



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 02:24 PM EDT

PDB ID : 9Z35 / pdb_00009z35
Title : RT XFEL structure of two-flash state of Photosystem II (2F, S3 rich) at 1.93 Angstrom obtained from anomalous data at 9.5 keV
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Minnetian, N.M.; Zhang, M.
Deposited on : 2025-11-05
Resolution : 1.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

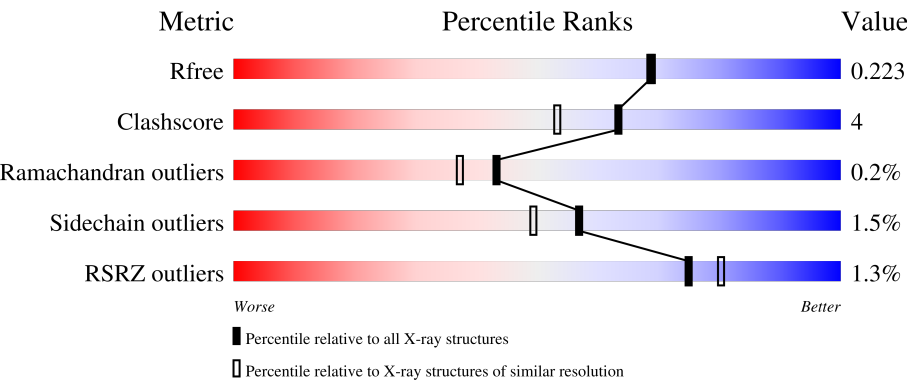
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.93 Å.

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



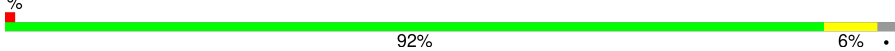
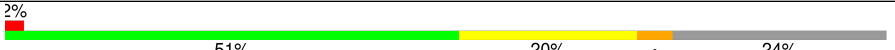
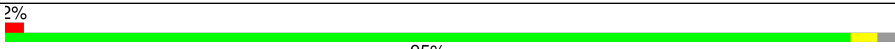
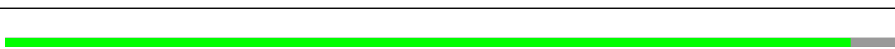
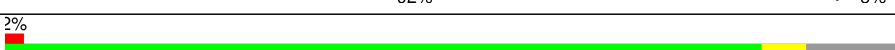
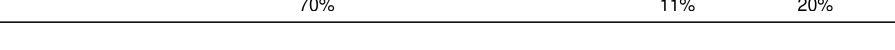
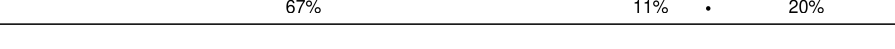
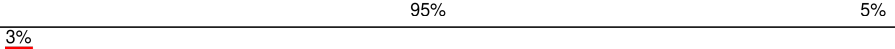
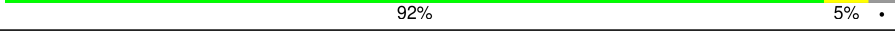
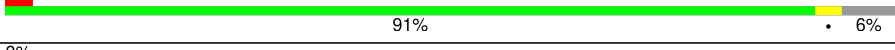
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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

Mol	Chain	Length	Quality of chain
1	A	344	92%6%.
1	a	344	90%6%..
2	B	510	% 92%7%.
2	b	510	% 91%7%.

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	HEC	V	201	X	-	-	-
36	HEC	v	201	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54713 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	69	0
			3152	2055	520	558	19			
1	a	334	Total	C	N	O	S	0	69	0
			3149	2052	520	558	19			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3509	2302	586	607	14			
3	c	451	Total	C	N	O	S	0	12	0
			3583	2343	602	624	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	10	0
			2805	1859	456	478	12			
4	d	341	Total	C	N	O	S	0	11	0
			2811	1863	456	480	12			

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

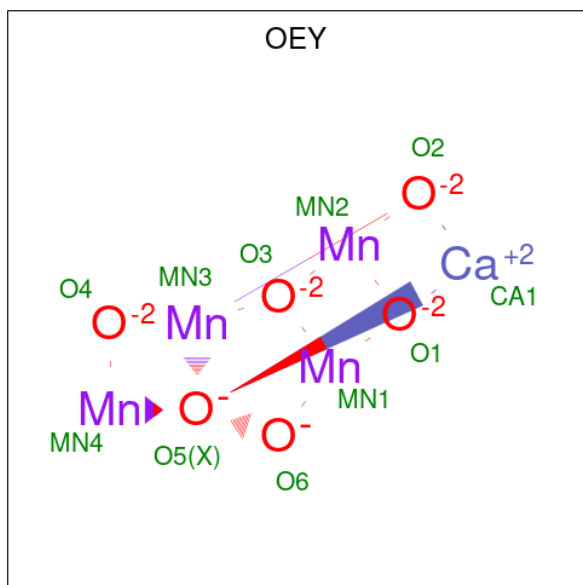
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	28	Total	C	N	O	0	0	0
			221	151	38	32			

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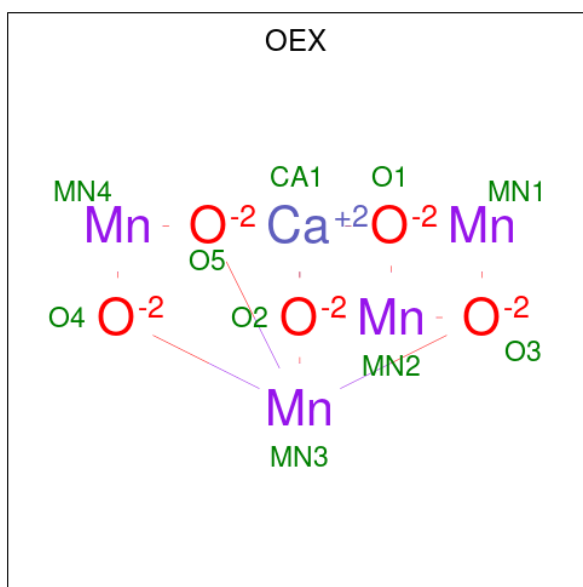
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	r	28	Total	C	N	O	0	0	0
			221	151	38	32			

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
21	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

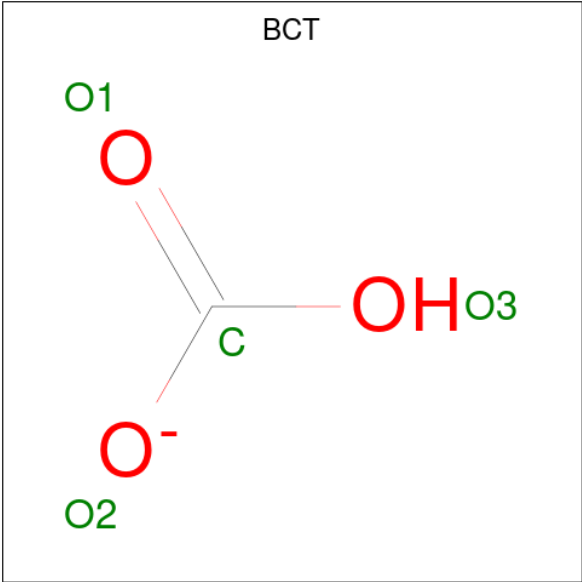
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

