



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 02:54 PM EDT

PDB ID : 9Z69 / pdb_00009z69
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2 rich) at 1.98 Angstrom obtained from conventional data at 9.5 keV
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Minnetian, N.M.; Zhang, M.
Deposited on : 2025-11-14
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

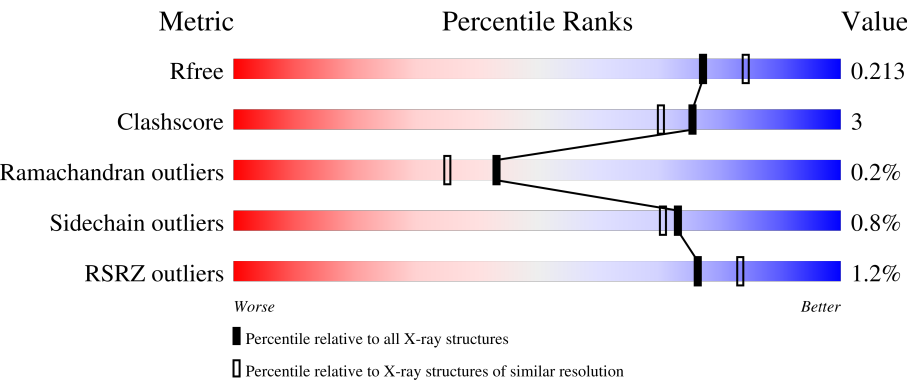
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



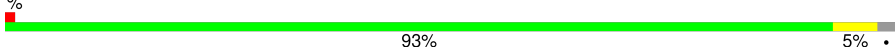
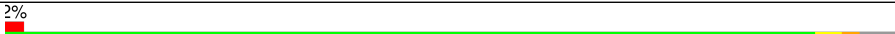
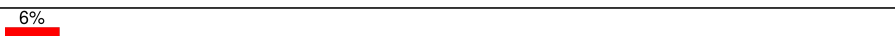
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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

Mol	Chain	Length	Quality of chain
1	A	344	91%6%.
1	a	344	91%6%.
2	B	510	% 94%..
2	b	510	% 95%..

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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 104563 atoms, of which 52080 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5091	1717	2469	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5081	1714	2462	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	H	N	O	S	0	7	0
			7903	2637	3887	670	696	13			
2	b	505	Total	C	H	N	O	S	0	1	0
			7826	2614	3842	665	692	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6773	2249	3347	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6918	2290	3418	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	H	N	O	S	0	0	0
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	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	H	N	O	0	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O		0	0	0
			600	197	304	47	52				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0	0
			523	171	267	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3700	1168	1830	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3720	1170	1846	317	383	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
14	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			995	328	516	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

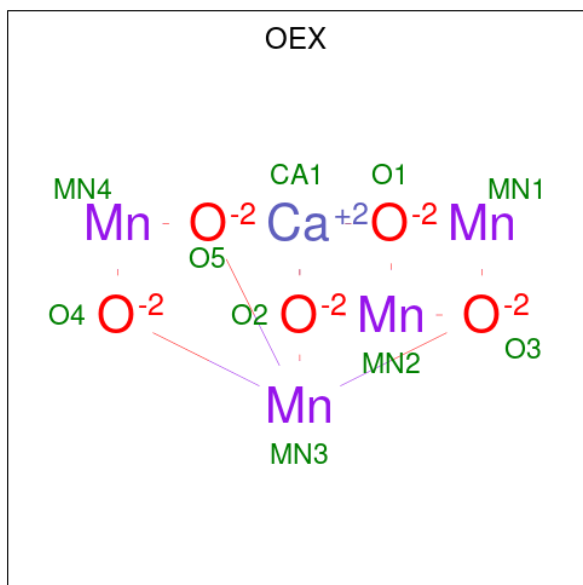
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

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

- Molecule 21 is CA-MN4-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).

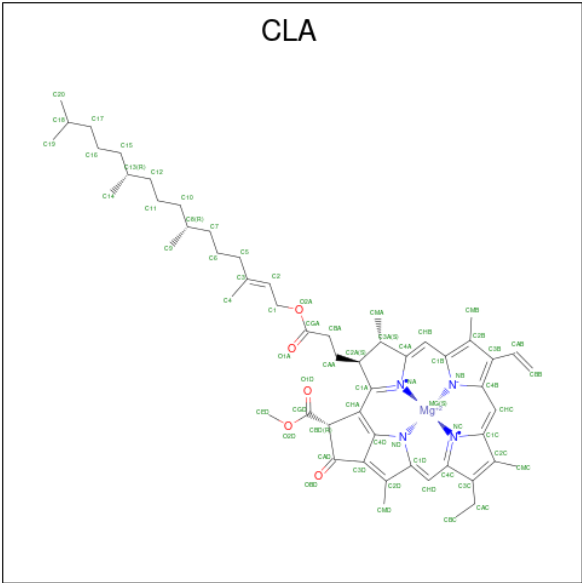
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		

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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	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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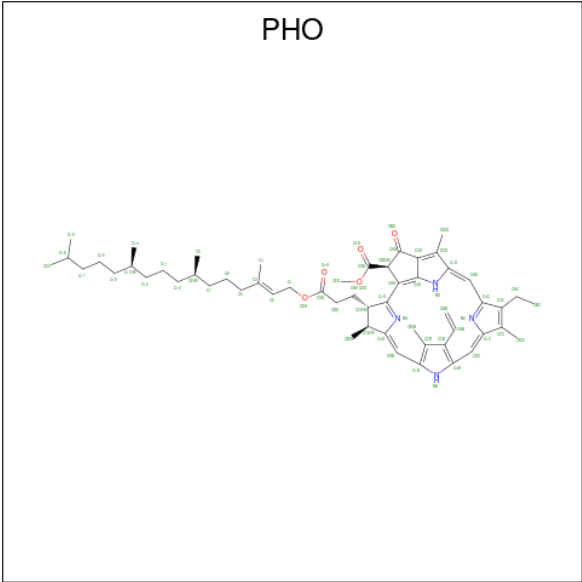
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4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

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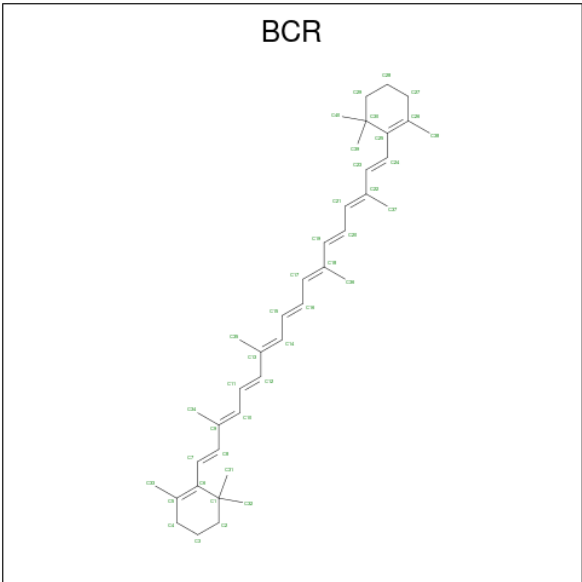
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



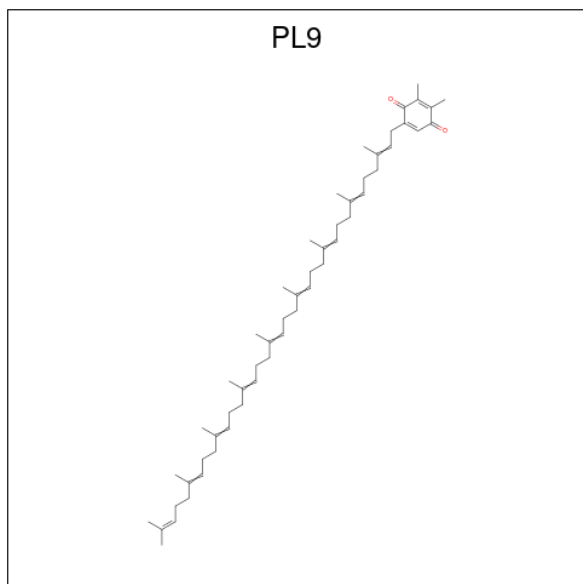
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

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



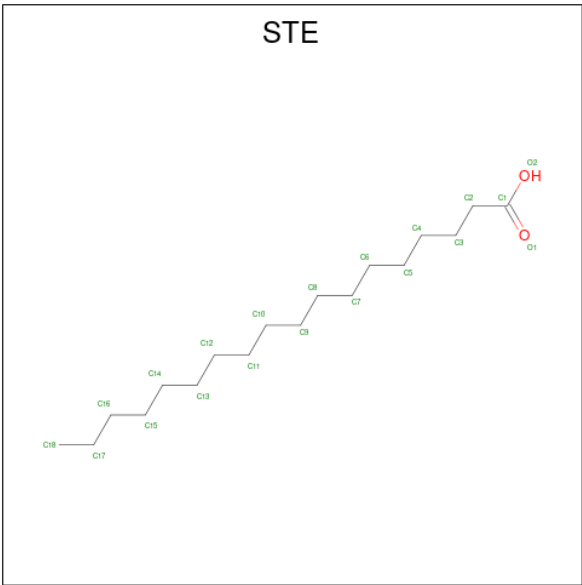
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	D	1	Total	C	H	0	0
			96	40	56		
26	H	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	T	1	Total	C	H	0	0
			96	40	56		
26	a	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	h	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	t	1	Total	C	H	0	0
			96	40	56		

- 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	H	O	0	0
			135	53	80	2		
27	D	1	Total	C	H	O	0	0
			135	53	80	2		
27	a	1	Total	C	H	O	0	0
			135	53	80	2		
27	d	1	Total	C	H	O	0	0
			135	53	80	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	H		0	0
			23	9	14			
28	A	1	Total	C	H		0	0
			23	8	15			
28	A	1	Total	C	H		0	0
			50	17	33			
28	A	1	Total	C	H		0	0
			32	11	21			
28	B	1	Total	C	H	O	0	0
			43	15	26	2		
28	B	1	Total	C	H	O	0	0
			46	16	28	2		
28	B	1	Total	C	H	O	0	0
			28	10	16	2		
28	B	1	Total	C	H		0	0
			41	15	26			
28	C	1	Total	C	H	O	0	0
			34	12	20	2		
28	C	1	Total	C	H		0	0
			11	5	6			
28	C	1	Total	C	H		0	0
			17	7	10			
28	C	1	Total	C	H		0	0
			26	10	16			
28	C	1	Total	C	H	O	0	0
			28	10	16	2		
28	C	1	Total	C	H		0	0
			47	16	31			

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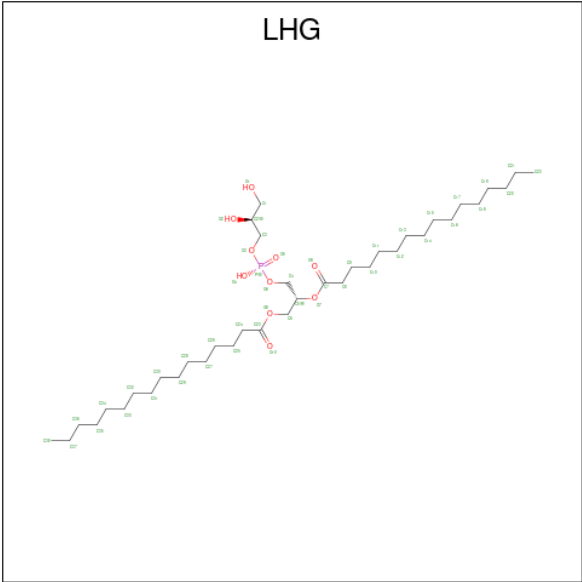
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C H 41 14 27	0	0
28	D	1	Total C H O 55 18 35 2	0	0
28	E	1	Total C H 35 12 23	0	0
28	E	1	Total C H O 55 18 35 2	0	0
28	H	1	Total C H 53 18 35	0	0
28	H	1	Total C H 26 9 17	0	0
28	I	1	Total C H O 43 15 26 2	0	0
28	I	1	Total C H O 37 13 22 2	0	0
28	J	1	Total C H O 28 10 16 2	0	0
28	K	1	Total C H 41 14 27	0	0
28	M	1	Total C H O 37 13 22 2	0	0
28	M	1	Total C H 26 10 16	0	0
28	M	1	Total C H 44 15 29	0	0
28	T	1	Total C H 47 16 31	0	0
28	Z	1	Total C H 50 17 33	0	0
28	R	1	Total C H O 28 10 16 2	0	0
28	a	1	Total C H O 28 10 16 2	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	b	1	Total C H O 40 14 24 2	0	0
28	b	1	Total C H 26 10 16	0	0
28	b	1	Total C H 32 11 21	0	0

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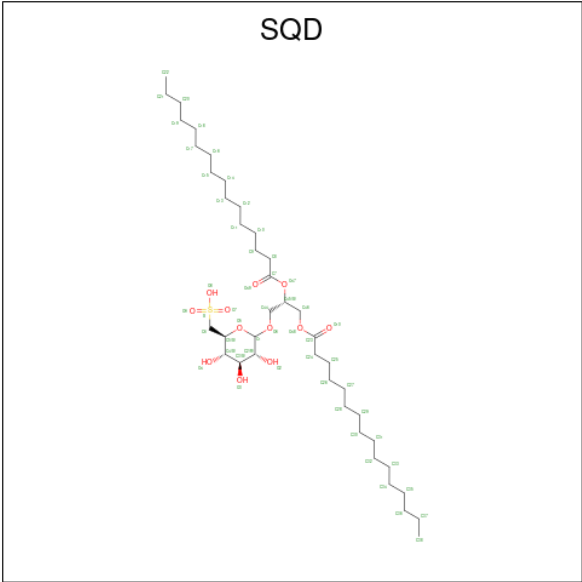
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	c	1	Total	C	H		0	0
			35	13	22			
28	c	1	Total	C	H		0	0
			53	18	35			
28	d	1	Total	C	H	O	0	0
			55	18	35	2		
28	d	1	Total	C	H	O	0	0
			55	18	35	2		
28	d	1	Total	C	H	O	0	0
			55	18	35	2		
28	e	1	Total	C	H		0	0
			26	9	17			
28	e	1	Total	C	H		0	0
			26	9	17			
28	e	1	Total	C	H	O	0	0
			31	11	18	2		
28	f	1	Total	C	H		0	0
			23	8	15			
28	h	1	Total	C	H		0	0
			29	10	19			
28	i	1	Total	C	H	O	0	0
			28	10	16	2		
28	i	1	Total	C	H		0	0
			14	6	8			
28	j	1	Total	C	H	O	0	0
			28	10	16	2		
28	j	1	Total	C	H		0	0
			47	16	31			
28	k	1	Total	C	H	O	0	0
			34	12	20	2		
28	m	1	Total	C	H	O	0	0
			28	10	16	2		
28	m	1	Total	C	H		0	0
			53	18	35			
28	t	1	Total	C	H	O	0	0
			34	12	20	2		
28	t	1	Total	C	H		0	0
			26	10	16			
28	z	1	Total	C	H		0	0
			23	9	14			

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



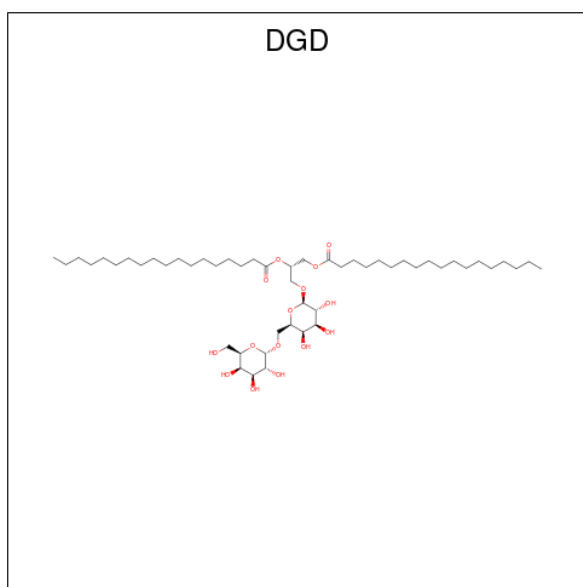
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
29	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
29	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



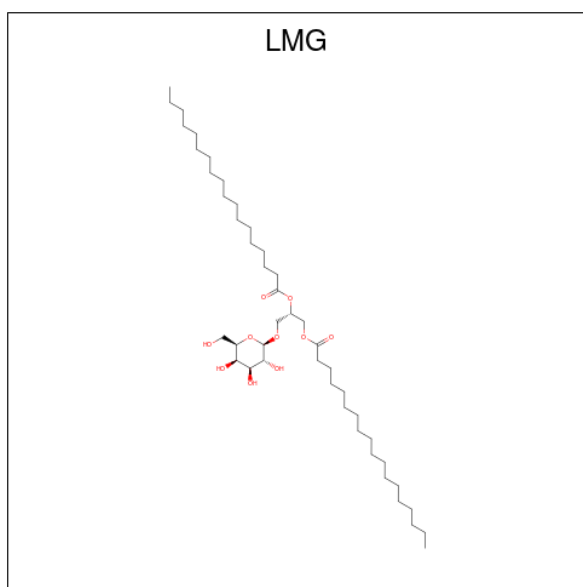
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	S	0	0
			95	30	52	12	1		
30	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
30	D	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
30	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	b	1	Total	C	H	O	S	0	0
			113	36	64	12	1		
30	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			162	51	96	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



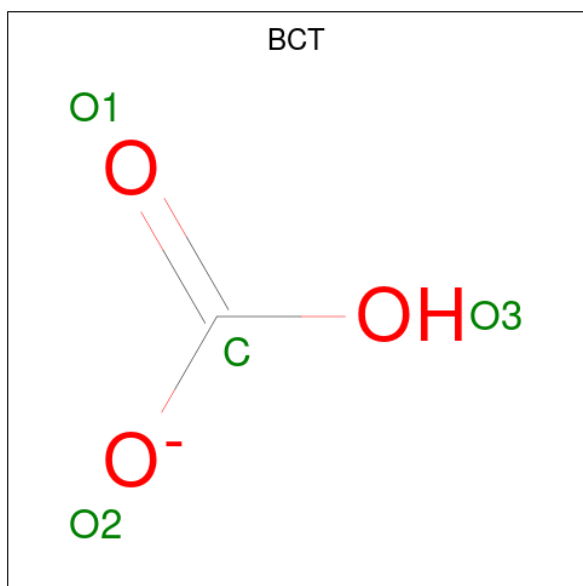
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			105	35	60	10		
32	C	1	Total	C	H	O	0	0
			76	26	40	10		
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	D	1	Total	C	H	O	0	0
			120	40	70	10		
32	D	1	Total	C	H	O	0	0
			123	41	72	10		
32	M	1	Total	C	H	O	0	0
			123	41	72	10		
32	a	1	Total	C	H	O	0	0
			141	45	86	10		
32	a	1	Total	C	H	O	0	0
			117	39	68	10		
32	b	1	Total	C	H	O	0	0
			141	45	86	10		
32	c	1	Total	C	H	O	0	0
			71	25	41	5		
32	c	1	Total	C	H	O	0	0
			108	36	62	10		
32	c	1	Total	C	H	O	0	0
			117	38	69	10		
32	d	1	Total	C	H	O	0	0
			102	34	58	10		

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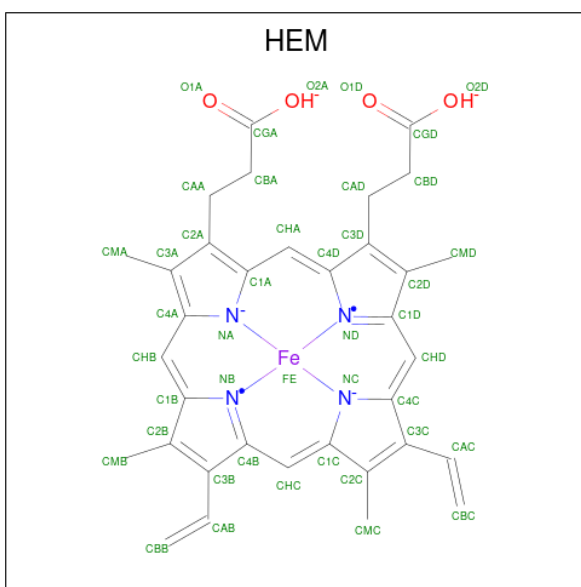
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	m	1	Total	C	H	O	0	0
			123	41	72	10		

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



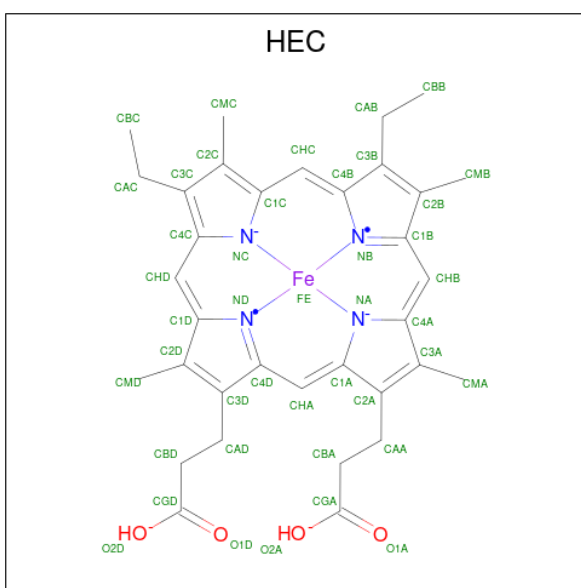
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	d	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

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



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	130	Total O 130 130	0	0
36	B	208	Total O 208 208	0	0
36	C	180	Total O 180 180	0	0
36	D	137	Total O 137 137	0	0
36	E	26	Total O 26 26	0	0
36	F	8	Total O 8 8	0	0
36	H	30	Total O 30 30	0	0
36	I	17	Total O 17 17	0	0
36	J	14	Total O 14 14	0	0
36	K	8	Total O 8 8	0	0
36	L	8	Total O 8 8	0	0
36	M	5	Total O 5 5	0	0
36	O	100	Total O 100 100	0	0
36	T	8	Total O 8 8	0	0
36	U	46	Total O 46 46	0	0
36	V	71	Total O 71 71	0	0
36	X	18	Total O 18 18	0	0
36	R	3	Total O 3 3	0	0
36	a	119	Total O 119 119	0	0
36	b	190	Total O 190 190	0	0
36	c	158	Total O 158 158	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	d	126	Total 126	O 126	0	0
36	e	19	Total 19	O 19	0	0
36	f	6	Total 6	O 6	0	0
36	h	20	Total 20	O 20	0	0
36	i	12	Total 12	O 12	0	0
36	j	7	Total 7	O 7	0	0
36	k	8	Total 8	O 8	0	0
36	l	11	Total 11	O 11	0	0
36	m	9	Total 9	O 9	0	0
36	o	109	Total 109	O 109	0	0
36	t	9	Total 9	O 9	0	0
36	u	53	Total 53	O 53	0	0
36	v	52	Total 52	O 52	0	0
36	y	3	Total 3	O 3	0	0
36	x	10	Total 10	O 10	0	0
36	z	3	Total 3	O 3	0	0
36	r	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1

Chain A: 

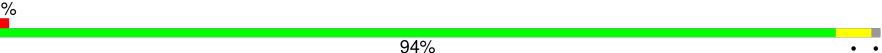


- Molecule 1: Photosystem II protein D1 1

Chain a: 

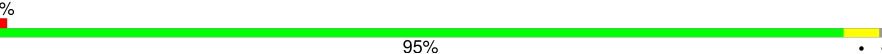


- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



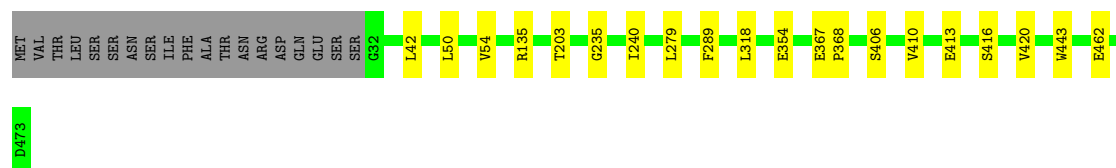
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 

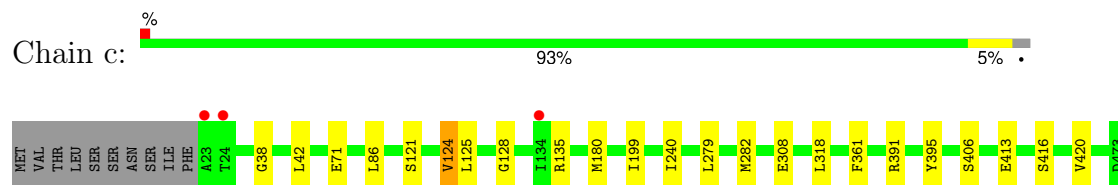


- Molecule 3: Photosystem II CP43 reaction center protein

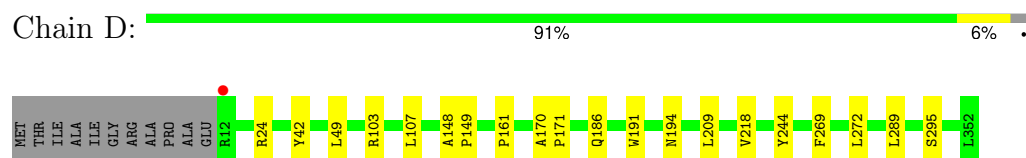
Chain C: 



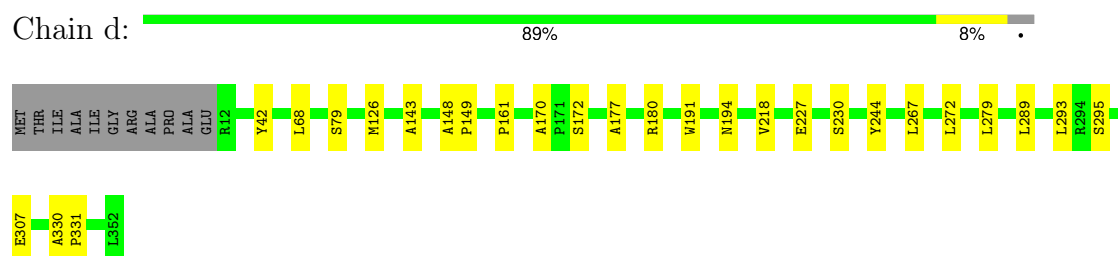
- Molecule 3: Photosystem II CP43 reaction center protein



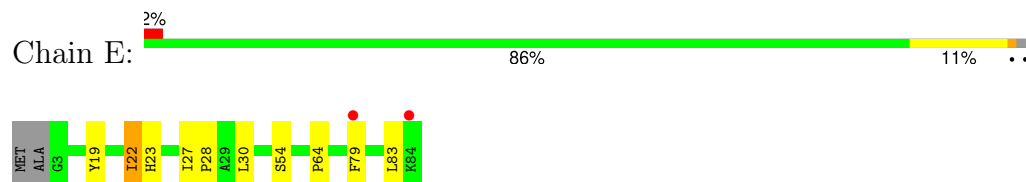
- Molecule 4: Photosystem II D2 protein



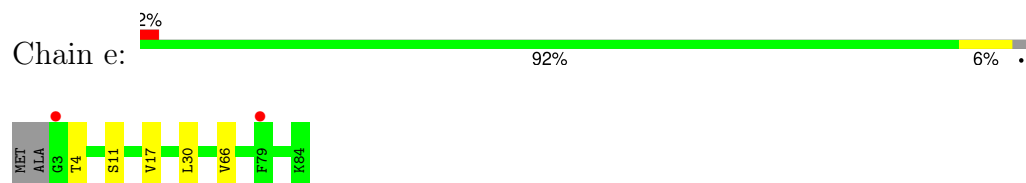
- Molecule 4: Photosystem II D2 protein



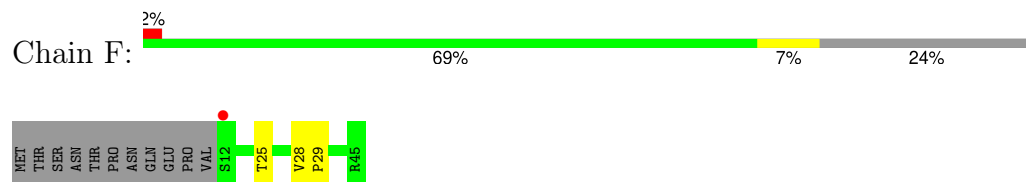
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

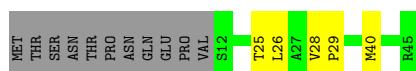


- Molecule 6: Cytochrome b559 subunit beta

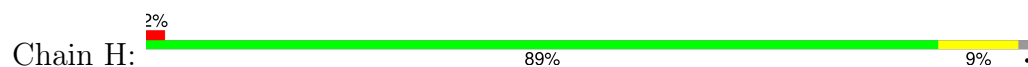


- Molecule 6: Cytochrome b559 subunit beta

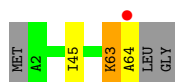
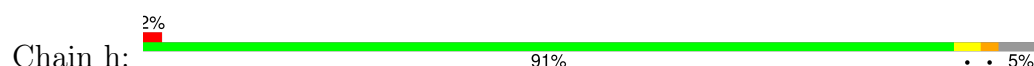




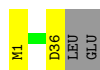
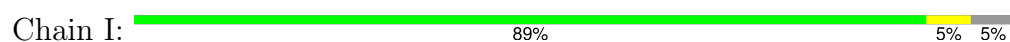
- Molecule 7: Photosystem II reaction center protein H



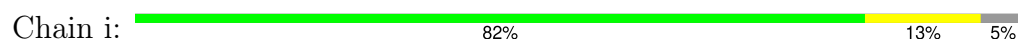
- Molecule 7: Photosystem II reaction center protein H



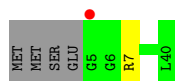
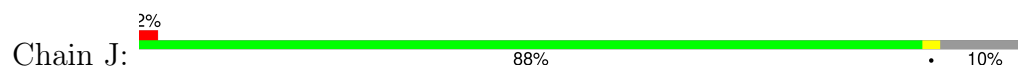
- Molecule 8: Photosystem II reaction center protein I



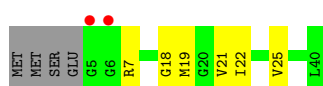
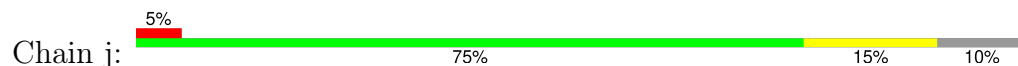
- Molecule 8: Photosystem II reaction center protein I



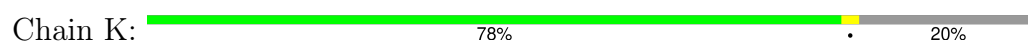
- Molecule 9: Photosystem II reaction center protein J

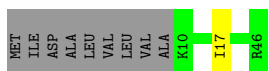


- Molecule 9: Photosystem II reaction center protein J

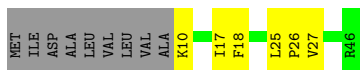


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

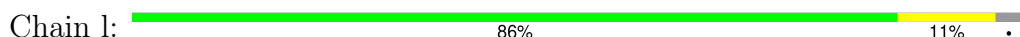


- Molecule 11: Photosystem II reaction center protein L

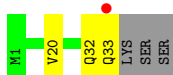
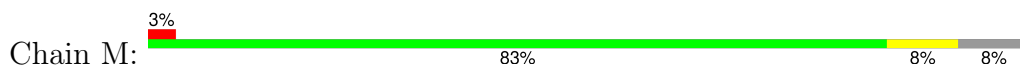


There are no outlier residues recorded for this chain.

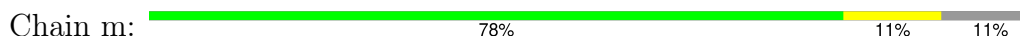
- Molecule 11: Photosystem II reaction center protein L



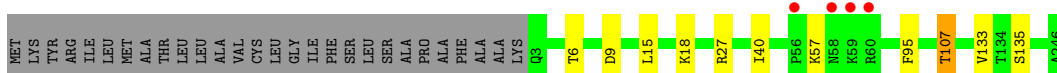
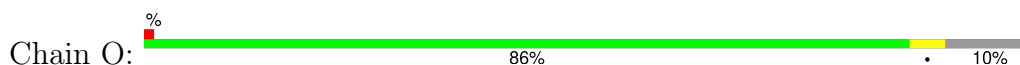
- Molecule 12: Photosystem II reaction center protein M



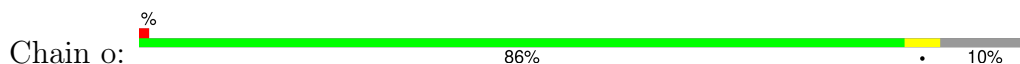
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



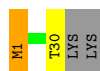
- Molecule 13: Photosystem II manganese-stabilizing polypeptide





- Molecule 14: Photosystem II reaction center protein T

Chain T: 88% 6%



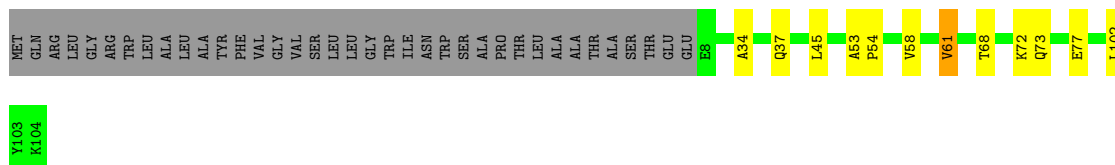
- Molecule 14: Photosystem II reaction center protein T

Chain t: 6% 91% 6%



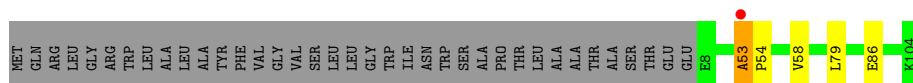
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 63% 8% 28%



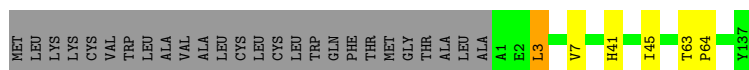
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 69% 28% 3%



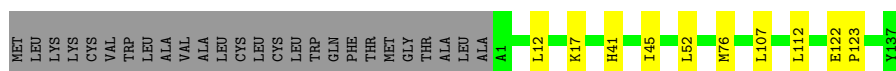
- Molecule 16: Cytochrome c-550

Chain V: 80% 16% 4%

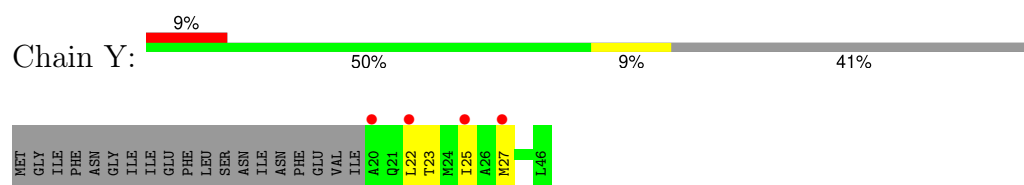


- Molecule 16: Cytochrome c-550

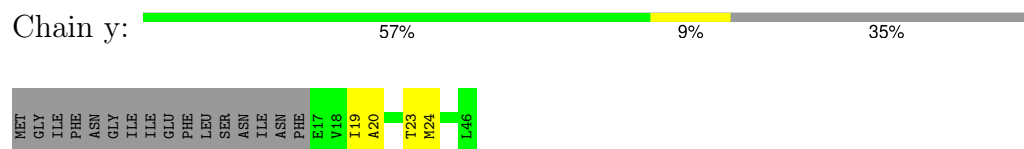
Chain v: 78% 6% 16%



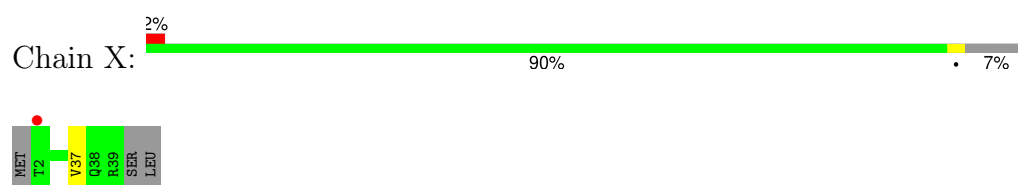
- Molecule 17: Photosystem II reaction center protein Ycf12



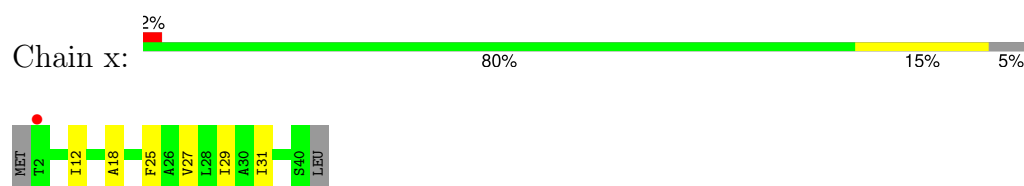
• Molecule 17: Photosystem II reaction center protein Ycf12



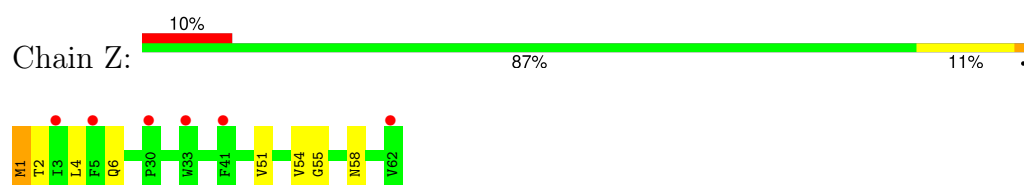
• Molecule 18: Photosystem II reaction center X protein



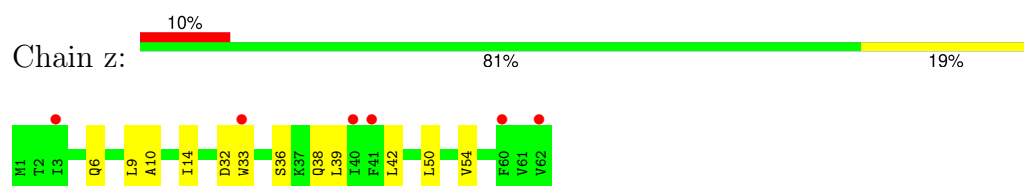
• Molecule 18: Photosystem II reaction center X protein



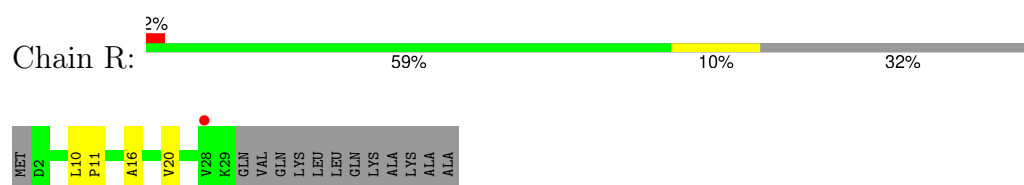
• Molecule 19: Photosystem II reaction center protein Z



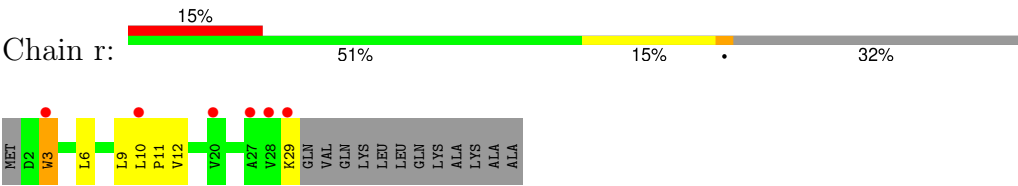
• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.55Å 222.83Å 309.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.44 – 1.98 37.44 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.44-1.98) 86.3 (37.44-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 1.98Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.173 , 0.213 0.173 , 0.213	Depositor DCC
R_{free} test set	4966 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	104563	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: STE, CLA, FE2, LMG, PHO, FME, HEC, SQD, DGD, OEX, HEM, BCR, BCT, LHG, PL9, CL

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	0.59	0/3692
1	a	0.36	0/2704	0.58	0/3688
2	B	0.35	0/4179	0.54	0/5693
2	b	0.32	0/4127	0.53	0/5623
3	C	0.34	0/3547	0.54	0/4830
3	c	0.32	0/3619	0.53	0/4926
4	D	0.35	0/2812	0.57	0/3832
4	d	0.33	0/2821	0.54	0/3844
5	E	0.29	0/688	0.51	0/940
5	e	0.27	0/683	0.48	0/932
6	F	0.28	0/284	0.48	0/387
6	f	0.28	0/284	0.52	0/387
7	H	0.32	0/517	0.53	0/705
7	h	0.28	0/505	0.49	0/689
8	I	0.31	0/293	0.51	0/396
8	i	0.33	0/293	0.45	0/396
9	J	0.28	0/263	0.44	0/356
9	j	0.28	0/263	0.46	0/356
10	K	0.28	0/303	0.50	0/416
10	k	0.25	0/303	0.43	0/416
11	L	0.37	0/311	0.54	0/422
11	l	0.35	0/303	0.49	0/412
12	M	0.36	0/249	0.59	0/341
12	m	0.37	0/244	0.52	0/334
13	O	0.34	0/1904	0.55	0/2585
13	o	0.36	0/1905	0.57	0/2583
14	T	0.37	0/257	0.55	0/349
14	t	0.34	0/255	0.48	0/346
15	U	0.31	0/785	0.54	0/1064
15	u	0.34	0/785	0.57	0/1064
16	V	0.35	0/1085	0.57	0/1473
16	v	0.31	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.27	0/197	0.39	0/264
17	y	0.22	0/219	0.45	0/294
18	X	0.28	0/284	0.50	0/384
18	x	0.24	0/289	0.42	0/391
19	Z	0.24	0/490	0.47	0/669
19	z	0.23	0/488	0.39	0/666
20	R	0.24	0/227	0.41	0/313
20	r	0.24	0/227	0.47	0/313
All	All	0.33	0/42784	0.54	0/58244

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
13	o	0	1
16	V	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide
13	o	152	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2469	2519	11	0
1	a	2619	2462	2510	15	0
2	B	4016	3887	3871	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3984	3842	3842	12	0
3	C	3426	3347	3343	11	1
3	c	3500	3418	3426	14	0
4	D	2717	2621	2621	16	0
4	d	2723	2627	2627	17	0
5	E	666	651	651	7	0
5	e	664	648	648	4	0
6	F	275	282	282	2	0
6	f	275	282	282	6	0
7	H	505	528	528	6	1
7	h	493	514	514	2	0
8	I	296	311	311	1	0
8	i	296	311	311	2	0
9	J	257	268	268	0	0
9	j	257	268	268	4	0
10	K	293	305	305	4	0
10	k	293	305	305	7	0
11	L	304	316	316	0	0
11	l	296	304	304	1	0
12	M	256	267	269	3	0
12	m	251	267	267	5	0
13	O	1870	1830	1830	7	0
13	o	1874	1846	1846	6	0
14	T	258	261	261	2	0
14	t	256	256	256	1	0
15	U	774	773	773	6	0
15	u	774	773	773	5	0
16	V	1064	1071	1073	2	0
16	v	1064	1071	1073	4	0
17	Y	196	217	217	2	0
17	y	218	241	241	2	0
18	X	281	312	312	1	0
18	x	286	316	314	5	0
19	Z	479	516	516	5	0
19	z	477	509	509	9	0
20	R	221	238	238	2	0
20	r	221	238	238	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	2	0	0	0	0
24	A	249	264	264	6	0
24	B	1035	1139	1139	17	0
24	C	839	922	922	9	0
24	D	130	144	144	1	0
24	a	260	288	288	2	0
24	b	1035	1139	1139	13	0
24	c	839	919	919	9	0
24	d	130	144	144	1	0
25	A	64	74	74	0	0
25	D	64	74	74	0	0
25	a	64	74	74	0	0
25	d	64	74	74	1	0
26	A	40	56	56	1	0
26	B	120	168	168	3	0
26	C	80	112	112	4	0
26	D	40	56	56	5	0
26	H	40	56	56	4	0
26	K	80	112	112	2	0
26	T	40	56	56	4	0
26	a	40	56	56	0	0
26	b	120	168	168	4	0
26	c	80	112	112	0	0
26	d	40	56	56	5	0
26	h	40	56	56	5	0
26	k	80	112	112	4	0
26	t	40	56	56	2	0
27	A	55	80	80	2	0
27	D	55	80	80	0	0
27	a	55	80	80	2	0
27	d	55	80	80	0	0
28	A	45	83	83	2	0
28	B	62	96	96	0	0
28	C	78	126	126	0	0
28	D	20	35	35	0	0
28	E	32	58	58	0	0
28	H	27	52	52	1	0
28	I	32	48	48	0	0
28	J	12	16	16	0	0
28	K	14	27	27	0	0
28	M	40	67	67	0	0
28	R	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	T	16	31	31	1	0
28	Z	17	33	33	0	0
28	a	12	16	16	0	0
28	b	57	96	96	2	0
28	c	31	57	57	1	0
28	d	60	105	105	3	0
28	e	31	52	52	0	0
28	f	8	15	15	0	0
28	h	10	19	19	0	0
28	i	18	24	24	0	0
28	j	28	47	47	0	0
28	k	14	20	20	0	0
28	m	30	51	51	0	0
28	t	24	36	36	0	0
28	z	9	14	14	0	0
29	A	49	74	74	1	0
29	D	145	215	215	2	0
29	L	49	74	74	3	0
29	d	137	199	199	1	0
29	e	42	57	57	1	0
29	l	49	74	74	1	0
30	A	43	52	53	0	0
30	B	54	77	78	2	0
30	D	88	115	117	1	0
30	a	108	154	156	1	0
30	b	49	64	65	0	0
30	f	41	48	49	0	0
31	A	66	96	96	1	0
31	C	186	246	246	0	0
31	H	62	82	82	0	0
31	c	186	246	246	1	0
31	h	62	82	82	0	0
32	B	45	60	60	2	0
32	C	132	172	172	2	0
32	D	101	142	142	6	0
32	M	51	72	72	1	0
32	a	104	154	154	2	0
32	b	55	86	86	0	0
32	c	124	172	172	1	0
32	d	44	58	58	0	0
32	m	51	72	72	4	0
33	D	4	1	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	d	4	1	1	0	0
34	F	43	30	30	4	0
34	f	43	30	30	4	0
35	V	43	30	30	0	0
35	v	43	30	30	0	0
36	A	130	0	0	2	0
36	B	208	0	0	0	0
36	C	180	0	0	0	0
36	D	137	0	0	2	0
36	E	26	0	0	0	0
36	F	8	0	0	0	0
36	H	30	0	0	0	0
36	I	17	0	0	0	0
36	J	14	0	0	0	0
36	K	8	0	0	0	0
36	L	8	0	0	0	0
36	M	5	0	0	0	0
36	O	100	0	0	1	0
36	R	3	0	0	0	0
36	T	8	0	0	1	0
36	U	46	0	0	0	0
36	V	71	0	0	0	0
36	X	18	0	0	0	0
36	a	119	0	0	0	0
36	b	190	0	0	2	0
36	c	158	0	0	1	0
36	d	126	0	0	1	0
36	e	19	0	0	0	0
36	f	6	0	0	0	0
36	h	20	0	0	0	0
36	i	12	0	0	1	0
36	j	7	0	0	0	0
36	k	8	0	0	0	0
36	l	11	0	0	0	0
36	m	9	0	0	1	0
36	o	109	0	0	1	0
36	r	4	0	0	0	0
36	t	9	0	0	0	0
36	u	53	0	0	0	0
36	v	52	0	0	0	0
36	x	10	0	0	0	0
36	y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	z	3	0	0	0	0
All	All	52483	52080	52178	312	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:613:CLA:H192	29:d:408:LHG:H223	1.38	1.05
26:t:101:BCR:HC8	26:t:101:BCR:H311	1.61	0.83
34:f:101:HEM:HHD	34:f:101:HEM:HBC2	1.65	0.79
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.66	0.78
26:H:101:BCR:HC8	26:H:101:BCR:H331	1.66	0.77
24:A:605:CLA:H191	29:D:410:LHG:H162	1.65	0.77
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.68	0.76
26:D:405:BCR:H23C	26:D:405:BCR:H392	1.69	0.74
24:B:604:CLA:H43	24:B:605:CLA:H2	1.69	0.73
29:L:101:LHG:H383	32:M:101:LMG:C43	2.20	0.71
15:u:53:ALA:HB1	15:u:54:PRO:CD	2.20	0.71
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.72	0.71
26:t:101:BCR:H23C	26:t:101:BCR:H382	1.75	0.69
24:d:404:CLA:H92	18:x:18:ALA:HB2	1.74	0.69
5:e:30:LEU:HD11	34:f:101:HEM:CBB	2.23	0.69
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.75	0.68
13:O:107:THR:HG22	36:O:340:HOH:O	1.94	0.67
15:U:58:VAL:O	15:U:61:VAL:HG22	1.94	0.66
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.30	0.65
19:Z:2:THR:HG22	19:Z:6:GLN:NE2	2.11	0.65
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.79	0.65
36:A:749:HOH:O	13:O:107:THR:HG21	1.99	0.63
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.81	0.63
18:x:27:VAL:O	18:x:31:ILE:HD12	1.98	0.63
26:K:101:BCR:H321	26:K:101:BCR:HC8	1.81	0.62
19:z:10:ALA:O	19:z:14:ILE:HD12	2.00	0.61
3:c:279:LEU:HD23	3:c:282:MET:HE3	1.82	0.61
26:h:101:BCR:HC8	26:h:101:BCR:H331	1.82	0.61
24:C:502:CLA:H61	24:C:512:CLA:H42	1.83	0.61
34:F:101:HEM:HBB2	34:F:101:HEM:HMB1	1.83	0.61
24:c:509:CLA:H43	24:c:509:CLA:O1A	2.00	0.61
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:38:GLN:O	19:z:42:LEU:HD13	2.02	0.60
3:c:318:LEU:C	3:c:318:LEU:HD23	2.27	0.60
4:d:267:LEU:C	4:d:267:LEU:HD23	2.26	0.60
2:B:241:SER:HB3	24:B:612:CLA:HED3	1.82	0.60
5:e:30:LEU:HD11	34:f:101:HEM:HBB2	1.85	0.58
24:A:606:CLA:H91	32:D:408:LMG:C25	2.33	0.58
24:C:505:CLA:HBB1	24:C:505:CLA:HMB3	1.86	0.58
10:k:10:LYS:N	10:k:10:LYS:HE2	2.18	0.58
19:Z:2:THR:HG22	19:Z:6:GLN:HE21	1.68	0.57
24:b:602:CLA:H43	7:h:45:ILE:HG22	1.86	0.57
26:d:405:BCR:H23C	26:d:405:BCR:H392	1.85	0.57
4:D:194:ASN:HA	4:D:295:SER:OG	2.05	0.57
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.40	0.57
26:H:101:BCR:H331	26:H:101:BCR:C8	2.31	0.57
24:A:606:CLA:H91	32:D:408:LMG:C24	2.35	0.56
26:k:101:BCR:H321	26:k:101:BCR:HC8	1.88	0.56
1:a:200:LEU:HD13	31:c:521:DGD:HAT2	1.88	0.56
4:d:126:MET:HE3	4:d:143:ALA:O	2.06	0.56
19:Z:51:VAL:O	19:Z:54:VAL:O	2.25	0.55
27:A:610:PL9:H502	30:D:409:SQD:H381	1.87	0.55
24:b:613:CLA:H142	32:m:101:LMG:C25	2.36	0.55
13:o:84:GLU:CD	13:o:86:LYS:NZ	2.64	0.55
5:E:54:SER:HB2	5:E:83:LEU:HD13	1.89	0.55
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.42	0.55
24:C:509:CLA:H141	24:C:509:CLA:H171	1.88	0.54
4:d:272:LEU:C	4:d:272:LEU:HD23	2.33	0.54
26:C:514:BCR:H331	26:C:514:BCR:C8	2.37	0.54
26:h:101:BCR:H331	26:h:101:BCR:C8	2.38	0.54
24:b:614:CLA:C19	12:m:13:LEU:HD13	2.38	0.53
15:u:86:GLU:H	15:u:86:GLU:CD	2.16	0.53
10:K:17:ILE:N	10:K:17:ILE:HD12	2.22	0.53
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.43	0.53
1:a:265:PHE:CD2	1:a:271:LEU:HD23	2.44	0.53
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.43	0.53
24:B:601:CLA:H52	28:H:103:STE:H162	1.90	0.53
24:B:605:CLA:HHC	24:B:605:CLA:HBB1	1.92	0.52
13:O:27:ARG:O	13:O:27:ARG:HG2	2.09	0.52
32:a:614:LMG:C10	32:a:614:LMG:O8	2.57	0.52
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.91	0.52
10:k:18:PHE:CE2	19:z:9:LEU:HD23	2.44	0.52
34:F:101:HEM:HBB2	34:F:101:HEM:CMB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:30:THR:HG21	36:T:208:HOH:O	2.08	0.52
7:h:63:LYS:O	7:h:64:ALA:HB2	2.10	0.52
26:k:101:BCR:H333	26:k:102:BCR:C12	2.39	0.52
2:B:371:THR:HG23	2:B:372:ASP:O	2.09	0.52
26:T:101:BCR:H382	26:T:101:BCR:H23C	1.92	0.52
24:c:505:CLA:H142	36:i:210:HOH:O	2.10	0.52
3:C:135:ARG:O	3:C:135:ARG:HD3	2.09	0.52
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.91	0.52
4:d:307:GLU:HG3	36:d:552:HOH:O	2.10	0.52
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.92	0.51
2:B:52:LEU:HD12	13:o:59:LYS:HE2	1.92	0.51
24:b:614:CLA:H121	24:b:614:CLA:H91	1.92	0.51
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.25	0.51
24:c:501:CLA:H192	24:c:507:CLA:HBB1	1.91	0.51
2:B:172:TYR:OH	7:H:63:LYS:HE2	2.11	0.51
28:A:617:STE:H181	28:A:618:STE:C14	2.41	0.51
13:o:84:GLU:CD	13:o:86:LYS:HZ3	2.17	0.51
3:C:406:SER:HA	3:C:420:VAL:HG23	1.93	0.50
3:c:279:LEU:HD23	3:c:282:MET:CE	2.40	0.50
26:D:405:BCR:H331	26:D:405:BCR:C8	2.41	0.50
2:B:104:SER:OG	30:B:622:SQD:H221	2.11	0.50
4:D:209:LEU:HD23	4:D:209:LEU:C	2.37	0.50
1:a:249:VAL:HG12	2:b:491:VAL:HG21	1.94	0.50
24:c:513:CLA:H191	28:c:517:STE:C1	2.42	0.50
15:u:53:ALA:CB	15:u:54:PRO:CD	2.89	0.50
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.94	0.49
1:a:271:LEU:HD21	27:a:610:PL9:HC71	1.93	0.49
2:B:117:TYR:CD1	7:H:3:ARG:NH1	2.80	0.49
4:D:272:LEU:C	4:D:272:LEU:HD23	2.38	0.49
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.95	0.49
19:Z:1:MET:HE3	19:Z:4:LEU:HD12	1.94	0.49
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.49
24:A:605:CLA:HMB1	24:A:605:CLA:HBB1	1.95	0.48
28:A:617:STE:H181	28:A:618:STE:H141	1.95	0.48
3:c:71:GLU:HB3	3:c:86:LEU:HD22	1.94	0.48
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	1.96	0.48
26:b:619:BCR:H331	26:b:619:BCR:C8	2.43	0.48
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.96	0.48
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.48
24:B:611:CLA:C14	29:L:101:LHG:H382	2.44	0.48
10:k:17:ILE:CD1	19:z:6:GLN:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:32:GLN:C	36:m:202:HOH:O	2.56	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.49	0.48
2:B:75:TRP:HB3	32:a:614:LMG:HC8	1.96	0.48
20:r:29:LYS:HD3	20:r:29:LYS:C	2.39	0.47
2:b:486:LEU:HD11	2:b:490:GLN:NE2	2.29	0.47
3:c:180:MET:HG2	3:c:199:ILE:O	2.13	0.47
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.96	0.47
1:a:183:MET:HA	24:a:605:CLA:HMD1	1.95	0.47
17:y:20:ALA:O	17:y:24:MET:HG2	2.14	0.47
32:C:517:LMG:O2	32:C:517:LMG:HC71	2.13	0.47
4:D:170:ALA:HB1	4:D:171:PRO:HD2	1.95	0.47
3:c:180:MET:HE1	32:c:523:LMG:HC72	1.95	0.47
3:c:391[B]:ARG:HD2	3:c:395:TYR:CZ	2.49	0.47
28:d:413:STE:H52	18:x:12:ILE:HG21	1.96	0.47
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.96	0.47
4:d:79:SER:HA	4:d:172:SER:HB3	1.96	0.47
13:o:54:GLU:HG3	13:o:66:VAL:HG13	1.97	0.47
2:b:62:VAL:HB	24:b:605:CLA:HED3	1.97	0.47
15:U:73:GLN:O	15:U:77:GLU:HG2	2.16	0.47
3:c:42:LEU:HD21	24:c:511:CLA:H2A	1.97	0.47
1:A:227:THR:HB	1:A:231:GLU:HG3	1.97	0.46
26:d:405:BCR:H383	9:j:25:VAL:HG21	1.98	0.46
3:C:279:LEU:HD12	24:C:509:CLA:HED2	1.96	0.46
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.46
24:c:513:CLA:HBB1	24:c:513:CLA:HMB3	1.96	0.46
27:A:610:PL9:H251	29:A:613:LHG:H223	1.98	0.46
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.04	0.46
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.98	0.46
29:l:101:LHG:H271	12:m:22:LEU:HD21	1.98	0.46
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.97	0.46
24:a:605:CLA:HBB1	24:a:605:CLA:HMB3	1.97	0.46
26:T:101:BCR:C8	26:T:101:BCR:H321	2.44	0.46
2:b:505:ARG:O	2:b:506:ARG:HB2	2.16	0.46
12:M:32:GLN:O	12:M:33:GLN:CB	2.64	0.46
19:z:36:SER:HA	19:z:39:LEU:HD23	1.98	0.46
3:c:135:ARG:NE	36:c:603:HOH:O	2.48	0.46
1:A:183:MET:HA	24:A:605:CLA:HMD1	1.98	0.46
7:H:17:GLU:OE2	7:H:20:LYS:CE	2.64	0.46
15:U:34:ALA:O	15:U:37:GLN:HG3	2.16	0.45
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.98	0.45
2:b:287:ARG:HD3	36:b:793:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:5:LEU:HD13	13:o:10:ILE:HD11	1.98	0.45
26:C:514:BCR:H331	26:C:514:BCR:HC8	1.98	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.45
5:E:22[A]:ILE:HD12	5:E:23:HIS:CE1	2.51	0.45
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.98	0.45
24:b:614:CLA:H141	32:m:101:LMG:C43	2.46	0.45
24:B:614:CLA:H62	24:B:614:CLA:H41	1.73	0.45
32:B:620:LMG:O6	32:D:407:LMG:HC3	2.16	0.45
7:H:6:TRP:CZ2	7:H:10:ILE:HD11	2.51	0.45
13:o:39:ARG:HD2	36:o:355:HOH:O	2.14	0.45
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.32	0.45
2:B:86:ILE:HD13	2:B:87:ASP:N	2.32	0.45
26:D:405:BCR:H20C	26:D:405:BCR:H361	1.85	0.45
10:k:18:PHE:HE2	19:z:9:LEU:HD23	1.82	0.45
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.99	0.45
18:x:27:VAL:HG12	18:x:31:ILE:CD1	2.47	0.45
3:c:38:GLY:HA3	24:c:511:CLA:HMD2	1.98	0.44
10:k:17:ILE:HD11	19:z:6:GLN:HG2	1.99	0.44
16:v:41:HIS:HA	16:v:45:ILE:O	2.18	0.44
2:B:86:ILE:HD13	2:B:87:ASP:H	1.81	0.44
1:a:84:PRO:HA	1:a:112:TYR:CG	2.53	0.44
3:C:50:LEU:O	3:C:54:VAL:HG23	2.17	0.44
13:O:133:VAL:C	13:O:135:SER:H	2.25	0.44
3:C:410:VAL:HG22	3:C:413[B]:GLU:HG2	1.99	0.44
24:C:513:CLA:HBB1	24:C:513:CLA:HMB3	2.00	0.44
32:D:408:LMG:H112	36:D:529:HOH:O	2.18	0.44
26:b:618:BCR:H20C	26:b:618:BCR:H361	1.81	0.44
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.52	0.44
9:j:18:GLY:O	9:j:21:VAL:HG22	2.17	0.44
26:C:514:BCR:H24C	26:C:514:BCR:H371	1.82	0.44
4:D:269:PHE:CG	29:D:413:LHG:HC12	2.53	0.44
26:T:101:BCR:H321	26:T:101:BCR:HC8	1.99	0.44
3:C:410:VAL:CG2	3:C:413[B]:GLU:HG2	2.48	0.44
19:z:50:LEU:O	19:z:54:VAL:HG23	2.18	0.43
6:f:26:LEU:O	6:f:29:PRO:HD2	2.18	0.43
32:D:407:LMG:H122	36:D:510:HOH:O	2.18	0.43
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.53	0.43
5:E:64:PRO:HB2	5:E:79:PHE:CD2	2.53	0.43
2:B:117:TYR:CE1	7:H:3:ARG:NH1	2.87	0.43
4:D:186:GLN:HB2	24:D:403:CLA:HBC1	2.01	0.43
8:I:36:ASP:OD1	8:I:36:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:17:VAL:HG23	9:j:7:ARG:HB2	2.00	0.43
26:A:609:BCR:H24C	26:A:609:BCR:H371	1.92	0.43
10:k:10:LYS:HE2	10:k:10:LYS:CA	2.48	0.43
3:c:121:SER:O	3:c:124:VAL:HG13	2.19	0.43
26:d:405:BCR:H24C	26:d:405:BCR:H371	1.78	0.43
24:A:608:CLA:HED2	36:A:728:HOH:O	2.18	0.43
24:B:601:CLA:CBA	24:B:601:CLA:C2	2.97	0.43
1:a:201:GLY:HA3	1:a:286:THR:HB	2.01	0.43
6:f:28:VAL:CG2	6:f:29:PRO:HD3	2.46	0.43
5:E:30:LEU:HD11	34:F:101:HEM:HAB	2.00	0.43
3:c:128:GLY:HA3	24:c:513:CLA:C3C	2.49	0.43
20:r:3:TRP:CD1	20:r:3:TRP:C	2.96	0.43
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.01	0.42
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.01	0.42
5:e:11:SER:CB	29:e:102:LHG:HC32	2.48	0.42
20:r:9:LEU:O	20:r:12:VAL:HG22	2.18	0.42
1:A:161:TYR:CZ	1:A:165:GLN:HG3	2.54	0.42
24:B:601:CLA:H192	24:B:601:CLA:C12	2.50	0.42
24:B:612:CLA:HBB1	24:B:612:CLA:HMB1	2.01	0.42
24:b:609:CLA:C2B	26:h:101:BCR:H323	2.49	0.42
28:b:625:STE:C17	28:d:411:STE:H61	2.49	0.42
9:j:19:MET:HA	9:j:22:ILE:HD12	2.00	0.42
1:A:11:ALA:O	1:A:16:ARG:CZ	2.67	0.42
19:Z:55:GLY:HA2	19:Z:58:ASN:CB	2.50	0.42
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.02	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.01	0.42
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.01	0.42
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.02	0.42
16:V:3:LEU:HD23	16:V:3:LEU:HA	1.95	0.42
24:b:603:CLA:H2	24:b:605:CLA:H91	2.01	0.42
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.54	0.42
2:B:36:SER:OG	26:B:618:BCR:H362	2.19	0.42
4:D:42:TYR:CE1	6:F:25:THR:CG2	3.02	0.42
1:a:210:LEU:C	1:a:210:LEU:HD23	2.45	0.42
24:b:615:CLA:HHC	24:b:615:CLA:HBB1	2.01	0.42
26:h:101:BCR:H20C	26:h:101:BCR:H361	1.84	0.42
16:v:12:LEU:HD23	16:v:17:LYS:HD3	1.99	0.42
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.49	0.42
3:C:318:LEU:C	3:C:318:LEU:HD23	2.44	0.42
4:D:24:ARG:HD3	18:X:37:VAL:HG12	2.01	0.42
10:K:17:ILE:HD12	10:K:17:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:19:ILE:O	17:y:23:THR:HG22	2.20	0.42
30:B:622:SQD:H442	14:t:23:PHE:CD1	2.55	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.42
26:T:101:BCR:HC8	26:T:101:BCR:H311	2.01	0.42
19:z:32:ASP:O	19:z:33:TRP:C	2.63	0.42
24:B:601:CLA:H93	26:H:101:BCR:C40	2.50	0.42
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.50	0.42
8:i:12:VAL:O	8:i:16:VAL:HG23	2.20	0.42
10:k:25:LEU:N	10:k:26:PRO:CD	2.83	0.42
24:B:601:CLA:C2	24:B:601:CLA:HBA2	2.50	0.42
24:B:602:CLA:H141	24:B:602:CLA:H161	1.94	0.42
4:D:103:ARG:O	4:D:107:LEU:HG	2.20	0.42
4:d:279:LEU:HD22	25:d:402:PHO:HBC3	2.02	0.42
2:B:230:ARG:NH2	32:B:620:LMG:HC5	2.34	0.41
2:b:125:ASP:HB2	2:b:132:ALA:HB3	2.02	0.41
18:x:25:PHE:O	18:x:29:ILE:HG13	2.20	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.50	0.41
15:U:68:THR:O	15:U:72:LYS:HG3	2.20	0.41
31:A:615:DGD:HD5	2:b:75:TRP:HB3	2.01	0.41
14:T:1:FME:H	28:T:102:STE:C3	2.33	0.41
24:b:614:CLA:H192	32:m:101:LMG:C43	2.50	0.41
2:b:231:MET:HG2	24:b:610:CLA:HBC3	2.03	0.41
4:d:330:ALA:HB3	4:d:331:PRO:HD3	2.02	0.41
1:A:201:GLY:HA3	1:A:286:THR:HB	2.02	0.41
26:B:617:BCR:H382	26:B:617:BCR:H23C	2.02	0.41
26:D:405:BCR:H371	26:D:405:BCR:H24C	1.83	0.41
26:H:101:BCR:HC8	26:H:101:BCR:C33	2.44	0.41
24:B:605:CLA:H8	24:B:612:CLA:H193	2.03	0.41
24:B:610:CLA:HHC	24:B:610:CLA:CBB	2.51	0.41
24:C:505:CLA:HBC2	26:C:515:BCR:H341	2.02	0.41
13:O:15:LEU:HD23	13:O:18:LYS:HD3	2.02	0.41
8:i:27:ASP:N	8:i:28:PRO:CD	2.84	0.41
10:K:17:ILE:H	10:K:17:ILE:CD1	2.34	0.41
26:k:102:BCR:H371	26:k:102:BCR:H24C	1.80	0.41
1:a:271:LEU:HD21	27:a:610:PL9:C3	2.51	0.41
4:d:42:TYR:CZ	6:f:25:THR:CG2	3.04	0.41
26:d:405:BCR:H403	26:d:405:BCR:C23	2.51	0.41
2:B:67:ALA:HA	2:B:71:VAL:O	2.21	0.41
2:B:472:ARG:HG3	2:B:479[B]:PHE:CE2	2.56	0.41
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:603:CLA:H61	24:b:603:CLA:H41	1.91	0.41
11:l:20:GLY:O	11:l:24:ILE:HD12	2.21	0.41
4:D:49:LEU:HD13	26:D:405:BCR:C15	2.50	0.41
26:K:101:BCR:H20C	26:K:101:BCR:H361	1.92	0.41
30:a:613:SQD:H2	30:a:613:SQD:H61	2.03	0.41
2:b:157:HIS:CD2	2:b:157:HIS:C	2.98	0.41
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.09	0.41
4:d:180:ARG:C	4:d:180:ARG:HD3	2.46	0.41
16:v:122:GLU:N	16:v:123:PRO:HD2	2.36	0.41
2:B:386:ALA:HB3	15:U:102:LEU:HD22	2.02	0.40
3:C:367:GLU:N	3:C:368:PRO:CD	2.84	0.40
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.50	0.40
10:K:17:ILE:N	10:K:17:ILE:CD1	2.84	0.40
1:a:36:ILE:HD13	24:c:505:CLA:H143	2.03	0.40
2:b:373:LYS:HG3	36:b:706:HOH:O	2.20	0.40
4:d:68:LEU:HA	6:f:40:MET:SD	2.61	0.40
4:d:194:ASN:HA	4:d:295:SER:OG	2.21	0.40
26:d:405:BCR:H392	26:d:405:BCR:C23	2.51	0.40
26:h:101:BCR:H24C	26:h:101:BCR:H371	1.90	0.40
20:r:10:LEU:HB3	20:r:11:PRO:HD3	2.03	0.40
24:B:601:CLA:H192	24:B:601:CLA:H122	2.03	0.40
3:C:443:TRP:CE2	24:C:508:CLA:HMD2	2.56	0.40
16:V:41:HIS:HA	16:V:45:ILE:O	2.21	0.40
26:b:617:BCR:H313	32:m:101:LMG:H112	2.04	0.40
32:D:407:LMG:H132	32:D:407:LMG:H332	2.04	0.40
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.56	0.40
26:k:102:BCR:H20C	26:k:102:BCR:H361	1.94	0.40
24:B:611:CLA:H142	29:L:101:LHG:H382	2.02	0.40
26:B:619:BCR:H20C	26:B:619:BCR:H361	1.82	0.40
20:R:16:ALA:O	20:R:20:VAL:HG23	2.22	0.40
26:b:617:BCR:H24C	26:b:617:BCR:H371	1.93	0.40
28:b:625:STE:H171	28:d:411:STE:H61	2.03	0.40
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.57	0.40
32:C:521:LMG:O10	32:C:521:LMG:HC8	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:462:GLU:OE2	7:H:3:ARG:NH1[4_557]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	36	27
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	510/510 (100%)	503 (99%)	7 (1%)	0	100	100
2	b	504/510 (99%)	497 (99%)	7 (1%)	0	100	100
3	C	442/461 (96%)	434 (98%)	7 (2%)	1 (0%)	43	35
3	c	451/461 (98%)	441 (98%)	9 (2%)	1 (0%)	43	35
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	2 (3%)	1 (2%)	7	2
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	0
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	30 (100%)	0	0	100	100
13	O	243/272 (89%)	231 (95%)	11 (4%)	1 (0%)	30	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	236 (98%)	6 (2%)	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%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	4
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	9
16	v	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	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%)	57 (95%)	3 (5%)	0	100	100
20	R	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
20	r	26/41 (63%)	24 (92%)	2 (8%)	0	100	100
All	All	5234/5700 (92%)	5111 (98%)	115 (2%)	8 (0%)	43	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	64	PRO
3	c	416	SER
3	C	416	SER
7	h	63	LYS
15	u	53	ALA
9	J	7	ARG
13	O	57	LYS
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%)	269 (100%)	1 (0%)	84	82
1	a	269/280 (96%)	266 (99%)	3 (1%)	65	61
2	B	410/407 (101%)	408 (100%)	2 (0%)	81	79
2	b	403/407 (99%)	401 (100%)	2 (0%)	81	79
3	C	346/362 (96%)	343 (99%)	3 (1%)	70	67
3	c	354/362 (98%)	349 (99%)	5 (1%)	59	54
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	277/283 (98%)	273 (99%)	4 (1%)	59	54
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	29
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	29
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	53 (100%)	0	100	100
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	29 (97%)	1 (3%)	33	23
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	8
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	206/228 (90%)	205 (100%)	1 (0%)	81	79
13	o	207/228 (91%)	206 (100%)	1 (0%)	81	79
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	82 (98%)	2 (2%)	43	35
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	48
16	v	117/138 (85%)	115 (98%)	2 (2%)	53	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	22 (100%)	0	100	100
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	44
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	20 (91%)	2 (9%)	9	2
All	All	4324/4654 (93%)	4286 (99%)	38 (1%)	73	67

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
2	B	86	ILE
2	B	371	THR
3	C	240	ILE
3	C	289	PHE
3	C	354	GLU
5	E	22[A]	ILE
5	E	22[B]	ILE
13	O	107	THR
15	U	45	LEU
15	U	61	VAL
16	V	3	LEU
16	V	7	VAL
19	Z	1	MET
1	a	159	LEU
1	a	200	LEU
1	a	243	GLU
2	b	149	LEU
2	b	362	PHE
3	c	124	VAL
3	c	125	LEU
3	c	240	ILE
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	227[A]	GLU
4	d	227[B]	GLU

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Mol	Chain	Res	Type
4	d	230	SER
4	d	293	LEU
5	e	4	THR
5	e	66	VAL
10	k	27	VAL
11	l	21	LEU
11	l	30	LEU
13	o	49	THR
16	v	52	LEU
16	v	107	LEU
20	r	3	TRP
20	r	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
2	B	331	ASN
2	B	338	GLN
2	B	409	GLN
3	C	44	ASN
3	C	201	ASN
3	C	311	GLN
3	C	373	ASN
3	C	385	GLN
3	C	415	ASN
4	D	61	HIS
6	F	44	GLN
11	L	8	GLN
12	M	32	GLN
13	O	61	GLN
13	O	82	GLN
13	O	88	ASN
13	O	155	ASN
19	Z	6	GLN
20	R	22	ASN
1	a	165	GLN
2	b	409	GLN
2	b	490	GLN
2	b	497	GLN
3	c	28	GLN
3	c	44	ASN

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Mol	Chain	Res	Type
4	d	61	HIS
4	d	350	ASN
5	e	82	GLN
7	h	59	ASN
11	l	8	GLN
12	m	5	GLN
12	m	32	GLN
13	o	109	GLN
13	o	155	ASN
18	x	33	GLN
19	z	31	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.41	0	8,9,11	0.91	1 (12%)
14	FME	t	1	14	8,9,10	0.50	0	8,9,11	1.02	0
14	FME	T	1	14	8,9,10	0.40	0	8,9,11	1.11	1 (12%)
8	FME	i	1	8	8,9,10	0.42	0	8,9,11	0.87	1 (12%)
12	FME	m	1	12	8,9,10	0.41	0	8,9,11	0.87	0
12	FME	M	1	12	8,9,10	0.43	0	8,9,11	0.70	0

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

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

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	CG-CB-CA	2.29	119.87	112.87
8	I	1	FME	O-C-CA	-2.08	119.41	124.77
8	i	1	FME	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	603	2	69,73,73	1.45	7 (10%)	82,113,113	1.40	10 (12%)
31	DGD	h	102	-	63,63,67	0.63	0	77,77,81	0.95	6 (7%)
29	LHG	d	410	-	38,38,48	0.62	0	41,44,54	0.76	0
24	CLA	C	508	3	69,73,73	1.25	8 (11%)	82,113,113	1.27	7 (8%)
26	BCR	h	101	-	41,41,41	0.55	0	56,56,56	0.90	2 (3%)
28	STE	T	102	-	15,15,19	0.46	0	14,14,19	0.55	0
24	CLA	C	502	3	69,73,73	1.28	8 (11%)	82,113,113	1.33	7 (8%)
26	BCR	B	617	-	41,41,41	0.46	0	56,56,56	0.91	2 (3%)
28	STE	m	103	-	17,17,19	0.44	0	16,16,19	0.63	0
35	HEC	v	201	16	50,50,50	1.59	4 (8%)	68,82,82	1.25	7 (10%)
32	LMG	c	518	-	29,29,55	0.49	0	31,31,63	0.72	1 (3%)
32	LMG	D	407	-	50,50,55	0.48	0	58,58,63	1.27	6 (10%)
32	LMG	C	517	-	35,35,55	0.49	0	43,43,63	1.69	9 (20%)
24	CLA	B	613	2	69,73,73	1.36	7 (10%)	82,113,113	1.40	8 (9%)
28	STE	M	102	-	14,14,19	0.72	0	14,14,19	0.99	1 (7%)
28	STE	a	616	-	11,11,19	0.83	0	11,11,19	1.02	1 (9%)
28	STE	B	624	-	11,11,19	0.70	0	11,11,19	1.24	1 (9%)
29	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.68	0
26	BCR	b	618	-	41,41,41	0.52	0	56,56,56	0.93	3 (5%)
31	DGD	H	102	-	63,63,67	0.56	0	77,77,81	0.95	6 (7%)
24	CLA	C	506	3	69,73,73	1.29	11 (15%)	82,113,113	1.13	6 (7%)
24	CLA	c	502	3	69,73,73	1.13	5 (7%)	82,113,113	1.29	8 (9%)
28	STE	C	519	-	6,6,19	0.44	0	5,5,19	0.53	0
24	CLA	D	403	4	69,73,73	1.16	8 (11%)	82,113,113	1.12	8 (9%)
24	CLA	c	505	3	69,73,73	1.18	7 (10%)	82,113,113	1.22	4 (4%)
28	STE	k	103	-	13,13,19	0.69	0	13,13,19	1.06	0
30	SQD	b	620	-	47,49,54	1.67	10 (21%)	57,60,65	2.03	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	614	2	69,73,73	1.32	10 (14%)	82,113,113	1.30	7 (8%)
26	BCR	B	618	-	41,41,41	0.56	0	56,56,56	0.88	2 (3%)
24	CLA	c	508	3	68,72,73	1.32	9 (13%)	80,111,113	1.31	7 (8%)
28	STE	z	101	-	8,8,19	0.45	0	7,7,19	0.56	0
25	PHO	A	607	-	58,69,69	1.92	11 (18%)	55,99,99	1.59	7 (12%)
31	DGD	c	521	-	63,63,67	0.54	1 (1%)	77,77,81	0.79	2 (2%)
28	STE	Z	101	-	16,16,19	0.47	0	15,15,19	0.54	0
26	BCR	b	617	-	41,41,41	0.48	0	56,56,56	0.98	2 (3%)
24	CLA	C	512	3	69,73,73	1.52	10 (14%)	82,113,113	1.40	10 (12%)
32	LMG	d	412	-	44,44,55	0.51	0	52,52,63	0.72	1 (1%)
28	STE	A	617	-	16,16,19	0.45	0	15,15,19	0.57	0
32	LMG	C	525	-	48,48,55	0.50	0	56,56,63	0.71	1 (1%)
28	STE	K	103	-	13,13,19	0.37	0	12,12,19	0.77	0
32	LMG	b	622	-	55,55,55	0.50	0	63,63,63	1.19	9 (14%)
24	CLA	B	614	2	69,73,73	1.24	7 (10%)	82,113,113	1.32	11 (13%)
28	STE	j	101	-	11,11,19	0.85	0	11,11,19	1.35	2 (18%)
24	CLA	B	607	36	69,73,73	1.31	8 (11%)	82,113,113	1.31	6 (7%)
24	CLA	b	613	2	69,73,73	1.16	9 (13%)	82,113,113	1.27	9 (10%)
24	CLA	C	509	3	69,73,73	1.13	5 (7%)	82,113,113	1.26	6 (7%)
24	CLA	C	503	3	69,73,73	1.27	9 (13%)	82,113,113	1.43	8 (9%)
24	CLA	b	601	36	69,73,73	1.27	7 (10%)	82,113,113	1.31	5 (6%)
27	PL9	d	406	-	55,55,55	1.17	5 (9%)	68,69,69	1.68	13 (19%)
24	CLA	C	501	3	69,73,73	1.39	8 (11%)	82,113,113	1.48	8 (9%)
27	PL9	D	406	-	55,55,55	1.30	7 (12%)	68,69,69	1.52	12 (17%)
28	STE	C	526	-	11,11,19	0.79	0	11,11,19	1.35	2 (18%)
24	CLA	C	507	36	69,73,73	1.07	4 (5%)	82,113,113	1.40	8 (9%)
28	STE	b	623	-	15,15,19	0.78	0	15,15,19	1.07	2 (13%)
24	CLA	B	604	2	69,73,73	1.39	9 (13%)	82,113,113	1.54	7 (8%)
24	CLA	b	616	2	64,68,73	1.21	6 (9%)	76,107,113	1.40	8 (10%)
28	STE	M	103	-	9,9,19	0.41	0	8,8,19	0.63	0
28	STE	b	624	-	9,9,19	0.37	0	8,8,19	0.72	0
24	CLA	d	404	4	69,73,73	1.34	7 (10%)	82,113,113	1.15	8 (9%)
28	STE	c	517	-	17,17,19	0.46	0	16,16,19	0.54	0
27	PL9	A	610	-	55,55,55	0.98	0	68,69,69	1.47	8 (11%)
24	CLA	A	612	36	69,73,73	1.26	8 (11%)	82,113,113	1.16	6 (7%)
24	CLA	c	512	3	69,73,73	1.19	9 (13%)	82,113,113	1.24	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	c	523	-	48,48,55	0.51	0	56,56,63	0.72	0
28	STE	e	101	-	8,8,19	0.48	0	7,7,19	0.42	0
28	STE	B	625	-	14,14,19	0.41	0	13,13,19	0.72	0
24	CLA	a	605	1	69,73,73	1.34	9 (13%)	82,113,113	1.49	9 (10%)
26	BCR	a	609	-	41,41,41	0.48	0	56,56,56	0.88	2 (3%)
28	STE	d	413	-	19,19,19	0.68	0	19,19,19	0.88	0
28	STE	I	101	-	16,16,19	0.84	0	16,16,19	0.92	1 (6%)
30	SQD	a	612	-	52,54,54	1.52	8 (15%)	62,65,65	2.07	12 (19%)
24	CLA	c	501	3	69,73,73	1.10	4 (5%)	82,113,113	1.23	6 (7%)
26	BCR	b	619	-	41,41,41	0.49	0	56,56,56	0.97	3 (5%)
28	STE	C	527	-	15,15,19	0.37	0	14,14,19	0.74	0
32	LMG	a	615	-	49,49,55	0.56	1 (2%)	57,57,63	0.92	3 (5%)
24	CLA	C	511	3	69,73,73	1.41	7 (10%)	82,113,113	1.36	4 (4%)
28	STE	J	101	-	11,11,19	0.67	0	11,11,19	1.23	1 (9%)
28	STE	b	625	-	10,10,19	0.45	0	9,9,19	0.66	0
29	LHG	A	613	-	48,48,48	0.58	0	51,54,54	0.58	1 (1%)
26	BCR	D	405	-	41,41,41	0.49	0	56,56,56	0.84	1 (1%)
24	CLA	b	606	2	69,73,73	1.50	5 (7%)	82,113,113	1.42	6 (7%)
28	STE	j	102	-	15,15,19	0.50	0	14,14,19	0.50	0
24	CLA	C	504	36	63,67,73	1.27	7 (11%)	74,105,113	1.26	11 (14%)
26	BCR	K	102	-	41,41,41	0.44	0	56,56,56	1.02	3 (5%)
26	BCR	C	515	-	41,41,41	0.42	0	56,56,56	0.70	0
28	STE	m	102	-	11,11,19	0.70	0	11,11,19	1.17	0
24	CLA	c	510	3	69,73,73	1.27	8 (11%)	82,113,113	1.25	8 (9%)
26	BCR	H	101	-	41,41,41	0.50	0	56,56,56	0.99	2 (3%)
28	STE	R	101	-	11,11,19	0.82	0	11,11,19	1.10	1 (9%)
28	STE	I	102	-	14,14,19	0.78	0	14,14,19	0.97	0
32	LMG	M	101	-	51,51,55	0.52	0	59,59,63	0.95	1 (1%)
28	STE	A	616	-	7,7,19	0.37	0	6,6,19	0.63	0
24	CLA	C	505	3	69,73,73	1.15	7 (10%)	82,113,113	1.40	9 (10%)
30	SQD	B	622	-	52,54,54	1.59	10 (19%)	62,65,65	1.97	15 (24%)
28	STE	f	103	-	7,7,19	0.41	0	6,6,19	0.60	0
24	CLA	b	612	2	69,73,73	1.28	8 (11%)	82,113,113	1.18	7 (8%)
29	LHG	d	408	-	48,48,48	0.55	0	51,54,54	0.75	1 (1%)
30	SQD	a	613	-	52,54,54	1.61	8 (15%)	62,65,65	1.37	8 (12%)
31	DGD	C	522	-	63,63,67	0.60	1 (1%)	77,77,81	0.97	5 (6%)
30	SQD	f	102	-	39,41,54	1.69	7 (17%)	49,52,65	2.04	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	e	102	-	41,41,48	0.60	0	44,47,54	0.58	0
24	CLA	B	601	36	69,73,73	1.53	9 (13%)	82,113,113	1.45	7 (8%)
24	CLA	B	606	2	69,73,73	1.45	7 (10%)	82,113,113	1.39	9 (10%)
26	BCR	k	102	-	41,41,41	0.49	0	56,56,56	0.89	1 (1%)
28	STE	C	516	-	13,13,19	0.83	0	13,13,19	0.85	0
24	CLA	b	609	2	69,73,73	1.18	6 (8%)	82,113,113	1.36	11 (13%)
28	STE	i	101	-	11,11,19	0.75	0	11,11,19	1.05	0
28	STE	A	611	-	8,8,19	0.43	0	7,7,19	0.58	0
26	BCR	c	515	-	41,41,41	0.44	0	56,56,56	0.87	2 (3%)
30	SQD	D	412	-	50,52,54	1.61	8 (16%)	60,63,65	1.97	13 (21%)
32	LMG	D	408	-	51,51,55	0.49	0	59,59,63	0.77	0
31	DGD	C	524	-	63,63,67	0.60	1 (1%)	77,77,81	0.80	2 (2%)
28	STE	E	102	-	19,19,19	0.68	0	19,19,19	0.90	1 (5%)
33	BCT	D	401	22	3,3,3	0.79	0	2,3,3	2.49	1 (50%)
27	PL9	a	610	-	55,55,55	1.02	4 (7%)	68,69,69	1.56	11 (16%)
28	STE	B	623	-	17,17,19	0.65	0	17,17,19	1.02	0
28	STE	t	103	-	9,9,19	0.43	0	8,8,19	0.64	0
28	STE	D	414	-	19,19,19	0.61	0	19,19,19	1.16	0
30	SQD	A	614	-	41,43,54	1.80	9 (21%)	51,54,65	1.56	8 (15%)
35	HEC	V	201	16	50,50,50	1.56	4 (8%)	68,82,82	1.32	8 (11%)
24	CLA	b	607	36	69,73,73	1.36	6 (8%)	82,113,113	1.20	6 (7%)
24	CLA	b	608	2	69,73,73	1.10	8 (11%)	82,113,113	1.13	4 (4%)
24	CLA	B	605	2	69,73,73	1.23	6 (8%)	82,113,113	1.28	10 (12%)
24	CLA	c	509	3	69,73,73	1.12	6 (8%)	82,113,113	1.44	5 (6%)
34	HEM	F	101	5,6	50,50,50	1.35	6 (12%)	67,82,82	1.12	5 (7%)
31	DGD	c	519	-	63,63,67	0.61	0	77,77,81	0.85	3 (3%)
28	STE	H	104	-	8,8,19	0.41	0	7,7,19	0.49	0
24	CLA	C	513	3	69,73,73	1.47	9 (13%)	82,113,113	1.37	7 (8%)
25	PHO	d	402	-	58,69,69	2.20	13 (22%)	55,99,99	1.68	10 (18%)
24	CLA	B	616	2	64,68,73	1.30	6 (9%)	76,107,113	1.47	10 (13%)
24	CLA	c	507	36	69,73,73	1.11	6 (8%)	82,113,113	1.34	8 (9%)
29	LHG	D	413	-	48,48,48	0.56	0	51,54,54	0.94	3 (5%)
28	STE	c	516	-	12,12,19	0.44	0	11,11,19	0.62	0
24	CLA	a	611	36	69,73,73	1.32	8 (11%)	82,113,113	1.27	9 (10%)
32	LMG	B	620	-	45,45,55	0.51	0	53,53,63	0.92	2 (3%)
24	CLA	c	511	3	69,73,73	1.50	6 (8%)	82,113,113	1.46	7 (8%)
24	CLA	A	608	1	58,62,73	1.28	7 (12%)	68,99,113	1.35	6 (8%)

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	1.24	9 (13%)	82,113,113	1.37	9 (10%)
28	STE	C	520	-	9,9,19	0.44	0	8,8,19	0.60	0
24	CLA	c	503	3	69,73,73	1.32	6 (8%)	82,113,113	1.38	6 (7%)
32	LMG	C	521	-	48,48,55	0.53	0	56,56,63	0.83	1 (1%)
21	OEX	A	601	36,3,1	0,14,14	-	-	-		
24	CLA	b	604	2	69,73,73	1.13	6 (8%)	82,113,113	1.49	14 (17%)
24	CLA	b	615	2	69,73,73	1.42	9 (13%)	82,113,113	1.32	7 (8%)
24	CLA	b	602	2	69,73,73	1.17	8 (11%)	82,113,113	1.39	10 (12%)
28	STE	t	102	-	13,13,19	0.67	0	13,13,19	1.31	2 (15%)
29	LHG	D	410	-	48,48,48	0.63	1 (2%)	51,54,54	0.87	0
21	OEX	a	601	36,3,1	0,14,14	-	-	-		
24	CLA	a	606	36	69,73,73	1.17	7 (10%)	82,113,113	1.26	8 (9%)
26	BCR	C	514	-	41,41,41	0.42	0	56,56,56	0.75	1 (1%)
28	STE	d	407	-	19,19,19	0.74	0	19,19,19	0.87	1 (5%)
31	DGD	C	523	-	63,63,67	0.64	1 (1%)	77,77,81	0.78	1 (1%)
28	STE	A	618	-	10,10,19	0.37	0	9,9,19	0.77	0
30	SQD	D	409	-	34,36,54	1.55	4 (11%)	42,45,65	2.10	9 (21%)
24	CLA	D	404	4	69,73,73	1.30	9 (13%)	82,113,113	1.26	7 (8%)
28	STE	h	103	-	9,9,19	0.43	0	8,8,19	0.63	0
28	STE	e	103	-	8,8,19	0.42	0	7,7,19	0.61	0
26	BCR	k	101	-	41,41,41	0.46	0	56,56,56	0.77	1 (1%)
24	CLA	b	610	36	69,73,73	1.39	7 (10%)	82,113,113	1.20	9 (10%)
24	CLA	b	603	2	69,73,73	1.18	6 (8%)	82,113,113	1.47	11 (13%)
26	BCR	t	101	-	41,41,41	0.51	0	56,56,56	1.14	4 (7%)
24	CLA	B	602	2	69,73,73	1.21	7 (10%)	82,113,113	1.29	6 (7%)
24	CLA	c	506	3	69,73,73	1.34	11 (15%)	82,113,113	1.13	7 (8%)
29	LHG	D	411	-	46,46,48	0.57	0	49,52,54	0.67	2 (4%)
28	STE	e	104	-	12,12,19	0.71	0	12,12,19	1.10	1 (8%)
26	BCR	c	514	-	41,41,41	0.41	0	56,56,56	0.72	0
28	STE	E	101	-	11,11,19	0.40	0	10,10,19	0.62	0
34	HEM	f	101	5,6	50,50,50	1.47	8 (16%)	67,82,82	1.33	7 (10%)
26	BCR	A	609	-	41,41,41	0.44	0	56,56,56	0.71	0
24	CLA	c	504	36	64,68,73	1.25	9 (14%)	76,107,113	1.34	10 (13%)
25	PHO	a	607	-	58,69,69	2.06	11 (18%)	55,99,99	1.64	13 (23%)
29	LHG	L	101	-	48,48,48	0.54	0	51,54,54	0.85	2 (3%)
31	DGD	A	615	-	67,67,67	0.53	0	81,81,81	1.12	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	a	614	-	55,55,55	0.58	0	63,63,63	1.40	10 (15%)
29	LHG	d	409	-	48,48,48	0.54	0	51,54,54	0.73	2 (3%)
24	CLA	d	403	4	69,73,73	1.21	7 (10%)	82,113,113	1.30	5 (6%)
24	CLA	B	608	2	69,73,73	1.15	6 (8%)	82,113,113	1.39	11 (13%)
28	STE	b	621	-	19,19,19	0.63	0	19,19,19	0.98	1 (5%)
24	CLA	B	610	36	69,73,73	1.33	7 (10%)	82,113,113	1.44	10 (12%)
26	BCR	T	101	-	41,41,41	0.54	0	56,56,56	0.89	1 (1%)
28	STE	H	103	-	17,17,19	0.43	0	16,16,19	0.69	0
24	CLA	b	611	2	69,73,73	1.20	7 (10%)	82,113,113	1.28	7 (8%)
28	STE	C	518	-	4,4,19	0.46	0	3,3,19	0.36	0
24	CLA	c	513	3	69,73,73	1.21	7 (10%)	82,113,113	1.16	7 (8%)
33	BCT	d	401	22	3,3,3	0.79	0	2,3,3	2.17	1 (50%)
24	CLA	a	608	1	69,73,73	1.15	6 (8%)	82,113,113	1.21	8 (9%)
26	BCR	d	405	-	41,41,41	0.54	0	56,56,56	0.95	4 (7%)
24	CLA	A	606	36	69,73,73	1.21	6 (8%)	82,113,113	1.36	8 (9%)
28	STE	i	102	-	5,5,19	0.38	0	4,4,19	0.49	0
24	CLA	C	510	3	69,73,73	1.27	9 (13%)	82,113,113	1.43	8 (9%)
28	STE	d	411	-	19,19,19	0.66	0	19,19,19	0.83	0
32	LMG	m	101	-	51,51,55	0.51	0	59,59,63	0.96	4 (6%)
31	DGD	c	520	-	63,63,67	0.53	0	77,77,81	0.80	3 (3%)
32	LMG	c	522	-	46,46,55	0.50	0	54,54,63	0.66	0
28	STE	C	528	-	13,13,19	0.44	0	12,12,19	0.57	0
28	STE	M	104	-	14,14,19	0.37	0	13,13,19	0.76	0
26	BCR	B	619	-	41,41,41	0.41	0	56,56,56	0.80	1 (1%)
24	CLA	B	609	2	69,73,73	1.19	4 (5%)	82,113,113	1.31	7 (8%)
28	STE	B	621	-	16,16,19	0.68	0	16,16,19	1.08	0
25	PHO	D	402	-	58,69,69	1.99	10 (17%)	55,99,99	1.69	10 (18%)
24	CLA	B	615	2	69,73,73	1.64	10 (14%)	82,113,113	1.36	5 (6%)
24	CLA	A	605	1	69,73,73	1.20	5 (7%)	82,113,113	1.13	7 (8%)
24	CLA	B	611	2	69,73,73	1.24	9 (13%)	82,113,113	1.25	6 (7%)
24	CLA	b	605	2	69,73,73	1.09	6 (8%)	82,113,113	1.32	9 (10%)
26	BCR	K	101	-	41,41,41	0.47	0	56,56,56	0.86	1 (1%)

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	B	603	2	-	2/39/115/115	-
31	DGD	h	102	-	-	17/51/91/95	0/2/2/2
29	LHG	d	410	-	-	8/43/43/53	-
24	CLA	C	508	3	-	3/39/115/115	-
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
28	STE	T	102	-	-	7/13/13/17	-
24	CLA	C	502	3	-	6/39/115/115	-
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
28	STE	m	103	-	-	7/15/15/17	-
35	HEC	v	201	16	1/1/7/7	4/14/54/54	-
32	LMG	c	518	-	-	7/31/31/70	-
32	LMG	D	407	-	-	16/45/65/70	0/1/1/1
32	LMG	C	517	-	-	13/30/50/70	0/1/1/1
24	CLA	B	613	2	-	10/39/115/115	-
28	STE	M	102	-	-	4/12/12/17	-
28	STE	a	616	-	-	4/9/9/17	-
28	STE	B	624	-	-	3/9/9/17	-
29	LHG	l	101	-	-	18/53/53/53	-
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
24	CLA	C	506	3	-	12/39/115/115	-
24	CLA	c	502	3	-	6/39/115/115	-
28	STE	C	519	-	-	0/4/4/17	-
24	CLA	D	403	4	-	3/39/115/115	-
24	CLA	c	505	3	-	6/39/115/115	-
28	STE	k	103	-	-	4/11/11/17	-
30	SQD	b	620	-	-	16/44/64/69	0/1/1/1
24	CLA	b	614	2	-	13/39/115/115	-
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	CLA	c	508	3	-	2/38/114/115	-
28	STE	z	101	-	-	3/6/6/17	-
25	PHO	A	607	-	-	1/37/103/103	0/5/6/6
31	DGD	c	521	-	-	15/51/91/95	0/2/2/2
28	STE	Z	101	-	-	3/14/14/17	-
26	BCR	b	617	-	-	0/29/63/63	0/2/2/2
24	CLA	C	512	3	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	d	412	-	-	10/39/59/70	0/1/1/1
28	STE	A	617	-	-	9/14/14/17	-
32	LMG	C	525	-	-	11/43/63/70	0/1/1/1
28	STE	K	103	-	-	7/11/11/17	-
32	LMG	b	622	-	-	25/50/70/70	0/1/1/1
24	CLA	B	614	2	-	10/39/115/115	-
28	STE	j	101	-	-	3/9/9/17	-
24	CLA	B	607	36	-	2/39/115/115	-
24	CLA	b	613	2	-	2/39/115/115	-
24	CLA	C	509	3	-	11/39/115/115	-
24	CLA	C	503	3	-	1/39/115/115	-
24	CLA	b	601	36	-	14/39/115/115	-
27	PL9	d	406	-	-	8/53/73/73	0/1/1/1
24	CLA	C	501	3	-	4/39/115/115	-
27	PL9	D	406	-	-	6/53/73/73	0/1/1/1
28	STE	C	526	-	-	2/9/9/17	-
24	CLA	C	507	36	-	9/39/115/115	-
28	STE	b	623	-	-	4/13/13/17	-
24	CLA	B	604	2	-	6/39/115/115	-
24	CLA	b	616	2	-	5/33/109/115	-
28	STE	M	103	-	-	5/7/7/17	-
28	STE	b	624	-	-	3/7/7/17	-
24	CLA	d	404	4	-	9/39/115/115	-
28	STE	c	517	-	-	8/15/15/17	-
27	PL9	A	610	-	-	22/53/73/73	0/1/1/1
24	CLA	A	612	36	-	3/39/115/115	-
24	CLA	c	512	3	-	15/39/115/115	-
32	LMG	c	523	-	-	15/43/63/70	0/1/1/1
28	STE	e	101	-	-	3/6/6/17	-
28	STE	B	625	-	-	4/12/12/17	-
24	CLA	a	605	1	-	5/39/115/115	-
26	BCR	a	609	-	-	0/29/63/63	0/2/2/2
28	STE	d	413	-	-	8/17/17/17	-
28	STE	I	101	-	-	6/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	a	612	-	-	20/49/69/69	0/1/1/1
24	CLA	c	501	3	-	2/39/115/115	-
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
28	STE	C	527	-	-	4/13/13/17	-
32	LMG	a	615	-	-	18/44/64/70	0/1/1/1
24	CLA	C	511	3	-	2/39/115/115	-
28	STE	J	101	-	-	4/9/9/17	-
28	STE	b	625	-	-	4/8/8/17	-
29	LHG	A	613	-	-	14/53/53/53	-
26	BCR	D	405	-	-	2/29/63/63	0/2/2/2
24	CLA	b	606	2	-	6/39/115/115	-
28	STE	j	102	-	-	6/13/13/17	-
24	CLA	C	504	36	-	8/32/108/115	-
26	BCR	K	102	-	-	4/29/63/63	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
28	STE	m	102	-	-	4/9/9/17	-
24	CLA	c	510	3	-	7/39/115/115	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
28	STE	R	101	-	-	4/9/9/17	-
28	STE	I	102	-	-	4/12/12/17	-
32	LMG	M	101	-	-	20/46/66/70	0/1/1/1
28	STE	A	616	-	-	3/5/5/17	-
24	CLA	C	505	3	-	9/39/115/115	-
30	SQD	B	622	-	-	23/49/69/69	0/1/1/1
28	STE	f	103	-	-	4/5/5/17	-
24	CLA	b	612	2	-	4/39/115/115	-
29	LHG	d	408	-	-	19/53/53/53	-
30	SQD	a	613	-	-	20/49/69/69	0/1/1/1
31	DGD	C	522	-	-	18/51/91/95	0/2/2/2
30	SQD	f	102	-	-	12/36/56/69	0/1/1/1
29	LHG	e	102	-	-	22/46/46/53	-
24	CLA	B	601	36	-	12/39/115/115	-
24	CLA	B	606	2	-	8/39/115/115	-
26	BCR	k	102	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	C	516	-	-	7/11/11/17	-
24	CLA	b	609	2	-	3/39/115/115	-
28	STE	i	101	-	-	6/9/9/17	-
28	STE	A	611	-	-	3/6/6/17	-
26	BCR	c	515	-	-	1/29/63/63	0/2/2/2
30	SQD	D	412	-	-	18/47/67/69	0/1/1/1
32	LMG	D	408	-	-	13/46/66/70	0/1/1/1
31	DGD	C	524	-	-	12/51/91/95	0/2/2/2
35	HEC	V	201	16	1/1/7/7	6/14/54/54	-
28	STE	E	102	-	-	10/17/17/17	-
27	PL9	a	610	-	-	14/53/73/73	0/1/1/1
28	STE	B	623	-	-	11/15/15/17	-
28	STE	t	103	-	-	2/7/7/17	-
28	STE	D	414	-	-	6/17/17/17	-
30	SQD	A	614	-	-	14/38/58/69	0/1/1/1
24	CLA	b	607	36	-	9/39/115/115	-
24	CLA	b	608	2	-	7/39/115/115	-
24	CLA	B	605	2	-	6/39/115/115	-
24	CLA	c	509	3	-	13/39/115/115	-
34	HEM	F	101	5,6	-	3/14/54/54	-
31	DGD	c	519	-	-	24/51/91/95	0/2/2/2
28	STE	H	104	-	-	4/6/6/17	-
24	CLA	C	513	3	-	11/39/115/115	-
25	PHO	d	402	-	-	0/37/103/103	0/5/6/6
24	CLA	B	616	2	-	6/33/109/115	-
24	CLA	c	507	36	-	7/39/115/115	-
29	LHG	D	413	-	-	20/53/53/53	-
28	STE	c	516	-	-	6/10/10/17	-
24	CLA	a	611	36	-	4/39/115/115	-
32	LMG	B	620	-	-	15/40/60/70	0/1/1/1
24	CLA	c	511	3	-	4/39/115/115	-
24	CLA	A	608	1	-	3/26/102/115	-
24	CLA	B	612	2	-	7/39/115/115	-
28	STE	C	520	-	-	5/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	503	3	-	6/39/115/115	-
32	LMG	C	521	-	-	18/43/63/70	0/1/1/1
24	CLA	b	604	2	-	8/39/115/115	-
24	CLA	b	615	2	-	2/39/115/115	-
24	CLA	b	602	2	-	4/39/115/115	-
28	STE	t	102	-	-	3/11/11/17	-
29	LHG	D	410	-	-	15/53/53/53	-
24	CLA	a	606	36	-	4/39/115/115	-
26	BCR	C	514	-	-	3/29/63/63	0/2/2/2
28	STE	d	407	-	-	7/17/17/17	-
31	DGD	C	523	-	-	17/51/91/95	0/2/2/2
28	STE	A	618	-	-	5/8/8/17	-
30	SQD	D	409	-	-	18/28/48/69	0/1/1/1
24	CLA	D	404	4	-	4/39/115/115	-
28	STE	h	103	-	-	3/7/7/17	-
28	STE	e	103	-	-	3/6/6/17	-
26	BCR	k	101	-	-	4/29/63/63	0/2/2/2
24	CLA	b	610	36	-	5/39/115/115	-
24	CLA	b	603	2	-	6/39/115/115	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
24	CLA	B	602	2	-	3/39/115/115	-
24	CLA	c	506	3	-	12/39/115/115	-
29	LHG	D	411	-	-	15/51/51/53	-
28	STE	e	104	-	-	3/10/10/17	-
26	BCR	c	514	-	-	3/29/63/63	0/2/2/2
28	STE	E	101	-	-	4/9/9/17	-
34	HEM	f	101	5,6	-	4/14/54/54	-
26	BCR	A	609	-	-	0/29/63/63	0/2/2/2
24	CLA	c	504	36	-	6/33/109/115	-
25	PHO	a	607	-	-	3/37/103/103	0/5/6/6
29	LHG	L	101	-	-	12/53/53/53	-
31	DGD	A	615	-	-	24/55/95/95	0/2/2/2
32	LMG	a	614	-	-	21/50/70/70	0/1/1/1
29	LHG	d	409	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	403	4	-	7/39/115/115	-
24	CLA	B	608	2	-	2/39/115/115	-
28	STE	b	621	-	-	8/17/17/17	-
24	CLA	B	610	36	-	6/39/115/115	-
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
28	STE	H	103	-	-	8/15/15/17	-
24	CLA	b	611	2	-	7/39/115/115	-
28	STE	C	518	-	-	1/2/2/17	-
24	CLA	c	513	3	-	13/39/115/115	-
24	CLA	a	608	1	-	12/39/115/115	-
26	BCR	d	405	-	-	0/29/63/63	0/2/2/2
24	CLA	A	606	36	-	5/39/115/115	-
28	STE	i	102	-	-	1/3/3/17	-
24	CLA	C	510	3	-	9/39/115/115	-
28	STE	d	411	-	-	8/17/17/17	-
32	LMG	m	101	-	-	14/46/66/70	0/1/1/1
31	DGD	c	520	-	-	17/51/91/95	0/2/2/2
32	LMG	c	522	-	-	17/41/61/70	0/1/1/1
28	STE	C	528	-	-	6/11/11/17	-
28	STE	M	104	-	-	7/12/12/17	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	B	609	2	-	4/39/115/115	-
28	STE	B	621	-	-	5/14/14/17	-
25	PHO	D	402	-	-	1/37/103/103	0/5/6/6
24	CLA	B	615	2	-	15/39/115/115	-
24	CLA	A	605	1	-	6/39/115/115	-
24	CLA	B	611	2	-	4/39/115/115	-
24	CLA	b	605	2	-	6/39/115/115	-
26	BCR	K	101	-	-	4/29/63/63	0/2/2/2

