C14-C13-C15-C16
24	B	602	CLA	C11-C12-C13-C14
24	B	605	CLA	C11-C10-C8-C9
24	B	613	CLA	C6-C7-C8-C9
24	B	616	CLA	C6-C7-C8-C9
24	C	502	CLA	C14-C13-C15-C16
24	C	506	CLA	C14-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C9
24	b	614	CLA	C11-C12-C13-C14
24	c	507	CLA	C11-C12-C13-C14
24	c	511	CLA	C14-C13-C15-C16
28	A	618	STE	C7-C8-C9-C10
24	C	508	CLA	C11-C10-C8-C7
24	c	505	CLA	C11-C12-C13-C15
28	C	528	STE	C13-C14-C15-C16
32	h	101	DGD	C2B-C3B-C4B-C5B
30	a	614	SQD	C32-C33-C34-C35
31	B	622	LHG	C19-C20-C21-C22
32	C	522	DGD	CDA-CEA-CFA-CGA
30	a	614	SQD	C2-C1-O6-C44
32	C	522	DGD	C2E-C1E-O5D-C6D
28	A	611	STE	C1-C2-C3-C4
29	c	522	LMG	C15-C16-C17-C18
30	A	615	SQD	C10-C11-C12-C13
24	c	506	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
28	C	526	STE	C3-C4-C5-C6
24	C	513	CLA	C10-C11-C12-C13
29	M	101	LMG	O7-C8-C9-O8
31	e	103	LHG	O7-C5-C6-O8
24	c	509	CLA	CAA-CBA-CGA-O2A
32	H	102	DGD	O2G-C1B-C2B-C3B
28	M	102	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	C	524	LMG	C13-C14-C15-C16
31	D	411	LHG	C26-C27-C28-C29
24	b	608	CLA	C16-C17-C18-C19
31	D	412	LHG	C26-C27-C28-C29
32	h	101	DGD	O2G-C1B-C2B-C3B
28	m	102	STE	C1-C2-C3-C4
30	D	410	SQD	C24-C25-C26-C27
29	C	524	LMG	C40-C41-C42-C43
24	b	609	CLA	C16-C17-C18-C20
28	f	102	STE	C15-C16-C17-C18
24	c	506	CLA	C8-C10-C11-C12
29	B	625	LMG	C7-C8-C9-O8
32	c	519	DGD	C4E-C5E-C6E-O5E
31	D	411	LHG	C33-C34-C35-C36
29	D	408	LMG	C35-C36-C37-C38
28	H	103	STE	C11-C10-C9-C8
29	c	522	LMG	C16-C17-C18-C19
29	b	622	LMG	C8-C7-O1-C1
24	B	601	CLA	C15-C16-C17-C18
24	B	615	CLA	C10-C11-C12-C13
29	C	517	LMG	C17-C18-C19-C20
31	a	612	LHG	C32-C33-C34-C35
31	l	101	LHG	C11-C10-C9-C8
24	B	601	CLA	C4-C3-C5-C6
24	c	506	CLA	C4-C3-C5-C6
32	H	102	DGD	C9B-CAB-CBB-CCB
29	d	411	LMG	C15-C16-C17-C18
29	m	101	LMG	C18-C19-C20-C21
30	D	410	SQD	C45-C44-O6-C1
24	b	614	CLA	C16-C17-C18-C20
31	e	103	LHG	C25-C26-C27-C28
24	C	509	CLA	C14-C13-C15-C16
24	b	603	CLA	C6-C7-C8-C9
24	C	507	CLA	O1D-CGD-O2D-CED
28	H	104	STE	C15-C16-C17-C18
24	B	605	CLA	C4B-C3B-CAB-CBB
24	B	609	CLA	C4B-C3B-CAB-CBB
24	B	615	CLA	C4B-C3B-CAB-CBB
24	C	502	CLA	C4B-C3B-CAB-CBB
24	B	611	CLA	C15-C16-C17-C18
24	C	511	CLA	CBA-CGA-O2A-C1
24	b	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	b	607	CLA	O1A-CGA-O2A-C1
30	b	620	SQD	C15-C16-C17-C18
24	B	601	CLA	C2-C3-C5-C6
28	T	102	STE	C11-C10-C9-C8
31	d	408	LHG	C29-C30-C31-C32
29	m	101	LMG	C21-C22-C23-C24
24	C	511	CLA	C6-C7-C8-C10
24	C	512	CLA	C11-C10-C8-C7
24	c	502	CLA	C11-C12-C13-C15
24	c	506	CLA	C6-C7-C8-C10
28	d	407	STE	C3-C4-C5-C6
29	M	101	LMG	O9-C10-O7-C8
29	M	101	LMG	C10-C11-C12-C13
24	C	511	CLA	O1A-CGA-O2A-C1
24	b	614	CLA	O1A-CGA-O2A-C1
24	B	601	CLA	C3A-C2A-CAA-CBA
24	B	609	CLA	C4-C3-C5-C6
24	C	512	CLA	C4-C3-C5-C6
27	A	610	PL9	C40-C39-C41-C42
29	B	625	LMG	C20-C21-C22-C23
24	c	509	CLA	C2-C3-C5-C6
24	a	606	CLA	C2C-C3C-CAC-CBC
35	v	201	HEC	C2B-C3B-CAB-CBB
30	a	613	SQD	C19-C20-C21-C22
32	C	522	DGD	O6E-C1E-O5D-C6D
24	C	511	CLA	C3-C5-C6-C7
25	a	607	PHO	C10-C11-C12-C13
32	C	523	DGD	O6D-C5D-C6D-O5D
29	c	521	LMG	C31-C32-C33-C34
24	B	613	CLA	C2-C1-O2A-CGA
24	B	616	CLA	C2-C1-O2A-CGA
26	H	101	BCR	C9-C10-C11-C12
26	T	101	BCR	C13-C14-C15-C16
24	D	405	CLA	C10-C11-C12-C13
24	c	512	CLA	C8-C10-C11-C12
32	c	520	DGD	C2B-C3B-C4B-C5B
24	A	605	CLA	C4C-C3C-CAC-CBC
28	C	526	STE	C5-C6-C7-C8
28	H	103	STE	C11-C12-C13-C14
24	c	507	CLA	C16-C17-C18-C20
28	d	407	STE	O1-C1-C2-C3
34	e	102	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C11-C12-C13-C14
24	B	606	CLA	C11-C12-C13-C14
24	B	607	CLA	C11-C12-C13-C14
24	B	608	CLA	C6-C7-C8-C9
24	C	501	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
24	c	502	CLA	C11-C12-C13-C14
24	c	506	CLA	C6-C7-C8-C9
24	c	507	CLA	C6-C7-C8-C9
24	c	513	CLA	C6-C7-C8-C9
25	a	607	PHO	C11-C10-C8-C9
25	a	607	PHO	C14-C13-C15-C16
30	A	615	SQD	C18-C19-C20-C21
30	B	623	SQD	C14-C15-C16-C17
32	H	102	DGD	CAA-CBA-CCA-CDA
31	L	101	LHG	C5-C6-O8-C23
28	H	104	STE	C10-C11-C12-C13
31	a	612	LHG	C24-C25-C26-C27
29	A	612	LMG	C31-C32-C33-C34
31	a	612	LHG	C29-C30-C31-C32
35	v	201	HEC	CAD-CBD-CGD-O1D
35	v	201	HEC	C2C-C3C-CAC-CBC
24	B	613	CLA	CBD-CGD-O2D-CED
28	A	618	STE	C4-C5-C6-C7
31	d	408	LHG	C10-C11-C12-C13
24	b	610	CLA	C2A-CAA-CBA-CGA
24	b	604	CLA	C1A-C2A-CAA-CBA
28	X	101	STE	C13-C14-C15-C16
28	B	626	STE	C6-C7-C8-C9
28	C	528	STE	C11-C12-C13-C14
24	c	502	CLA	C2B-C3B-CAB-CBB
26	A	609	BCR	C5-C6-C7-C8
26	A	609	BCR	C23-C24-C25-C26
26	A	609	BCR	C23-C24-C25-C30
26	C	514	BCR	C23-C24-C25-C26
26	J	101	BCR	C5-C6-C7-C8
26	t	101	BCR	C1-C6-C7-C8
30	A	613	SQD	C16-C17-C18-C19
28	d	407	STE	O2-C1-C2-C3
24	C	512	CLA	C2-C3-C5-C6
24	C	510	CLA	O1D-CGD-O2D-CED
24	A	605	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C12-C13-C15-C16
24	B	610	CLA	C11-C12-C13-C15
24	C	502	CLA	C12-C13-C15-C16
24	C	505	CLA	C12-C13-C15-C16
24	b	601	CLA	C11-C12-C13-C15
24	b	616	CLA	C11-C10-C8-C7
24	c	506	CLA	C12-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C7
25	a	607	PHO	C6-C7-C8-C10
31	A	614	LHG	C18-C19-C20-C21
30	B	623	SQD	C31-C32-C33-C34
35	v	201	HEC	C4C-C3C-CAC-CBC
31	e	103	LHG	C15-C16-C17-C18
24	C	505	CLA	C8-C10-C11-C12
28	B	627	STE	C6-C7-C8-C9
31	L	101	LHG	C15-C16-C17-C18
28	C	520	STE	C3-C4-C5-C6
35	v	201	HEC	CAD-CBD-CGD-O2D
24	B	606	CLA	O1D-CGD-O2D-CED
29	M	101	LMG	C35-C36-C37-C38
28	z	702	STE	C12-C13-C14-C15
29	B	620	LMG	C20-C21-C22-C23
24	C	513	CLA	C2-C3-C5-C6
27	a	611	PL9	C12-C11-C9-C8
24	C	506	CLA	C15-C16-C17-C18
28	I	102	STE	O1-C1-C2-C3
28	d	410	STE	O2-C1-C2-C3
24	b	614	CLA	CBA-CGA-O2A-C1
29	M	101	LMG	C11-C10-O7-C8
24	A	605	CLA	C14-C13-C15-C16
24	b	605	CLA	C11-C12-C13-C14
28	C	519	STE	C4-C5-C6-C7
29	m	101	LMG	C13-C14-C15-C16
24	B	614	CLA	C16-C17-C18-C19
24	b	601	CLA	C16-C17-C18-C20
29	D	409	LMG	C12-C13-C14-C15
30	a	613	SQD	C25-C26-C27-C28
28	I	102	STE	O2-C1-C2-C3
29	c	521	LMG	C36-C37-C38-C39
28	T	102	STE	C3-C4-C5-C6
27	A	610	PL9	C12-C11-C9-C10
27	A	610	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
28	B	627	STE	O2-C1-C2-C3
24	a	606	CLA	C4C-C3C-CAC-CBC
24	b	610	CLA	CBD-CGD-O2D-CED
29	a	615	LMG	C29-C30-C31-C32
29	A	612	LMG	C13-C14-C15-C16
32	c	518	DGD	C4B-C5B-C6B-C7B
30	a	614	SQD	C31-C32-C33-C34
31	d	408	LHG	C30-C31-C32-C33
31	d	409	LHG	C4-C5-C6-O8
35	V	201	HEC	CAD-CBD-CGD-O2D
27	a	611	PL9	C11-C12-C13-C14
24	C	501	CLA	C2A-CAA-CBA-CGA
34	e	102	HEM	CAD-CBD-CGD-O2D
24	B	603	CLA	C4-C3-C5-C6
27	A	610	PL9	C25-C24-C26-C27
28	d	413	STE	O2-C1-C2-C3
24	B	606	CLA	C16-C17-C18-C19
24	c	510	CLA	C10-C11-C12-C13
24	d	402	CLA	C15-C16-C17-C18
30	D	410	SQD	C33-C34-C35-C36
24	C	504	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	C4B-C3B-CAB-CBB
28	Z	101	STE	C5-C6-C7-C8
32	H	102	DGD	CCA-CDA-CEA-CFA
24	c	512	CLA	O1D-CGD-O2D-CED
24	b	603	CLA	CBA-CGA-O2A-C1
28	d	410	STE	O1-C1-C2-C3
29	c	522	LMG	C4-C5-C6-O5
32	c	518	DGD	C9A-CAA-CBA-CCA
24	c	502	CLA	C16-C17-C18-C20
24	B	611	CLA	C4-C3-C5-C6
24	c	504	CLA	C8-C10-C11-C12
24	B	602	CLA	C11-C10-C8-C7
24	B	615	CLA	C12-C13-C15-C16
28	h	103	STE	C9-C10-C11-C12
30	f	101	SQD	C30-C31-C32-C33
28	d	413	STE	O1-C1-C2-C3
31	l	101	LHG	C30-C31-C32-C33
30	A	613	SQD	C26-C27-C28-C29
24	b	604	CLA	C13-C15-C16-C17
28	J	102	STE	C1-C2-C3-C4
28	B	621	STE	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	B	604	CLA	C11-C12-C13-C14
24	a	609	CLA	C6-C7-C8-C9
24	c	512	CLA	C14-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C14
32	H	102	DGD	C9A-CAA-CBA-CCA
29	M	101	LMG	C8-C7-O1-C1
29	m	101	LMG	C8-C7-O1-C1
32	h	101	DGD	C1A-C2A-C3A-C4A
31	e	103	LHG	C13-C14-C15-C16
35	V	201	HEC	CAD-CBD-CGD-O1D
24	b	603	CLA	O1A-CGA-O2A-C1
24	B	603	CLA	C3-C5-C6-C7
30	A	613	SQD	C11-C12-C13-C14
28	b	624	STE	C13-C14-C15-C16
24	b	606	CLA	C4-C3-C5-C6
24	c	509	CLA	C3A-C2A-CAA-CBA
28	Z	101	STE	C2-C3-C4-C5
29	B	620	LMG	C31-C32-C33-C34
24	c	504	CLA	C10-C11-C12-C13
24	c	512	CLA	O2A-C1-C2-C3
28	b	621	STE	C9-C10-C11-C12
28	A	618	STE	C11-C12-C13-C14
26	c	515	BCR	C15-C16-C17-C18
28	B	627	STE	O1-C1-C2-C3
25	D	402	PHO	C8-C10-C11-C12
29	C	524	LMG	C31-C32-C33-C34
24	B	611	CLA	C2-C3-C5-C6
28	b	621	STE	C12-C13-C14-C15
29	b	622	LMG	C13-C14-C15-C16
31	L	101	LHG	C29-C30-C31-C32
31	e	103	LHG	C2-C3-O3-P
28	B	621	STE	C2-C3-C4-C5
28	f	103	STE	C13-C14-C15-C16
24	B	603	CLA	C10-C11-C12-C13
24	c	505	CLA	C8-C10-C11-C12
27	d	406	PL9	C42-C43-C44-C45
30	D	410	SQD	C28-C29-C30-C31
28	d	407	STE	C7-C8-C9-C10
28	B	621	STE	O1-C1-C2-C3
26	C	515	BCR	C13-C14-C15-C16
26	x	101	BCR	C9-C10-C11-C12
28	C	525	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
24	b	616	CLA	C10-C11-C12-C13
28	J	102	STE	O2-C1-C2-C3
32	c	518	DGD	CBA-CCA-CDA-CEA
24	B	612	CLA	C11-C12-C13-C14
24	B	615	CLA	C11-C10-C8-C9
24	C	502	CLA	C11-C10-C8-C9
24	a	609	CLA	C11-C10-C8-C9
24	c	504	CLA	C6-C7-C8-C9
24	d	404	CLA	C14-C13-C15-C16
29	a	615	LMG	C16-C17-C18-C19
24	B	609	CLA	C2-C3-C5-C6
24	c	501	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C6-C7-C8-C10
24	B	604	CLA	C11-C12-C13-C15
24	B	614	CLA	C11-C12-C13-C15
24	a	609	CLA	C6-C7-C8-C10
24	a	609	CLA	C11-C10-C8-C7
24	b	605	CLA	C11-C12-C13-C15
24	d	402	CLA	C11-C12-C13-C15
24	B	605	CLA	C2B-C3B-CAB-CBB
24	B	609	CLA	C2B-C3B-CAB-CBB
24	B	615	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C5-C6-C7-C8
26	C	514	BCR	C23-C24-C25-C30
26	T	101	BCR	C5-C6-C7-C8
24	B	613	CLA	C13-C15-C16-C17
24	b	613	CLA	CAA-CBA-CGA-O2A
29	a	615	LMG	C30-C31-C32-C33
24	A	605	CLA	C2-C1-O2A-CGA
24	D	404	CLA	C2-C1-O2A-CGA
24	a	605	CLA	C2-C1-O2A-CGA
24	b	613	CLA	C2-C1-O2A-CGA
28	d	412	STE	C11-C10-C9-C8
24	C	510	CLA	CBD-CGD-O2D-CED
31	D	411	LHG	C28-C29-C30-C31
31	l	101	LHG	C5-C6-O8-C23
28	f	102	STE	C12-C13-C14-C15
30	a	614	SQD	C10-C11-C12-C13
29	B	625	LMG	O7-C10-C11-C12
28	C	527	STE	C6-C7-C8-C9
28	z	703	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	B	623	SQD	O47-C7-C8-C9
32	c	520	DGD	C6A-C7A-C8A-C9A
28	J	102	STE	O1-C1-C2-C3
24	b	601	CLA	CAA-CBA-CGA-O2A
24	b	608	CLA	C4-C3-C5-C6
28	h	103	STE	C11-C10-C9-C8
27	d	406	PL9	C13-C14-C16-C17
24	B	613	CLA	O1D-CGD-O2D-CED
31	A	614	LHG	C27-C28-C29-C30
28	a	616	STE	C6-C7-C8-C9
28	z	703	STE	C1-C2-C3-C4
32	C	521	DGD	O2G-C1B-C2B-C3B
31	D	411	LHG	C30-C31-C32-C33
32	H	102	DGD	CBB-CCB-CDB-CEB
24	B	601	CLA	C6-C7-C8-C9
24	B	607	CLA	C11-C10-C8-C9
24	B	613	CLA	CAA-CBA-CGA-O2A
29	c	521	LMG	O7-C10-C11-C12
32	c	518	DGD	O2G-C1B-C2B-C3B
28	C	525	STE	C6-C7-C8-C9
29	C	524	LMG	O1-C7-C8-C9
31	l	101	LHG	C17-C18-C19-C20
24	A	606	CLA	C10-C11-C12-C13
24	B	601	CLA	C4B-C3B-CAB-CBB
24	B	602	CLA	C1A-C2A-CAA-CBA
24	C	508	CLA	C1A-C2A-CAA-CBA
32	C	523	DGD	C7B-C8B-C9B-CAB
32	C	521	DGD	O6E-C1E-O5D-C6D
29	C	524	LMG	O7-C10-C11-C12
29	D	408	LMG	C39-C40-C41-C42
24	c	506	CLA	C2-C3-C5-C6
26	H	101	BCR	C17-C18-C19-C20
26	c	515	BCR	C13-C14-C15-C16
26	t	101	BCR	C9-C10-C11-C12
24	B	601	CLA	CBD-CGD-O2D-CED
24	C	507	CLA	CBD-CGD-O2D-CED
28	f	102	STE	C13-C14-C15-C16
32	C	521	DGD	C3A-C4A-C5A-C6A
28	A	619	STE	C14-C15-C16-C17
35	v	201	HEC	C4B-C3B-CAB-CBB
32	C	523	DGD	C1A-C2A-C3A-C4A
24	c	505	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	A	613	SQD	O47-C7-C8-C9
28	i	102	STE	C7-C8-C9-C10
31	D	412	LHG	O1-C1-C2-C3
31	d	408	LHG	C1-C2-C3-O3
24	C	508	CLA	C8-C10-C11-C12
24	C	511	CLA	C2-C1-O2A-CGA
24	C	512	CLA	C2-C1-O2A-CGA
32	c	520	DGD	C7A-C8A-C9A-CAA
24	B	604	CLA	C12-C13-C15-C16
24	D	404	CLA	C11-C10-C8-C7
24	D	405	CLA	C11-C10-C8-C7
24	b	605	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C10-C8-C7
24	c	502	CLA	C12-C13-C15-C16
24	c	509	CLA	C12-C13-C15-C16
24	c	512	CLA	C11-C12-C13-C15
24	c	512	CLA	C12-C13-C15-C16
35	V	201	HEC	C2B-C3B-CAB-CBB
28	B	626	STE	C5-C6-C7-C8
29	C	524	LMG	C38-C39-C40-C41
28	d	412	STE	C9-C10-C11-C12
25	a	607	PHO	O2A-C1-C2-C3
28	C	516	STE	C7-C8-C9-C10
28	E	103	STE	C3-C4-C5-C6
28	A	611	STE	C6-C7-C8-C9
30	a	614	SQD	C16-C17-C18-C19
28	X	101	STE	O2-C1-C2-C3
34	F	101	HEM	CAD-CBD-CGD-O1D
30	f	101	SQD	O47-C7-C8-C9
24	A	606	CLA	C15-C16-C17-C18
24	d	402	CLA	C4C-C3C-CAC-CBC
24	B	608	CLA	O1A-CGA-O2A-C1
29	A	612	LMG	C18-C19-C20-C21
31	D	411	LHG	C14-C15-C16-C17
24	B	608	CLA	CBA-CGA-O2A-C1
30	A	615	SQD	C24-C23-O48-C46
28	M	102	STE	C5-C6-C7-C8
24	B	608	CLA	C3-C5-C6-C7
24	B	608	CLA	C11-C12-C13-C14
24	C	505	CLA	C14-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C9
24	b	601	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	b	614	CLA	C14-C13-C15-C16
25	a	607	PHO	C6-C7-C8-C9
32	c	518	DGD	O1B-C1B-C2B-C3B
28	J	102	STE	C7-C8-C9-C10
31	B	622	LHG	C10-C11-C12-C13
26	H	101	BCR	C36-C18-C19-C20
24	b	613	CLA	CAA-CBA-CGA-O1A
28	I	101	STE	C12-C13-C14-C15
31	e	103	LHG	C14-C15-C16-C17
24	c	505	CLA	O1A-CGA-O2A-C1
32	C	521	DGD	O1B-C1B-C2B-C3B
28	z	702	STE	C15-C16-C17-C18
30	a	613	SQD	C45-C44-O6-C1
30	b	620	SQD	C45-C44-O6-C1
30	A	615	SQD	O10-C23-O48-C46
31	d	409	LHG	O7-C5-C6-O8
32	C	521	DGD	C2A-C3A-C4A-C5A
28	C	516	STE	O2-C1-C2-C3
29	B	625	LMG	O9-C10-C11-C12
29	C	524	LMG	O9-C10-C11-C12
30	B	623	SQD	O49-C7-C8-C9
28	j	101	STE	C5-C6-C7-C8
30	B	623	SQD	C10-C11-C12-C13
24	d	404	CLA	C16-C17-C18-C20
27	a	611	PL9	C39-C41-C42-C43
28	H	104	STE	C12-C13-C14-C15
24	B	613	CLA	CAA-CBA-CGA-O1A
24	b	601	CLA	CAA-CBA-CGA-O1A
24	B	605	CLA	C8-C10-C11-C12
29	c	522	LMG	O8-C28-C29-C30
24	D	404	CLA	C3-C5-C6-C7
28	C	519	STE	C2-C3-C4-C5
29	c	521	LMG	O9-C10-C11-C12
32	H	102	DGD	C8A-C9A-CAA-CBA
24	c	510	CLA	CAA-CBA-CGA-O2A
24	b	611	CLA	C3-C5-C6-C7
24	B	611	CLA	C13-C15-C16-C17
30	b	620	SQD	C24-C25-C26-C27
24	C	506	CLA	C2-C1-O2A-CGA
24	d	403	CLA	C2-C1-O2A-CGA
28	I	101	STE	O2-C1-C2-C3
24	B	601	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	B	612	CLA	CAA-CBA-CGA-O2A
24	C	510	CLA	CAA-CBA-CGA-O2A
29	D	408	LMG	O8-C28-C29-C30
31	l	101	LHG	O7-C7-C8-C9
24	C	513	CLA	C16-C17-C18-C19
24	d	404	CLA	C16-C17-C18-C19
28	I	101	STE	C10-C11-C12-C13
24	B	610	CLA	C2A-CAA-CBA-CGA
31	a	612	LHG	C15-C16-C17-C18
28	X	101	STE	O1-C1-C2-C3
28	A	619	STE	C13-C14-C15-C16
29	a	615	LMG	O8-C28-C29-C30
31	D	412	LHG	C10-C11-C12-C13
24	c	501	CLA	CAA-CBA-CGA-O2A
28	C	516	STE	O1-C1-C2-C3
28	i	101	STE	O1-C1-C2-C3
34	F	101	HEM	CAD-CBD-CGD-O2D
27	a	611	PL9	C37-C38-C39-C41
30	A	613	SQD	O49-C7-C8-C9
31	L	101	LHG	C17-C18-C19-C20
32	c	518	DGD	C6B-C7B-C8B-C9B
31	L	101	LHG	C24-C25-C26-C27

There are no ring outliers.

144 monomers are involved in 265 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	507	CLA	4	0
24	b	607	CLA	1	0
26	J	101	BCR	4	0
32	A	616	DGD	3	0
28	z	703	STE	1	0
29	D	409	LMG	3	0
24	B	602	CLA	1	0
24	b	613	CLA	4	0
24	b	605	CLA	2	0
24	c	513	CLA	2	0
28	j	101	STE	1	0
24	c	511	CLA	4	0
26	H	101	BCR	3	0
24	c	509	CLA	1	0
26	C	514	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	519	STE	1	0
28	z	702	STE	1	0
24	B	610	CLA	2	0
24	b	611	CLA	1	0
28	I	102	STE	2	0
28	X	101	STE	3	0
24	b	609	CLA	1	0
26	C	515	BCR	4	0
26	B	617	BCR	2	0
32	H	102	DGD	2	0
24	B	613	CLA	2	0
24	C	505	CLA	2	0
24	C	508	CLA	2	0
28	C	527	STE	1	0
29	a	615	LMG	2	0
26	B	619	BCR	2	0
24	D	403	CLA	3	0
24	B	615	CLA	1	0
32	h	101	DGD	3	0
28	A	618	STE	1	0
34	F	101	HEM	2	0
24	B	606	CLA	2	0
24	C	507	CLA	1	0
28	e	104	STE	1	0
32	c	518	DGD	1	0
24	B	614	CLA	3	0
24	C	504	CLA	1	0
25	a	608	PHO	2	0
24	b	615	CLA	5	0
31	e	103	LHG	1	0
34	e	102	HEM	3	0
31	D	412	LHG	4	0
24	C	502	CLA	1	0
29	B	620	LMG	4	0
24	b	604	CLA	3	0
28	M	102	STE	1	0
24	A	608	CLA	1	0
24	b	614	CLA	3	0
24	C	512	CLA	1	0
27	d	406	PL9	1	0
31	D	411	LHG	1	0
28	d	412	STE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	609	CLA	4	0
24	b	606	CLA	2	0
30	a	613	SQD	2	0
28	C	526	STE	1	0
28	l	102	STE	1	0
24	b	601	CLA	3	0
27	A	610	PL9	9	0
28	d	410	STE	4	0
29	A	612	LMG	1	0
29	C	524	LMG	1	0
31	a	612	LHG	3	0
28	H	103	STE	2	0
24	c	501	CLA	3	0
24	b	610	CLA	1	0
24	B	609	CLA	2	0
26	a	610	BCR	1	0
24	d	404	CLA	1	0
27	a	611	PL9	8	0
28	h	103	STE	2	0
30	D	410	SQD	1	0
28	E	103	STE	2	0
29	B	625	LMG	3	0
30	a	614	SQD	3	0
28	d	407	STE	5	0
24	A	605	CLA	3	0
24	B	604	CLA	3	0
24	c	506	CLA	2	0
24	c	512	CLA	5	0
24	c	510	CLA	2	0
30	A	613	SQD	2	0
29	D	408	LMG	9	0
24	c	504	CLA	1	0
24	C	513	CLA	2	0
24	B	608	CLA	3	0
24	A	606	CLA	4	0
28	i	101	STE	1	0
32	C	522	DGD	3	0
30	b	620	SQD	2	0
26	c	514	BCR	1	0
31	B	622	LHG	4	0
24	B	612	CLA	3	0
24	b	612	CLA	3	0

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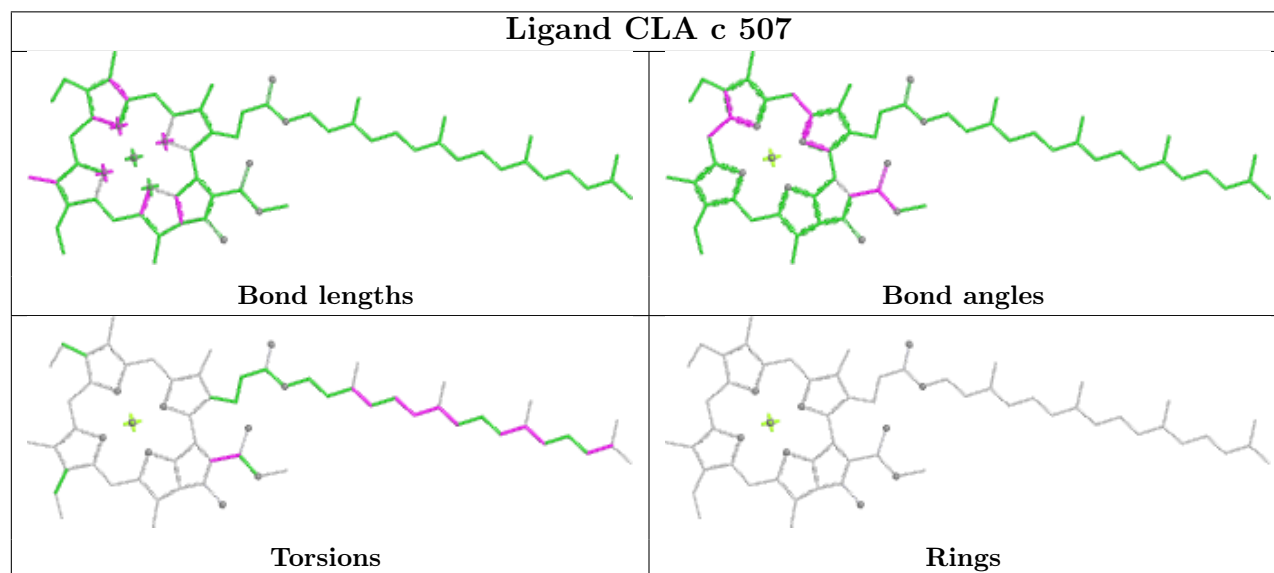
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24	D	404	CLA	1	0
24	C	503	CLA	1	0
25	A	607	PHO	1	0
28	B	628	STE	2	0
26	T	101	BCR	2	0
27	D	407	PL9	1	0
30	A	615	SQD	1	0
31	L	101	LHG	3	0
29	c	522	LMG	3	0
24	C	509	CLA	1	0
24	D	405	CLA	1	0
28	B	626	STE	2	0
30	B	623	SQD	3	0
24	d	402	CLA	1	0
32	c	519	DGD	2	0
26	B	618	BCR	3	0
28	T	102	STE	2	0
24	B	603	CLA	1	0
24	a	606	CLA	3	0
31	A	614	LHG	2	0
24	d	403	CLA	3	0
26	d	405	BCR	1	0
24	C	506	CLA	1	0
24	b	602	CLA	4	0
28	A	619	STE	3	0
26	x	101	BCR	3	0
26	b	618	BCR	2	0
26	c	517	BCR	1	0
29	m	101	LMG	1	0
24	C	511	CLA	3	0
24	B	616	CLA	1	0
29	M	101	LMG	4	0
30	f	101	SQD	1	0
24	c	502	CLA	1	0
31	l	101	LHG	2	0
29	b	622	LMG	1	0
24	c	508	CLA	3	0
26	D	406	BCR	3	0
26	A	609	BCR	2	0
24	b	616	CLA	4	0
24	B	605	CLA	4	0

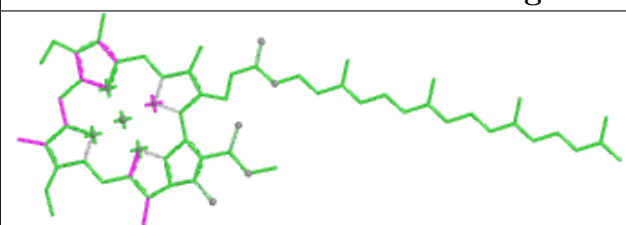
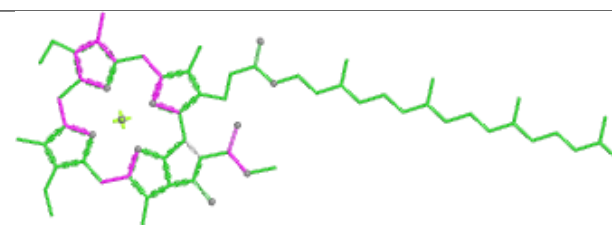
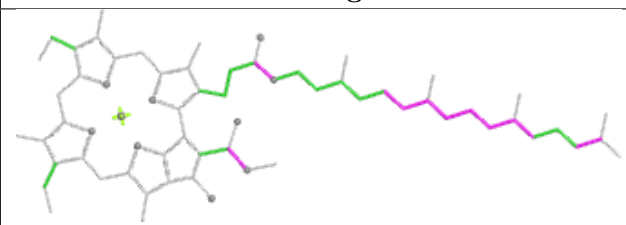
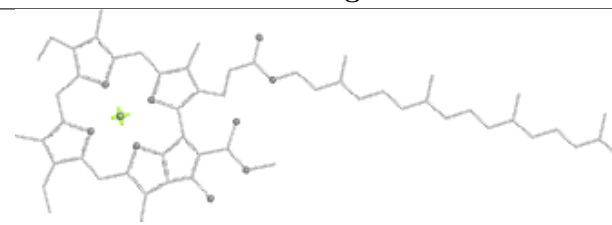
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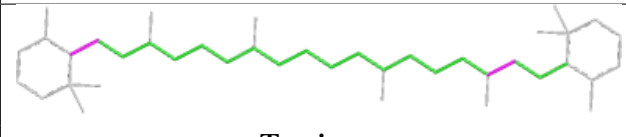
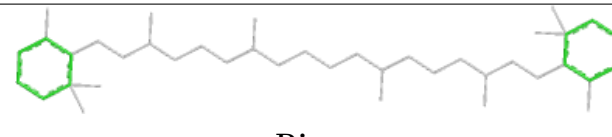
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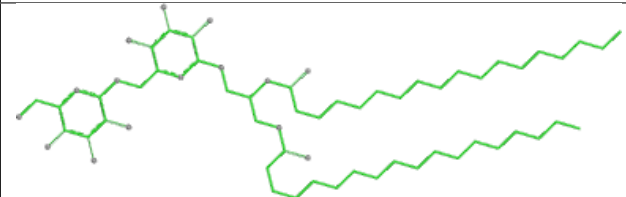
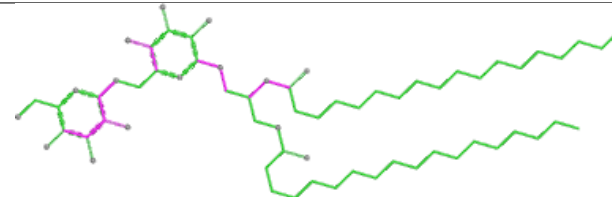
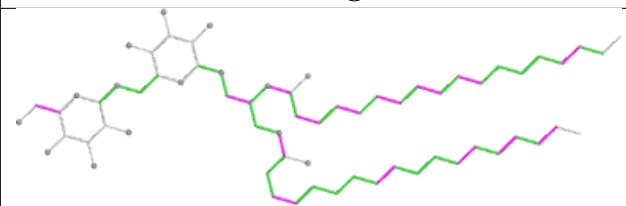
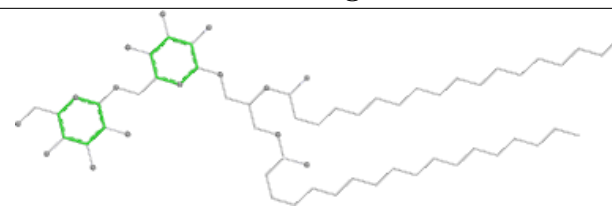
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	t	101	BCR	7	0
32	C	523	DGD	1	0
24	B	611	CLA	1	0

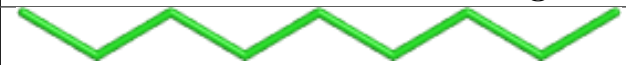
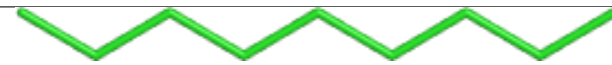
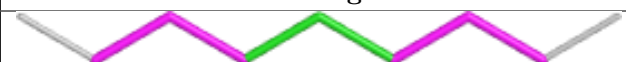
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



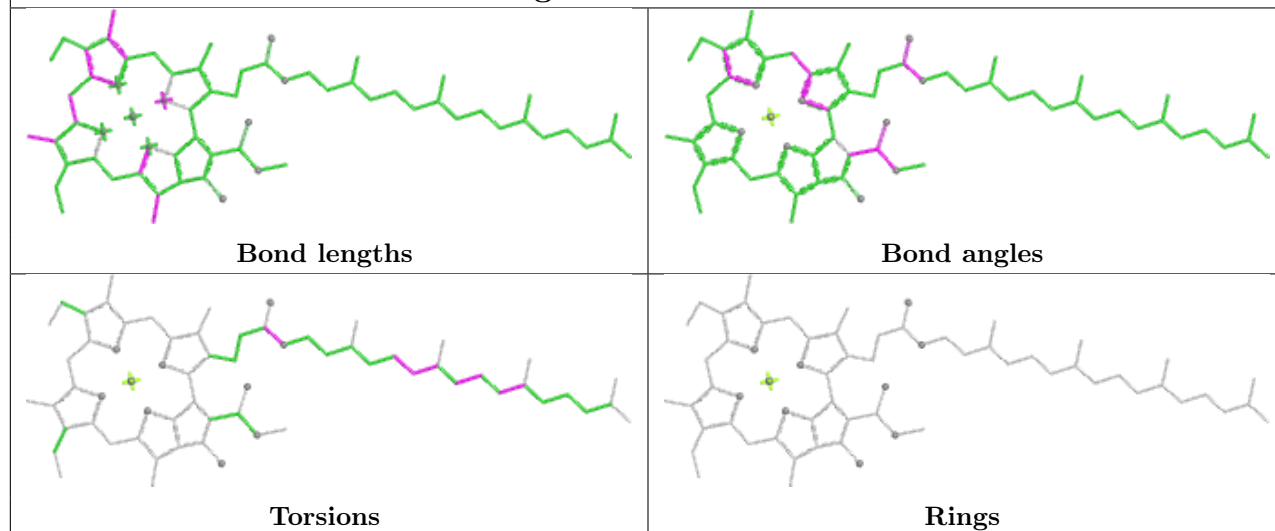
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

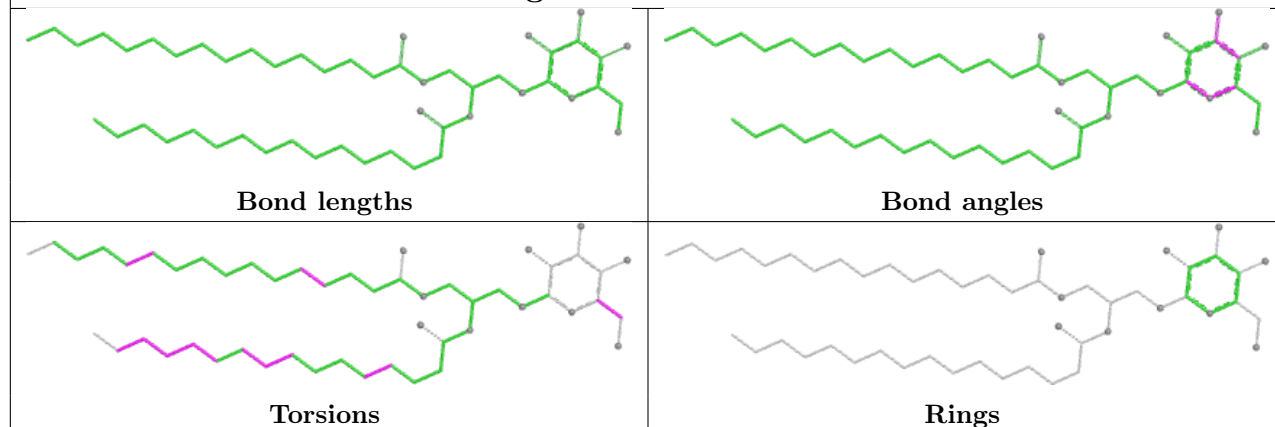
Ligand DGD A 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE z 703	
	
Bond lengths	Bond angles
	
Torsions	Rings

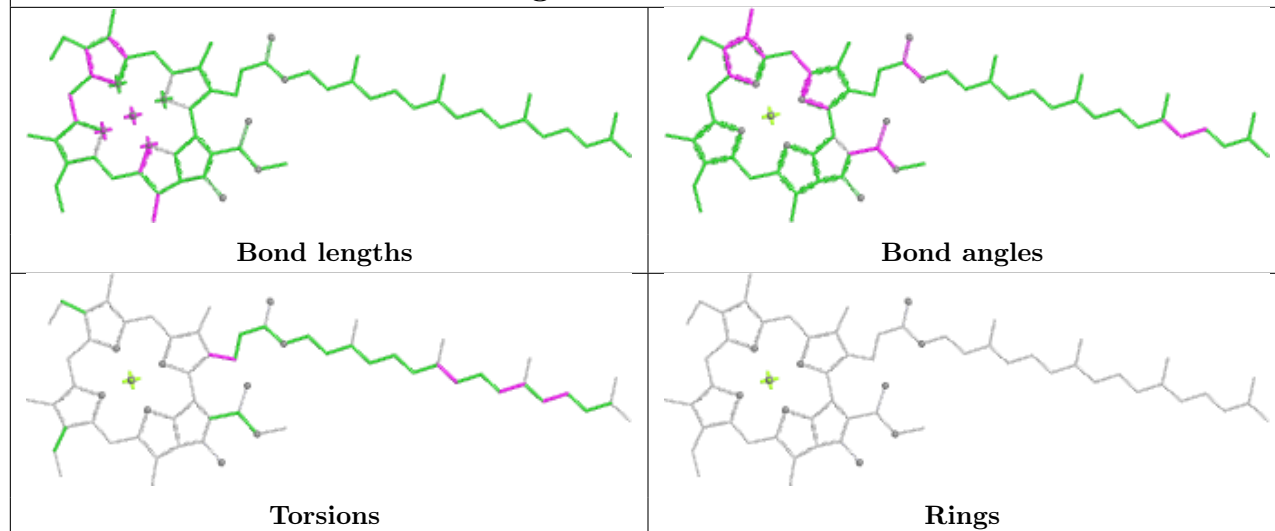
Ligand CLA b 603

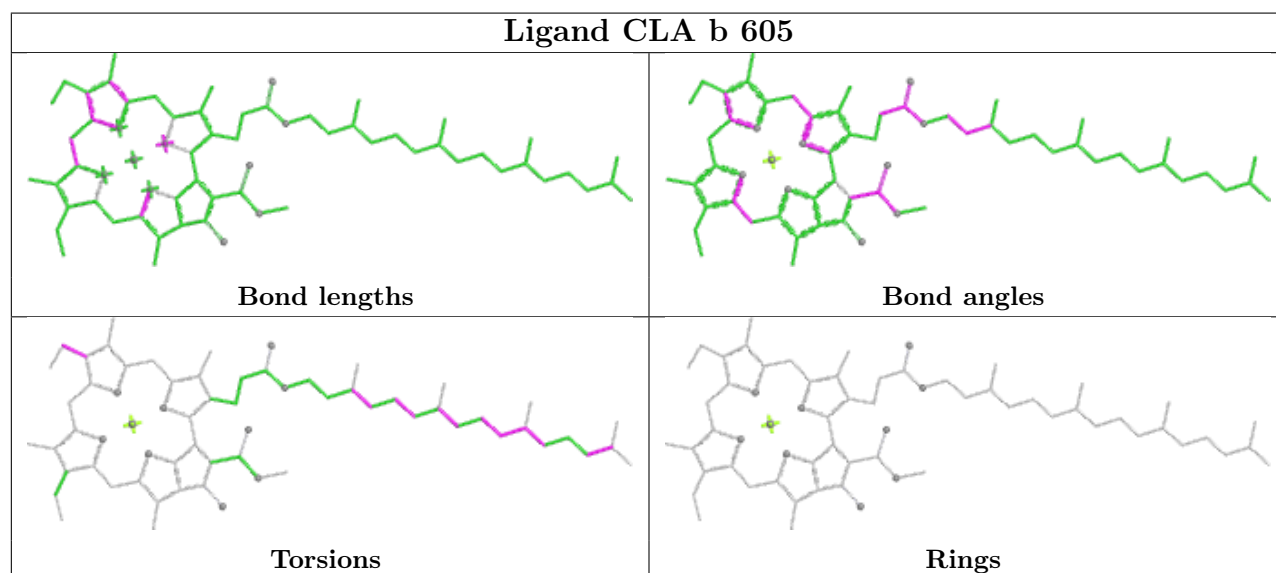
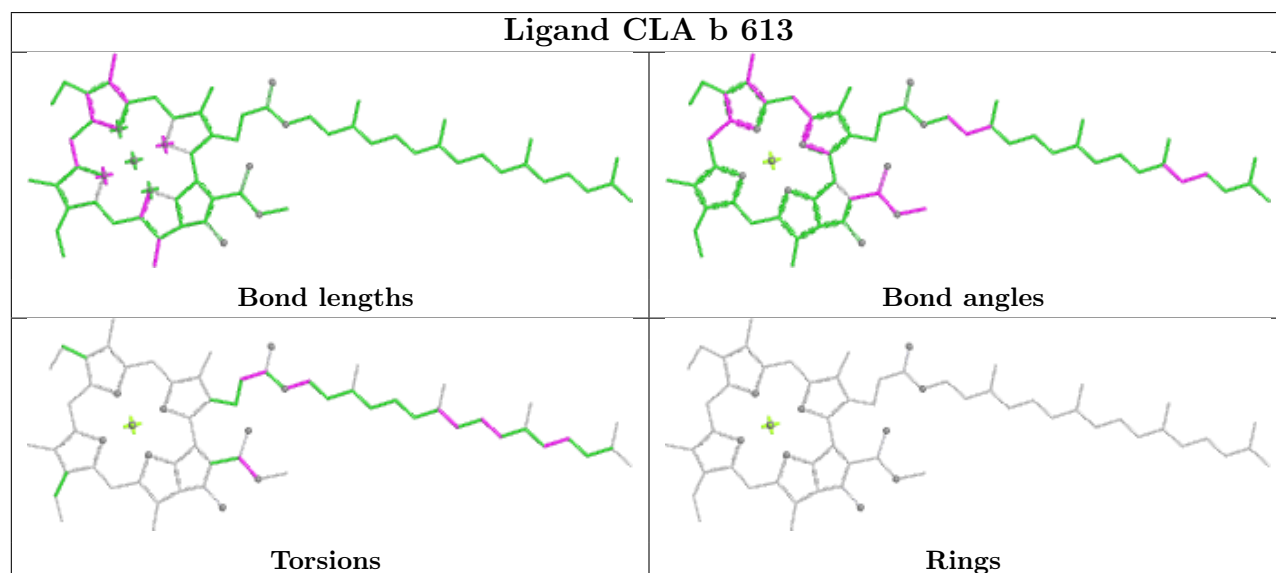
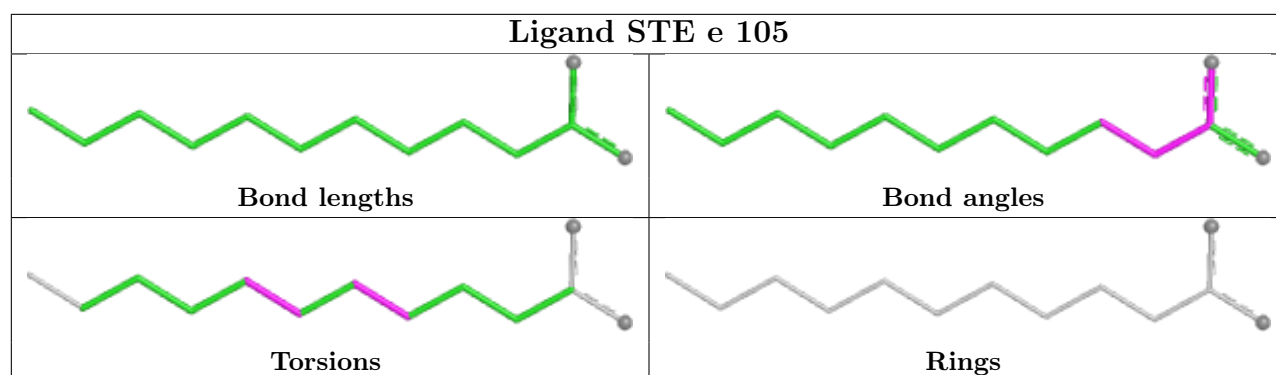


Ligand LMG D 409

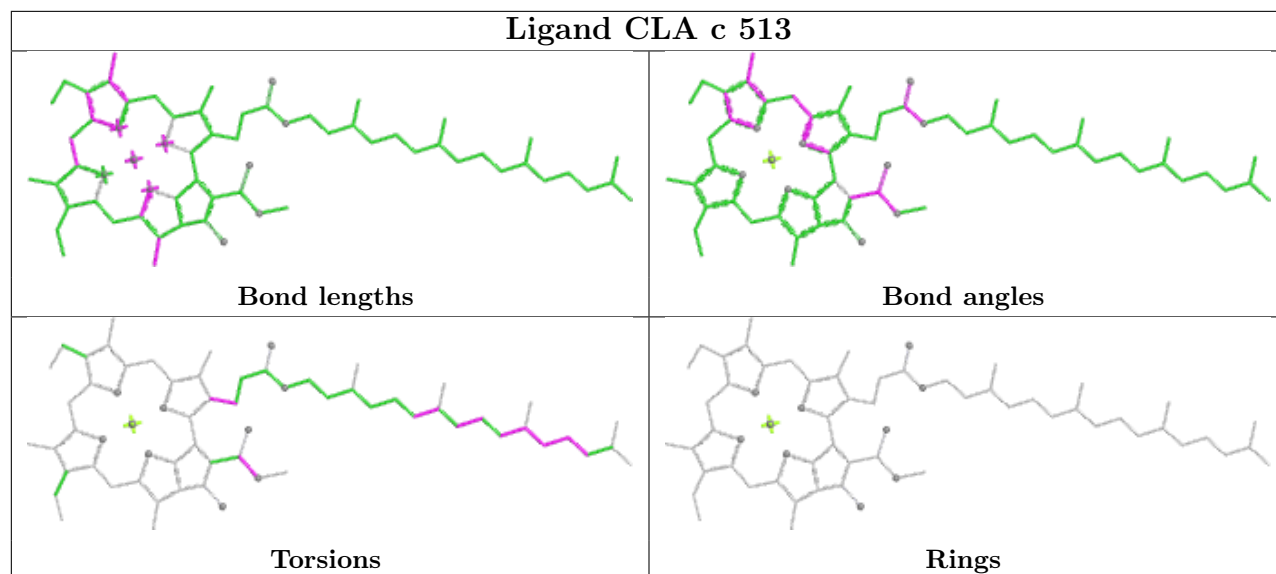


Ligand CLA B 602

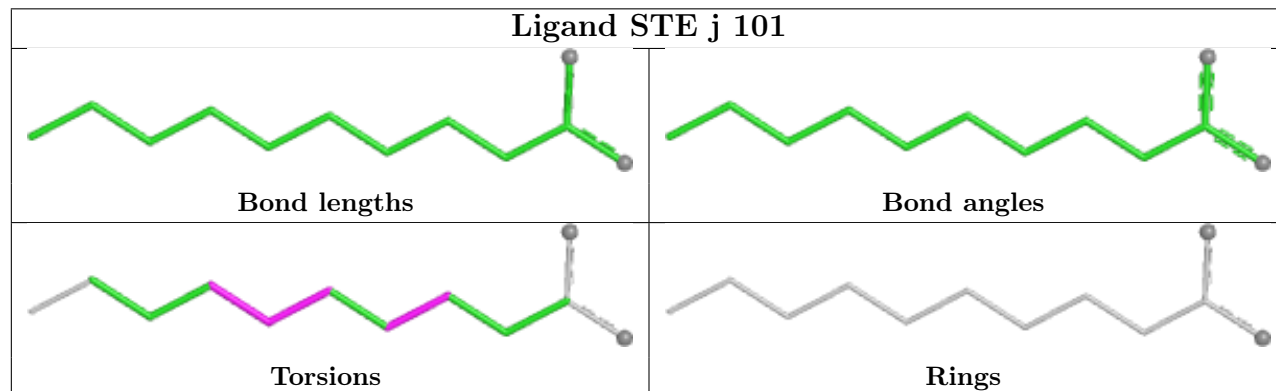




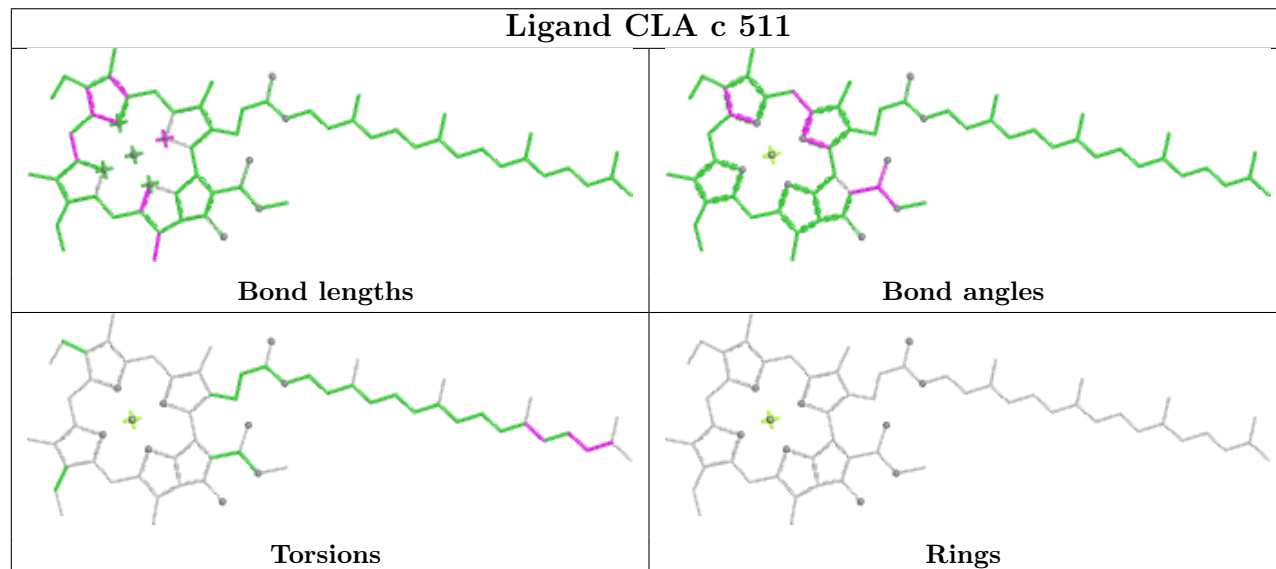
Ligand CLA c 513

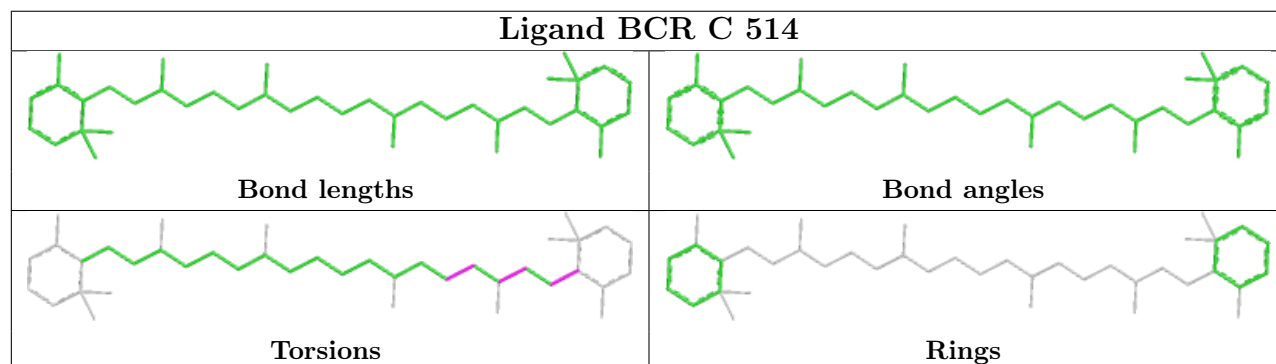
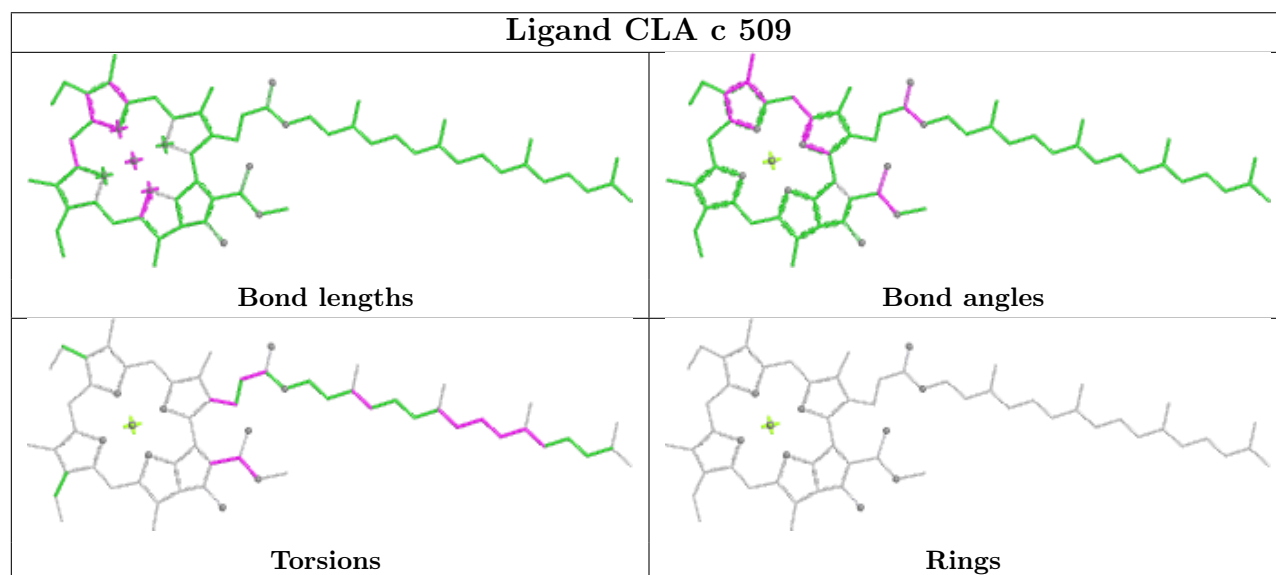
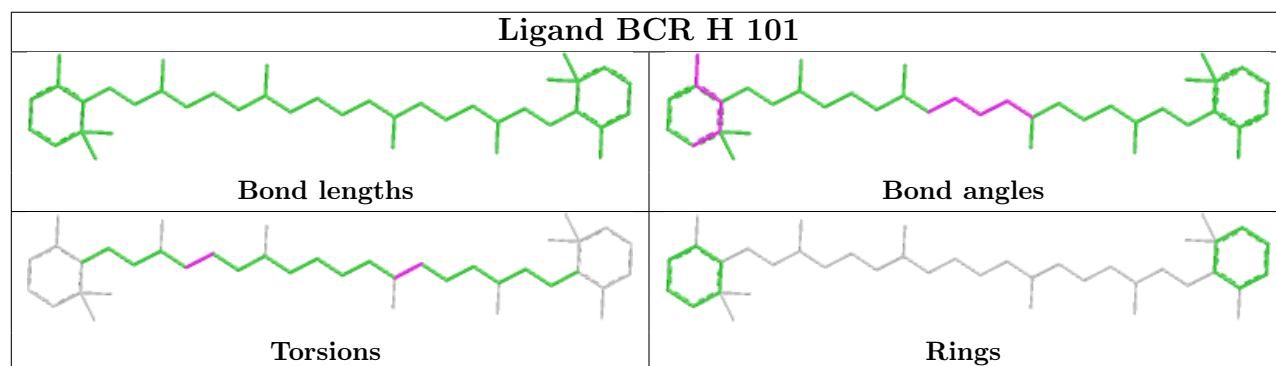
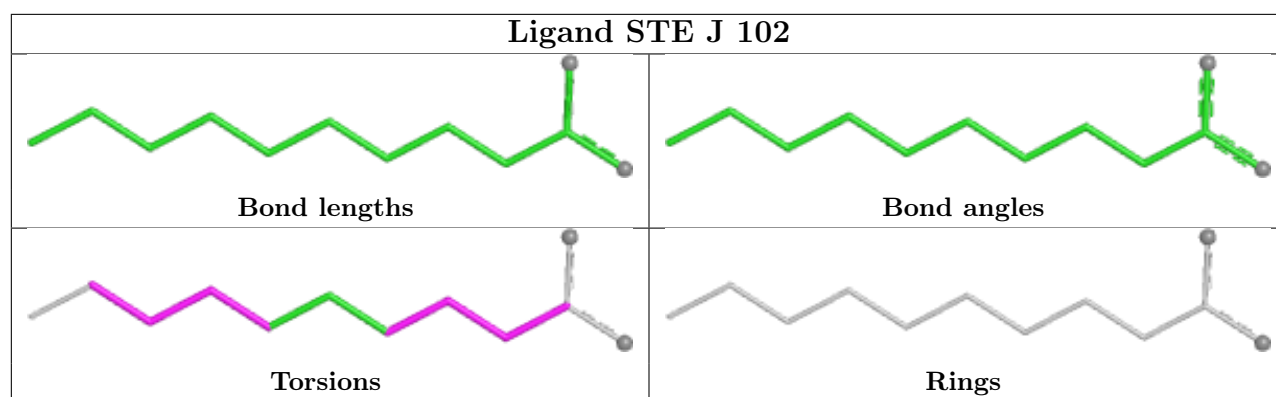


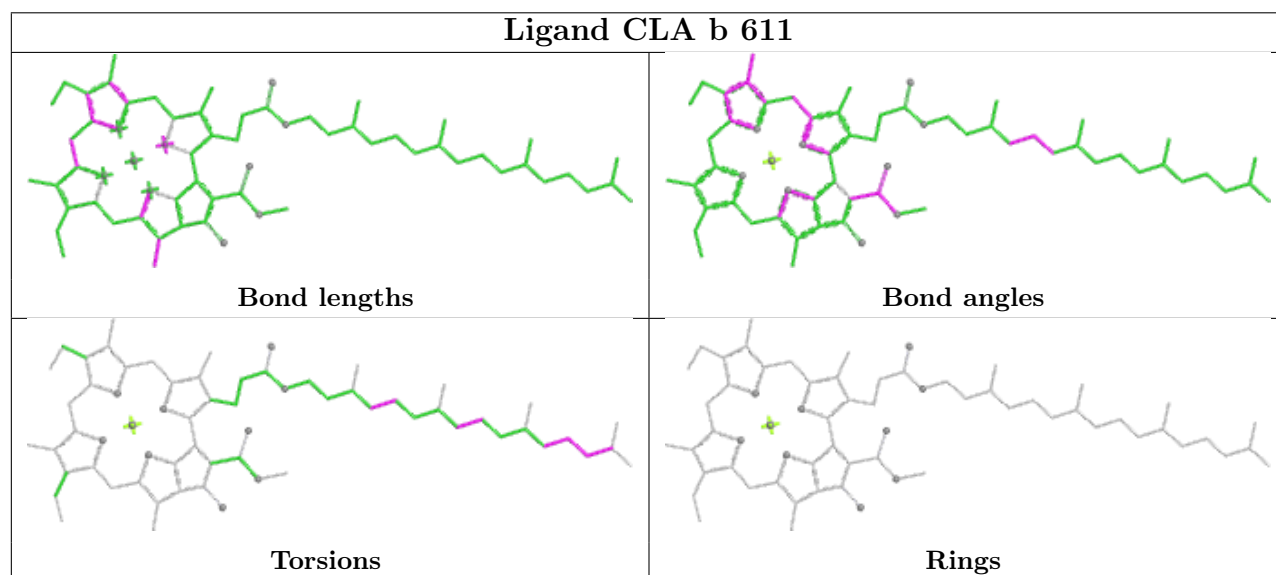
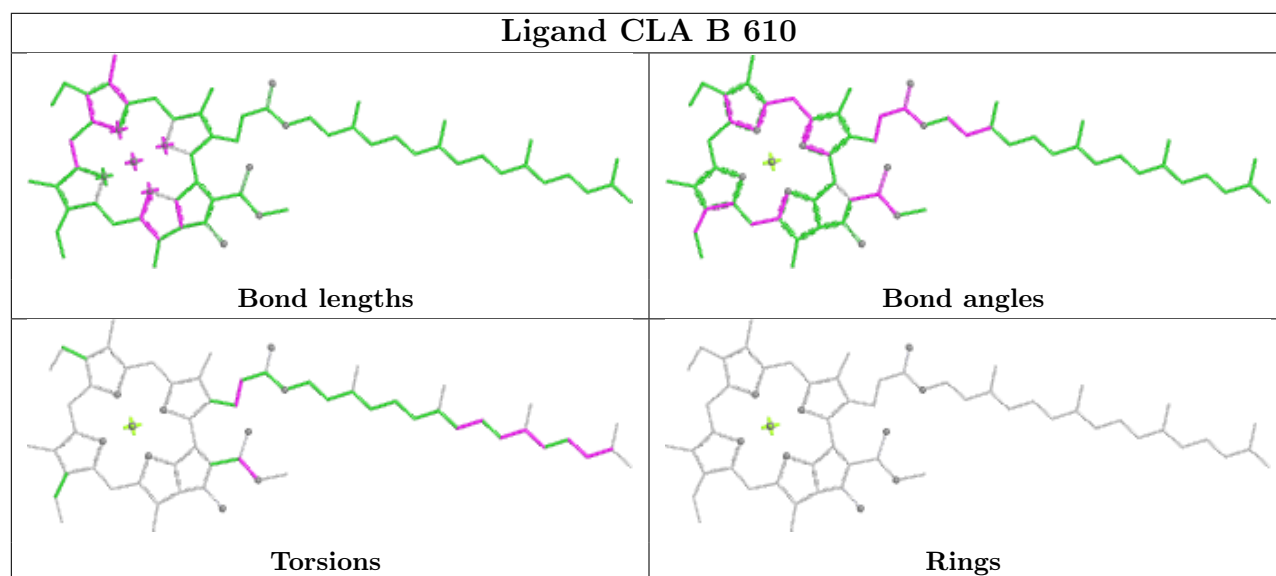
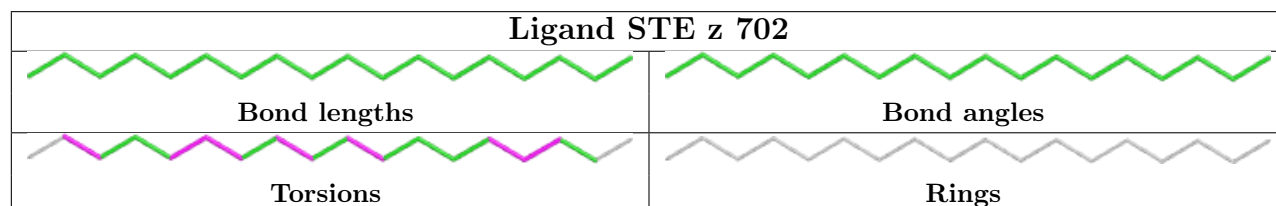
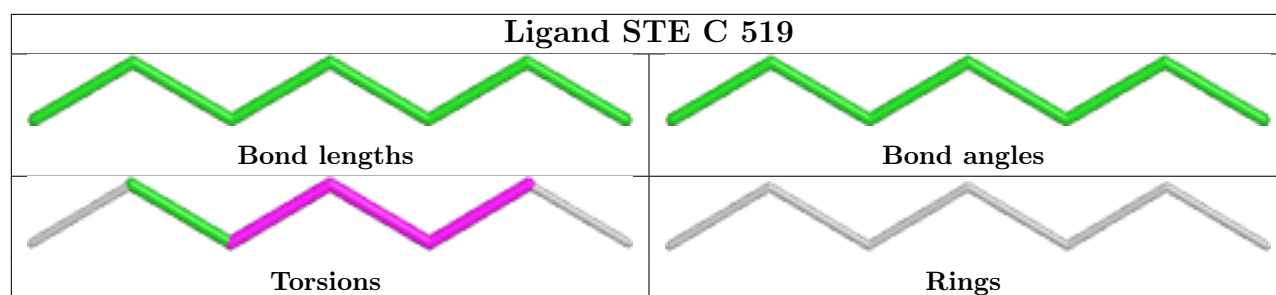
Ligand STE j 101

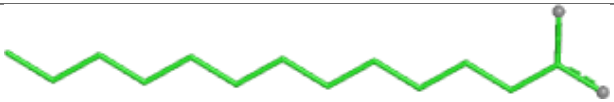
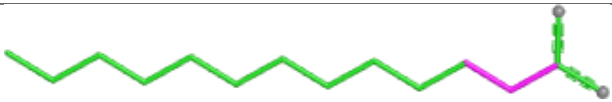
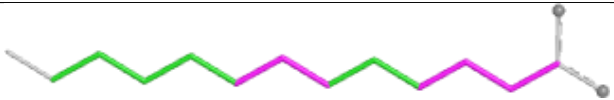
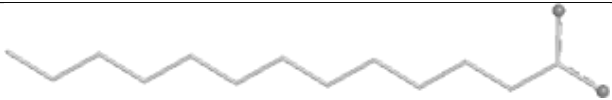


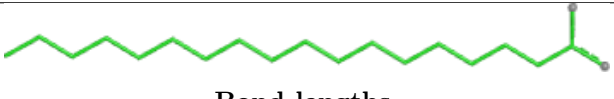
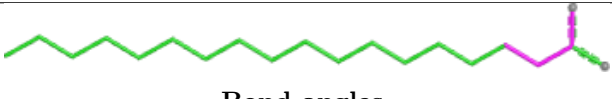
Ligand CLA c 511

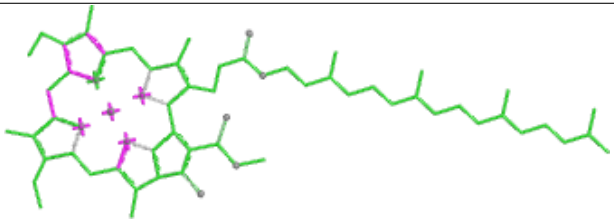
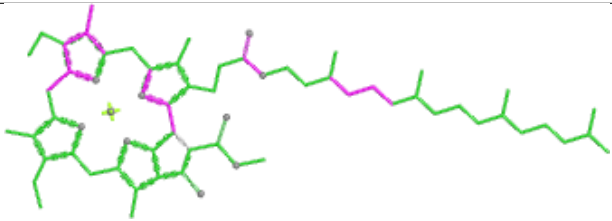
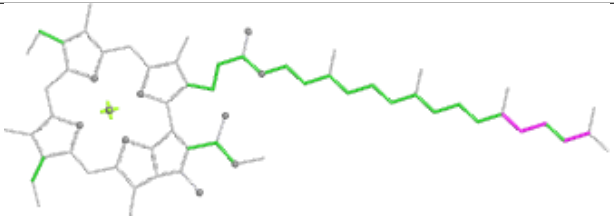
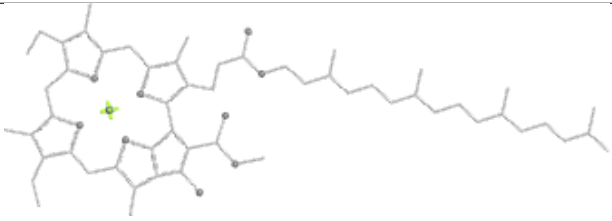


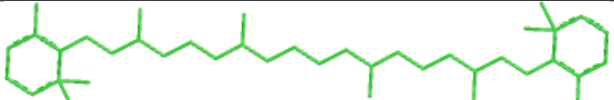
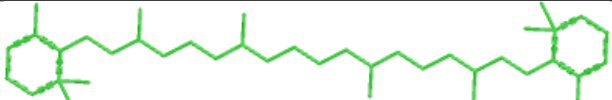
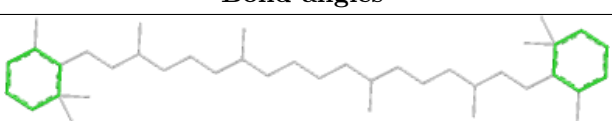


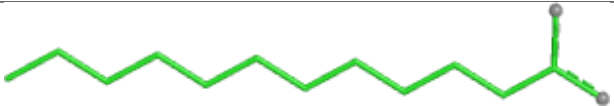
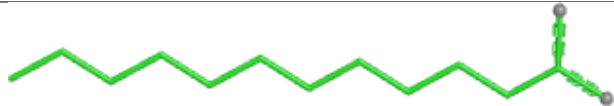
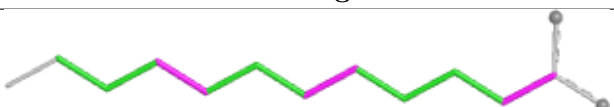
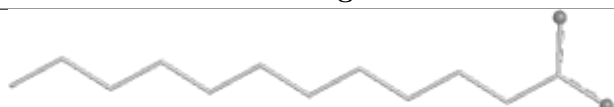


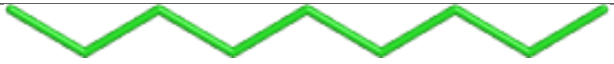
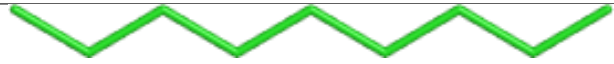
Ligand STE I 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

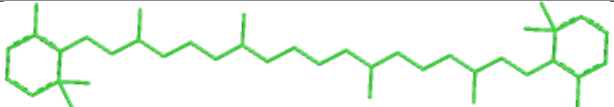
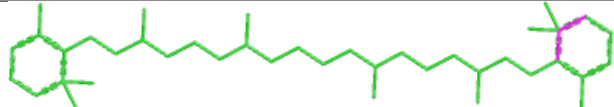
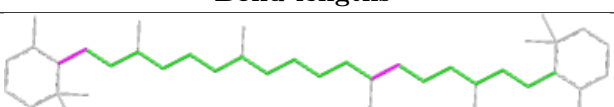
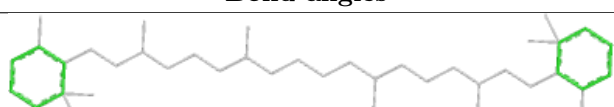
Ligand STE X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

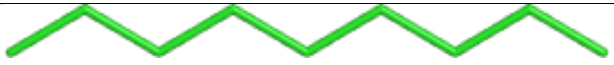
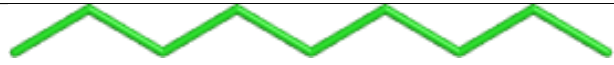
Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

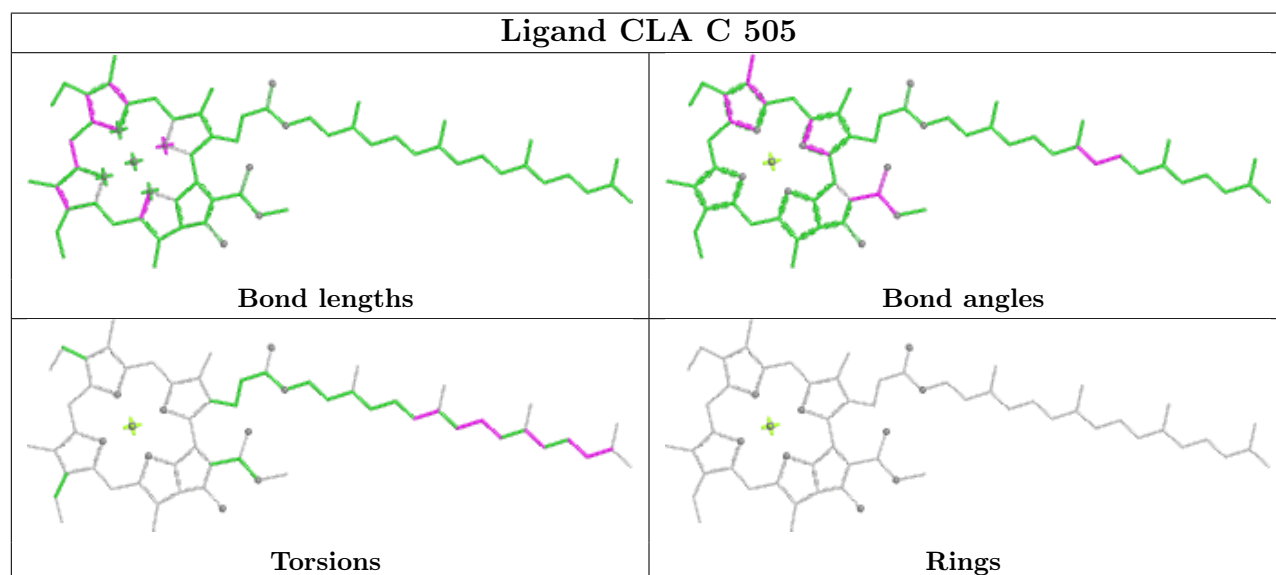
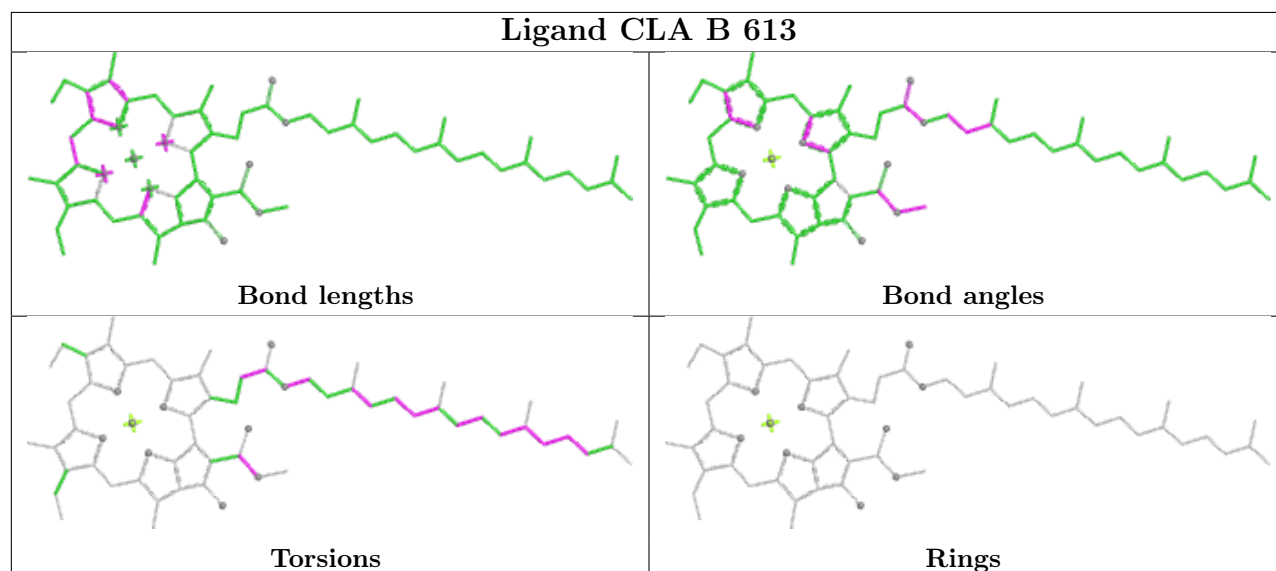
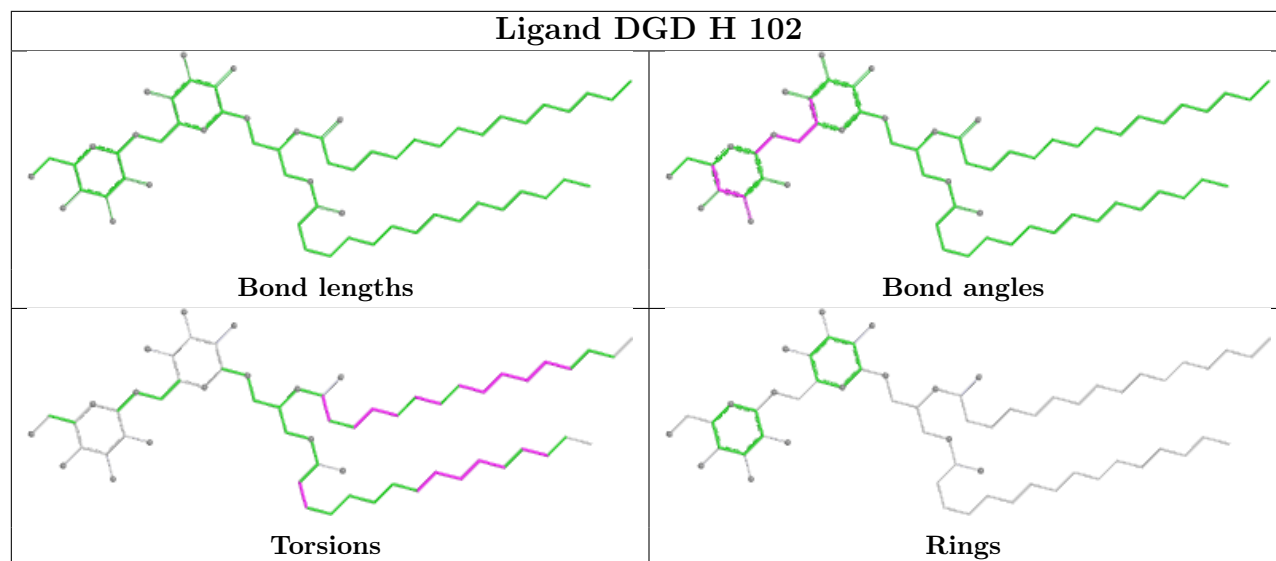
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

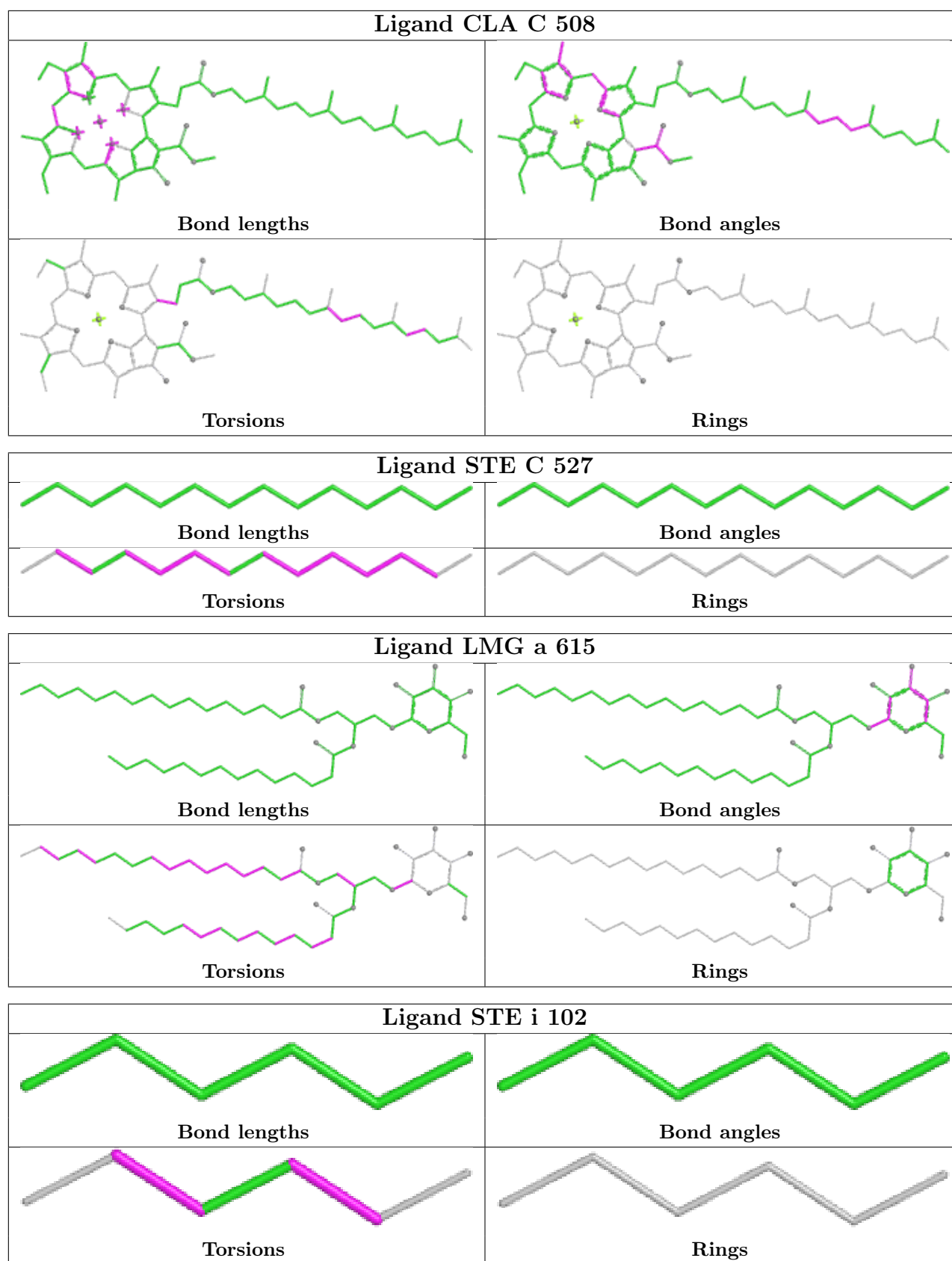
Ligand STE d 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

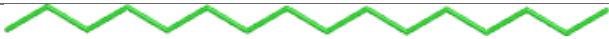
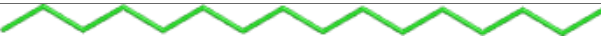
Ligand STE A 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