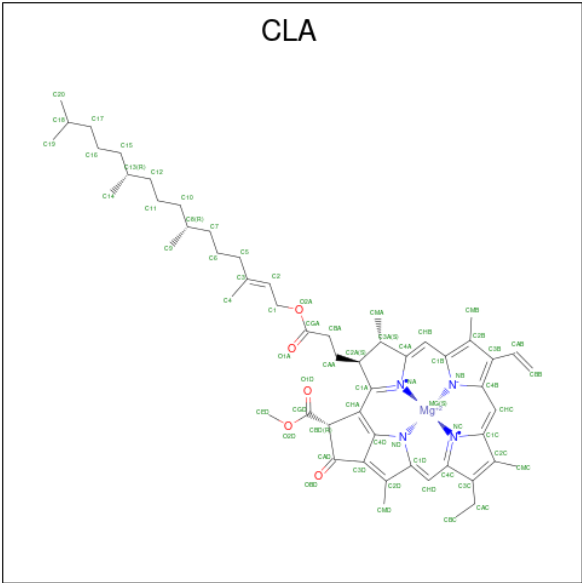
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

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



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

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
26	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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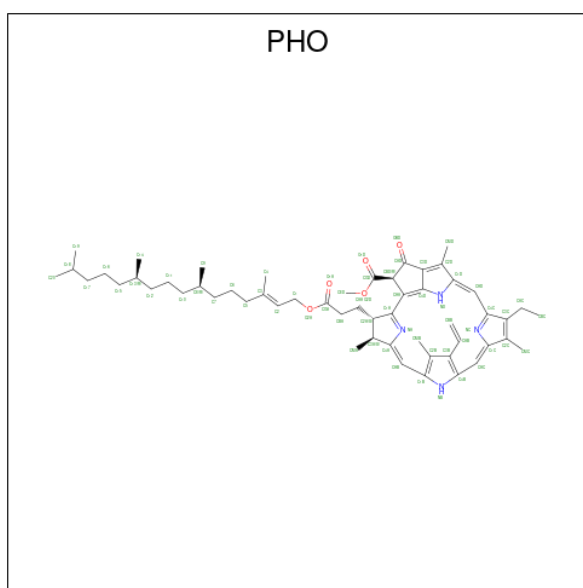
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
26	b	1	Total 65	C 55	Mg 1	N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

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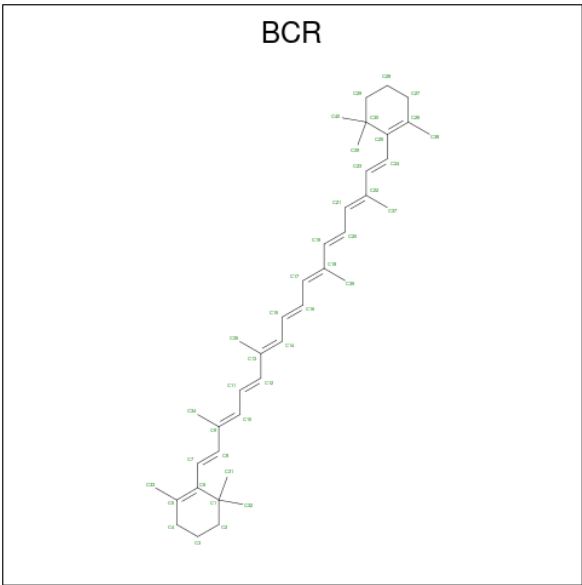
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
26	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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



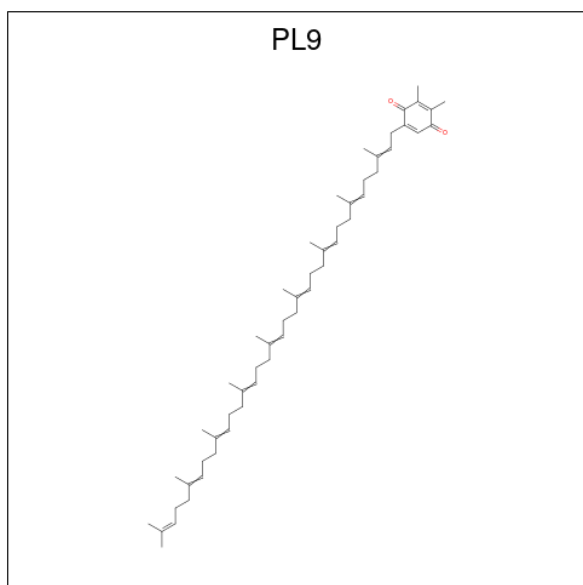
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	D	1	Total C 40 40	0	0
28	H	1	Total C 40 40	0	0
28	K	1	Total C 40 40	0	0
28	T	1	Total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

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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



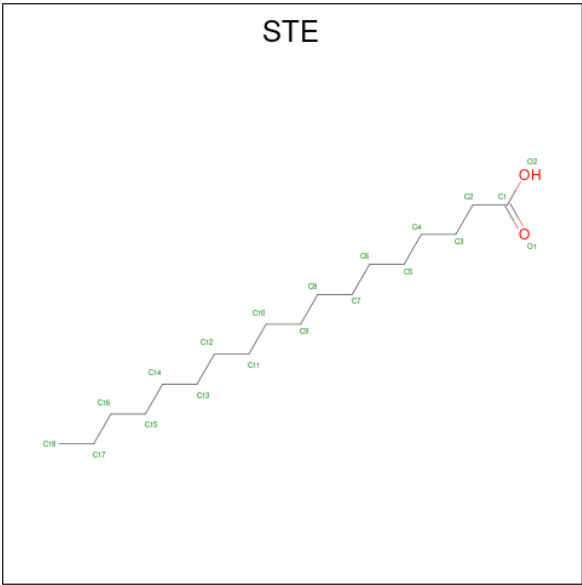
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 55 53 2	0	0
29	D	1	Total C O 55 53 2	0	0

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

- Molecule 30 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	C	1	Total C 7 7	0	0
30	C	1	Total C 10 10	0	0
30	C	1	Total C O 12 10 2	0	0
30	C	1	Total C 16 16	0	0
30	C	1	Total C 14 14	0	0
30	D	1	Total C O 20 18 2	0	0
30	D	1	Total C 9 9	0	0
30	E	1	Total C O 12 10 2	0	0
30	E	1	Total C 12 12	0	0
30	E	1	Total C O 20 18 2	0	0
30	H	1	Total C 18 18	0	0
30	I	1	Total C O 17 15 2	0	0
30	I	1	Total C O 15 13 2	0	0
30	J	1	Total C O 12 10 2	0	0
30	K	1	Total C 14 14	0	0
30	M	1	Total C O 15 13 2	0	0
30	M	1	Total C 10 10	0	0
30	T	1	Total C 16 16	0	0
30	T	1	Total C 15 15	0	0
30	Z	1	Total C 17 17	0	0
30	a	1	Total C O 12 10 2	0	0