All (667) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	PHO	C1B-C2B	10.33	1.50	1.39
25	a	607	PHO	C1B-C2B	9.10	1.49	1.39
25	d	402	PHO	C3B-C4B	8.91	1.50	1.41
24	b	606	CLA	MG-NA	8.89	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	402	PHO	C1B-C2B	8.50	1.48	1.39
24	c	511	CLA	MG-NA	7.81	2.24	2.06
25	a	607	PHO	C3B-C4B	7.62	1.49	1.41
25	A	607	PHO	C3B-C4B	7.50	1.49	1.41
25	A	607	PHO	C1B-C2B	7.41	1.47	1.39
25	D	402	PHO	C3B-C4B	7.39	1.49	1.41
35	v	201	HEC	C3D-C2D	7.33	1.52	1.36
24	B	606	CLA	MG-NA	7.12	2.23	2.06
24	b	610	CLA	MG-NB	-6.92	1.92	2.05
24	C	511	CLA	MG-NA	6.88	2.22	2.06
35	V	201	HEC	C3D-C2D	6.60	1.51	1.36
24	d	404	CLA	MG-ND	-6.19	1.93	2.05
24	b	615	CLA	MG-NA	6.17	2.20	2.06
24	b	607	CLA	MG-NA	6.12	2.20	2.06
24	B	603	CLA	MG-NA	6.11	2.20	2.06
24	B	615	CLA	MG-NB	6.06	2.17	2.05
24	B	601	CLA	MG-NA	6.01	2.20	2.06
24	C	512	CLA	MG-NB	5.98	2.17	2.05
24	C	513	CLA	MG-NA	5.76	2.20	2.06
24	C	513	CLA	MG-ND	5.46	2.16	2.05
24	c	503	CLA	MG-NA	5.40	2.19	2.06
24	B	615	CLA	MG-NA	5.34	2.19	2.06
34	f	101	HEM	FE-NA	5.28	2.12	1.95
24	a	611	CLA	MG-NA	5.27	2.18	2.06
35	V	201	HEC	FE-ND	5.09	2.10	1.94
24	C	501	CLA	MG-NA	5.00	2.18	2.06
24	B	603	CLA	MG-ND	4.99	2.15	2.05
30	D	409	SQD	O48-C23	4.86	1.47	1.33
24	B	613	CLA	MG-NC	4.84	2.17	2.06
30	A	614	SQD	O48-C23	4.74	1.47	1.33
30	D	412	SQD	O48-C23	4.74	1.47	1.33
30	f	102	SQD	O48-C23	4.71	1.47	1.33
24	B	612	CLA	MG-NA	4.71	2.17	2.06
24	B	601	CLA	MG-NB	-4.61	1.96	2.05
24	b	611	CLA	MG-NA	4.57	2.17	2.06
30	B	622	SQD	O48-C23	4.55	1.46	1.33
24	B	604	CLA	MG-NC	4.54	2.17	2.06
30	a	613	SQD	O48-C23	4.51	1.46	1.33
24	C	502	CLA	MG-NA	4.51	2.17	2.06
24	c	510	CLA	MG-NA	4.50	2.17	2.06
24	A	606	CLA	MG-NA	4.42	2.16	2.06
30	a	612	SQD	O48-C23	4.41	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	404	CLA	MG-NC	4.39	2.16	2.06
24	C	503	CLA	MG-NA	4.34	2.16	2.06
24	B	607	CLA	MG-NA	4.32	2.16	2.06
24	C	506	CLA	MG-NA	4.29	2.16	2.06
24	C	501	CLA	C1D-ND	4.28	1.43	1.37
24	b	603	CLA	MG-NA	4.23	2.16	2.06
24	c	506	CLA	MG-ND	-4.19	1.97	2.05
24	B	609	CLA	MG-NA	4.19	2.16	2.06
25	A	607	PHO	C1D-C2D	4.18	1.44	1.39
24	b	612	CLA	MG-NA	4.18	2.16	2.06
25	a	607	PHO	C1D-C2D	4.17	1.44	1.39
30	b	620	SQD	O48-C23	4.15	1.45	1.33
24	B	616	CLA	C1D-ND	4.12	1.43	1.37
24	D	404	CLA	C1D-ND	4.12	1.43	1.37
24	C	512	CLA	MG-NC	4.08	2.16	2.06
24	B	604	CLA	MG-NA	4.04	2.15	2.06
24	B	614	CLA	C1D-ND	4.03	1.43	1.37
30	a	612	SQD	O47-C45	-4.03	1.37	1.46
24	B	610	CLA	MG-NA	4.02	2.15	2.06
24	B	616	CLA	MG-NC	3.99	2.15	2.06
24	a	605	CLA	C1D-ND	3.99	1.43	1.37
24	c	504	CLA	MG-ND	-3.96	1.97	2.05
24	B	604	CLA	C1D-ND	3.95	1.43	1.37
24	b	609	CLA	MG-NA	3.94	2.15	2.06
24	B	605	CLA	MG-NA	3.94	2.15	2.06
24	B	610	CLA	C1D-ND	3.94	1.43	1.37
27	D	406	PL9	C6-C1	-3.94	1.42	1.48
30	a	613	SQD	O5-C1	3.93	1.52	1.41
24	c	506	CLA	MG-NC	3.93	2.15	2.06
24	b	614	CLA	C1D-ND	3.92	1.43	1.37
24	B	615	CLA	C1D-ND	3.90	1.43	1.37
34	F	101	HEM	FE-NC	3.90	2.08	1.95
24	a	605	CLA	MG-NB	3.88	2.13	2.05
24	A	608	CLA	MG-ND	-3.88	1.98	2.05
25	D	402	PHO	C1D-C2D	3.85	1.43	1.39
30	A	614	SQD	O5-C1	3.83	1.51	1.41
24	A	612	CLA	C1D-ND	3.83	1.42	1.37
30	b	620	SQD	O5-C1	3.79	1.51	1.41
24	c	511	CLA	C1D-ND	3.79	1.42	1.37
24	B	615	CLA	MG-ND	-3.78	1.98	2.05
24	A	605	CLA	MG-NB	3.78	2.13	2.05
24	b	601	CLA	C1D-ND	3.78	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	MG-NA	3.74	2.15	2.06
24	B	610	CLA	MG-NB	-3.74	1.98	2.05
24	B	603	CLA	MG-NB	-3.73	1.98	2.05
24	C	505	CLA	C1D-ND	3.72	1.42	1.37
30	a	613	SQD	O47-C45	-3.69	1.37	1.46
25	d	402	PHO	C1D-C2D	3.69	1.43	1.39
30	B	622	SQD	O47-C45	-3.67	1.38	1.46
24	B	607	CLA	C1D-ND	3.67	1.42	1.37
24	b	612	CLA	C1D-ND	3.66	1.42	1.37
30	f	102	SQD	O47-C7	3.66	1.44	1.34
24	d	403	CLA	MG-NA	3.65	2.14	2.06
24	B	602	CLA	C1D-ND	3.61	1.42	1.37
24	B	611	CLA	MG-NA	3.61	2.14	2.06
24	c	505	CLA	MG-NA	3.60	2.14	2.06
24	B	606	CLA	C1D-ND	3.58	1.42	1.37
30	D	412	SQD	O47-C45	-3.57	1.38	1.46
24	c	508	CLA	MG-NB	3.56	2.12	2.05
24	C	502	CLA	C1D-ND	3.56	1.42	1.37
24	b	614	CLA	C4B-NB	3.56	1.42	1.37
24	C	504	CLA	MG-NA	3.56	2.14	2.06
27	d	406	PL9	C3-C4	-3.55	1.44	1.49
24	B	601	CLA	C4B-NB	3.55	1.42	1.37
24	b	613	CLA	C1D-ND	3.55	1.42	1.37
24	a	605	CLA	MG-NC	3.55	2.14	2.06
30	b	620	SQD	C24-C23	3.53	1.60	1.50
24	C	501	CLA	C4B-NB	3.51	1.42	1.37
30	B	622	SQD	O47-C7	3.51	1.44	1.34
24	C	508	CLA	C1B-C2B	3.50	1.51	1.43
27	D	406	PL9	C52-C5	-3.50	1.43	1.50
24	B	601	CLA	C1D-ND	3.50	1.42	1.37
24	B	609	CLA	C1D-ND	3.49	1.42	1.37
24	A	605	CLA	C1D-ND	3.48	1.42	1.37
24	a	608	CLA	C1D-ND	3.46	1.42	1.37
24	c	508	CLA	C1D-ND	3.46	1.42	1.37
24	A	612	CLA	C4B-NB	3.45	1.42	1.37
24	c	513	CLA	MG-NA	3.45	2.14	2.06
30	A	614	SQD	O47-C45	-3.45	1.38	1.46
24	c	502	CLA	C1D-ND	3.44	1.42	1.37
30	b	620	SQD	O47-C7	3.43	1.44	1.34
24	B	613	CLA	C1D-ND	3.42	1.42	1.37
24	C	510	CLA	MG-NB	3.41	2.12	2.05
24	c	503	CLA	C1D-ND	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	412	SQD	C24-C23	3.41	1.60	1.50
30	f	102	SQD	O47-C45	-3.40	1.38	1.46
30	A	614	SQD	O47-C7	3.39	1.43	1.34
24	b	607	CLA	C1D-ND	3.38	1.42	1.37
24	b	615	CLA	MG-NB	3.38	2.12	2.05
24	C	505	CLA	MG-NA	3.37	2.14	2.06
24	c	510	CLA	C1D-ND	3.37	1.42	1.37
30	D	409	SQD	O5-C1	3.37	1.50	1.41
24	b	616	CLA	C1D-ND	3.37	1.42	1.37
24	C	510	CLA	C1D-ND	3.36	1.42	1.37
24	a	606	CLA	C4B-NB	3.36	1.42	1.37
30	D	409	SQD	C24-C23	3.33	1.60	1.50
24	B	610	CLA	C4B-NB	3.33	1.42	1.37
24	b	612	CLA	MG-NB	-3.33	1.99	2.05
30	a	613	SQD	O47-C7	3.30	1.43	1.34
30	a	612	SQD	O5-C1	3.30	1.50	1.41
24	C	506	CLA	MG-NB	3.30	2.12	2.05
24	B	602	CLA	C4B-NB	3.29	1.42	1.37
24	C	512	CLA	C1D-ND	3.29	1.42	1.37
27	a	610	PL9	C53-C6	-3.29	1.44	1.50
24	C	509	CLA	C1D-ND	3.28	1.42	1.37
24	c	506	CLA	C1D-ND	3.28	1.42	1.37
24	b	601	CLA	C4B-NB	3.25	1.42	1.37
24	d	403	CLA	C1B-C2B	3.24	1.50	1.43
24	B	605	CLA	C1D-ND	3.23	1.42	1.37
24	B	613	CLA	C4B-NB	3.23	1.42	1.37
24	c	504	CLA	C4B-NB	3.22	1.42	1.37
24	c	507	CLA	C1D-ND	3.22	1.42	1.37
24	b	615	CLA	C1D-ND	3.22	1.42	1.37
24	b	606	CLA	C1B-C2B	3.22	1.50	1.43
25	a	607	PHO	C4D-CHA	3.21	1.44	1.39
24	A	606	CLA	C1B-C2B	3.20	1.50	1.43
30	A	614	SQD	C24-C23	3.19	1.60	1.50
24	C	512	CLA	C4B-NB	3.19	1.42	1.37
24	B	601	CLA	MG-ND	3.17	2.12	2.05
24	A	612	CLA	C3B-C4B	3.17	1.51	1.42
24	c	506	CLA	C4B-NB	3.16	1.42	1.37
24	C	504	CLA	C4B-NB	3.16	1.42	1.37
35	v	201	HEC	FE-ND	3.16	2.04	1.94
24	c	513	CLA	C1D-ND	3.14	1.42	1.37
24	c	503	CLA	C4B-NB	3.13	1.42	1.37
24	B	608	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	3.13	1.42	1.37
24	C	511	CLA	C4B-NB	3.12	1.42	1.37
30	D	412	SQD	O5-C1	3.12	1.49	1.41
24	b	601	CLA	C1B-C2B	3.12	1.50	1.43
24	B	615	CLA	C1B-C2B	3.12	1.50	1.43
24	A	612	CLA	CHC-C1C	3.11	1.44	1.38
24	c	513	CLA	C1B-C2B	3.11	1.50	1.43
24	c	512	CLA	C1D-ND	3.11	1.41	1.37
24	b	602	CLA	C1D-ND	3.10	1.41	1.37
24	b	604	CLA	MG-NA	3.10	2.13	2.06
24	B	612	CLA	C1B-C2B	3.08	1.50	1.43
30	b	620	SQD	O47-C45	-3.07	1.39	1.46
24	C	513	CLA	C1D-ND	3.06	1.41	1.37
24	d	403	CLA	C1D-ND	3.06	1.41	1.37
24	a	608	CLA	C1B-C2B	3.05	1.50	1.43
24	C	506	CLA	C1D-ND	3.05	1.41	1.37
27	d	406	PL9	C46-C44	-3.05	1.45	1.51
30	f	102	SQD	O5-C1	3.05	1.49	1.41
24	A	608	CLA	C1D-ND	3.04	1.41	1.37
24	b	616	CLA	MG-NA	3.04	2.13	2.06
30	f	102	SQD	C24-C23	3.04	1.59	1.50
24	C	504	CLA	C1D-ND	3.04	1.41	1.37
24	a	611	CLA	C4B-NB	3.03	1.41	1.37
24	C	513	CLA	C1B-C2B	3.03	1.50	1.43
24	C	510	CLA	C1B-C2B	3.03	1.50	1.43
24	A	605	CLA	C1B-C2B	3.03	1.50	1.43
24	b	602	CLA	C1B-C2B	3.02	1.50	1.43
24	b	602	CLA	C4B-NB	3.02	1.41	1.37
34	F	101	HEM	FE-NA	3.02	2.05	1.95
25	D	402	PHO	C4D-ND	-3.02	1.34	1.38
24	c	505	CLA	C4B-NB	3.02	1.41	1.37
24	a	606	CLA	C1D-ND	3.00	1.41	1.37
24	C	508	CLA	MG-NC	2.99	2.13	2.06
24	B	613	CLA	MG-NA	2.99	2.13	2.06
24	b	612	CLA	C4B-NB	2.99	1.41	1.37
24	d	404	CLA	C1D-ND	2.98	1.41	1.37
24	b	610	CLA	C1D-ND	2.97	1.41	1.37
25	d	402	PHO	C4D-CHA	2.97	1.44	1.39
30	B	622	SQD	C24-C23	2.97	1.59	1.50
24	d	404	CLA	C1B-C2B	2.97	1.50	1.43
24	C	511	CLA	C1B-C2B	2.97	1.50	1.43
24	a	605	CLA	C1B-C2B	2.96	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C1D-ND	2.96	1.41	1.37
24	B	611	CLA	C1B-C2B	2.95	1.50	1.43
24	c	509	CLA	C1B-C2B	2.95	1.50	1.43
24	c	513	CLA	C4B-NB	2.94	1.41	1.37
35	v	201	HEC	FE-NA	2.93	2.04	1.95
24	B	601	CLA	C1B-C2B	2.93	1.50	1.43
24	b	604	CLA	C1D-ND	2.93	1.41	1.37
24	B	614	CLA	MG-NA	2.93	2.13	2.06
24	B	603	CLA	C1D-ND	2.93	1.41	1.37
24	b	610	CLA	C1B-C2B	2.93	1.50	1.43
24	c	501	CLA	C1B-C2B	2.92	1.50	1.43
24	b	616	CLA	C1B-C2B	2.92	1.50	1.43
24	B	610	CLA	C1B-C2B	2.92	1.50	1.43
24	B	615	CLA	C4B-NB	2.92	1.41	1.37
30	D	412	SQD	O47-C7	2.92	1.42	1.34
24	B	615	CLA	MG-NC	2.91	2.13	2.06
30	B	622	SQD	O5-C1	2.91	1.49	1.41
24	B	613	CLA	C1B-C2B	2.90	1.49	1.43
24	B	614	CLA	C4B-NB	2.89	1.41	1.37
24	B	607	CLA	C1B-C2B	2.89	1.49	1.43
24	b	614	CLA	MG-NA	2.89	2.13	2.06
24	C	512	CLA	MG-ND	-2.88	2.00	2.05
24	C	507	CLA	C1B-C2B	2.88	1.49	1.43
24	c	502	CLA	C1B-C2B	2.88	1.49	1.43
24	C	512	CLA	MG-NA	2.88	2.13	2.06
24	d	404	CLA	C4B-NB	2.87	1.41	1.37
24	C	503	CLA	MG-NC	2.87	2.13	2.06
24	c	501	CLA	C1D-ND	2.87	1.41	1.37
30	a	613	SQD	C24-C23	2.86	1.59	1.50
24	D	403	CLA	C1B-C2B	2.86	1.49	1.43
24	B	605	CLA	C4B-NB	2.85	1.41	1.37
27	D	406	PL9	C3-C4	-2.85	1.45	1.49
24	C	512	CLA	CHC-C1C	2.85	1.44	1.38
24	C	509	CLA	C1B-C2B	2.85	1.49	1.43
24	B	607	CLA	C4B-NB	2.84	1.41	1.37
24	b	615	CLA	C1B-C2B	2.83	1.49	1.43
30	a	612	SQD	C24-C23	2.83	1.58	1.50
24	C	511	CLA	C1D-ND	2.83	1.41	1.37
24	C	504	CLA	C3B-C4B	2.82	1.50	1.42
24	b	604	CLA	C4B-NB	2.82	1.41	1.37
24	a	611	CLA	C1D-ND	2.82	1.41	1.37
24	a	611	CLA	C1B-C2B	2.82	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	CHC-C1C	2.82	1.44	1.38
24	C	503	CLA	C4B-NB	2.81	1.41	1.37
25	a	607	PHO	CMB-C2B	-2.81	1.46	1.51
24	b	615	CLA	CMD-C2D	-2.80	1.45	1.50
24	b	611	CLA	C4B-NB	2.79	1.41	1.37
24	A	612	CLA	C1B-C2B	2.79	1.49	1.43
24	b	612	CLA	C1B-C2B	2.79	1.49	1.43
24	c	510	CLA	C1B-C2B	2.79	1.49	1.43
24	c	512	CLA	MG-NB	2.79	2.11	2.05
24	b	615	CLA	C3B-C4B	2.79	1.50	1.42
24	C	503	CLA	C1D-ND	2.78	1.41	1.37
24	B	606	CLA	C4B-NB	2.78	1.41	1.37
24	c	509	CLA	C1D-ND	2.78	1.41	1.37
24	C	507	CLA	C1D-ND	2.77	1.41	1.37
24	c	508	CLA	CHC-C1C	2.77	1.44	1.38
24	C	508	CLA	C1D-ND	2.77	1.41	1.37
24	b	614	CLA	MG-NC	2.77	2.12	2.06
24	b	601	CLA	MG-NA	2.77	2.12	2.06
24	D	403	CLA	MG-NB	2.76	2.11	2.05
24	c	503	CLA	C1B-C2B	2.76	1.49	1.43
24	c	505	CLA	C1D-ND	2.76	1.41	1.37
24	b	603	CLA	C4B-NB	2.75	1.41	1.37
24	C	502	CLA	C1B-C2B	2.75	1.49	1.43
24	b	605	CLA	C1B-C2B	2.75	1.49	1.43
24	B	605	CLA	C3B-C4B	2.74	1.50	1.42
24	c	502	CLA	MG-NA	2.74	2.12	2.06
24	c	511	CLA	C4B-NB	2.74	1.41	1.37
24	c	508	CLA	C4B-NB	2.74	1.41	1.37
24	C	501	CLA	MG-ND	-2.74	2.00	2.05
24	c	510	CLA	C4B-NB	2.74	1.41	1.37
24	B	608	CLA	C1D-ND	2.73	1.41	1.37
24	c	507	CLA	C1B-C2B	2.73	1.49	1.43
24	B	607	CLA	MG-ND	-2.73	2.00	2.05
24	B	605	CLA	CHC-C1C	2.73	1.44	1.38
24	B	616	CLA	C1B-C2B	2.73	1.49	1.43
24	c	511	CLA	C1B-C2B	2.73	1.49	1.43
24	C	504	CLA	CHC-C1C	2.73	1.44	1.38
25	d	402	PHO	C4D-ND	-2.72	1.34	1.38
24	b	615	CLA	C4B-NB	2.72	1.41	1.37
24	C	503	CLA	C1B-C2B	2.72	1.49	1.43
24	b	614	CLA	C3B-C4B	2.72	1.50	1.42
24	B	616	CLA	MG-ND	2.72	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C1B-C2B	2.72	1.49	1.43
25	D	402	PHO	C3A-C2A	-2.71	1.52	1.54
24	a	606	CLA	CHC-C1C	2.71	1.43	1.38
24	D	403	CLA	CMD-C2D	-2.71	1.45	1.50
25	D	402	PHO	C3B-C2B	-2.70	1.36	1.40
24	B	602	CLA	MG-NA	2.70	2.12	2.06
24	a	608	CLA	C4B-NB	2.70	1.41	1.37
34	F	101	HEM	CAC-C3C	2.70	1.54	1.47
34	f	101	HEM	CAC-C3C	2.70	1.54	1.47
24	b	611	CLA	C1B-C2B	2.70	1.49	1.43
24	c	508	CLA	C1B-C2B	2.70	1.49	1.43
24	C	505	CLA	C1B-C2B	2.70	1.49	1.43
24	b	609	CLA	C1B-C2B	2.70	1.49	1.43
24	b	613	CLA	C4B-NB	2.69	1.41	1.37
24	c	508	CLA	C3B-C4B	2.69	1.50	1.42
24	B	608	CLA	MG-NA	2.69	2.12	2.06
24	b	603	CLA	C1D-ND	2.69	1.41	1.37
24	b	610	CLA	C4B-NB	2.68	1.41	1.37
25	A	607	PHO	C4D-CHA	2.68	1.43	1.39
24	c	508	CLA	MG-NC	2.68	2.12	2.06
24	A	606	CLA	C4B-NB	2.68	1.41	1.37
24	b	604	CLA	C1B-C2B	2.68	1.49	1.43
24	B	605	CLA	C1B-C2B	2.68	1.49	1.43
25	d	402	PHO	CMD-C2D	-2.68	1.46	1.51
24	B	612	CLA	MG-NC	-2.67	1.99	2.06
25	D	402	PHO	CMD-C2D	-2.67	1.46	1.51
24	a	606	CLA	C1B-C2B	2.67	1.49	1.43
24	A	608	CLA	C1B-C2B	2.66	1.49	1.43
25	A	607	PHO	C3D-C4D	2.66	1.44	1.41
25	A	607	PHO	CBD-CGD	-2.65	1.49	1.52
24	C	502	CLA	MG-NB	-2.65	2.00	2.05
24	C	501	CLA	C3B-C4B	2.65	1.50	1.42
30	a	612	SQD	O47-C7	2.65	1.41	1.34
24	a	605	CLA	MG-NA	2.65	2.12	2.06
24	B	603	CLA	C1B-C2B	2.64	1.49	1.43
24	B	611	CLA	C4B-NB	2.64	1.41	1.37
24	B	602	CLA	C1B-C2B	2.64	1.49	1.43
24	b	614	CLA	CHC-C1C	2.64	1.43	1.38
24	C	502	CLA	C4B-NB	2.64	1.41	1.37
24	b	607	CLA	C1B-C2B	2.63	1.49	1.43
24	B	608	CLA	C1B-C2B	2.63	1.49	1.43
24	c	506	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	406	PL9	C7-C8	-2.62	1.46	1.50
24	C	511	CLA	C3B-C4B	2.62	1.50	1.42
25	D	402	PHO	C4D-CHA	2.62	1.43	1.39
24	c	504	CLA	C1D-ND	2.61	1.41	1.37
25	D	402	PHO	CMC-C2C	-2.61	1.46	1.50
24	b	606	CLA	C1D-ND	2.61	1.41	1.37
24	b	606	CLA	C4B-NB	2.60	1.41	1.37
25	a	607	PHO	CAC-C3C	-2.60	1.47	1.51
24	C	512	CLA	C3B-C4B	2.60	1.50	1.42
24	c	512	CLA	CHC-C1C	2.59	1.43	1.38
24	B	604	CLA	CHC-C1C	2.59	1.43	1.38
34	F	101	HEM	CAB-C3B	2.59	1.54	1.47
24	b	608	CLA	C3B-C4B	2.59	1.50	1.42
25	a	607	PHO	CBD-CGD	-2.59	1.49	1.52
24	C	510	CLA	C3B-C4B	2.59	1.50	1.42
24	c	512	CLA	C1B-C2B	2.58	1.49	1.43
24	b	613	CLA	C1B-C2B	2.57	1.49	1.43
24	d	403	CLA	CMB-C2B	-2.57	1.45	1.50
24	d	404	CLA	CMD-C2D	-2.57	1.45	1.50
24	b	601	CLA	CHC-C1C	2.57	1.43	1.38
24	c	505	CLA	C1B-C2B	2.56	1.49	1.43
24	B	606	CLA	CMB-C2B	-2.56	1.45	1.50
24	a	605	CLA	C3B-C4B	2.56	1.50	1.42
34	f	101	HEM	CAB-C3B	2.55	1.54	1.47
24	b	609	CLA	C1D-ND	2.55	1.41	1.37
24	C	501	CLA	CHC-C1C	2.54	1.43	1.38
24	A	612	CLA	MG-NB	2.54	2.10	2.05
24	B	611	CLA	MG-ND	-2.54	2.00	2.05
30	A	614	SQD	O7-S	2.53	1.52	1.45
25	d	402	PHO	CMC-C2C	-2.52	1.46	1.50
27	a	610	PL9	C3-C4	-2.52	1.45	1.49
27	D	406	PL9	C5-C4	-2.52	1.38	1.47
24	a	605	CLA	CHC-C1C	2.52	1.43	1.38
24	B	614	CLA	MG-ND	-2.52	2.00	2.05
24	c	513	CLA	C3B-C4B	2.50	1.50	1.42
24	B	609	CLA	C1B-C2B	2.50	1.49	1.43
24	C	510	CLA	C4B-NB	2.49	1.41	1.37
24	b	614	CLA	C1B-C2B	2.49	1.49	1.43
24	C	506	CLA	C4B-NB	2.49	1.41	1.37
24	C	508	CLA	C3B-C4B	2.49	1.50	1.42
24	B	613	CLA	CMD-C2D	-2.48	1.45	1.50
24	c	506	CLA	CHC-C1C	2.48	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	CMC-C2C	-2.48	1.45	1.50
29	D	410	LHG	O7-C5	-2.47	1.40	1.46
24	b	603	CLA	CMC-C2C	-2.47	1.45	1.50
24	b	607	CLA	MG-NB	-2.47	2.00	2.05
24	B	608	CLA	C3B-C4B	2.47	1.49	1.42
24	b	602	CLA	MG-NA	2.46	2.12	2.06
30	a	613	SQD	O7-S	2.46	1.52	1.45
24	D	403	CLA	C4B-NB	2.46	1.41	1.37
24	B	604	CLA	C1B-C2B	2.46	1.48	1.43
24	a	605	CLA	C4B-NB	2.45	1.41	1.37
24	b	611	CLA	C1D-ND	2.45	1.41	1.37
24	a	606	CLA	C3B-C4B	2.45	1.49	1.42
24	c	504	CLA	C1B-C2B	2.45	1.48	1.43
24	b	607	CLA	C4B-NB	2.45	1.41	1.37
24	C	501	CLA	C1B-C2B	2.44	1.48	1.43
24	c	505	CLA	CHC-C1C	2.44	1.43	1.38
25	A	607	PHO	C3A-C2A	-2.44	1.52	1.54
24	C	508	CLA	C4B-NB	2.44	1.41	1.37
24	c	510	CLA	MG-NB	-2.44	2.00	2.05
24	b	612	CLA	CHC-C1C	2.43	1.43	1.38
24	B	604	CLA	C3B-C4B	2.43	1.49	1.42
24	b	603	CLA	C1B-C2B	2.42	1.48	1.43
24	c	508	CLA	MG-NA	2.42	2.12	2.06
25	D	402	PHO	CMB-C2B	-2.42	1.46	1.51
24	b	608	CLA	C1B-C2B	2.42	1.48	1.43
35	V	201	HEC	CMB-C2B	2.42	1.55	1.50
34	f	101	HEM	C3B-C2B	-2.42	1.32	1.37
30	b	620	SQD	O9-S	2.42	1.51	1.45
24	C	506	CLA	C1B-C2B	2.42	1.48	1.43
24	b	601	CLA	C3B-C4B	2.42	1.49	1.42
30	a	613	SQD	O9-S	2.42	1.51	1.45
24	C	512	CLA	C1B-C2B	2.41	1.48	1.43
25	a	607	PHO	C4D-ND	-2.41	1.34	1.38
24	c	512	CLA	C4B-NB	2.41	1.41	1.37
24	D	404	CLA	MG-NB	-2.41	2.01	2.05
24	d	403	CLA	C3B-C4B	2.41	1.49	1.42
24	c	512	CLA	C3B-C4B	2.40	1.49	1.42
24	b	609	CLA	C4B-NB	2.40	1.41	1.37
24	c	505	CLA	C3B-C4B	2.40	1.49	1.42
24	B	602	CLA	MG-NC	2.40	2.12	2.06
24	b	602	CLA	MG-NB	2.40	2.10	2.05
24	a	608	CLA	MG-NA	2.39	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	CMD-C2D	-2.39	1.45	1.50
35	V	201	HEC	FE-NB	2.39	2.02	1.94
24	b	605	CLA	C3B-C4B	2.39	1.49	1.42
24	B	612	CLA	C4B-NB	2.39	1.41	1.37
24	b	604	CLA	C3B-C4B	2.39	1.49	1.42
24	c	501	CLA	C4B-NB	2.38	1.41	1.37
30	A	614	SQD	O9-S	2.38	1.51	1.45
27	d	406	PL9	C53-C6	-2.38	1.45	1.50
24	C	513	CLA	MG-NB	-2.38	2.01	2.05
24	B	607	CLA	CMB-C2B	-2.37	1.45	1.50
25	a	607	PHO	CMC-C2C	-2.37	1.46	1.50
25	a	607	PHO	C3D-C4D	2.37	1.44	1.41
30	a	613	SQD	O5-C5	2.37	1.50	1.44
24	b	608	CLA	C1D-ND	2.37	1.41	1.37
24	b	616	CLA	C4B-NB	2.37	1.41	1.37
24	C	505	CLA	C4B-NB	2.36	1.41	1.37
24	b	613	CLA	MG-NA	2.36	2.11	2.06
24	C	502	CLA	CMB-C2B	-2.36	1.45	1.50
24	A	606	CLA	CMD-C2D	-2.36	1.45	1.50
24	B	613	CLA	MG-ND	-2.36	2.01	2.05
24	B	615	CLA	CHC-C1C	2.36	1.43	1.38
24	B	615	CLA	C1B-NB	-2.36	1.34	1.37
24	C	505	CLA	C3B-C4B	2.36	1.49	1.42
24	B	609	CLA	C4B-NB	2.35	1.41	1.37
24	b	605	CLA	C4B-NB	2.35	1.41	1.37
25	A	607	PHO	C4D-ND	-2.35	1.35	1.38
24	C	509	CLA	C3B-C4B	2.35	1.49	1.42
24	D	404	CLA	C4B-NB	2.35	1.40	1.37
24	b	606	CLA	C3B-C4B	2.34	1.49	1.42
24	b	615	CLA	CHC-C1C	2.34	1.43	1.38
24	D	403	CLA	CHC-C1C	2.34	1.43	1.38
24	a	611	CLA	MG-NC	2.34	2.11	2.06
30	A	614	SQD	O5-C5	2.34	1.50	1.44
24	d	403	CLA	C4B-NB	2.33	1.40	1.37
27	D	406	PL9	C10-C9	-2.33	1.45	1.50
24	A	608	CLA	C4B-NB	2.33	1.40	1.37
24	b	611	CLA	CMD-C2D	-2.33	1.46	1.50
24	C	507	CLA	C4B-NB	2.32	1.40	1.37
24	b	611	CLA	CHC-C1C	2.32	1.43	1.38
24	C	513	CLA	C4B-NB	2.32	1.40	1.37
24	b	612	CLA	CMC-C2C	-2.32	1.46	1.50
24	b	609	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	523	DGD	O3G-C3G	-2.31	1.39	1.43
24	C	508	CLA	CHC-C1C	2.31	1.43	1.38
25	A	607	PHO	CMD-C2D	-2.31	1.47	1.51
30	B	622	SQD	C8-C7	2.31	1.57	1.50
24	B	615	CLA	CMB-C2B	-2.31	1.46	1.50
24	a	611	CLA	CHC-C1C	2.31	1.43	1.38
24	C	503	CLA	C3B-C4B	2.31	1.49	1.42
24	c	509	CLA	C3B-C4B	2.30	1.49	1.42
24	B	612	CLA	CMC-C2C	-2.30	1.46	1.50
24	c	502	CLA	CMD-C2D	-2.30	1.46	1.50
24	c	511	CLA	CHC-C1C	2.30	1.43	1.38
24	C	513	CLA	C3B-C4B	2.30	1.49	1.42
24	c	507	CLA	MG-NB	-2.29	2.01	2.05
24	a	608	CLA	MG-NB	-2.29	2.01	2.05
24	B	612	CLA	C3B-C4B	2.29	1.49	1.42
24	c	512	CLA	CMD-C2D	-2.29	1.46	1.50
31	C	524	DGD	O2G-C2G	-2.28	1.41	1.46
24	C	506	CLA	CHC-C1C	2.28	1.43	1.38
32	a	615	LMG	O1-C7	-2.27	1.39	1.43
24	b	608	CLA	CMD-C2D	-2.27	1.46	1.50
24	b	608	CLA	CHC-C1C	2.27	1.43	1.38
24	B	601	CLA	C3B-C4B	2.27	1.49	1.42
24	C	507	CLA	C1B-NB	-2.26	1.34	1.37
24	a	611	CLA	C3B-C4B	2.26	1.49	1.42
24	b	602	CLA	C3B-C4B	2.26	1.49	1.42
24	B	610	CLA	C3B-C4B	2.26	1.49	1.42
24	A	606	CLA	C1D-ND	2.25	1.40	1.37
35	v	201	HEC	CMA-C3A	2.25	1.55	1.50
30	b	620	SQD	O7-S	2.25	1.51	1.45
24	b	601	CLA	O2A-CGA	2.25	1.39	1.33
24	B	611	CLA	MG-NB	2.25	2.10	2.05
24	C	503	CLA	CHC-C1C	2.25	1.43	1.38
24	c	507	CLA	CMC-C2C	-2.25	1.46	1.50
24	c	502	CLA	C4B-NB	2.24	1.40	1.37
25	A	607	PHO	CMC-C2C	-2.24	1.47	1.50
30	D	412	SQD	C8-C7	2.24	1.57	1.50
24	D	404	CLA	C1B-C2B	2.24	1.48	1.43
24	C	509	CLA	O2D-CGD	2.24	1.38	1.33
24	C	501	CLA	CMB-C2B	-2.24	1.46	1.50
24	C	504	CLA	C1B-C2B	2.24	1.48	1.43
24	b	602	CLA	CMD-C2D	-2.23	1.46	1.50
24	a	605	CLA	O2D-CED	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3B-C4B	2.23	1.49	1.42
24	c	504	CLA	CHC-C1C	2.23	1.43	1.38
24	b	611	CLA	C3B-C4B	2.23	1.49	1.42
24	b	613	CLA	CHC-C1C	2.23	1.42	1.38
24	c	504	CLA	C1B-NB	-2.22	1.34	1.37
24	B	614	CLA	CHC-C1C	2.22	1.42	1.38
24	D	404	CLA	MG-ND	-2.22	2.01	2.05
24	c	513	CLA	CMB-C2B	-2.21	1.46	1.50
24	b	613	CLA	C3B-C4B	2.21	1.49	1.42
27	a	610	PL9	C46-C44	2.21	1.55	1.51
24	A	608	CLA	CMB-C2B	-2.21	1.46	1.50
24	C	512	CLA	CMB-C2B	-2.21	1.46	1.50
24	B	614	CLA	MG-NC	2.21	2.11	2.06
30	f	102	SQD	O9-S	2.21	1.51	1.45
24	D	403	CLA	C1D-ND	2.21	1.40	1.37
24	B	614	CLA	CMB-C2B	-2.20	1.46	1.50
24	A	605	CLA	C3B-C4B	2.20	1.49	1.42
24	B	602	CLA	CMB-C2B	-2.20	1.46	1.50
24	b	612	CLA	C3B-C4B	2.20	1.49	1.42
24	C	506	CLA	C3B-C4B	2.20	1.49	1.42
34	f	101	HEM	C2A-C3A	-2.20	1.33	1.38
24	A	612	CLA	CMD-C2D	-2.20	1.46	1.50
24	d	404	CLA	CMC-C2C	-2.20	1.46	1.50
24	c	509	CLA	C4B-NB	2.20	1.40	1.37
24	b	616	CLA	CHC-C1C	2.20	1.42	1.38
24	b	610	CLA	CMB-C2B	-2.19	1.46	1.50
24	D	404	CLA	CMB-C2B	-2.19	1.46	1.50
24	D	403	CLA	MG-NA	2.18	2.11	2.06
24	a	611	CLA	CMB-C2B	-2.18	1.46	1.50
24	b	608	CLA	CMB-C2B	-2.18	1.46	1.50
24	c	504	CLA	MG-NC	2.18	2.11	2.06
24	b	608	CLA	C4B-NB	2.18	1.40	1.37
24	c	506	CLA	C3B-C4B	2.18	1.49	1.42
24	C	505	CLA	CMC-C2C	-2.18	1.46	1.50
34	f	101	HEM	CMA-C3A	2.18	1.55	1.50
24	B	611	CLA	MG-NC	-2.18	2.01	2.06
24	D	404	CLA	CMD-C2D	-2.17	1.46	1.50
24	C	511	CLA	CHC-C1C	2.17	1.42	1.38
24	b	613	CLA	CMC-C2C	-2.17	1.46	1.50
24	b	613	CLA	CMB-C2B	-2.16	1.46	1.50
24	c	505	CLA	CMB-C2B	-2.16	1.46	1.50
25	d	402	PHO	C3B-C2B	-2.16	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C3B-C4B	2.16	1.49	1.42
24	c	509	CLA	CMD-C2D	-2.16	1.46	1.50
24	B	612	CLA	C3D-C4D	2.16	1.49	1.44
24	c	511	CLA	C3B-C4B	2.15	1.49	1.42
24	B	608	CLA	C3D-C4D	2.15	1.49	1.44
24	b	607	CLA	C3B-C4B	2.15	1.49	1.42
24	C	510	CLA	CMD-C2D	-2.15	1.46	1.50
27	d	406	PL9	C41-C39	-2.15	1.46	1.51
24	c	507	CLA	CMB-C2B	-2.15	1.46	1.50
24	B	601	CLA	CMB-C2B	-2.14	1.46	1.50
25	d	402	PHO	CAC-C3C	-2.14	1.48	1.51
24	c	504	CLA	C3B-C4B	2.14	1.49	1.42
24	C	506	CLA	CMC-C2C	-2.14	1.46	1.50
24	B	602	CLA	C3B-C4B	2.14	1.49	1.42
27	D	406	PL9	C11-C9	-2.14	1.46	1.51
31	C	522	DGD	O3G-C3G	-2.14	1.40	1.43
24	C	505	CLA	CHC-C1C	2.13	1.42	1.38
25	d	402	PHO	CMB-C2B	-2.13	1.47	1.51
24	C	503	CLA	CMD-C2D	-2.13	1.46	1.50
24	C	511	CLA	CMB-C2B	-2.13	1.46	1.50
30	D	412	SQD	O6-C1	-2.12	1.36	1.40
24	d	404	CLA	C3B-C4B	2.12	1.48	1.42
24	B	606	CLA	C3B-C4B	2.12	1.48	1.42
24	b	610	CLA	MG-NC	2.12	2.11	2.06
27	a	610	PL9	C46-C47	2.12	1.60	1.53
30	B	622	SQD	O9-S	2.12	1.51	1.45
30	A	614	SQD	C46-C45	2.11	1.57	1.50
34	f	101	HEM	CMC-C2C	2.11	1.55	1.50
24	C	510	CLA	MG-NA	2.11	2.11	2.06
24	A	608	CLA	CMD-C2D	-2.11	1.46	1.50
24	c	509	CLA	C1B-NB	-2.11	1.35	1.37
24	B	611	CLA	CMD-C2D	-2.11	1.46	1.50
24	C	513	CLA	CMB-C2B	-2.10	1.46	1.50
24	b	616	CLA	MG-ND	2.10	2.10	2.05
24	C	513	CLA	CHC-C4B	-2.10	1.34	1.39
24	c	512	CLA	CMB-C2B	-2.10	1.46	1.50
24	B	606	CLA	CHC-C1C	2.10	1.42	1.38
30	B	622	SQD	O7-S	2.10	1.51	1.45
30	D	412	SQD	O9-S	2.10	1.51	1.45
24	c	513	CLA	CHC-C1C	2.10	1.42	1.38
30	a	612	SQD	O9-S	2.10	1.51	1.45
25	A	607	PHO	CMB-C2B	-2.09	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	CHC-C1C	2.09	1.42	1.38
24	b	615	CLA	CMB-C2B	-2.09	1.46	1.50
24	b	613	CLA	CMD-C2D	-2.09	1.46	1.50
24	B	616	CLA	MG-NB	-2.09	2.01	2.05
24	B	601	CLA	CHC-C1C	2.09	1.42	1.38
24	c	510	CLA	C3B-C4B	2.09	1.48	1.42
24	B	603	CLA	CMB-C2B	-2.09	1.46	1.50
24	C	504	CLA	CMB-C2B	-2.09	1.46	1.50
24	B	603	CLA	C3D-C4D	2.09	1.48	1.44
24	B	607	CLA	CHC-C1C	2.08	1.42	1.38
24	B	604	CLA	MG-NB	2.08	2.09	2.05
25	d	402	PHO	O2D-CGD	2.08	1.38	1.33
34	F	101	HEM	C2A-C3A	-2.07	1.33	1.38
30	b	620	SQD	O5-C5	2.07	1.49	1.44
24	b	614	CLA	MG-NB	-2.07	2.01	2.05
24	c	510	CLA	CMB-C2B	-2.07	1.46	1.50
24	c	510	CLA	CMC-C2C	-2.07	1.46	1.50
24	c	512	CLA	CMC-C2C	-2.07	1.46	1.50
24	B	611	CLA	C3B-C4B	2.06	1.48	1.42
30	B	622	SQD	C44-C45	2.06	1.57	1.50
24	C	509	CLA	CMB-C2B	-2.06	1.46	1.50
30	B	622	SQD	C46-C45	2.06	1.57	1.50
34	F	101	HEM	CMD-C2D	2.06	1.55	1.50
24	b	608	CLA	CMC-C2C	-2.06	1.46	1.50
24	D	404	CLA	CMC-C2C	-2.05	1.46	1.50
24	C	506	CLA	O2D-CGD	2.05	1.38	1.33
24	a	606	CLA	MG-NA	2.05	2.11	2.06
24	B	616	CLA	C3B-C4B	2.05	1.48	1.42
24	b	602	CLA	CHC-C1C	2.05	1.42	1.38
30	a	612	SQD	O7-S	2.05	1.50	1.45
25	d	402	PHO	C4C-NC	2.05	1.44	1.37
24	B	604	CLA	C4B-NB	2.05	1.40	1.37
24	c	504	CLA	CMB-C2B	-2.05	1.46	1.50
24	c	503	CLA	CMC-C2C	-2.05	1.46	1.50
24	A	606	CLA	C3B-C4B	2.04	1.48	1.42
34	f	101	HEM	FE-NB	2.04	2.01	1.94
24	C	510	CLA	MG-NC	2.04	2.11	2.06
24	c	503	CLA	CMB-C2B	-2.04	1.46	1.50
24	C	508	CLA	C1D-C2D	2.04	1.49	1.45
24	b	614	CLA	CMB-C2B	-2.04	1.46	1.50
24	a	606	CLA	CMB-C2B	-2.04	1.46	1.50
24	c	506	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	MG-ND	-2.03	2.01	2.05
24	A	612	CLA	CMB-C2B	-2.03	1.46	1.50
24	c	508	CLA	CMD-C2D	-2.03	1.46	1.50
24	B	610	CLA	MG-ND	-2.03	2.01	2.05
30	b	620	SQD	C25-C24	2.03	1.59	1.52
24	C	502	CLA	CMC-C2C	-2.03	1.46	1.50
24	c	506	CLA	C1B-NB	-2.03	1.35	1.37
24	c	501	CLA	C3B-C4B	2.02	1.48	1.42
24	c	506	CLA	CMD-C2D	-2.02	1.46	1.50
30	f	102	SQD	C44-C45	2.02	1.57	1.50
30	b	620	SQD	C44-C45	2.02	1.57	1.50
24	b	609	CLA	CMB-C2B	-2.02	1.46	1.50
24	C	503	CLA	O2D-CED	-2.02	1.40	1.45
30	D	409	SQD	O9-S	2.02	1.50	1.45
24	b	604	CLA	CHC-C1C	2.02	1.42	1.38
24	B	604	CLA	C1D-C2D	2.02	1.49	1.45
24	c	507	CLA	C4B-NB	2.02	1.40	1.37
24	C	506	CLA	C3D-C4D	2.02	1.48	1.44
31	c	521	DGD	O3G-C3G	-2.02	1.40	1.43
25	a	607	PHO	CMD-C2D	-2.01	1.47	1.51
24	A	608	CLA	CMC-C2C	-2.01	1.46	1.50
24	b	605	CLA	MG-NA	2.01	2.11	2.06
24	b	605	CLA	C1D-ND	2.01	1.40	1.37
24	b	603	CLA	CMD-C2D	-2.01	1.46	1.50
27	d	406	PL9	C52-C5	-2.01	1.46	1.50
24	b	605	CLA	CHC-C4B	-2.01	1.34	1.39
24	b	614	CLA	O2D-CED	-2.01	1.40	1.45
30	a	612	SQD	O6-C1	-2.01	1.36	1.40
24	A	605	CLA	MG-ND	-2.01	2.01	2.05
24	c	506	CLA	CMC-C2C	-2.01	1.46	1.50
24	B	607	CLA	CMD-C2D	-2.00	1.46	1.50
24	a	608	CLA	C3B-C4B	2.00	1.48	1.42
25	d	402	PHO	C3D-CAD	-2.00	1.44	1.47

All (894) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O6-C1-C2	8.66	121.42	108.27
24	B	601	CLA	C4A-NA-C1A	8.42	110.52	106.68
24	C	510	CLA	C4A-NA-C1A	8.40	110.51	106.68
24	B	604	CLA	C4A-NA-C1A	8.23	110.44	106.68
24	a	605	CLA	C4A-NA-C1A	8.21	110.42	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	612	SQD	O6-C1-C2	8.13	120.62	108.27
24	c	511	CLA	C4A-NA-C1A	8.08	110.37	106.68
24	B	615	CLA	C4A-NA-C1A	7.87	110.27	106.68
24	C	511	CLA	C4A-NA-C1A	7.80	110.24	106.68
30	b	620	SQD	O6-C1-C2	7.74	120.03	108.27
24	b	606	CLA	C4A-NA-C1A	7.66	110.17	106.68
24	b	601	CLA	C4A-NA-C1A	7.54	110.12	106.68
24	C	507	CLA	C4A-NA-C1A	7.41	110.06	106.68
24	d	403	CLA	C4A-NA-C1A	7.28	110.00	106.68
24	C	501	CLA	C4A-NA-C1A	7.22	109.97	106.68
24	c	509	CLA	C4A-NA-C1A	7.20	109.96	106.68
24	c	503	CLA	C4A-NA-C1A	7.15	109.94	106.68
24	B	606	CLA	C4A-NA-C1A	7.11	109.92	106.68
24	B	607	CLA	C4A-NA-C1A	7.03	109.89	106.68
24	C	503	CLA	C4A-NA-C1A	6.99	109.87	106.68
24	c	502	CLA	C4A-NA-C1A	6.84	109.80	106.68
30	a	612	SQD	C1-O5-C5	-6.81	100.42	113.72
24	B	613	CLA	C4A-NA-C1A	6.67	109.72	106.68
24	B	616	CLA	C4A-NA-C1A	6.57	109.67	106.68
24	B	612	CLA	C4A-NA-C1A	6.47	109.63	106.68
24	C	508	CLA	C4A-NA-C1A	6.45	109.62	106.68
24	b	615	CLA	C4A-NA-C1A	6.45	109.62	106.68
30	D	412	SQD	C1-O5-C5	-6.42	101.18	113.72
24	c	507	CLA	C4A-NA-C1A	6.37	109.59	106.68
30	D	412	SQD	O6-C1-C2	6.37	117.94	108.27
24	b	614	CLA	C4A-NA-C1A	6.34	109.57	106.68
25	d	402	PHO	C4D-CHA-CBD	-6.33	105.42	108.45
24	c	508	CLA	C4A-NA-C1A	6.23	109.52	106.68
32	a	614	LMG	O1-C1-C2	6.22	117.71	108.27
30	B	622	SQD	C1-O5-C5	-6.21	101.60	113.72
24	C	505	CLA	C4A-NA-C1A	6.16	109.49	106.68
24	B	608	CLA	C4A-NA-C1A	6.16	109.49	106.68
27	a	610	PL9	C7-C3-C4	6.14	121.97	116.91
24	C	512	CLA	C4A-NA-C1A	6.11	109.47	106.68
24	C	502	CLA	C4A-NA-C1A	6.11	109.47	106.68
24	B	610	CLA	C4A-NA-C1A	6.04	109.43	106.68
25	A	607	PHO	C4D-CHA-CBD	-6.04	105.56	108.45
24	C	513	CLA	C4A-NA-C1A	5.97	109.40	106.68
27	A	610	PL9	C7-C3-C4	5.92	121.79	116.91
24	a	606	CLA	C4A-NA-C1A	5.91	109.37	106.68
24	b	613	CLA	C4A-NA-C1A	5.89	109.36	106.68
24	c	513	CLA	C4A-NA-C1A	5.85	109.35	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	622	SQD	O6-C1-C2	5.78	117.05	108.27
24	C	509	CLA	C4A-NA-C1A	5.67	109.27	106.68
24	b	603	CLA	C4A-NA-C1A	5.64	109.25	106.68
24	B	609	CLA	C4A-NA-C1A	5.53	109.20	106.68
24	b	616	CLA	C4A-NA-C1A	5.52	109.20	106.68
24	c	501	CLA	C4A-NA-C1A	5.51	109.19	106.68
24	b	605	CLA	C4A-NA-C1A	5.40	109.14	106.68
27	d	406	PL9	C7-C3-C4	5.38	121.34	116.91
24	B	603	CLA	C4A-NA-C1A	5.38	109.13	106.68
24	c	505	CLA	C4A-NA-C1A	5.36	109.13	106.68
24	c	504	CLA	C4A-NA-C1A	5.34	109.12	106.68
24	b	607	CLA	C4A-NA-C1A	5.34	109.11	106.68
30	f	102	SQD	O6-C1-C2	5.33	116.38	108.27
24	A	608	CLA	C4A-NA-C1A	5.27	109.08	106.68
24	c	510	CLA	C4A-NA-C1A	5.23	109.06	106.68
24	D	404	CLA	C4A-NA-C1A	5.21	109.06	106.68
24	b	602	CLA	C4A-NA-C1A	5.02	108.97	106.68
30	D	409	SQD	O5-C1-C2	-4.96	100.19	110.37
30	f	102	SQD	O9-S-O7	-4.92	97.84	113.82
25	a	607	PHO	C4D-CHA-CBD	-4.90	106.10	108.45
24	C	501	CLA	O2D-CGD-O1D	-4.84	114.43	123.85
35	v	201	HEC	C1D-ND-C4D	4.80	110.89	105.21
24	B	602	CLA	C4A-NA-C1A	4.79	108.86	106.68
24	B	610	CLA	O2D-CGD-O1D	-4.79	114.53	123.85
30	f	102	SQD	C1-O5-C5	-4.76	104.42	113.72
25	D	402	PHO	C4D-CHA-CBD	-4.75	106.18	108.45
24	A	606	CLA	O2D-CGD-CBD	4.75	119.54	111.23
24	A	606	CLA	O2D-CGD-O1D	-4.72	114.65	123.85
25	D	402	PHO	CBC-CAC-C3C	4.71	119.61	112.87
30	A	614	SQD	O7-S-C6	4.68	113.74	106.76
24	b	609	CLA	C4A-NA-C1A	4.67	108.81	106.68
35	V	201	HEC	C1D-ND-C4D	4.62	110.67	105.21
32	C	517	LMG	C4-C3-C2	4.60	118.91	110.83
24	C	512	CLA	C3B-C4B-NB	-4.60	106.43	110.53
24	c	512	CLA	C4A-NA-C1A	4.58	108.77	106.68
30	B	622	SQD	O47-C7-C8	4.57	121.38	111.48
24	b	603	CLA	O2D-CGD-O1D	-4.56	114.97	123.85
31	A	615	DGD	O5D-C1E-C2E	4.53	115.14	108.27
27	a	610	PL9	C7-C3-C2	-4.49	118.10	123.39
24	b	616	CLA	O2D-CGD-O1D	-4.47	115.14	123.85
24	b	604	CLA	C4A-NA-C1A	4.45	108.71	106.68
27	D	406	PL9	C7-C3-C4	4.45	120.57	116.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	412	SQD	O7-S-C6	4.44	113.38	106.76
24	c	506	CLA	C4A-NA-C1A	4.41	108.69	106.68
32	C	517	LMG	O6-C5-C4	4.39	117.61	109.70
32	D	407	LMG	O6-C1-C2	-4.39	101.36	110.37
24	b	604	CLA	C1-C2-C3	-4.38	119.02	126.20
30	B	622	SQD	O48-C23-C24	4.38	125.20	111.83
24	a	611	CLA	C4A-NA-C1A	4.38	108.68	106.68
30	D	412	SQD	C1-C2-C3	-4.34	100.87	110.01
25	D	402	PHO	O2D-CGD-O1D	-4.34	115.40	123.85
24	B	611	CLA	C4A-NA-C1A	4.32	108.65	106.68
31	A	615	DGD	C3G-O3G-C1D	4.31	123.04	113.80
24	B	614	CLA	C4A-NA-C1A	4.31	108.64	106.68
24	C	513	CLA	O2D-CGD-O1D	-4.24	115.59	123.85
27	d	406	PL9	C40-C39-C41	4.23	122.58	115.23
24	b	615	CLA	C3B-C4B-NB	-4.23	106.75	110.53
24	c	509	CLA	CHB-C4A-NA	4.23	130.50	124.40
30	A	614	SQD	O47-C7-C8	4.20	120.57	111.48
24	B	604	CLA	C3B-C4B-NB	-4.19	106.79	110.53
24	A	606	CLA	C4A-NA-C1A	4.17	108.58	106.68
30	f	102	SQD	O9-S-C6	4.17	112.97	106.76
25	D	402	PHO	O1D-CGD-CBD	4.16	131.03	124.72
30	a	612	SQD	C1-C2-C3	-4.15	101.27	110.01
24	b	603	CLA	O2D-CGD-CBD	4.14	118.47	111.23
25	d	402	PHO	CBC-CAC-C3C	4.11	118.76	112.87
24	A	612	CLA	C3B-C4B-NB	-4.11	106.86	110.53
30	a	613	SQD	O7-S-C6	4.11	112.89	106.76
24	c	509	CLA	O2A-CGA-O1A	-4.04	113.53	123.63
24	b	602	CLA	O2D-CGD-CBD	4.03	118.28	111.23
30	D	412	SQD	O47-C7-C8	4.02	120.18	111.48
30	f	102	SQD	O7-S-C6	4.01	112.75	106.76
24	b	602	CLA	O2D-CGD-O1D	-4.01	116.05	123.85
34	f	101	HEM	CBD-CAD-C3D	-4.00	101.48	112.53
24	B	608	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
24	b	608	CLA	CHB-C4A-NA	3.99	130.16	124.40
24	A	612	CLA	C4A-NA-C1A	3.99	108.50	106.68
24	C	507	CLA	O2D-CGD-O1D	-3.98	116.09	123.85
25	a	607	PHO	C2B-C1B-NB	-3.97	106.56	109.43
24	b	612	CLA	C3B-C4B-NB	-3.94	107.01	110.53
27	D	406	PL9	C37-C38-C39	-3.94	118.62	127.62
25	A	607	PHO	CMA-C3A-C4A	-3.93	106.14	114.61
24	C	501	CLA	C3B-C4B-NB	-3.92	107.03	110.53
24	b	606	CLA	O2D-CGD-O1D	-3.91	116.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	605	CLA	C3B-C4B-NB	-3.88	107.06	110.53
24	C	504	CLA	C4A-NA-C1A	3.88	108.45	106.68
24	c	505	CLA	C3B-C4B-NB	-3.87	107.07	110.53
24	B	606	CLA	O2D-CGD-O1D	-3.87	116.31	123.85
26	b	619	BCR	C38-C26-C25	-3.87	120.26	124.48
32	D	407	LMG	O1-C1-C2	3.87	114.14	108.27
24	c	501	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
32	a	614	LMG	C1-C2-C3	-3.86	101.90	110.01
27	d	406	PL9	C37-C38-C39	-3.86	118.80	127.62
30	f	102	SQD	O5-C1-C2	-3.86	102.45	110.37
30	a	612	SQD	C3-C4-C5	3.85	117.22	110.23
32	C	517	LMG	C7-O1-C1	3.85	122.05	113.80
24	b	611	CLA	C4A-NA-C1A	3.83	108.43	106.68
25	a	607	PHO	CMA-C3A-C4A	-3.83	106.36	114.61
24	C	505	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
24	b	610	CLA	C4A-NA-C1A	3.83	108.42	106.68
24	B	602	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
24	a	608	CLA	C4A-NA-C1A	3.82	108.42	106.68
24	b	611	CLA	C3B-C4B-NB	-3.82	107.12	110.53
24	B	603	CLA	C3B-C4B-NB	-3.80	107.14	110.53
30	A	614	SQD	O5-C5-C4	3.79	116.52	109.70
24	C	506	CLA	C3B-C4B-NB	-3.77	107.17	110.53
25	d	402	PHO	CMA-C3A-C4A	-3.77	106.49	114.61
25	A	607	PHO	CMB-C2B-C3B	3.74	132.15	124.68
24	B	614	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
24	C	504	CLA	C3B-C4B-NB	-3.72	107.21	110.53
30	b	620	SQD	O5-C1-C2	-3.71	102.74	110.37
24	B	613	CLA	C1-C2-C3	-3.71	120.13	126.20
30	b	620	SQD	O9-S-C6	3.70	112.28	106.76
24	c	508	CLA	C3B-C4B-NB	-3.70	107.23	110.53
32	b	622	LMG	C1-O6-C5	-3.69	106.52	113.72
26	b	618	BCR	C2-C1-C6	3.68	115.79	110.44
24	A	605	CLA	C4A-NA-C1A	3.68	108.36	106.68
30	D	412	SQD	O9-S-O7	-3.68	101.86	113.82
32	D	407	LMG	O6-C5-C4	3.65	116.28	109.70
27	d	406	PL9	C7-C3-C2	-3.65	119.09	123.39
24	b	604	CLA	C3B-C4B-NB	-3.64	107.28	110.53
24	C	506	CLA	C4A-NA-C1A	3.64	108.34	106.68
30	b	620	SQD	O9-S-O7	-3.62	102.04	113.82
24	d	404	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
32	M	101	LMG	O1-C7-C8	-3.57	102.13	110.82
24	C	510	CLA	C3B-C4B-NB	-3.57	107.34	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O9-S-C6	3.56	112.07	106.76
25	a	607	PHO	C1-C2-C3	-3.55	120.38	126.20
24	B	614	CLA	C3B-C4B-NB	-3.55	107.36	110.53
30	b	620	SQD	O7-S-C6	3.54	112.05	106.76
24	a	611	CLA	C3B-C4B-NB	-3.54	107.37	110.53
24	a	605	CLA	O1D-CGD-CBD	3.54	131.51	124.52
24	C	502	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
24	b	601	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
30	A	614	SQD	O9-S-O7	-3.53	102.33	113.82
30	b	620	SQD	C1-C2-C3	-3.52	102.60	110.01
25	d	402	PHO	C2B-C1B-NB	-3.52	106.89	109.43
30	D	412	SQD	O5-C1-C2	-3.52	103.14	110.37
24	B	605	CLA	O1D-CGD-CBD	3.51	131.45	124.52
24	C	508	CLA	C3B-C4B-NB	-3.50	107.40	110.53
24	C	512	CLA	CHB-C4A-NA	3.50	129.45	124.40
27	A	610	PL9	C7-C3-C2	-3.49	119.27	123.39
24	b	611	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
24	b	607	CLA	C3B-C4B-NB	-3.48	107.42	110.53
26	t	101	BCR	C31-C1-C6	3.48	115.71	110.24
24	b	605	CLA	C1-C2-C3	-3.48	120.49	126.20
24	B	601	CLA	C3B-C4B-NB	-3.46	107.44	110.53
34	F	101	HEM	CBD-CAD-C3D	-3.45	103.00	112.53
27	d	406	PL9	C42-C43-C44	-3.42	119.80	127.62
24	b	614	CLA	C3B-C4B-NB	-3.42	107.48	110.53
24	c	512	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
24	A	605	CLA	CHB-C4A-NA	3.41	129.33	124.40
24	c	511	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
30	b	620	SQD	C3-C4-C5	3.38	116.37	110.23
24	C	513	CLA	O2D-CGD-CBD	3.38	117.14	111.23
30	B	622	SQD	C3-C4-C5	3.37	116.34	110.23
24	B	605	CLA	C3B-C4B-NB	-3.37	107.52	110.53
29	D	413	LHG	C6-C5-C4	3.36	119.63	111.78
24	B	604	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
32	b	622	LMG	C3-C4-C5	-3.36	104.14	110.23
27	D	406	PL9	C27-C28-C29	-3.35	119.96	127.62
24	C	503	CLA	C7-C6-C5	-3.35	104.34	113.26
32	b	622	LMG	C8-O7-C10	3.34	125.78	117.80
24	b	612	CLA	C4A-NA-C1A	3.33	108.20	106.68
24	D	403	CLA	C3B-C4B-NB	-3.31	107.57	110.53
24	C	501	CLA	O2D-CGD-CBD	3.31	117.02	111.23
24	a	608	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
30	b	620	SQD	O48-C23-O10	-3.31	115.35	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	O2D-CGD-CBD	3.31	117.01	111.23
24	B	612	CLA	C3B-C4B-NB	-3.30	107.58	110.53
30	b	620	SQD	O48-C23-C24	3.29	121.86	111.83
24	B	610	CLA	CHB-C4A-NA	3.27	129.11	124.40
30	a	613	SQD	C3-C4-C5	3.27	116.15	110.23
33	D	401	BCT	O2-C-O1	3.26	128.00	119.68
30	b	620	SQD	O2-C2-C1	3.24	117.80	110.08
25	a	607	PHO	OBD-CAD-CBD	-3.24	121.07	125.82
24	B	616	CLA	O2A-CGA-O1A	-3.23	115.54	123.63
32	D	407	LMG	C8-O7-C10	3.22	125.51	117.80
24	A	608	CLA	O2D-CGD-CBD	3.22	116.86	111.23
30	a	613	SQD	O9-S-O7	-3.22	103.35	113.82
24	B	616	CLA	C3B-C4B-NB	-3.22	107.66	110.53
30	a	613	SQD	O47-C7-C8	3.22	118.44	111.48
27	a	610	PL9	C37-C38-C39	-3.22	120.26	127.62
24	b	612	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
24	B	612	CLA	O2A-CGA-O1A	-3.21	115.60	123.63
24	B	616	CLA	CAC-C3C-C4C	3.20	128.95	124.79
24	b	602	CLA	CHB-C4A-NA	3.19	129.01	124.40
24	B	605	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
24	B	615	CLA	CHB-C4A-NA	3.18	128.99	124.40
24	b	604	CLA	C6-C7-C8	-3.18	105.40	115.97
30	f	102	SQD	O5-C5-C4	3.18	115.42	109.70
24	c	507	CLA	CHB-C4A-NA	3.17	128.98	124.40
24	C	511	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
24	b	609	CLA	O1D-CGD-CBD	3.17	130.77	124.52
24	c	504	CLA	CMB-C2B-C1B	-3.16	120.60	125.42
30	D	409	SQD	O8-S-C6	3.16	112.08	105.97
32	m	101	LMG	O1-C7-C8	-3.16	103.12	110.82
31	C	522	DGD	C3D-C4D-C5D	-3.16	104.50	110.23
27	d	406	PL9	C32-C33-C34	-3.16	120.39	127.62
24	B	601	CLA	C1-O2A-CGA	3.16	124.29	116.65
28	j	101	STE	O2-C1-C2	3.15	123.95	114.00
24	C	512	CLA	C6-C5-C3	-3.15	105.80	113.47
24	C	502	CLA	C3B-C4B-NB	-3.15	107.72	110.53
24	c	502	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
24	B	611	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
24	a	608	CLA	C4-C3-C5	3.14	120.67	115.23
32	C	517	LMG	C9-C8-C7	3.13	119.09	111.78
24	c	506	CLA	C3B-C4B-NB	-3.13	107.73	110.53
30	a	612	SQD	C44-O6-C1	-3.13	107.09	113.80
30	D	409	SQD	O48-C23-C24	3.13	121.37	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	CHB-C4A-NA	3.13	128.91	124.40
30	D	409	SQD	C1-O5-C5	-3.13	107.62	113.72
24	a	608	CLA	O2D-CGD-CBD	3.12	116.69	111.23
30	a	612	SQD	O9-S-C6	3.12	111.42	106.76
24	B	605	CLA	C4A-NA-C1A	3.12	108.10	106.68
30	B	622	SQD	O9-S-O7	-3.12	103.68	113.82
24	b	608	CLA	C3B-C4B-NB	-3.12	107.75	110.53
30	a	612	SQD	O47-C7-C8	3.11	118.22	111.48
24	C	513	CLA	O2A-CGA-O1A	-3.11	115.84	123.63
24	C	505	CLA	C3B-C4B-NB	-3.11	107.75	110.53
30	b	620	SQD	O47-C7-C8	3.10	118.19	111.48
24	c	505	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
24	B	604	CLA	CHB-C4A-NA	3.10	128.87	124.40
24	b	613	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
34	F	101	HEM	CHC-C4B-NB	3.09	127.74	124.42
24	c	510	CLA	C3B-C4B-NB	-3.08	107.78	110.53
25	A	607	PHO	C3B-C4B-NB	-3.08	105.46	107.46
24	c	512	CLA	C3B-C4B-NB	-3.07	107.79	110.53
31	C	522	DGD	C3G-O3G-C1D	3.06	120.36	113.80
24	d	403	CLA	CHB-C4A-NA	3.06	128.81	124.40
30	B	622	SQD	O7-S-C6	3.05	111.32	106.76
34	F	101	HEM	CBA-CAA-C2A	-3.05	104.09	112.53
24	c	510	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	b	616	CLA	C3B-C4B-NB	-3.05	107.81	110.53
24	b	603	CLA	C3B-C4B-NB	-3.04	107.82	110.53
30	a	612	SQD	O9-S-O7	-3.03	103.96	113.82
24	C	507	CLA	CHB-C4A-NA	3.03	128.78	124.40
24	a	606	CLA	C3B-C4B-NB	-3.03	107.82	110.53
24	B	608	CLA	C3B-C4B-NB	-3.03	107.83	110.53
27	D	406	PL9	C12-C13-C14	-3.02	120.71	127.62
24	b	616	CLA	O2D-CGD-CBD	3.02	116.51	111.23
24	B	610	CLA	C3B-C4B-NB	-3.02	107.84	110.53
24	c	512	CLA	CHB-C4A-NA	3.02	128.75	124.40
31	A	615	DGD	C4E-C3E-C2E	-3.01	105.54	110.83
35	V	201	HEC	CBD-CAD-C3D	-3.01	104.20	112.53
24	c	512	CLA	C1-C2-C3	-3.00	121.28	126.20
30	a	612	SQD	O8-S-C6	3.00	111.76	105.97
24	C	503	CLA	C3B-C4B-NB	-2.99	107.86	110.53
25	d	402	PHO	O1D-CGD-CBD	2.99	129.26	124.72
24	C	512	CLA	C1-C2-C3	-2.97	121.33	126.20
30	a	613	SQD	O8-S-C6	2.97	111.71	105.97
27	D	406	PL9	C22-C23-C24	-2.97	120.83	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	O2A-CGA-O1A	-2.97	116.21	123.63
24	D	403	CLA	CHB-C4A-NA	2.96	128.67	124.40
32	b	622	LMG	O2-C2-C1	-2.95	103.03	110.08
24	B	606	CLA	C3B-C4B-NB	-2.95	107.89	110.53
24	B	603	CLA	CHC-C4B-NB	2.95	128.47	124.05
24	C	501	CLA	CHB-C1B-NB	2.95	128.47	124.05
34	f	101	HEM	CBA-CAA-C2A	-2.94	104.39	112.53
31	H	102	DGD	C3G-O3G-C1D	2.93	120.09	113.80
32	C	517	LMG	O6-C1-C2	-2.93	104.35	110.37
31	h	102	DGD	O3E-C3E-C2E	-2.93	103.47	110.38
24	A	608	CLA	O2A-CGA-O1A	-2.92	116.32	123.63
24	b	613	CLA	CHB-C4A-NA	2.92	128.61	124.40
24	B	601	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	b	604	CLA	CHB-C4A-NA	2.89	128.57	124.40
24	c	513	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
24	b	601	CLA	C3B-C4B-NB	-2.89	107.95	110.53
30	a	612	SQD	O5-C1-C2	-2.88	104.45	110.37
24	B	609	CLA	C3B-C4B-NB	-2.88	107.96	110.53
32	C	517	LMG	O3-C3-C2	-2.88	103.59	110.38
24	d	404	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
24	B	614	CLA	CMB-C2B-C1B	-2.87	121.04	125.42
24	D	404	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
24	B	609	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
24	B	611	CLA	CHB-C4A-NA	2.87	128.54	124.40
24	B	610	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
24	c	508	CLA	CHB-C4A-NA	2.86	128.53	124.40
26	B	617	BCR	C29-C30-C25	2.85	114.58	110.44
24	c	503	CLA	C3B-C4B-NB	-2.85	107.99	110.53
25	D	402	PHO	CAA-C2A-C3A	-2.85	105.31	113.00
24	b	610	CLA	CHC-C4B-NB	2.84	128.31	124.05
32	m	101	LMG	O3-C3-C2	-2.84	103.69	110.38
24	A	606	CLA	CHB-C4A-NA	2.83	128.48	124.40
25	A	607	PHO	CMA-C3A-C2A	-2.83	103.21	114.13
24	C	501	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
24	b	608	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
25	D	402	PHO	CMA-C3A-C2A	-2.83	103.22	114.13
24	B	609	CLA	CHC-C4B-NB	2.82	128.29	124.05
24	B	611	CLA	O2D-CGD-CBD	2.82	116.17	111.23
24	c	511	CLA	C3B-C4B-NB	-2.82	108.01	110.53
27	a	610	PL9	C27-C28-C29	-2.82	121.17	127.62
31	A	615	DGD	O2E-C2E-C3E	2.82	117.02	110.38
24	B	610	CLA	O2D-CGD-CBD	2.81	116.15	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C2-C1-C6	2.81	114.53	110.44
27	D	406	PL9	C7-C8-C9	-2.81	121.99	126.83
24	b	610	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
30	f	102	SQD	O47-C7-C8	2.80	121.22	110.93
24	b	605	CLA	C4-C3-C5	2.80	120.08	115.23
24	c	509	CLA	O2A-CGA-CBA	2.80	120.36	111.83
24	c	507	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
24	b	602	CLA	C1-C2-C3	-2.78	121.64	126.20
24	B	603	CLA	O2D-CGD-CBD	2.78	116.09	111.23
24	c	501	CLA	O2D-CGD-CBD	2.78	116.09	111.23
32	a	614	LMG	C8-O7-C10	2.78	124.45	117.80
29	D	413	LHG	O7-C5-C4	-2.78	98.37	108.34
24	B	604	CLA	O2D-CGD-CBD	2.78	116.09	111.23
30	A	614	SQD	O48-C23-C24	2.78	120.30	111.83
24	B	604	CLA	C1-O2A-CGA	-2.78	109.93	116.65
24	b	610	CLA	C3B-C4B-NB	-2.77	108.05	110.53
24	a	606	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	B	612	CLA	O1D-CGD-CBD	2.77	129.99	124.52
24	c	511	CLA	O2D-CGD-CBD	2.77	116.08	111.23
24	a	606	CLA	O2D-CGD-CBD	2.77	116.08	111.23
24	c	501	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	b	609	CLA	C6-C5-C3	2.76	120.20	113.47
24	c	504	CLA	C3B-C4B-NB	-2.76	108.06	110.53
24	D	403	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
24	b	611	CLA	O2D-CGD-CBD	2.75	116.04	111.23
30	a	612	SQD	O48-C23-C24	2.75	120.22	111.83
24	b	616	CLA	CHB-C4A-NA	2.75	128.37	124.40
24	b	606	CLA	O2D-CGD-CBD	2.75	116.03	111.23
24	C	509	CLA	C1-C2-C3	-2.75	121.70	126.20
24	B	601	CLA	O2A-CGA-O1A	-2.74	116.76	123.63
24	B	614	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
24	B	614	CLA	C1-C2-C3	-2.74	121.70	126.20
24	b	609	CLA	CHB-C4A-NA	2.73	128.35	124.40
27	a	610	PL9	C22-C23-C24	-2.73	121.37	127.62
24	A	608	CLA	C4-C3-C5	2.73	119.97	115.23
24	B	616	CLA	CHC-C4B-NB	2.73	128.15	124.05
34	f	101	HEM	CHB-C1B-NB	2.73	127.74	124.37
24	B	612	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	B	602	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
24	B	606	CLA	O1D-CGD-CBD	2.72	129.88	124.52
24	b	615	CLA	CHB-C4A-NA	2.72	128.32	124.40
24	A	605	CLA	C3B-C4B-NB	-2.69	108.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	C11-C12-C13	-2.69	107.01	115.97
27	d	406	PL9	C27-C28-C29	-2.69	121.46	127.62
24	d	403	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
26	K	102	BCR	C39-C30-C25	-2.69	106.03	110.24
24	C	504	CLA	C4-C3-C5	2.68	119.88	115.23
32	b	622	LMG	O1-C1-C2	-2.68	104.20	108.27
24	b	610	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
24	a	608	CLA	O2A-CGA-O1A	-2.67	116.96	123.63
24	A	612	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
24	A	612	CLA	O2D-CGD-CBD	2.66	115.88	111.23
24	C	505	CLA	CAC-C3C-C4C	2.65	128.24	124.79
27	A	610	PL9	C40-C39-C41	2.65	119.83	115.23
24	b	607	CLA	CED-O2D-CGD	2.65	121.93	115.92
31	h	102	DGD	O6E-C5E-C4E	2.65	114.47	109.70
24	b	603	CLA	CHD-C1D-ND	-2.64	121.08	124.80
32	d	412	LMG	O3-C3-C4	2.64	116.60	110.38
24	b	614	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
27	D	406	PL9	C7-C3-C2	-2.64	120.28	123.39
30	b	620	SQD	O8-S-C6	2.64	111.06	105.97
24	c	510	CLA	CHB-C4A-NA	2.64	128.20	124.40
33	d	401	BCT	O2-C-O1	2.63	126.42	119.68
31	H	102	DGD	O3D-C3D-C4D	2.63	116.57	110.38
24	c	504	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
27	A	610	PL9	O2-C1-C2	-2.63	115.86	121.83
24	C	510	CLA	CHB-C4A-NA	2.62	128.19	124.40
24	A	608	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
24	b	611	CLA	O2A-CGA-O1A	-2.62	117.08	123.63
24	C	503	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
24	B	612	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
24	b	601	CLA	CHB-C4A-NA	2.61	128.17	124.40
32	D	407	LMG	C1-C2-C3	-2.61	104.52	110.01
24	B	609	CLA	O1D-CGD-CBD	2.61	129.67	124.52
26	a	609	BCR	C39-C30-C25	-2.60	106.16	110.24
24	B	608	CLA	C6-C7-C8	-2.60	107.31	115.97
24	C	511	CLA	O2D-CGD-CBD	2.60	115.78	111.23
30	A	614	SQD	C1-O5-C5	2.60	118.80	113.72
24	b	604	CLA	CMA-C3A-C4A	2.60	118.76	111.77
24	b	612	CLA	CHC-C4B-NB	2.60	127.95	124.05
24	B	614	CLA	CMB-C2B-C3B	2.60	132.65	126.55
24	B	608	CLA	CHB-C4A-NA	2.59	128.14	124.40
31	c	521	DGD	C3G-O3G-C1D	2.59	119.35	113.80
24	b	602	CLA	C3B-C4B-NB	-2.59	108.22	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	614	LMG	O2-C2-C1	2.59	116.24	110.08
24	b	603	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
31	c	519	DGD	C3D-C4D-C5D	-2.59	105.54	110.23
24	B	615	CLA	C3B-C4B-NB	-2.59	108.22	110.53
24	b	612	CLA	O2A-CGA-O1A	-2.58	117.16	123.63
24	C	505	CLA	O1D-CGD-CBD	2.58	129.62	124.52
24	A	606	CLA	CED-O2D-CGD	-2.58	110.06	115.92
32	C	517	LMG	C8-O7-C10	2.58	123.97	117.80
30	f	102	SQD	O48-C23-C24	2.58	119.70	111.83
31	H	102	DGD	C3D-C4D-C5D	-2.58	105.56	110.23
24	b	610	CLA	CAA-CBA-CGA	-2.58	105.89	113.21
24	B	603	CLA	O2A-CGA-O1A	-2.58	117.19	123.63
24	c	504	CLA	CHB-C4A-NA	2.57	128.11	124.40
30	B	622	SQD	O5-C1-C2	-2.57	105.09	110.37
24	B	613	CLA	CHA-C1A-NA	-2.57	120.58	126.39
26	k	101	BCR	C23-C22-C21	-2.56	114.97	119.01
26	t	101	BCR	C36-C18-C19	2.56	122.00	118.09
25	D	402	PHO	C2B-C1B-NB	-2.56	107.58	109.43
31	h	102	DGD	O3E-C3E-C4E	2.56	116.42	110.38
28	C	526	STE	C3-C2-C1	-2.56	107.83	114.51
24	C	512	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
24	b	609	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
24	B	602	CLA	C3B-C4B-NB	-2.55	108.26	110.53
34	f	101	HEM	C3B-C2B-C1B	2.55	108.32	106.41
24	c	508	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
35	V	201	HEC	C1D-C2D-C3D	-2.54	104.31	106.98
24	B	608	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
24	d	404	CLA	CHB-C4A-NA	2.53	128.06	124.40
25	d	402	PHO	O2D-CGD-O1D	-2.53	118.92	123.85
24	a	606	CLA	CHD-C1D-ND	-2.53	121.24	124.80
24	b	611	CLA	CHD-C1D-ND	-2.53	121.24	124.80
30	f	102	SQD	C1-C2-C3	-2.53	104.69	110.01
24	C	502	CLA	C4D-CHA-C1A	2.53	124.26	121.24
24	c	510	CLA	O1D-CGD-CBD	2.53	129.50	124.52
25	d	402	PHO	C1-C2-C3	-2.52	122.06	126.20
24	c	504	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
24	B	611	CLA	C3B-C4B-NB	-2.52	108.28	110.53
26	c	515	BCR	C3-C4-C5	2.52	118.55	114.06
24	a	611	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	B	622	SQD	O48-C23-O10	-2.52	117.32	123.63
24	c	503	CLA	C7-C6-C5	-2.52	106.56	113.26
24	C	507	CLA	CHD-C1D-ND	-2.52	121.26	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	610	PL9	O2-C1-C6	2.51	124.48	120.48
24	b	608	CLA	O2D-CGD-CBD	2.51	115.62	111.23
35	v	201	HEC	CBA-CAA-C2A	-2.51	105.59	112.53
32	C	517	LMG	O4-C4-C5	2.51	115.50	109.32
24	B	615	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
24	B	602	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	D	402	PHO	C3B-C4B-NB	-2.50	105.83	107.46
24	C	507	CLA	C3B-C4B-NB	-2.50	108.30	110.53
26	k	102	BCR	C7-C8-C9	-2.50	122.54	126.23
24	B	607	CLA	CHB-C4A-NA	2.50	128.00	124.40
32	a	614	LMG	O7-C8-C9	2.50	117.30	108.34
24	b	614	CLA	C4-C3-C5	2.49	119.56	115.23
24	c	504	CLA	C4-C3-C5	2.49	119.56	115.23
32	B	620	LMG	C8-O7-C10	2.49	123.75	117.80
30	b	620	SQD	O5-C5-C4	2.48	114.17	109.70
24	c	507	CLA	C3B-C4B-NB	-2.48	108.32	110.53
30	B	622	SQD	C44-O6-C1	-2.48	108.49	113.80
25	d	402	PHO	CMA-C3A-C2A	-2.48	104.57	114.13
30	a	613	SQD	O6-C1-C2	2.48	112.03	108.27
24	c	506	CLA	CHB-C4A-NA	2.47	127.97	124.40
26	K	101	BCR	C1-C6-C5	-2.47	119.26	122.64
26	T	101	BCR	C38-C26-C27	-2.47	108.33	113.60
24	B	614	CLA	O1D-CGD-CBD	2.47	129.39	124.52
24	c	502	CLA	C3B-C4B-NB	-2.47	108.33	110.53
24	a	611	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
26	B	619	BCR	C29-C30-C25	2.46	114.02	110.44
30	D	412	SQD	O47-C7-O49	-2.46	117.95	123.70
31	c	519	DGD	C6D-O5D-C1E	2.46	119.08	113.80
24	b	609	CLA	C7-C6-C5	-2.46	106.70	113.26
24	C	505	CLA	C11-C10-C8	-2.46	107.79	115.97
24	a	608	CLA	CHB-C4A-NA	2.46	127.95	124.40
27	a	610	PL9	O2-C1-C6	2.45	124.38	120.48
24	C	508	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
24	c	508	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
24	B	603	CLA	CHD-C1D-ND	-2.45	121.36	124.80
24	B	606	CLA	CHB-C1B-NB	2.45	127.72	124.05
26	c	515	BCR	C2-C1-C6	2.44	113.99	110.44
35	V	201	HEC	CMD-C2D-C1D	2.44	128.85	125.03
35	V	201	HEC	CHB-C4A-NA	2.44	127.11	124.45
27	D	406	PL9	C32-C33-C34	-2.44	122.04	127.62
32	b	622	LMG	O6-C5-C6	2.44	112.48	106.44
26	K	102	BCR	C29-C30-C25	2.44	113.98	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	404	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	B	605	CLA	CHD-C1D-ND	-2.44	121.37	124.80
24	B	607	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
24	c	510	CLA	C1-C2-C3	-2.43	122.21	126.20
24	B	610	CLA	O1D-CGD-CBD	2.43	129.32	124.52
25	a	607	PHO	OBD-CAD-C3D	2.43	131.69	127.89
24	B	603	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	B	603	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
24	B	603	CLA	C4-C3-C5	2.43	119.44	115.23
30	B	622	SQD	O8-S-C6	2.43	110.66	105.97
26	B	618	BCR	C2-C1-C6	2.42	113.96	110.44
24	c	513	CLA	CHB-C4A-NA	2.42	127.90	124.40
31	C	522	DGD	O2E-C2E-C3E	2.42	116.09	110.38
27	a	610	PL9	O2-C1-C2	-2.42	116.32	121.83
31	c	520	DGD	C3D-C4D-C5D	-2.42	105.84	110.23
24	d	403	CLA	C4-C3-C5	2.41	119.41	115.23
24	B	610	CLA	C1-C2-C3	-2.41	122.25	126.20
27	d	406	PL9	C7-C8-C9	-2.41	122.68	126.83
24	b	614	CLA	C1-C2-C3	-2.41	122.25	126.20
24	B	613	CLA	C2A-C1A-CHA	2.41	128.04	123.87
24	C	513	CLA	CHB-C4A-NA	2.40	127.87	124.40
32	C	517	LMG	C9-O8-C28	2.40	125.90	117.12
27	a	610	PL9	O1-C4-C3	-2.40	118.20	120.73
24	b	609	CLA	C3B-C4B-NB	-2.40	108.39	110.53
24	C	503	CLA	C14-C13-C15	-2.39	102.74	111.27
26	B	618	BCR	C8-C9-C10	-2.39	115.25	119.01
26	H	101	BCR	C16-C17-C18	-2.39	123.93	127.28
24	c	504	CLA	CMB-C2B-C3B	2.39	132.17	126.55
24	a	611	CLA	O2D-CGD-CBD	2.39	115.40	111.23
32	m	101	LMG	O1-C1-C2	-2.38	104.65	108.27
26	K	102	BCR	C27-C26-C25	-2.38	119.49	122.70
24	B	607	CLA	C4-C3-C5	2.38	119.36	115.23
24	d	404	CLA	C1-C2-C3	-2.38	122.31	126.20
28	B	624	STE	O2-C1-C2	2.37	121.50	114.00
28	b	623	STE	O2-C1-C2	2.37	121.49	114.00
24	B	605	CLA	CED-O2D-CGD	2.37	121.29	115.92
24	a	605	CLA	CMB-C2B-C3B	2.37	132.12	126.55
27	d	406	PL9	C22-C23-C24	-2.37	122.20	127.62
35	v	201	HEC	CHD-C1D-ND	2.37	127.29	124.37
24	c	503	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	b	605	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	c	506	CLA	C1-O2A-CGA	2.36	122.37	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	O1D-CGD-CBD	2.36	129.18	124.52
24	b	604	CLA	C4-C3-C5	2.36	119.33	115.23
25	D	402	PHO	O2D-CGD-CBD	2.36	113.54	110.95
24	B	616	CLA	C1-C2-C3	-2.36	122.33	126.20
25	a	607	PHO	C3B-C4B-NB	-2.36	105.93	107.46
24	a	605	CLA	CHB-C4A-NA	2.36	127.81	124.40
26	b	618	BCR	C4-C5-C6	-2.36	119.52	122.70
24	a	606	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
29	A	613	LHG	C6-C5-C4	2.35	117.27	111.78
31	C	522	DGD	O1G-C1G-C2G	-2.35	101.62	108.40
32	a	615	LMG	O6-C1-O1	-2.35	104.49	110.04
28	t	102	STE	O2-C1-C2	2.35	121.42	114.00
27	A	610	PL9	C30-C29-C28	-2.35	117.60	123.63
29	L	101	LHG	O7-C5-C4	-2.34	99.93	108.34
30	B	622	SQD	C25-C24-C23	-2.34	105.11	113.69
28	I	101	STE	O2-C1-C2	2.34	121.39	114.00
24	c	504	CLA	O2D-CGD-CBD	2.34	115.32	111.23
24	C	504	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
24	B	605	CLA	C4-C3-C5	2.34	119.29	115.23
30	b	620	SQD	C1-O5-C5	-2.34	109.16	113.72
24	c	506	CLA	O1D-CGD-CBD	2.34	129.13	124.52
26	b	617	BCR	C19-C18-C17	-2.34	115.33	119.01
28	C	526	STE	O2-C1-C2	2.34	121.38	114.00
34	F	101	HEM	CHD-C4C-C3C	2.34	129.15	125.21
31	h	102	DGD	O5D-C1E-C2E	2.33	111.82	108.27
26	d	405	BCR	C33-C5-C6	-2.33	121.94	124.48
24	C	507	CLA	O2D-CGD-CBD	2.33	115.31	111.23
32	a	614	LMG	O4-C4-C5	2.33	115.07	109.32
24	C	508	CLA	O2D-CGD-CBD	2.33	115.30	111.23
30	a	613	SQD	O5-C5-C4	2.33	113.89	109.70
24	c	506	CLA	O2D-CGD-O1D	-2.32	119.32	123.85
27	A	610	PL9	C22-C23-C24	-2.32	122.31	127.62
24	b	615	CLA	CHA-C4D-ND	2.32	137.34	132.55
24	b	603	CLA	CMA-C3A-C4A	2.32	118.02	111.77
24	b	604	CLA	C1D-ND-C4D	2.32	107.94	106.31
24	d	404	CLA	CHA-C1A-NA	-2.32	121.13	126.39
24	a	605	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
28	t	102	STE	C3-C2-C1	-2.32	108.45	114.51
24	B	616	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
25	d	402	PHO	C4A-C3A-C2A	2.32	105.05	102.84
24	b	613	CLA	CED-O2D-CGD	2.32	121.17	115.92
29	d	408	LHG	C6-C5-C4	2.32	117.19	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	101	HEM	CAB-C3B-C2B	-2.32	120.90	128.43
30	f	102	SQD	C3-C4-C5	2.31	114.43	110.23
24	C	501	CLA	CED-O2D-CGD	-2.31	110.67	115.92
24	b	602	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
29	D	411	LHG	O4-P-O5	2.31	123.18	112.44
27	a	610	PL9	C42-C43-C44	-2.31	122.35	127.62
24	B	609	CLA	CMB-C2B-C3B	2.30	131.97	126.55
24	b	611	CLA	CHD-C1D-C2D	2.30	130.28	125.49
25	D	402	PHO	CMA-C3A-C4A	-2.30	109.65	114.61
24	B	604	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
24	c	506	CLA	C4-C3-C2	-2.30	117.73	123.63
24	b	601	CLA	O1D-CGD-CBD	2.29	129.04	124.52
32	c	518	LMG	C8-O7-C10	2.29	123.28	117.80
24	c	513	CLA	O2D-CGD-CBD	2.29	115.24	111.23
24	c	503	CLA	CHC-C4B-NB	2.29	127.48	124.05
24	B	601	CLA	CHC-C4B-NB	2.29	127.48	124.05
24	c	510	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
24	C	506	CLA	CHB-C4A-NA	2.28	127.70	124.40
24	c	507	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
27	D	406	PL9	C40-C39-C38	-2.28	117.76	123.63
24	b	603	CLA	CHC-C4B-NB	2.28	127.47	124.05
24	C	511	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	A	607	PHO	C1-C2-C3	-2.28	122.47	126.20
24	B	614	CLA	CHB-C4A-NA	2.28	127.69	124.40
24	b	602	CLA	C6-C5-C3	-2.28	107.92	113.47
24	c	502	CLA	C1-O2A-CGA	2.27	122.15	116.65
24	c	510	CLA	C7-C6-C5	-2.27	107.20	113.26
24	b	603	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
24	a	611	CLA	CHA-C1A-NA	-2.27	121.26	126.39
26	d	405	BCR	C7-C8-C9	-2.27	122.88	126.23
26	D	405	BCR	C32-C1-C6	2.27	113.80	110.24
24	d	404	CLA	C3B-C4B-NB	-2.27	108.51	110.53
24	B	608	CLA	CHB-C1B-NB	2.27	127.45	124.05
24	c	511	CLA	CHB-C1B-NB	2.27	127.45	124.05
24	a	611	CLA	C2A-C1A-CHA	2.27	127.80	123.87
24	B	608	CLA	O1D-CGD-CBD	2.27	128.99	124.52
24	C	502	CLA	O1D-CGD-CBD	2.26	128.99	124.52
27	a	610	PL9	C32-C33-C34	-2.26	122.44	127.62
28	J	101	STE	O2-C1-C2	2.26	121.15	114.00
32	a	614	LMG	C7-O1-C1	2.26	118.64	113.80
24	d	404	CLA	C4A-NA-C1A	2.26	107.71	106.68
30	a	613	SQD	C9-C8-C7	-2.26	105.42	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	522	DGD	C3G-C2G-C1G	-2.26	106.52	111.78
24	b	607	CLA	CHA-C4D-ND	2.26	137.20	132.55
24	C	513	CLA	CHD-C1D-ND	-2.26	121.63	124.80
24	B	616	CLA	CHB-C4A-NA	2.25	127.65	124.40
27	a	610	PL9	C40-C39-C41	2.25	119.14	115.23
24	b	604	CLA	CAC-C3C-C4C	2.25	127.72	124.79
25	a	607	PHO	CMA-C3A-C2A	-2.25	105.43	114.13
24	A	605	CLA	C17-C16-C15	-2.25	103.19	113.28
24	b	615	CLA	C11-C12-C13	-2.25	108.49	115.97
27	d	406	PL9	C8-C7-C3	2.25	117.84	112.03
24	b	610	CLA	CHA-C1A-NA	-2.25	121.31	126.39
24	D	403	CLA	CHD-C1D-C2D	2.24	130.16	125.49
24	a	605	CLA	CAC-C3C-C4C	2.24	127.71	124.79
26	a	609	BCR	C33-C5-C6	-2.24	122.04	124.48
32	a	614	LMG	O6-C1-C2	-2.24	105.76	110.37
25	a	607	PHO	C4A-C3A-C2A	2.24	104.97	102.84
24	C	504	CLA	CHB-C4A-NA	2.24	127.63	124.40
31	A	615	DGD	O4E-C4E-C5E	2.24	114.84	109.32
24	c	513	CLA	C3B-C4B-NB	-2.24	108.53	110.53
24	B	601	CLA	CHB-C1B-NB	2.24	127.40	124.05
25	A	607	PHO	C2B-C1B-NB	-2.23	107.81	109.43
26	d	405	BCR	C30-C25-C26	-2.23	119.59	122.64
25	d	402	PHO	O2A-CGA-O1A	-2.23	118.05	123.63
28	e	104	STE	O2-C1-C2	2.23	121.05	114.00
24	d	404	CLA	O2D-CGD-CBD	2.23	115.13	111.23
24	b	610	CLA	C1-C2-C3	-2.23	122.55	126.20
31	A	615	DGD	C2G-O2G-C1B	2.23	123.13	117.80
31	H	102	DGD	O3E-C3E-C2E	-2.23	105.13	110.38
24	B	605	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
24	C	510	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
24	a	611	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
30	D	412	SQD	O8-S-C6	2.22	110.26	105.97
24	c	511	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
24	a	605	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
30	D	412	SQD	C3-C4-C5	2.22	114.25	110.23
24	b	616	CLA	CHC-C4B-NB	2.22	127.38	124.05
29	d	409	LHG	O4-P-O5	2.22	122.76	112.44
28	j	101	STE	O2-C1-O1	-2.22	117.63	123.33
26	b	619	BCR	C29-C30-C25	2.22	113.66	110.44
24	c	502	CLA	O1D-CGD-CBD	2.21	128.89	124.52
24	D	404	CLA	CHC-C4B-NB	2.21	127.37	124.05
32	b	622	LMG	O5-C6-C5	-2.21	103.79	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
24	B	605	CLA	C4D-C3D-CAD	-2.21	105.70	108.11
35	v	201	HEC	CHA-C4D-ND	2.21	126.80	124.42
27	d	406	PL9	O2-C1-C2	-2.21	116.80	121.83
24	b	603	CLA	CHD-C4C-NC	2.21	127.66	124.23
24	b	613	CLA	C1-C2-C3	-2.21	122.58	126.20
24	B	606	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
24	c	509	CLA	C1-O2A-CGA	-2.20	111.31	116.65
24	b	615	CLA	O2D-CGD-CBD	2.20	115.08	111.23
24	C	506	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
32	a	615	LMG	O7-C8-C7	-2.20	100.44	108.34
24	C	512	CLA	CMA-C3A-C4A	-2.20	105.85	111.77
27	D	406	PL9	C47-C48-C49	-2.20	120.30	127.64
24	c	513	CLA	CGD-CBD-CAD	-2.20	103.73	110.85
30	D	409	SQD	O8-S-O9	-2.20	105.90	111.40
24	c	501	CLA	CHD-C1D-ND	-2.20	121.71	124.80
27	d	406	PL9	O2-C1-C6	2.19	123.97	120.48
24	C	510	CLA	C11-C12-C13	-2.19	108.67	115.97
24	C	513	CLA	CHD-C1D-C2D	2.19	130.05	125.49
26	b	617	BCR	C29-C30-C25	2.19	113.62	110.44
24	B	614	CLA	CHB-C1B-NB	2.19	127.34	124.05
24	C	504	CLA	CHB-C1B-NB	2.19	127.34	124.05
24	a	608	CLA	CHC-C4B-NB	2.19	127.33	124.05
24	B	608	CLA	CMB-C2B-C3B	2.19	131.70	126.55
30	a	612	SQD	C9-C8-C7	-2.19	105.68	113.69
24	b	610	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	b	612	CLA	C11-C12-C13	-2.18	108.70	115.97
27	D	406	PL9	C8-C7-C3	2.18	117.68	112.03
24	B	607	CLA	C2A-C1A-CHA	2.18	127.66	123.87
24	C	508	CLA	CHD-C1D-ND	-2.18	121.73	124.80
31	H	102	DGD	O3E-C3E-C4E	2.18	115.52	110.38
27	d	406	PL9	C12-C13-C14	-2.18	122.63	127.62
24	B	610	CLA	CHC-C4B-NB	2.18	127.32	124.05
24	c	507	CLA	CHC-C4B-NB	2.18	127.32	124.05
30	B	622	SQD	C46-C45-C44	-2.18	106.71	111.78
24	B	606	CLA	CHA-C1A-NA	-2.18	121.46	126.39
24	C	509	CLA	CED-O2D-CGD	2.18	120.85	115.92
30	B	622	SQD	C1-C2-C3	-2.18	105.43	110.01
24	c	502	CLA	CMB-C2B-C3B	2.17	131.66	126.55
31	c	520	DGD	C3G-O3G-C1D	2.17	118.45	113.80
24	A	606	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
24	A	612	CLA	C17-C16-C15	-2.17	103.56	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
24	B	605	CLA	CHB-C1B-NB	2.17	127.30	124.05
30	f	102	SQD	C46-C45-C44	-2.17	106.73	111.78
24	D	403	CLA	O2D-CGD-O1D	-2.16	119.63	123.85
31	h	102	DGD	C3D-C4D-C5D	-2.16	106.31	110.23
24	D	403	CLA	C2D-C1D-ND	-2.16	107.98	110.13
30	D	412	SQD	O6-C44-C45	-2.16	105.56	110.82
24	B	613	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	c	501	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	b	605	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
24	C	508	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
24	b	605	CLA	CHD-C1D-ND	-2.16	121.77	124.80
32	C	525	LMG	O1-C7-C8	-2.15	105.58	110.82
24	C	502	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	c	502	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
24	B	606	CLA	CHA-C4D-ND	2.15	136.98	132.55
24	b	613	CLA	C2A-C3A-C4A	2.15	105.34	101.87
25	a	607	PHO	CMD-C2D-C3D	2.15	128.97	124.68
24	b	607	CLA	CHC-C4B-NB	2.15	127.27	124.05
24	B	613	CLA	CHC-C4B-NB	2.15	127.27	124.05
34	F	101	HEM	CHB-C1B-NB	2.14	127.02	124.37
26	h	101	BCR	C2-C1-C6	2.14	113.55	110.44
24	B	614	CLA	CHA-C4D-ND	2.14	136.97	132.55
28	b	623	STE	O2-C1-O1	-2.14	117.82	123.33
31	h	102	DGD	C6D-C5D-C4D	2.14	116.56	112.07
24	A	606	CLA	C7-C6-C5	-2.14	107.56	113.26
24	c	507	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	c	521	DGD	C3D-C4D-C5D	-2.14	106.35	110.23
35	V	201	HEC	CAD-CBD-CGD	-2.14	107.99	113.67
24	b	609	CLA	C5-C3-C2	2.14	125.97	121.17
24	A	605	CLA	CED-O2D-CGD	2.14	120.76	115.92
30	A	614	SQD	O8-S-C6	2.14	110.09	105.97
24	C	504	CLA	C6-C5-C3	2.13	118.67	113.47
24	b	602	CLA	CHD-C1D-ND	-2.13	121.80	124.80
24	C	505	CLA	C6-C7-C8	-2.13	108.88	115.97
32	a	614	LMG	O8-C9-C8	2.13	114.54	108.40
25	a	607	PHO	CMB-C2B-C3B	2.13	128.94	124.68
30	A	614	SQD	C3-C4-C5	2.13	114.09	110.23
24	C	506	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
24	B	612	CLA	CMD-C2D-C3D	2.13	132.57	127.69
24	b	613	CLA	C3B-C4B-NB	-2.13	108.63	110.53
26	b	618	BCR	C38-C26-C27	-2.13	109.06	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	V	201	HEC	CHD-C4C-NC	2.13	127.71	123.86
24	d	403	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
24	B	612	CLA	C1-C2-C3	-2.12	122.72	126.20
28	a	616	STE	O2-C1-C2	2.12	120.70	114.00
24	b	605	CLA	CHB-C4A-NA	2.12	127.46	124.40
24	b	614	CLA	CHB-C1B-NB	2.12	127.23	124.05
24	A	612	CLA	CHB-C4A-NA	2.12	127.46	124.40
28	M	102	STE	O2-C1-C2	2.12	120.69	114.00
24	b	614	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
24	A	606	CLA	C3B-C4B-NB	-2.12	108.64	110.53
24	C	504	CLA	CHD-C4C-NC	2.12	127.51	124.23
31	c	519	DGD	C3G-O3G-C1D	2.12	118.33	113.80
32	a	614	LMG	C9-O8-C28	2.12	124.85	117.12
24	a	608	CLA	C3B-C4B-NB	-2.11	108.64	110.53
24	c	508	CLA	C1-C2-C3	-2.11	122.74	126.20
24	b	609	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
24	C	509	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
24	C	512	CLA	CHA-C1A-NA	-2.11	121.62	126.39
24	b	613	CLA	C7-C6-C5	-2.11	107.65	113.26
24	C	504	CLA	CED-O2D-CGD	2.10	120.69	115.92
24	b	606	CLA	CHB-C4A-NA	2.10	127.44	124.40
24	B	608	CLA	O2D-CGD-CBD	2.10	114.91	111.23
32	b	622	LMG	O6-C1-O1	2.10	115.01	110.04
35	v	201	HEC	CAD-CBD-CGD	-2.10	108.09	113.67
27	D	406	PL9	C50-C49-C48	-2.10	116.35	122.66
24	B	609	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
24	C	510	CLA	CMB-C2B-C3B	2.10	131.48	126.55
24	c	508	CLA	C7-C6-C5	-2.09	107.68	113.26
30	D	412	SQD	O4-C4-C3	-2.09	105.44	110.38
24	b	603	CLA	CMB-C2B-C3B	2.09	131.47	126.55
24	D	403	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	b	609	CLA	CHD-C4C-NC	2.09	127.47	124.23
24	D	403	CLA	C4A-NA-C1A	2.09	107.63	106.68
24	b	616	CLA	CHD-C1D-ND	-2.09	121.86	124.80
28	d	407	STE	O2-C1-C2	2.09	120.61	114.00
24	b	609	CLA	CMB-C2B-C3B	2.09	131.47	126.55
24	b	604	CLA	C6-C5-C3	-2.09	108.38	113.47
24	c	512	CLA	CHC-C1C-NC	2.09	127.45	124.31
30	D	412	SQD	O48-C23-C24	2.09	118.20	111.83
24	C	510	CLA	CHD-C1D-ND	-2.09	121.87	124.80
34	f	101	HEM	O1A-CGA-CBA	-2.08	116.48	123.09
24	c	502	CLA	CHB-C4A-NA	2.08	127.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	622	SQD	C9-C8-C7	-2.08	106.06	113.69
24	b	606	CLA	C3B-C4B-NB	-2.08	108.67	110.53
24	A	605	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	C	507	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	b	604	CLA	CED-O2D-CGD	2.08	120.63	115.92
24	b	604	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
32	D	407	LMG	O2-C2-C3	2.08	115.28	110.38
26	C	514	BCR	C7-C8-C9	-2.08	123.16	126.23
24	b	612	CLA	C1-C2-C3	-2.08	122.80	126.20
24	b	607	CLA	CHA-C1A-NA	-2.07	121.69	126.39
24	B	611	CLA	C1-C2-C3	-2.07	122.80	126.20
24	a	606	CLA	CHD-C4C-NC	2.07	127.45	124.23
24	C	512	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
24	B	613	CLA	C4D-CHA-C1A	2.07	123.72	121.24
24	c	505	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
24	C	509	CLA	CHA-C1A-NA	-2.07	121.71	126.39
24	C	506	CLA	CMB-C2B-C3B	2.07	131.41	126.55
28	b	621	STE	O2-C1-C2	2.07	120.53	114.00
31	H	102	DGD	O3D-C3D-C2D	-2.07	105.50	110.38
24	B	615	CLA	CHA-C4D-ND	2.07	136.81	132.55
24	C	504	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
24	C	507	CLA	O1D-CGD-CBD	2.07	128.59	124.52
24	C	504	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
32	m	101	LMG	O6-C1-C2	2.06	114.61	110.37
29	D	413	LHG	O3-P-O5	-2.06	100.75	108.94
30	D	409	SQD	O5-C5-C4	2.06	113.42	109.70
24	C	503	CLA	CHB-C1B-NB	2.06	127.14	124.05
24	b	602	CLA	CHD-C1D-C2D	2.06	129.78	125.49
25	a	607	PHO	O2A-CGA-O1A	-2.06	118.47	123.63
24	C	502	CLA	C16-C17-C18	-2.06	106.73	115.94
35	V	201	HEC	C2A-C1A-NA	-2.06	108.33	110.32
24	c	511	CLA	C2D-C1D-ND	-2.06	108.09	110.13
24	a	605	CLA	O2D-CGD-CBD	-2.06	107.63	111.23
26	d	405	BCR	C39-C30-C25	-2.06	107.01	110.24
31	C	523	DGD	O4E-C4E-C5E	2.06	114.39	109.32
24	B	608	CLA	CHD-C1D-ND	-2.06	121.91	124.80
35	v	201	HEC	CBD-CAD-C3D	-2.06	106.84	112.53
32	C	521	LMG	C8-O7-C10	2.06	122.72	117.80
24	b	615	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
30	D	409	SQD	C1-C2-C3	-2.05	105.69	110.01
32	a	615	LMG	C9-C8-C7	2.05	116.58	111.78
24	b	605	CLA	CAC-C3C-C4C	2.05	127.46	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	615	DGD	O4E-C4E-C3E	-2.05	105.54	110.38
24	B	606	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	b	613	CLA	C16-C15-C13	-2.05	109.15	115.97
24	b	605	CLA	O1A-CGA-CBA	2.05	131.80	123.78
28	R	101	STE	O2-C1-C2	2.05	120.47	114.00
29	d	409	LHG	C5-O7-C7	2.05	122.70	117.80
24	C	508	CLA	CHB-C4A-NA	2.04	127.35	124.40
24	b	616	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
24	c	503	CLA	C11-C12-C13	-2.04	109.19	115.97
24	C	505	CLA	O1A-CGA-CBA	2.04	131.76	123.78
24	b	604	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
24	B	603	CLA	C16-C15-C13	-2.04	109.19	115.97
24	D	404	CLA	CHA-C4D-ND	2.04	136.75	132.55
24	A	605	CLA	CAC-C3C-C4C	2.04	127.44	124.79
24	C	503	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
28	E	102	STE	O2-C1-C2	2.04	120.43	114.00
24	B	612	CLA	CAC-C3C-C4C	2.03	127.44	124.79
25	a	607	PHO	CAA-C2A-C3A	-2.03	107.50	113.00
35	v	201	HEC	CHB-C1B-NB	2.03	126.61	124.42
24	B	610	CLA	CHA-C1A-NA	-2.03	121.79	126.39
24	b	606	CLA	CHB-C1B-NB	2.03	127.10	124.05
32	b	622	LMG	O3-C3-C4	2.03	115.17	110.38
24	B	607	CLA	C3B-C4B-NB	-2.03	108.72	110.53
24	C	501	CLA	O1D-CGD-CBD	2.03	128.52	124.52
26	B	617	BCR	C33-C5-C6	-2.03	122.27	124.48
24	D	404	CLA	CHA-C1A-NA	-2.02	121.81	126.39
26	t	101	BCR	C37-C22-C21	2.02	126.09	122.82
24	A	608	CLA	CHB-C4A-NA	2.02	127.32	124.40
24	a	611	CLA	CAC-C3C-C4C	2.02	127.42	124.79
29	L	101	LHG	O6-P-O5	-2.02	100.93	108.94
24	B	616	CLA	C1-O2A-CGA	-2.02	111.76	116.65
32	B	620	LMG	O6-C5-C4	2.02	113.33	109.70
24	C	512	CLA	C2A-C3A-C4A	2.02	105.13	101.87
31	C	524	DGD	O3E-C3E-C2E	-2.01	105.63	110.38
24	D	404	CLA	CHB-C1B-NB	2.01	127.07	124.05
29	D	411	LHG	O7-C7-C8	2.01	115.84	111.48
24	c	504	CLA	O1A-CGA-CBA	2.01	131.65	123.78
34	f	101	HEM	C3B-C4B-NB	-2.01	108.02	109.47
26	b	619	BCR	C38-C26-C27	-2.01	109.31	113.60
26	h	101	BCR	C33-C5-C6	2.01	126.68	124.48
31	C	524	DGD	O6E-C5E-C6E	2.01	111.41	106.44
31	c	520	DGD	O4E-C4E-C5E	2.01	114.27	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	610	PL9	C15-C14-C16	-2.00	111.75	115.23
24	C	510	CLA	C11-C10-C8	-2.00	109.31	115.97
26	t	101	BCR	C38-C26-C27	-2.00	109.33	113.60
24	B	616	CLA	O2D-CGD-CBD	2.00	114.73	111.23
30	b	620	SQD	C46-O48-C23	-2.00	109.80	117.12
24	c	507	CLA	C4-C3-C5	2.00	118.70	115.23
24	a	606	CLA	CHD-C1D-C2D	2.00	129.65	125.49

All (2) chirality outliers are listed below:

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

All (1528) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CBA-CGA-O2A-C1
24	B	601	CLA	O1A-CGA-O2A-C1
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	b	605	CLA	C11-C10-C8-C9
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	509	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
24	c	513	CLA	CBD-CGD-O2D-CED
26	K	101	BCR	C1-C6-C7-C8
26	K	101	BCR	C5-C6-C7-C8
26	K	101	BCR	C21-C22-C23-C24
26	K	102	BCR	C7-C8-C9-C10
26	k	101	BCR	C1-C6-C7-C8
26	k	101	BCR	C21-C22-C23-C24
27	A	610	PL9	C27-C28-C29-C30
27	A	610	PL9	C27-C28-C29-C31
27	A	610	PL9	C37-C38-C39-C41
27	D	406	PL9	C32-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
27	a	610	PL9	C17-C18-C19-C21
27	a	610	PL9	C22-C23-C24-C25
27	a	610	PL9	C24-C26-C27-C28
27	a	610	PL9	C32-C33-C34-C35
27	a	610	PL9	C47-C48-C49-C50
27	d	406	PL9	C32-C33-C34-C35
27	d	406	PL9	C32-C33-C34-C36
27	d	406	PL9	C42-C43-C44-C45
29	D	410	LHG	C3-O3-P-O4
29	D	410	LHG	C3-O3-P-O6
29	D	413	LHG	C3-O3-P-O4
29	D	413	LHG	C3-O3-P-O6
29	L	101	LHG	C4-O6-P-O3
29	L	101	LHG	C4-O6-P-O4
29	d	408	LHG	O1-C1-C2-C3
29	d	408	LHG	C1-C2-C3-O3
29	d	409	LHG	C3-O3-P-O6
29	e	102	LHG	C3-O3-P-O5
29	e	102	LHG	C3-O3-P-O6
29	l	101	LHG	C4-O6-P-O3
29	l	101	LHG	C4-O6-P-O4
29	l	101	LHG	C4-O6-P-O5
30	A	614	SQD	O5-C5-C6-S
30	B	622	SQD	O5-C1-O6-C44
30	B	622	SQD	O6-C44-C45-O47
30	B	622	SQD	O49-C7-O47-C45
30	B	622	SQD	O10-C23-O48-C46
30	B	622	SQD	C24-C23-O48-C46
30	D	409	SQD	O5-C1-O6-C44
30	a	613	SQD	O5-C5-C6-S
30	a	613	SQD	C5-C6-S-O7
30	a	613	SQD	C5-C6-S-O8
30	a	613	SQD	C5-C6-S-O9
30	b	620	SQD	C8-C7-O47-C45
30	f	102	SQD	C2-C1-O6-C44
30	f	102	SQD	O5-C1-O6-C44
31	A	615	DGD	C2B-C1B-O2G-C2G
32	C	517	LMG	C2-C1-O1-C7
32	C	521	LMG	O9-C10-O7-C8
32	C	521	LMG	C11-C10-O7-C8
32	D	407	LMG	C2-C1-O1-C7
32	D	407	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
32	D	407	LMG	C11-C10-O7-C8
32	c	518	LMG	O1-C7-C8-C9
32	c	518	LMG	O1-C7-C8-O7
24	b	616	CLA	CBD-CGD-O2D-CED
32	B	620	LMG	O10-C28-O8-C9
27	A	610	PL9	C47-C48-C49-C51
27	a	610	PL9	C47-C48-C49-C51
32	B	620	LMG	C29-C28-O8-C9
24	b	601	CLA	CBD-CGD-O2D-CED
30	f	102	SQD	O10-C23-O48-C46
30	b	620	SQD	O49-C7-O47-C45
31	A	615	DGD	O1B-C1B-O2G-C2G
24	b	601	CLA	C3-C5-C6-C7
24	c	513	CLA	C3-C5-C6-C7
30	b	620	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
32	C	517	LMG	C29-C28-O8-C9
30	B	622	SQD	C8-C7-O47-C45
24	A	608	CLA	C4-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	a	608	CLA	C4-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	a	608	CLA	C2-C3-C5-C6
24	c	513	CLA	O1D-CGD-O2D-CED
24	B	616	CLA	CBA-CGA-O2A-C1
30	D	409	SQD	C24-C23-O48-C46
27	a	610	PL9	C22-C23-C24-C26
26	C	514	BCR	C15-C16-C17-C18
30	D	409	SQD	O10-C23-O48-C46
31	A	615	DGD	O1A-C1A-O1G-C1G
32	C	517	LMG	O10-C28-O8-C9
32	D	407	LMG	O9-C10-O7-C8
27	A	610	PL9	C47-C48-C49-C50
24	B	615	CLA	C3-C5-C6-C7
24	C	512	CLA	C3-C5-C6-C7
29	D	410	LHG	O2-C2-C3-O3
29	D	413	LHG	O2-C2-C3-O3
29	d	408	LHG	O2-C2-C3-O3
31	A	615	DGD	C2A-C1A-O1G-C1G
30	b	620	SQD	O10-C23-O48-C46
32	c	523	LMG	C11-C10-O7-C8
24	b	616	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	A	615	DGD	O6E-C5E-C6E-O5E
31	h	102	DGD	O6E-C5E-C6E-O5E
24	B	603	CLA	C4-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	B	614	CLA	C4-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
27	A	610	PL9	C35-C34-C36-C37
24	A	608	CLA	C2-C3-C5-C6
24	B	605	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
27	A	610	PL9	C33-C34-C36-C37
24	B	614	CLA	C13-C15-C16-C17
24	B	616	CLA	O1A-CGA-O2A-C1
27	A	610	PL9	C19-C21-C22-C23
27	A	610	PL9	C39-C41-C42-C43
27	a	610	PL9	C39-C41-C42-C43
32	C	521	LMG	O6-C1-O1-C7
24	B	612	CLA	CBD-CGD-O2D-CED
31	C	522	DGD	O6E-C5E-C6E-O5E
35	V	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C2C-C3C-CAC-CBC
32	b	622	LMG	O6-C5-C6-O5
28	d	411	STE	C5-C6-C7-C8
28	C	526	STE	C2-C3-C4-C5
32	c	523	LMG	O9-C10-O7-C8
29	D	410	LHG	C1-C2-C3-O3
29	D	413	LHG	C1-C2-C3-O3
24	C	513	CLA	CBA-CGA-O2A-C1
32	D	407	LMG	C29-C28-O8-C9
32	a	614	LMG	C29-C28-O8-C9
32	b	622	LMG	C4-C5-C6-O5
24	b	601	CLA	O1D-CGD-O2D-CED
24	B	603	CLA	C2-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
27	D	406	PL9	C47-C48-C49-C51
24	C	506	CLA	C3-C5-C6-C7
24	B	604	CLA	C11-C10-C8-C9
24	B	605	CLA	C6-C7-C8-C9
24	B	606	CLA	C11-C12-C13-C14
24	B	613	CLA	C11-C12-C13-C14
24	B	615	CLA	C6-C7-C8-C9
24	C	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	D	404	CLA	C11-C12-C13-C14
24	b	606	CLA	C14-C13-C15-C16
24	b	610	CLA	C14-C13-C15-C16
24	c	512	CLA	C6-C7-C8-C9
28	d	411	STE	C3-C4-C5-C6
32	a	614	LMG	O10-C28-O8-C9
26	K	101	BCR	C37-C22-C23-C24
26	K	102	BCR	C7-C8-C9-C34
26	k	101	BCR	C37-C22-C23-C24
35	v	201	HEC	C4C-C3C-CAC-CBC
32	b	622	LMG	O9-C10-O7-C8
32	b	622	LMG	C11-C10-O7-C8
30	a	613	SQD	O6-C44-C45-O47
32	a	614	LMG	O7-C8-C9-O8
24	b	605	CLA	C5-C6-C7-C8
29	l	101	LHG	C7-C8-C9-C10
30	D	412	SQD	C23-C24-C25-C26
24	B	604	CLA	CBD-CGD-O2D-CED
24	C	501	CLA	CBD-CGD-O2D-CED
27	a	610	PL9	C17-C18-C19-C20
24	B	613	CLA	C8-C10-C11-C12
24	b	601	CLA	C8-C10-C11-C12
29	d	408	LHG	C7-C8-C9-C10
31	c	521	DGD	C1A-C2A-C3A-C4A
27	A	610	PL9	C12-C13-C14-C16
24	C	503	CLA	C5-C6-C7-C8
24	c	509	CLA	CBD-CGD-O2D-CED
24	B	611	CLA	C12-C13-C15-C16
24	B	613	CLA	C11-C10-C8-C7
24	c	506	CLA	CBA-CGA-O2A-C1
35	V	201	HEC	C4C-C3C-CAC-CBC
24	A	606	CLA	C13-C15-C16-C17
30	D	409	SQD	C23-C24-C25-C26
28	C	516	STE	C1-C2-C3-C4
28	i	101	STE	C1-C2-C3-C4
29	e	102	LHG	C23-C24-C25-C26
30	a	612	SQD	C7-C8-C9-C10
32	D	407	LMG	C10-C11-C12-C13
32	D	407	LMG	O10-C28-O8-C9
24	C	512	CLA	C10-C11-C12-C13
24	a	608	CLA	C13-C15-C16-C17
24	b	609	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	C13-C15-C16-C17
24	C	506	CLA	C13-C15-C16-C17
24	c	503	CLA	C8-C10-C11-C12
24	c	506	CLA	C13-C15-C16-C17
30	D	412	SQD	C7-C8-C9-C10
32	a	614	LMG	C10-C11-C12-C13
32	c	522	LMG	C28-C29-C30-C31
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	506	CLA	O1A-CGA-O2A-C1
32	a	614	LMG	O6-C1-O1-C7
24	B	601	CLA	C8-C10-C11-C12
24	B	602	CLA	C8-C10-C11-C12
24	B	615	CLA	C5-C6-C7-C8
24	C	506	CLA	C8-C10-C11-C12
24	a	608	CLA	C5-C6-C7-C8
24	c	513	CLA	C13-C15-C16-C17
29	d	409	LHG	O2-C2-C3-O3
32	b	622	LMG	C28-C29-C30-C31
24	b	602	CLA	C13-C15-C16-C17
24	b	616	CLA	C8-C10-C11-C12
27	A	610	PL9	C32-C33-C34-C35
24	b	614	CLA	C10-C11-C12-C13
29	d	410	LHG	C23-C24-C25-C26
32	m	101	LMG	C28-C29-C30-C31
24	A	606	CLA	C15-C16-C17-C18
24	a	605	CLA	C15-C16-C17-C18
24	b	606	CLA	C15-C16-C17-C18
24	b	611	CLA	C13-C15-C16-C17
24	c	508	CLA	C8-C10-C11-C12
24	C	513	CLA	CBD-CGD-O2D-CED
31	A	615	DGD	C4E-C5E-C6E-O5E
24	c	507	CLA	C5-C6-C7-C8
29	d	409	LHG	C1-C2-C3-O3
24	b	606	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C5-C6-C7-C8
24	b	607	CLA	C10-C11-C12-C13
24	b	613	CLA	C13-C15-C16-C17
24	b	614	CLA	C13-C15-C16-C17
24	B	611	CLA	C8-C10-C11-C12
24	C	509	CLA	C8-C10-C11-C12
24	a	611	CLA	C15-C16-C17-C18
24	b	607	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	c	503	CLA	C5-C6-C7-C8
24	c	507	CLA	C4-C3-C5-C6
32	a	614	LMG	C11-C10-O7-C8
30	B	622	SQD	C2-C1-O6-C44
31	C	523	DGD	C2E-C1E-O5D-C6D
32	a	615	LMG	C2-C1-O1-C7
32	b	622	LMG	C2-C1-O1-C7
24	B	601	CLA	C16-C17-C18-C20
24	B	606	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C20
24	b	605	CLA	C10-C11-C12-C13
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	609	CLA	C15-C16-C17-C18
32	d	412	LMG	C28-C29-C30-C31
30	b	620	SQD	C46-C45-O47-C7
24	A	612	CLA	C16-C17-C18-C20
24	a	608	CLA	C16-C17-C18-C19
24	c	511	CLA	C16-C17-C18-C19
28	C	516	STE	C11-C10-C9-C8
29	A	613	LHG	C27-C28-C29-C30
25	D	402	PHO	C2C-C3C-CAC-CBC
24	c	507	CLA	C2-C3-C5-C6
30	A	614	SQD	O6-C44-C45-O47
30	D	409	SQD	O6-C44-C45-C46
24	c	512	CLA	CBA-CGA-O2A-C1
31	c	519	DGD	C1B-C2B-C3B-C4B
32	C	525	LMG	C28-C29-C30-C31
24	c	506	CLA	C2-C1-O2A-CGA
24	B	606	CLA	C16-C17-C18-C20
24	C	502	CLA	C16-C17-C18-C20
24	C	507	CLA	C16-C17-C18-C19
24	a	608	CLA	C16-C17-C18-C20
24	c	503	CLA	C16-C17-C18-C20
24	c	511	CLA	C16-C17-C18-C20
30	a	612	SQD	C31-C32-C33-C34
31	c	519	DGD	C8A-C9A-CAA-CBA
31	c	519	DGD	C7B-C8B-C9B-CAB
32	C	521	LMG	C33-C34-C35-C36
32	b	622	LMG	C18-C19-C20-C21
28	c	516	STE	C2-C3-C4-C5
28	m	102	STE	C2-C3-C4-C5
29	d	409	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	A	615	DGD	CDA-CEA-CFA-CGA
31	C	523	DGD	C5A-C6A-C7A-C8A
31	h	102	DGD	CAA-CBA-CCA-CDA
32	M	101	LMG	C30-C31-C32-C33
32	m	101	LMG	C12-C13-C14-C15
32	C	517	LMG	C28-C29-C30-C31
35	V	201	HEC	C2B-C3B-CAB-CBB
28	E	101	STE	C9-C10-C11-C12
29	A	613	LHG	C32-C33-C34-C35
31	C	522	DGD	CCA-CDA-CEA-CFA
31	c	519	DGD	C5B-C6B-C7B-C8B
31	c	521	DGD	C4B-C5B-C6B-C7B
32	a	614	LMG	C38-C39-C40-C41
28	A	618	STE	C13-C14-C15-C16
28	C	528	STE	C11-C12-C13-C14
28	d	407	STE	C7-C8-C9-C10
29	A	613	LHG	C13-C14-C15-C16
29	d	410	LHG	C32-C33-C34-C35
30	A	614	SQD	C10-C11-C12-C13
30	b	620	SQD	C14-C15-C16-C17
31	C	524	DGD	C5A-C6A-C7A-C8A
31	H	102	DGD	CCB-CDB-CEB-CFB
32	c	518	LMG	C32-C33-C34-C35
32	d	412	LMG	C37-C38-C39-C40
29	d	408	LHG	O1-C1-C2-O2
30	D	409	SQD	C45-C44-O6-C1
28	J	101	STE	C5-C6-C7-C8
28	c	517	STE	C7-C8-C9-C10
28	t	102	STE	C6-C7-C8-C9
29	l	101	LHG	C14-C15-C16-C17
31	c	519	DGD	C5A-C6A-C7A-C8A
31	c	519	DGD	C3B-C4B-C5B-C6B
31	h	102	DGD	C7B-C8B-C9B-CAB
28	Z	101	STE	C2-C3-C4-C5
28	B	623	STE	C5-C6-C7-C8
28	i	101	STE	C5-C6-C7-C8
32	b	622	LMG	C21-C22-C23-C24
24	B	614	CLA	C16-C17-C18-C20
24	C	507	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C19
29	D	413	LHG	C29-C30-C31-C32
31	c	520	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
32	D	408	LMG	C30-C31-C32-C33
24	B	602	CLA	C13-C15-C16-C17
24	B	606	CLA	C15-C16-C17-C18
24	C	508	CLA	C11-C10-C8-C7
24	b	606	CLA	C6-C7-C8-C10
28	B	625	STE	C11-C10-C9-C8
31	c	519	DGD	C3A-C4A-C5A-C6A
32	c	518	LMG	C30-C31-C32-C33
28	E	102	STE	C1-C2-C3-C4
28	A	611	STE	C4-C5-C6-C7
28	A	618	STE	C10-C11-C12-C13
28	C	527	STE	C4-C5-C6-C7
28	c	517	STE	C9-C10-C11-C12
31	C	523	DGD	CAB-CBB-CCB-CDB
31	C	524	DGD	CAB-CBB-CCB-CDB
31	H	102	DGD	C4B-C5B-C6B-C7B
31	c	520	DGD	C8A-C9A-CAA-CBA
32	B	620	LMG	C32-C33-C34-C35
24	B	612	CLA	O1D-CGD-O2D-CED
28	Z	101	STE	C5-C6-C7-C8
29	d	408	LHG	C16-C17-C18-C19
29	d	408	LHG	C27-C28-C29-C30
29	l	101	LHG	C11-C12-C13-C14
31	C	524	DGD	C6A-C7A-C8A-C9A
32	a	615	LMG	C36-C37-C38-C39
28	b	623	STE	C1-C2-C3-C4
31	c	520	DGD	C1B-C2B-C3B-C4B
30	b	620	SQD	C11-C10-C9-C8
24	B	615	CLA	C16-C17-C18-C20
24	C	502	CLA	C16-C17-C18-C19
28	c	516	STE	C7-C8-C9-C10
32	C	521	LMG	C16-C17-C18-C19
32	a	614	LMG	O9-C10-O7-C8
28	e	104	STE	C4-C5-C6-C7
29	e	102	LHG	C26-C27-C28-C29
30	a	612	SQD	C24-C23-O48-C46
30	a	612	SQD	C44-C45-C46-O48
28	B	623	STE	C10-C11-C12-C13
28	C	520	STE	C7-C8-C9-C10
28	I	101	STE	C7-C8-C9-C10
28	c	517	STE	C11-C10-C9-C8
30	a	613	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	f	102	SQD	C25-C26-C27-C28
31	c	519	DGD	C6A-C7A-C8A-C9A
28	B	625	STE	C7-C8-C9-C10
28	E	102	STE	C3-C4-C5-C6
28	H	103	STE	C4-C5-C6-C7
28	J	101	STE	C6-C7-C8-C9
29	A	613	LHG	C28-C29-C30-C31
29	D	411	LHG	C15-C16-C17-C18
29	L	101	LHG	C17-C18-C19-C20
29	d	408	LHG	C12-C13-C14-C15
29	l	101	LHG	C16-C17-C18-C19
30	D	412	SQD	C16-C17-C18-C19
30	a	612	SQD	C12-C13-C14-C15
31	C	522	DGD	CAA-CBA-CCA-CDA
31	c	519	DGD	C9A-CAA-CBA-CCA
31	c	520	DGD	CAA-CBA-CCA-CDA
31	h	102	DGD	CCA-CDA-CEA-CFA
32	a	614	LMG	C22-C23-C24-C25
28	C	528	STE	C7-C8-C9-C10
29	d	408	LHG	C17-C18-C19-C20
29	d	409	LHG	C11-C12-C13-C14
31	h	102	DGD	C2B-C3B-C4B-C5B
28	d	407	STE	C5-C6-C7-C8
30	D	412	SQD	C12-C13-C14-C15
32	B	620	LMG	C33-C34-C35-C36
32	M	101	LMG	C17-C18-C19-C20
28	T	102	STE	C9-C10-C11-C12
29	l	101	LHG	C34-C35-C36-C37
31	C	523	DGD	CCA-CDA-CEA-CFA
32	D	408	LMG	C17-C18-C19-C20
32	c	523	LMG	C30-C31-C32-C33
24	C	512	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C1-C6-C7-C8
26	B	617	BCR	C5-C6-C7-C8
26	D	405	BCR	C23-C24-C25-C26
26	D	405	BCR	C23-C24-C25-C30
26	H	101	BCR	C5-C6-C7-C8
26	T	101	BCR	C23-C24-C25-C26
26	h	101	BCR	C5-C6-C7-C8
26	k	101	BCR	C5-C6-C7-C8
26	t	101	BCR	C23-C24-C25-C26
28	C	520	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	T	102	STE	C4-C5-C6-C7
29	D	413	LHG	C17-C18-C19-C20
31	A	615	DGD	C9A-CAA-CBA-CCA
32	B	620	LMG	C29-C30-C31-C32
28	E	102	STE	C5-C6-C7-C8
29	D	411	LHG	C29-C30-C31-C32
30	B	622	SQD	C33-C34-C35-C36
30	a	613	SQD	C9-C10-C11-C12
32	D	408	LMG	C13-C14-C15-C16
24	c	512	CLA	O1A-CGA-O2A-C1
27	A	610	PL9	C4-C3-C7-C8
28	C	527	STE	C5-C6-C7-C8
28	e	101	STE	C11-C12-C13-C14
28	k	103	STE	C7-C8-C9-C10
32	C	521	LMG	C32-C33-C34-C35
28	E	102	STE	C7-C8-C9-C10
28	b	621	STE	C11-C12-C13-C14
30	D	412	SQD	C24-C25-C26-C27
31	C	522	DGD	C4B-C5B-C6B-C7B
32	M	101	LMG	C13-C14-C15-C16
32	c	522	LMG	C36-C37-C38-C39
24	B	615	CLA	C10-C11-C12-C13
28	K	103	STE	C14-C15-C16-C17
30	D	412	SQD	C33-C34-C35-C36
31	A	615	DGD	C4A-C5A-C6A-C7A
31	c	521	DGD	C3A-C4A-C5A-C6A
31	c	521	DGD	C5B-C6B-C7B-C8B
32	C	521	LMG	C31-C32-C33-C34
31	C	522	DGD	O6D-C5D-C6D-O5D
28	B	624	STE	C5-C6-C7-C8
28	I	101	STE	C11-C10-C9-C8
32	b	622	LMG	C29-C30-C31-C32
28	d	411	STE	C14-C15-C16-C17
32	a	615	LMG	O6-C1-O1-C7
32	b	622	LMG	O6-C1-O1-C7
29	e	102	LHG	C11-C12-C13-C14
29	l	101	LHG	C10-C11-C12-C13
31	A	615	DGD	CEB-CFB-CGB-CHB
28	K	103	STE	C10-C11-C12-C13
28	h	103	STE	C12-C13-C14-C15
31	C	523	DGD	CCB-CDB-CEB-CFB
32	M	101	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	b	622	LMG	C15-C16-C17-C18
28	K	103	STE	C6-C7-C8-C9
30	a	612	SQD	C9-C10-C11-C12
30	a	612	SQD	C33-C34-C35-C36
31	h	102	DGD	C5B-C6B-C7B-C8B
32	c	523	LMG	C15-C16-C17-C18
29	D	411	LHG	C33-C34-C35-C36
32	c	522	LMG	C4-C5-C6-O5
24	B	613	CLA	C15-C16-C17-C18
24	a	608	CLA	C10-C11-C12-C13
32	D	408	LMG	C14-C15-C16-C17
32	a	614	LMG	C29-C30-C31-C32
32	b	622	LMG	C17-C18-C19-C20
28	B	623	STE	C1-C2-C3-C4
28	C	527	STE	C7-C8-C9-C10
30	b	620	SQD	C16-C17-C18-C19
30	f	102	SQD	C30-C31-C32-C33
31	C	523	DGD	C6A-C7A-C8A-C9A
31	c	520	DGD	C5D-C6D-O5D-C1E
32	a	614	LMG	C8-C7-O1-C1
31	c	520	DGD	C8B-C9B-CAB-CBB
31	h	102	DGD	C7A-C8A-C9A-CAA
24	B	601	CLA	C16-C17-C18-C19
28	R	101	STE	C3-C4-C5-C6
31	H	102	DGD	C8A-C9A-CAA-CBA
32	c	523	LMG	C37-C38-C39-C40
24	b	601	CLA	C10-C11-C12-C13
24	c	509	CLA	C10-C11-C12-C13
28	j	101	STE	C5-C6-C7-C8
32	C	525	LMG	C17-C18-C19-C20
24	b	608	CLA	C2C-C3C-CAC-CBC
30	a	612	SQD	C27-C28-C29-C30
30	a	612	SQD	O10-C23-O48-C46
24	B	612	CLA	C10-C11-C12-C13
24	d	404	CLA	C5-C6-C7-C8
28	c	517	STE	C3-C4-C5-C6
29	e	102	LHG	O6-C4-C5-O7
28	K	103	STE	C12-C13-C14-C15
28	b	621	STE	C13-C14-C15-C16
32	B	620	LMG	C34-C35-C36-C37
24	a	606	CLA	C15-C16-C17-C18
24	b	607	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	B	609	CLA	C16-C17-C18-C20
28	A	617	STE	C5-C6-C7-C8
32	D	407	LMG	C31-C32-C33-C34
29	d	409	LHG	C33-C34-C35-C36
30	B	622	SQD	C25-C26-C27-C28
28	m	102	STE	C1-C2-C3-C4
30	A	614	SQD	C11-C12-C13-C14
31	H	102	DGD	C6B-C7B-C8B-C9B
32	D	408	LMG	C12-C13-C14-C15
28	M	102	STE	C5-C6-C7-C8
28	h	103	STE	C11-C12-C13-C14
30	b	620	SQD	C29-C30-C31-C32
31	c	519	DGD	C2B-C3B-C4B-C5B
32	C	521	LMG	C12-C13-C14-C15
32	a	615	LMG	C30-C31-C32-C33
28	T	102	STE	C11-C12-C13-C14
30	a	613	SQD	C18-C19-C20-C21
31	A	615	DGD	C4B-C5B-C6B-C7B
28	C	528	STE	C14-C15-C16-C17
31	A	615	DGD	CCA-CDA-CEA-CFA
31	C	522	DGD	C5B-C6B-C7B-C8B
32	c	523	LMG	C36-C37-C38-C39
28	b	623	STE	C11-C10-C9-C8
30	B	622	SQD	C11-C12-C13-C14
30	B	622	SQD	C16-C17-C18-C19
32	b	622	LMG	C19-C20-C21-C22
32	c	523	LMG	O6-C5-C6-O5
28	C	528	STE	C9-C10-C11-C12
28	H	103	STE	C6-C7-C8-C9
27	a	610	PL9	C21-C22-C23-C24
31	C	523	DGD	C1B-C2B-C3B-C4B
28	j	102	STE	C4-C5-C6-C7
29	A	613	LHG	C14-C15-C16-C17
31	c	519	DGD	O6E-C5E-C6E-O5E
28	E	102	STE	C11-C12-C13-C14
28	j	101	STE	C4-C5-C6-C7
29	d	408	LHG	C14-C15-C16-C17
31	c	520	DGD	C6A-C7A-C8A-C9A
32	m	101	LMG	C17-C18-C19-C20
32	b	622	LMG	C10-C11-C12-C13
28	B	623	STE	C2-C3-C4-C5
28	H	104	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	t	102	STE	C11-C10-C9-C8
28	z	101	STE	C2-C3-C4-C5
30	a	612	SQD	C14-C15-C16-C17
32	D	408	LMG	C35-C36-C37-C38
32	M	101	LMG	C14-C15-C16-C17
24	B	616	CLA	C3-C5-C6-C7
31	C	524	DGD	C3A-C4A-C5A-C6A
31	H	102	DGD	C5A-C6A-C7A-C8A
32	b	622	LMG	C39-C40-C41-C42
24	c	513	CLA	C1A-C2A-CAA-CBA
32	D	408	LMG	O6-C5-C6-O5
31	C	523	DGD	O6E-C1E-O5D-C6D
29	d	408	LHG	C30-C31-C32-C33
30	A	614	SQD	C11-C10-C9-C8
30	D	412	SQD	C11-C10-C9-C8
31	C	524	DGD	C3B-C4B-C5B-C6B
29	d	410	LHG	C25-C26-C27-C28
28	M	102	STE	C2-C3-C4-C5
28	m	103	STE	C10-C11-C12-C13
32	m	101	LMG	C15-C16-C17-C18
28	C	516	STE	C5-C6-C7-C8
32	b	622	LMG	C13-C14-C15-C16
32	d	412	LMG	C34-C35-C36-C37
24	B	615	CLA	C6-C7-C8-C10
24	C	511	CLA	C6-C7-C8-C10
24	C	512	CLA	C11-C12-C13-C15
24	b	604	CLA	C12-C13-C15-C16
24	b	606	CLA	C12-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C15
24	c	513	CLA	C12-C13-C15-C16
24	d	404	CLA	C11-C12-C13-C15
29	D	410	LHG	C11-C10-C9-C8
24	b	601	CLA	C16-C17-C18-C19
28	H	103	STE	C11-C10-C9-C8
30	a	613	SQD	C30-C31-C32-C33
24	C	509	CLA	C10-C11-C12-C13
32	D	408	LMG	C10-C11-C12-C13
30	D	412	SQD	C11-C12-C13-C14
31	c	519	DGD	C6B-C7B-C8B-C9B
31	C	522	DGD	C4D-C5D-C6D-O5D
28	b	621	STE	C3-C4-C5-C6
28	d	407	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	h	102	DGD	C8B-C9B-CAB-CBB
32	B	620	LMG	C31-C32-C33-C34
24	B	612	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
24	b	601	CLA	C11-C12-C13-C14
24	b	603	CLA	C6-C7-C8-C9
24	b	607	CLA	C6-C7-C8-C9
24	b	611	CLA	C11-C12-C13-C14
24	d	404	CLA	C11-C12-C13-C14
28	i	102	STE	C11-C10-C9-C8
30	f	102	SQD	C33-C34-C35-C36
28	f	103	STE	C11-C12-C13-C14
28	m	102	STE	C6-C7-C8-C9
30	D	409	SQD	C2-C1-O6-C44
32	d	412	LMG	O6-C5-C6-O5
29	A	613	LHG	C4-C5-C6-O8
30	a	612	SQD	O6-C44-C45-C46
30	a	613	SQD	O6-C44-C45-C46
31	c	519	DGD	O1G-C1G-C2G-C3G
32	a	614	LMG	C7-C8-C9-O8
32	a	615	LMG	O1-C7-C8-C9
28	A	617	STE	C2-C3-C4-C5
29	l	101	LHG	C32-C33-C34-C35
30	b	620	SQD	C18-C19-C20-C21
28	J	101	STE	C2-C3-C4-C5
30	D	412	SQD	C15-C16-C17-C18
29	e	102	LHG	O2-C2-C3-O3
31	h	102	DGD	C4E-C5E-C6E-O5E
28	k	103	STE	C6-C7-C8-C9
32	C	521	LMG	C39-C40-C41-C42
28	d	411	STE	C1-C2-C3-C4
24	C	510	CLA	C16-C17-C18-C19
29	d	409	LHG	C17-C18-C19-C20
32	C	517	LMG	C16-C17-C18-C19
32	b	622	LMG	C32-C33-C34-C35
28	E	102	STE	C13-C14-C15-C16
31	c	521	DGD	C4A-C5A-C6A-C7A
28	M	104	STE	C13-C14-C15-C16
32	c	522	LMG	C12-C13-C14-C15
24	C	509	CLA	C5-C6-C7-C8
24	c	503	CLA	C15-C16-C17-C18
24	c	510	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	B	623	STE	C9-C10-C11-C12
29	D	413	LHG	C25-C26-C27-C28
29	D	413	LHG	C7-C8-C9-C10
29	d	408	LHG	C29-C30-C31-C32
31	C	524	DGD	CBA-CCA-CDA-CEA
27	a	610	PL9	C43-C44-C46-C47
28	A	617	STE	C10-C11-C12-C13
28	I	102	STE	C5-C6-C7-C8
28	M	103	STE	C6-C7-C8-C9
32	C	525	LMG	C37-C38-C39-C40
28	M	102	STE	C4-C5-C6-C7
31	A	615	DGD	C7B-C8B-C9B-CAB
32	B	620	LMG	O6-C5-C6-O5
29	D	411	LHG	C16-C17-C18-C19
30	A	614	SQD	C14-C15-C16-C17
28	b	625	STE	C12-C13-C14-C15
28	i	101	STE	C4-C5-C6-C7
32	B	620	LMG	C10-C11-C12-C13
28	k	103	STE	C5-C6-C7-C8
31	C	523	DGD	CBA-CCA-CDA-CEA
24	C	512	CLA	O2A-C1-C2-C3
32	a	614	LMG	C9-C8-O7-C10
32	m	101	LMG	C14-C15-C16-C17
24	C	508	CLA	C15-C16-C17-C18
28	E	102	STE	C12-C13-C14-C15
30	D	409	SQD	C25-C26-C27-C28
31	H	102	DGD	C7A-C8A-C9A-CAA
31	c	521	DGD	C5A-C6A-C7A-C8A
32	B	620	LMG	C15-C16-C17-C18
32	C	521	LMG	C35-C36-C37-C38
32	D	407	LMG	C32-C33-C34-C35
32	d	412	LMG	C35-C36-C37-C38
29	d	408	LHG	C13-C14-C15-C16
32	m	101	LMG	C10-C11-C12-C13
29	A	613	LHG	C17-C18-C19-C20
28	A	616	STE	C12-C13-C14-C15
28	C	520	STE	C11-C10-C9-C8
32	a	615	LMG	C17-C18-C19-C20
32	c	522	LMG	C29-C30-C31-C32
32	c	522	LMG	C29-C28-O8-C9
24	B	604	CLA	O1D-CGD-O2D-CED
24	c	509	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	D	414	STE	C7-C8-C9-C10
28	f	103	STE	C12-C13-C14-C15
31	C	522	DGD	CBA-CCA-CDA-CEA
31	H	102	DGD	CDA-CEA-CFA-CGA
28	D	414	STE	C10-C11-C12-C13
30	D	409	SQD	C34-C35-C36-C37
24	B	610	CLA	C16-C17-C18-C20
29	D	410	LHG	C15-C16-C17-C18
29	D	413	LHG	C31-C32-C33-C34
29	D	413	LHG	C24-C25-C26-C27
29	D	413	LHG	C28-C29-C30-C31
30	D	409	SQD	C27-C28-C29-C30
30	a	612	SQD	O47-C45-C46-O48
31	C	523	DGD	CDA-CEA-CFA-CGA
28	m	103	STE	C6-C7-C8-C9
32	c	522	LMG	C40-C41-C42-C43
28	j	101	STE	C2-C3-C4-C5
28	j	102	STE	C5-C6-C7-C8
29	D	413	LHG	C27-C28-C29-C30
29	L	101	LHG	C11-C12-C13-C14
32	c	523	LMG	C34-C35-C36-C37
31	c	521	DGD	CDA-CEA-CFA-CGA
28	A	617	STE	C13-C14-C15-C16
28	c	516	STE	C5-C6-C7-C8
28	e	104	STE	C3-C4-C5-C6
29	D	410	LHG	C18-C19-C20-C21
30	D	409	SQD	C32-C33-C34-C35
29	e	102	LHG	C7-C8-C9-C10
32	C	525	LMG	C30-C31-C32-C33
28	A	616	STE	C11-C12-C13-C14
28	D	414	STE	C4-C5-C6-C7
28	c	516	STE	C6-C7-C8-C9
32	C	525	LMG	C32-C33-C34-C35
28	A	611	STE	C1-C2-C3-C4
32	m	101	LMG	C40-C41-C42-C43
27	A	610	PL9	C42-C43-C44-C45
24	b	608	CLA	C4C-C3C-CAC-CBC
29	L	101	LHG	C13-C14-C15-C16
31	A	615	DGD	C8A-C9A-CAA-CBA
24	C	513	CLA	C8-C10-C11-C12
31	H	102	DGD	C3B-C4B-C5B-C6B
30	D	409	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
24	B	614	CLA	C8-C10-C11-C12
24	b	614	CLA	C16-C17-C18-C19
28	B	621	STE	C12-C13-C14-C15
32	a	615	LMG	C40-C41-C42-C43
31	A	615	DGD	CAA-CBA-CCA-CDA
32	M	101	LMG	C16-C17-C18-C19
24	b	612	CLA	C3-C5-C6-C7
24	A	612	CLA	C14-C13-C15-C16
24	B	613	CLA	C11-C10-C8-C9
24	C	507	CLA	C11-C10-C8-C9
24	C	507	CLA	C11-C12-C13-C14
24	C	508	CLA	C11-C10-C8-C9
24	C	510	CLA	C11-C10-C8-C9
24	C	511	CLA	C6-C7-C8-C9
24	C	512	CLA	C11-C12-C13-C14
24	b	601	CLA	C11-C10-C8-C9
24	b	604	CLA	C14-C13-C15-C16
24	b	611	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C9
24	c	506	CLA	C11-C12-C13-C14
24	c	508	CLA	C14-C13-C15-C16
24	c	513	CLA	C14-C13-C15-C16
32	M	101	LMG	C38-C39-C40-C41
24	c	512	CLA	C15-C16-C17-C18
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	512	CLA	C4B-C3B-CAB-CBB
31	C	522	DGD	C2B-C3B-C4B-C5B
32	M	101	LMG	C19-C20-C21-C22
28	e	101	STE	C15-C16-C17-C18
35	V	201	HEC	C4B-C3B-CAB-CBB
29	D	411	LHG	C11-C12-C13-C14
24	b	614	CLA	C16-C17-C18-C20
28	A	617	STE	C7-C8-C9-C10
29	d	410	LHG	C26-C27-C28-C29
31	C	522	DGD	C2E-C1E-O5D-C6D
28	B	621	STE	C3-C4-C5-C6
28	C	527	STE	C12-C13-C14-C15
28	t	102	STE	C3-C4-C5-C6
29	l	101	LHG	C15-C16-C17-C18
30	D	409	SQD	C31-C32-C33-C34
31	H	102	DGD	C5B-C6B-C7B-C8B
32	D	408	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	b	622	LMG	C16-C17-C18-C19
28	C	520	STE	C9-C10-C11-C12
29	d	408	LHG	C19-C20-C21-C22
29	e	102	LHG	O6-C4-C5-C6
31	H	102	DGD	O2G-C1B-C2B-C3B
24	B	604	CLA	C6-C7-C8-C10
24	B	606	CLA	C11-C12-C13-C15
24	B	612	CLA	C12-C13-C15-C16
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	C	507	CLA	C11-C12-C13-C15
24	C	510	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C10-C8-C7
24	b	601	CLA	C11-C12-C13-C15
24	b	603	CLA	C6-C7-C8-C10
24	b	607	CLA	C6-C7-C8-C10
24	b	611	CLA	C11-C12-C13-C15
24	c	504	CLA	C11-C10-C8-C7
28	C	528	STE	C15-C16-C17-C18
32	c	522	LMG	O6-C5-C6-O5
28	d	407	STE	C4-C5-C6-C7
32	a	615	LMG	C10-C11-C12-C13
28	t	103	STE	C7-C8-C9-C10
24	c	503	CLA	C16-C17-C18-C19
28	C	520	STE	C6-C7-C8-C9
28	M	104	STE	C5-C6-C7-C8
29	D	411	LHG	C14-C15-C16-C17
28	E	102	STE	C14-C15-C16-C17
28	B	625	STE	C12-C13-C14-C15
28	M	104	STE	C11-C10-C9-C8
31	h	102	DGD	O2G-C1B-C2B-C3B
28	c	516	STE	C9-C10-C11-C12
28	e	101	STE	C14-C15-C16-C17
32	D	407	LMG	C13-C14-C15-C16
28	A	617	STE	C6-C7-C8-C9
28	A	618	STE	C14-C15-C16-C17
30	b	620	SQD	C11-C12-C13-C14
24	C	501	CLA	O1D-CGD-O2D-CED
26	k	102	BCR	C9-C10-C11-C12
26	K	102	BCR	C37-C22-C23-C24
26	c	514	BCR	C36-C18-C19-C20
24	b	610	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
32	c	522	LMG	C17-C18-C19-C20
28	d	411	STE	C10-C11-C12-C13
28	b	624	STE	C7-C8-C9-C10
31	c	519	DGD	CCA-CDA-CEA-CFA
32	D	407	LMG	C29-C30-C31-C32
32	C	525	LMG	C40-C41-C42-C43
32	m	101	LMG	C38-C39-C40-C41
28	J	101	STE	C7-C8-C9-C10
29	D	411	LHG	C35-C36-C37-C38
29	L	101	LHG	C26-C27-C28-C29
30	A	614	SQD	C9-C10-C11-C12
32	c	522	LMG	C38-C39-C40-C41
29	e	102	LHG	C4-C5-C6-O8
30	A	614	SQD	O6-C44-C45-C46
30	B	622	SQD	O6-C44-C45-C46
32	C	517	LMG	C7-C8-C9-O8
32	a	615	LMG	C7-C8-C9-O8
27	A	610	PL9	C32-C33-C34-C36
28	B	621	STE	C10-C11-C12-C13
24	B	609	CLA	C16-C17-C18-C19
28	m	103	STE	C2-C3-C4-C5
28	A	611	STE	C3-C4-C5-C6
28	b	621	STE	C11-C10-C9-C8
32	a	615	LMG	C19-C20-C21-C22
24	c	512	CLA	C13-C15-C16-C17
28	D	414	STE	C3-C4-C5-C6
28	d	413	STE	C3-C4-C5-C6
29	d	409	LHG	C14-C15-C16-C17
31	C	522	DGD	CAB-CBB-CCB-CDB
24	c	509	CLA	C4-C3-C5-C6
28	z	101	STE	C3-C4-C5-C6
28	f	103	STE	C15-C16-C17-C18
29	l	101	LHG	C27-C28-C29-C30
24	C	506	CLA	C16-C17-C18-C20
31	c	519	DGD	O6D-C5D-C6D-O5D
28	b	621	STE	C7-C8-C9-C10
29	e	102	LHG	C9-C10-C11-C12
26	C	514	BCR	C5-C6-C7-C8
30	f	102	SQD	C23-C24-C25-C26
24	B	606	CLA	C5-C6-C7-C8
28	I	102	STE	C6-C7-C8-C9
30	a	613	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	C16-C17-C18-C20
24	b	601	CLA	C16-C17-C18-C20
29	e	102	LHG	O7-C5-C6-O8
30	D	412	SQD	O6-C44-C45-O47
30	a	612	SQD	O6-C44-C45-O47
32	a	615	LMG	O1-C7-C8-O7
32	c	523	LMG	O1-C7-C8-O7
27	a	610	PL9	C4-C3-C7-C8
28	M	104	STE	C11-C12-C13-C14
29	d	410	LHG	C27-C28-C29-C30
31	C	523	DGD	C2A-C3A-C4A-C5A
27	d	406	PL9	C15-C14-C16-C17
28	H	103	STE	C7-C8-C9-C10
28	c	517	STE	C6-C7-C8-C9
32	M	101	LMG	C37-C38-C39-C40
32	d	412	LMG	C31-C32-C33-C34
30	D	409	SQD	C45-C46-O48-C23
24	c	509	CLA	C2-C3-C5-C6
28	H	103	STE	C15-C16-C17-C18
28	j	102	STE	C10-C11-C12-C13
24	C	513	CLA	C16-C17-C18-C20
28	A	617	STE	C14-C15-C16-C17
28	B	624	STE	C2-C3-C4-C5
28	d	413	STE	C10-C11-C12-C13
28	a	616	STE	C1-C2-C3-C4
24	C	513	CLA	O1D-CGD-O2D-CED
24	A	606	CLA	C11-C10-C8-C9
24	B	604	CLA	C6-C7-C8-C9
29	D	411	LHG	C12-C13-C14-C15
32	D	407	LMG	C33-C34-C35-C36
32	m	101	LMG	C30-C31-C32-C33
28	d	411	STE	C11-C12-C13-C14
30	D	412	SQD	C13-C14-C15-C16
31	C	523	DGD	C7B-C8B-C9B-CAB
28	B	623	STE	C13-C14-C15-C16
29	L	101	LHG	C19-C20-C21-C22
24	A	612	CLA	C16-C17-C18-C19
24	B	610	CLA	C16-C17-C18-C19
24	B	615	CLA	C16-C17-C18-C19
27	a	610	PL9	C44-C46-C47-C48
31	A	615	DGD	CFB-CGB-CHB-CIB
32	B	620	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	C	521	LMG	C17-C18-C19-C20
30	B	622	SQD	C13-C14-C15-C16
30	f	102	SQD	C31-C32-C33-C34
28	A	618	STE	C11-C10-C9-C8
30	a	613	SQD	C19-C20-C21-C22
24	C	509	CLA	C3-C5-C6-C7
32	M	101	LMG	C40-C41-C42-C43
27	d	406	PL9	C38-C39-C41-C42
24	B	610	CLA	C8-C10-C11-C12
28	H	103	STE	C13-C14-C15-C16
29	L	101	LHG	C33-C34-C35-C36
29	L	101	LHG	C10-C11-C12-C13
29	e	102	LHG	C27-C28-C29-C30
32	C	521	LMG	C38-C39-C40-C41
24	a	608	CLA	C15-C16-C17-C18
28	A	616	STE	C14-C15-C16-C17
29	d	408	LHG	C24-C25-C26-C27
31	C	524	DGD	CAA-CBA-CCA-CDA
24	B	614	CLA	C16-C17-C18-C19
24	C	506	CLA	C16-C17-C18-C19
24	C	513	CLA	C16-C17-C18-C19
28	B	623	STE	C4-C5-C6-C7
29	l	101	LHG	C17-C18-C19-C20
31	h	102	DGD	C6B-C7B-C8B-C9B
24	A	606	CLA	C11-C10-C8-C7
24	C	505	CLA	C6-C7-C8-C10
24	a	606	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C15
24	d	403	CLA	C11-C12-C13-C15
24	d	404	CLA	C12-C13-C15-C16
30	B	622	SQD	C27-C28-C29-C30
28	M	104	STE	C9-C10-C11-C12
30	B	622	SQD	C9-C10-C11-C12
31	c	520	DGD	C3A-C4A-C5A-C6A
24	B	616	CLA	C5-C6-C7-C8
26	c	514	BCR	C17-C18-C19-C20
26	c	515	BCR	C21-C22-C23-C24
31	c	521	DGD	CCA-CDA-CEA-CFA
32	C	517	LMG	C14-C15-C16-C17
31	C	523	DGD	C2G-C3G-O3G-C1D
31	C	523	DGD	C5D-C6D-O5D-C1E
31	c	520	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
24	B	613	CLA	C13-C15-C16-C17
32	D	407	LMG	C30-C31-C32-C33
32	c	522	LMG	C39-C40-C41-C42
32	c	522	LMG	O10-C28-O8-C9
28	b	621	STE	C12-C13-C14-C15
28	j	102	STE	C7-C8-C9-C10
30	B	622	SQD	C28-C29-C30-C31
29	D	413	LHG	C23-C24-C25-C26
28	I	101	STE	C5-C6-C7-C8
31	c	519	DGD	C4B-C5B-C6B-C7B
30	B	622	SQD	C46-C45-O47-C7
32	C	517	LMG	C7-C8-O7-C10
32	D	407	LMG	C7-C8-O7-C10
28	T	102	STE	C13-C14-C15-C16
29	D	410	LHG	C25-C26-C27-C28
31	H	102	DGD	C9B-CAB-CBB-CCB
24	c	502	CLA	C16-C17-C18-C19
28	d	413	STE	C6-C7-C8-C9
29	l	101	LHG	C12-C13-C14-C15
28	E	101	STE	C11-C10-C9-C8
24	a	611	CLA	C13-C15-C16-C17
24	c	506	CLA	C8-C10-C11-C12
30	a	612	SQD	C15-C16-C17-C18
28	m	102	STE	C7-C8-C9-C10
31	C	522	DGD	O6E-C1E-O5D-C6D
31	c	521	DGD	C7A-C8A-C9A-CAA
32	d	412	LMG	C10-C11-C12-C13
34	F	101	HEM	C4C-C3C-CAC-CBC
34	f	101	HEM	C4B-C3B-CAB-CBB
34	f	101	HEM	C4C-C3C-CAC-CBC
24	b	608	CLA	C16-C17-C18-C19
24	b	604	CLA	C3-C5-C6-C7
29	A	613	LHG	C29-C30-C31-C32
24	C	506	CLA	C4-C3-C5-C6
28	H	104	STE	C11-C12-C13-C14
30	A	614	SQD	C18-C19-C20-C21
28	b	623	STE	C9-C10-C11-C12
30	D	412	SQD	C25-C26-C27-C28
31	A	615	DGD	O1G-C1G-C2G-O2G
31	c	519	DGD	O1G-C1G-C2G-O2G
32	a	615	LMG	O7-C8-C9-O8
24	A	606	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	D	404	CLA	C13-C15-C16-C17
24	b	607	CLA	C11-C12-C13-C14
28	t	103	STE	C4-C5-C6-C7
28	M	104	STE	C10-C11-C12-C13
28	M	104	STE	C14-C15-C16-C17
28	c	517	STE	C13-C14-C15-C16
28	d	413	STE	C11-C12-C13-C14
28	e	103	STE	C14-C15-C16-C17
29	e	102	LHG	C13-C14-C15-C16
31	C	524	DGD	C7B-C8B-C9B-CAB
28	f	103	STE	C14-C15-C16-C17
30	a	612	SQD	C32-C33-C34-C35
32	c	523	LMG	C32-C33-C34-C35
24	C	512	CLA	C13-C15-C16-C17
24	b	601	CLA	C13-C15-C16-C17
24	d	404	CLA	C10-C11-C12-C13
28	C	526	STE	C4-C5-C6-C7
32	c	522	LMG	C34-C35-C36-C37
29	D	411	LHG	C17-C18-C19-C20
28	B	625	STE	C6-C7-C8-C9
28	a	616	STE	C5-C6-C7-C8
28	d	413	STE	C4-C5-C6-C7
31	c	520	DGD	C9B-CAB-CBB-CCB
24	B	601	CLA	C2-C1-O2A-CGA
31	c	520	DGD	C2E-C1E-O5D-C6D
24	c	505	CLA	C16-C17-C18-C20
29	e	102	LHG	C2-C3-O3-P
29	l	101	LHG	C26-C27-C28-C29
32	a	615	LMG	C8-C9-O8-C28
24	b	605	CLA	C4-C3-C5-C6
24	c	502	CLA	C16-C17-C18-C20
28	d	413	STE	C7-C8-C9-C10
28	T	102	STE	C3-C4-C5-C6
32	d	412	LMG	C12-C13-C14-C15
32	m	101	LMG	C22-C23-C24-C25
28	I	102	STE	C9-C10-C11-C12
32	m	101	LMG	C31-C32-C33-C34
24	b	610	CLA	C4C-C3C-CAC-CBC
30	a	613	SQD	C10-C11-C12-C13
32	B	620	LMG	C19-C20-C21-C22
24	C	504	CLA	C4B-C3B-CAB-CBB
27	d	406	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
26	K	102	BCR	C21-C22-C23-C24
24	c	506	CLA	C15-C16-C17-C18
28	b	621	STE	C4-C5-C6-C7
30	a	613	SQD	C15-C16-C17-C18
28	M	103	STE	C1-C2-C3-C4
24	b	603	CLA	CBD-CGD-O2D-CED
30	a	613	SQD	C27-C28-C29-C30
28	B	623	STE	C6-C7-C8-C9
28	H	103	STE	C12-C13-C14-C15
31	c	520	DGD	C7B-C8B-C9B-CAB
24	B	615	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	B	616	CLA	C11-C10-C8-C7
24	C	504	CLA	C11-C10-C8-C7
24	C	506	CLA	C12-C13-C15-C16
24	b	602	CLA	C12-C13-C15-C16
24	b	603	CLA	C11-C10-C8-C7
24	b	608	CLA	C11-C12-C13-C15
24	b	614	CLA	C11-C10-C8-C7
24	c	505	CLA	C6-C7-C8-C10
24	c	506	CLA	C11-C10-C8-C7
24	c	510	CLA	C11-C10-C8-C7
29	d	410	LHG	C31-C32-C33-C34
24	d	404	CLA	C16-C17-C18-C19
24	B	605	CLA	C13-C15-C16-C17
31	C	522	DGD	C8A-C9A-CAA-CBA
32	D	408	LMG	C39-C40-C41-C42
31	c	519	DGD	CDB-CEB-CFB-CGB
29	A	613	LHG	C12-C13-C14-C15
24	b	608	CLA	C13-C15-C16-C17
28	K	103	STE	C5-C6-C7-C8
28	z	101	STE	C4-C5-C6-C7
32	M	101	LMG	C35-C36-C37-C38
24	C	505	CLA	C6-C7-C8-C9
24	a	606	CLA	C14-C13-C15-C16
24	a	608	CLA	C11-C12-C13-C14
24	d	404	CLA	C14-C13-C15-C16
28	T	102	STE	C10-C11-C12-C13
28	Z	101	STE	C13-C14-C15-C16
31	c	519	DGD	C4D-C5D-C6D-O5D
28	C	516	STE	C3-C4-C5-C6
32	d	412	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	d	413	STE	C5-C6-C7-C8
29	d	410	LHG	C30-C31-C32-C33
31	c	521	DGD	C3B-C4B-C5B-C6B
32	C	517	LMG	O7-C8-C9-O8
24	C	505	CLA	C8-C10-C11-C12
31	c	520	DGD	C5A-C6A-C7A-C8A
30	D	412	SQD	O6-C44-C45-C46
31	A	615	DGD	O1G-C1G-C2G-C3G
32	c	523	LMG	O1-C7-C8-C9
24	C	506	CLA	C15-C16-C17-C18
28	b	625	STE	C11-C10-C9-C8
24	B	601	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	b	604	CLA	C13-C15-C16-C17
32	M	101	LMG	C39-C40-C41-C42
24	D	403	CLA	C2C-C3C-CAC-CBC
29	d	409	LHG	C19-C20-C21-C22
31	c	521	DGD	C8A-C9A-CAA-CBA
24	c	502	CLA	O1A-CGA-O2A-C1
28	b	624	STE	C5-C6-C7-C8
30	B	622	SQD	C26-C27-C28-C29
24	B	601	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O1D
26	C	514	BCR	C13-C14-C15-C16
29	D	413	LHG	C3-O3-P-O5
29	L	101	LHG	C4-O6-P-O5
29	d	409	LHG	C3-O3-P-O5
29	d	409	LHG	C4-O6-P-O4
29	e	102	LHG	C3-O3-P-O4
32	a	615	LMG	C39-C40-C41-C42
24	C	504	CLA	C2B-C3B-CAB-CBB
24	C	506	CLA	C2-C3-C5-C6
27	A	610	PL9	C28-C29-C31-C32
29	D	411	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
29	d	410	LHG	C2-C3-O3-P
29	D	410	LHG	C11-C12-C13-C14
24	b	608	CLA	C16-C17-C18-C20
24	c	504	CLA	C11-C12-C13-C15
28	k	103	STE	C11-C10-C9-C8
28	B	621	STE	C5-C6-C7-C8
28	d	407	STE	C14-C15-C16-C17
32	D	407	LMG	C16-C17-C18-C19
30	A	614	SQD	C7-C8-C9-C10
29	d	408	LHG	C26-C27-C28-C29
31	C	522	DGD	C4E-C5E-C6E-O5E
32	C	521	LMG	C9-C8-O7-C10
28	b	623	STE	C10-C11-C12-C13
29	D	413	LHG	C26-C27-C28-C29
31	C	522	DGD	CBB-CCB-CDB-CEB
24	c	512	CLA	C8-C10-C11-C12
29	D	410	LHG	C29-C30-C31-C32
30	a	613	SQD	C11-C12-C13-C14
31	c	519	DGD	C8B-C9B-CAB-CBB
26	h	101	BCR	C9-C10-C11-C12
24	B	611	CLA	C11-C12-C13-C14
24	C	513	CLA	C11-C12-C13-C14
24	b	608	CLA	C11-C12-C13-C14
24	b	614	CLA	C11-C12-C13-C14
24	c	505	CLA	C6-C7-C8-C9
24	c	510	CLA	C11-C10-C8-C9
30	D	412	SQD	C28-C29-C30-C31
24	B	604	CLA	C11-C10-C8-C7
24	c	512	CLA	C6-C7-C8-C10
25	a	607	PHO	C6-C7-C8-C10
24	b	612	CLA	C10-C11-C12-C13
24	C	510	CLA	C10-C11-C12-C13
24	c	502	CLA	CBA-CGA-O2A-C1
30	D	412	SQD	C29-C30-C31-C32
28	D	414	STE	C5-C6-C7-C8
24	c	505	CLA	C8-C10-C11-C12
32	C	525	LMG	C15-C16-C17-C18
27	A	610	PL9	C38-C39-C41-C42
29	A	613	LHG	C24-C25-C26-C27
31	H	102	DGD	CBA-CCA-CDA-CEA
24	c	504	CLA	C11-C12-C13-C14
28	M	103	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	A	613	LHG	C18-C19-C20-C21
29	e	102	LHG	O9-C7-O7-C5
32	D	408	LMG	C31-C32-C33-C34
29	A	613	LHG	O7-C5-C6-O8
24	c	509	CLA	CAA-CBA-CGA-O2A
29	d	409	LHG	C11-C10-C9-C8
28	D	414	STE	C9-C10-C11-C12
28	i	101	STE	C6-C7-C8-C9
31	h	102	DGD	C1A-C2A-C3A-C4A
29	e	102	LHG	C8-C7-O7-C5
32	M	101	LMG	C36-C37-C38-C39
29	d	408	LHG	C25-C26-C27-C28
29	d	408	LHG	C18-C19-C20-C21
31	H	102	DGD	C8B-C9B-CAB-CBB
28	B	621	STE	C9-C10-C11-C12
24	B	601	CLA	C13-C15-C16-C17
32	a	614	LMG	C15-C16-C17-C18
24	b	604	CLA	C4-C3-C5-C6
28	H	104	STE	C15-C16-C17-C18
30	D	409	SQD	O48-C23-C24-C25
24	C	512	CLA	C15-C16-C17-C18
24	b	604	CLA	C16-C17-C18-C19
24	B	616	CLA	C11-C10-C8-C9
24	b	602	CLA	C14-C13-C15-C16
24	b	614	CLA	C11-C10-C8-C9
24	c	506	CLA	C11-C10-C8-C9
31	C	524	DGD	O6D-C5D-C6D-O5D
24	A	605	CLA	C2C-C3C-CAC-CBC
28	C	528	STE	C12-C13-C14-C15
31	C	524	DGD	C4B-C5B-C6B-C7B
28	A	618	STE	C15-C16-C17-C18
31	h	102	DGD	CDB-CEB-CFB-CGB
32	b	622	LMG	C35-C36-C37-C38
30	a	613	SQD	C33-C34-C35-C36
29	d	409	LHG	C18-C19-C20-C21
32	C	525	LMG	C29-C28-O8-C9
31	A	615	DGD	C1B-C2B-C3B-C4B
24	c	501	CLA	C2A-CAA-CBA-CGA
24	C	510	CLA	C4-C3-C5-C6
24	b	605	CLA	C2-C3-C5-C6
24	B	610	CLA	C15-C16-C17-C18
29	D	410	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	D	410	LHG	C30-C31-C32-C33
24	c	513	CLA	C8-C10-C11-C12
30	D	409	SQD	C29-C30-C31-C32
32	m	101	LMG	C29-C30-C31-C32
24	C	510	CLA	C6-C7-C8-C10
32	C	525	LMG	O10-C28-O8-C9
31	C	523	DGD	C8B-C9B-CAB-CBB
28	A	617	STE	C9-C10-C11-C12
29	D	413	LHG	C32-C33-C34-C35
29	e	102	LHG	C11-C10-C9-C8
31	c	521	DGD	C9A-CAA-CBA-CCA
32	a	615	LMG	C31-C32-C33-C34
31	h	102	DGD	CBA-CCA-CDA-CEA
32	C	521	LMG	C34-C35-C36-C37
24	b	615	CLA	C16-C17-C18-C19
31	C	524	DGD	CDB-CEB-CFB-CGB
30	B	622	SQD	C10-C11-C12-C13
28	T	102	STE	C6-C7-C8-C9
28	b	624	STE	C4-C5-C6-C7
30	A	614	SQD	C17-C18-C19-C20
26	c	514	BCR	C13-C14-C15-C16
24	B	607	CLA	C3-C5-C6-C7
29	l	101	LHG	C29-C30-C31-C32
32	C	525	LMG	C18-C19-C20-C21
24	B	605	CLA	C8-C10-C11-C12
29	L	101	LHG	C35-C36-C37-C38
35	v	201	HEC	CAD-CBD-CGD-O1D
29	e	102	LHG	C1-C2-C3-O3
27	A	610	PL9	C24-C26-C27-C28
24	B	609	CLA	C13-C15-C16-C17
28	E	101	STE	C10-C11-C12-C13
31	H	102	DGD	CCA-CDA-CEA-CFA
24	B	615	CLA	C11-C10-C8-C9
24	D	403	CLA	C11-C10-C8-C9
24	b	603	CLA	C11-C10-C8-C9
24	c	511	CLA	C11-C10-C8-C9
29	D	410	LHG	C12-C13-C14-C15
30	B	622	SQD	C31-C32-C33-C34
29	D	413	LHG	O1-C1-C2-C3
29	d	409	LHG	C16-C17-C18-C19
29	D	410	LHG	C32-C33-C34-C35
29	D	413	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	c	519	DGD	O1G-C1A-C2A-C3A
32	C	521	LMG	C7-C8-O7-C10
24	b	602	CLA	C8-C10-C11-C12
31	C	522	DGD	C6A-C7A-C8A-C9A
29	D	413	LHG	C19-C20-C21-C22
24	C	509	CLA	C16-C17-C18-C19
24	A	608	CLA	C6-C7-C8-C9
27	d	406	PL9	C13-C14-C16-C17
28	e	103	STE	C12-C13-C14-C15
24	c	509	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	C15-C16-C17-C18
30	a	612	SQD	C24-C25-C26-C27
30	D	412	SQD	C34-C35-C36-C37
24	B	615	CLA	C2B-C3B-CAB-CBB
28	d	413	STE	C9-C10-C11-C12
32	M	101	LMG	C10-C11-C12-C13
32	c	518	LMG	C29-C28-O8-C9
28	m	103	STE	C11-C12-C13-C14
32	C	521	LMG	C37-C38-C39-C40
30	f	102	SQD	C28-C29-C30-C31
24	b	607	CLA	C16-C17-C18-C20
24	c	510	CLA	O1D-CGD-O2D-CED
28	a	616	STE	O2-C1-C2-C3
24	c	513	CLA	C4-C3-C5-C6
27	D	406	PL9	C40-C39-C41-C42
27	D	406	PL9	C45-C44-C46-C47
32	C	517	LMG	C29-C30-C31-C32
28	j	102	STE	C11-C12-C13-C14
24	C	510	CLA	C2-C3-C5-C6
30	a	613	SQD	C12-C13-C14-C15
31	c	521	DGD	C1B-C2B-C3B-C4B
24	c	513	CLA	CBA-CGA-O2A-C1
24	b	604	CLA	C11-C12-C13-C15
24	b	614	CLA	C11-C12-C13-C15
24	c	507	CLA	C11-C12-C13-C15
24	c	513	CLA	C11-C10-C8-C7
27	D	406	PL9	C47-C48-C49-C50
29	A	613	LHG	C25-C26-C27-C28
31	A	615	DGD	O2G-C2G-C3G-O3G
29	l	101	LHG	C24-C25-C26-C27
32	C	525	LMG	C39-C40-C41-C42
24	b	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	m	101	LMG	C35-C36-C37-C38
28	a	616	STE	O1-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O2D
24	c	510	CLA	CBD-CGD-O2D-CED
27	A	610	PL9	C22-C23-C24-C26
34	F	101	HEM	CAD-CBD-CGD-O1D
28	c	517	STE	C10-C11-C12-C13
30	b	620	SQD	C12-C13-C14-C15
32	c	523	LMG	C28-C29-C30-C31
24	C	510	CLA	C6-C7-C8-C9
24	a	608	CLA	C6-C7-C8-C9
29	D	411	LHG	C27-C28-C29-C30
24	a	605	CLA	C2C-C3C-CAC-CBC
28	C	516	STE	C9-C10-C11-C12
24	c	512	CLA	C4-C3-C5-C6
24	C	507	CLA	C5-C6-C7-C8
24	b	611	CLA	C10-C11-C12-C13
30	b	620	SQD	C25-C26-C27-C28
30	b	620	SQD	C28-C29-C30-C31
24	b	615	CLA	C16-C17-C18-C20
28	I	101	STE	C2-C3-C4-C5
27	A	610	PL9	C42-C43-C44-C46
32	c	518	LMG	O10-C28-O8-C9
32	m	101	LMG	C37-C38-C39-C40
31	A	615	DGD	C1G-C2G-C3G-O3G
31	C	523	DGD	CDB-CEB-CFB-CGB
34	F	101	HEM	CAD-CBD-CGD-O2D
24	d	403	CLA	C2C-C3C-CAC-CBC
24	C	509	CLA	C16-C17-C18-C20
32	a	615	LMG	C12-C13-C14-C15
32	C	521	LMG	C14-C15-C16-C17
28	d	407	STE	O2-C1-C2-C3
30	f	102	SQD	C27-C28-C29-C30
24	B	615	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C4B-C3B-CAB-CBB
30	D	412	SQD	C30-C31-C32-C33
32	c	518	LMG	O8-C28-C29-C30
30	f	102	SQD	C32-C33-C34-C35
31	c	519	DGD	C4A-C5A-C6A-C7A
24	A	605	CLA	C16-C17-C18-C19
24	C	501	CLA	C16-C17-C18-C20
29	D	410	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	A	607	PHO	CHA-CBD-CGD-O1D
24	A	605	CLA	C4C-C3C-CAC-CBC
24	C	512	CLA	C8-C10-C11-C12
28	d	411	STE	C7-C8-C9-C10
32	d	412	LMG	C33-C34-C35-C36
28	b	625	STE	C13-C14-C15-C16
29	D	411	LHG	C13-C14-C15-C16
29	d	409	LHG	C26-C27-C28-C29
24	B	613	CLA	C16-C17-C18-C19
24	C	513	CLA	C13-C15-C16-C17
30	a	612	SQD	C23-C24-C25-C26
24	c	512	CLA	C2-C3-C5-C6
24	B	608	CLA	C15-C16-C17-C18
24	C	509	CLA	C13-C15-C16-C17
24	C	509	CLA	C12-C13-C15-C16
32	B	620	LMG	C30-C31-C32-C33
28	d	407	STE	O1-C1-C2-C3
32	c	523	LMG	C12-C13-C14-C15
26	k	102	BCR	C7-C8-C9-C10
24	A	605	CLA	C14-C13-C15-C16
24	B	601	CLA	C14-C13-C15-C16
24	B	611	CLA	C14-C13-C15-C16
24	B	615	CLA	C14-C13-C15-C16
24	C	506	CLA	C14-C13-C15-C16
24	C	513	CLA	C14-C13-C15-C16
24	c	509	CLA	C11-C10-C8-C9
28	m	103	STE	C9-C10-C11-C12
30	a	612	SQD	C5-C6-S-O8
24	B	612	CLA	C8-C10-C11-C12
24	B	610	CLA	C2A-CAA-CBA-CGA
24	B	613	CLA	C2-C1-O2A-CGA
24	b	616	CLA	C2-C1-O2A-CGA
24	d	403	CLA	C2-C1-O2A-CGA
30	B	622	SQD	C18-C19-C20-C21
32	C	521	LMG	C40-C41-C42-C43
32	b	622	LMG	C34-C35-C36-C37
27	a	610	PL9	C20-C19-C21-C22
29	e	102	LHG	C19-C20-C21-C22
31	h	102	DGD	O1B-C1B-C2B-C3B
28	E	102	STE	O2-C1-C2-C3
24	c	512	CLA	O2A-C1-C2-C3
32	b	622	LMG	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
32	B	620	LMG	C16-C17-C18-C19
31	c	520	DGD	C6B-C7B-C8B-C9B
32	D	407	LMG	O8-C28-C29-C30
24	c	505	CLA	C10-C11-C12-C13
28	B	623	STE	O2-C1-C2-C3
31	C	524	DGD	CBB-CCB-CDB-CEB
28	e	104	STE	C2-C3-C4-C5
24	a	605	CLA	C4C-C3C-CAC-CBC
32	B	620	LMG	C18-C19-C20-C21
27	A	610	PL9	C21-C22-C23-C24
28	m	103	STE	C15-C16-C17-C18
31	c	520	DGD	O6E-C1E-O5D-C6D
28	R	101	STE	C2-C3-C4-C5
24	c	513	CLA	O1A-CGA-O2A-C1
29	d	408	LHG	C33-C34-C35-C36
28	R	101	STE	C5-C6-C7-C8
24	a	611	CLA	C2C-C3C-CAC-CBC
29	D	411	LHG	C24-C25-C26-C27
32	a	614	LMG	C34-C35-C36-C37
24	D	404	CLA	C4-C3-C5-C6
28	E	102	STE	O1-C1-C2-C3
26	k	102	BCR	C19-C20-C21-C22
28	B	623	STE	O1-C1-C2-C3
30	D	412	SQD	C27-C28-C29-C30
28	C	516	STE	C6-C7-C8-C9
31	c	520	DGD	C9A-CAA-CBA-CCA
28	j	102	STE	C13-C14-C15-C16
30	a	613	SQD	C13-C14-C15-C16
24	B	606	CLA	C11-C10-C8-C9
24	B	615	CLA	C11-C12-C13-C14
24	C	504	CLA	C11-C10-C8-C9
24	a	608	CLA	C14-C13-C15-C16
24	a	605	CLA	C16-C17-C18-C19
32	b	622	LMG	C33-C34-C35-C36
32	b	622	LMG	O8-C28-C29-C30
31	H	102	DGD	O1B-C1B-C2B-C3B
35	V	201	HEC	CAD-CBD-CGD-O1D
35	V	201	HEC	CAD-CBD-CGD-O2D
29	D	411	LHG	C31-C32-C33-C34
32	C	517	LMG	O7-C10-C11-C12
28	i	101	STE	O2-C1-C2-C3
32	a	614	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	L	101	LHG	C5-C6-O8-C23
24	A	605	CLA	C12-C13-C15-C16
24	B	613	CLA	C11-C12-C13-C15
24	a	608	CLA	C6-C7-C8-C10
24	b	605	CLA	C11-C10-C8-C7
24	c	509	CLA	C11-C10-C8-C7
24	A	605	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C2B-C3B-CAB-CBB
24	a	605	CLA	C2B-C3B-CAB-CBB
24	c	501	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
30	A	614	SQD	C15-C16-C17-C18
24	D	403	CLA	C2-C1-O2A-CGA
24	c	512	CLA	C2-C1-O2A-CGA
24	d	404	CLA	O1A-CGA-O2A-C1
28	K	103	STE	C11-C12-C13-C14
29	D	413	LHG	C18-C19-C20-C21
32	a	614	LMG	C40-C41-C42-C43
31	c	520	DGD	C1A-C2A-C3A-C4A
30	D	409	SQD	C24-C25-C26-C27
24	B	614	CLA	C5-C6-C7-C8
34	f	101	HEM	CAD-CBD-CGD-O1D
28	H	103	STE	C1-C2-C3-C4
24	C	505	CLA	C10-C11-C12-C13
31	h	102	DGD	CAB-CBB-CCB-CDB
31	c	521	DGD	CBA-CCA-CDA-CEA
24	b	603	CLA	C2A-CAA-CBA-CGA
30	a	613	SQD	C23-C24-C25-C26
28	B	624	STE	C4-C5-C6-C7
24	B	607	CLA	C13-C15-C16-C17
24	B	615	CLA	C13-C15-C16-C17
32	M	101	LMG	O8-C28-C29-C30
32	c	523	LMG	O8-C28-C29-C30
28	K	103	STE	C7-C8-C9-C10
28	d	411	STE	C4-C5-C6-C7
28	e	103	STE	C15-C16-C17-C18
32	b	622	LMG	C38-C39-C40-C41
31	c	521	DGD	C7B-C8B-C9B-CAB
28	C	518	STE	C3-C4-C5-C6
24	b	616	CLA	C10-C11-C12-C13
32	M	101	LMG	O10-C28-O8-C9
30	A	614	SQD	C4-C5-C6-S

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C4-C3-C5-C6
24	c	511	CLA	C3-C5-C6-C7
31	A	615	DGD	C6B-C7B-C8B-C9B
24	D	404	CLA	C10-C11-C12-C13
28	H	104	STE	C14-C15-C16-C17
28	h	103	STE	C14-C15-C16-C17
24	B	610	CLA	C14-C13-C15-C16
24	C	509	CLA	C14-C13-C15-C16
24	c	503	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C12-C13-C14
31	c	519	DGD	O2G-C1B-C2B-C3B
32	a	615	LMG	C29-C30-C31-C32
24	a	606	CLA	C4B-C3B-CAB-CBB
24	b	601	CLA	C4B-C3B-CAB-CBB
28	I	101	STE	O1-C1-C2-C3
28	M	103	STE	C3-C4-C5-C6
32	a	614	LMG	C24-C25-C26-C27
24	C	505	CLA	C4-C3-C5-C6
24	c	510	CLA	CAA-CBA-CGA-O2A
32	c	522	LMG	O7-C10-C11-C12
27	D	406	PL9	C36-C37-C38-C39
24	d	403	CLA	C16-C17-C18-C20
24	B	612	CLA	CAA-CBA-CGA-O2A
24	b	613	CLA	CAA-CBA-CGA-O2A
24	b	601	CLA	O1A-CGA-O2A-C1
30	a	612	SQD	C5-C6-S-O7
24	C	506	CLA	C2-C1-O2A-CGA
24	B	601	CLA	C12-C13-C15-C16
24	B	605	CLA	C6-C7-C8-C10
24	C	512	CLA	C12-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C7
24	b	611	CLA	C12-C13-C15-C16
32	M	101	LMG	C29-C28-O8-C9
28	m	103	STE	C14-C15-C16-C17
30	b	620	SQD	C17-C18-C19-C20
24	c	509	CLA	C16-C17-C18-C19
24	a	611	CLA	C4C-C3C-CAC-CBC
32	M	101	LMG	C7-C8-O7-C10
31	A	615	DGD	C5A-C6A-C7A-C8A
28	i	101	STE	O1-C1-C2-C3
30	a	612	SQD	C16-C17-C18-C19
24	B	614	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	C	501	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
24	B	613	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C20
27	d	406	PL9	C36-C37-C38-C39
32	c	522	LMG	C16-C17-C18-C19
31	C	522	DGD	O2G-C1B-C2B-C3B
29	e	102	LHG	C12-C13-C14-C15
24	b	601	CLA	CBA-CGA-O2A-C1
28	I	101	STE	O2-C1-C2-C3
27	A	610	PL9	C15-C14-C16-C17
27	A	610	PL9	C20-C19-C21-C22
24	b	610	CLA	C15-C16-C17-C18
24	b	612	CLA	C8-C10-C11-C12
24	b	614	CLA	C8-C10-C11-C12
24	c	505	CLA	C16-C17-C18-C19
32	a	614	LMG	O7-C10-C11-C12
28	b	625	STE	C10-C11-C12-C13
29	A	613	LHG	C10-C11-C12-C13
32	c	522	LMG	C15-C16-C17-C18
31	A	615	DGD	CBA-CCA-CDA-CEA
24	d	404	CLA	CBA-CGA-O2A-C1
28	M	103	STE	C7-C8-C9-C10
28	I	102	STE	C2-C3-C4-C5
31	h	102	DGD	C9A-CAA-CBA-CCA
29	l	101	LHG	O7-C7-C8-C9
24	b	604	CLA	C11-C12-C13-C14
24	c	513	CLA	C11-C10-C8-C9
24	d	403	CLA	C11-C12-C13-C14
25	a	607	PHO	C6-C7-C8-C9
31	c	519	DGD	O1B-C1B-C2B-C3B
32	b	622	LMG	O10-C28-C29-C30
30	A	614	SQD	O47-C7-C8-C9
24	c	506	CLA	C10-C11-C12-C13
28	M	102	STE	O2-C1-C2-C3
34	f	101	HEM	CAD-CBD-CGD-O2D
32	a	615	LMG	C14-C15-C16-C17
24	c	510	CLA	CAA-CBA-CGA-O1A
32	M	101	LMG	O10-C28-C29-C30
32	c	523	LMG	O10-C28-C29-C30
32	D	408	LMG	C11-C12-C13-C14
29	d	409	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
28	c	516	STE	C4-C5-C6-C7
26	H	101	BCR	C7-C8-C9-C10
32	C	517	LMG	O9-C10-C11-C12
28	E	101	STE	C14-C15-C16-C17
30	b	620	SQD	O6-C44-C45-O47
32	D	408	LMG	C18-C19-C20-C21
32	c	522	LMG	O9-C10-C11-C12
24	B	608	CLA	C13-C15-C16-C17
31	C	523	DGD	C5B-C6B-C7B-C8B
32	M	101	LMG	O1-C7-C8-C9
28	A	617	STE	C11-C10-C9-C8
24	B	609	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
25	a	607	PHO	CAD-CBD-CGD-O2D
28	b	621	STE	C10-C11-C12-C13
32	C	517	LMG	O6-C1-O1-C7
24	C	506	CLA	O1A-CGA-O2A-C1
32	a	614	LMG	C14-C15-C16-C17
28	C	516	STE	O2-C1-C2-C3
29	D	411	LHG	C30-C31-C32-C33
24	C	505	CLA	C2-C3-C5-C6
24	b	611	CLA	C15-C16-C17-C18
28	R	101	STE	O2-C1-C2-C3
31	C	522	DGD	O1B-C1B-C2B-C3B
30	B	622	SQD	C29-C30-C31-C32
24	C	505	CLA	CAA-CBA-CGA-O2A
24	b	612	CLA	CAA-CBA-CGA-O2A
32	a	614	LMG	C30-C31-C32-C33
30	B	622	SQD	C35-C36-C37-C38
28	c	517	STE	C2-C3-C4-C5
30	D	409	SQD	C30-C31-C32-C33
28	B	623	STE	C11-C10-C9-C8

There are no ring outliers.

88 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	508	CLA	1	0
26	h	101	BCR	5	0
28	T	102	STE	1	0
24	C	502	CLA	1	0

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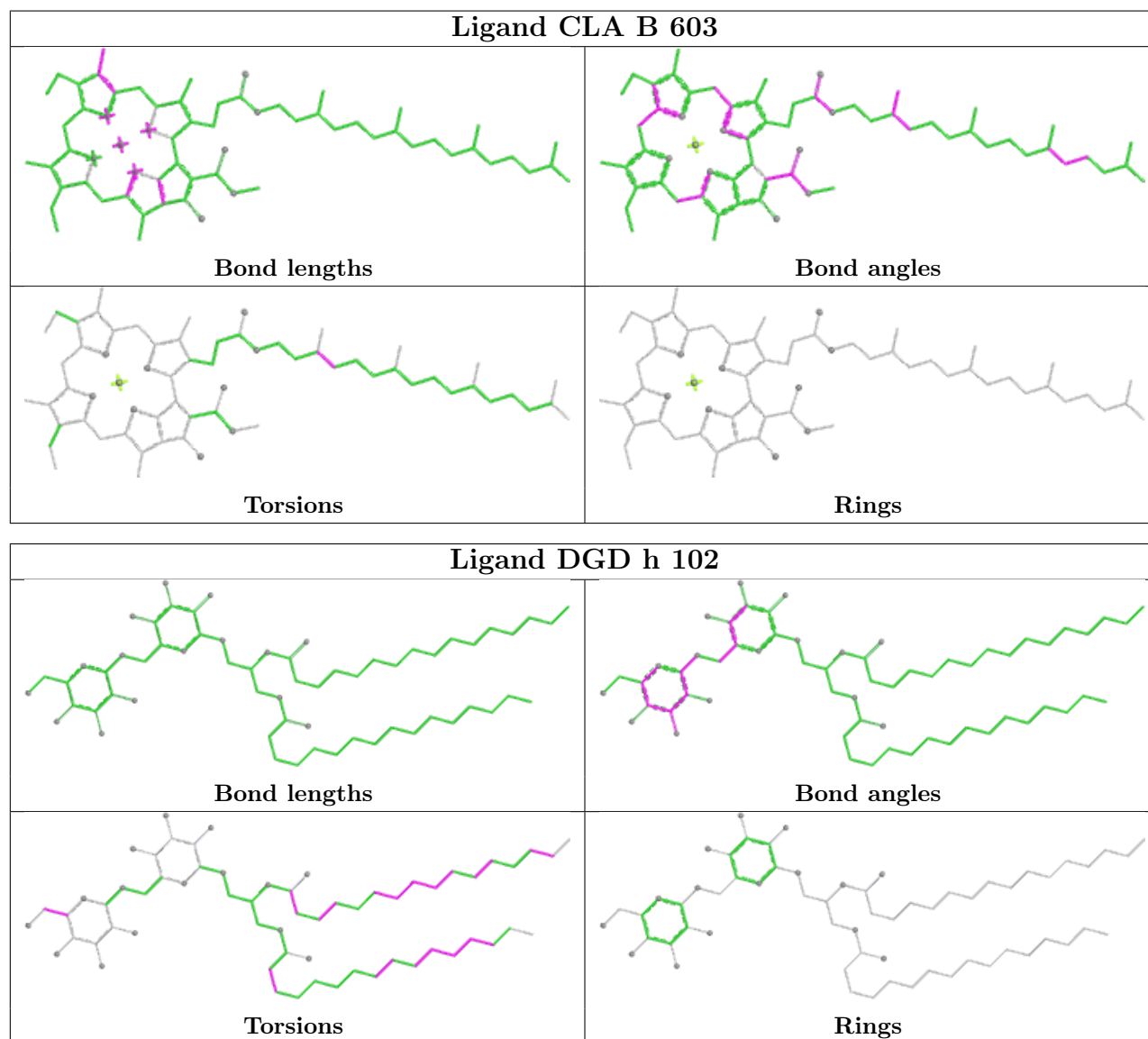
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	617	BCR	1	0
32	D	407	LMG	3	0
32	C	517	LMG	1	0
24	B	613	CLA	1	0
29	l	101	LHG	1	0
26	b	618	BCR	1	0
24	D	403	CLA	1	0
24	c	505	CLA	2	0
24	b	614	CLA	4	0
26	B	618	BCR	1	0
31	c	521	DGD	1	0
26	b	617	BCR	2	0
24	C	512	CLA	1	0
28	A	617	STE	2	0
24	B	614	CLA	1	0
24	b	613	CLA	2	0
24	C	509	CLA	3	0
24	B	604	CLA	1	0
24	d	404	CLA	1	0
28	c	517	STE	1	0
27	A	610	PL9	2	0
32	c	523	LMG	1	0
24	a	605	CLA	2	0
28	d	413	STE	1	0
24	c	501	CLA	1	0
26	b	619	BCR	1	0
24	C	511	CLA	1	0
28	b	625	STE	2	0
29	A	613	LHG	1	0
26	D	405	BCR	5	0
26	C	515	BCR	1	0
26	H	101	BCR	4	0
32	M	101	LMG	1	0
24	C	505	CLA	2	0
30	B	622	SQD	2	0
29	d	408	LHG	1	0
30	a	613	SQD	1	0
29	e	102	LHG	1	0
24	B	601	CLA	6	0
26	k	102	BCR	3	0
24	b	609	CLA	1	0
32	D	408	LMG	3	0

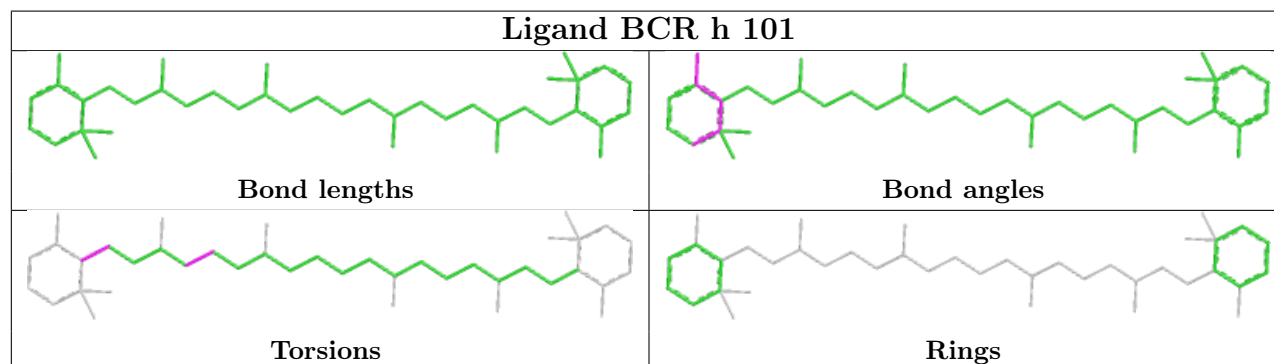
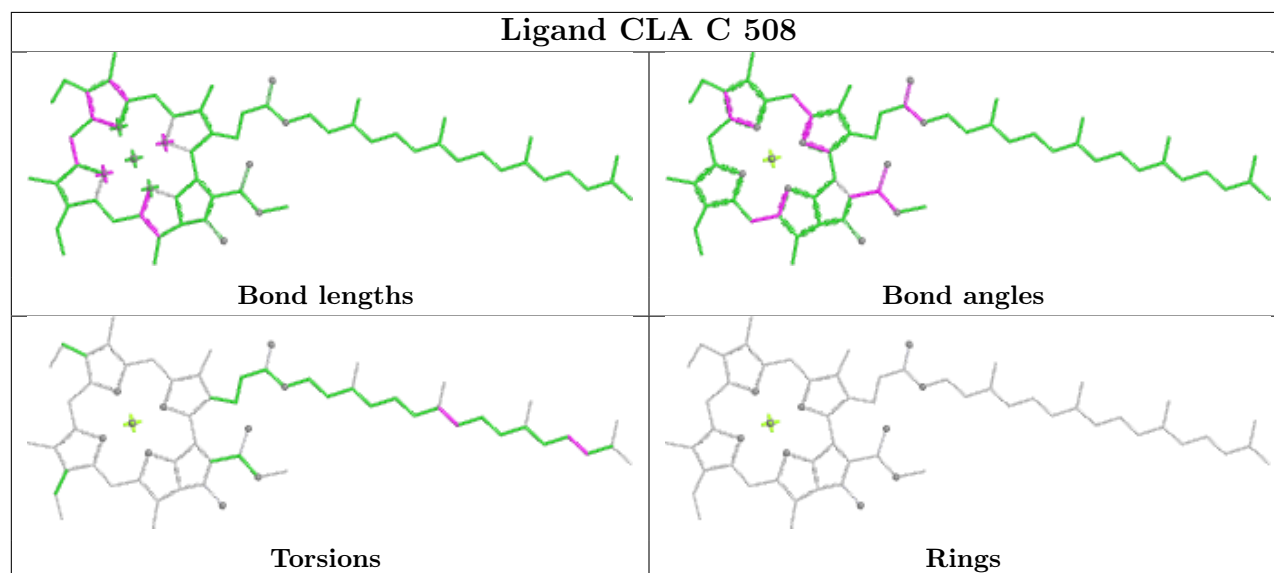
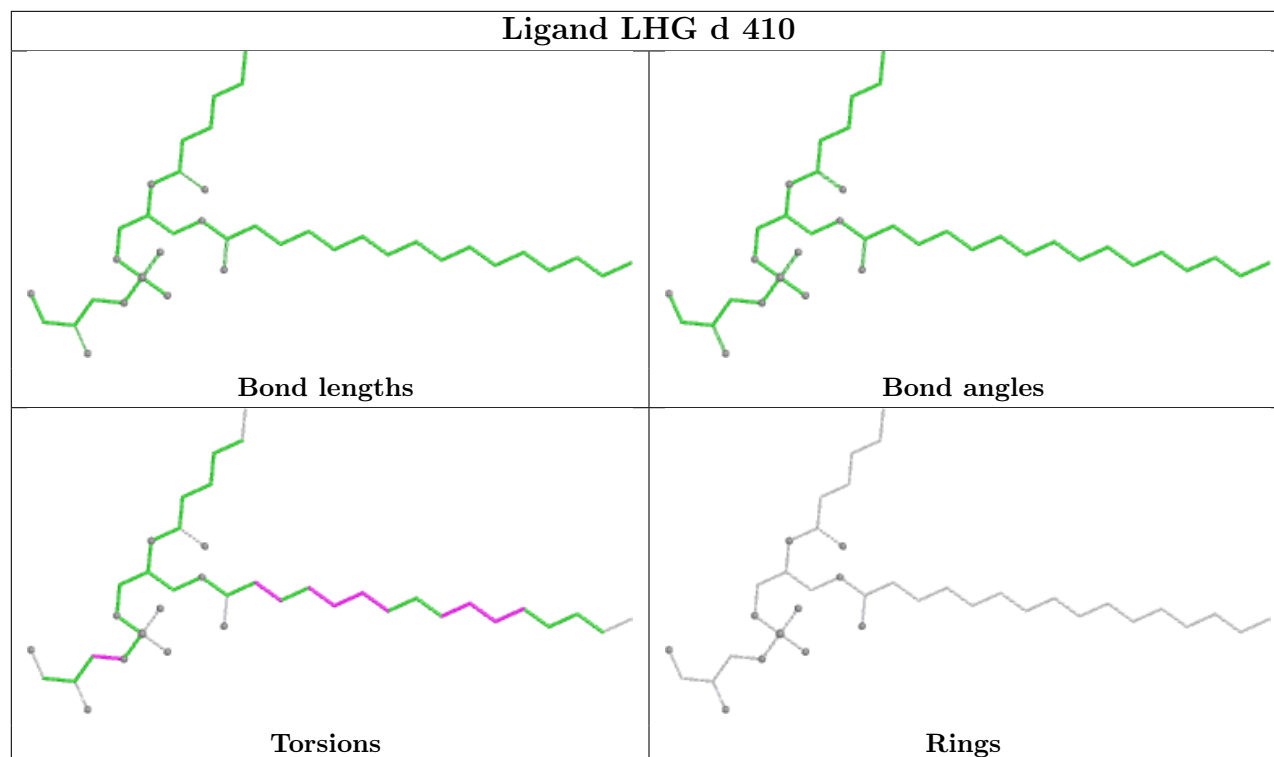
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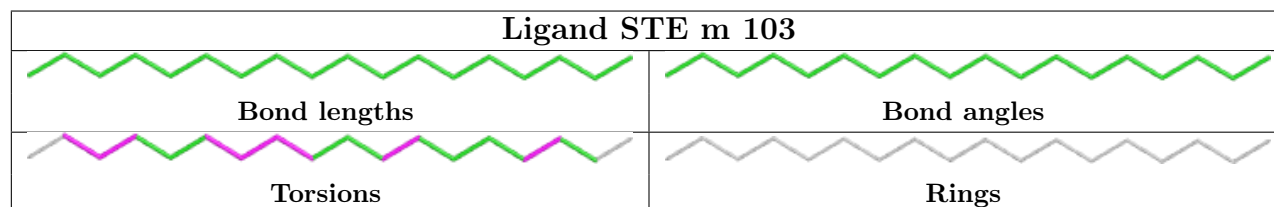
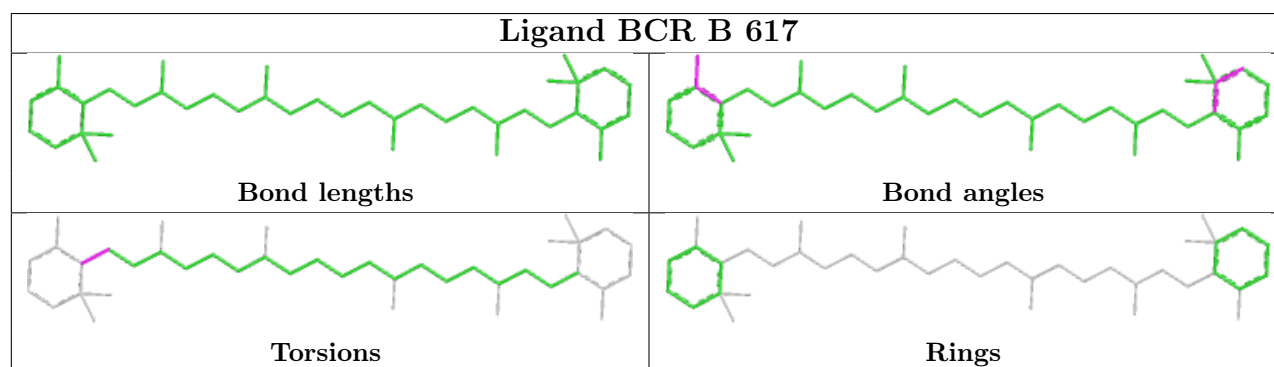
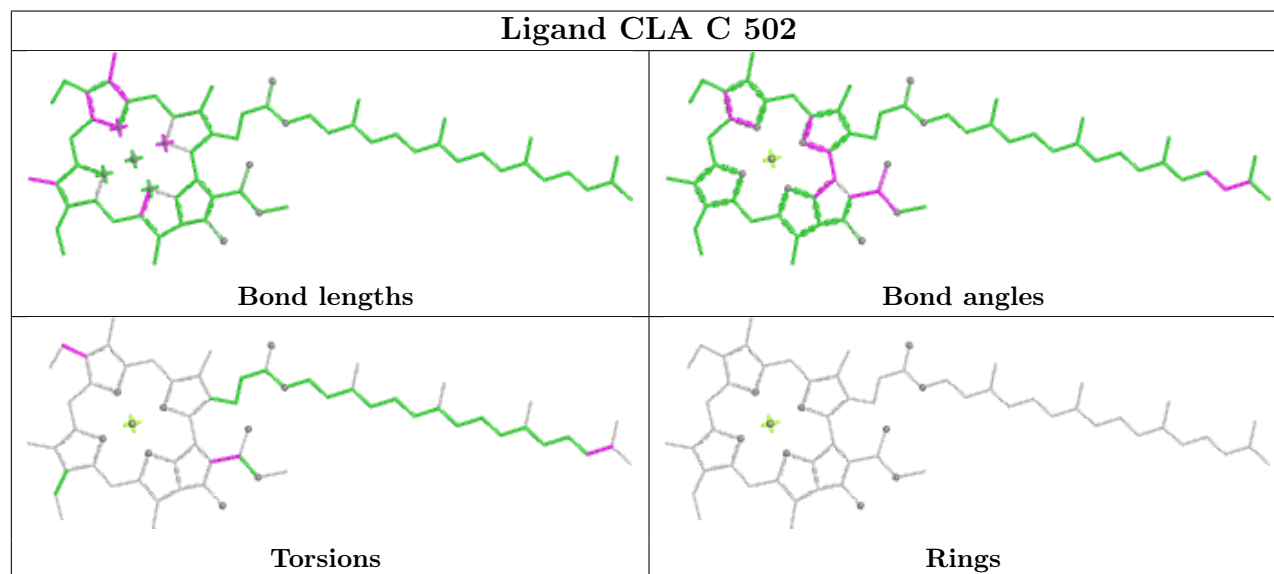
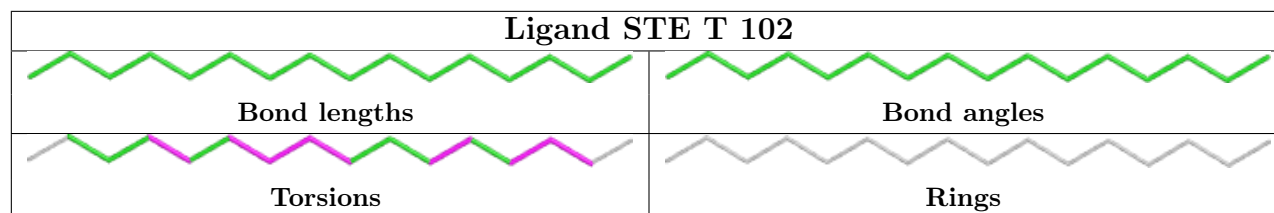
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	610	PL9	2	0
24	B	605	CLA	3	0
24	c	509	CLA	1	0
34	F	101	HEM	4	0
24	C	513	CLA	1	0
25	d	402	PHO	1	0
24	c	507	CLA	1	0
29	D	413	LHG	1	0
32	B	620	LMG	2	0
24	c	511	CLA	2	0
24	A	608	CLA	1	0
24	B	612	CLA	3	0
32	C	521	LMG	1	0
24	b	615	CLA	1	0
24	b	602	CLA	1	0
29	D	410	LHG	1	0
26	C	514	BCR	3	0
28	A	618	STE	2	0
30	D	409	SQD	1	0
26	k	101	BCR	2	0
24	b	610	CLA	1	0
24	b	603	CLA	2	0
26	t	101	BCR	2	0
24	B	602	CLA	1	0
34	f	101	HEM	4	0
26	A	609	BCR	1	0
29	L	101	LHG	3	0
31	A	615	DGD	1	0
32	a	614	LMG	2	0
24	B	610	CLA	1	0
26	T	101	BCR	4	0
28	H	103	STE	1	0
24	c	513	CLA	3	0
26	d	405	BCR	5	0
24	A	606	CLA	2	0
28	d	411	STE	2	0
32	m	101	LMG	4	0
26	B	619	BCR	1	0
24	A	605	CLA	3	0
24	B	611	CLA	2	0
24	b	605	CLA	2	0
26	K	101	BCR	2	0

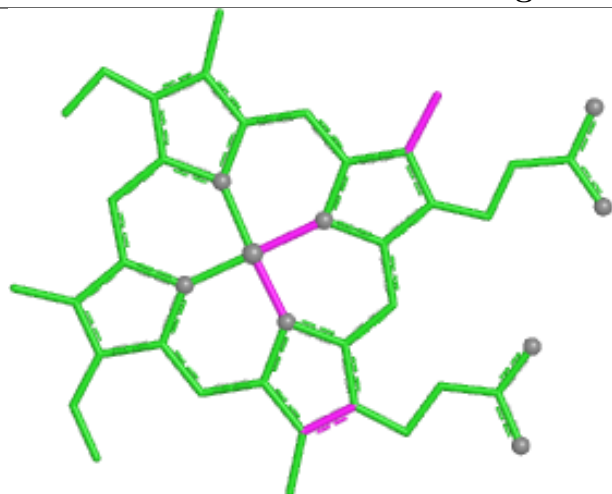
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



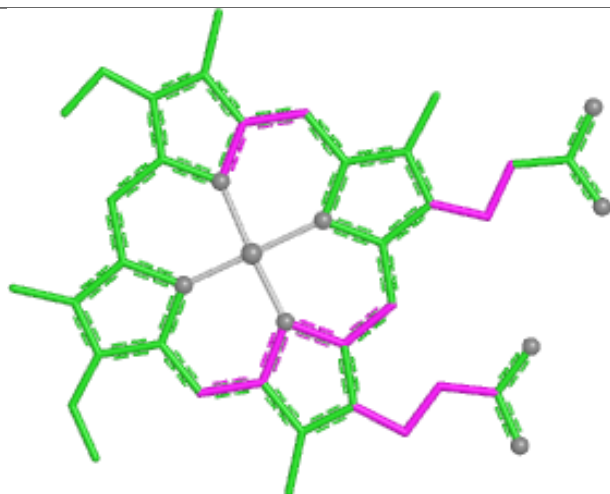




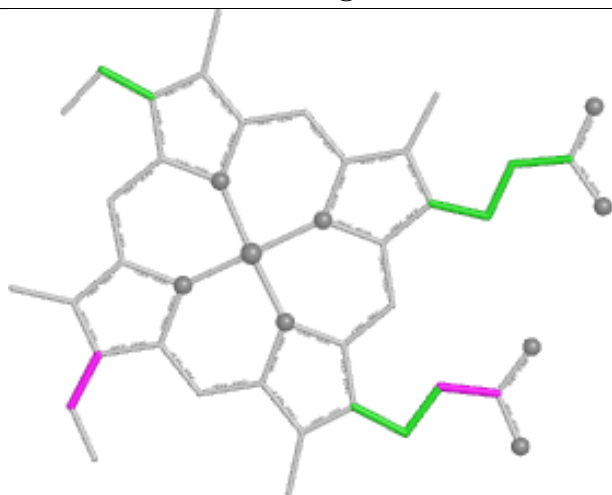
Ligand HEC v 201



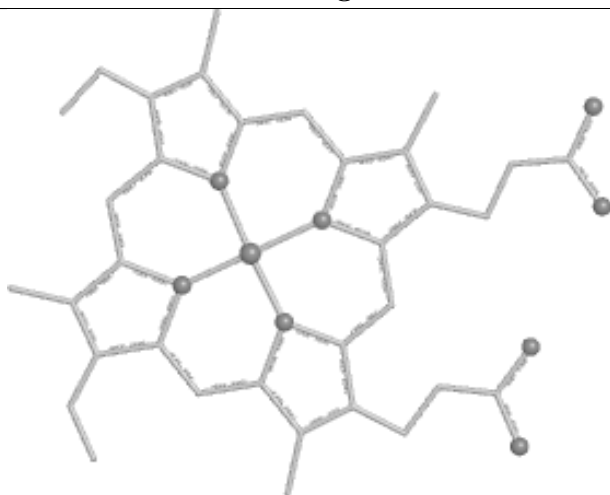
Bond lengths



Bond angles

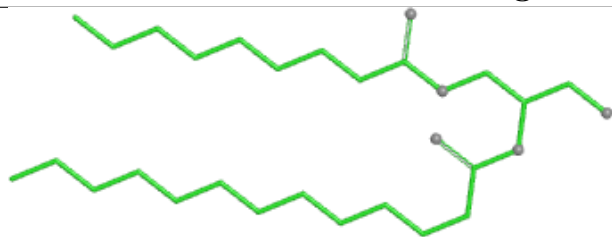


Torsions

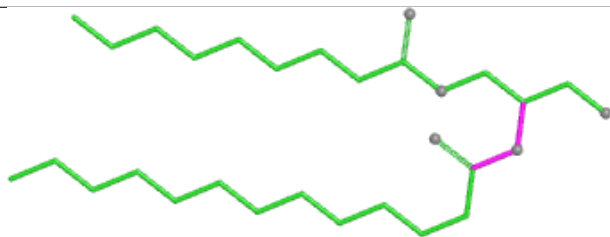


Rings

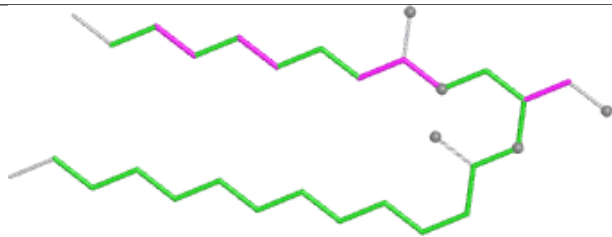
Ligand LMG c 518



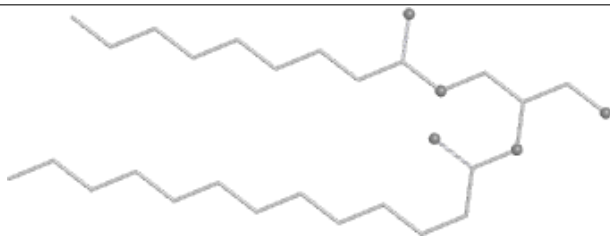
Bond lengths



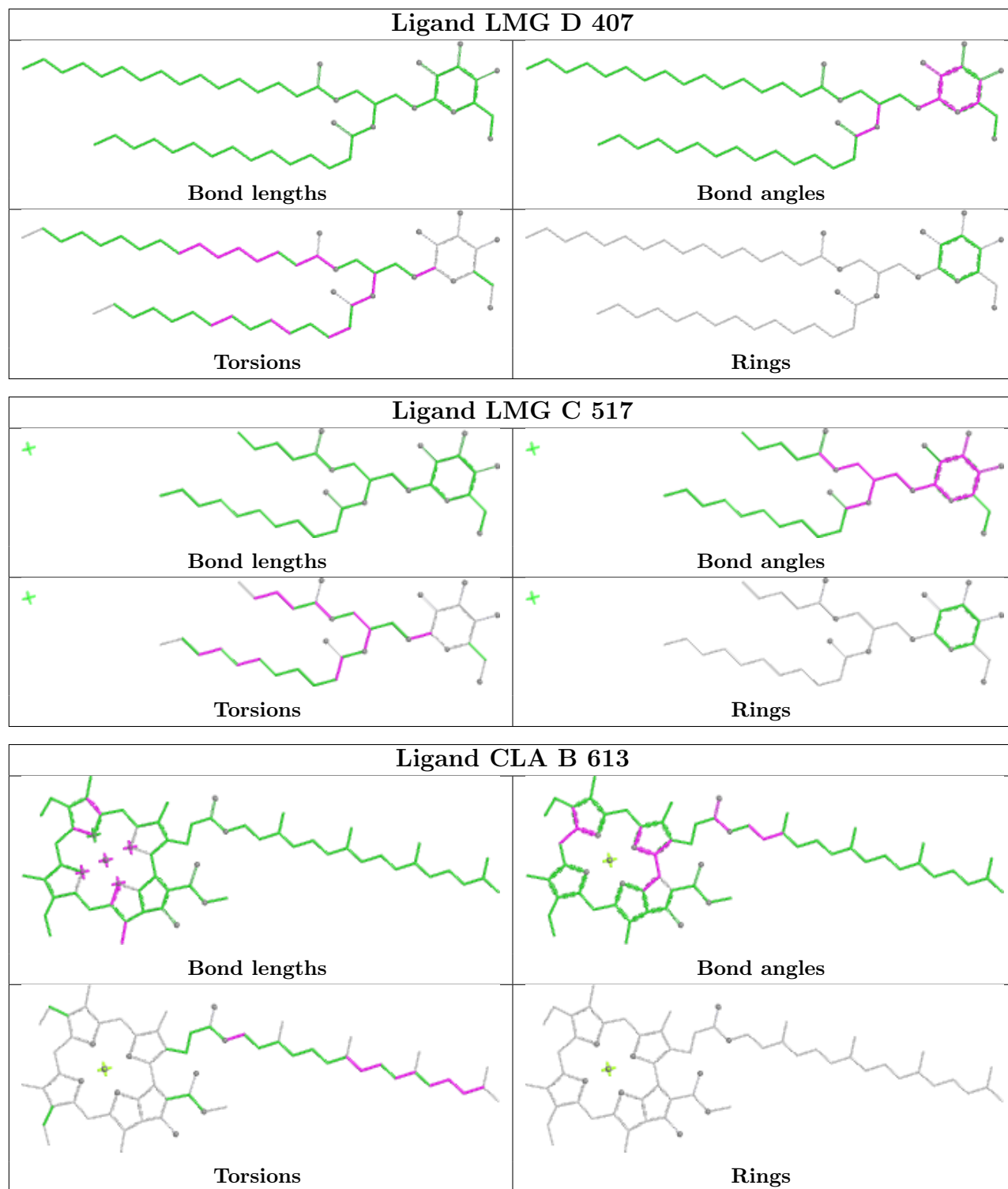
Bond angles

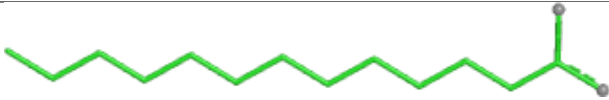
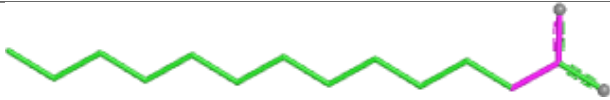
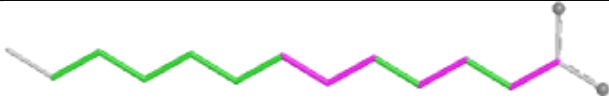
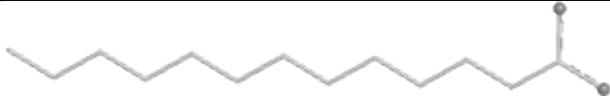


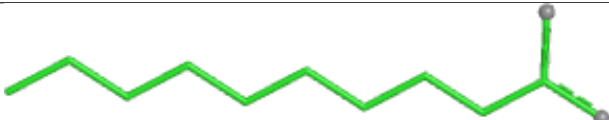
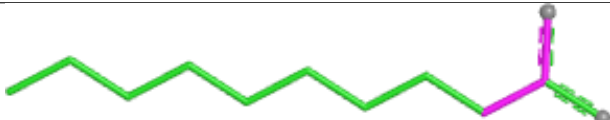
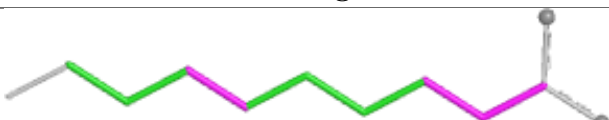
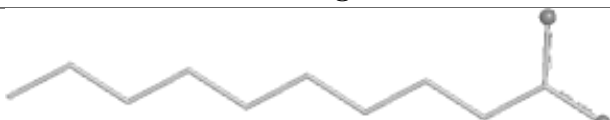
Torsions

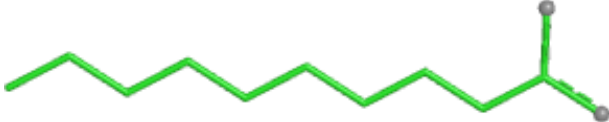
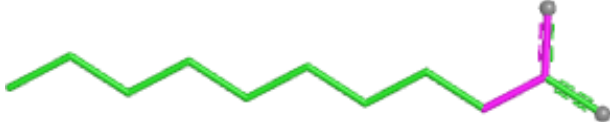
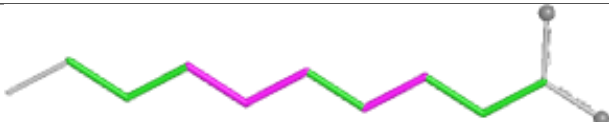
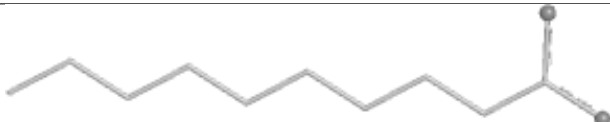


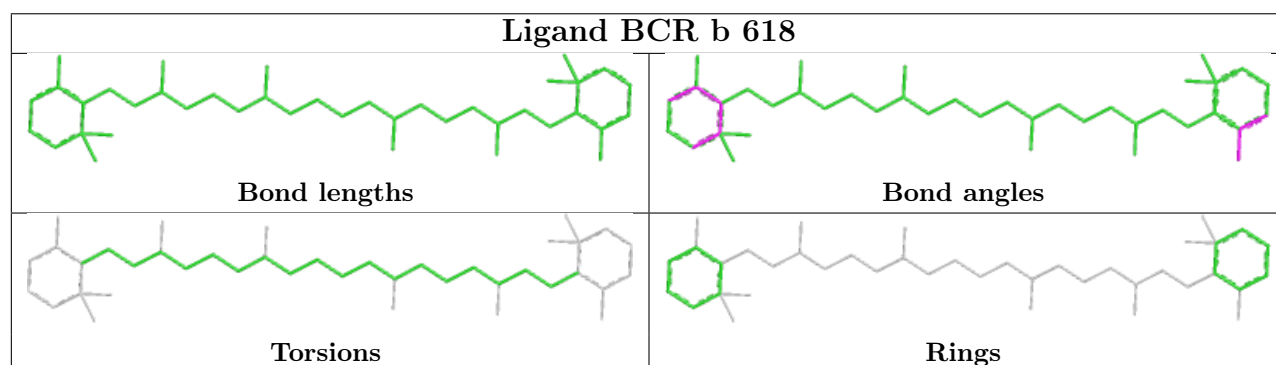
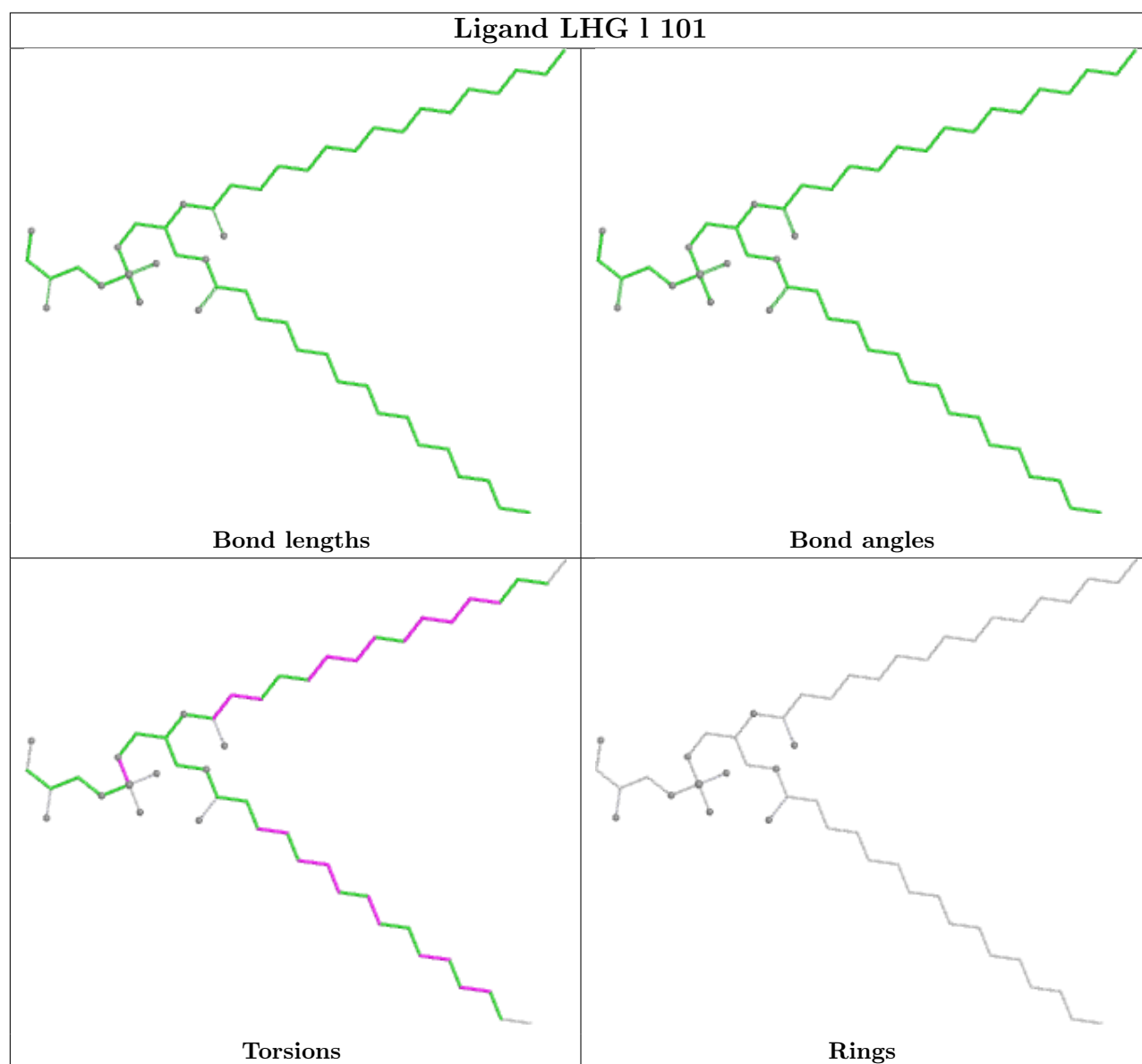
Rings

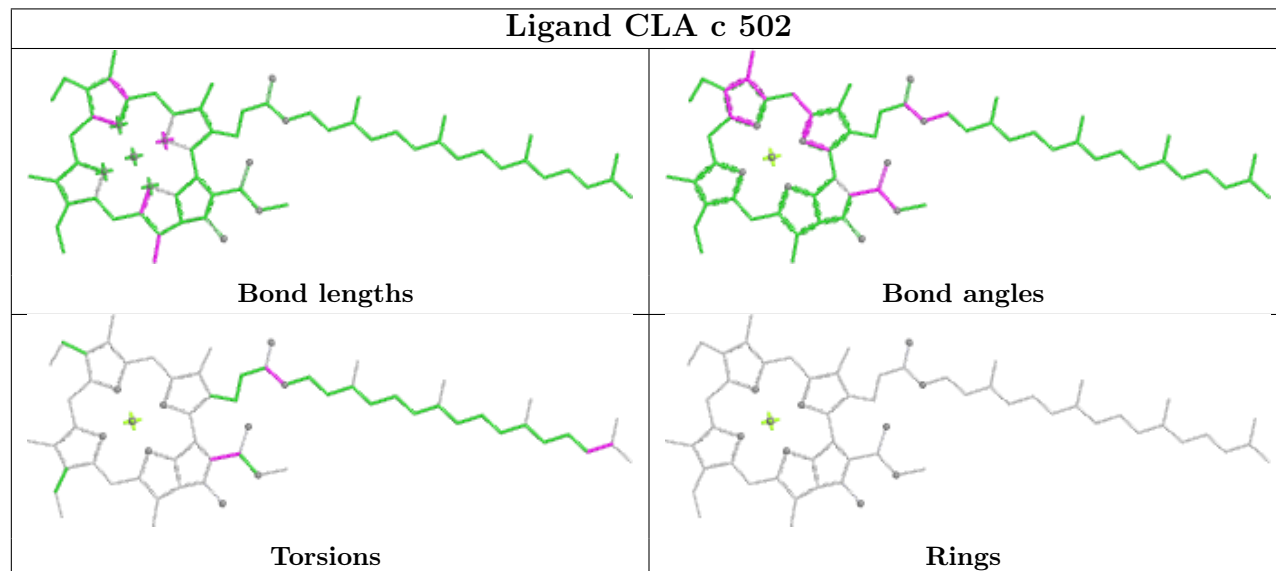
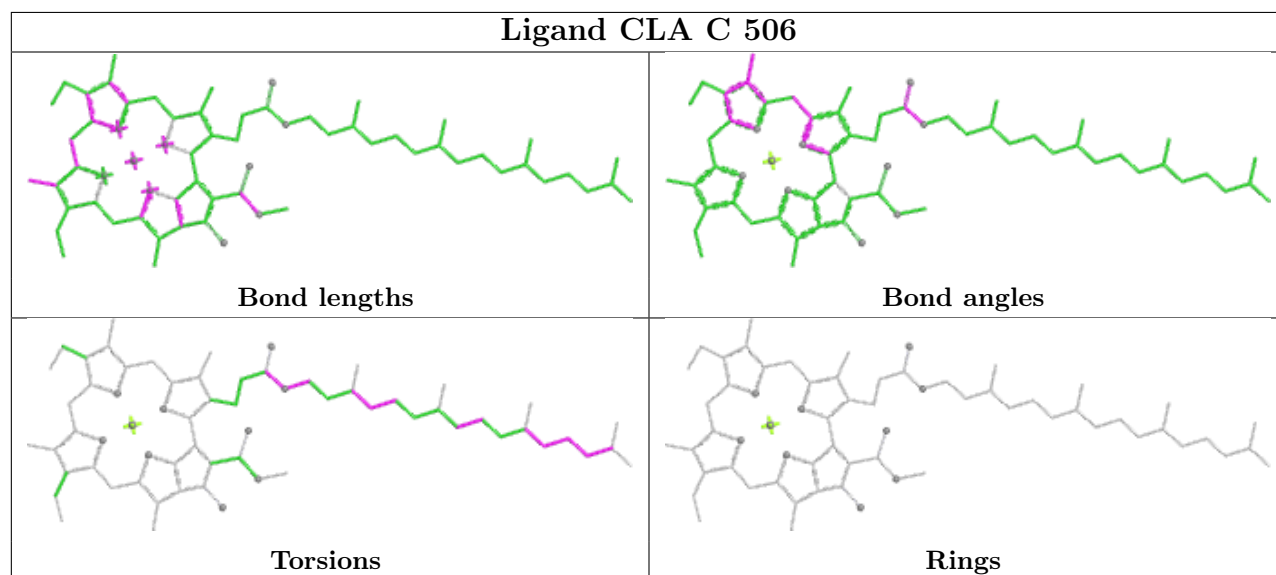
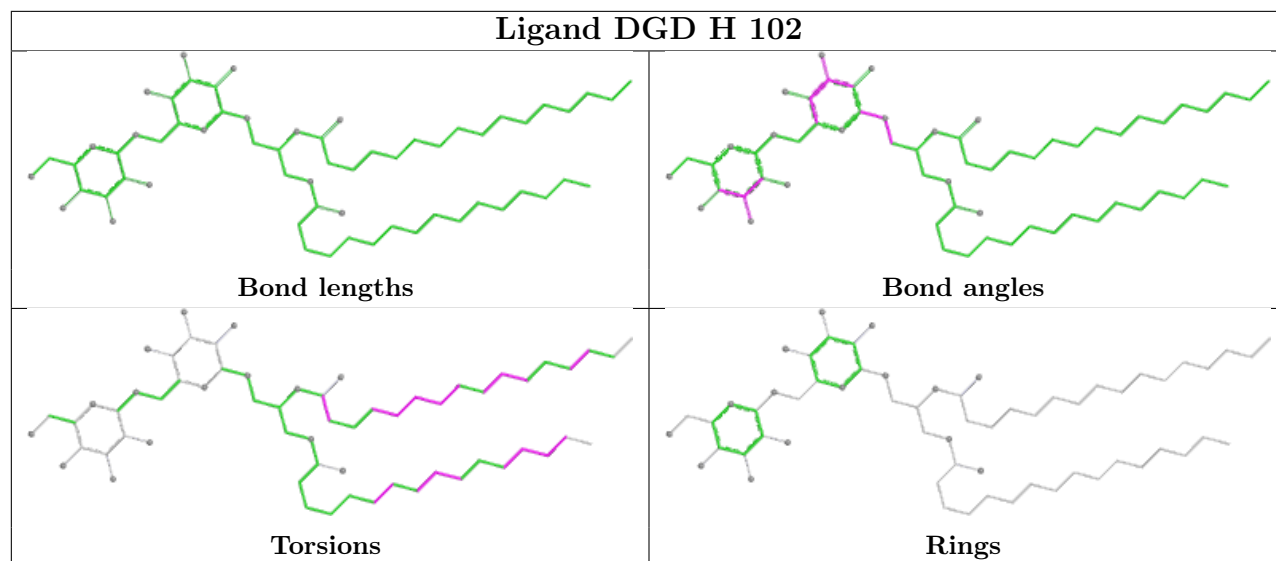


Ligand STE M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

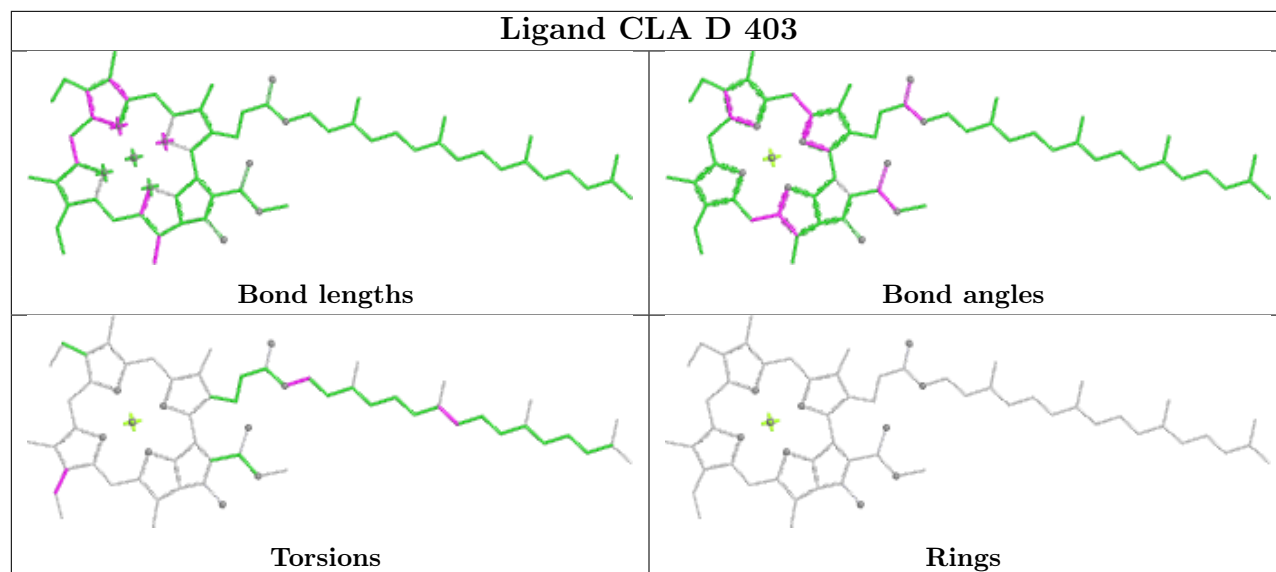
Ligand STE a 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE B 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

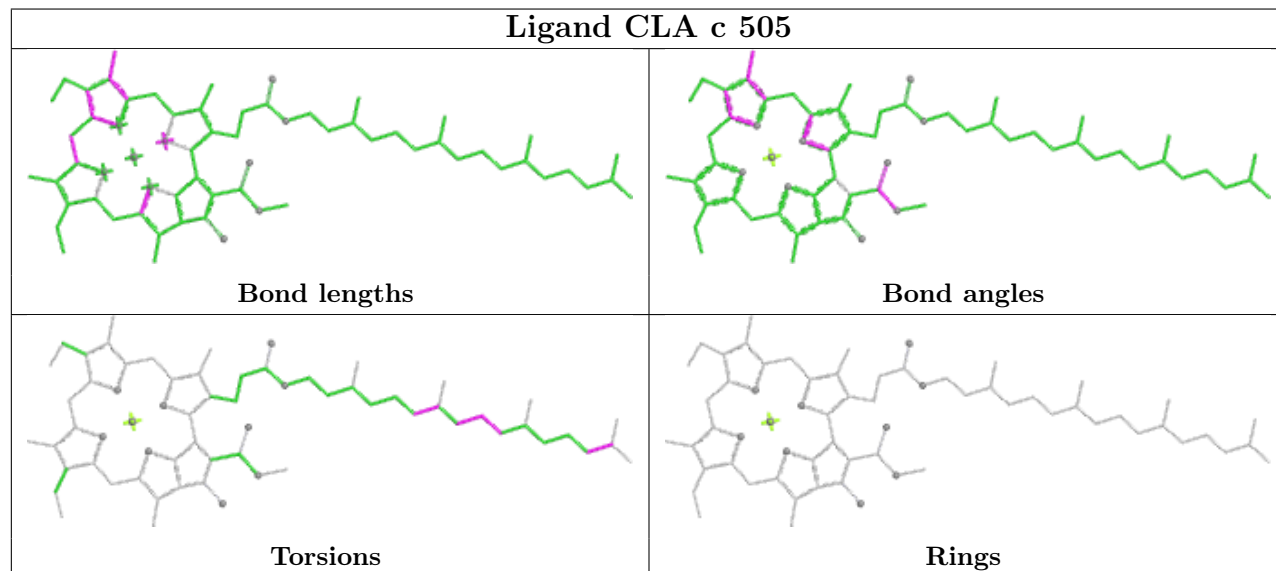




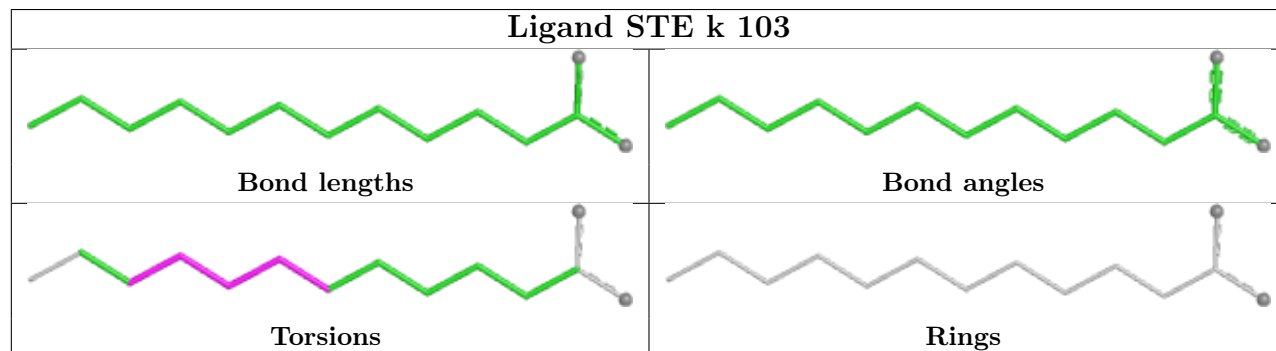
Ligand CLA D 403

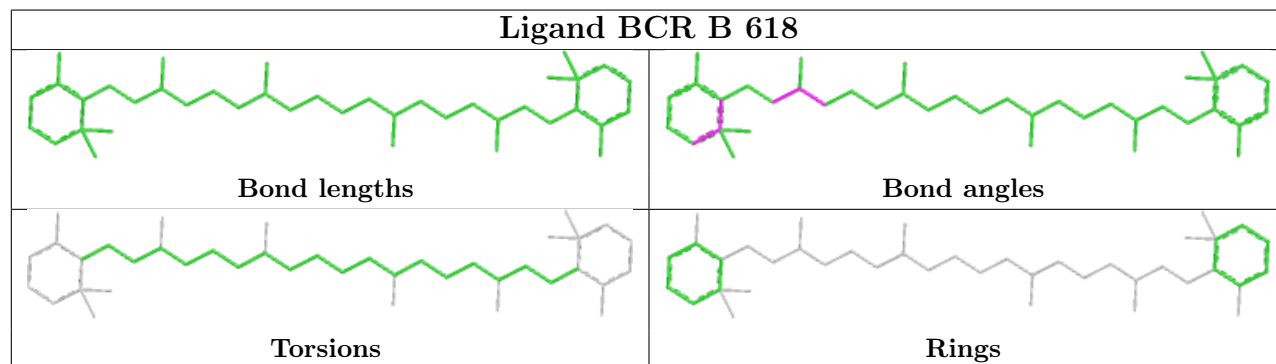
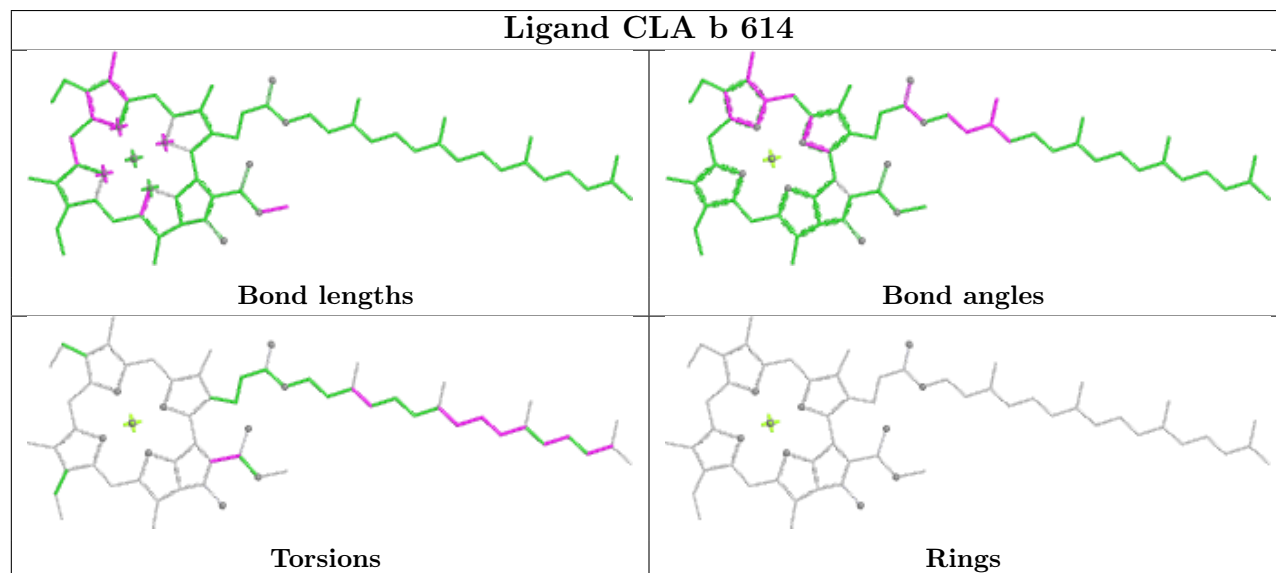
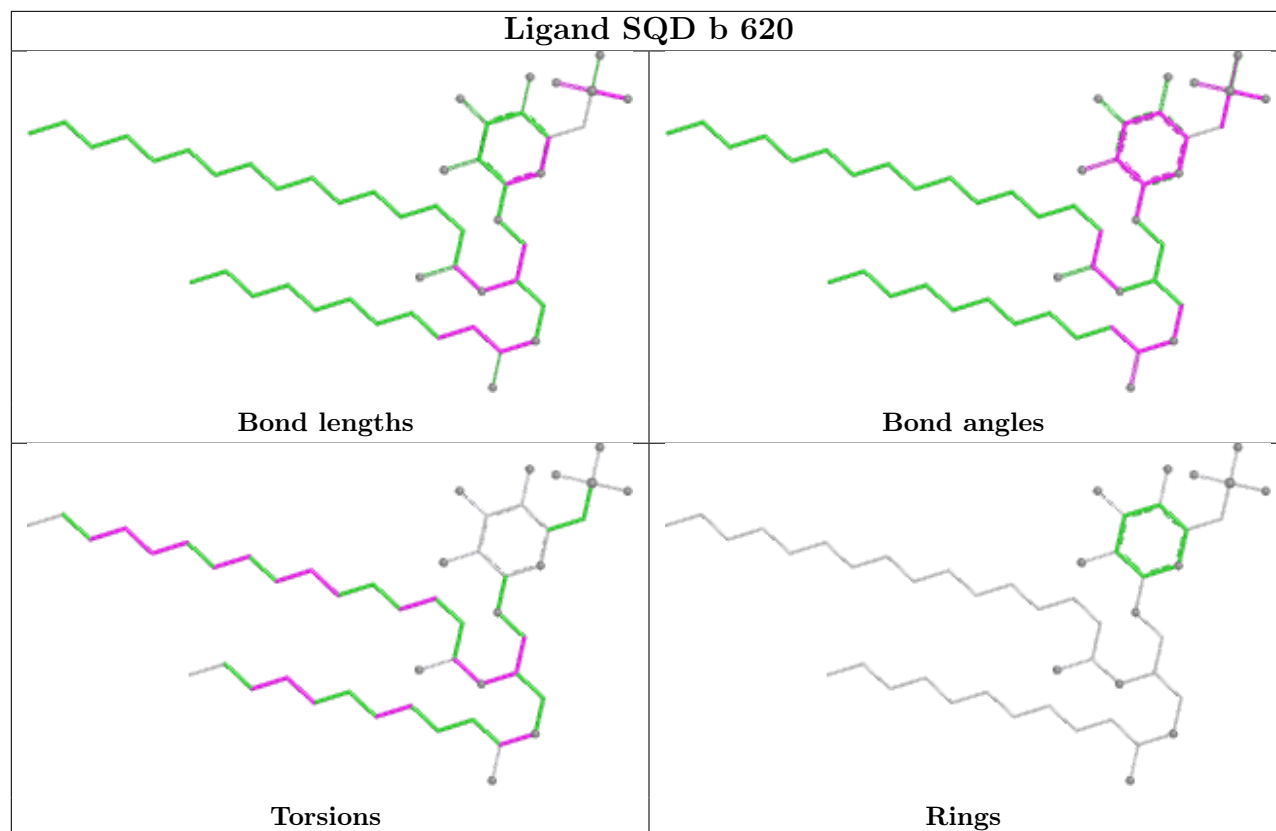


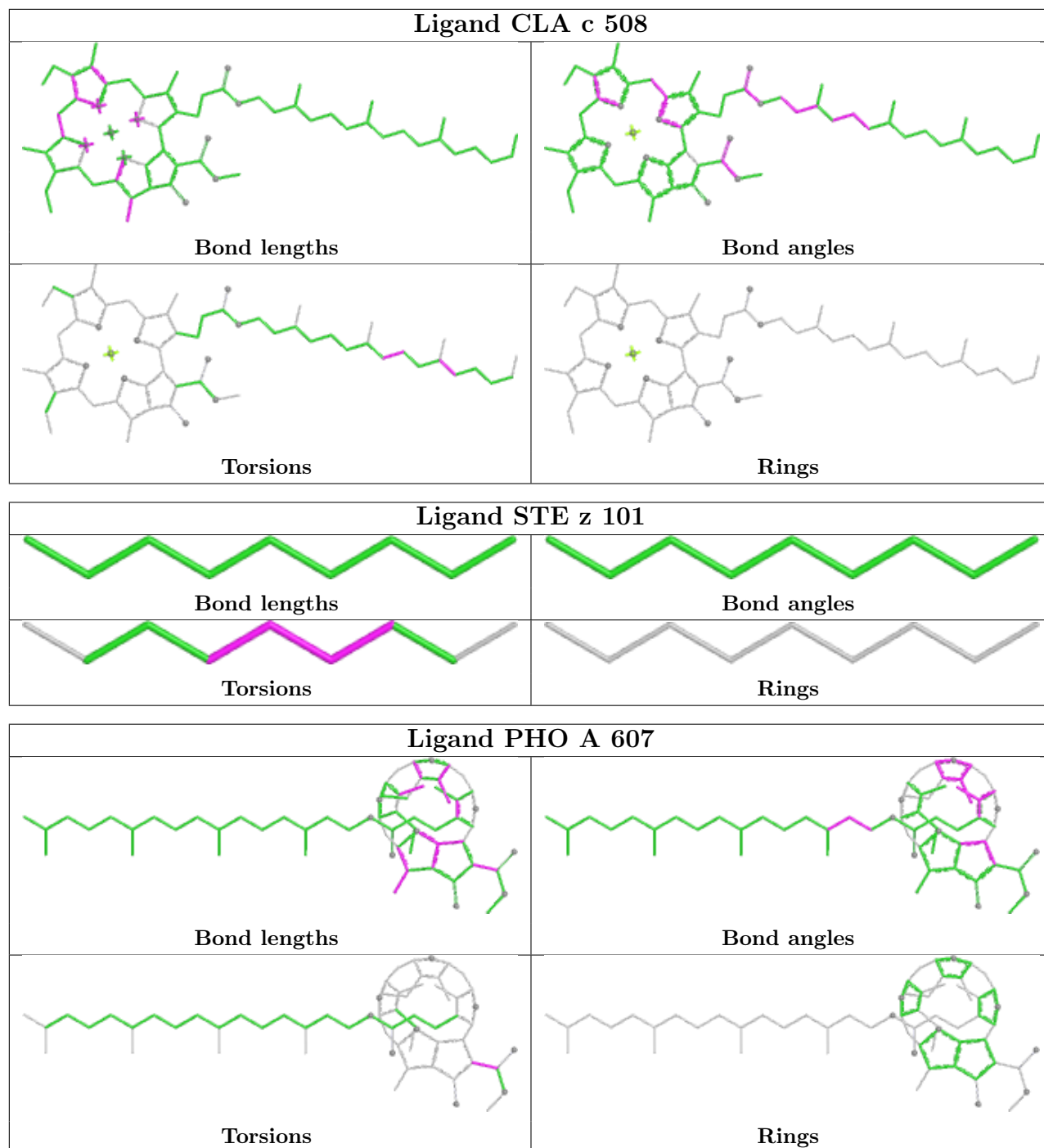
Ligand CLA c 505

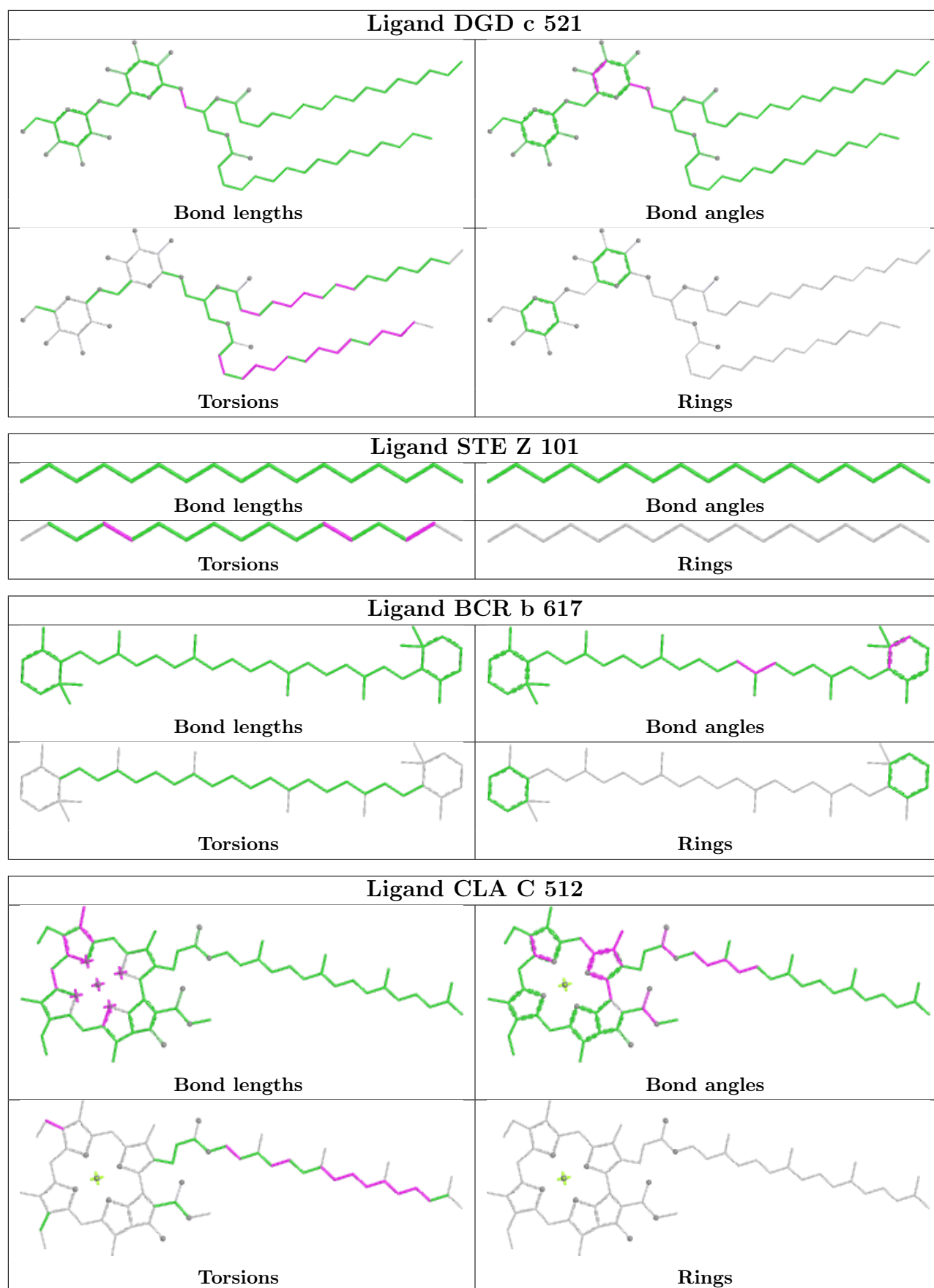


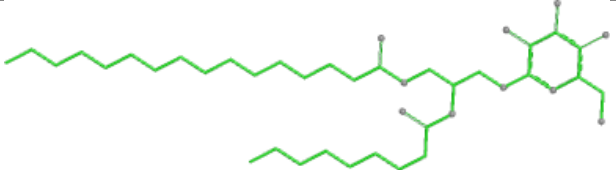
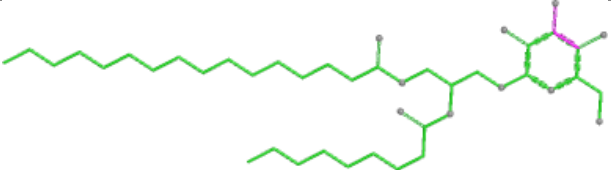
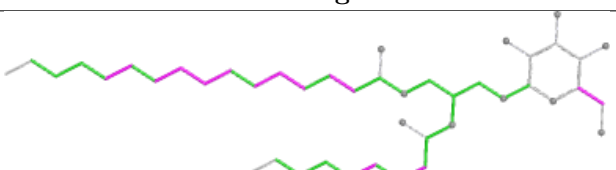
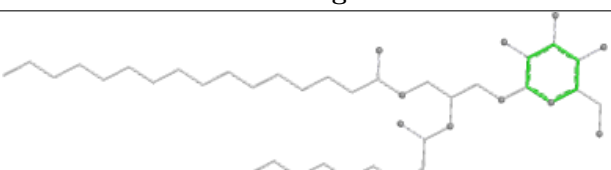
Ligand STE k 103