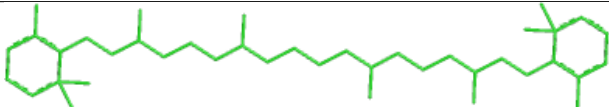
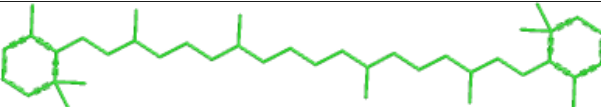
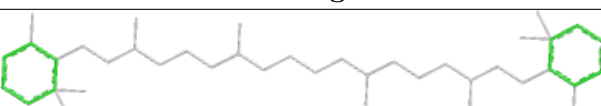
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

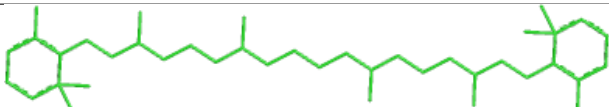
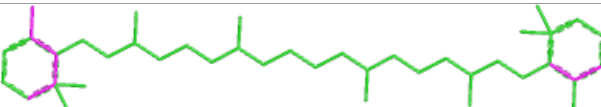
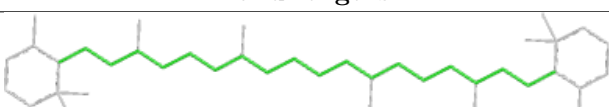
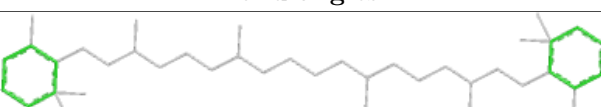
Ligand STE e 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

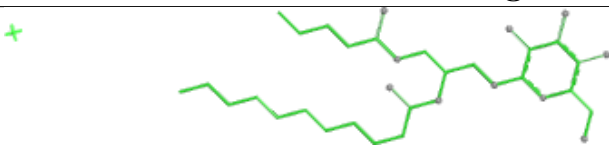
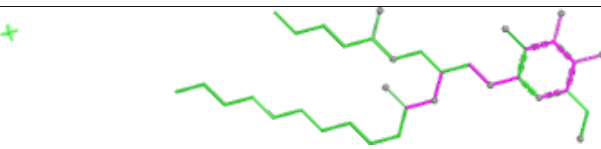
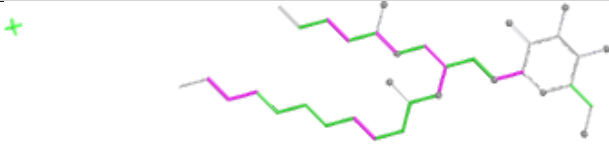
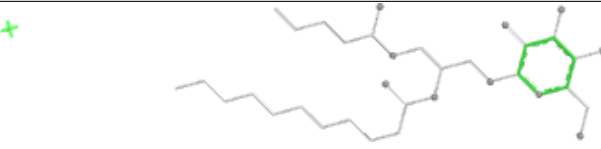


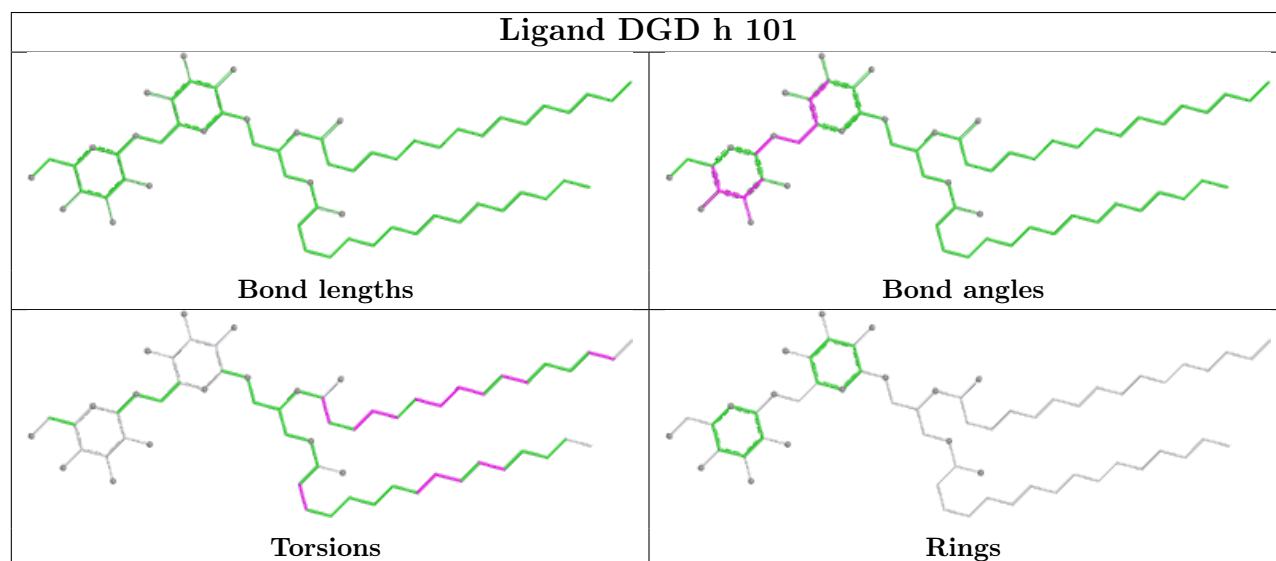
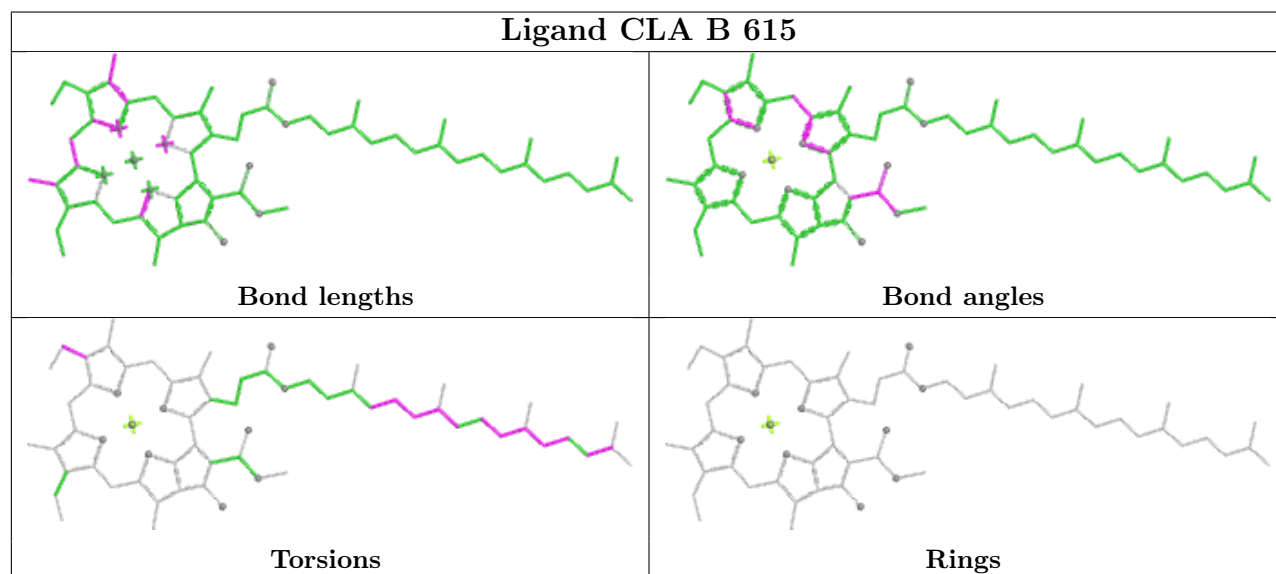
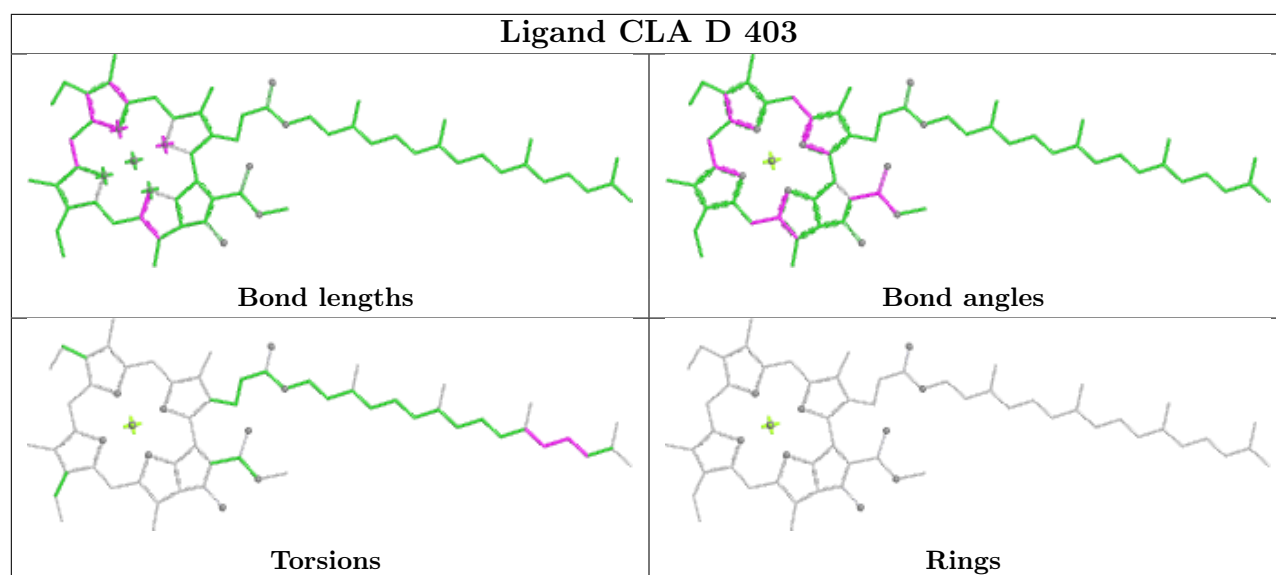


Ligand STE f 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

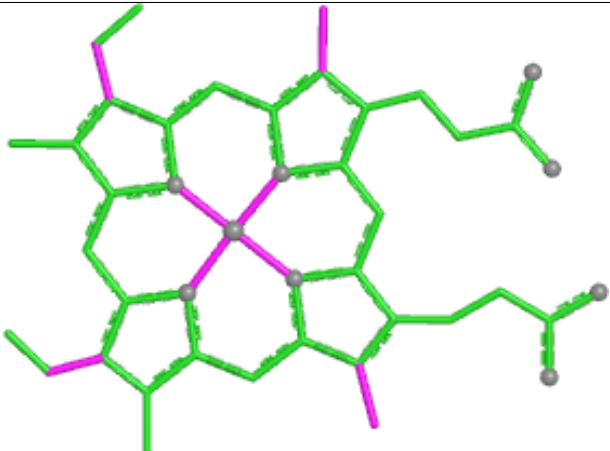
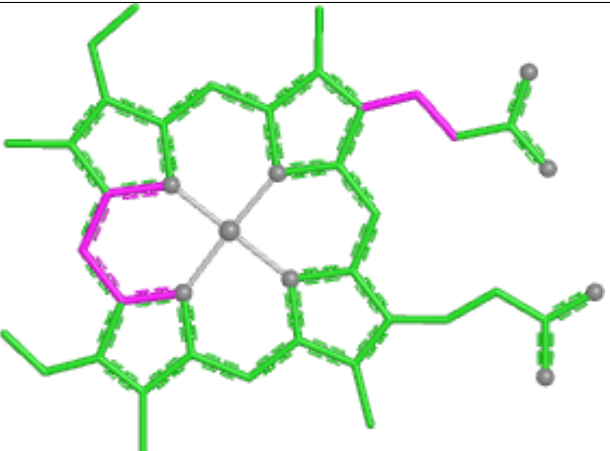
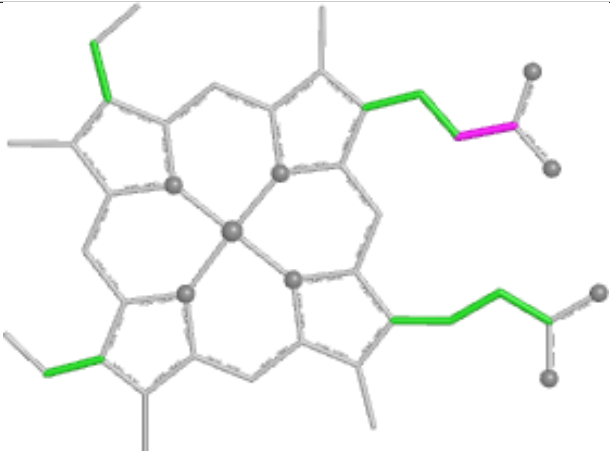
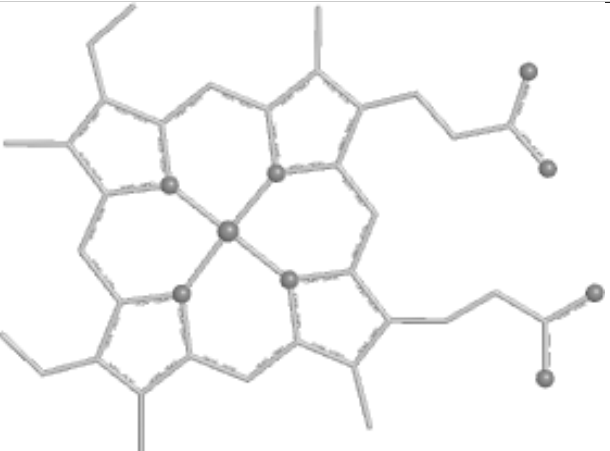
Ligand BCR b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

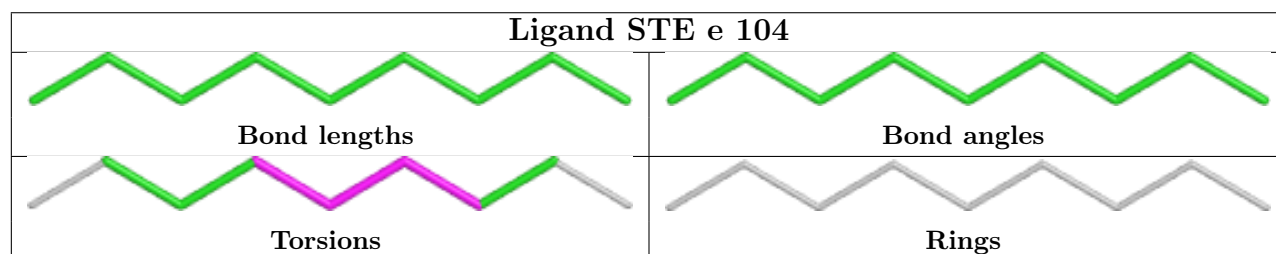
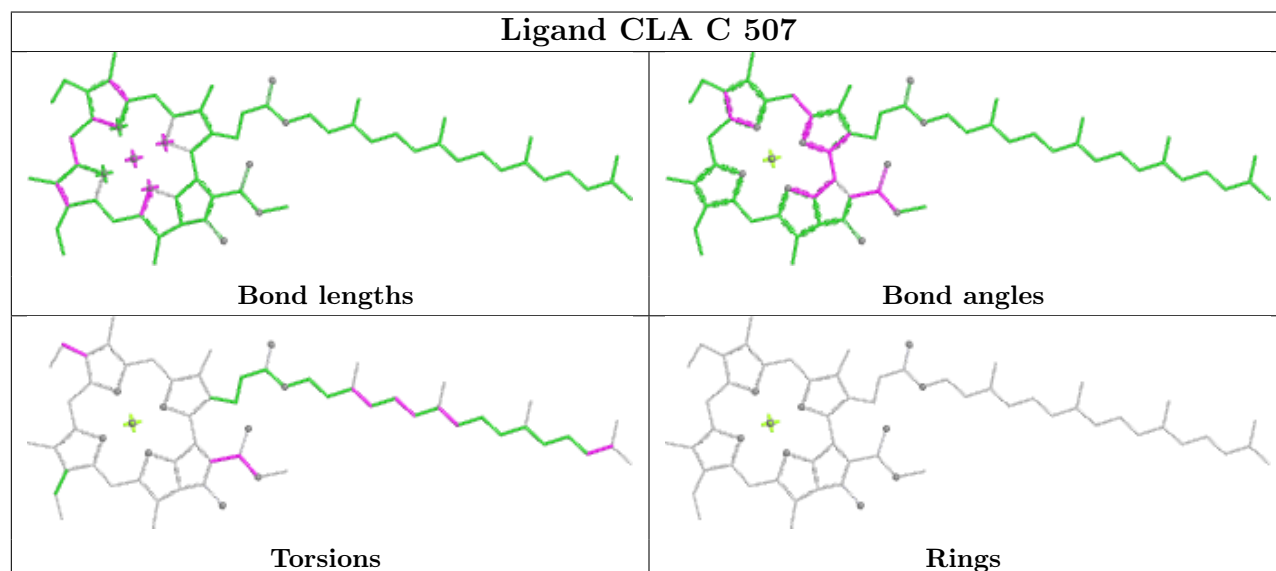
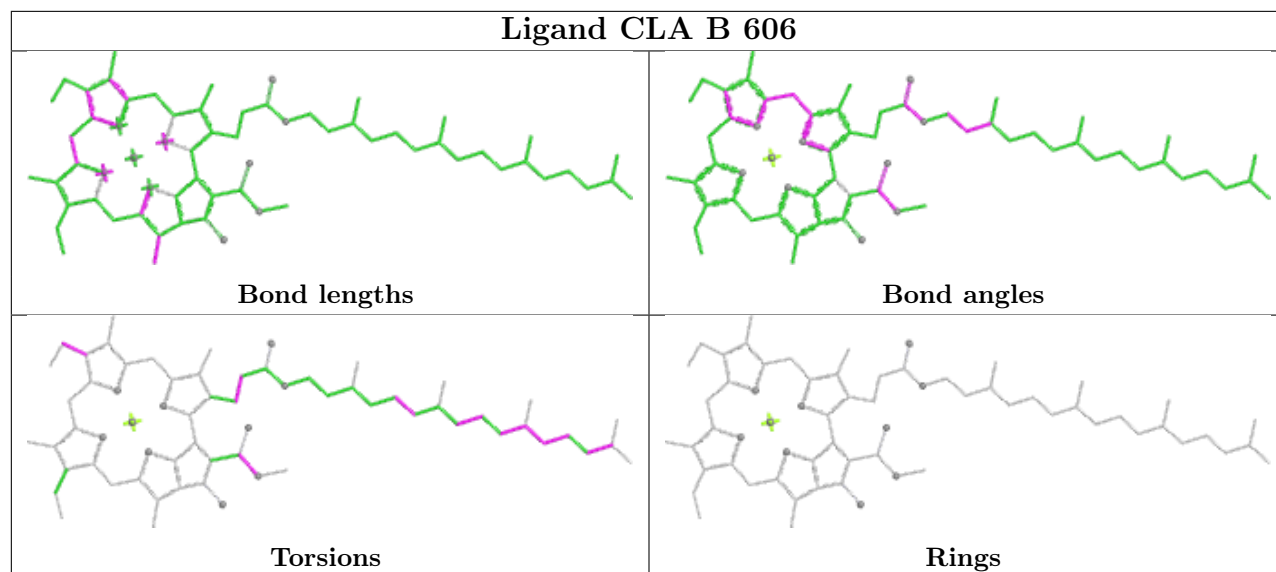
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

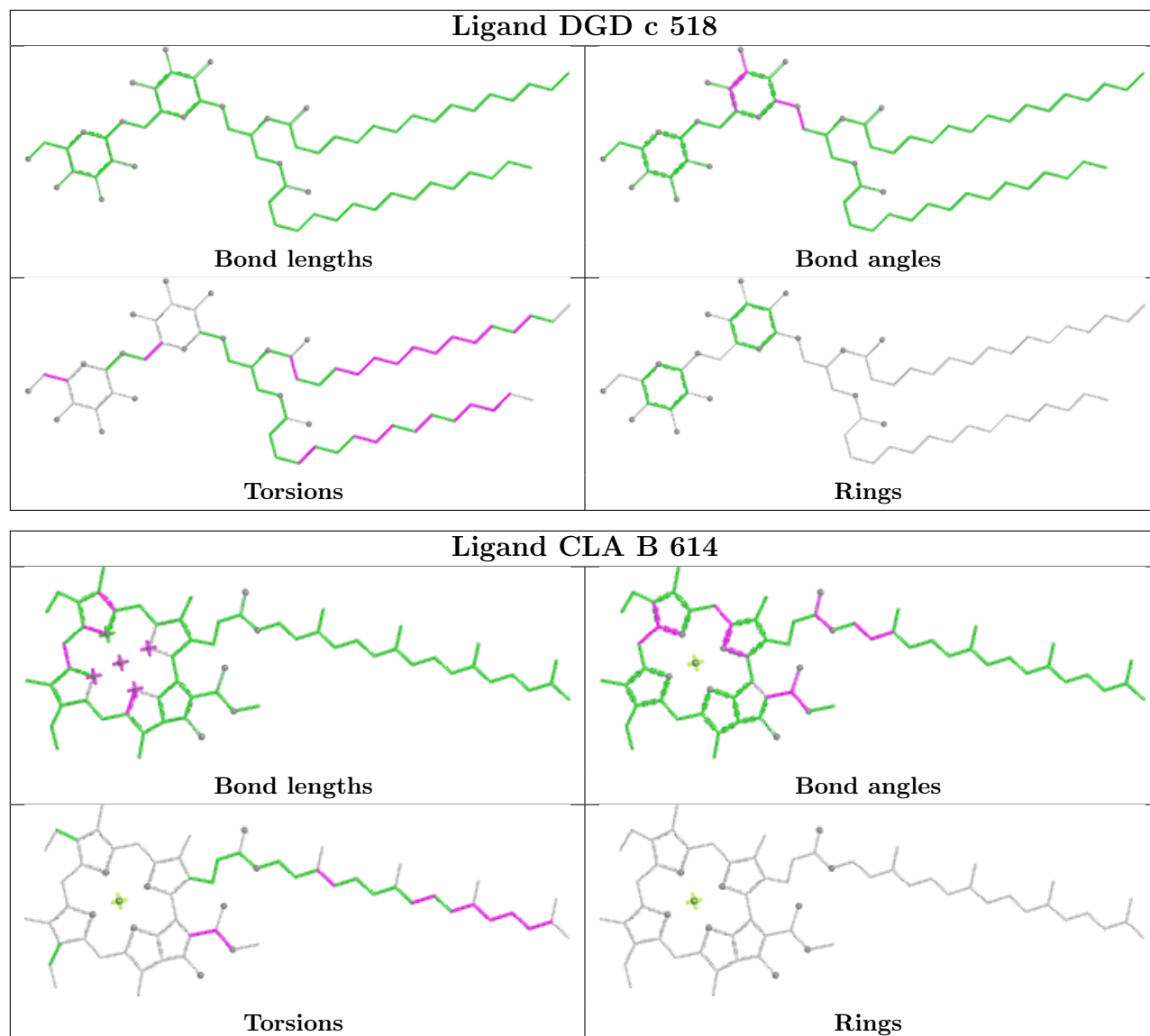
Ligand LMG C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings



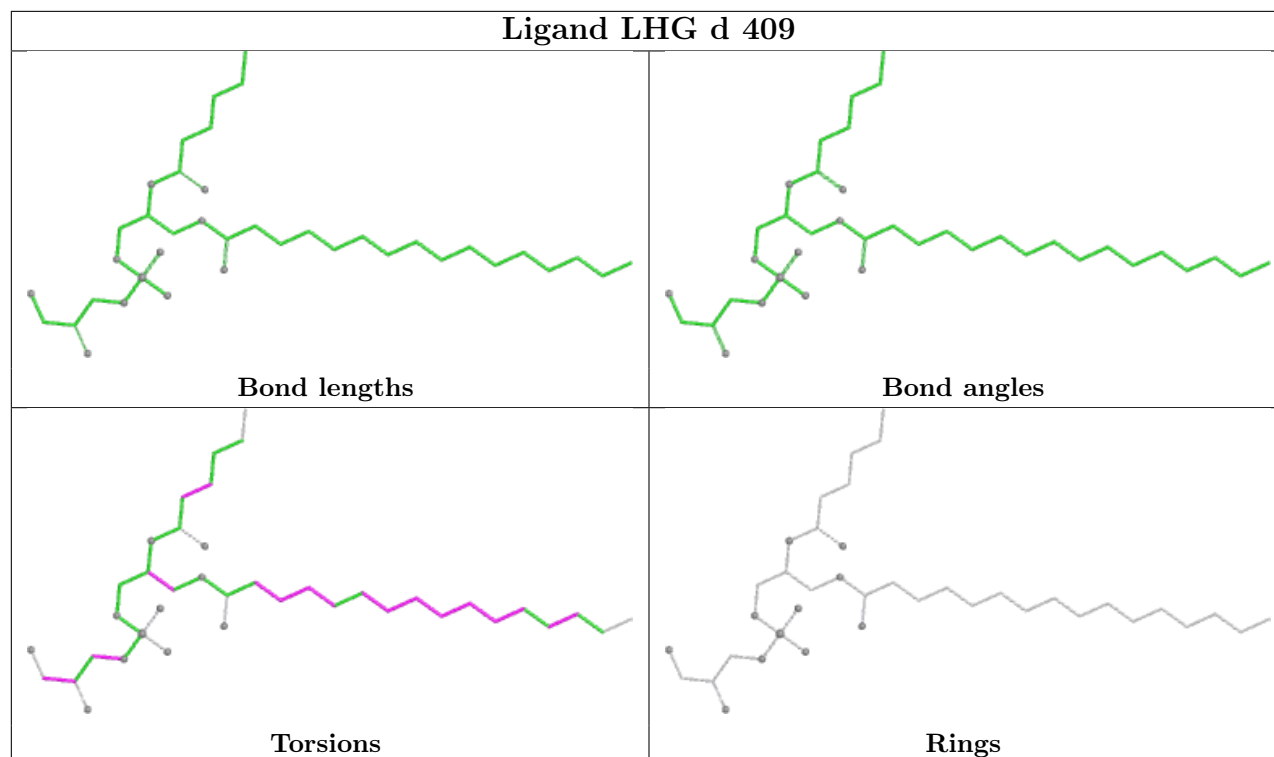
Ligand STE A 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM F 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

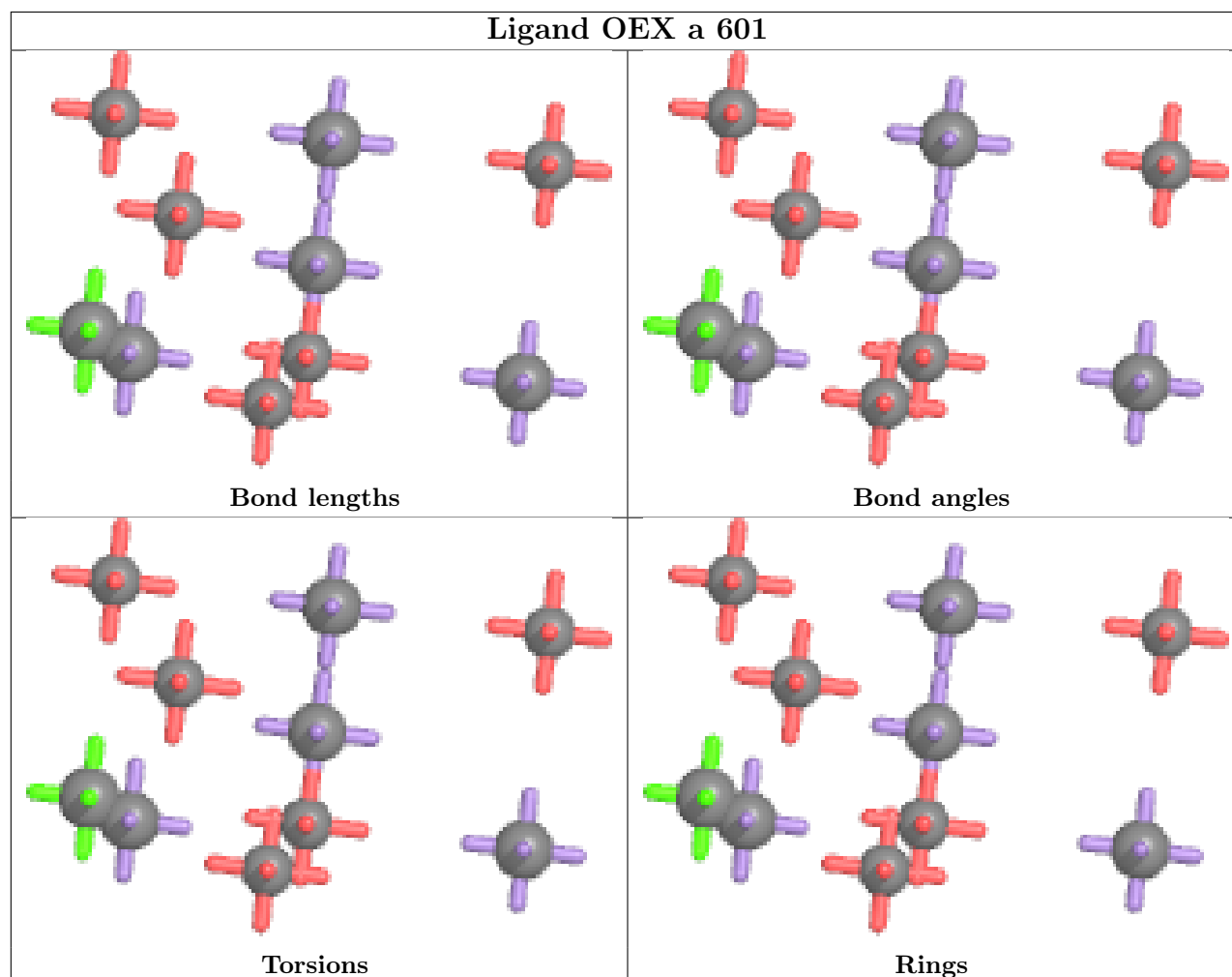




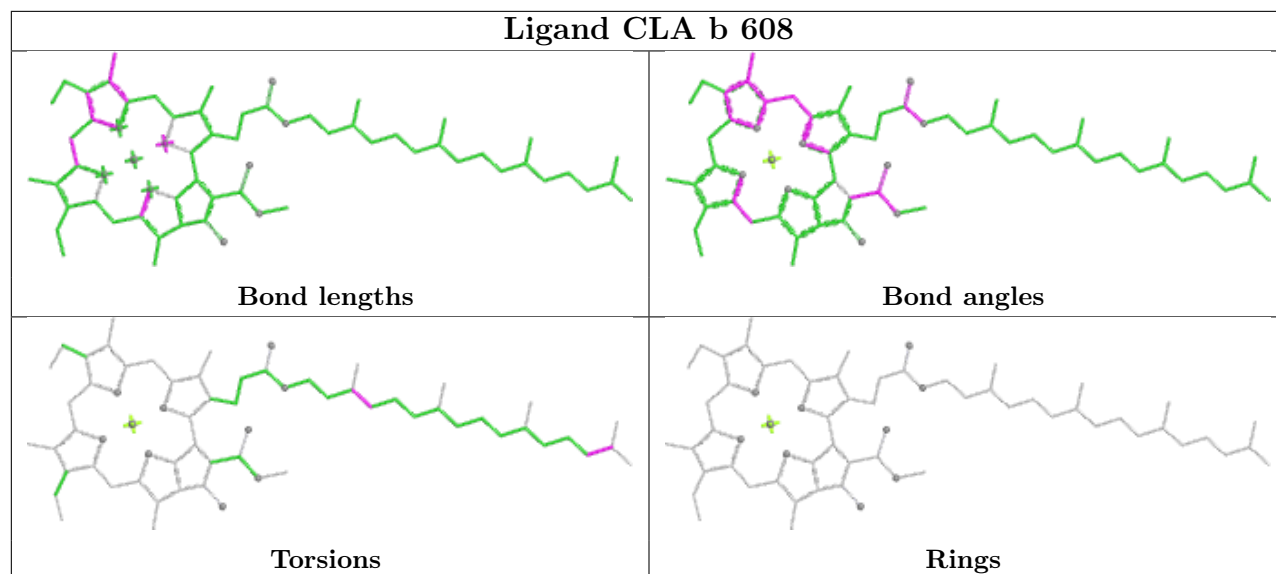
Ligand LHG d 409



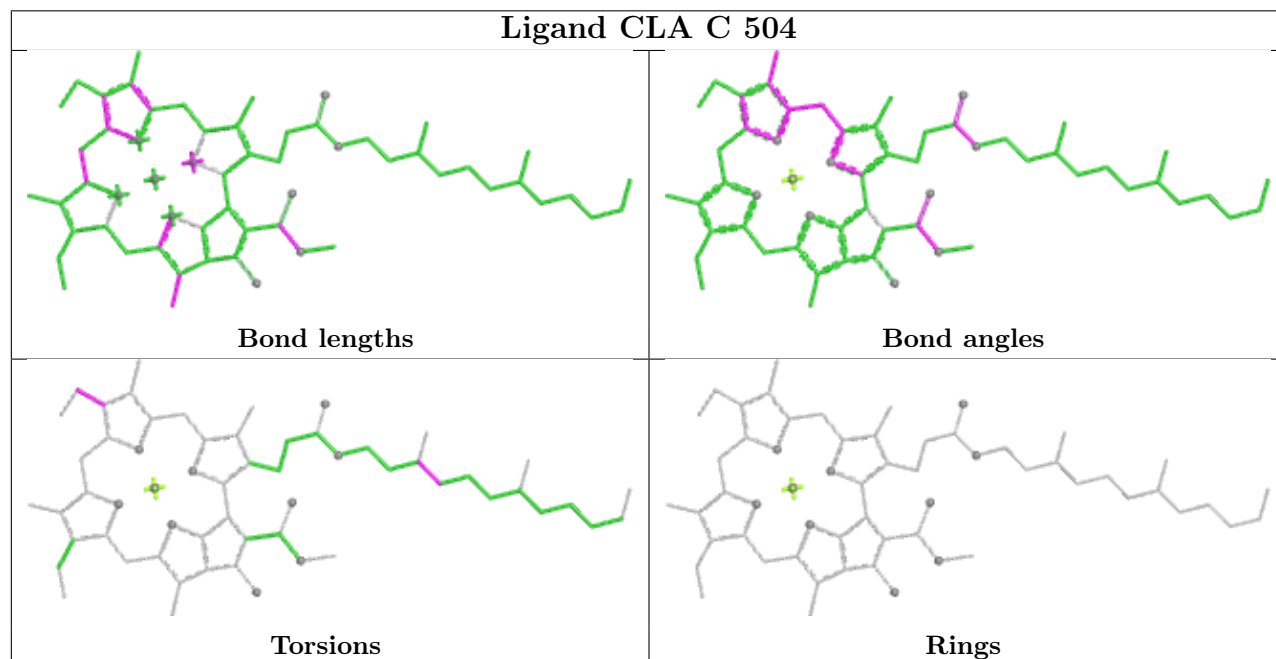
Ligand OEX a 601



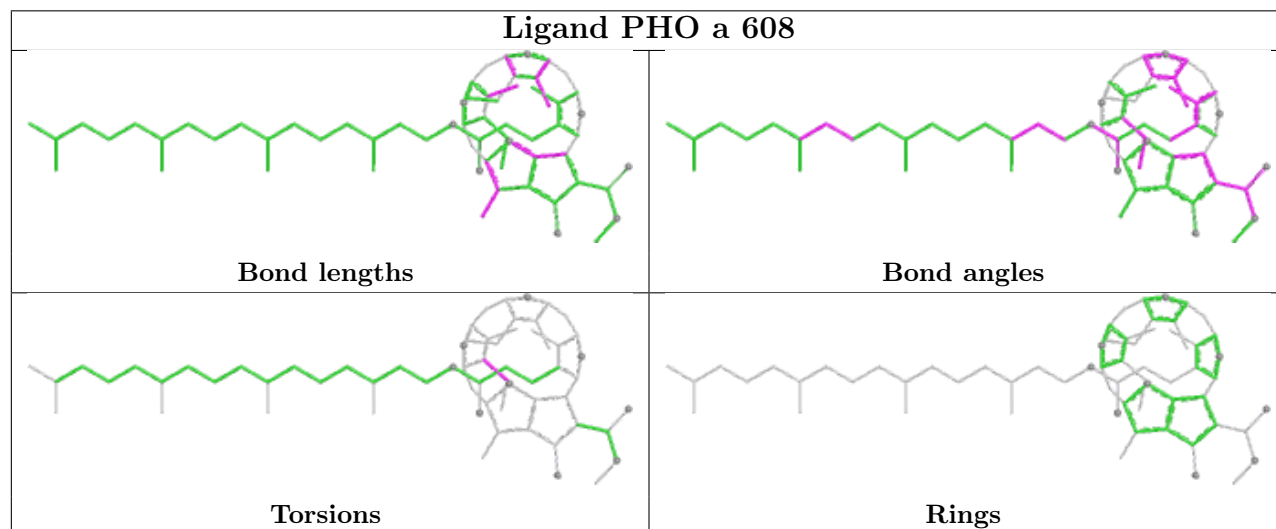
Ligand CLA b 608



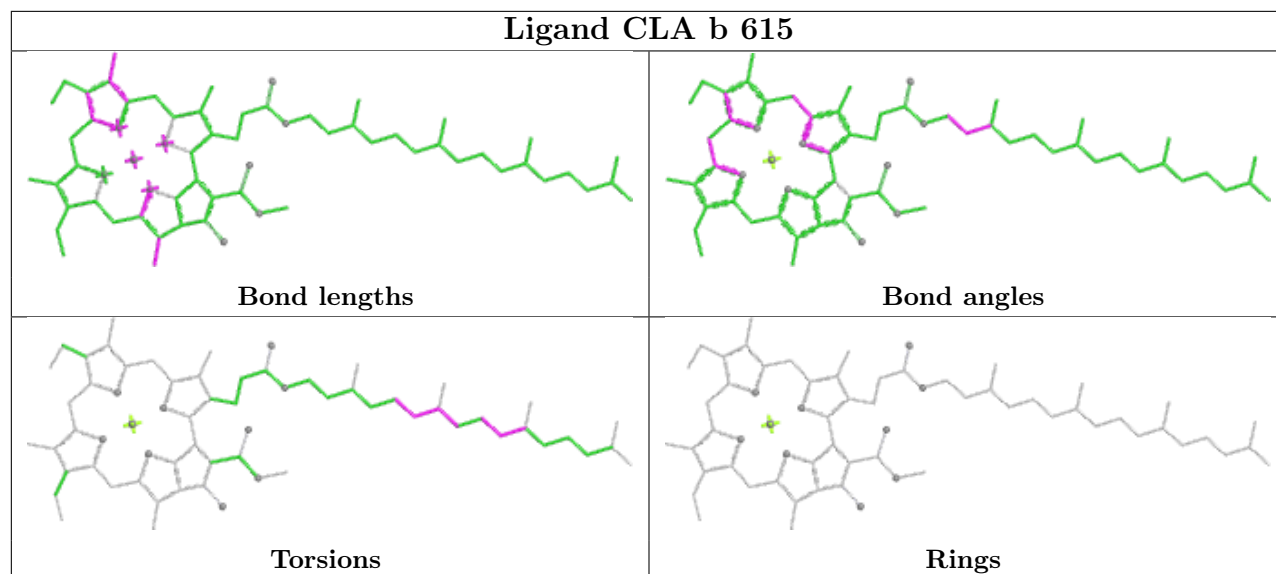
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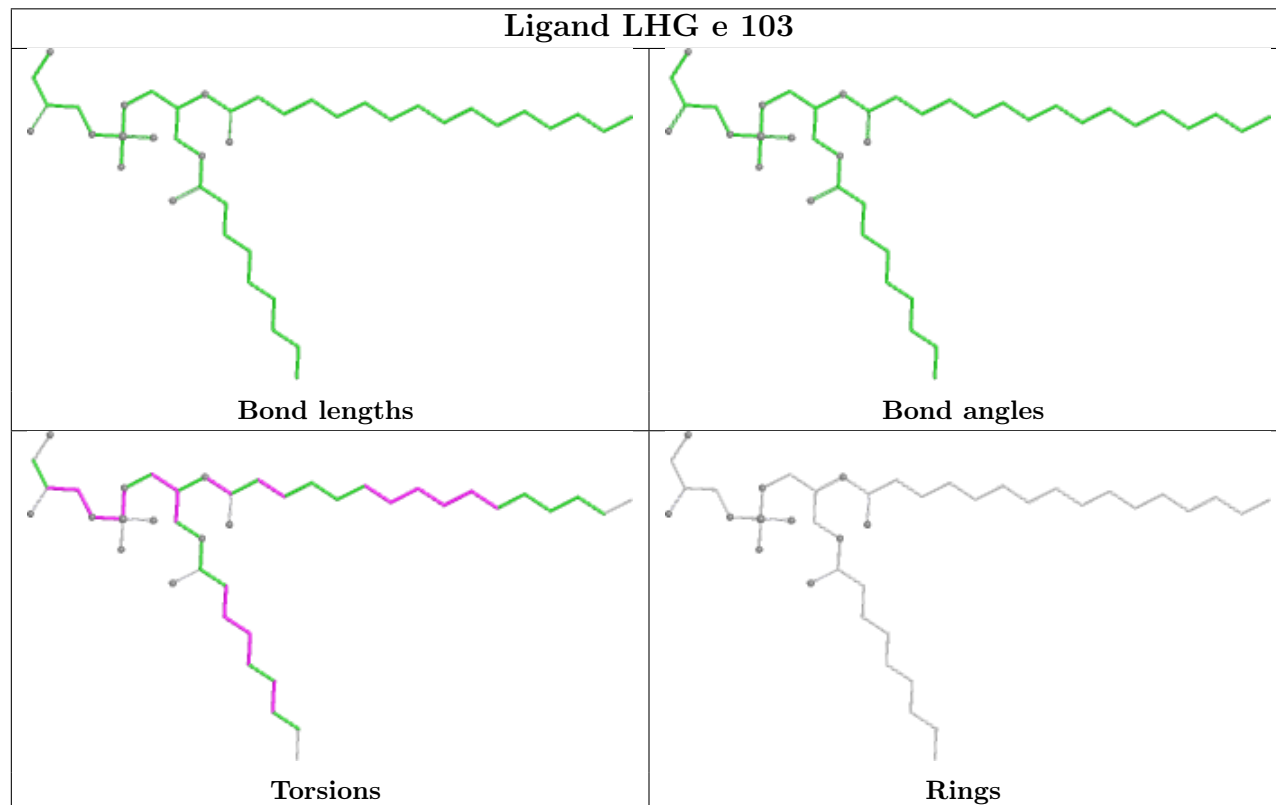
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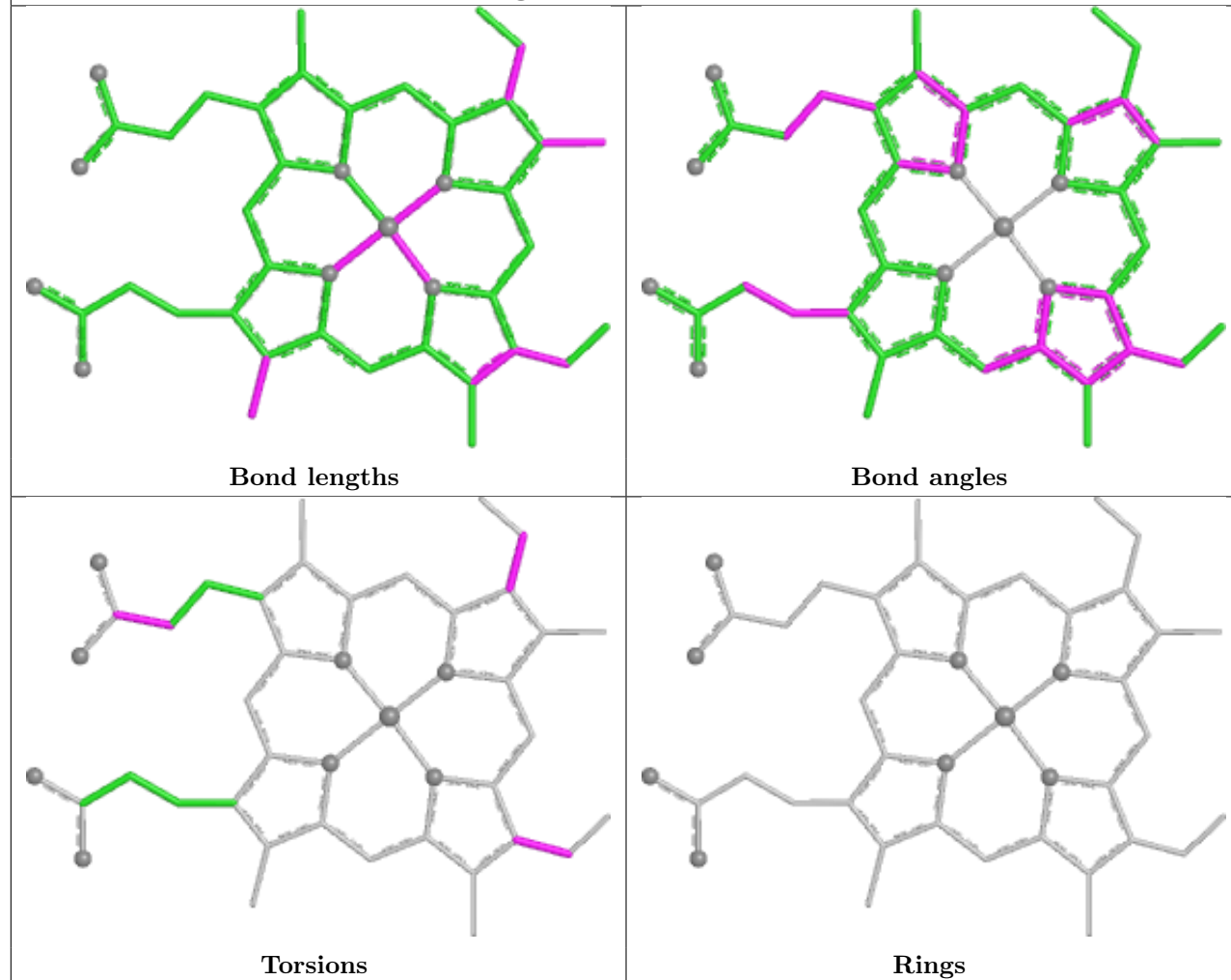
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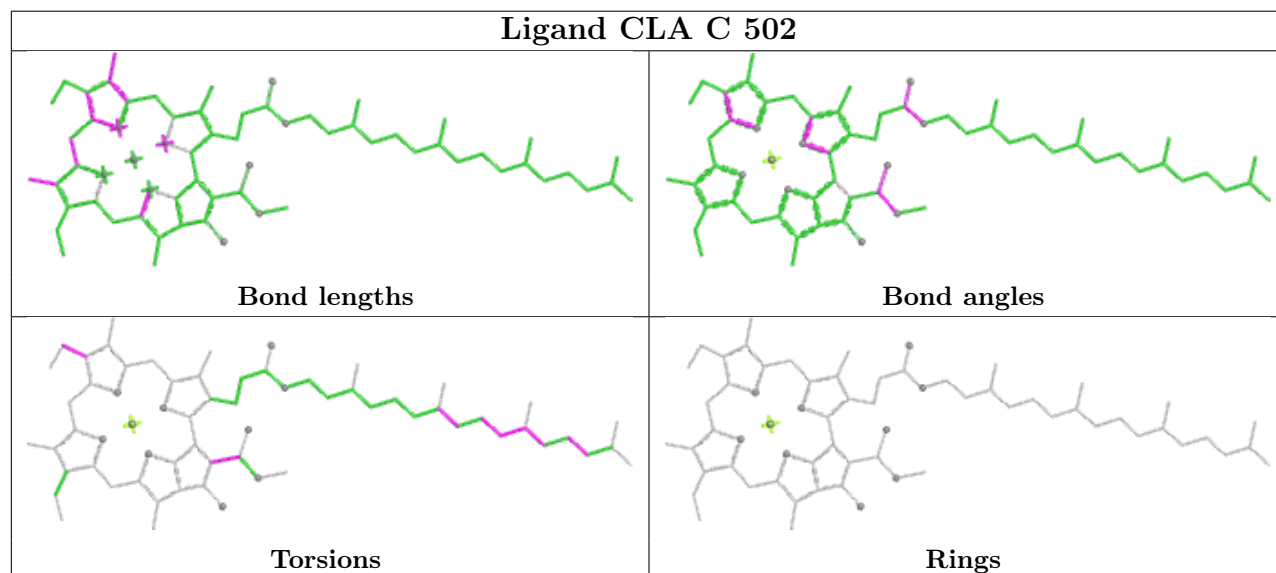
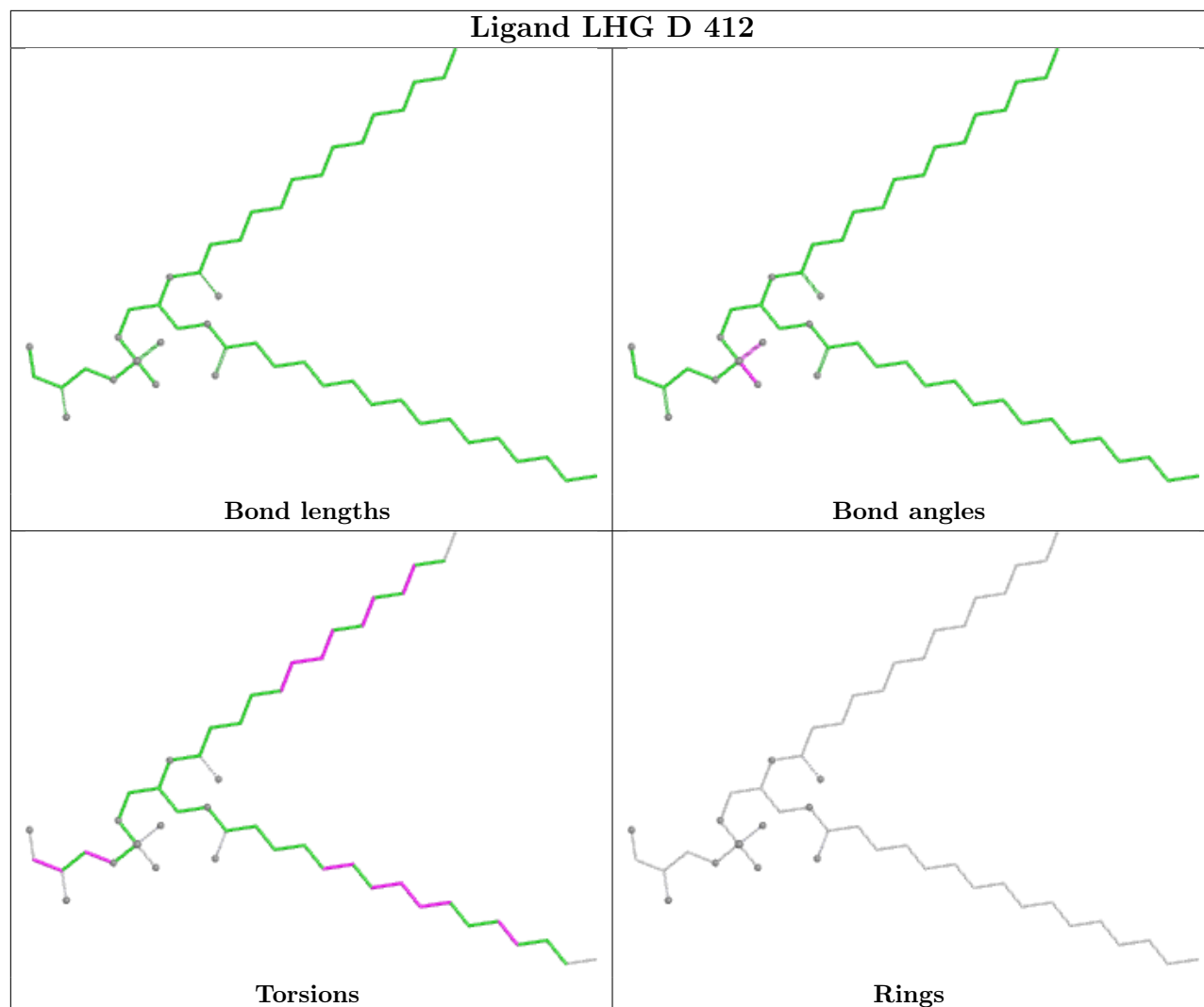


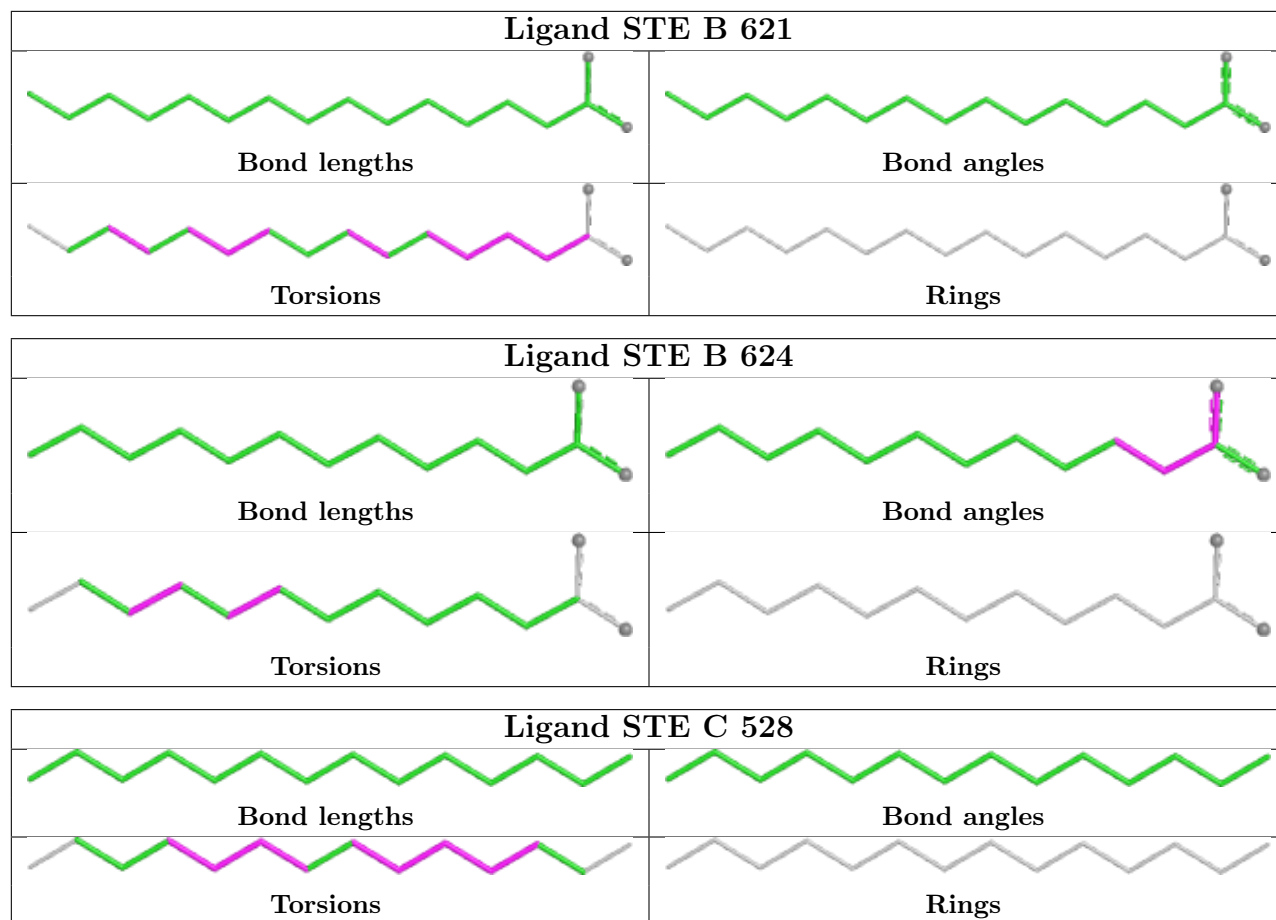
Ligand LHG e 103

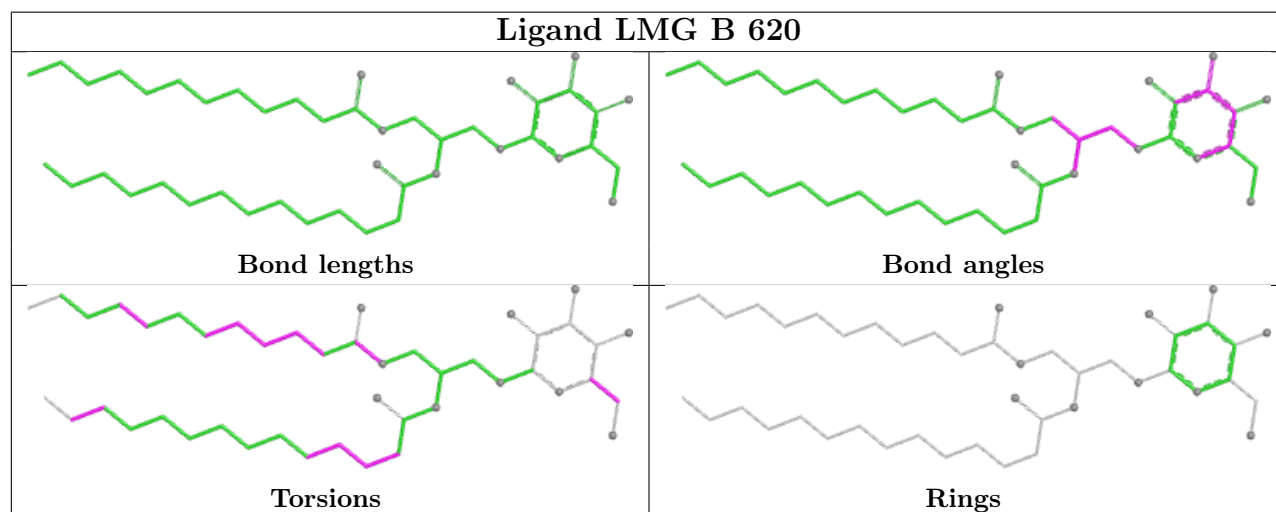
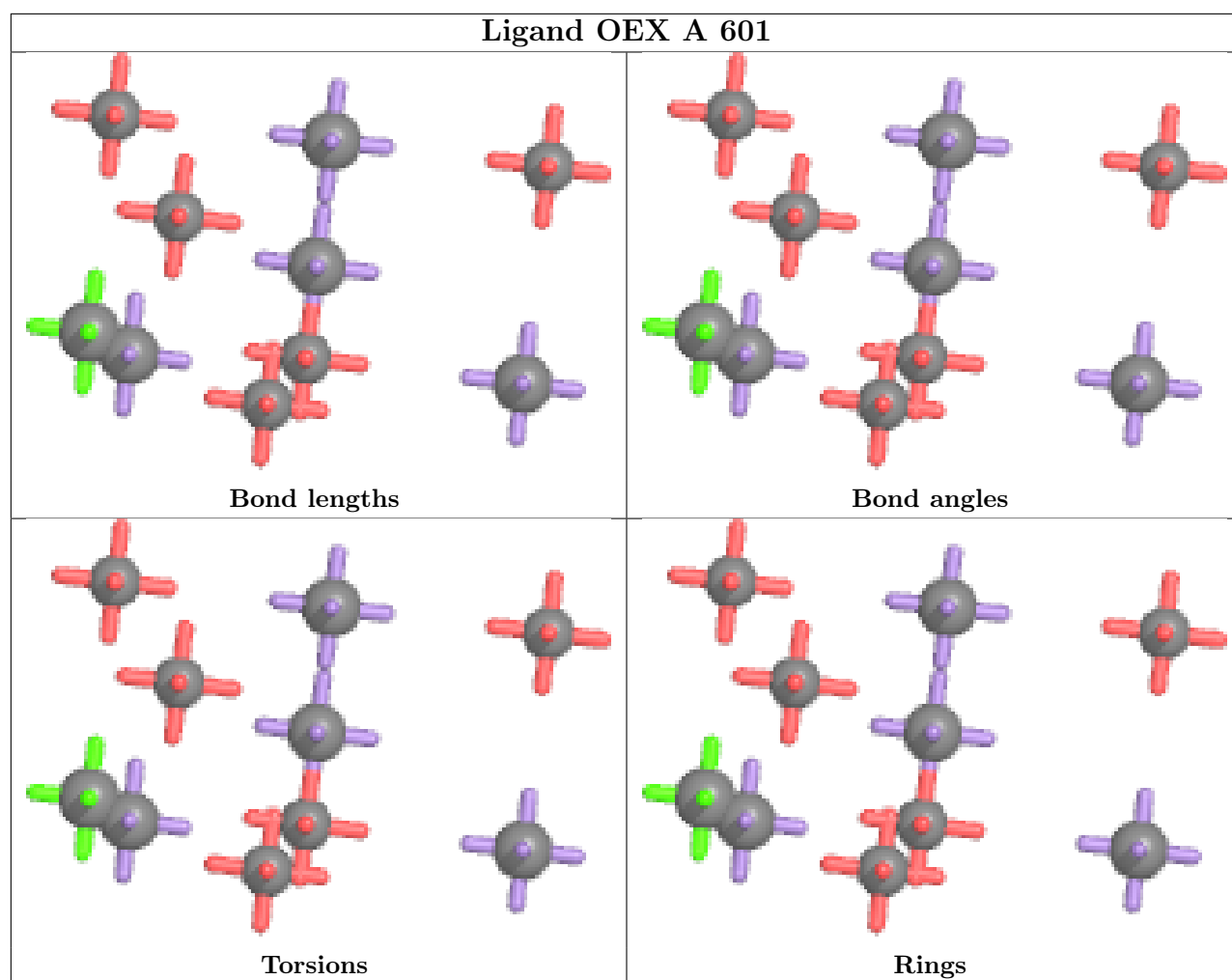


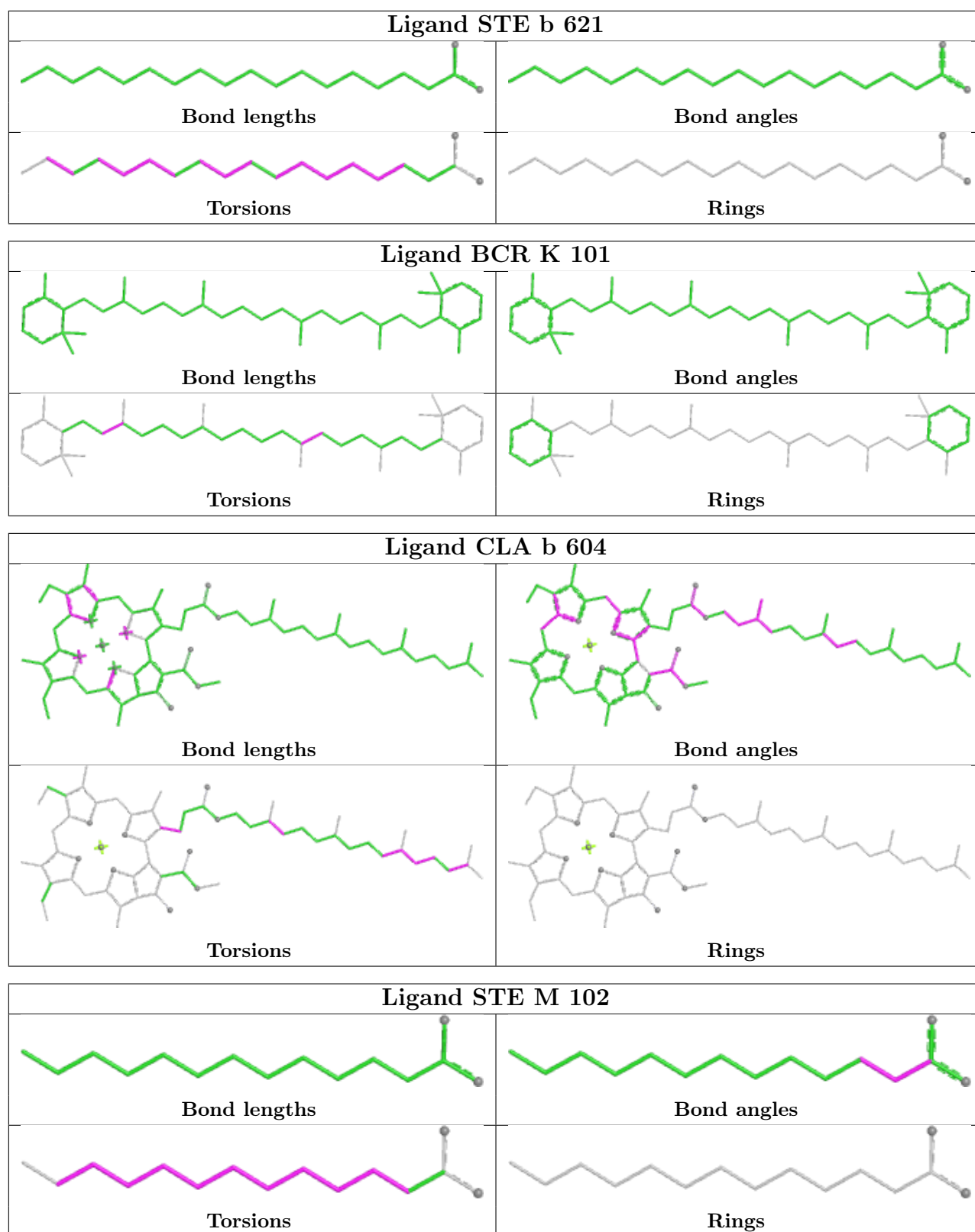
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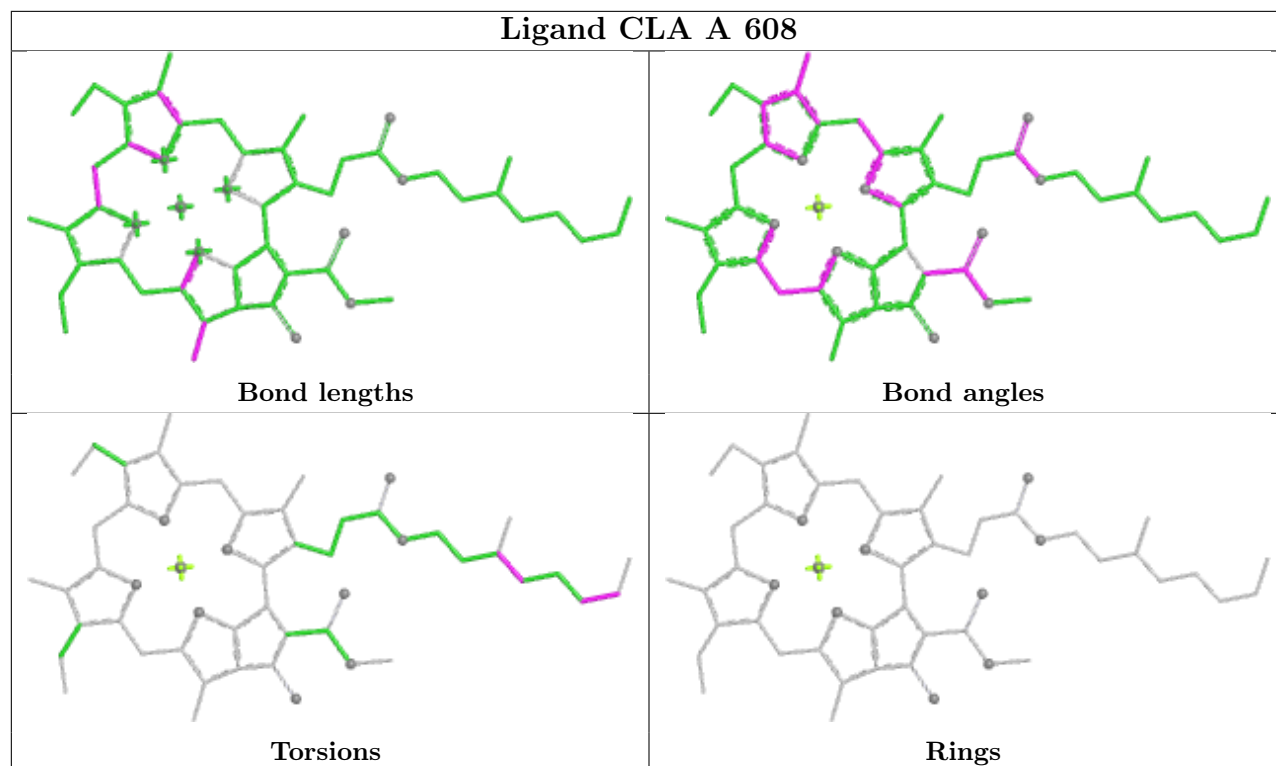




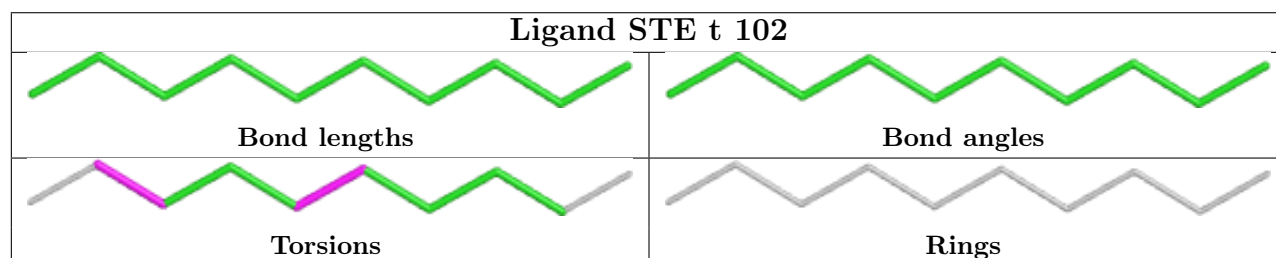




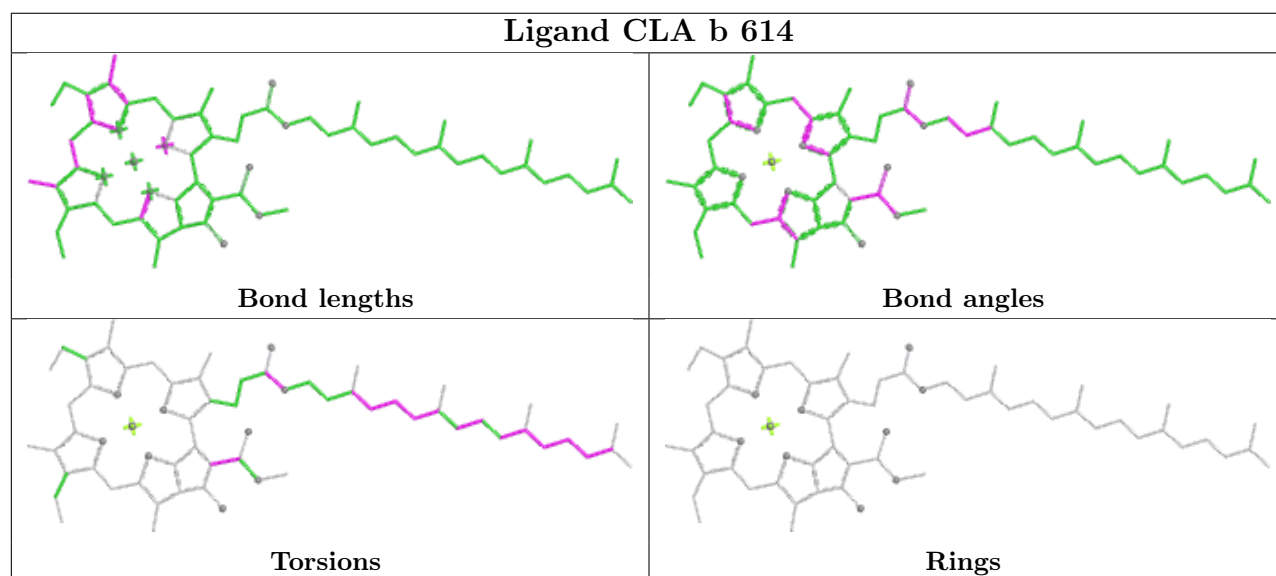
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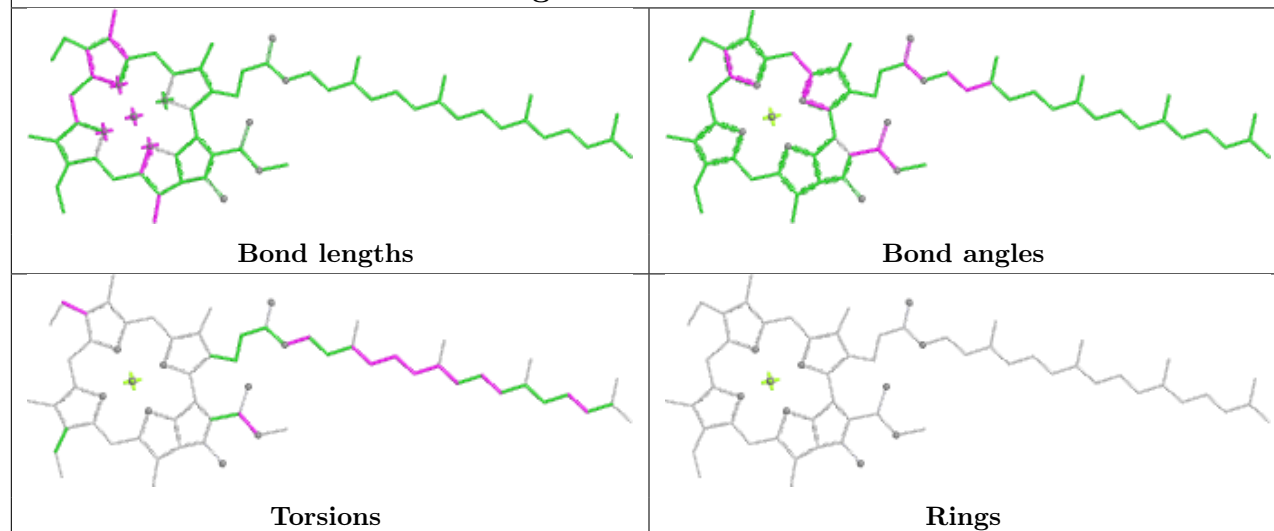
Ligand STE t 102



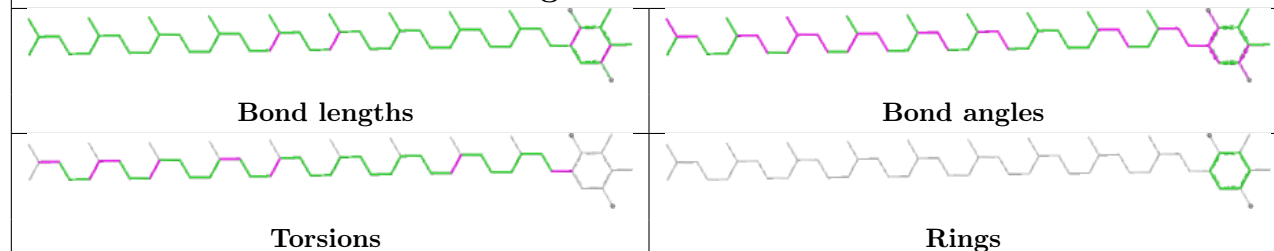
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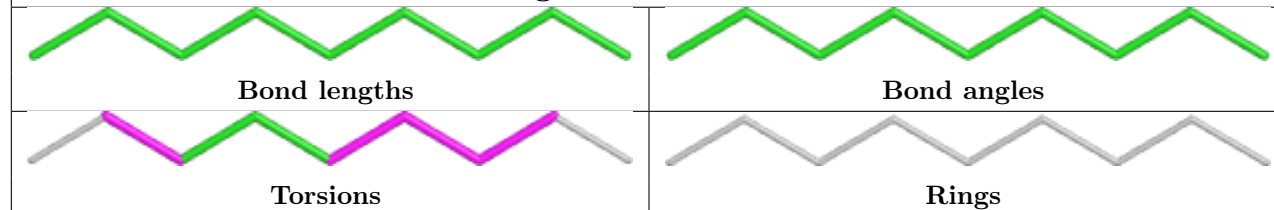
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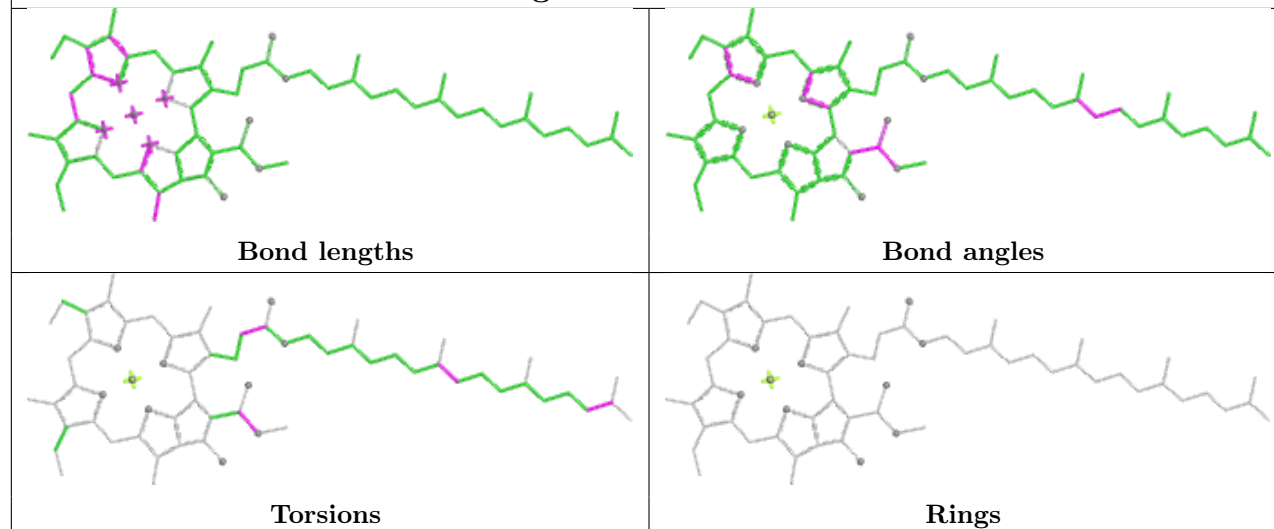
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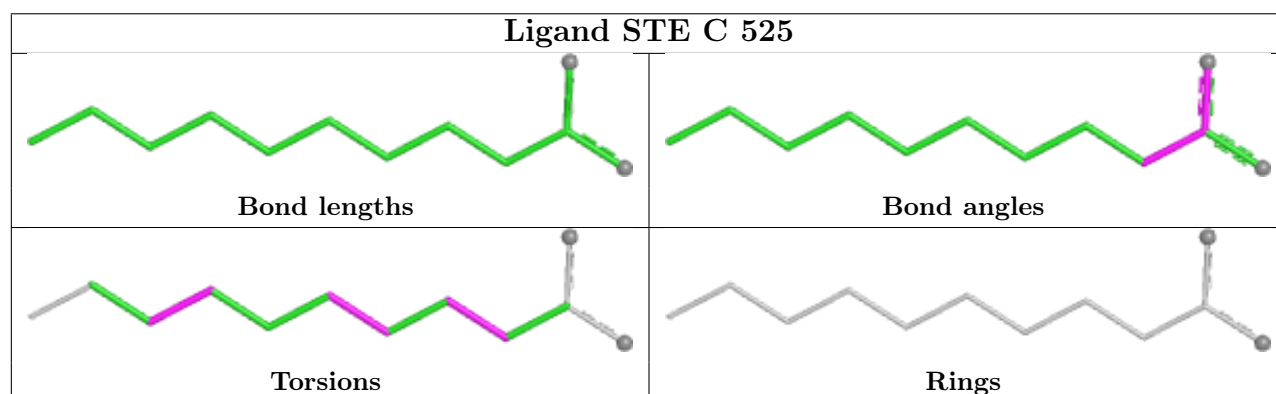
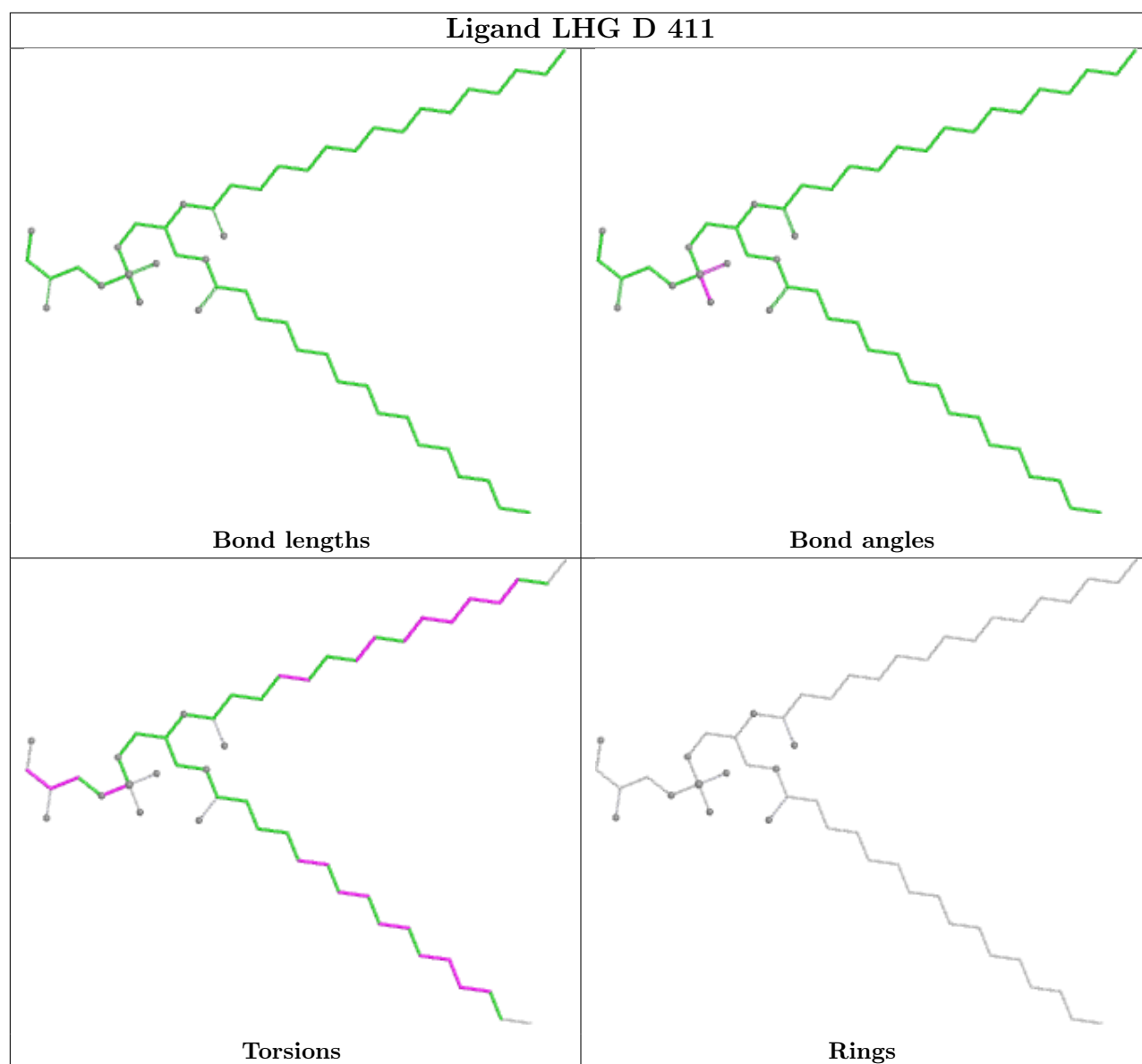