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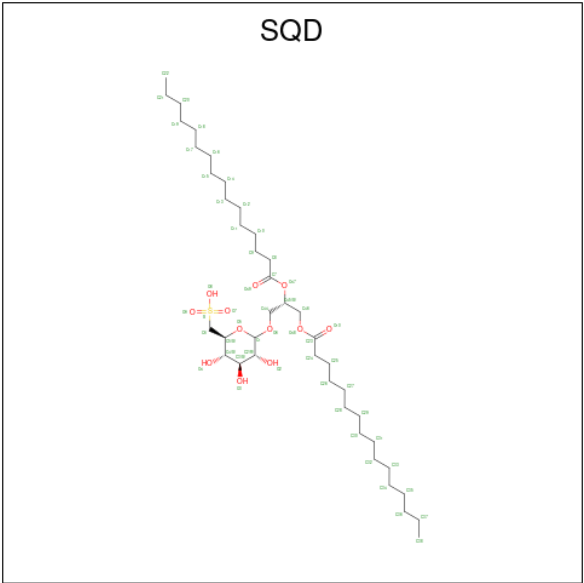
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C 15 15	0	0
30	b	1	Total C O 20 18 2	0	0
30	b	1	Total C O 16 14 2	0	0
30	b	1	Total C 10 10	0	0
30	b	1	Total C 11 11	0	0
30	c	1	Total C 13 13	0	0
30	c	1	Total C 18 18	0	0
30	d	1	Total C O 20 18 2	0	0
30	d	1	Total C O 20 18 2	0	0
30	d	1	Total C O 20 18 2	0	0
30	e	1	Total C 9 9	0	0
30	e	1	Total C 9 9	0	0
30	e	1	Total C O 13 11 2	0	0
30	f	1	Total C 8 8	0	0
30	h	1	Total C 10 10	0	0
30	i	1	Total C O 12 10 2	0	0
30	i	1	Total C 6 6	0	0
30	j	1	Total C O 12 10 2	0	0
30	j	1	Total C 16 16	0	0
30	k	1	Total C O 14 12 2	0	0
30	m	1	Total C O 12 10 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	m	1	Total C 18 18	0	0
30	t	1	Total C O 14 12 2	0	0
30	t	1	Total C 10 10	0	0
30	z	1	Total C 9 9	0	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



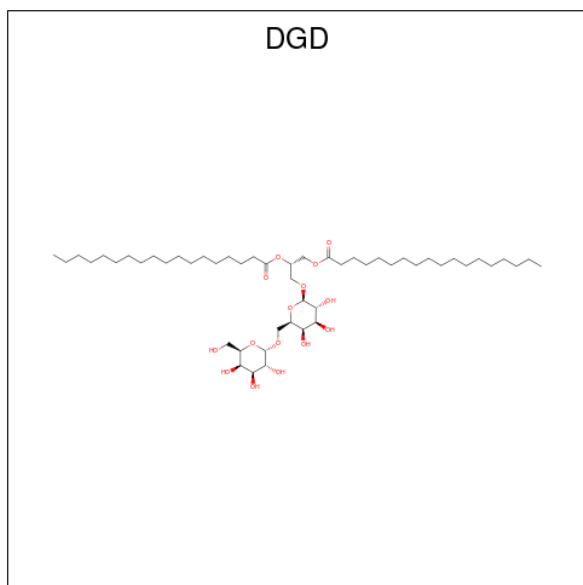
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O S 52 39 12 1	0	0
31	A	1	Total C O S 43 30 12 1	0	0
31	B	1	Total C O S 54 41 12 1	0	0
31	F	1	Total C O S 36 25 10 1	0	0
31	a	1	Total C O S 54 41 12 1	0	0
31	a	1	Total C O S 54 41 12 1	0	0
31	b	1	Total C O S 49 36 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	f	1	Total	C	O	S	0	0
			41	28	12	1		

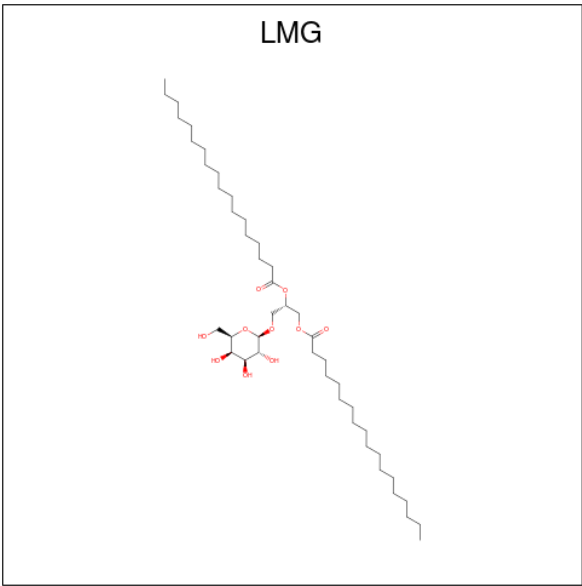
- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: C₄₅H₈₆O₁₀).



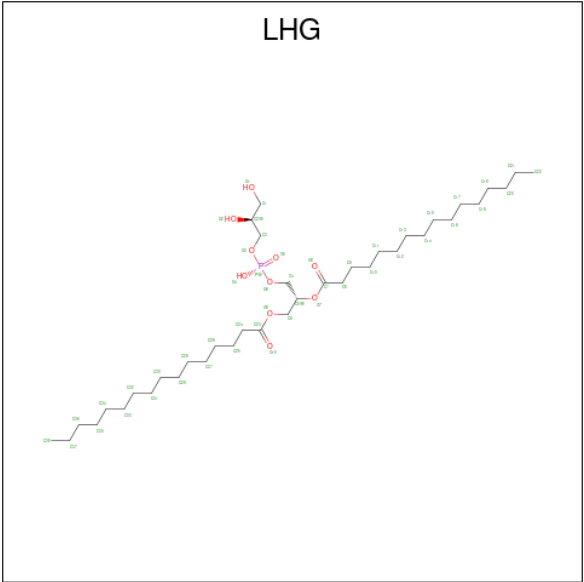
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			45	35	10		
33	C	1	Total	C	O	0	0
			36	26	10		
33	C	1	Total	C	O	0	0
			48	38	10		
33	C	1	Total	C	O	0	0
			48	38	10		
33	D	1	Total	C	O	0	0
			50	40	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	M	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	d	1	Total	C	O	0	0
			44	34	10		
33	m	1	Total	C	O	0	0
			51	41	10		

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



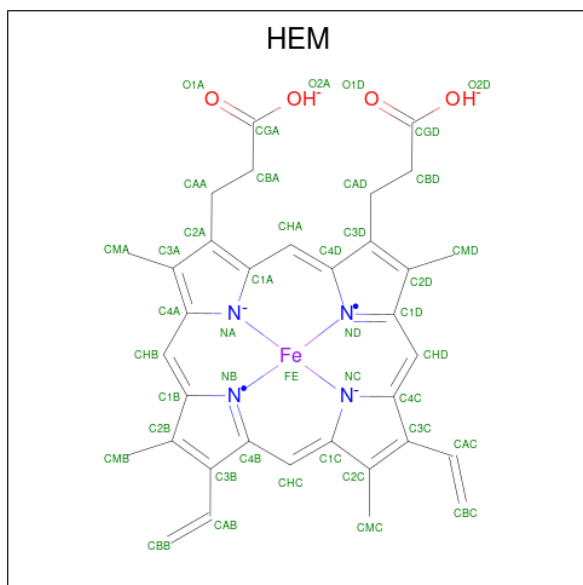
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			47	36	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	E	1	Total	C	O	P	0	0
			49	38	10	1		
34	a	1	Total	C	O	P	0	0
			42	31	10	1		
34	d	1	Total	C	O	P	0	0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