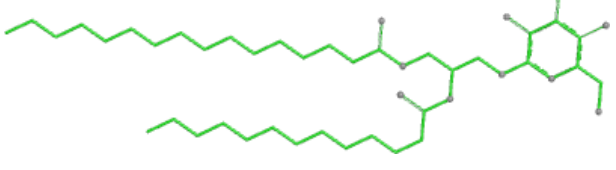
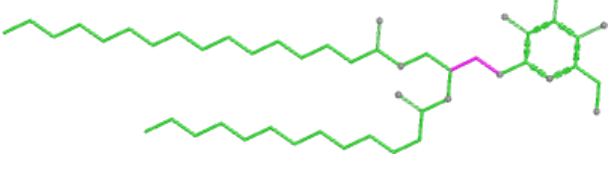
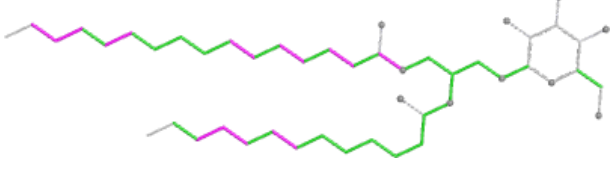
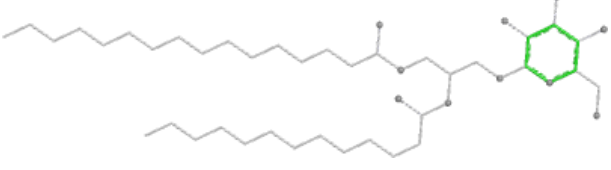


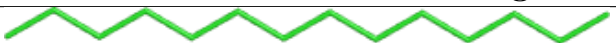
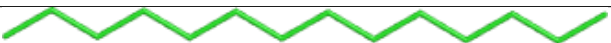


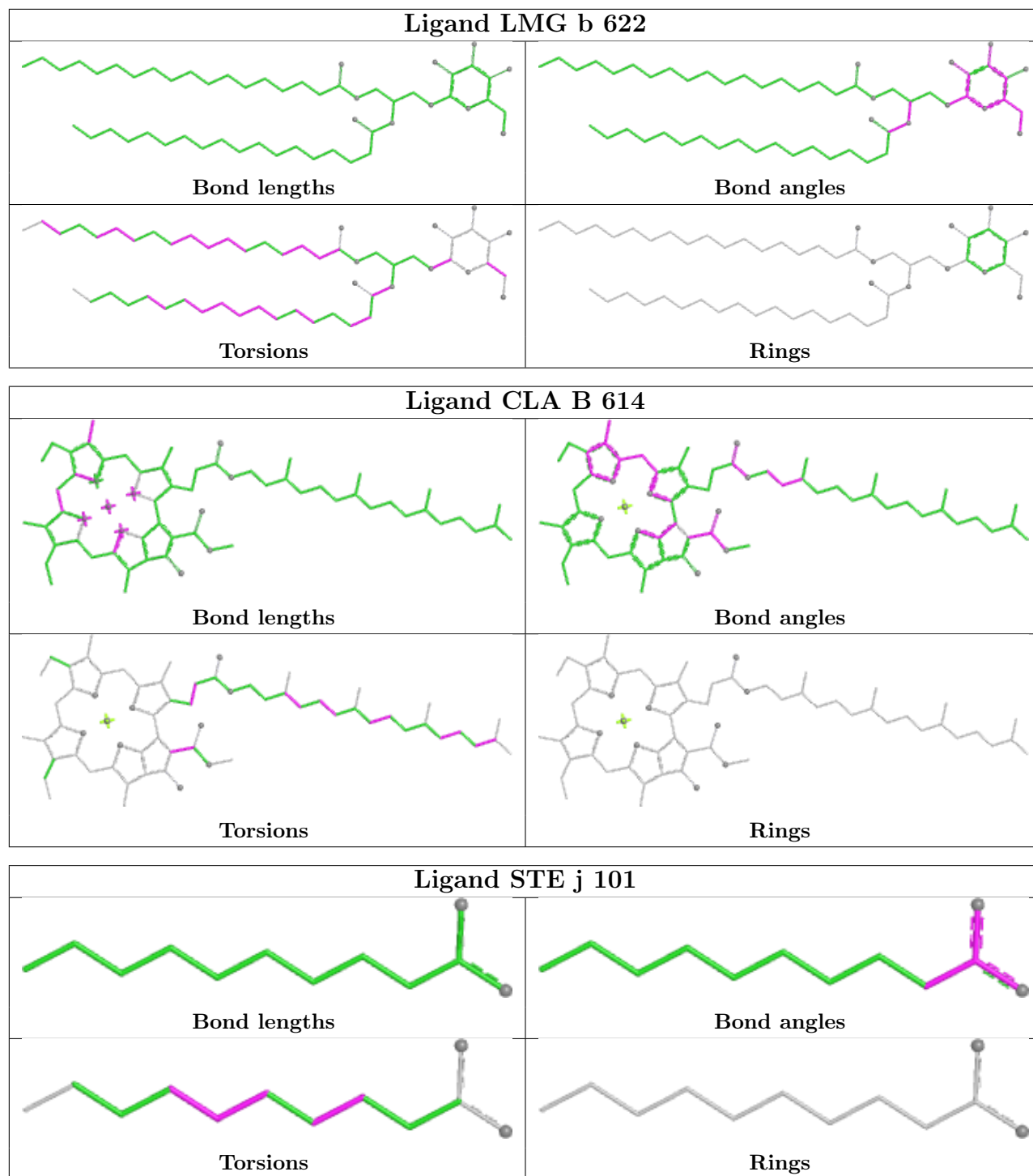


Ligand LMG d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

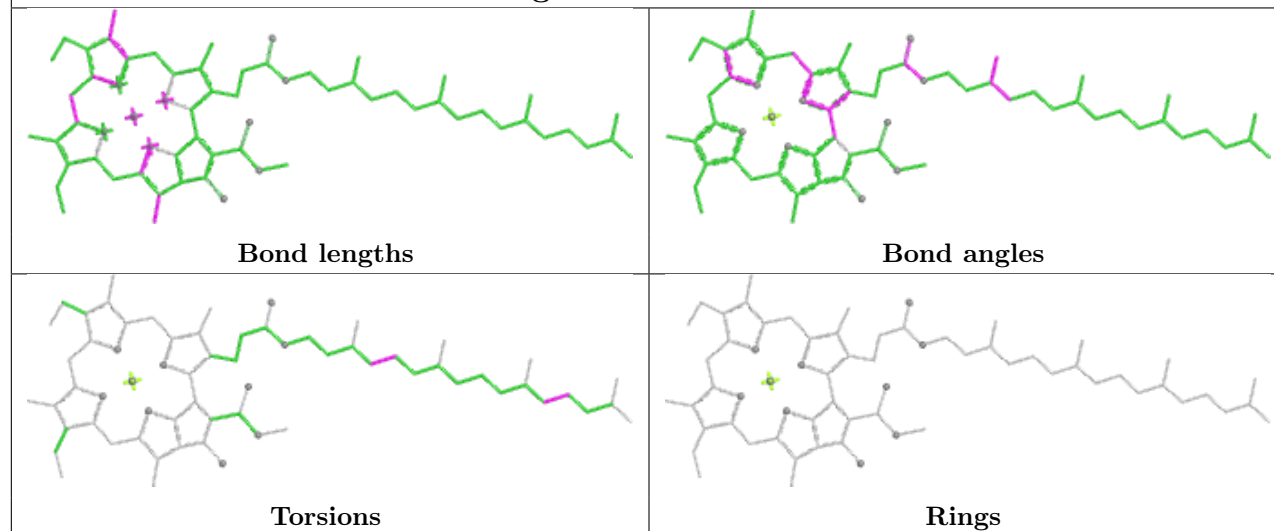
Ligand STE A 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG C 525	
 Bond lengths	 Bond angles
 Torsions	 Rings

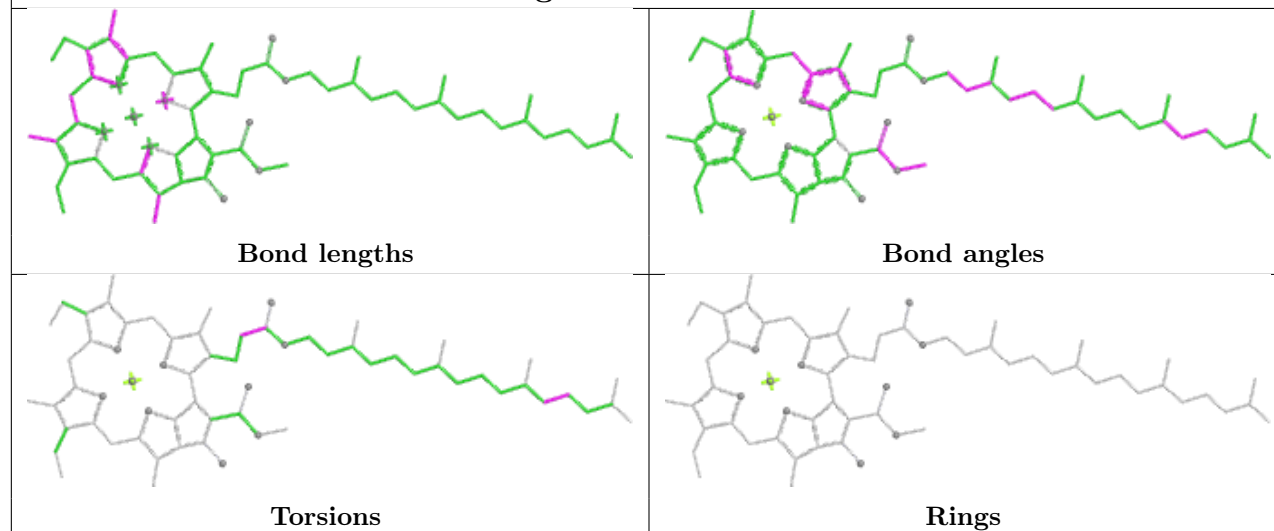
Ligand STE K 103	
 Bond lengths	 Bond angles
 Torsions	 Rings



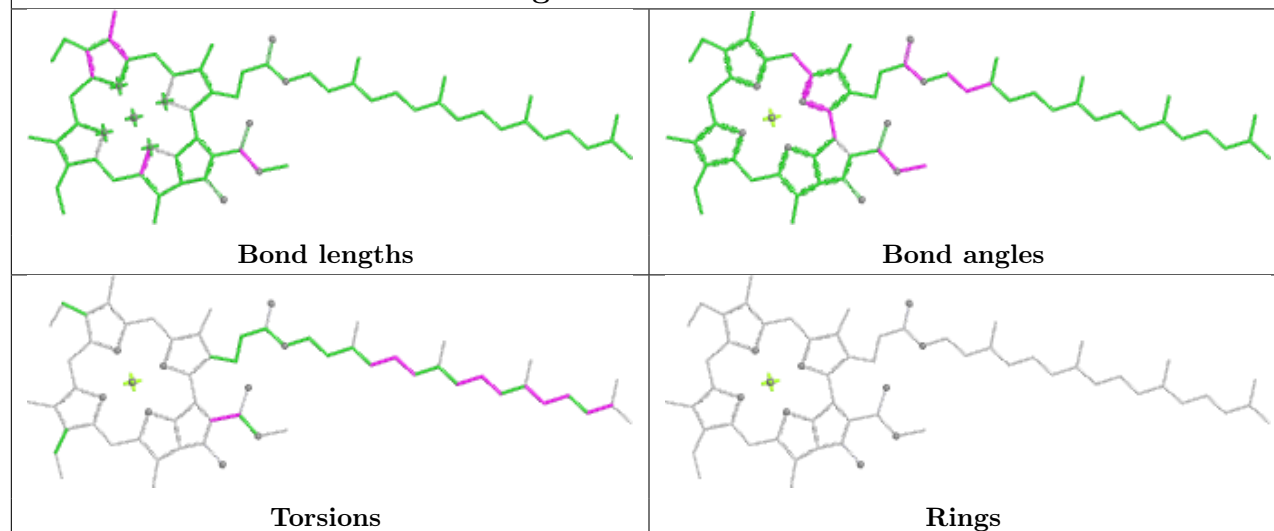
Ligand CLA B 607

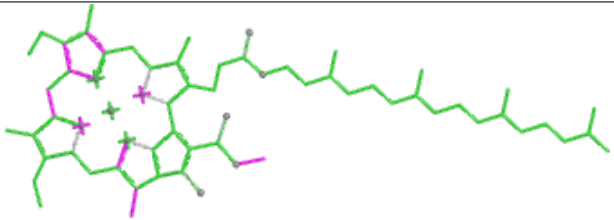
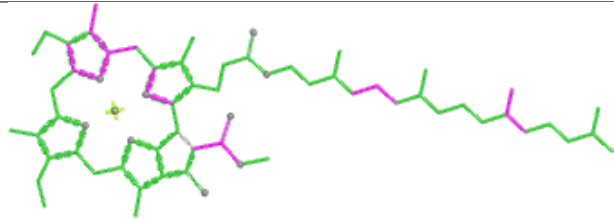
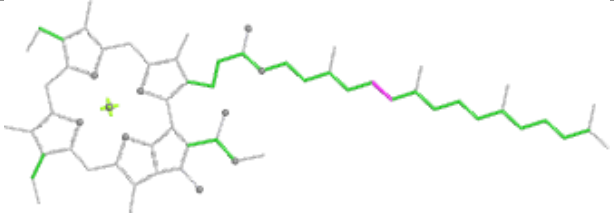
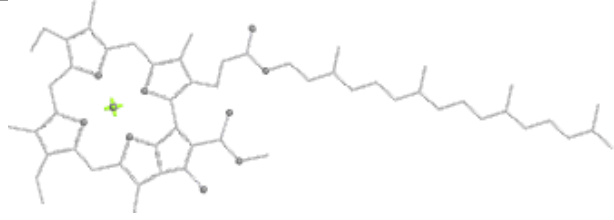


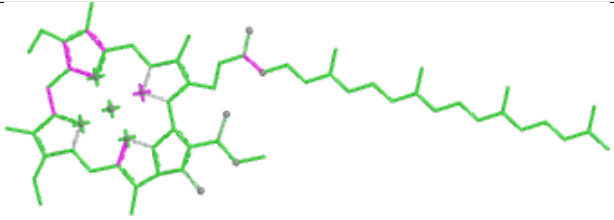
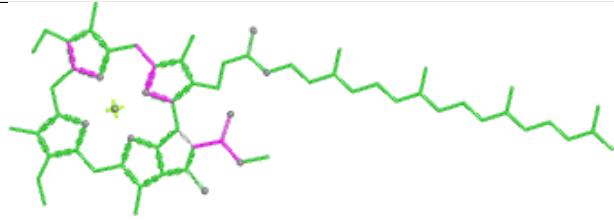
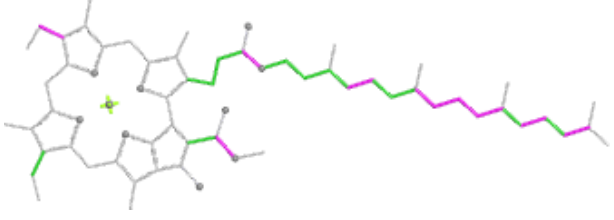
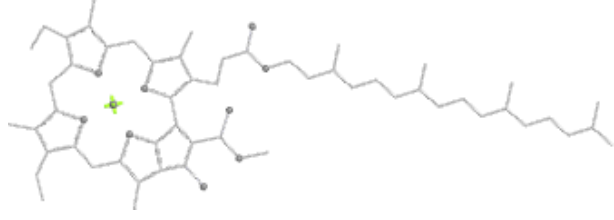
Ligand CLA b 613

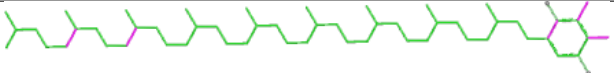
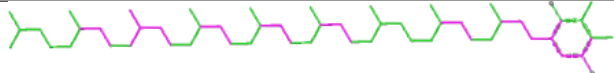


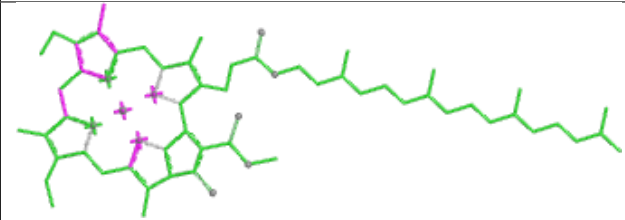
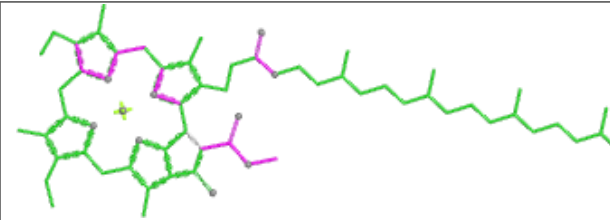
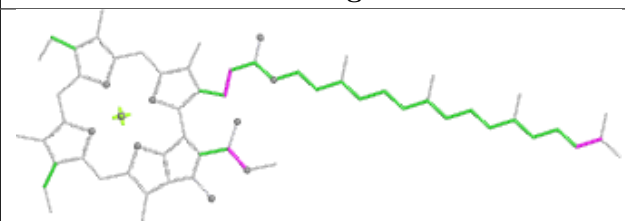
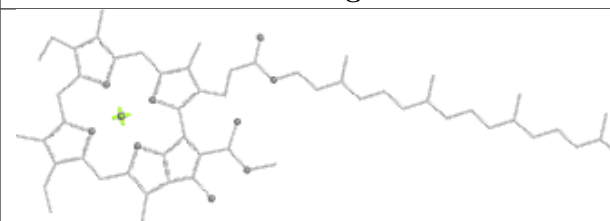
Ligand CLA C 509

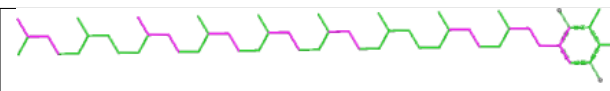


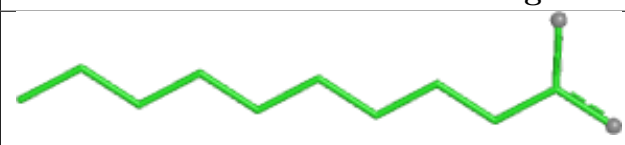
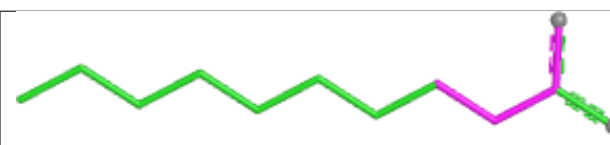
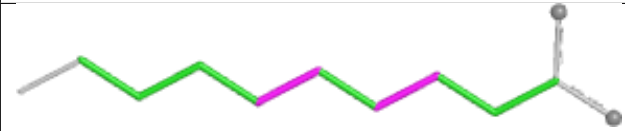
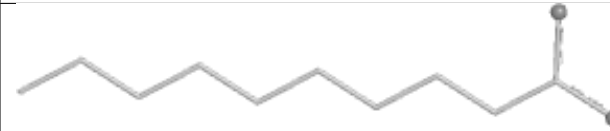
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

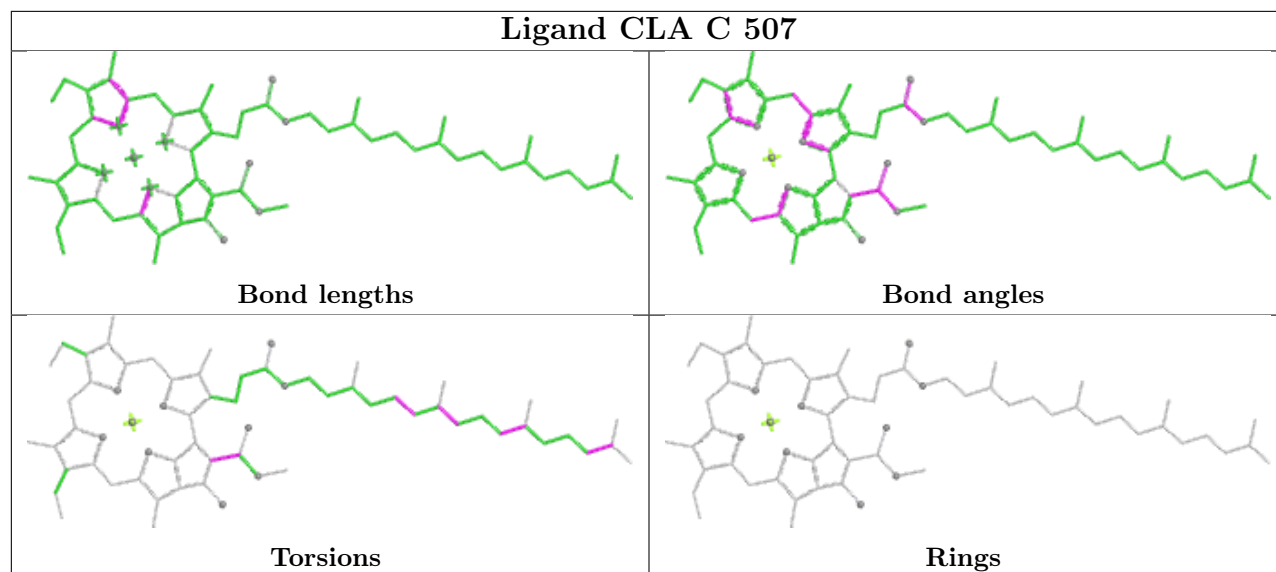
Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

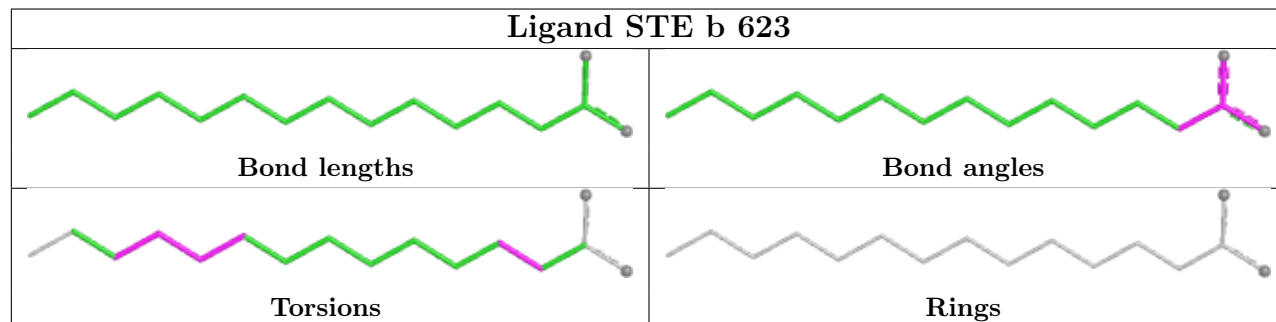
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE C 526	
	
Bond lengths	Bond angles
	
Torsions	Rings

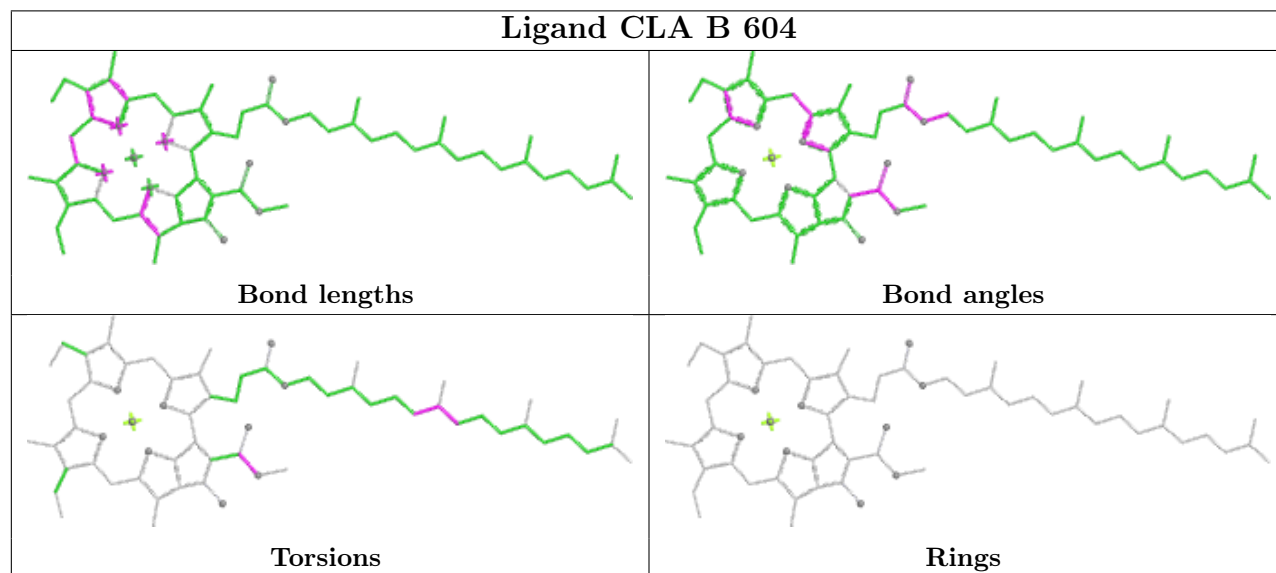
Ligand CLA C 507



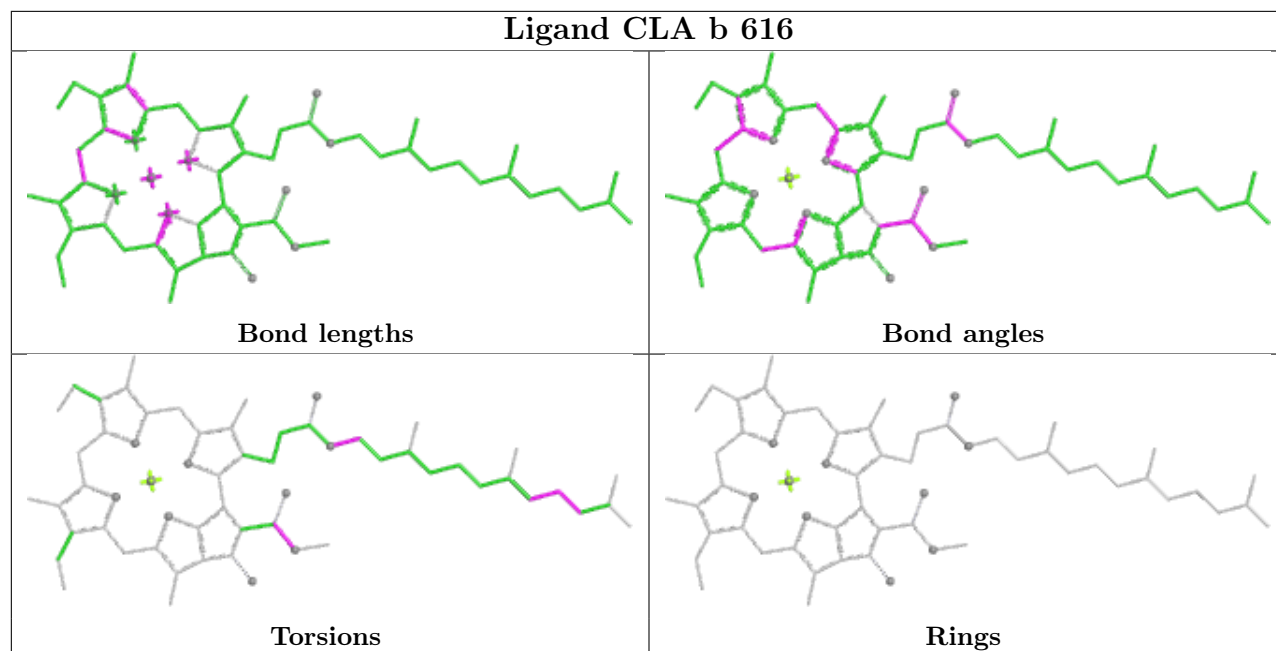
Ligand STE b 623



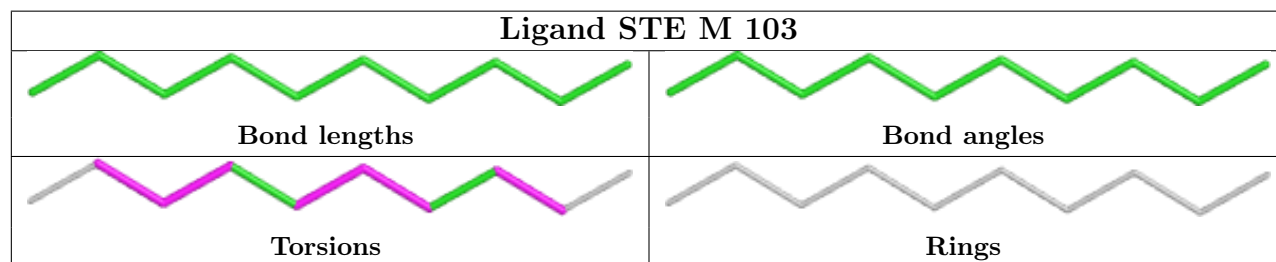
Ligand CLA B 604



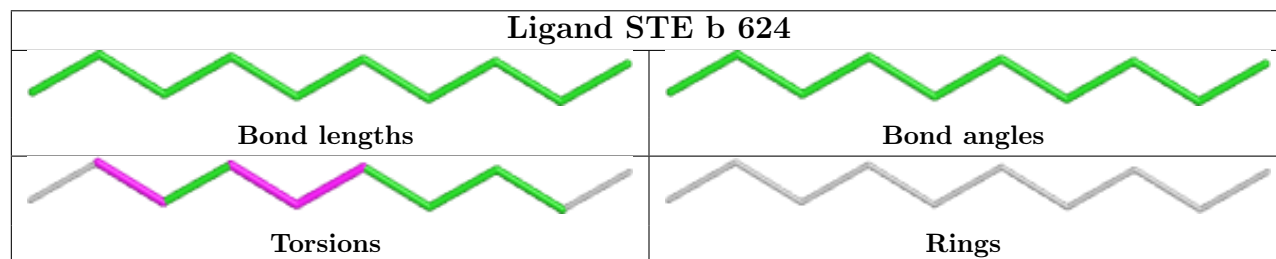
Ligand CLA b 616



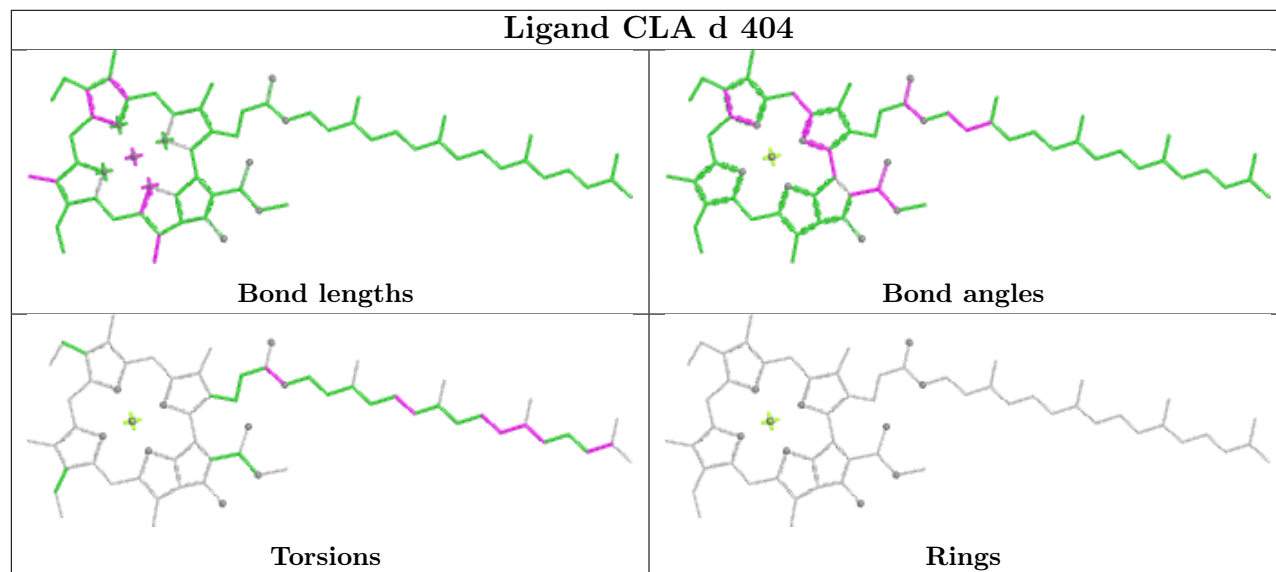
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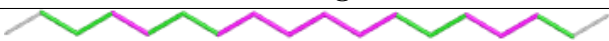


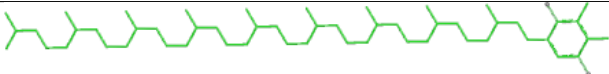
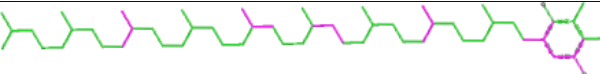
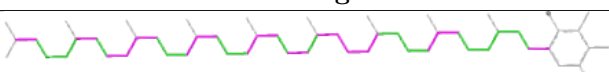
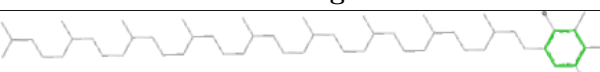
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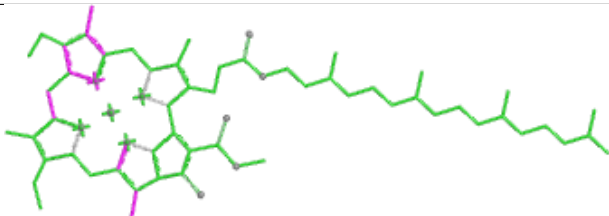
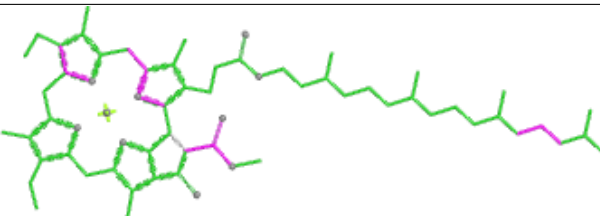
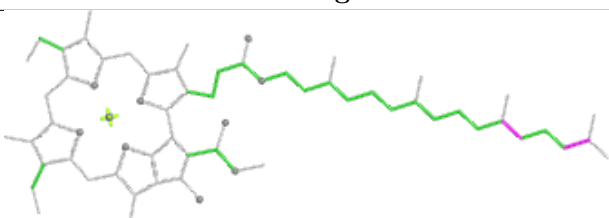
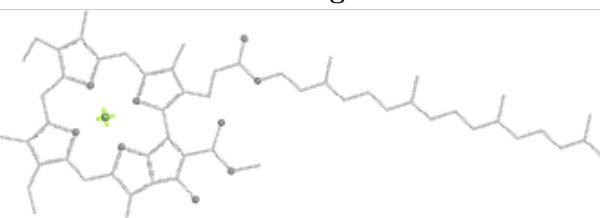


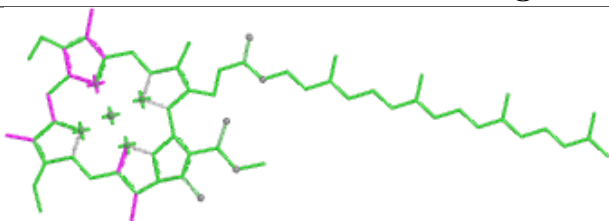
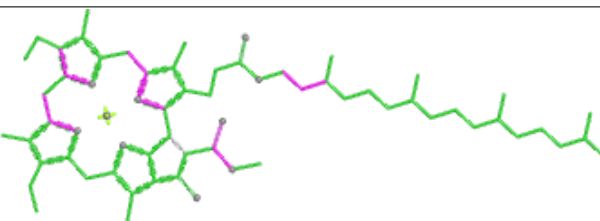
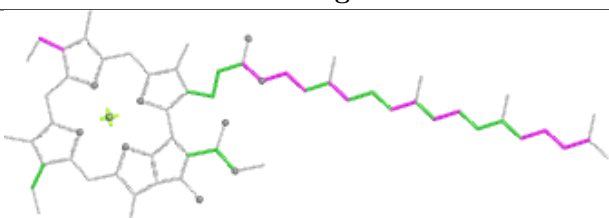
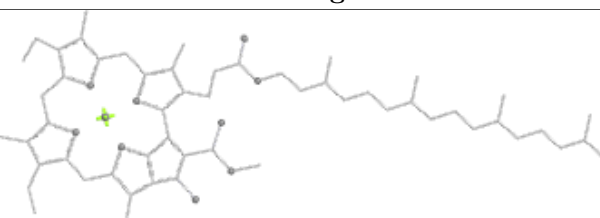
Ligand CLA d 404

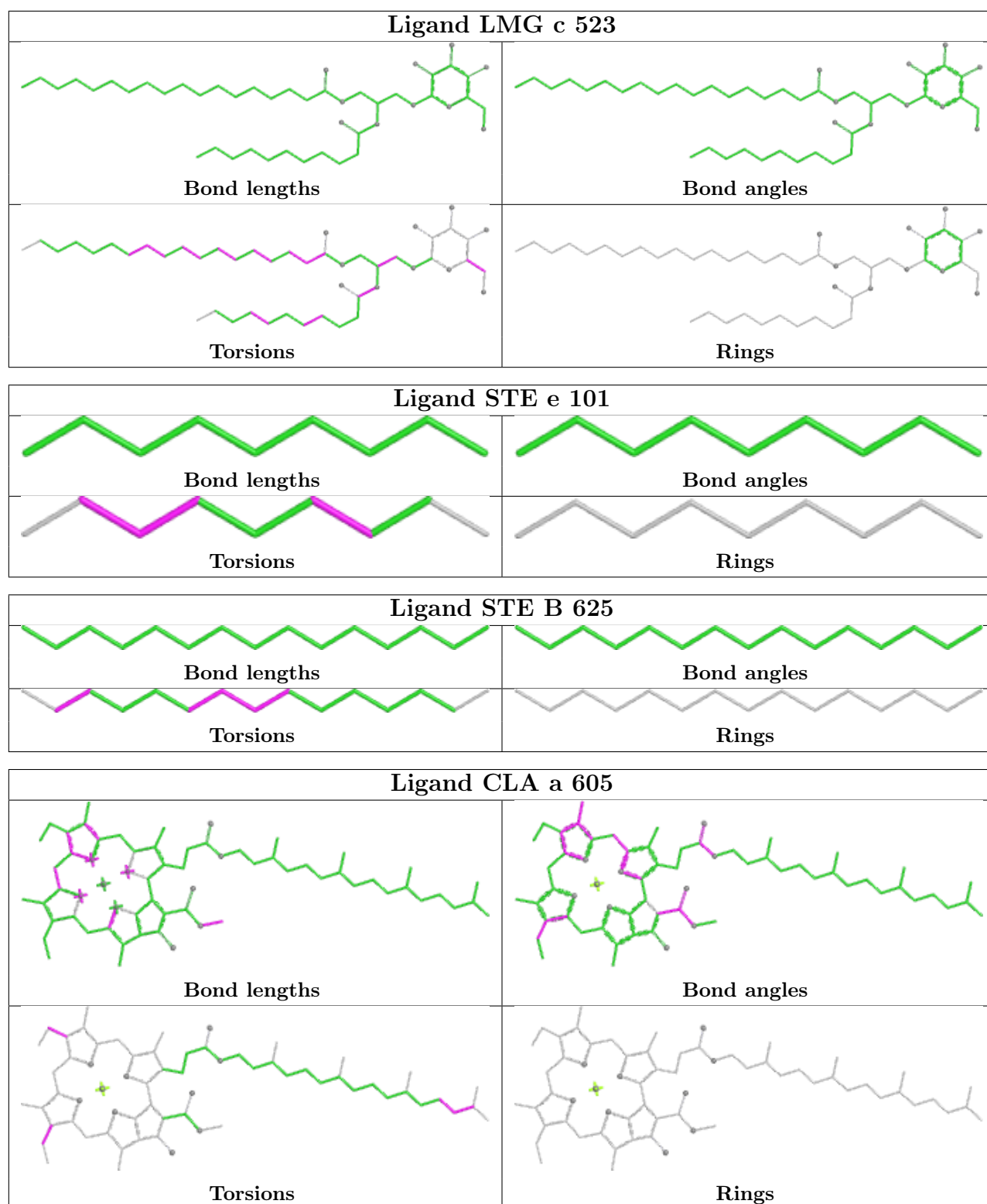


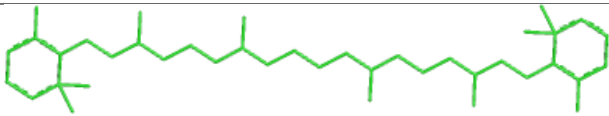
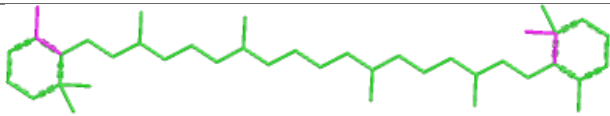
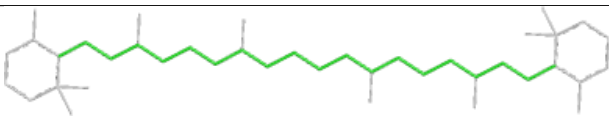
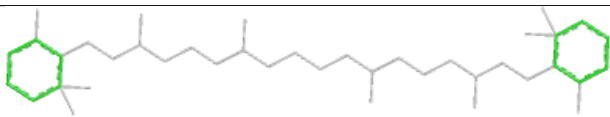
Ligand STE c 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

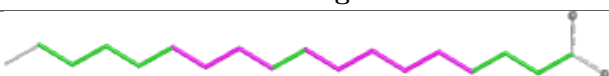
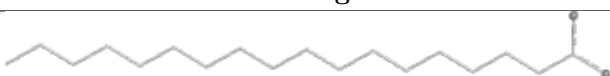
Ligand PL9 A 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

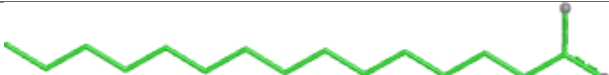
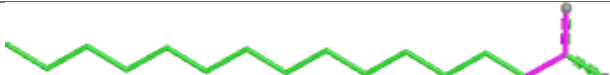
Ligand CLA A 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

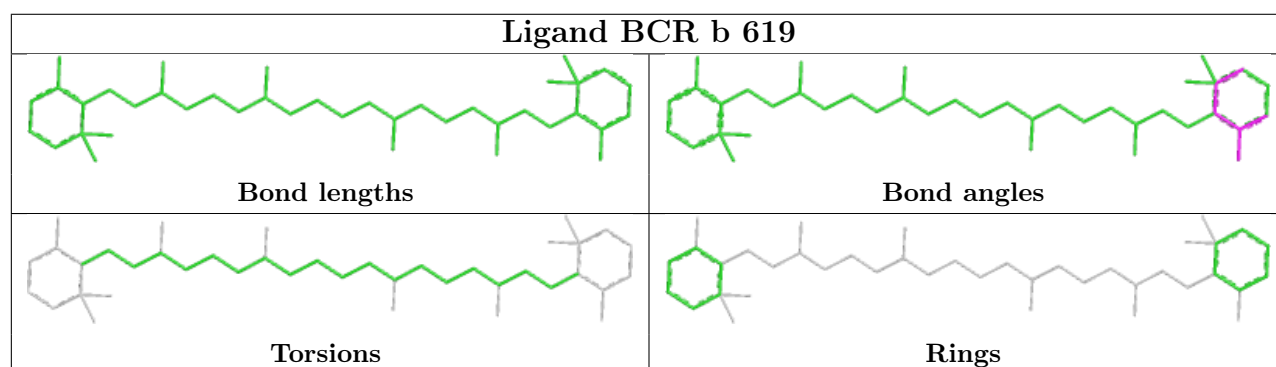
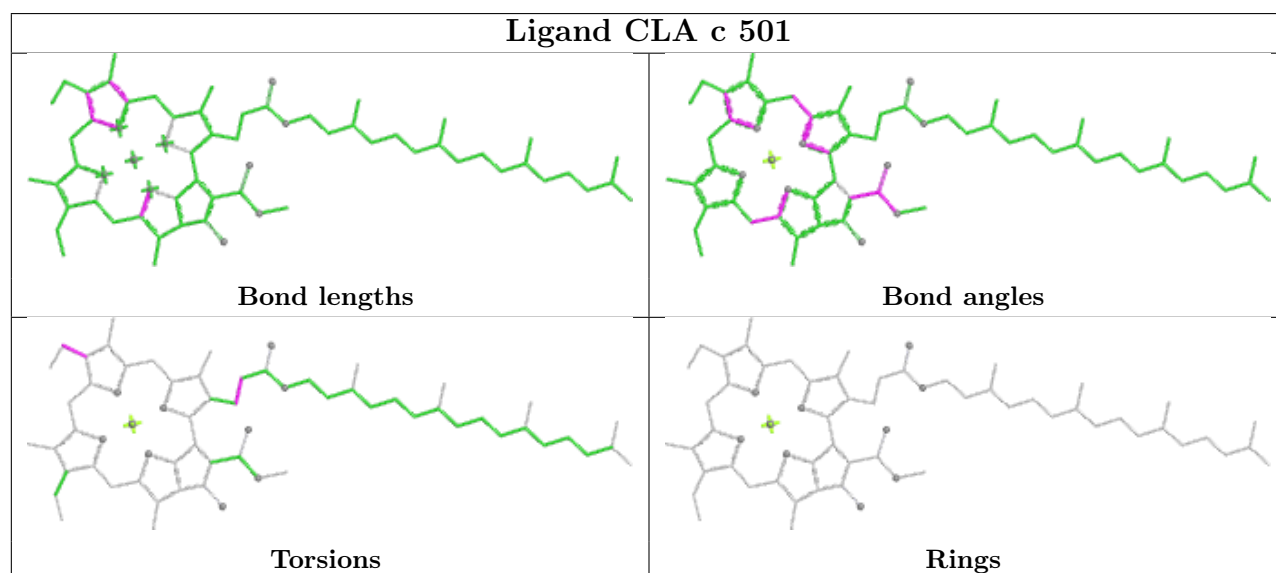
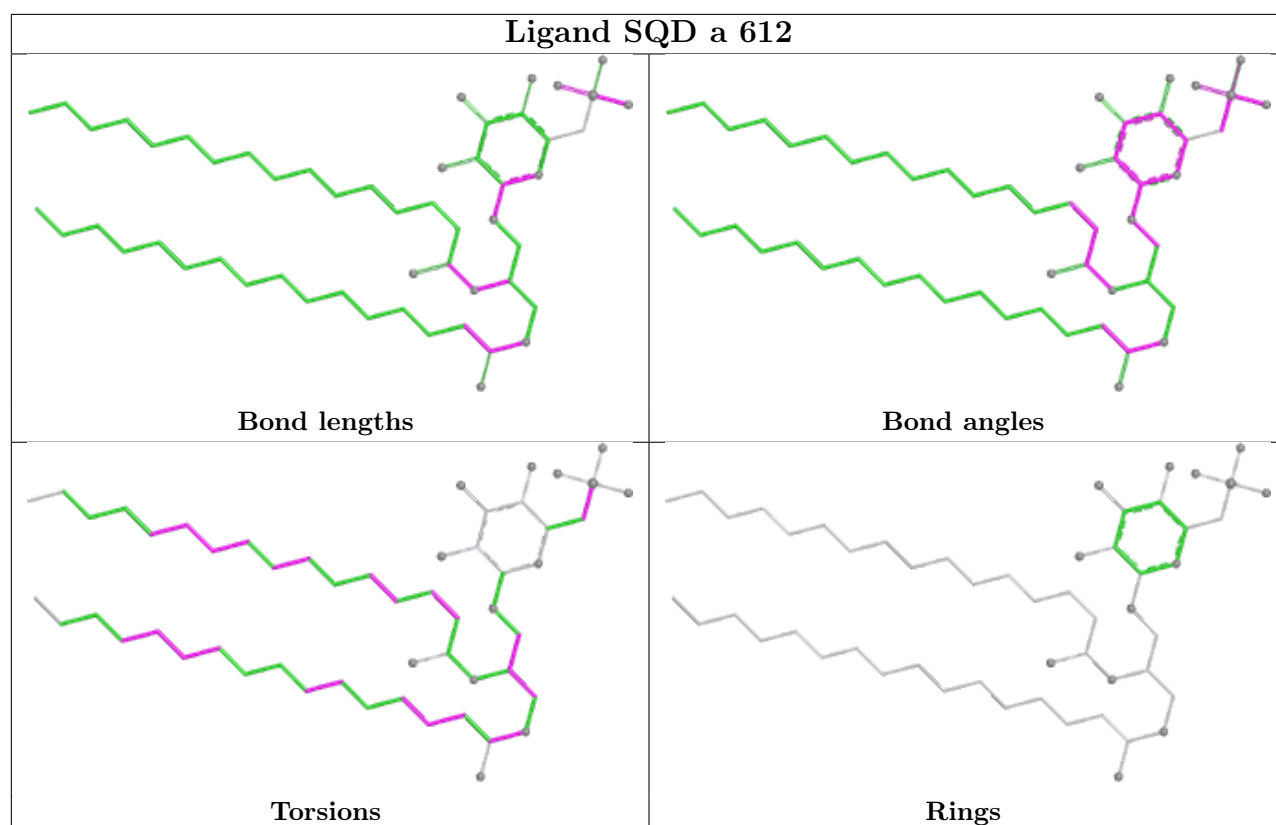
Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

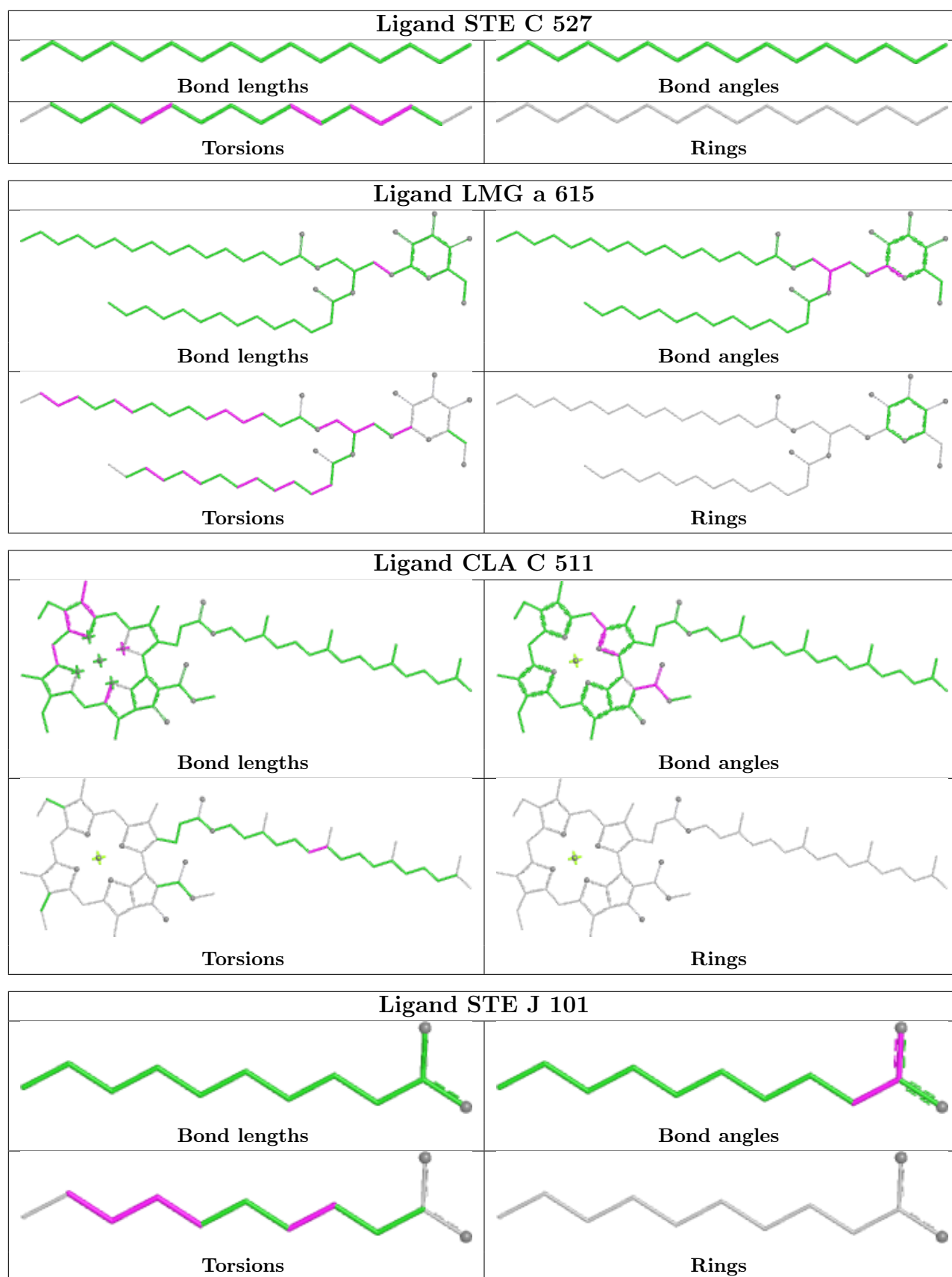


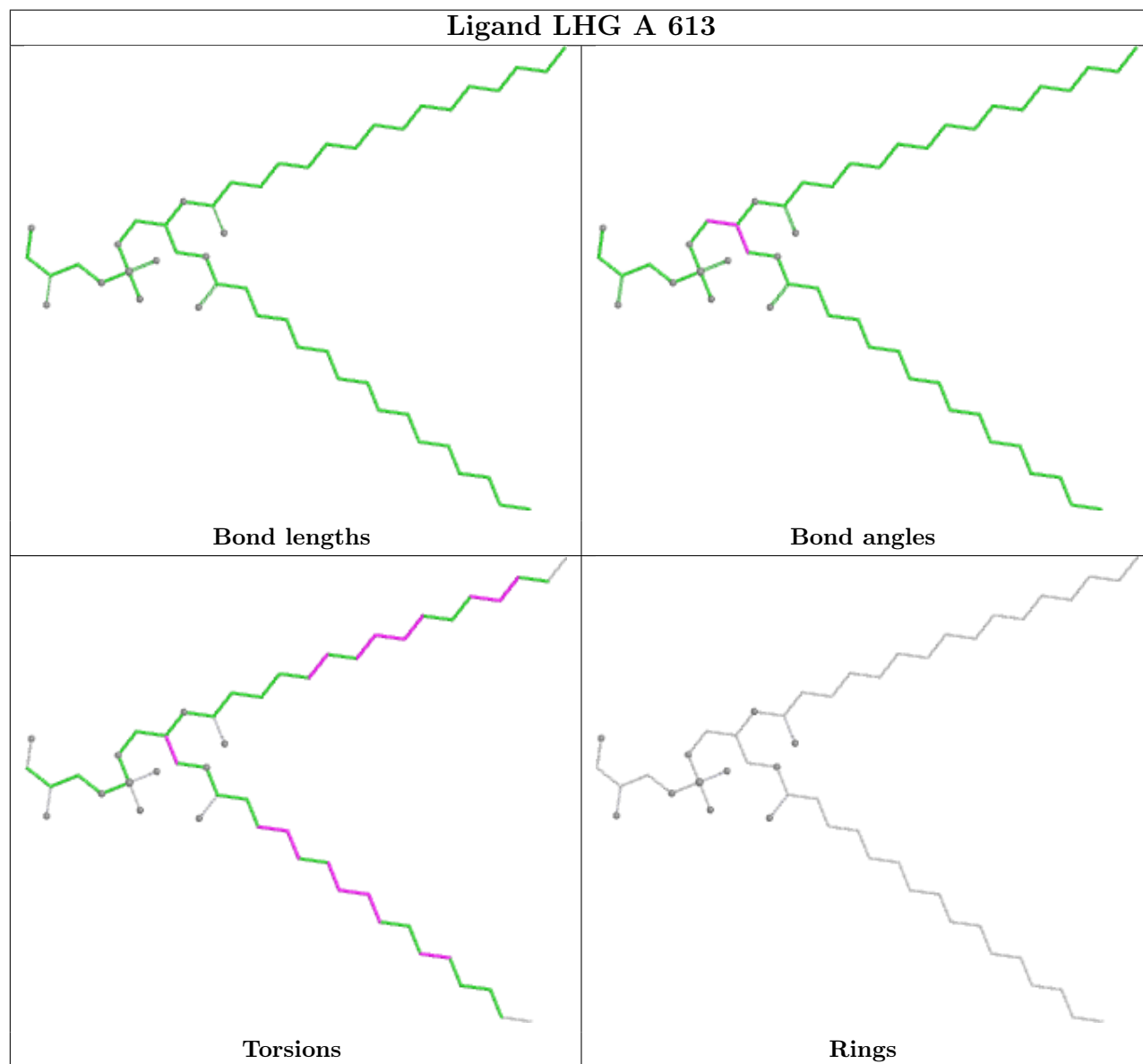
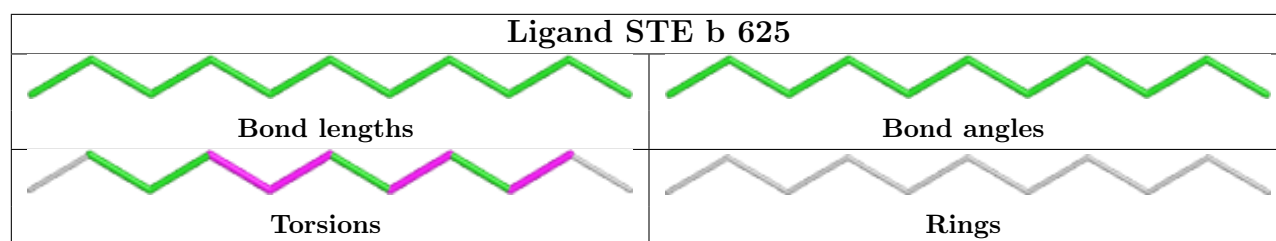
Ligand BCR a 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

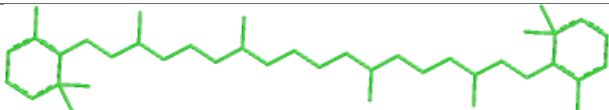
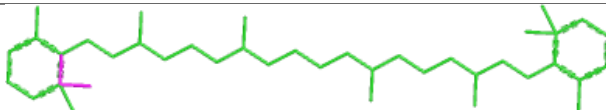
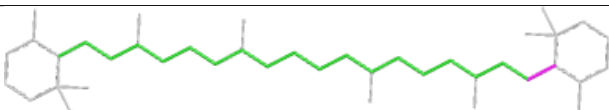
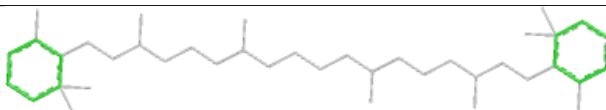
Ligand STE d 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

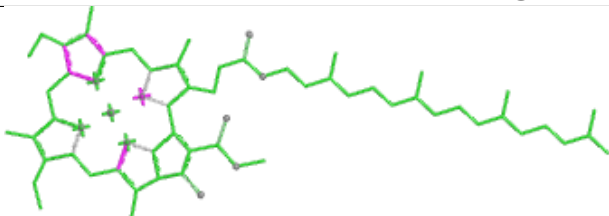
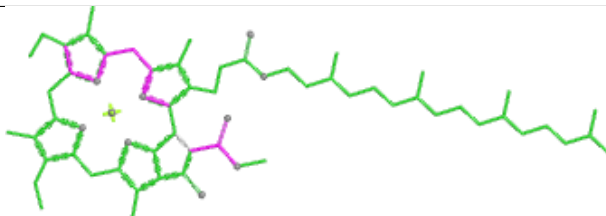
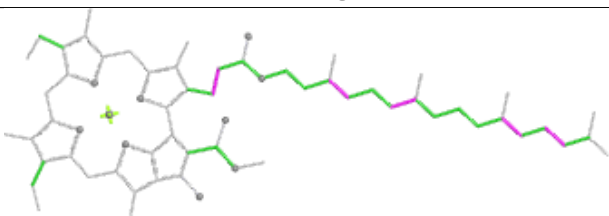
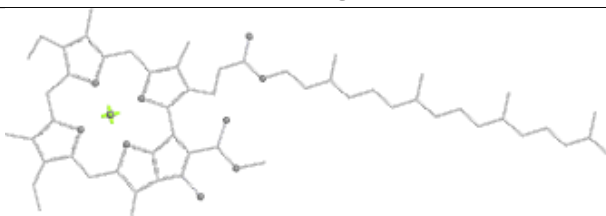
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

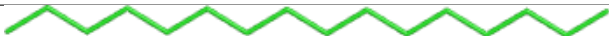
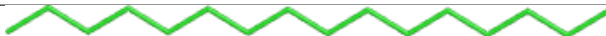
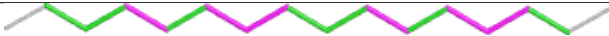


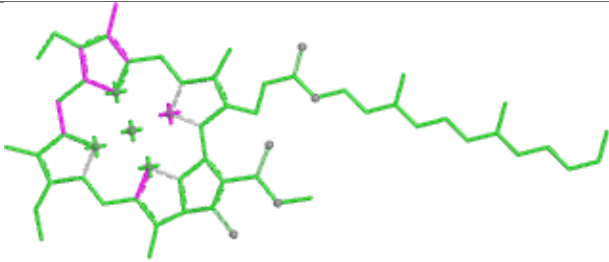
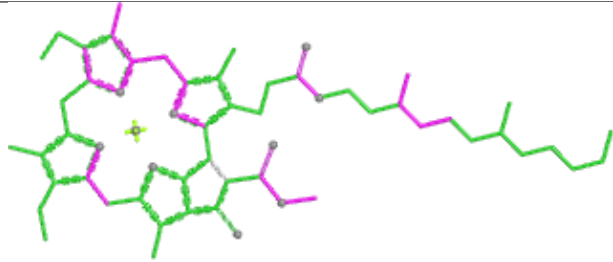
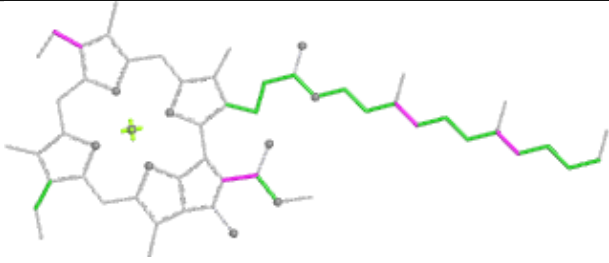
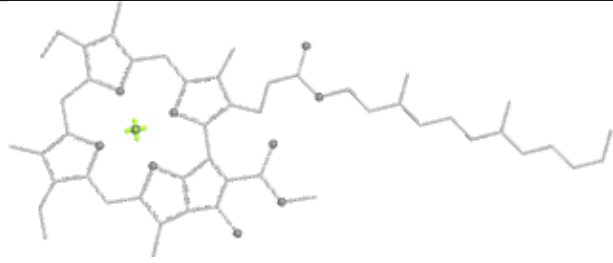


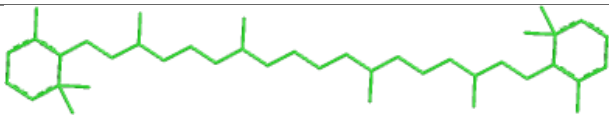
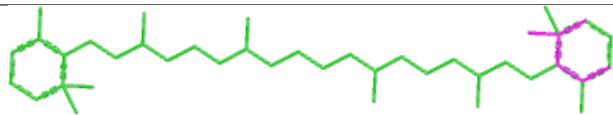
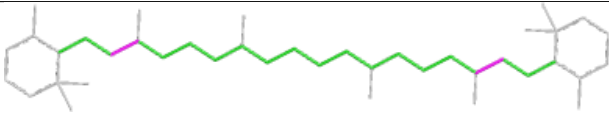
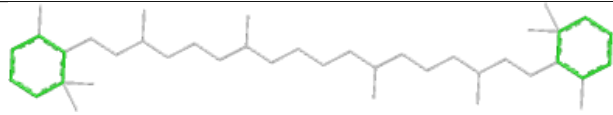


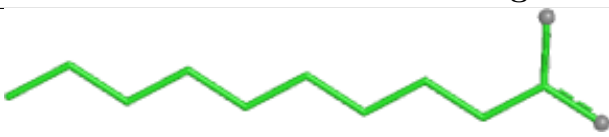
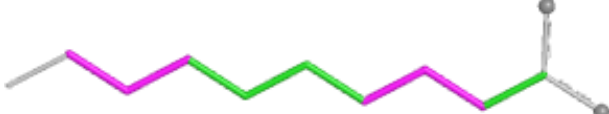
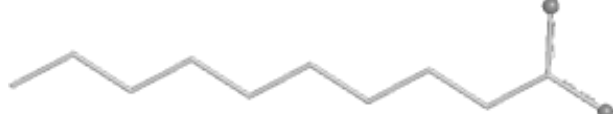
Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

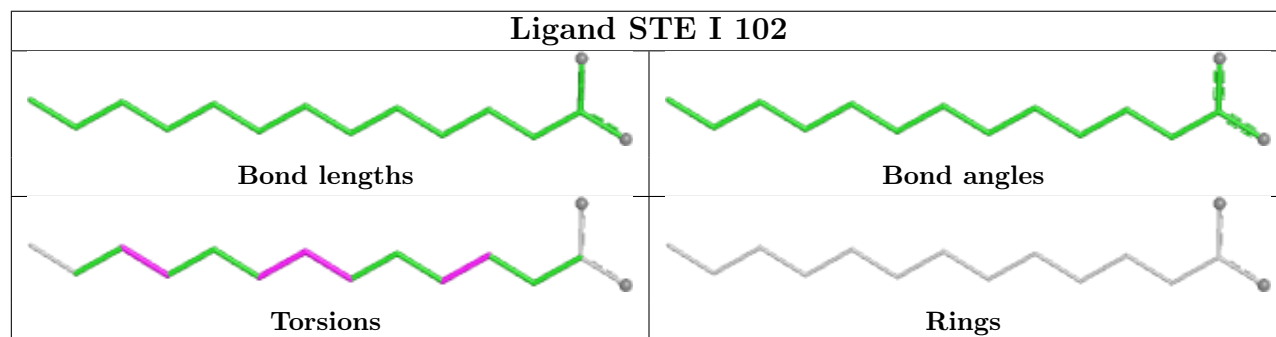
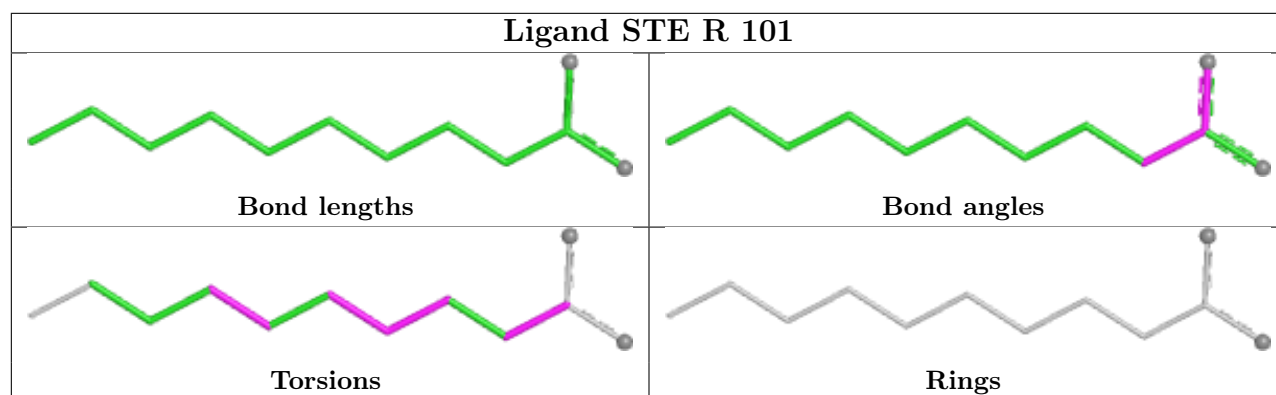
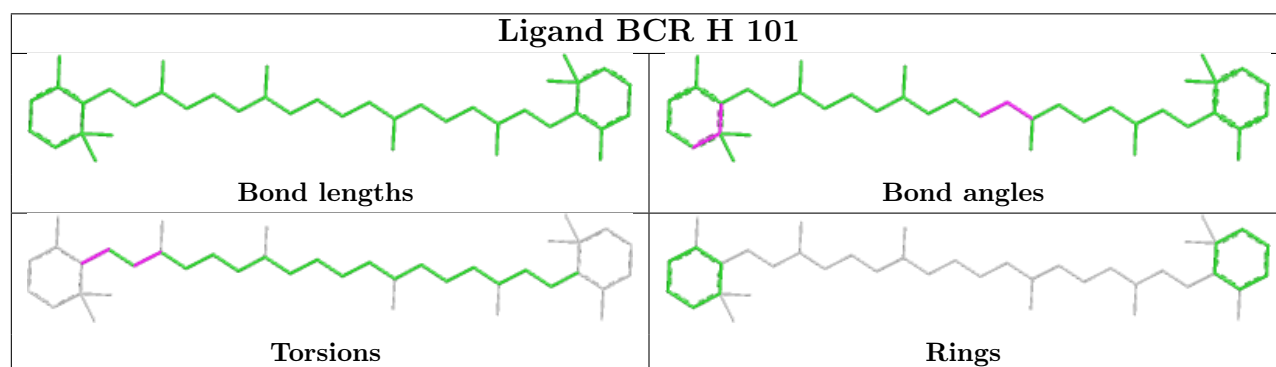
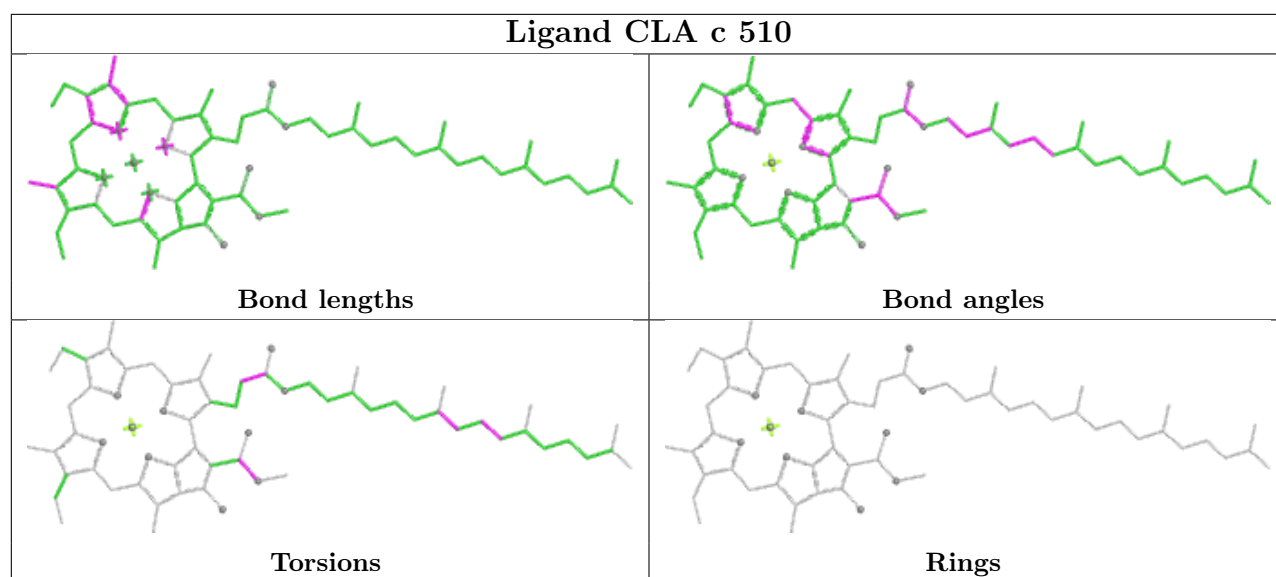
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

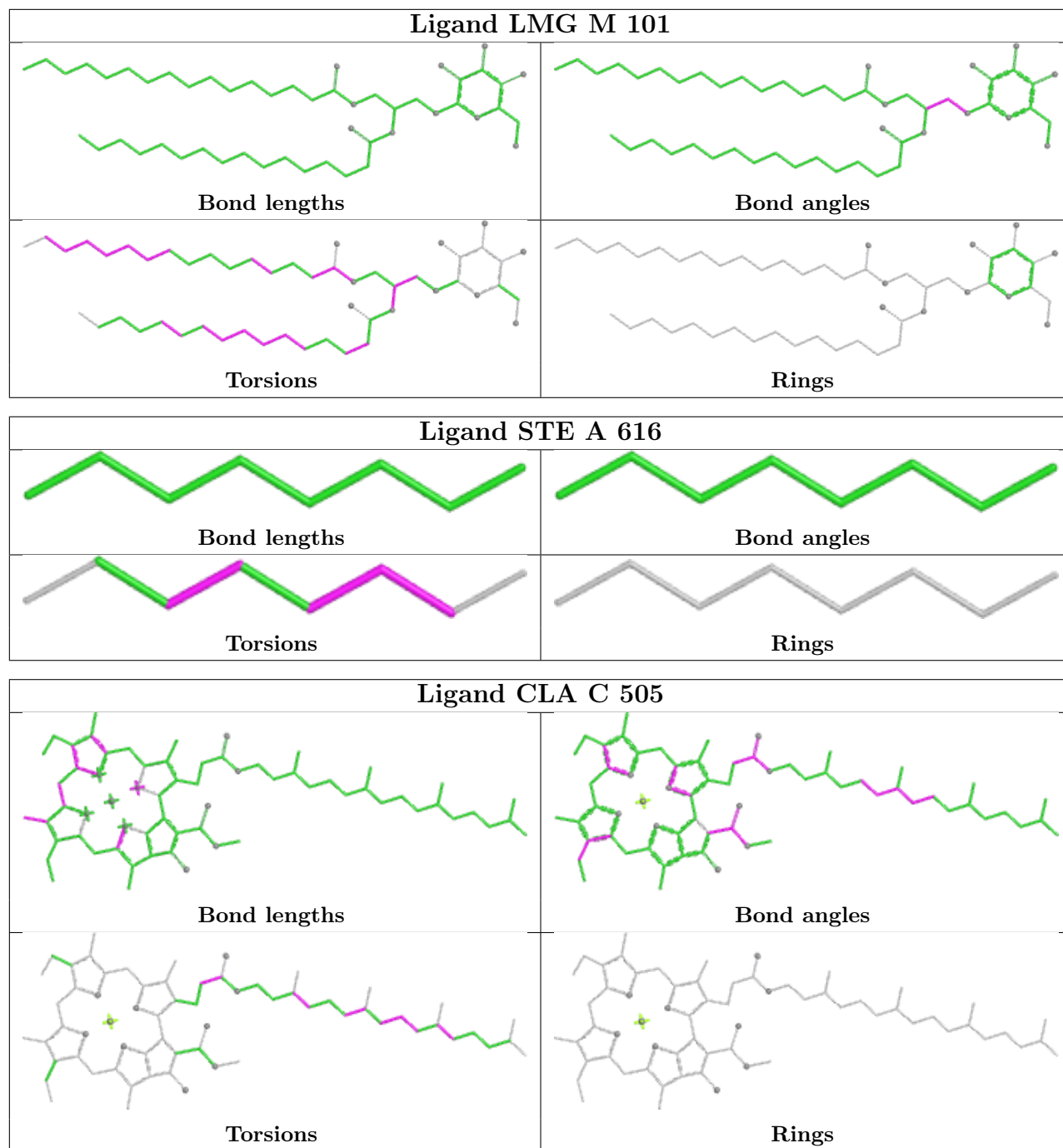
Ligand STE j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

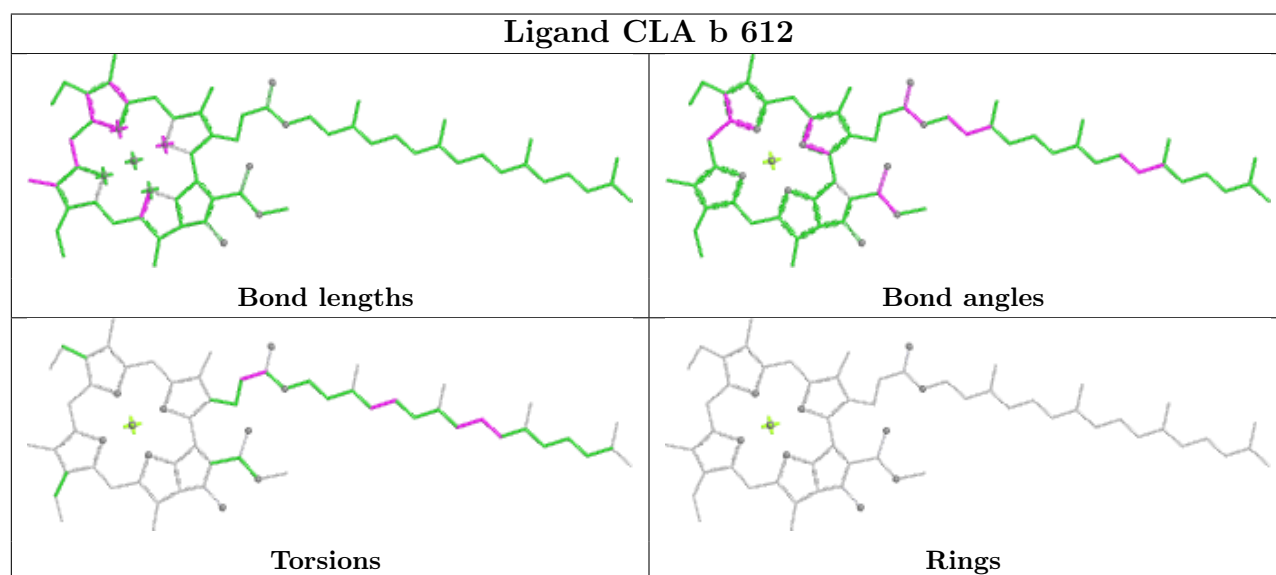
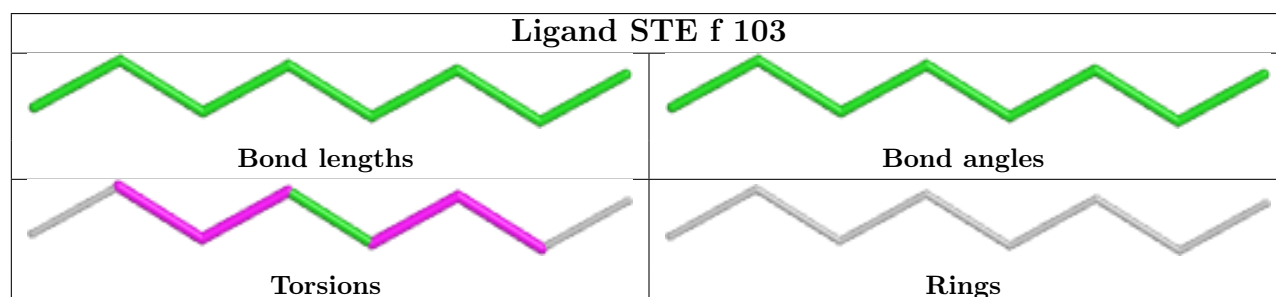
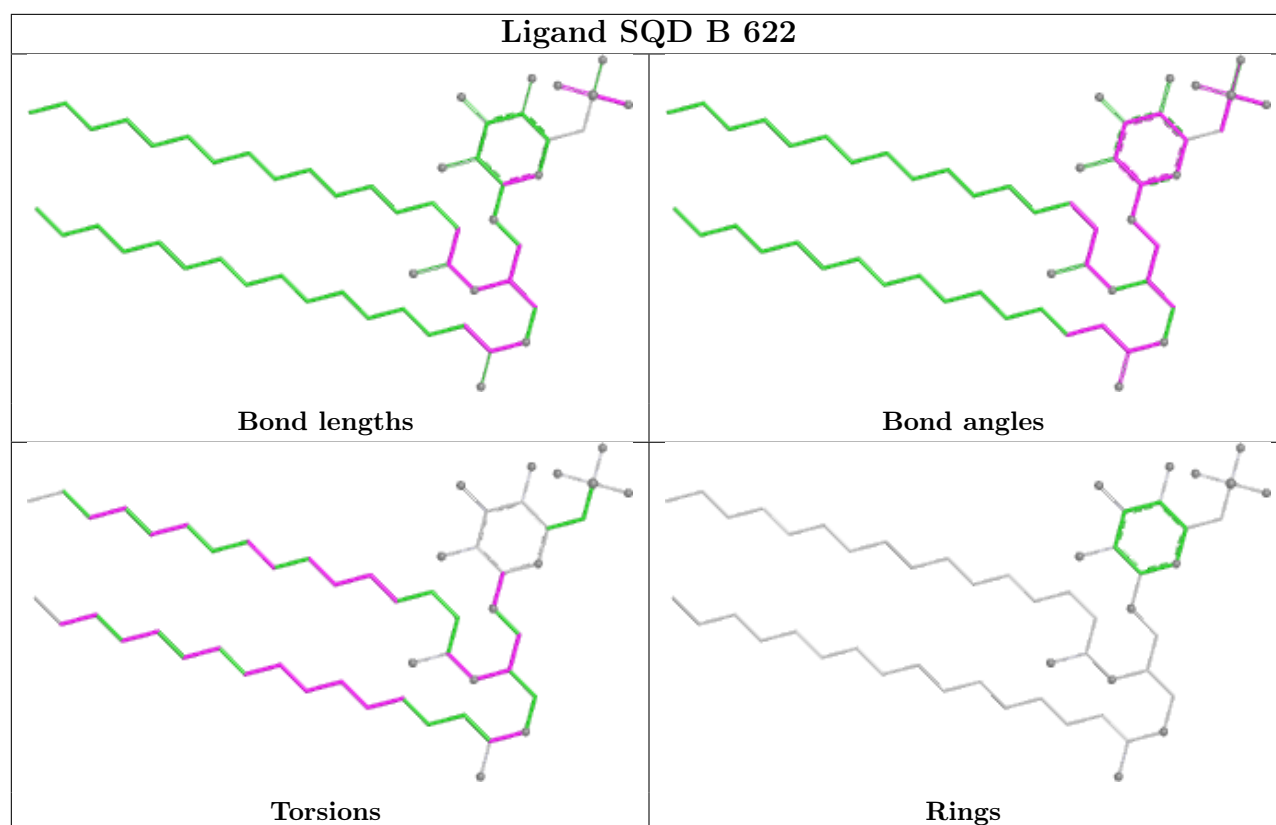
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

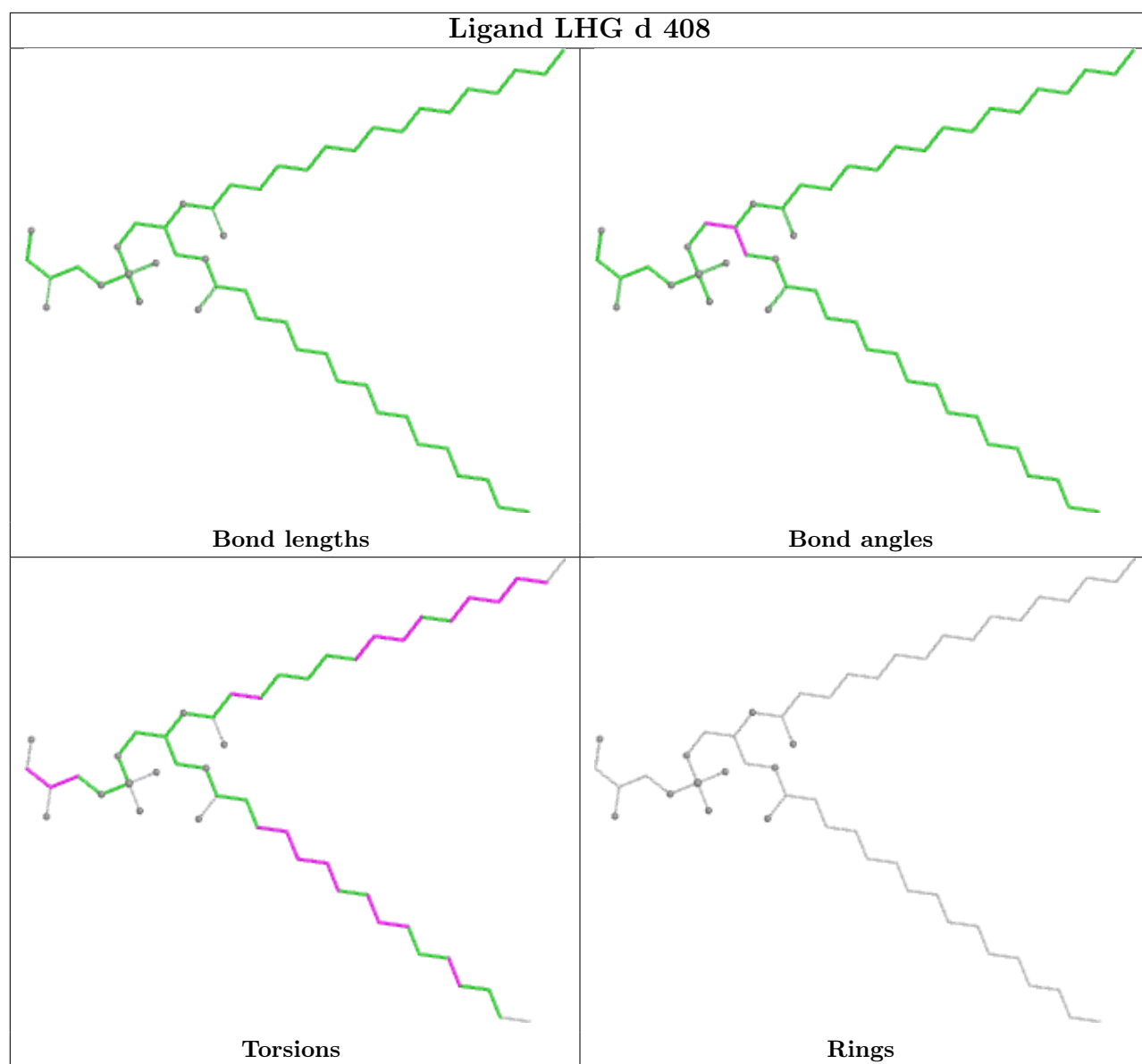
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

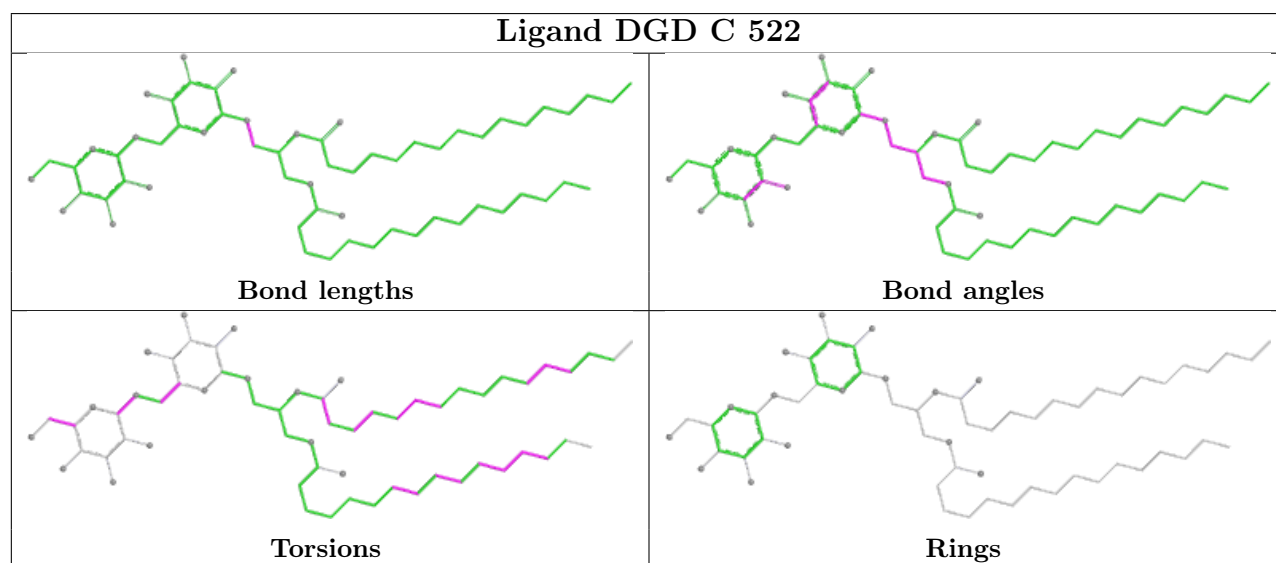
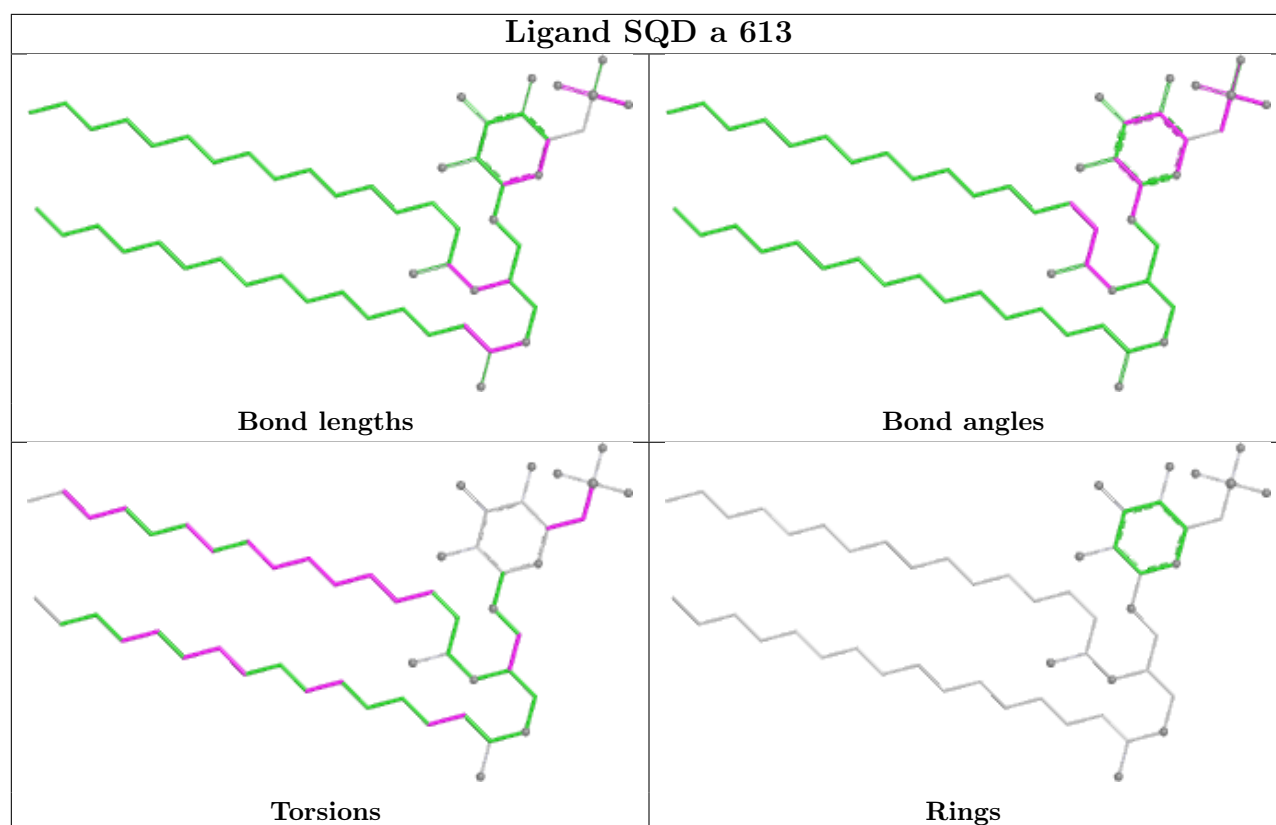
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Bond lengths	Bond angles
	
Torsions	Rings

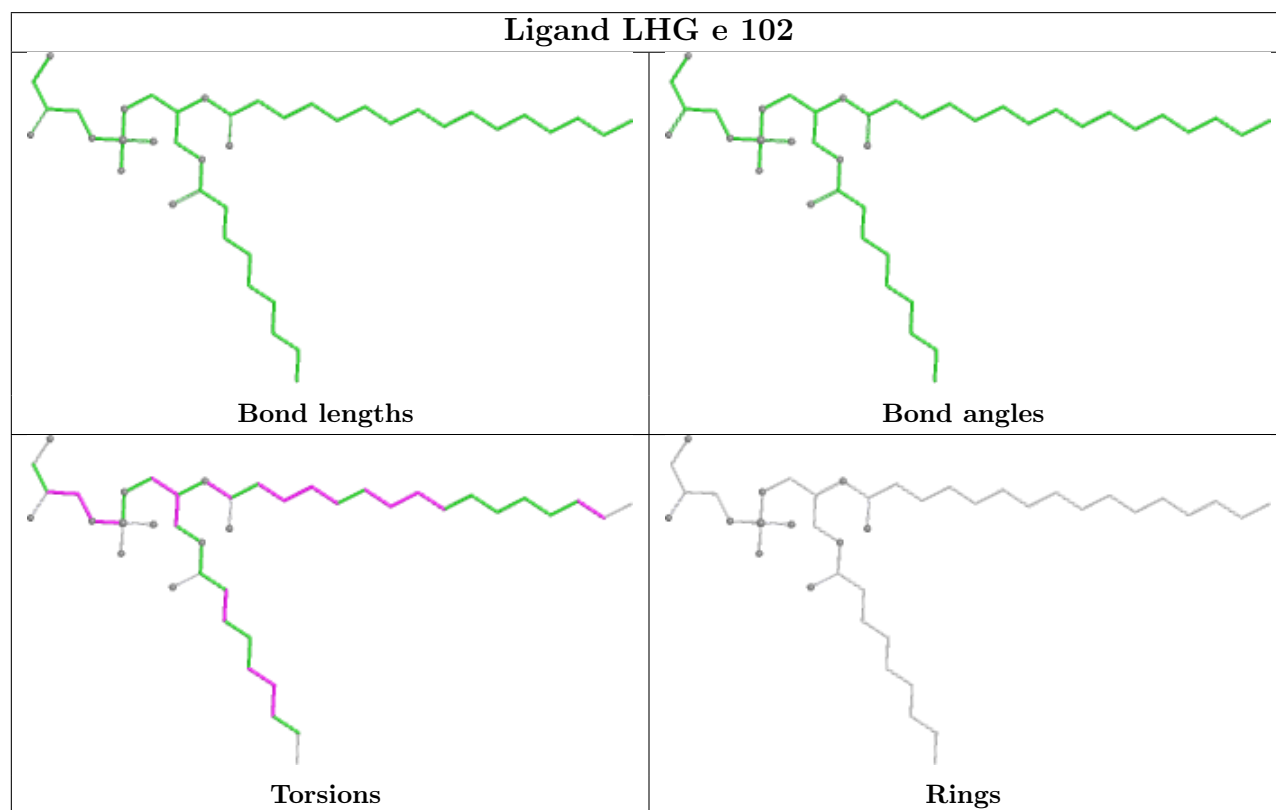
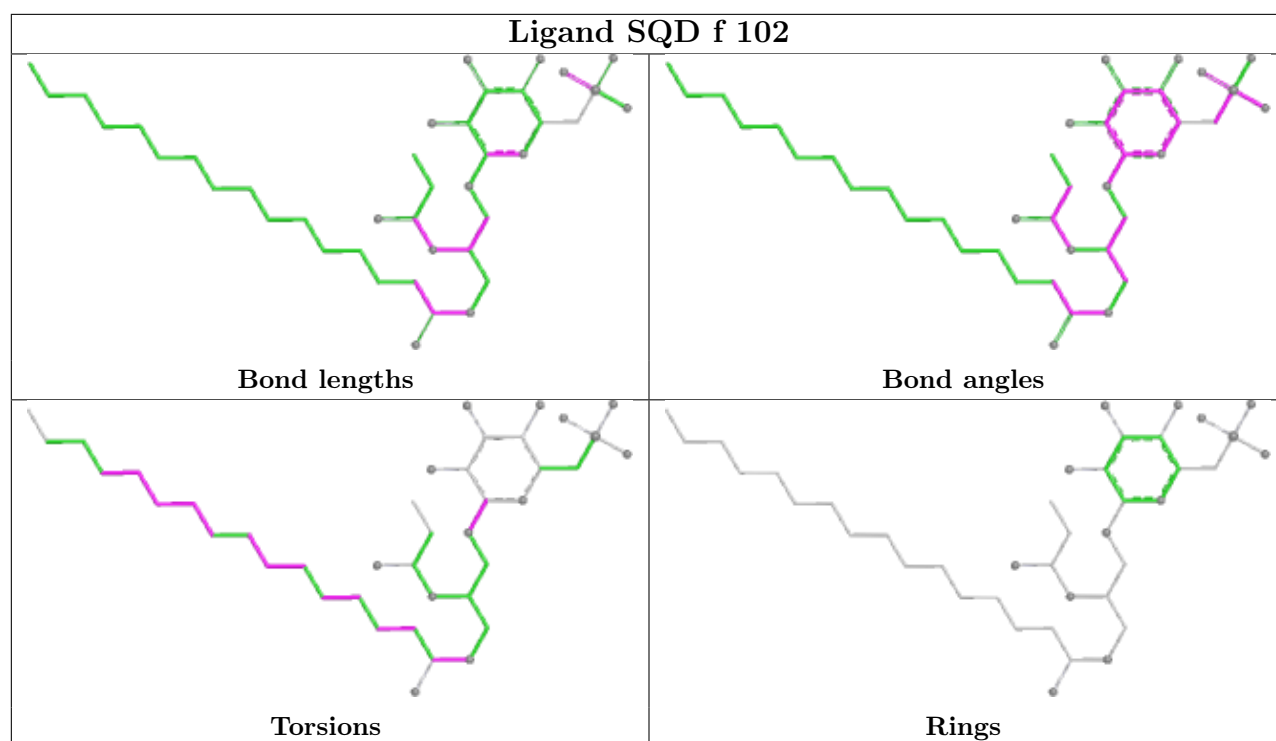


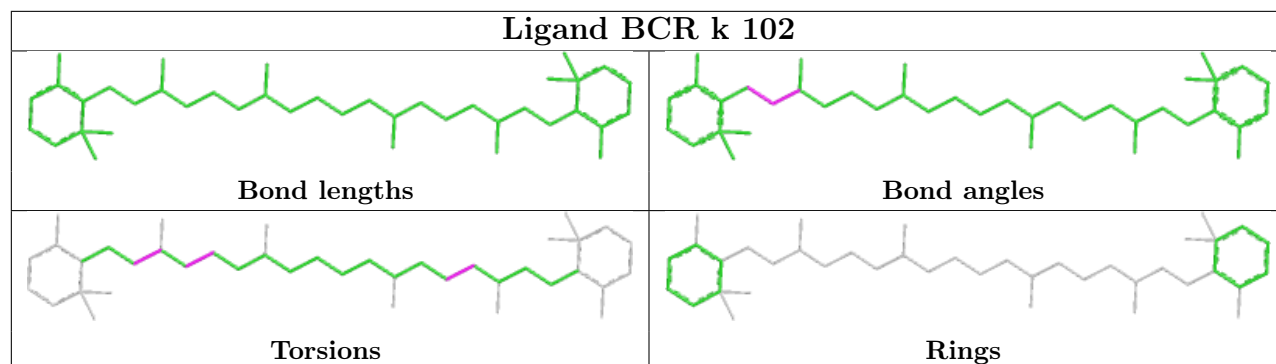
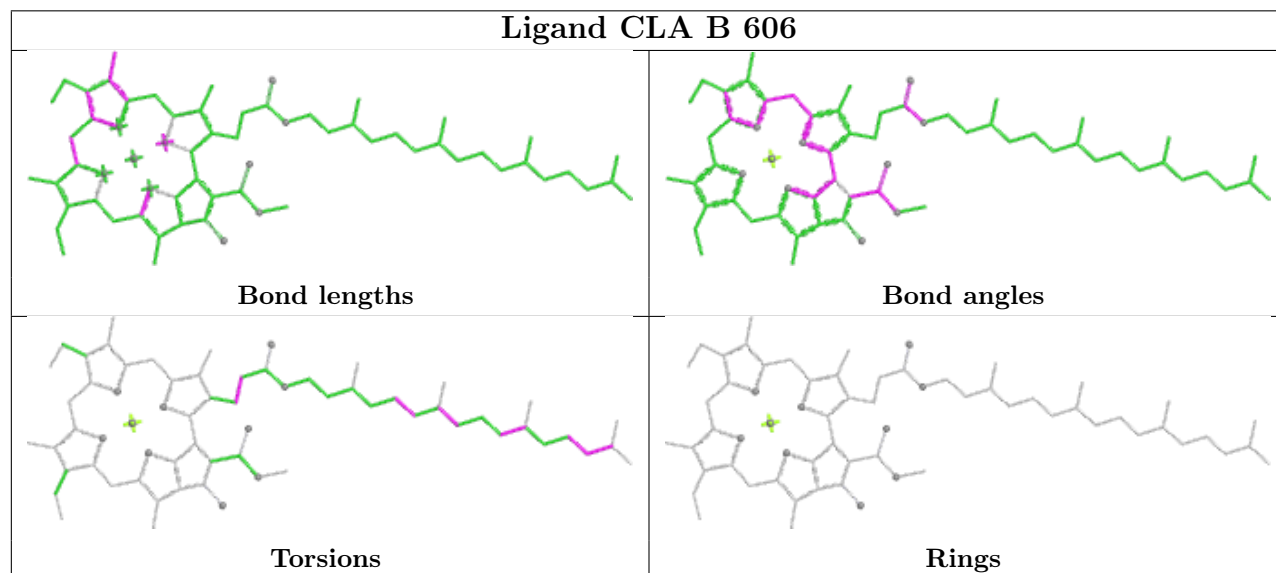
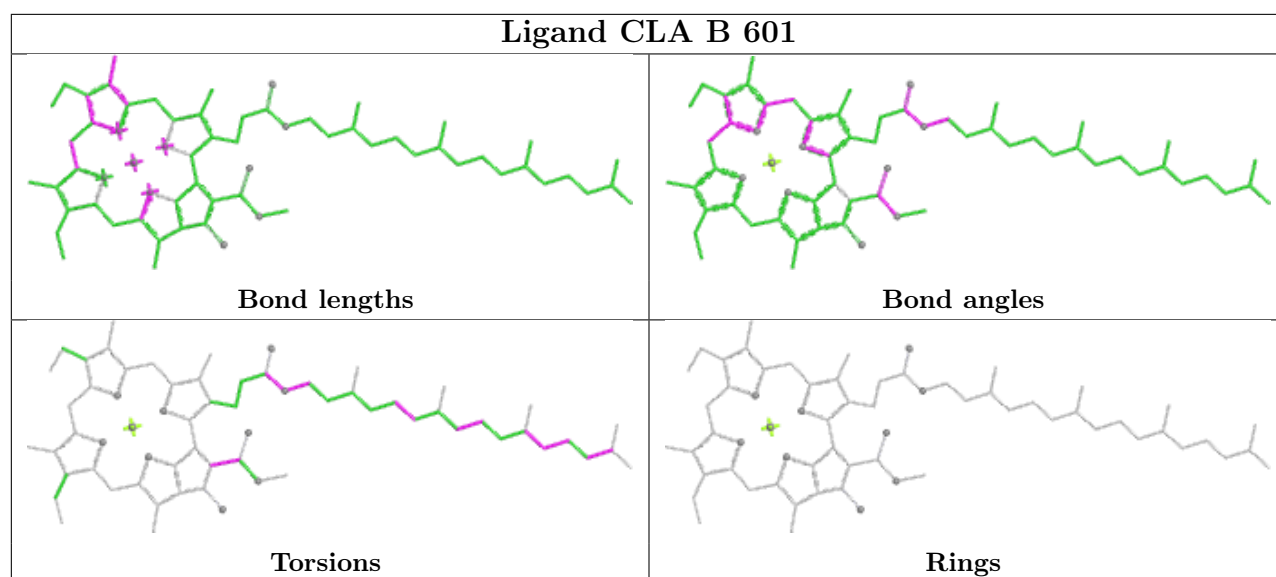


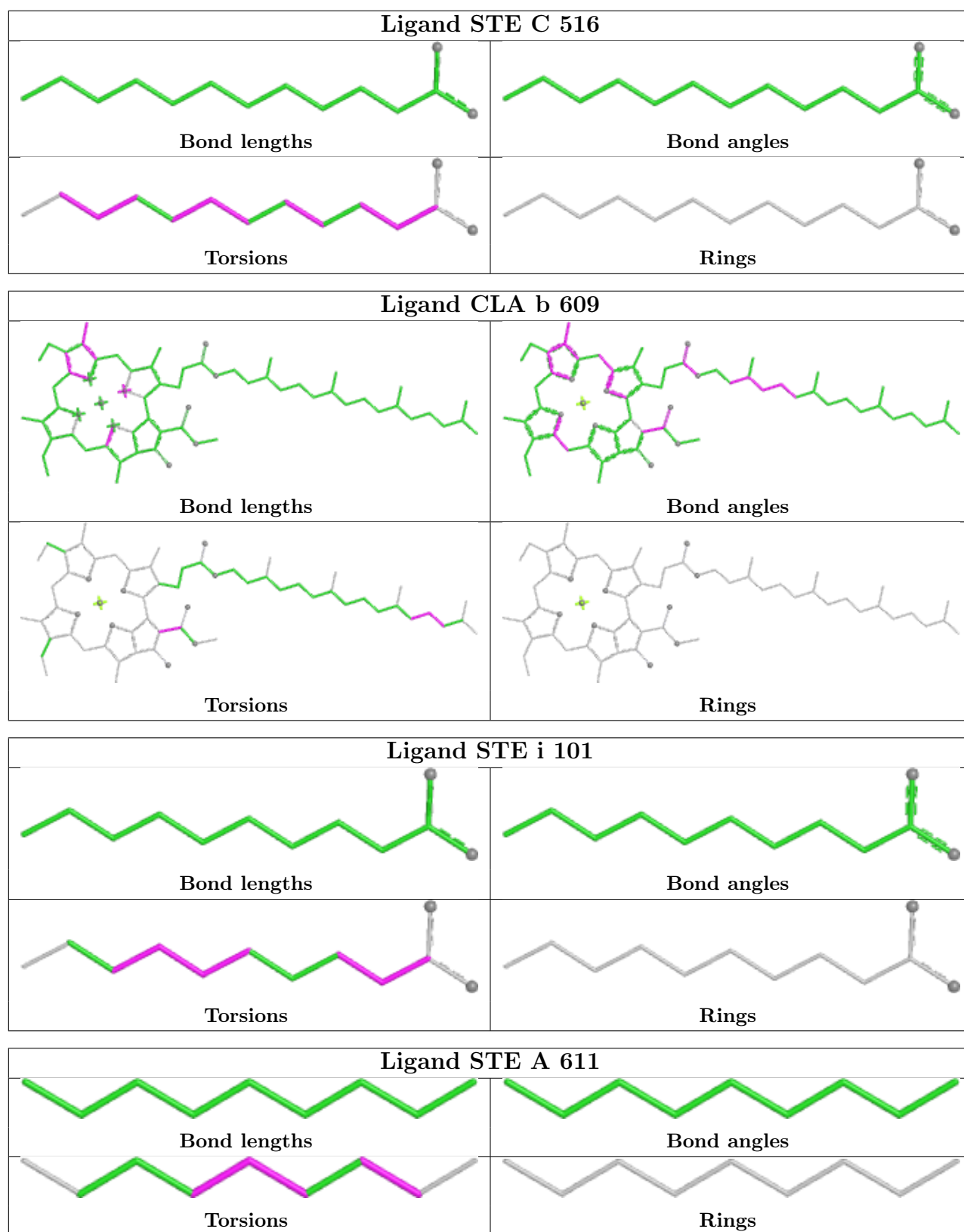




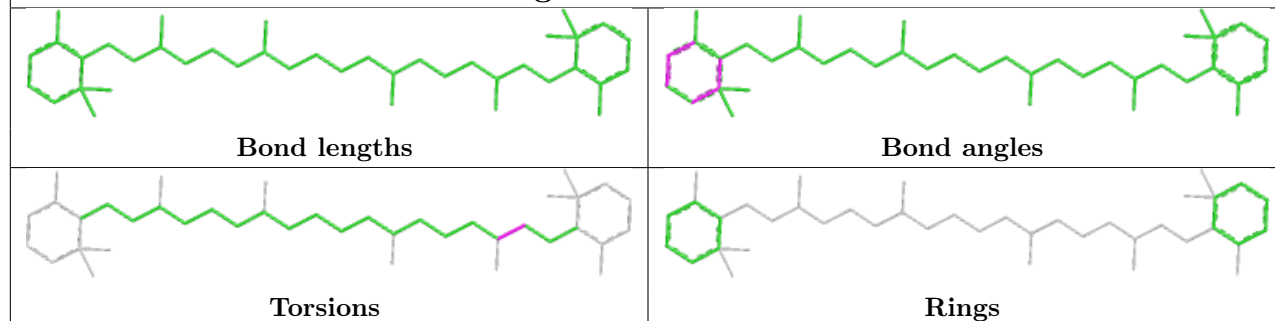




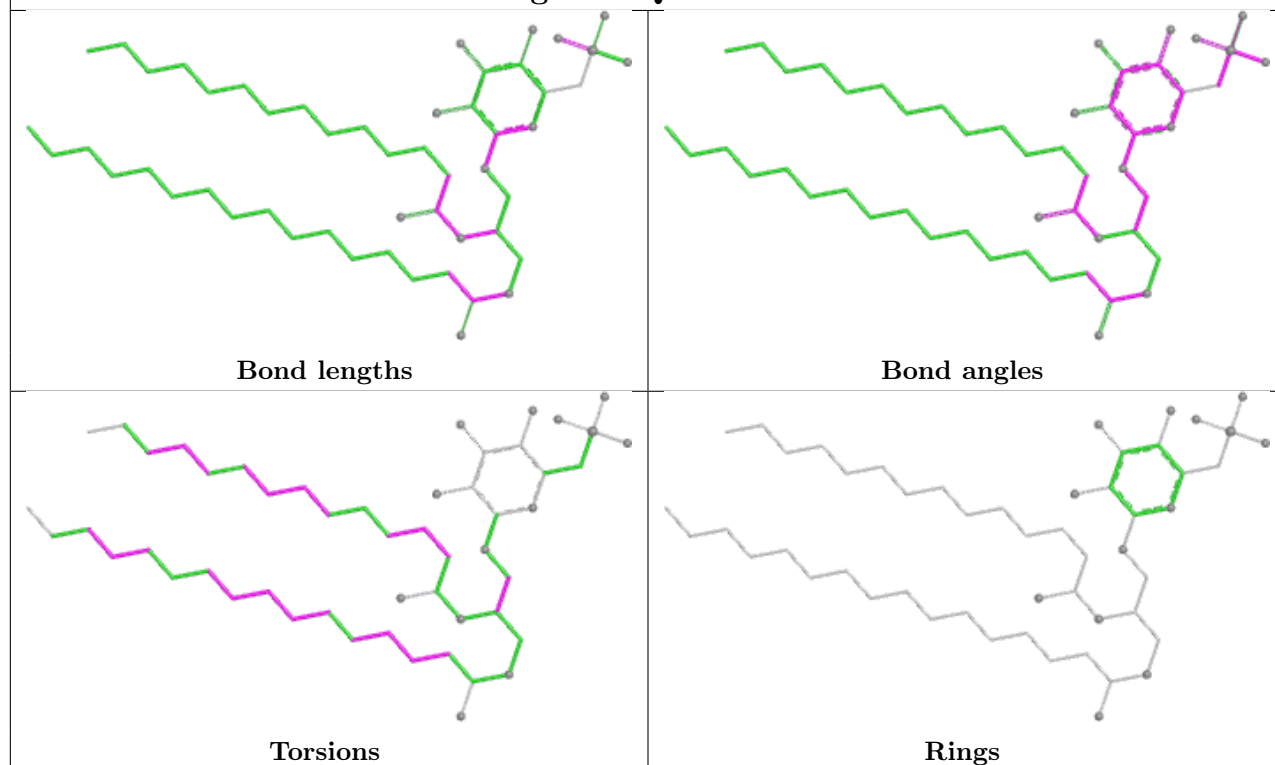




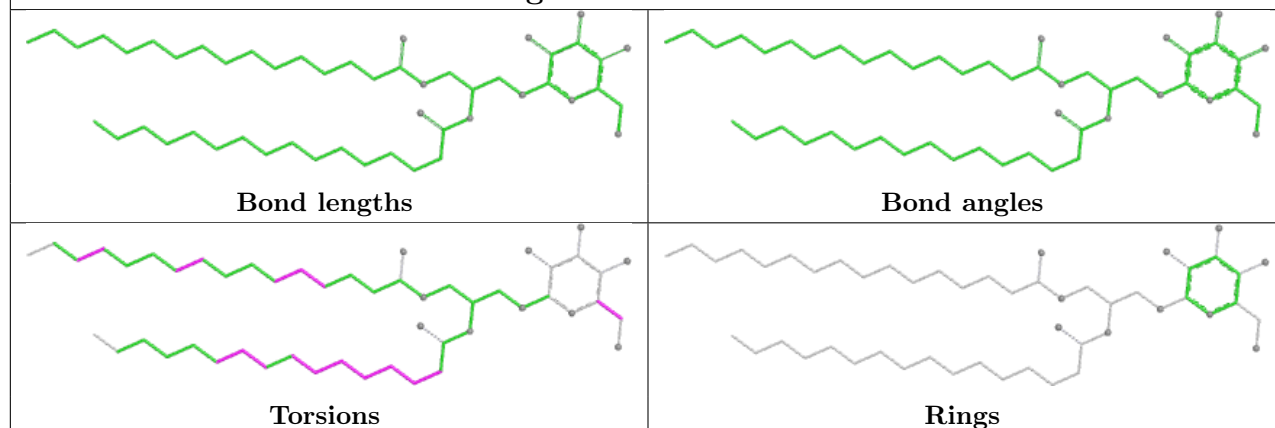
Ligand BCR c 515

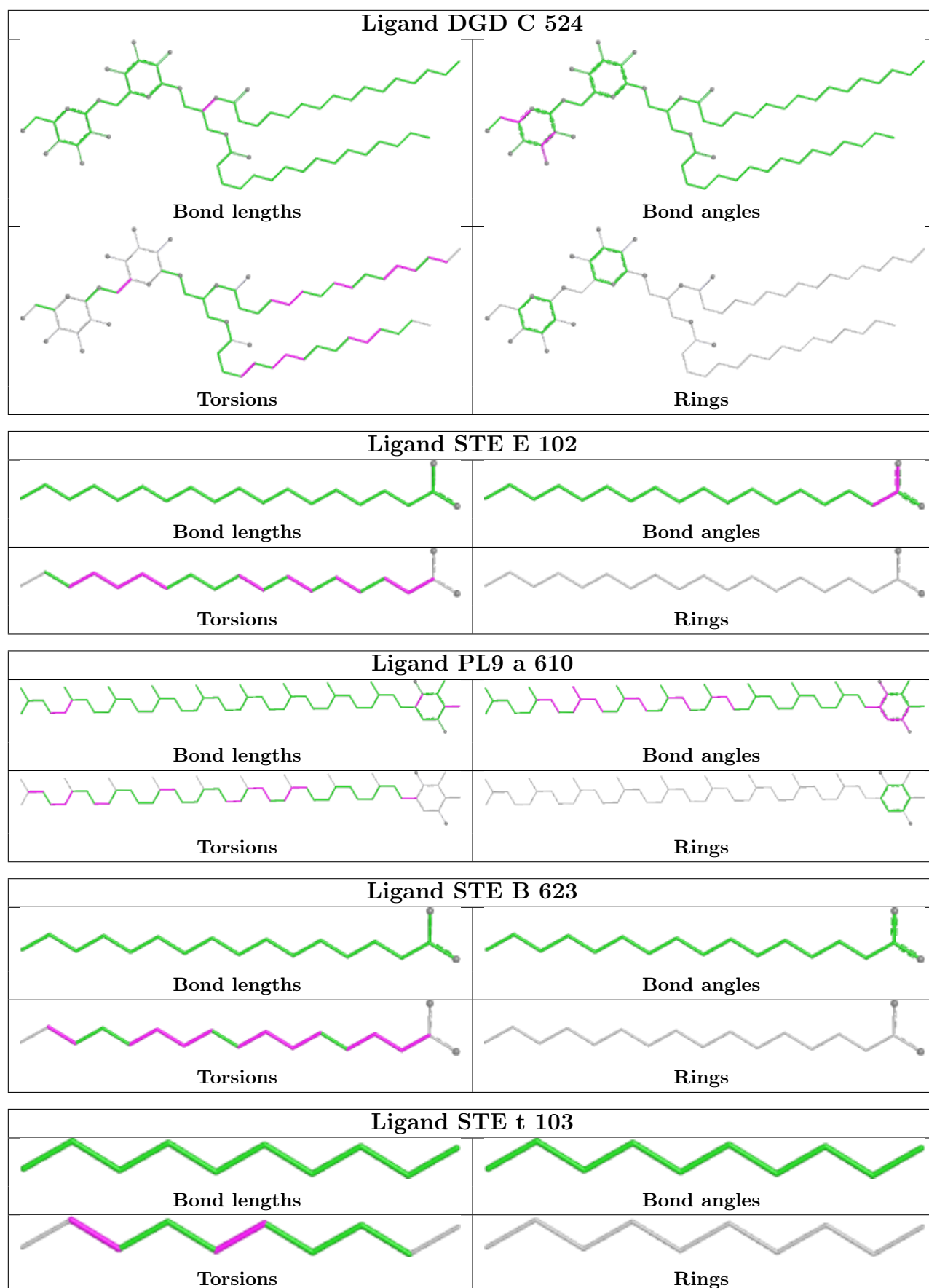


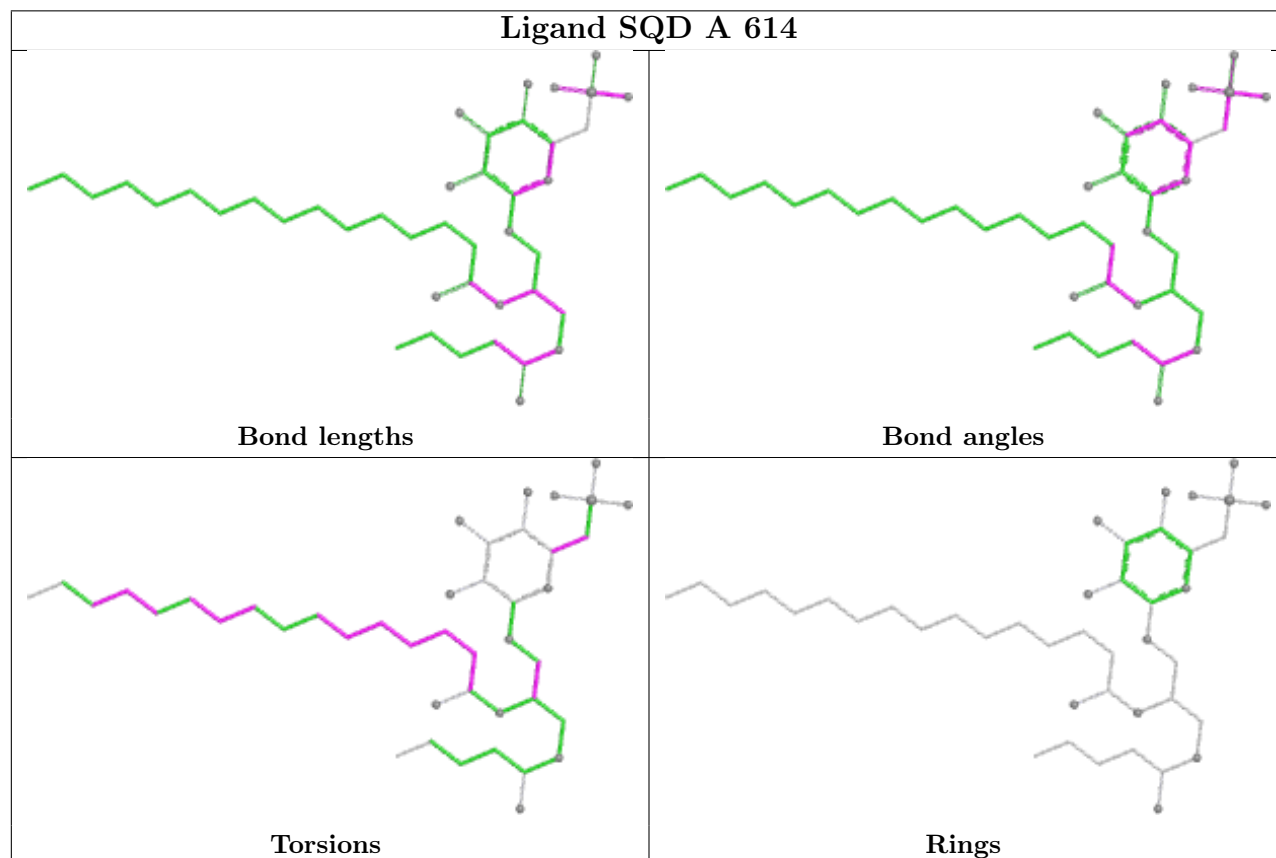
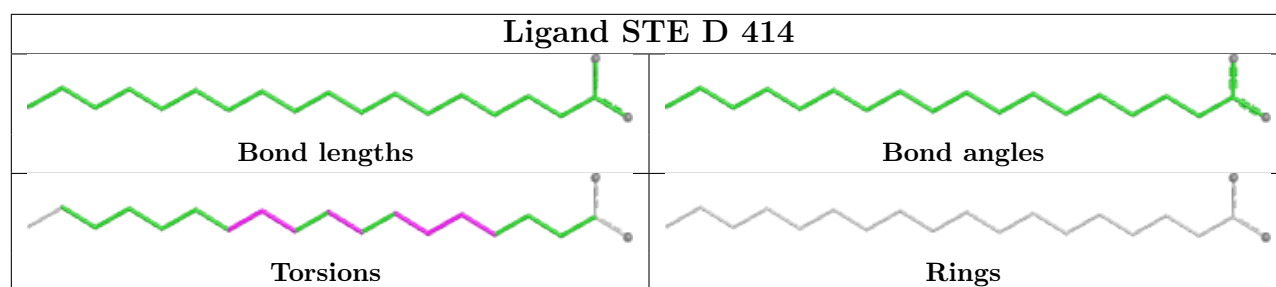
Ligand SQD D 412