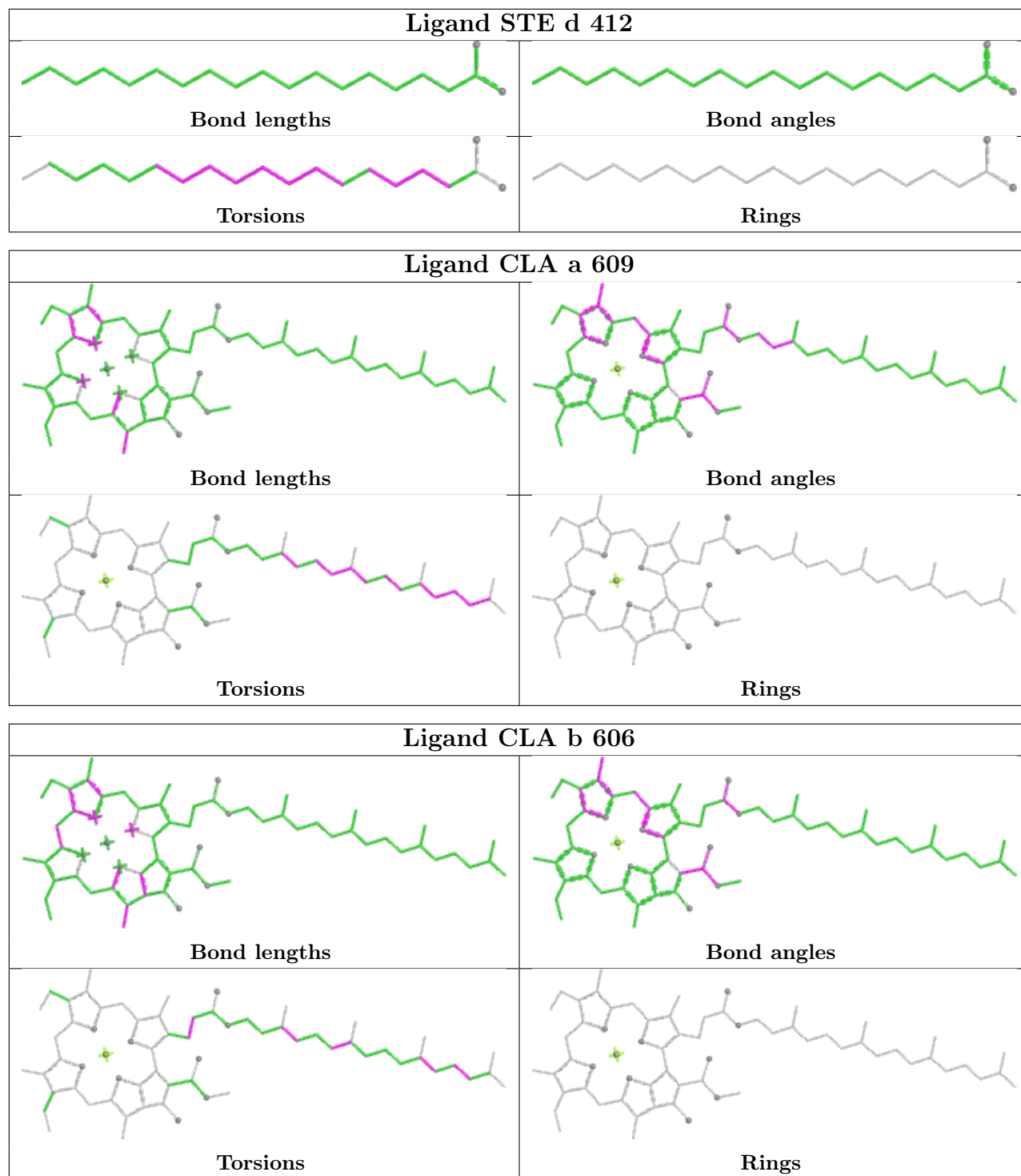
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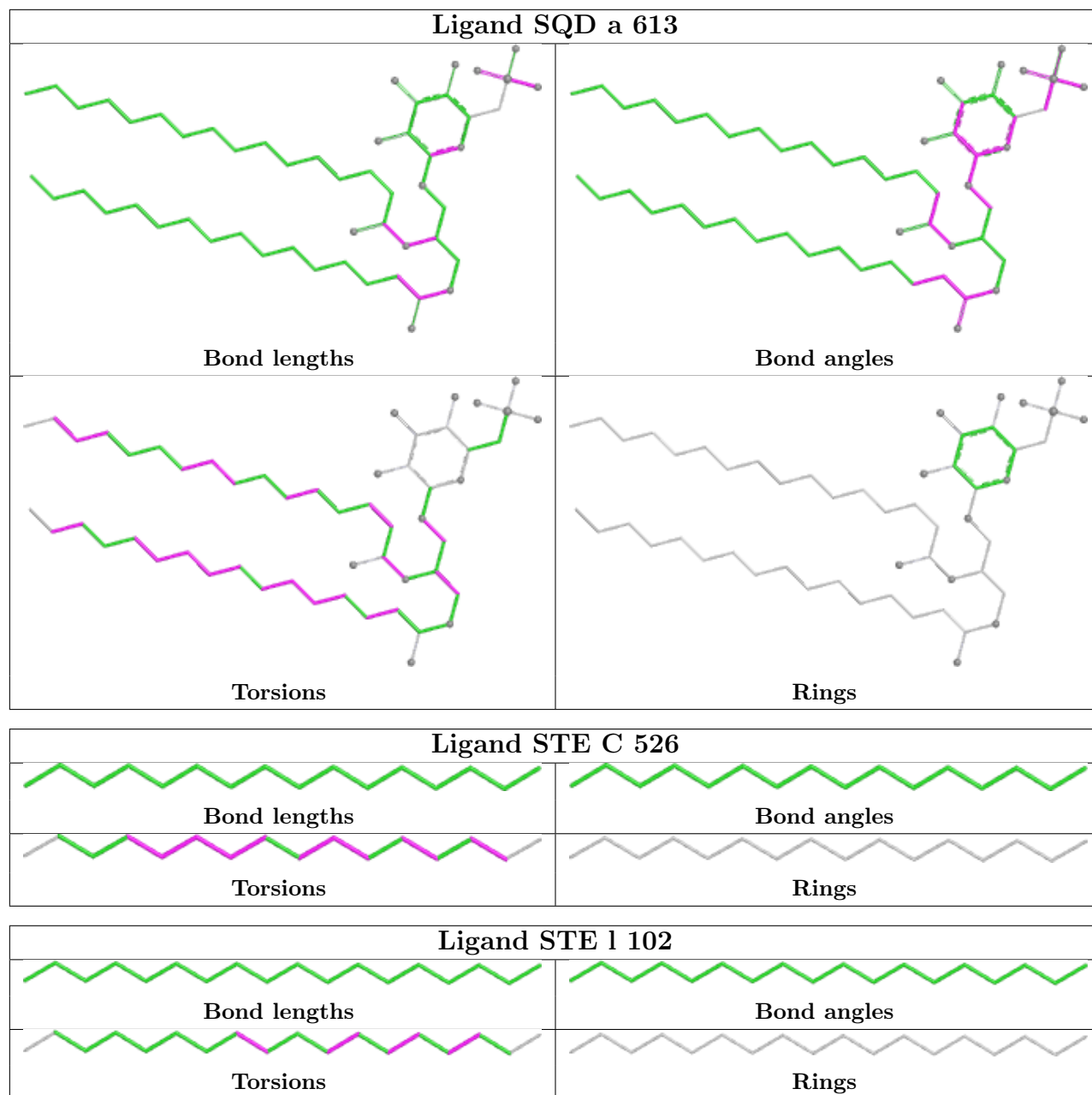


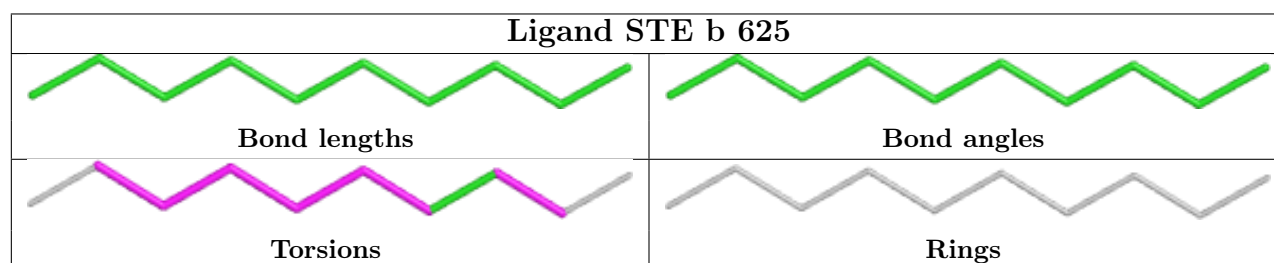
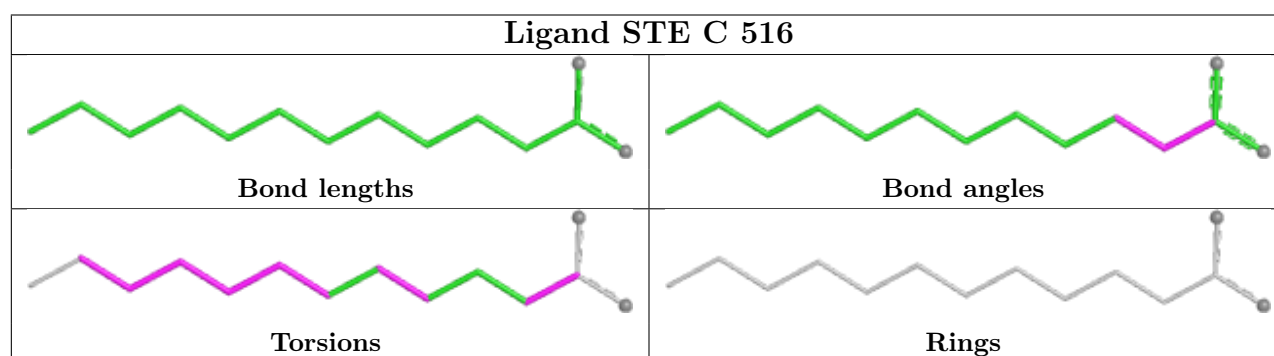
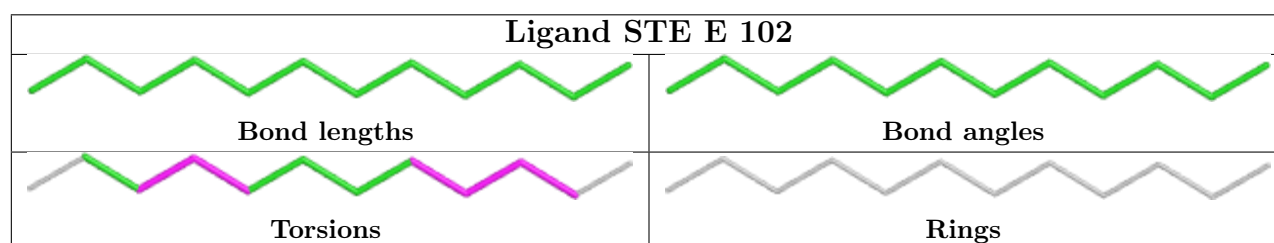
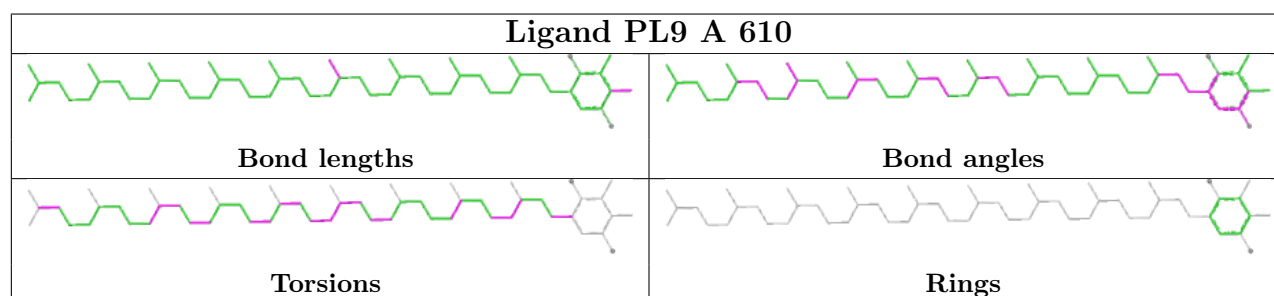
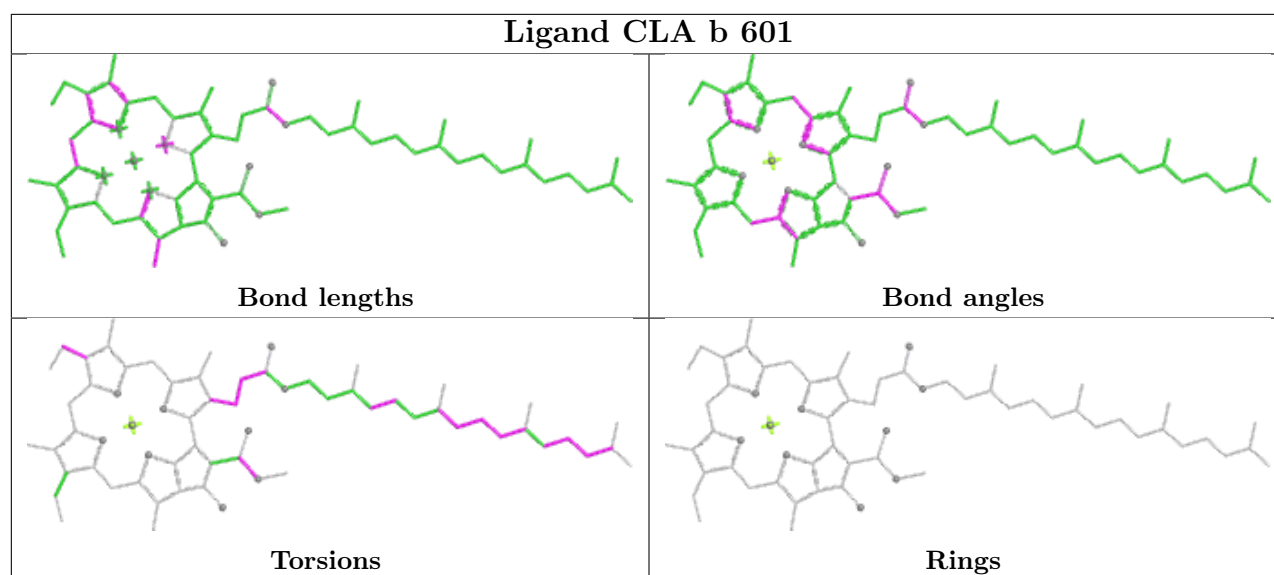
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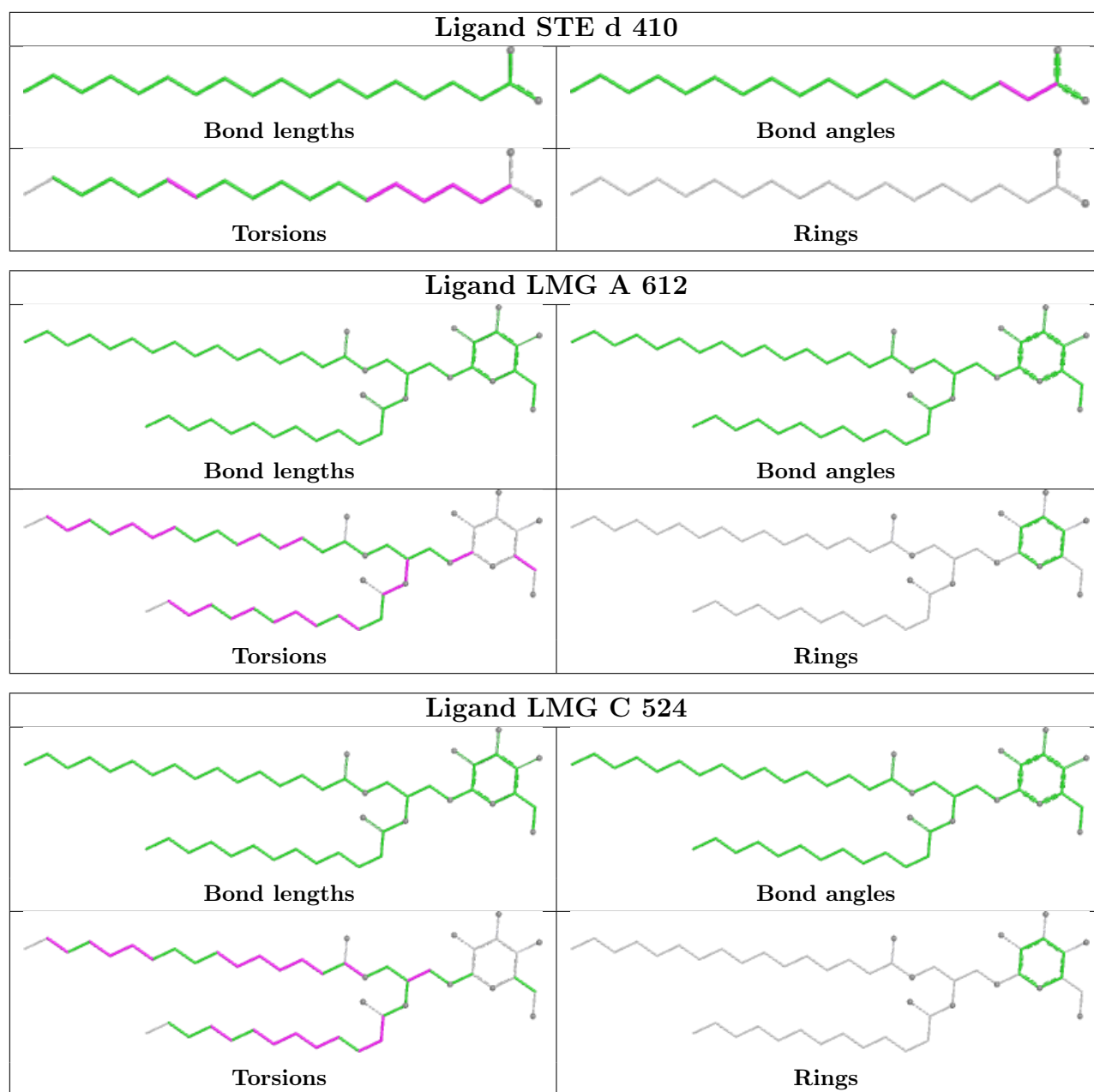


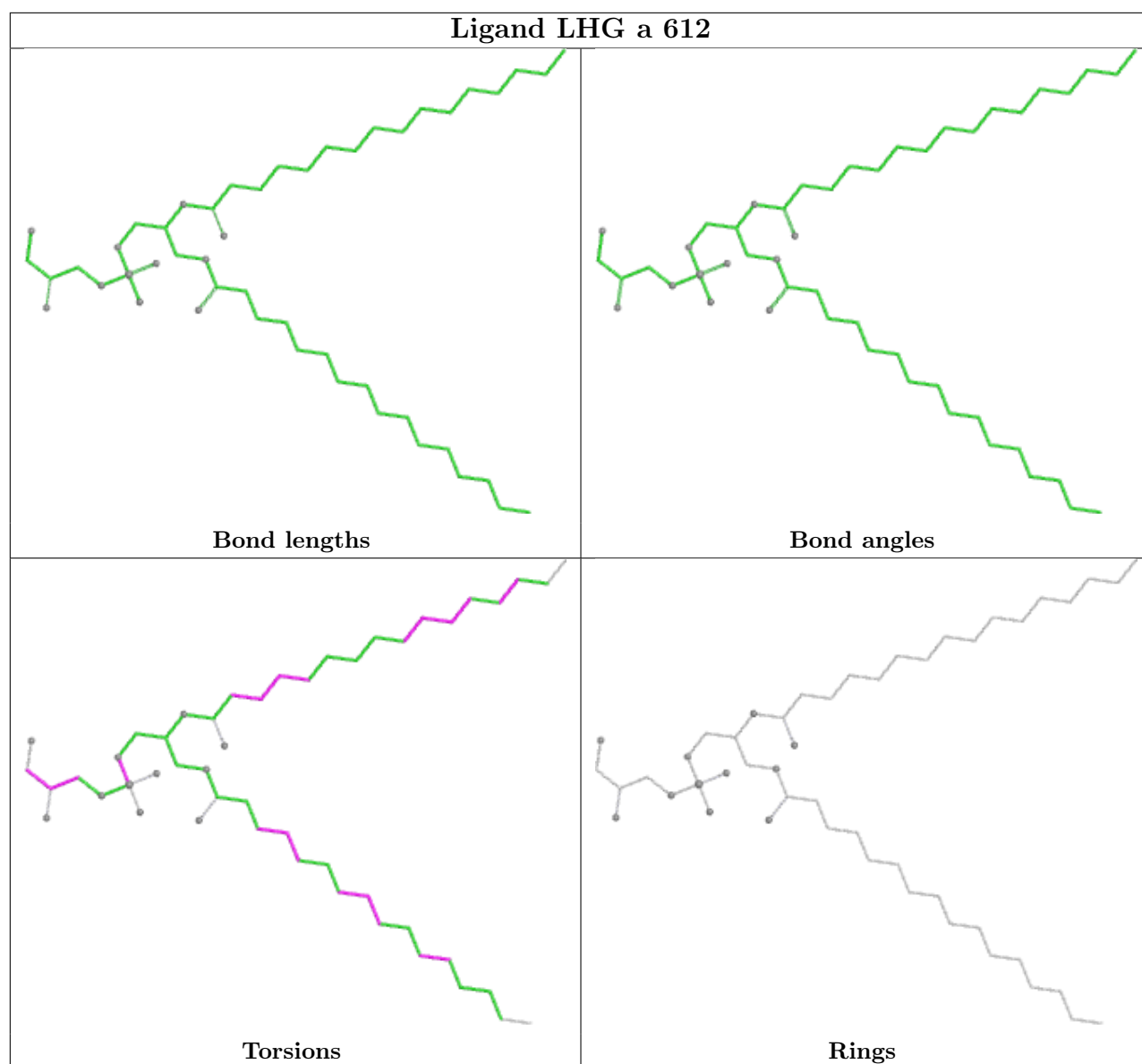


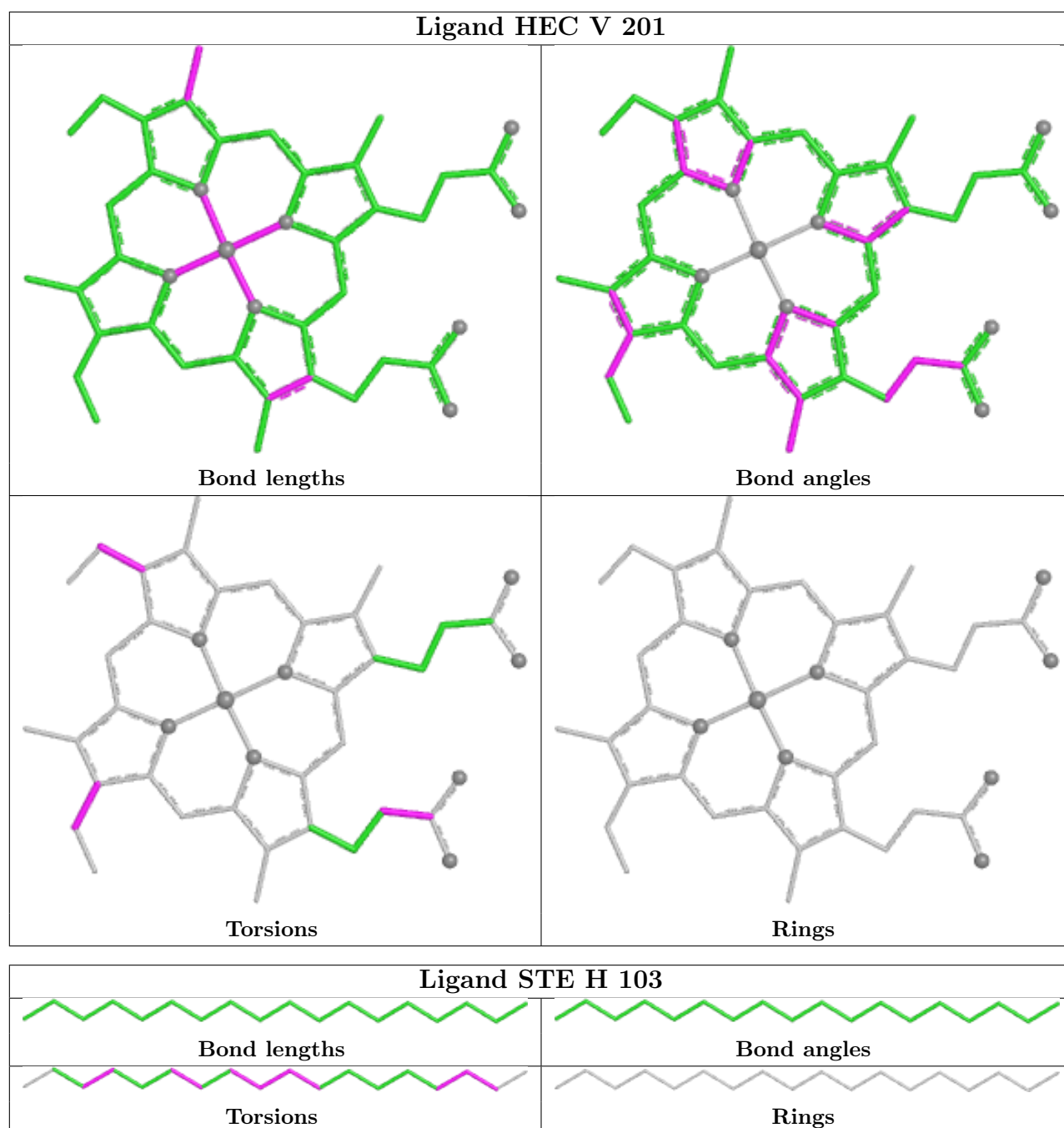




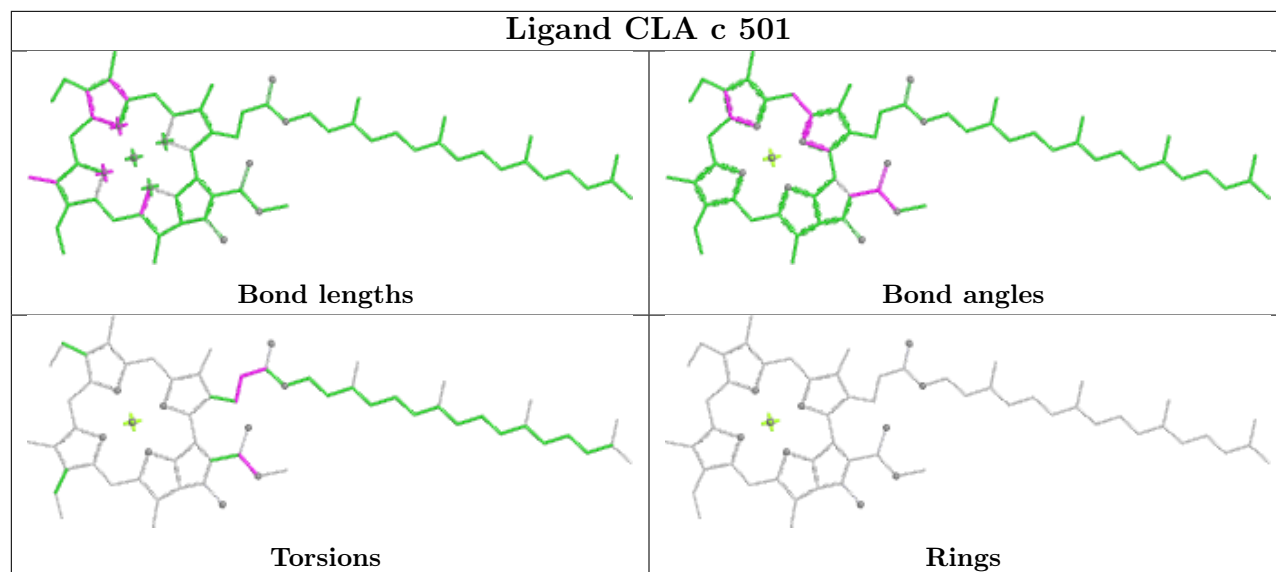




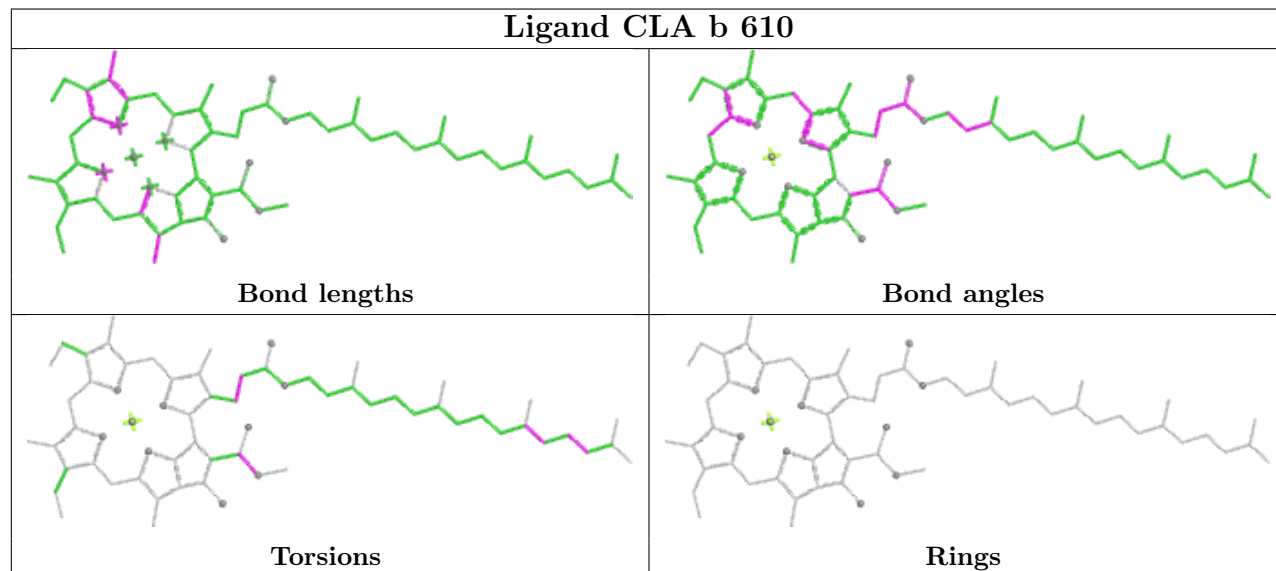




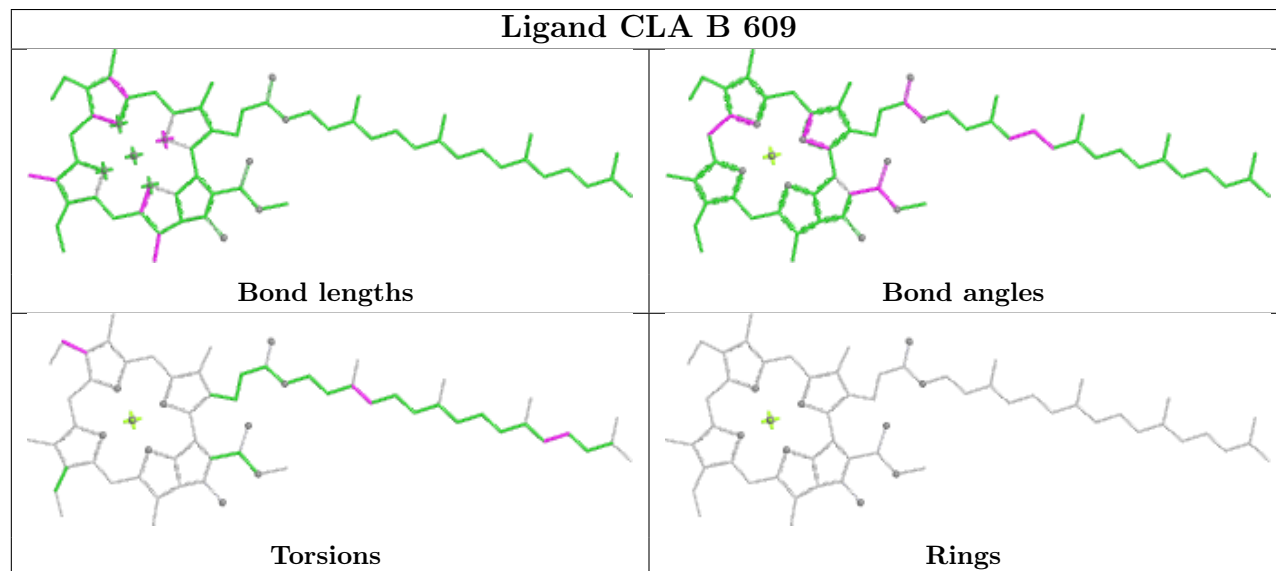
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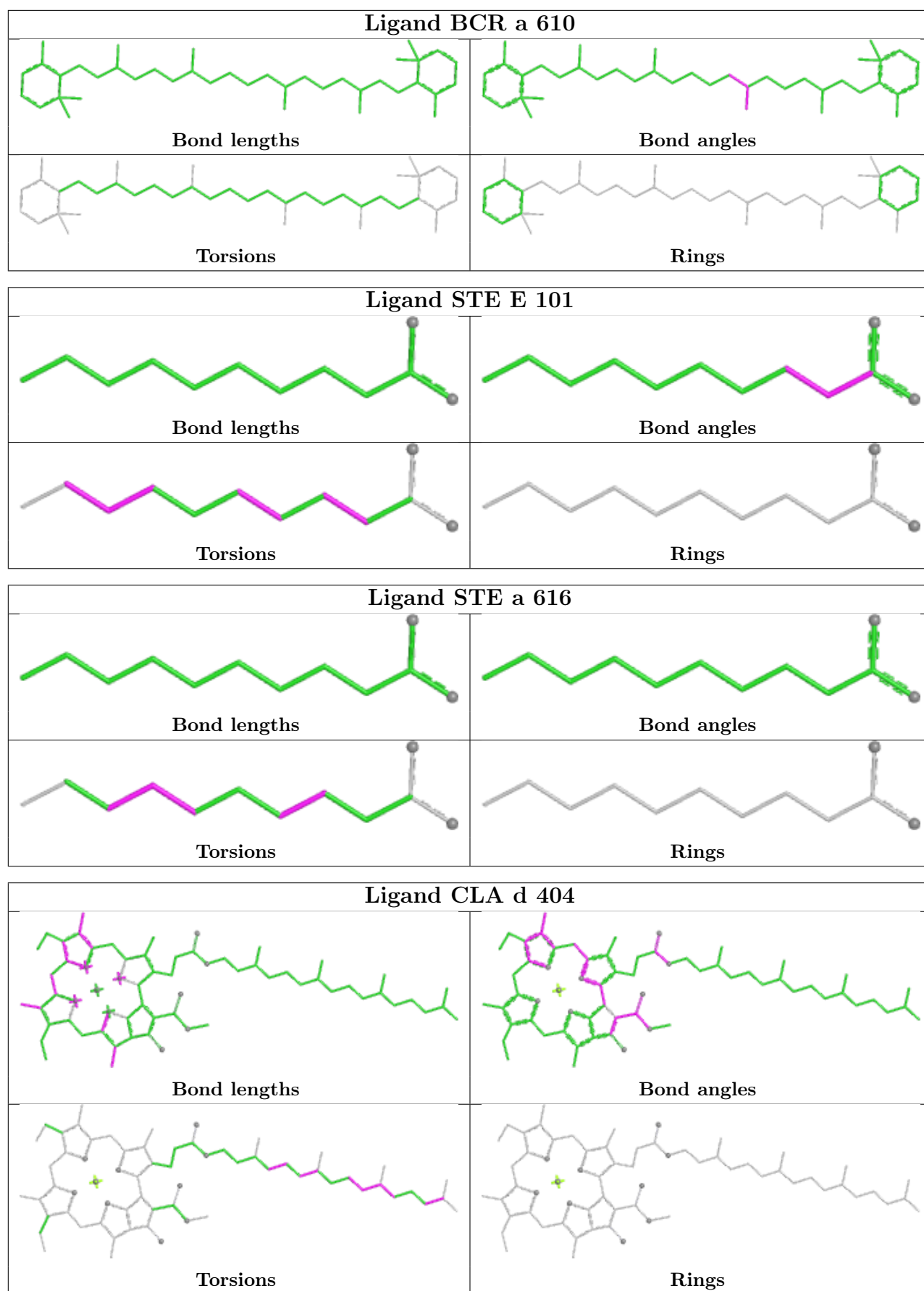


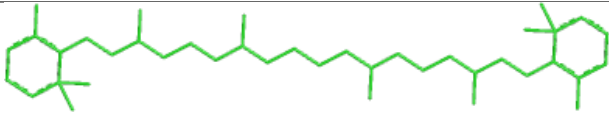
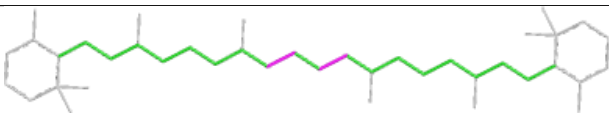
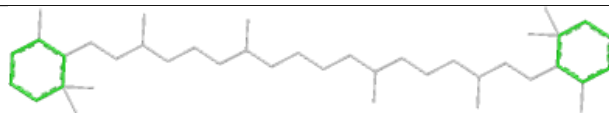
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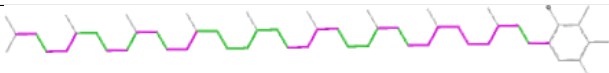


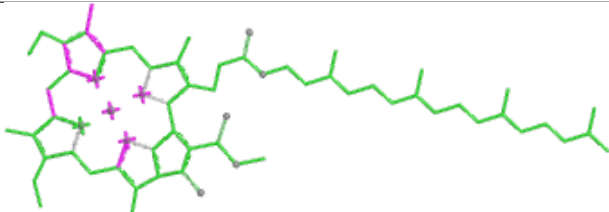
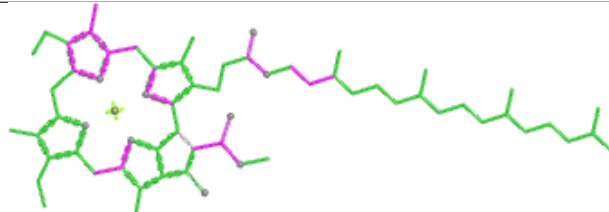
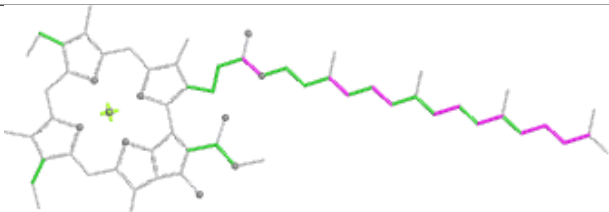
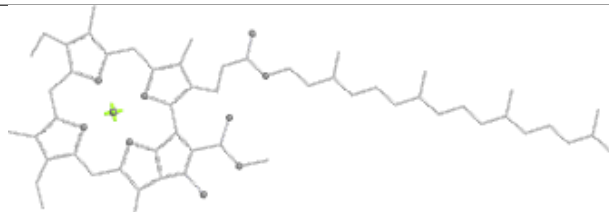
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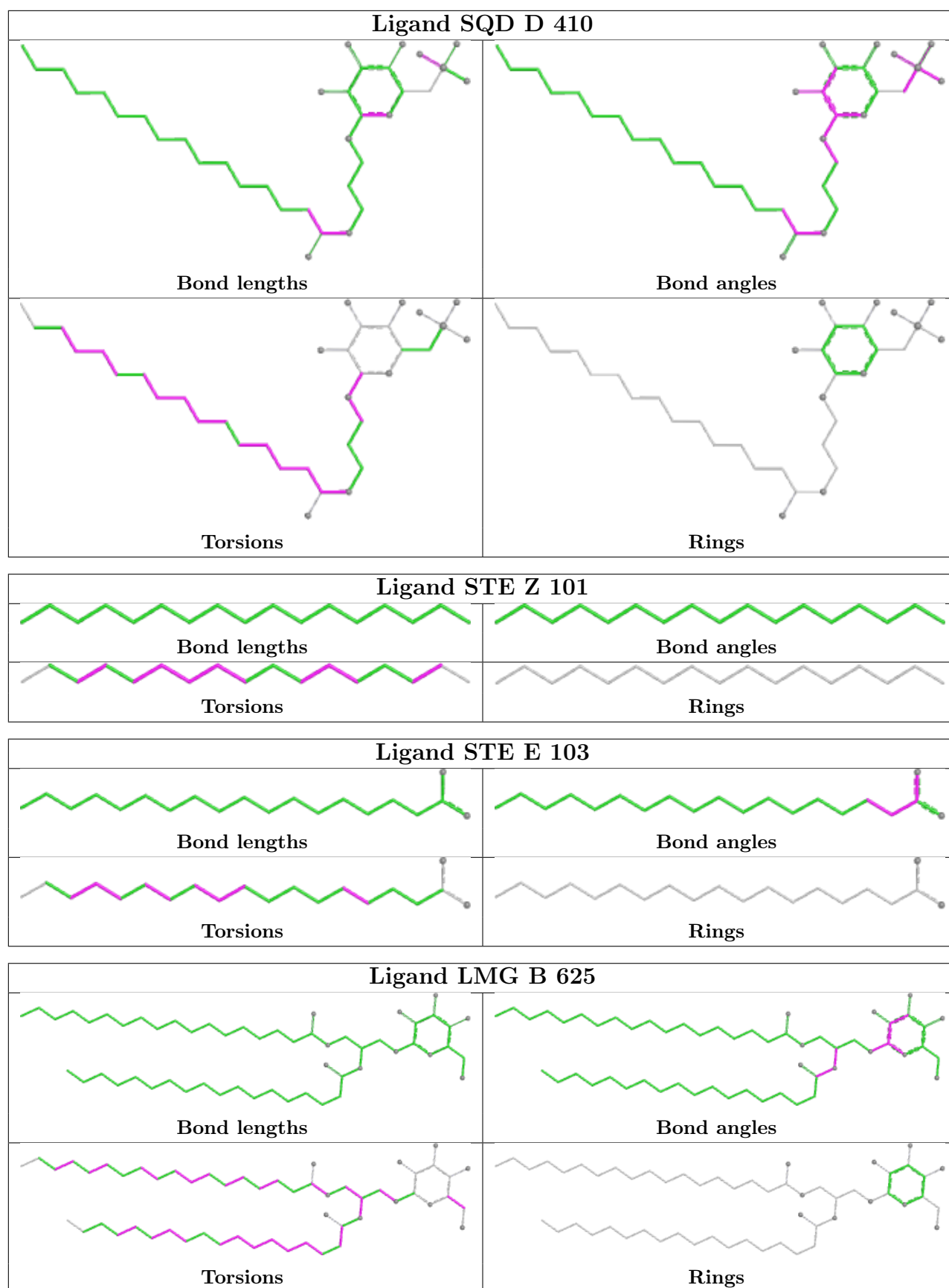


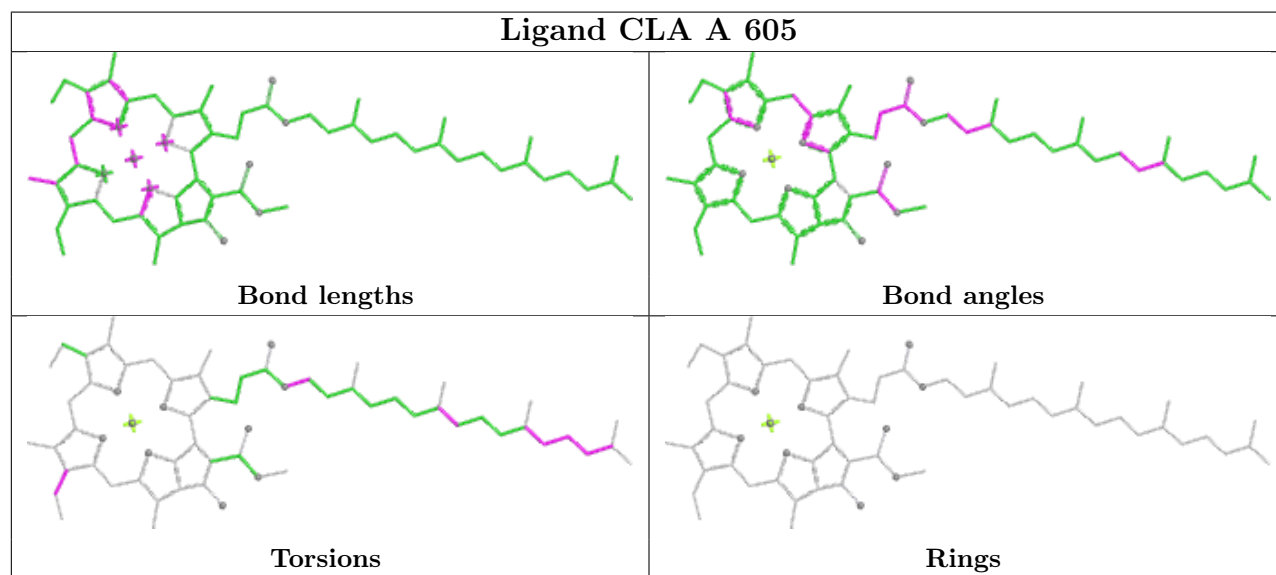
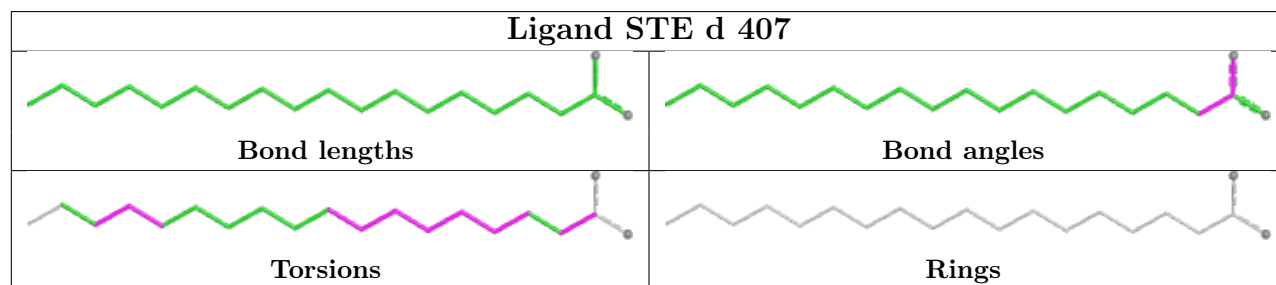
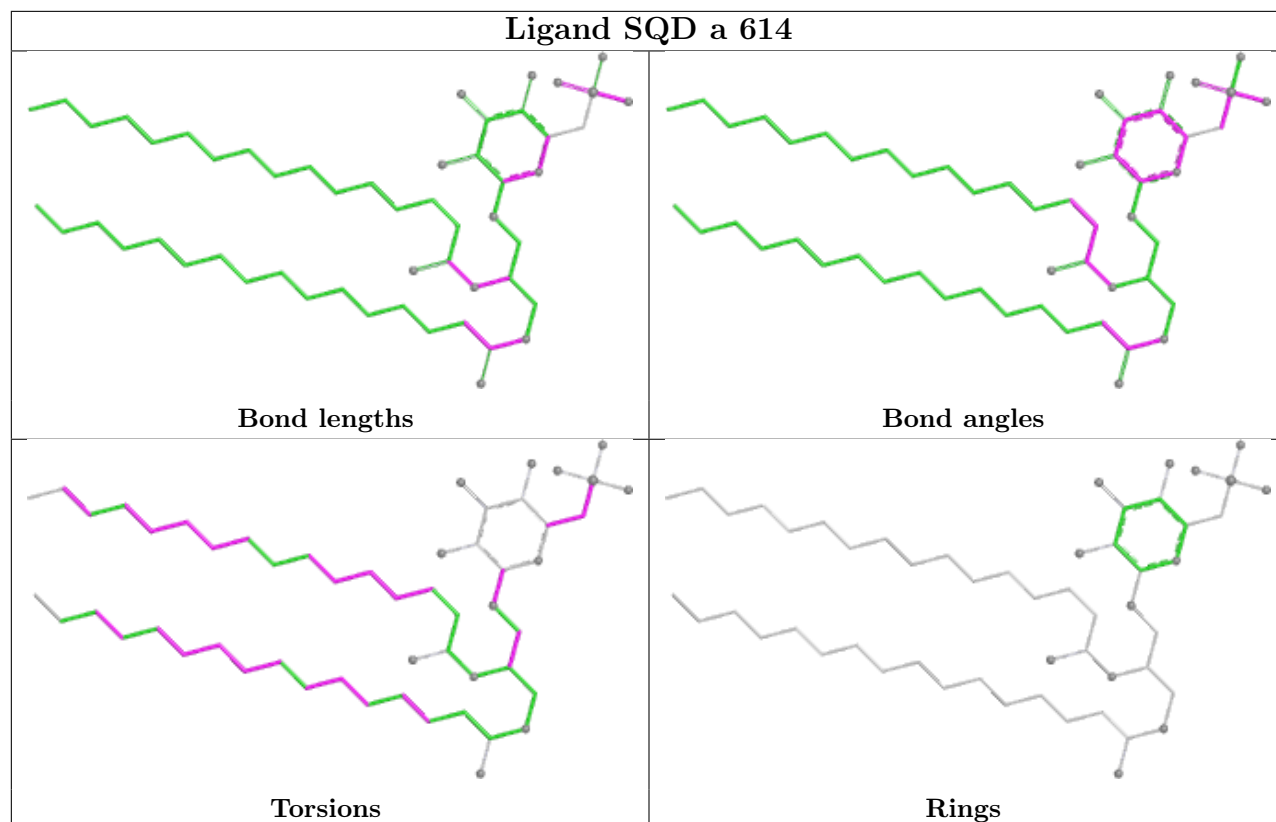
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

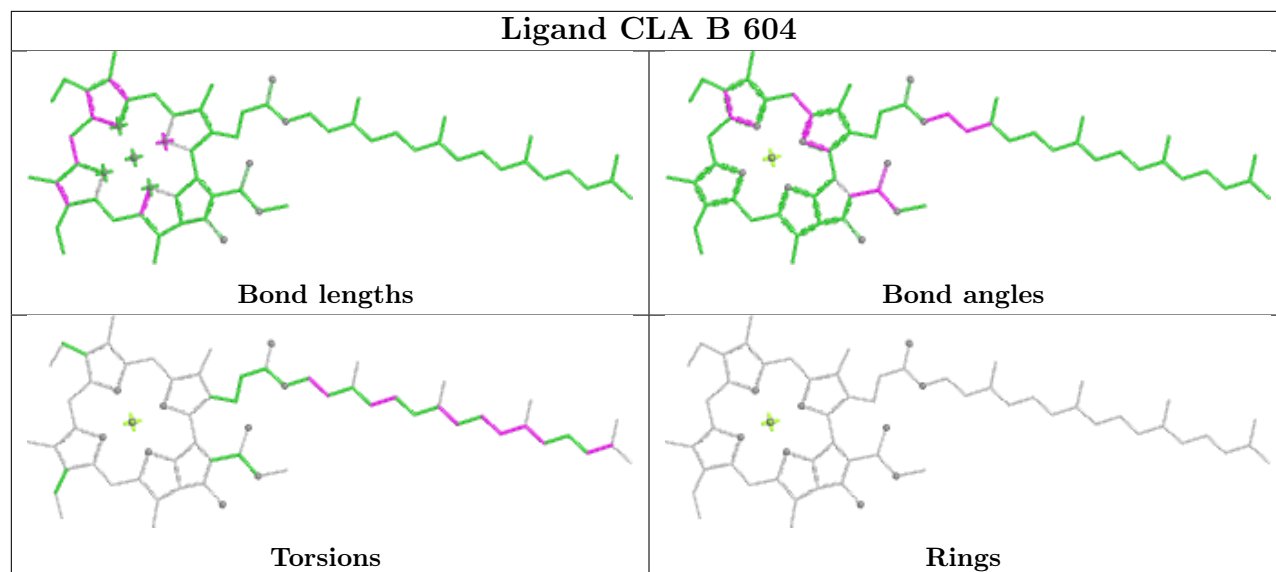
Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE h 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

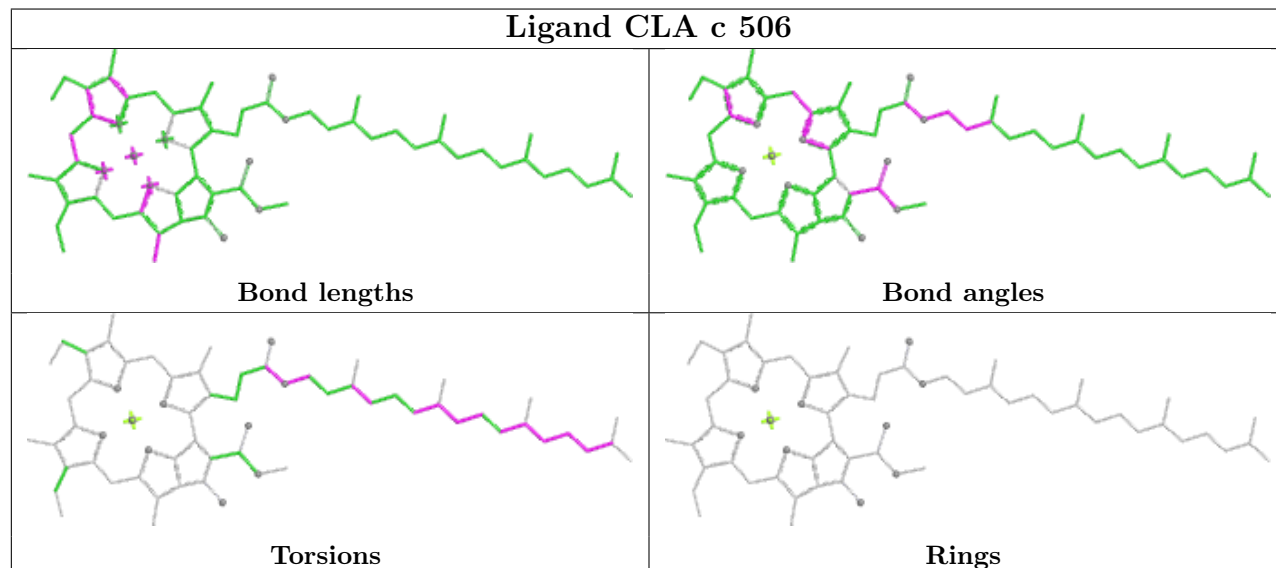




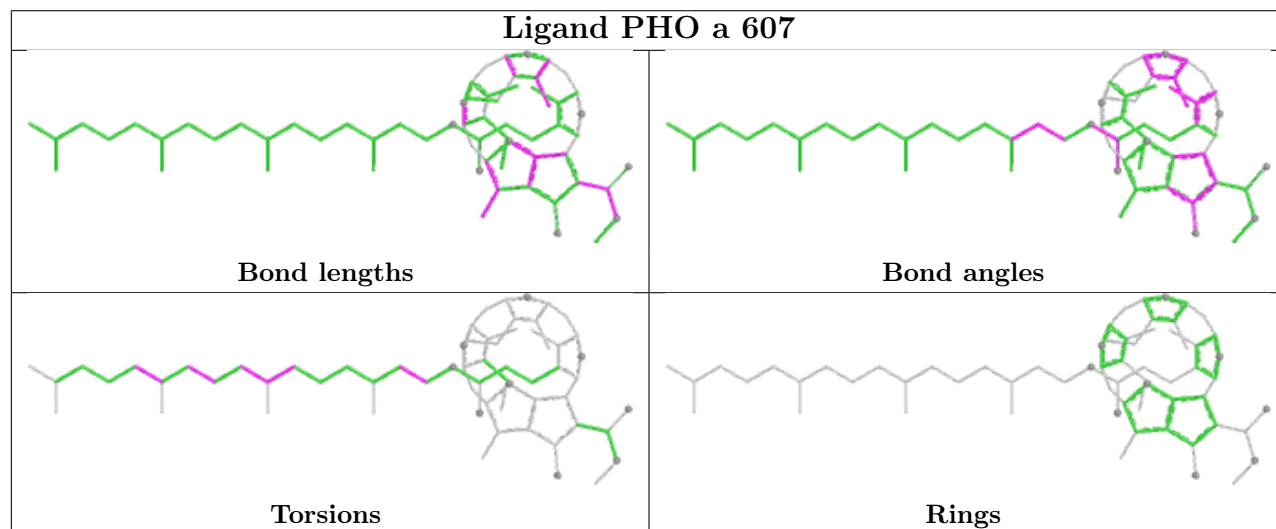
Ligand CLA B 604



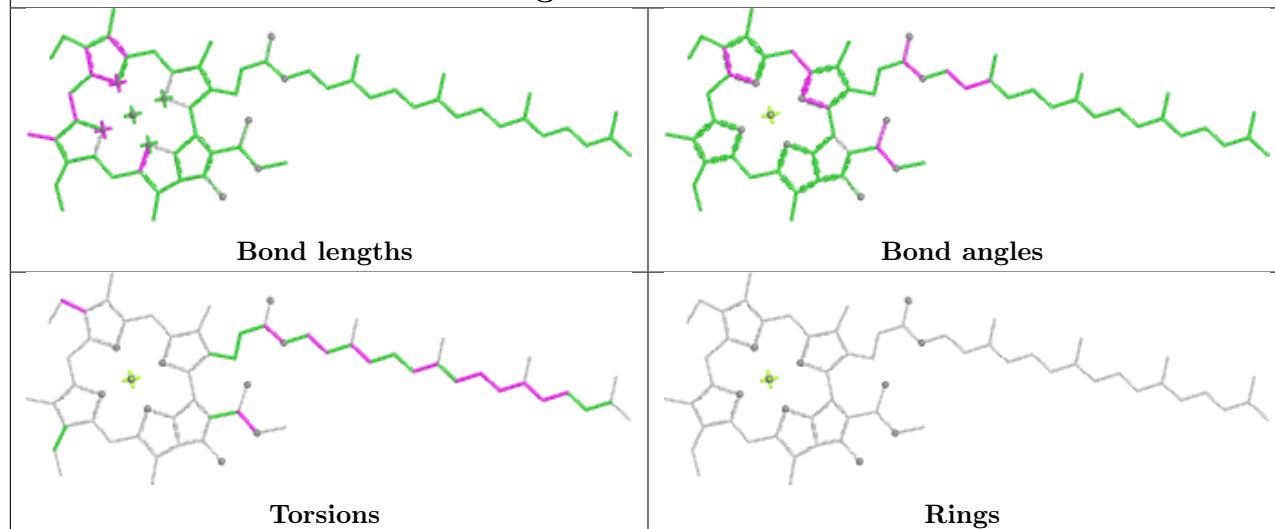
Ligand CLA c 506



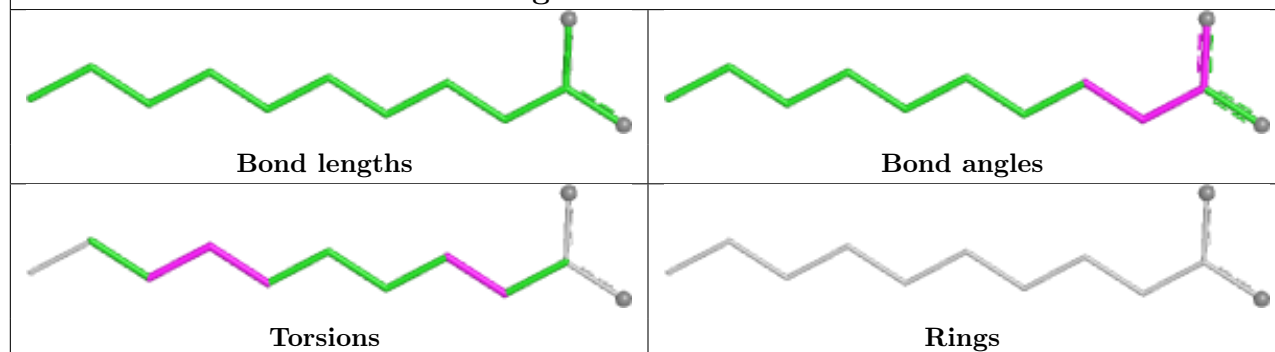
Ligand PHO a 607



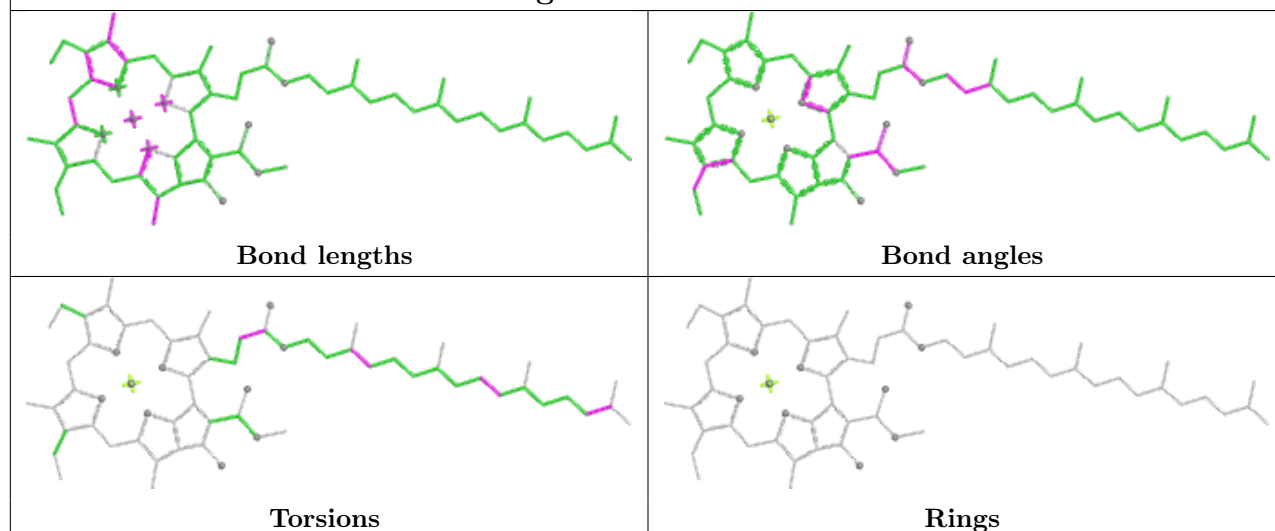
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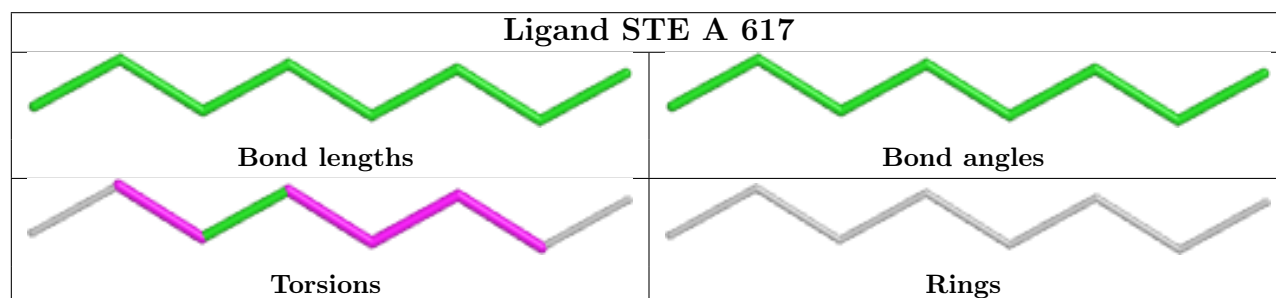
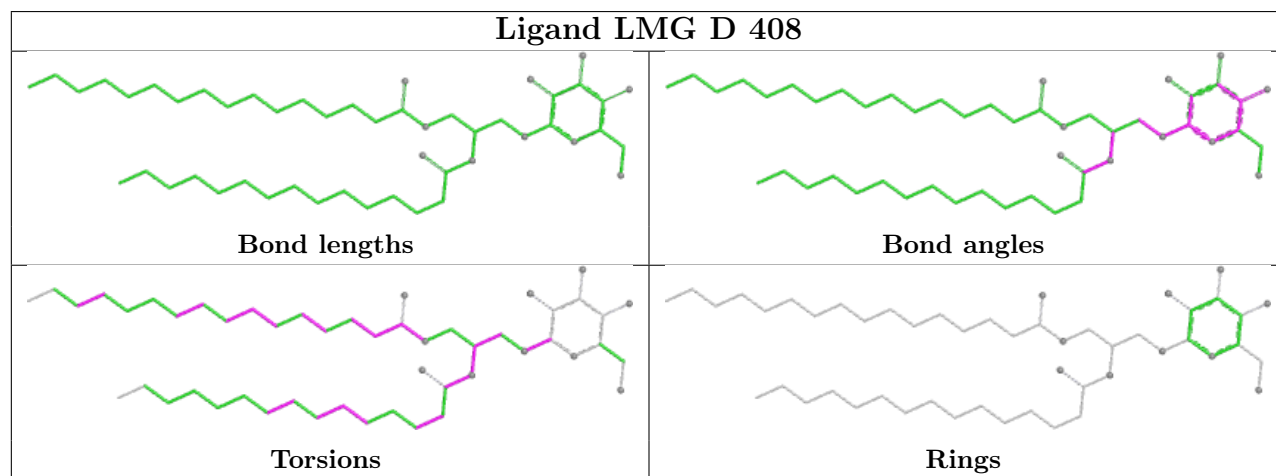
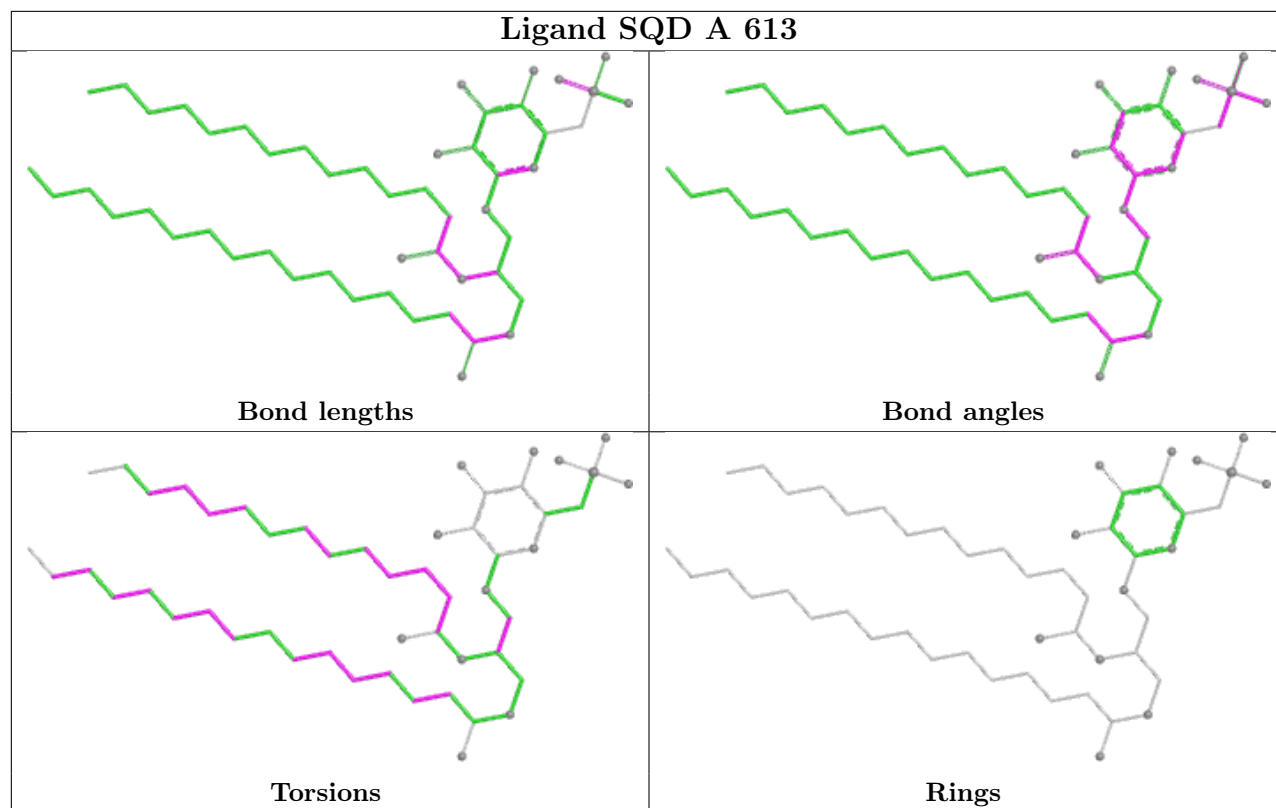


Ligand STE m 102

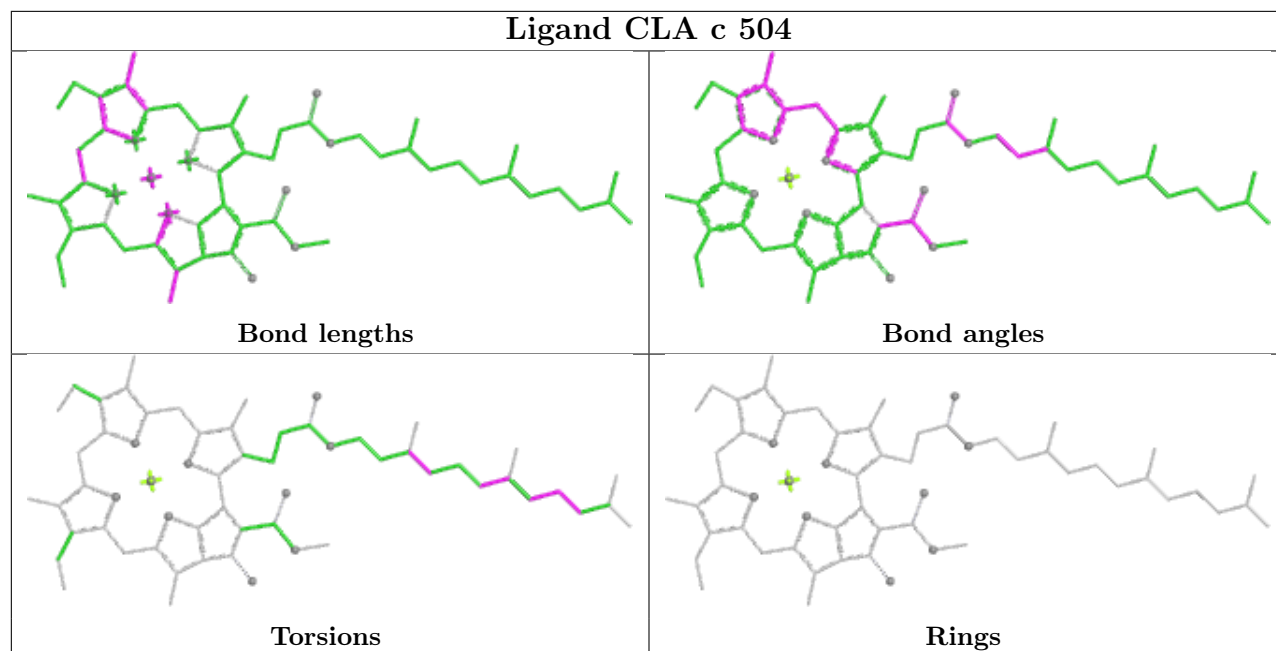


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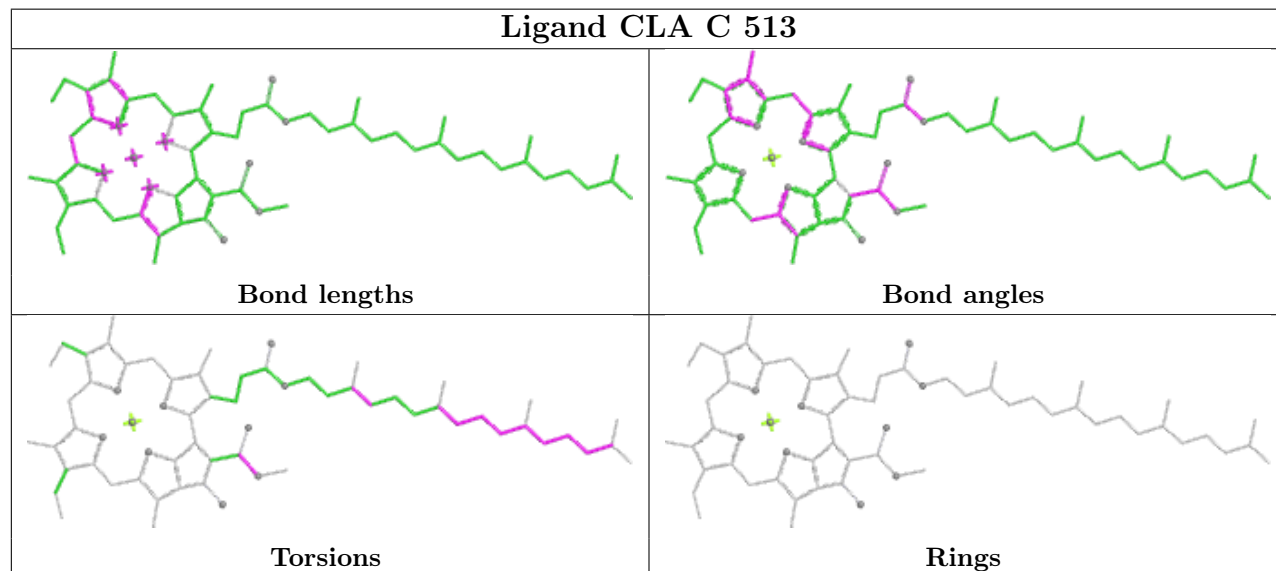




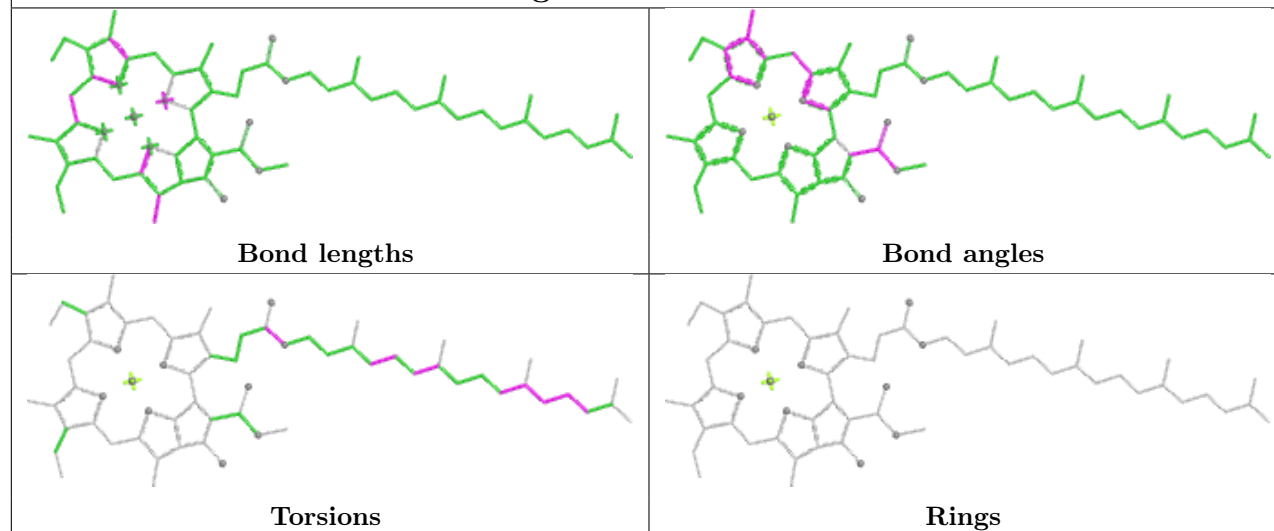
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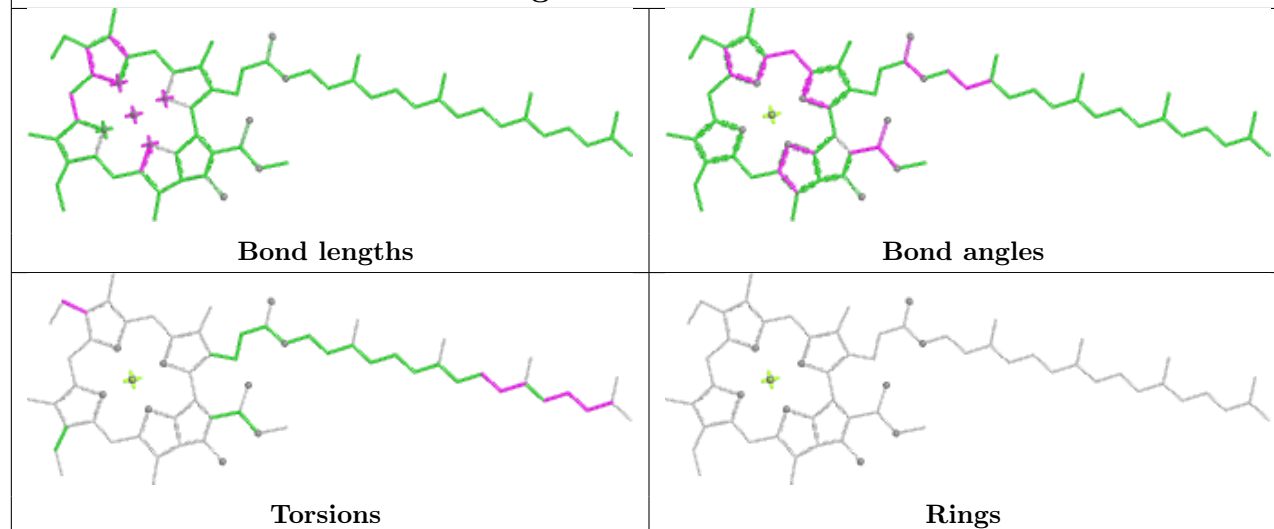
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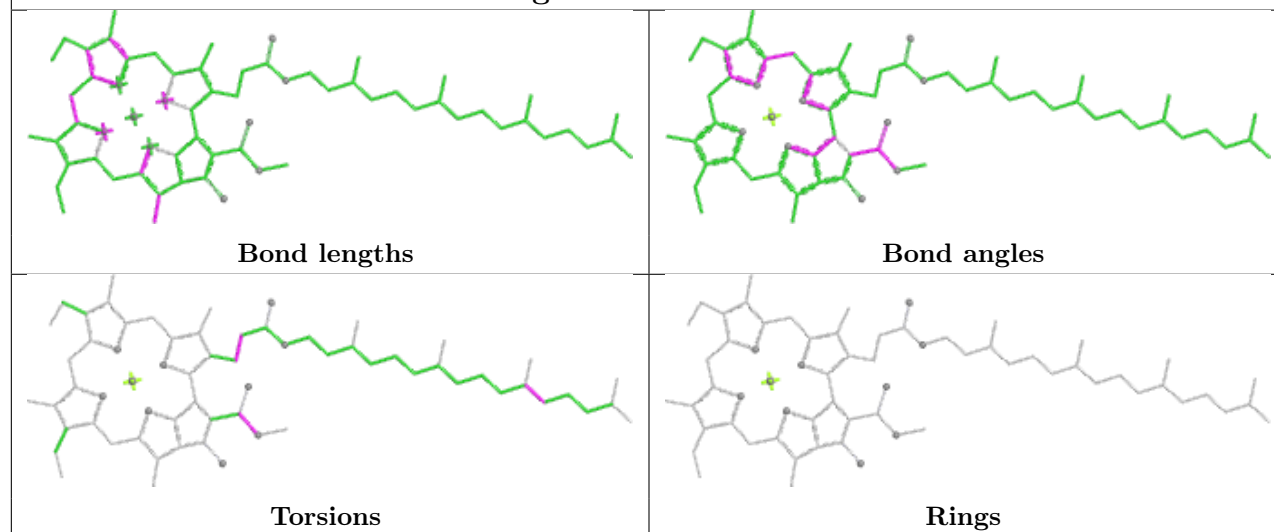
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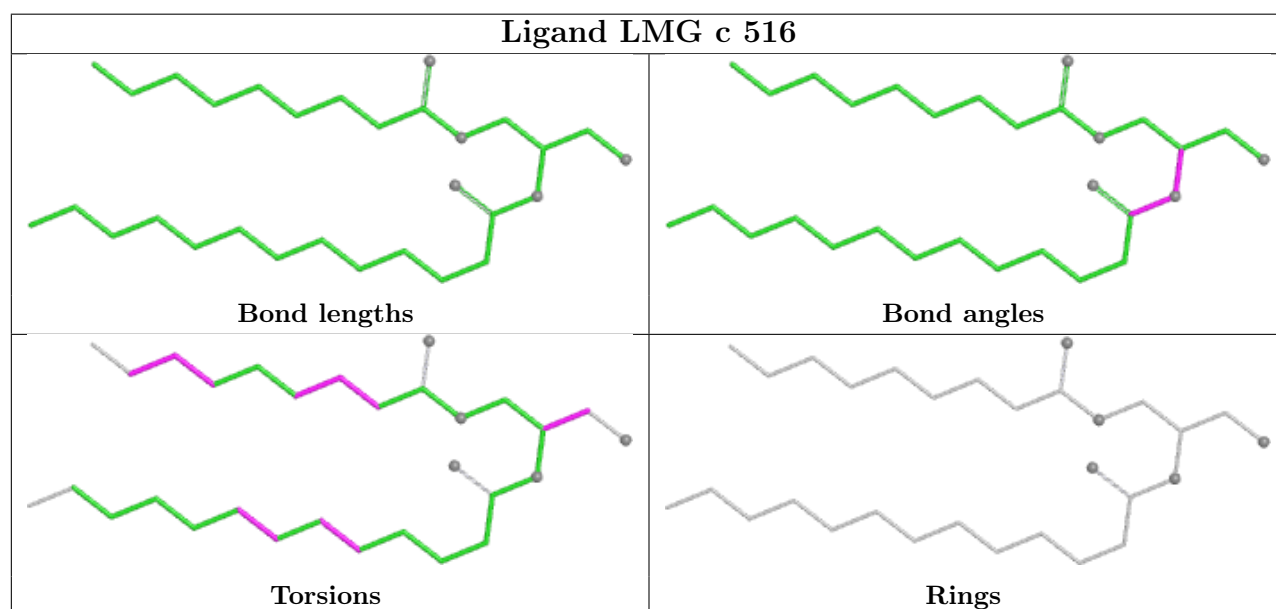
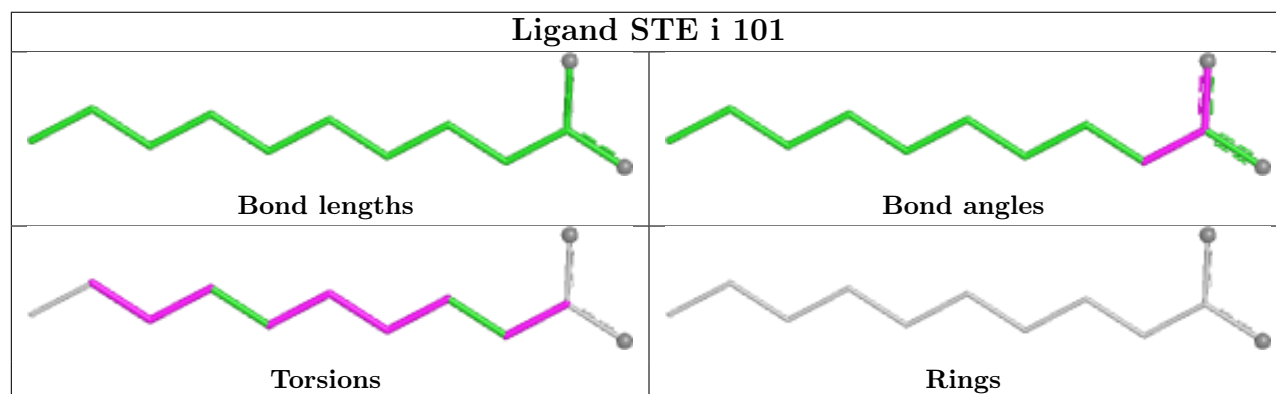
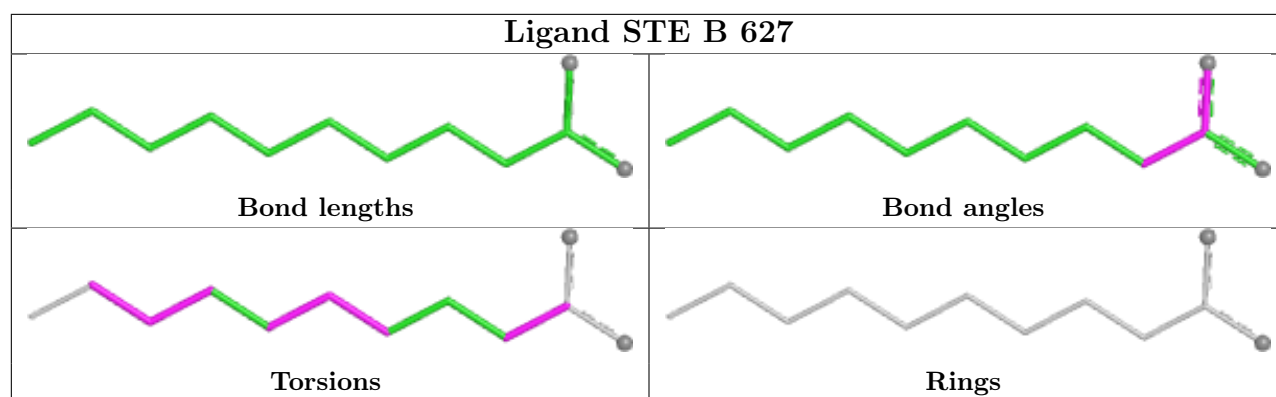