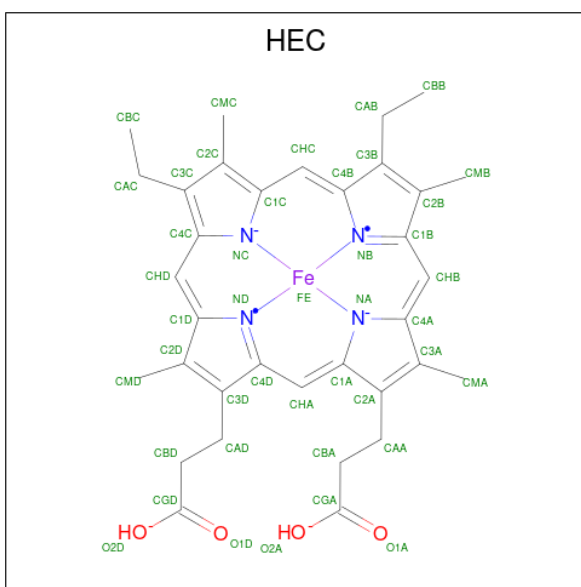
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	1	1	Total	C	O	P	0	0
			49	38	10	1		

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





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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	180	Total O 184 184	0	4
37	B	318	Total O 318 318	0	0
37	C	253	Total O 253 253	0	0
37	D	156	Total O 156 156	0	0
37	E	43	Total O 43 43	0	0
37	F	17	Total O 17 17	0	0
37	H	40	Total O 40 40	0	0
37	I	17	Total O 17 17	0	0
37	J	12	Total O 12 12	0	0
37	K	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	10	Total 10	O 10	0	0
37	M	14	Total 14	O 14	0	0
37	O	146	Total 146	O 146	0	0
37	T	14	Total 14	O 14	0	0
37	U	69	Total 69	O 69	0	0
37	V	97	Total 97	O 97	0	0
37	Y	9	Total 9	O 9	0	0
37	X	14	Total 14	O 14	0	0
37	Z	8	Total 8	O 8	0	0
37	R	1	Total 1	O 1	0	0
37	a	150	Total 154	O 154	0	4
37	b	280	Total 280	O 280	0	0
37	c	224	Total 224	O 224	0	0
37	d	177	Total 177	O 177	0	0
37	e	27	Total 27	O 27	0	0
37	f	10	Total 10	O 10	0	0
37	h	31	Total 31	O 31	0	0
37	i	13	Total 13	O 13	0	0
37	j	10	Total 10	O 10	0	0
37	k	10	Total 10	O 10	0	0
37	l	16	Total 16	O 16	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	14	Total 14	O 14	0	0
37	o	163	Total 163	O 163	0	0
37	t	13	Total 13	O 13	0	0
37	u	86	Total 86	O 86	0	0
37	v	71	Total 71	O 71	0	0
37	y	6	Total 6	O 6	0	0
37	x	9	Total 9	O 9	0	0
37	z	8	Total 8	O 8	0	0
37	r	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

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

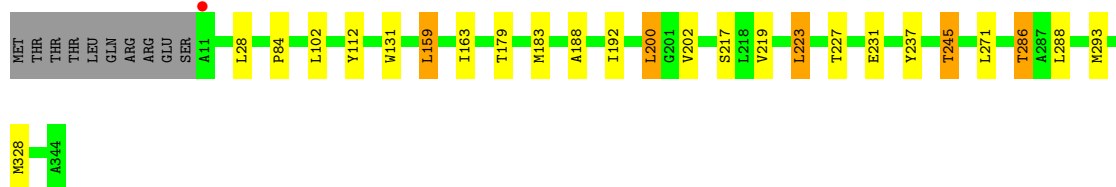
- Molecule 1: Photosystem II protein D1 1

Chain A: 

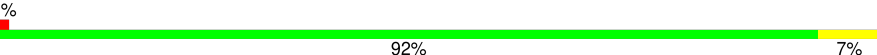


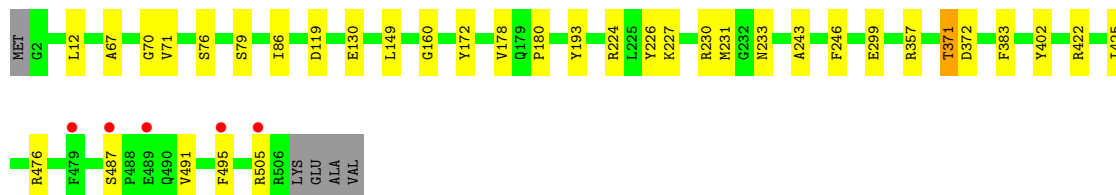
- Molecule 1: Photosystem II protein D1 1

Chain a: 

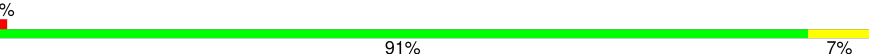


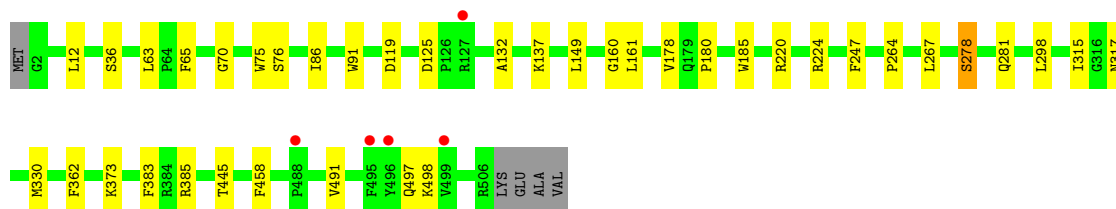
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

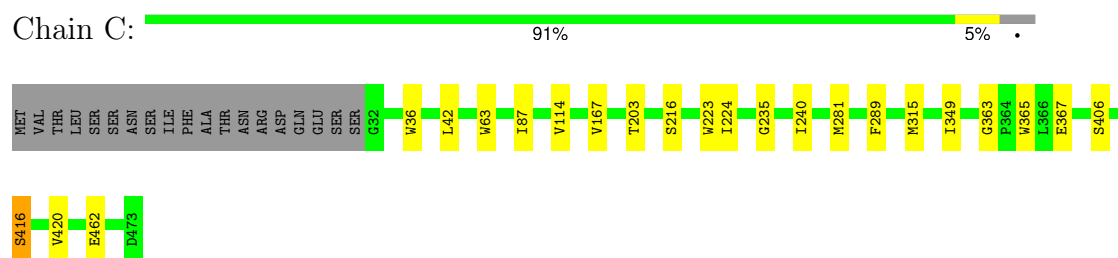


- Molecule 2: Photosystem II CP47 reaction center protein

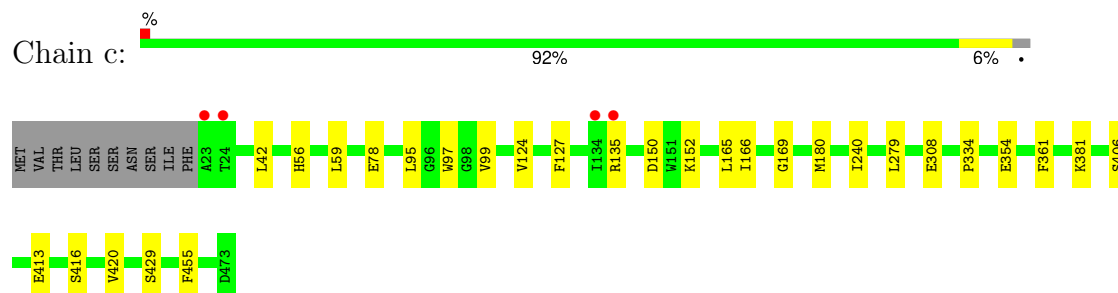
Chain b: 