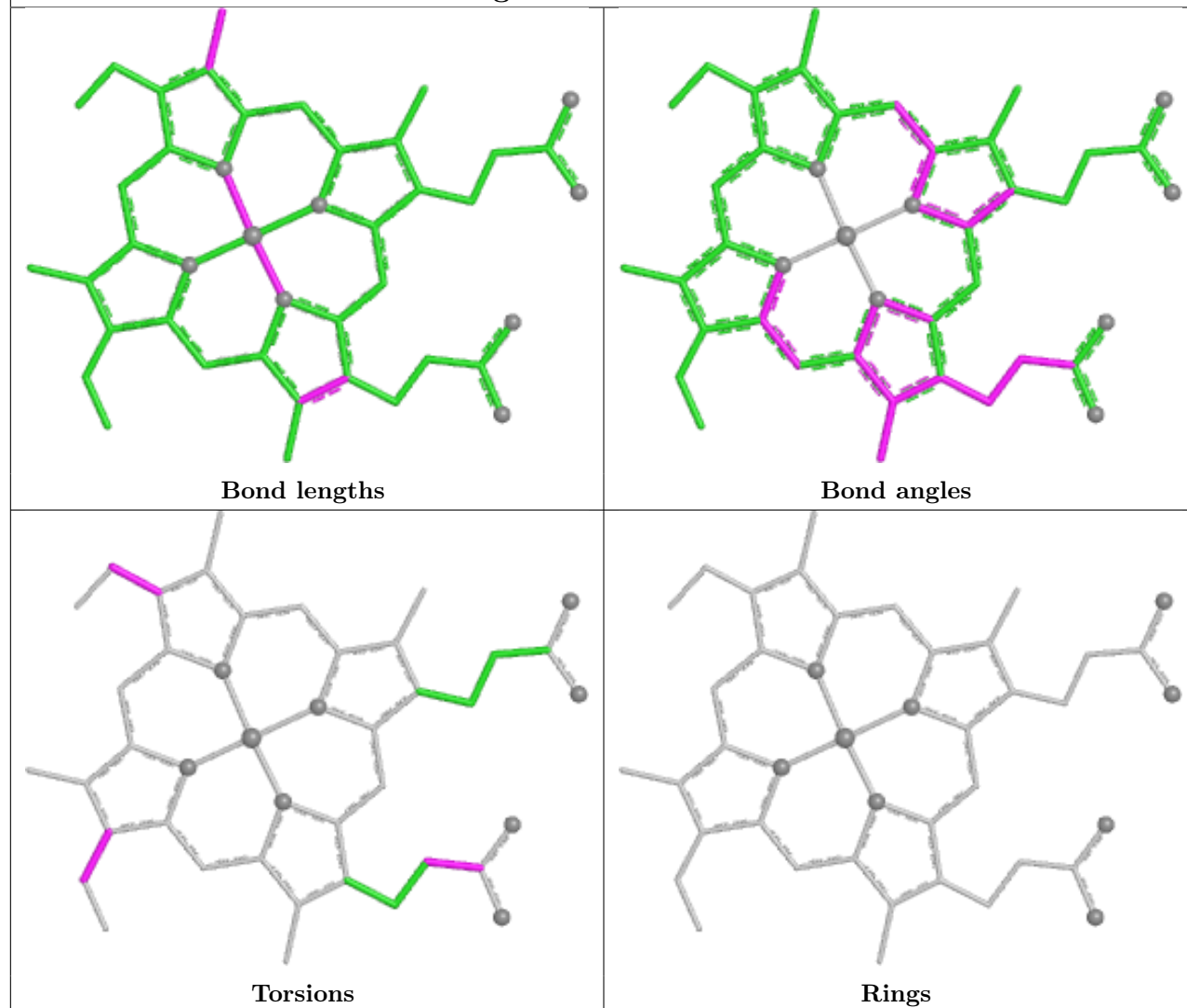
Ligand LMG D 408



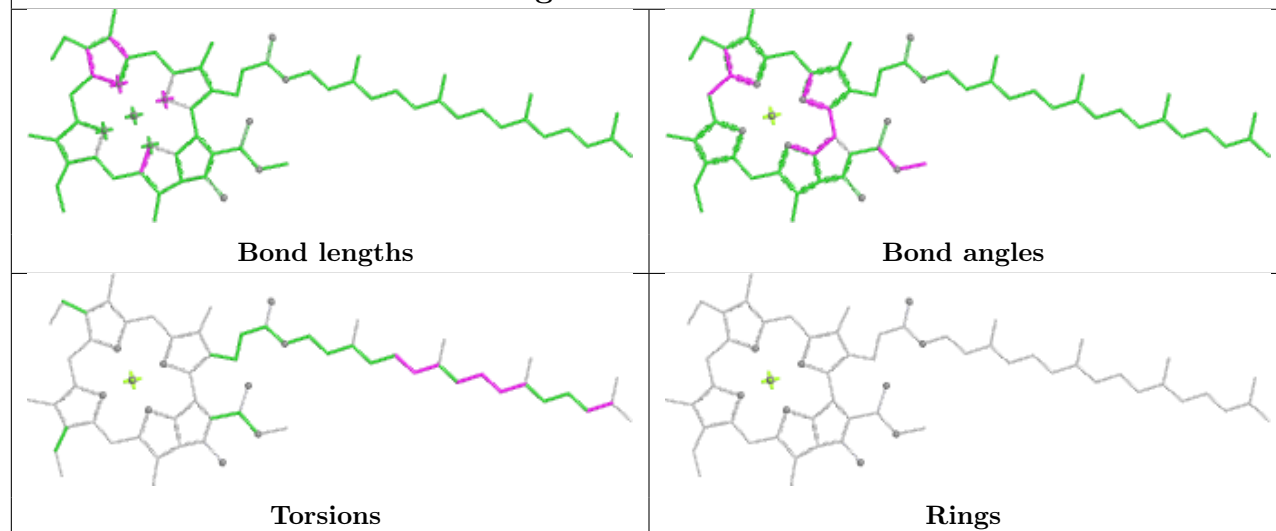




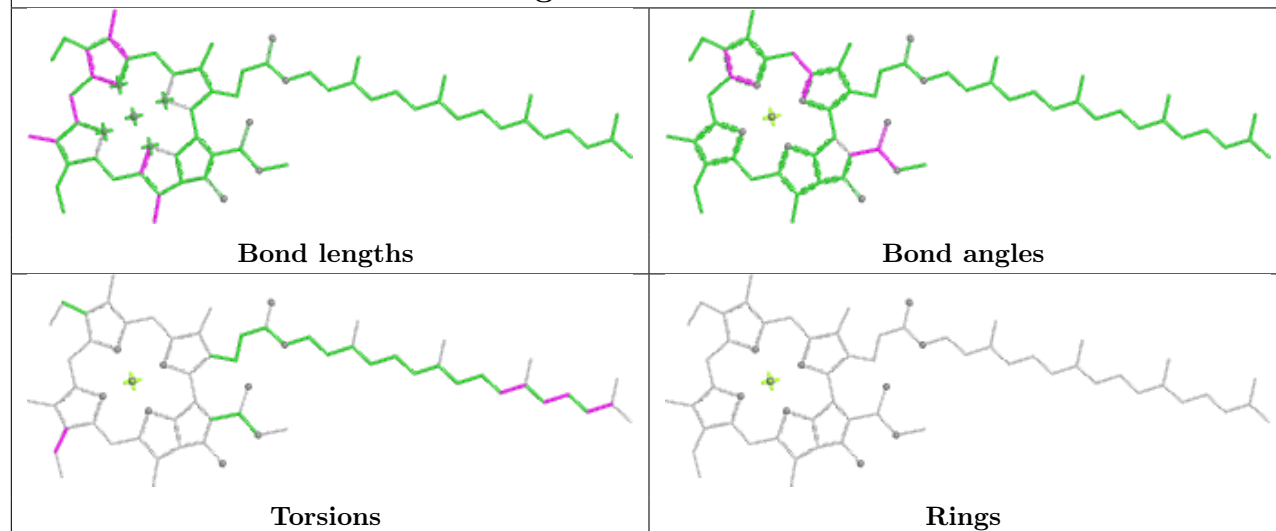
Ligand HEC V 201



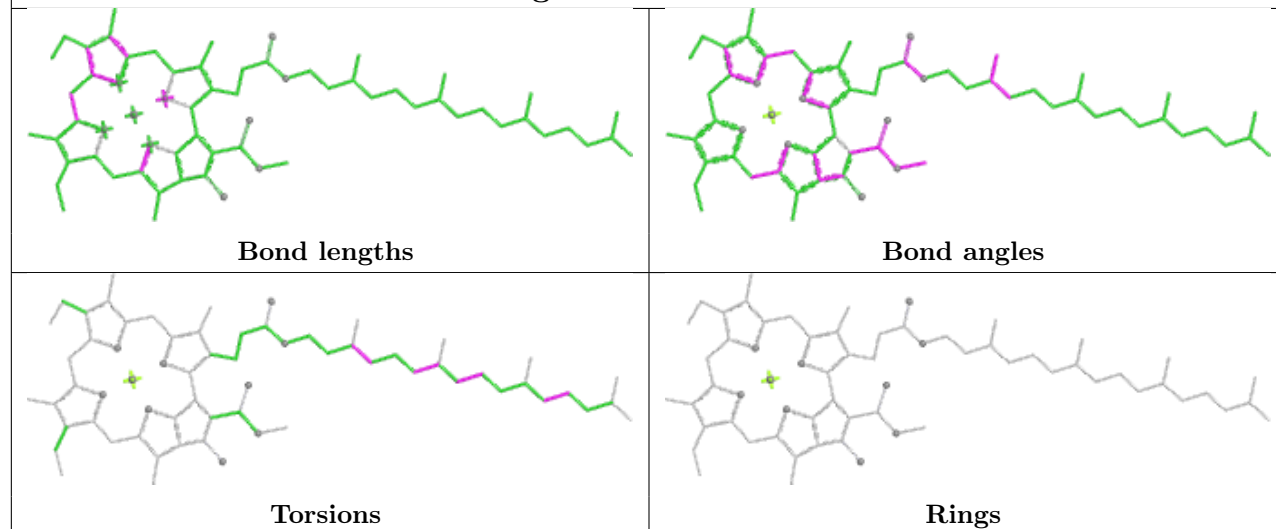
Ligand CLA b 607



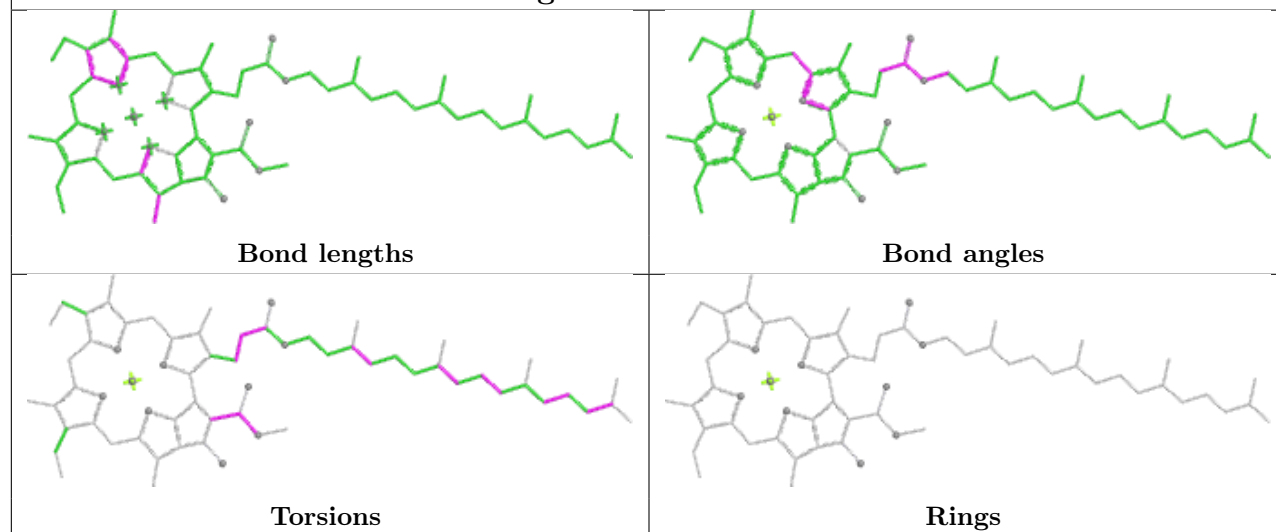
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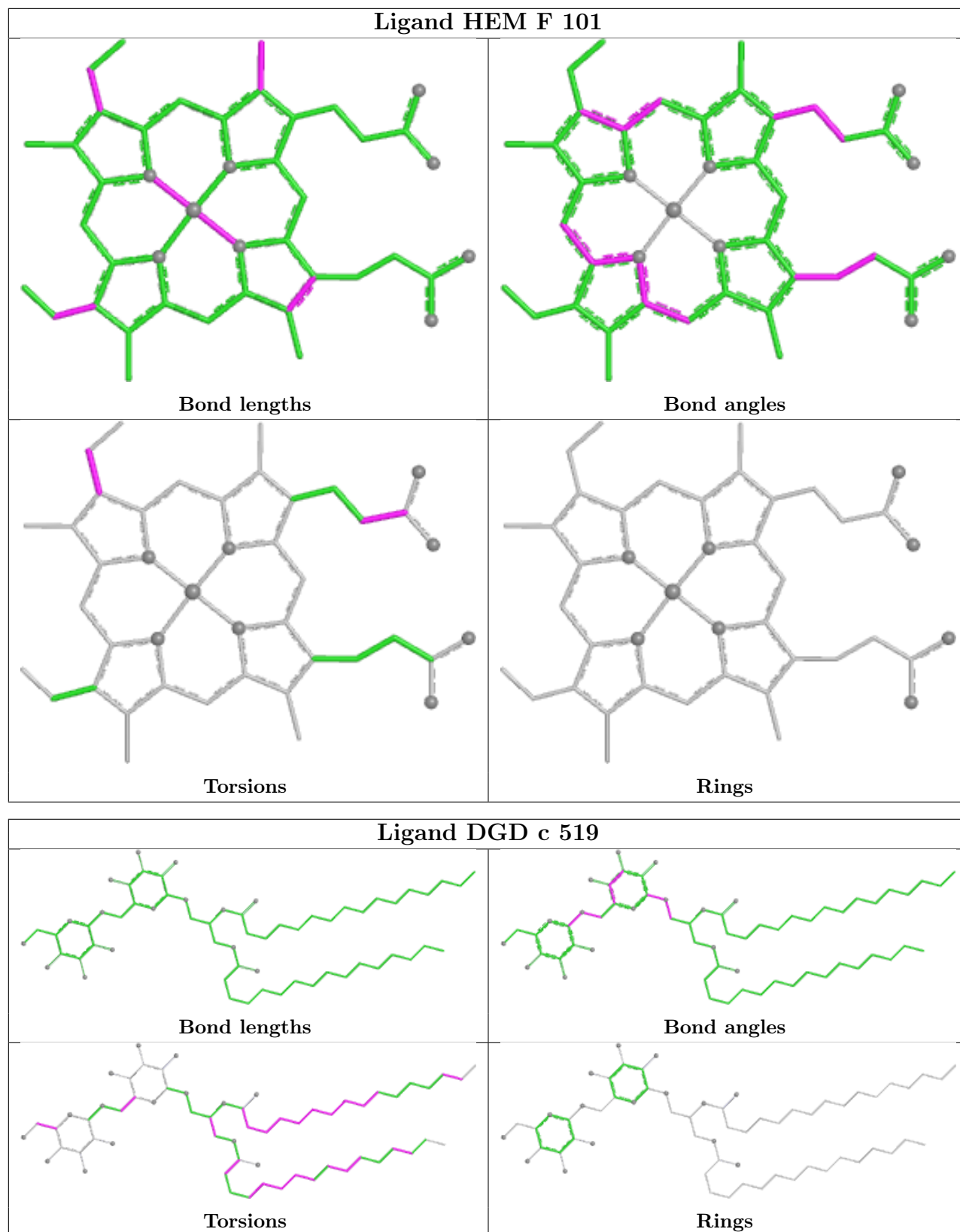


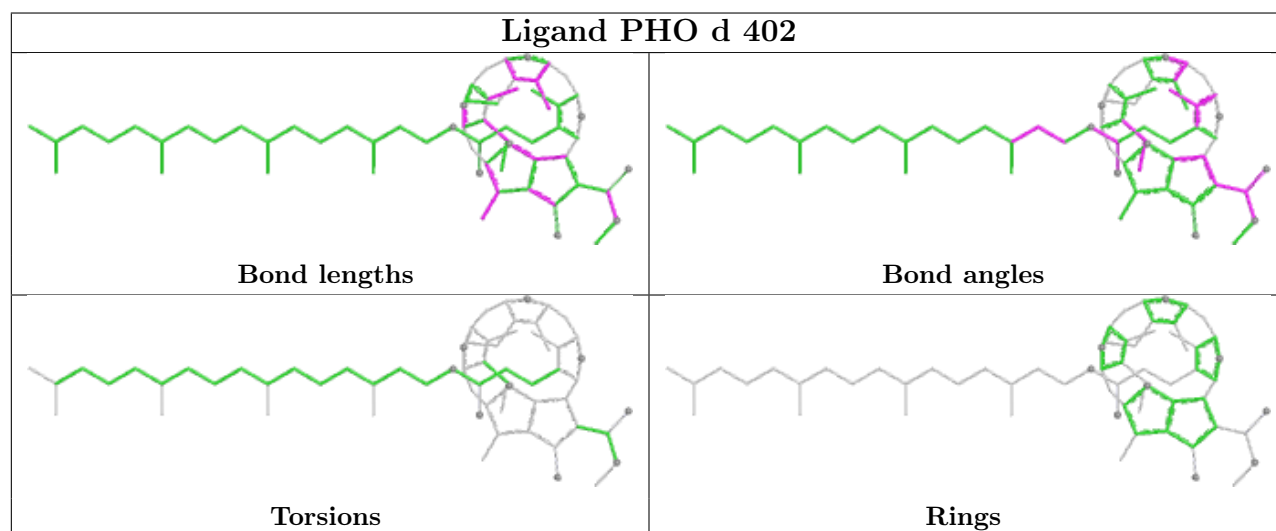
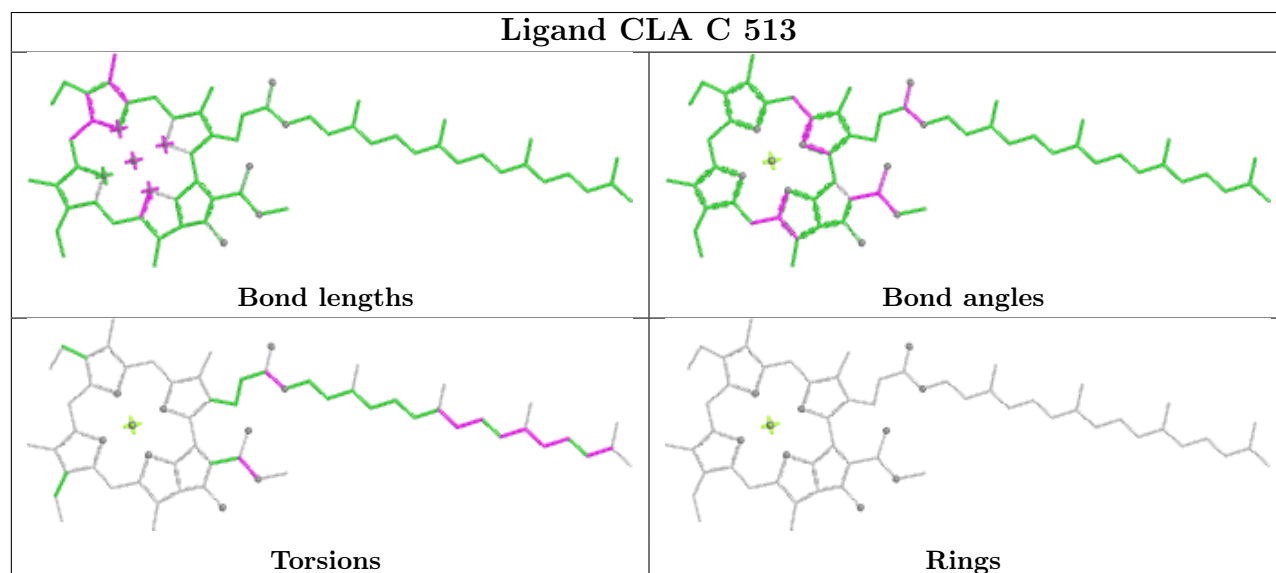
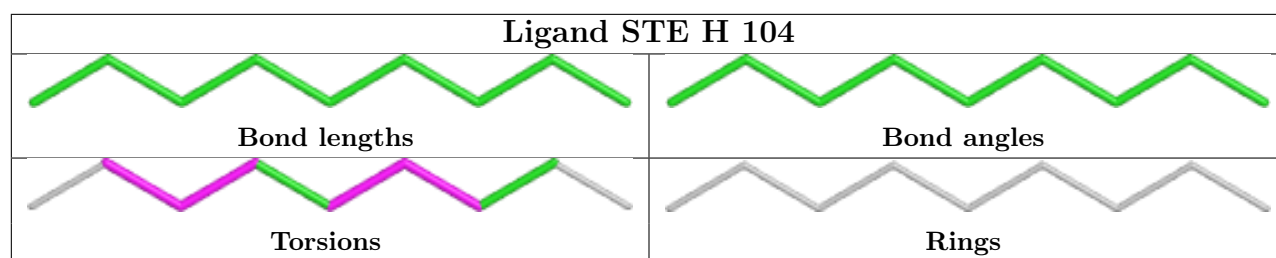
Ligand CLA B 605



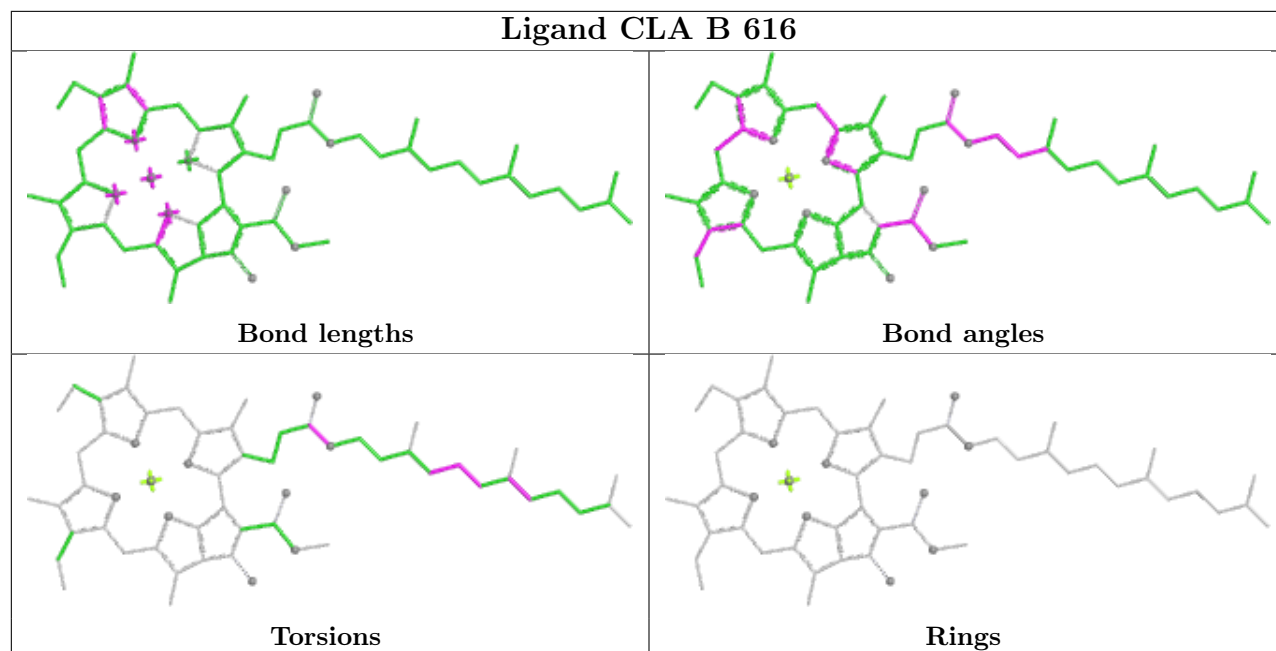
Ligand CLA c 509



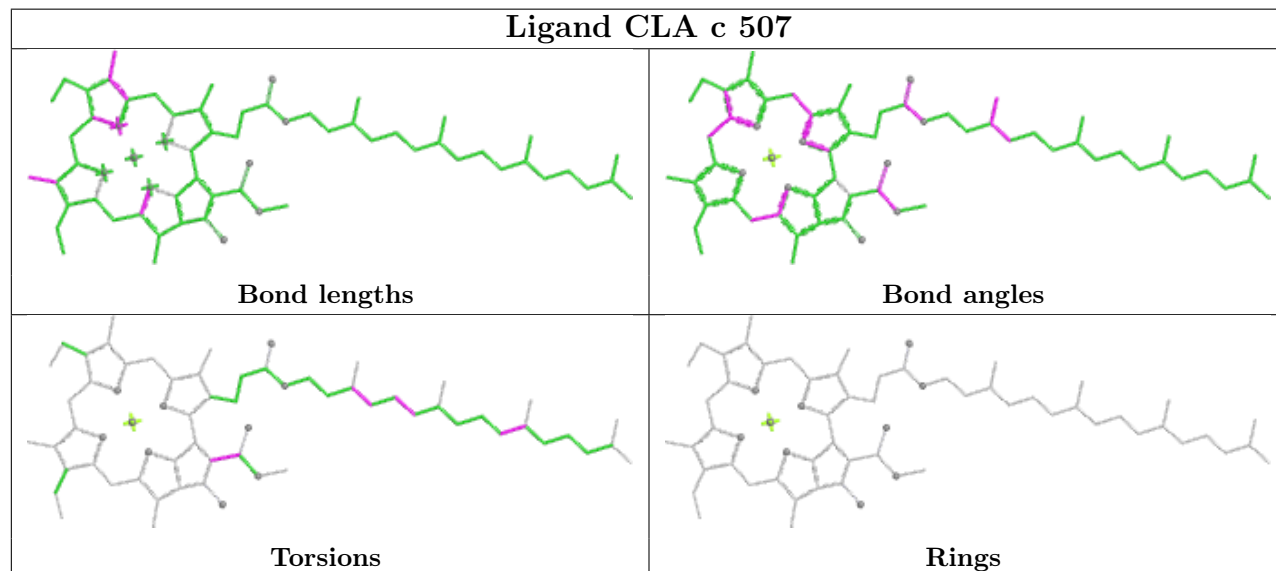


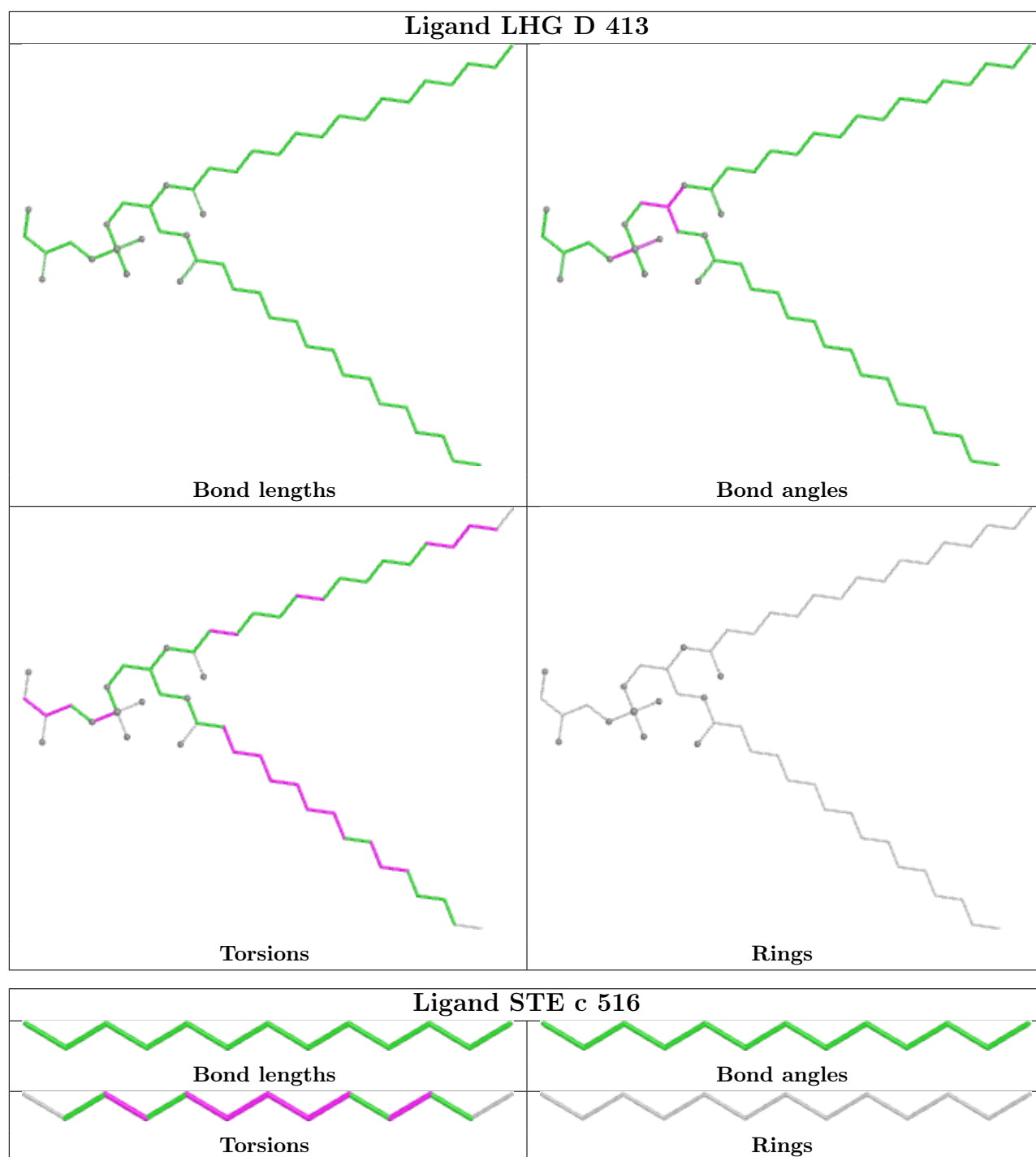


Ligand CLA B 616

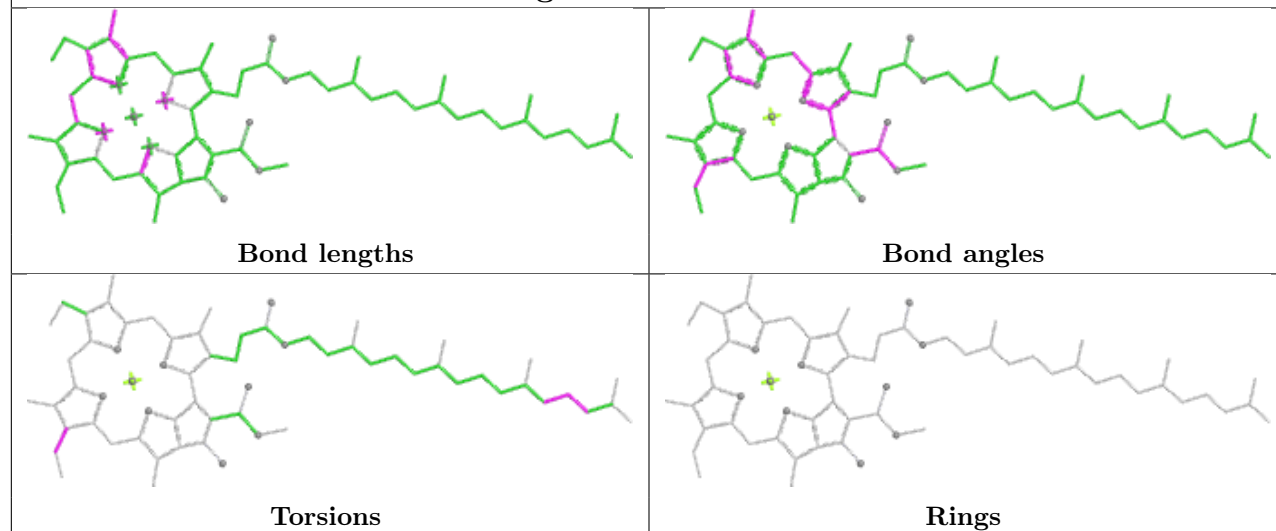


Ligand CLA c 507





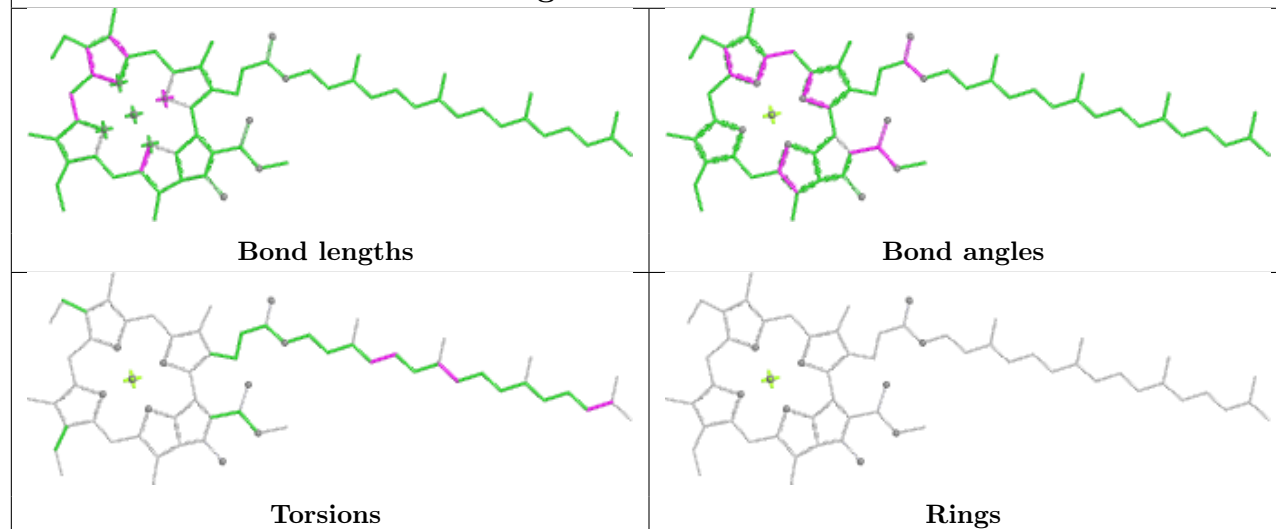
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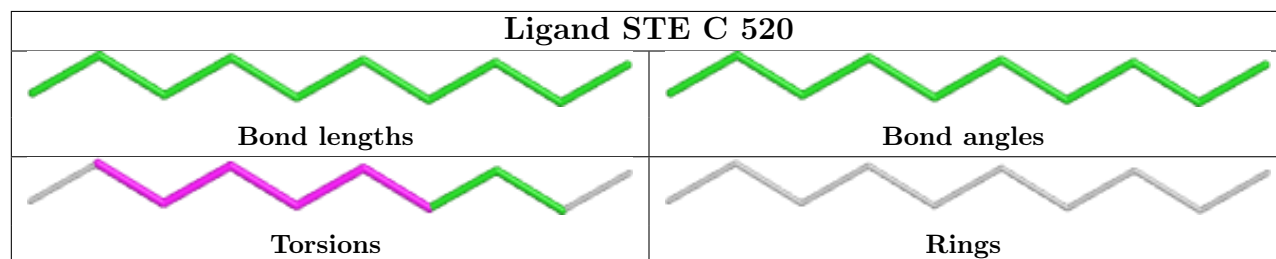
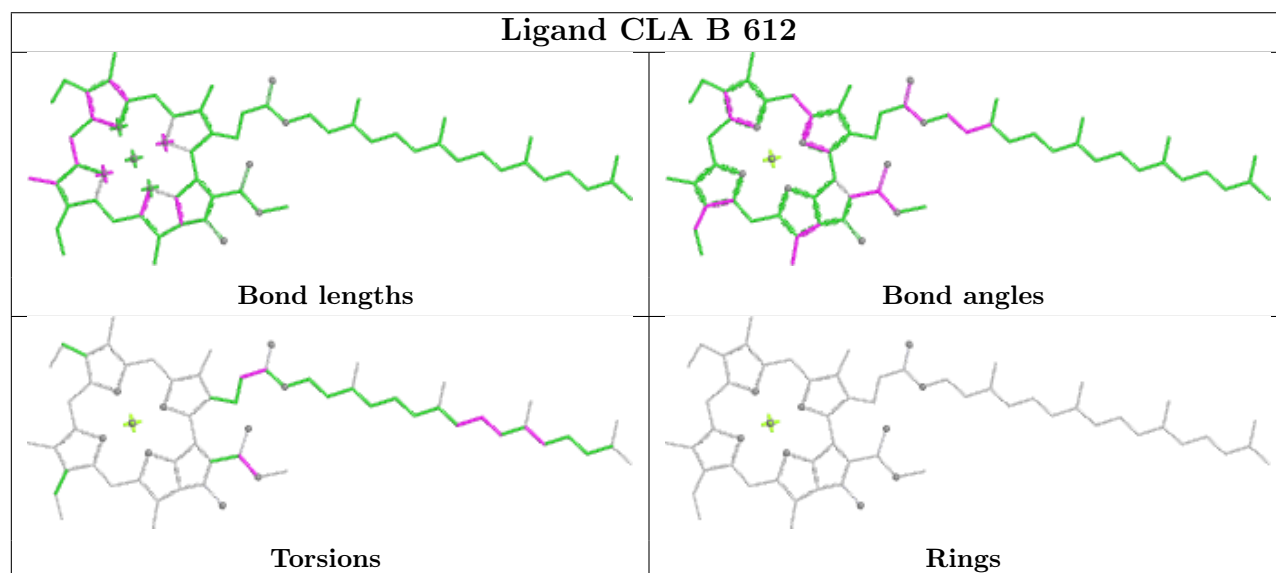
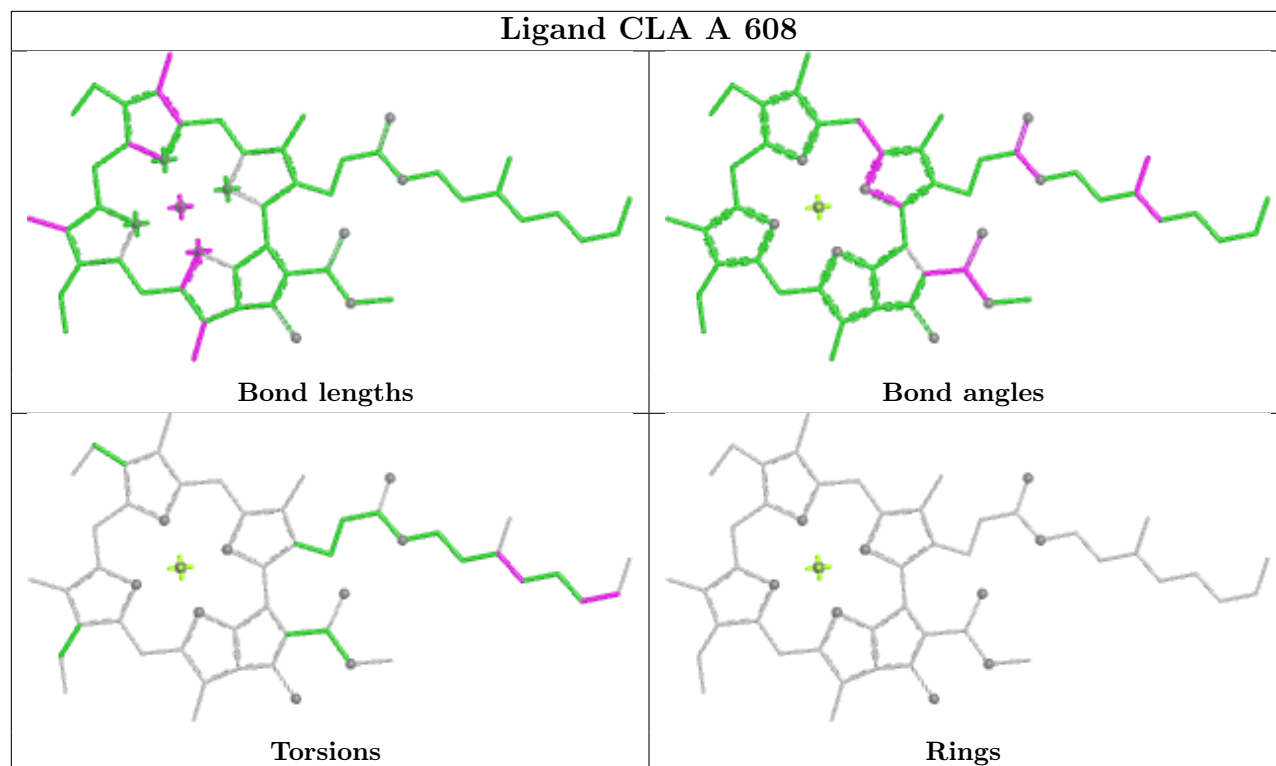


Ligand LMG B 620

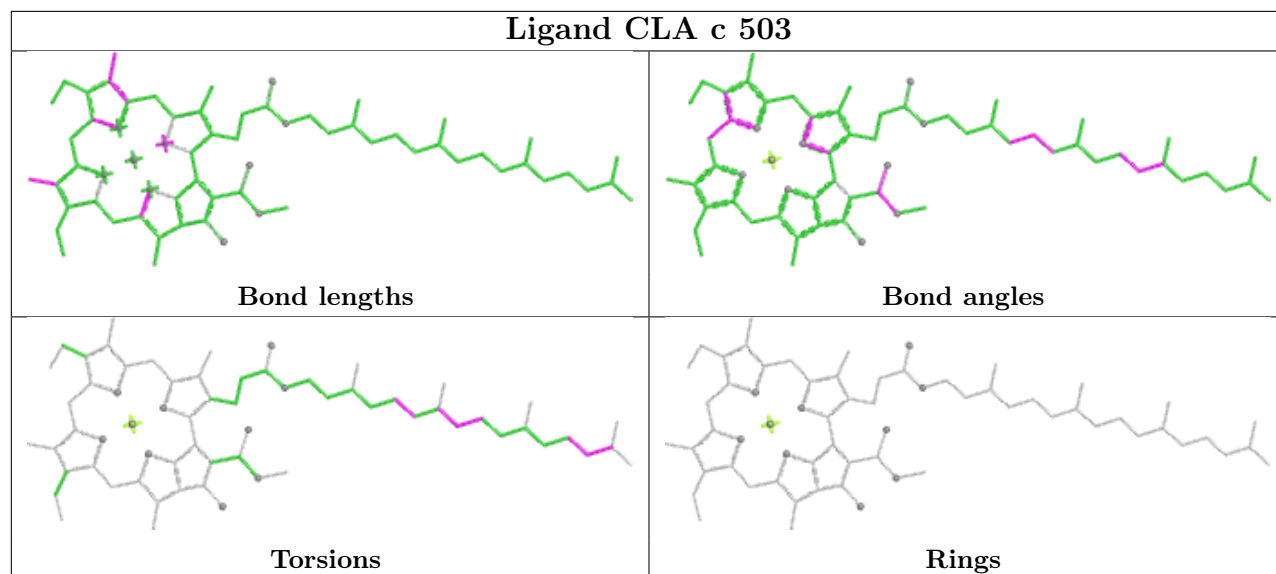


Ligand CLA c 511

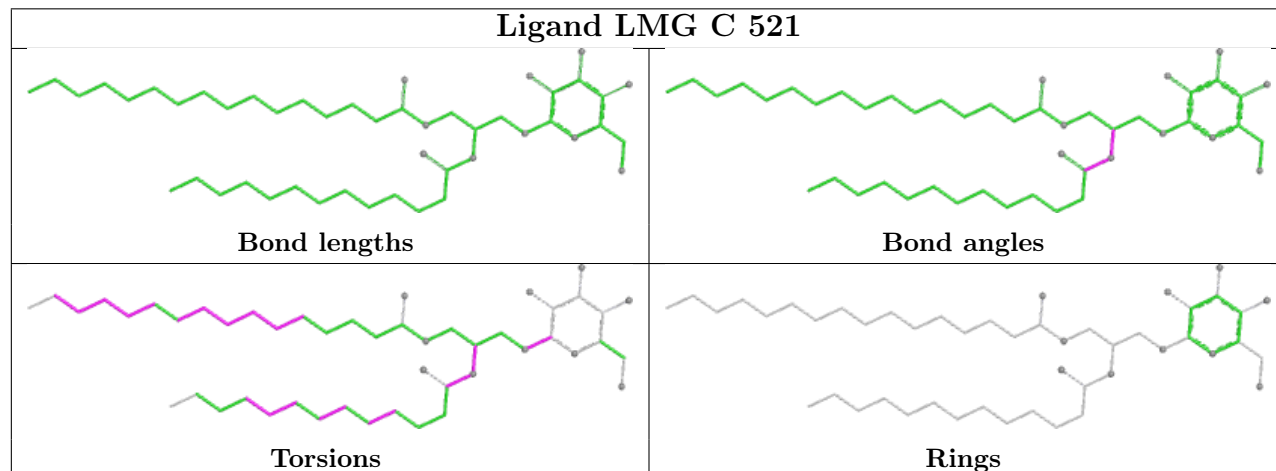


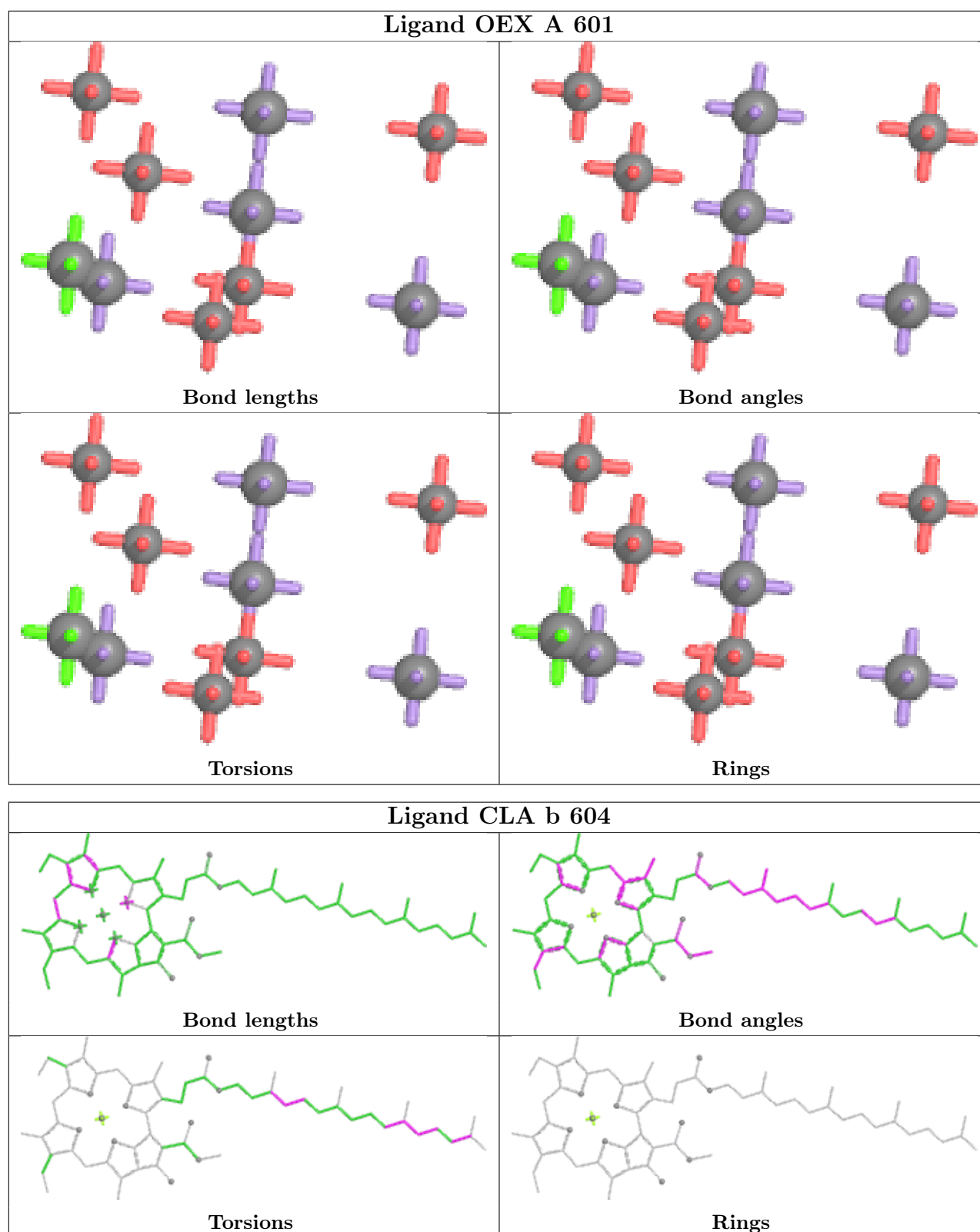


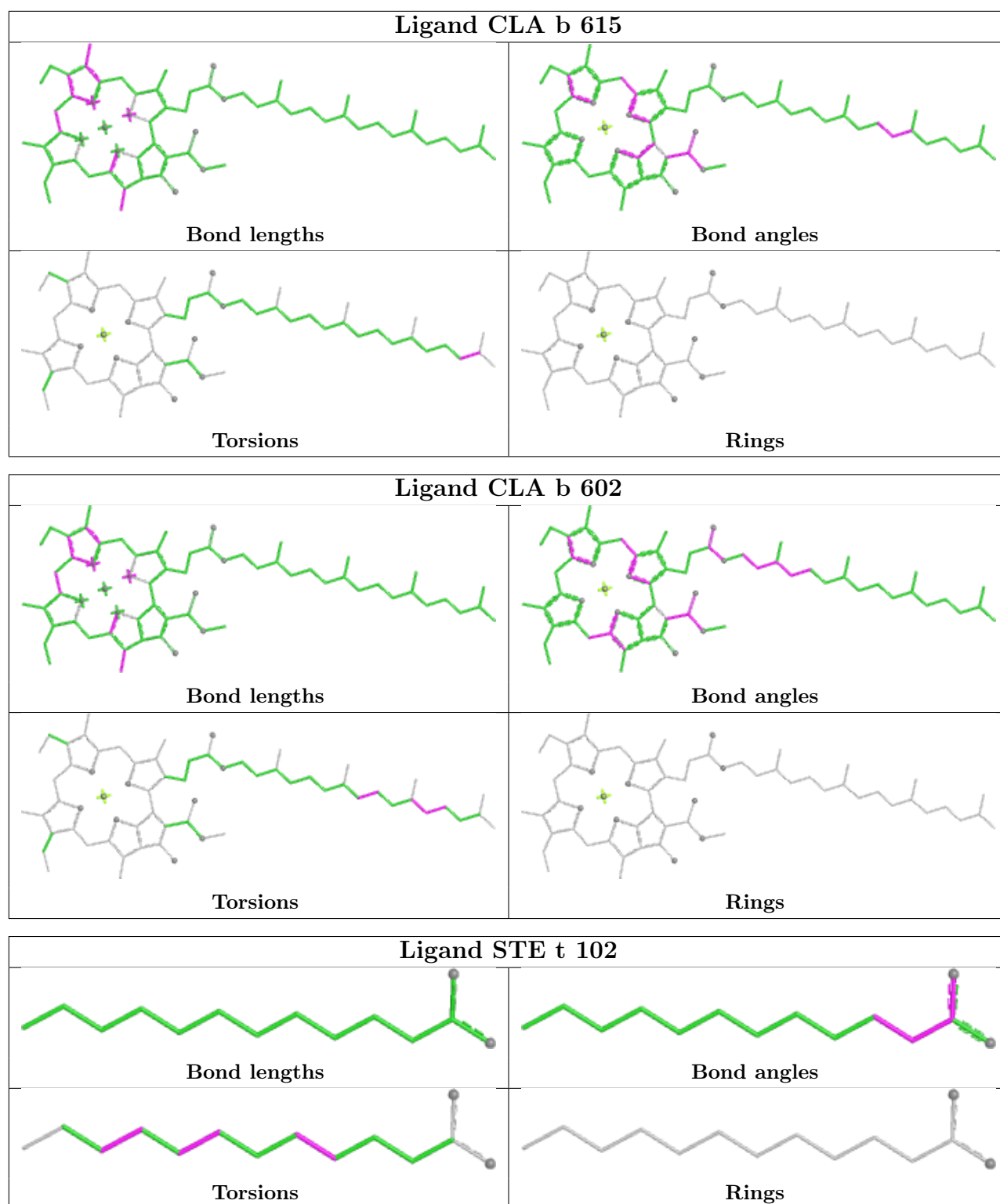
Ligand CLA c 503

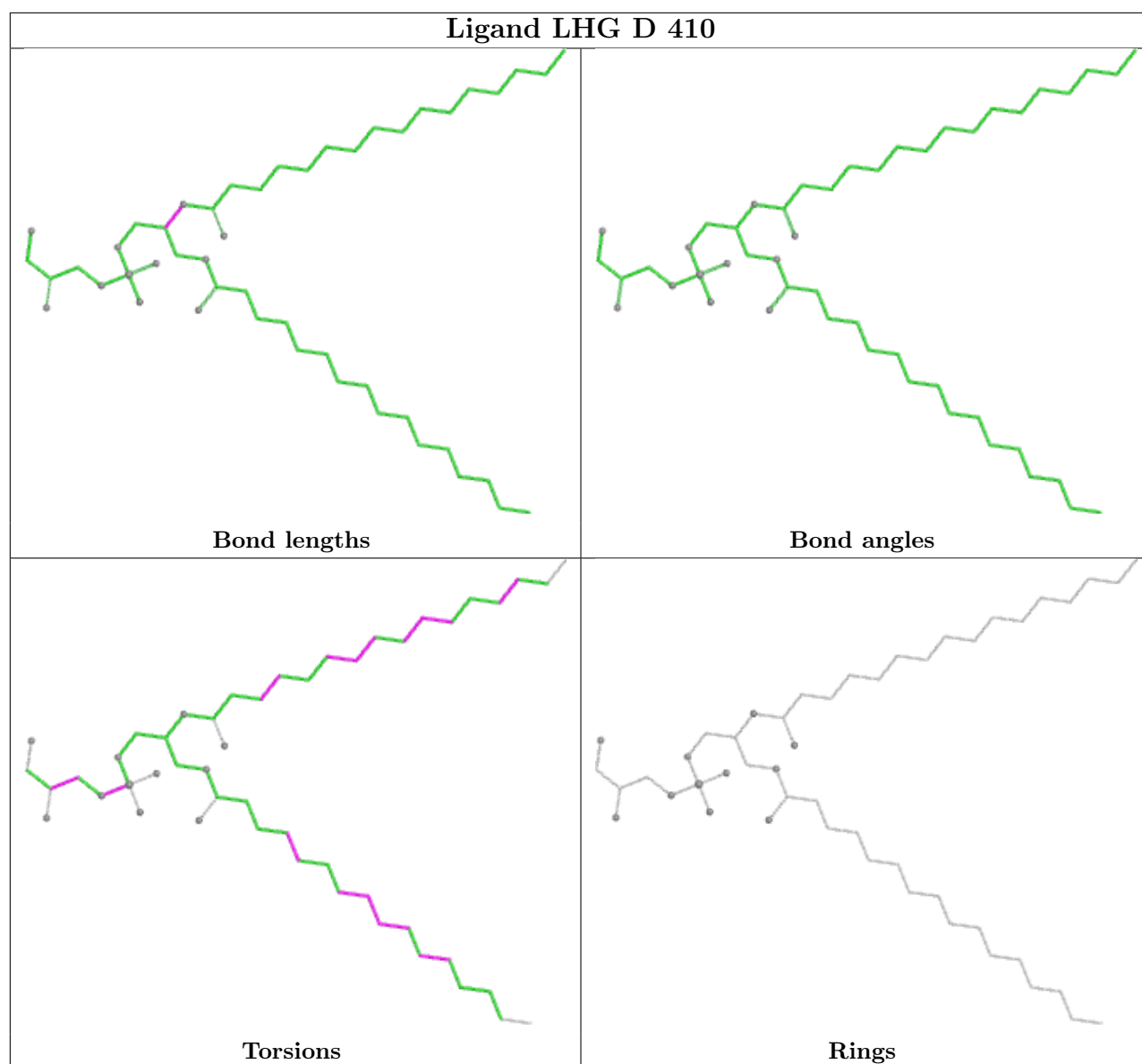


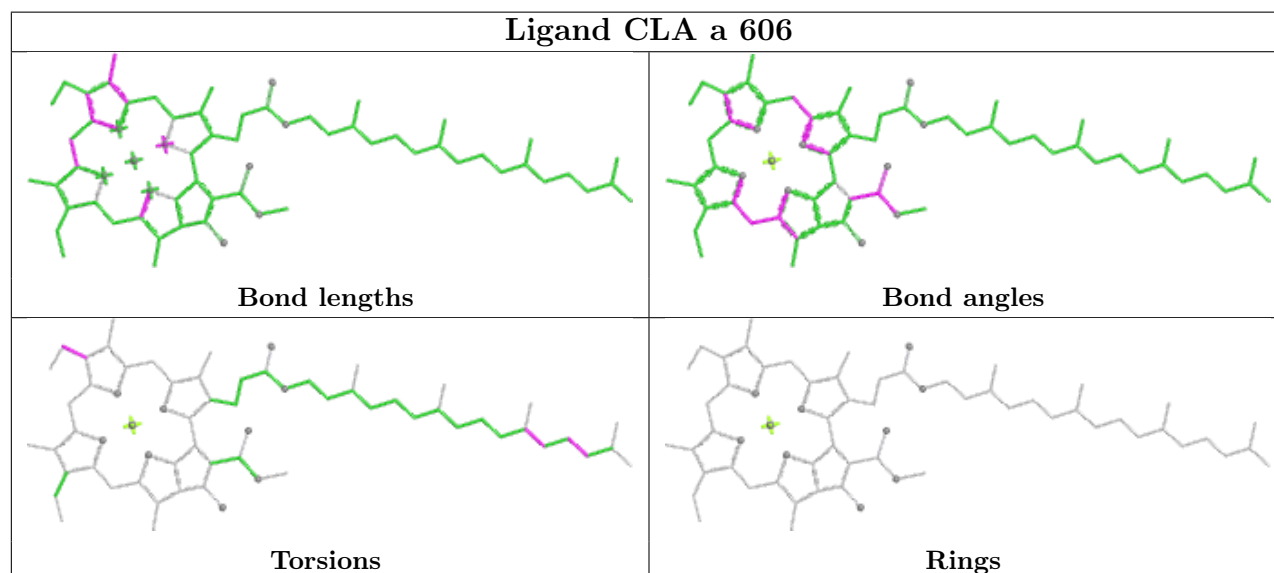
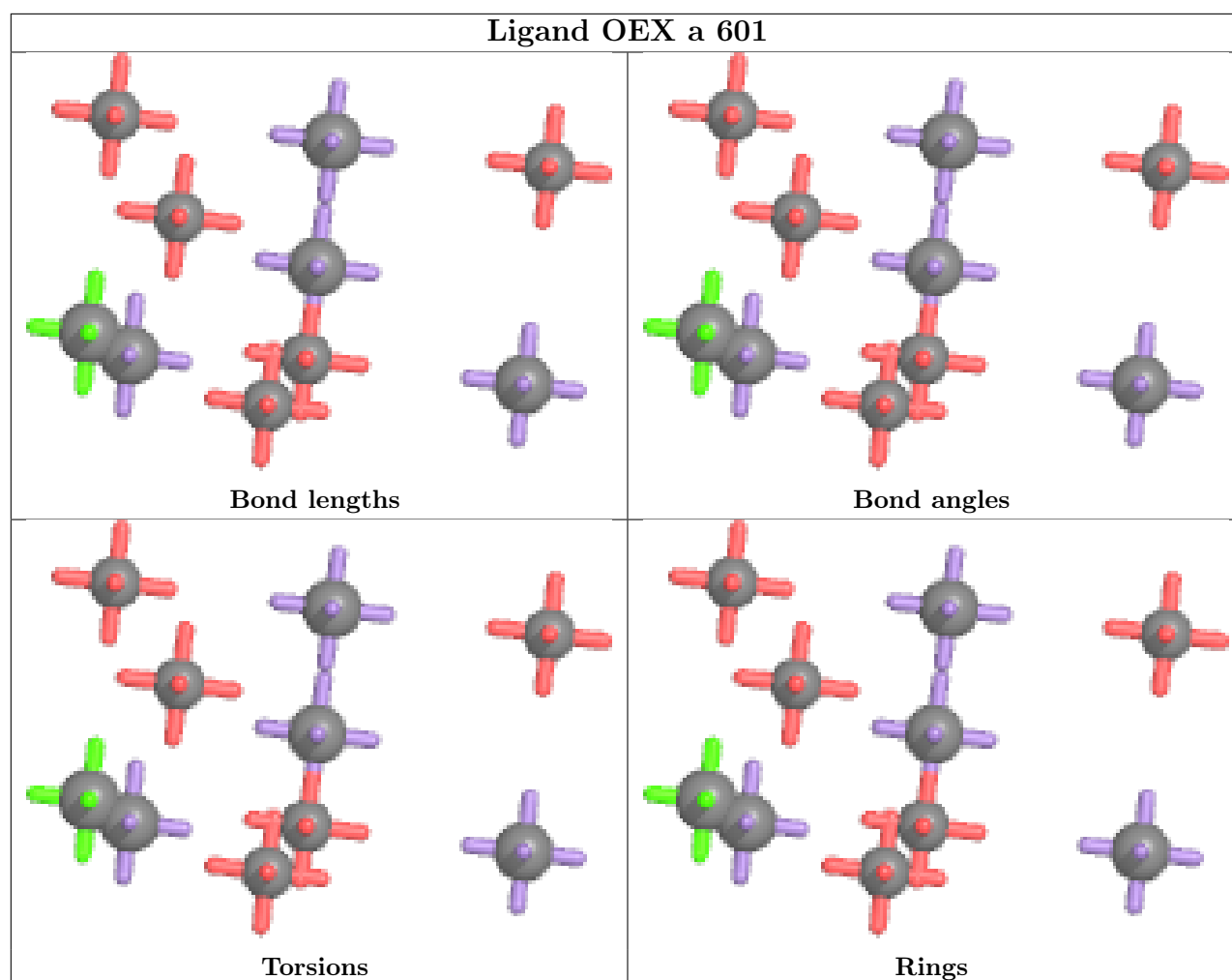
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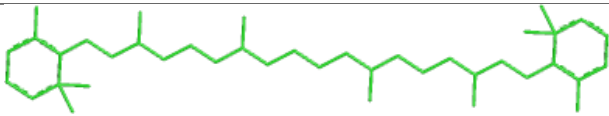
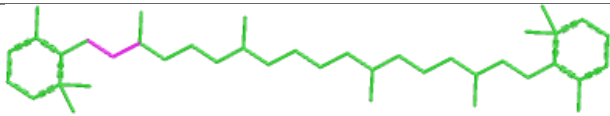
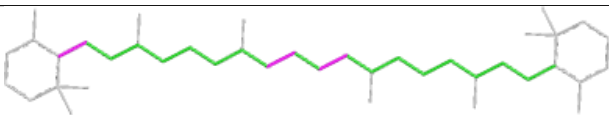
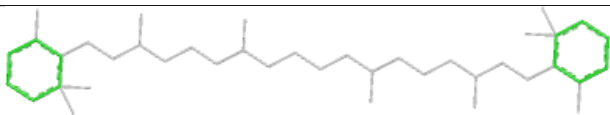


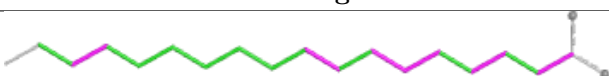
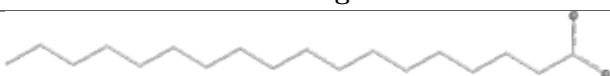


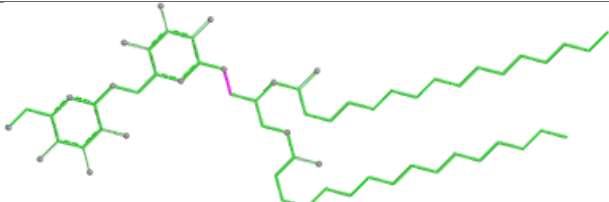
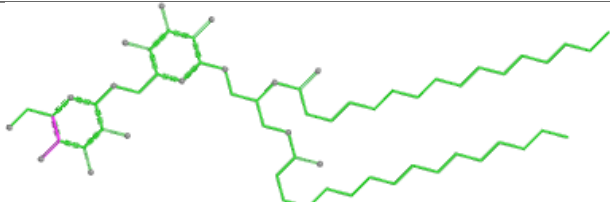
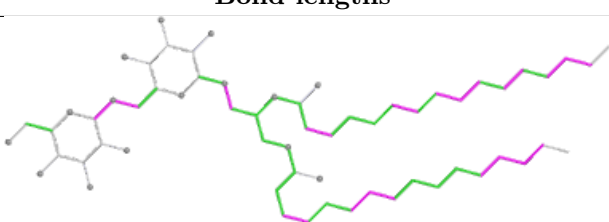
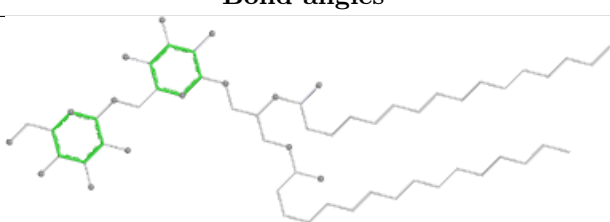


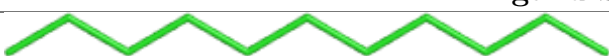
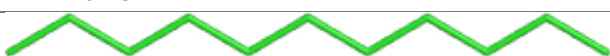
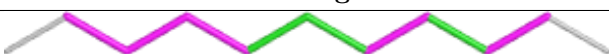


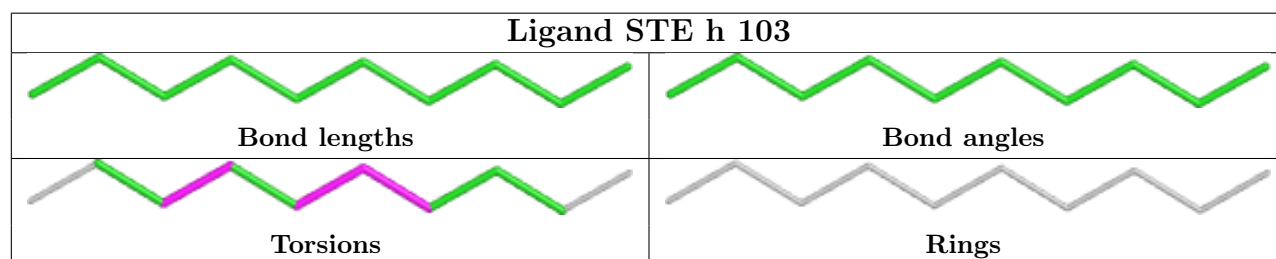
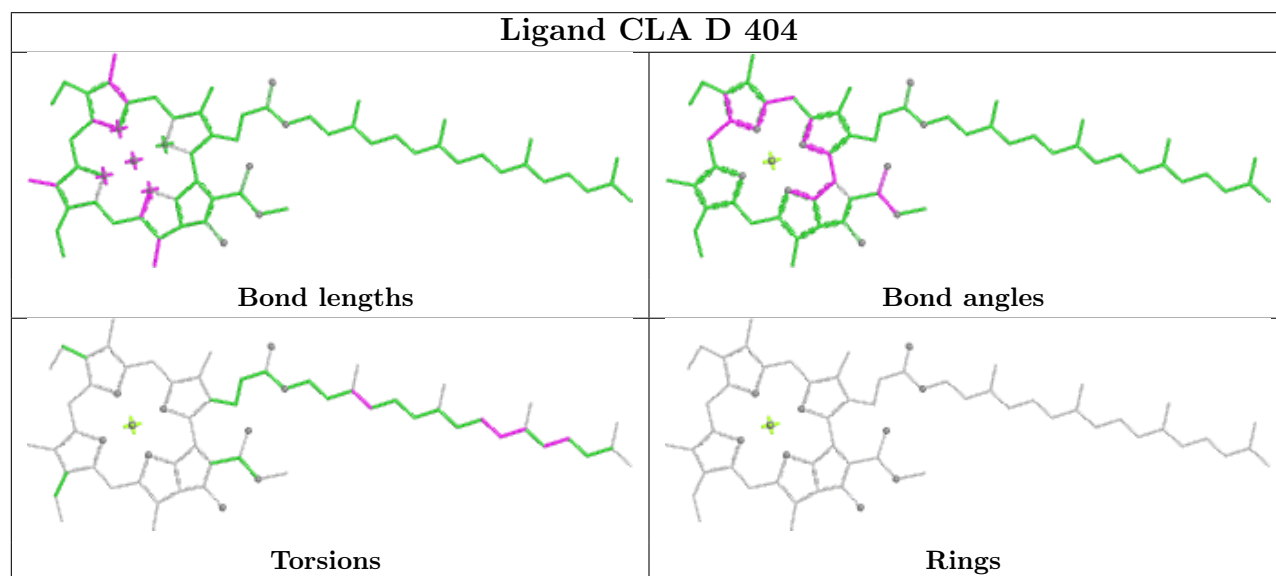
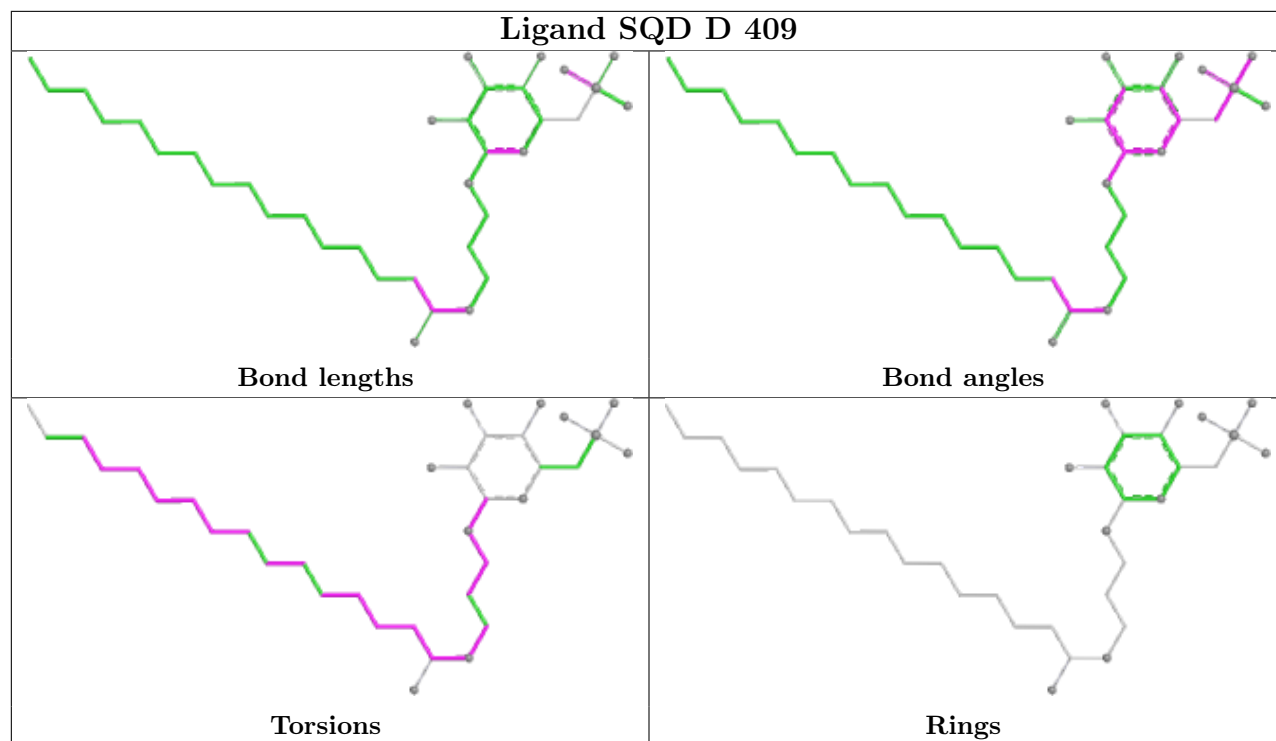


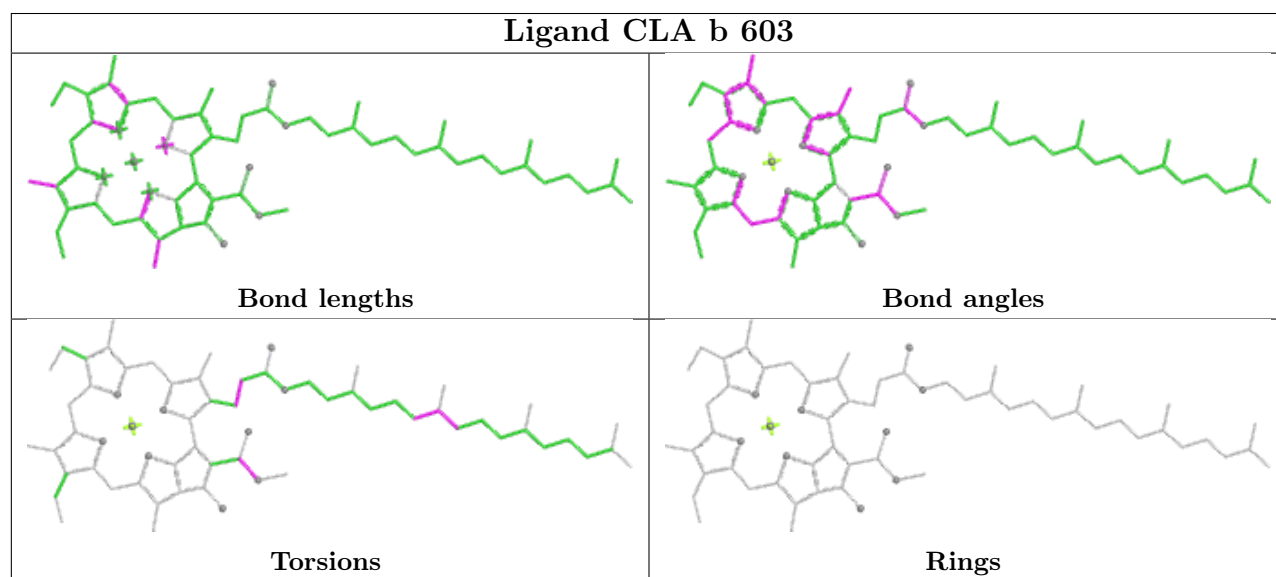
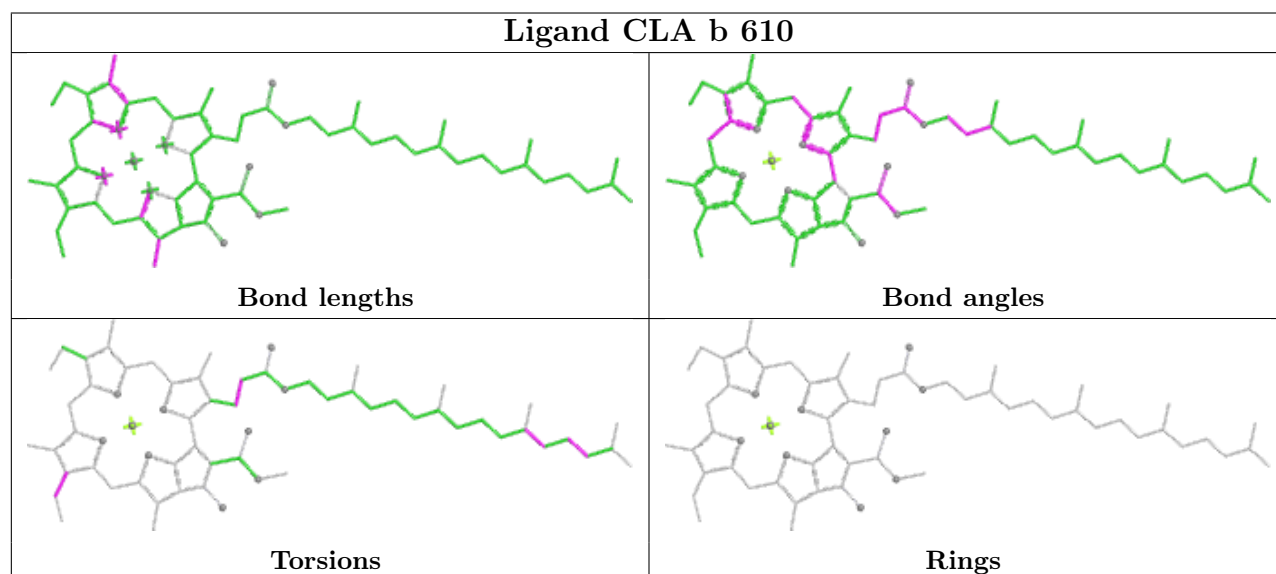
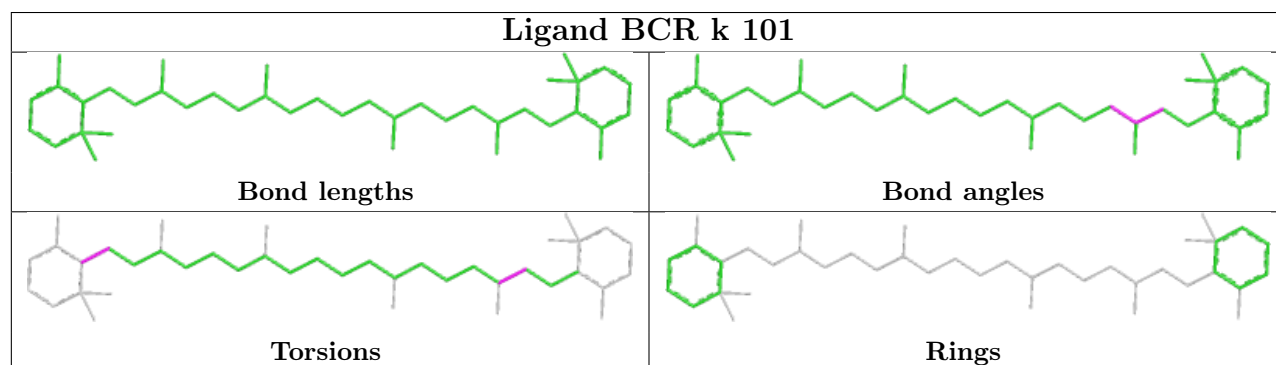
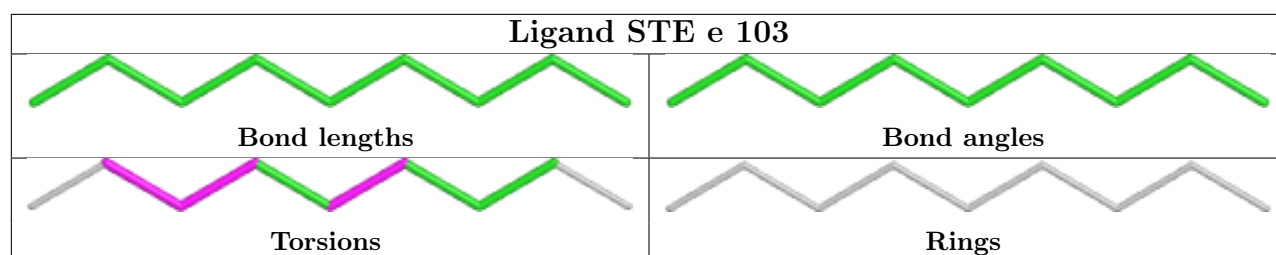
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

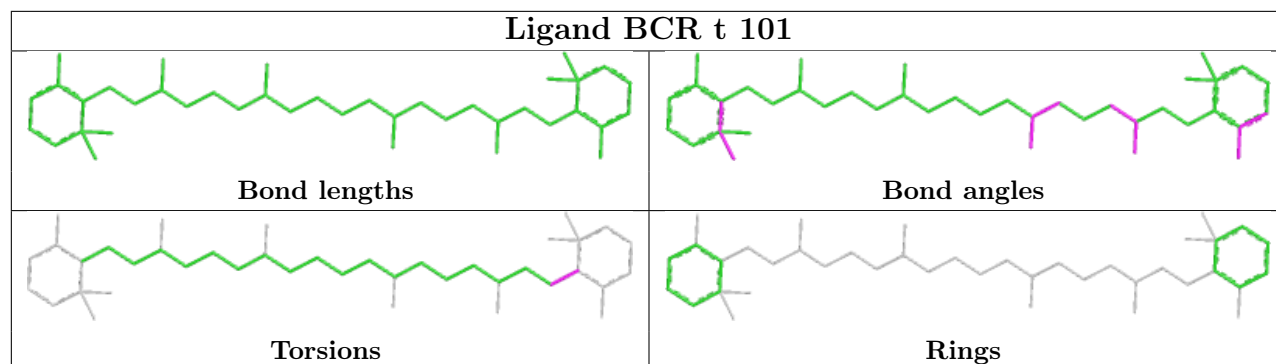
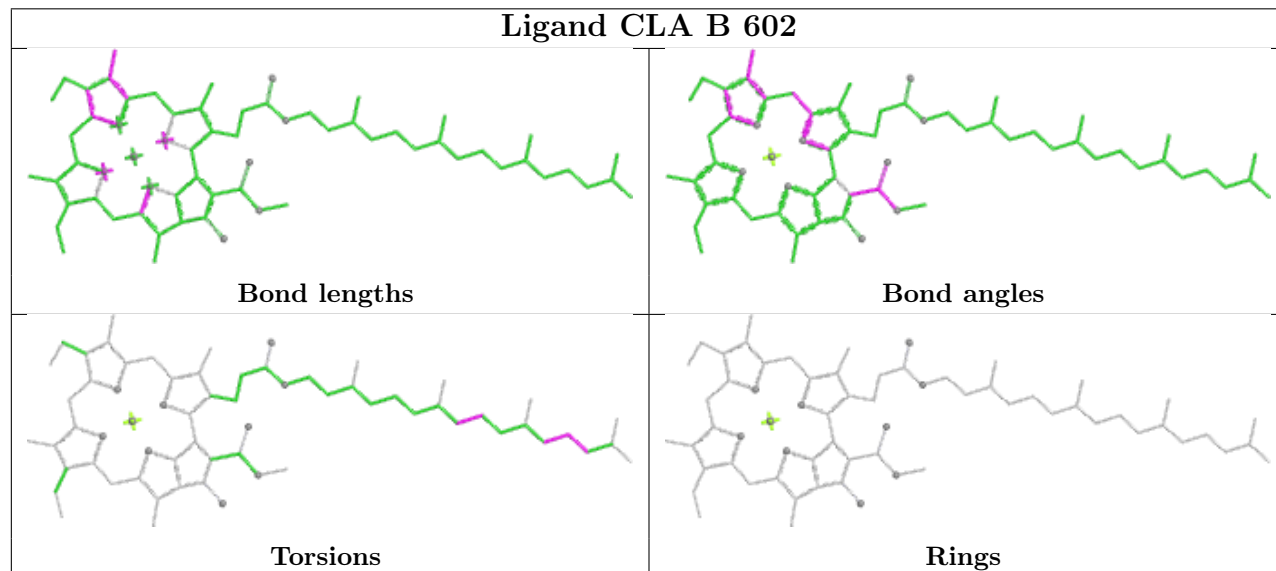
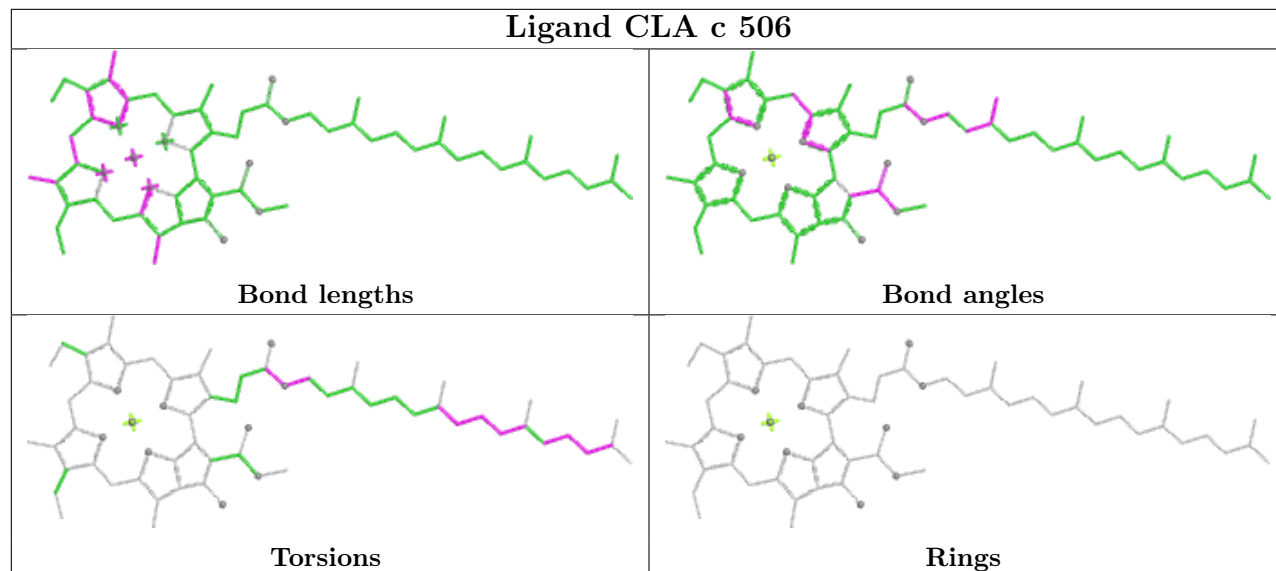
Ligand STE d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

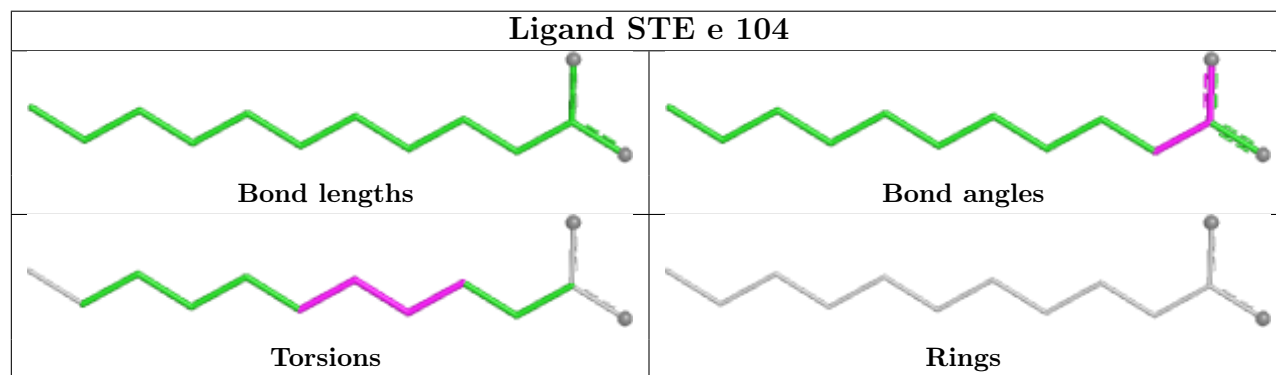
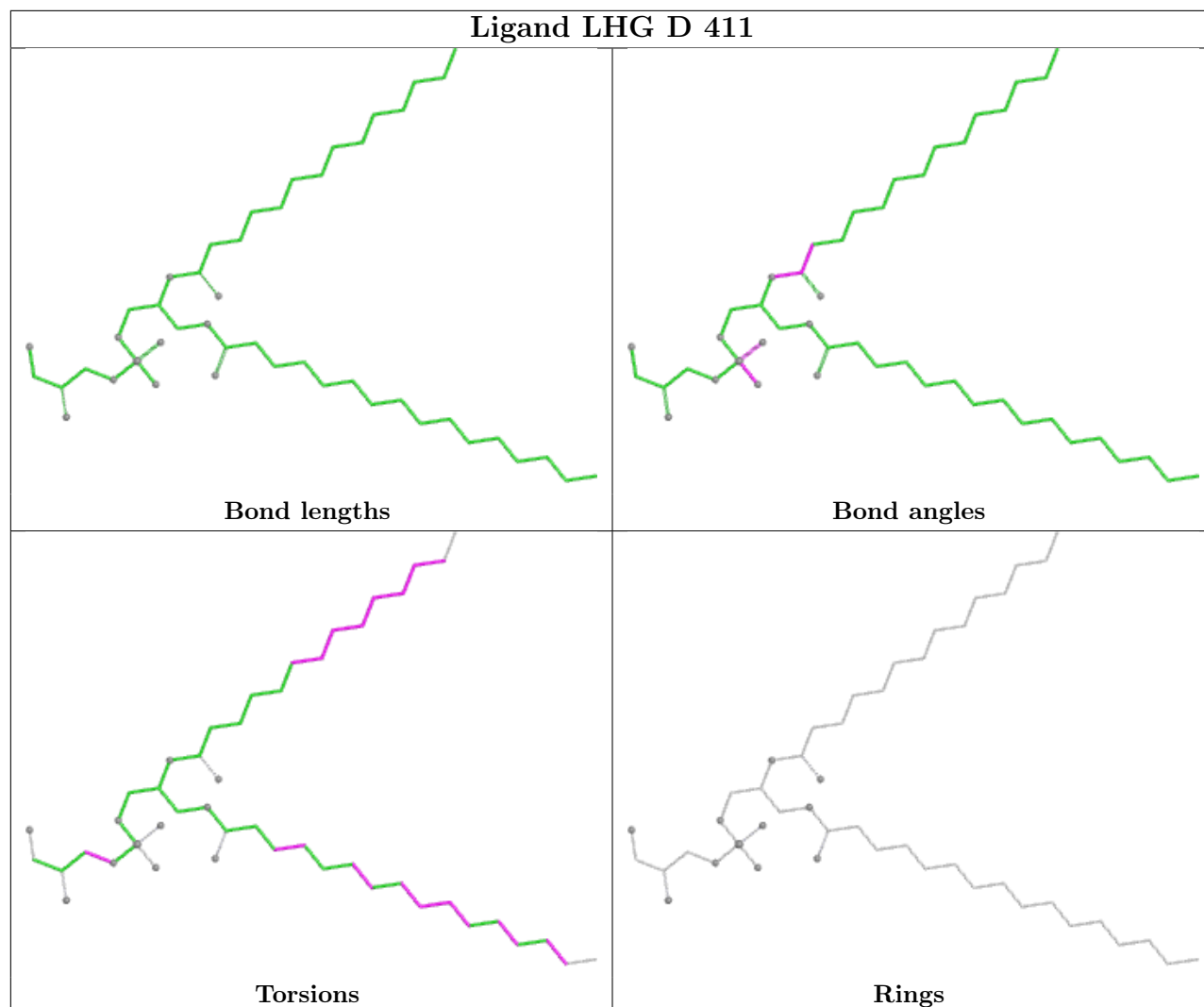
Ligand DGD C 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

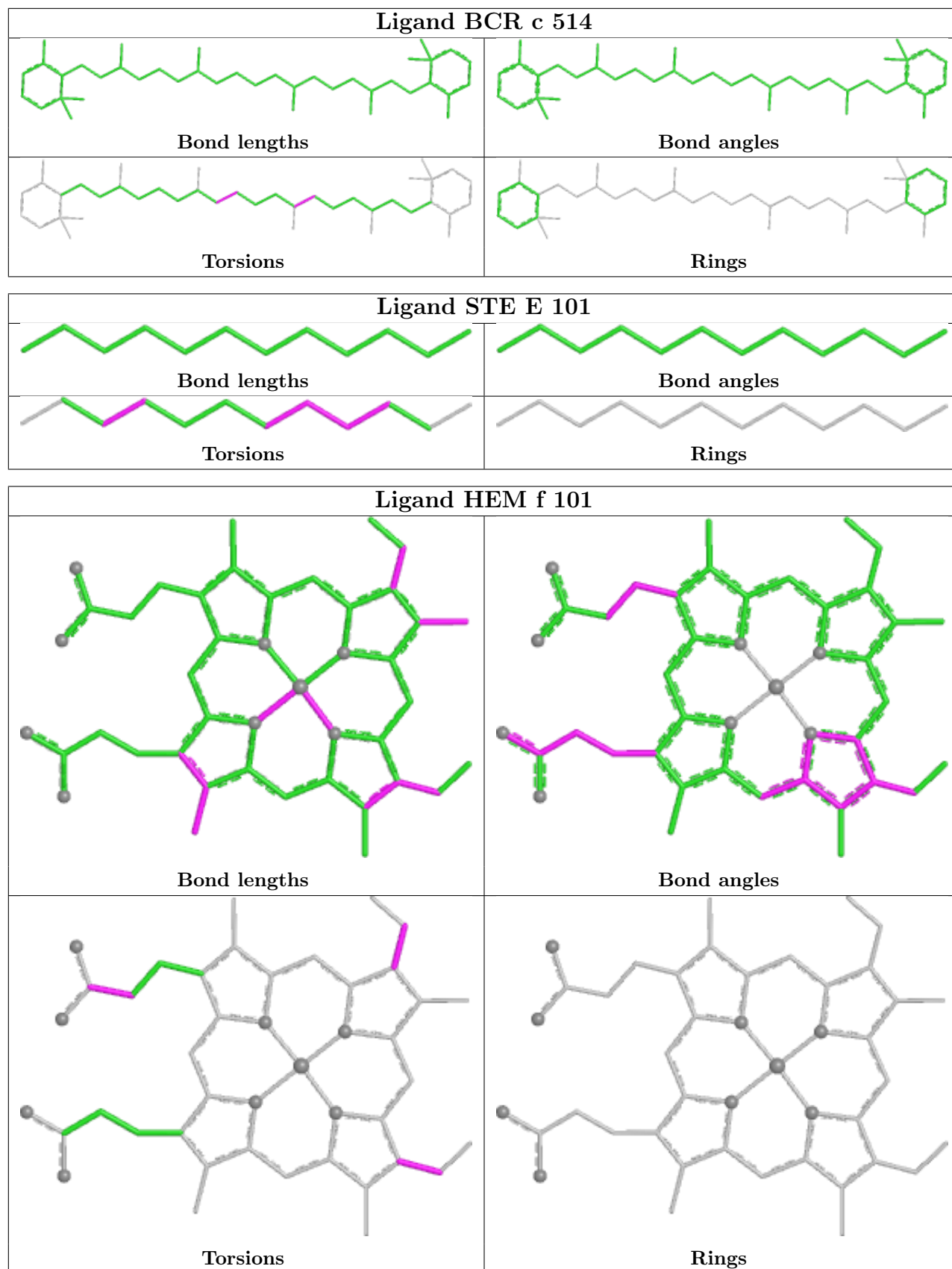
Ligand STE A 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



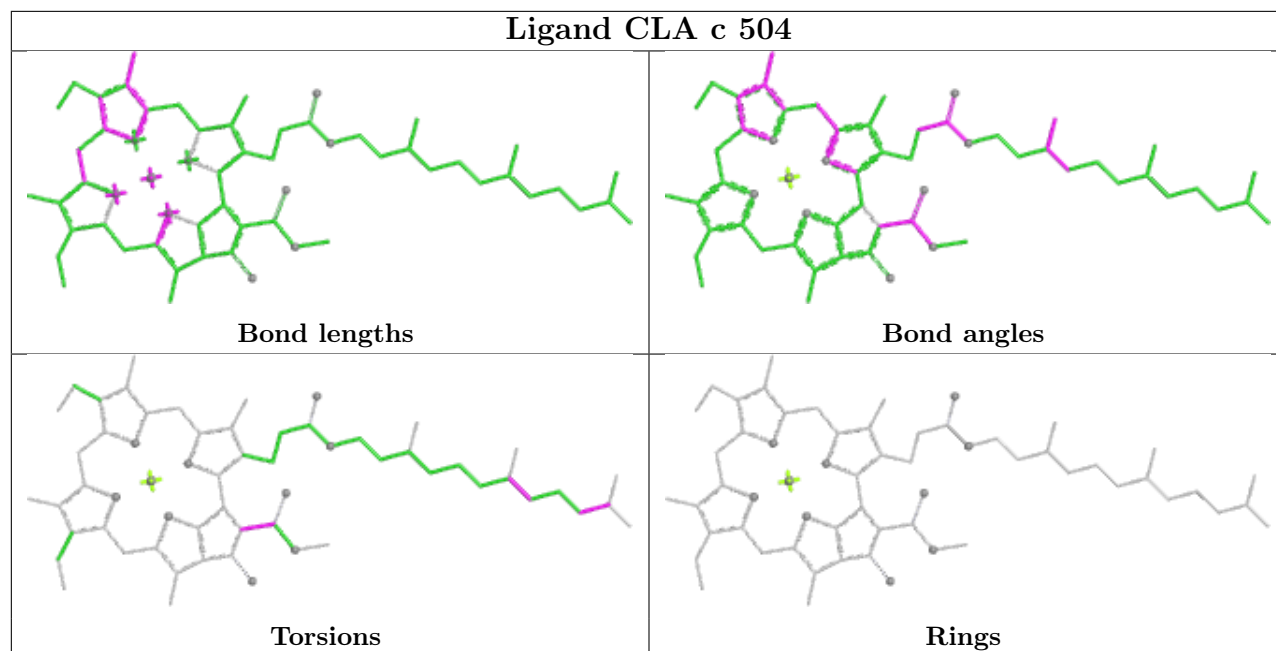


Ligand BCR t 101**Ligand CLA B 602****Ligand CLA c 506**

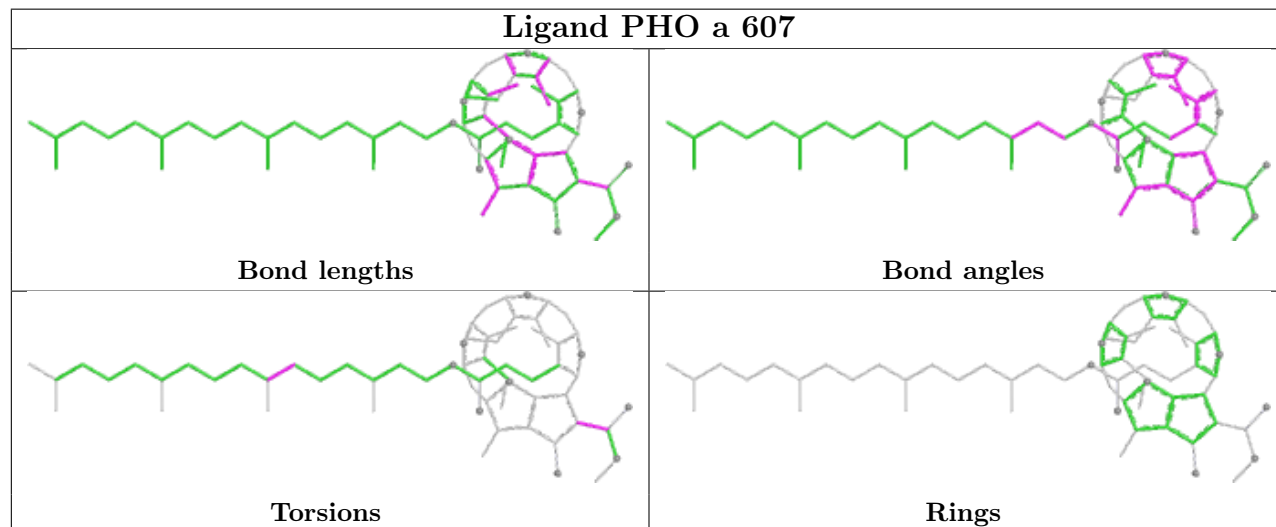


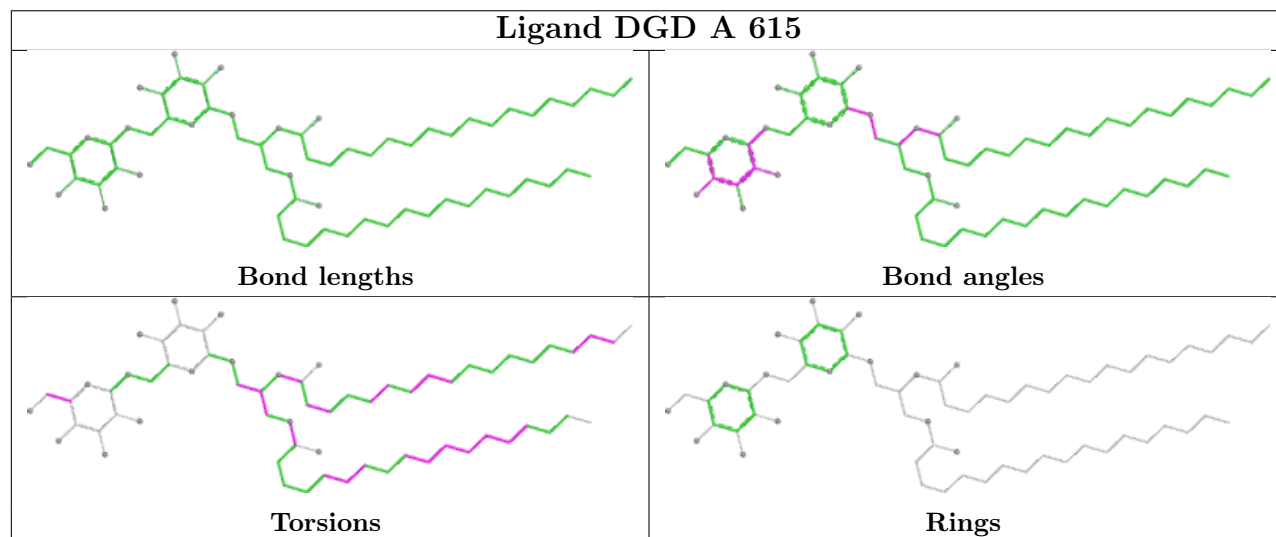
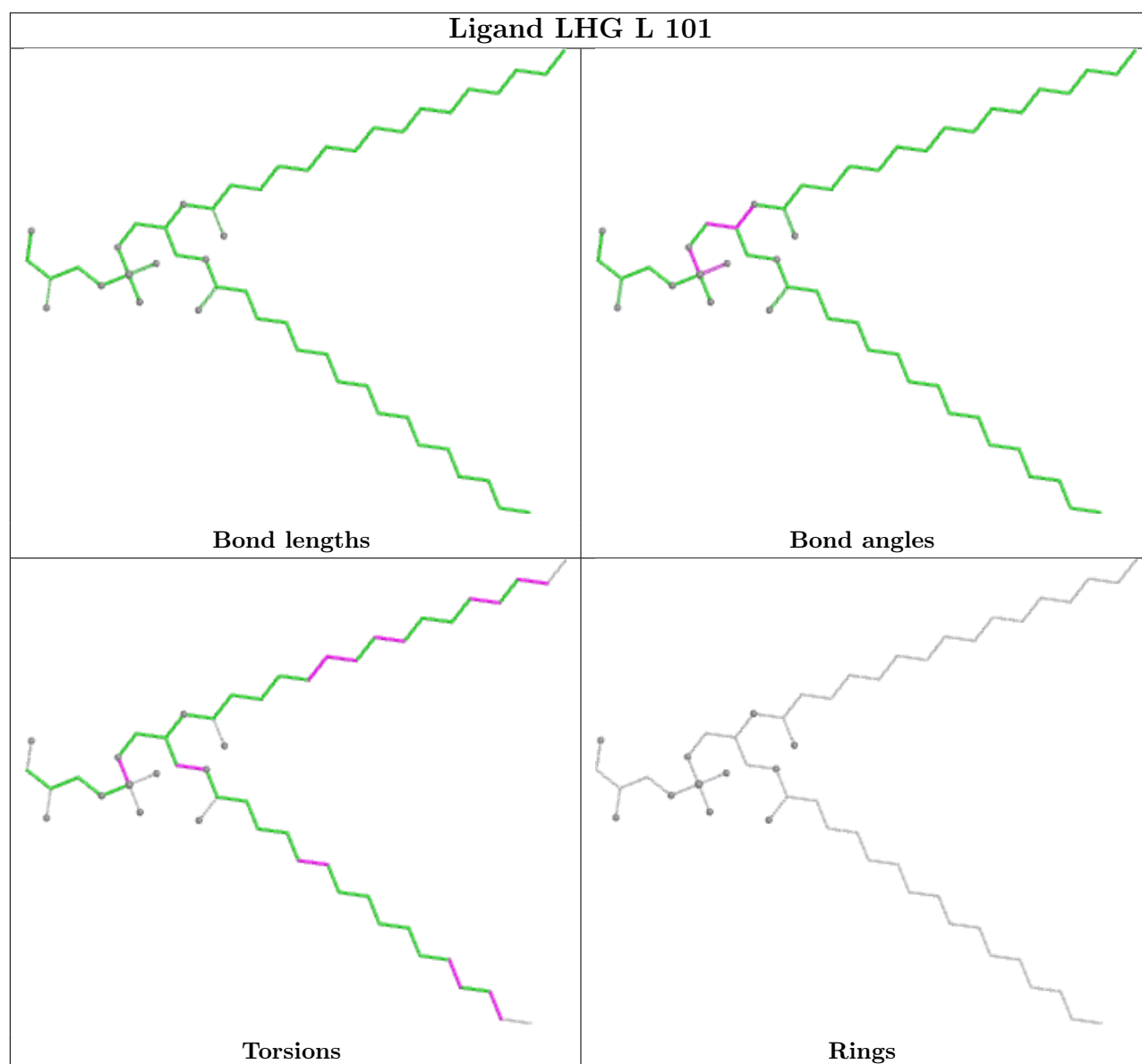


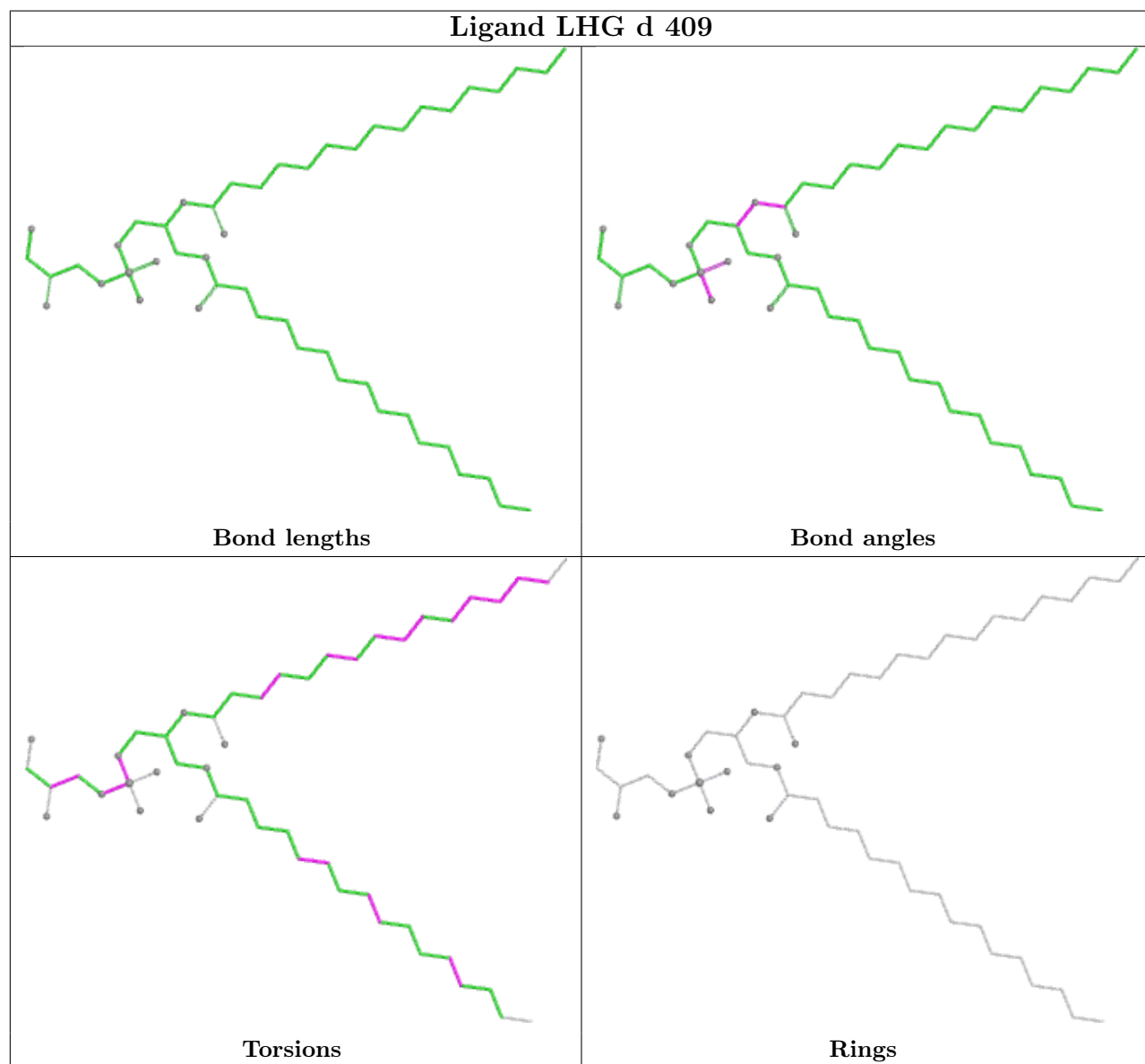
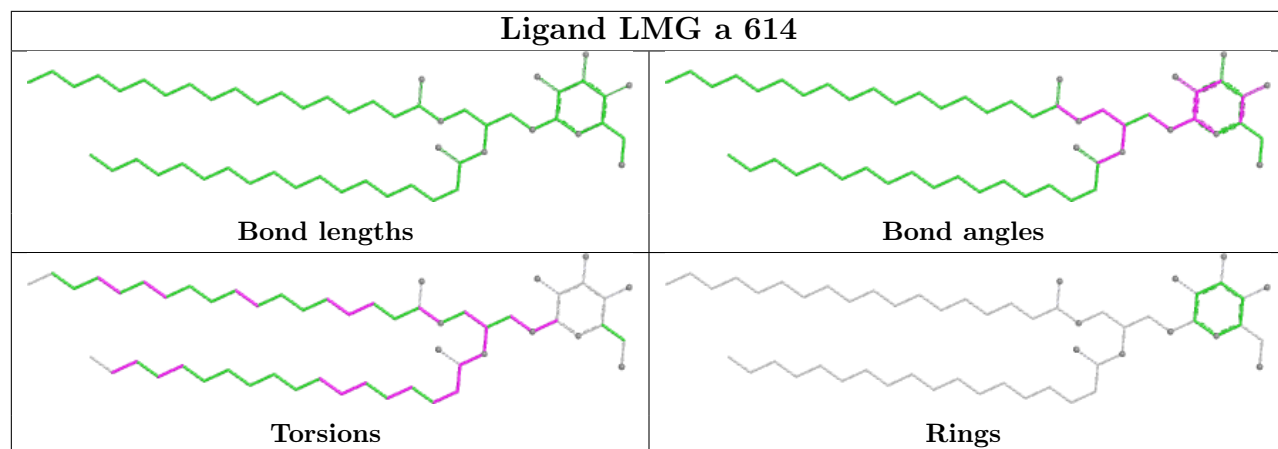
Ligand CLA c 504