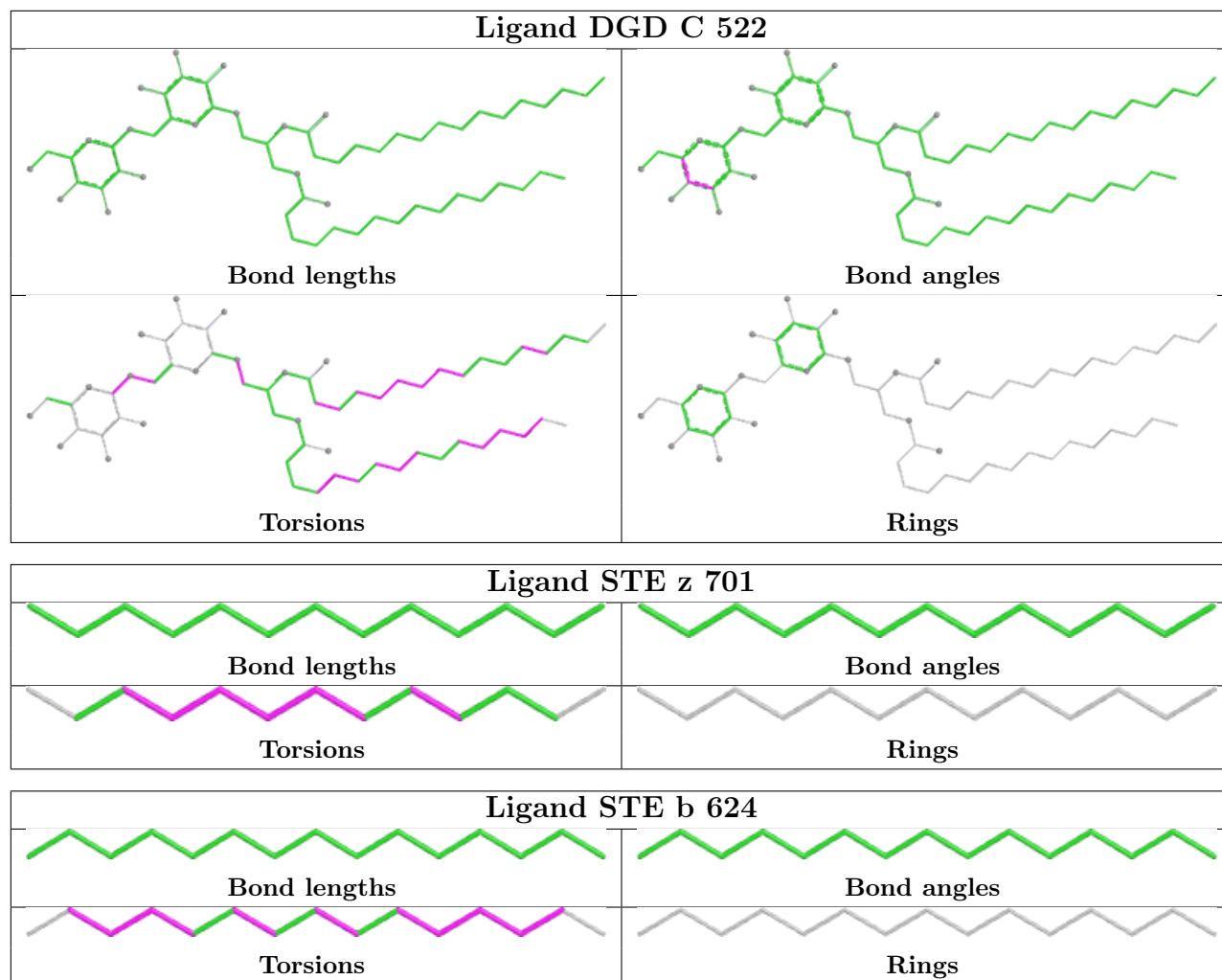
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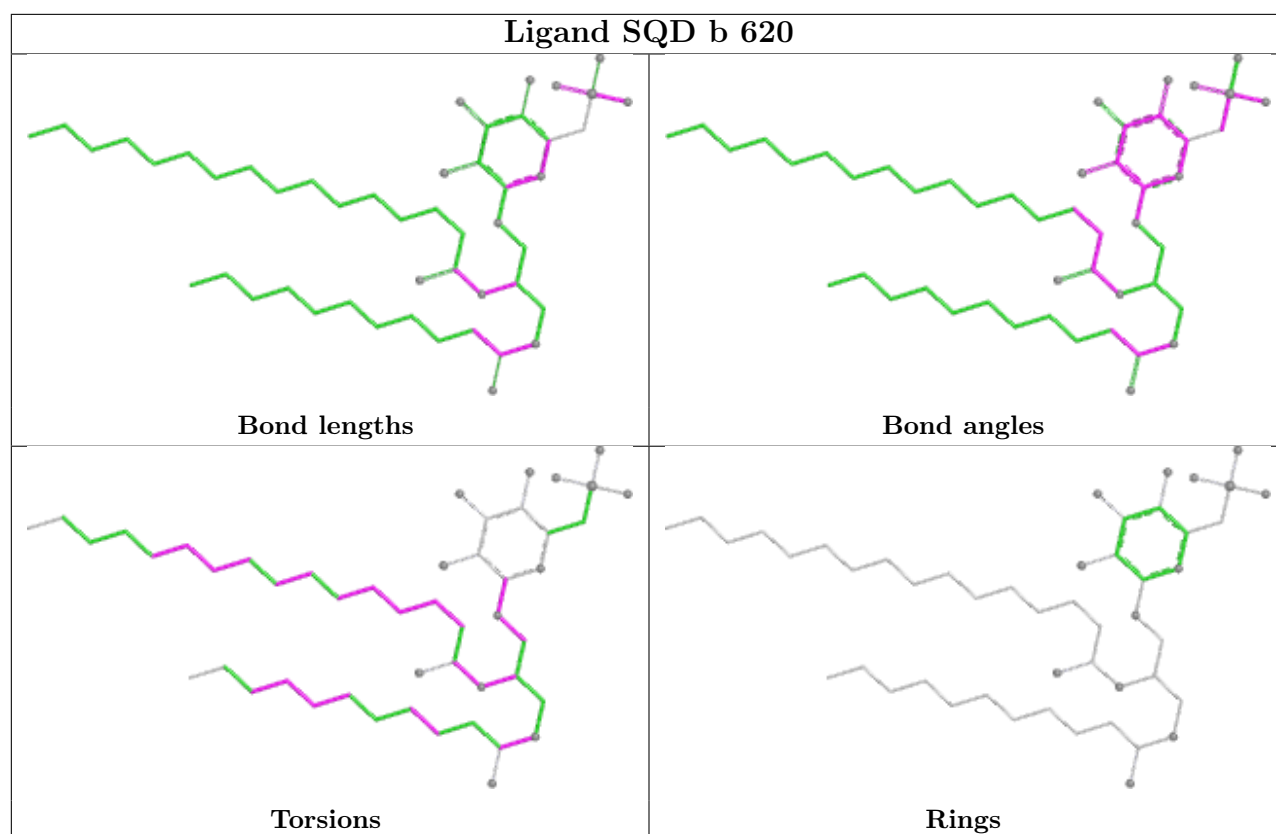


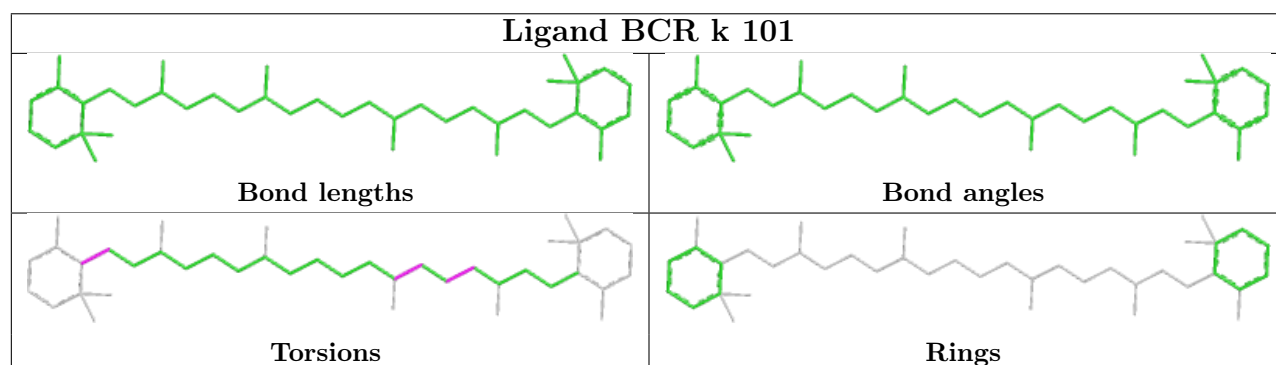
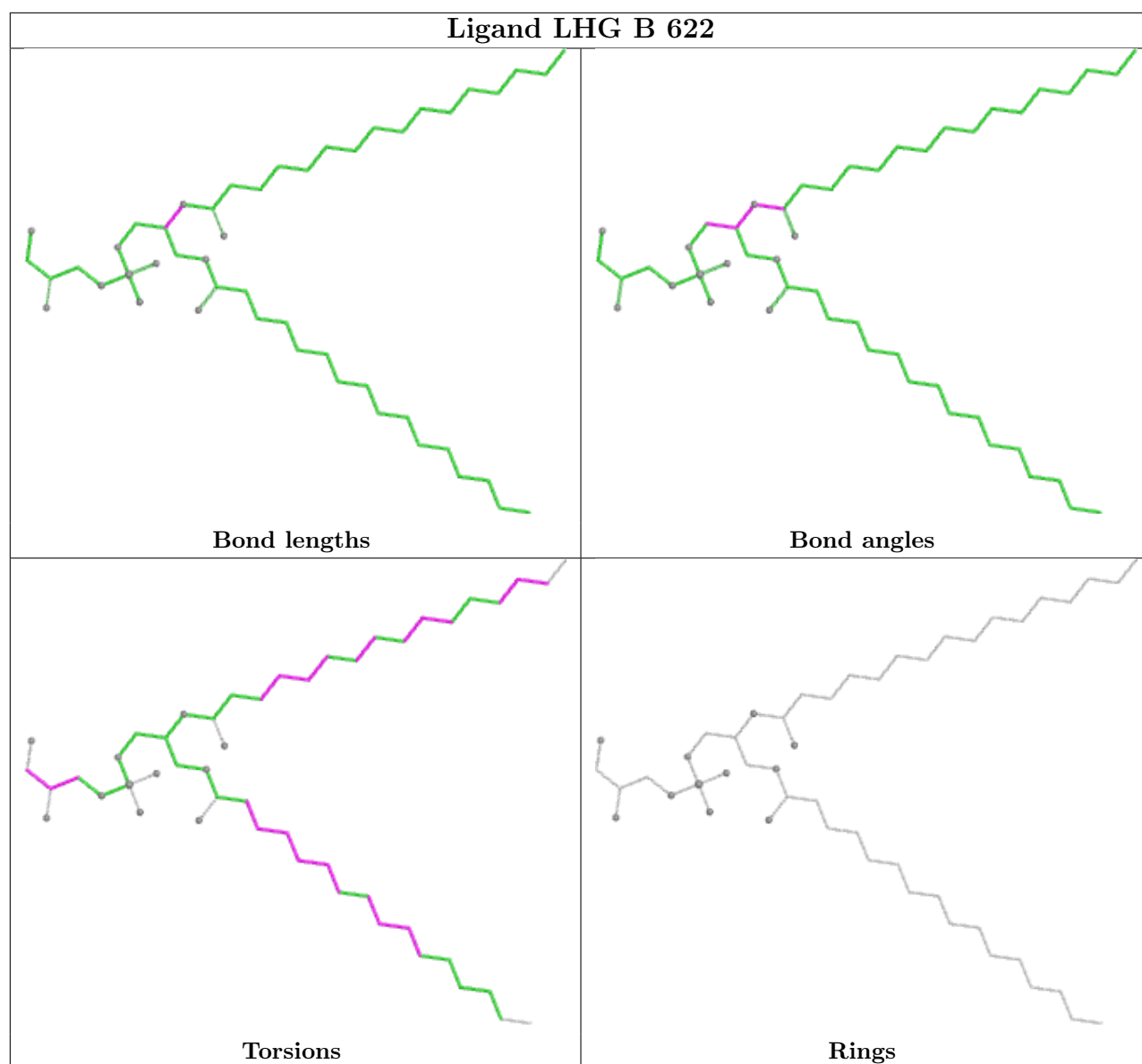
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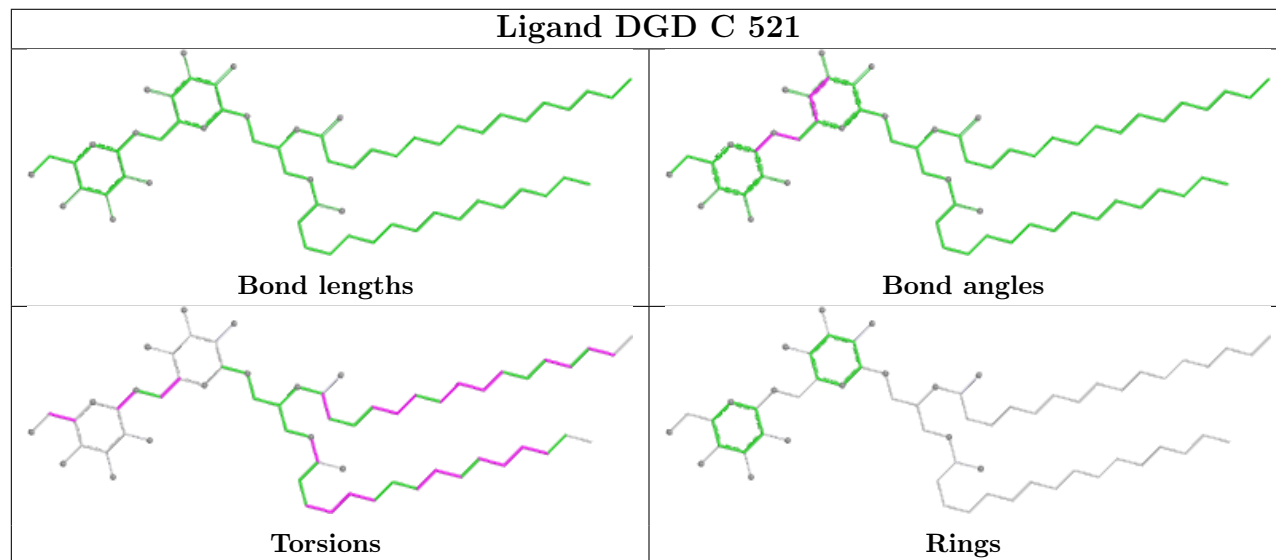
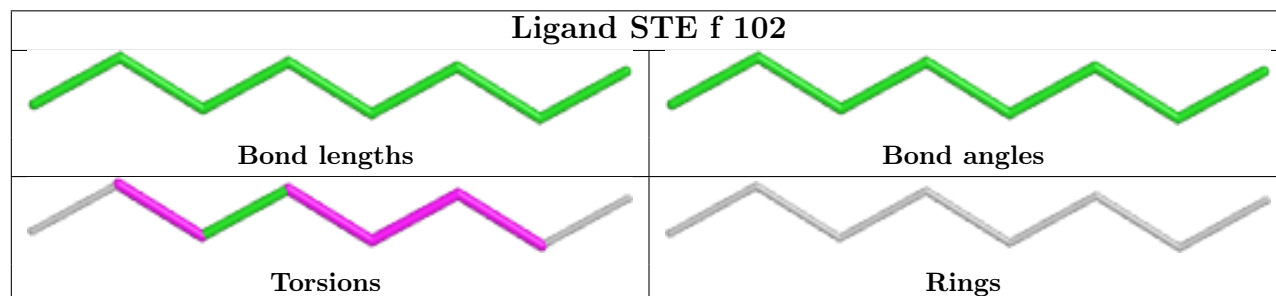
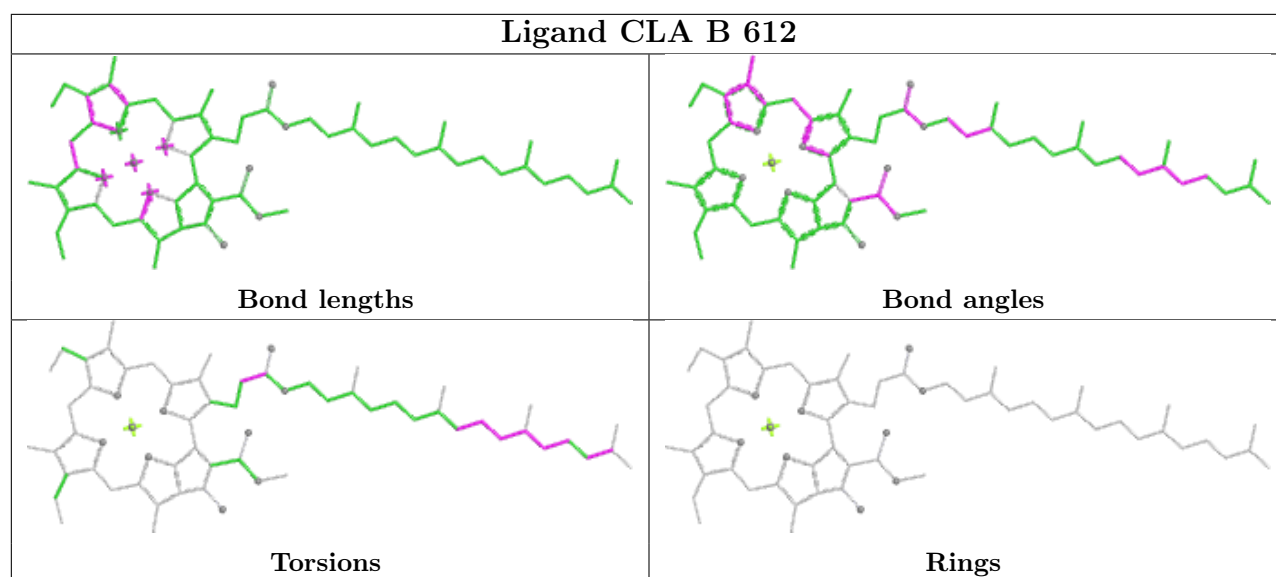




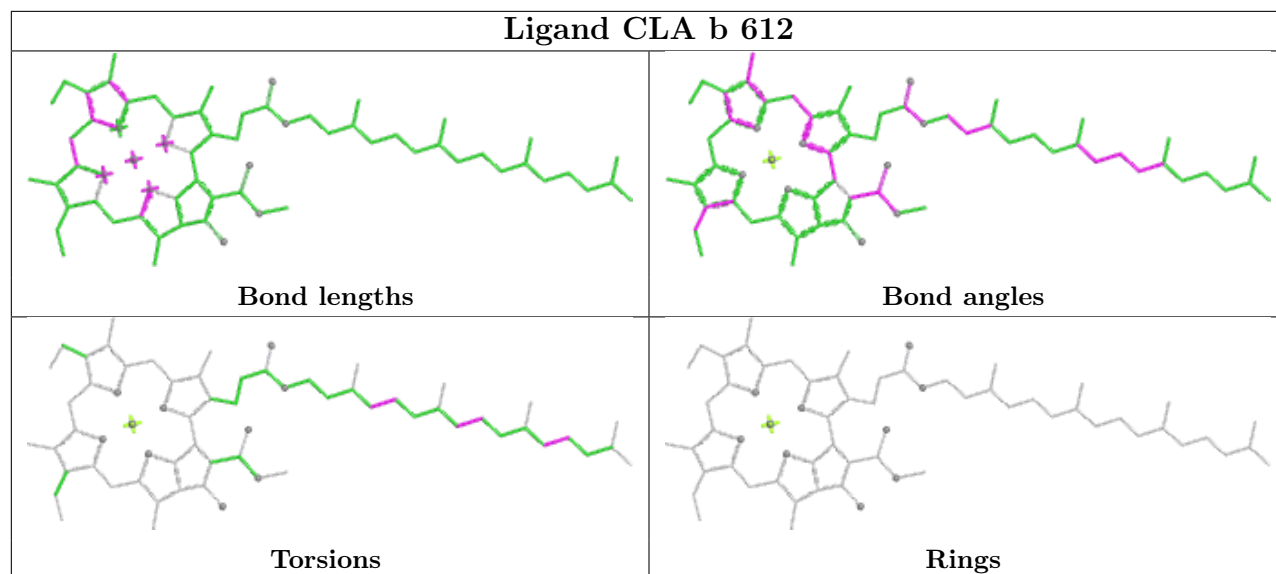




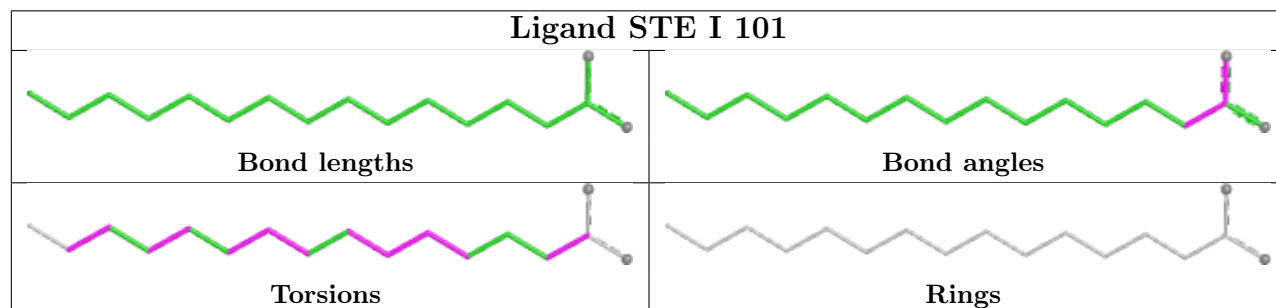




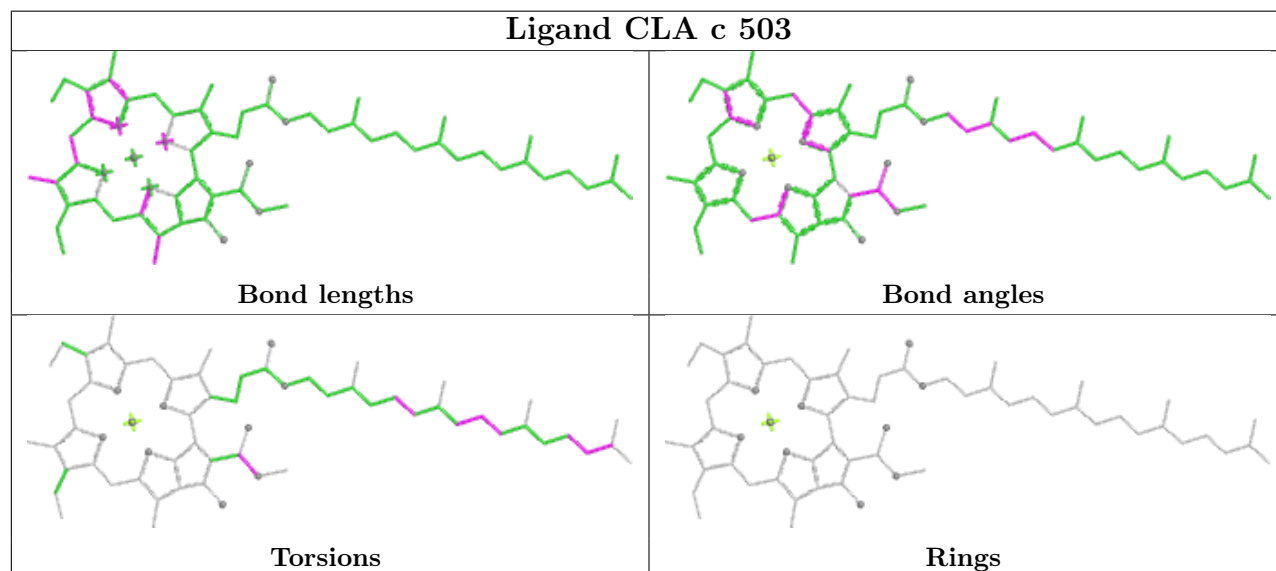
Ligand CLA b 612

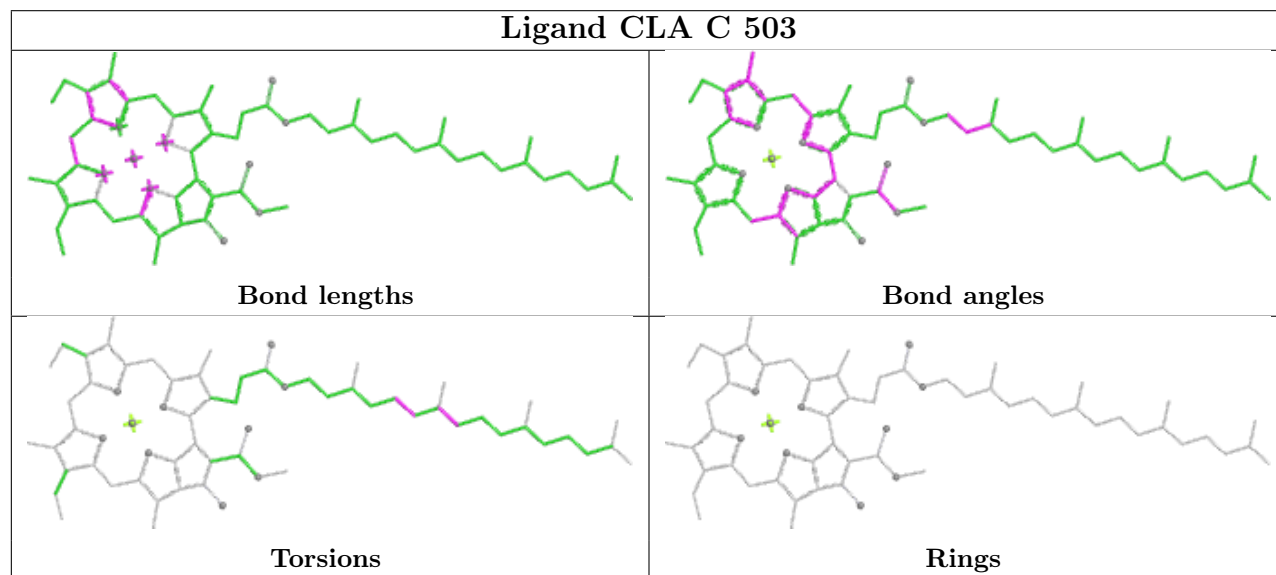
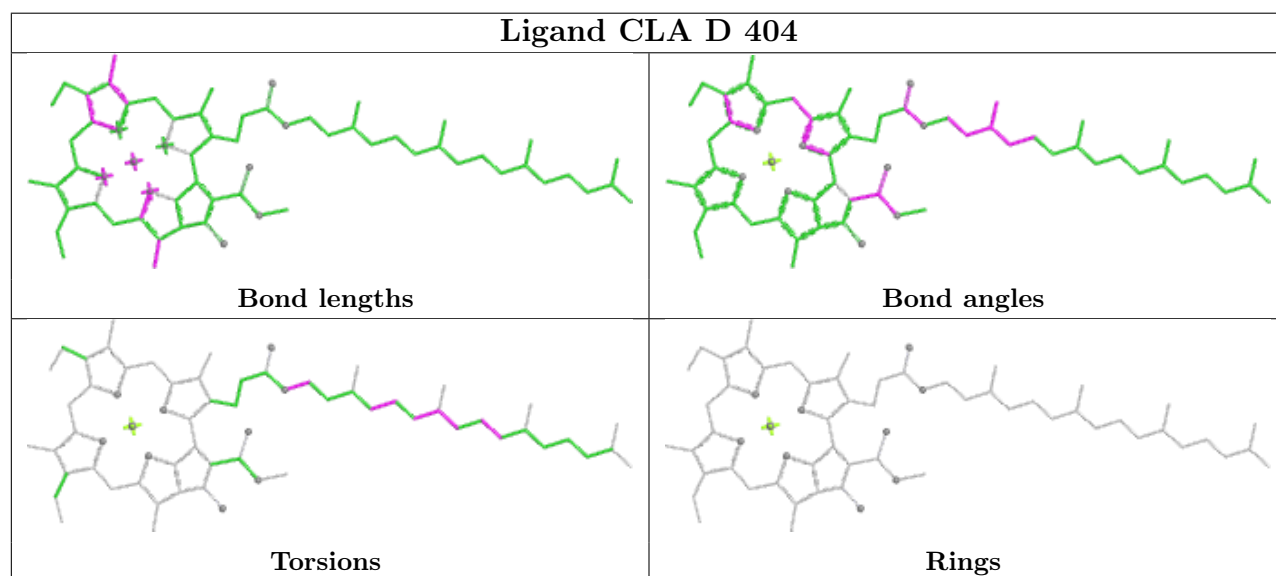
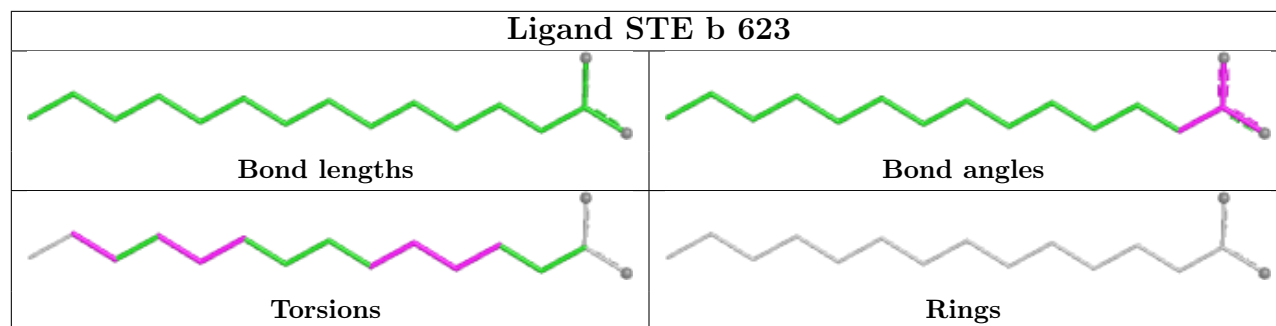


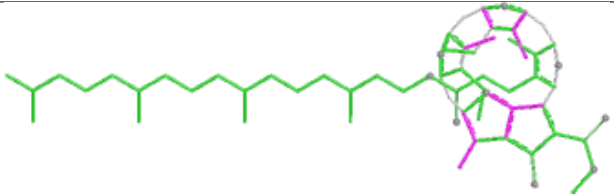
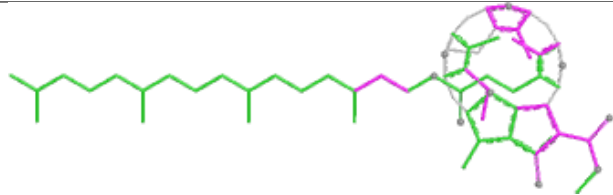
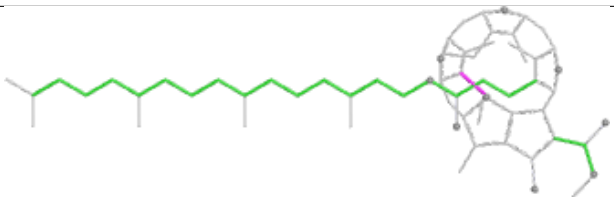
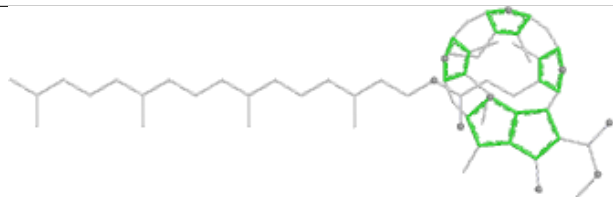
Ligand STE I 101



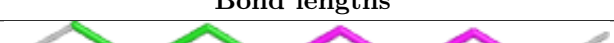
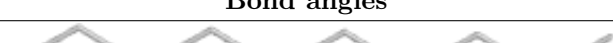
Ligand CLA c 503

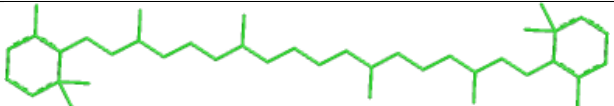
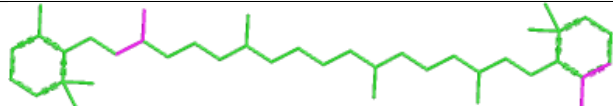
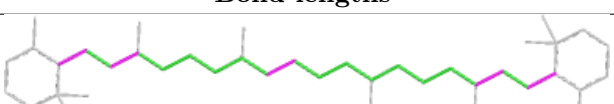
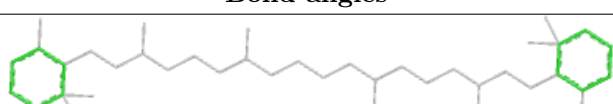


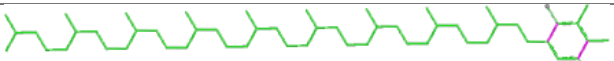
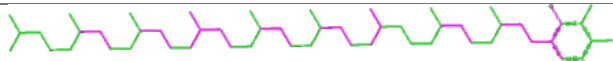
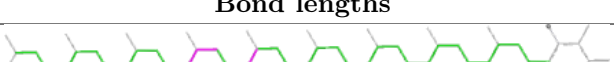
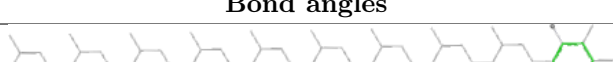


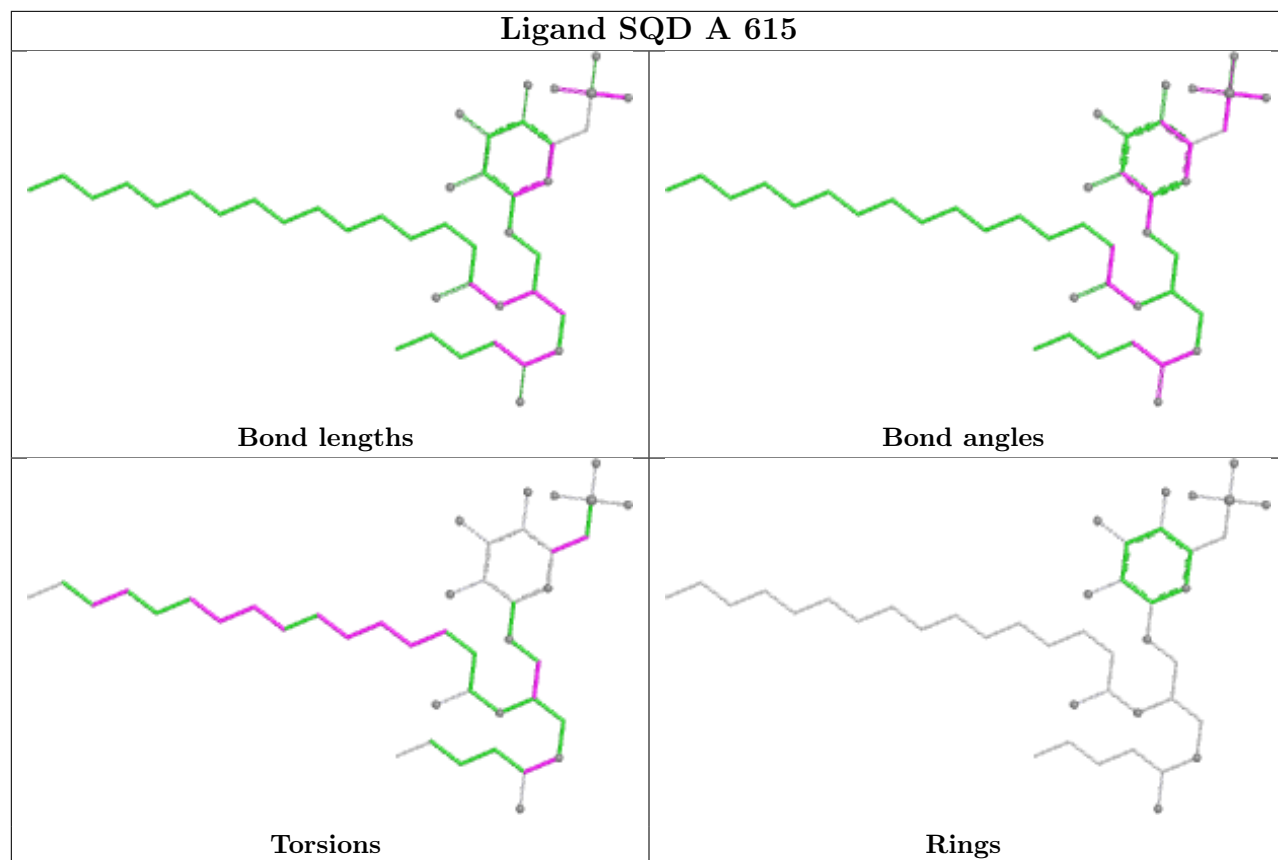
Ligand PHO A 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

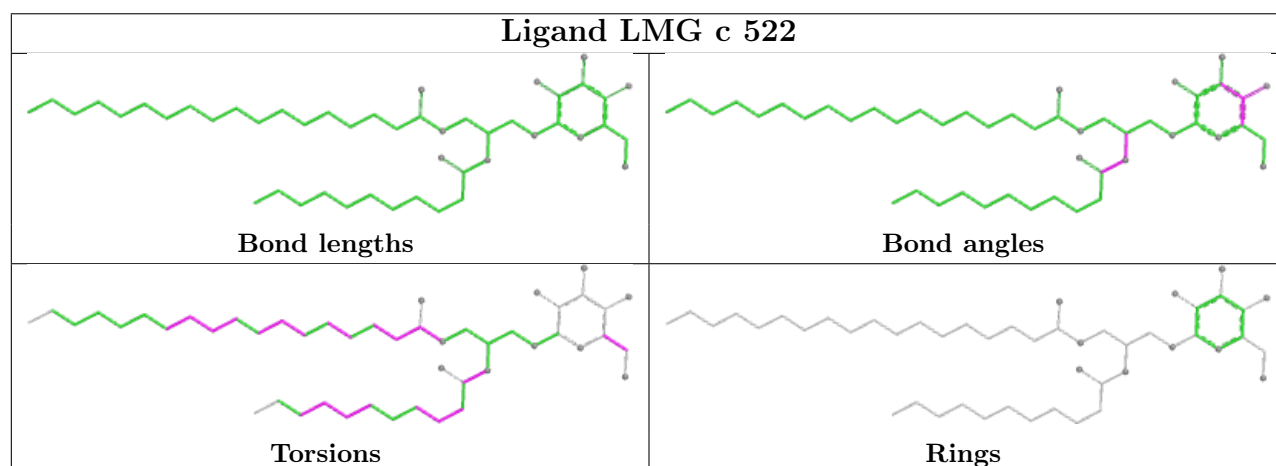
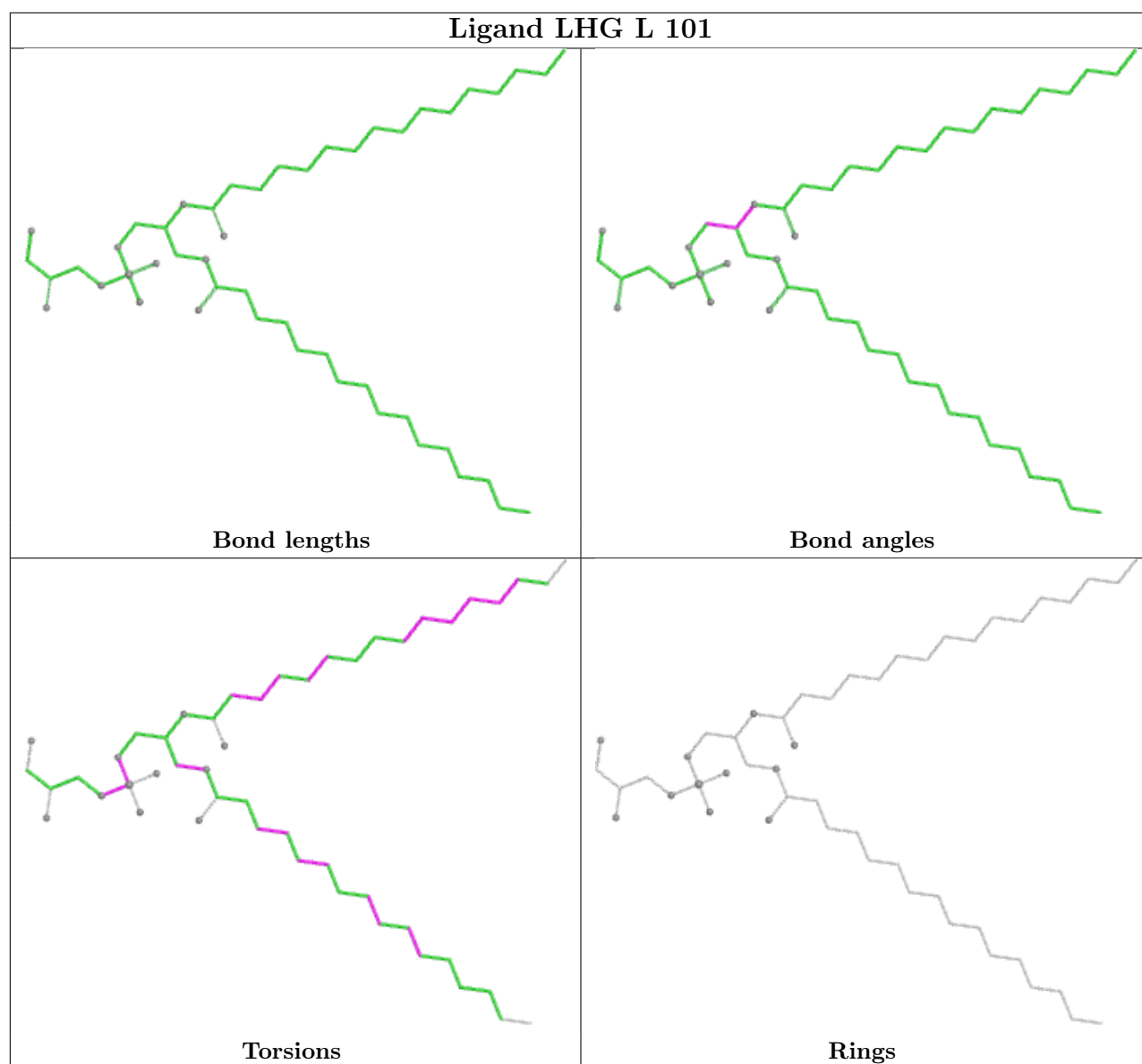
Ligand STE B 628	
	
Bond lengths	Bond angles
	
Torsions	Rings

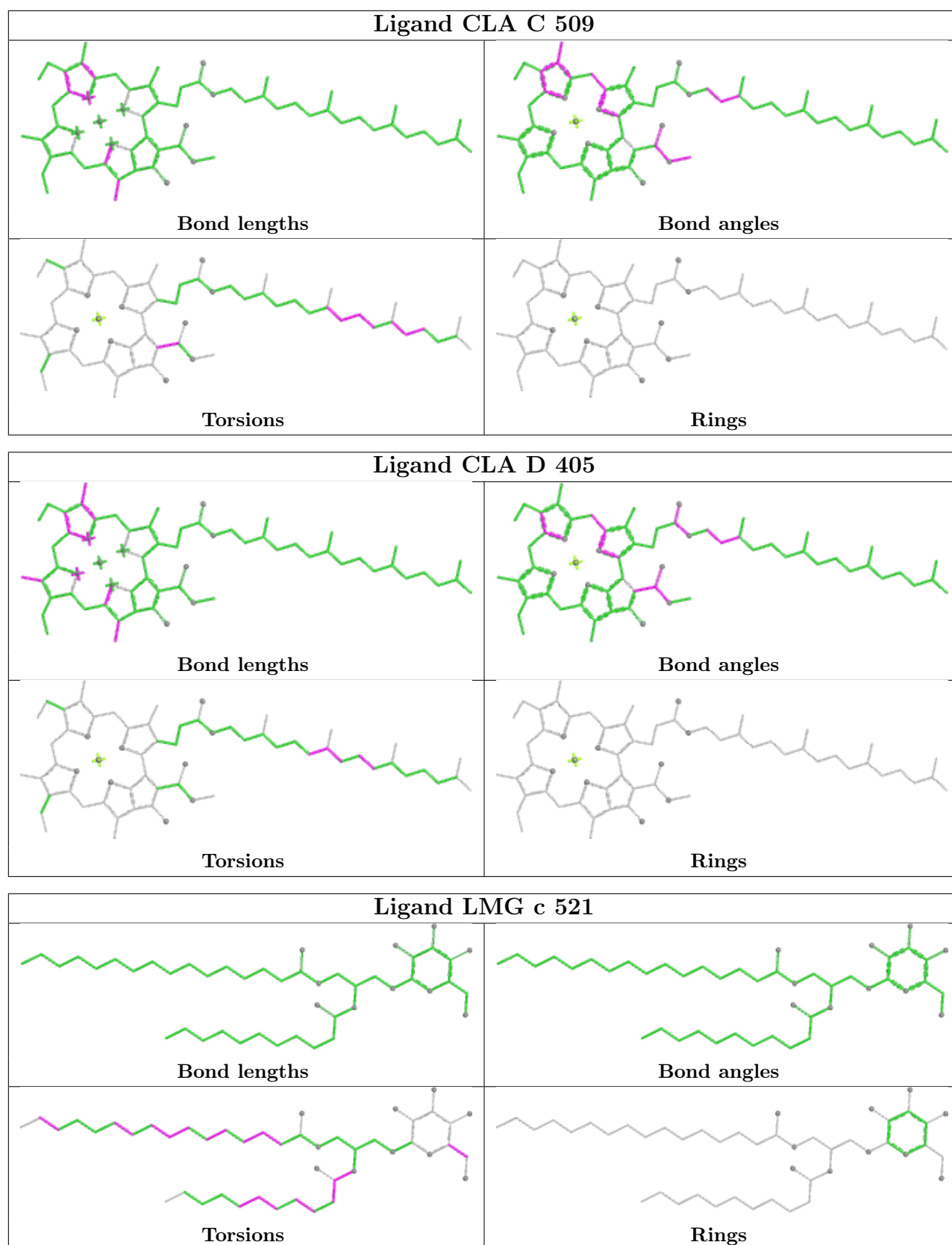
Ligand STE h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

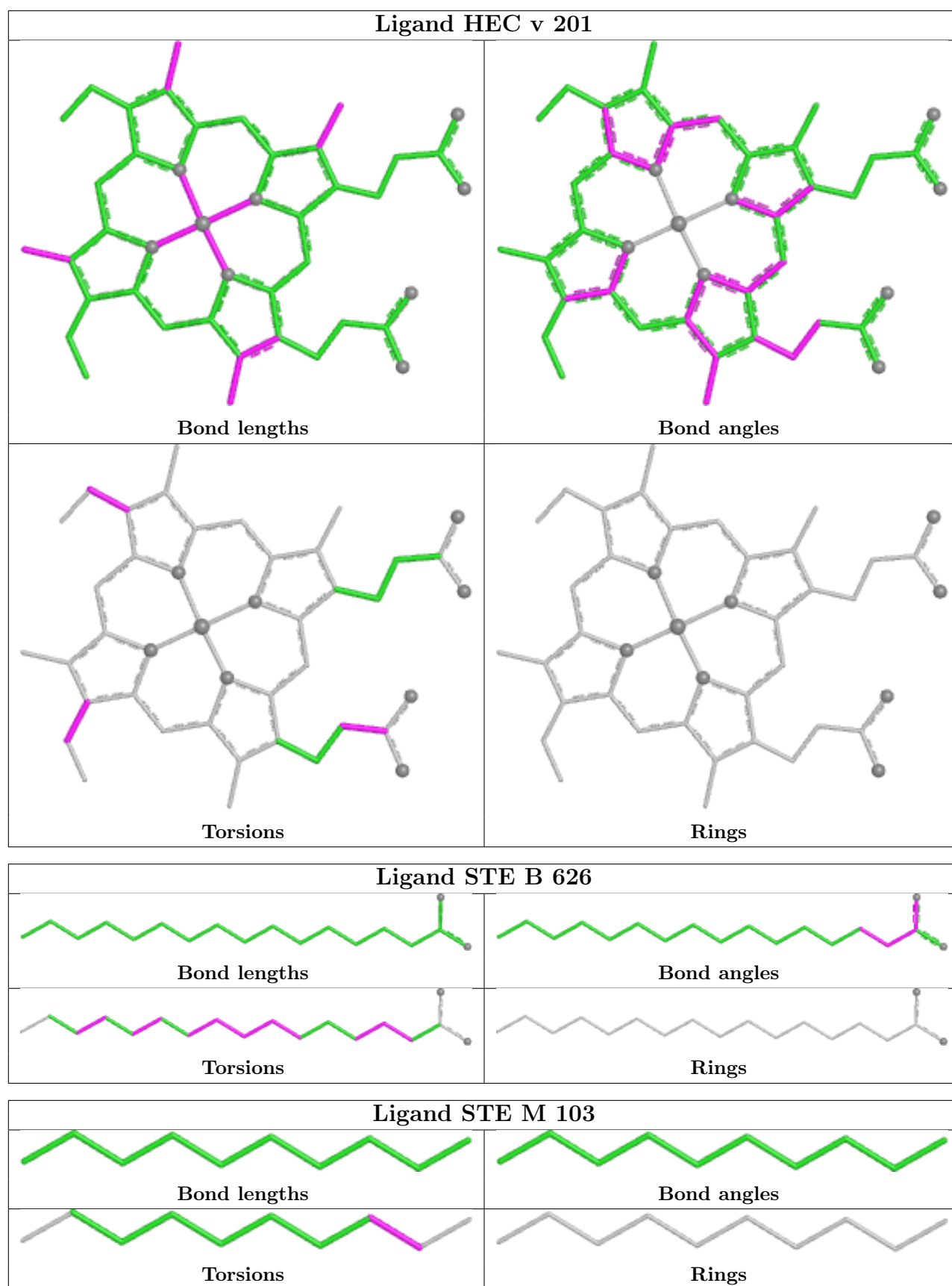
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

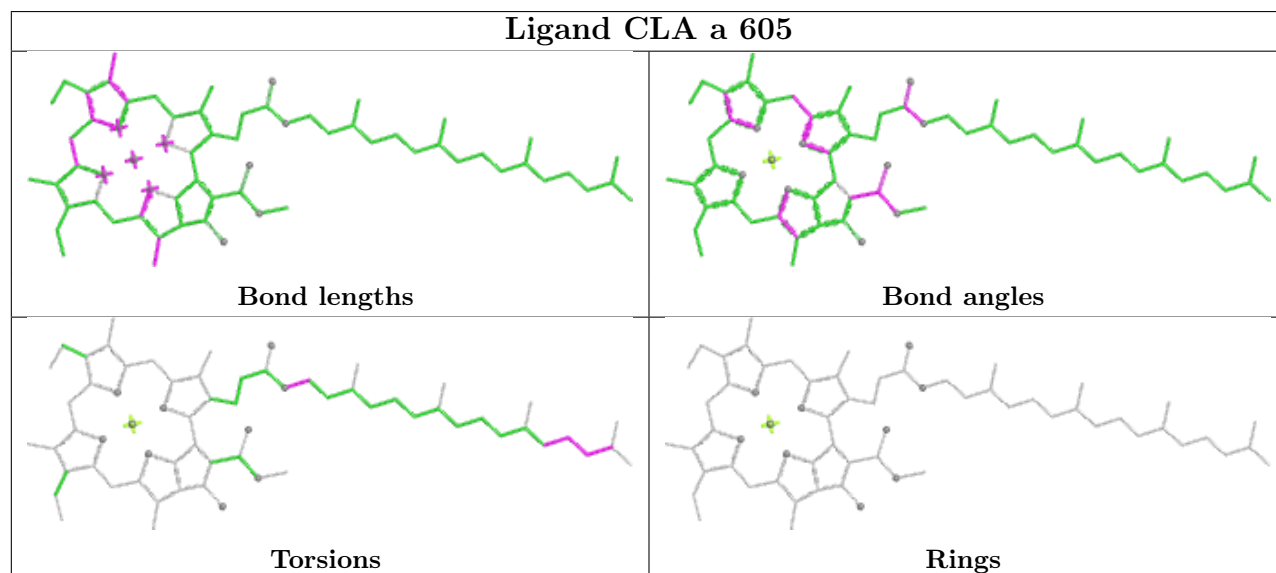
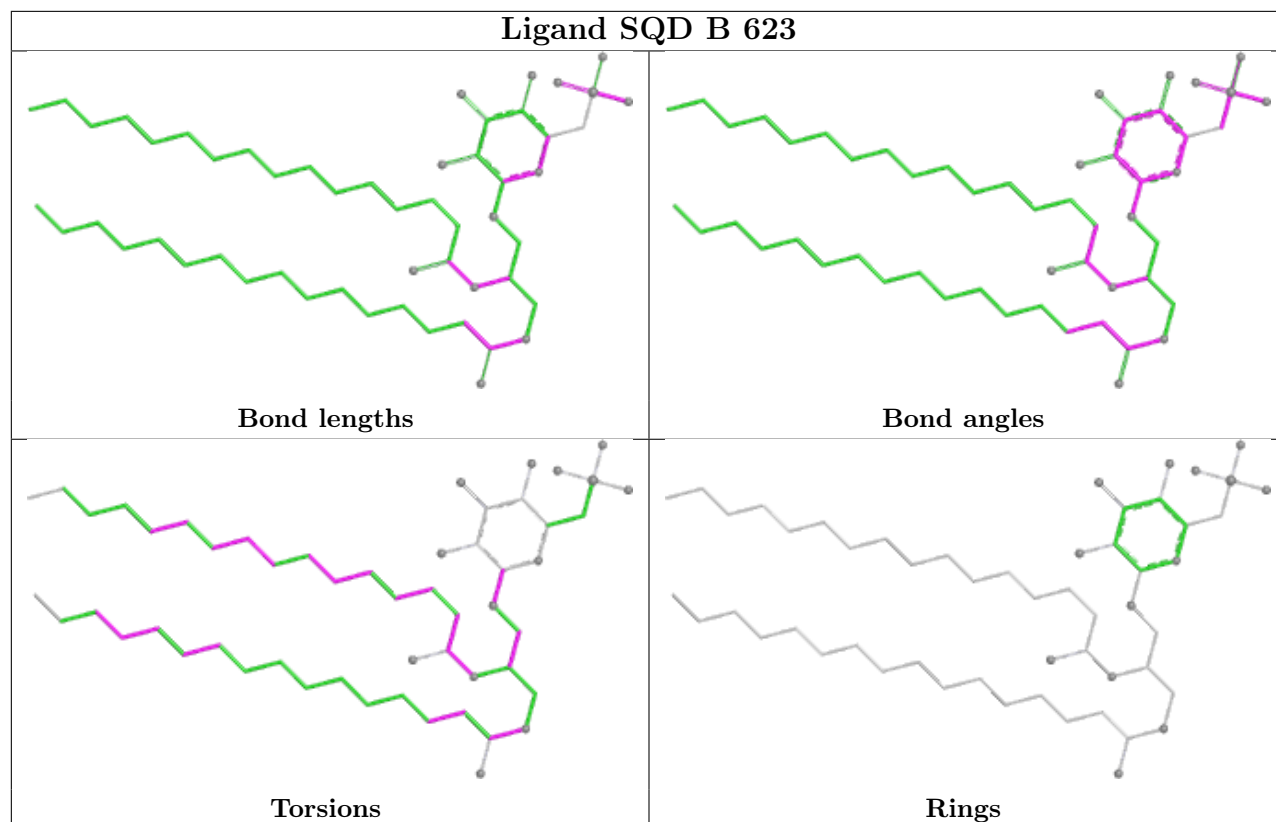
Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



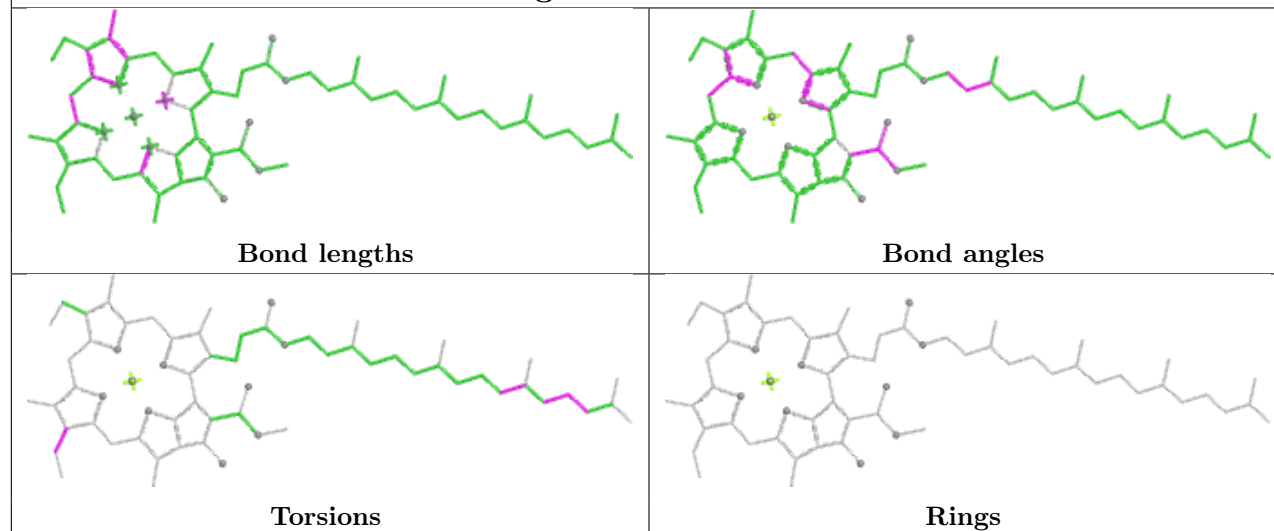




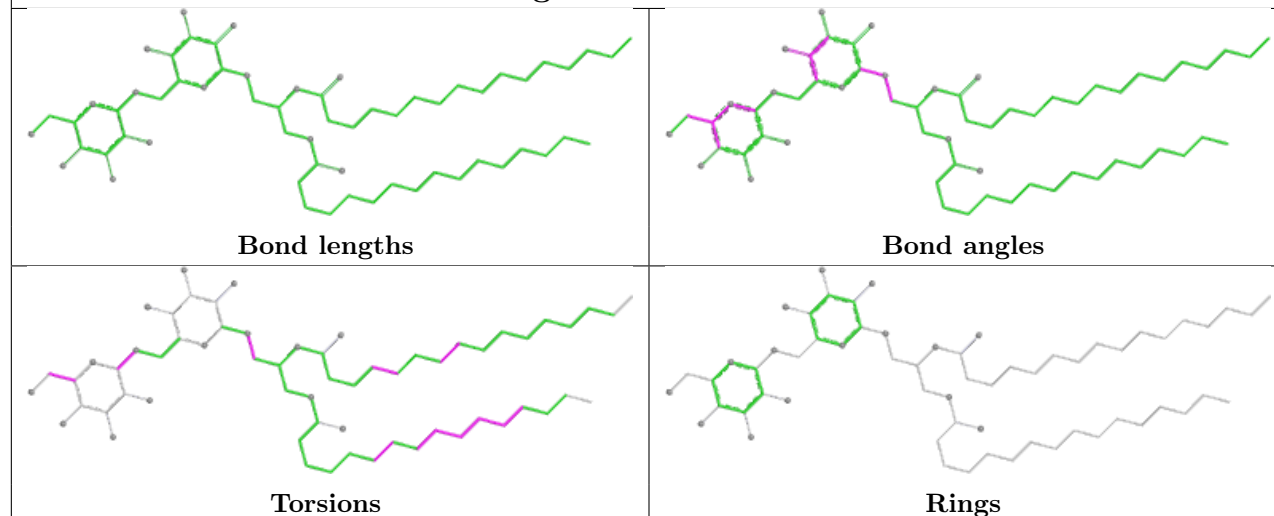




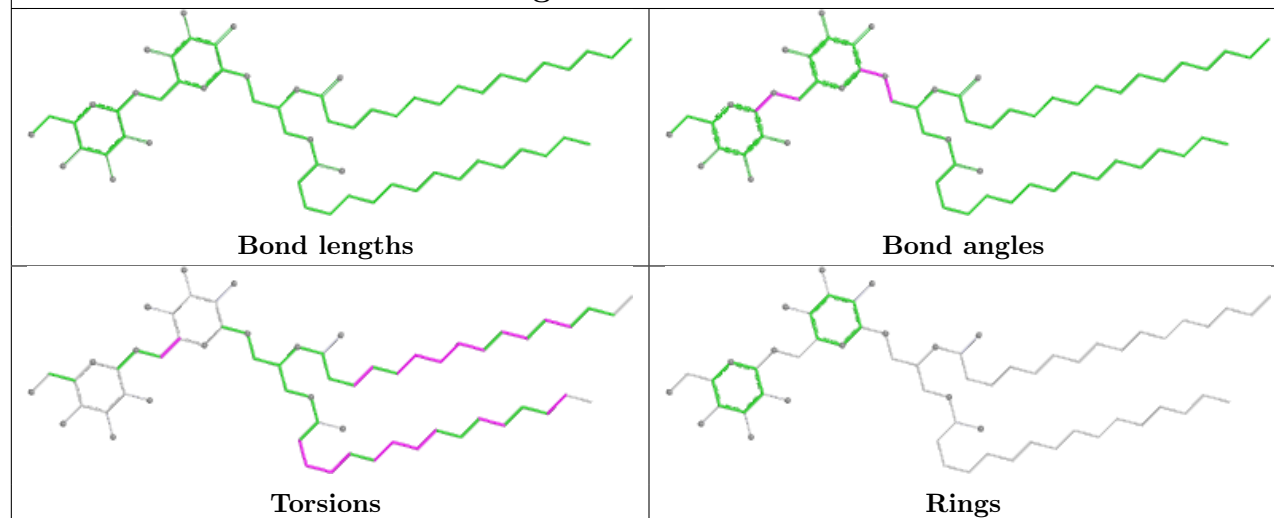
Ligand CLA d 402

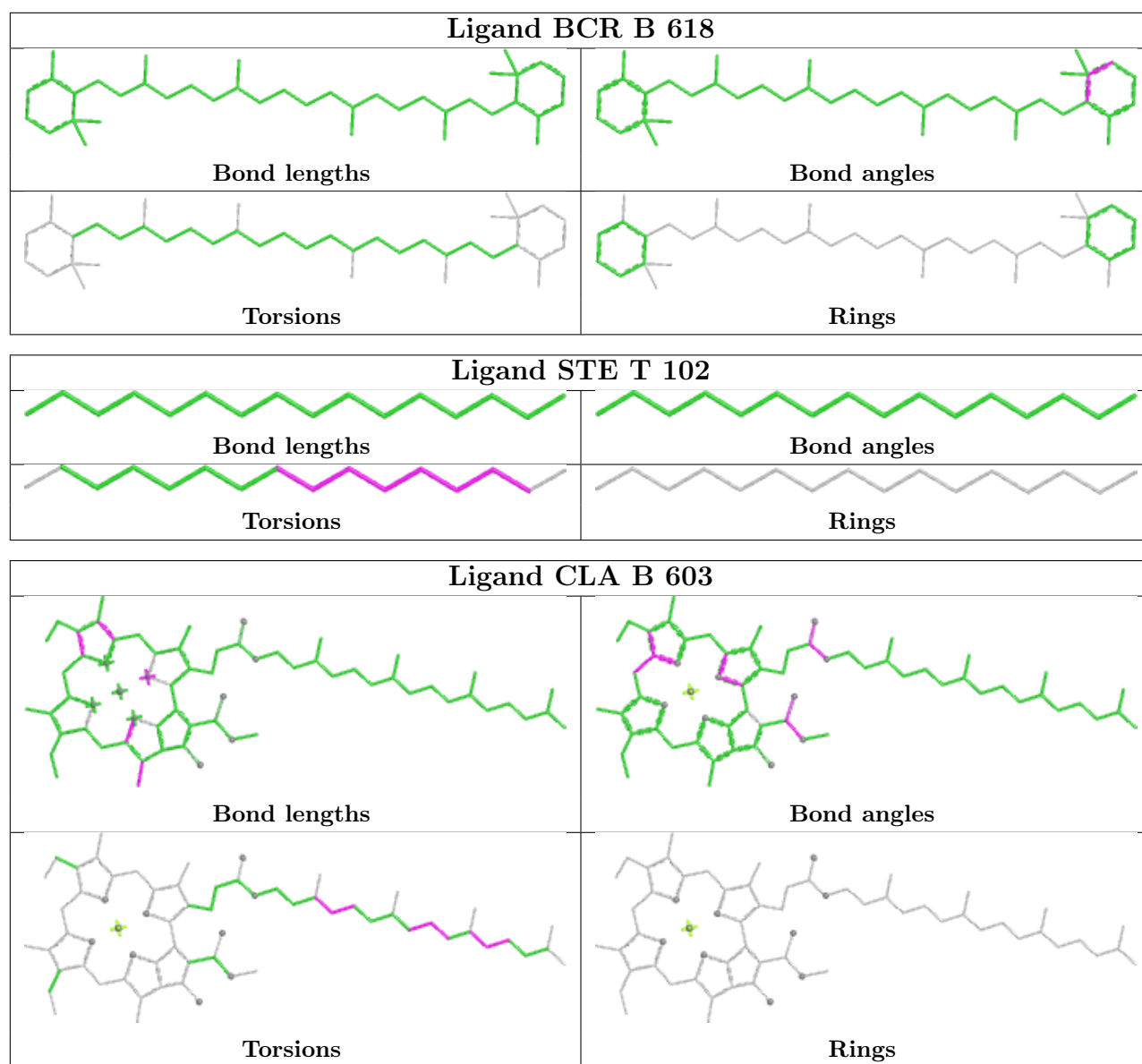


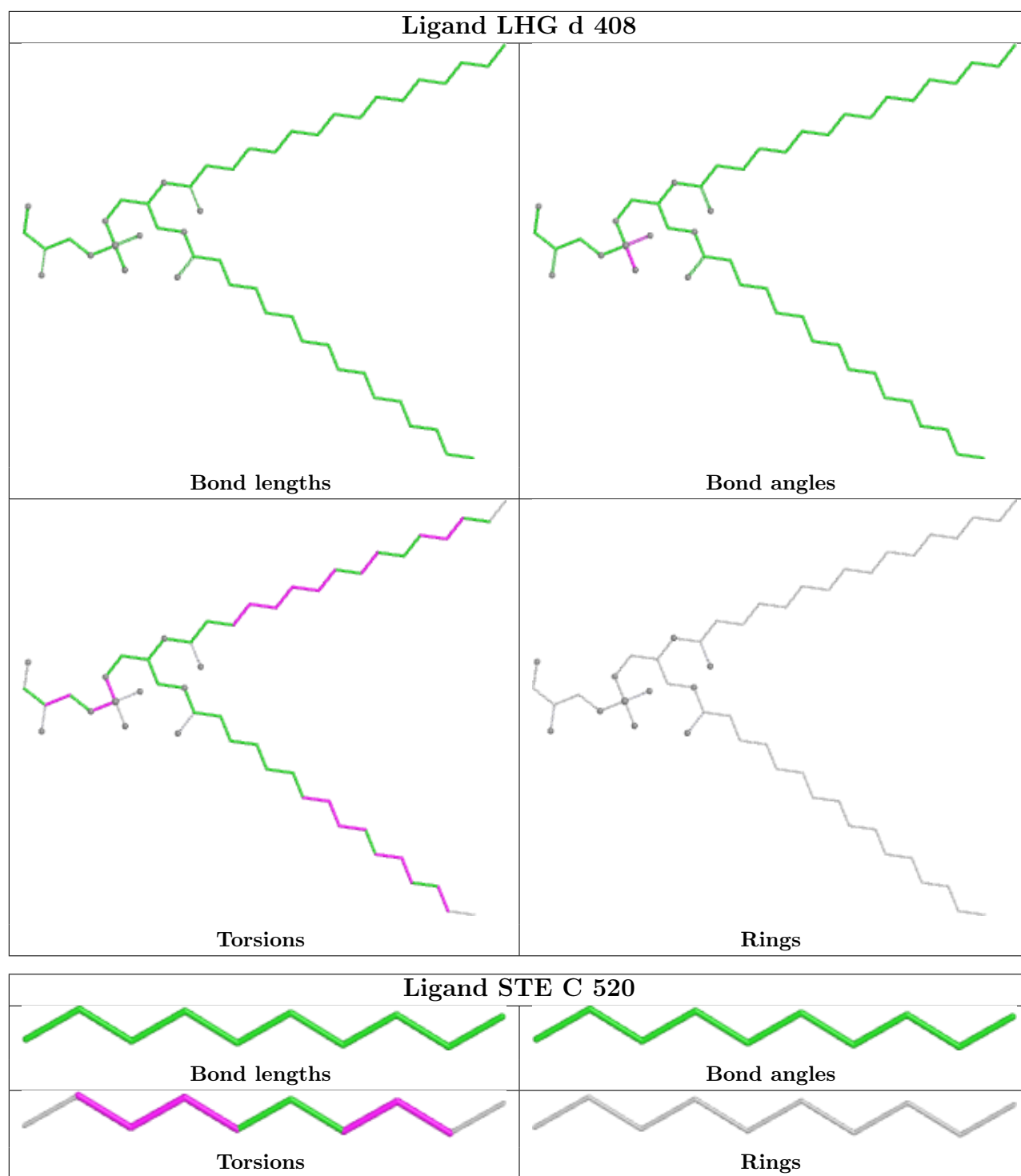
Ligand DGD c 519

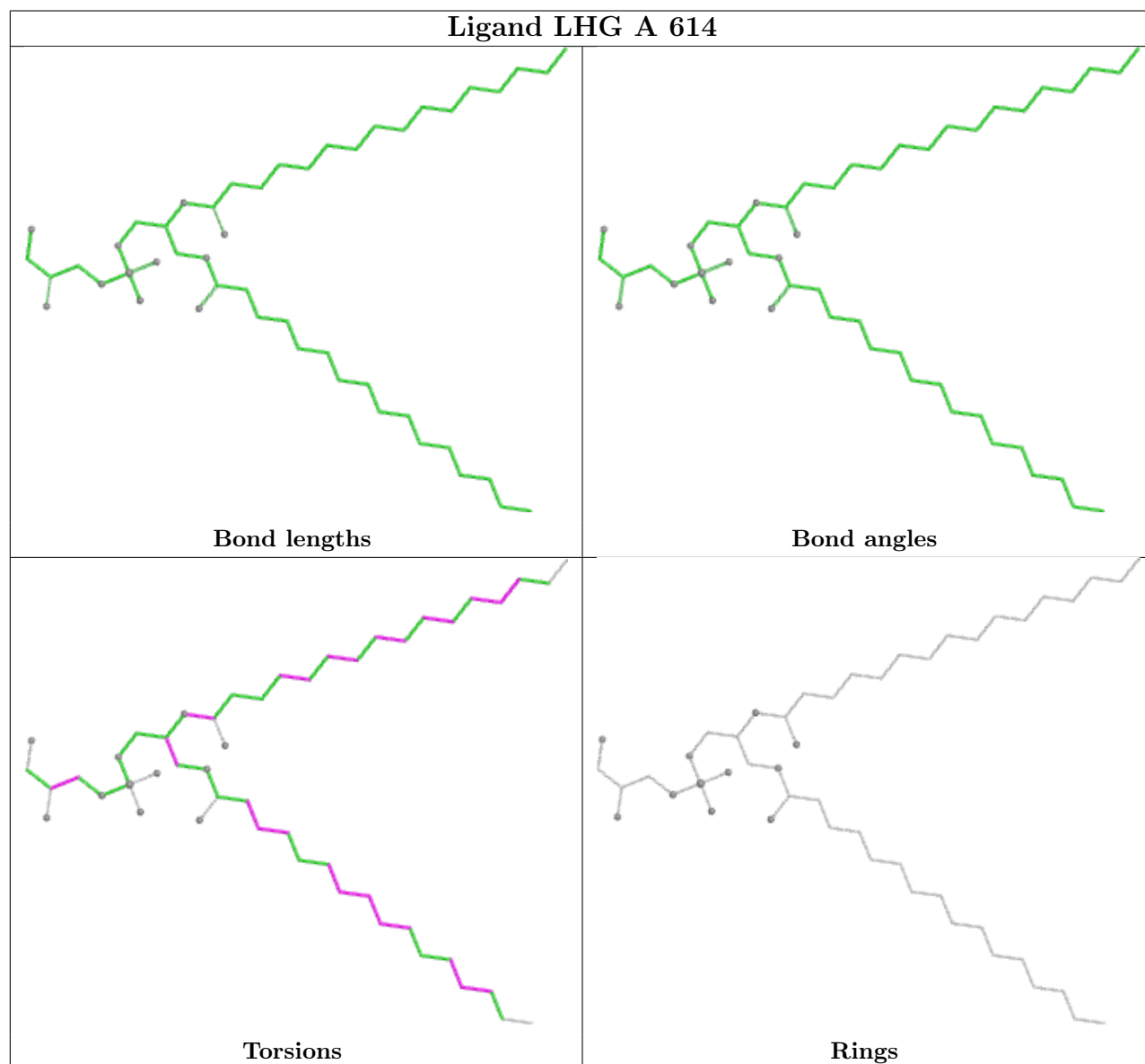
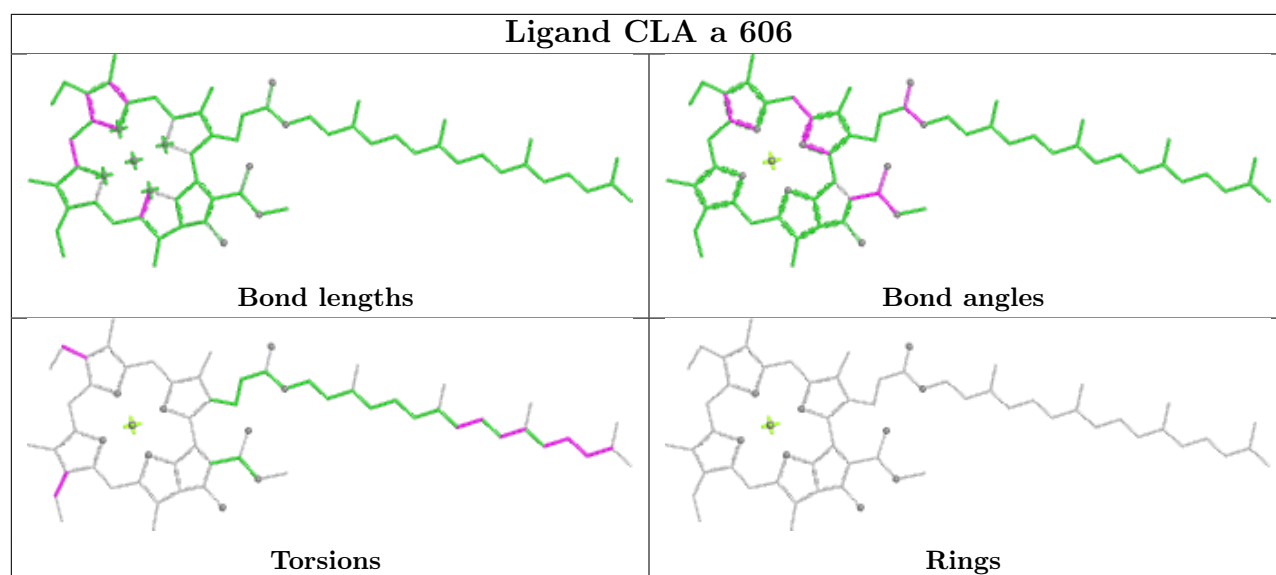


Ligand DGD c 520

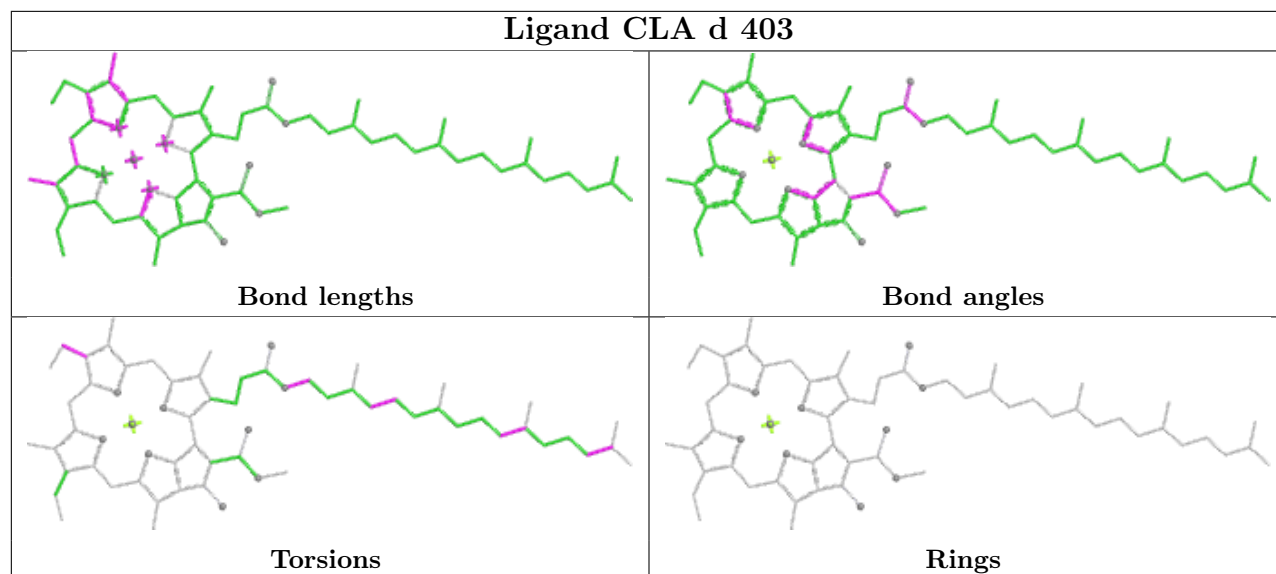




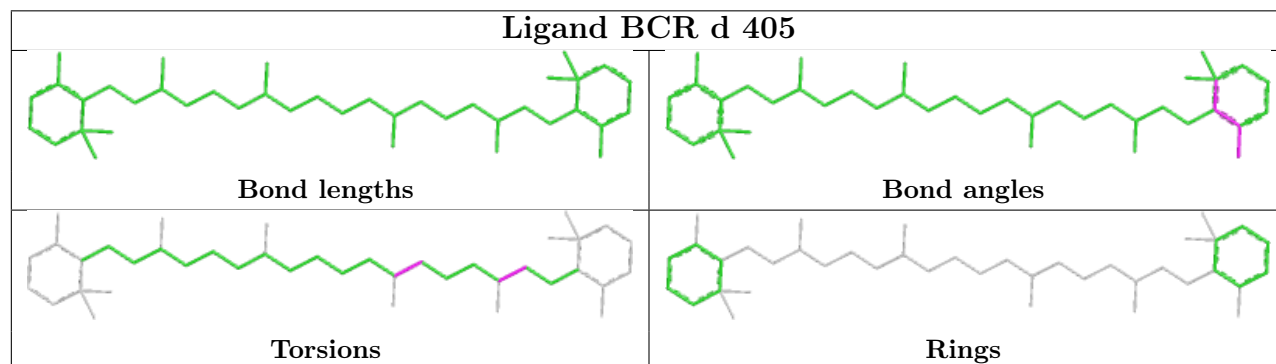




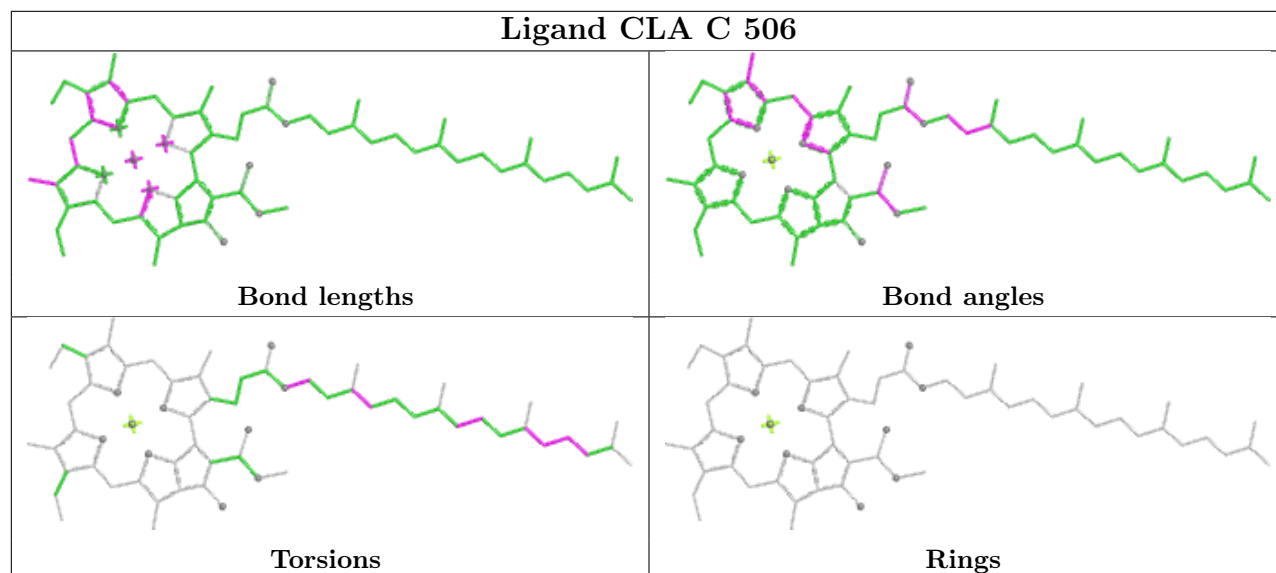
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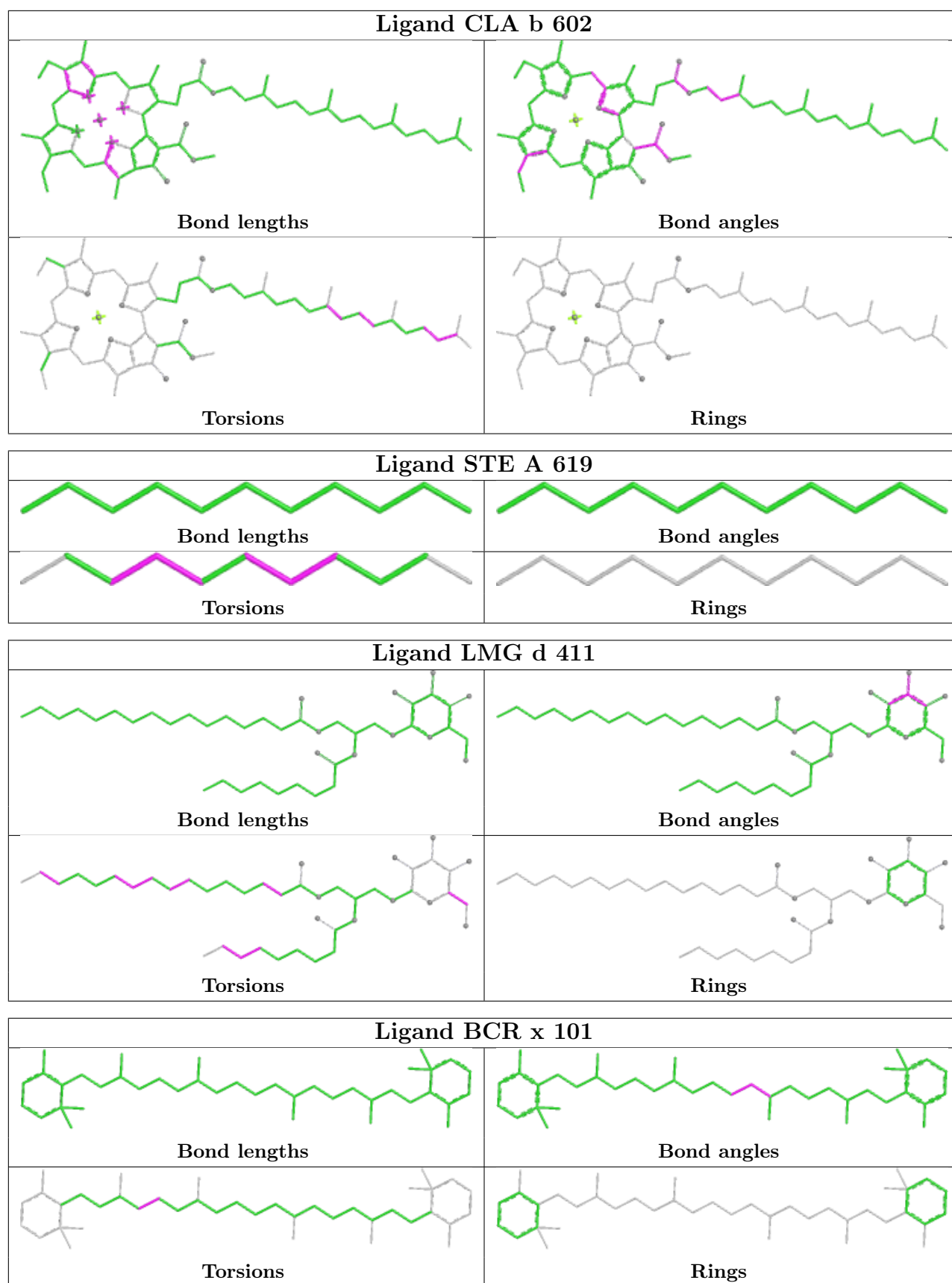


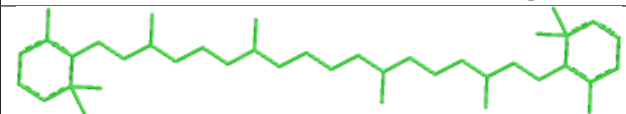
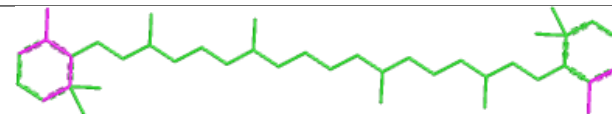
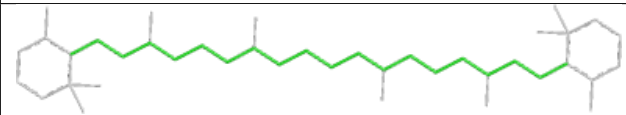
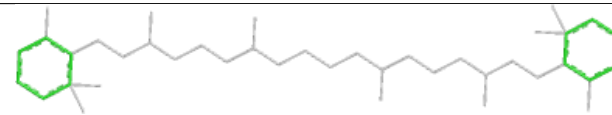
Ligand BCR d 405

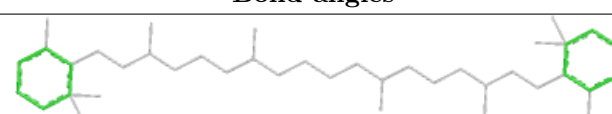


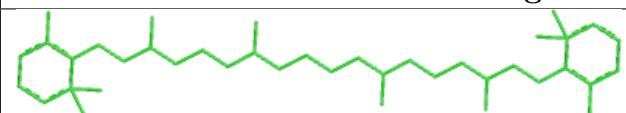
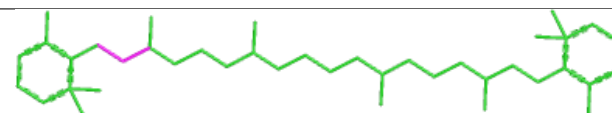
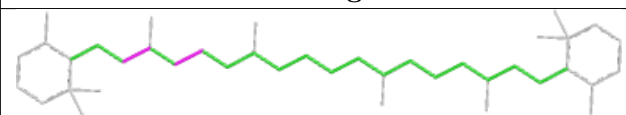
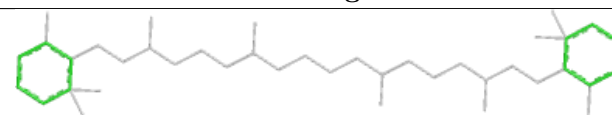
Ligand CLA C 506

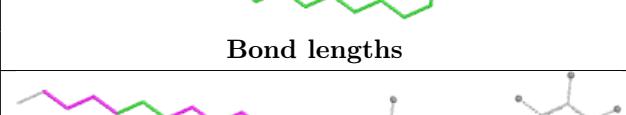
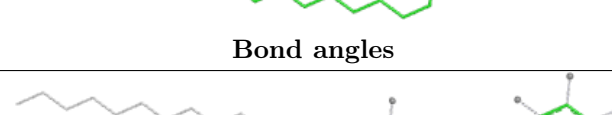