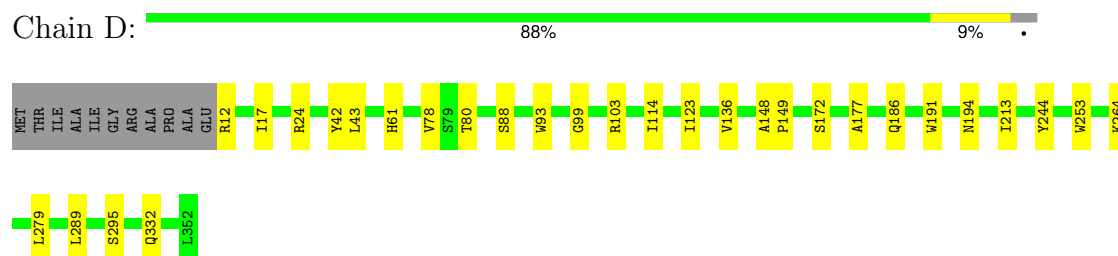
- Molecule 3: Photosystem II CP43 reaction center protein



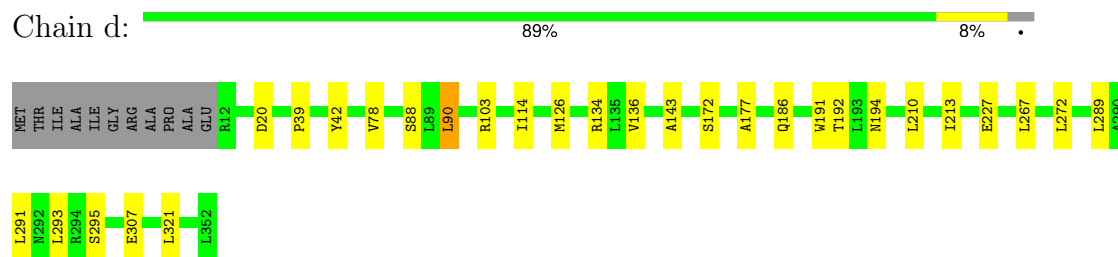
- Molecule 3: Photosystem II CP43 reaction center protein



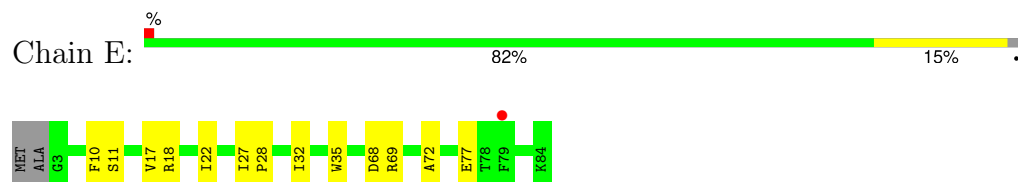
- Molecule 4: Photosystem II D2 protein



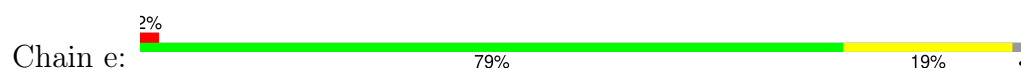
- Molecule 4: Photosystem II D2 protein



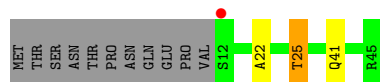
- Molecule 5: Cytochrome b559 subunit alpha



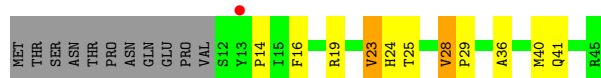
- Molecule 5: Cytochrome b559 subunit alpha



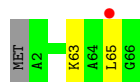
- Molecule 6: Cytochrome b559 subunit beta



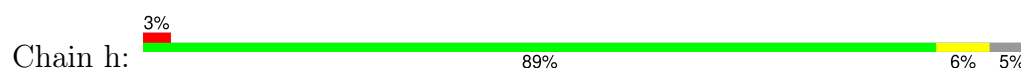
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



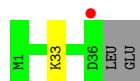
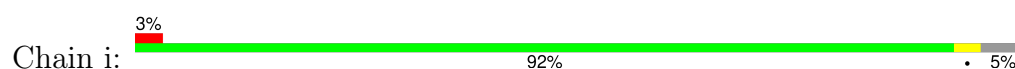
- Molecule 7: Photosystem II reaction center protein H



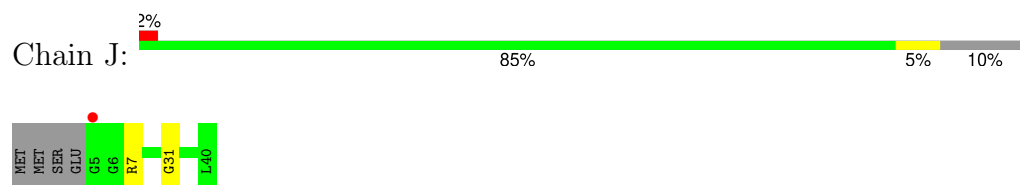
- Molecule 8: Photosystem II reaction center protein I



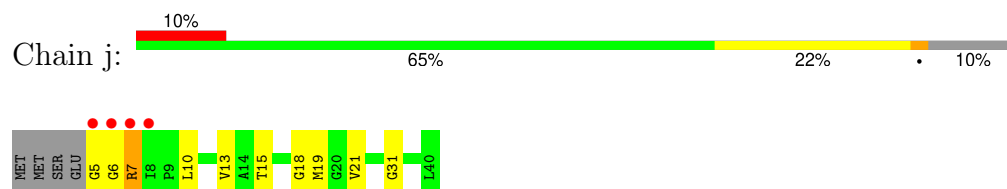
- Molecule 8: Photosystem II reaction center protein I



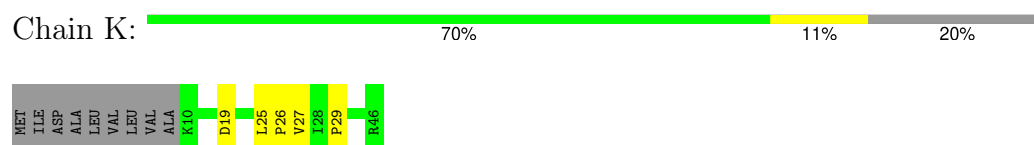
- Molecule 9: Photosystem II reaction center protein J