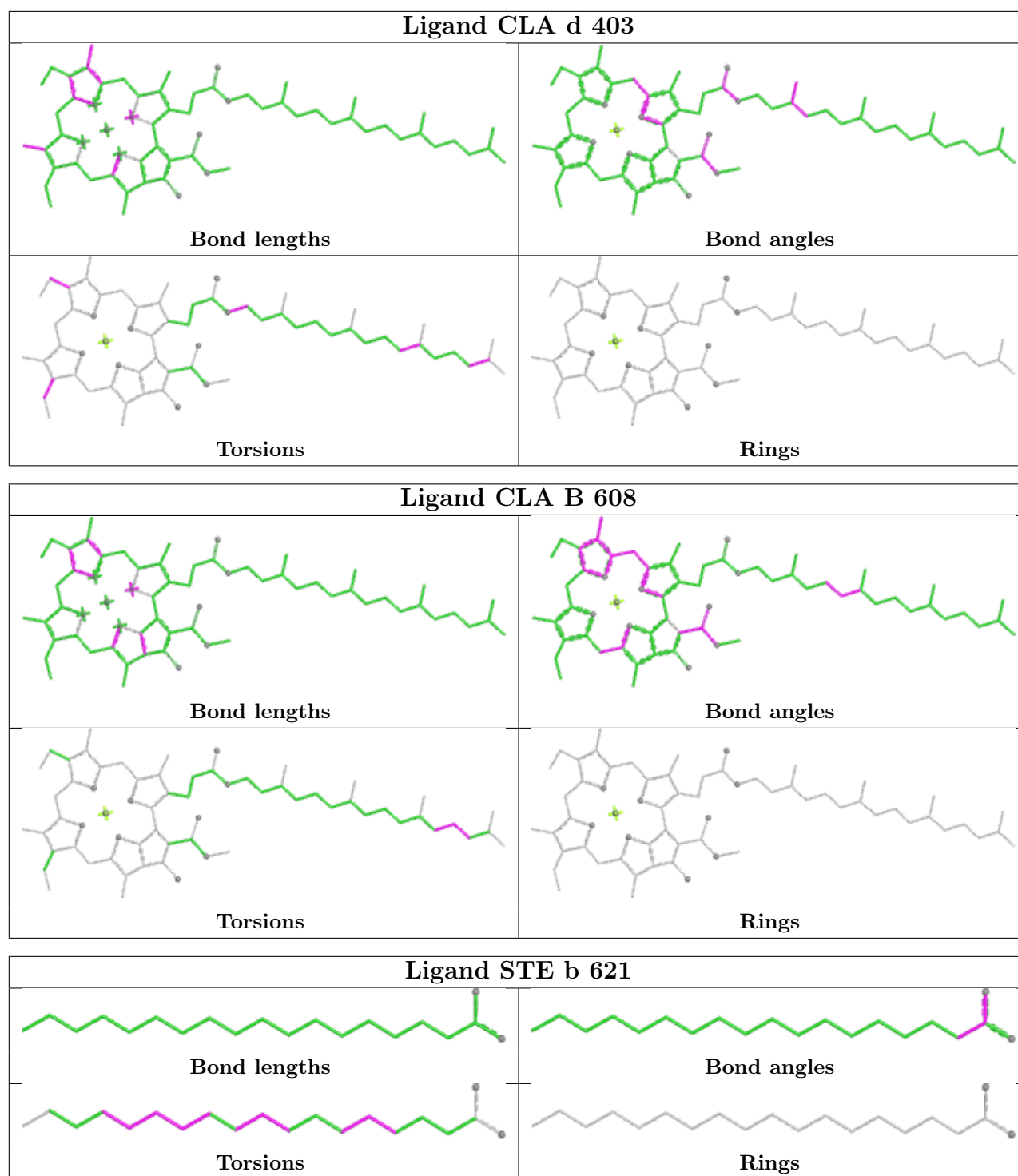


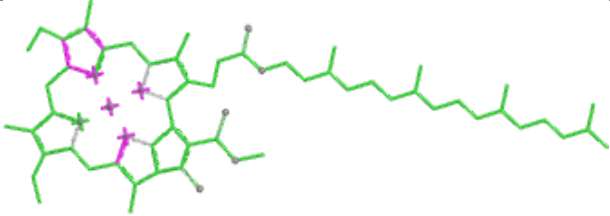
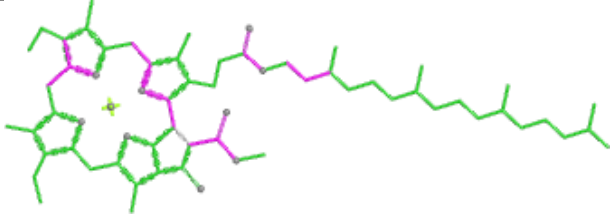
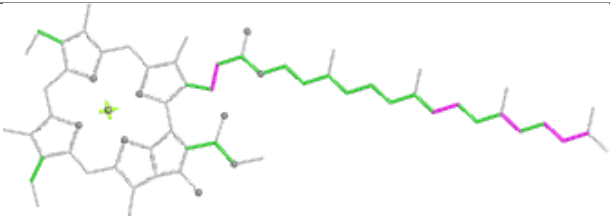
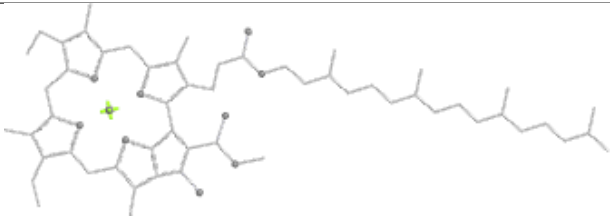
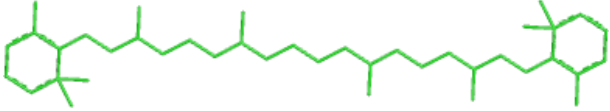
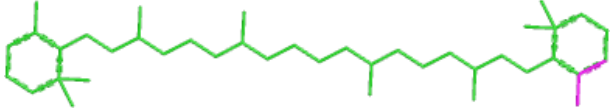
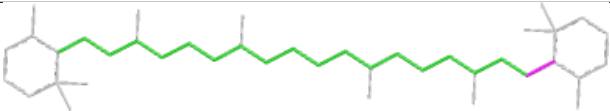
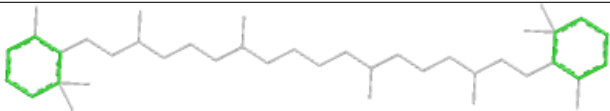
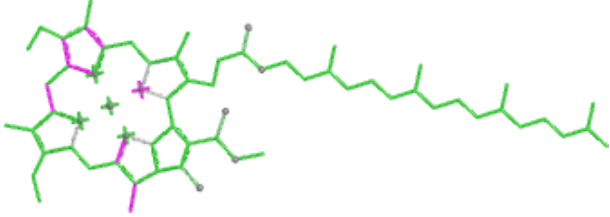
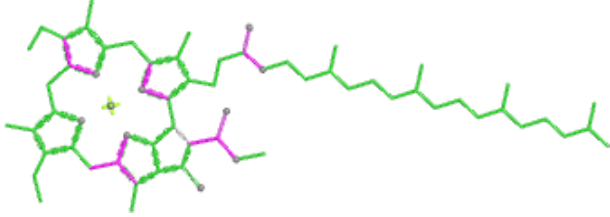
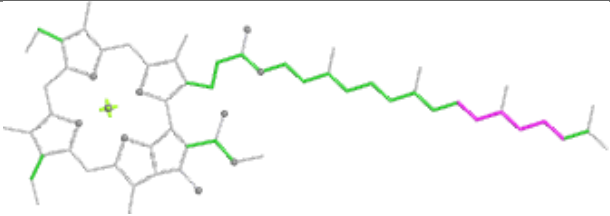
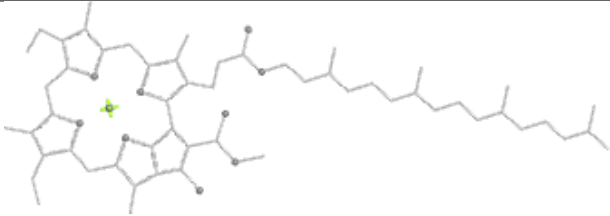
Ligand PHO a 607



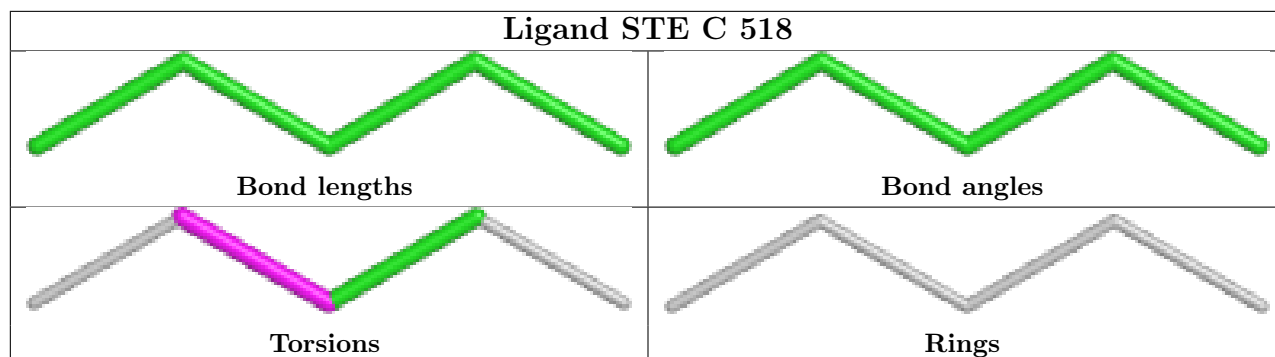




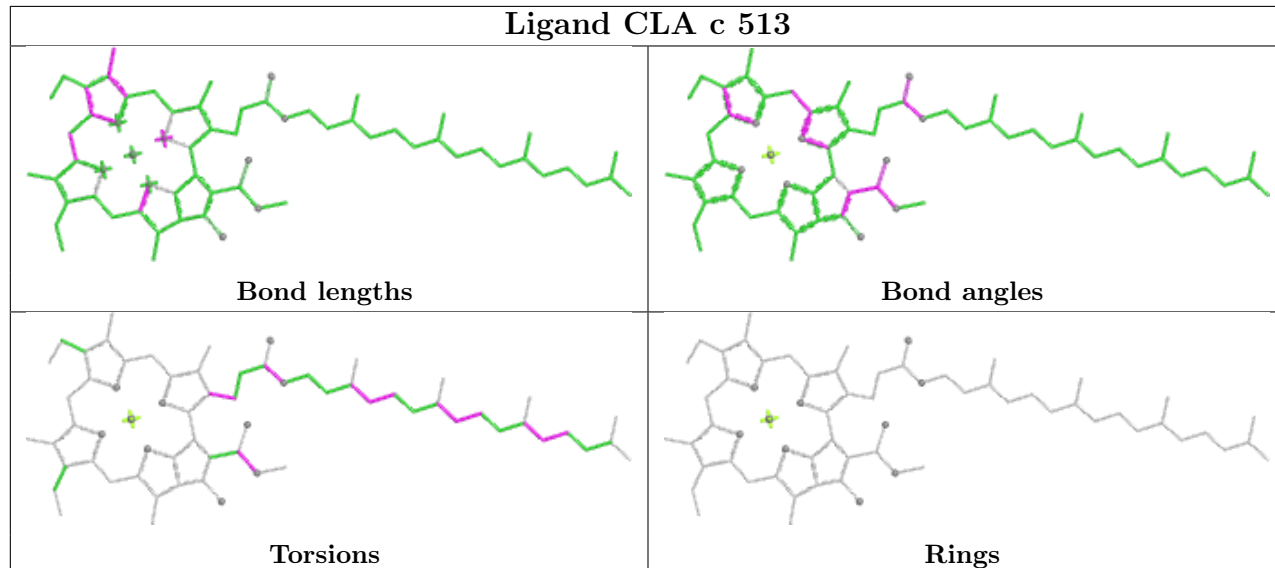


Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

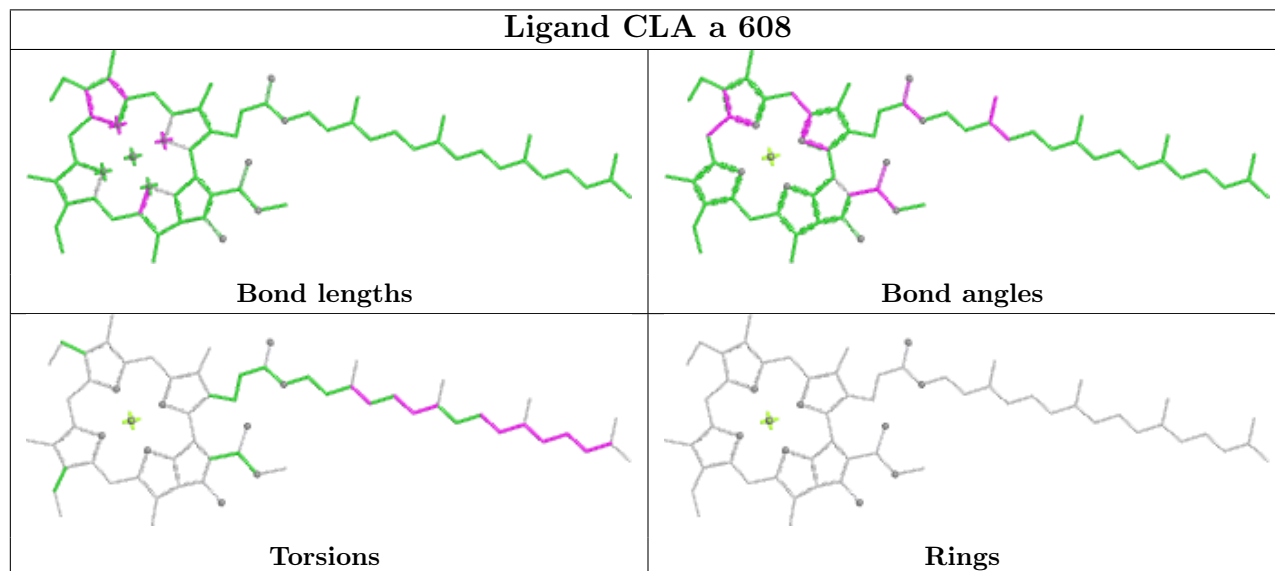
Ligand STE C 518

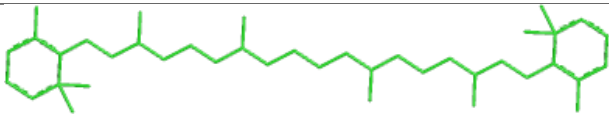
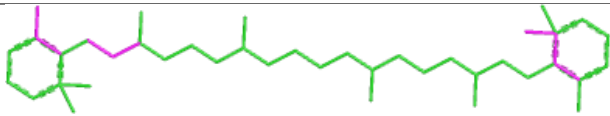
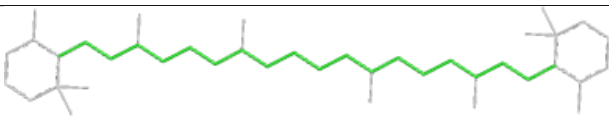
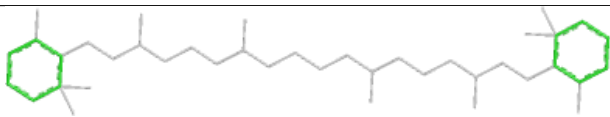


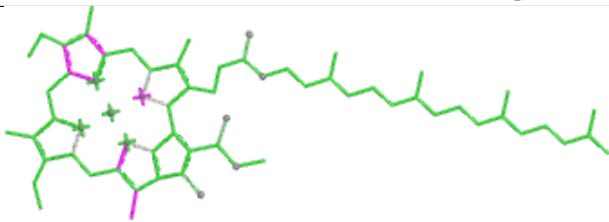
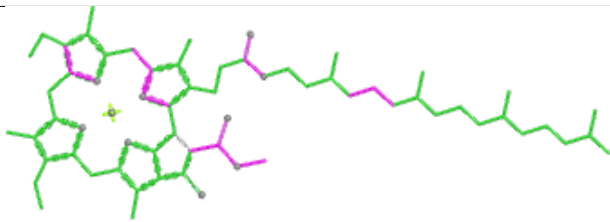
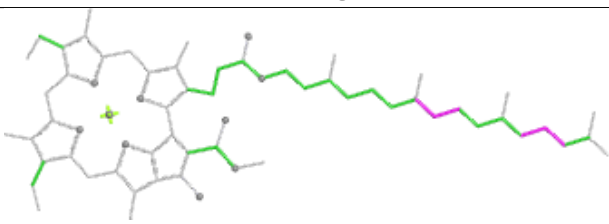
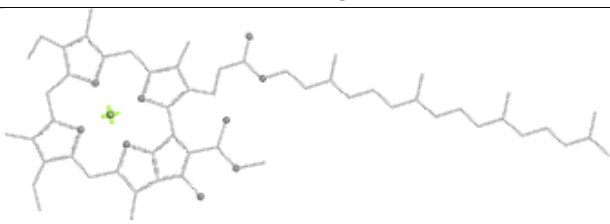
Ligand CLA c 513

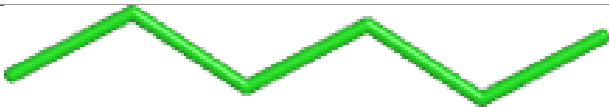
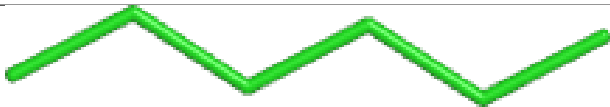


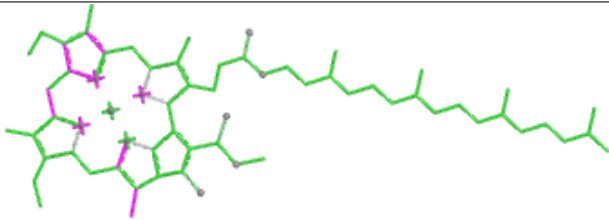
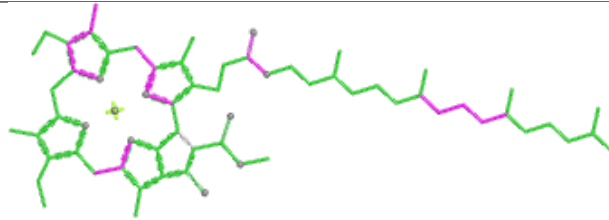
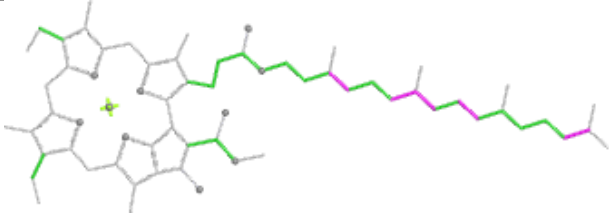
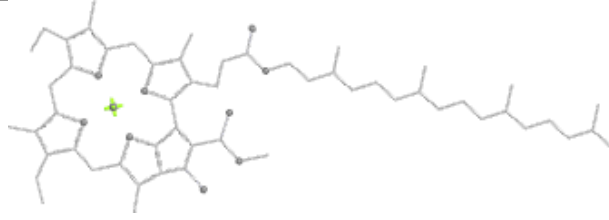
Ligand CLA a 608

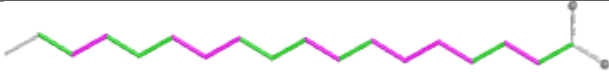
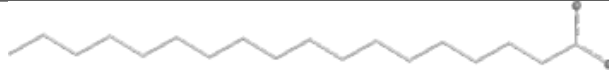


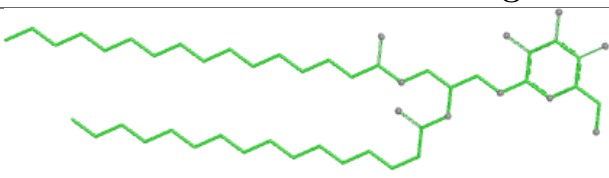
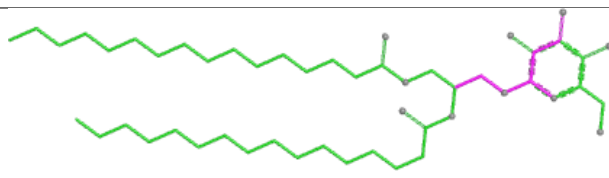
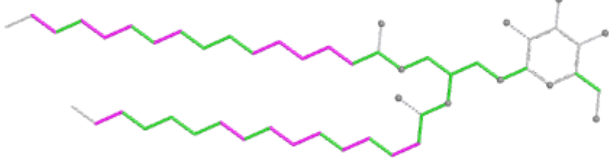
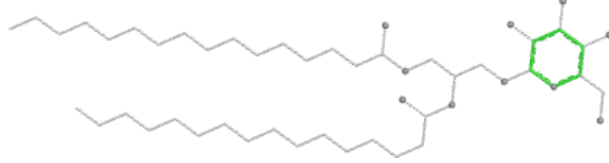
Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

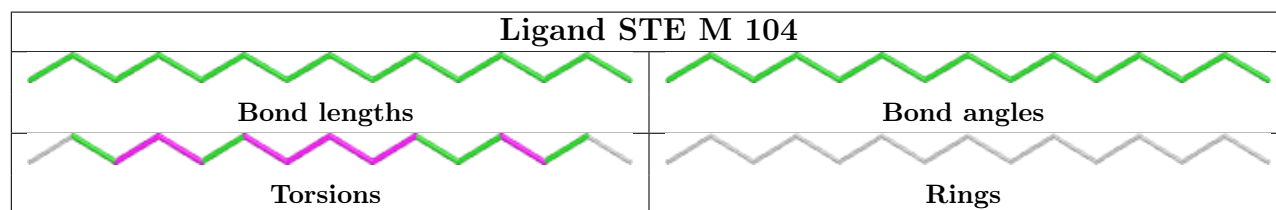
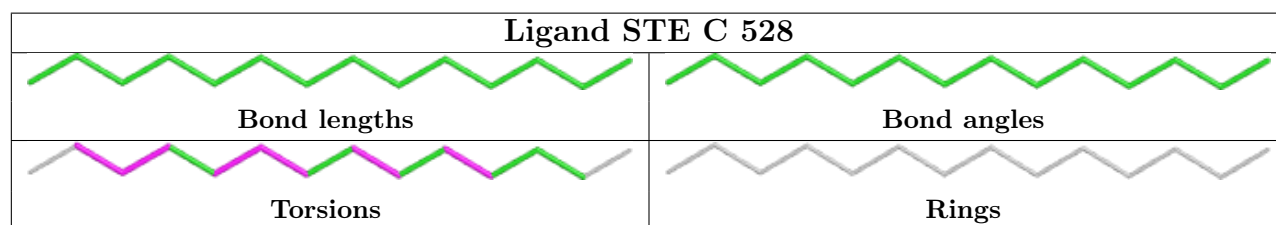
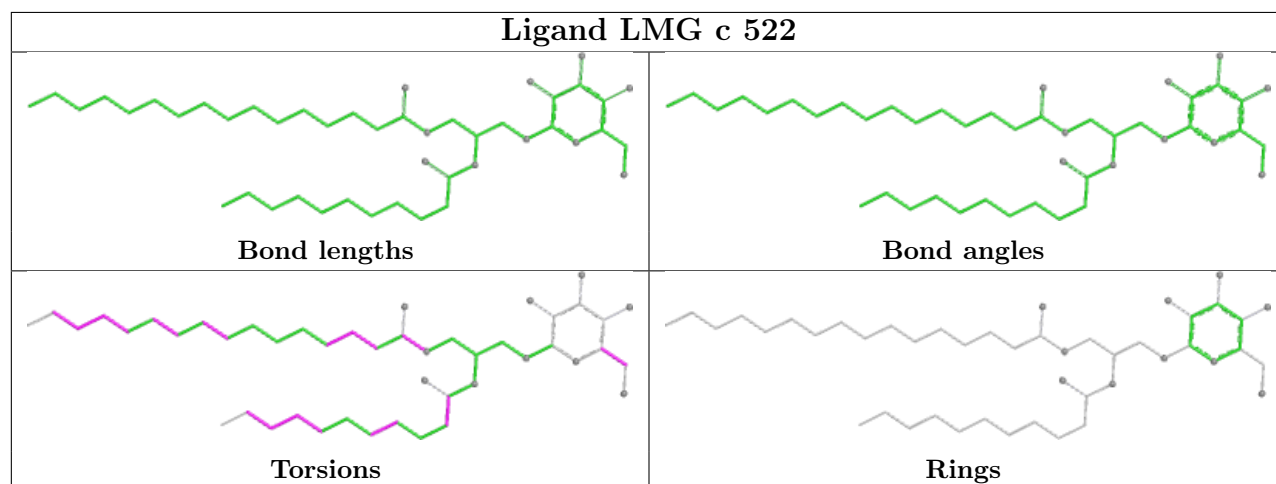
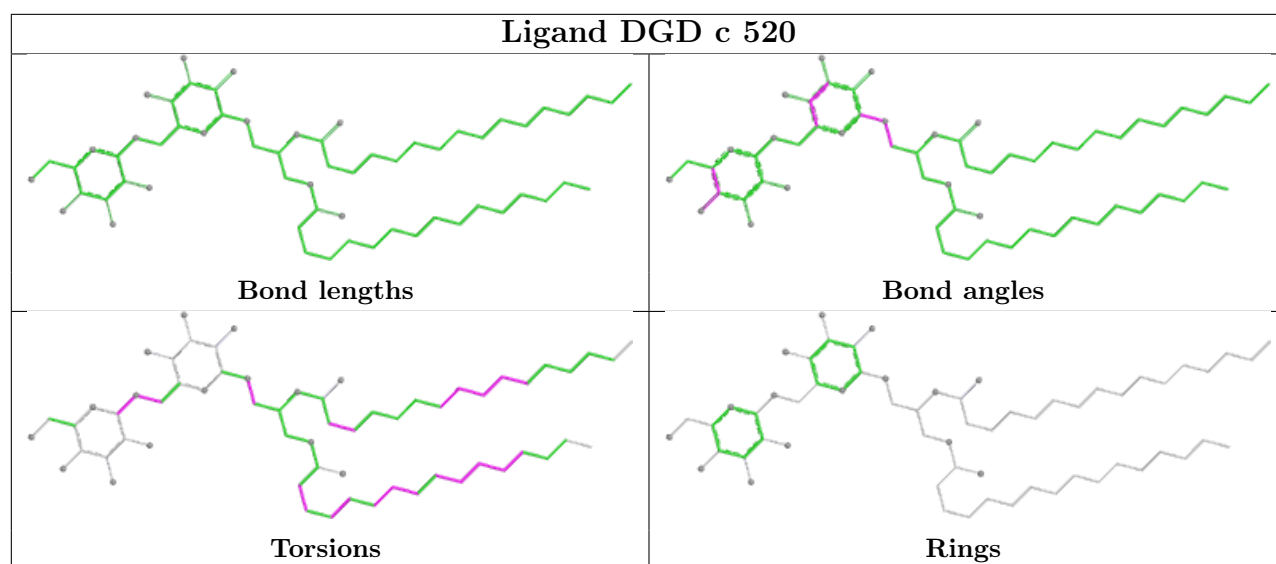
Ligand CLA A 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

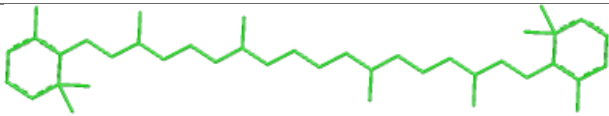
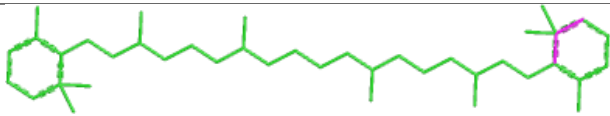
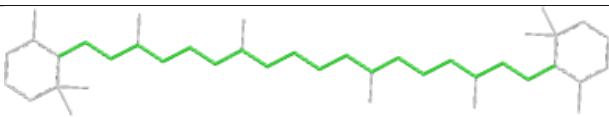
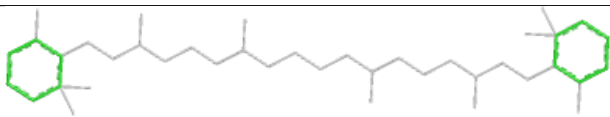
Ligand STE i 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

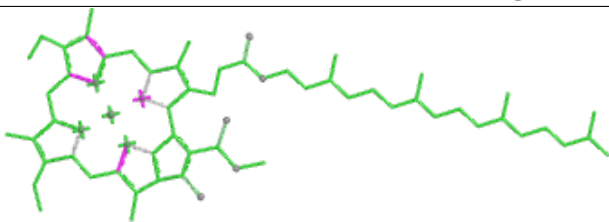
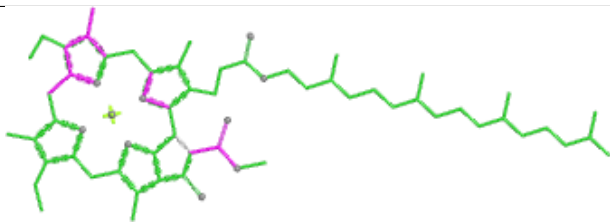
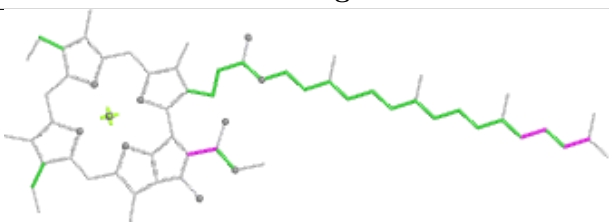
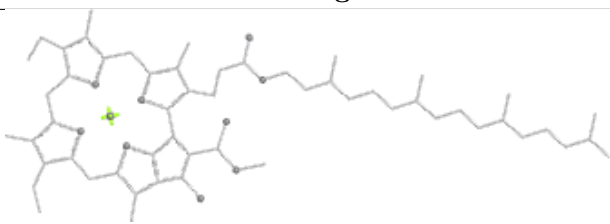
Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

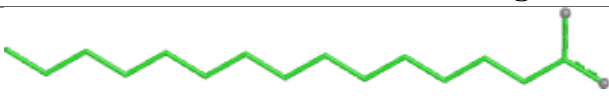
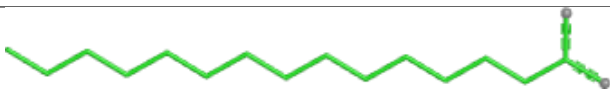
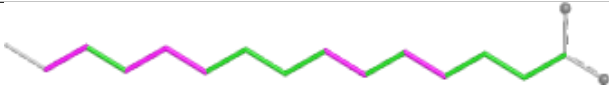
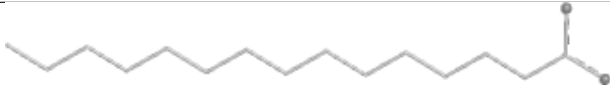
Ligand STE d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

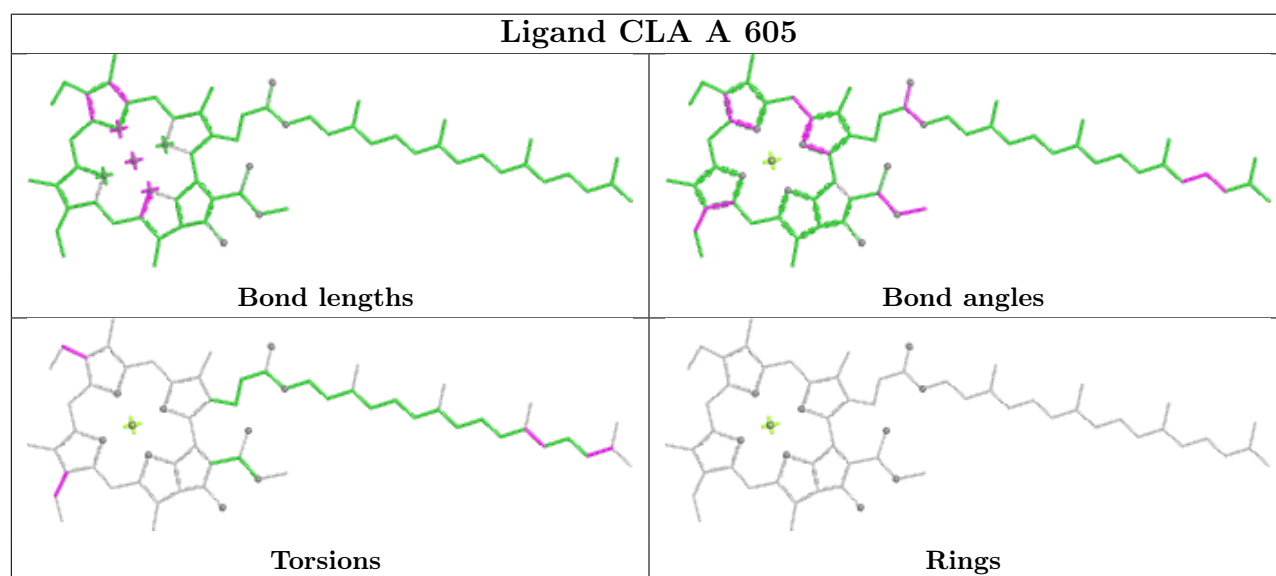
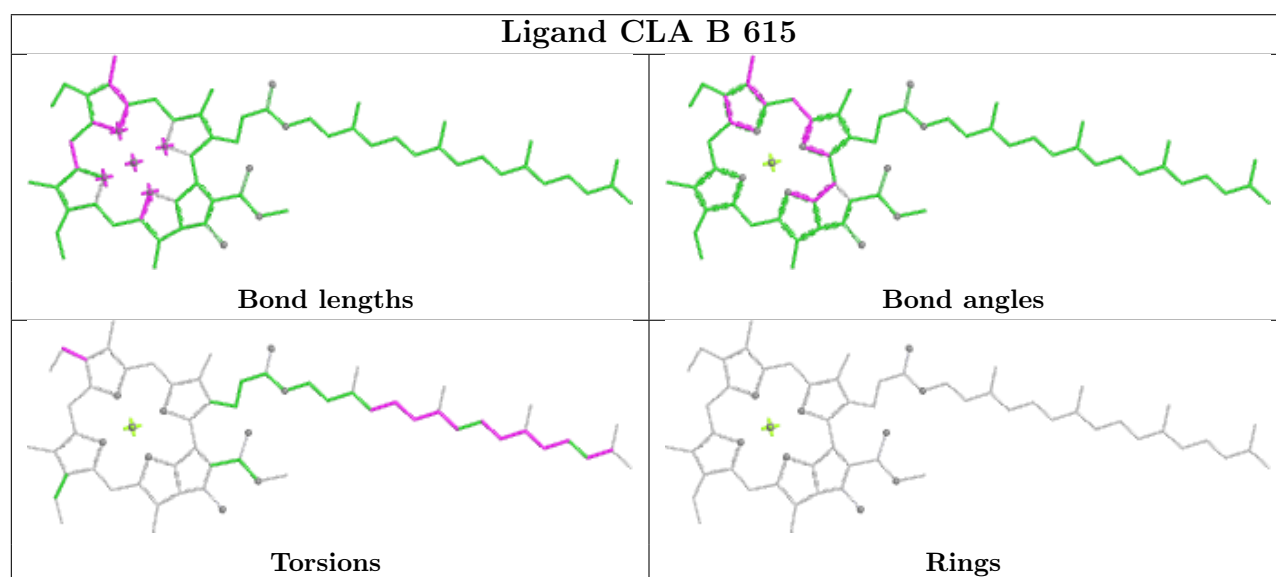
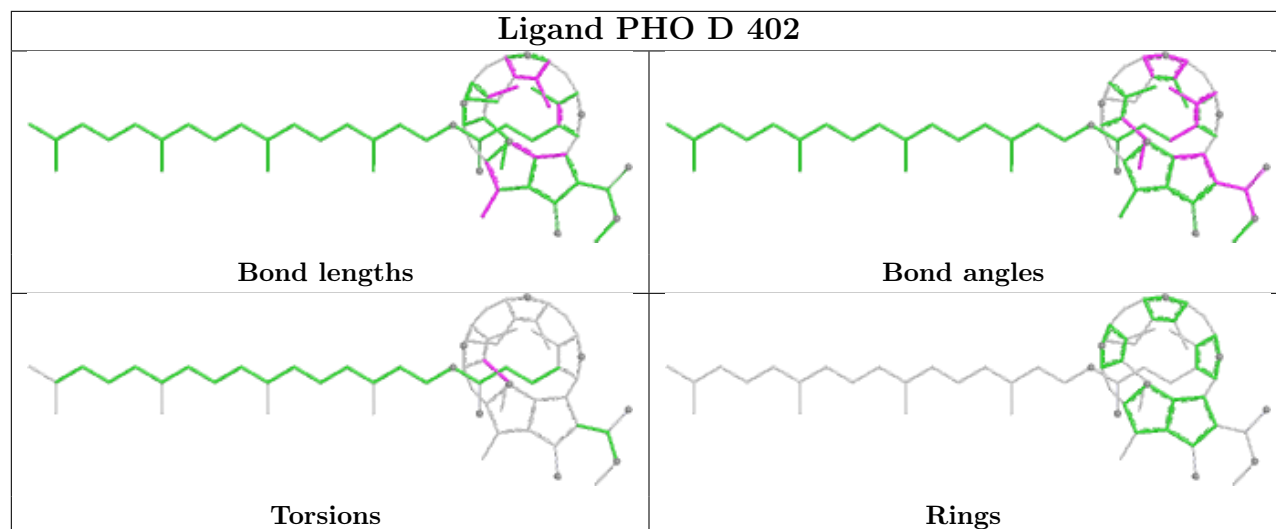
Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

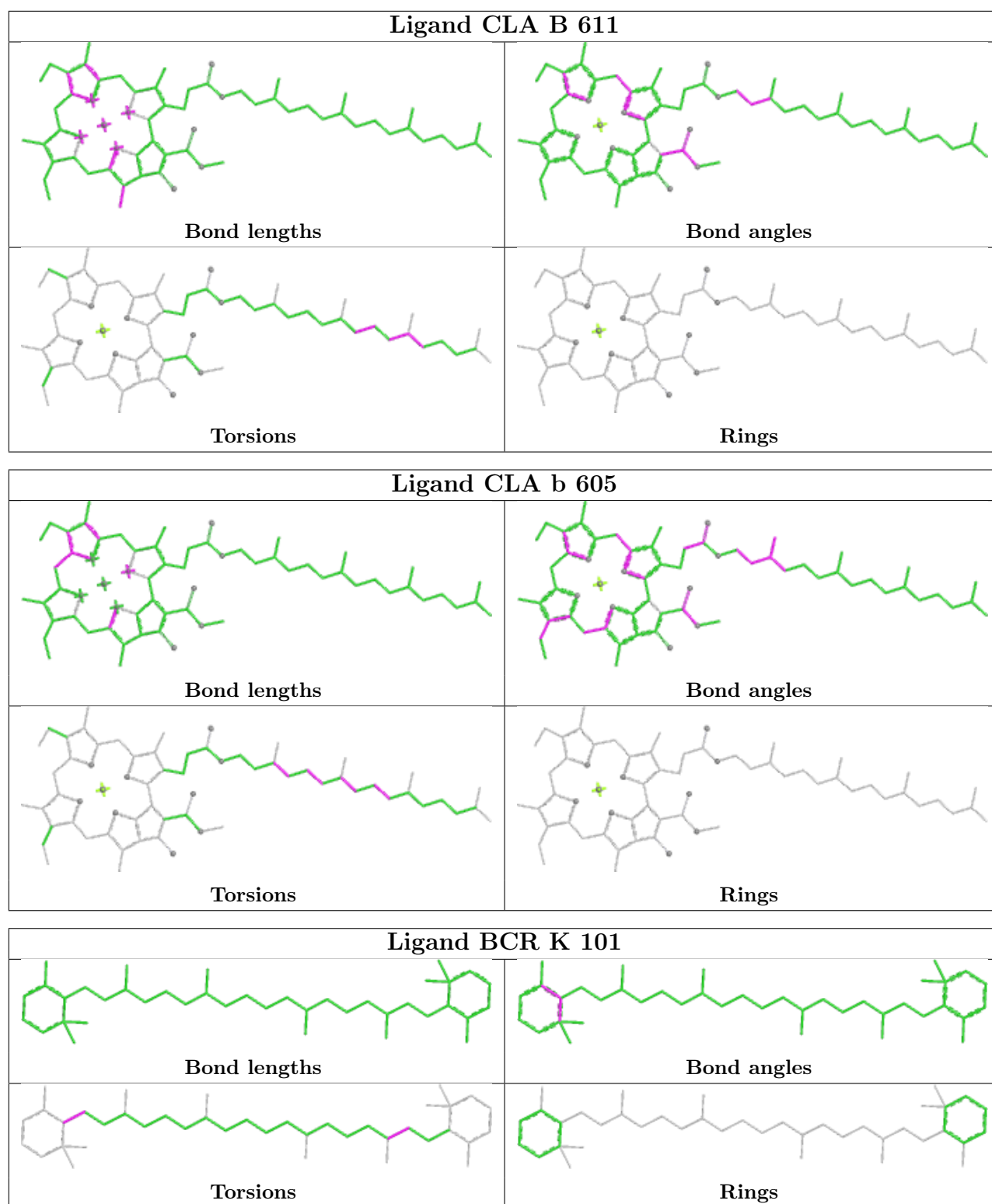


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 621	
	
Bond lengths	Bond angles
	
Torsions	Rings





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%)	-0.61	1 (0%) 90 93	26, 32, 50, 87	0
1	a	334/344 (97%)	-0.46	1 (0%) 90 93	26, 35, 58, 82	0
2	B	505/510 (99%)	-0.37	5 (0%) 79 86	20, 36, 62, 99	5 (0%)
2	b	505/510 (99%)	-0.26	3 (0%) 85 90	28, 40, 72, 104	1 (0%)
3	C	442/461 (95%)	-0.37	0 100 100	18, 39, 55, 84	1 (0%)
3	c	451/461 (97%)	-0.17	3 (0%) 84 89	21, 44, 64, 104	2 (0%)
4	D	341/352 (96%)	-0.59	1 (0%) 90 93	25, 33, 49, 80	0
4	d	341/352 (96%)	-0.42	0 100 100	27, 38, 61, 81	1 (0%)
5	E	82/84 (97%)	0.37	2 (2%) 59 69	31, 54, 69, 85	1 (1%)
5	e	82/84 (97%)	0.41	2 (2%) 59 69	44, 62, 80, 96	0
6	F	34/45 (75%)	-0.03	1 (2%) 53 63	38, 45, 64, 88	0
6	f	34/45 (75%)	0.29	0 100 100	47, 53, 79, 93	0
7	H	65/66 (98%)	-0.17	1 (1%) 72 80	34, 44, 62, 77	0
7	h	63/66 (95%)	0.26	1 (1%) 70 79	42, 53, 68, 71	0
8	I	35/38 (92%)	-0.30	0 100 100	36, 43, 70, 80	0
8	i	35/38 (92%)	-0.07	0 100 100	37, 46, 79, 96	0
9	J	36/40 (90%)	0.13	1 (2%) 55 65	37, 52, 83, 102	0
9	j	36/40 (90%)	0.33	2 (5%) 30 38	43, 59, 94, 97	0
10	K	37/46 (80%)	0.14	0 100 100	44, 54, 73, 77	0
10	k	37/46 (80%)	0.23	0 100 100	50, 59, 74, 85	0
11	L	37/37 (100%)	-0.53	0 100 100	29, 34, 67, 72	0
11	l	36/37 (97%)	-0.51	0 100 100	29, 35, 74, 83	0
12	M	32/36 (88%)	-0.19	1 (3%) 51 61	32, 37, 59, 77	0
12	m	31/36 (86%)	-0.34	0 100 100	32, 39, 53, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.14	4 (1%) 70 79	26, 45, 82, 139	1 (0%)
13	o	244/272 (89%)	-0.09	4 (1%) 70 79	29, 44, 84, 134	0
14	T	29/32 (90%)	-0.45	0 100 100	30, 36, 59, 78	0
14	t	29/32 (90%)	-0.26	2 (6%) 23 30	30, 36, 69, 84	0
15	U	97/134 (72%)	-0.13	0 100 100	34, 46, 71, 100	0
15	u	97/134 (72%)	-0.17	1 (1%) 79 86	33, 44, 63, 93	0
16	V	137/163 (84%)	-0.32	0 100 100	31, 43, 58, 75	0
16	v	137/163 (84%)	-0.06	0 100 100	36, 50, 72, 89	0
17	Y	27/46 (58%)	1.25	4 (14%) 5 7	57, 75, 99, 106	0
17	y	30/46 (65%)	0.66	0 100 100	61, 75, 94, 95	0
18	X	38/41 (92%)	0.20	1 (2%) 57 67	42, 53, 74, 87	0
18	x	39/41 (95%)	0.27	1 (2%) 57 67	49, 62, 84, 96	0
19	Z	62/62 (100%)	0.92	6 (9%) 13 19	56, 70, 117, 128	0
19	z	62/62 (100%)	0.84	6 (9%) 13 19	59, 74, 117, 135	0
20	R	28/41 (68%)	0.76	1 (3%) 46 56	60, 74, 84, 103	0
20	r	28/41 (68%)	1.43	6 (21%) 2 2	71, 90, 107, 110	0
All	All	5293/5700 (92%)	-0.21	61 (1%) 76 83	18, 41, 75, 139	12 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	6.2
20	r	29	LYS	4.5
19	Z	62	VAL	4.4
14	t	30	THR	4.4
19	z	33	TRP	4.3
17	Y	20	ALA	3.9
17	Y	22	LEU	3.9
3	c	23	ALA	3.8
19	Z	33	TRP	3.8
7	h	64	ALA	3.8
2	B	479[A]	PHE	3.7
14	t	29	ILE	3.6
1	a	11	ALA	3.6
13	o	59	LYS	3.3
17	Y	25	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	79	PHE	3.2
12	M	33	GLN	3.2
20	r	3	TRP	3.1
13	O	56	PRO	2.9
3	c	24	THR	2.8
20	r	20	VAL	2.8
5	E	84	LYS	2.8
15	u	53	ALA	2.8
9	J	5	GLY	2.8
1	A	11	ALA	2.7
20	r	28	VAL	2.7
18	X	2	THR	2.6
2	b	495	PHE	2.5
20	R	28	VAL	2.5
13	o	57	LYS	2.5
2	b	488	PRO	2.5
5	e	3	GLY	2.4
2	B	495	PHE	2.4
5	e	79	PHE	2.4
20	r	27	ALA	2.4
7	H	66	GLY	2.4
2	B	294	SER	2.4
3	c	134	ILE	2.3
19	z	40	ILE	2.3
13	O	58	ASN	2.3
19	Z	30	PRO	2.3
13	o	63	ALA	2.3
4	D	12	ARG	2.3
19	z	60	PHE	2.3
13	O	59	LYS	2.2
19	z	62	VAL	2.2
9	j	6	GLY	2.2
13	O	60	ARG	2.2
19	Z	3	ILE	2.1
2	B	490	GLN	2.1
6	F	12	SER	2.1
19	Z	5	PHE	2.1
19	Z	41	PHE	2.1
19	z	3	ILE	2.1
9	j	5	GLY	2.1
19	z	41	PHE	2.1
2	b	84	THR	2.1

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Mol	Chain	Res	Type	RSRZ
20	r	10	LEU	2.1
17	Y	27	MET	2.0
18	x	2	THR	2.0
2	B	499	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	34,49,70,70	0
14	FME	t	1	10/11	0.95	0.07	31,46,65,65	0
12	FME	M	1	10/11	0.96	0.09	37,46,66,72	0
8	FME	i	1	10/11	0.97	0.07	38,47,58,62	0
8	FME	I	1	10/11	0.97	0.07	39,49,64,65	0
12	FME	m	1	10/11	0.98	0.06	35,47,71,77	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
28	STE	C	520	10/20	0.55	0.25	51,79,95,97	0
28	STE	j	102	16/20	0.63	0.23	60,80,105,106	0
28	STE	e	101	9/20	0.64	0.25	60,78,92,94	0
28	STE	i	101	12/20	0.66	0.14	63,95,115,122	0
28	STE	K	103	14/20	0.68	0.17	59,76,99,101	0
28	STE	I	101	17/20	0.68	0.16	53,76,84,88	0
28	STE	c	517	18/20	0.70	0.19	61,83,102,103	0
28	STE	C	528	14/20	0.71	0.19	60,85,108,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	A	617	17/20	0.72	0.14	54,74,81,88	0
28	STE	C	518	5/20	0.72	0.24	54,61,73,73	0
28	STE	b	625	11/20	0.74	0.20	54,68,82,82	0
28	STE	C	519	7/20	0.75	0.21	57,68,79,79	0
28	STE	H	103	18/20	0.75	0.17	48,74,94,95	0
28	STE	A	618	11/20	0.75	0.15	56,72,88,88	0
32	LMG	c	518	30/55	0.75	0.17	45,80,107,111	0
28	STE	E	101	12/20	0.76	0.19	63,80,107,108	0
29	LHG	e	102	42/49	0.76	0.17	59,85,116,130	0
32	LMG	D	407	50/55	0.76	0.15	41,72,115,121	0
28	STE	b	624	10/20	0.76	0.18	51,61,69,73	0
28	STE	E	102	20/20	0.78	0.14	47,69,87,96	0
28	STE	A	611	9/20	0.78	0.17	62,76,86,93	0
28	STE	Z	101	17/20	0.78	0.20	51,74,99,102	0
28	STE	C	516	14/20	0.79	0.17	53,69,83,83	0
28	STE	B	625	15/20	0.79	0.21	47,64,79,94	0
28	STE	I	102	15/20	0.80	0.18	50,64,85,88	0
28	STE	a	616	12/20	0.80	0.13	51,76,81,91	0
28	STE	T	102	16/20	0.80	0.17	42,58,96,100	0
32	LMG	C	517	36/55	0.80	0.14	49,63,81,87	0
28	STE	e	103	9/20	0.80	0.16	53,72,83,87	0
32	LMG	b	622	55/55	0.80	0.16	50,74,94,104	0
28	STE	h	103	10/20	0.80	0.18	63,77,88,91	0
32	LMG	c	523	48/55	0.80	0.15	53,80,104,114	0
29	LHG	A	613	49/49	0.81	0.14	51,74,109,113	0
28	STE	b	623	16/20	0.81	0.17	49,63,85,91	0
28	STE	i	102	6/20	0.81	0.17	55,73,76,76	0
28	STE	c	516	13/20	0.81	0.16	56,75,83,84	0
32	LMG	a	614	55/55	0.81	0.14	41,64,84,96	0
28	STE	k	103	14/20	0.81	0.13	57,74,93,94	0
28	STE	t	103	10/20	0.81	0.18	48,69,77,80	0
28	STE	z	101	9/20	0.81	0.22	56,70,80,82	0
28	STE	e	104	13/20	0.82	0.17	73,88,96,99	0
32	LMG	B	620	45/55	0.82	0.15	38,59,98,116	0
27	PL9	a	610	55/55	0.83	0.16	38,70,87,91	0
28	STE	f	103	8/20	0.83	0.17	56,69,79,81	0
28	STE	d	411	20/20	0.83	0.13	50,68,91,92	0
27	PL9	A	610	55/55	0.84	0.16	35,68,88,90	0
28	STE	H	104	9/20	0.84	0.14	53,66,82,83	0
31	DGD	A	615	66/66	0.84	0.13	50,69,105,114	0
28	STE	B	624	12/20	0.84	0.13	52,68,78,81	0
28	STE	j	101	12/20	0.84	0.14	49,64,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	C	526	12/20	0.85	0.15	40,52,63,63	0
28	STE	M	104	15/20	0.85	0.15	46,63,93,95	0
28	STE	R	101	12/20	0.85	0.15	57,74,87,87	0
30	SQD	a	613	54/54	0.85	0.12	45,63,101,118	0
30	SQD	A	614	43/54	0.86	0.11	44,61,102,117	0
28	STE	d	407	20/20	0.86	0.12	42,58,81,82	0
28	STE	M	103	10/20	0.87	0.14	45,57,64,75	0
28	STE	A	616	8/20	0.87	0.14	47,63,74,74	0
24	CLA	b	601	65/65	0.87	0.12	49,68,91,108	0
28	STE	M	102	15/20	0.87	0.10	38,50,65,70	0
32	LMG	C	521	48/55	0.87	0.12	43,60,74,84	0
28	STE	m	103	18/20	0.88	0.14	40,53,84,90	0
32	LMG	a	615	49/55	0.88	0.12	42,64,86,92	0
28	STE	J	101	12/20	0.88	0.12	49,62,66,70	0
28	STE	C	527	16/20	0.88	0.12	42,53,70,80	0
32	LMG	M	101	51/55	0.88	0.10	34,53,72,80	0
30	SQD	f	102	41/54	0.89	0.13	55,80,98,102	0
28	STE	b	621	20/20	0.89	0.11	37,59,72,76	0
28	STE	B	621	17/20	0.89	0.11	40,57,75,80	0
28	STE	d	413	20/20	0.89	0.11	39,57,70,72	0
28	STE	B	623	18/20	0.89	0.11	46,61,80,83	0
30	SQD	b	620	49/54	0.89	0.10	44,61,83,88	0
32	LMG	m	101	51/55	0.89	0.10	37,57,71,84	0
30	SQD	B	622	54/54	0.90	0.09	41,61,86,91	0
32	LMG	c	522	46/55	0.90	0.11	40,70,86,87	0
28	STE	t	102	14/20	0.91	0.09	42,52,67,67	0
28	STE	m	102	12/20	0.91	0.11	47,58,76,77	0
32	LMG	C	525	48/55	0.91	0.12	44,74,96,99	0
26	BCR	C	514	40/40	0.92	0.10	48,60,71,76	0
26	BCR	d	405	40/40	0.92	0.10	39,53,89,94	0
30	SQD	a	612	54/54	0.92	0.11	43,68,96,100	0
24	CLA	B	601	65/65	0.92	0.10	35,59,96,98	0
24	CLA	c	513	65/65	0.92	0.11	48,70,99,103	0
28	STE	D	414	20/20	0.93	0.09	36,50,73,81	0
26	BCR	k	102	40/40	0.93	0.10	43,55,71,74	0
26	BCR	B	618	40/40	0.93	0.08	27,41,53,55	0
24	CLA	c	512	65/65	0.93	0.10	43,60,92,94	0
30	SQD	D	409	36/54	0.93	0.11	43,71,90,93	0
30	SQD	D	412	52/54	0.93	0.10	31,61,87,94	0
26	BCR	H	101	40/40	0.93	0.08	32,45,59,62	0
26	BCR	K	101	40/40	0.93	0.09	40,54,72,76	0
26	BCR	c	514	40/40	0.93	0.10	51,64,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	513	65/65	0.93	0.09	43,66,99,103	0
26	BCR	h	101	40/40	0.93	0.09	41,53,72,73	0
26	BCR	k	101	40/40	0.93	0.09	46,59,71,75	0
31	DGD	c	520	62/66	0.94	0.09	35,53,94,100	0
31	DGD	h	102	62/66	0.94	0.08	35,50,62,64	0
26	BCR	C	515	40/40	0.94	0.08	28,42,54,60	0
29	LHG	d	408	49/49	0.94	0.10	38,53,74,82	0
26	BCR	c	515	40/40	0.94	0.09	32,47,63,63	0
26	BCR	b	619	40/40	0.94	0.09	32,49,67,70	0
31	DGD	C	523	62/66	0.94	0.10	32,50,107,118	0
32	LMG	D	408	51/55	0.94	0.11	30,61,87,92	0
26	BCR	B	617	40/40	0.95	0.07	29,41,52,55	0
27	PL9	d	406	55/55	0.95	0.07	27,38,45,47	0
24	CLA	B	606	65/65	0.95	0.08	25,37,76,81	0
26	BCR	B	619	40/40	0.95	0.07	30,45,64,70	0
24	CLA	C	510	65/65	0.95	0.07	33,44,64,77	0
24	CLA	b	606	65/65	0.95	0.08	29,41,79,85	0
26	BCR	D	405	40/40	0.95	0.10	33,47,83,99	0
31	DGD	H	102	62/66	0.95	0.08	31,45,60,67	0
24	CLA	b	616	60/65	0.95	0.09	32,45,90,94	0
24	CLA	c	503	65/65	0.95	0.07	35,46,56,59	0
26	BCR	K	102	40/40	0.95	0.08	42,53,70,70	0
26	BCR	T	101	40/40	0.95	0.07	30,40,59,59	0
26	BCR	b	617	40/40	0.95	0.07	30,43,53,57	0
26	BCR	b	618	40/40	0.95	0.07	28,44,59,63	0
24	CLA	c	506	65/65	0.95	0.09	36,51,96,103	0
24	CLA	c	509	65/65	0.95	0.08	34,48,65,68	0
24	CLA	c	511	65/65	0.95	0.08	40,56,72,75	0
29	LHG	D	413	49/49	0.95	0.09	31,47,72,76	0
24	CLA	C	511	65/65	0.95	0.08	32,51,65,71	0
29	LHG	d	410	39/49	0.95	0.09	32,48,71,80	0
24	CLA	C	512	65/65	0.95	0.08	39,54,89,99	0
24	CLA	d	404	65/65	0.95	0.09	33,49,94,97	0
25	PHO	D	402	64/64	0.95	0.06	24,33,40,45	0
32	LMG	d	412	44/55	0.95	0.09	37,55,83,94	0
25	PHO	d	402	64/64	0.95	0.07	30,38,46,53	0
24	CLA	C	504	59/65	0.96	0.07	29,42,92,96	0
29	LHG	D	411	47/49	0.96	0.09	31,52,87,94	0
24	CLA	c	504	60/65	0.96	0.07	33,44,82,87	0
24	CLA	c	505	65/65	0.96	0.07	29,44,75,85	0
29	LHG	d	409	49/49	0.96	0.07	30,44,58,69	0
24	CLA	C	505	65/65	0.96	0.07	27,40,69,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	507	65/65	0.96	0.07	33,47,61,64	0
24	CLA	c	508	64/65	0.96	0.09	35,46,98,111	0
26	BCR	t	101	40/40	0.96	0.06	27,41,53,58	0
24	CLA	C	506	65/65	0.96	0.10	31,46,93,100	0
27	PL9	D	406	55/55	0.96	0.06	22,34,46,51	0
24	CLA	c	510	65/65	0.96	0.07	33,47,63,68	0
24	CLA	C	507	65/65	0.96	0.06	27,42,61,66	0
24	CLA	C	509	65/65	0.96	0.07	31,45,61,74	0
24	CLA	B	609	65/65	0.96	0.06	27,37,57,66	0
24	CLA	B	610	65/65	0.96	0.06	23,34,43,46	0
31	DGD	C	522	62/66	0.96	0.08	24,44,90,94	0
25	PHO	A	607	64/64	0.96	0.06	21,30,38,44	0
31	DGD	C	524	62/66	0.96	0.08	29,51,86,98	0
24	CLA	B	614	65/65	0.96	0.07	24,37,81,95	0
31	DGD	c	519	62/66	0.96	0.09	24,45,81,97	0
25	PHO	a	607	64/64	0.96	0.06	24,32,40,44	0
31	DGD	c	521	62/66	0.96	0.09	31,54,91,96	0
24	CLA	B	616	60/65	0.96	0.08	27,40,94,104	0
26	BCR	A	609	40/40	0.96	0.06	27,39,46,49	0
24	CLA	a	606	65/65	0.96	0.09	28,42,101,108	0
24	CLA	a	608	65/65	0.96	0.09	23,37,83,96	0
24	CLA	C	501	65/65	0.96	0.06	27,38,52,58	0
24	CLA	b	602	65/65	0.96	0.08	28,44,62,67	0
24	CLA	b	605	65/65	0.96	0.06	26,37,51,54	0
24	CLA	C	502	65/65	0.96	0.06	29,40,55,61	0
24	CLA	b	608	65/65	0.96	0.06	30,43,62,66	0
24	CLA	b	609	65/65	0.96	0.07	32,47,68,72	0
24	CLA	b	610	65/65	0.96	0.07	30,41,51,52	0
24	CLA	b	614	65/65	0.96	0.08	28,40,85,92	0
26	BCR	a	609	40/40	0.96	0.06	27,37,49,51	0
24	CLA	b	615	65/65	0.96	0.07	27,44,68,77	0
24	CLA	C	503	65/65	0.96	0.06	33,42,50,57	0
24	CLA	c	502	65/65	0.96	0.07	30,43,60,69	0
33	BCT	D	401	4/4	0.96	0.07	28,32,36,43	0
24	CLA	B	612	65/65	0.97	0.07	21,34,47,56	0
24	CLA	b	611	65/65	0.97	0.06	25,36,56,59	0
24	CLA	b	612	65/65	0.97	0.06	25,37,49,54	0
24	CLA	b	613	65/65	0.97	0.07	25,36,82,86	0
24	CLA	B	613	65/65	0.97	0.06	22,33,75,80	0
24	CLA	B	603	65/65	0.97	0.07	25,35,64,65	0
24	CLA	B	615	65/65	0.97	0.07	26,40,62,69	0
24	CLA	c	501	65/65	0.97	0.07	31,43,56,60	0

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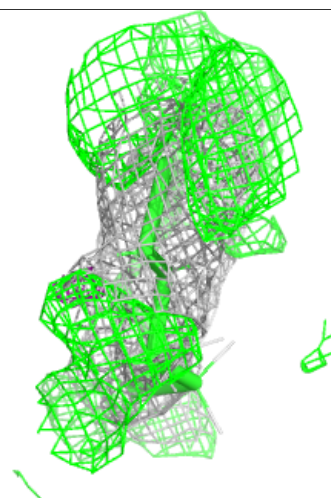
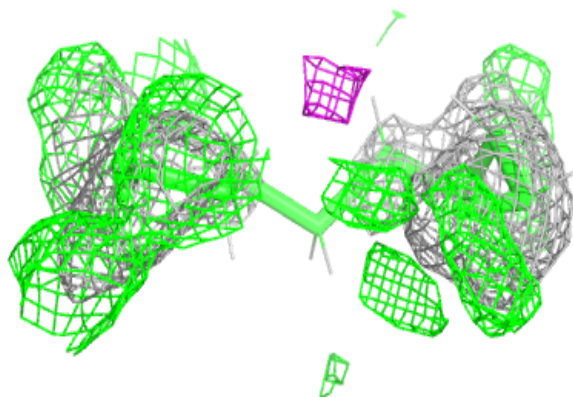
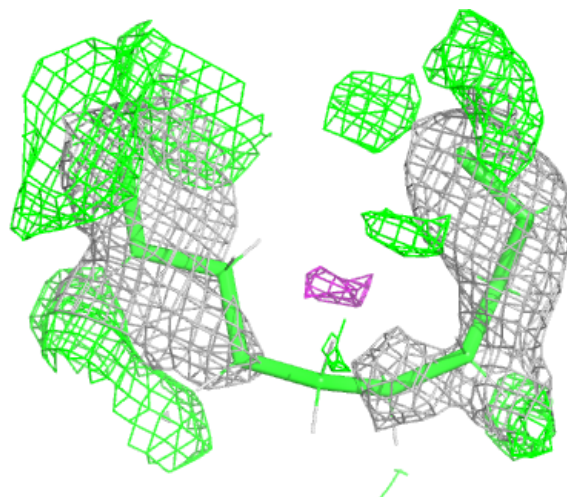
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	604	65/65	0.97	0.07	22,34,74,82	0
24	CLA	D	404	65/65	0.97	0.08	27,42,115,134	0
24	CLA	a	605	65/65	0.97	0.06	22,31,50,60	0
24	CLA	B	605	65/65	0.97	0.06	22,34,49,51	0
29	LHG	D	410	49/49	0.97	0.06	27,41,52,55	0
24	CLA	A	612	65/65	0.97	0.06	22,29,49,58	0
24	CLA	a	611	65/65	0.97	0.06	23,31,49,56	0
29	LHG	L	101	49/49	0.97	0.07	30,44,63,75	0
24	CLA	B	607	65/65	0.97	0.07	22,36,64,77	0
24	CLA	B	608	65/65	0.97	0.06	25,36,58,62	0
24	CLA	b	603	65/65	0.97	0.06	28,38,67,74	0
24	CLA	b	604	65/65	0.97	0.07	24,37,79,98	0
29	LHG	l	101	49/49	0.97	0.07	30,48,67,75	0
24	CLA	A	605	65/65	0.97	0.05	20,29,53,59	0
24	CLA	B	602	65/65	0.97	0.06	26,37,56,62	0
24	CLA	d	403	65/65	0.97	0.06	23,35,64,67	0
24	CLA	b	607	65/65	0.97	0.08	25,38,66,73	0
24	CLA	B	611	65/65	0.97	0.05	23,32,49,55	0
24	CLA	C	508	65/65	0.97	0.07	30,42,111,122	0
33	BCT	d	401	4/4	0.97	0.06	33,36,47,56	0
34	HEM	F	101	43/43	0.97	0.07	40,47,61,61	0
34	HEM	f	101	43/43	0.97	0.08	47,57,73,73	0
24	CLA	D	403	65/65	0.98	0.05	21,30,62,70	0
24	CLA	A	606	65/65	0.98	0.07	24,37,100,111	0
24	CLA	A	608	54/65	0.98	0.05	22,35,67,78	0
23	CL	a	603	1/1	0.99	0.03	29,29,29,29	0
35	HEC	V	201	43/43	0.99	0.05	27,34,41,42	0
35	HEC	v	201	43/43	0.99	0.05	30,37,49,49	0
21	OEX	a	601	10/10	1.00	0.02	24,27,30,31	0
22	FE2	A	602	1/1	1.00	0.01	29,29,29,29	0
22	FE2	a	602	1/1	1.00	0.03	35,35,35,35	0
23	CL	A	603	1/1	1.00	0.04	28,28,28,28	0
23	CL	A	604	1/1	1.00	0.03	29,29,29,29	0
21	OEX	A	601	10/10	1.00	0.02	25,27,30,32	0
23	CL	a	604	1/1	1.00	0.04	30,30,30,30	0

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

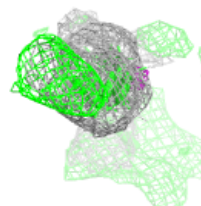
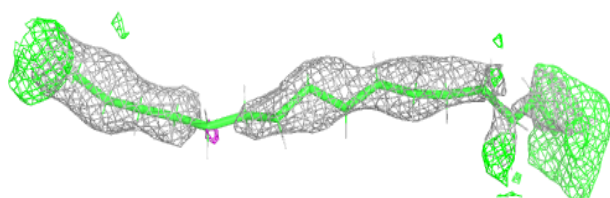
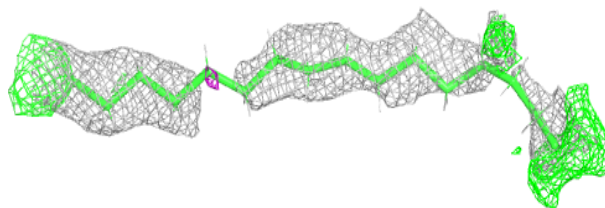
Electron density around STE C 520:

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

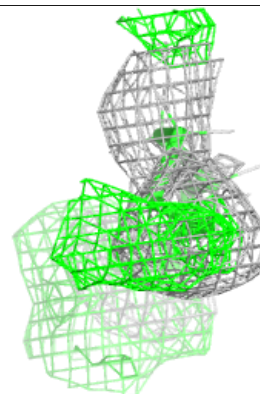
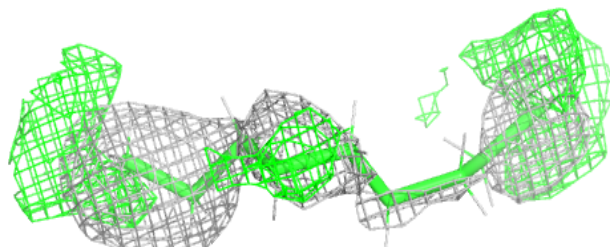
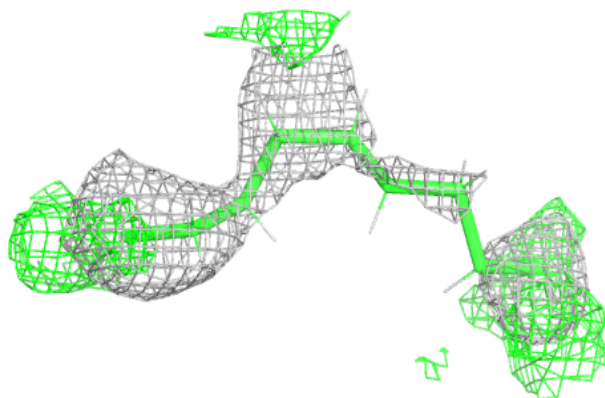


Electron density around STE j 102:

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

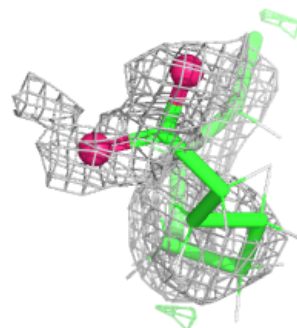
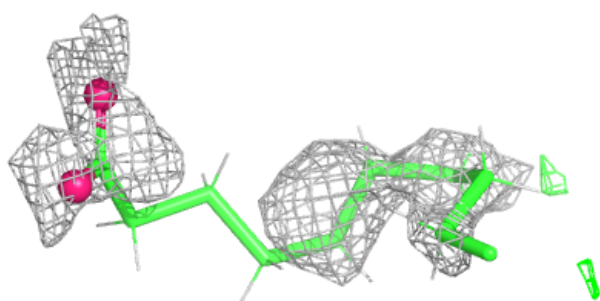
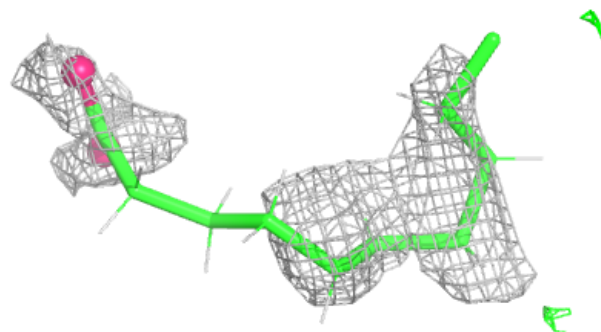
**Electron density around STE e 101:**

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

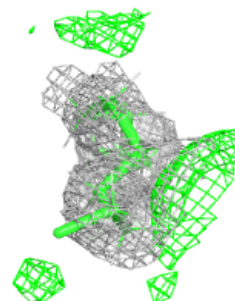
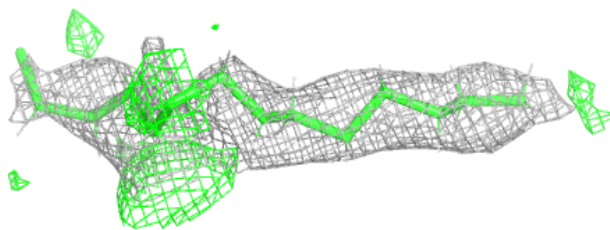
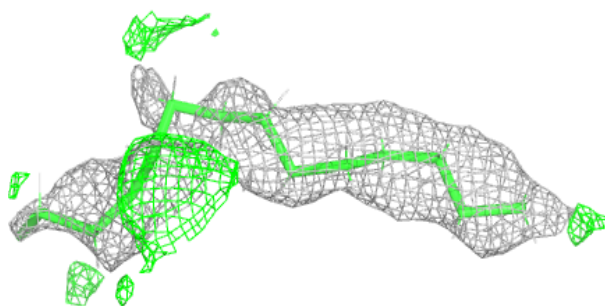


Electron density around STE i 101:

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

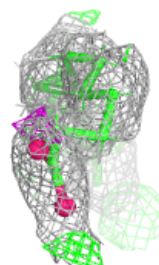
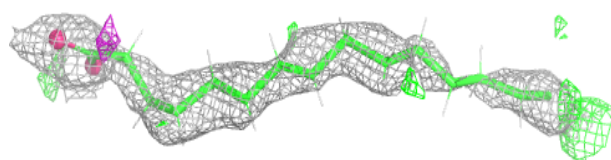
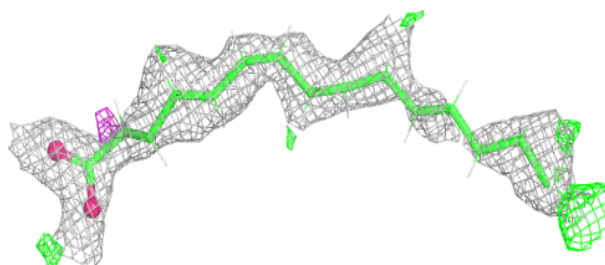
**Electron density around STE K 103:**

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

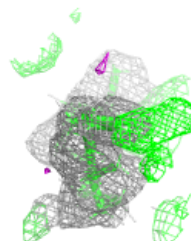
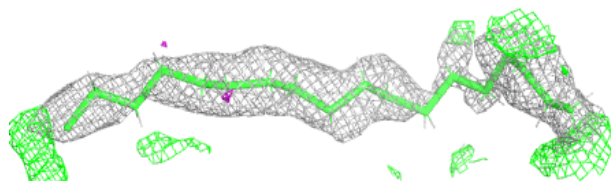
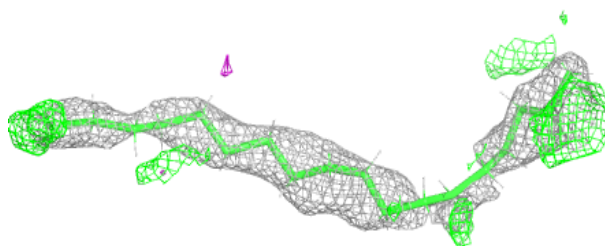


Electron density around STE I 101:

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

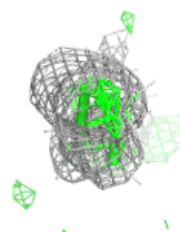
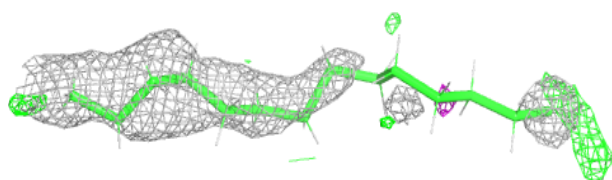
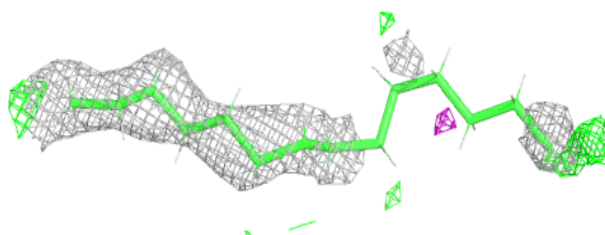
**Electron density around STE c 517:**

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

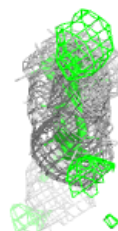
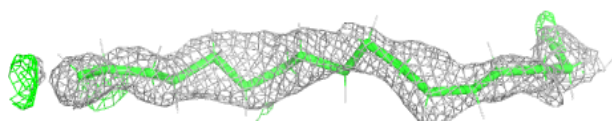
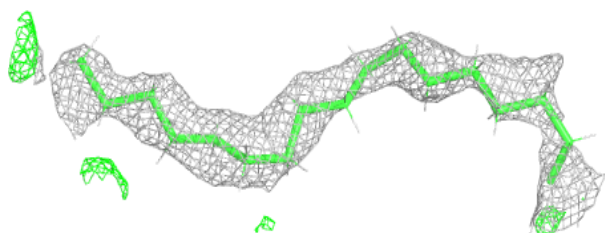


Electron density around STE C 528:

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

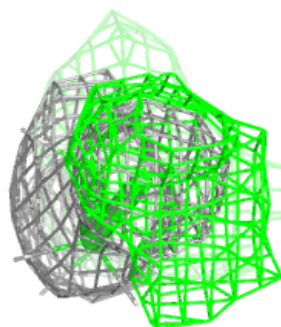
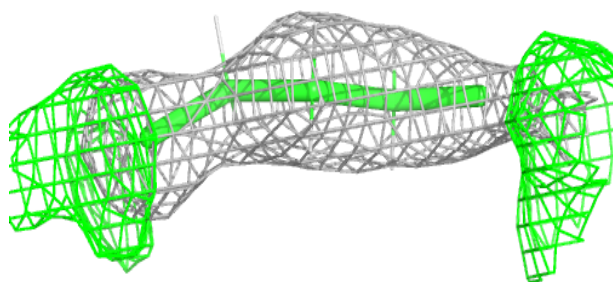
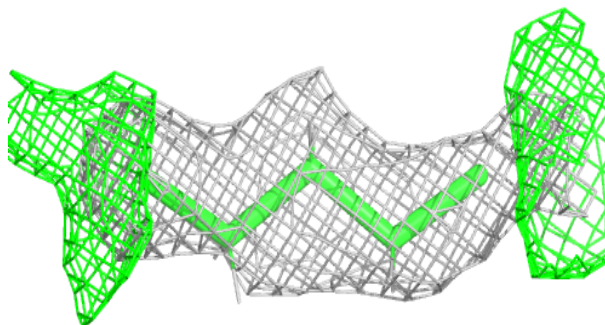
**Electron density around STE A 617:**

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

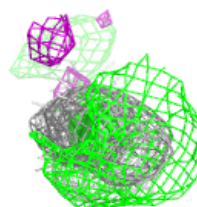
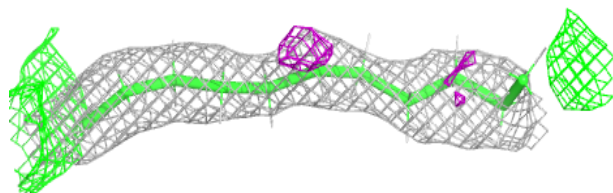
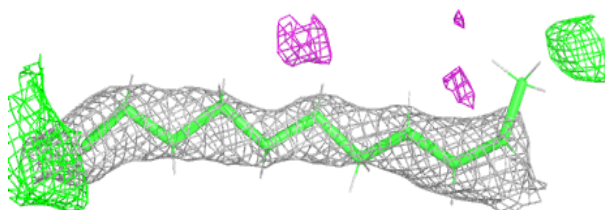


Electron density around STE C 518:

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

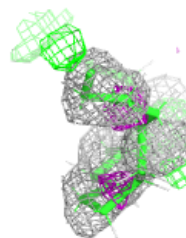
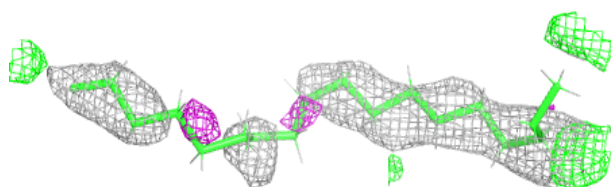
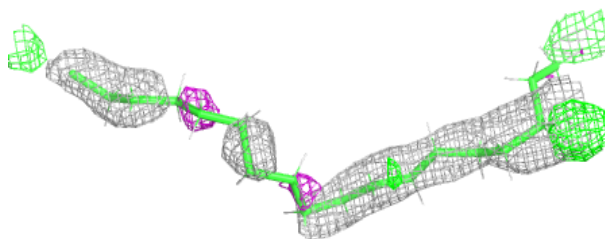
**Electron density around STE b 625:**

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

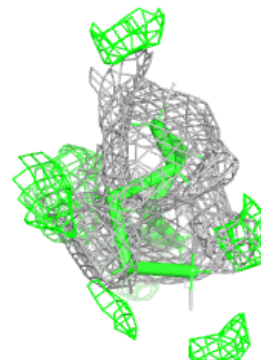
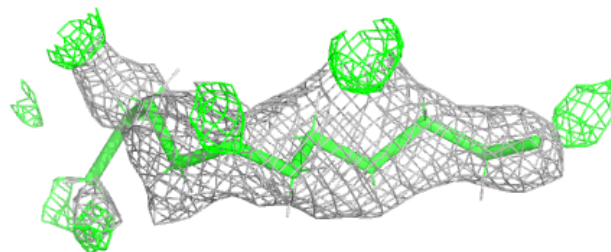
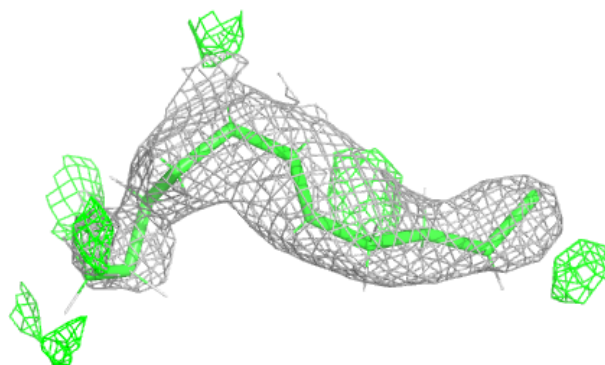


Electron density around STE H 103:

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

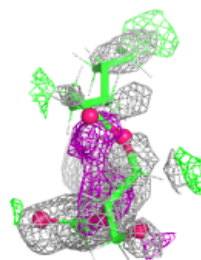
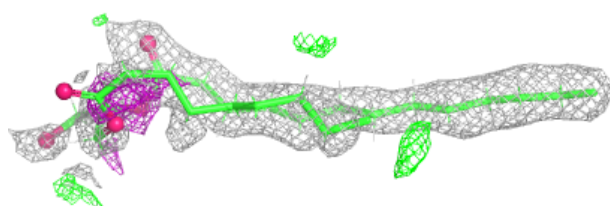
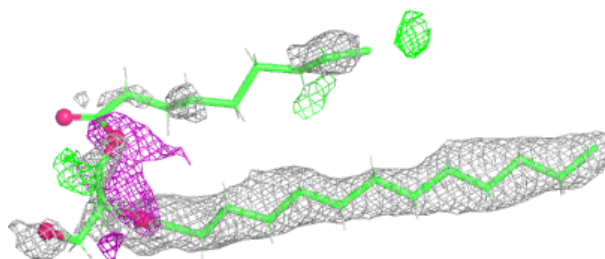
**Electron density around STE A 618:**

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

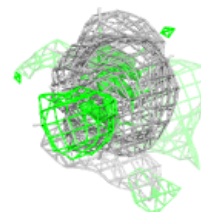
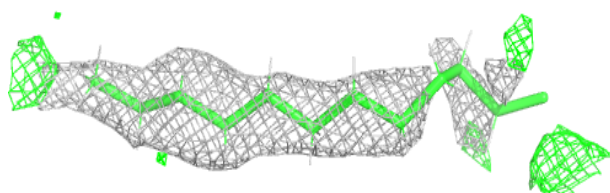
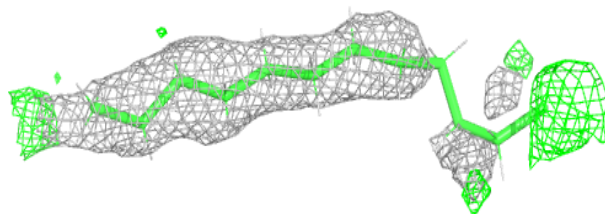


Electron density around LMG c 518:

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

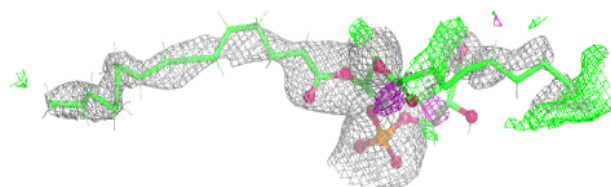
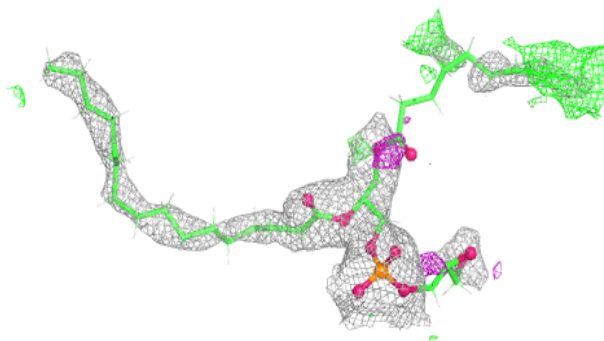
**Electron density around STE E 101:**

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

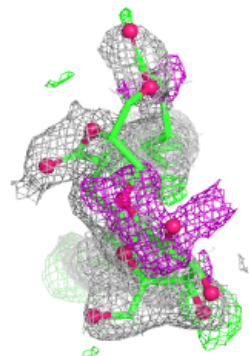
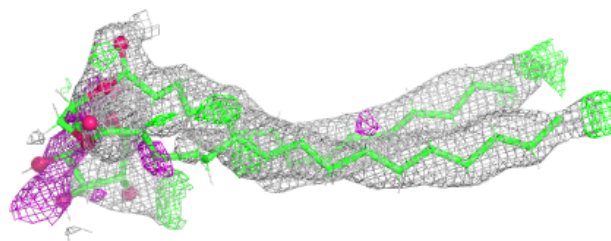
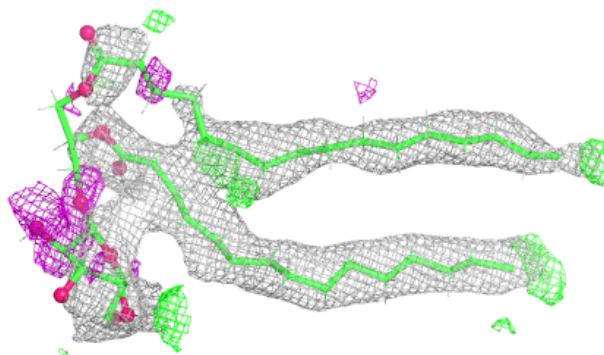


Electron density around LHG e 102:

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

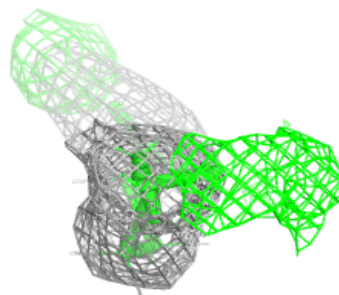
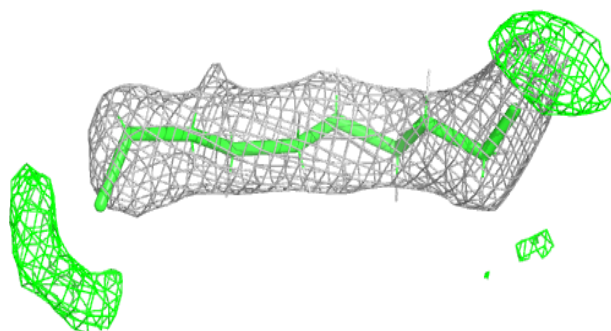
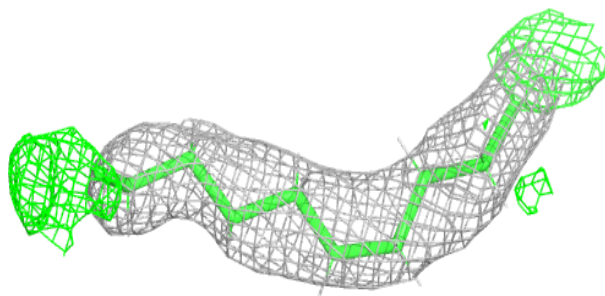
**Electron density around LMG D 407:**

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

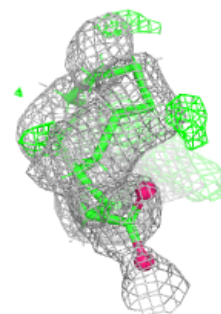
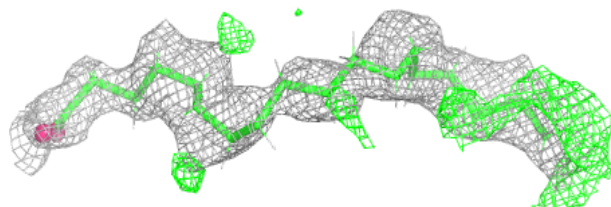
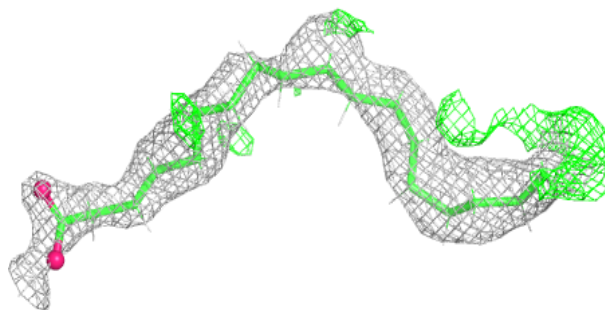


Electron density around STE b 624:

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

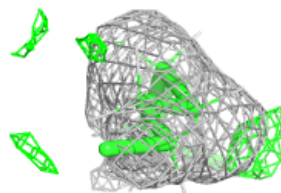
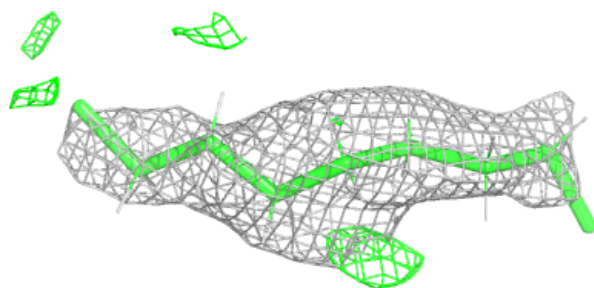
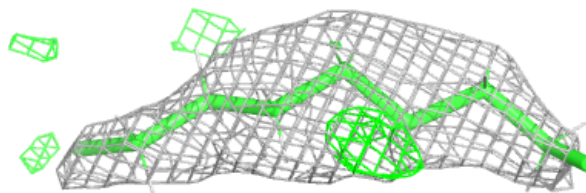
**Electron density around STE E 102:**

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

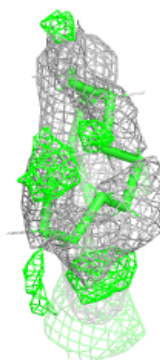
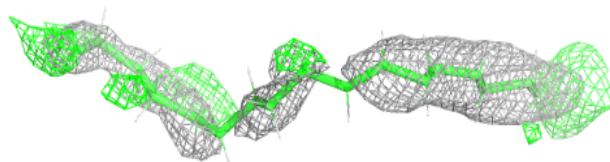
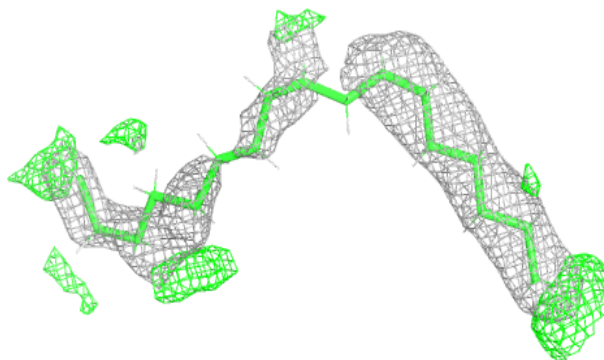


Electron density around STE A 611:

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

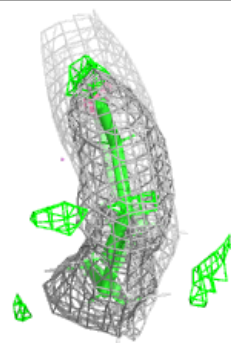
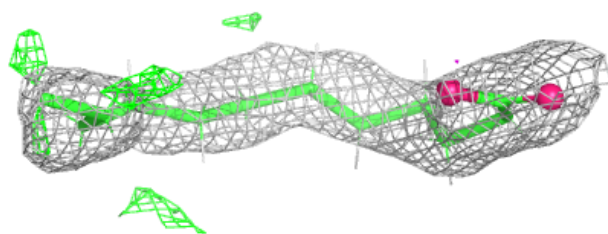
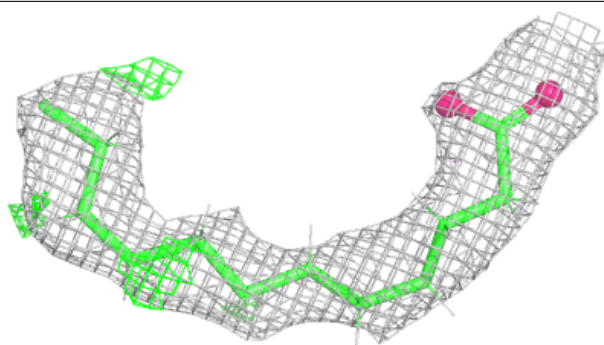
**Electron density around STE Z 101:**

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

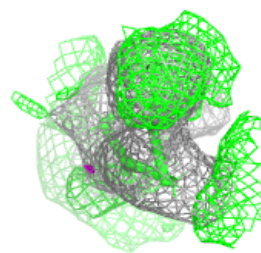
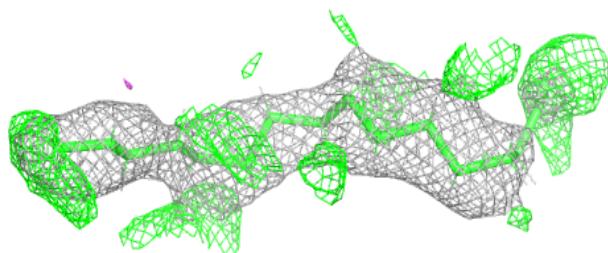
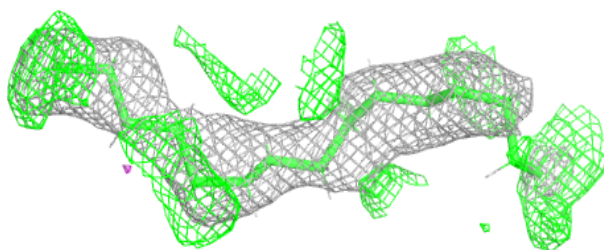


Electron density around STE C 516:

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

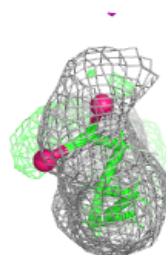
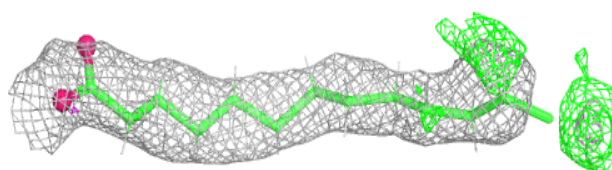
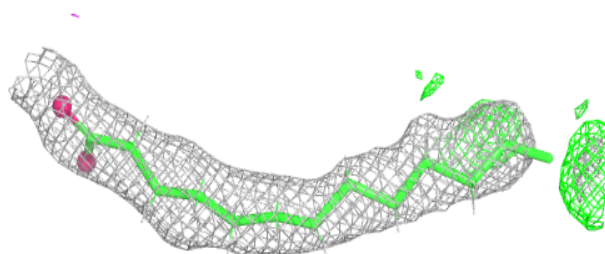
**Electron density around STE B 625:**

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

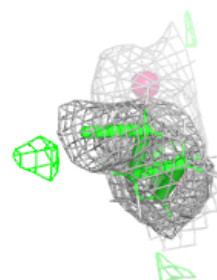
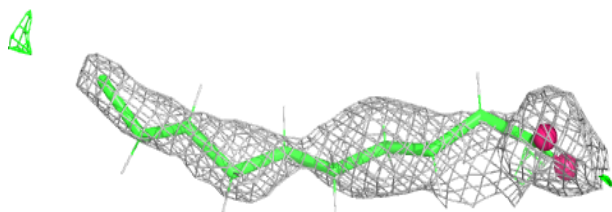
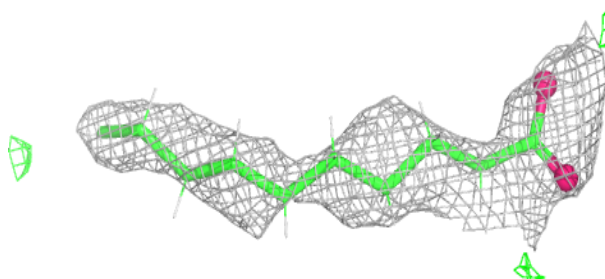


Electron density around STE I 102:

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

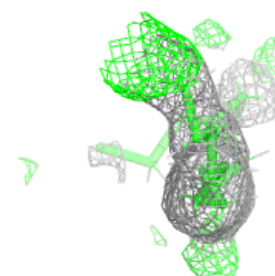
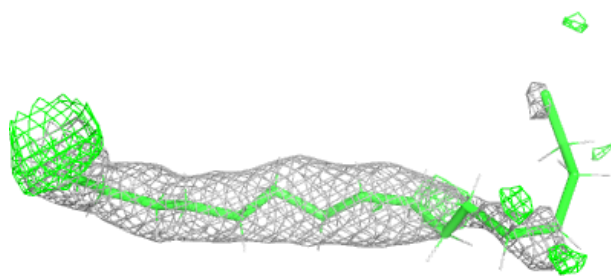
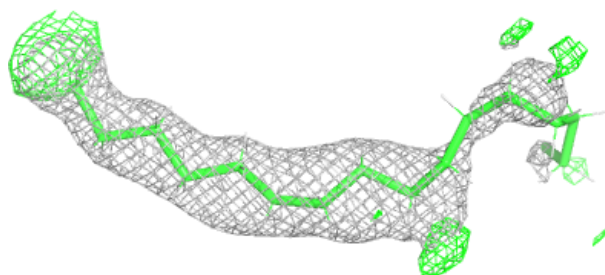
**Electron density around STE a 616:**

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

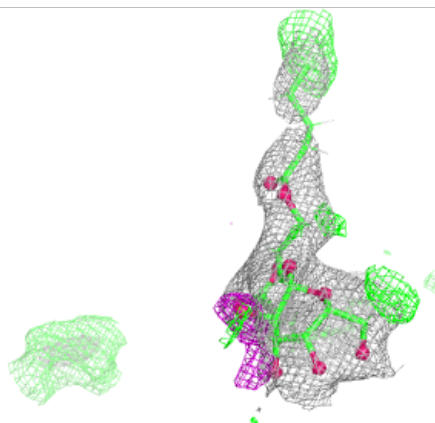
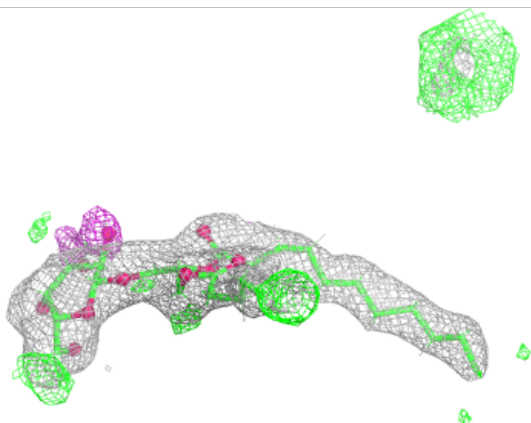
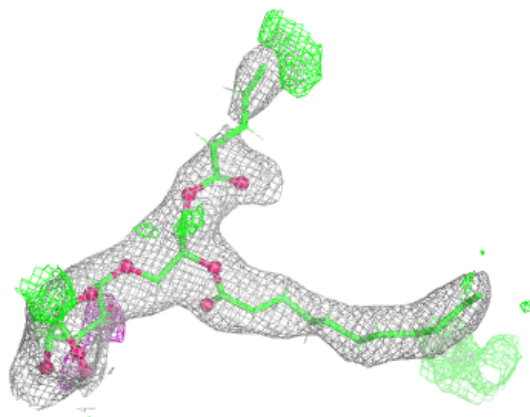


Electron density around STE T 102:

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

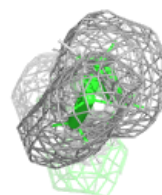
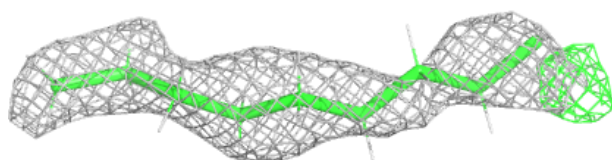
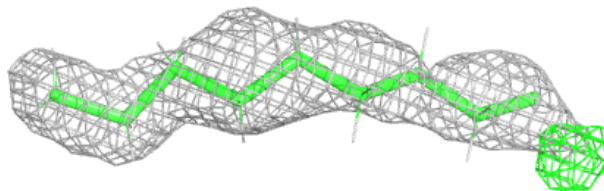
**Electron density around LMG C 517:**

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

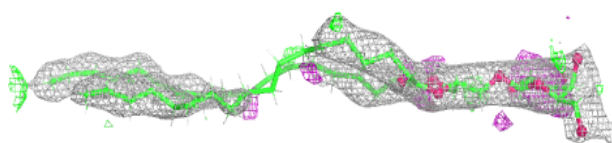
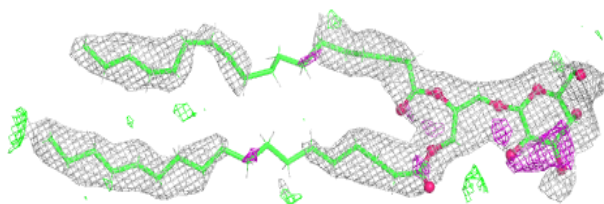


Electron density around STE e 103:

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

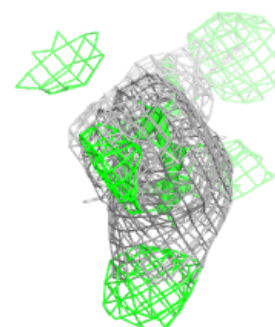
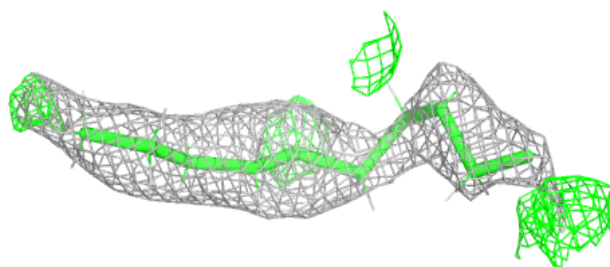
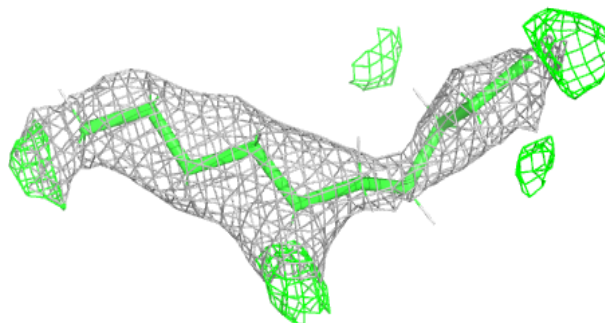
**Electron density around LMG b 622:**

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

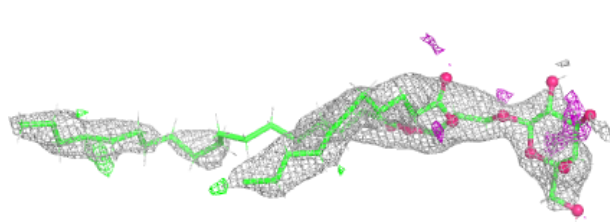
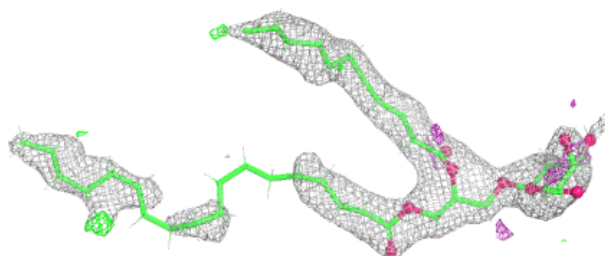


Electron density around STE h 103:

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

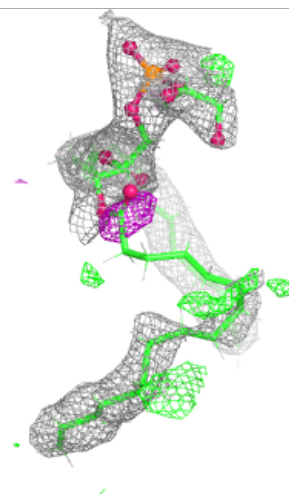
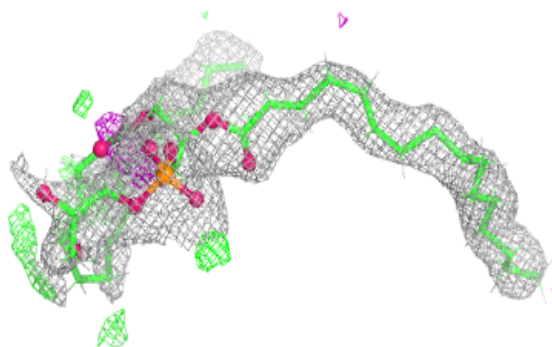
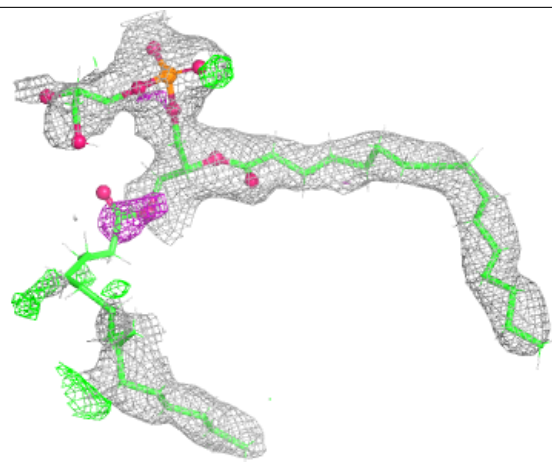
**Electron density around LMG c 523:**

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



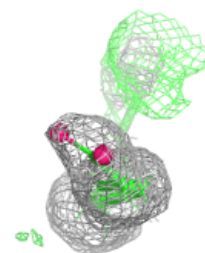
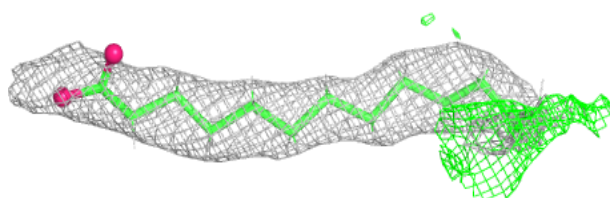
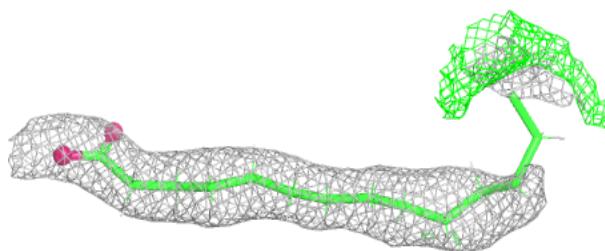
Electron density around LHG A 613:

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

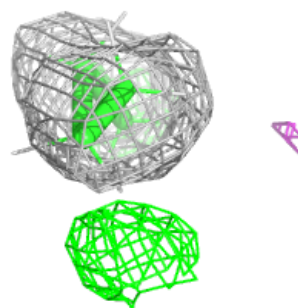
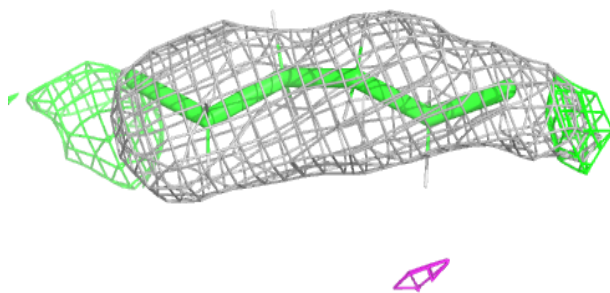
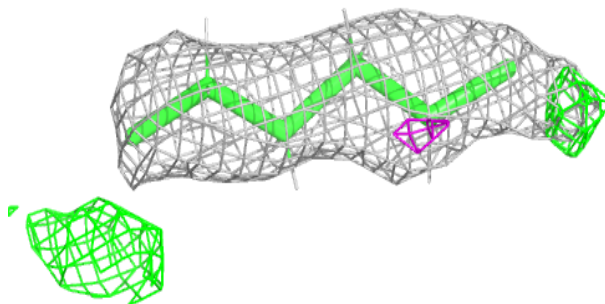


Electron density around STE b 623:

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

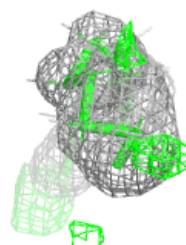
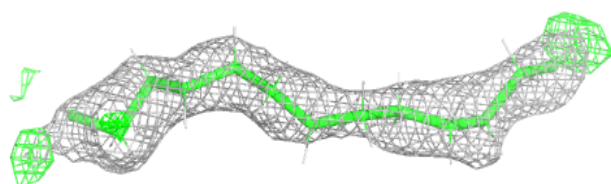
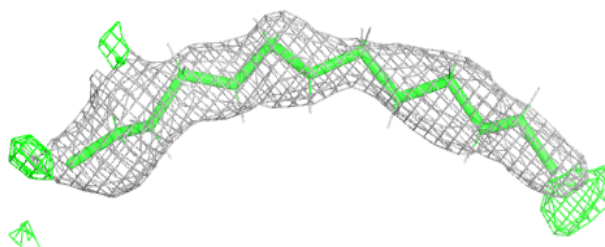
**Electron density around STE i 102:**

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

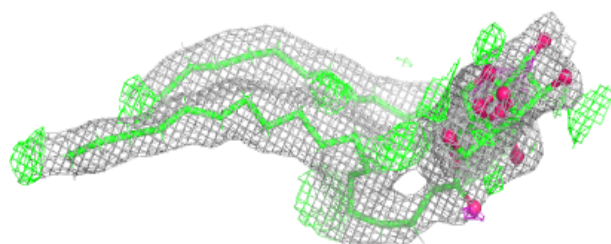
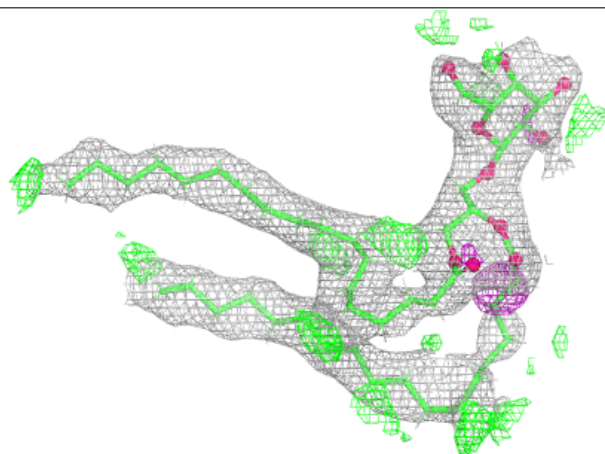


Electron density around STE c 516:

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

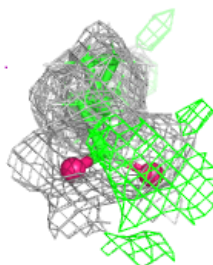
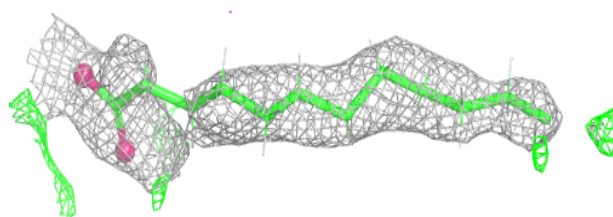
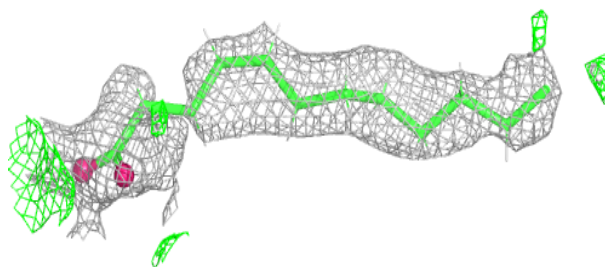
**Electron density around LMG a 614:**

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

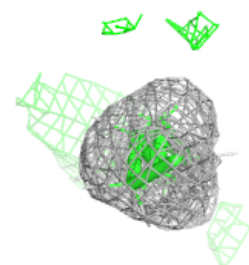
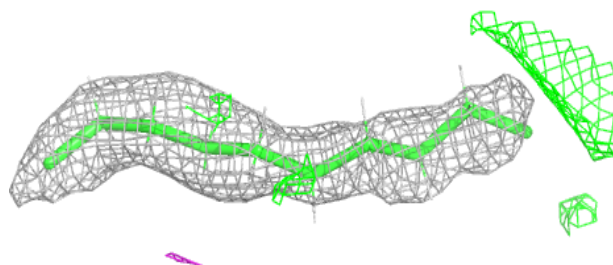
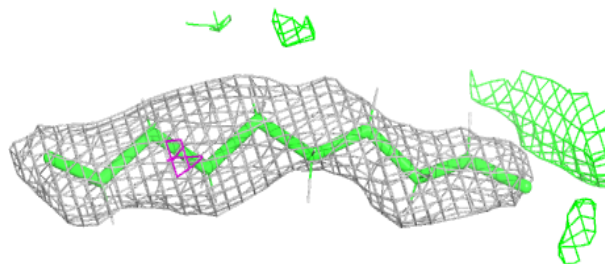


Electron density around STE k 103:

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

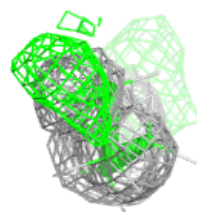
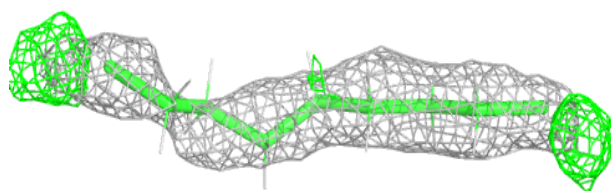
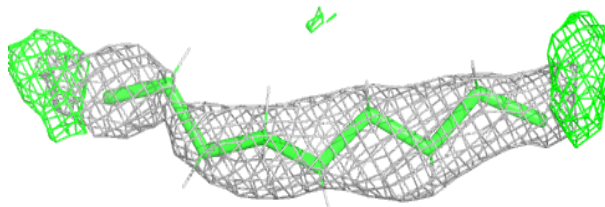
**Electron density around STE t 103:**

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

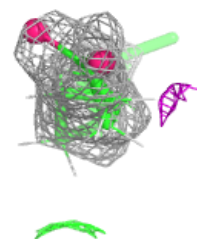
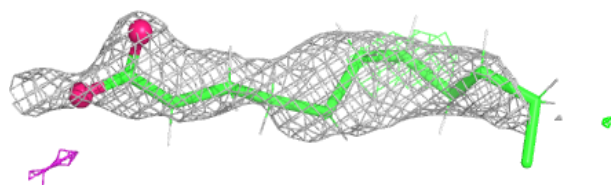
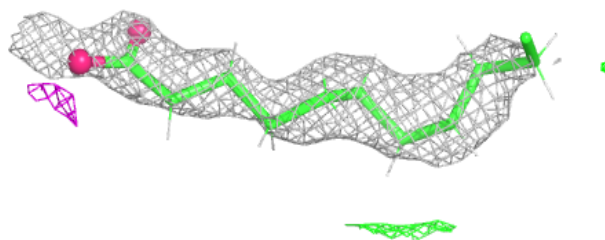


Electron density around STE z 101:

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

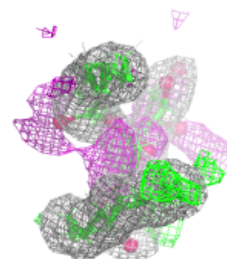
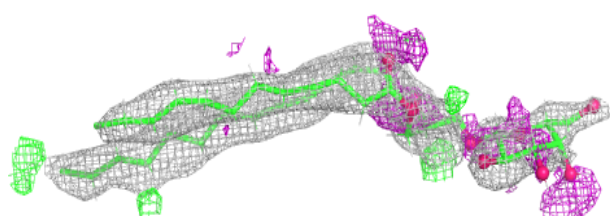
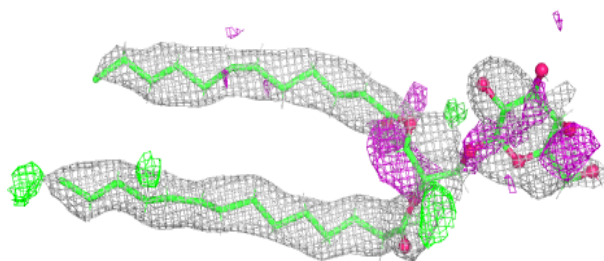
**Electron density around STE e 104:**

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

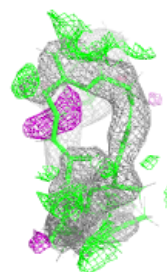
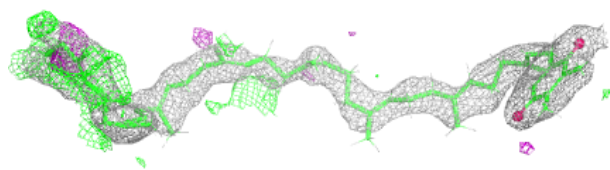
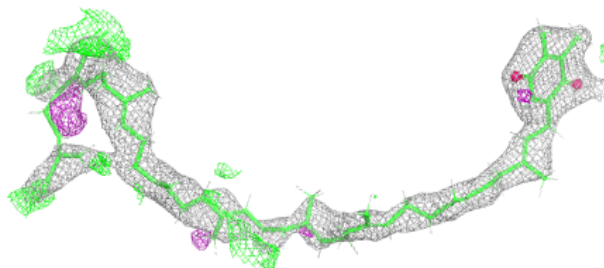