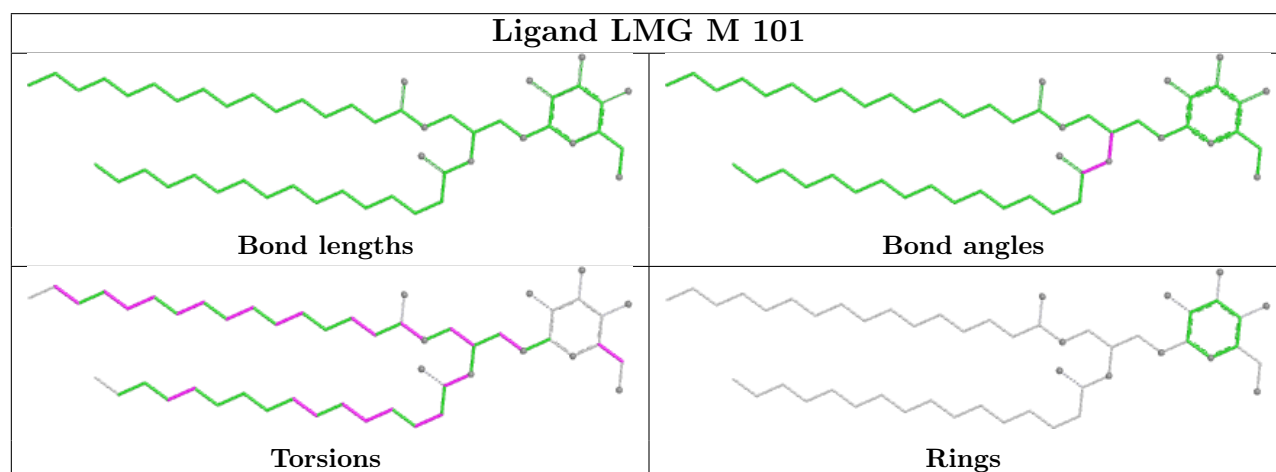
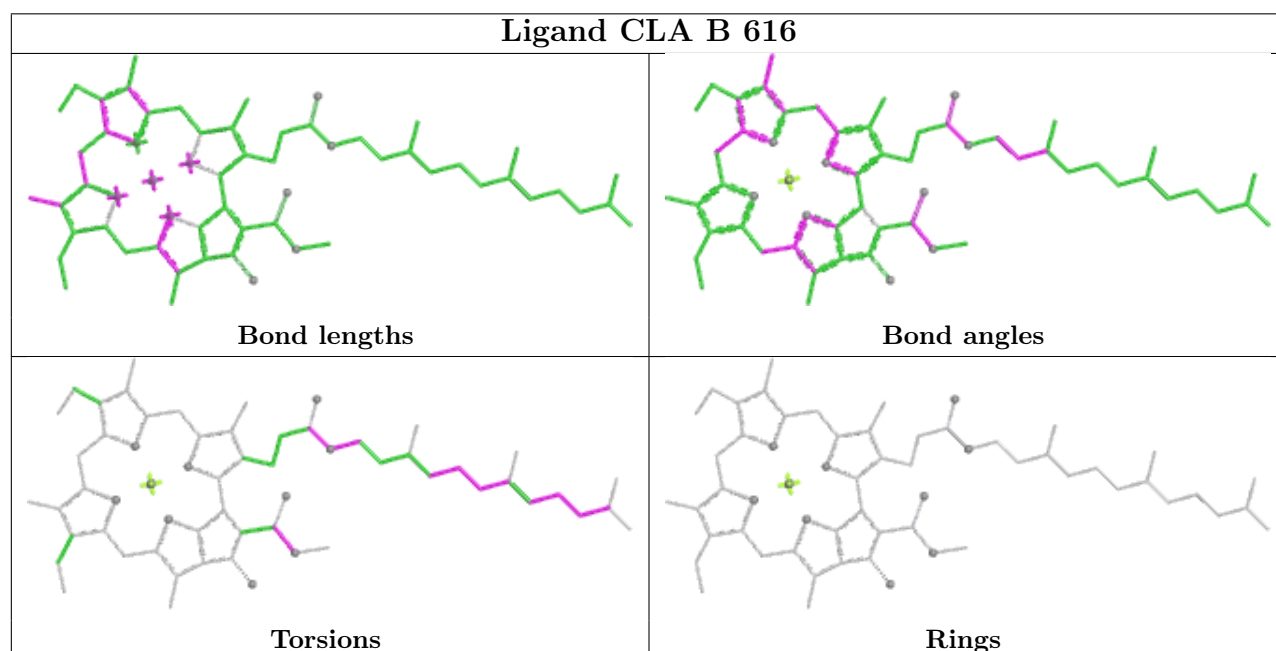
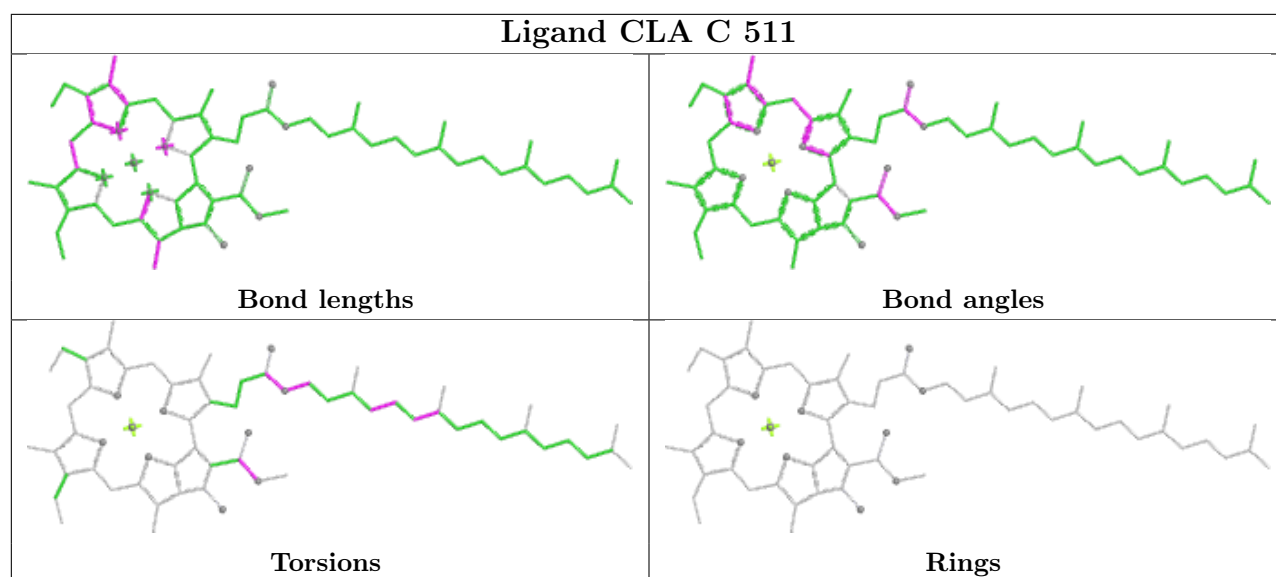


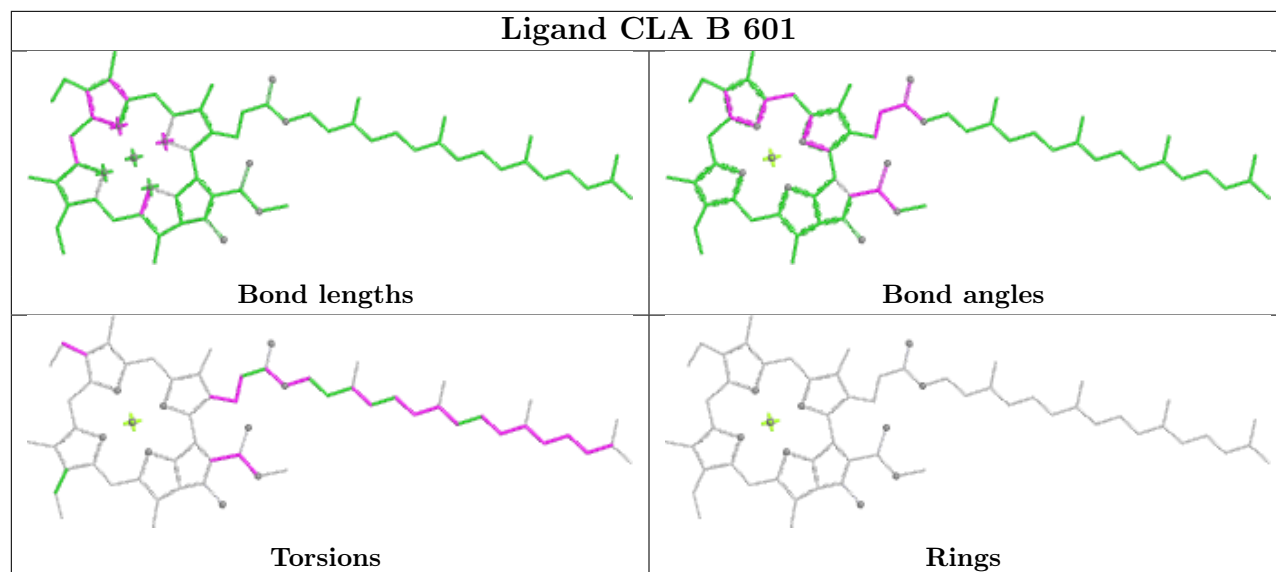
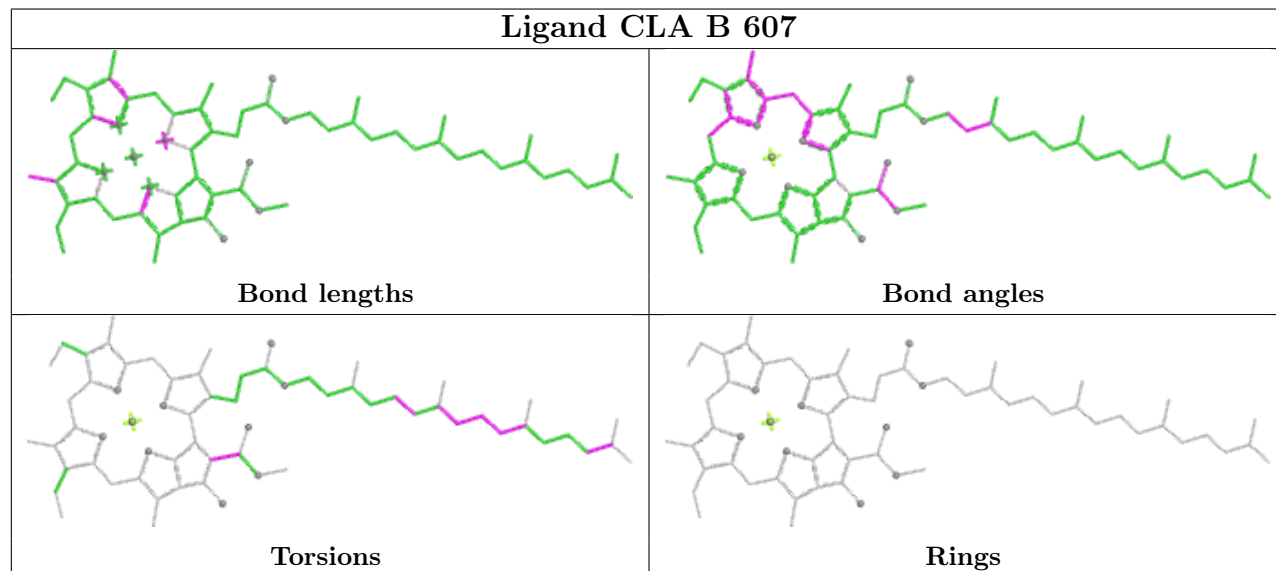
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

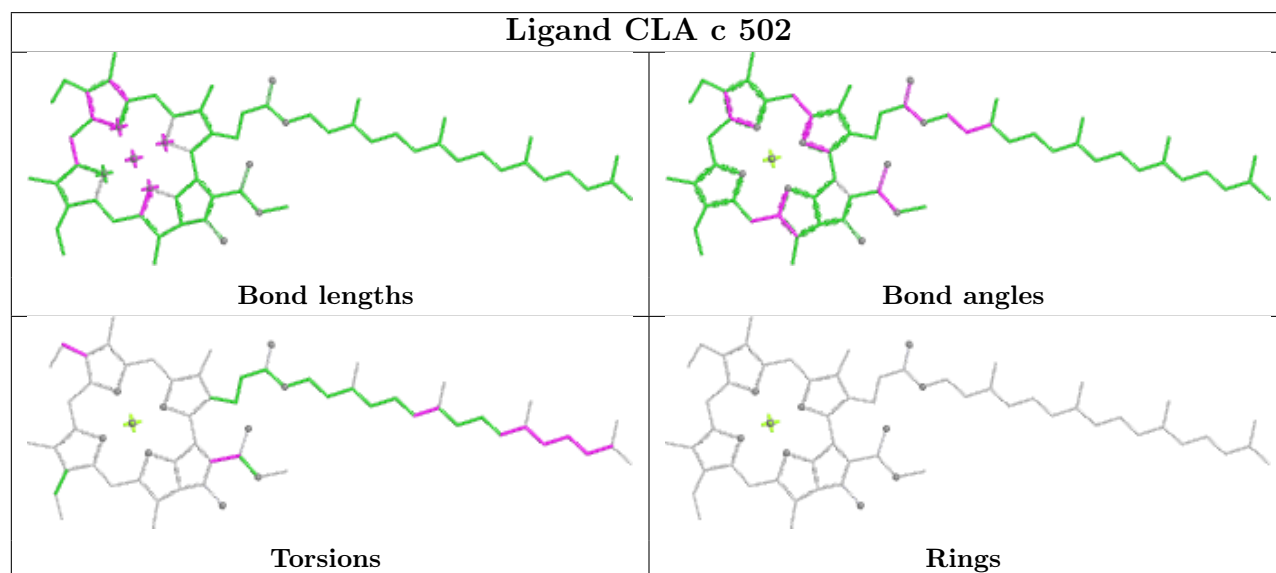
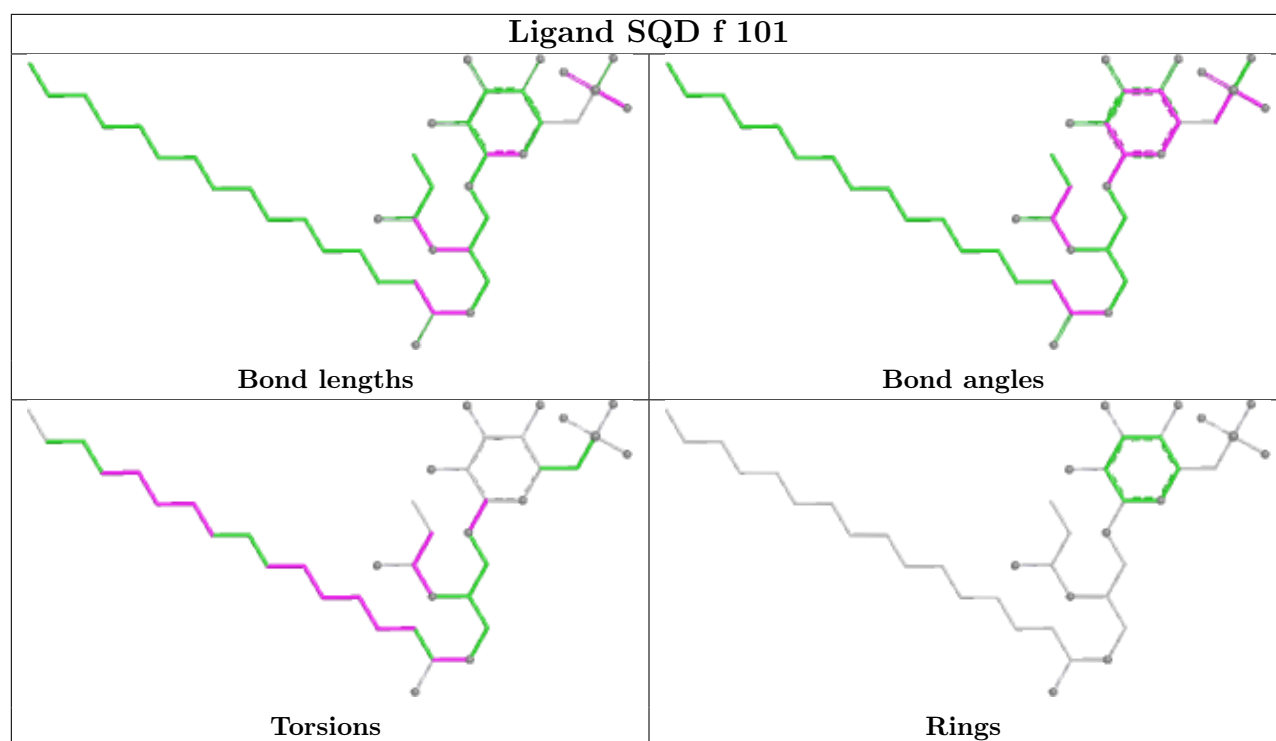
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

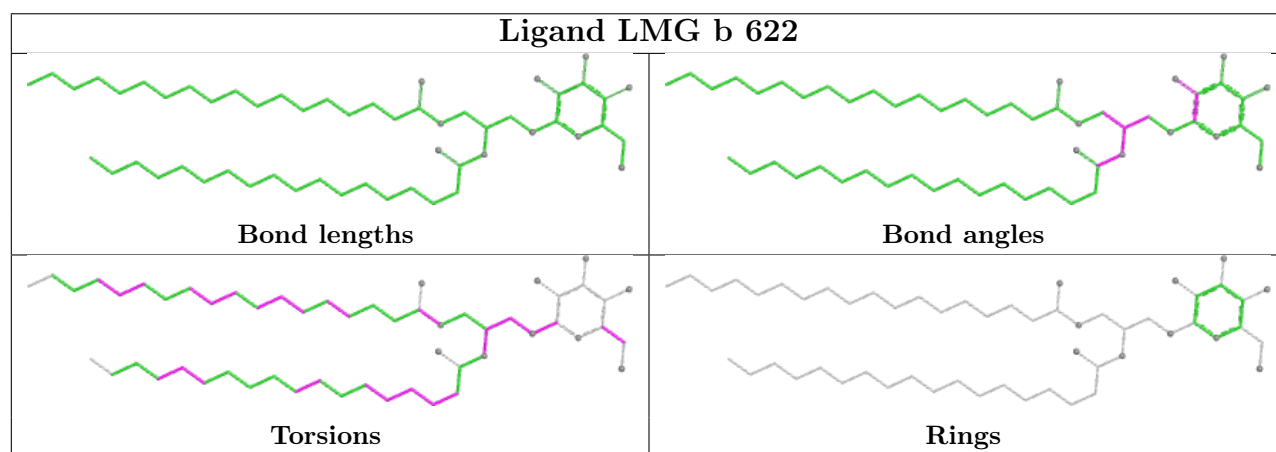
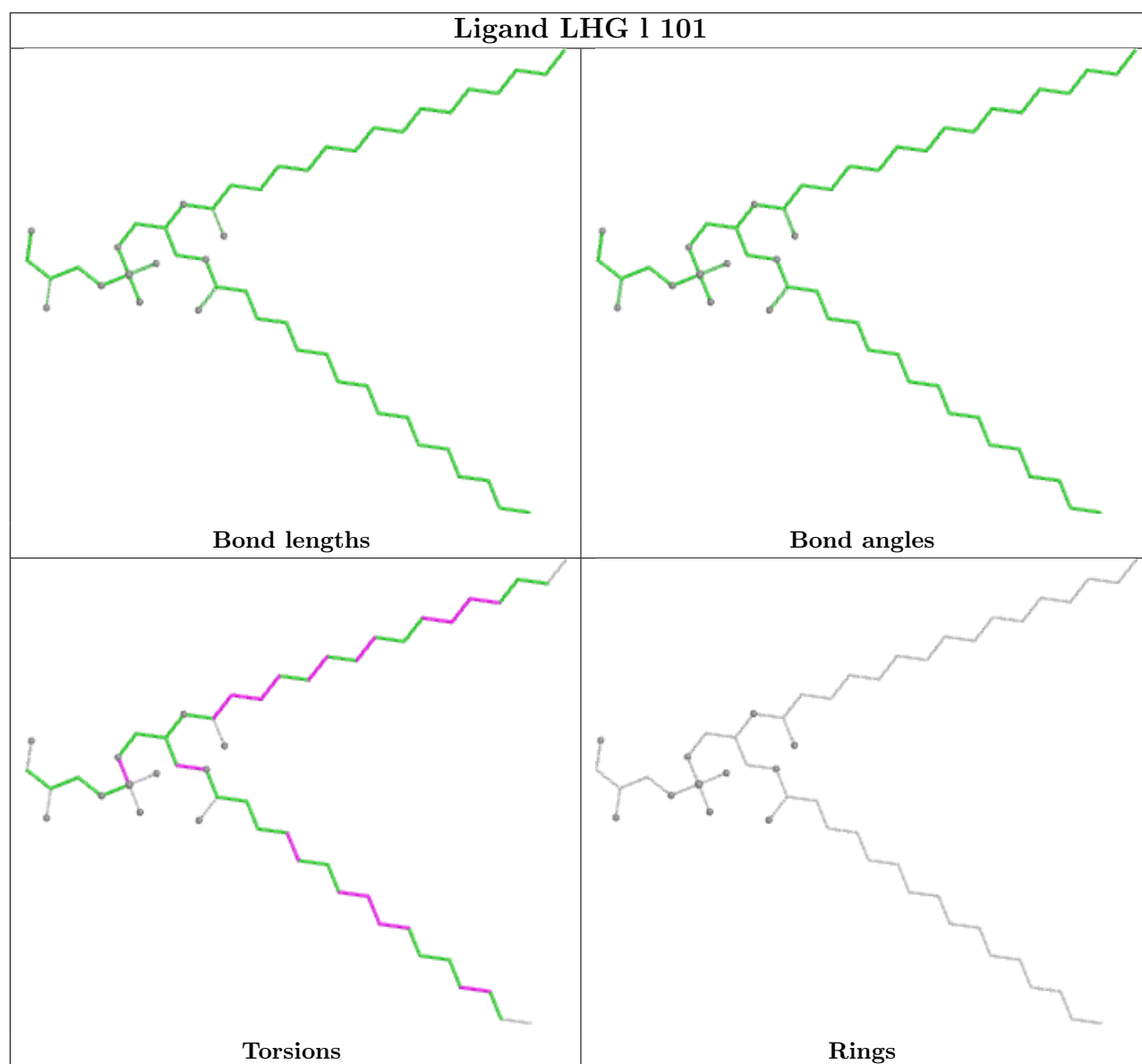
Ligand BCR c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

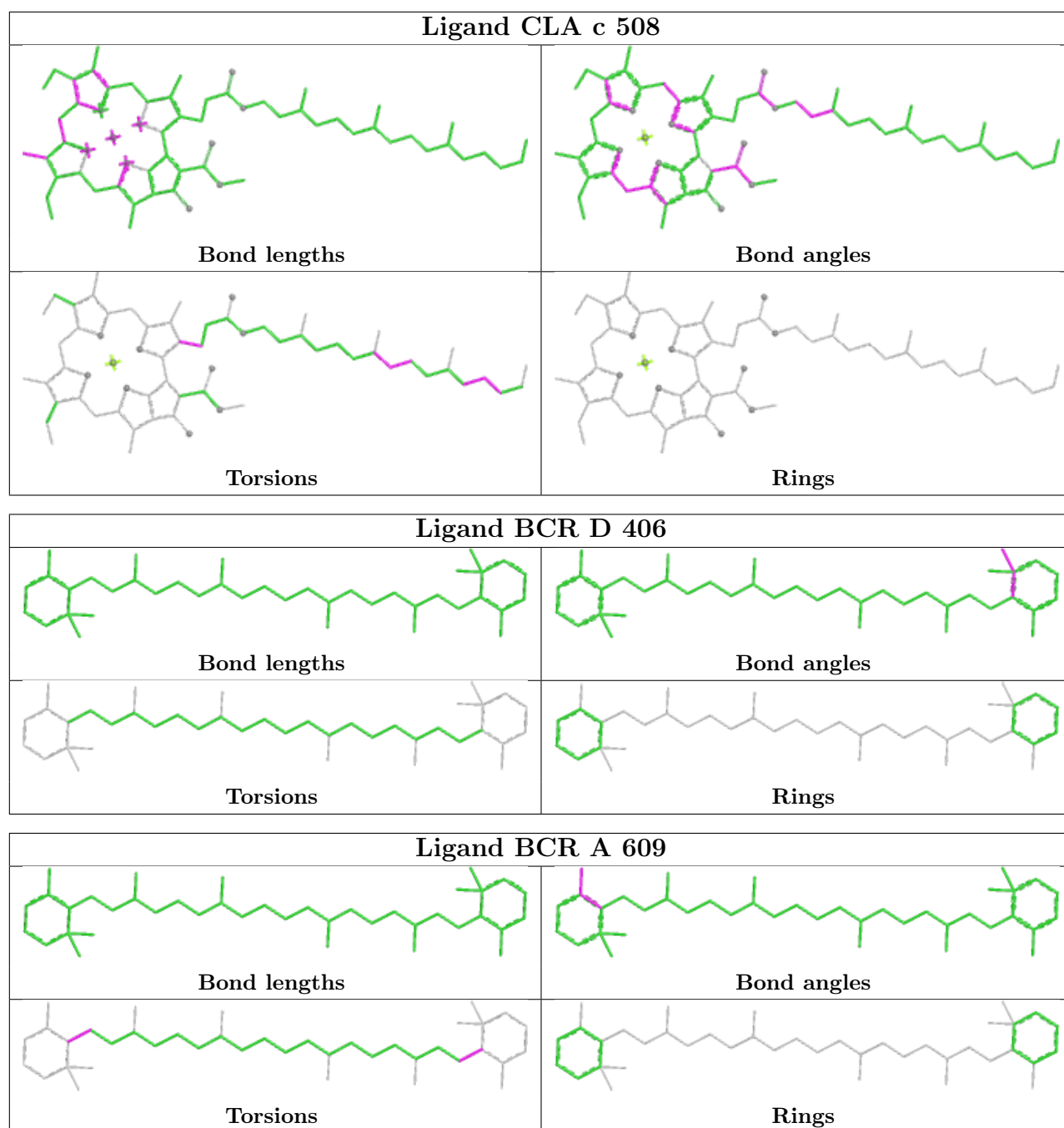
Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

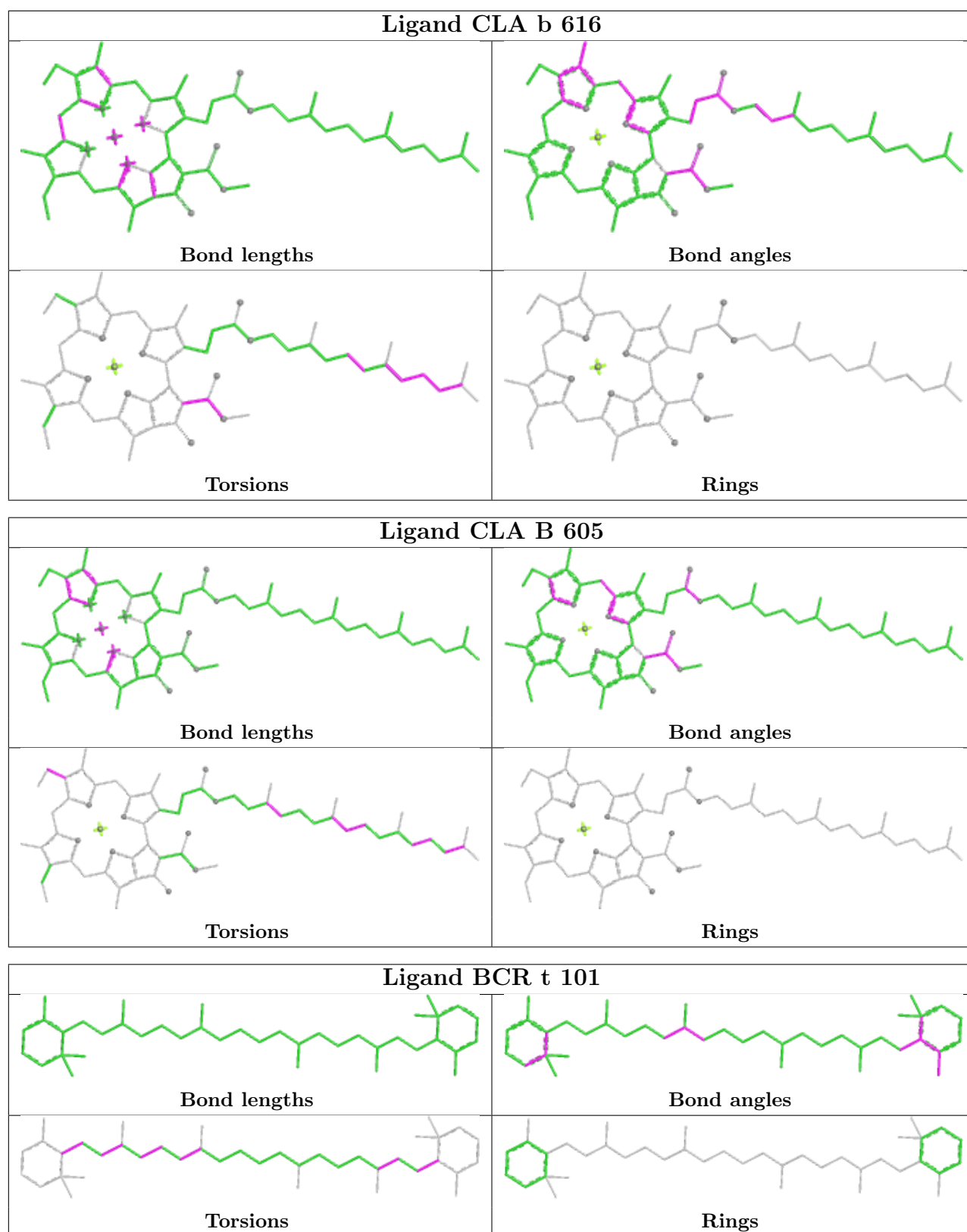


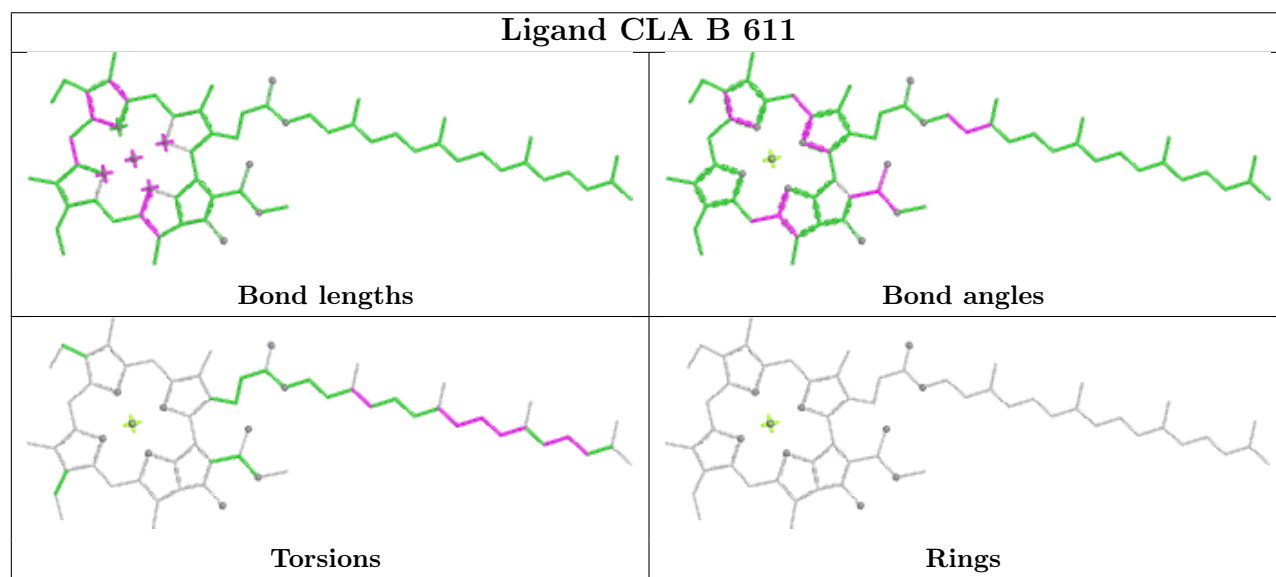
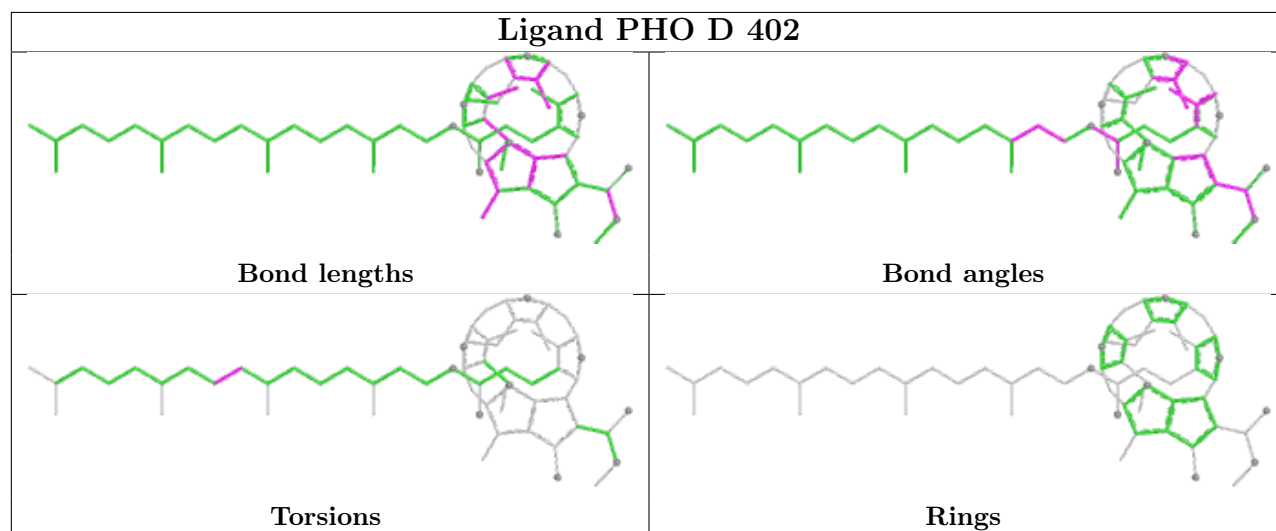
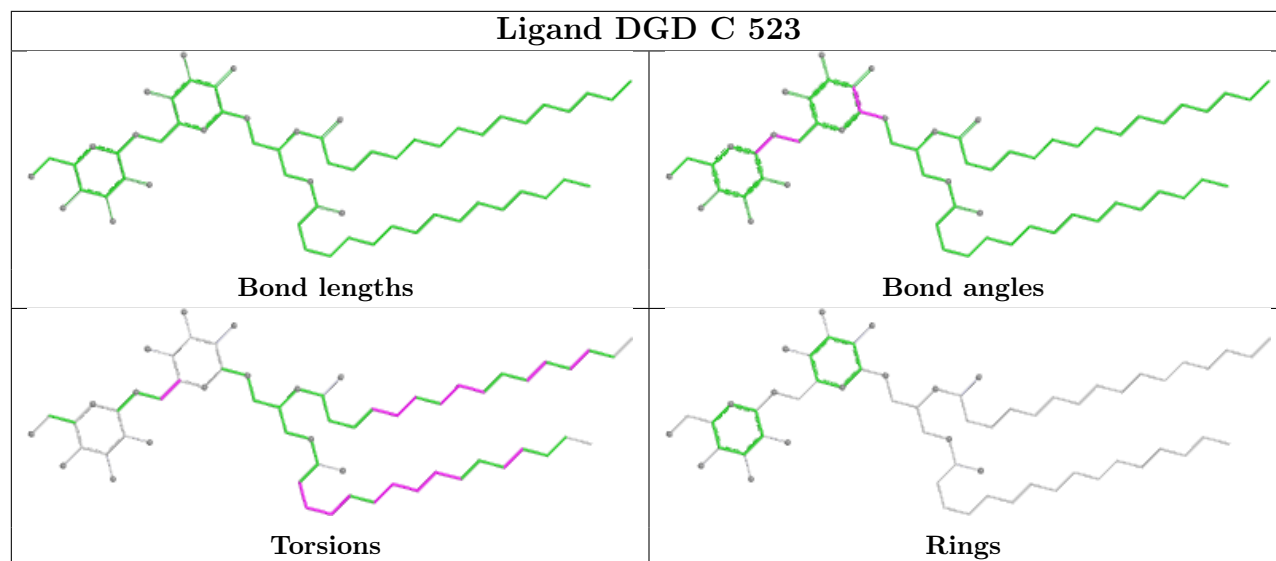
Ligand CLA B 601**Ligand CLA B 607**











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.20	2 (0%) 85 87	24, 30, 50, 79	0
1	a	334/344 (97%)	-0.08	3 (0%) 81 83	25, 32, 59, 78	0
2	B	505/510 (99%)	-0.07	7 (1%) 73 77	19, 33, 62, 89	5 (0%)
2	b	505/510 (99%)	0.07	11 (2%) 62 66	25, 37, 69, 110	1 (0%)
3	C	442/461 (95%)	0.04	2 (0%) 87 89	17, 38, 53, 76	1 (0%)
3	c	451/461 (97%)	0.16	7 (1%) 70 74	21, 41, 60, 96	2 (0%)
4	D	341/352 (96%)	-0.24	1 (0%) 90 91	25, 32, 49, 77	0
4	d	341/352 (96%)	-0.05	0 100 100	25, 36, 58, 79	1 (0%)
5	E	82/84 (97%)	0.68	3 (3%) 45 49	35, 53, 70, 84	1 (1%)
5	e	82/84 (97%)	0.82	7 (8%) 16 18	39, 60, 79, 85	0
6	F	34/45 (75%)	0.47	2 (5%) 28 32	37, 47, 60, 89	0
6	f	34/45 (75%)	0.60	0 100 100	44, 56, 75, 90	0
7	H	65/66 (98%)	0.26	1 (1%) 72 76	35, 42, 59, 77	0
7	h	63/66 (95%)	0.55	2 (3%) 50 54	41, 50, 61, 66	0
8	I	35/38 (92%)	0.10	1 (2%) 53 57	34, 39, 62, 76	0
8	i	35/38 (92%)	0.31	1 (2%) 53 57	33, 40, 70, 98	0
9	J	36/40 (90%)	0.59	2 (5%) 30 34	38, 55, 79, 89	0
9	j	36/40 (90%)	0.68	2 (5%) 30 34	40, 56, 86, 92	0
10	K	37/46 (80%)	0.68	0 100 100	46, 54, 69, 77	0
10	k	37/46 (80%)	0.67	0 100 100	50, 56, 75, 80	0
11	L	37/37 (100%)	-0.19	0 100 100	28, 30, 56, 67	0
11	l	36/37 (97%)	-0.28	0 100 100	28, 31, 61, 74	0
12	M	32/36 (88%)	0.07	1 (3%) 51 55	28, 33, 54, 74	0
12	m	31/36 (86%)	-0.16	0 100 100	30, 34, 51, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.11	6 (2%) 58 62	28, 41, 78, 119	1 (0%)
13	o	244/272 (89%)	0.15	3 (1%) 76 79	28, 41, 77, 126	0
14	T	29/32 (90%)	-0.05	2 (6%) 23 26	29, 33, 56, 71	0
14	t	29/32 (90%)	-0.03	2 (6%) 23 26	28, 33, 65, 79	0
15	U	97/134 (72%)	0.08	0 100 100	32, 42, 66, 93	0
15	u	97/134 (72%)	0.05	0 100 100	31, 40, 57, 86	0
16	V	137/163 (84%)	-0.01	0 100 100	31, 40, 55, 75	0
16	v	137/163 (84%)	0.33	1 (0%) 84 85	35, 47, 67, 85	0
17	Y	27/46 (58%)	1.80	11 (40%) 0 1	52, 75, 111, 119	0
17	y	30/46 (65%)	1.32	4 (13%) 7 8	63, 77, 96, 101	0
18	X	38/41 (92%)	0.63	3 (7%) 18 20	42, 54, 70, 78	0
18	x	39/41 (95%)	0.75	2 (5%) 33 37	47, 59, 83, 101	0
19	Z	62/62 (100%)	1.25	10 (16%) 4 5	56, 70, 110, 117	0
19	z	62/62 (100%)	1.39	8 (12%) 7 8	61, 72, 118, 127	0
20	R	28/41 (68%)	1.23	2 (7%) 22 25	63, 71, 88, 91	0
20	r	28/41 (68%)	1.63	8 (28%) 1 1	68, 84, 104, 121	0
All	All	5293/5700 (92%)	0.13	117 (2%) 62 66	17, 39, 73, 127	12 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	20	ALA	3.9
19	Z	33	TRP	3.9
19	z	33	TRP	3.9
20	r	29	LYS	3.8
20	r	28	VAL	3.7
17	Y	23	THR	3.5
5	e	79	PHE	3.5
19	Z	62	VAL	3.5
14	T	29	ILE	3.3
18	x	40	SER	3.3
17	Y	25	ILE	3.3
3	c	24	THR	3.3
13	o	58	ASN	3.3
3	c	147	PHE	3.2
3	c	23	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
5	E	79	PHE	3.1
17	Y	22	LEU	3.0
2	B	505	ARG	3.0
17	Y	28	ILE	3.0
2	b	488	PRO	3.0
2	b	496	TYR	3.0
1	a	11	ALA	2.9
2	B	499	VAL	2.9
2	b	495	PHE	2.9
1	A	11	ALA	2.9
2	b	486	LEU	2.9
2	b	494	GLY	2.9
19	z	40	ILE	2.8
7	H	65	LEU	2.8
20	R	28	VAL	2.8
14	t	30	THR	2.7
2	b	127	ARG	2.7
19	Z	30	PRO	2.7
2	B	479[A]	PHE	2.7
19	z	39	LEU	2.7
5	E	3	GLY	2.7
14	T	30	THR	2.7
2	B	496	TYR	2.7
17	y	45	ASN	2.7
19	z	3	ILE	2.7
9	j	5	GLY	2.6
17	Y	27	MET	2.6
9	J	5	GLY	2.6
5	E	29	ALA	2.6
6	F	12	SER	2.6
20	r	3	TRP	2.6
20	r	14	LEU	2.6
13	O	60	ARG	2.5
17	Y	21	GLN	2.5
7	h	21	VAL	2.5
9	j	6	GLY	2.5
3	C	142	GLU	2.5
13	O	56	PRO	2.5
17	y	22	LEU	2.5
20	r	26	TYR	2.5
9	J	6	GLY	2.5
19	z	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
19	Z	39	LEU	2.4
19	z	4	LEU	2.4
17	Y	26	ALA	2.4
19	Z	7	LEU	2.4
17	y	18	VAL	2.4
20	r	5	VAL	2.4
1	a	250	ALA	2.4
17	Y	46	LEU	2.4
18	x	37	VAL	2.4
19	Z	61	VAL	2.4
13	O	55	GLU	2.3
12	M	33	GLN	2.3
2	B	494	GLY	2.3
19	z	17	PHE	2.3
2	b	293	ALA	2.3
2	B	500	GLY	2.3
8	I	34	ARG	2.3
18	X	2	THR	2.3
5	e	21	VAL	2.2
19	z	27	TYR	2.2
13	O	61	GLN	2.2
6	F	16	PHE	2.2
5	e	22	ILE	2.2
14	t	29	ILE	2.2
2	b	499	VAL	2.2
3	C	32	GLY	2.2
4	D	229	ALA	2.2
13	o	3	GLN	2.2
3	c	204	LEU	2.2
18	X	39	ARG	2.2
3	c	143	TYR	2.2
16	v	35	TYR	2.2
13	O	57	LYS	2.2
17	Y	41	VAL	2.1
20	r	12	VAL	2.1
19	Z	32	ASP	2.1
2	B	495	PHE	2.1
5	e	14	ILE	2.1
19	Z	3	ILE	2.1
19	Z	59	PHE	2.1
2	b	491	VAL	2.1
2	b	502	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
13	o	57	LYS	2.1
17	y	34	MET	2.1
2	b	84	THR	2.1
3	c	134	ILE	2.1
5	e	3	GLY	2.1
20	R	7	VAL	2.1
20	r	27	ALA	2.1
5	e	4	THR	2.1
1	A	265	PHE	2.1
3	c	146	PHE	2.1
5	e	10	PHE	2.1
7	h	64	ALA	2.1
17	Y	24	MET	2.0
8	i	34	ARG	2.0
1	a	248	ILE	2.0
13	O	133	VAL	2.0
18	X	33	GLN	2.0
19	Z	57	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.90	0.10	32,37,48,64	0
12	FME	M	1	10/11	0.92	0.10	37,44,55,61	0
14	FME	T	1	10/11	0.93	0.10	31,39,51,68	0
8	FME	i	1	10/11	0.96	0.09	39,44,53,56	0
12	FME	m	1	10/11	0.96	0.08	30,45,65,65	0
8	FME	I	1	10/11	0.96	0.07	39,43,49,50	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
28	STE	i	101	12/20	0.58	0.18	66,83,93,94	0
28	STE	i	102	6/20	0.61	0.22	62,67,71,75	0
28	STE	H	103	18/20	0.65	0.23	56,73,76,80	0
28	STE	I	101	17/20	0.65	0.18	59,66,72,75	0
28	STE	e	105	13/20	0.66	0.21	75,83,89,91	0
28	STE	C	518	5/20	0.67	0.22	49,61,63,64	0
28	STE	f	103	16/20	0.67	0.21	63,75,84,87	0
28	STE	A	611	9/20	0.69	0.17	51,60,67,68	0
27	PL9	a	611	55/55	0.70	0.22	47,67,79,82	0
31	LHG	e	103	42/49	0.70	0.19	57,82,93,99	0
28	STE	h	103	11/20	0.71	0.23	60,63,64,69	0
28	STE	z	702	18/20	0.71	0.22	58,76,79,83	0
28	STE	C	520	10/20	0.71	0.21	59,67,73,83	0
28	STE	E	102	12/20	0.72	0.21	64,79,97,99	0
28	STE	d	413	14/20	0.72	0.18	55,61,85,91	0
29	LMG	D	408	50/55	0.72	0.19	41,66,92,97	0
28	STE	A	619	11/20	0.72	0.18	52,61,73,79	0
28	STE	B	627	12/20	0.73	0.17	44,57,66,68	0
27	PL9	A	610	55/55	0.73	0.22	43,65,86,89	0
29	LMG	c	516	30/55	0.73	0.18	49,73,96,97	0
31	LHG	A	614	49/49	0.73	0.18	49,78,100,112	0
28	STE	a	616	12/20	0.73	0.16	56,65,75,78	0
29	LMG	C	517	36/55	0.74	0.17	48,61,71,78	0
28	STE	C	516	14/20	0.74	0.20	51,63,69,69	0
28	STE	C	528	14/20	0.74	0.18	53,59,76,78	0
28	STE	C	519	7/20	0.74	0.20	53,56,61,67	0
28	STE	h	102	10/20	0.74	0.20	65,71,83,83	0
29	LMG	c	522	48/55	0.75	0.19	57,69,80,83	0
28	STE	A	618	17/20	0.75	0.16	51,61,67,69	0
28	STE	e	104	9/20	0.75	0.19	53,65,73,74	0
28	STE	f	102	8/20	0.76	0.22	58,61,66,75	0
29	LMG	B	625	55/55	0.77	0.15	39,56,70,78	0
28	STE	e	101	9/20	0.77	0.24	68,78,88,88	0
28	STE	E	103	20/20	0.77	0.17	47,66,73,76	0
29	LMG	b	622	55/55	0.77	0.20	50,66,79,83	0
32	DGD	A	616	66/66	0.77	0.16	46,57,73,80	0
28	STE	B	628	15/20	0.78	0.19	45,58,61,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	C	527	14/20	0.79	0.17	56,66,80,84	0
28	STE	d	410	20/20	0.79	0.16	50,63,80,83	0
29	LMG	B	620	45/55	0.80	0.16	34,58,76,83	0
28	STE	T	102	16/20	0.80	0.18	32,49,67,72	0
28	STE	t	102	10/20	0.80	0.16	46,52,56,57	0
28	STE	z	701	13/20	0.80	0.20	63,69,75,79	0
28	STE	b	623	16/20	0.80	0.20	52,59,76,82	0
28	STE	B	626	18/20	0.81	0.15	44,52,82,87	0
28	STE	I	102	15/20	0.81	0.17	46,51,64,67	0
28	STE	J	102	12/20	0.81	0.17	46,55,63,65	0
28	STE	C	525	12/20	0.82	0.17	38,44,51,52	0
24	CLA	b	601	65/65	0.82	0.13	50,65,82,90	0
30	SQD	A	615	43/54	0.83	0.12	40,53,81,87	0
30	SQD	a	614	54/54	0.83	0.14	38,59,83,88	0
28	STE	E	101	12/20	0.83	0.15	59,68,79,79	0
28	STE	Z	101	17/20	0.83	0.19	55,72,85,86	0
28	STE	b	624	15/20	0.83	0.17	46,54,73,75	0
29	LMG	c	521	46/55	0.84	0.14	49,66,75,80	0
29	LMG	C	524	48/55	0.85	0.16	44,68,83,85	0
28	STE	d	412	20/20	0.85	0.14	41,54,67,68	0
29	LMG	a	615	49/55	0.85	0.14	40,55,68,74	0
28	STE	m	102	12/20	0.85	0.14	43,46,69,76	0
28	STE	H	104	9/20	0.86	0.14	47,56,71,74	0
29	LMG	A	612	48/55	0.86	0.13	42,55,67,71	0
28	STE	X	101	20/20	0.86	0.13	37,50,67,75	0
28	STE	b	625	10/20	0.86	0.14	47,54,69,69	0
28	STE	j	101	12/20	0.86	0.14	51,60,67,68	0
24	CLA	B	601	65/65	0.86	0.13	42,54,79,86	0
28	STE	M	103	10/20	0.86	0.17	39,50,53,60	0
29	LMG	M	101	51/55	0.86	0.12	31,48,63,67	0
28	STE	b	621	20/20	0.86	0.14	40,53,62,62	0
26	BCR	J	101	40/40	0.87	0.13	41,53,59,65	0
28	STE	B	621	17/20	0.87	0.15	38,49,64,64	0
30	SQD	b	620	49/54	0.87	0.11	39,56,68,75	0
28	STE	C	526	16/20	0.87	0.14	42,50,56,62	0
28	STE	z	703	9/20	0.87	0.21	54,67,71,71	0
29	LMG	m	101	51/55	0.87	0.12	39,50,62,65	0
28	STE	d	407	20/20	0.88	0.13	39,52,75,78	0
28	STE	M	102	15/20	0.88	0.11	37,43,53,66	0
30	SQD	f	101	41/54	0.88	0.14	53,76,85,91	0
24	CLA	C	513	65/65	0.88	0.12	48,59,78,80	0
30	SQD	B	623	54/54	0.88	0.11	36,56,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	SQD	a	613	54/54	0.88	0.14	44,61,74,80	0
26	BCR	x	101	40/40	0.89	0.11	38,54,61,65	0
26	BCR	C	514	40/40	0.89	0.13	47,54,62,64	0
28	STE	B	624	14/20	0.89	0.10	34,44,56,60	0
24	CLA	c	513	65/65	0.89	0.13	50,60,83,85	0
26	BCR	d	405	40/40	0.89	0.13	34,48,80,88	0
26	BCR	k	101	40/40	0.89	0.13	46,58,64,69	0
30	SQD	D	410	36/54	0.89	0.14	47,68,80,83	0
28	STE	A	617	8/20	0.90	0.14	44,48,52,53	0
24	CLA	c	512	65/65	0.90	0.12	47,54,75,84	0
32	DGD	C	522	62/66	0.90	0.12	36,48,87,99	0
26	BCR	D	406	40/40	0.91	0.12	36,44,75,77	0
26	BCR	H	101	40/40	0.91	0.10	31,47,55,59	0
26	BCR	B	618	40/40	0.91	0.09	27,36,44,49	0
26	BCR	b	619	40/40	0.91	0.10	33,43,56,60	0
26	BCR	c	514	40/40	0.91	0.12	50,58,66,68	0
28	STE	l	102	18/20	0.91	0.12	36,42,64,65	0
24	CLA	C	511	65/65	0.91	0.11	38,48,60,64	0
32	DGD	H	102	62/66	0.91	0.10	33,40,51,55	0
32	DGD	c	519	62/66	0.91	0.11	39,50,77,80	0
32	DGD	h	101	62/66	0.91	0.11	37,44,53,53	0
26	BCR	b	618	40/40	0.92	0.09	26,38,45,46	0
26	BCR	B	619	40/40	0.92	0.09	29,39,50,52	0
24	CLA	c	511	65/65	0.92	0.11	43,53,62,66	0
26	BCR	c	517	40/40	0.92	0.12	46,53,62,67	0
24	CLA	C	503	65/65	0.92	0.09	35,43,47,52	0
31	LHG	a	612	49/49	0.92	0.12	36,47,59,63	0
29	LMG	d	411	44/55	0.92	0.11	40,49,71,75	0
24	CLA	C	512	65/65	0.92	0.11	43,50,78,84	0
30	SQD	A	613	52/54	0.92	0.11	32,53,80,84	0
26	BCR	t	101	40/40	0.92	0.08	26,34,42,44	0
29	LMG	D	409	51/55	0.92	0.12	32,47,72,81	0
24	CLA	c	503	65/65	0.92	0.10	34,44,48,54	0
26	BCR	A	609	40/40	0.93	0.08	26,34,40,41	0
26	BCR	c	515	40/40	0.93	0.10	31,44,52,54	0
26	BCR	B	617	40/40	0.93	0.09	26,38,43,44	0
24	CLA	b	606	65/65	0.93	0.09	29,36,62,69	0
24	CLA	C	508	65/65	0.93	0.11	33,39,87,95	0
24	CLA	c	504	60/65	0.93	0.10	31,44,74,77	0
26	BCR	C	515	40/40	0.93	0.10	30,39,48,51	0
24	CLA	C	510	65/65	0.93	0.09	35,41,53,62	0
24	CLA	a	605	65/65	0.93	0.08	25,30,37,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	PL9	d	406	55/55	0.93	0.09	25,33,39,45	0
31	LHG	d	409	39/49	0.93	0.11	34,43,64,70	0
24	CLA	C	502	65/65	0.93	0.09	33,38,53,56	0
26	BCR	K	101	40/40	0.93	0.11	42,49,57,64	0
26	BCR	T	101	40/40	0.93	0.09	29,38,48,50	0
26	BCR	b	617	40/40	0.93	0.08	30,38,43,48	0
25	PHO	A	607	64/64	0.93	0.08	28,33,37,42	0
32	DGD	c	520	62/66	0.93	0.11	33,47,69,83	0
25	PHO	a	608	64/64	0.93	0.08	32,38,44,51	0
33	BCT	D	401	4/4	0.93	0.09	33,34,37,38	0
33	BCT	d	401	4/4	0.93	0.08	36,38,46,49	0
24	CLA	b	616	60/65	0.94	0.10	28,38,78,85	0
24	CLA	c	502	65/65	0.94	0.08	33,41,50,56	0
24	CLA	B	616	60/65	0.94	0.09	25,34,72,79	0
24	CLA	C	504	59/65	0.94	0.09	32,42,73,80	0
24	CLA	c	505	65/65	0.94	0.09	31,39,54,60	0
24	CLA	c	506	65/65	0.94	0.10	35,44,75,81	0
24	CLA	c	507	65/65	0.94	0.08	31,41,50,53	0
24	CLA	c	508	64/65	0.94	0.10	34,41,80,94	0
24	CLA	c	509	65/65	0.94	0.10	35,43,59,60	0
24	CLA	c	510	65/65	0.94	0.09	37,44,54,57	0
24	CLA	C	506	65/65	0.94	0.10	33,42,75,79	0
31	LHG	B	622	49/49	0.94	0.11	29,40,56,60	0
31	LHG	D	412	47/49	0.94	0.12	32,40,75,77	0
24	CLA	C	501	65/65	0.94	0.08	26,33,43,47	0
24	CLA	a	609	65/65	0.94	0.10	22,29,71,77	0
24	CLA	d	404	65/65	0.94	0.10	33,39,74,79	0
24	CLA	C	509	65/65	0.94	0.09	31,40,57,61	0
32	DGD	C	521	62/66	0.94	0.10	26,36,69,73	0
24	CLA	b	605	65/65	0.94	0.08	25,34,43,48	0
32	DGD	C	523	62/66	0.94	0.10	33,41,70,89	0
24	CLA	B	606	65/65	0.94	0.09	24,34,58,65	0
27	PL9	D	407	55/55	0.94	0.08	22,31,38,41	0
24	CLA	b	609	65/65	0.94	0.08	32,41,54,63	0
24	CLA	b	610	65/65	0.94	0.09	29,35,43,46	0
24	CLA	b	614	65/65	0.94	0.09	26,34,63,71	0
24	CLA	b	615	65/65	0.94	0.08	30,37,51,54	0
34	HEM	e	102	43/43	0.94	0.11	49,59,69,77	0
24	CLA	B	610	65/65	0.95	0.08	23,30,39,41	0
24	CLA	b	602	65/65	0.95	0.09	32,37,54,57	0
24	CLA	b	603	65/65	0.95	0.09	27,32,55,62	0
24	CLA	b	604	65/65	0.95	0.09	24,31,59,71	0

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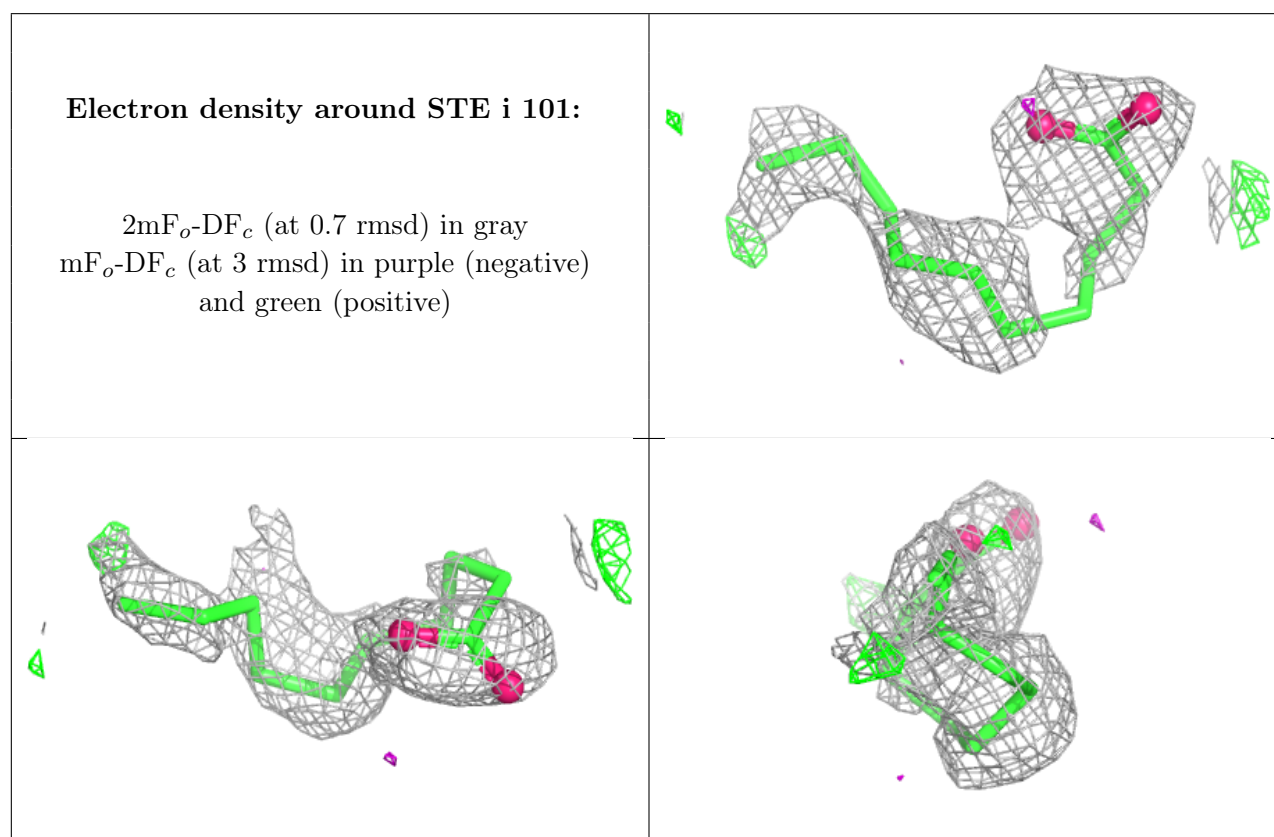
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	612	65/65	0.95	0.07	22,29,40,44	0
26	BCR	a	610	40/40	0.95	0.07	25,32,43,43	0
24	CLA	B	615	65/65	0.95	0.08	27,34,48,54	0
24	CLA	b	608	65/65	0.95	0.08	31,39,50,53	0
24	CLA	C	505	65/65	0.95	0.08	26,36,56,68	0
31	LHG	L	101	49/49	0.95	0.08	31,37,46,63	0
24	CLA	B	604	65/65	0.95	0.08	22,30,56,59	0
31	LHG	d	408	49/49	0.95	0.08	30,37,45,52	0
24	CLA	d	402	65/65	0.95	0.07	22,29,41,53	0
24	CLA	d	403	65/65	0.95	0.08	24,30,46,57	0
31	LHG	l	101	49/49	0.95	0.09	34,40,48,54	0
24	CLA	b	611	65/65	0.95	0.07	26,32,43,46	0
24	CLA	b	612	65/65	0.95	0.08	25,31,39,43	0
25	PHO	D	402	64/64	0.95	0.07	22,28,33,35	0
25	PHO	a	607	64/64	0.95	0.07	25,29,35,41	0
24	CLA	D	403	65/65	0.95	0.07	22,28,36,49	0
32	DGD	c	518	62/66	0.95	0.09	27,37,63,69	0
24	CLA	D	404	65/65	0.95	0.07	21,27,49,53	0
24	CLA	D	405	65/65	0.95	0.09	30,35,104,124	0
24	CLA	c	501	65/65	0.95	0.08	32,38,47,50	0
24	CLA	C	507	65/65	0.95	0.08	28,38,48,54	0
24	CLA	a	606	65/65	0.95	0.10	28,36,83,87	0
24	CLA	B	609	65/65	0.95	0.07	29,37,48,53	0
24	CLA	B	607	65/65	0.96	0.07	21,29,50,58	0
24	CLA	B	608	65/65	0.96	0.07	26,30,46,50	0
24	CLA	b	607	65/65	0.96	0.09	25,32,56,61	0
24	CLA	A	605	65/65	0.96	0.07	19,27,39,47	0
24	CLA	B	602	65/65	0.96	0.07	26,33,48,55	0
24	CLA	B	611	65/65	0.96	0.07	23,27,41,47	0
24	CLA	B	603	65/65	0.96	0.08	24,29,53,58	0
24	CLA	B	613	65/65	0.96	0.07	23,28,57,64	0
31	LHG	D	411	49/49	0.96	0.08	28,35,44,47	0
24	CLA	b	613	65/65	0.96	0.08	23,30,64,74	0
24	CLA	B	614	65/65	0.96	0.09	23,32,62,71	0
24	CLA	A	606	65/65	0.96	0.09	25,31,88,93	0
24	CLA	B	605	65/65	0.96	0.06	24,29,41,44	0
34	HEM	F	101	43/43	0.96	0.09	43,49,58,64	0
24	CLA	A	608	54/65	0.96	0.07	23,28,55,62	0
35	HEC	V	201	43/43	0.97	0.06	27,32,39,41	0
35	HEC	v	201	43/43	0.97	0.07	28,35,44,47	0
23	CL	a	604	1/1	0.98	0.08	32,32,32,32	0
22	FE2	a	602	1/1	0.98	0.03	43,43,43,43	0

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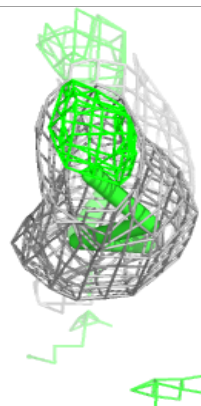
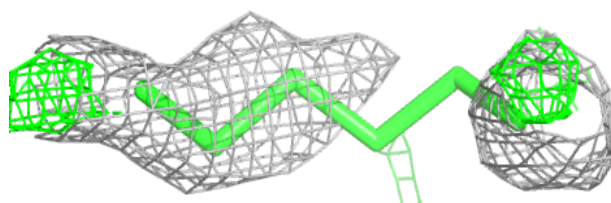
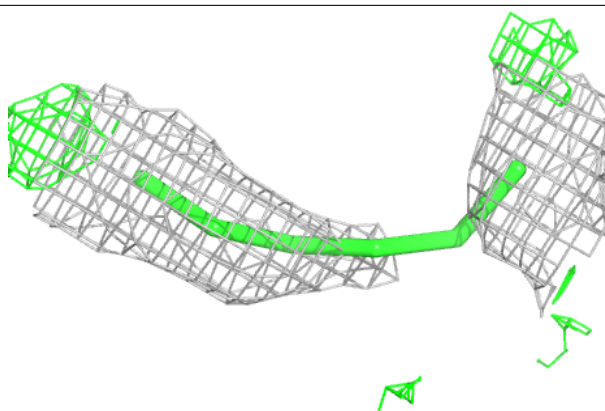
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CL	a	603	1/1	0.99	0.05	31,31,31,31	0
21	OEX	a	601	10/10	0.99	0.03	23,30,34,35	0
22	FE2	A	602	1/1	0.99	0.06	38,38,38,38	0
21	OEX	A	601	10/10	0.99	0.04	25,30,33,35	0
23	CL	A	603	1/1	0.99	0.03	29,29,29,29	0
23	CL	A	604	1/1	1.00	0.06	29,29,29,29	0

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

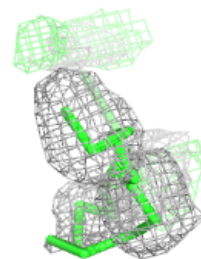
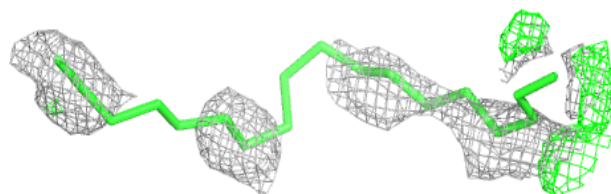
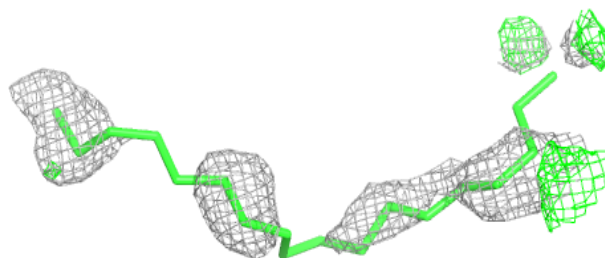


Electron density around STE i 102:

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

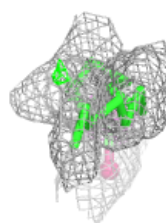
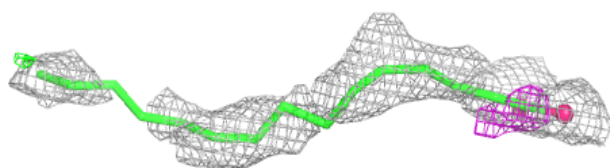
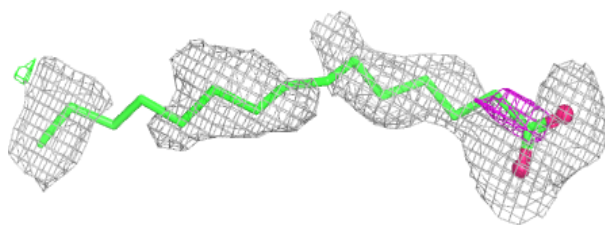
**Electron density around STE H 103:**

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

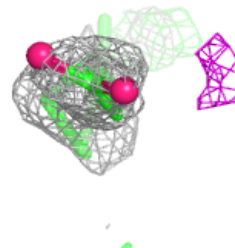
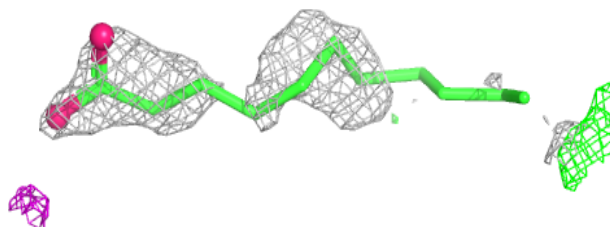
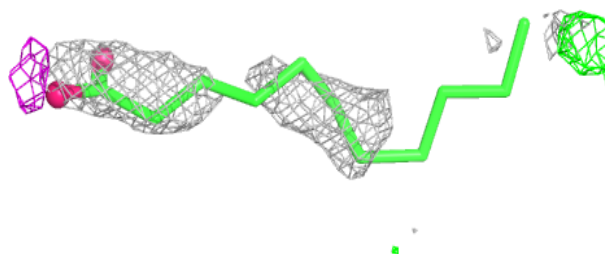


Electron density around STE I 101:

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

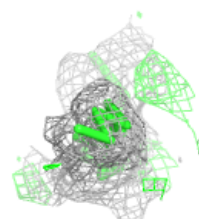
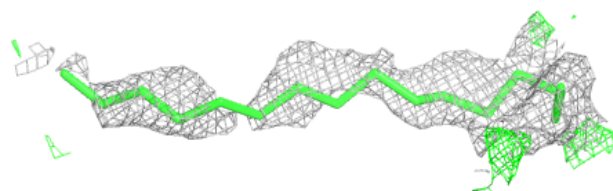
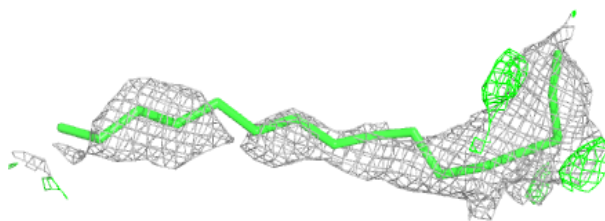
**Electron density around STE e 105:**

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

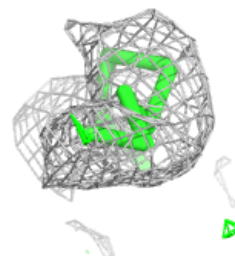
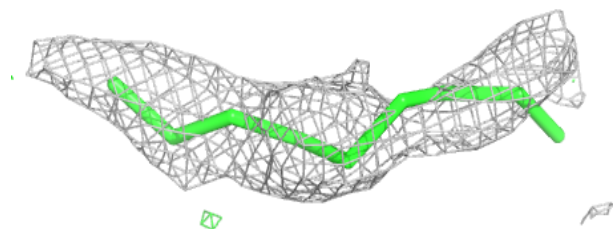
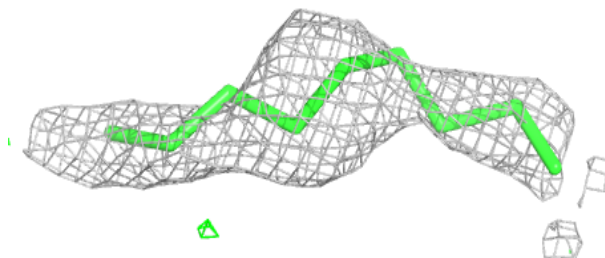


Electron density around STE f 103:

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

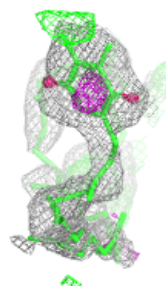
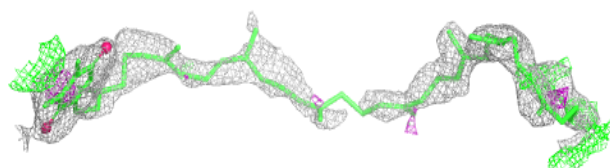
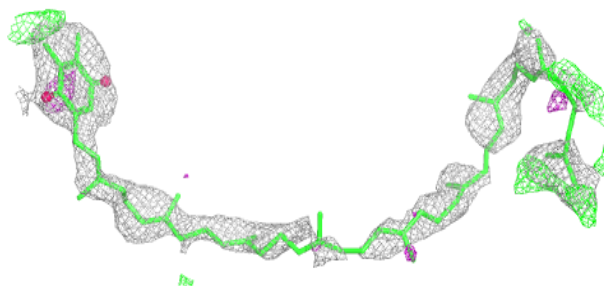
**Electron density around STE A 611:**

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

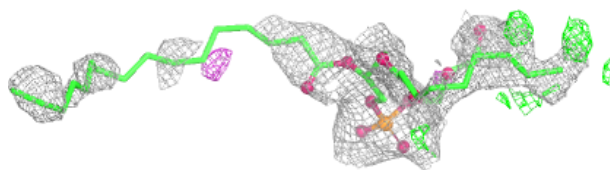
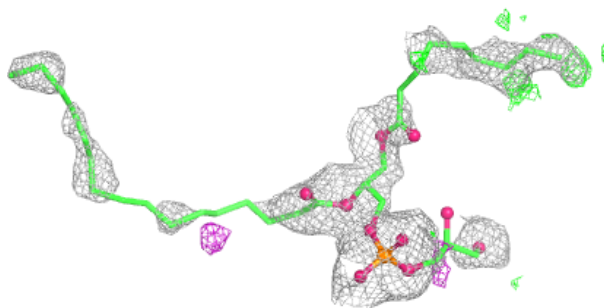


Electron density around PL9 a 611:

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

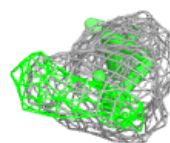
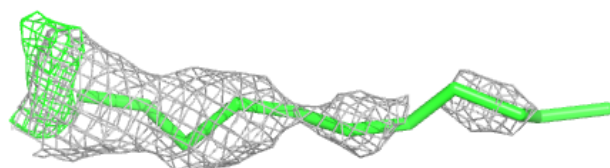
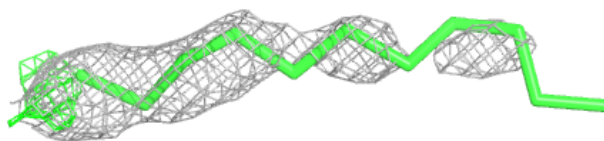
**Electron density around LHG e 103:**

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

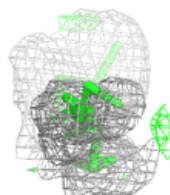
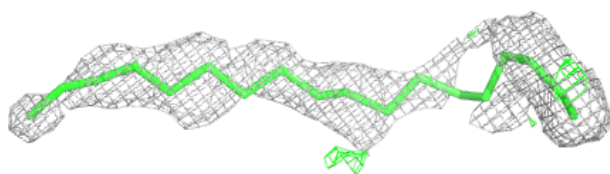
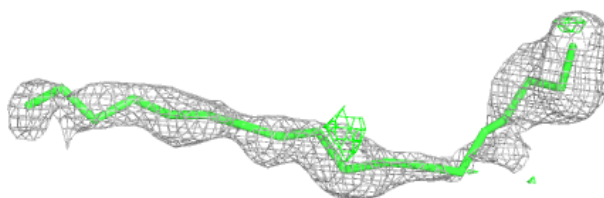


Electron density around STE h 103:

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

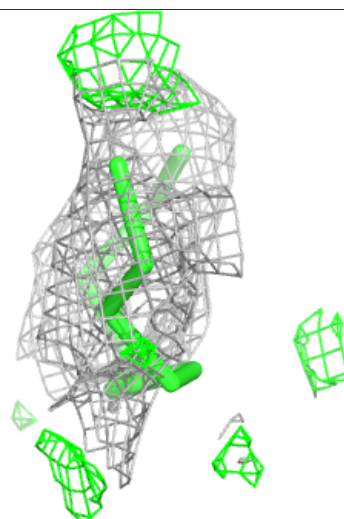
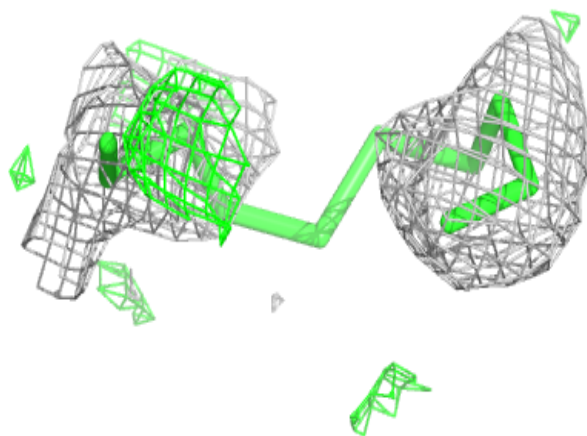
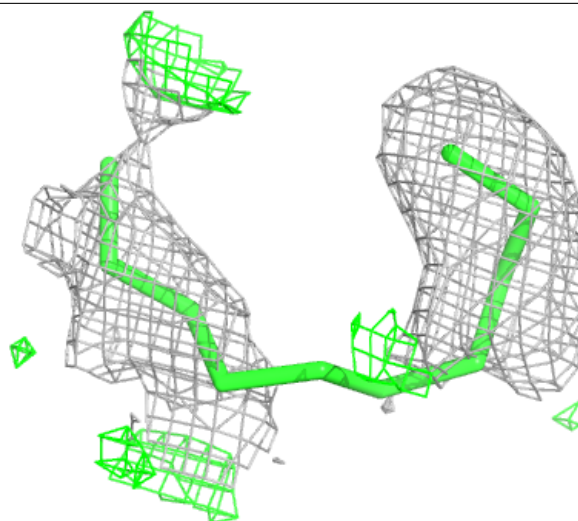
**Electron density around STE z 702:**

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



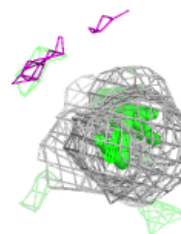
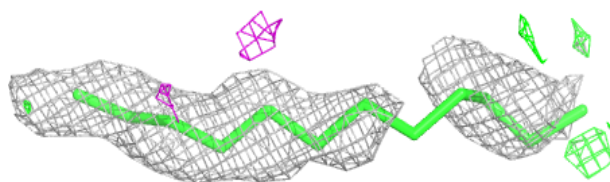
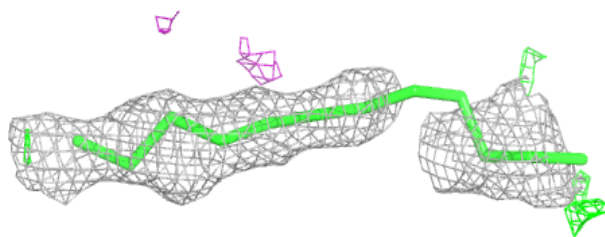
Electron density around STE C 520:

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

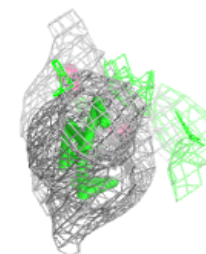
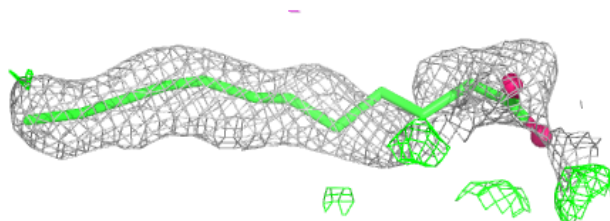
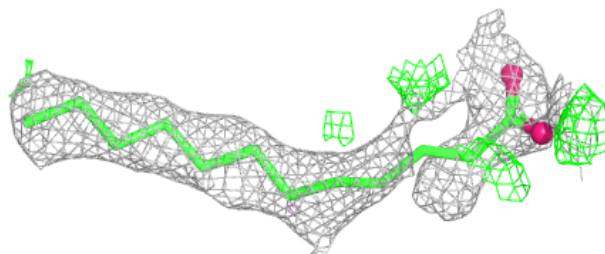


Electron density around STE E 102:

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and green (positive)

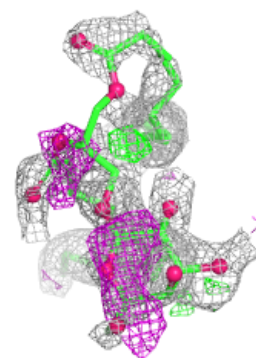
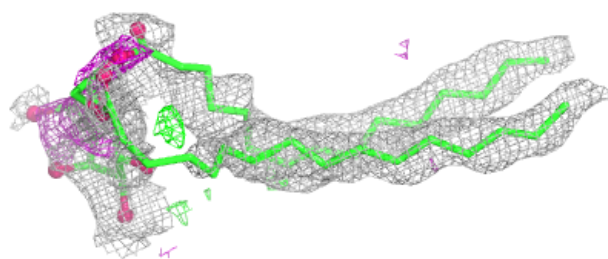
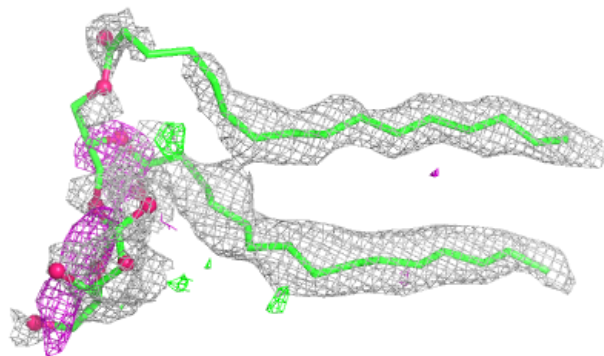
**Electron density around STE d 413:**

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

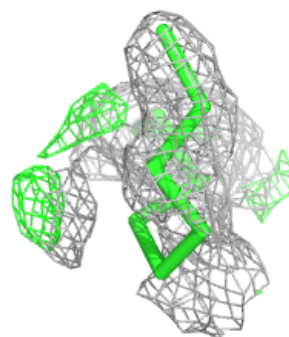
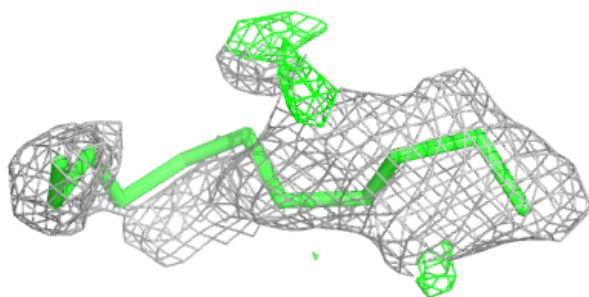
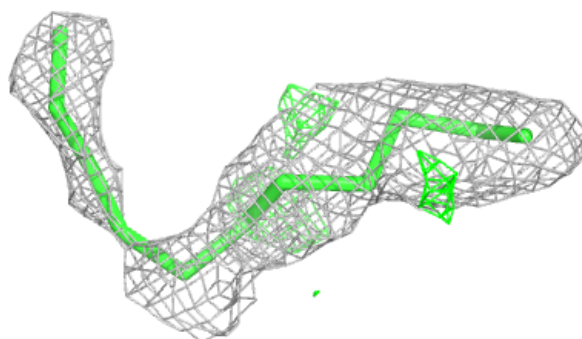


Electron density around LMG D 408:

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

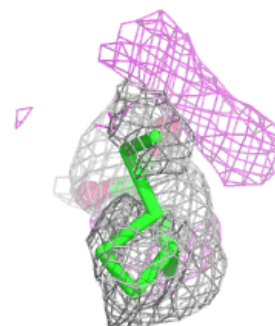
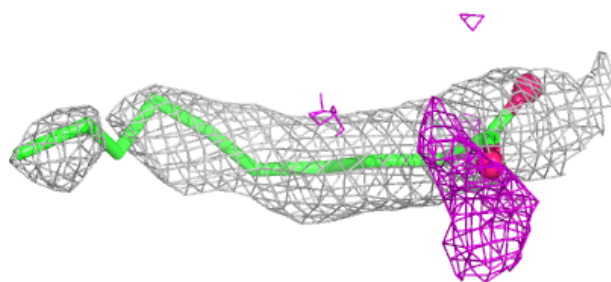
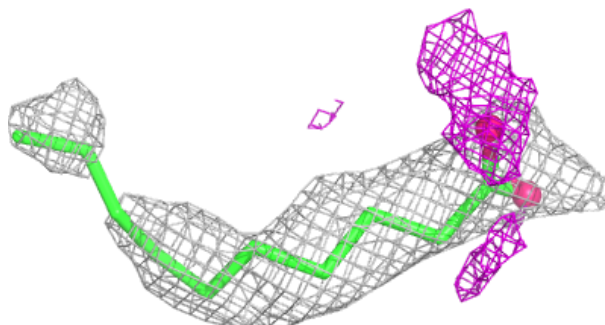
**Electron density around STE A 619:**

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

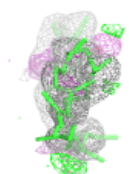
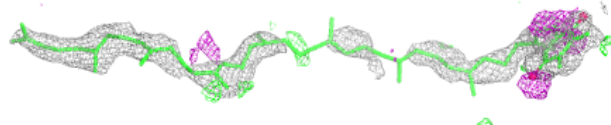
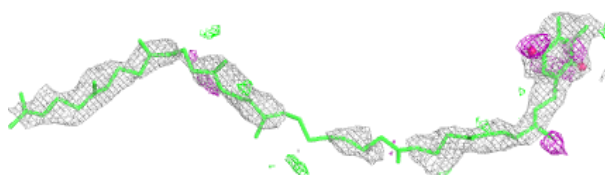


Electron density around STE B 627:

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

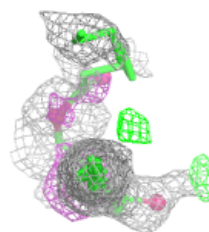
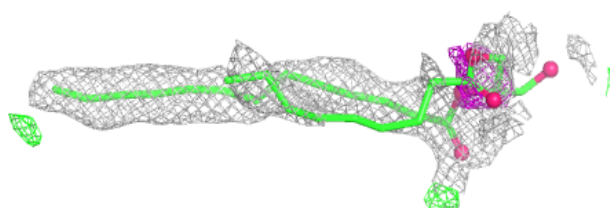
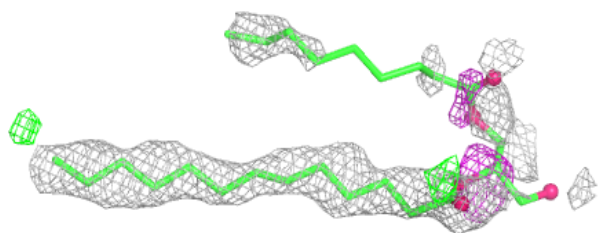
**Electron density around PL9 A 610:**