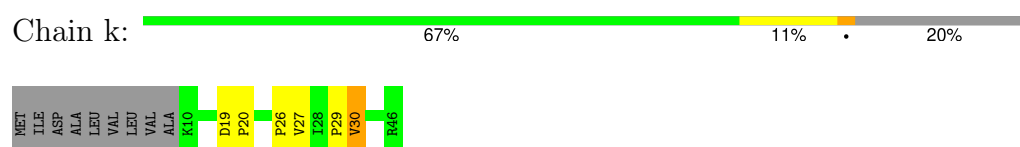
- Molecule 9: Photosystem II reaction center protein J



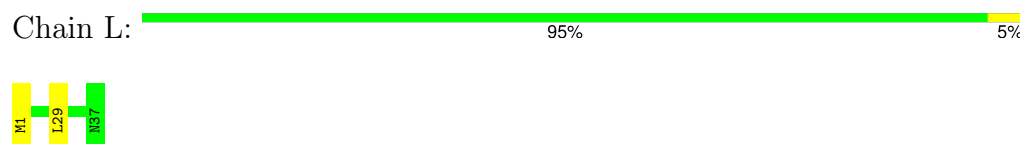
- Molecule 10: Photosystem II reaction center protein K



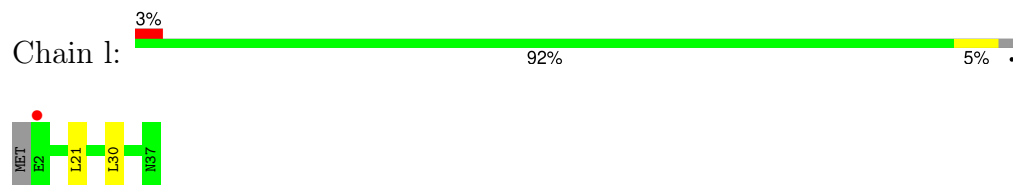
- Molecule 10: Photosystem II reaction center protein K



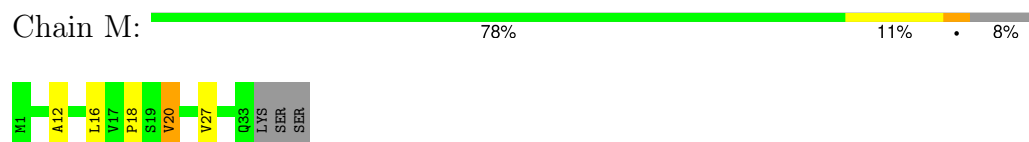
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



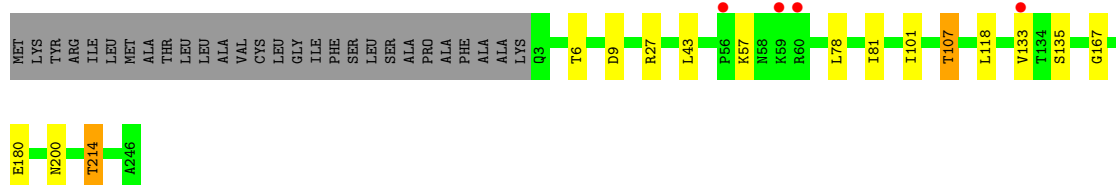
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 14% 11%



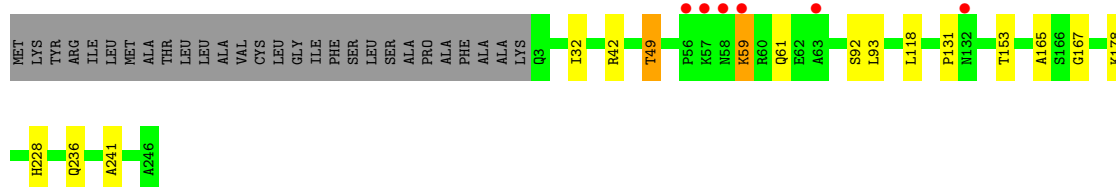
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  84% 5% 10%



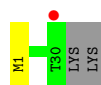
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  84% 5% 10%



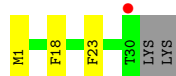
- Molecule 14: Photosystem II reaction center protein T

Chain T:  91% 3% 6%



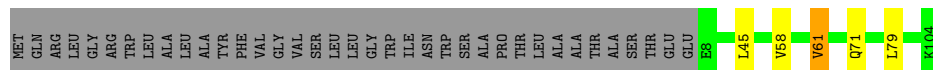
- Molecule 14: Photosystem II reaction center protein T

Chain t:  84% 9% 6%

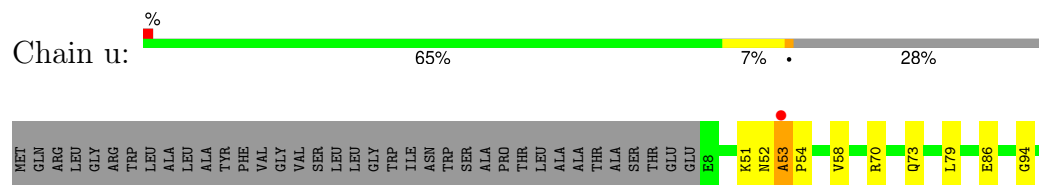


- Molecule 15: Photosystem II 12 kDa extrinsic protein

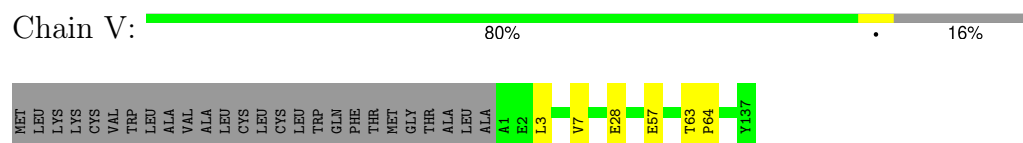
Chain U:  69% 28%



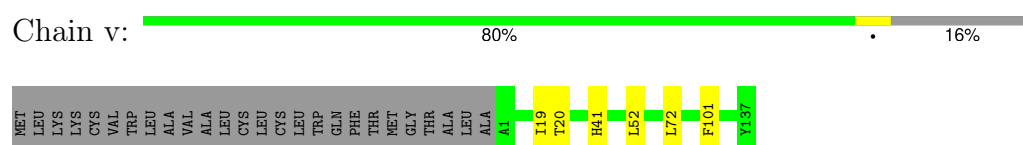
- Molecule 15: Photosystem II 12 kDa extrinsic protein