Electron density around LMG B 620:

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

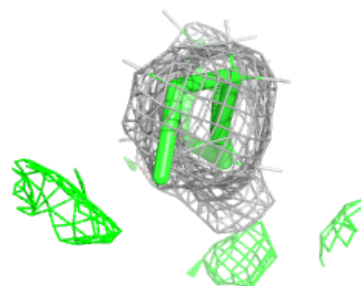
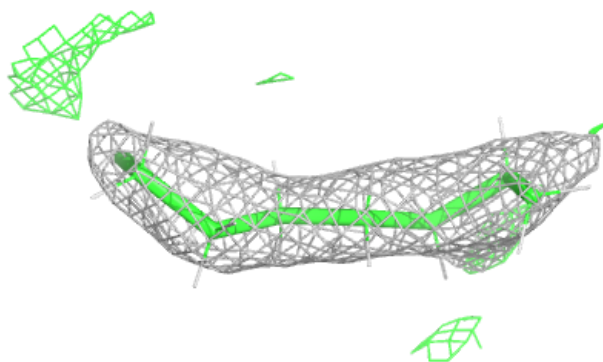
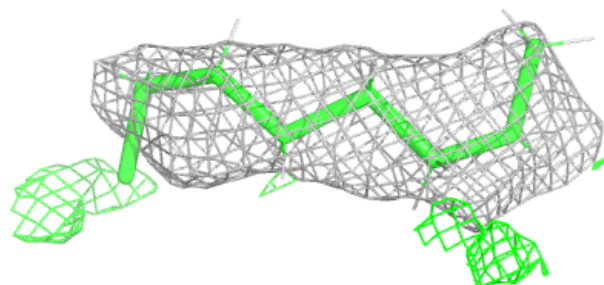
**Electron density around PL9 a 610:**

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

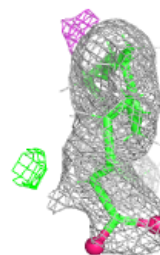
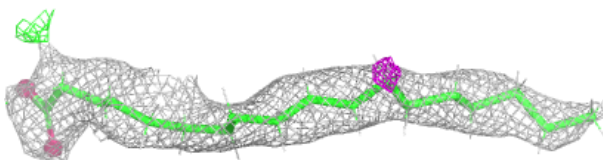
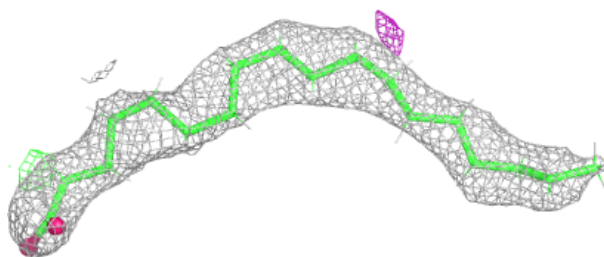


Electron density around STE f 103:

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

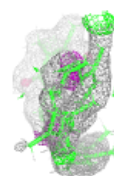
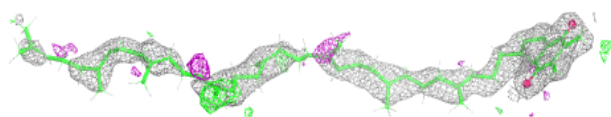
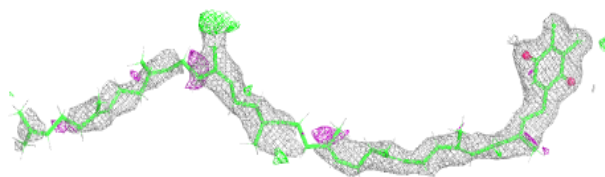
**Electron density around STE d 411:**

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

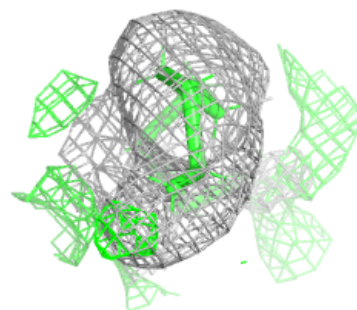
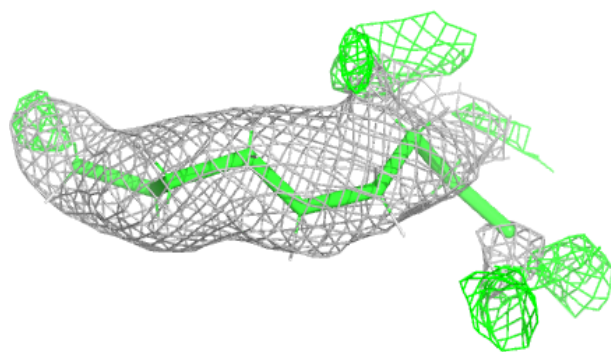
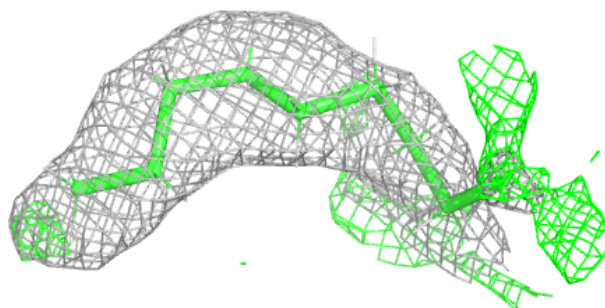


Electron density around PL9 A 610:

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

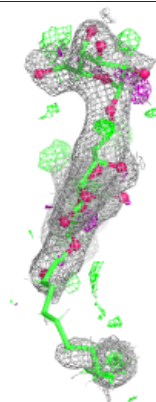
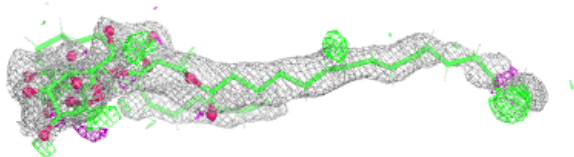
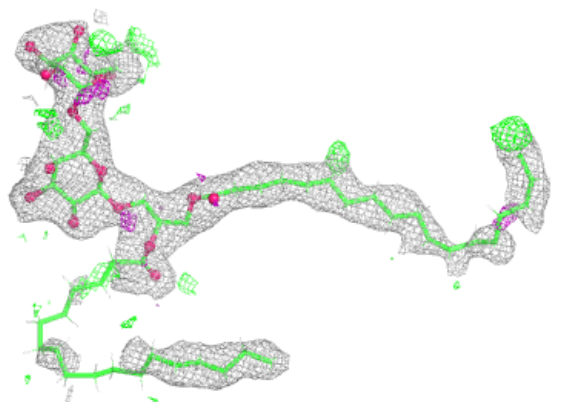
**Electron density around STE H 104:**

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

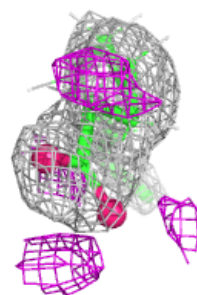
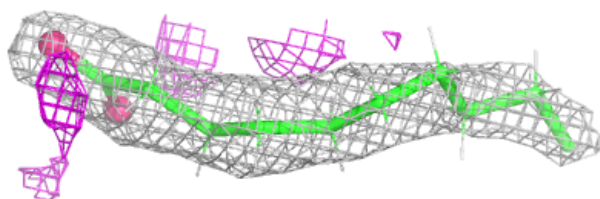
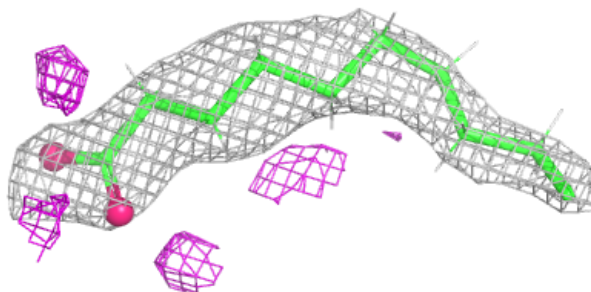


Electron density around DGD A 615:

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

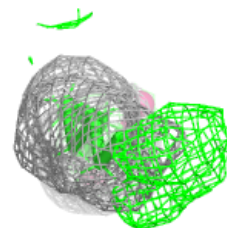
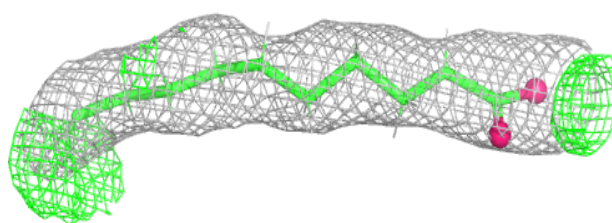
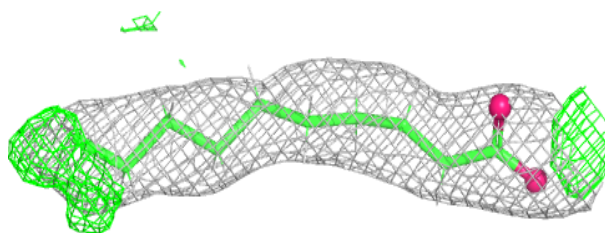
**Electron density around STE B 624:**

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

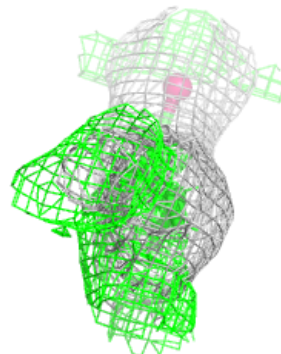
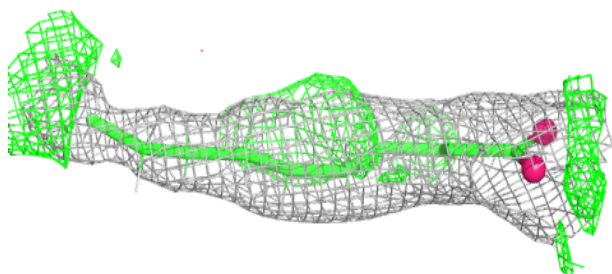
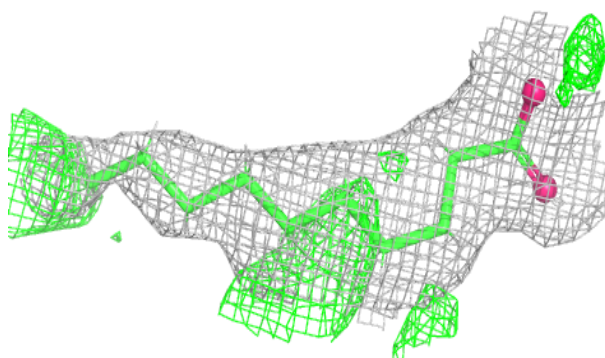


Electron density around STE j 101:

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

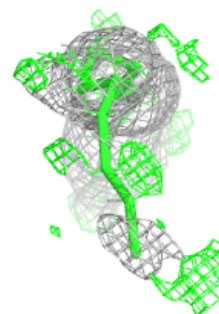
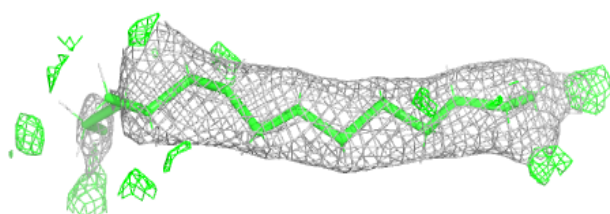
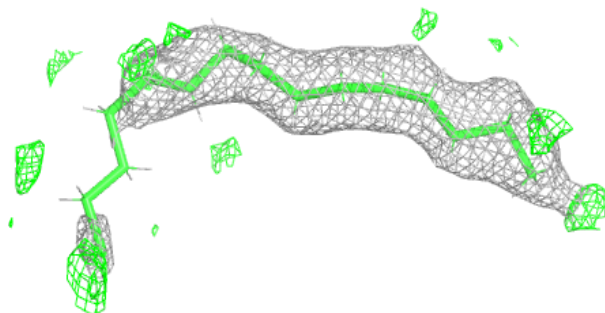
**Electron density around STE C 526:**

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

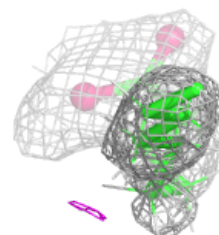
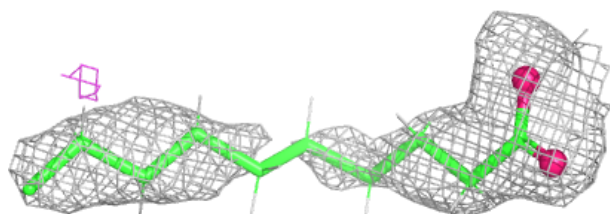
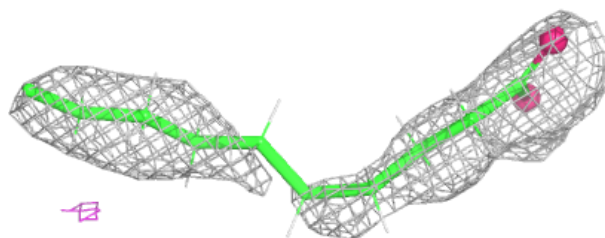


Electron density around STE M 104:

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

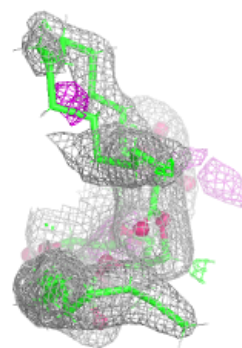
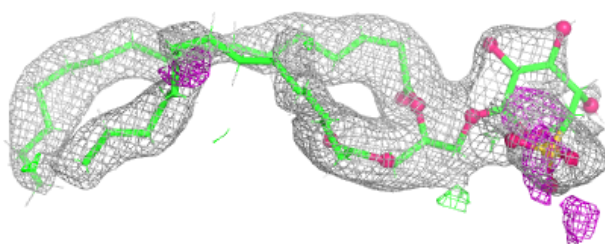
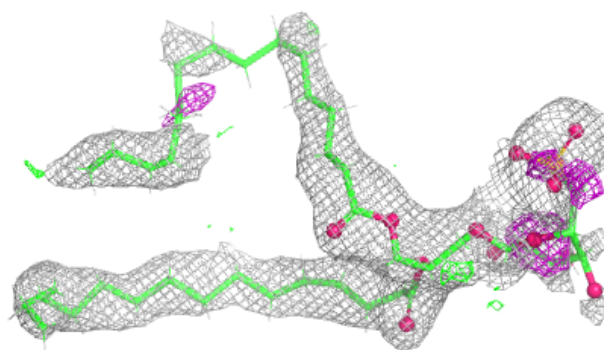
**Electron density around STE R 101:**

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

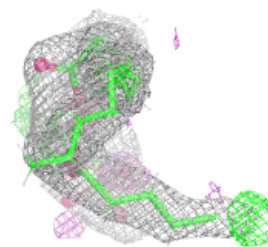
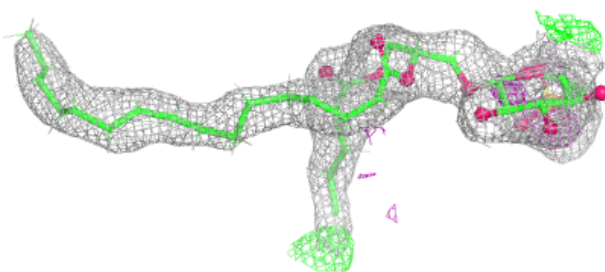
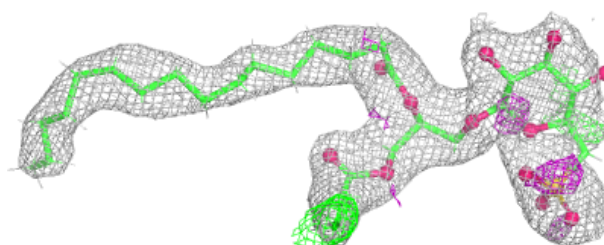


Electron density around SQD a 613:

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

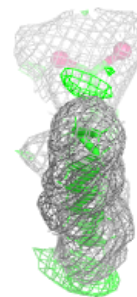
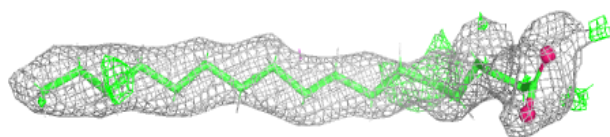
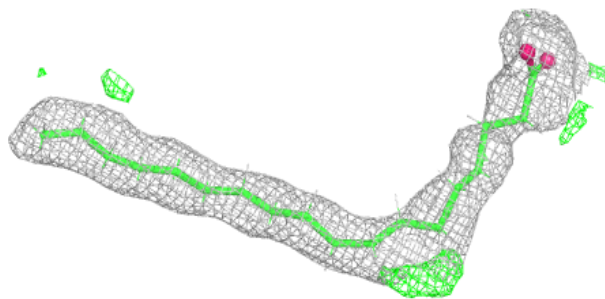
**Electron density around SQD A 614:**

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

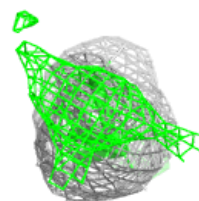
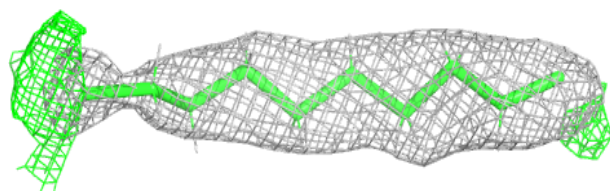
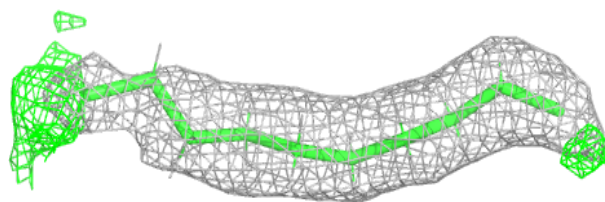


Electron density around STE d 407:

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

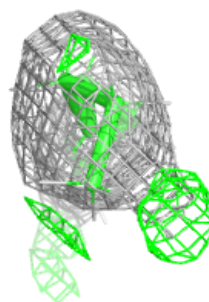
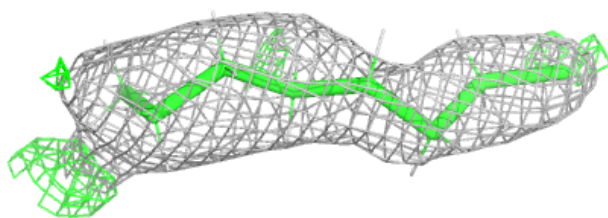
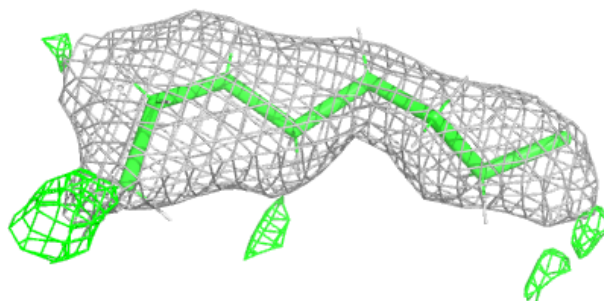
**Electron density around STE M 103:**

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

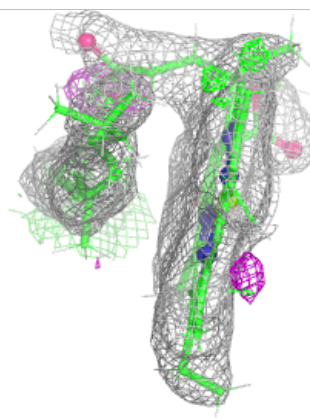
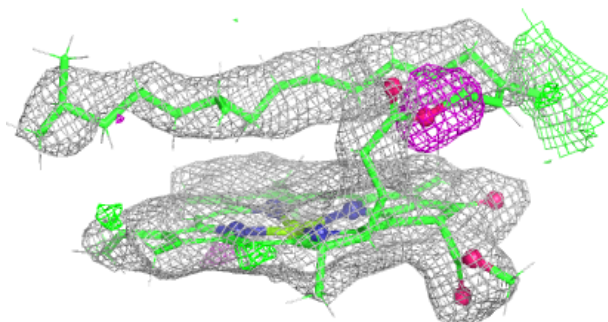
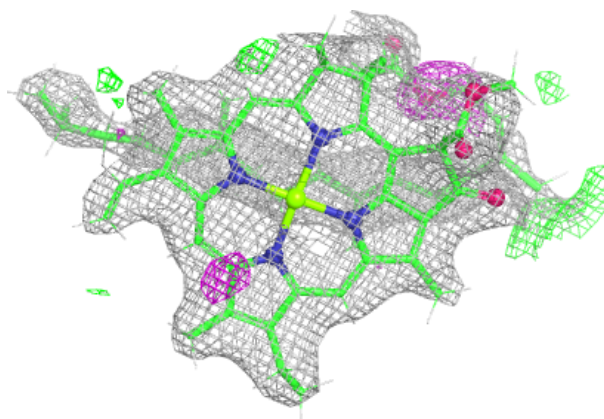


Electron density around STE A 616:

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

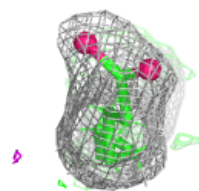
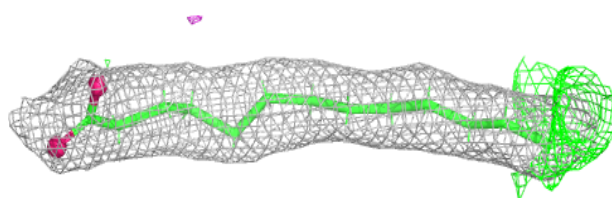
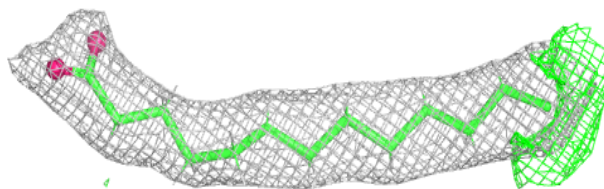
**Electron density around CLA b 601:**

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

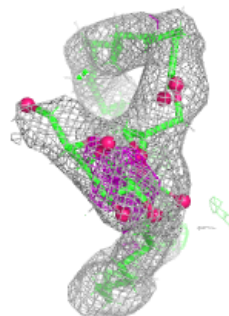
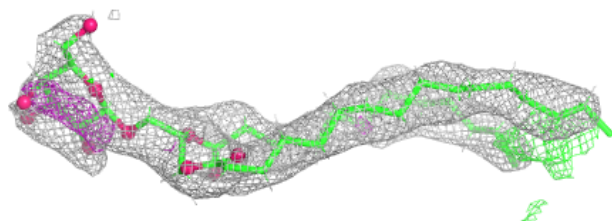
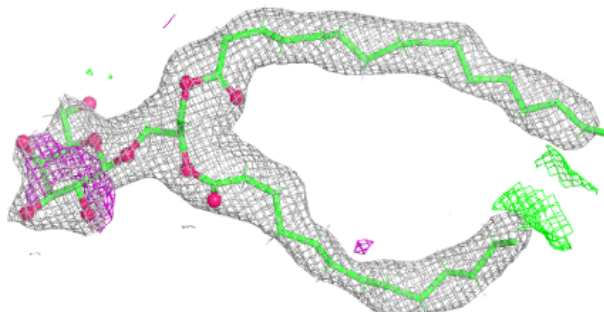


Electron density around STE M 102:

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

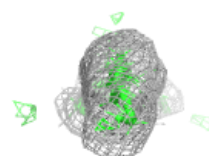
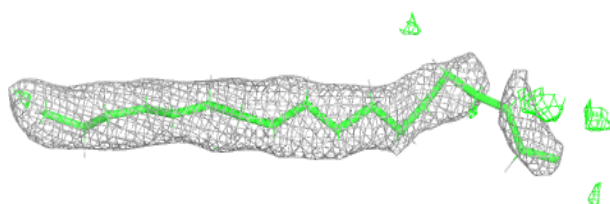
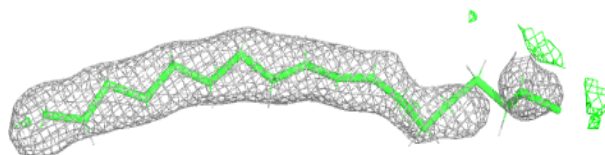
**Electron density around LMG C 521:**

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

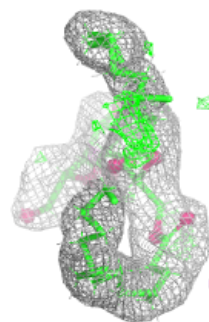
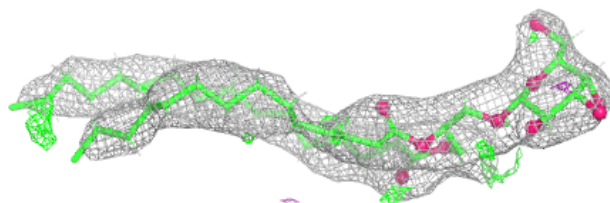
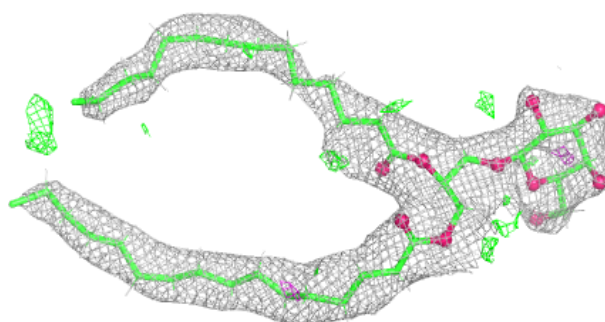


Electron density around STE m 103:

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

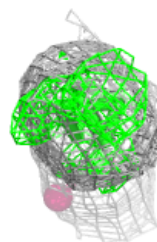
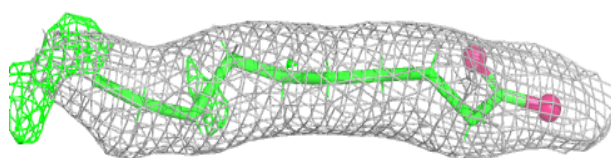
**Electron density around LMG a 615:**

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

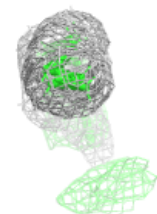
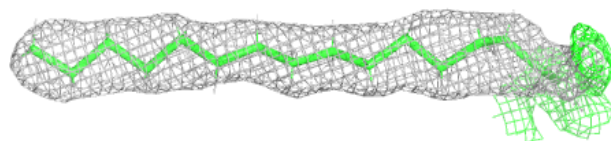
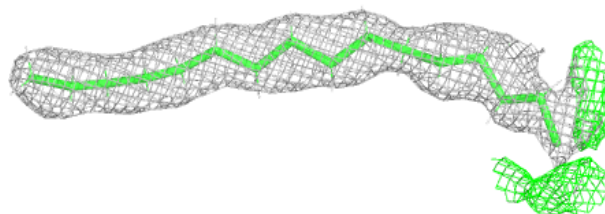


Electron density around STE J 101:

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

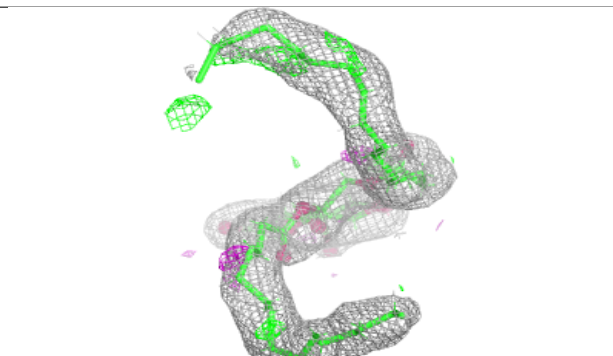
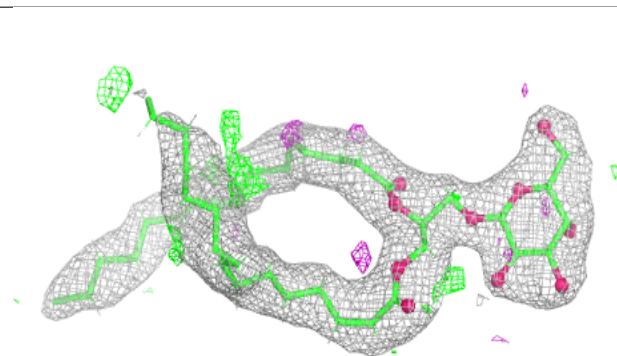
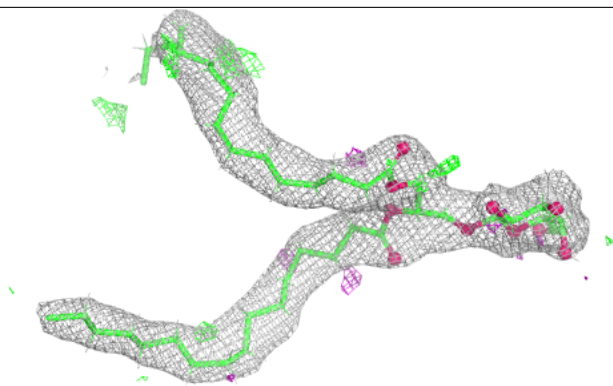
**Electron density around STE C 527:**

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

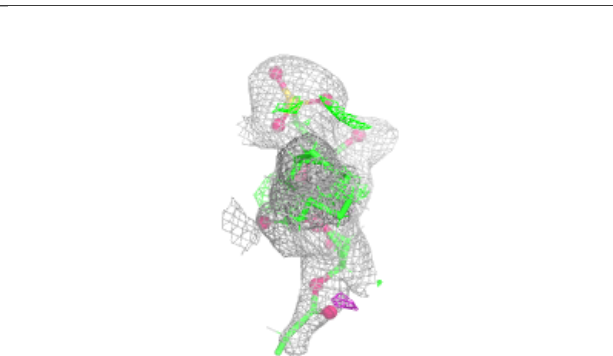
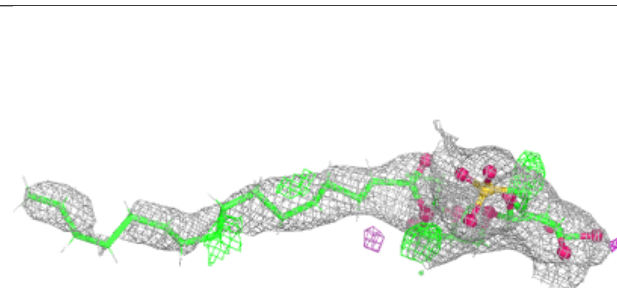
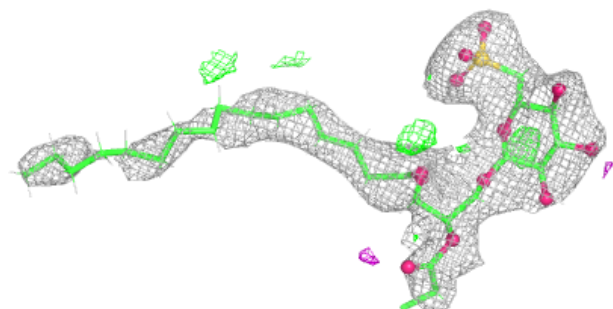


Electron density around LMG M 101:

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

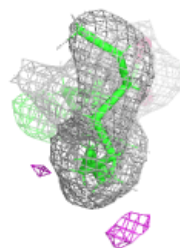
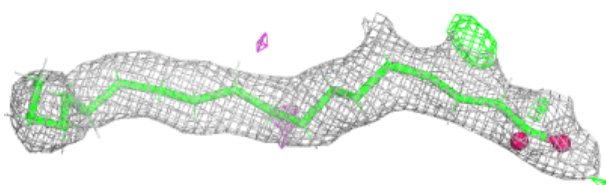
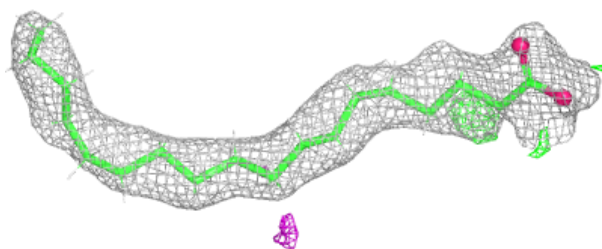
**Electron density around SQD f 102:**

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

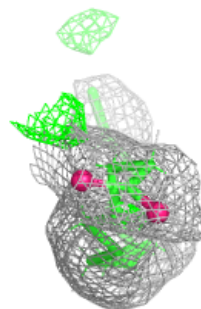
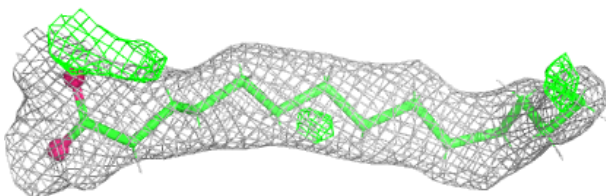
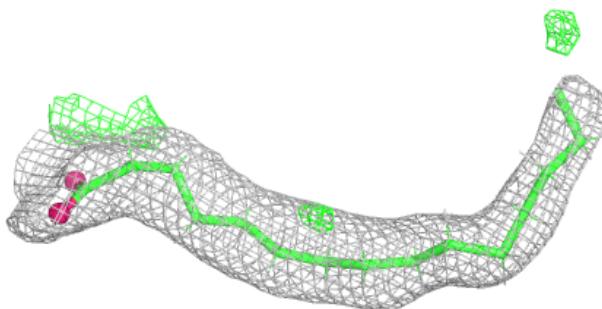


Electron density around STE b 621:

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

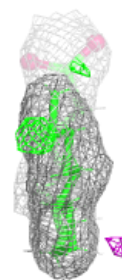
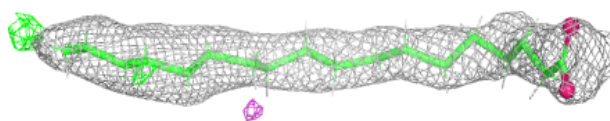
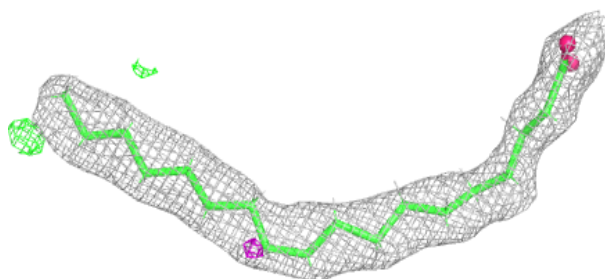
**Electron density around STE B 621:**

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

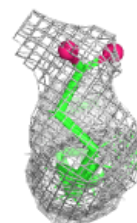
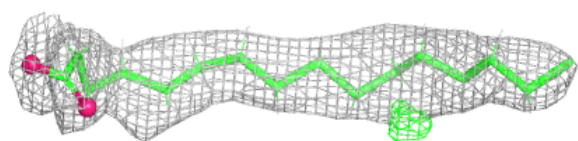
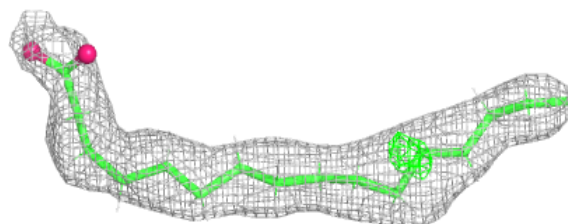


Electron density around STE d 413:

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

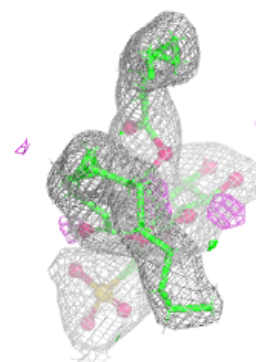
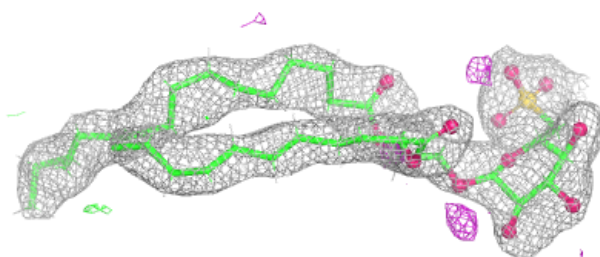
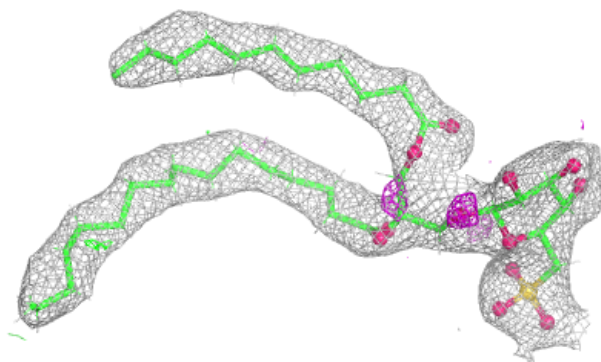
**Electron density around STE B 623:**

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

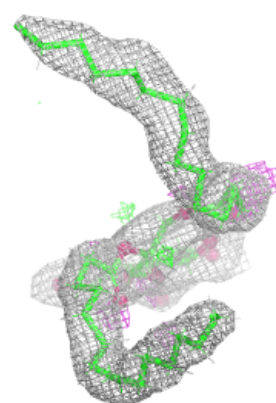
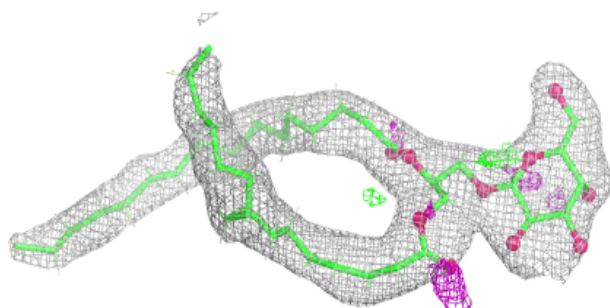
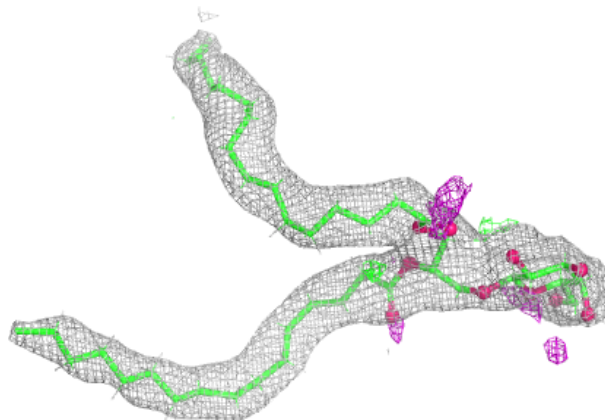


Electron density around SQD b 620:

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

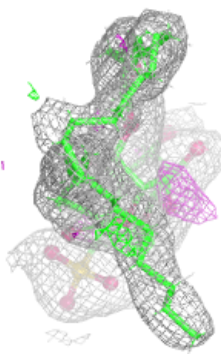
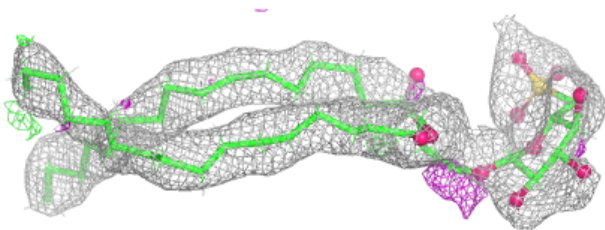
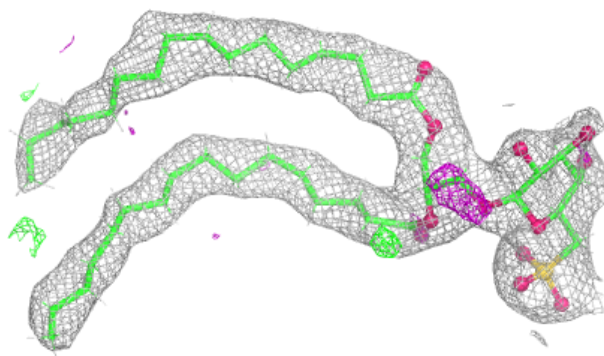
**Electron density around LMG m 101:**

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

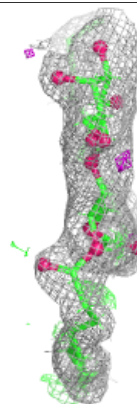
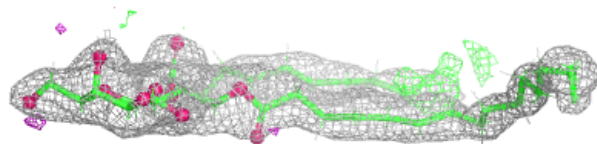
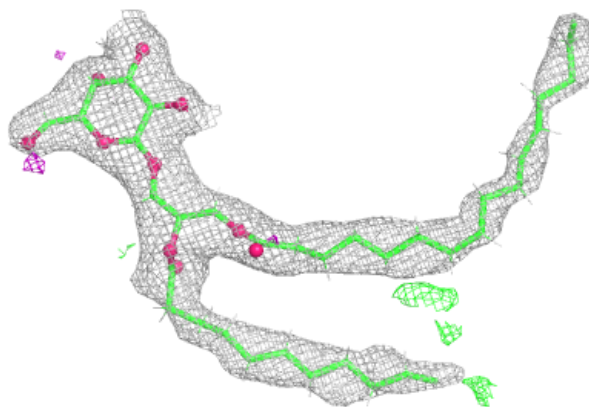


Electron density around SQD B 622:

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

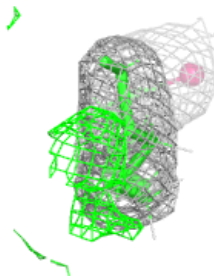
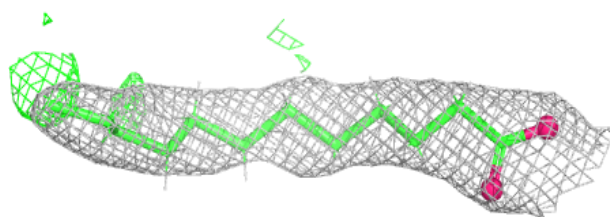
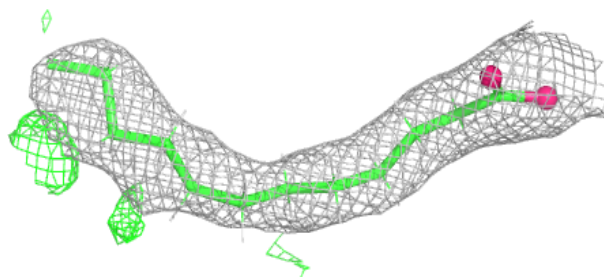
**Electron density around LMG c 522:**

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

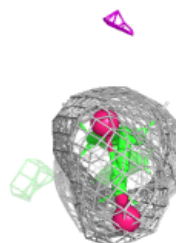
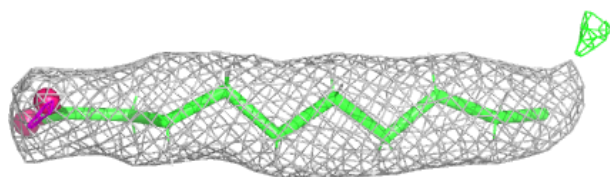
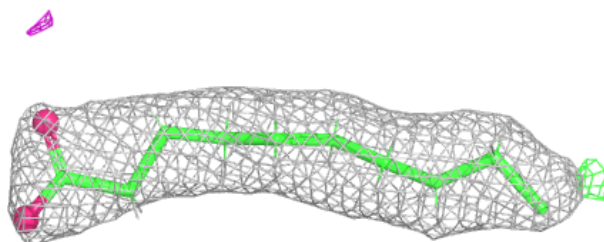


Electron density around STE t 102:

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

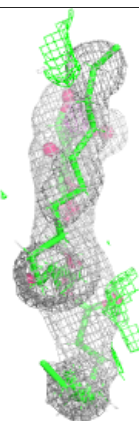
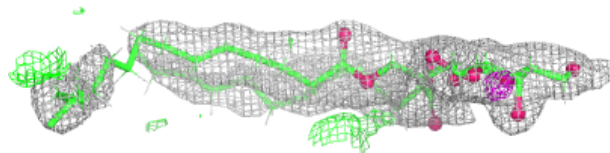
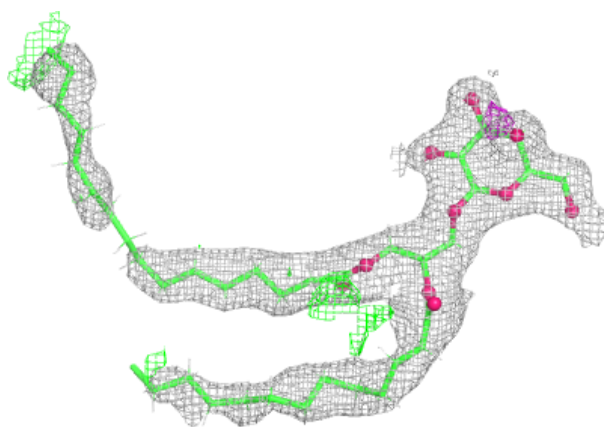
**Electron density around STE m 102:**

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

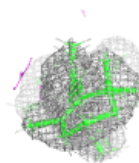
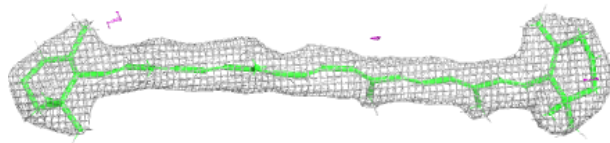
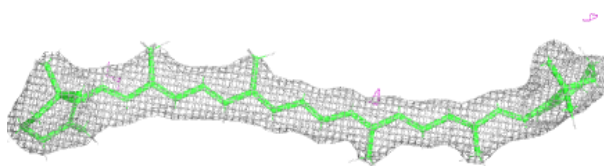


Electron density around LMG C 525:

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

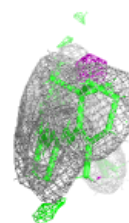
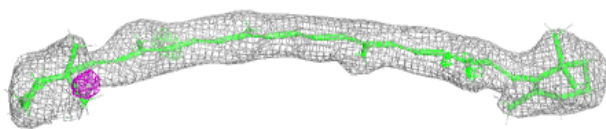
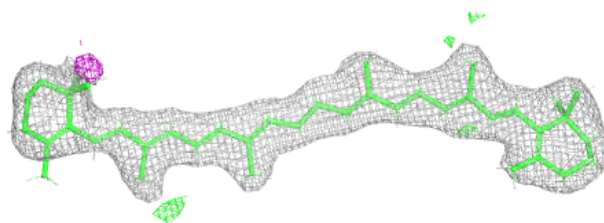
**Electron density around BCR C 514:**

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



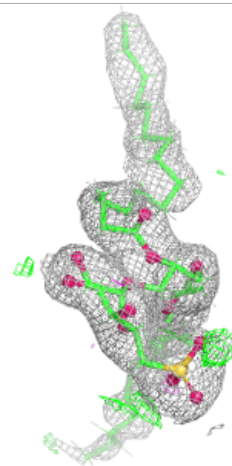
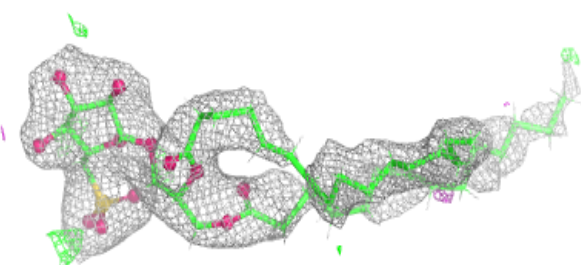
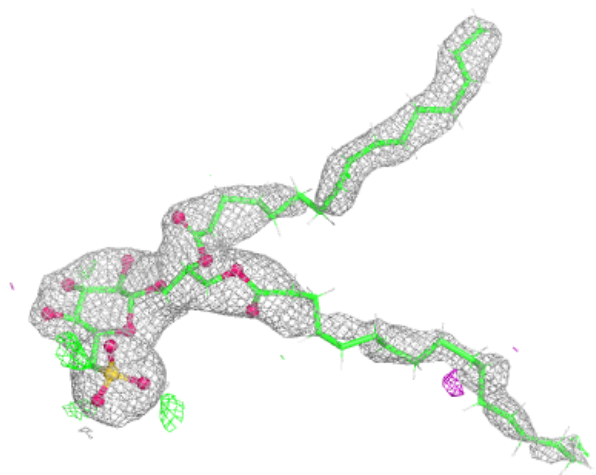
Electron density around BCR d 405:

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



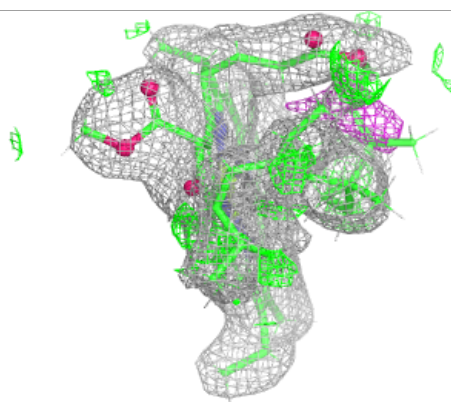
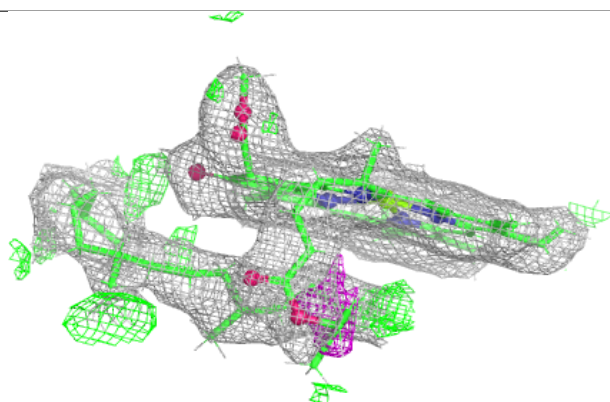
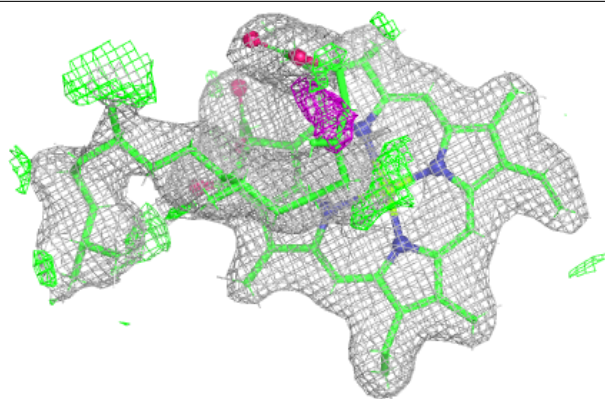
Electron density around SQD a 612:

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

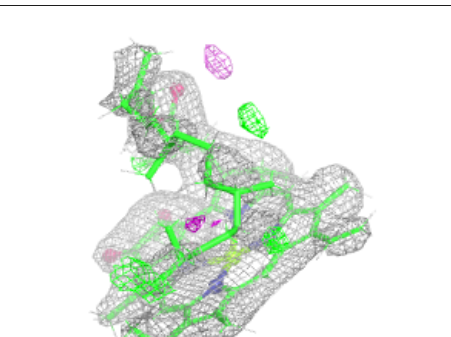
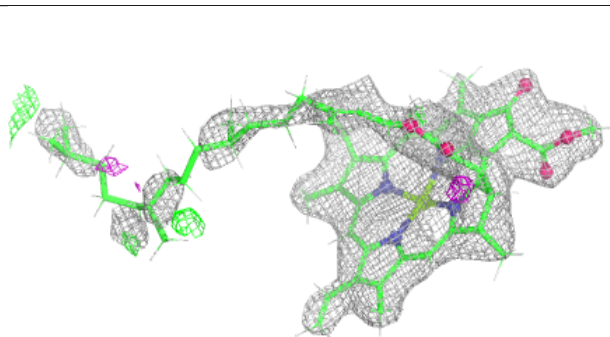
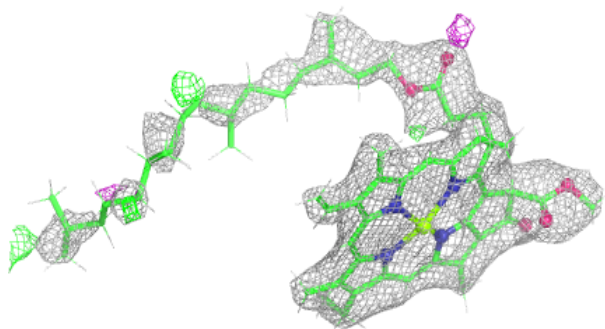


Electron density around CLA B 601:

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

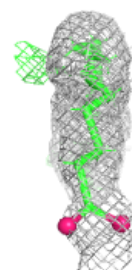
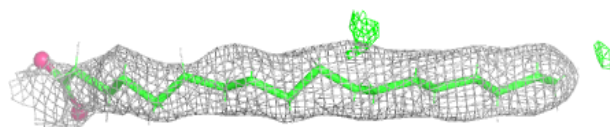
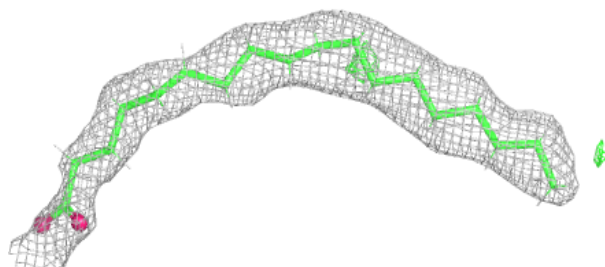
**Electron density around CLA c 513:**

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

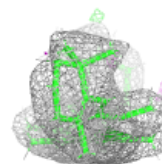
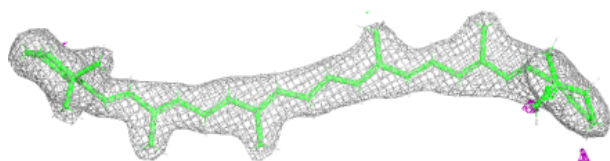
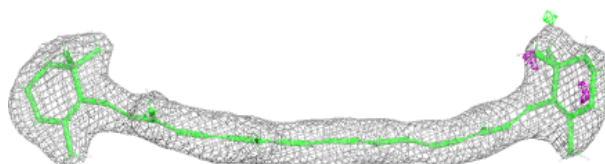


Electron density around STE D 414:

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

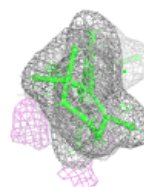
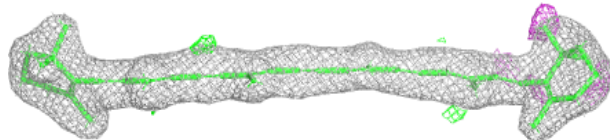
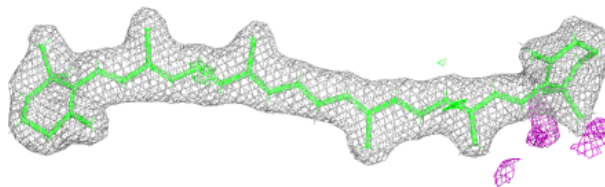
**Electron density around BCR k 102:**

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



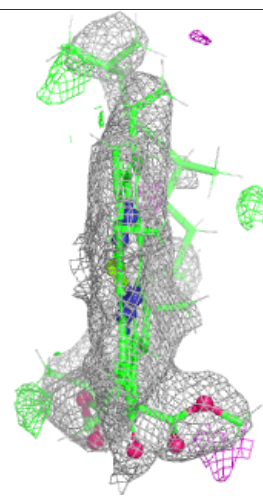
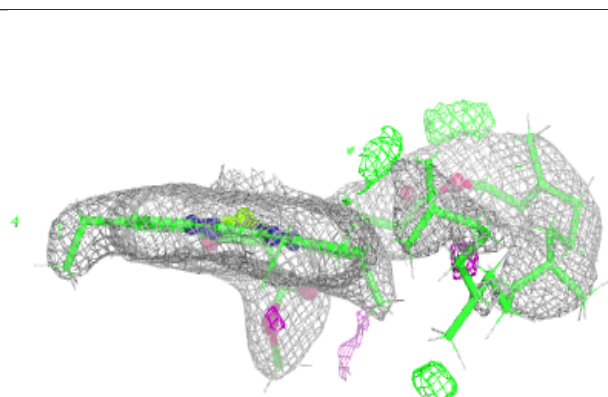
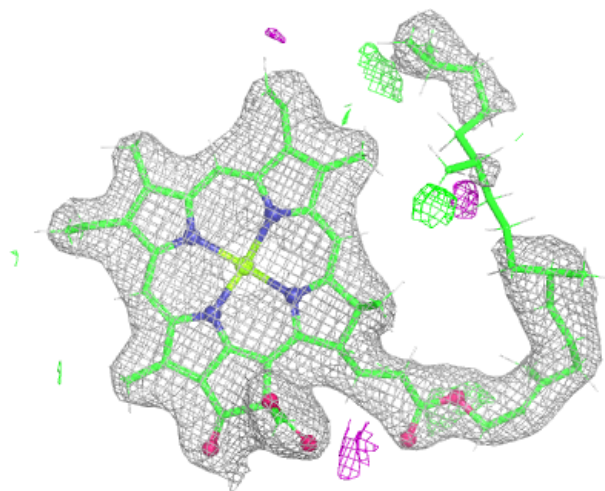
Electron density around BCR B 618:

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



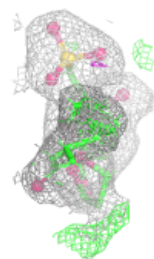
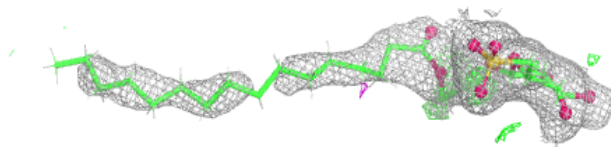
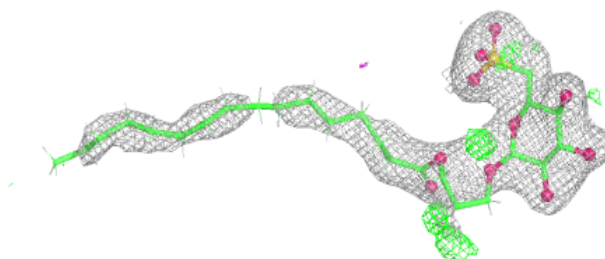
Electron density around CLA c 512:

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



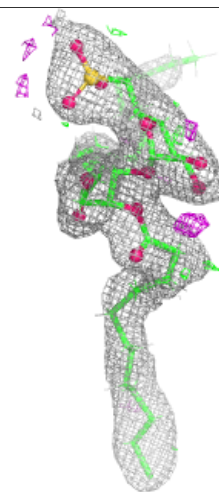
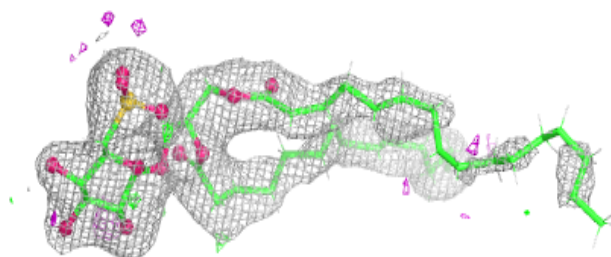
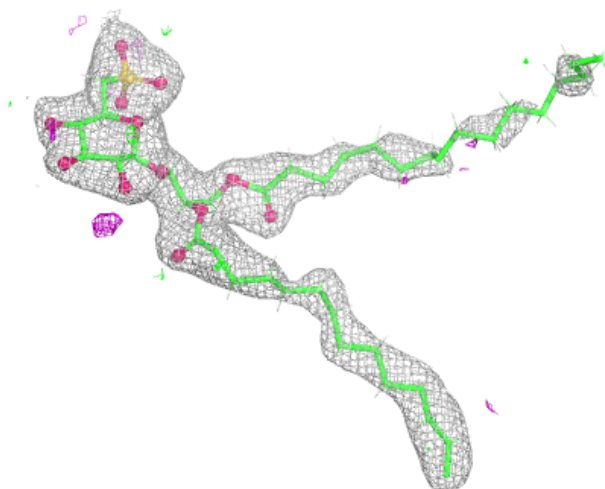
Electron density around SQD D 409:

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



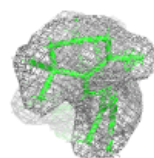
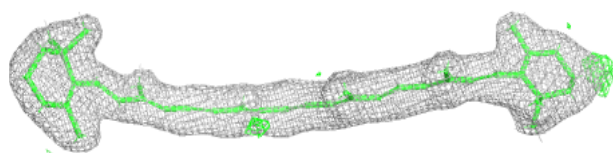
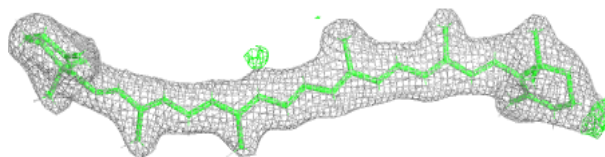
Electron density around SQD D 412:

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

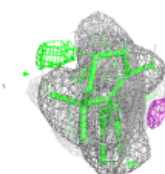
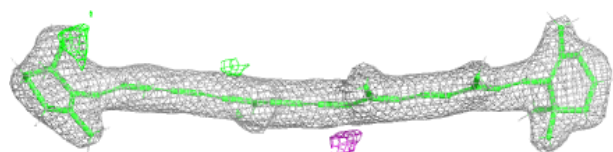
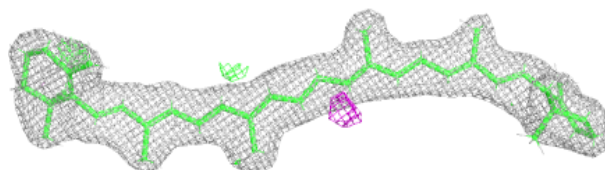


Electron density around BCR H 101:

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

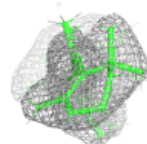
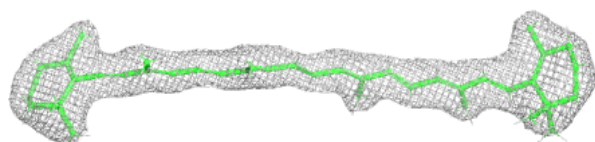
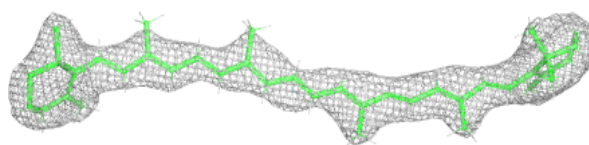
**Electron density around BCR K 101:**

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

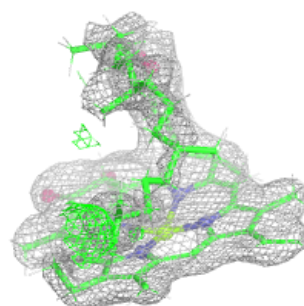
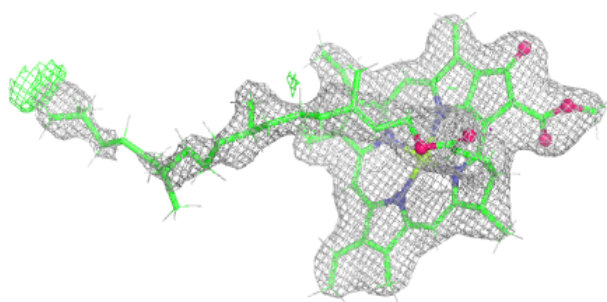
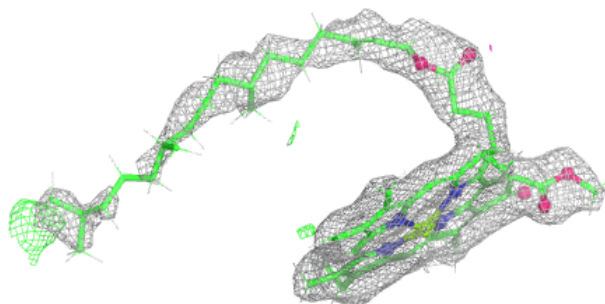


Electron density around BCR c 514:

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

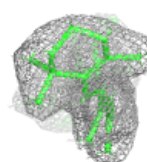
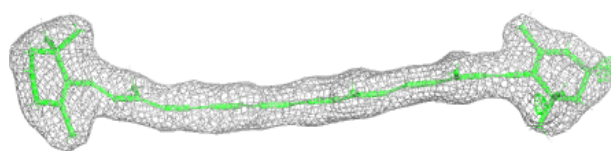
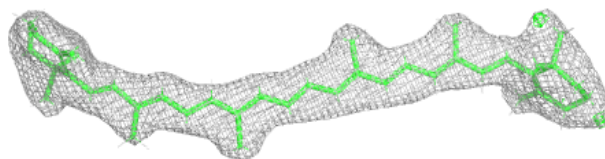
**Electron density around CLA C 513:**

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

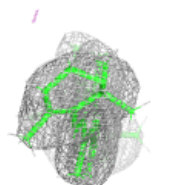
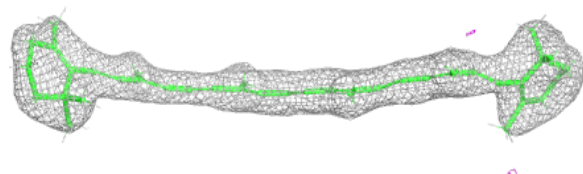
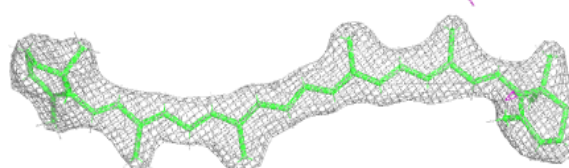


Electron density around BCR h 101:

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

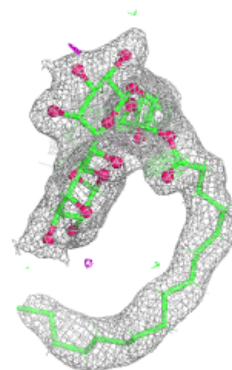
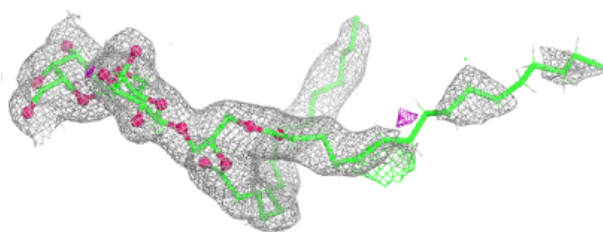
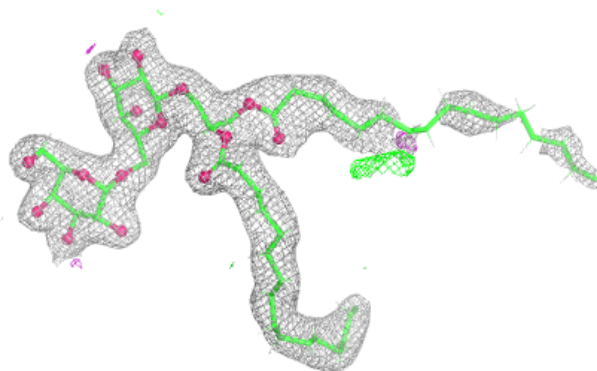
**Electron density around BCR k 101:**

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

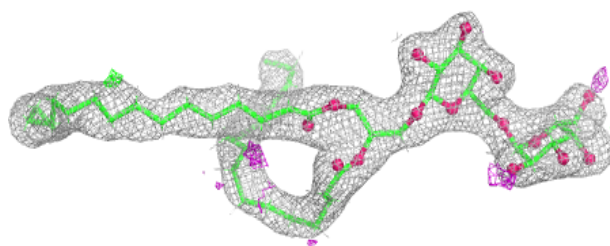
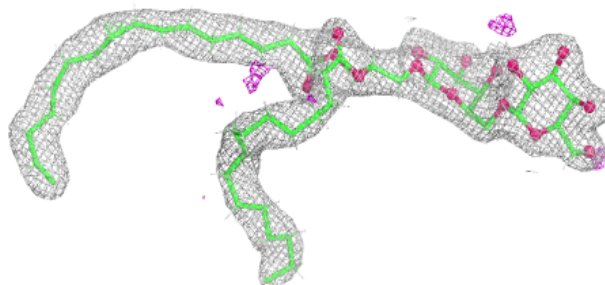


Electron density around DGD c 520:

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

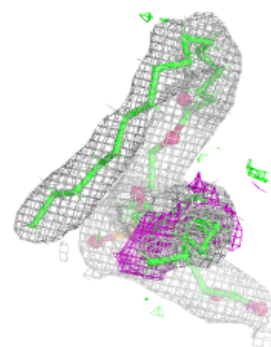
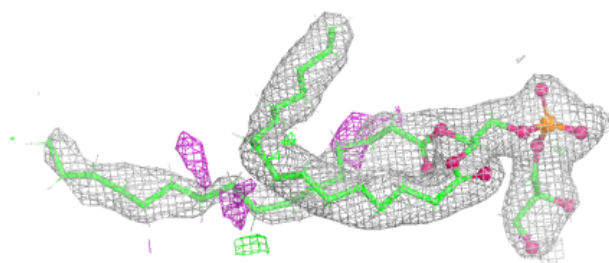
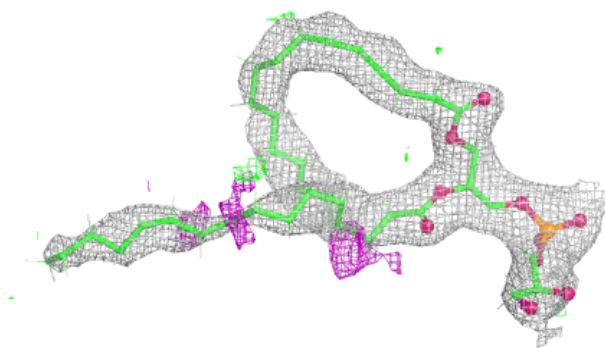
**Electron density around DGD h 102:**

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

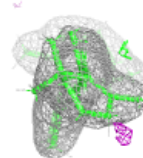
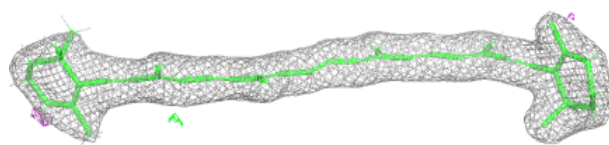
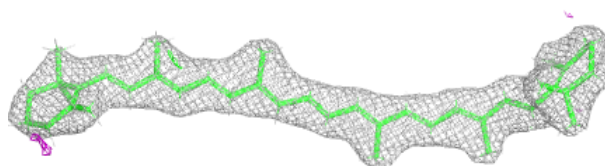


Electron density around LHG d 408:

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

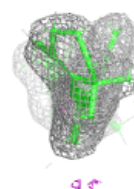
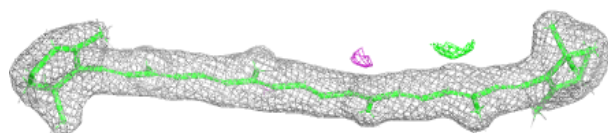
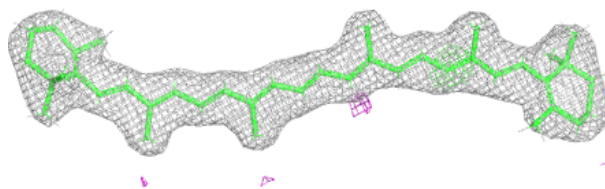
**Electron density around BCR c 515:**

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



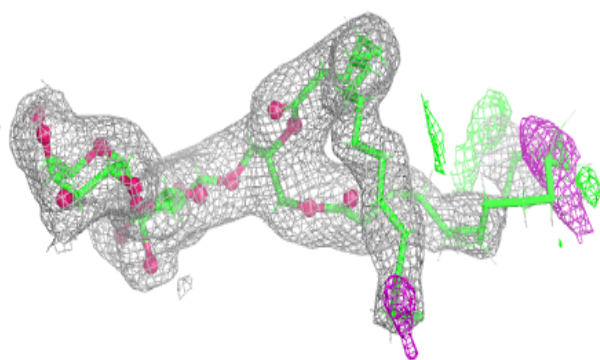
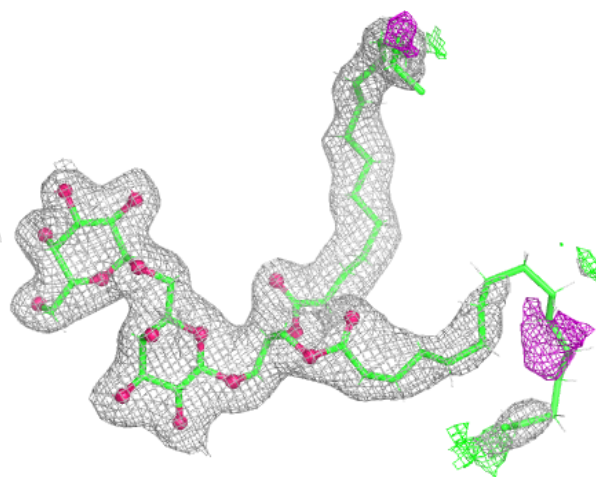
Electron density around BCR b 619:

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



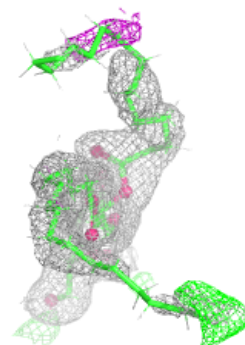
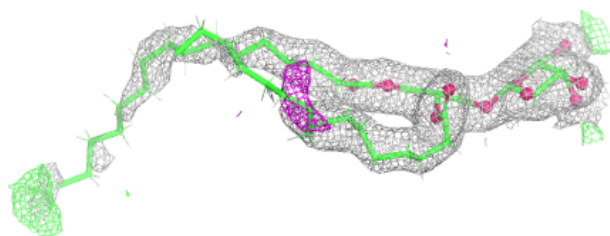
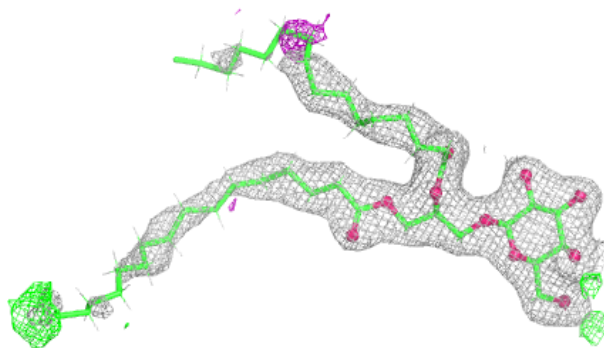
Electron density around DGD C 523:

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

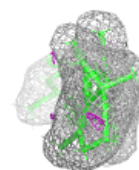
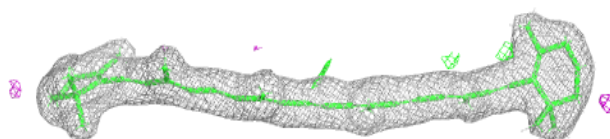
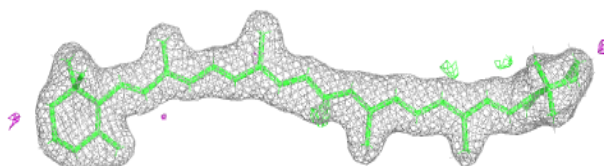


Electron density around LMG D 408:

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

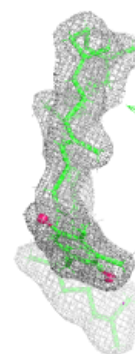
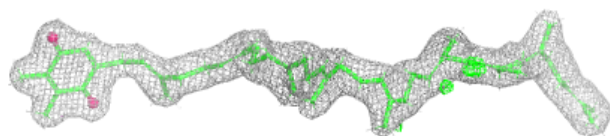
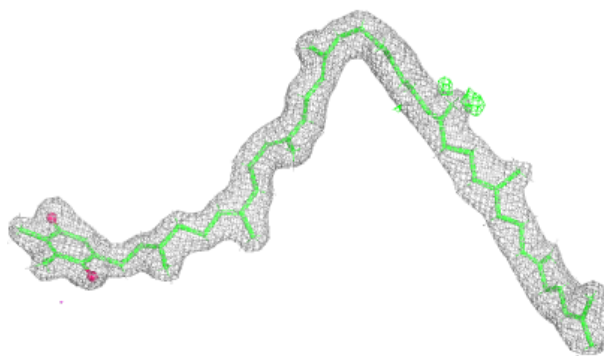
**Electron density around BCR B 617:**

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



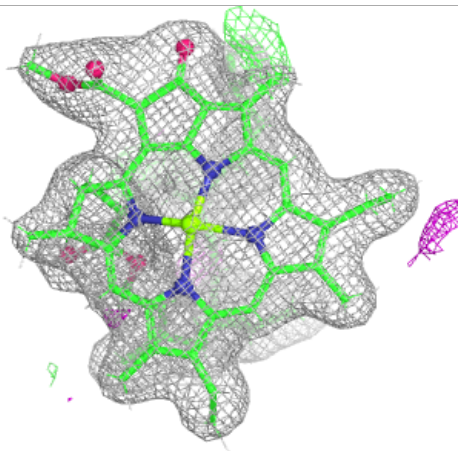
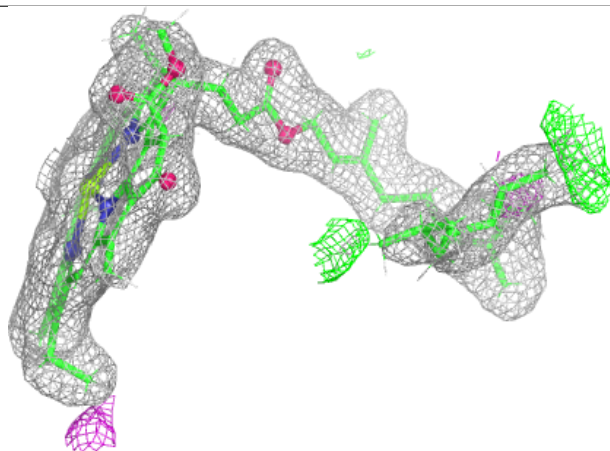
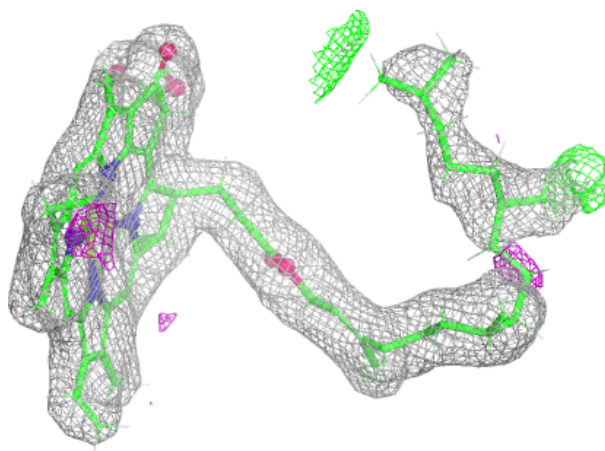
Electron density around PL9 d 406:

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



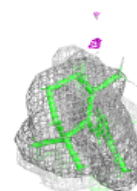
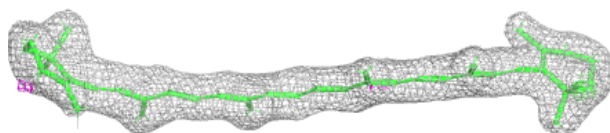
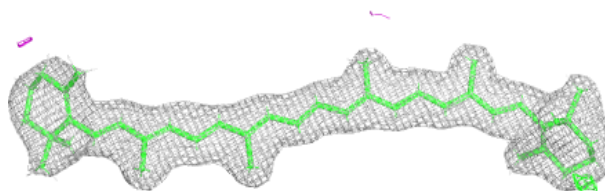
Electron density around CLA B 606:

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



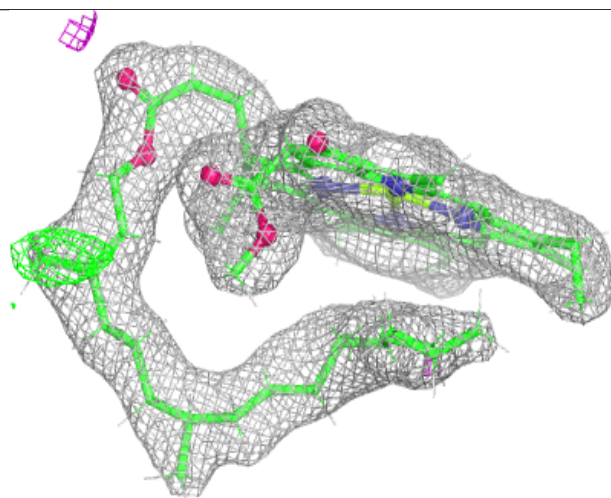
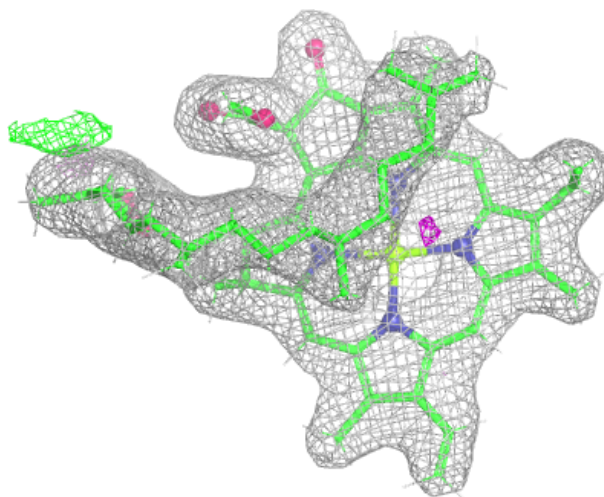
Electron density around BCR B 619:

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



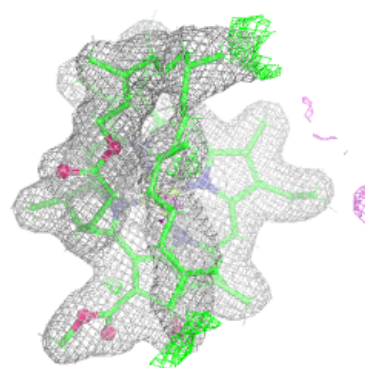
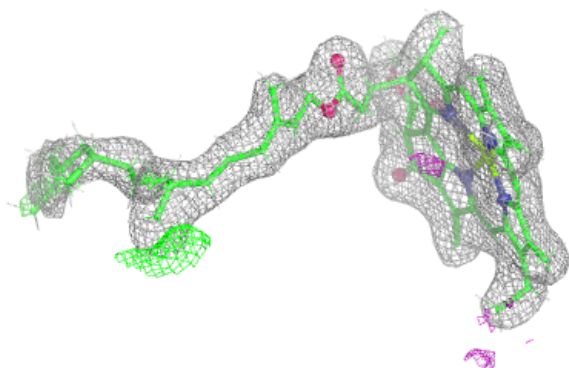
Electron density around CLA C 510:

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

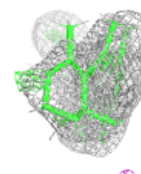
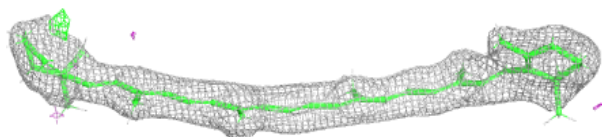
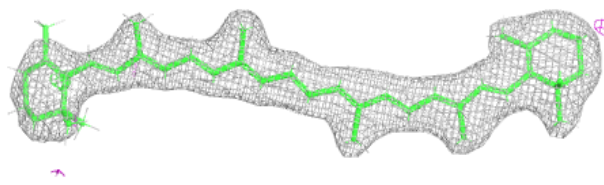


Electron density around CLA b 606:

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

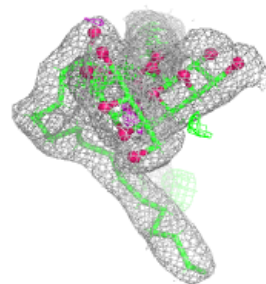
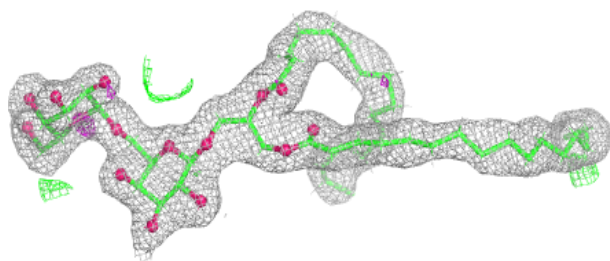
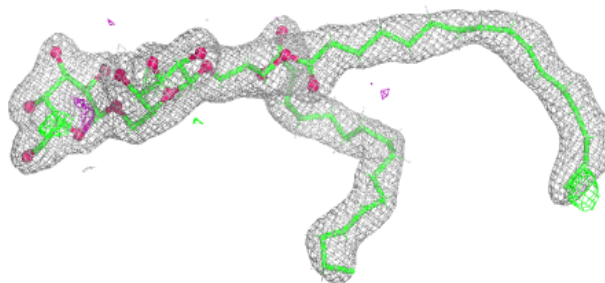
**Electron density around BCR D 405:**

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



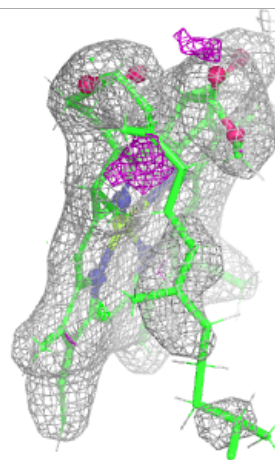
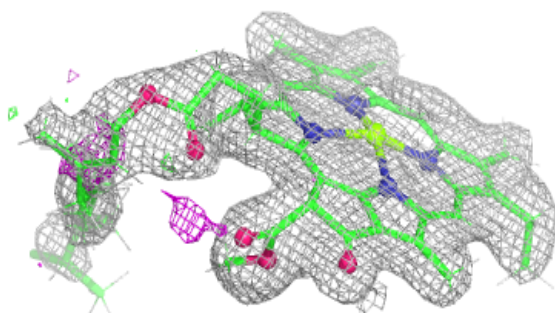
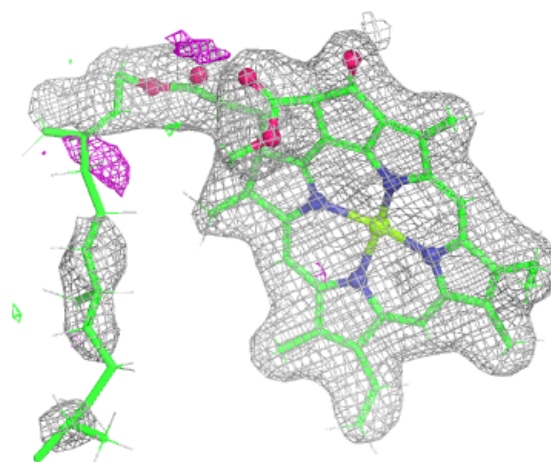
Electron density around DGD H 102:

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



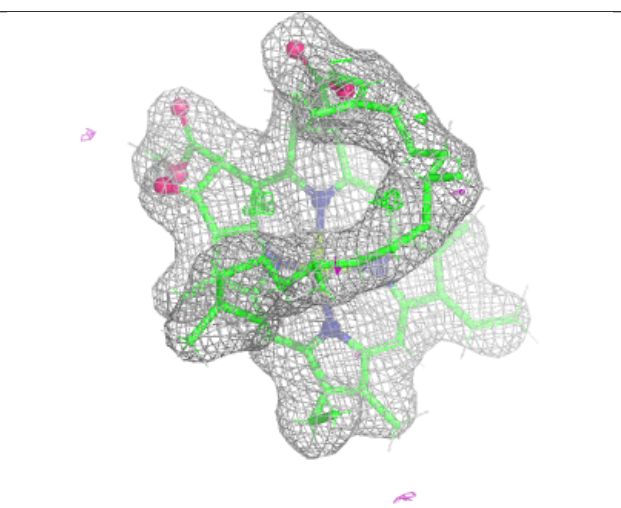
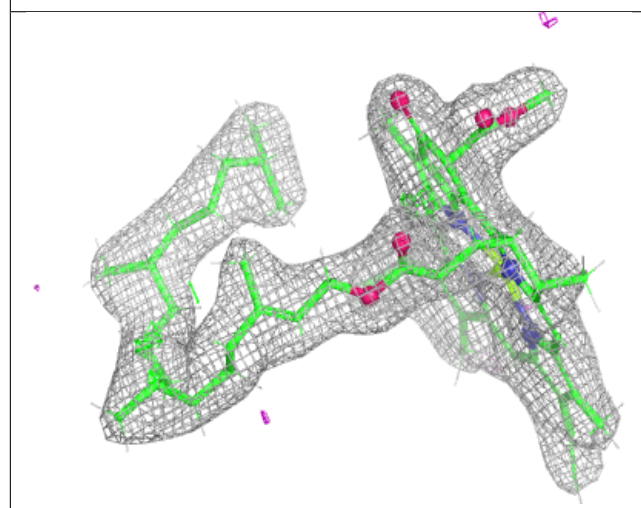
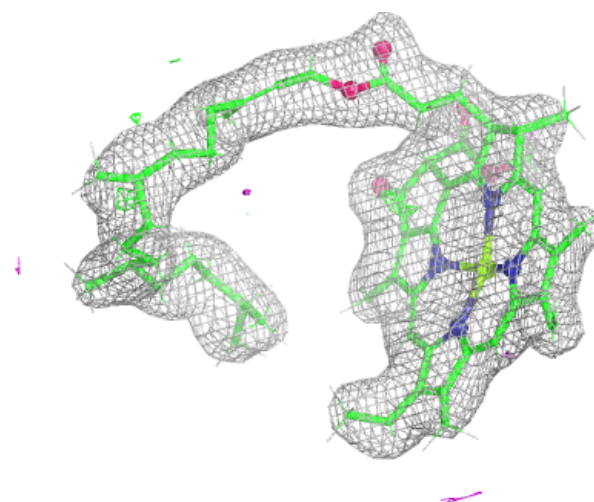
Electron density around CLA b 616:

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



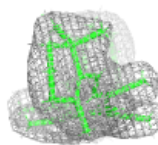
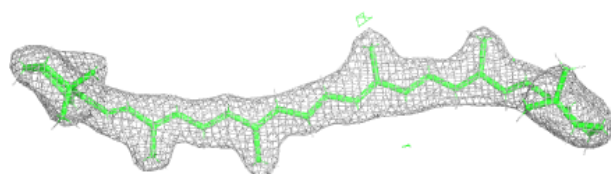
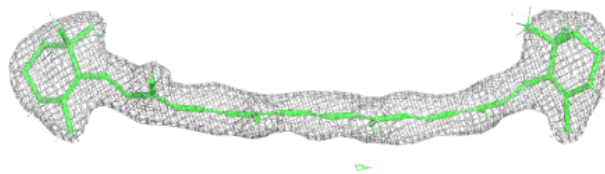
Electron density around CLA c 503:

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

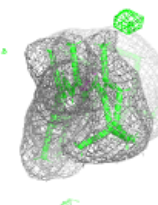
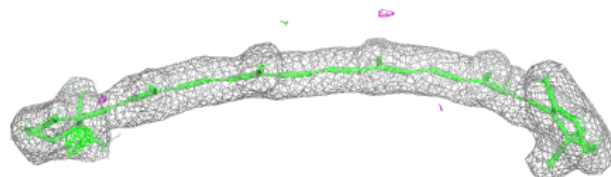
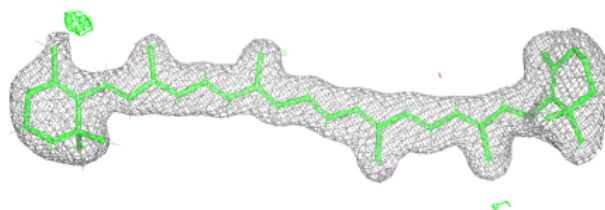


Electron density around BCR K 102:

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

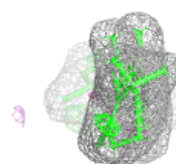
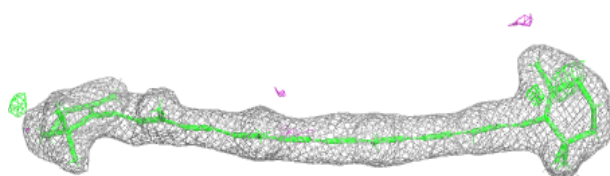
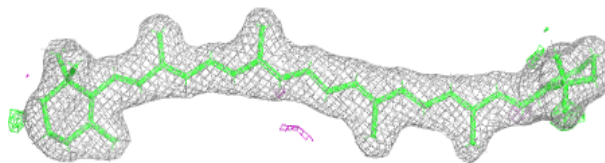
**Electron density around BCR T 101:**

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

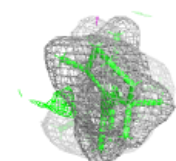
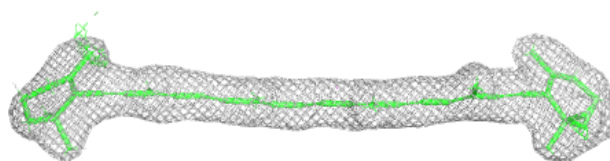
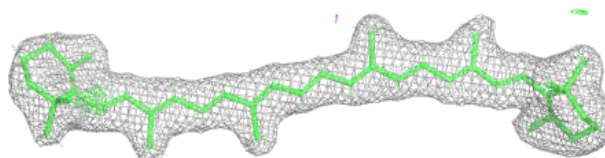


Electron density around BCR b 617:

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

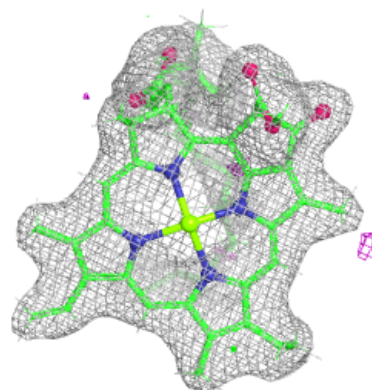
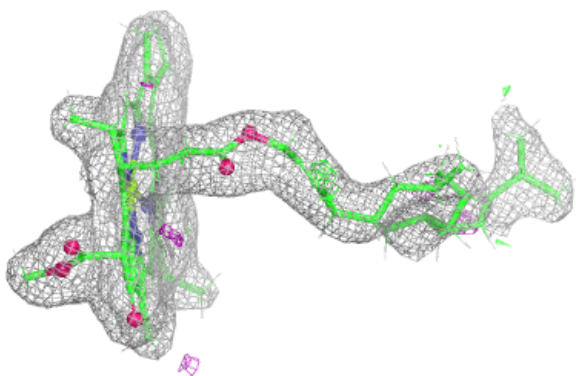
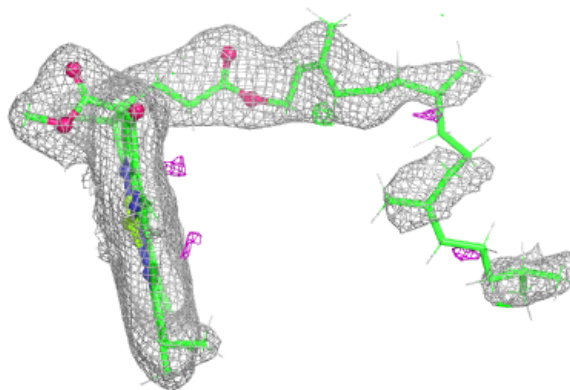
**Electron density around BCR b 618:**

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



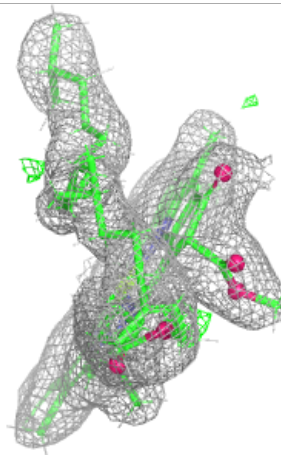
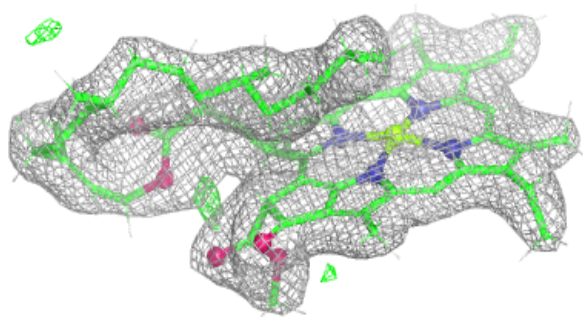
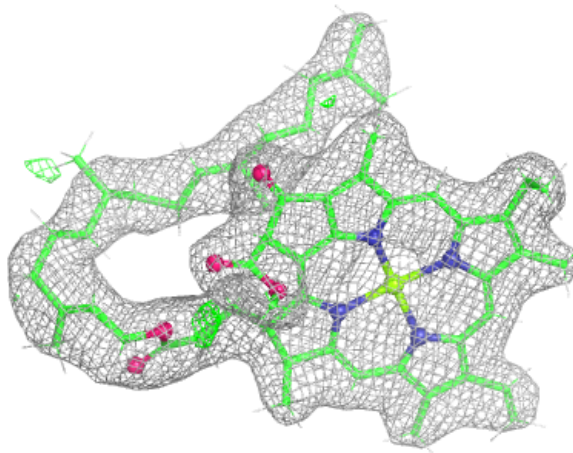
Electron density around CLA c 506:

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



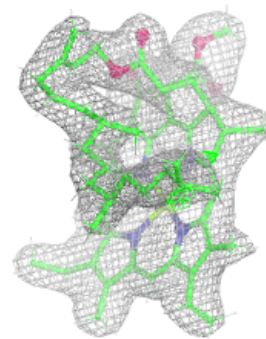
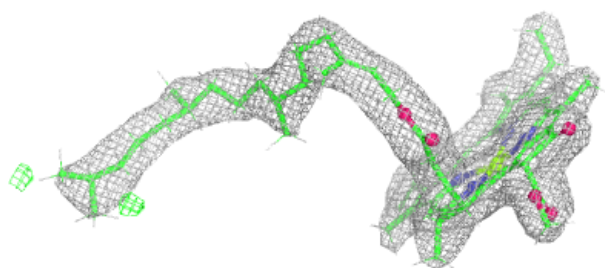
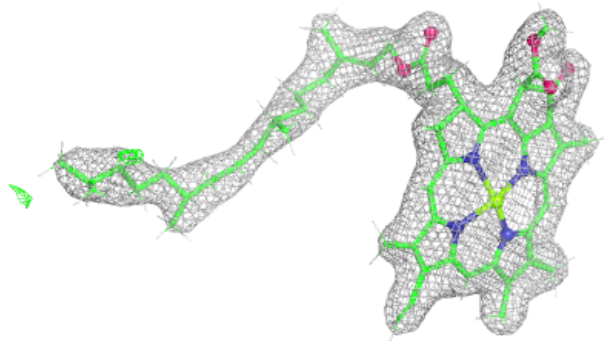
Electron density around CLA c 509:

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

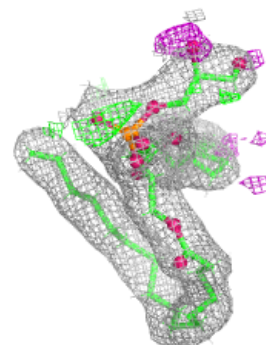
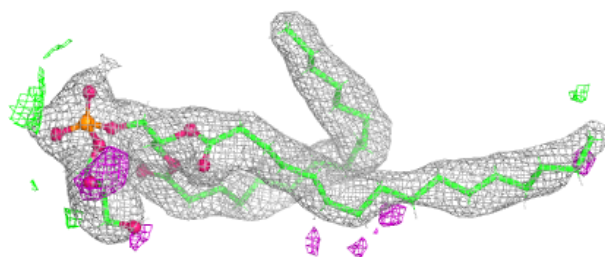
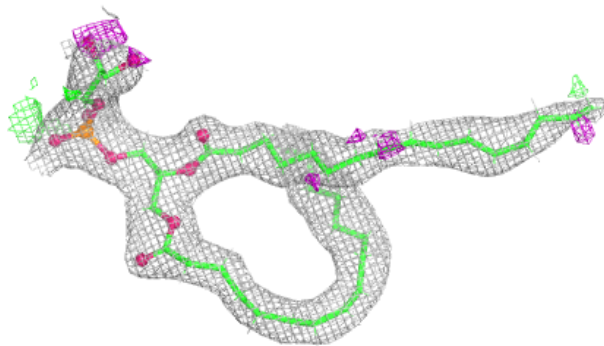


Electron density around CLA c 511:

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

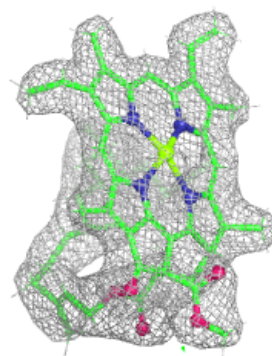
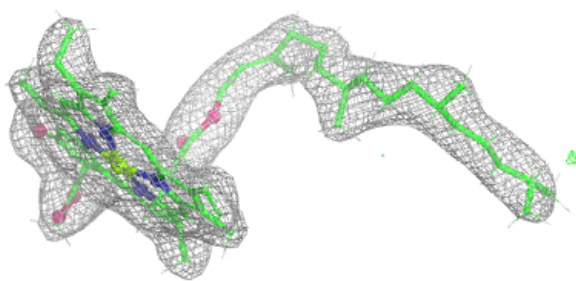
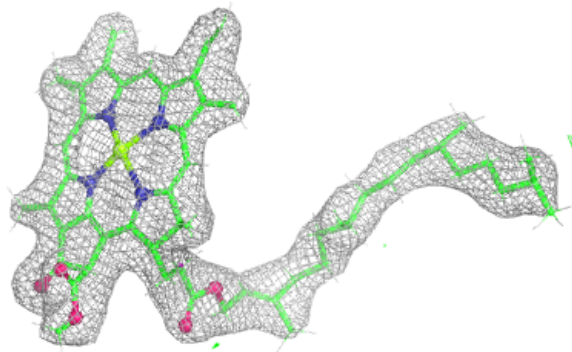
**Electron density around LHG D 413:**

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

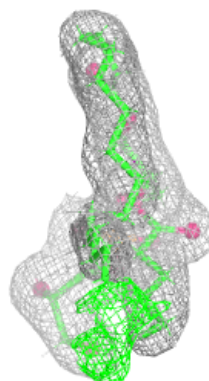
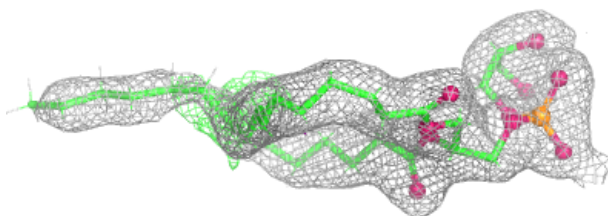
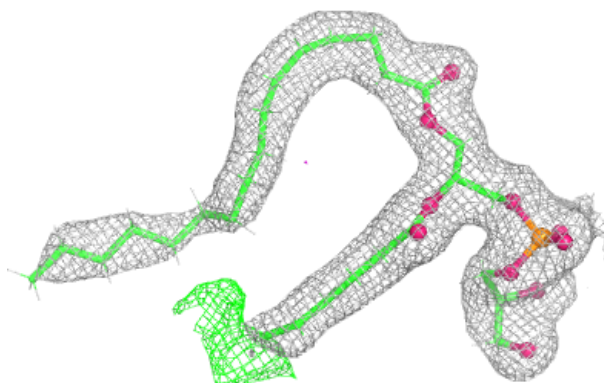


Electron density around CLA C 511:

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

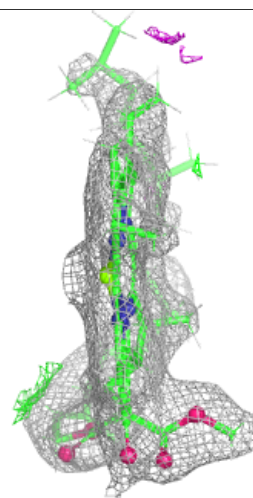
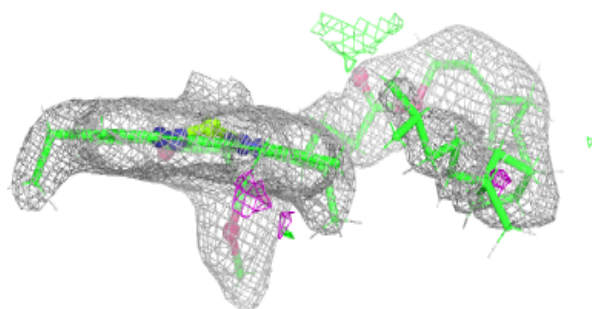
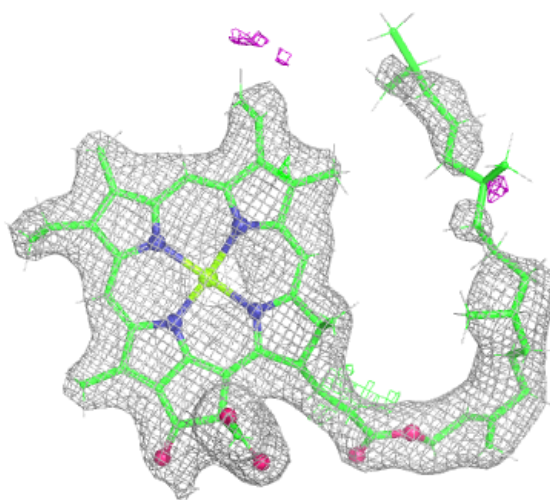
**Electron density around LHG d 410:**

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



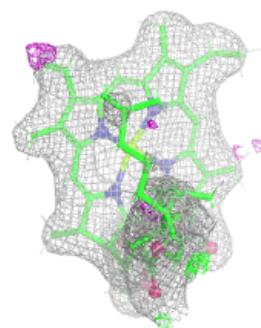
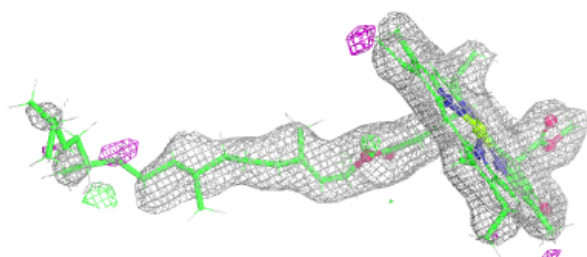
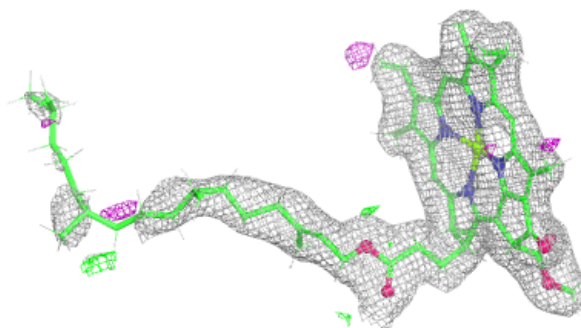
Electron density around CLA C 512:

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



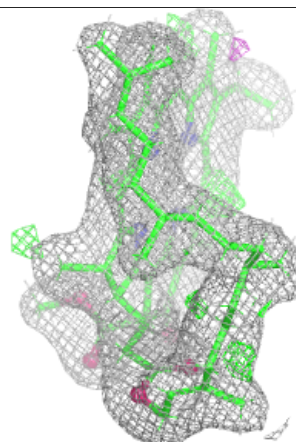
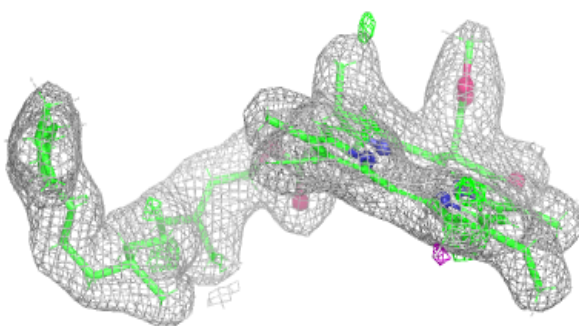
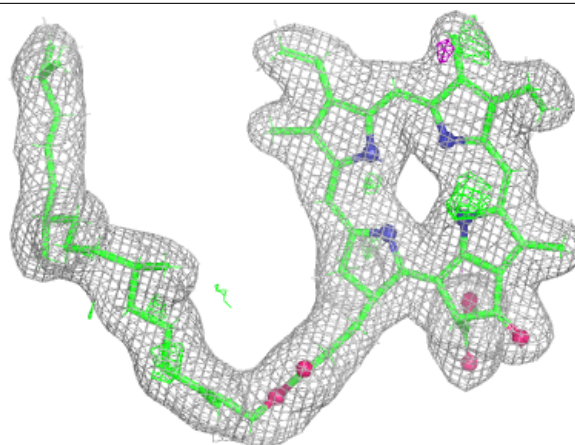
Electron density around CLA d 404:

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

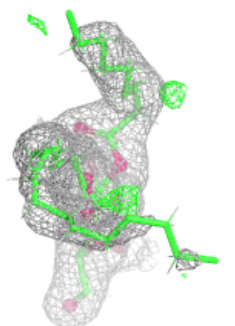
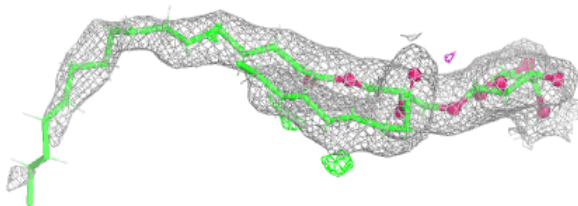
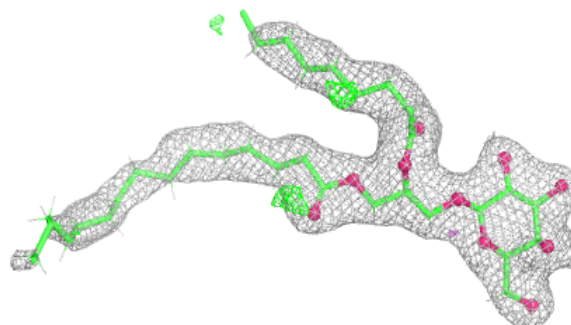


Electron density around PHO D 402:

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

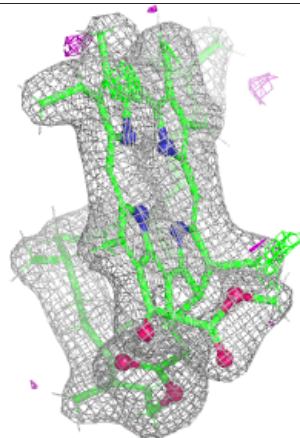
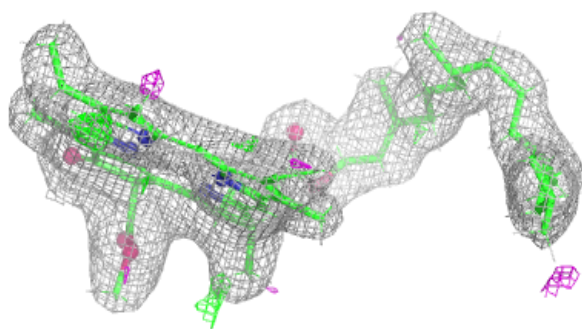
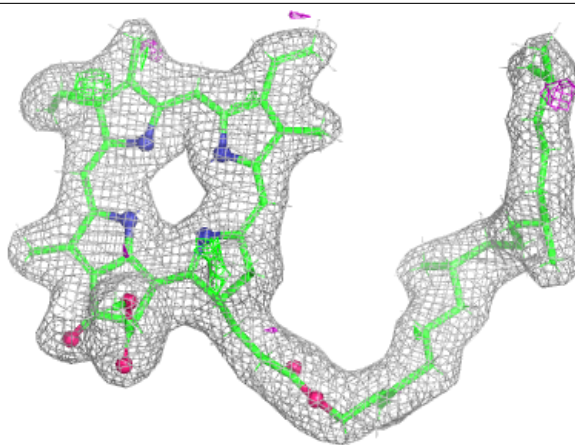
**Electron density around LMG d 412:**

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

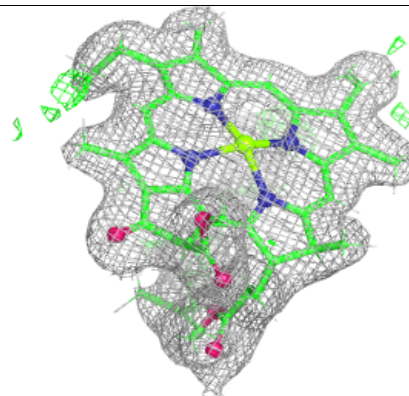
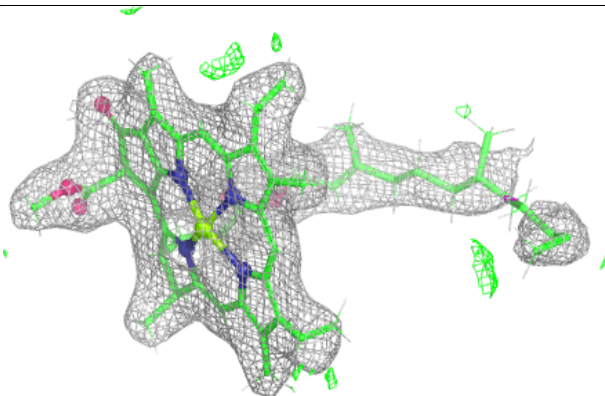
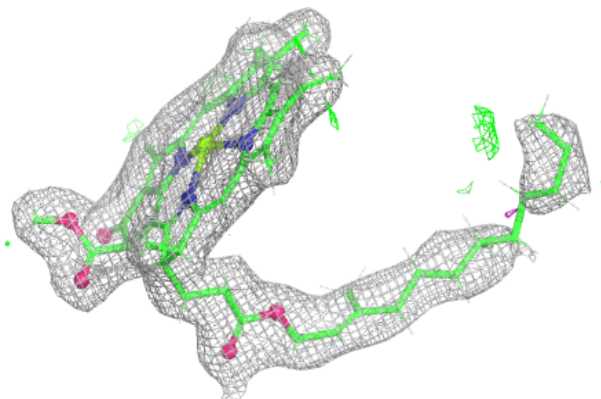


Electron density around PHO d 402:

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

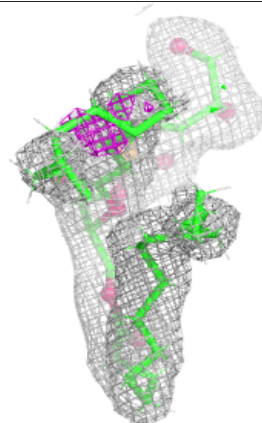
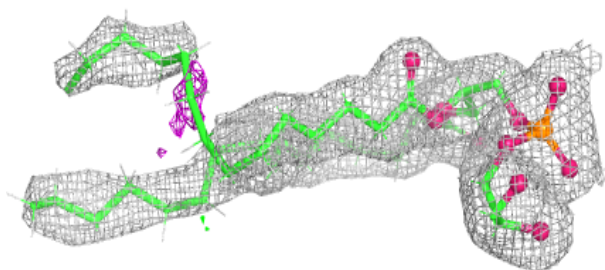
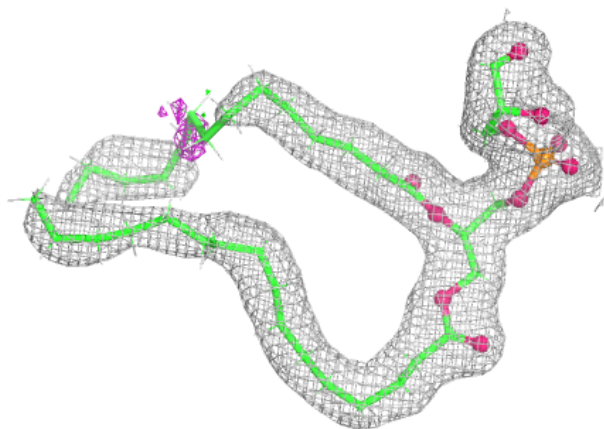
**Electron density around CLA C 504:**

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

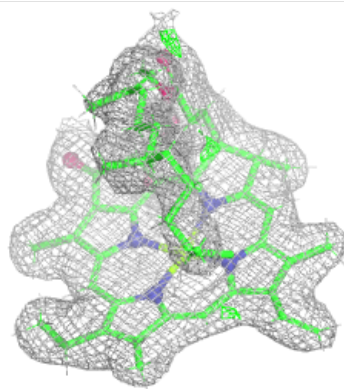
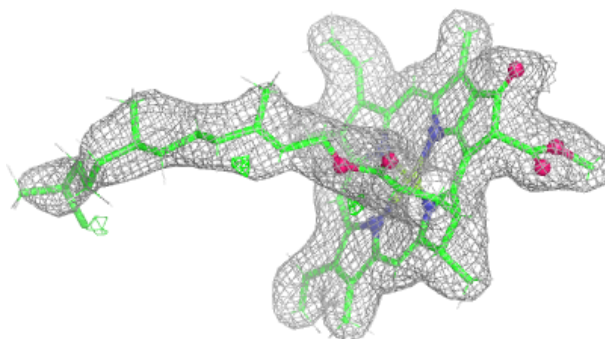
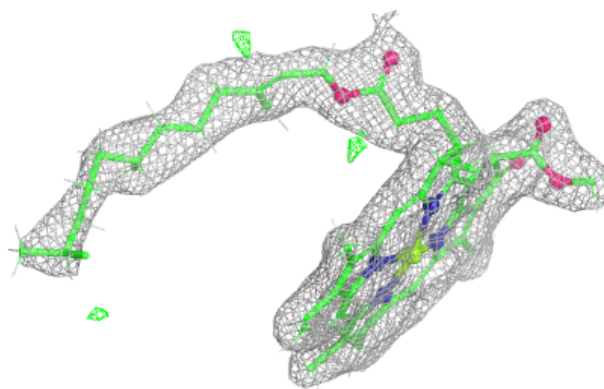