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

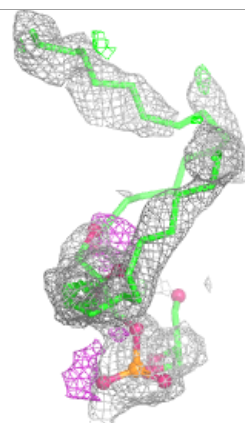
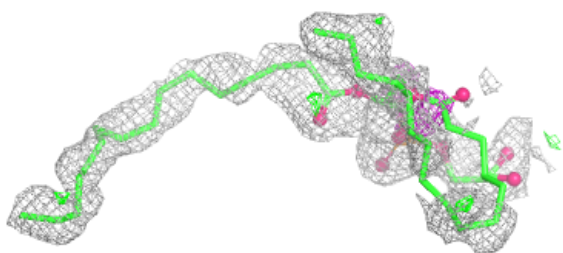
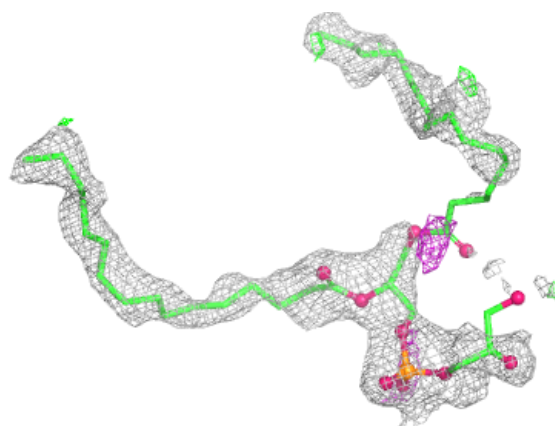


Electron density around LMG c 516:

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

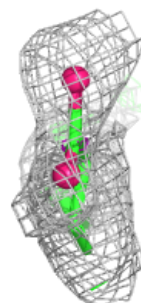
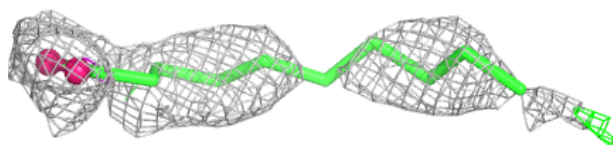
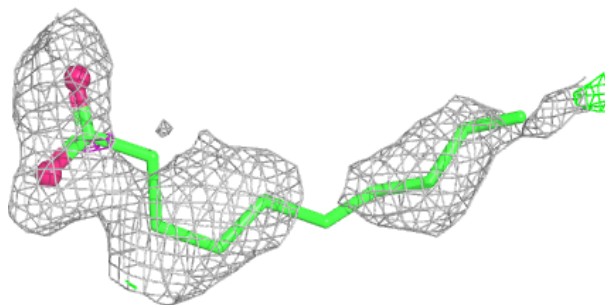
**Electron density around LHG A 614:**

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

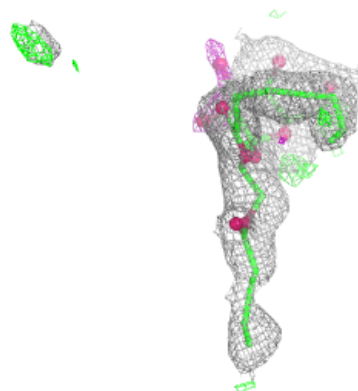
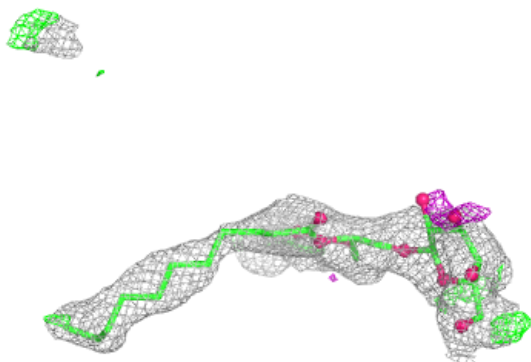
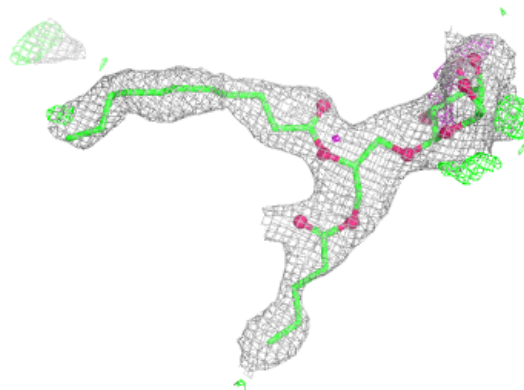


Electron density around STE a 616:

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

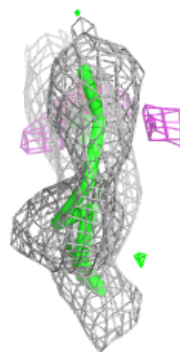
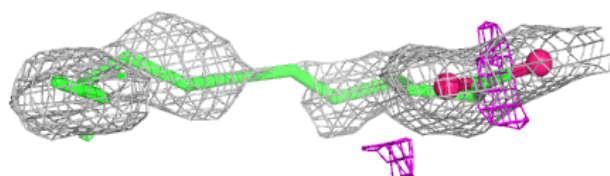
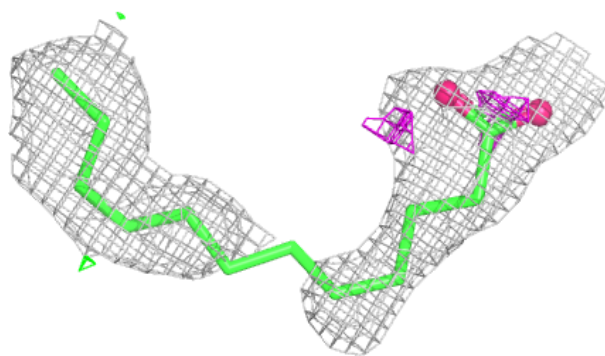
**Electron density around LMG C 517:**

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

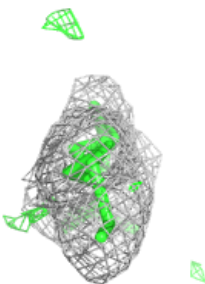
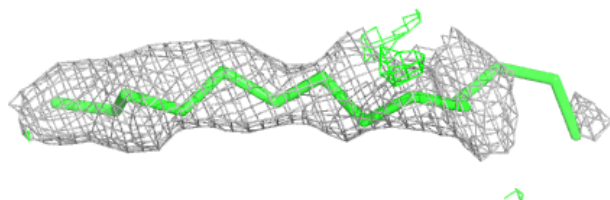
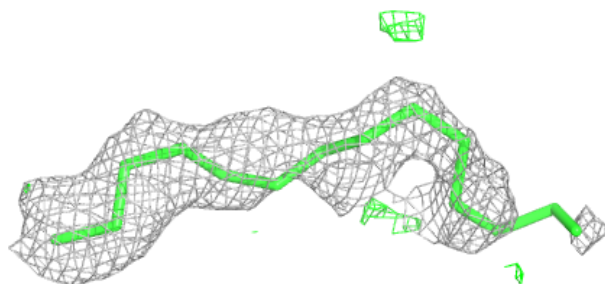


Electron density around STE C 516:

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

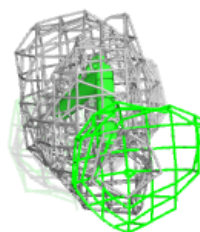
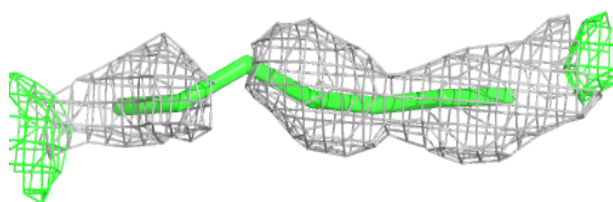
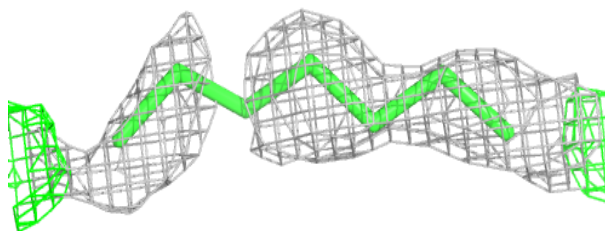
**Electron density around STE C 528:**

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

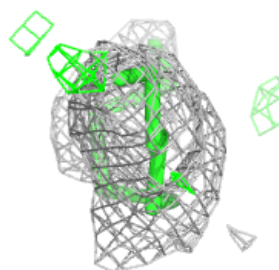
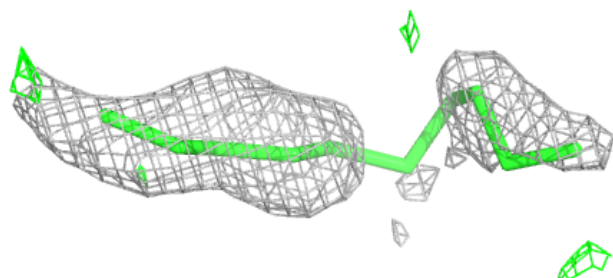
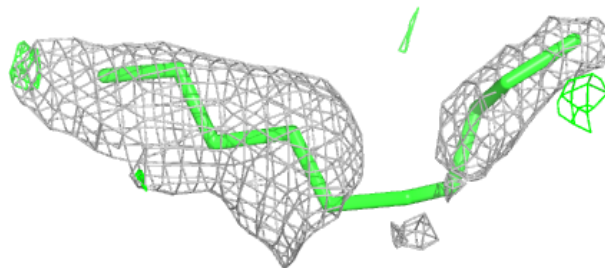


Electron density around STE C 519:

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

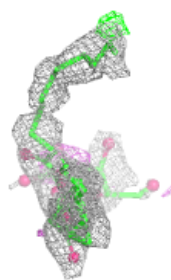
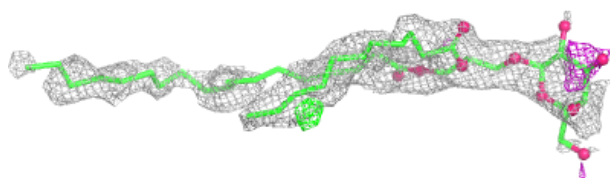
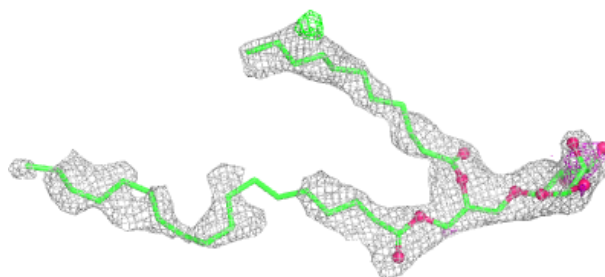
**Electron density around STE h 102:**

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

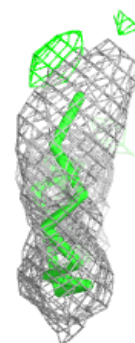
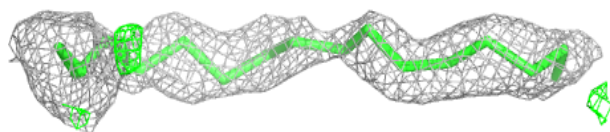
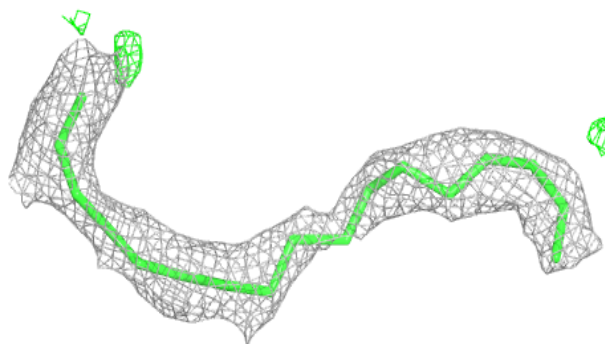


Electron density around LMG c 522:

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

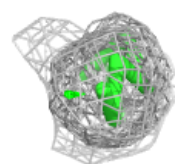
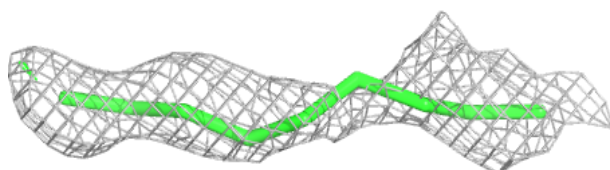
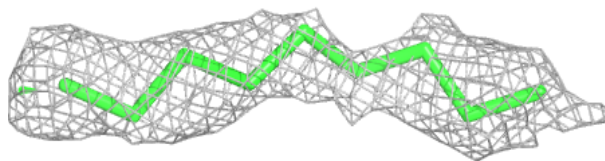
**Electron density around STE A 618:**

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

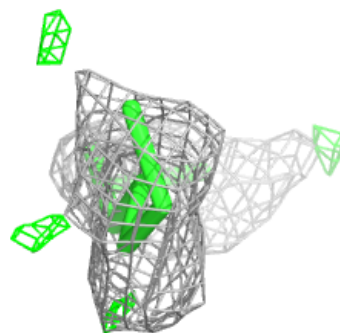
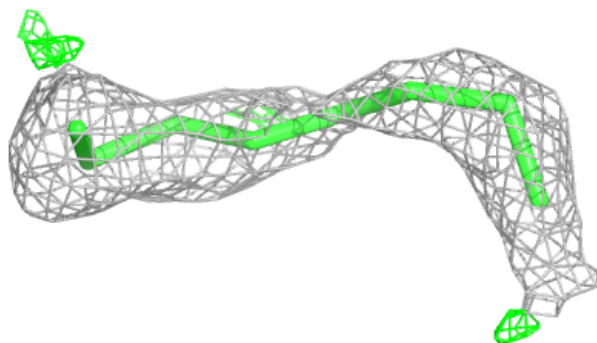
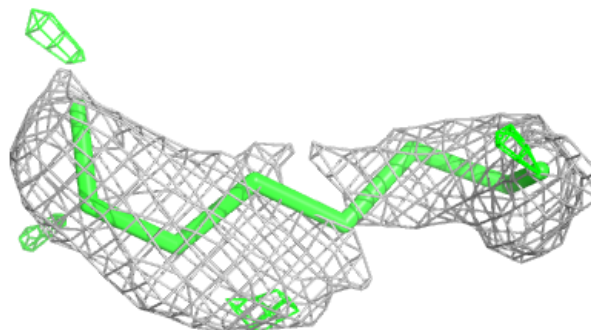


Electron density around STE e 104:

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

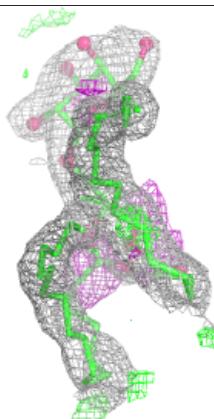
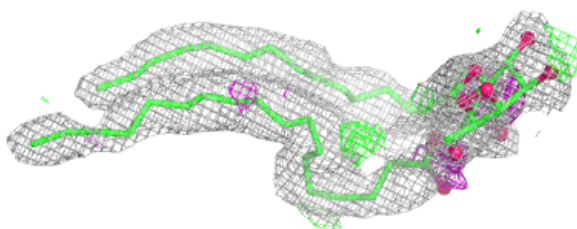
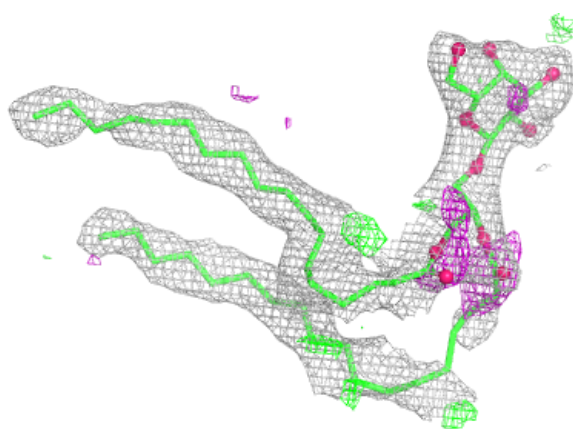
**Electron density around STE f 102:**

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

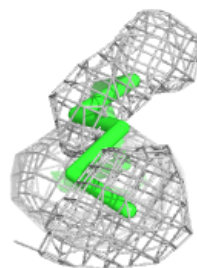
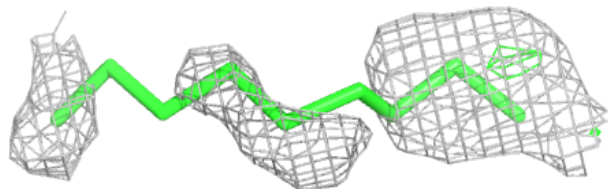
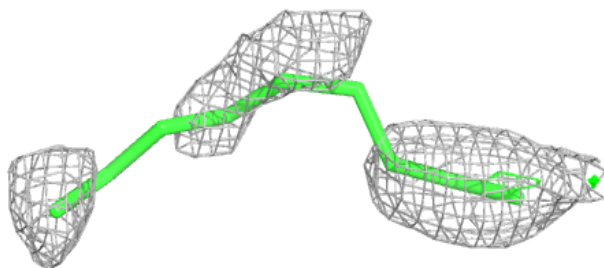


Electron density around LMG B 625:

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

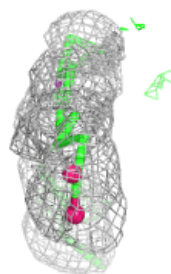
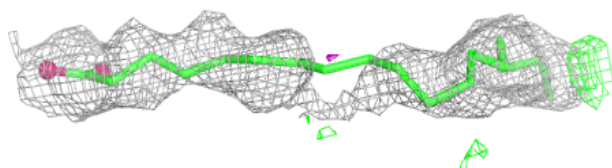
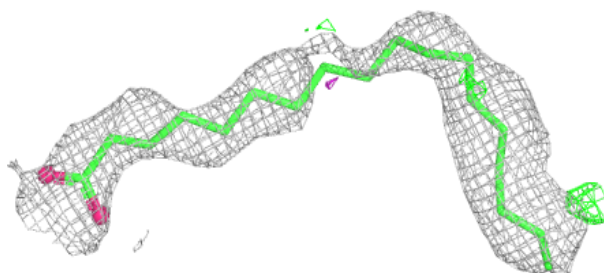
**Electron density around STE e 101:**

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

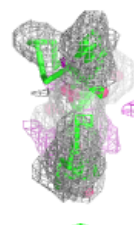
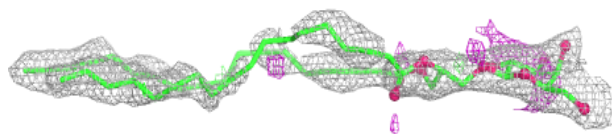
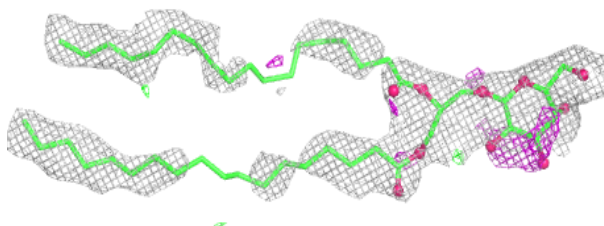


Electron density around STE E 103:

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

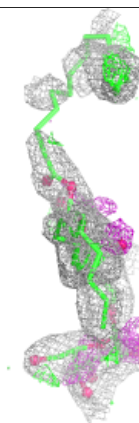
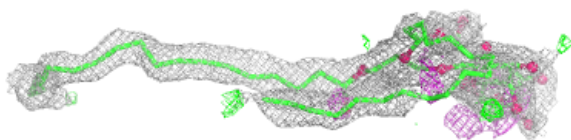
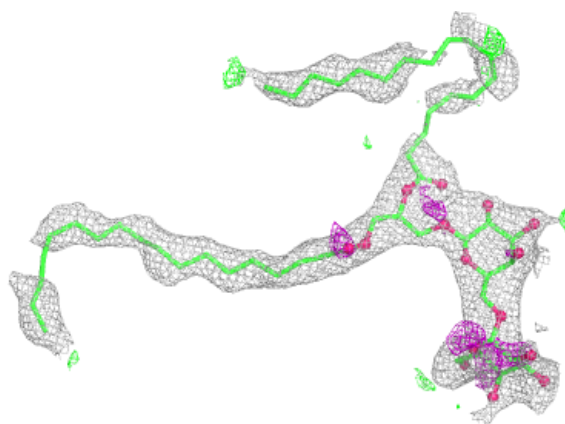
**Electron density around LMG b 622:**

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

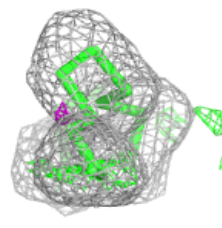
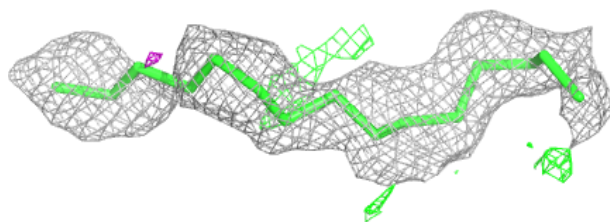
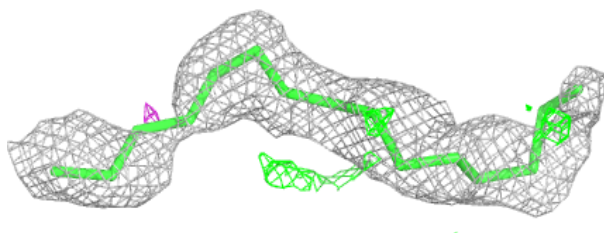


Electron density around DGD A 616:

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

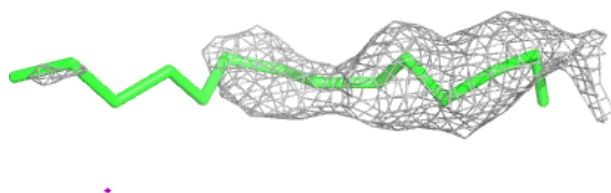
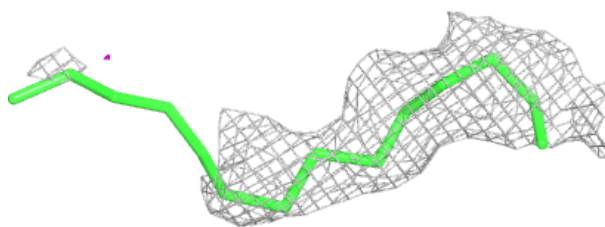
**Electron density around STE B 628:**

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

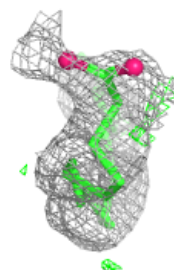
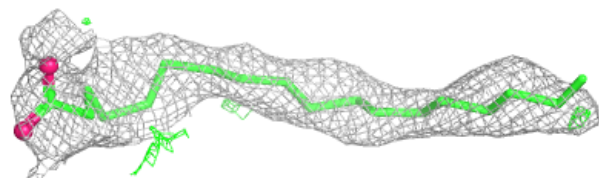
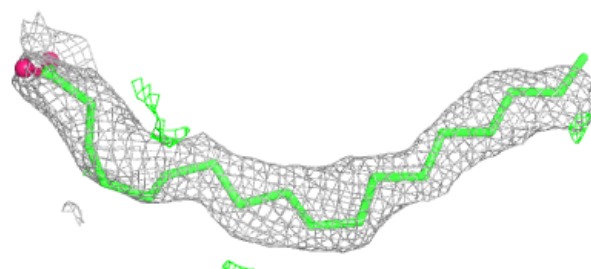


Electron density around STE C 527:

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

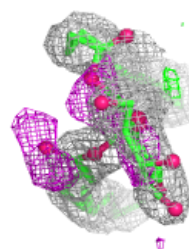
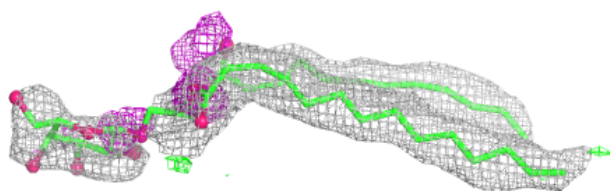
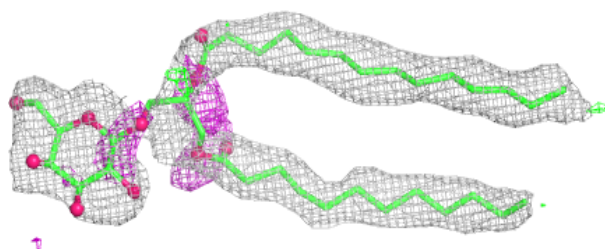
**Electron density around STE d 410:**

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

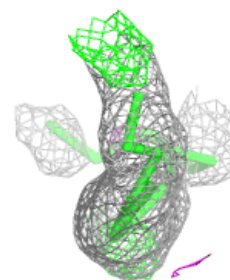
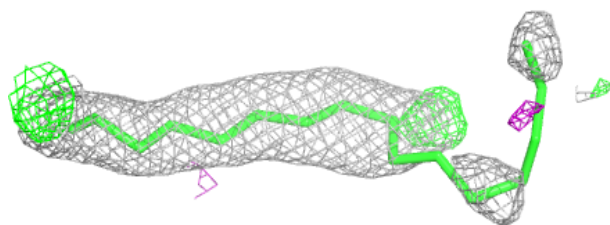
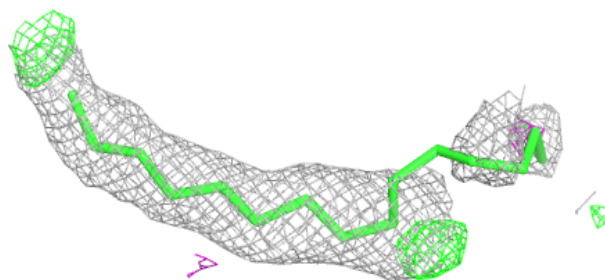


Electron density around LMG B 620:

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

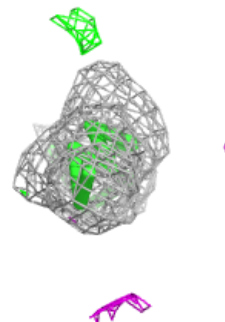
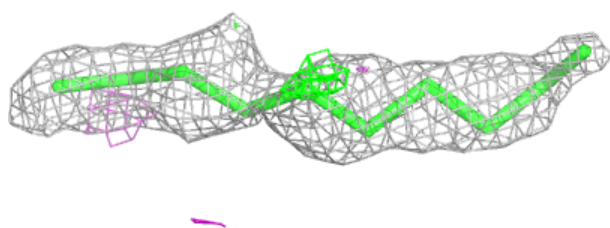
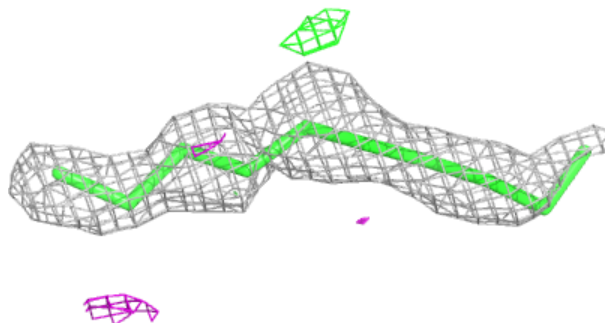
**Electron density around STE T 102:**

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

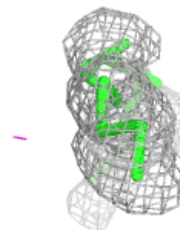
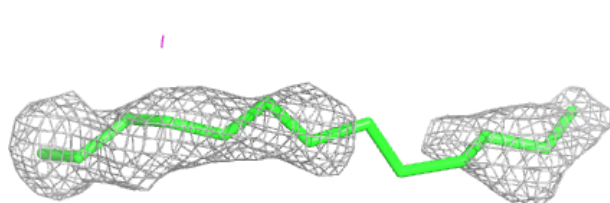
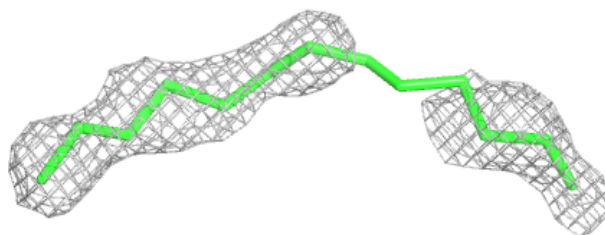


Electron density around STE t 102:

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

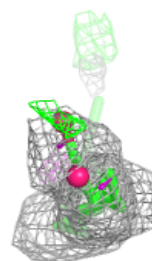
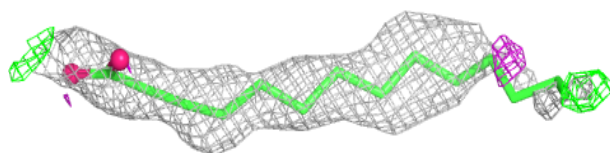
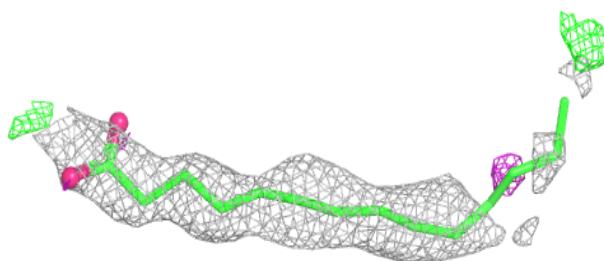
**Electron density around STE z 701:**

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

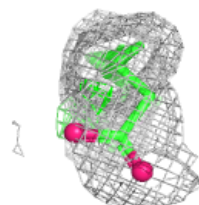
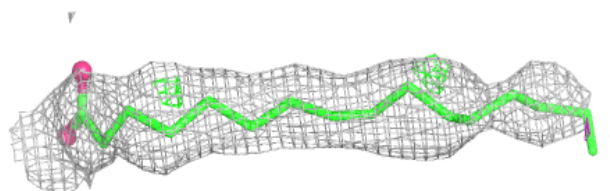
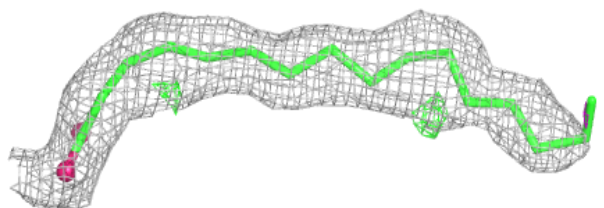


Electron density around STE b 623:

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

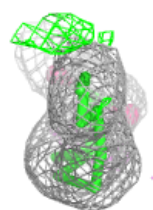
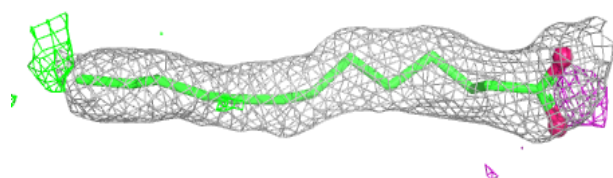
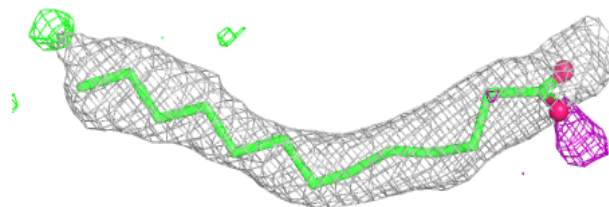
**Electron density around STE B 626:**

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

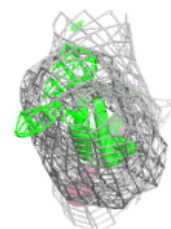
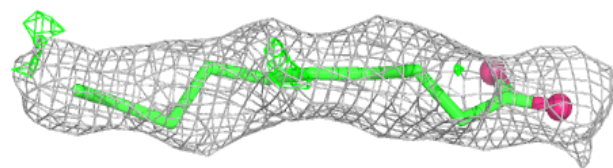
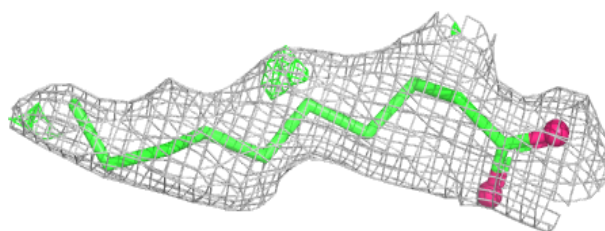


Electron density around STE I 102:

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

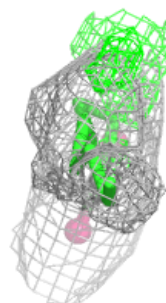
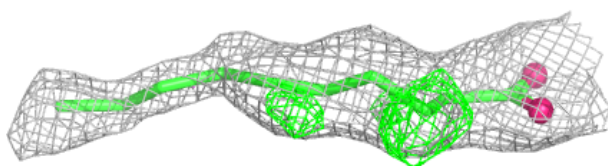
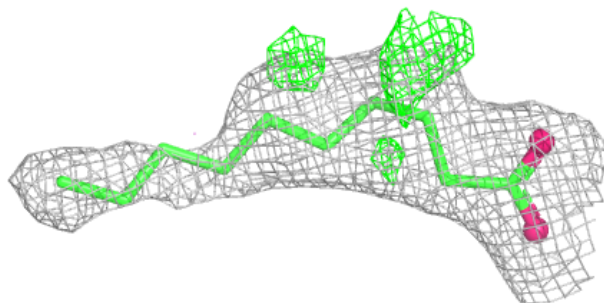
**Electron density around STE J 102:**

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

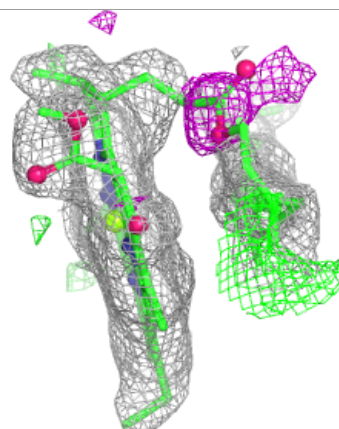
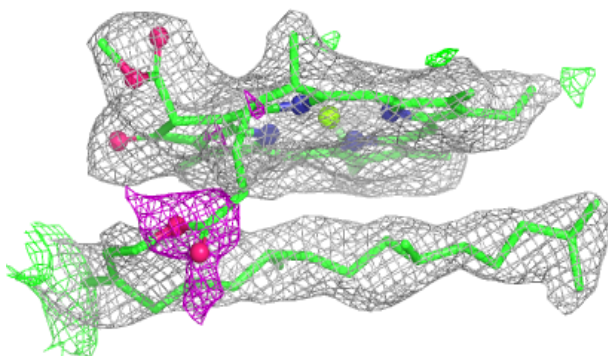
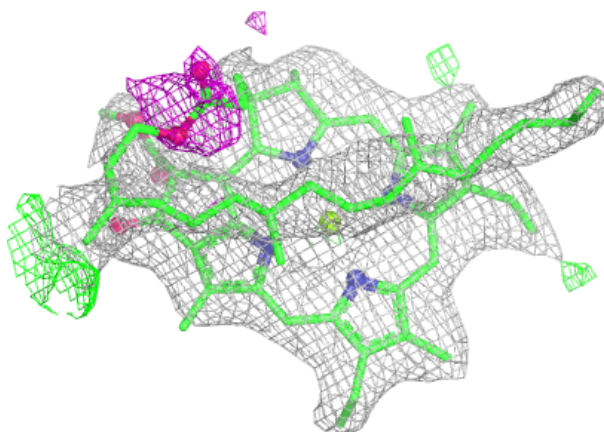


Electron density around STE C 525:

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

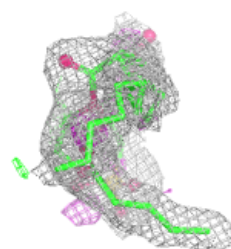
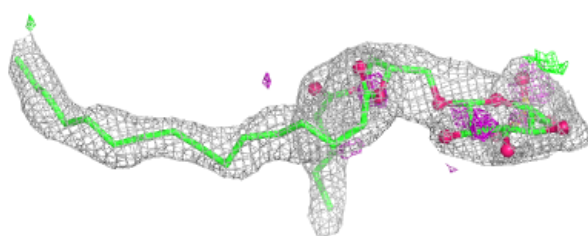
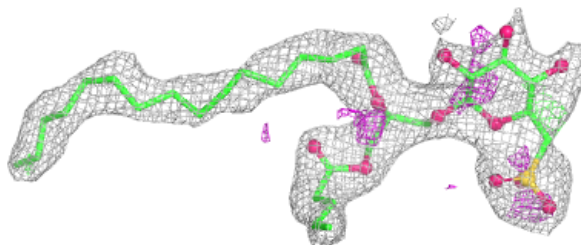
**Electron density around CLA b 601:**

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

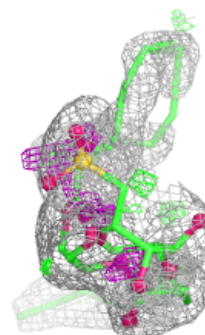
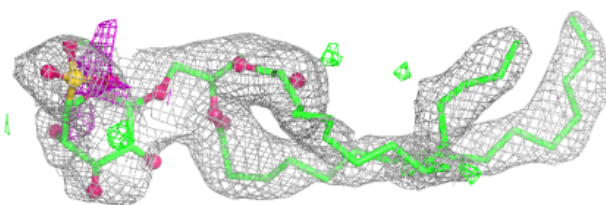
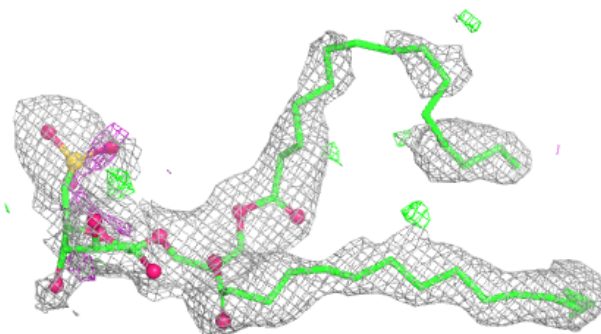


Electron density around SQD A 615:

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

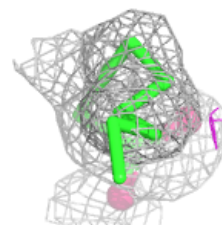
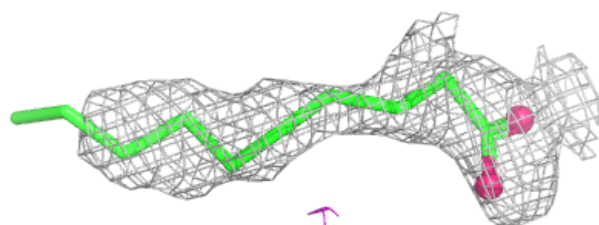
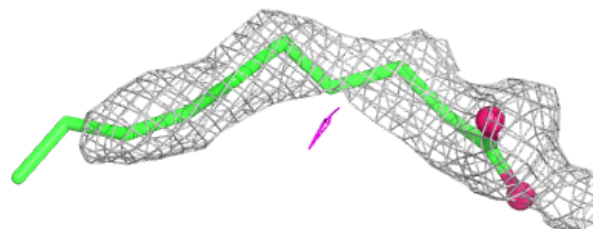
**Electron density around SQD a 614:**

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

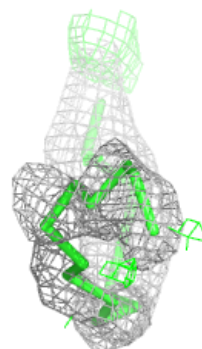
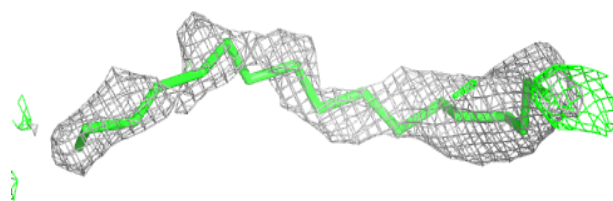
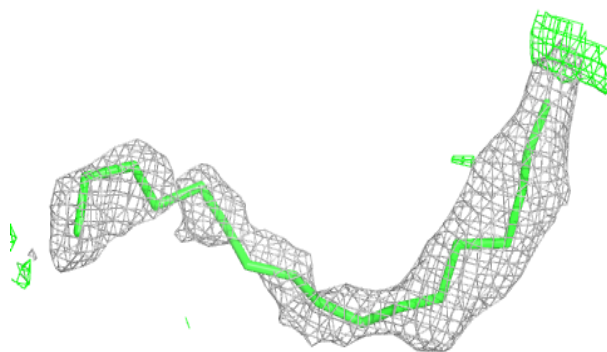


Electron density around STE E 101:

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

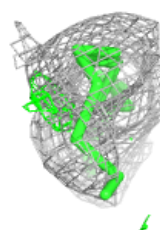
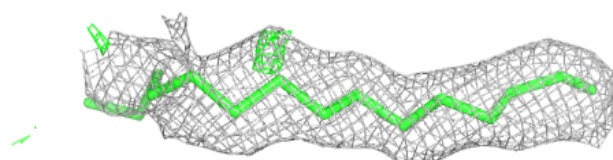
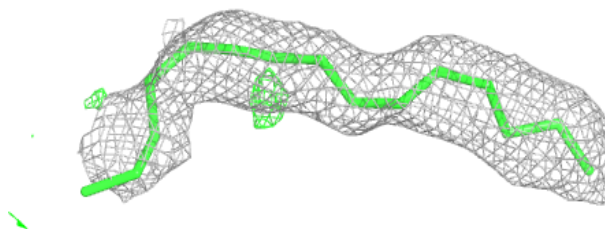
**Electron density around STE Z 101:**

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

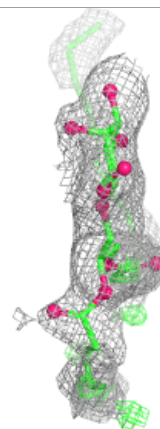
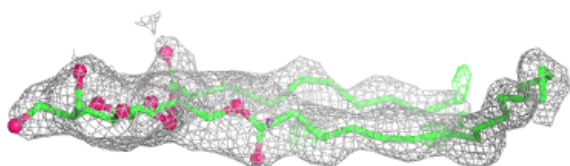
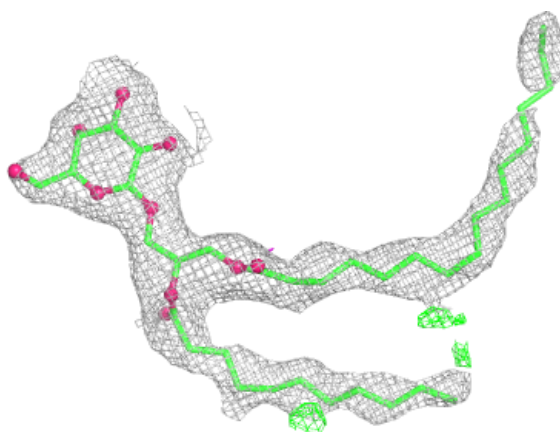


Electron density around STE b 624:

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

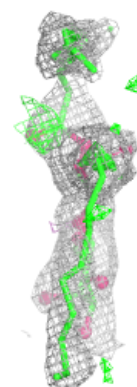
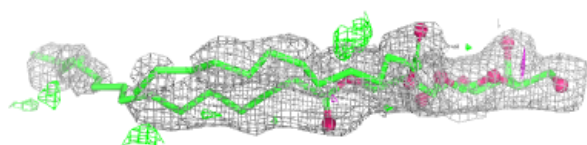
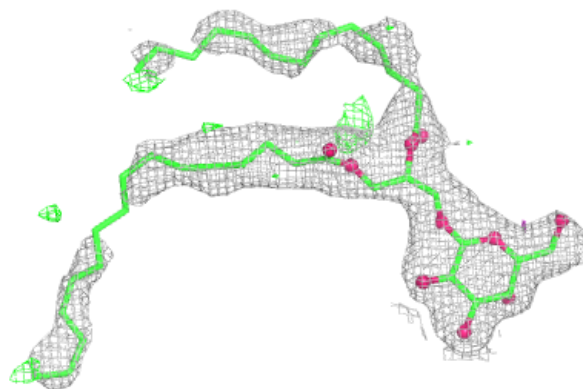
**Electron density around LMG c 521:**

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

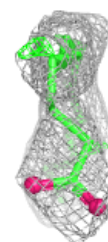
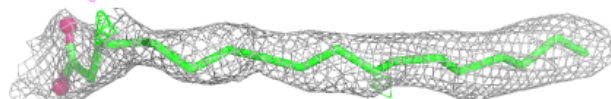
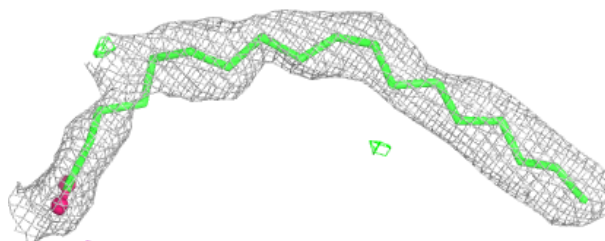


Electron density around LMG C 524:

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

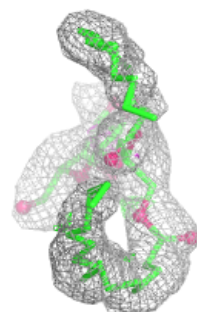
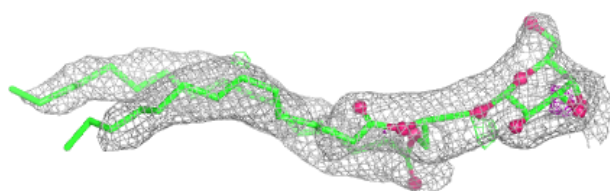
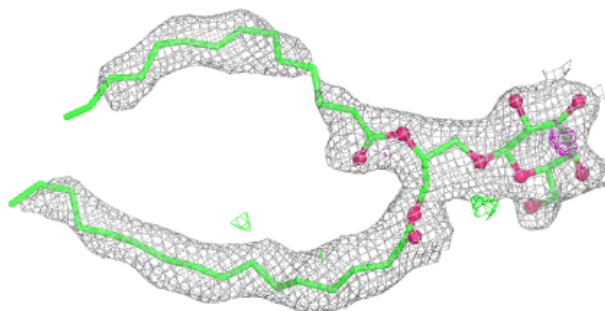
**Electron density around STE d 412:**

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

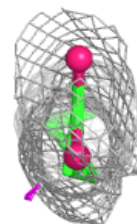
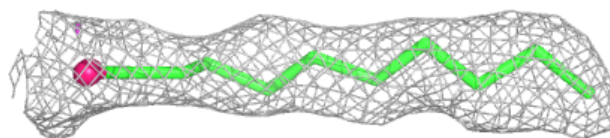
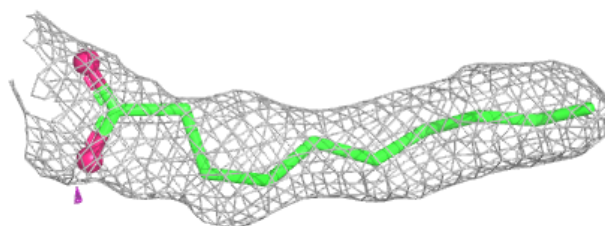


Electron density around LMG a 615:

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

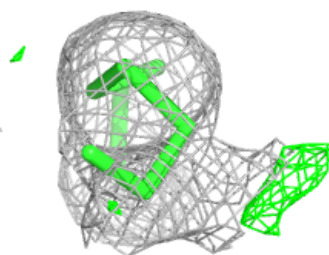
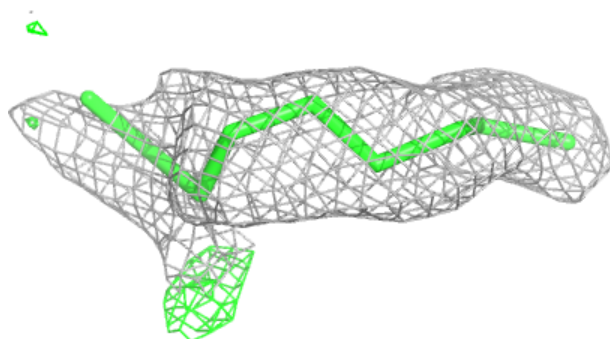
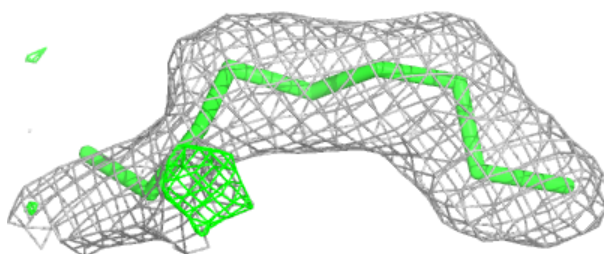
**Electron density around STE m 102:**

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

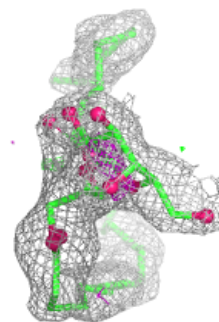
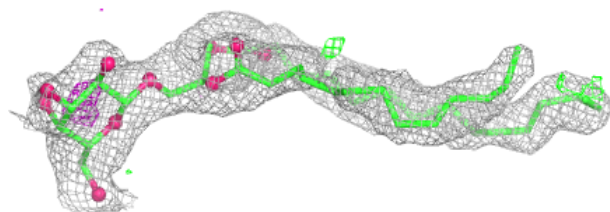
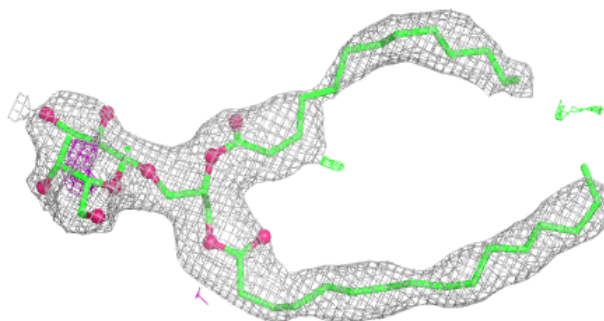


Electron density around STE H 104:

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

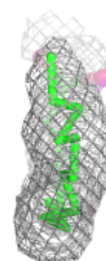
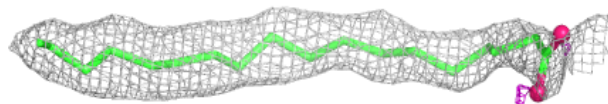
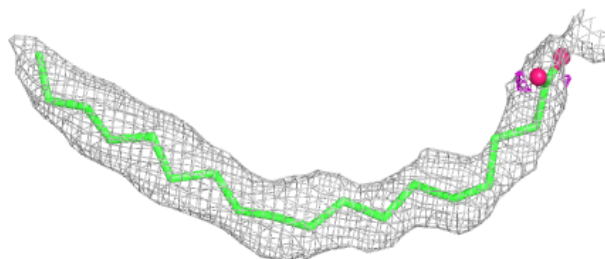
**Electron density around LMG A 612:**

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

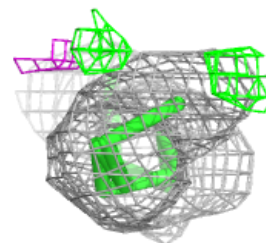
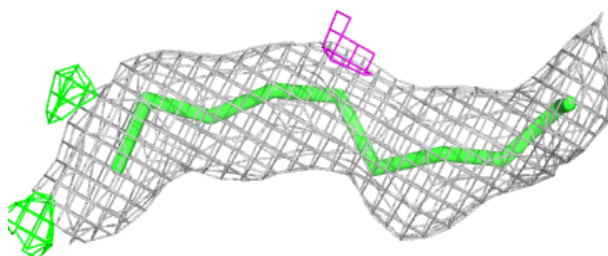
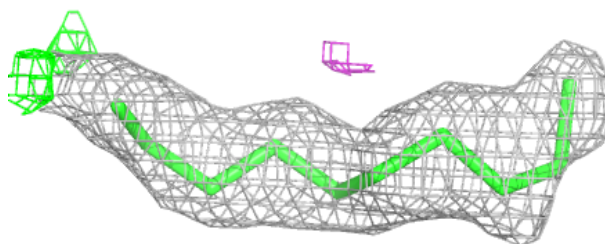


Electron density around STE X 101:

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

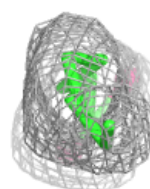
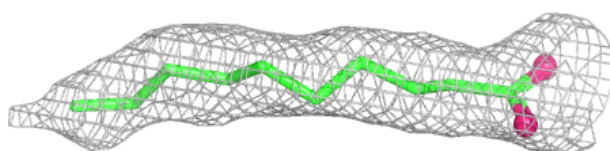
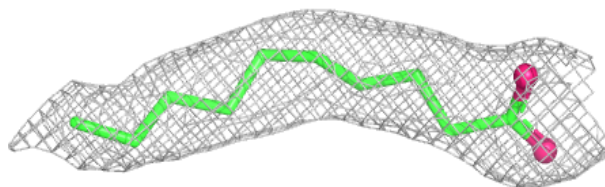
**Electron density around STE b 625:**

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

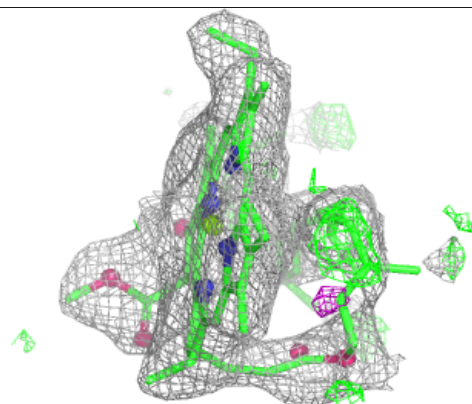
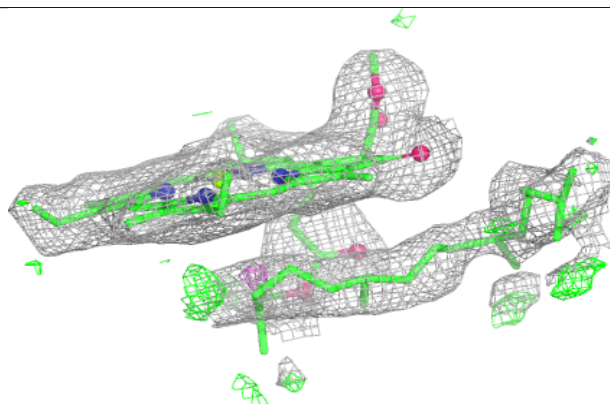
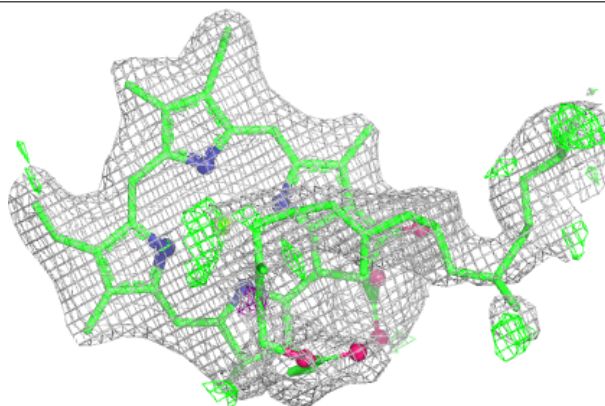


Electron density around STE j 101:

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

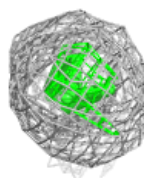
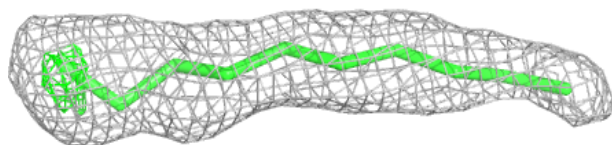
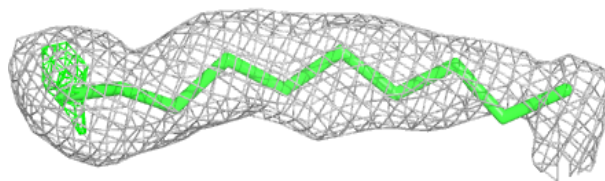
**Electron density around CLA B 601:**

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

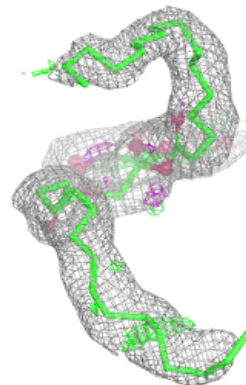
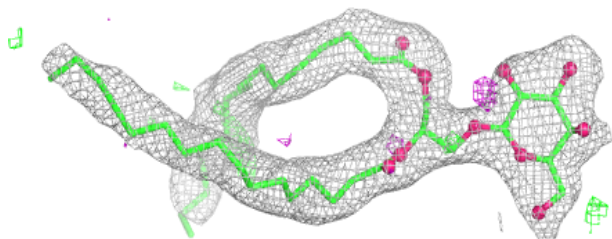
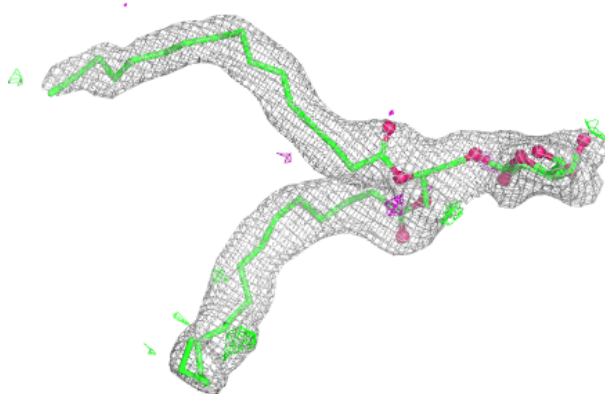


Electron density around STE M 103:

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

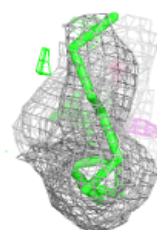
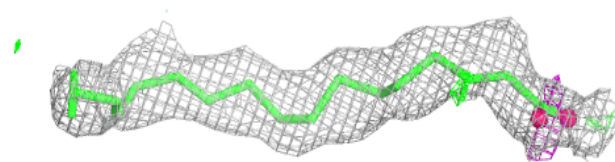
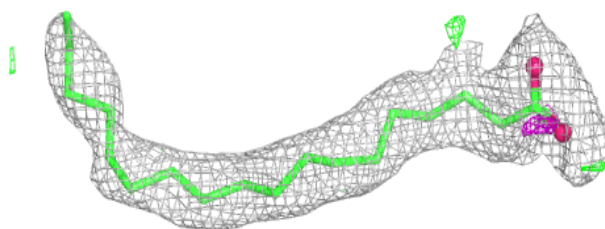
**Electron density around LMG M 101:**

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

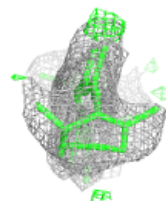
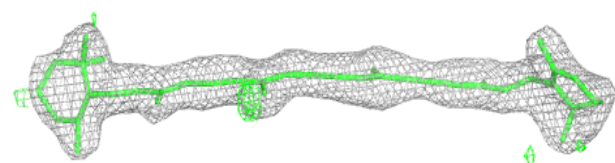
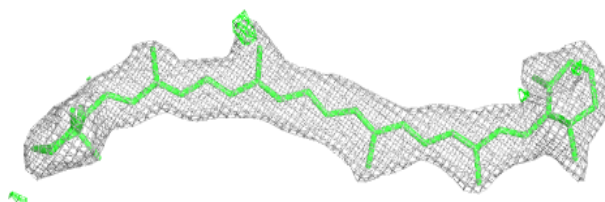


Electron density around STE b 621:

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

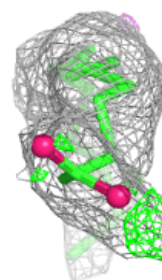
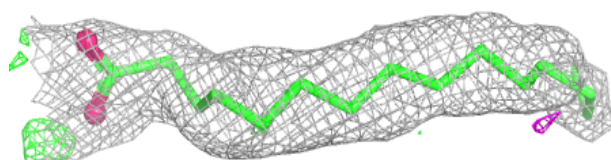
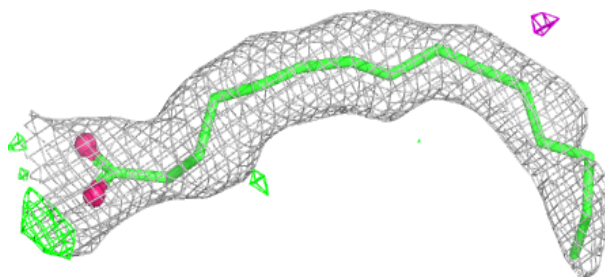
**Electron density around BCR J 101:**

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

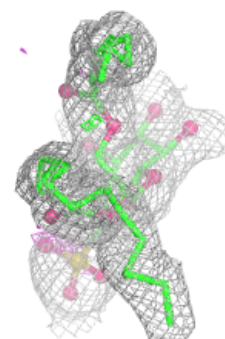
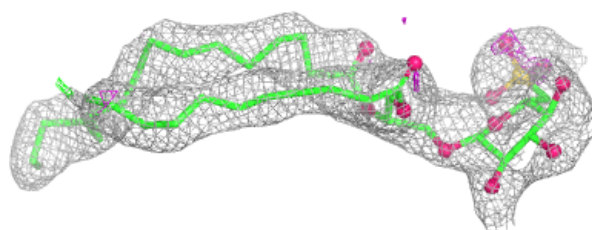
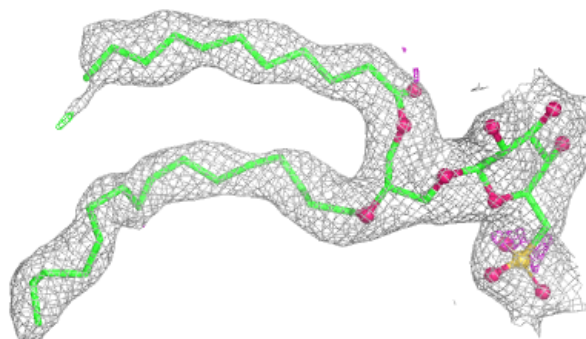


Electron density around STE B 621:

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

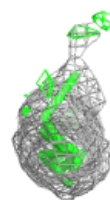
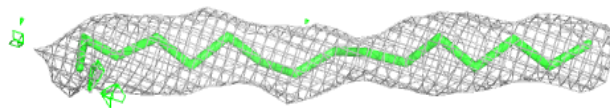
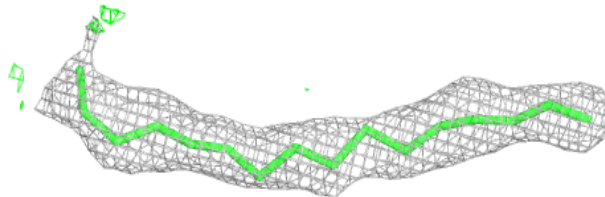
**Electron density around SQD b 620:**

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

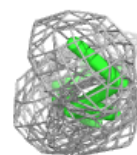
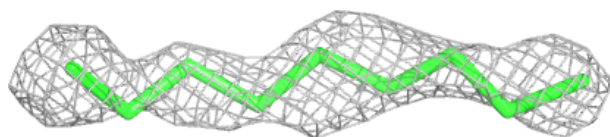
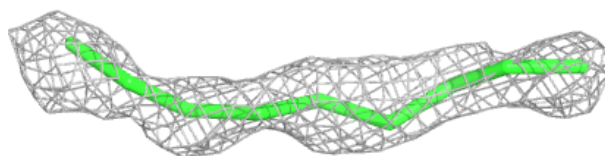


Electron density around STE C 526:

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

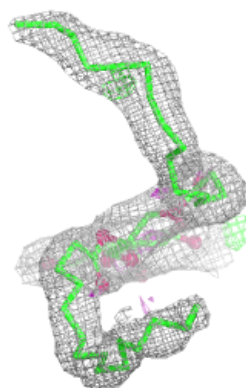
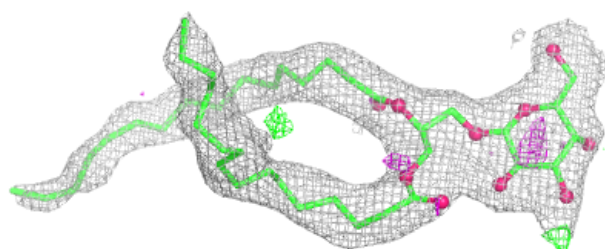
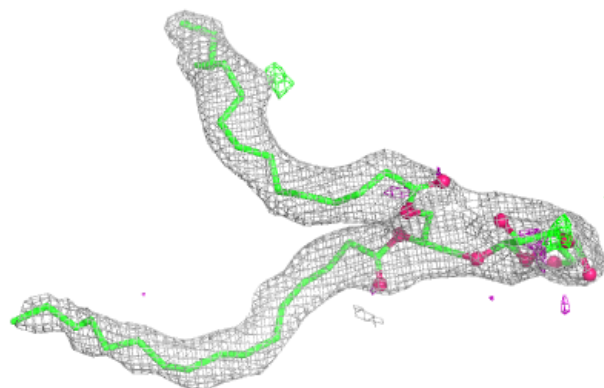
**Electron density around STE z 703:**

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

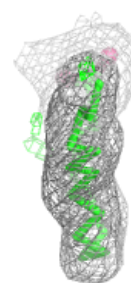
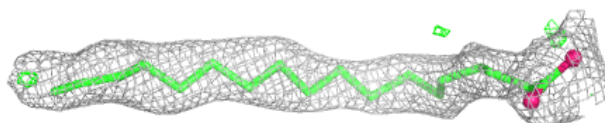
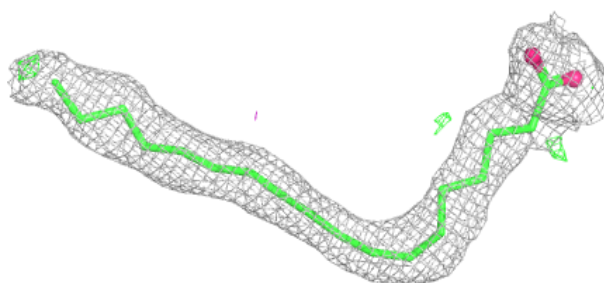


Electron density around LMG m 101:

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

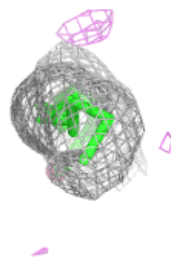
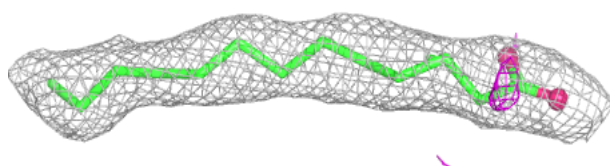
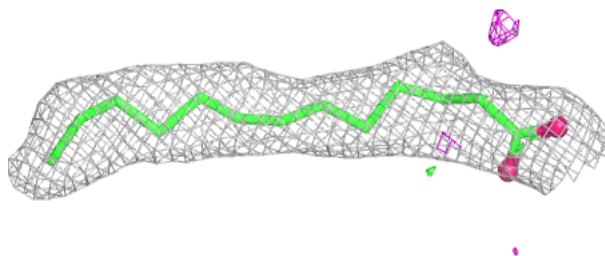
**Electron density around STE d 407:**

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

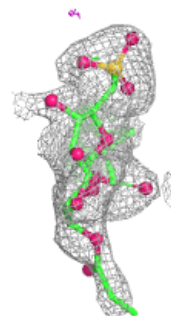
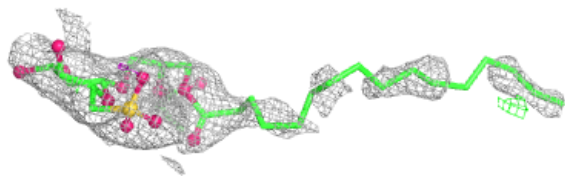
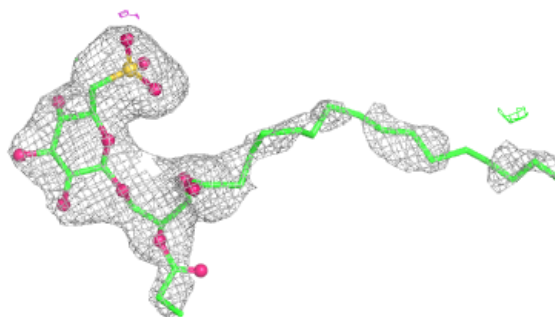


Electron density around STE M 102:

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

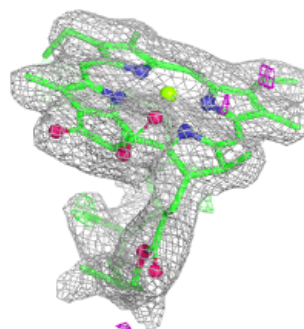
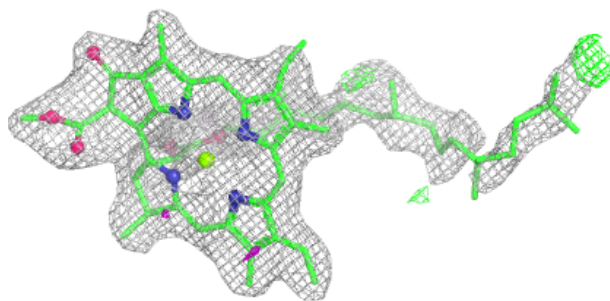
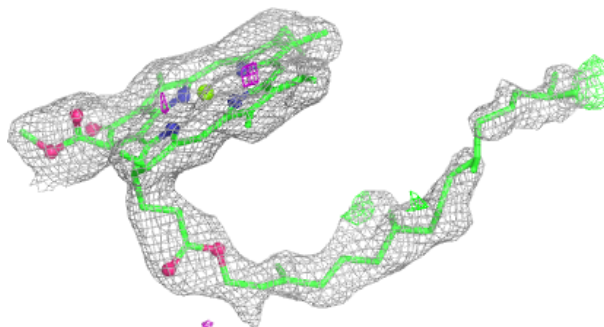
**Electron density around SQD f 101:**

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

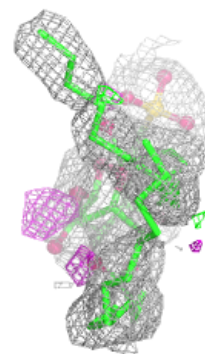
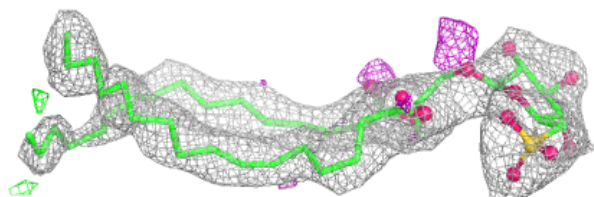
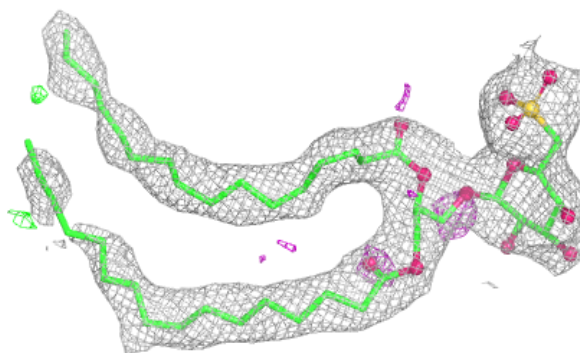


Electron density around CLA C 513:

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

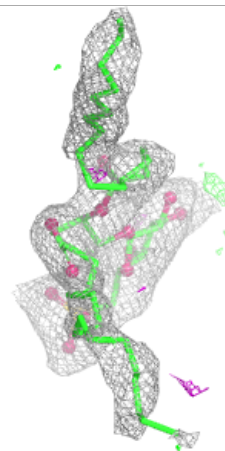
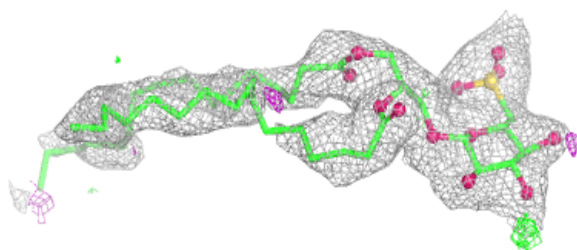
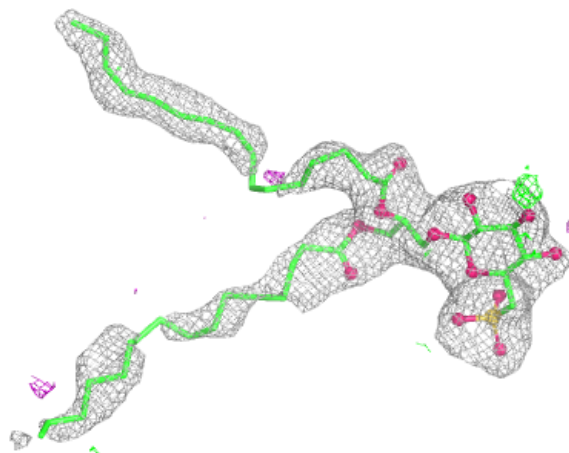
**Electron density around SQD B 623:**

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



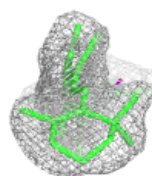
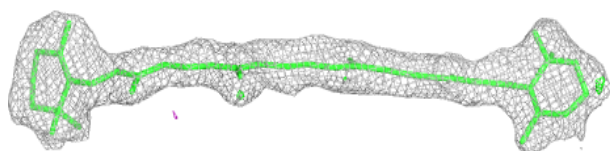
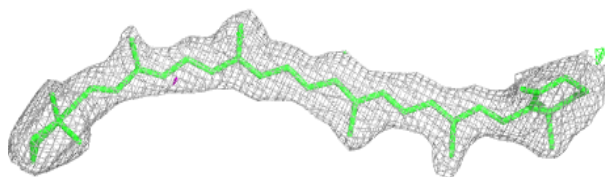
Electron density around SQD a 613:

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

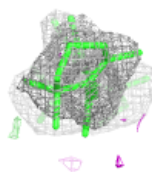
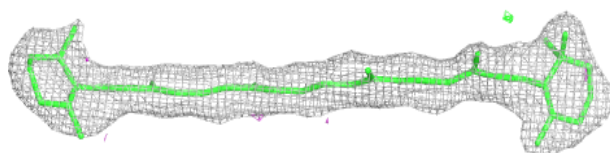
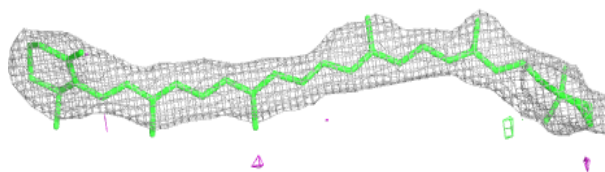


Electron density around BCR x 101:

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

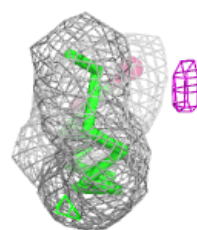
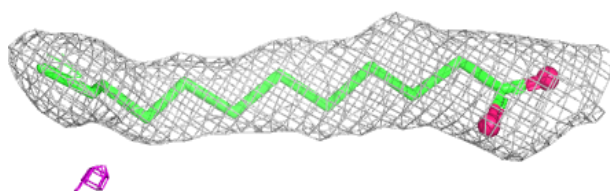
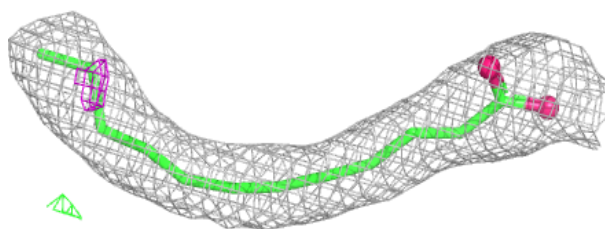
**Electron density around BCR C 514:**

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

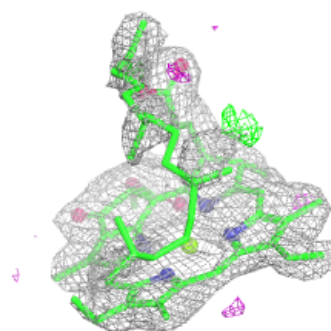
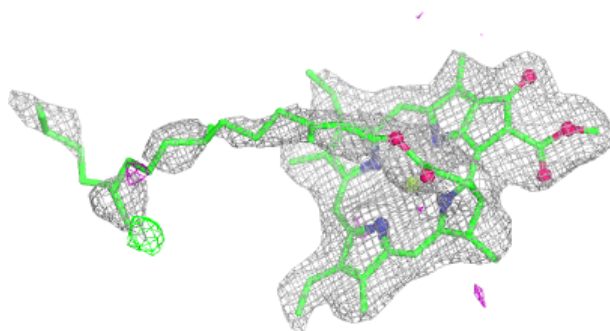
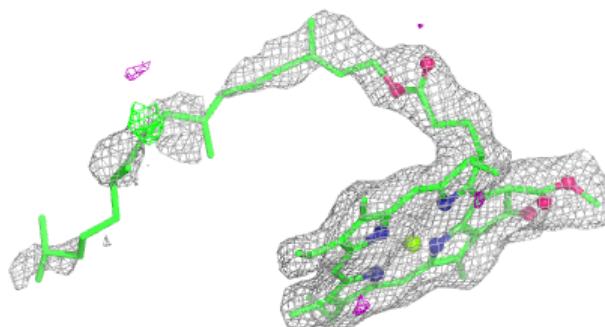


Electron density around STE B 624:

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

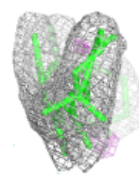
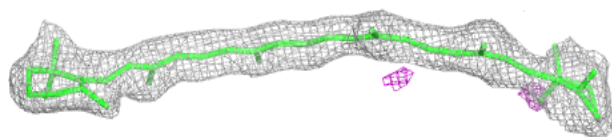
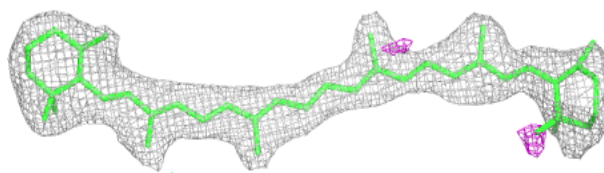
**Electron density around CLA c 513:**

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

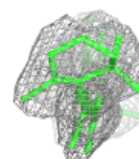
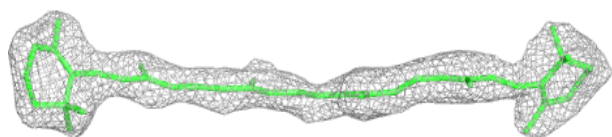
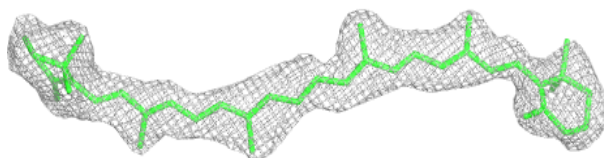


Electron density around BCR d 405:

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

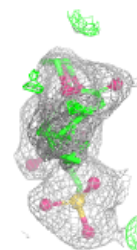
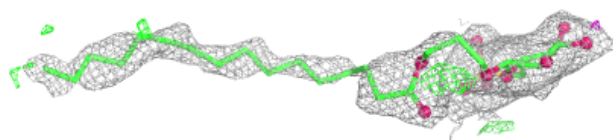
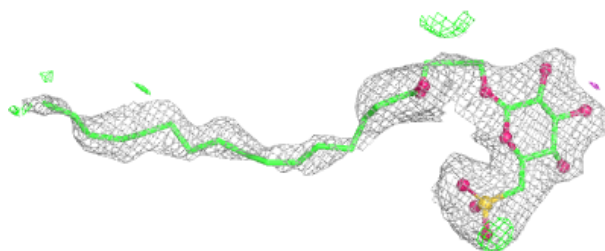
**Electron density around BCR k 101:**

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

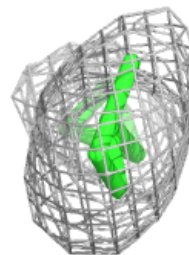
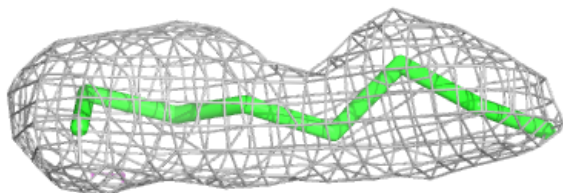
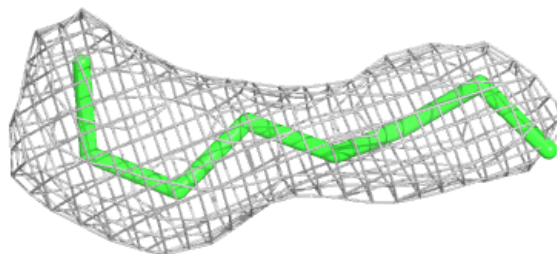


Electron density around SQD D 410:

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

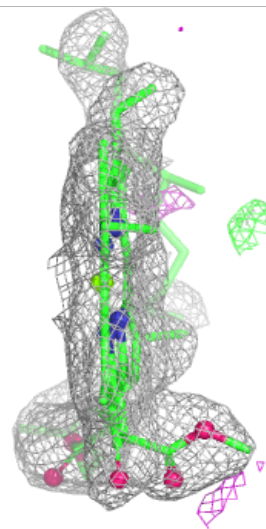
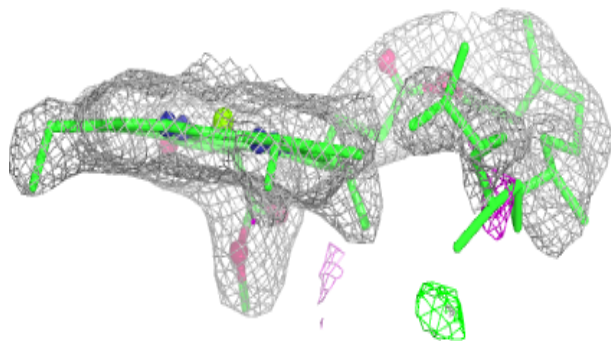
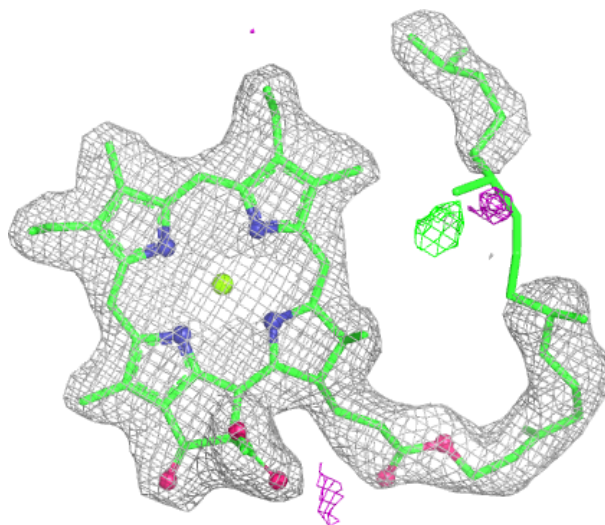
**Electron density around STE A 617:**

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



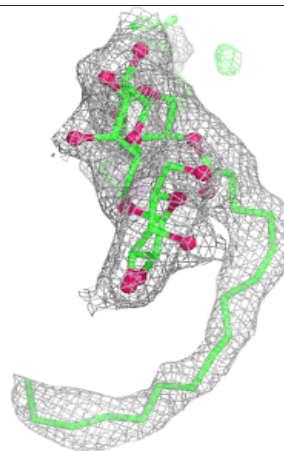
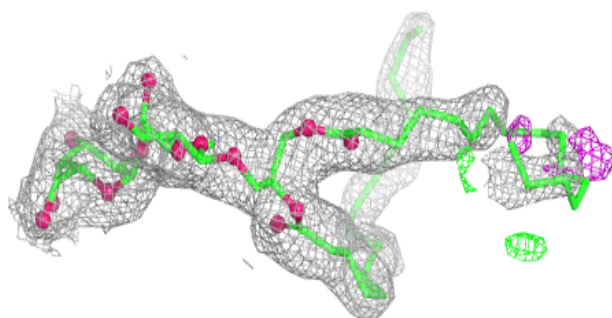
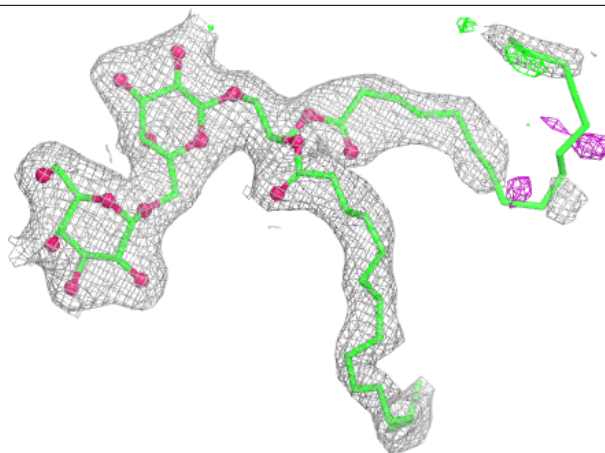
Electron density around CLA c 512:

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

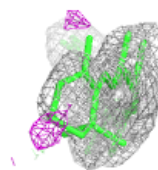
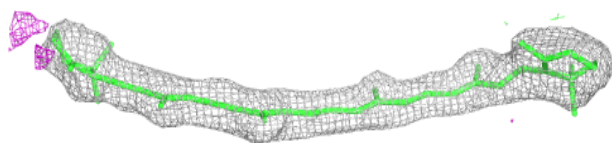
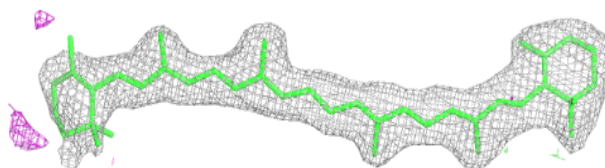