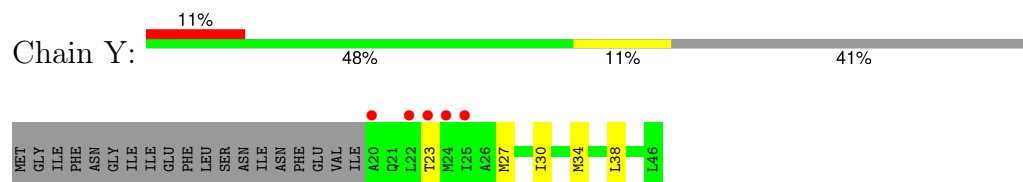
- Molecule 16: Cytochrome c-550



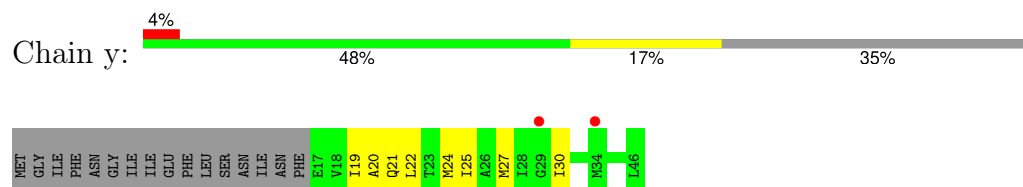
- Molecule 16: Cytochrome c-550



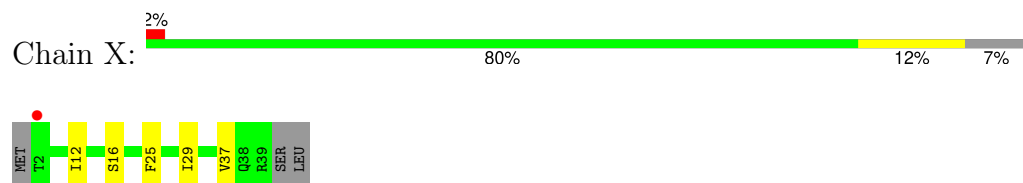
- Molecule 17: Photosystem II reaction center protein Ycf12



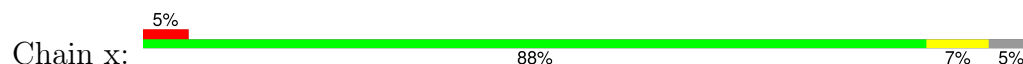
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

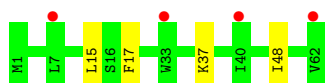


- Molecule 18: Photosystem II reaction center X protein

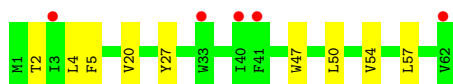
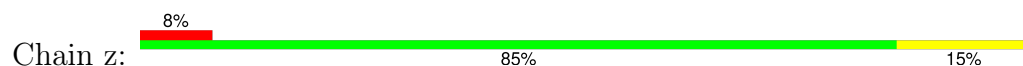




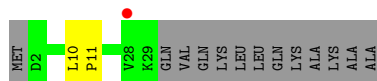
- Molecule 19: Photosystem II reaction center protein Z



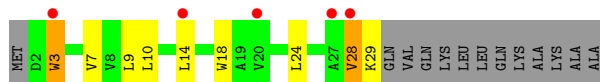
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.53Å 222.82Å 308.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.83 – 1.93 33.83 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.4 (33.83-1.93) 82.7 (33.83-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.28 (at 1.94Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.189 , 0.223 0.189 , 0.223	Depositor DCC
R_{free} test set	5354 reflections (0.85%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	54713	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: PL9, OEY, BCT, FME, STE, OEX, FE2, DGD, HEM, BCR, LMG, HEC, SQD, PHO, CLA, CL, LHG

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	0.31	0/3252	0.46	0/4430
1	a	0.30	0/3249	0.46	0/4426
2	B	0.31	0/4166	0.46	0/5675
2	b	0.29	0/4127	0.45	0/5623
3	C	0.29	0/3625	0.44	0/4935
3	c	0.28	0/3705	0.43	0/5042
4	D	0.32	0/2902	0.48	0/3951
4	d	0.30	0/2911	0.46	0/3963
5	E	0.25	0/688	0.44	0/940
5	e	0.23	0/683	0.42	0/932
6	F	0.27	0/284	0.44	0/387
6	f	0.24	0/284	0.46	0/387
7	H	0.30	0/517	0.47	0/705
7	h	0.25	0/505	0.43	0/689
8	I	0.27	0/293	0.44	0/396
8	i	0.26	0/293	0.36	0/396
9	J	0.24	0/263	0.38	0/356
9	j	0.23	0/263	0.40	0/356
10	K	0.25	0/303	0.44	0/416
10	k	0.23	0/303	0.37	0/416
11	L	0.32	0/311	0.43	0/422
11	l	0.31	0/303	0.42	0/412
12	M	0.30	0/249	0.51	0/341
12	m	0.30	0/244	0.46	0/334
13	O	0.29	0/1904	0.49	0/2585
13	o	0.29	0/1905	0.48	0/2583
14	T	0.30	0/257	0.48	0/349
14	t	0.28	0/255	0.38	0/346
15	U	0.25	0/785	0.43	0/1064
15	u	0.27	0/785	0.47	0/1064
16	V	0.28	0/1085	0.47	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.25	0/1085	0.41	0/1473
17	Y	0.18	0/197	0.34	0/264
17	y	0.20	0/219	0.35	0/294
18	X	0.25	0/284	0.36	0/384
18	x	0.20	0/289	0.32	0/391
19	Z	0.18	0/490	0.41	0/669
19	z	0.18	0/488	0.33	0/666
20	R	0.17	0/227	0.33	0/313
20	r	0.20	0/227	0.37	0/313
All	All	0.29	0/44205	0.45	0/60161