Electron density around LHG D 411:

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

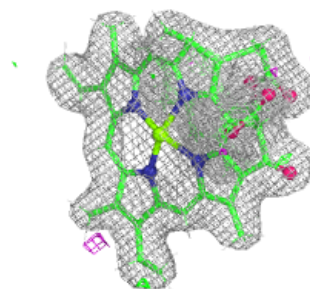
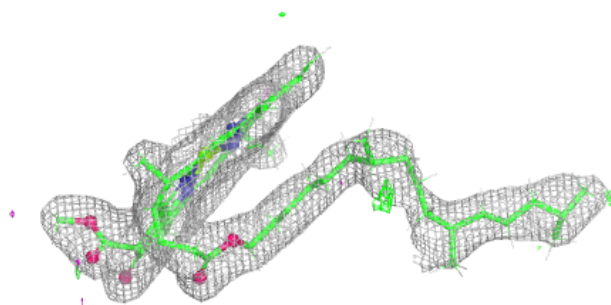
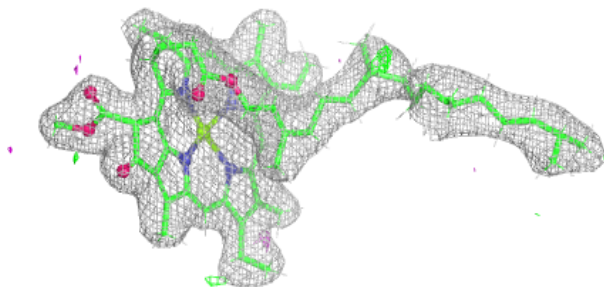
**Electron density around CLA c 504:**

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

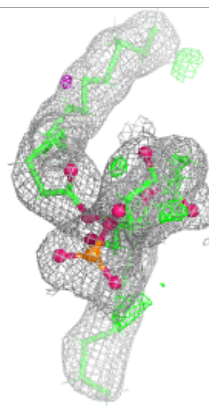
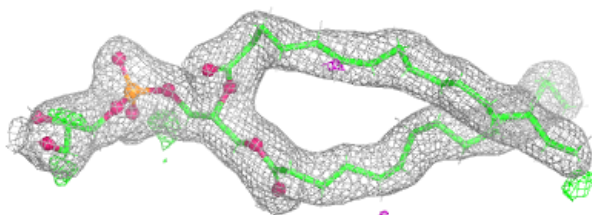
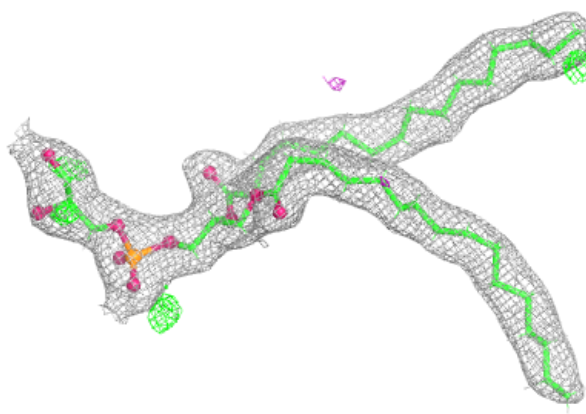


Electron density around CLA c 505:

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

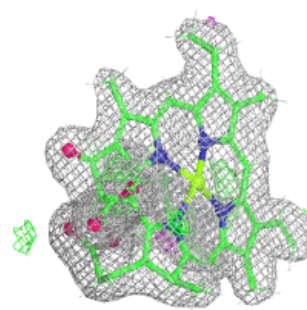
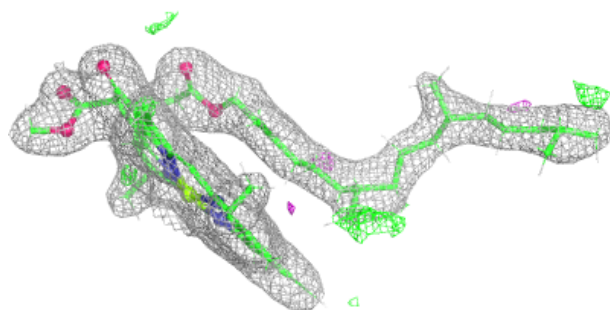
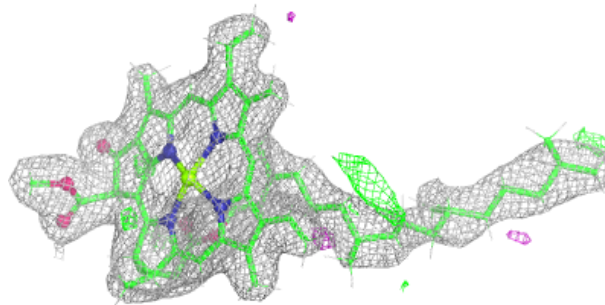
**Electron density around LHG d 409:**

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



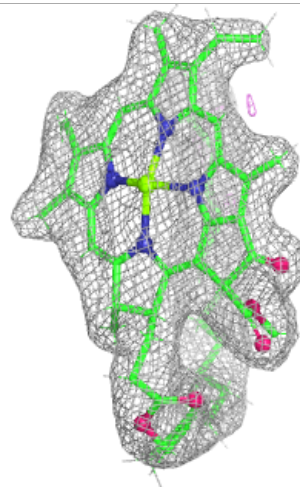
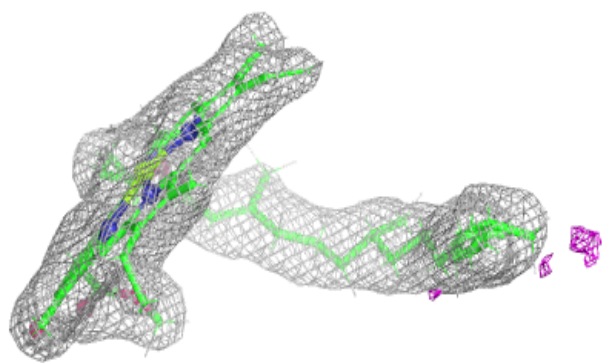
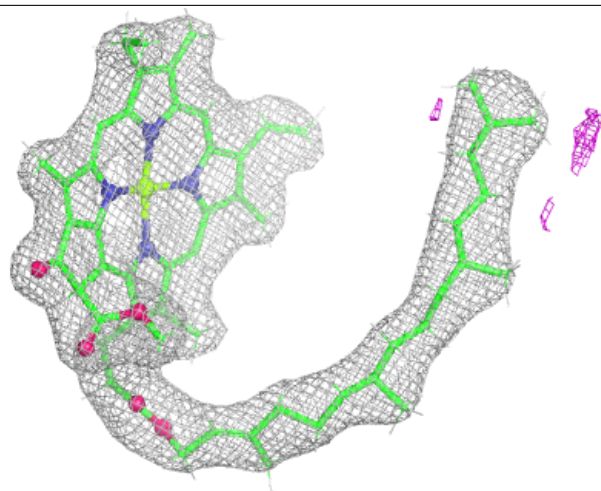
Electron density around CLA C 505:

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



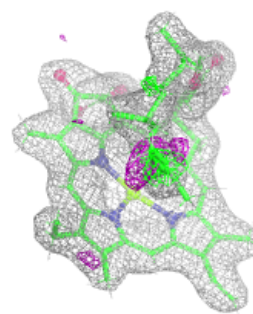
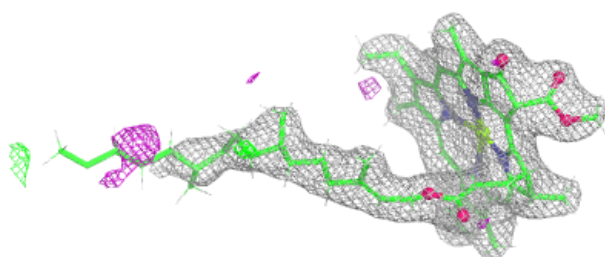
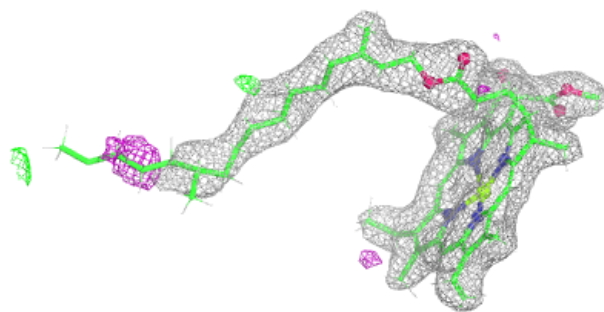
Electron density around CLA c 507:

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

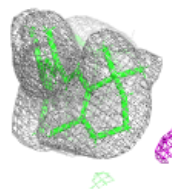
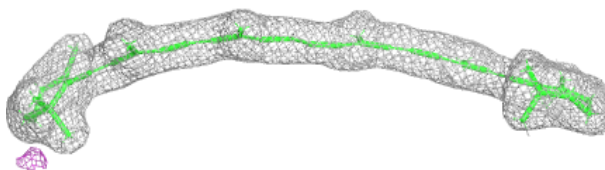
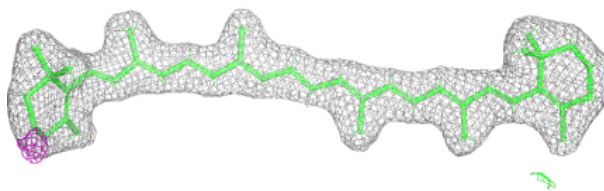


Electron density around CLA c 508:

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

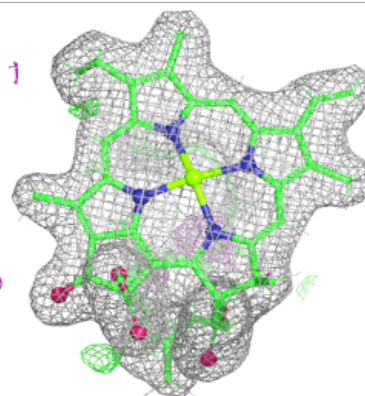
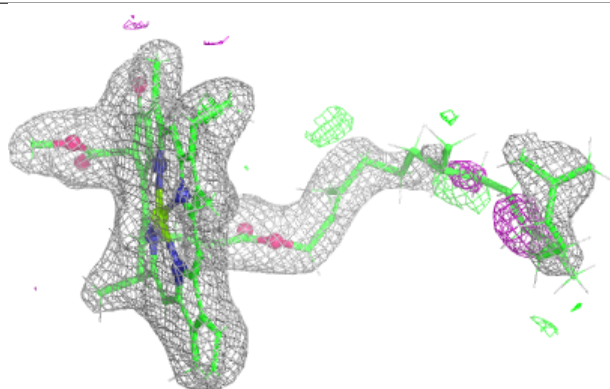
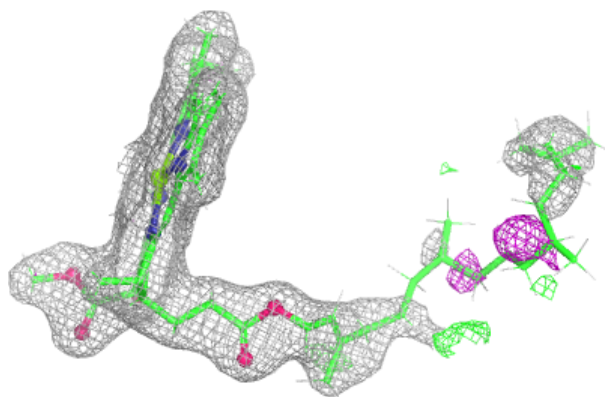
**Electron density around BCR t 101:**

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

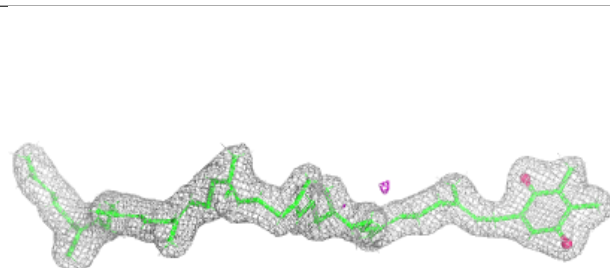
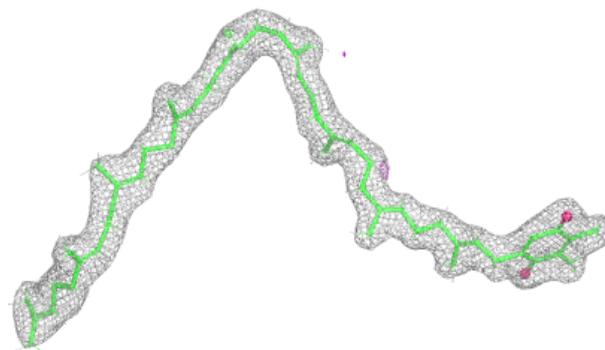


Electron density around CLA C 506:

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

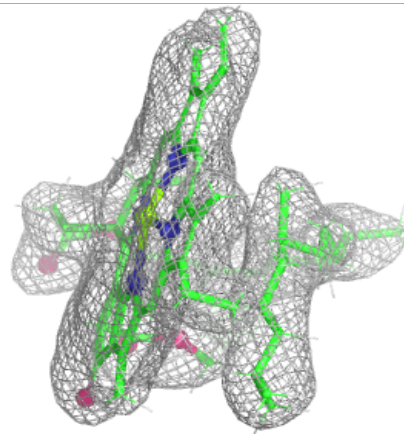
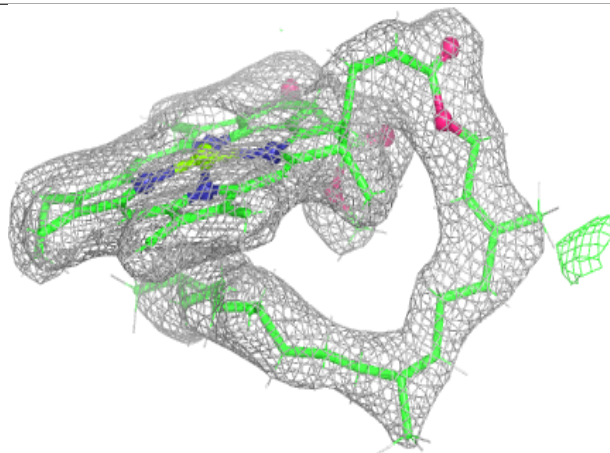
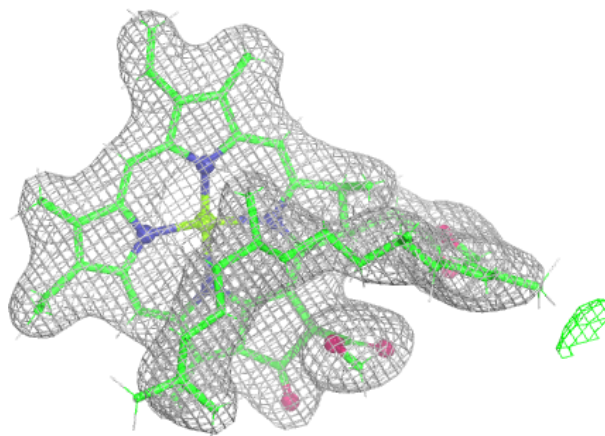
**Electron density around PL9 D 406:**

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



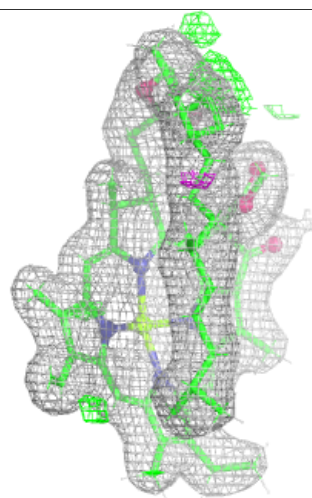
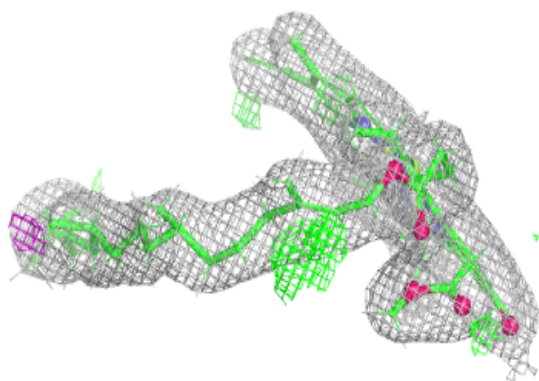
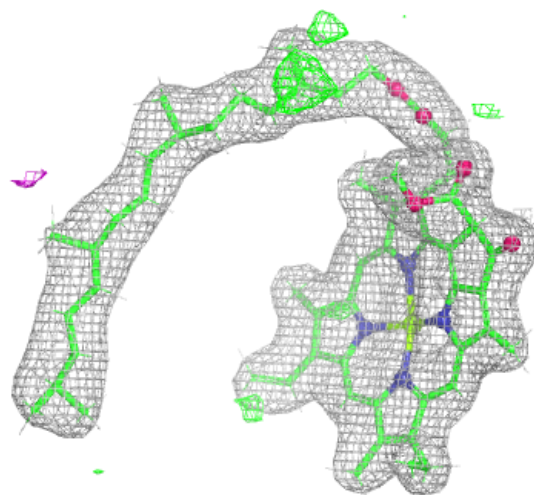
Electron density around CLA c 510:

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



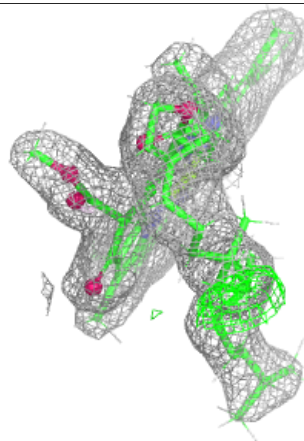
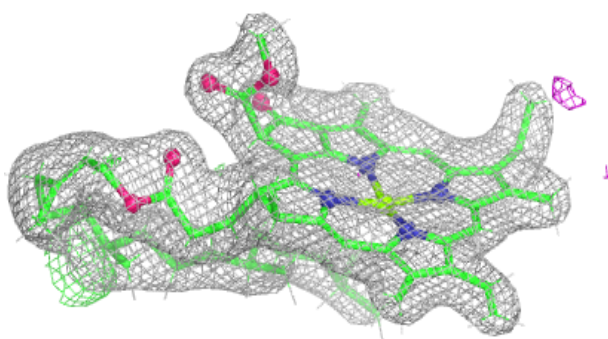
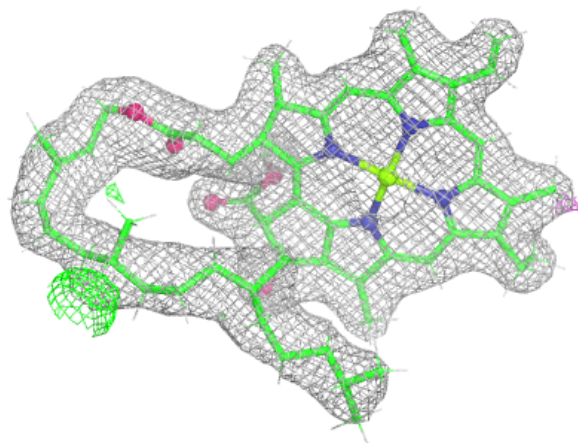
Electron density around CLA C 507:

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



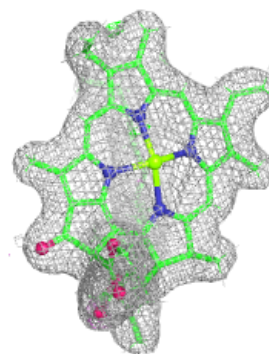
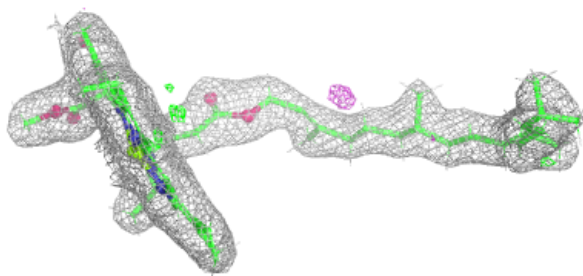
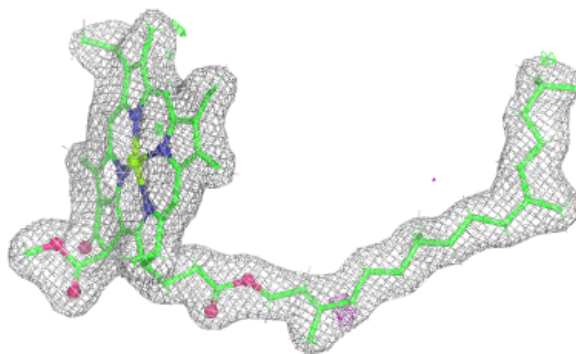
Electron density around CLA C 509:

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



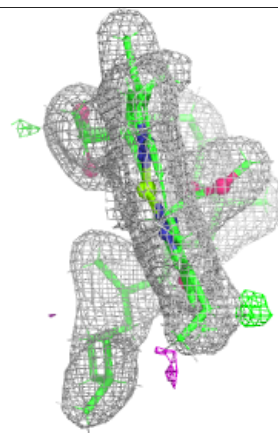
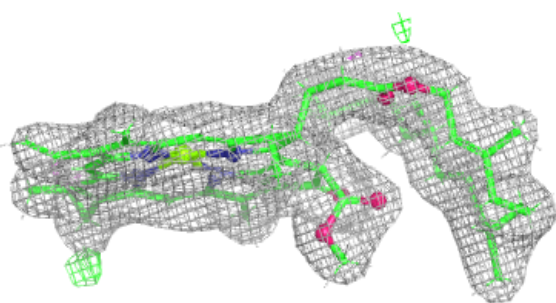
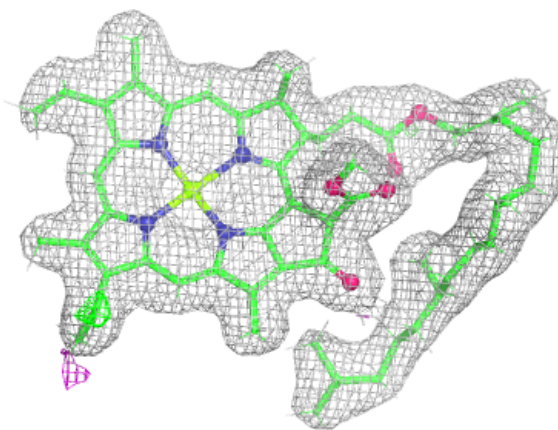
Electron density around CLA B 609:

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

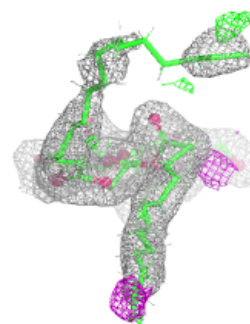
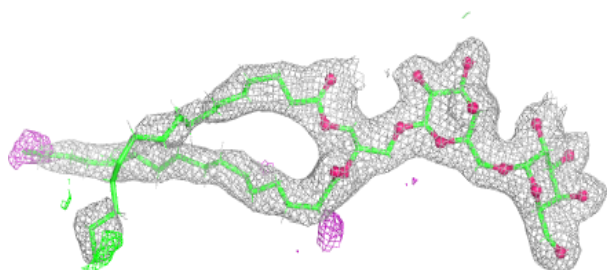
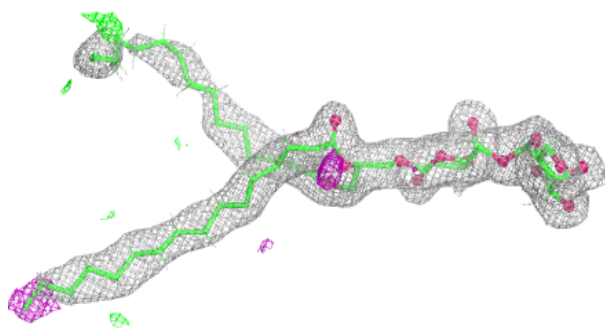


Electron density around CLA B 610:

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

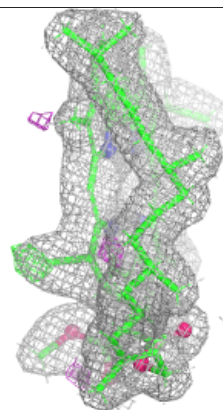
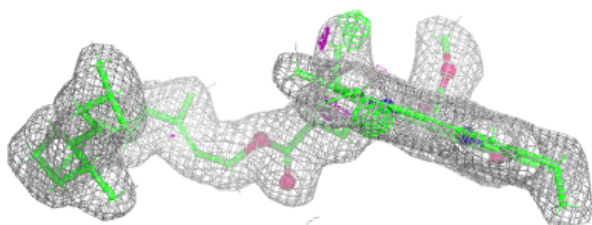
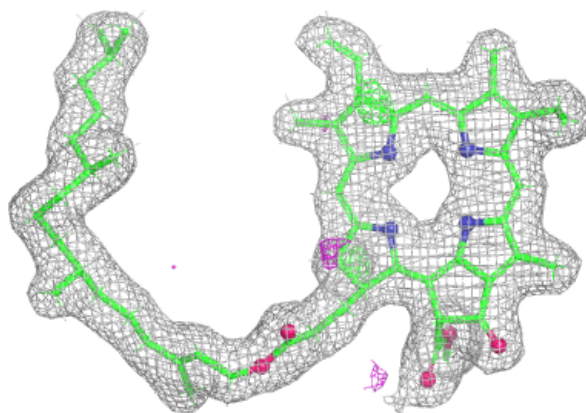
**Electron density around DGD C 522:**

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

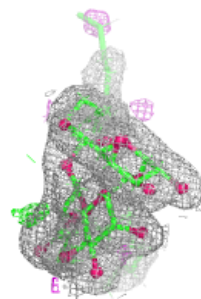
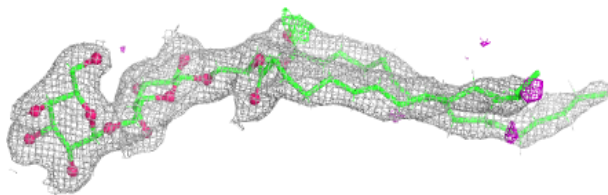
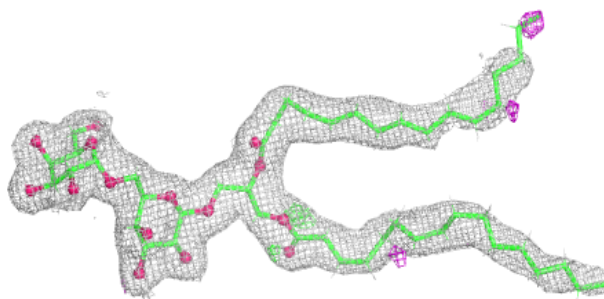


Electron density around PHO A 607:

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

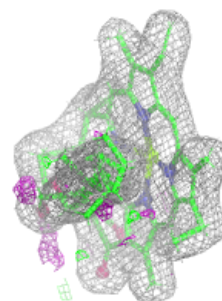
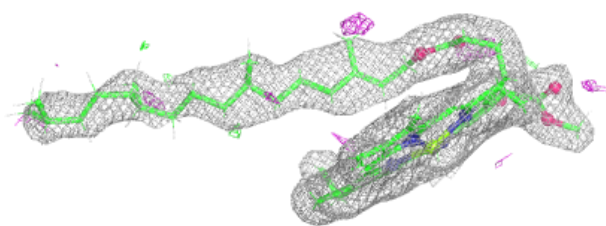
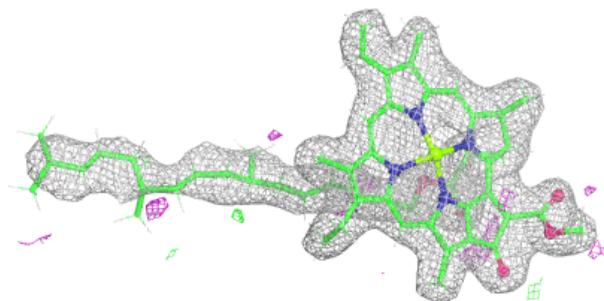
**Electron density around DGD C 524:**

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

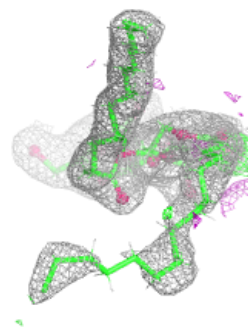
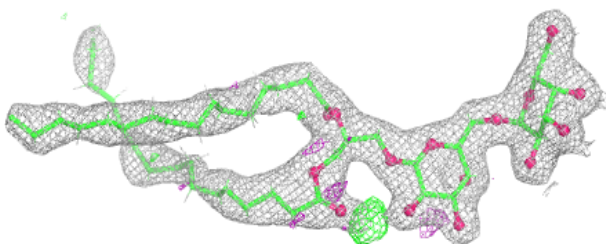
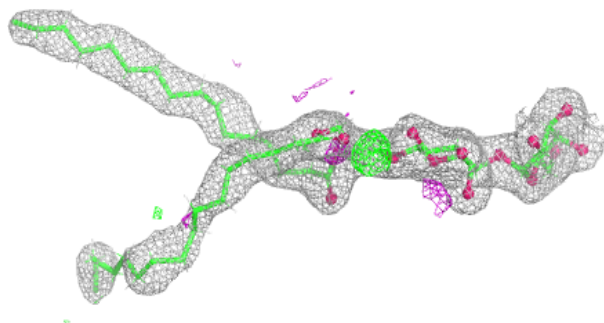


Electron density around CLA B 614:

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

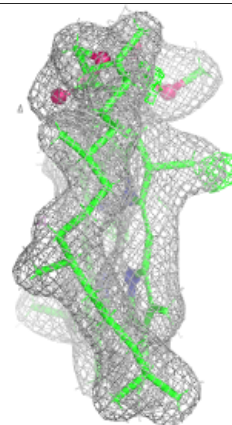
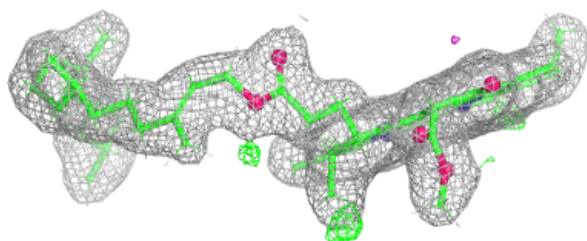
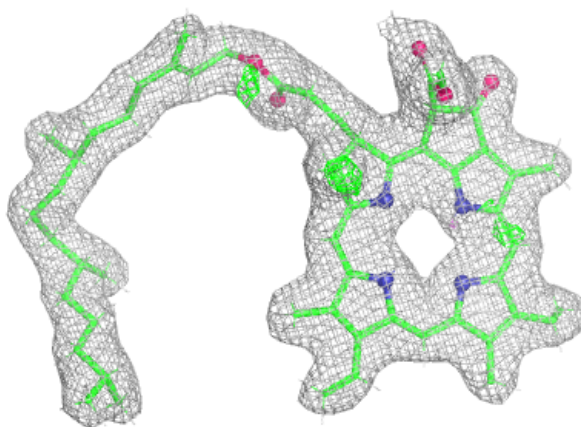
**Electron density around DGD c 519:**

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

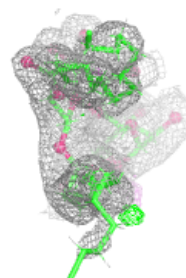
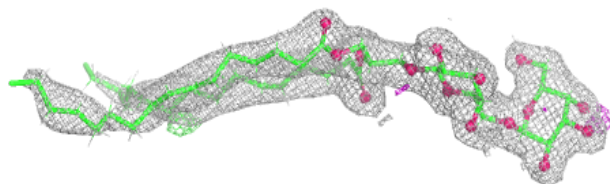
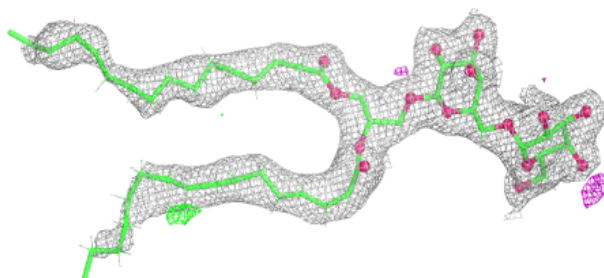


Electron density around PHO a 607:

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

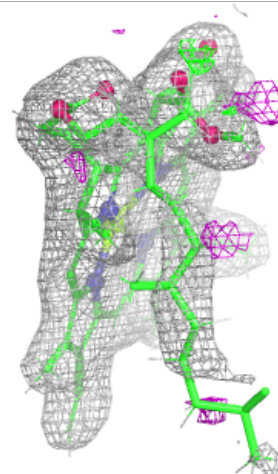
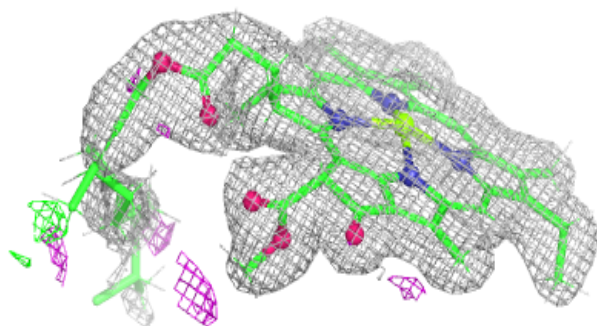
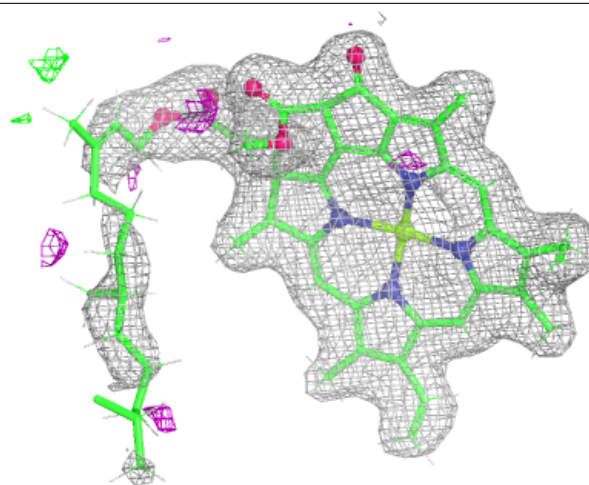
**Electron density around DGD c 521:**

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



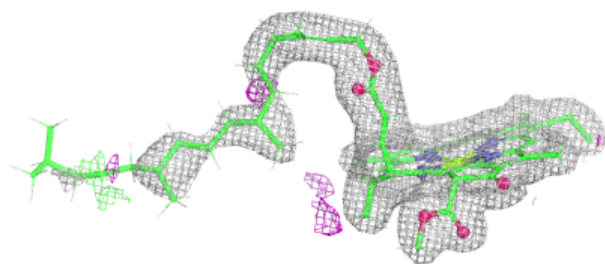
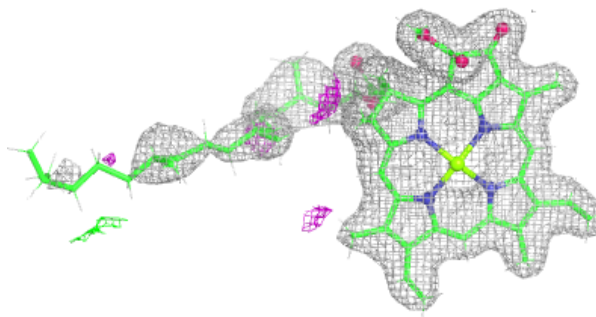
Electron density around CLA B 616:

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

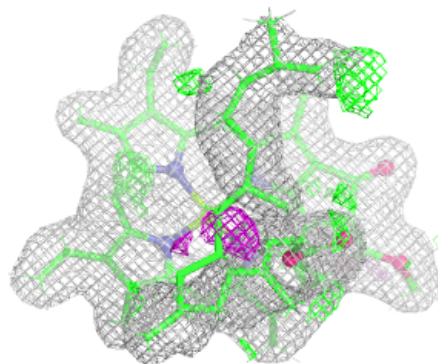
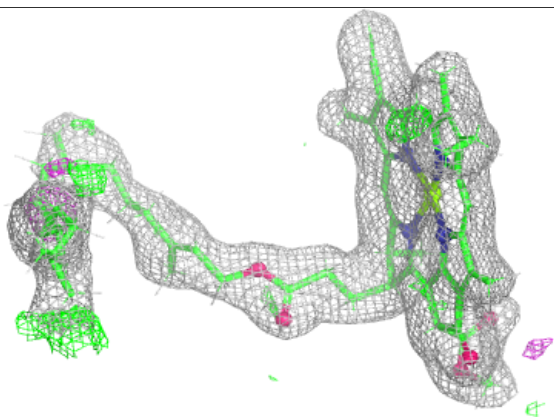
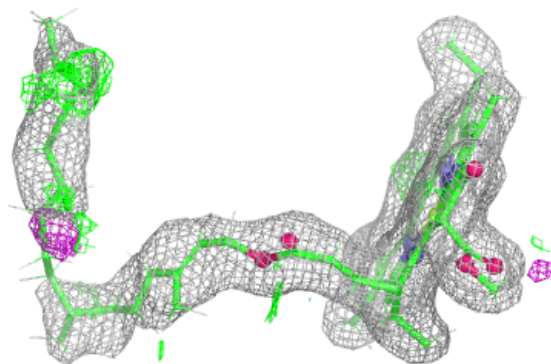


Electron density around CLA a 606:

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

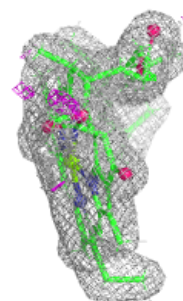
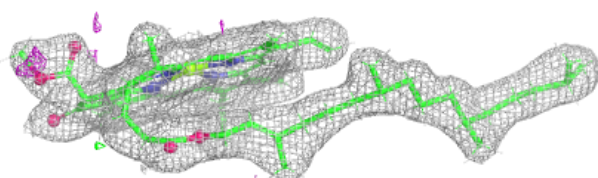
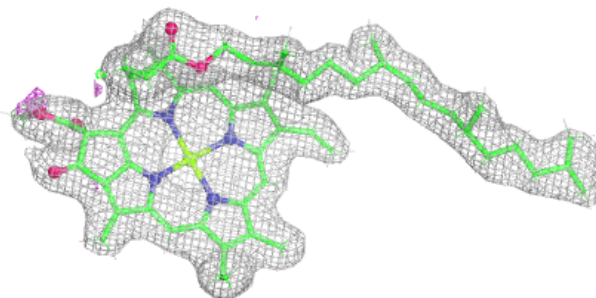
**Electron density around CLA a 608:**

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

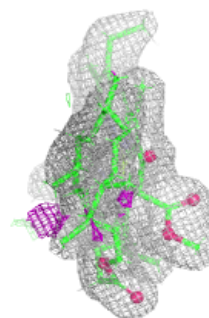
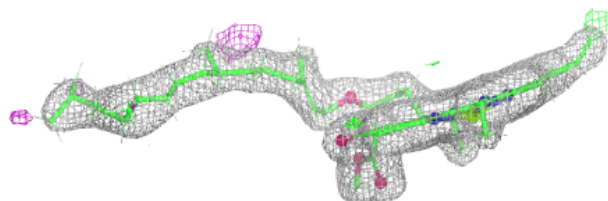
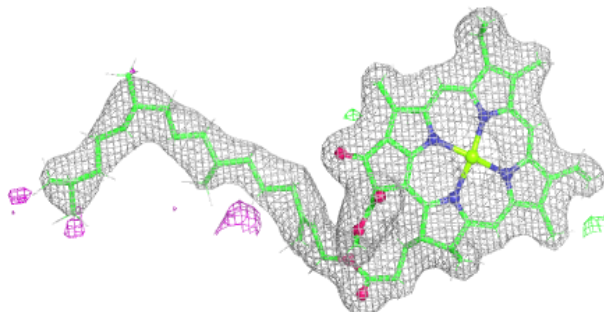


Electron density around CLA C 501:

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

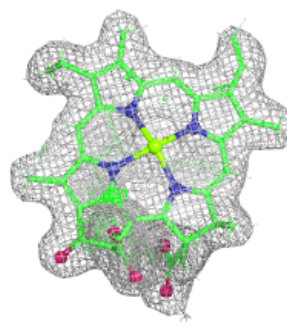
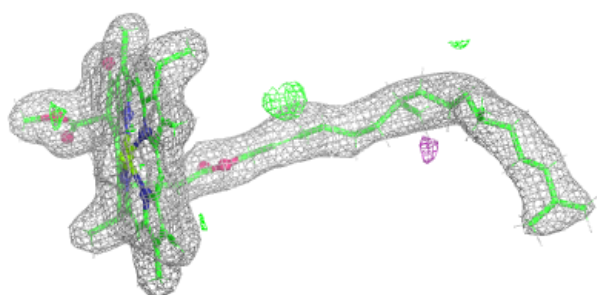
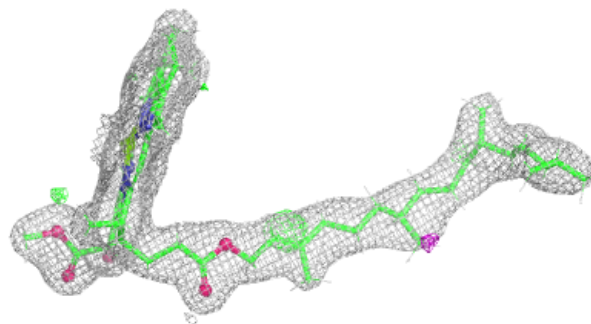
**Electron density around CLA b 602:**

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

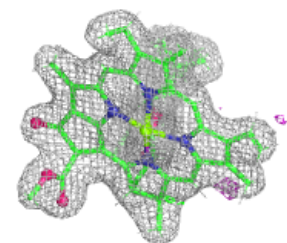
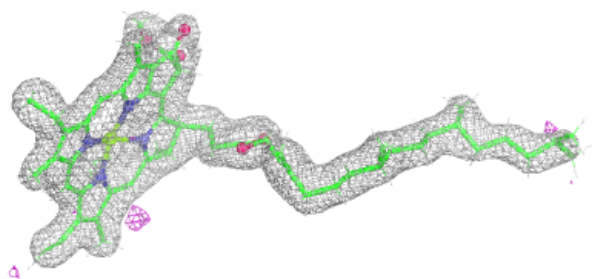
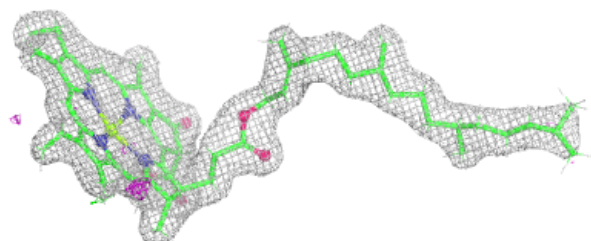


Electron density around CLA b 605:

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

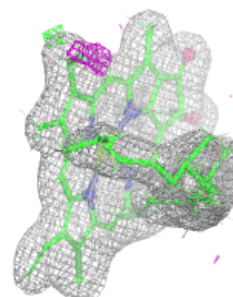
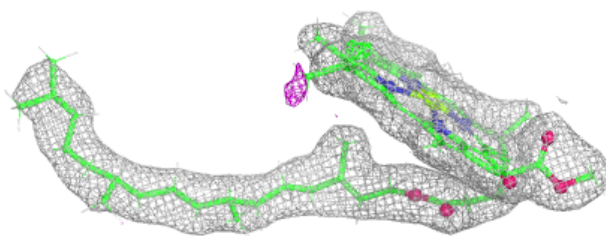
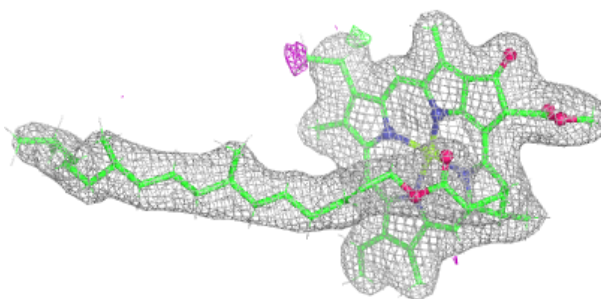
**Electron density around CLA C 502:**

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

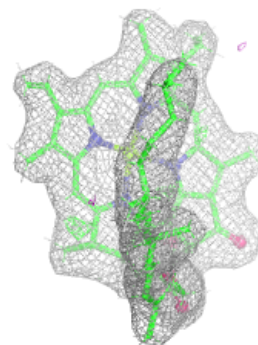
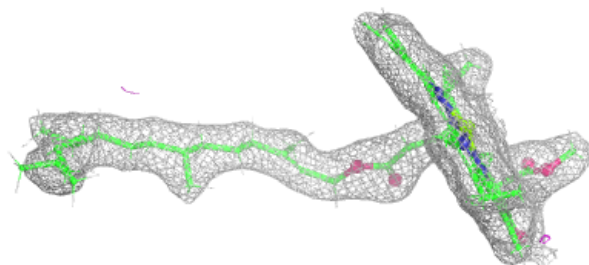
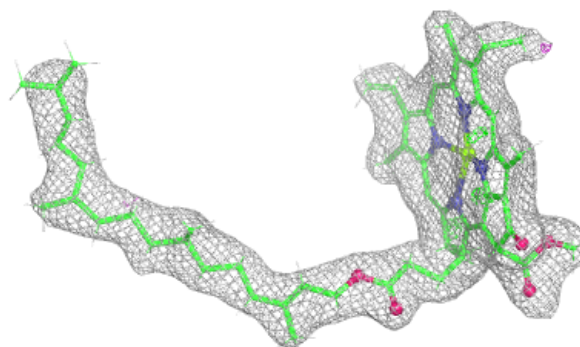


Electron density around CLA b 608:

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

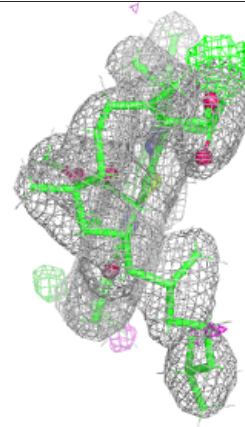
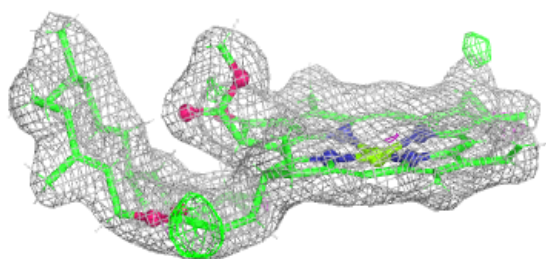
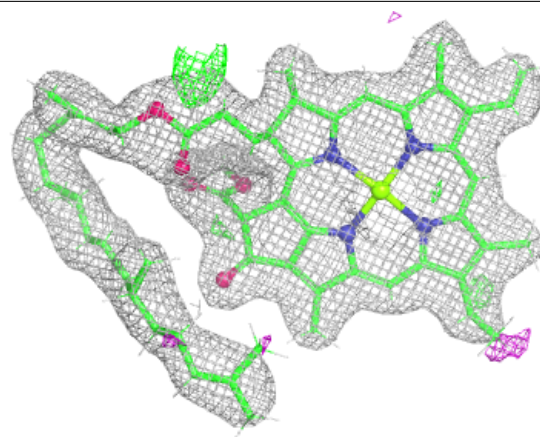
**Electron density around CLA b 609:**

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

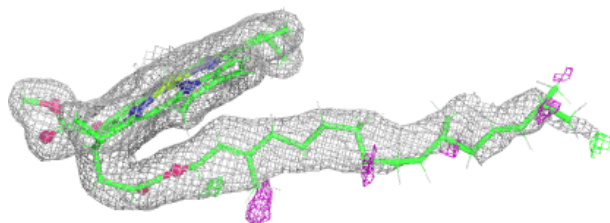
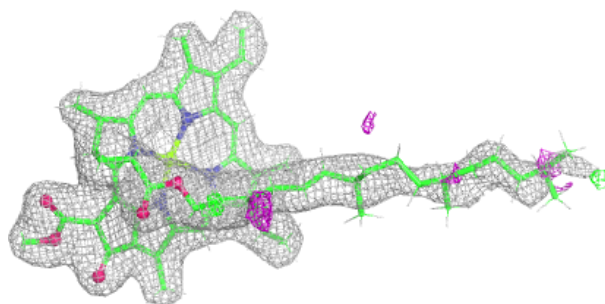


Electron density around CLA b 610:

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

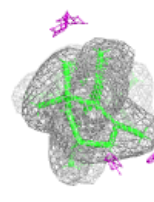
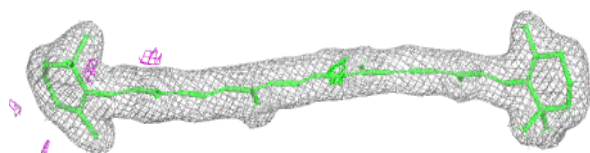
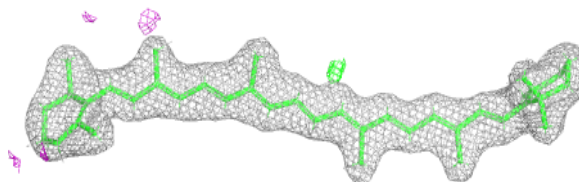
**Electron density around CLA b 614:**

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



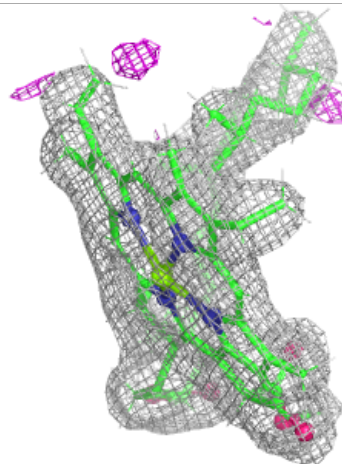
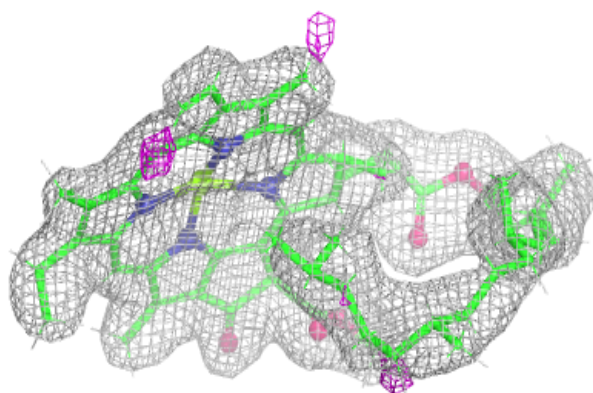
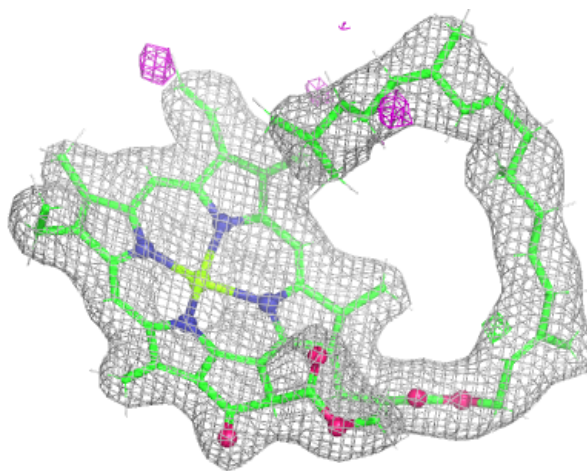
Electron density around BCR a 609:

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



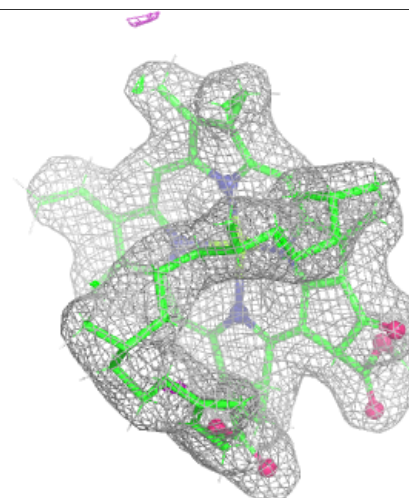
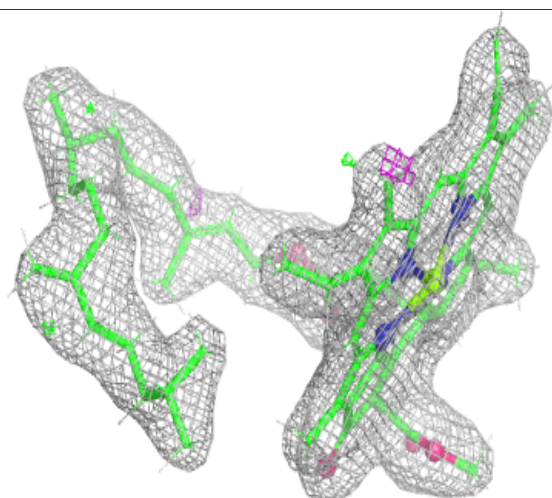
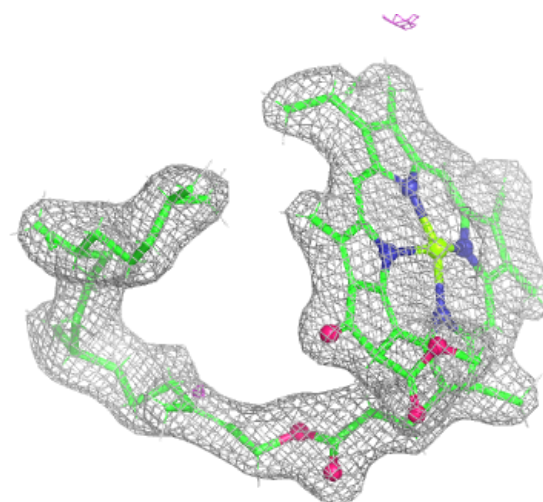
Electron density around CLA b 615:

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



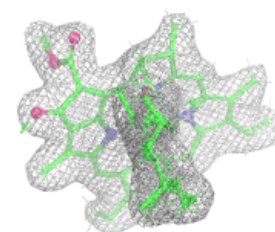
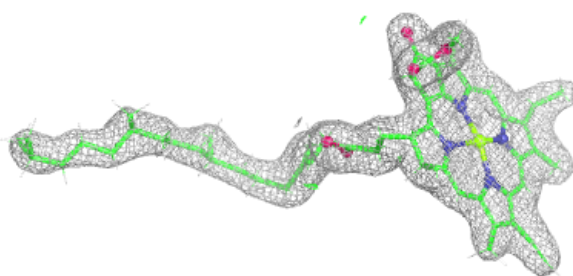
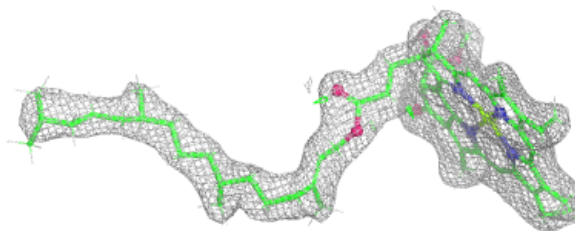
Electron density around CLA C 503:

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

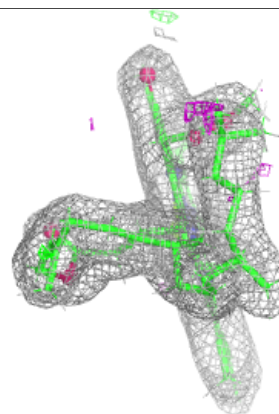
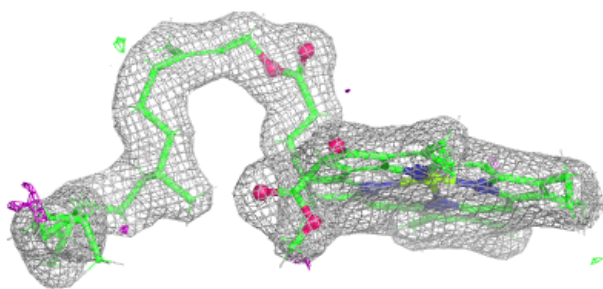
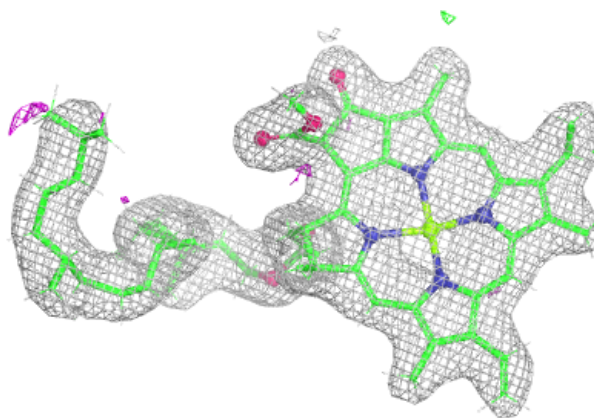


Electron density around CLA c 502:

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

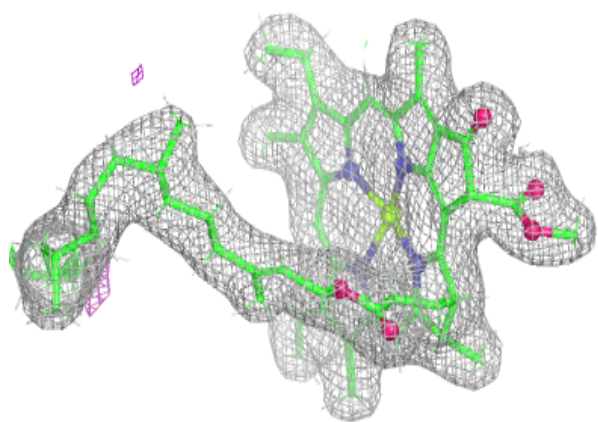
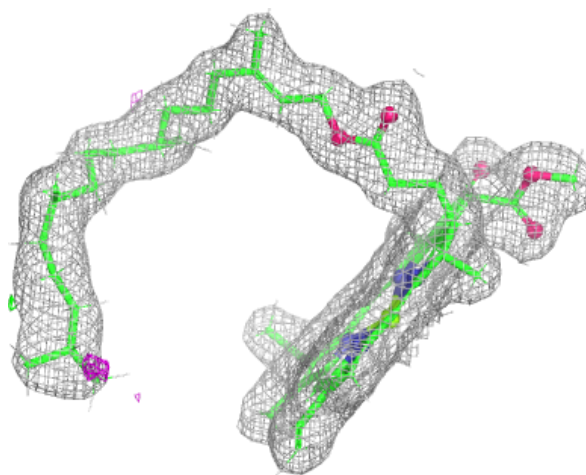
**Electron density around CLA B 612:**

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



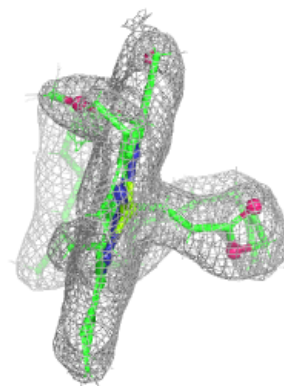
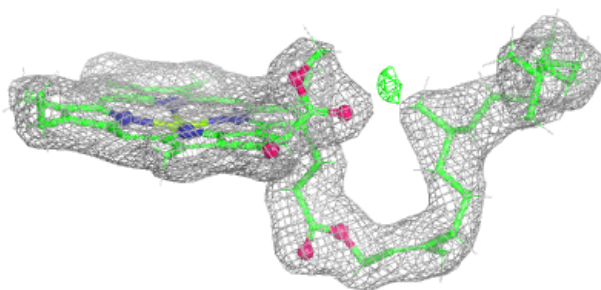
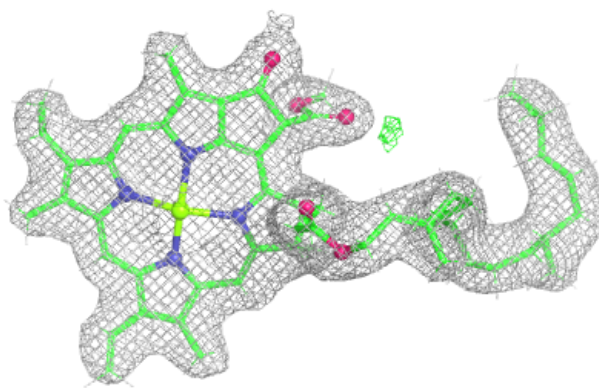
Electron density around CLA b 611:

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



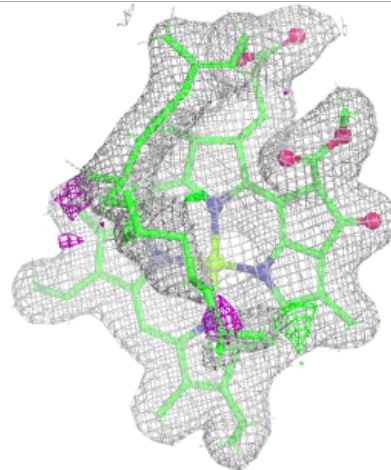
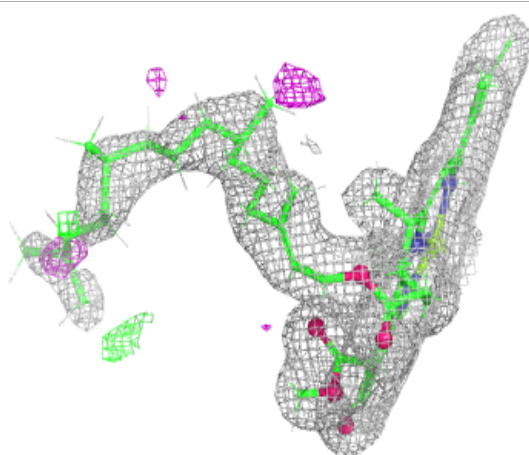
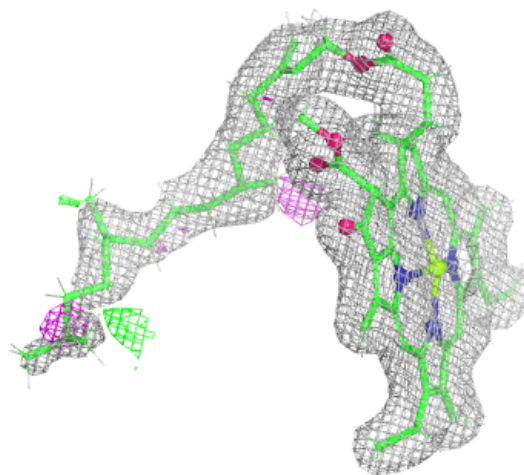
Electron density around CLA b 612:

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



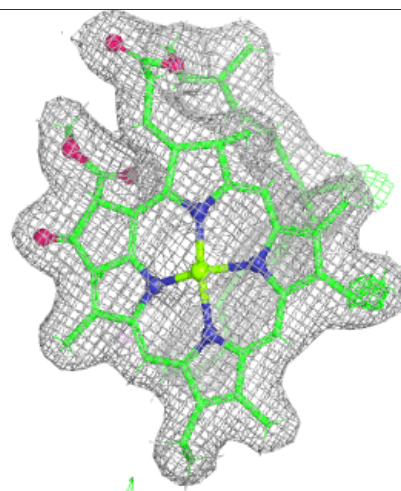
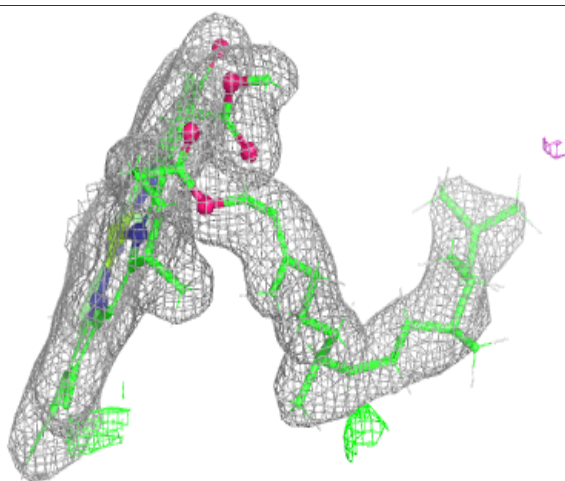
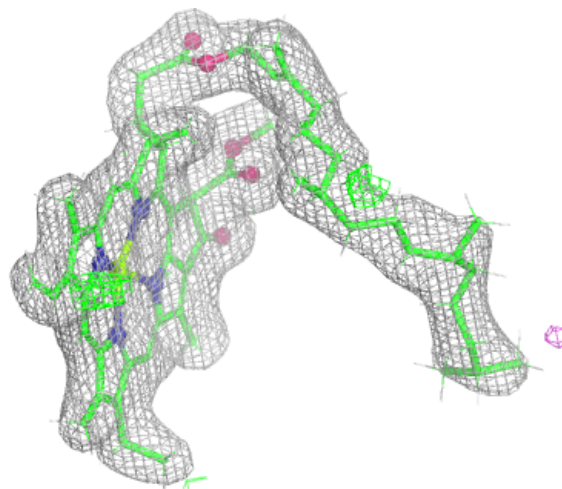
Electron density around CLA b 613:

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



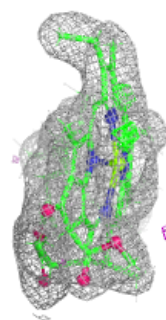
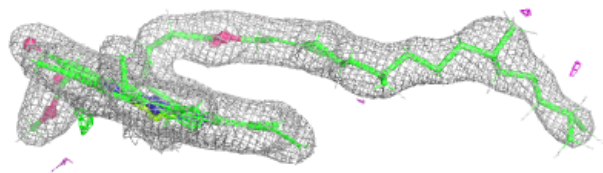
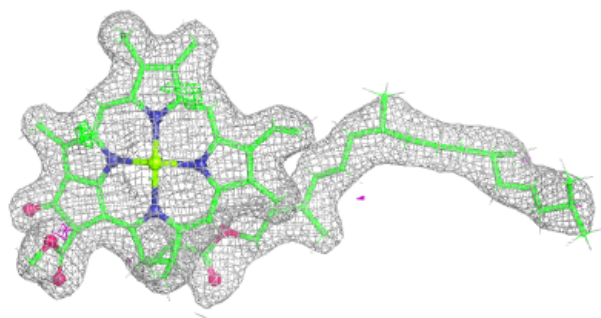
Electron density around CLA B 613:

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



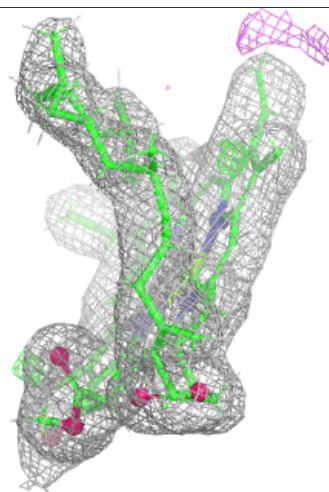
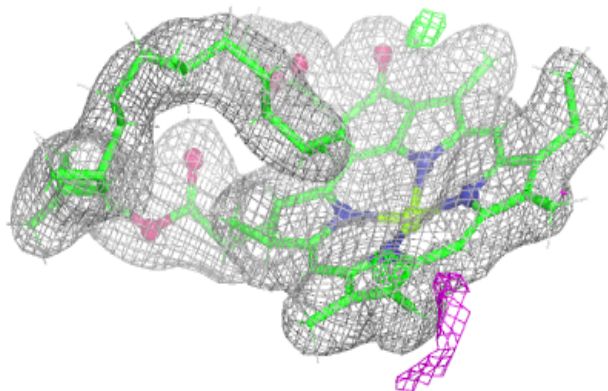
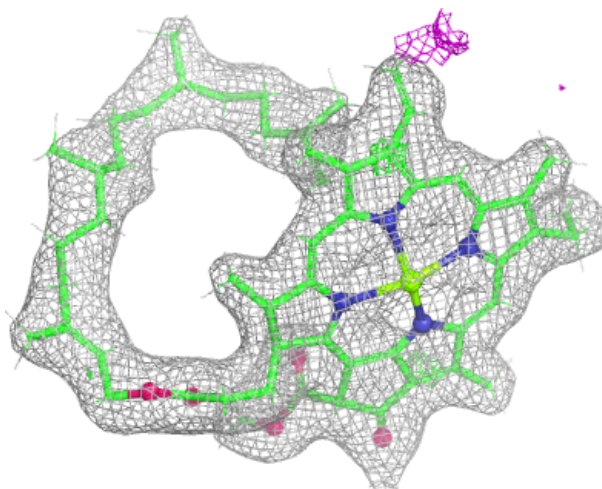
Electron density around CLA B 603:

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



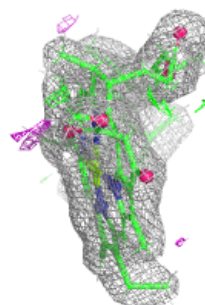
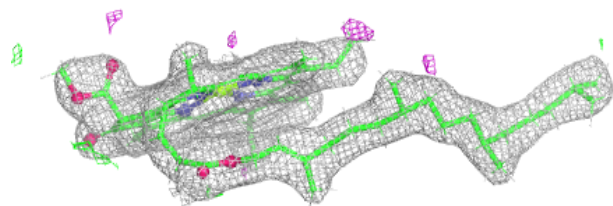
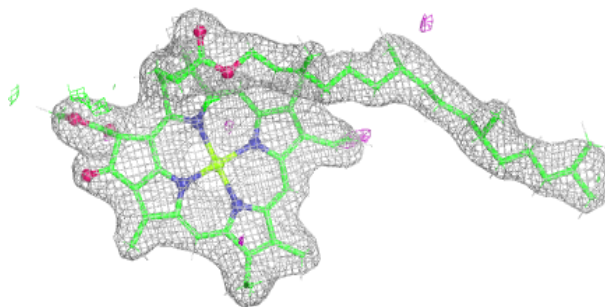
Electron density around CLA B 615:

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

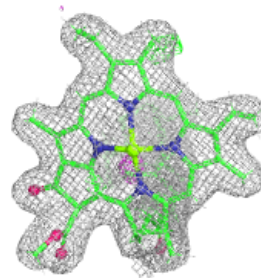
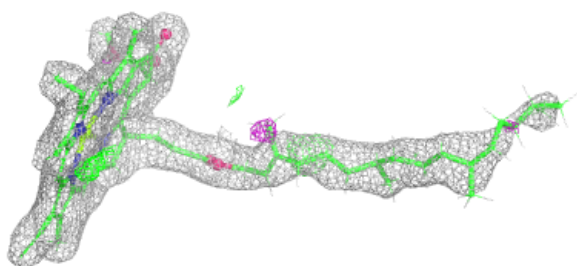
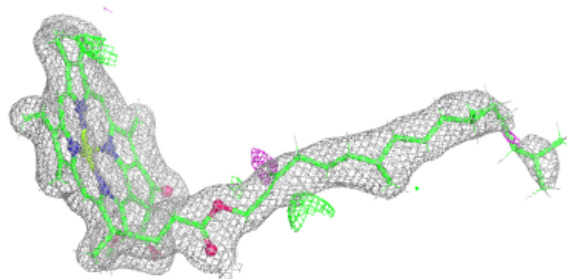


Electron density around CLA c 501:

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

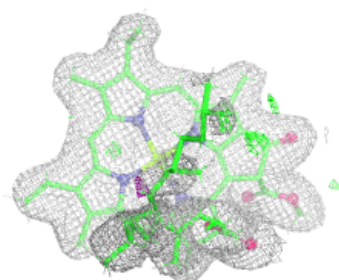
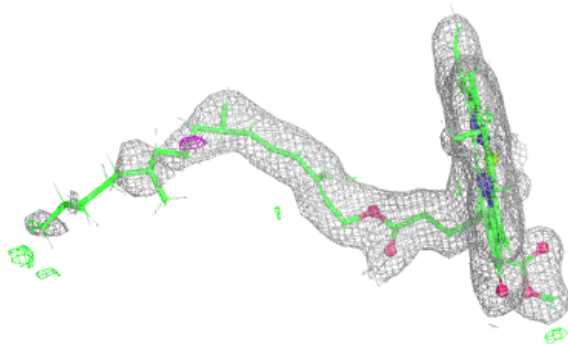
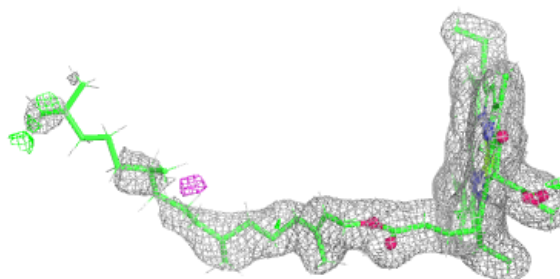
**Electron density around CLA B 604:**

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

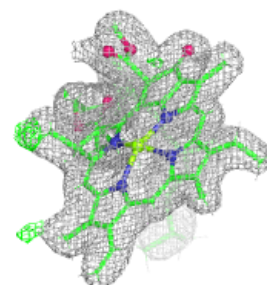
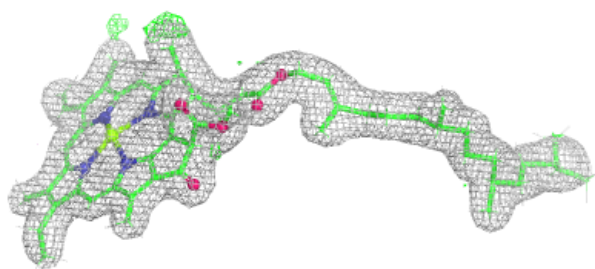
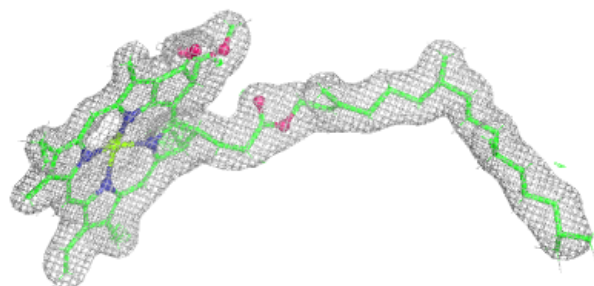


Electron density around CLA D 404:

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

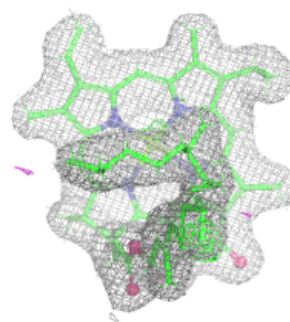
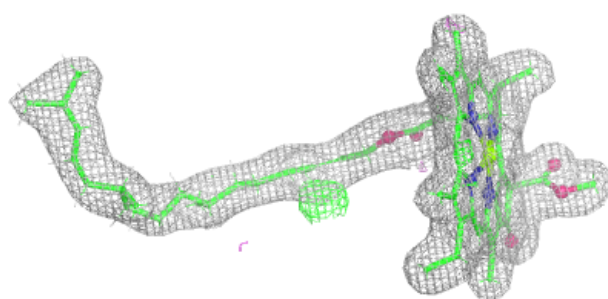
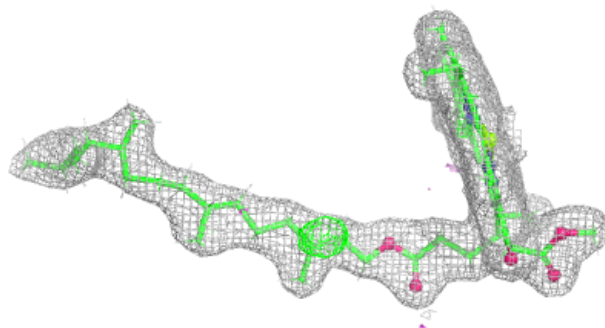
**Electron density around CLA a 605:**

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

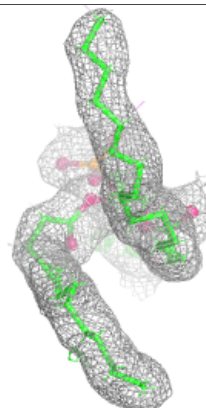
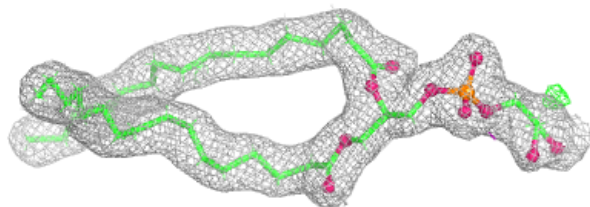
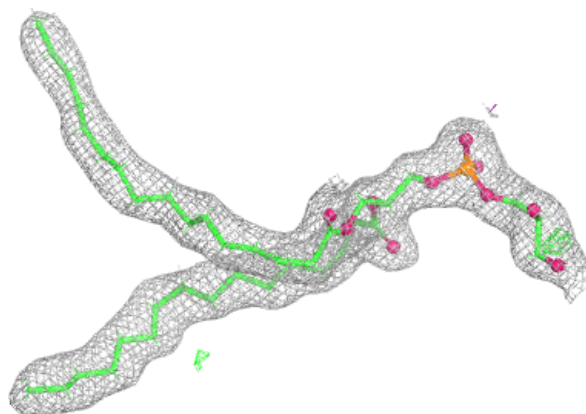


Electron density around CLA B 605:

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

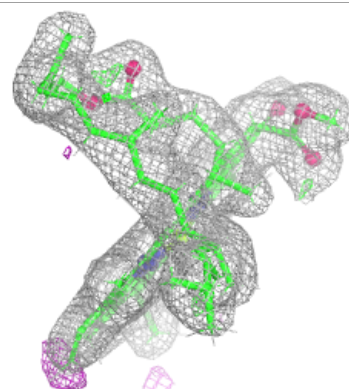
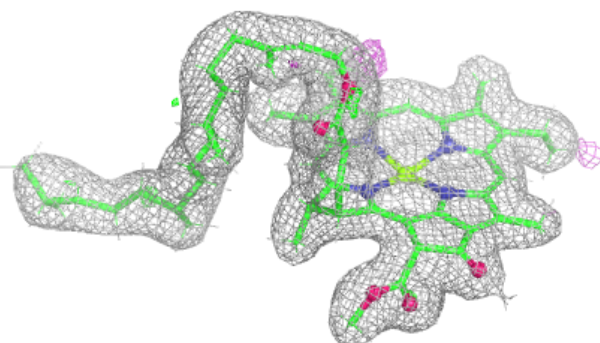
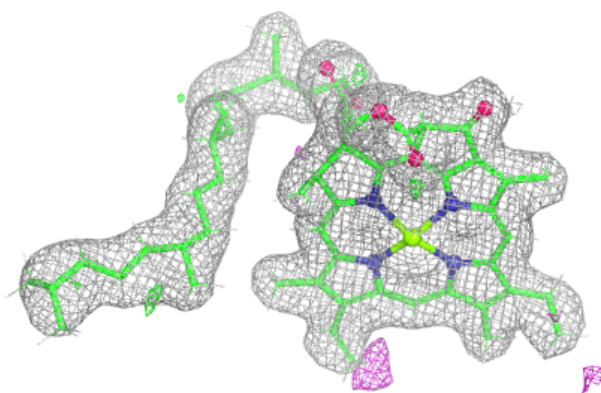
**Electron density around LHG D 410:**

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

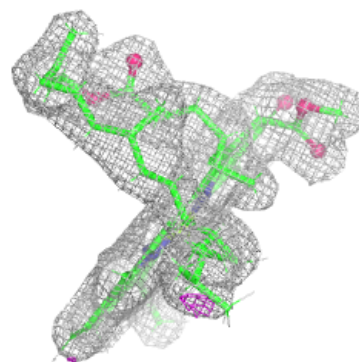
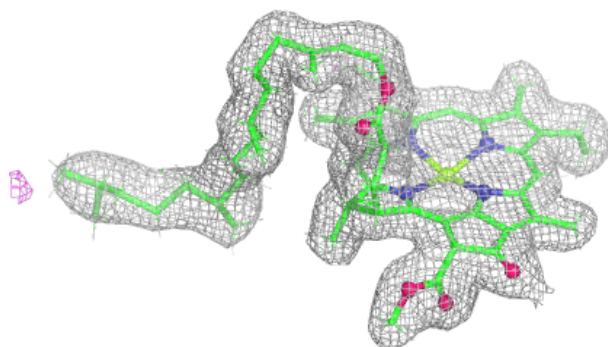
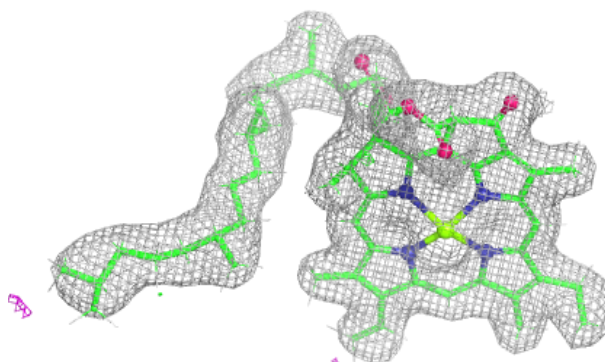


Electron density around CLA A 612:

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

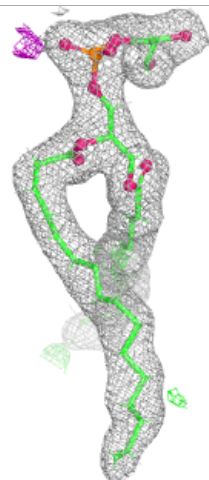
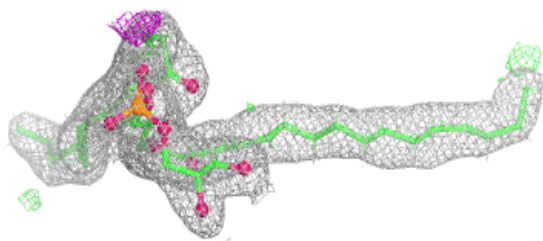
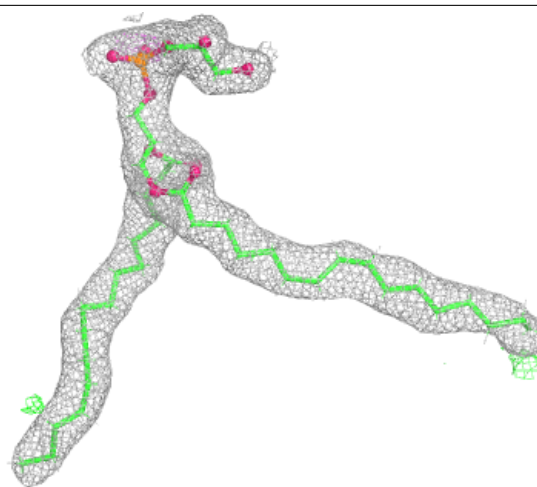
**Electron density around CLA a 611:**

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



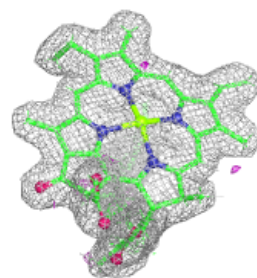
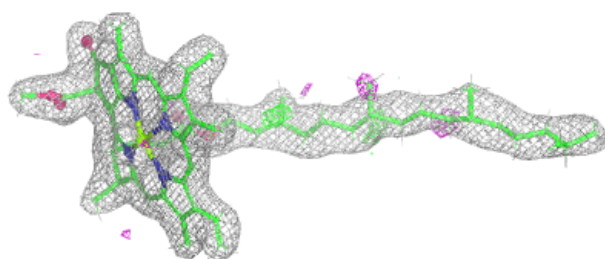
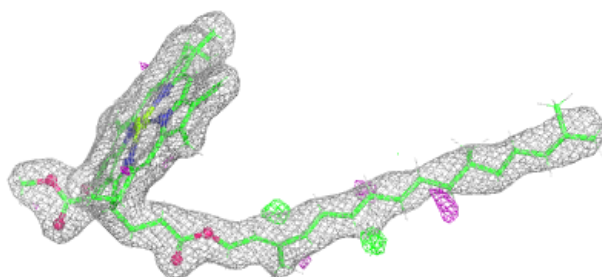
Electron density around LHG L 101:

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

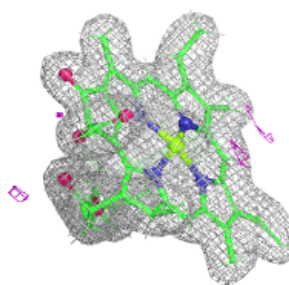
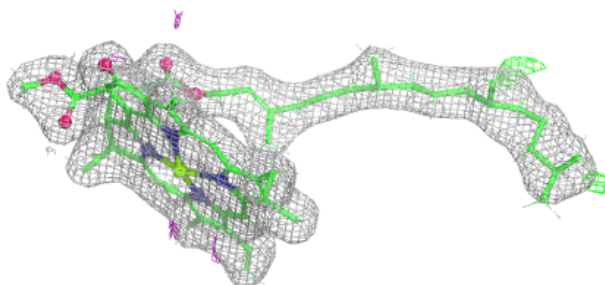
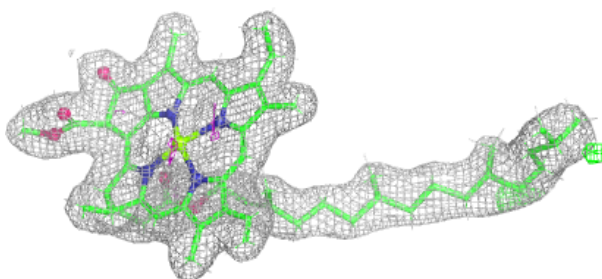


Electron density around CLA B 607:

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

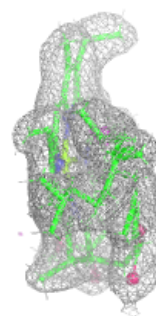
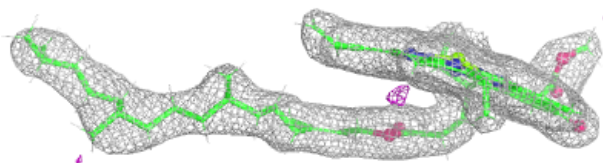
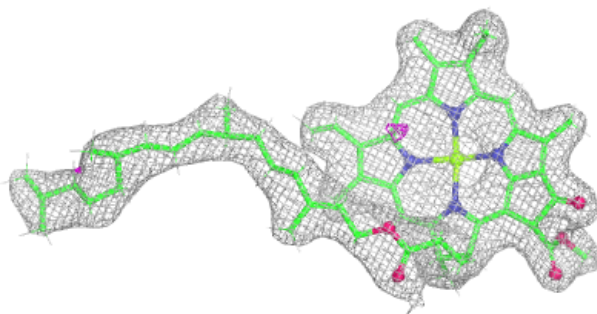
**Electron density around CLA B 608:**

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

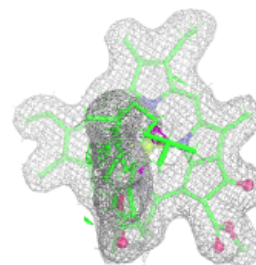
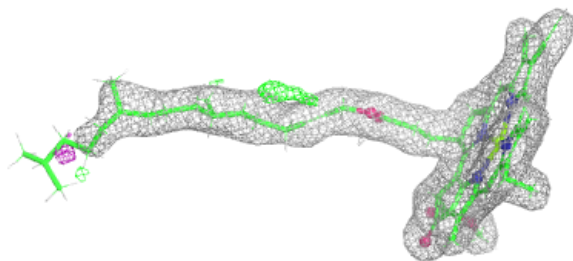
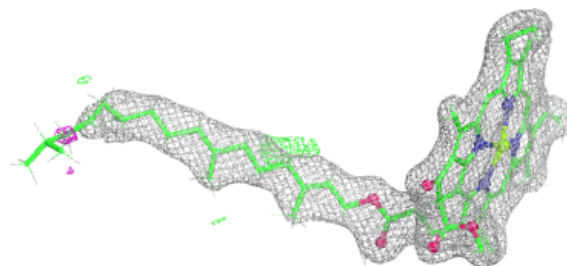


Electron density around CLA b 603:

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

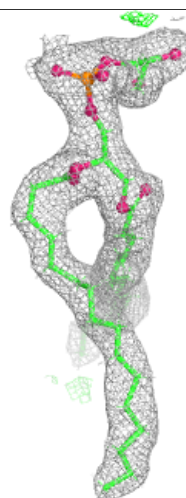
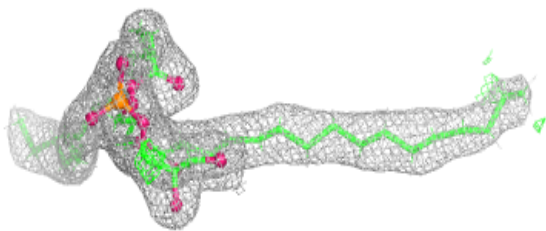
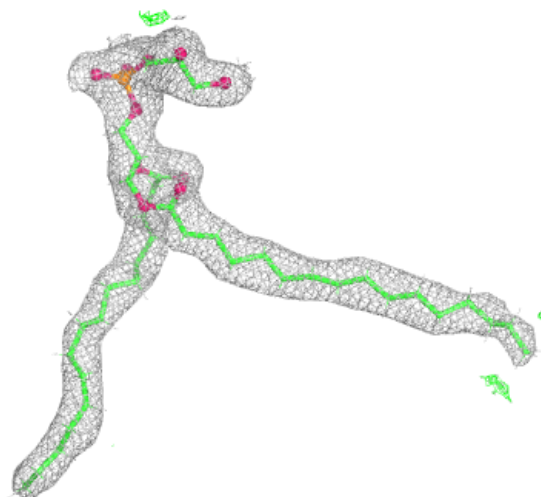
**Electron density around CLA b 604:**

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



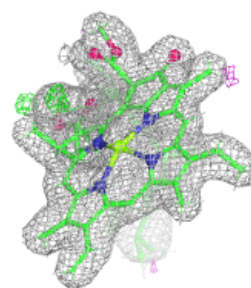
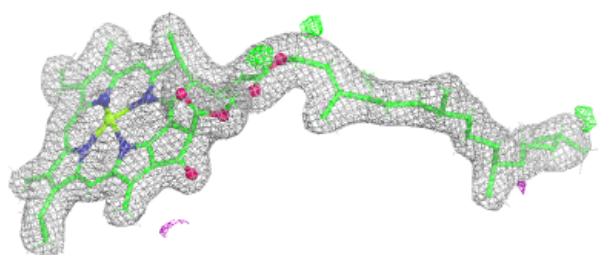
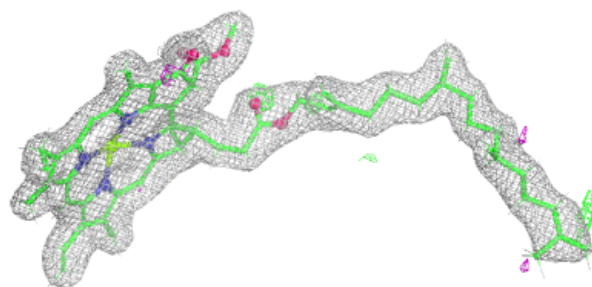
Electron density around LHG 1 101:

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

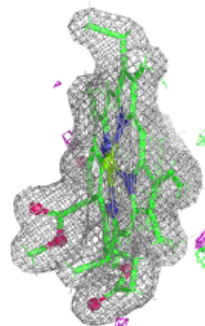
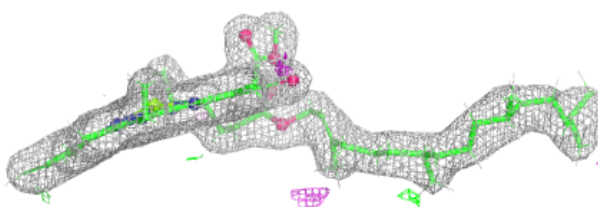
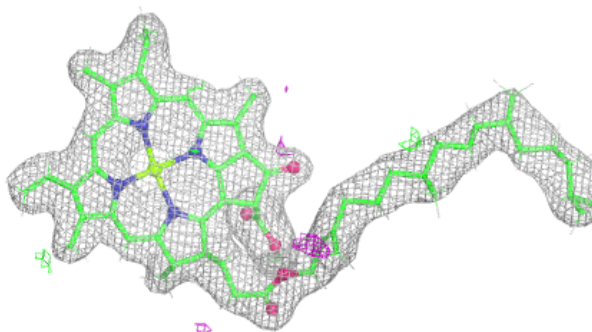


Electron density around CLA A 605:

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

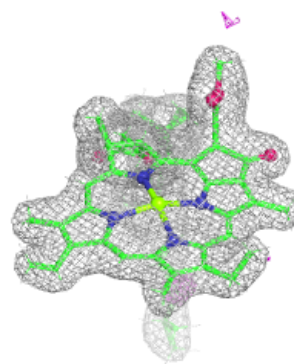
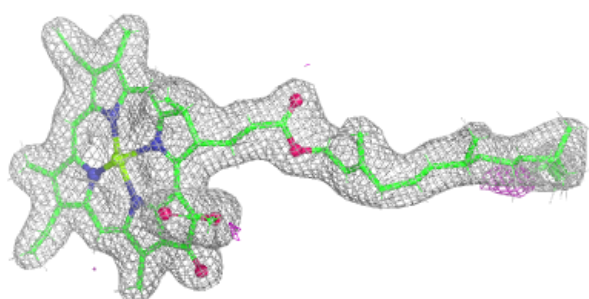
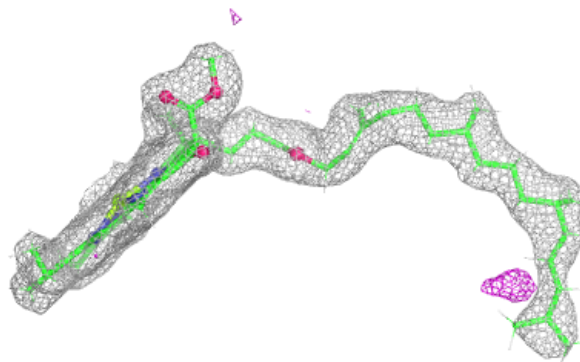
**Electron density around CLA B 602:**

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

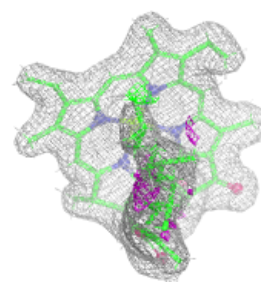
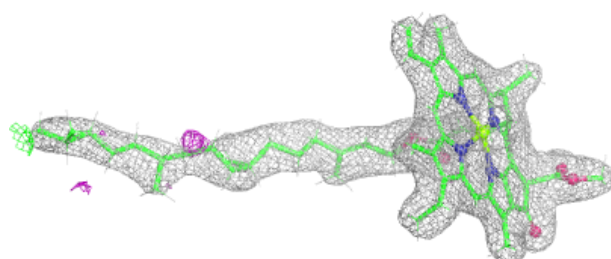
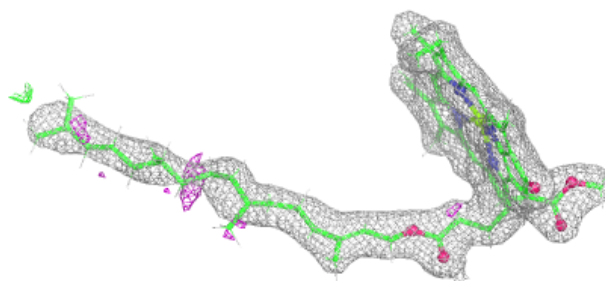


Electron density around CLA d 403:

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

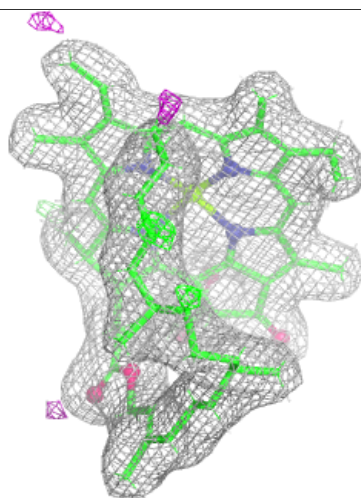
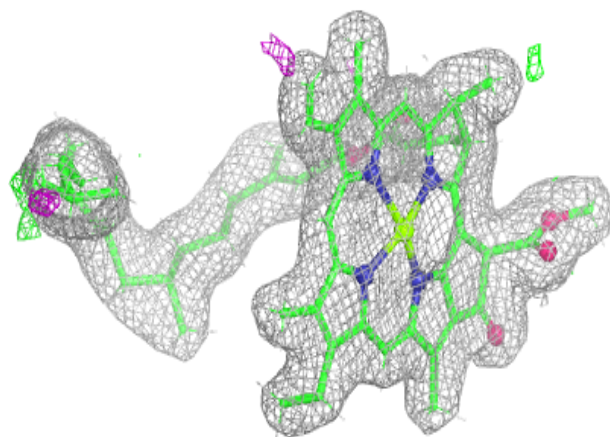
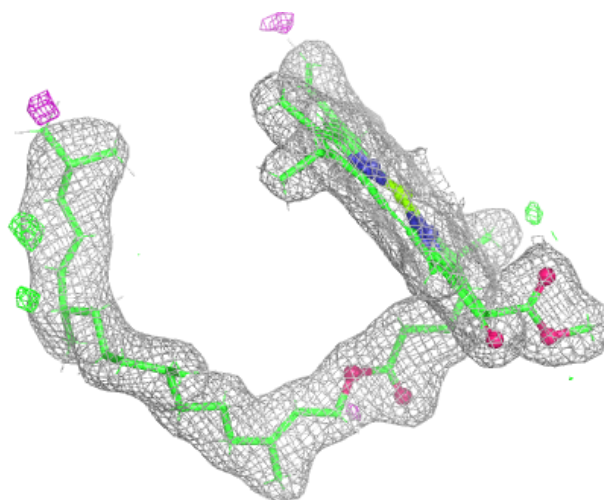
**Electron density around CLA b 607:**

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



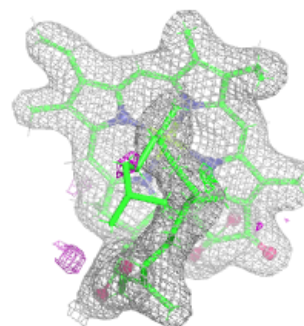
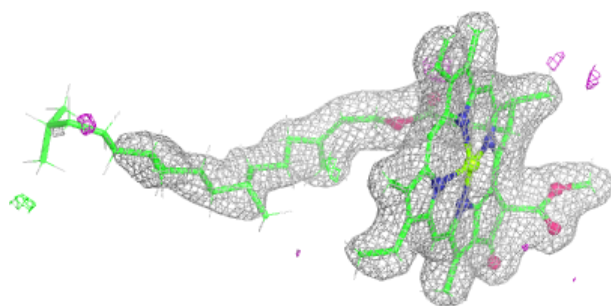
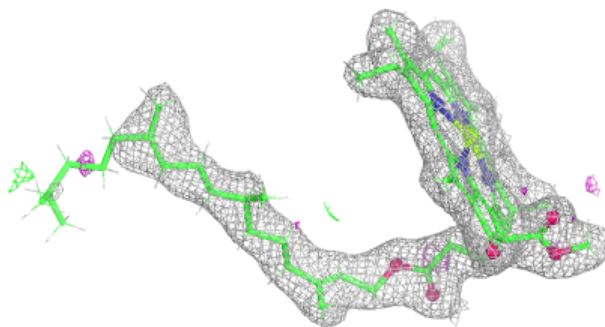
Electron density around CLA B 611:

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



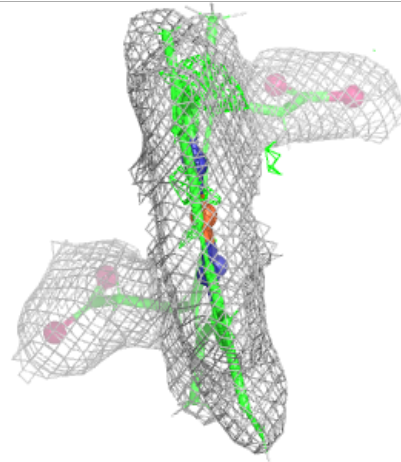
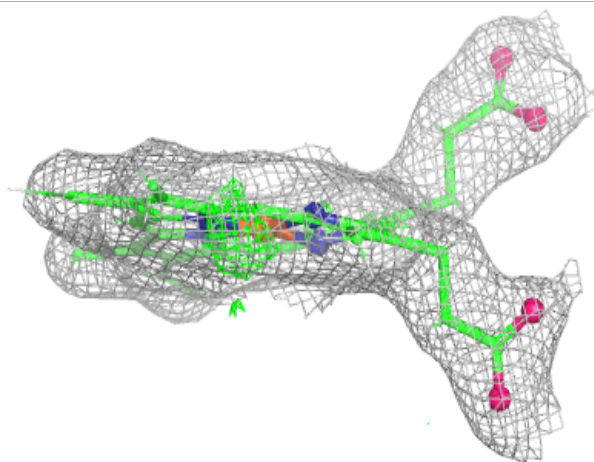
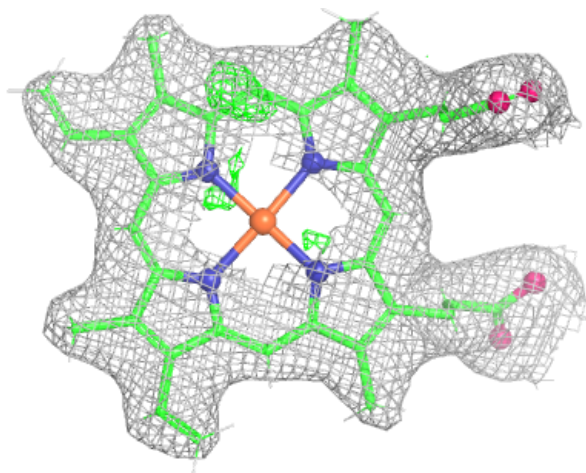
Electron density around CLA C 508:

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



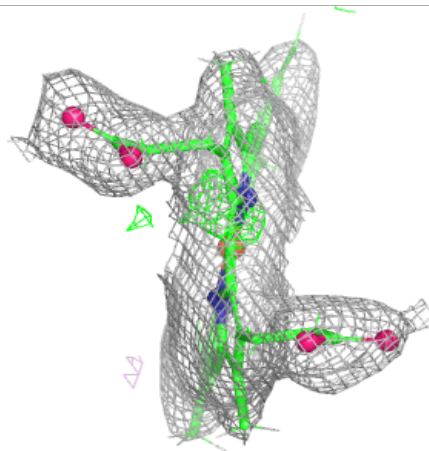
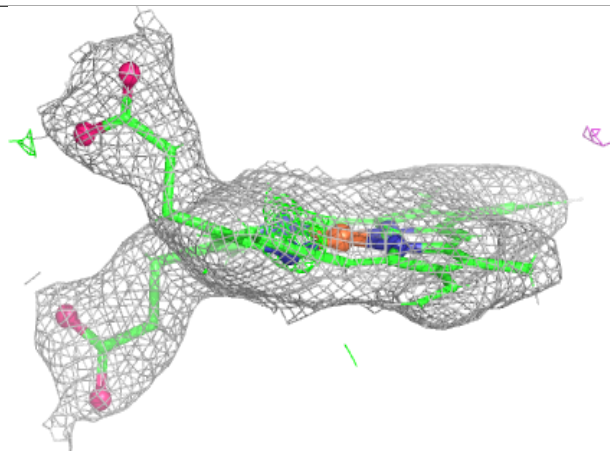
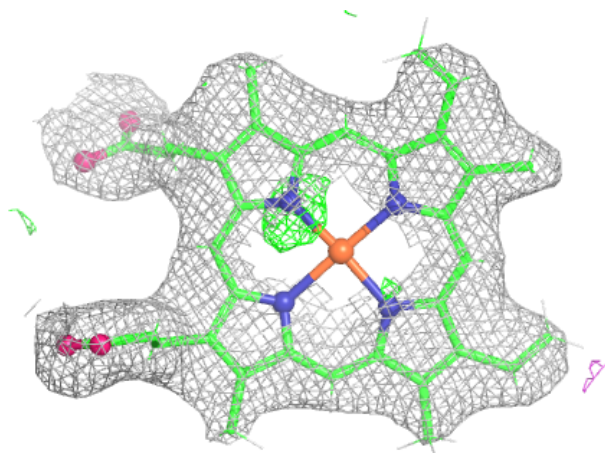
Electron density around HEM F 101:

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



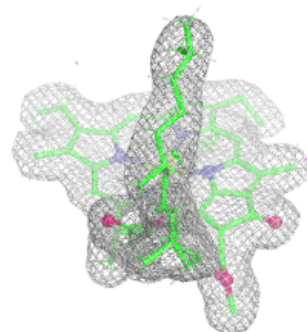
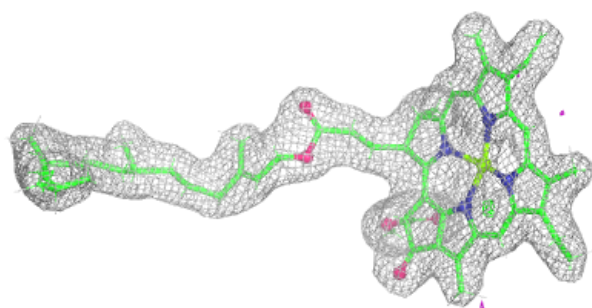
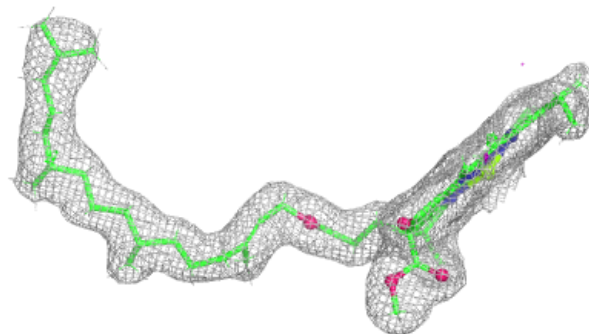
Electron density around HEM f 101:

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

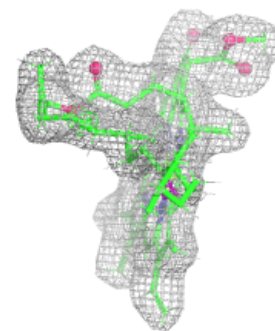
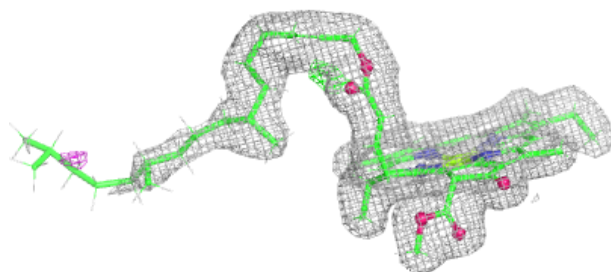
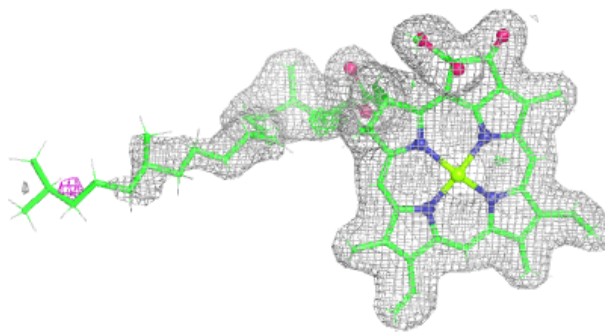


Electron density around CLA D 403:

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

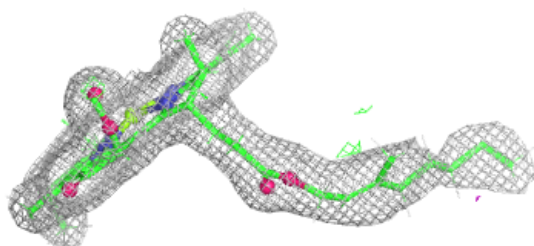
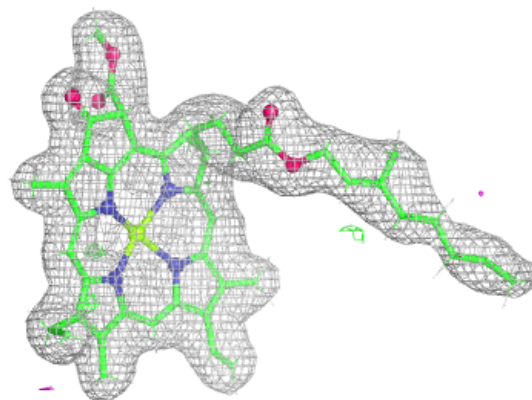
**Electron density around CLA A 606:**

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



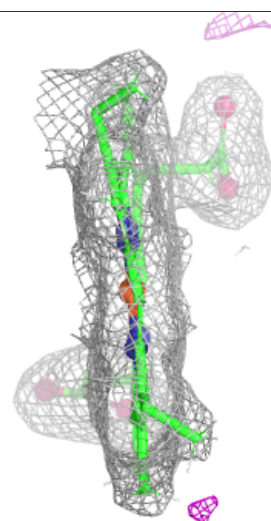
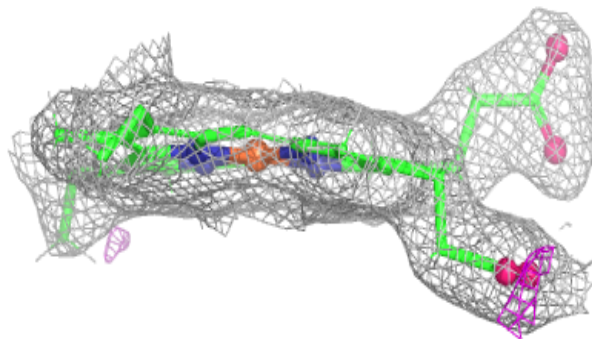
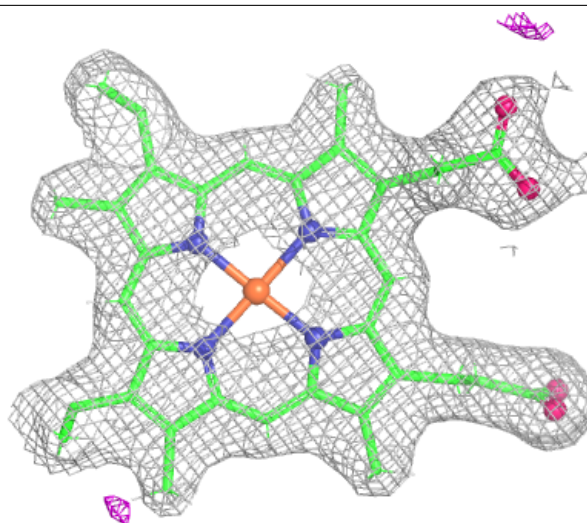
Electron density around CLA A 608:

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



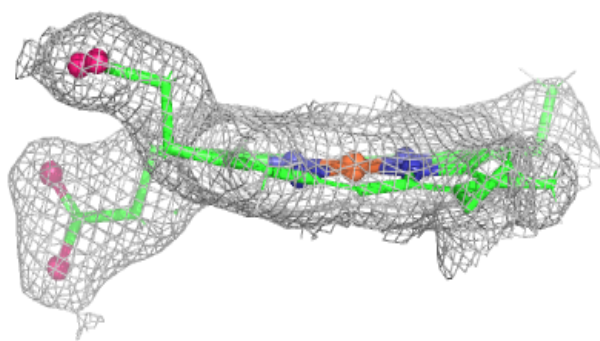
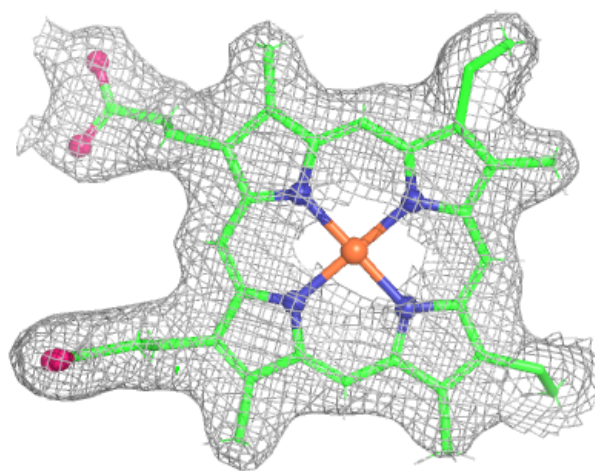
Electron density around HEC V 201:

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



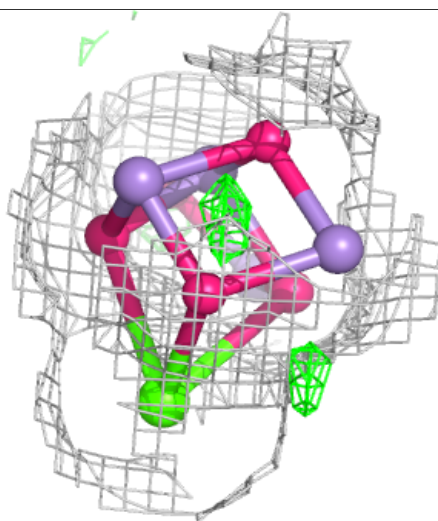
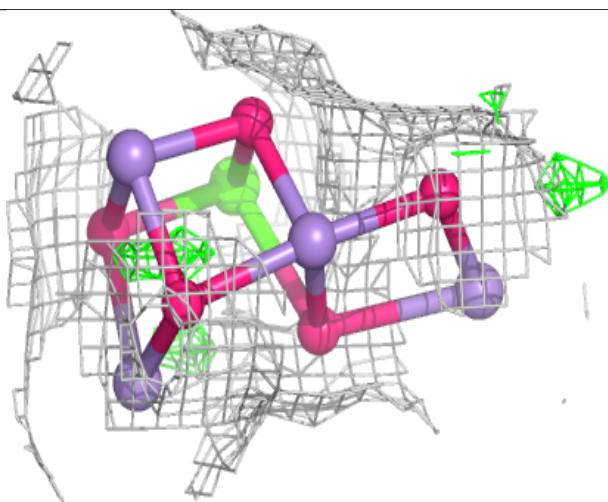
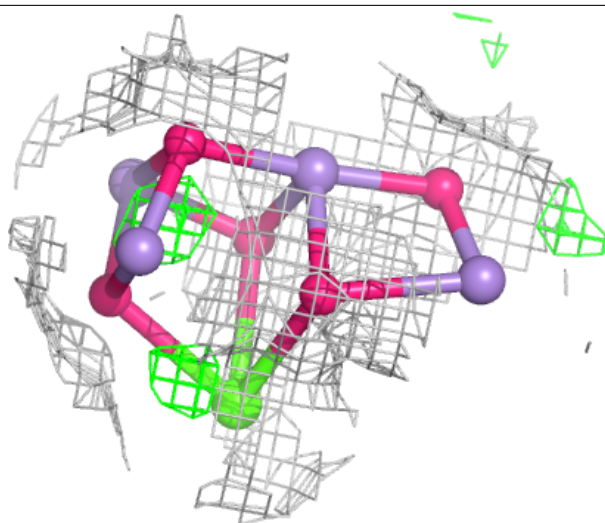
Electron density around HEC v 201:

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



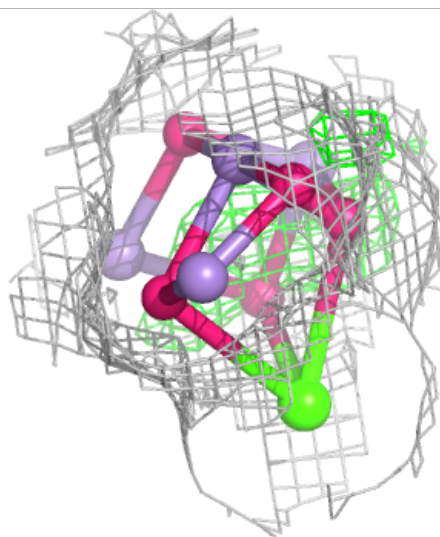
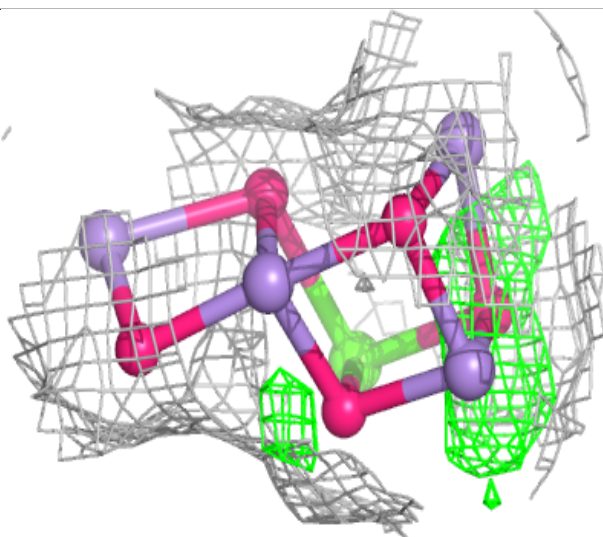
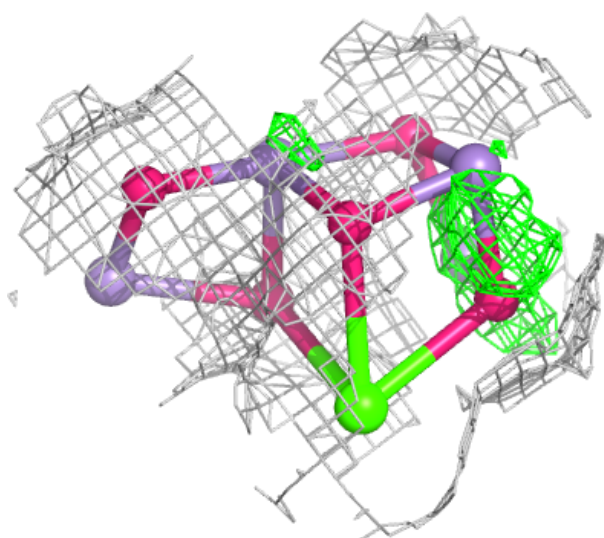
Electron density around OEX a 601:

$2mF_o-DF_c$ (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.