Electron density around DGD C 522:

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

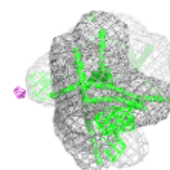
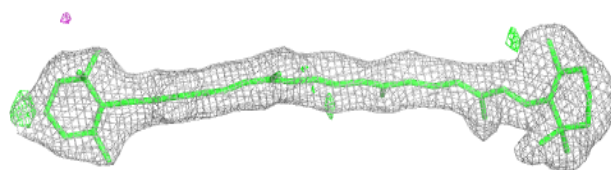
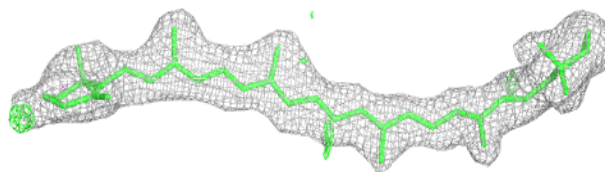
**Electron density around BCR D 406:**

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

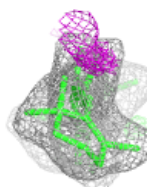
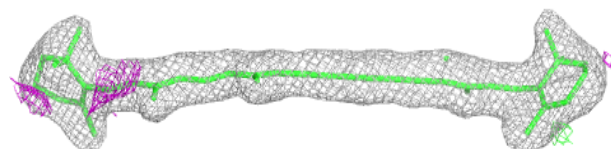
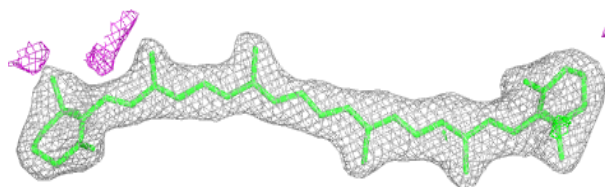


Electron density around BCR H 101:

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

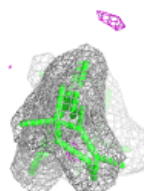
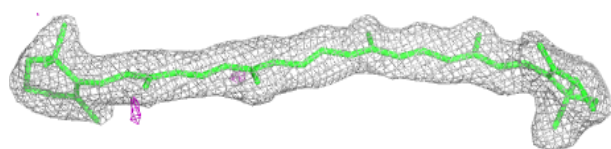
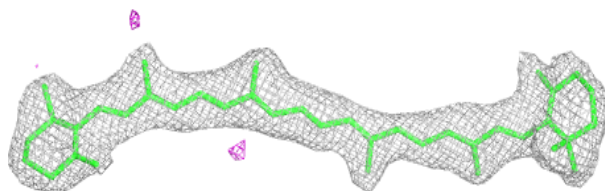
**Electron density around BCR B 618:**

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

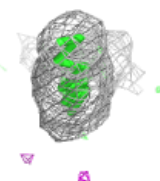
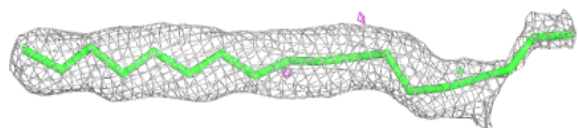
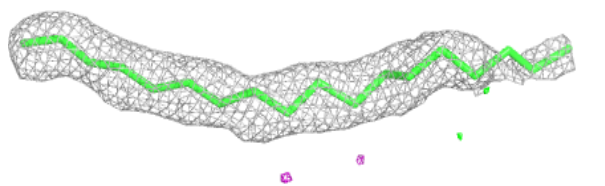


Electron density around BCR b 619:

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

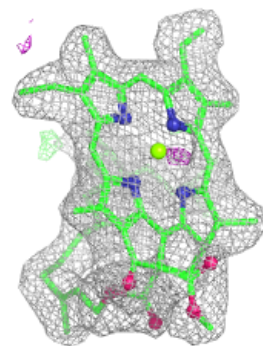
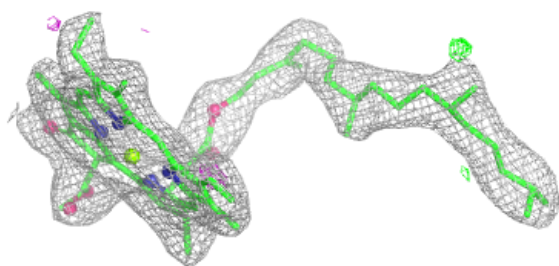
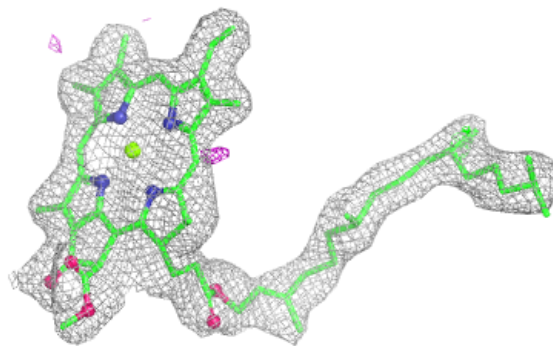
**Electron density around STE l 102:**

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

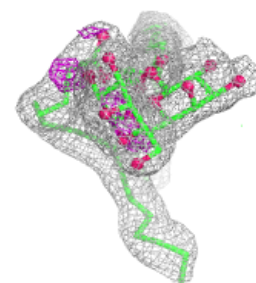
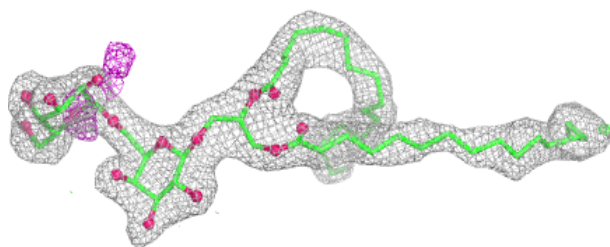
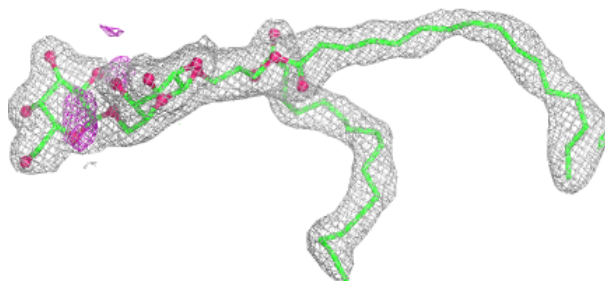


Electron density around CLA C 511:

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

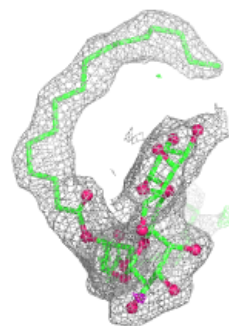
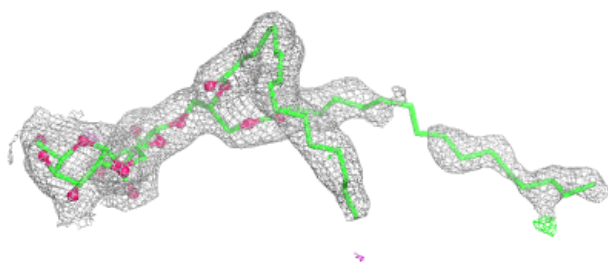
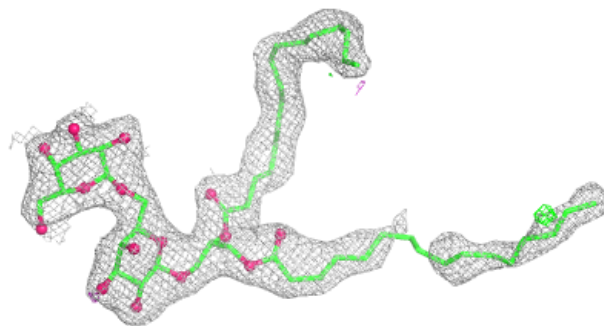
**Electron density around DGD H 102:**

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

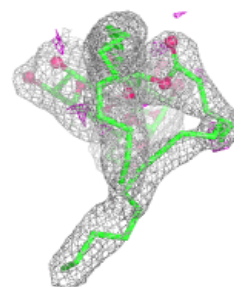
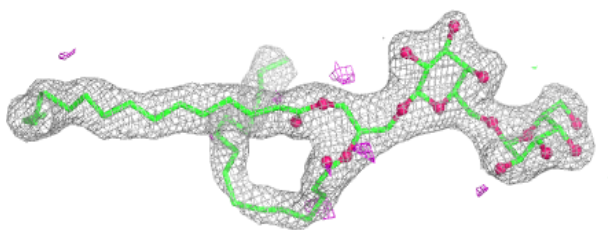
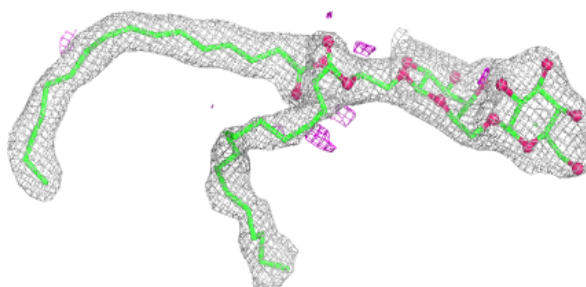


Electron density around DGD c 519:

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

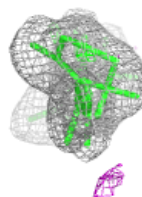
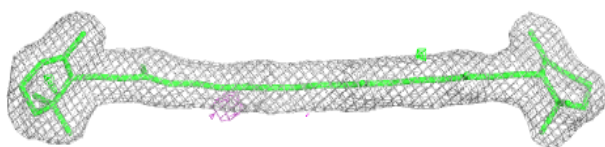
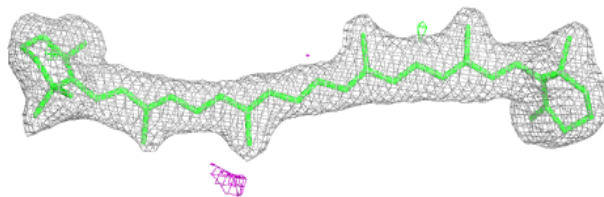
**Electron density around DGD h 101:**

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

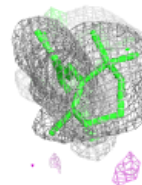
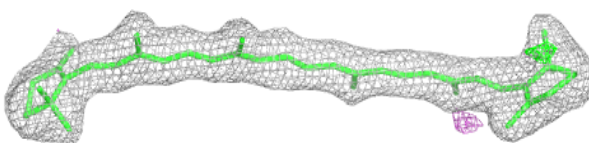
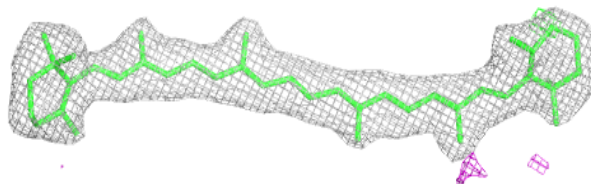


Electron density around BCR b 618:

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

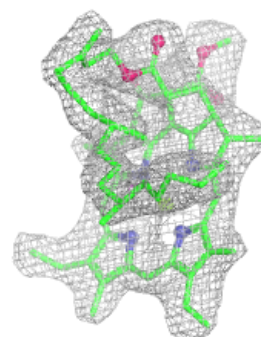
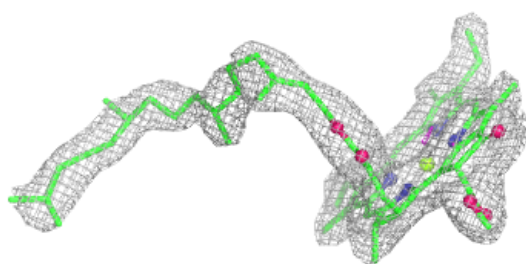
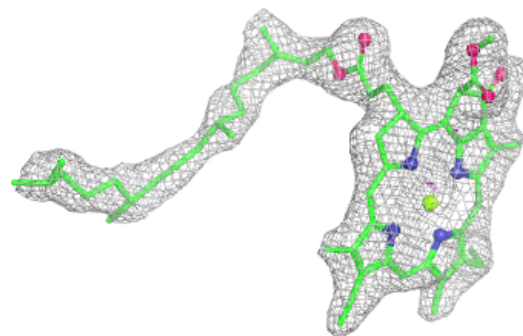
**Electron density around BCR B 619:**

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

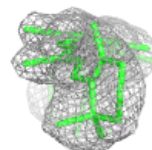
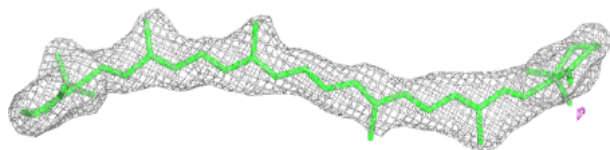
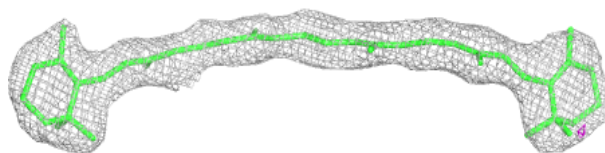


Electron density around CLA c 511:

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

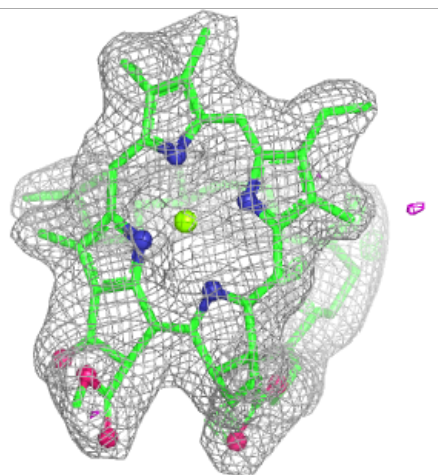
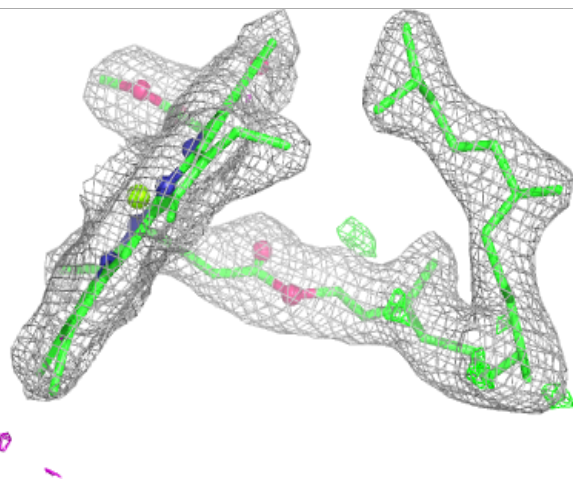
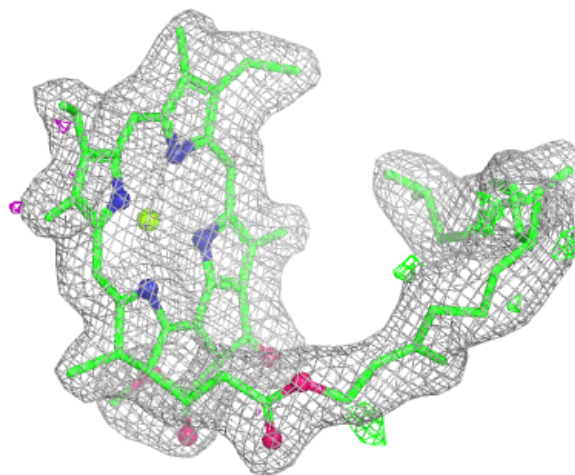
**Electron density around BCR c 517:**

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



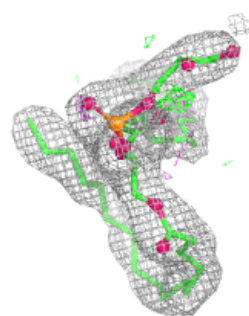
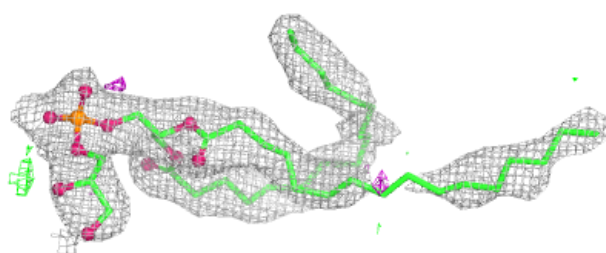
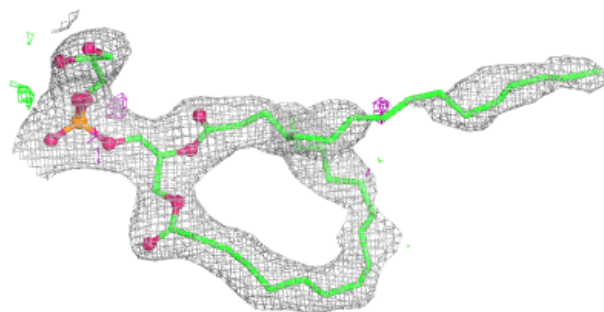
Electron density around CLA C 503:

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

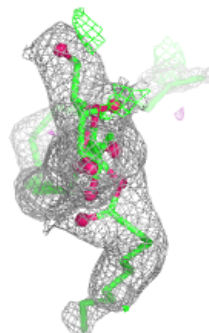
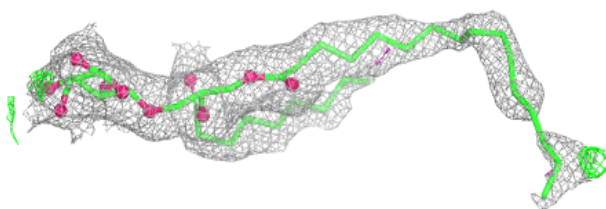
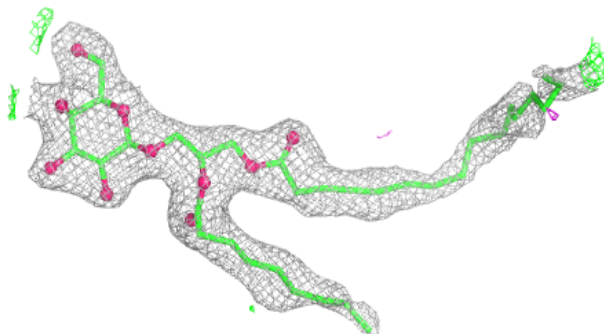


Electron density around LHG a 612:

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

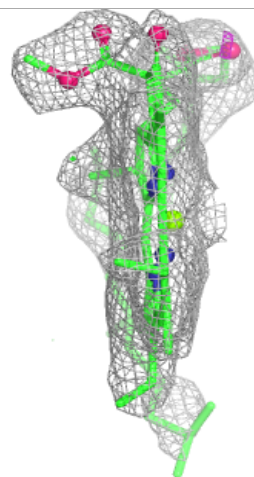
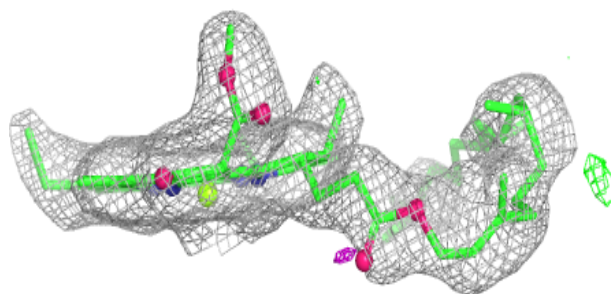
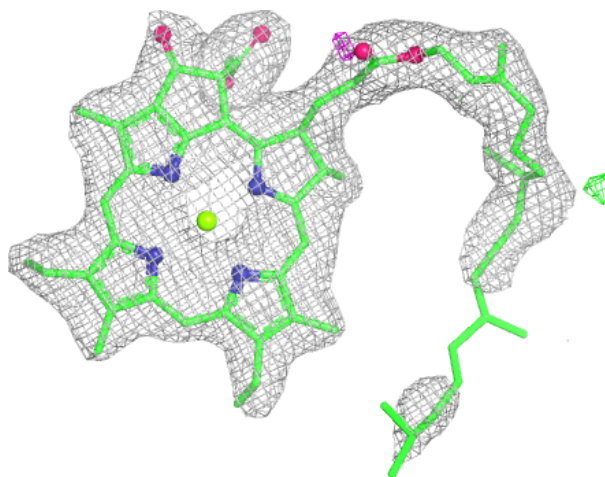
**Electron density around LMG d 411:**

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



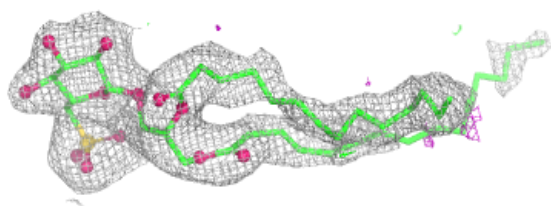
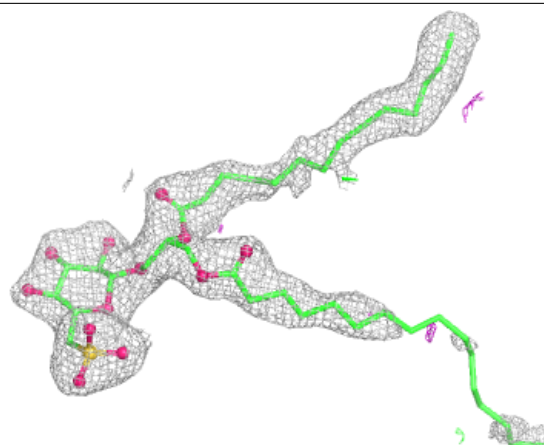
Electron density around CLA C 512:

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

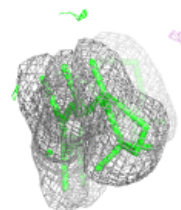
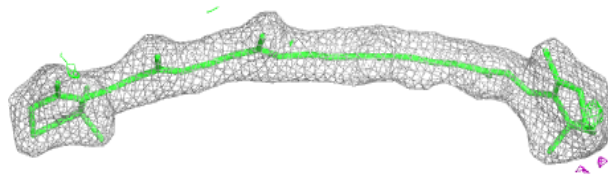
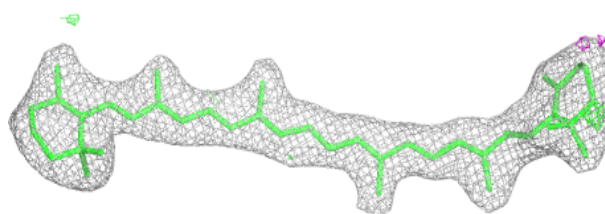


Electron density around SQD A 613:

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

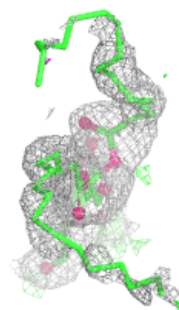
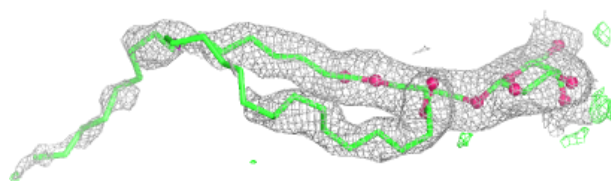
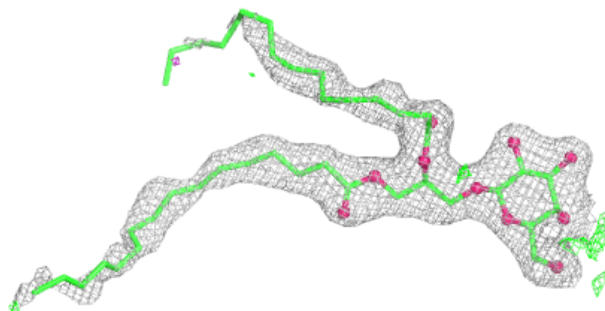
**Electron density around BCR t 101:**

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



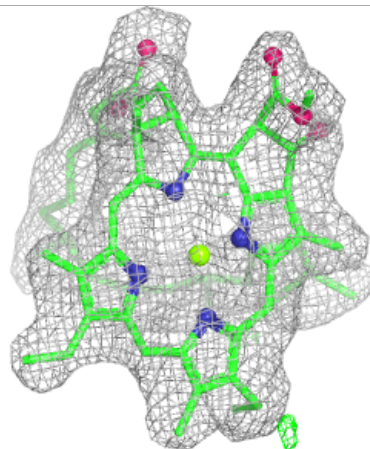
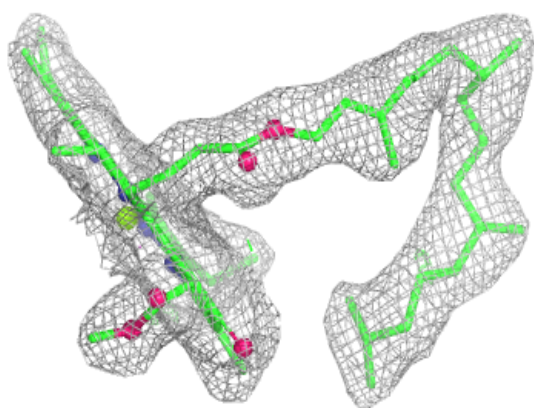
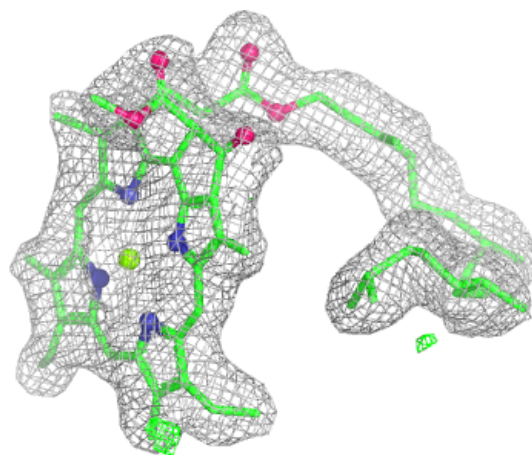
Electron density around LMG D 409:

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



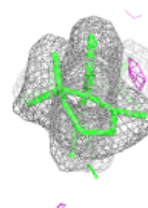
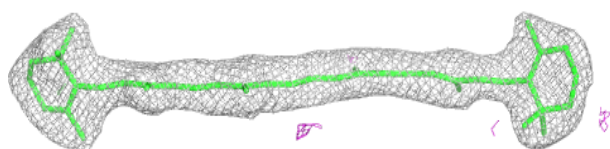
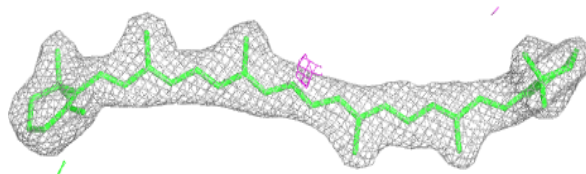
Electron density around CLA c 503:

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

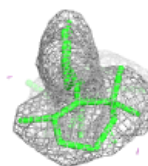
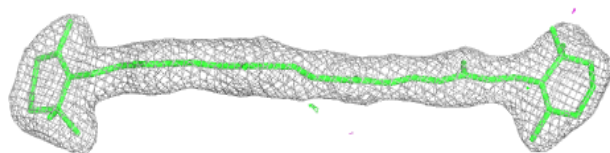
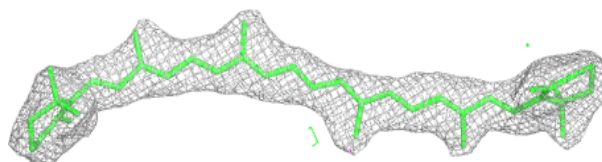


Electron density around BCR A 609:

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

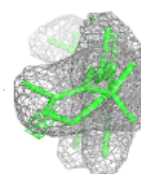
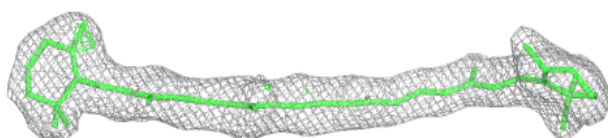
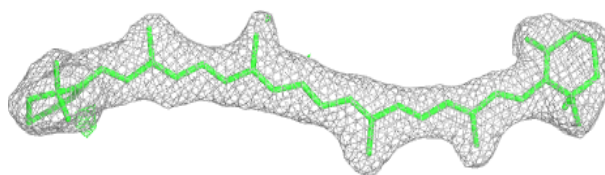
**Electron density around BCR c 515:**

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

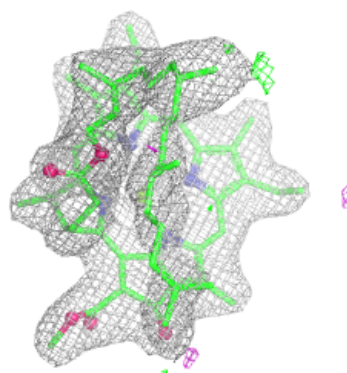
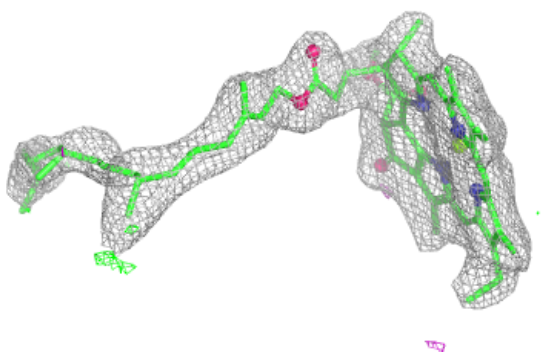
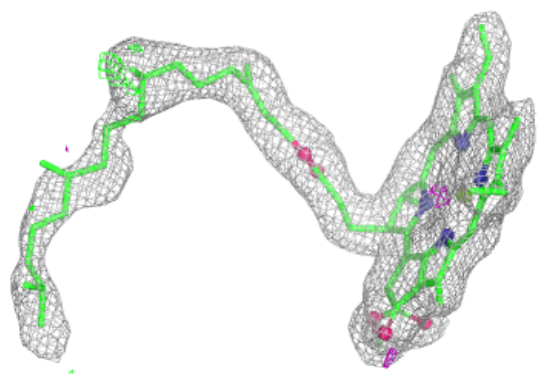


Electron density around BCR B 617:

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

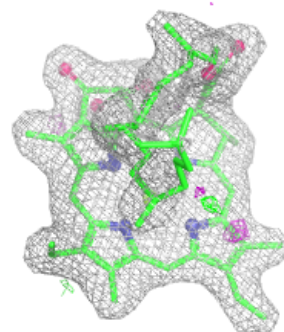
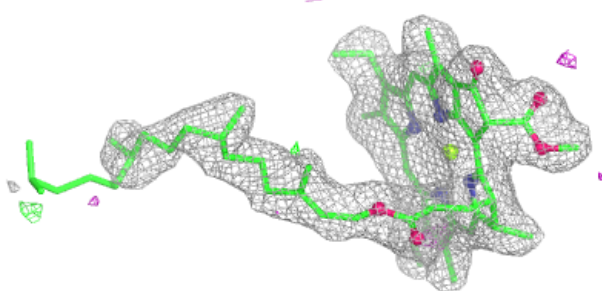
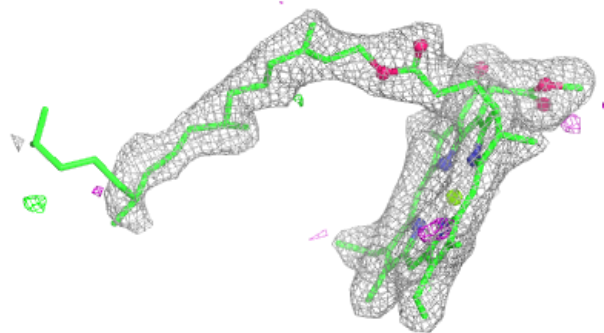
**Electron density around CLA b 606:**

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

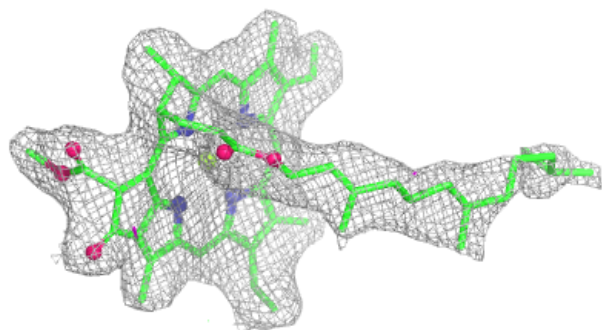
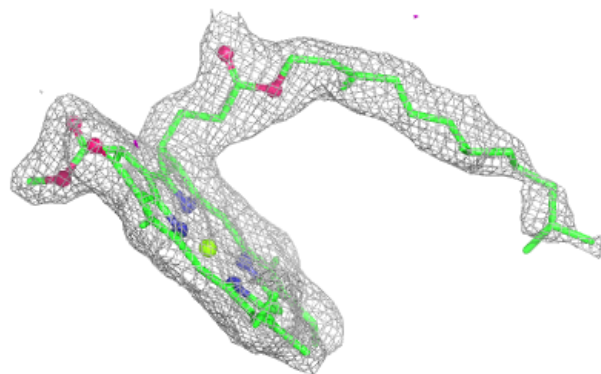


Electron density around CLA C 508:

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

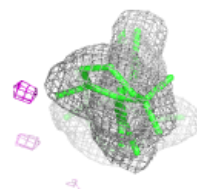
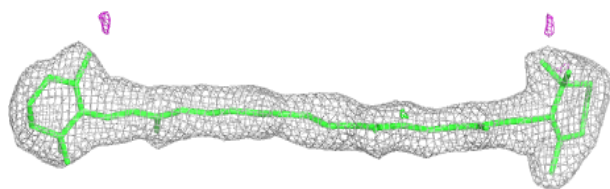
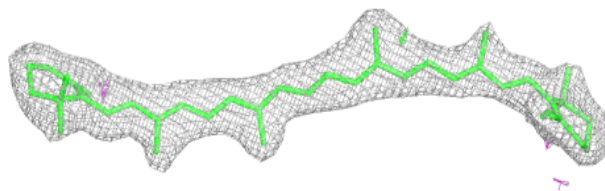
**Electron density around CLA c 504:**

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



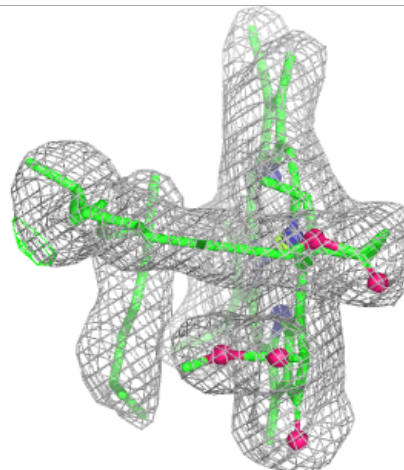
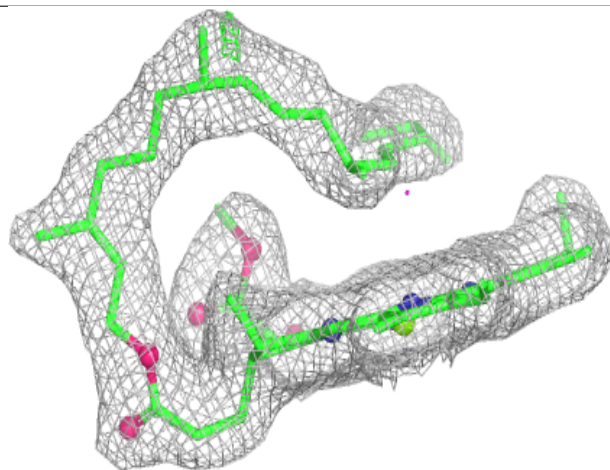
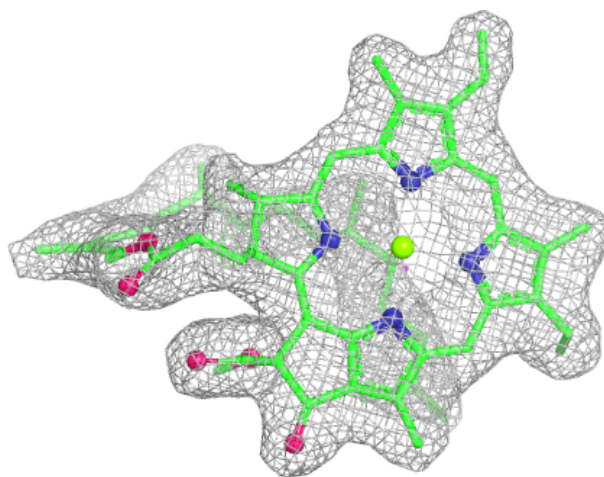
Electron density around BCR C 515:

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



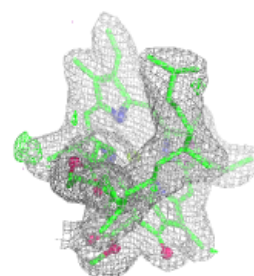
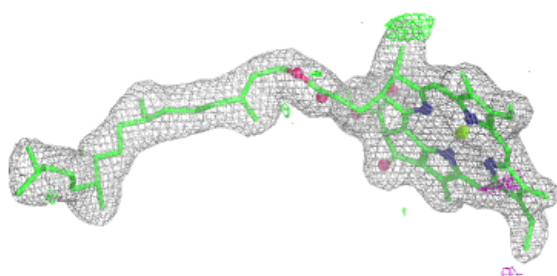
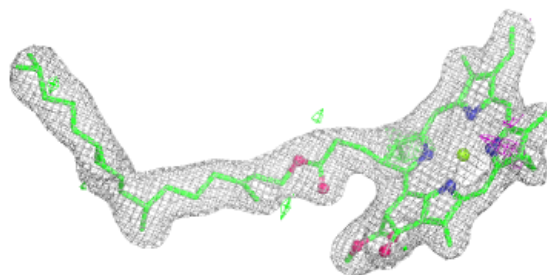
Electron density around CLA C 510:

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

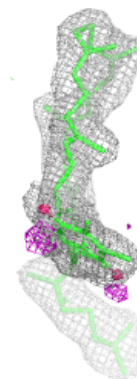
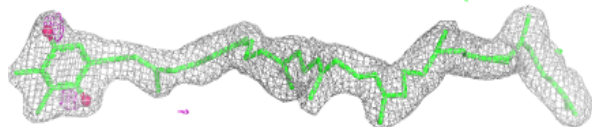
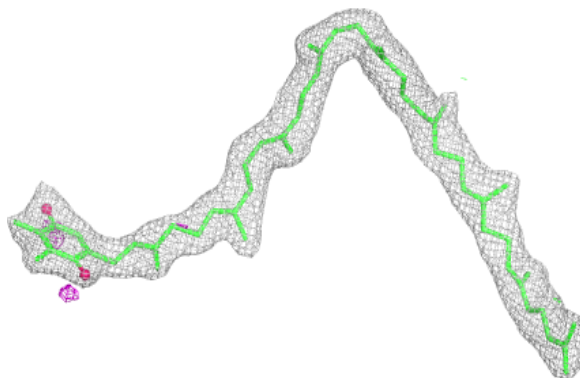


Electron density around CLA a 605:

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

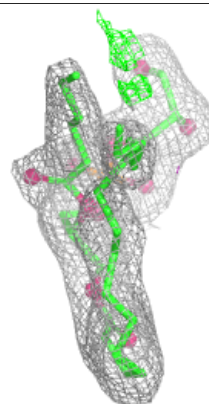
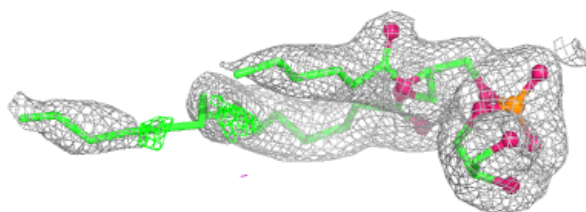
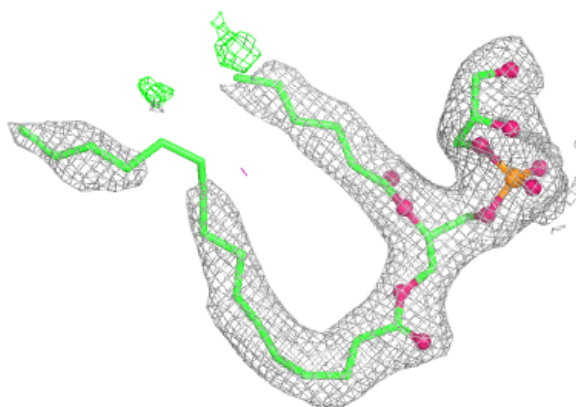
**Electron density around PL9 d 406:**

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

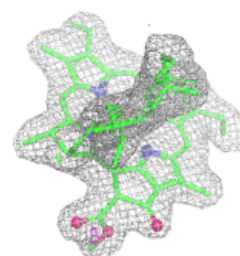
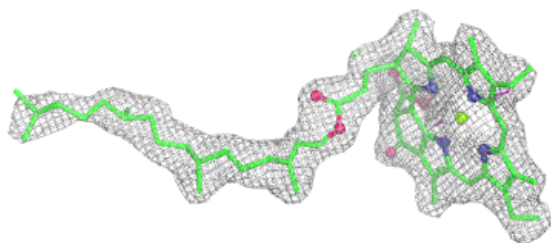
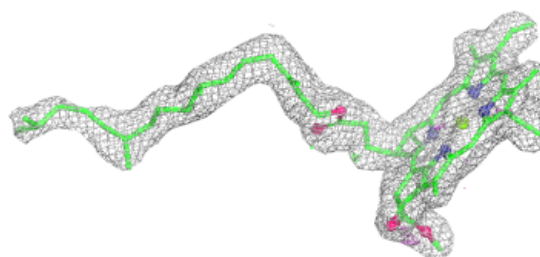


Electron density around LHG d 409:

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

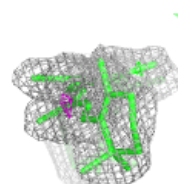
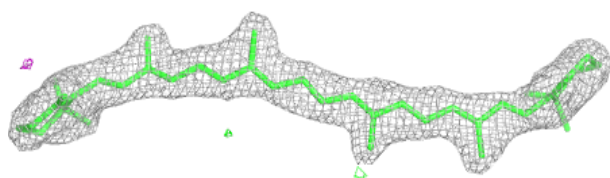
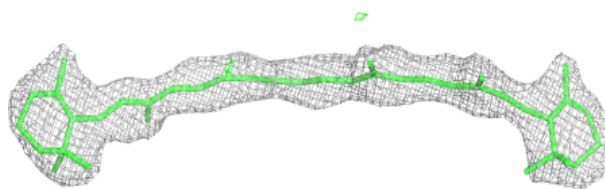
**Electron density around CLA C 502:**

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

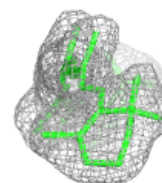
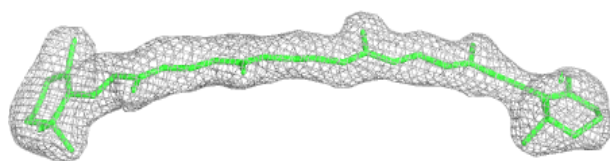
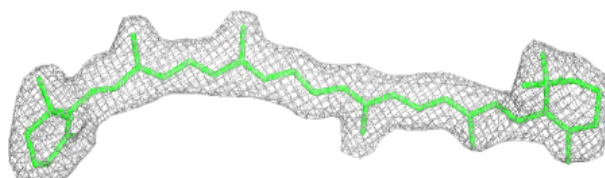


Electron density around BCR K 101:

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

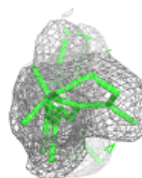
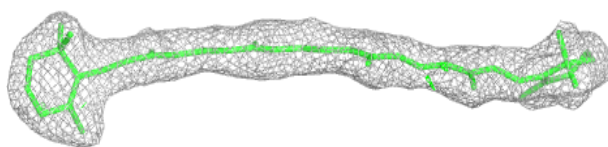
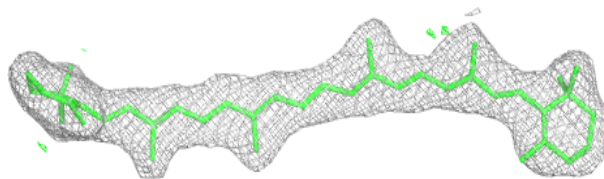
**Electron density around BCR T 101:**

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



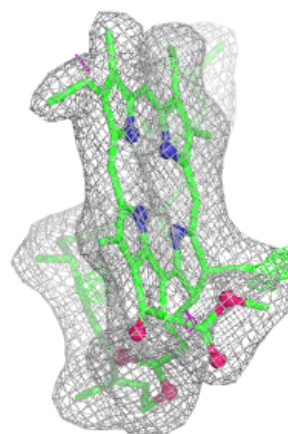
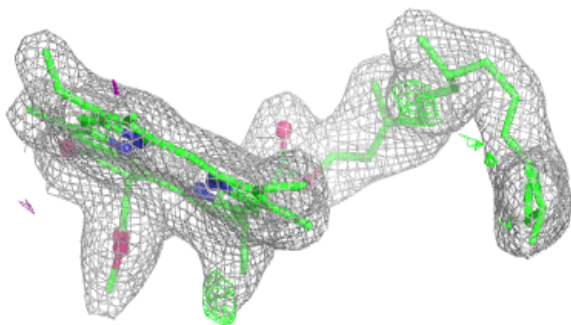
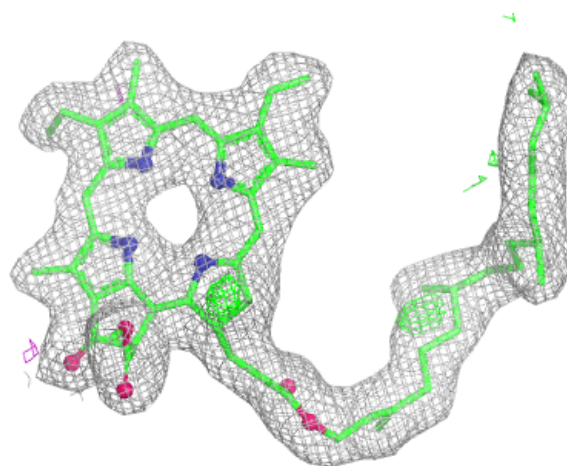
Electron density around BCR b 617:

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



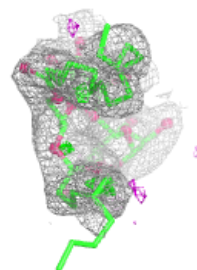
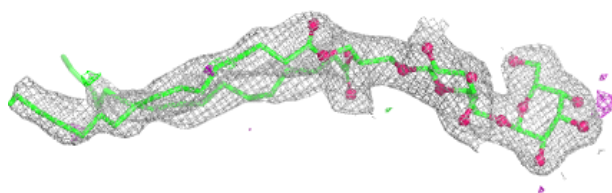
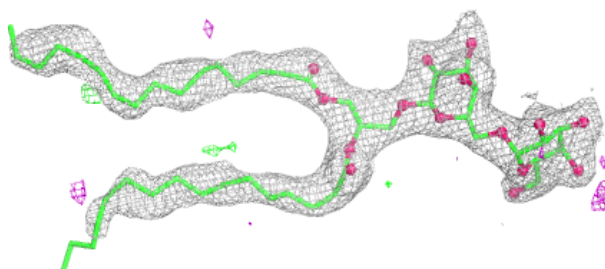
Electron density around PHO A 607:

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

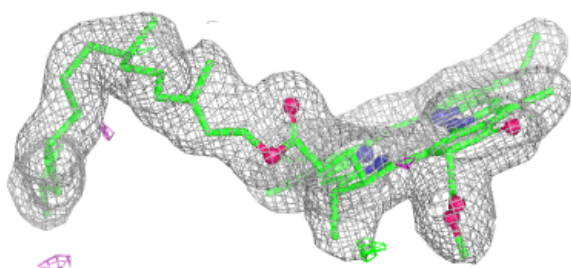
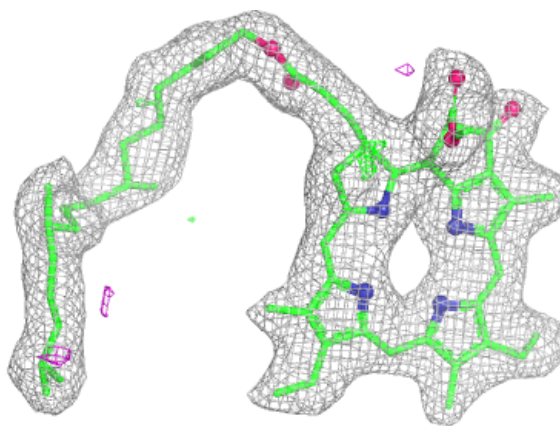


Electron density around DGD c 520:

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

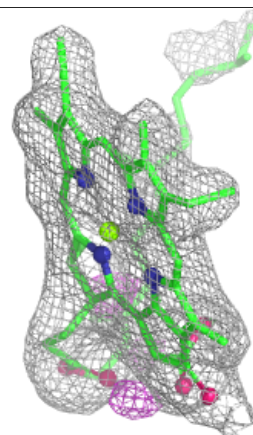
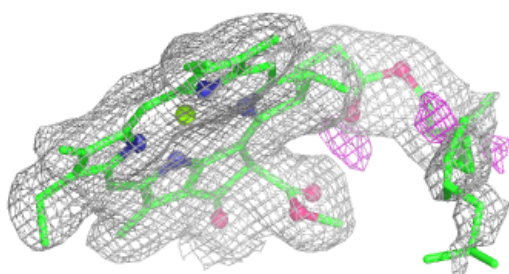
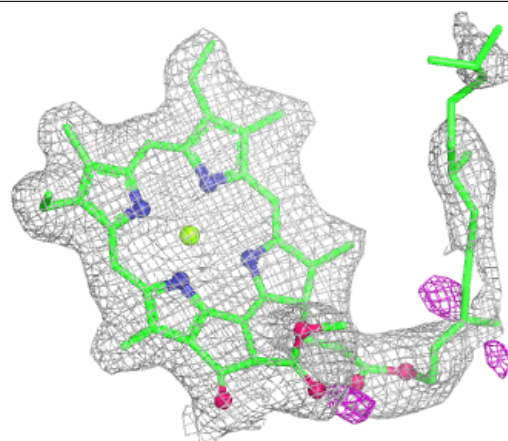
**Electron density around PHO a 608:**

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



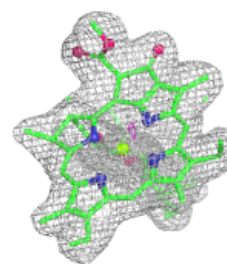
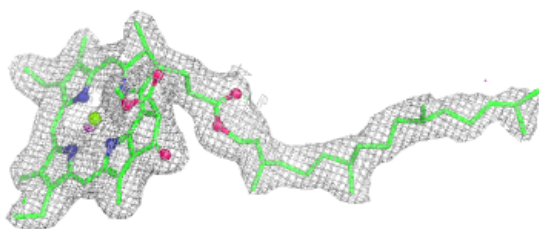
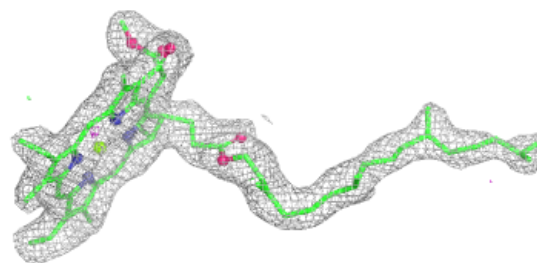
Electron density around CLA b 616:

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



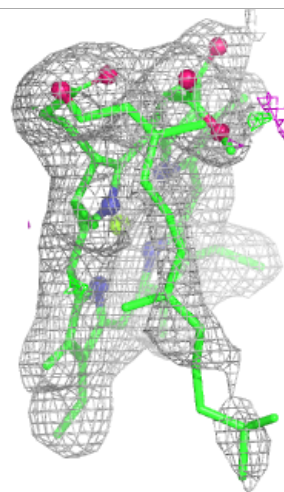
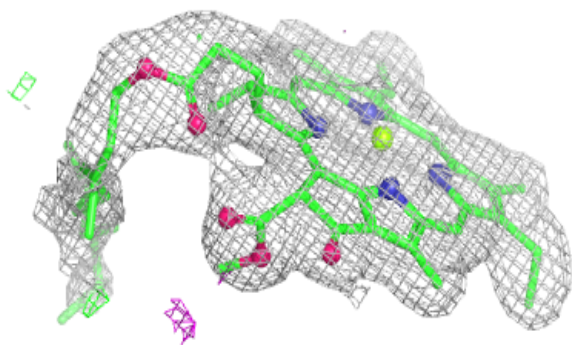
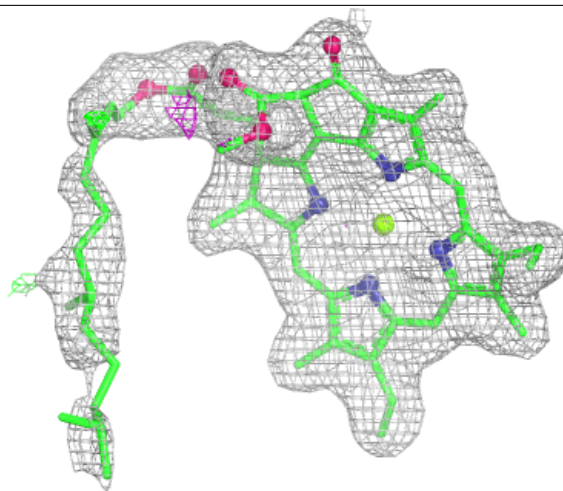
Electron density around CLA c 502:

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



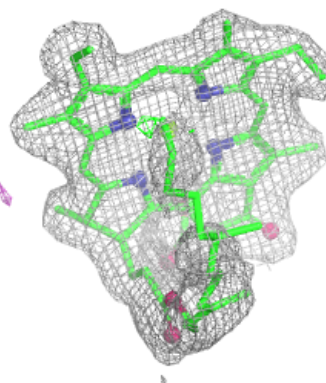
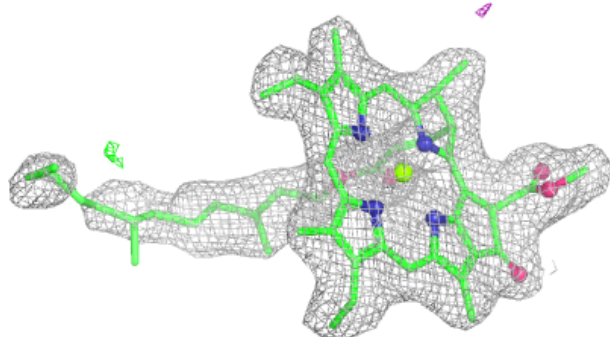
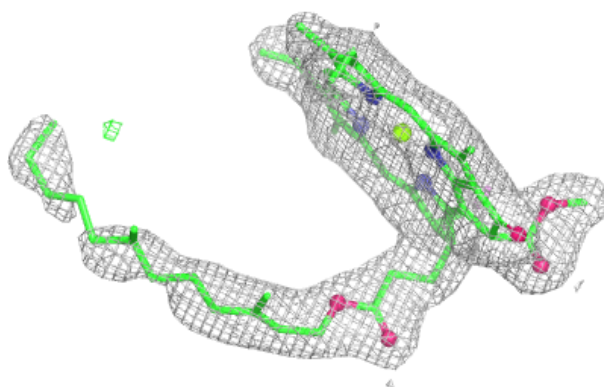
Electron density around CLA B 616:

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

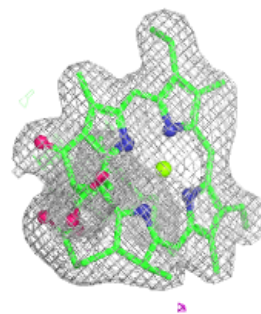
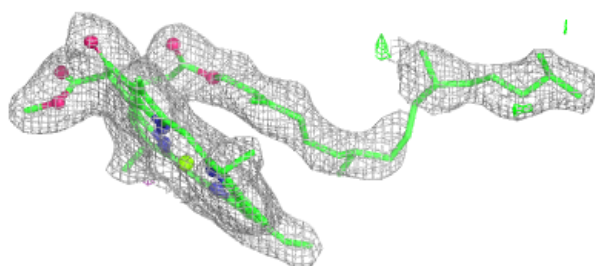
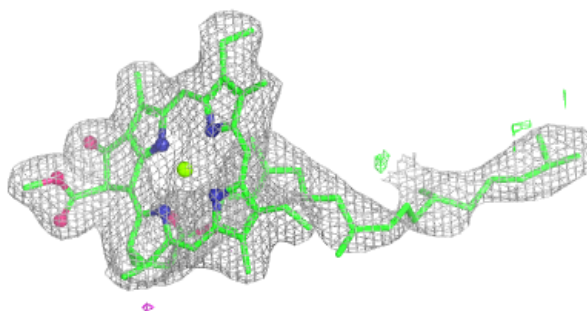


Electron density around CLA C 504:

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

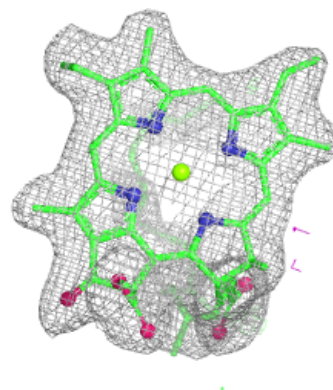
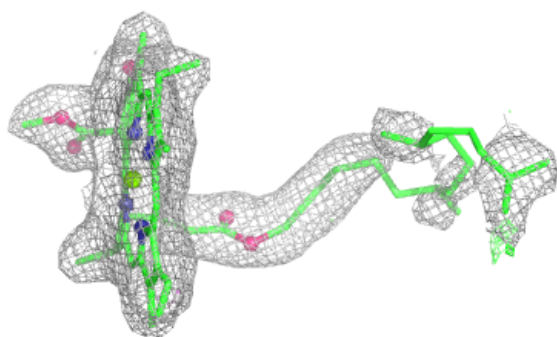
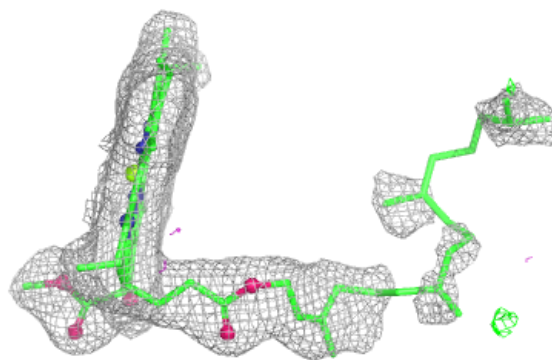
**Electron density around CLA c 505:**

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



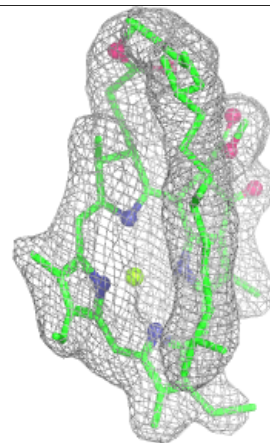
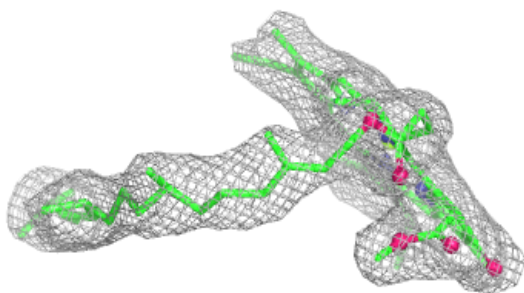
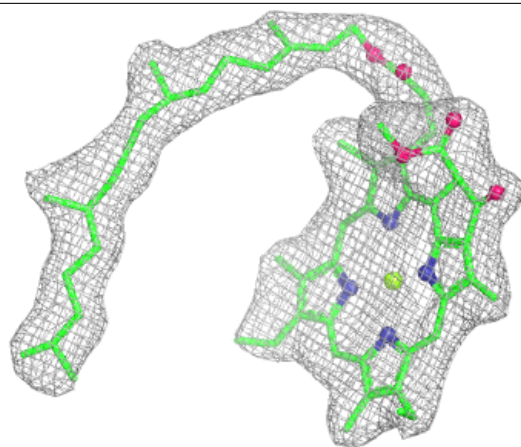
Electron density around CLA c 506:

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



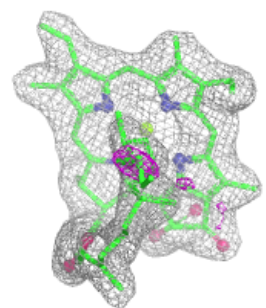
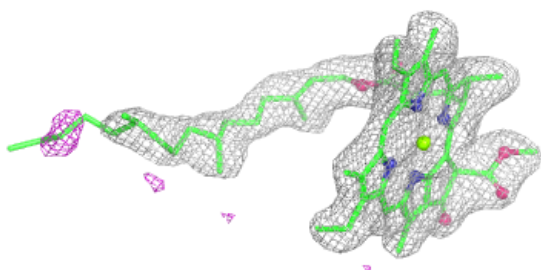
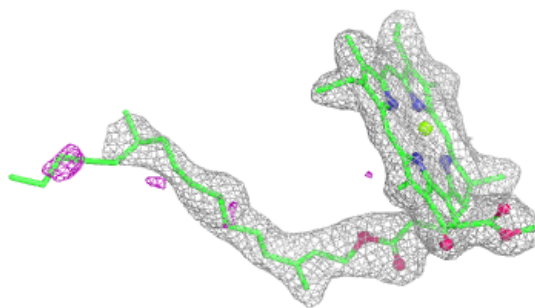
Electron density around CLA c 507:

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



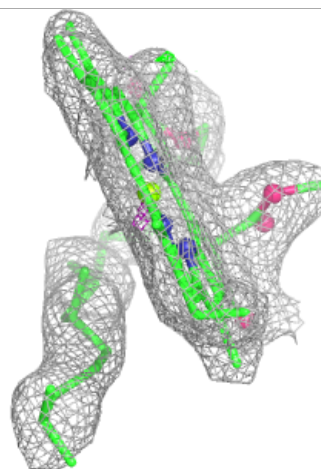
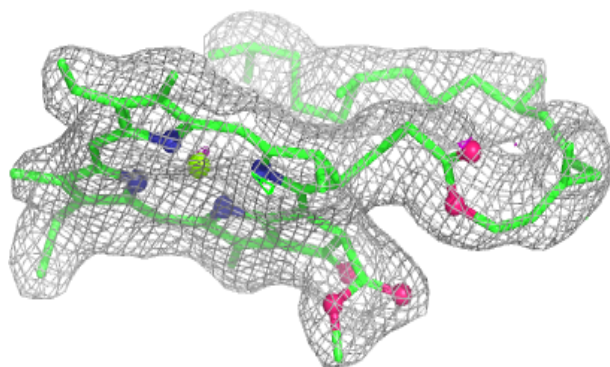
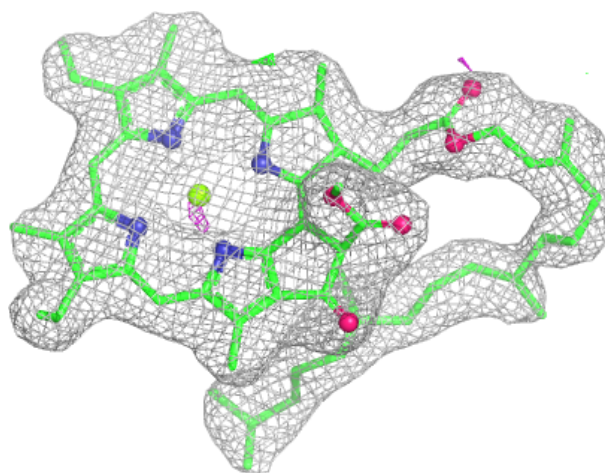
Electron density around CLA c 508:

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



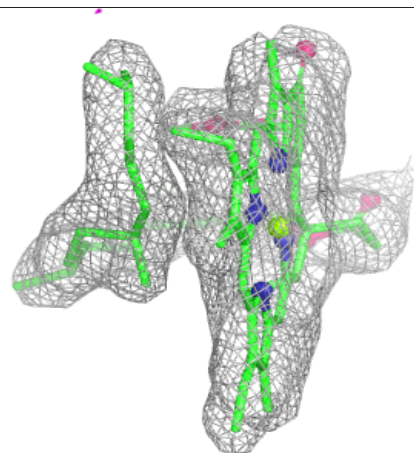
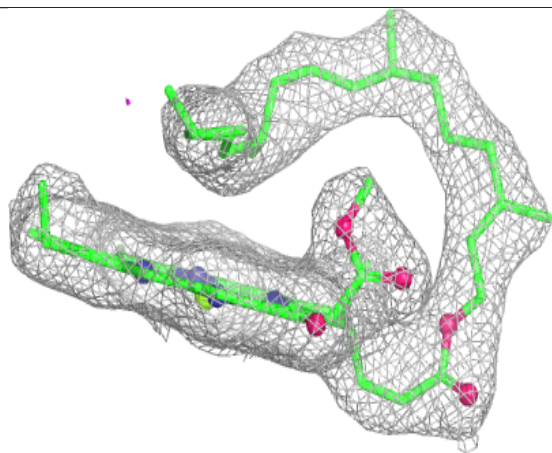
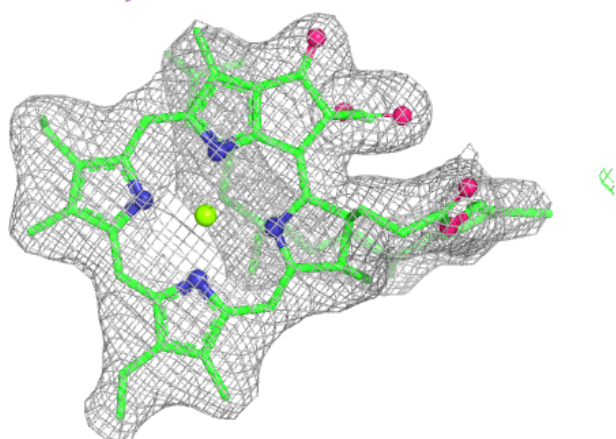
Electron density around CLA c 509:

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



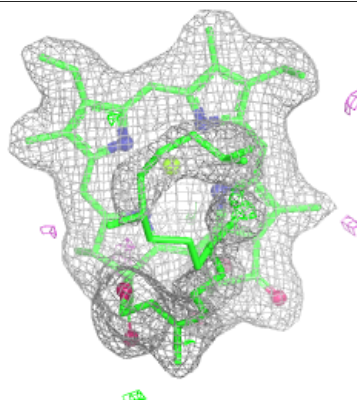
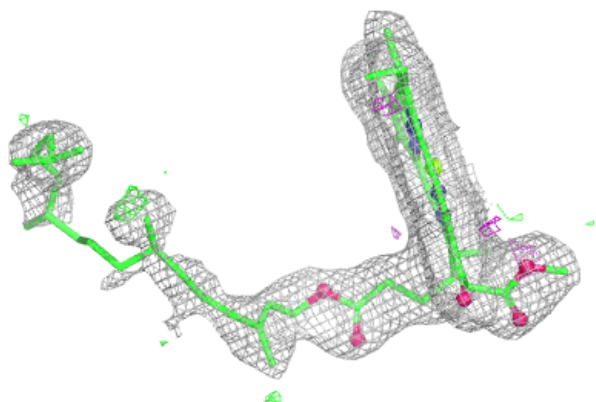
Electron density around CLA c 510:

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

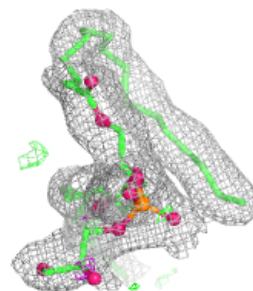
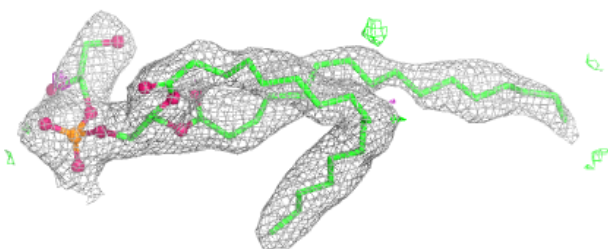
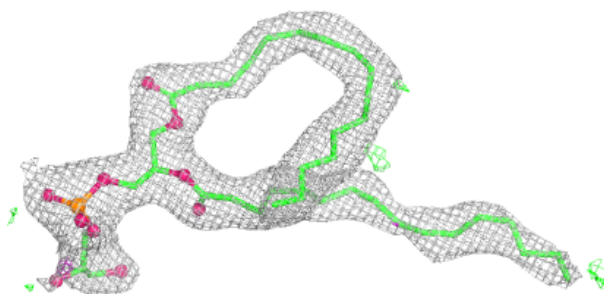


Electron density around CLA C 506:

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

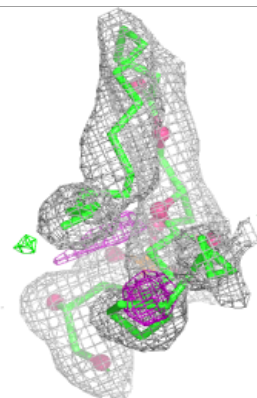
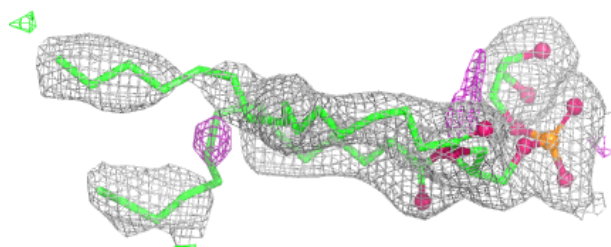
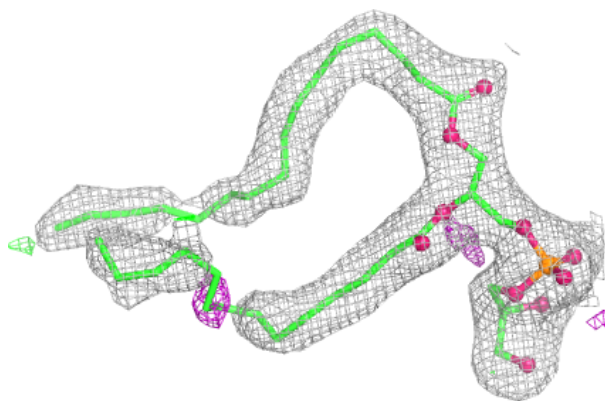
**Electron density around LHG B 622:**

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

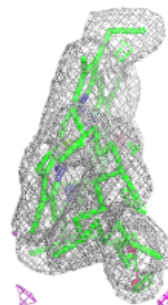
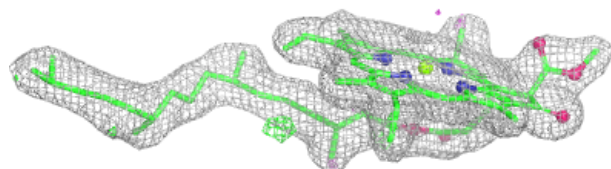
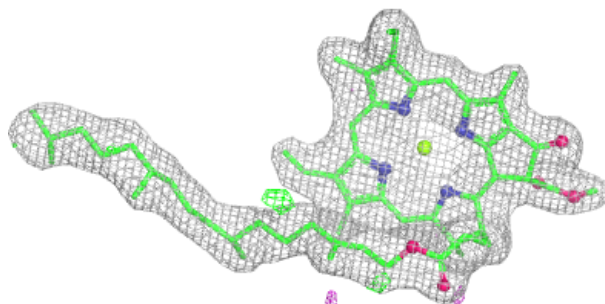


Electron density around LHG D 412:

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

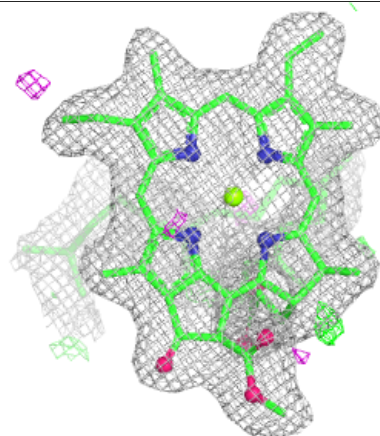
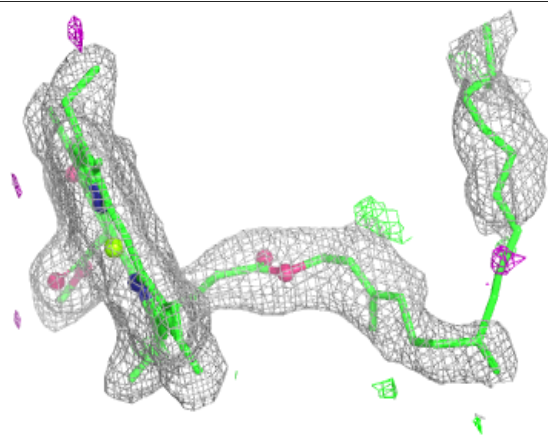
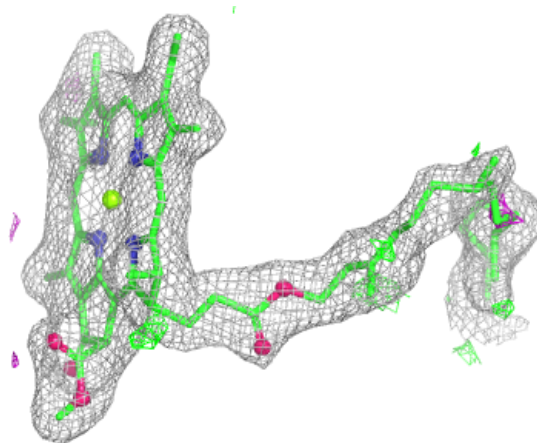
**Electron density around CLA C 501:**

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



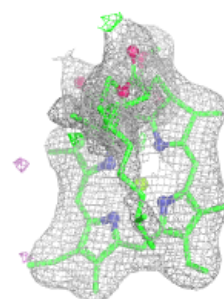
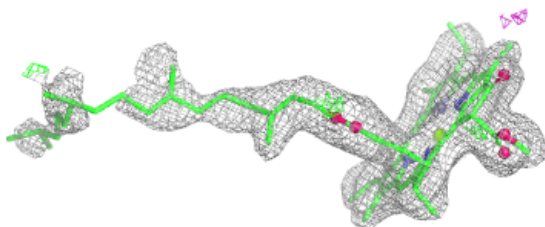
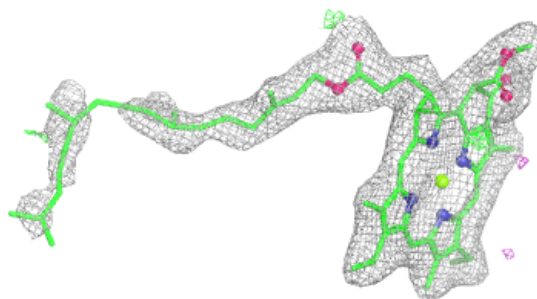
Electron density around CLA a 609:

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



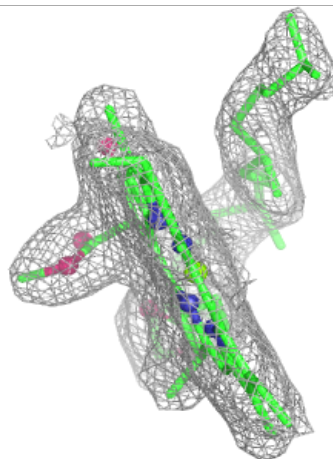
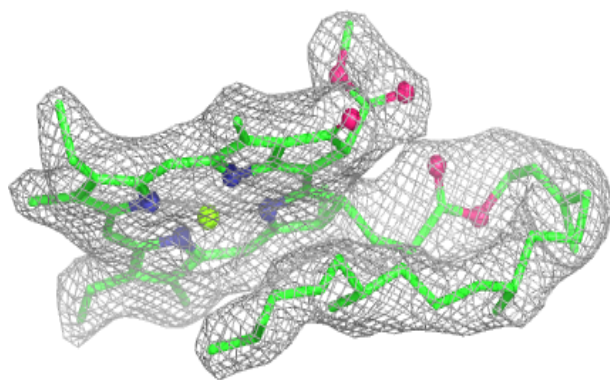
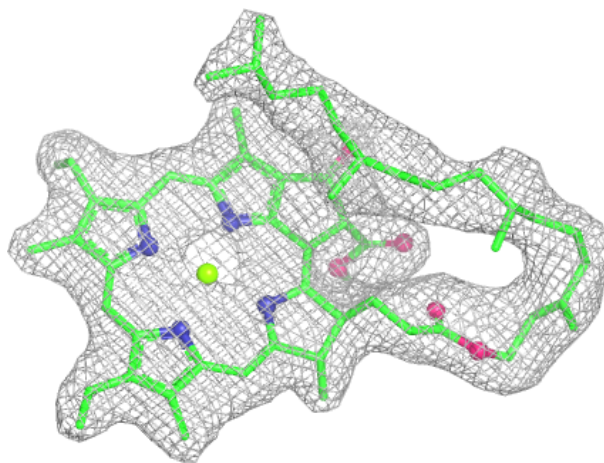
Electron density around CLA d 404:

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



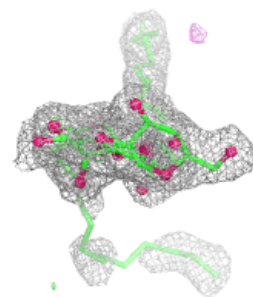
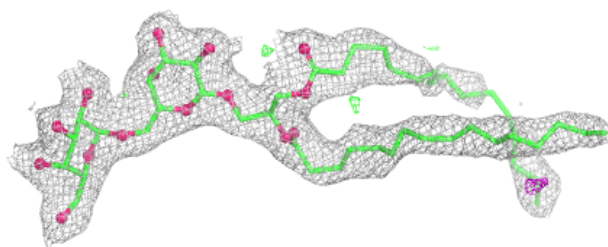
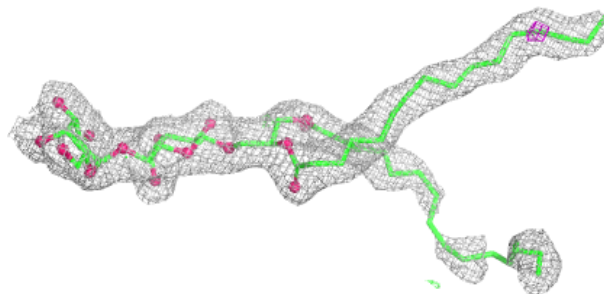
Electron density around CLA C 509:

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

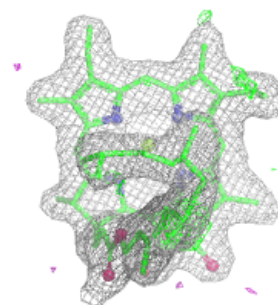
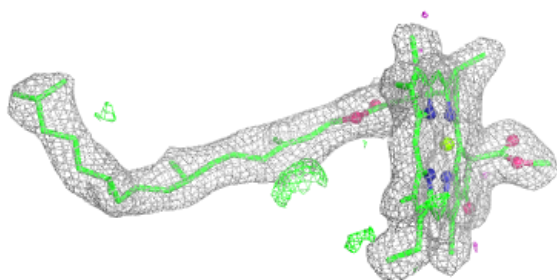
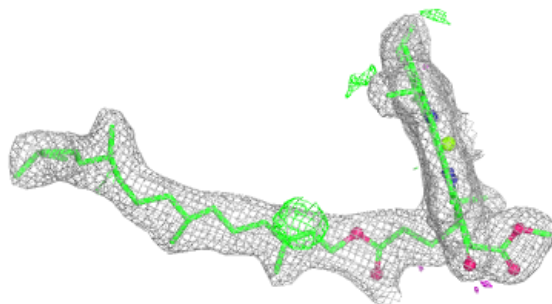


Electron density around DGD C 521:

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

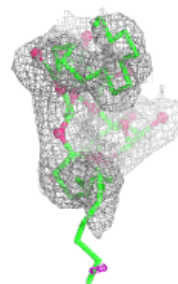
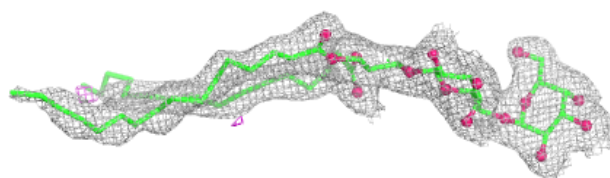
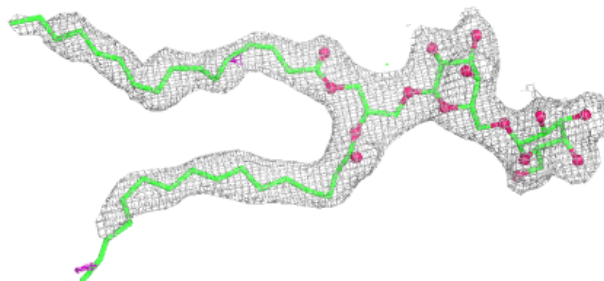
**Electron density around CLA b 605:**

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

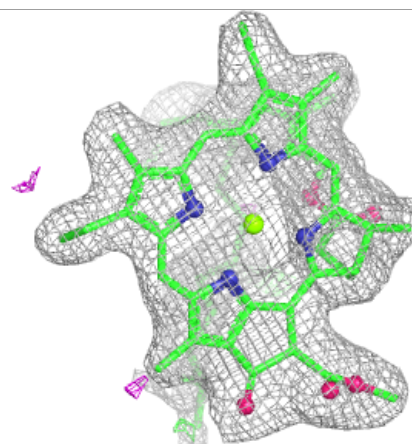
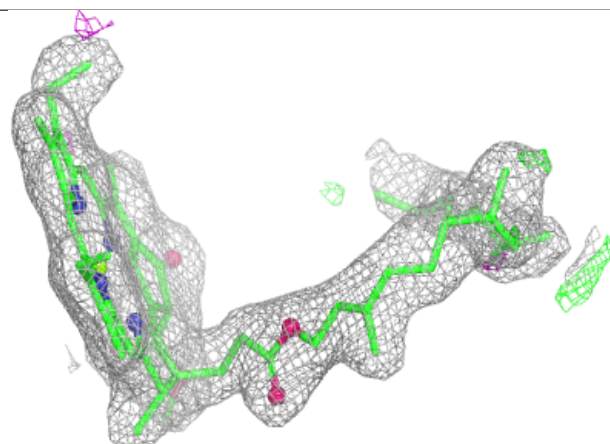
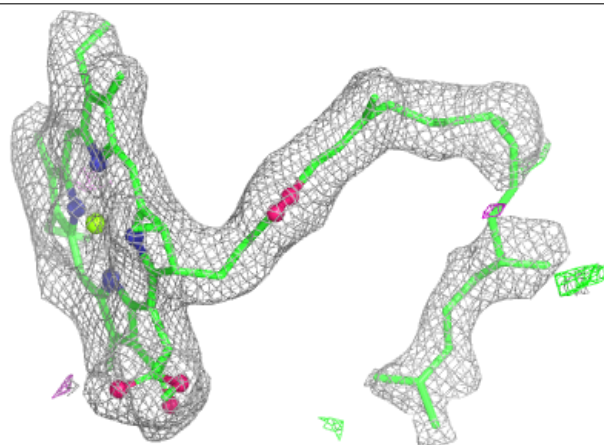


Electron density around DGD C 523:

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

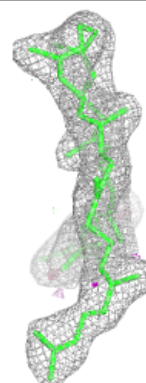
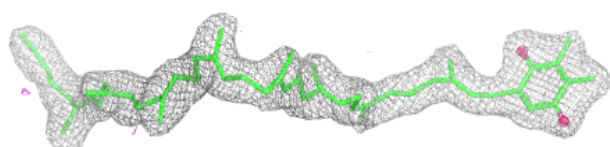
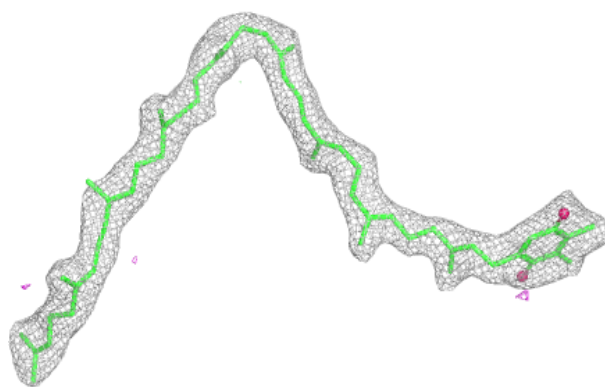
**Electron density around CLA B 606:**

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

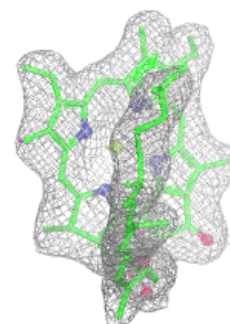
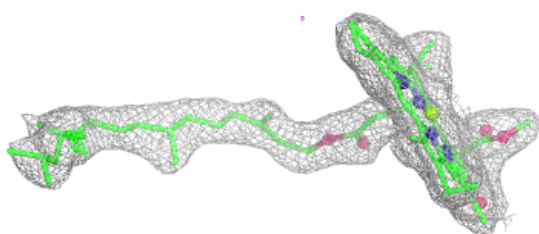
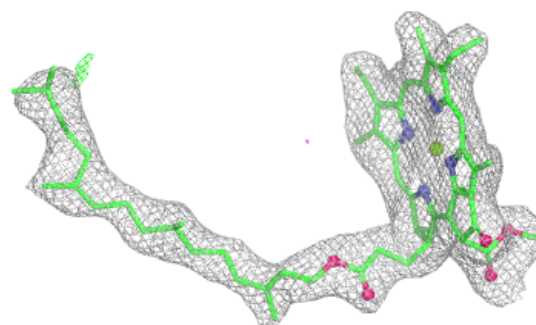


Electron density around PL9 D 407:

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

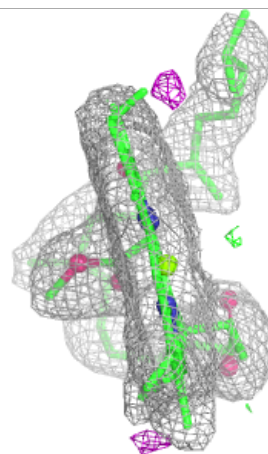
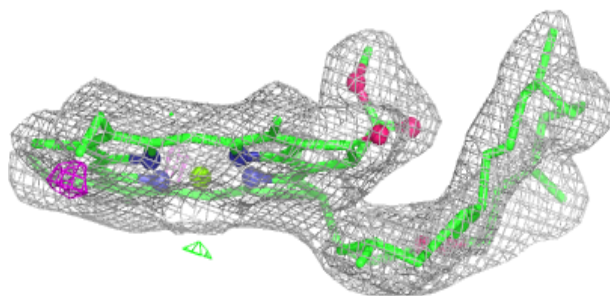
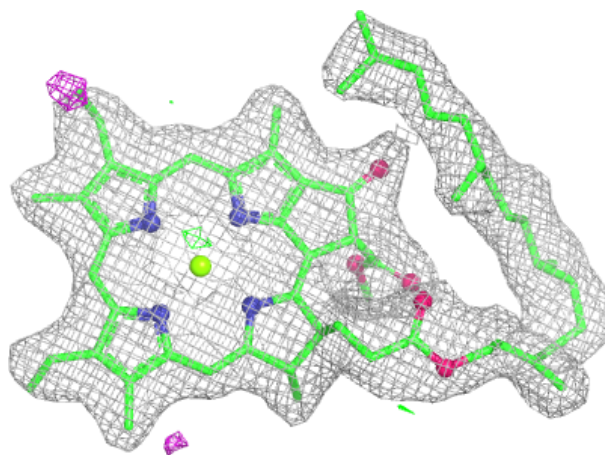
**Electron density around CLA b 609:**

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



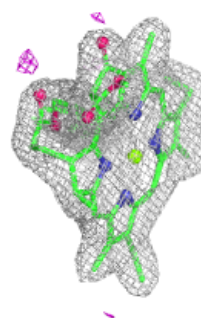
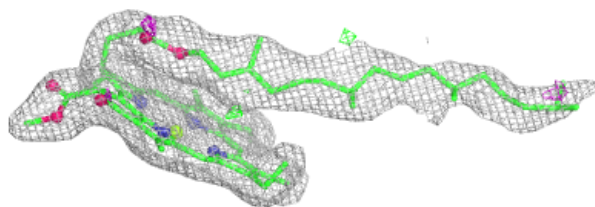
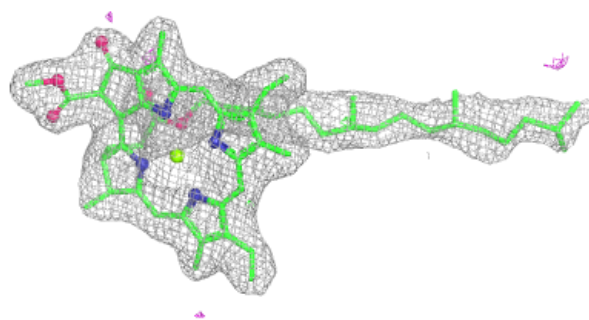
Electron density around CLA b 610:

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



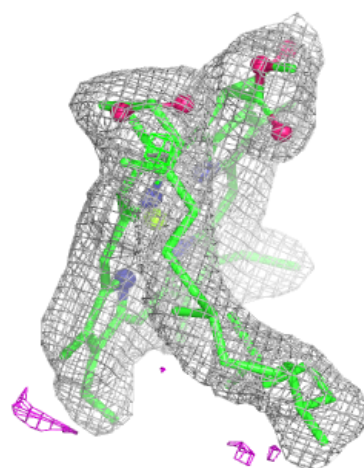
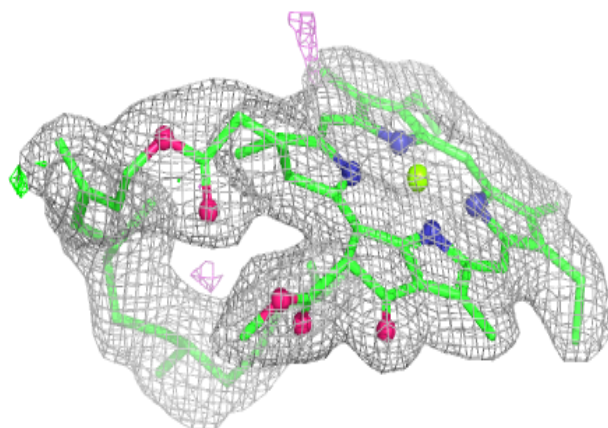
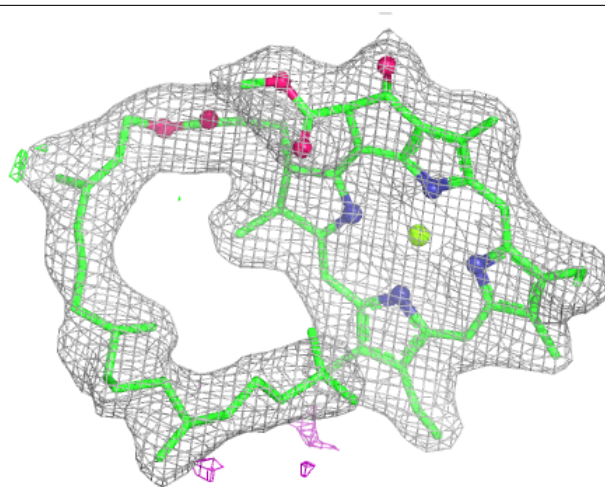
Electron density around CLA b 614:

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



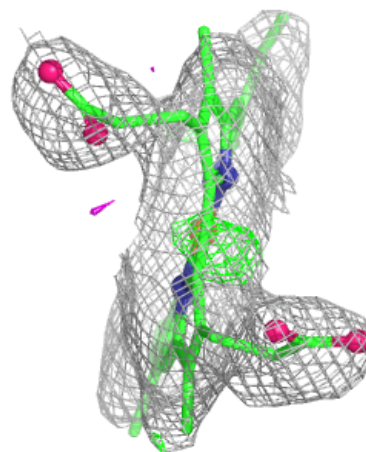
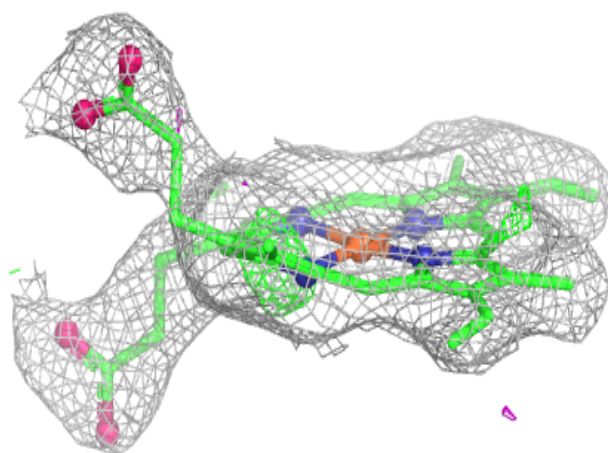
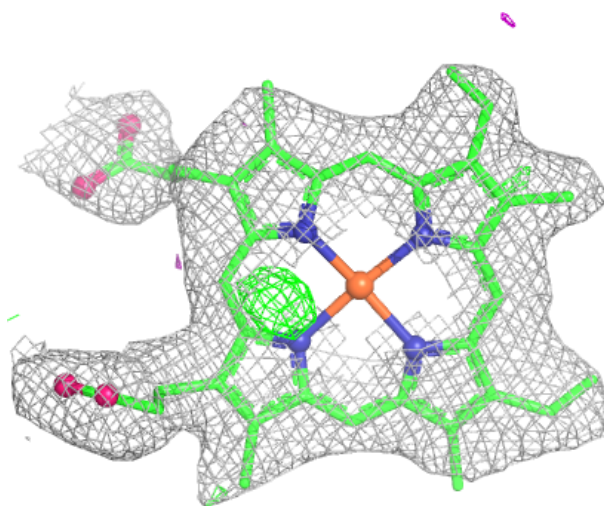
Electron density around CLA b 615:

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



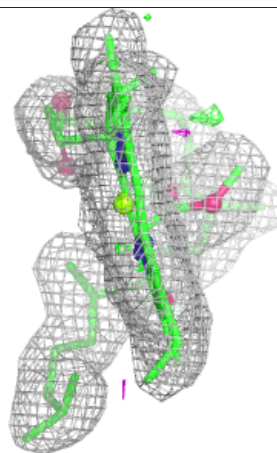
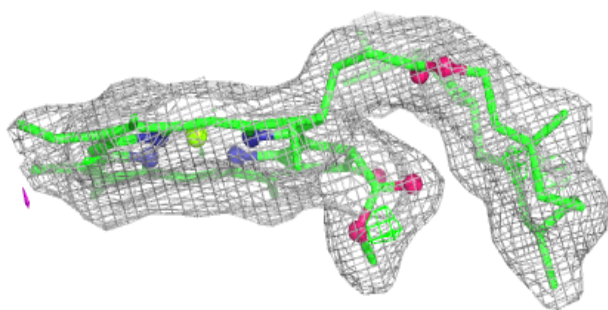
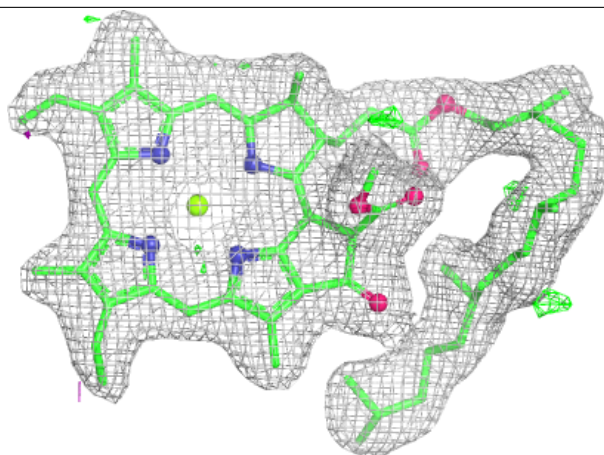
Electron density around HEM e 102:

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

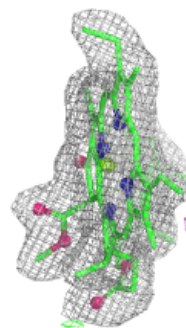
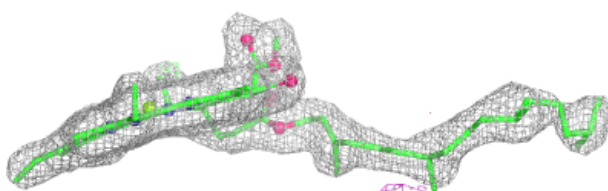
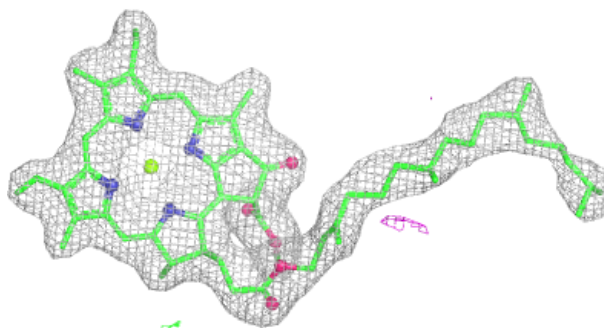


Electron density around CLA B 610:

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

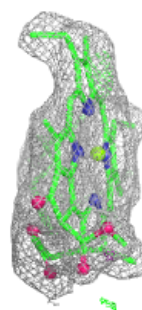
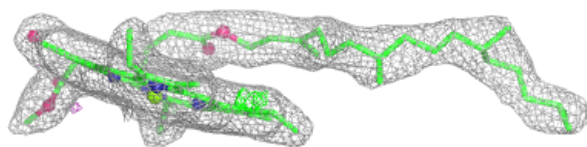
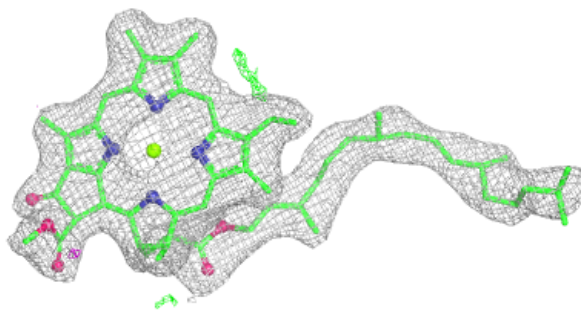
**Electron density around CLA b 602:**

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

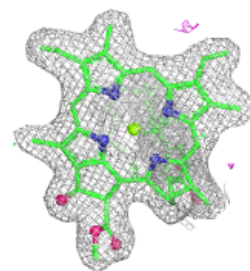
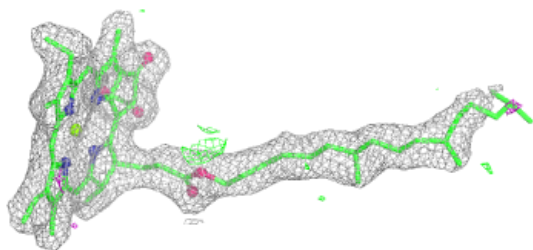
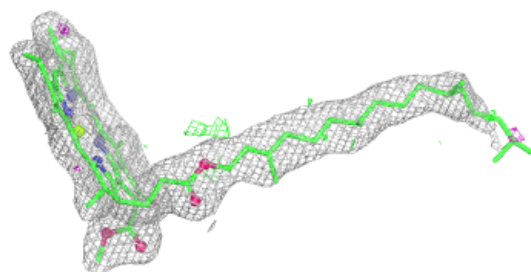


Electron density around CLA b 603:

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

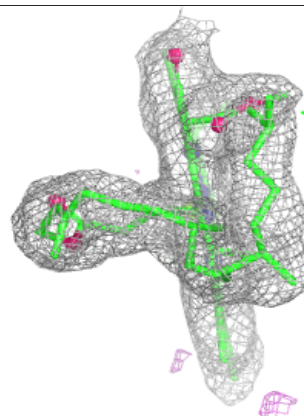
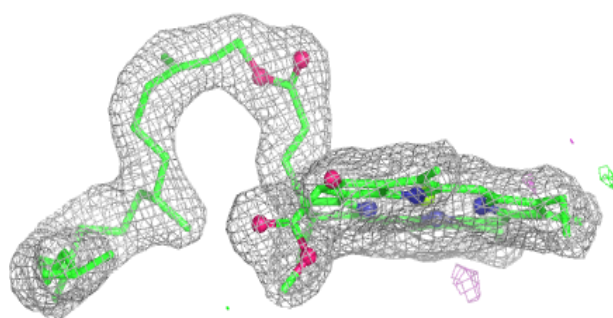
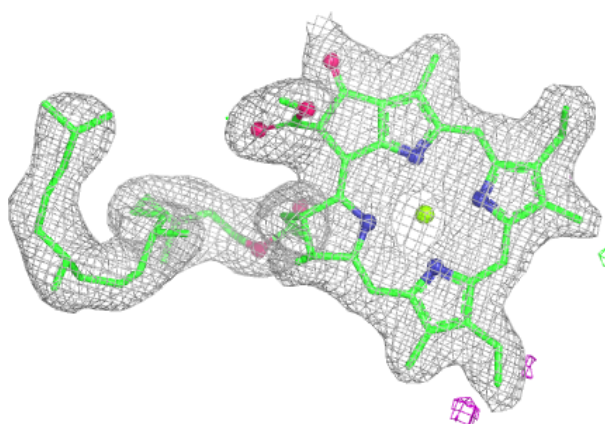
**Electron density around CLA b 604:**

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

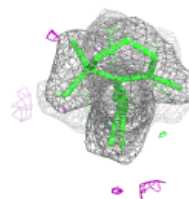
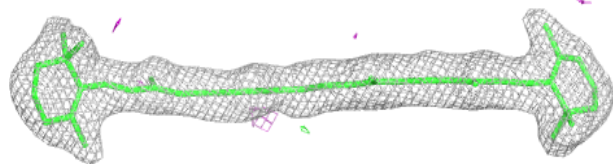
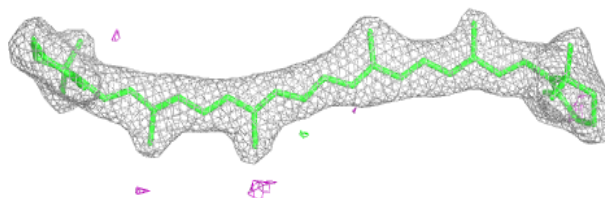


Electron density around CLA B 612:

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

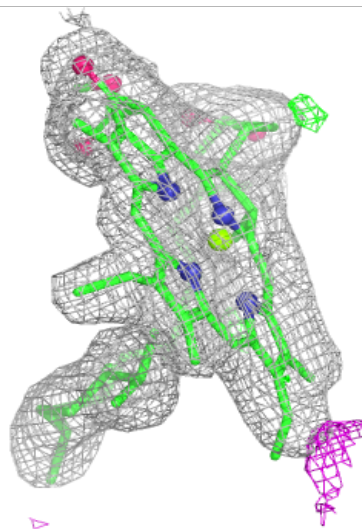
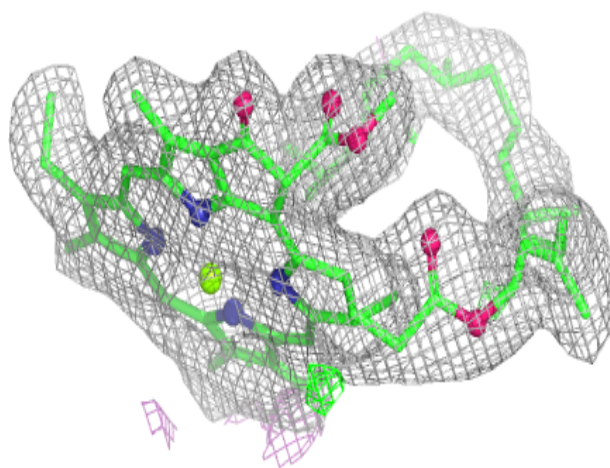
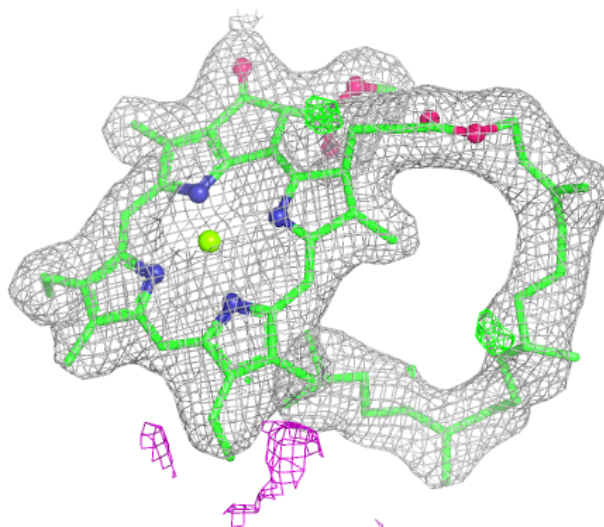
**Electron density around BCR a 610:**

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



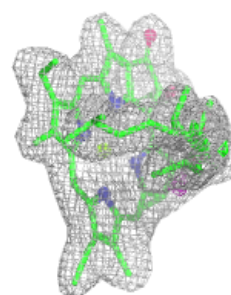
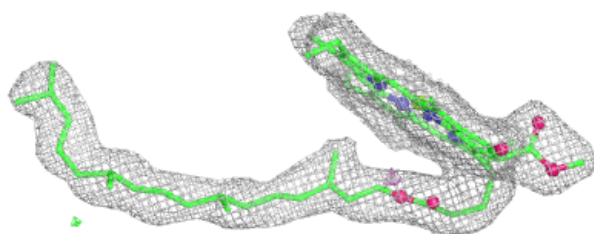
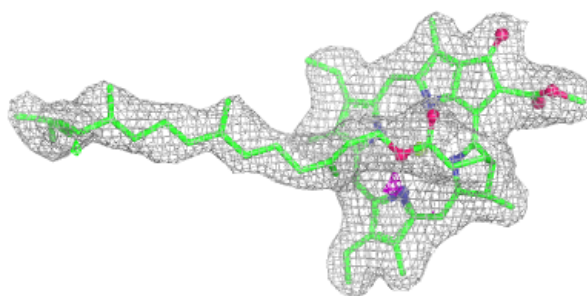
Electron density around CLA B 615:

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

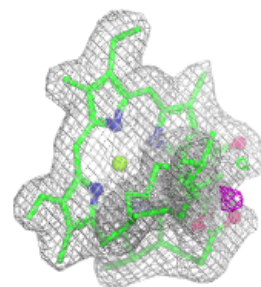
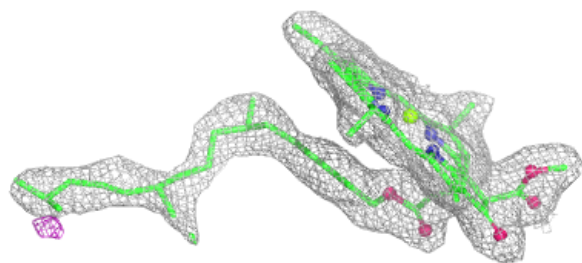
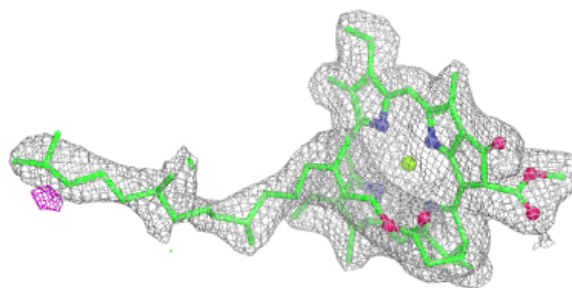


Electron density around CLA b 608:

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

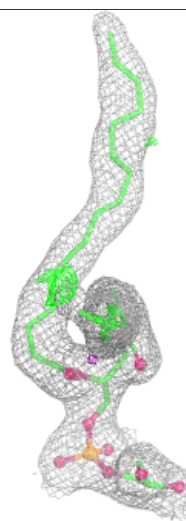
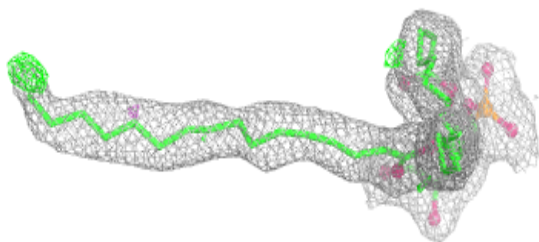
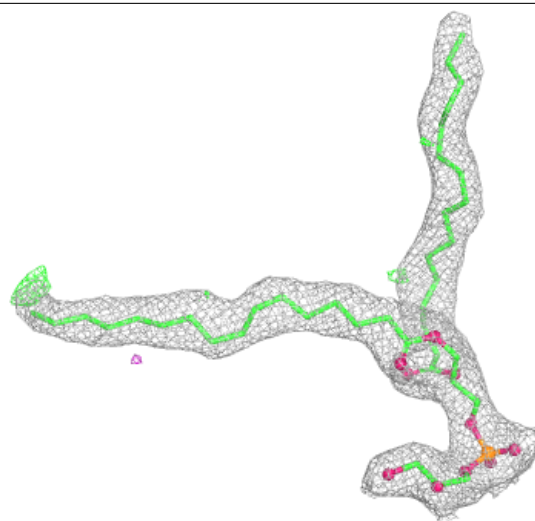
**Electron density around CLA C 505:**

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



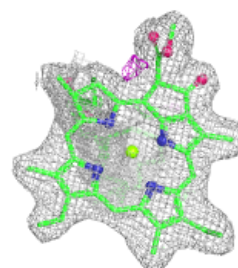
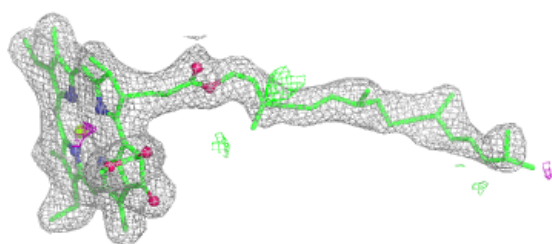
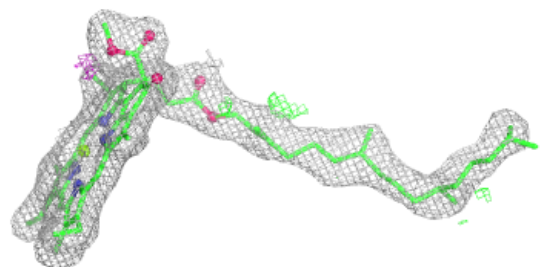
Electron density around LHG L 101:

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

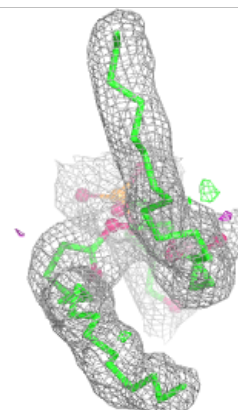
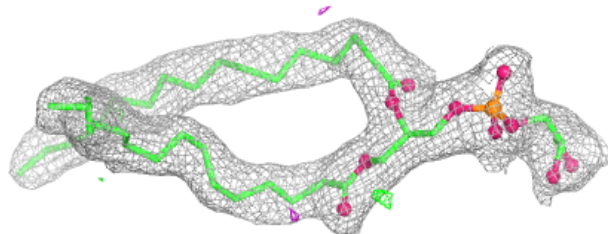
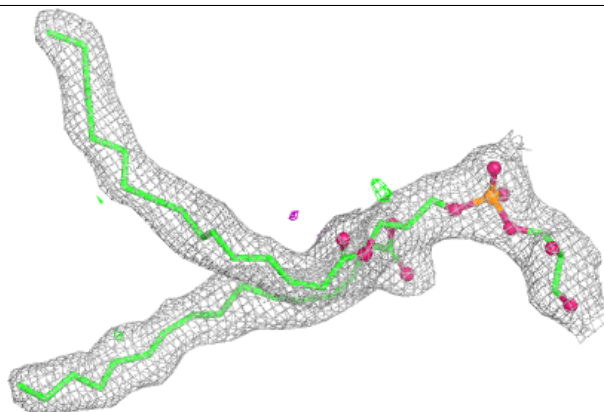


Electron density around CLA B 604:

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

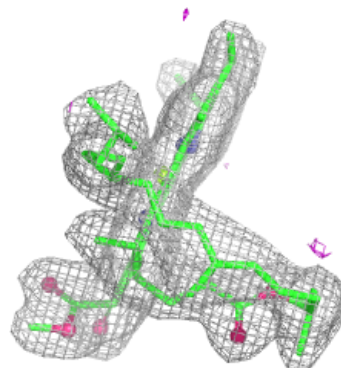
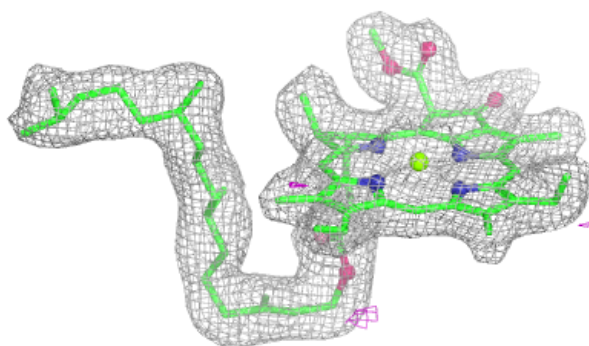
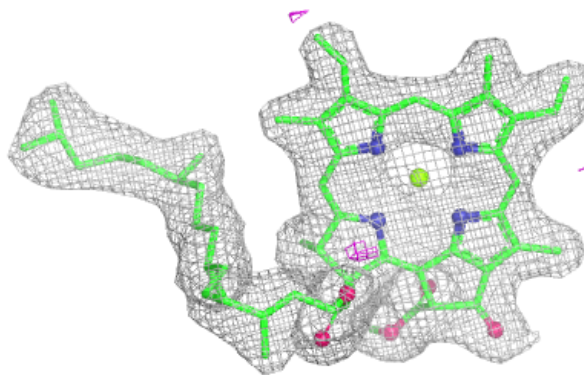
**Electron density around LHG d 408:**

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

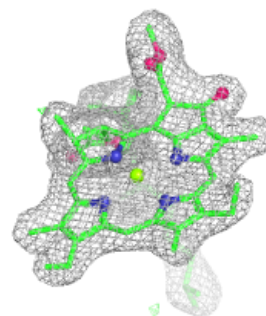
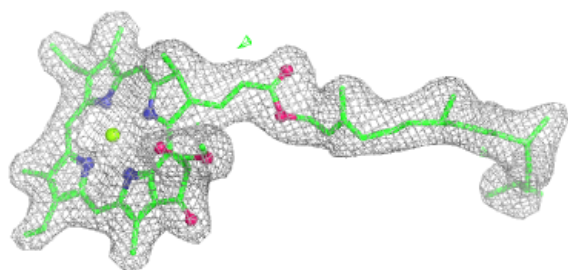
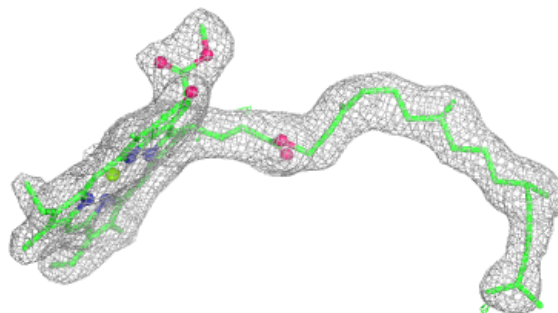


Electron density around CLA d 402:

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

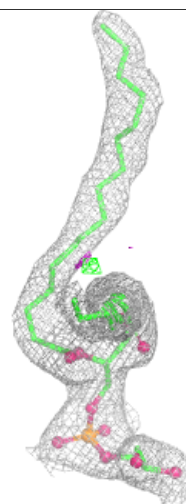
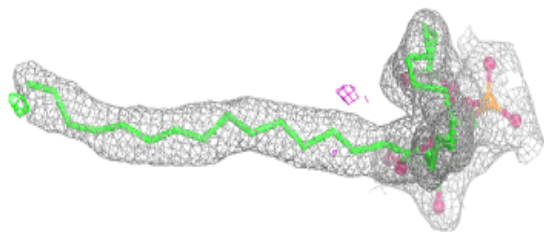
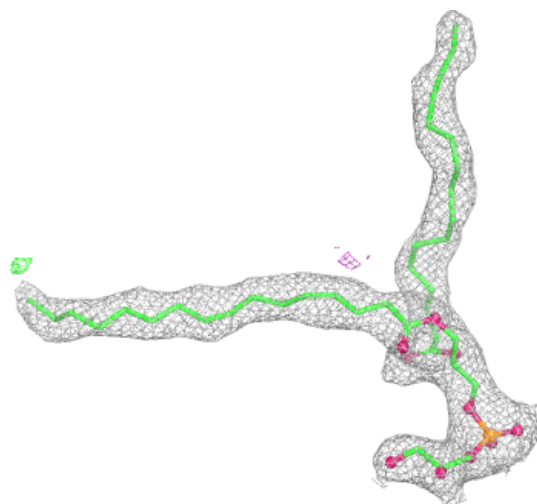
**Electron density around CLA d 403:**

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



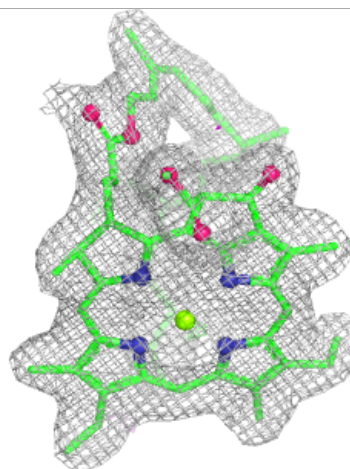
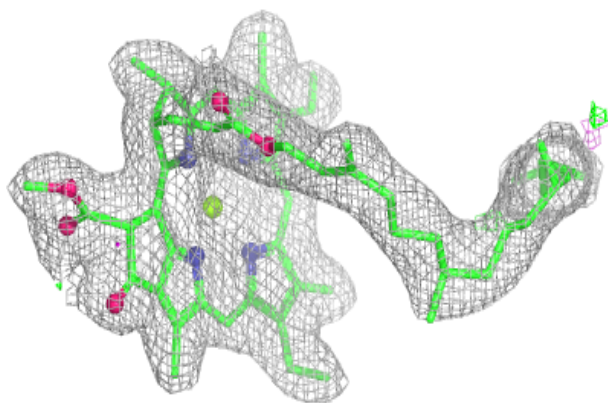
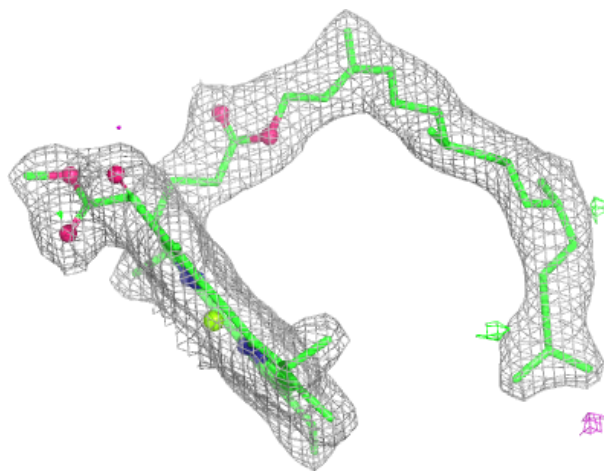
Electron density around LHG 1 101:

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



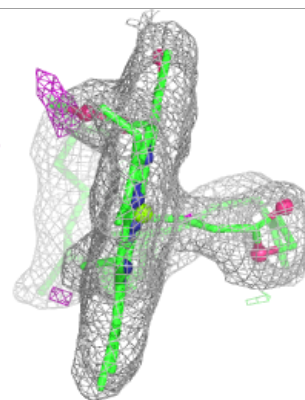
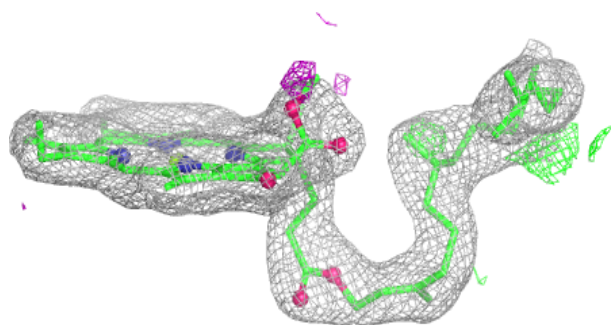
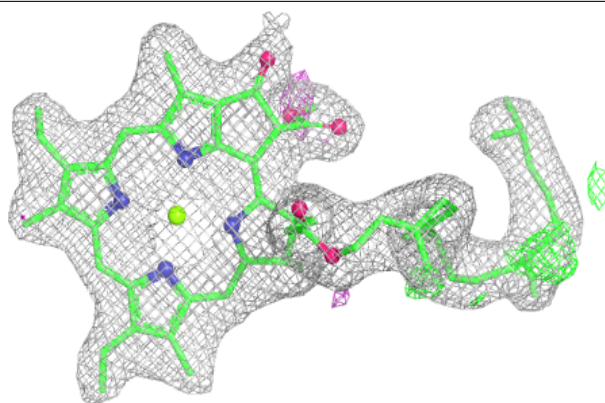
Electron density around CLA b 611:

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

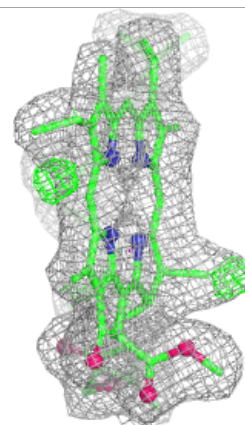
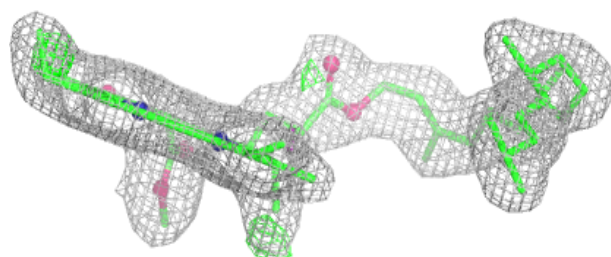
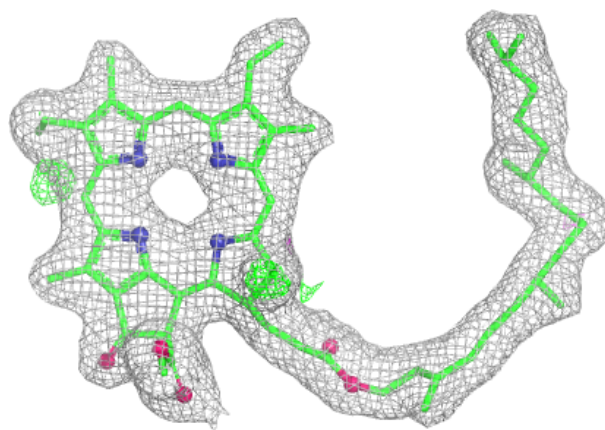


Electron density around CLA b 612:

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

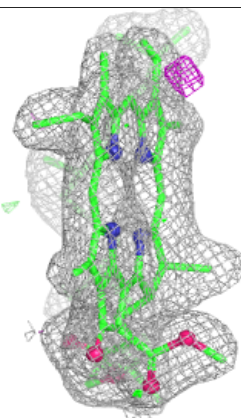
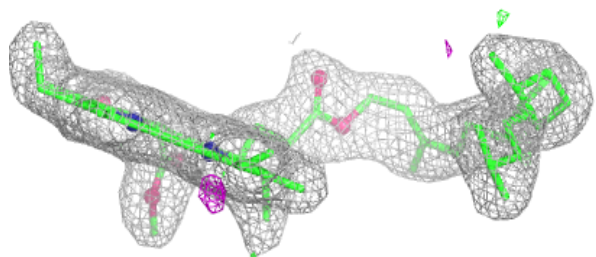
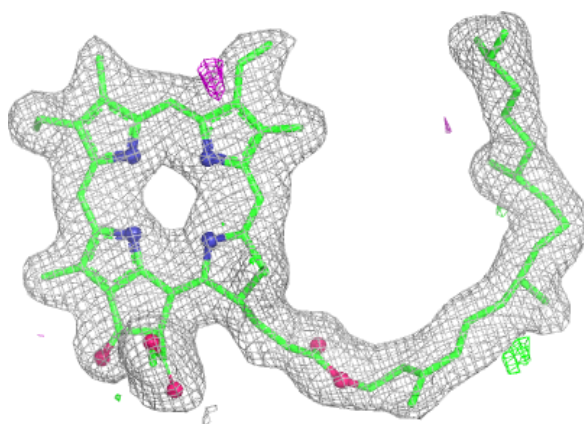
**Electron density around PHO D 402:**

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

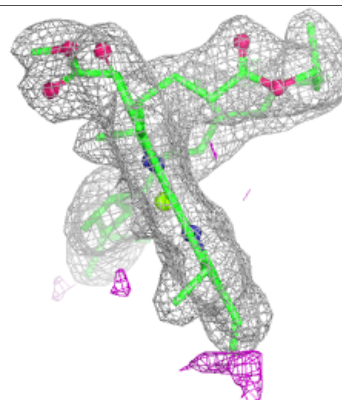
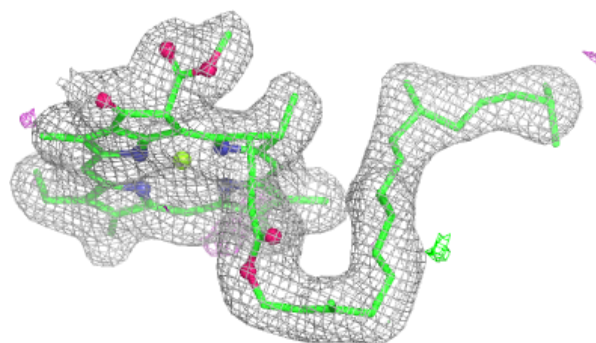
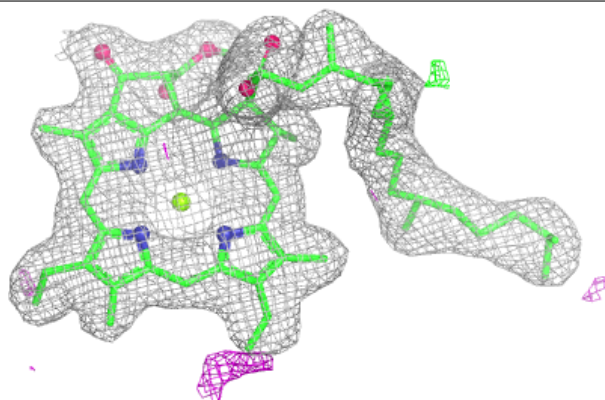


Electron density around PHO a 607:

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

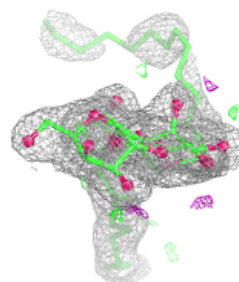
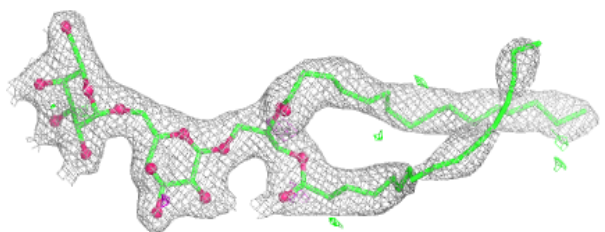
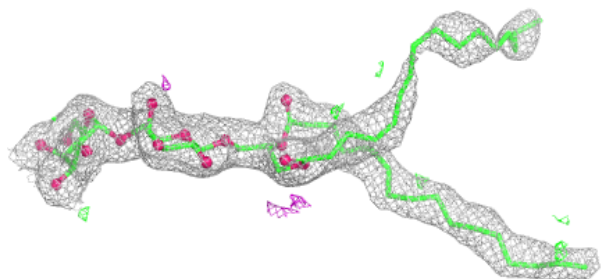
**Electron density around CLA D 403:**

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

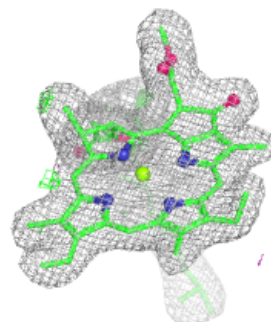
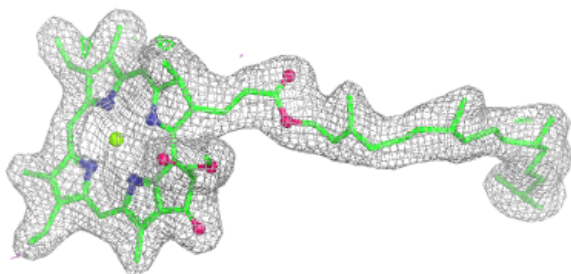
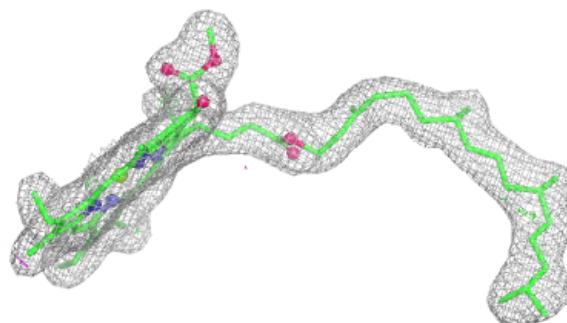


Electron density around DGD c 518:

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

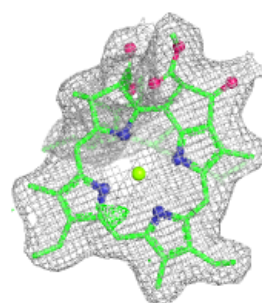
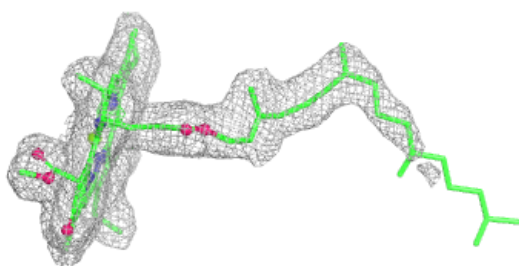
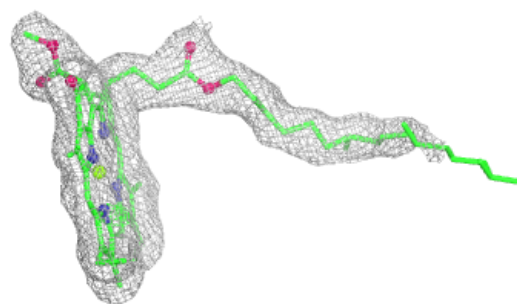
**Electron density around CLA D 404:**

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

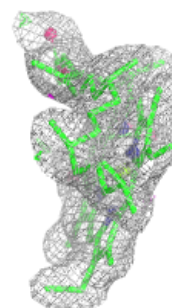
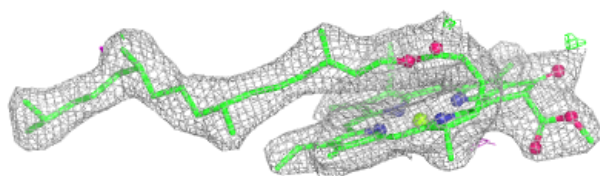
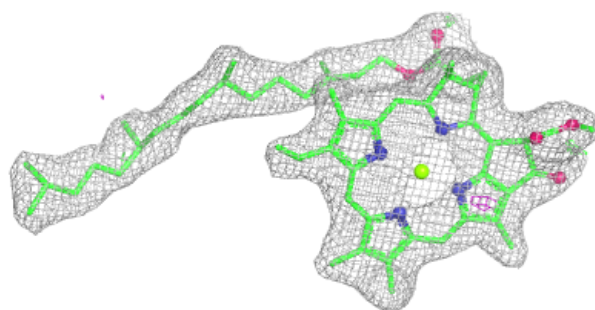


Electron density around CLA D 405:

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

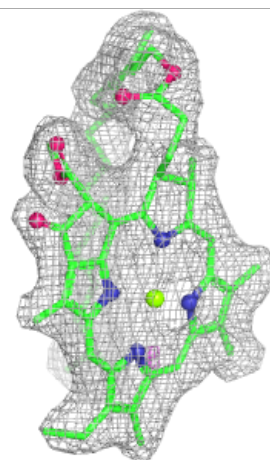
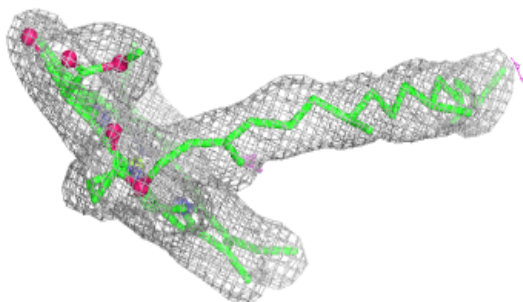
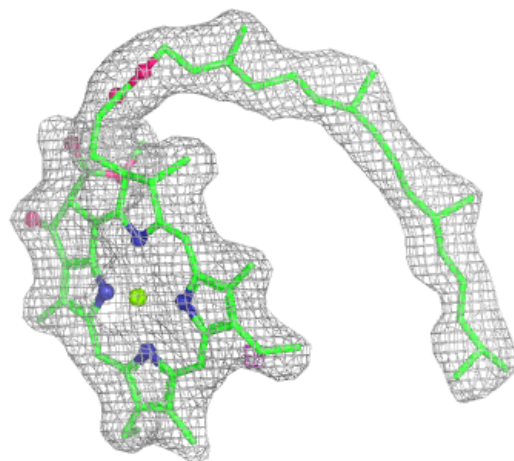
**Electron density around CLA c 501:**

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



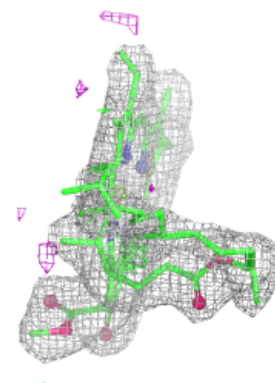
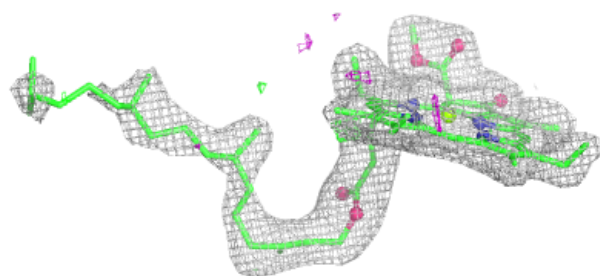
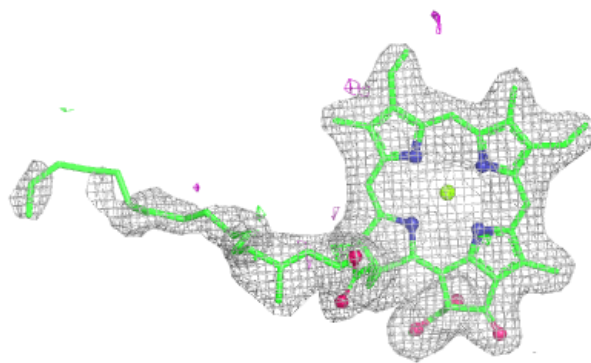
Electron density around CLA C 507:

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

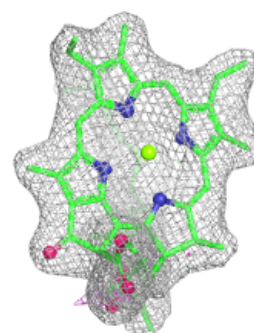
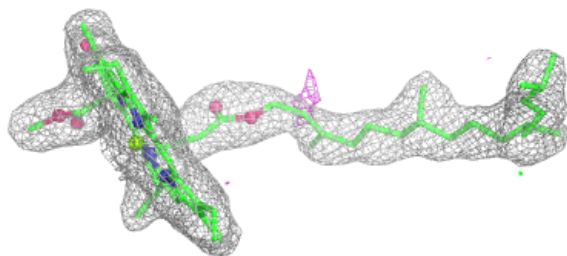
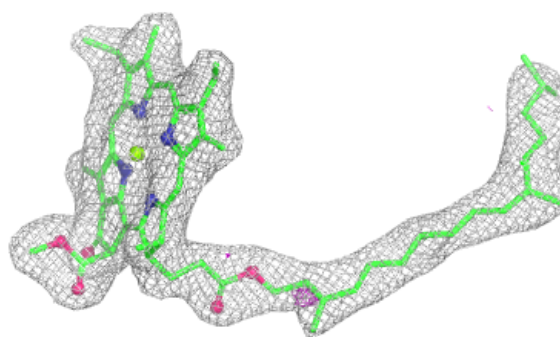


Electron density around CLA a 606:

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

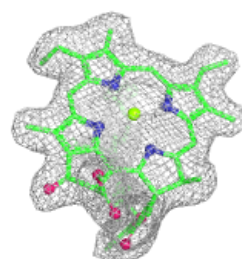
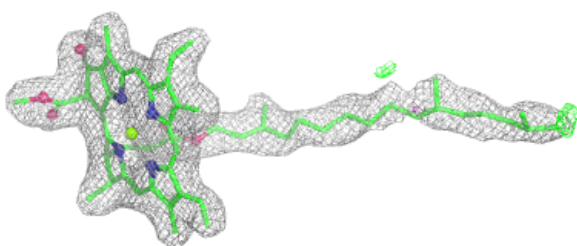
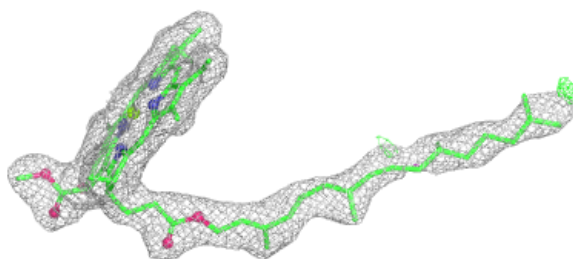
**Electron density around CLA B 609:**

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

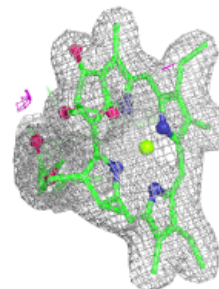
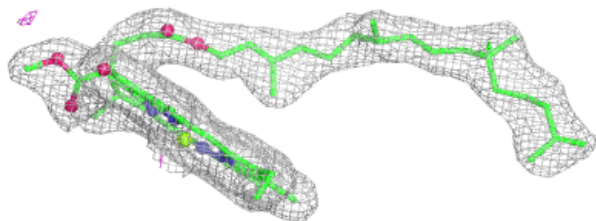
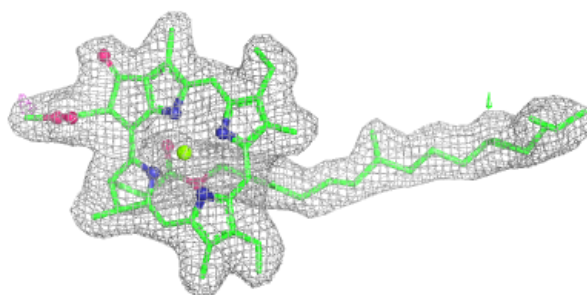


Electron density around CLA B 607:

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

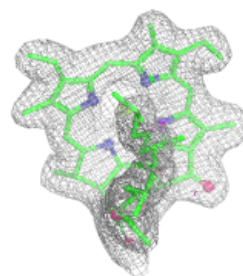
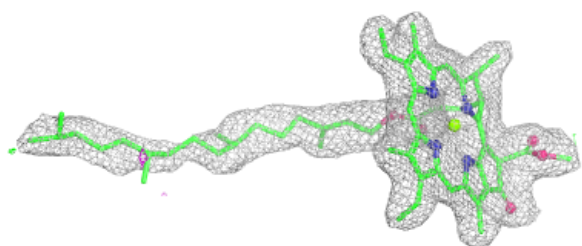
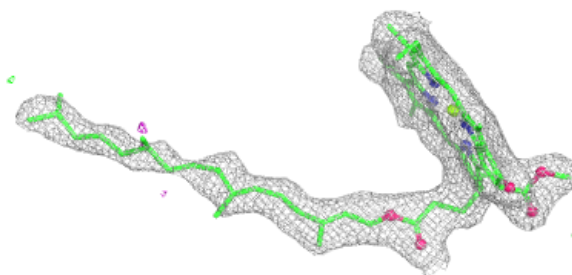
**Electron density around CLA B 608:**

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

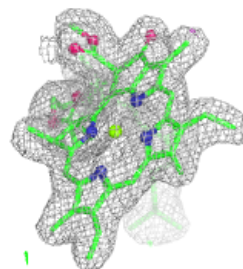
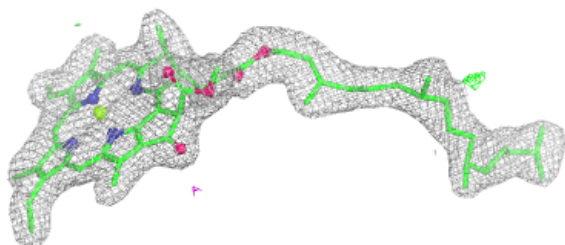
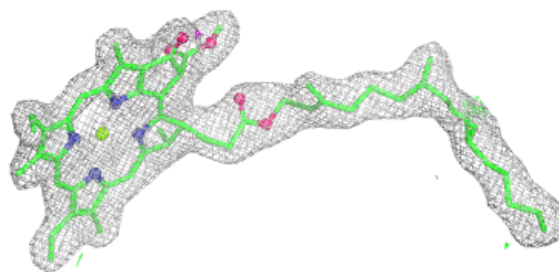


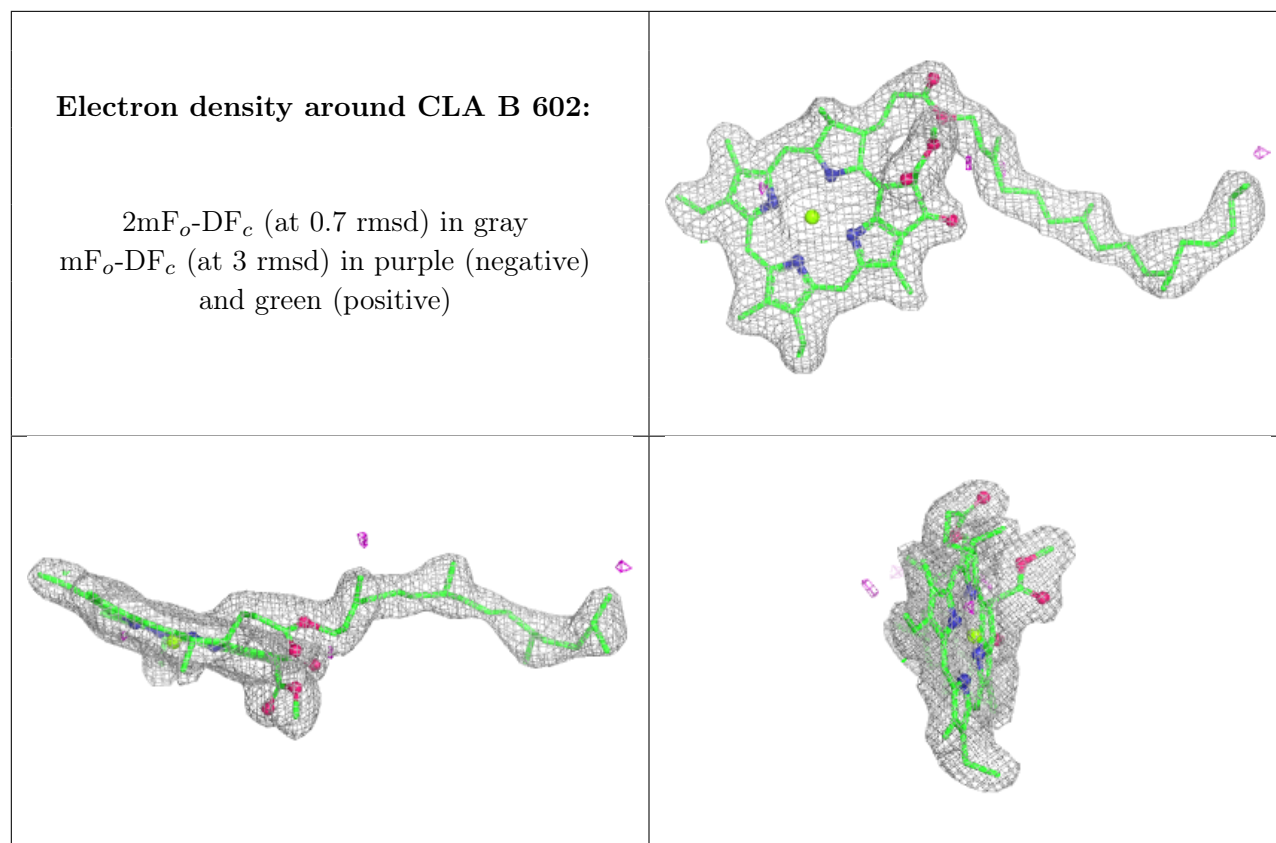
Electron density around CLA b 607:

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

**Electron density around CLA A 605:**

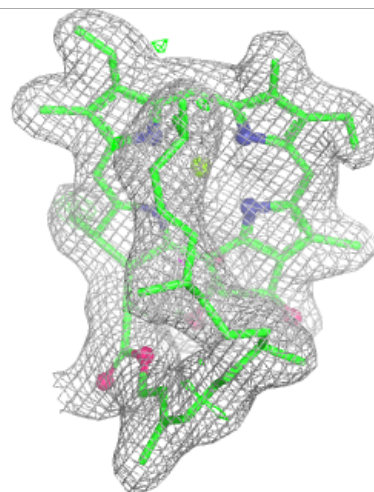
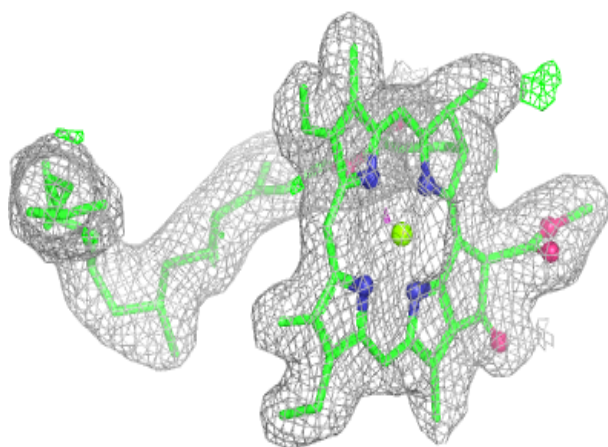
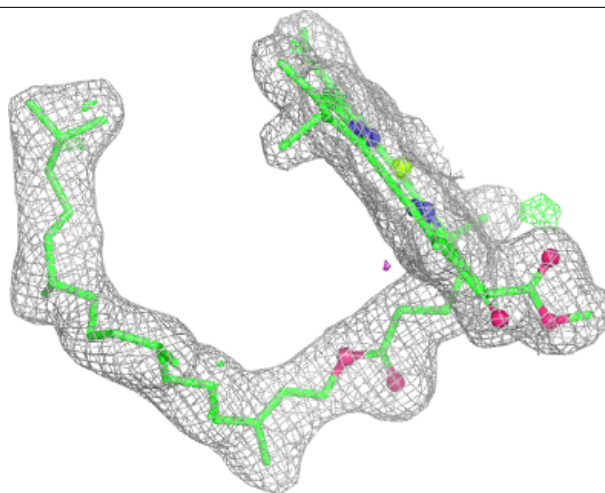
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





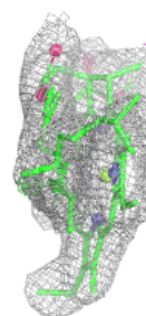
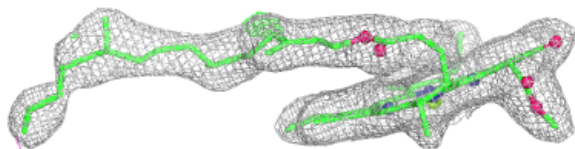
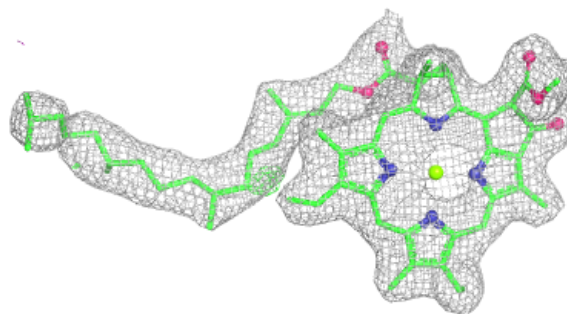
Electron density around CLA B 611:

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



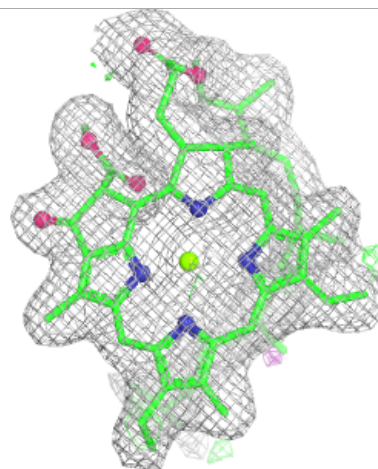
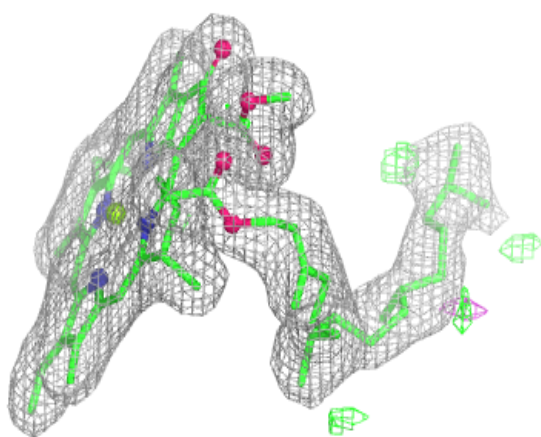
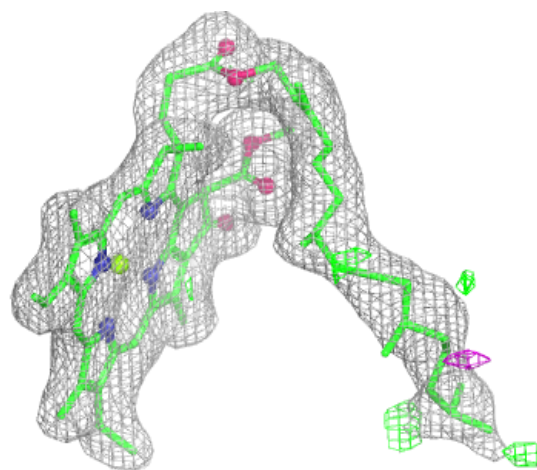
Electron density around CLA B 603:

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



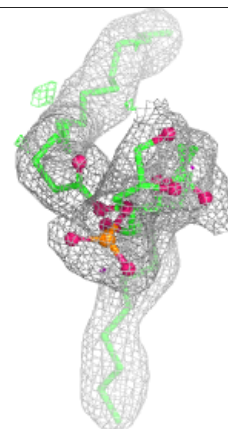
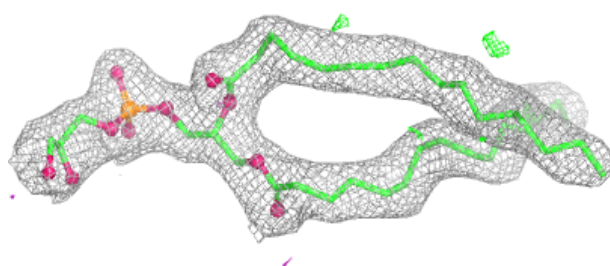
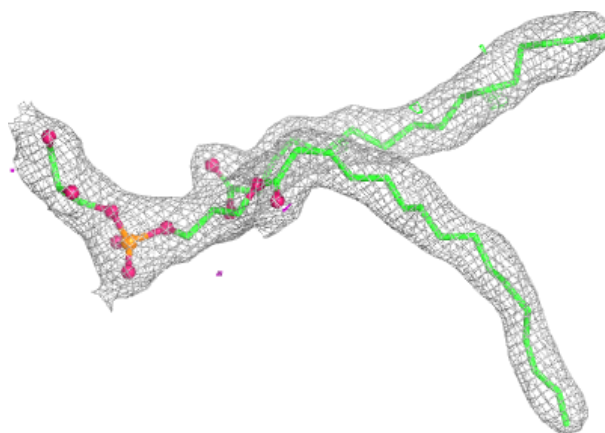
Electron density around CLA B 613:

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



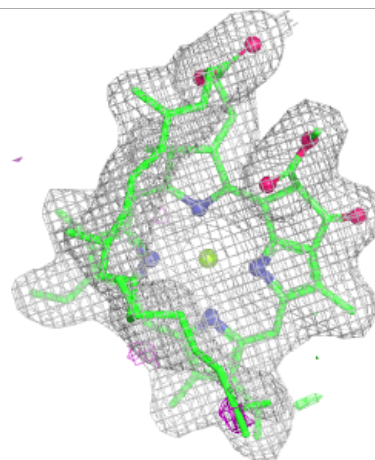
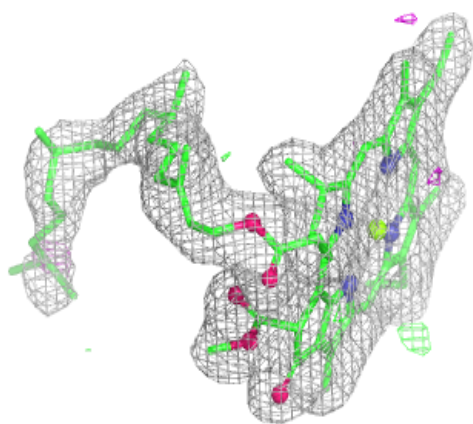
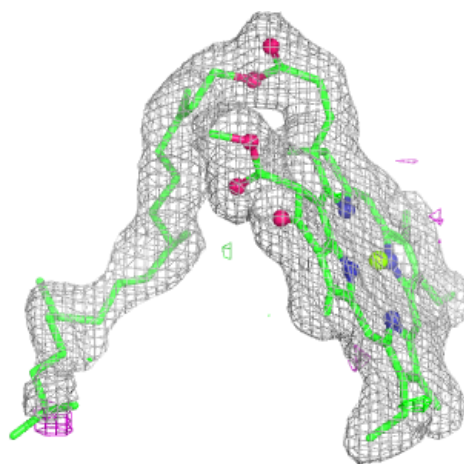
Electron density around LHG D 411:

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



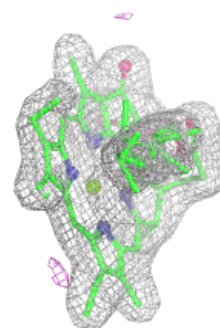
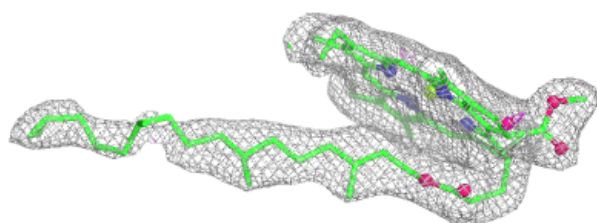
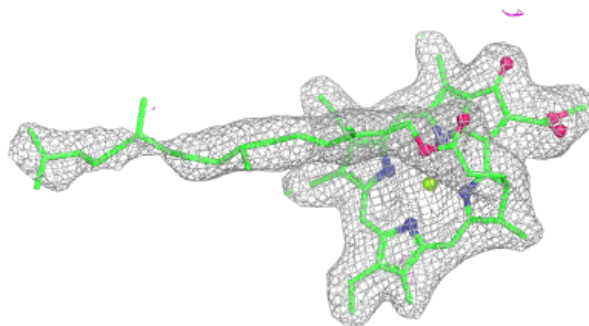
Electron density around CLA b 613:

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

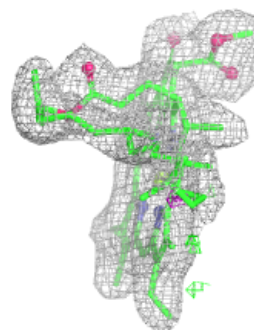
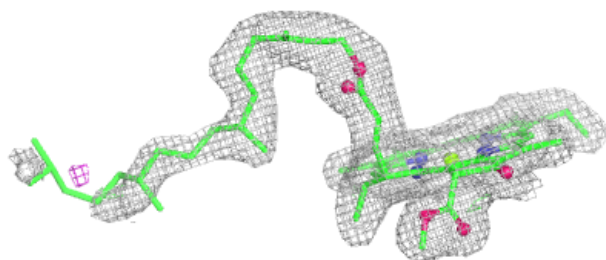
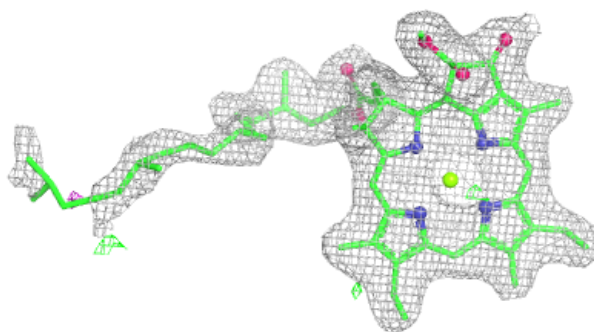


Electron density around CLA B 614:

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

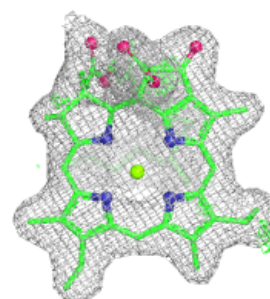
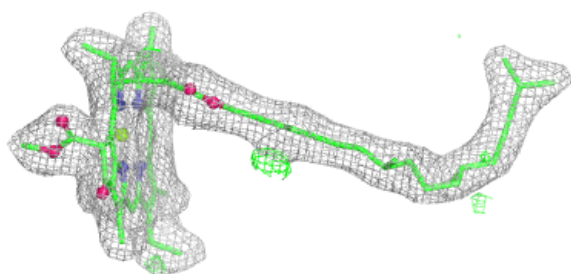
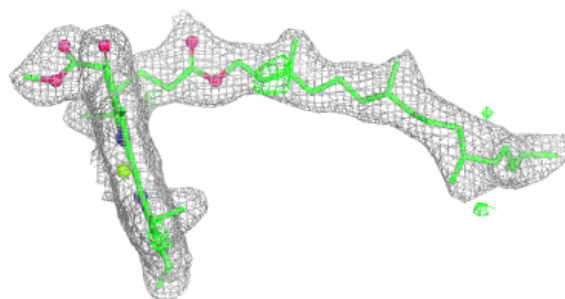
**Electron density around CLA A 606:**

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



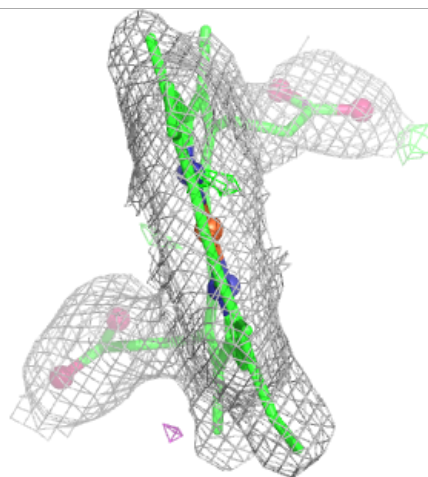
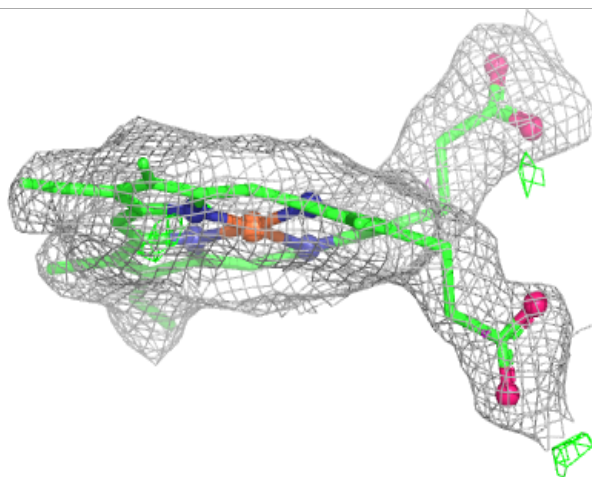
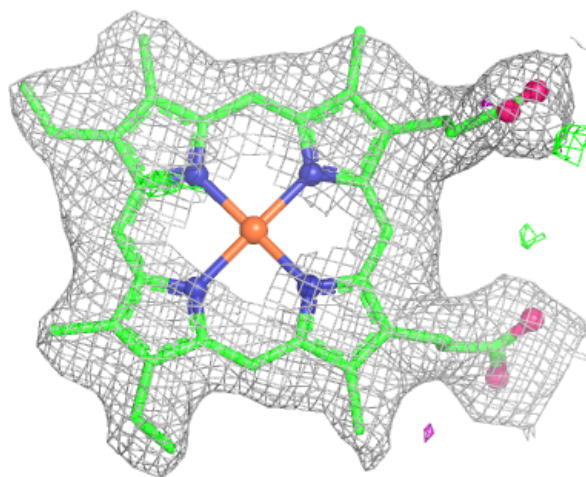
Electron density around CLA B 605:

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



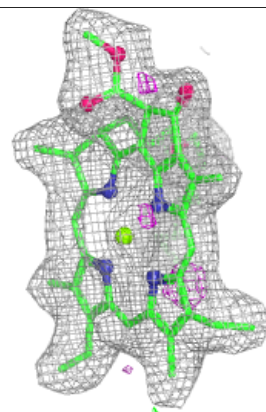
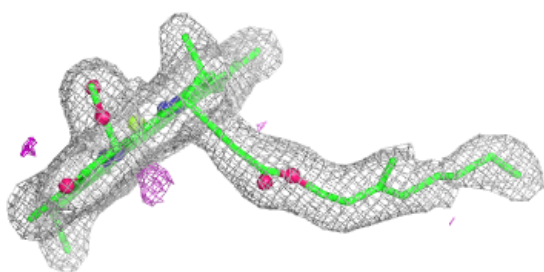
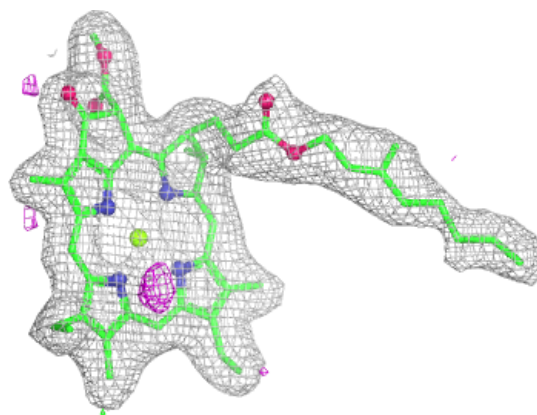
Electron density around HEM F 101:

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



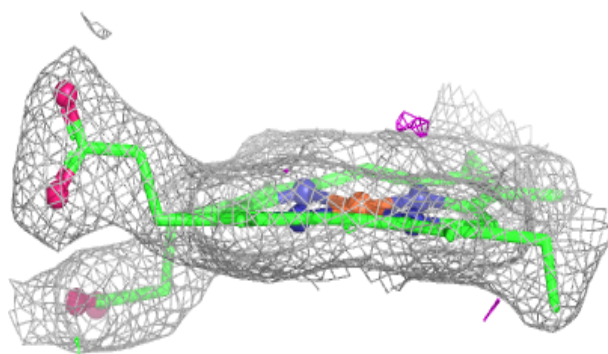
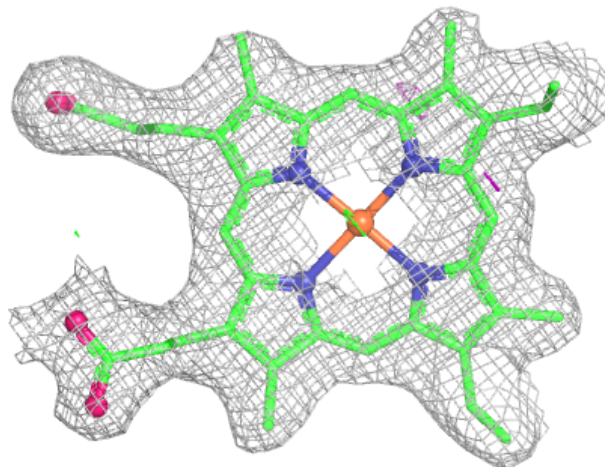
Electron density around CLA A 608:

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



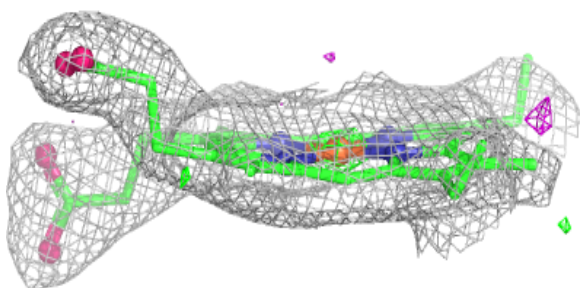
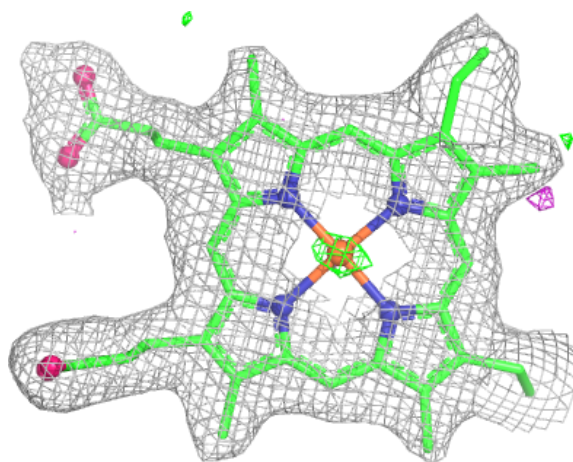
Electron density around HEC V 201:

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



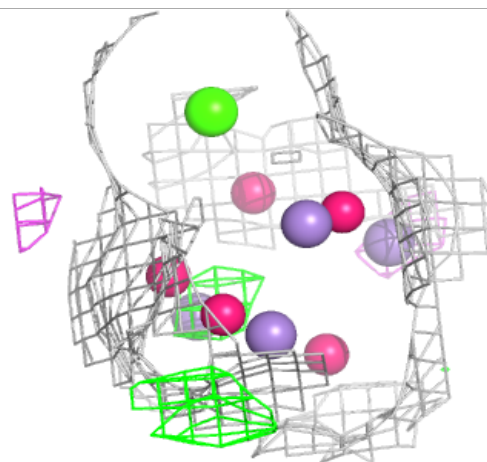
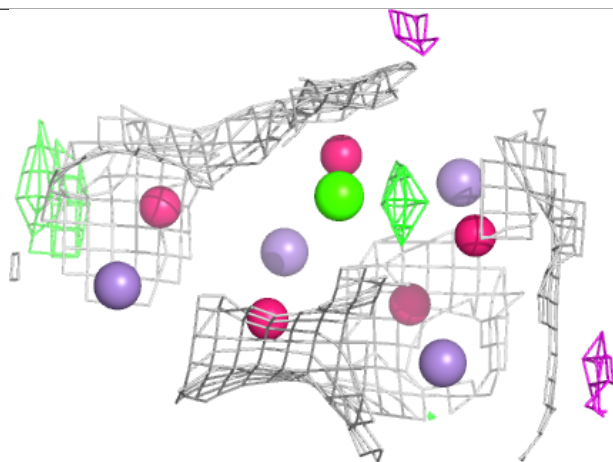
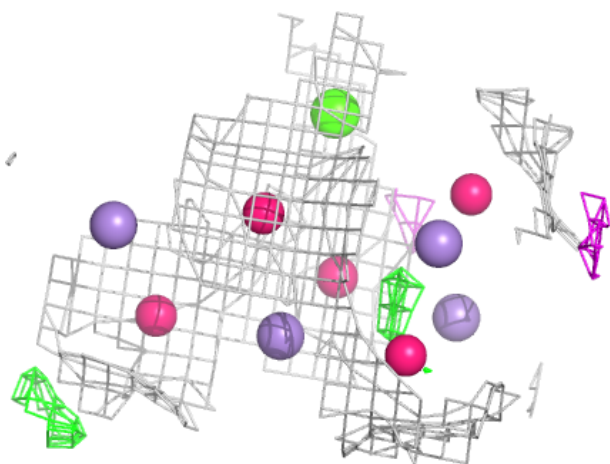
Electron density around HEC v 201:

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



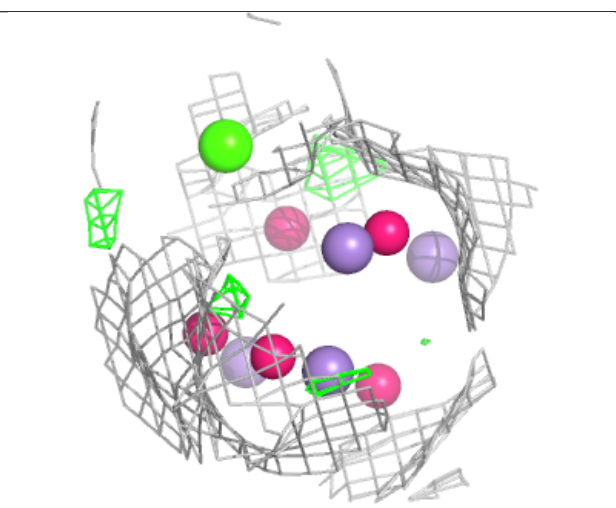
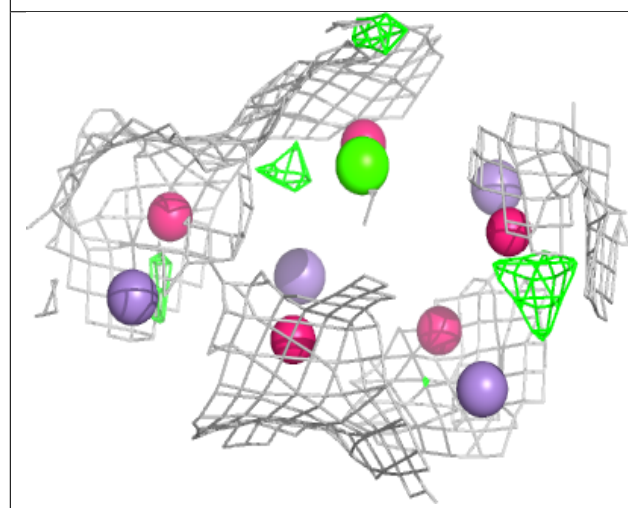
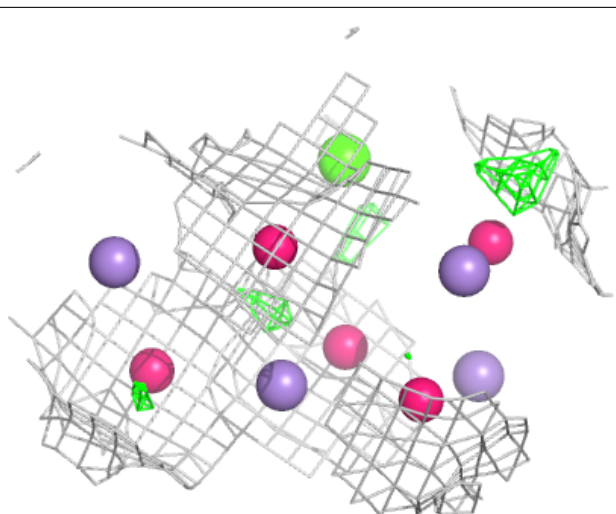
Electron density around OEX a 601:

$2mF_o-DF_c$ (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.