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3152	0	3015	13	0
1	a	3149	0	3006	20	0
2	B	4016	0	3883	27	0
2	b	3984	0	3842	32	0
3	C	3509	0	3426	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	17	0
4	D	2805	0	2702	21	0
4	d	2811	0	2708	20	0
5	E	666	0	651	13	0
5	e	664	0	648	14	0
6	F	275	0	282	3	0
6	f	275	0	282	9	0
7	H	505	0	528	3	0
7	h	493	0	514	3	0
8	I	296	0	311	0	0
8	i	296	0	311	1	0
9	J	257	0	268	1	0
9	j	257	0	268	11	0
10	K	293	0	305	3	0
10	k	293	0	305	3	0
11	L	304	0	316	2	0
11	l	296	0	304	0	0
12	M	256	0	269	4	0
12	m	251	0	267	3	0
13	O	1870	0	1830	10	0
13	o	1874	0	1846	11	0
14	T	258	0	261	1	0
14	t	256	0	256	3	0
15	U	774	0	773	3	0
15	u	774	0	773	7	0
16	V	1064	0	1073	2	0
16	v	1064	0	1073	4	0
17	Y	196	0	217	3	0
17	y	218	0	241	5	0
18	X	281	0	312	4	0
18	x	286	0	314	2	0
19	Z	479	0	516	4	0
19	z	477	0	509	8	0
20	R	221	0	238	1	0
20	r	221	0	238	5	0
21	A	11	0	0	1	0
21	a	11	0	0	0	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	4	0	1	0	0
25	a	4	0	1	0	0
26	A	249	0	264	13	0
26	B	1035	0	1139	28	0
26	C	839	0	922	15	0
26	D	130	0	144	3	0
26	a	260	0	288	6	0
26	b	1035	0	1139	22	0
26	c	839	0	919	15	0
26	d	130	0	144	4	0
27	A	64	0	74	0	0
27	D	64	0	74	2	0
27	a	64	0	74	0	0
27	d	64	0	74	0	0
28	A	40	0	56	0	0
28	B	120	0	168	2	0
28	C	120	0	168	5	0
28	D	40	0	56	1	0
28	H	40	0	56	2	0
28	K	40	0	56	0	0
28	T	40	0	56	3	0
28	a	40	0	56	1	0
28	b	120	0	168	4	0
28	c	80	0	112	1	0
28	d	40	0	56	1	0
28	k	80	0	112	2	0
28	t	40	0	56	3	0
28	x	40	0	56	3	0
29	A	55	0	80	6	0
29	D	55	0	80	1	0
29	a	55	0	80	3	0
29	d	55	0	80	1	0
30	A	45	0	83	3	0
30	B	47	0	70	3	0
30	C	78	0	126	4	0
30	D	29	0	52	4	0
30	E	44	0	74	5	0
30	H	18	0	35	4	0
30	I	32	0	48	1	0
30	J	12	0	16	0	0
30	K	14	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	M	25	0	38	0	0
30	T	31	0	60	4	0
30	Z	17	0	33	2	0
30	a	27	0	42	2	0
30	b	57	0	96	2	0
30	c	31	0	57	0	0
30	d	60	0	105	3	0
30	e	31	0	52	1	0
30	f	8	0	15	0	0
30	h	10	0	19	1	0
30	i	18	0	24	1	0
30	j	28	0	47	1	0
30	k	14	0	20	2	0
30	m	30	0	51	1	0
30	t	24	0	36	0	0
30	z	9	0	14	2	0
31	A	95	0	124	0	0
31	B	54	0	78	4	0
31	F	36	0	46	0	0
31	a	108	0	156	4	0
31	b	49	0	65	0	0
31	f	41	0	49	2	0
32	A	66	0	96	2	0
32	C	186	0	246	3	0
32	H	62	0	82	2	0
32	c	186	0	246	3	0
32	h	62	0	82	1	0
33	B	45	0	60	5	0
33	C	132	0	172	3	0
33	D	101	0	142	6	0
33	M	51	0	72	2	0
33	a	104	0	154	6	0
33	b	55	0	86	1	0
33	c	124	0	172	5	0
33	d	44	0	58	0	0
33	m	51	0	72	3	0
34	B	49	0	74	2	0
34	D	145	0	215	7	0
34	E	49	0	74	1	0
34	a	42	0	57	2	0
34	d	137	0	199	1	0
34	l	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	F	43	0	30	1	0
35	e	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	1	0
37	A	184	0	0	3	0
37	B	318	0	0	8	0
37	C	253	0	0	4	0
37	D	156	0	0	0	0
37	E	43	0	0	1	0
37	F	17	0	0	1	0
37	H	40	0	0	1	0
37	I	17	0	0	0	0
37	J	12	0	0	1	0
37	K	5	0	0	1	0
37	L	10	0	0	0	0
37	M	14	0	0	0	0
37	O	146	0	0	0	0
37	R	1	0	0	0	0
37	T	14	0	0	0	0
37	U	69	0	0	0	0
37	V	97	0	0	1	0
37	X	14	0	0	0	0
37	Y	9	0	0	0	0
37	Z	8	0	0	1	0
37	a	154	0	0	3	0
37	b	280	0	0	9	0
37	c	224	0	0	3	0
37	d	177	0	0	2	0
37	e	27	0	0	0	0
37	f	10	0	0	1	0
37	h	31	0	0	1	0
37	i	13	0	0	0	0
37	j	10	0	0	0	0
37	k	10	0	0	0	0
37	l	16	0	0	1	0
37	m	14	0	0	0	0
37	o	163	0	0	1	0
37	r	2	0	0	0	0
37	t	13	0	0	0	0
37	u	86	0	0	2	0
37	v	71	0	0	1	0
37	x	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	y	6	0	0	1	0
37	z	8	0	0	0	0
All	All	54713	0	53500	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (426) 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)
29:A:612:PL9:H361	6:F:25:THR:HG21	1.57	0.86
2:B:495:PHE:HD2	2:B:505:ARG:HH12	1.20	0.85
30:b:625:STE:H181	30:d:410:STE:H32	1.60	0.84
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.68	0.76
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.69	0.74
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.06	0.73
28:t:101:BCR:HC8	28:t:101:BCR:H311	1.70	0.73
30:I:102:STE:H22	26:b:606:CLA:H192	1.71	0.71
26:a:610:CLA:H111	26:a:610:CLA:H52	1.72	0.71
2:B:224:ARG:HD3	33:D:406:LMG:H292	1.71	0.71
30:A:619:STE:H182	30:A:620:STE:H141	1.73	0.71
26:C:513:CLA:H193	30:C:528:STE:H171	1.73	0.70
26:C:507:CLA:H191	30:C:529:STE:H122	1.72	0.69
26:b:615:CLA:H2	26:b:616:CLA:HBB2	1.74	0.69
26:B:604:CLA:H43	26:B:605:CLA:H2	1.75	0.69
33:C:526:LMG:H191	10:K:27:VAL:HG11	1.74	0.69
26:c:501:CLA:H192	26:c:507:CLA:HBB1	1.76	0.67
26:C:502:CLA:H61	26:C:512:CLA:H42	1.76	0.67
16:v:101:PHE:HB2	37:v:301:HOH:O	1.94	0.66
30:A:619:STE:H161	30:A:620:STE:H121	1.77	0.66
35:e:102:HEM:HHD	35:e:102:HEM:HBC2	1.78	0.65
1:a:102:LEU:H	33:a:617:LMG:H121	1.61	0.65
28:C:521:BCR:H322	19:Z:17:PHE:CE2	2.32	0.65
30:B:624:STE:H22	33:M:101:LMG:HC5	1.79	0.64
3:C:87:ILE:HD11	37:C:744:HOH:O	1.96	0.64
5:E:11:SER:HB3	30:E:103:STE:H122	1.80	0.64
26:b:602:CLA:H43	7:h:45:ILE:HG22	1.80	0.63
2:B:230:ARG:NH2	33:B:620:LMG:HC5	2.14	0.63
26:B:614:CLA:H112	31:B:623:SQD:H371	1.81	0.63
26:b:601:CLA:HAB	26:b:601:CLA:H172	1.80	0.62
31:a:614:SQD:H301	30:k:103:STE:H112	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:861:HOH:O	4:D:332:GLN:HG2	2.00	0.62
1:a:102:LEU:HB2	33:a:617:LMG:H112	1.82	0.62
28:C:521:BCR:HC8	28:C:521:BCR:H321	1.81	0.61
30:T:103:STE:H72	33:m:101:LMG:HC5	1.83	0.61
34:D:409:LHG:H141	34:D:409:LHG:H341	1.83	0.61
26:B:614:CLA:H13	33:M:101:LMG:H421	1.83	0.61
3:C:63:TRP:HZ2	37:C:744:HOH:O	1.83	0.61
2:b:497:GLN:HE22	18:x:38:GLN:H	1.48	0.61
26:A:608:CLA:H172	29:A:612:PL9:H261	1.82	0.60
15:u:86:GLU:H	15:u:86:GLU:CD	2.10	0.60
26:C:506:CLA:H8	28:C:515:BCR:H12C	1.83	0.60
33:B:620:LMG:HC91	33:D:406:LMG:H161	1.83	0.60
2:B:371:THR:HG23	2:B:372:ASP:O	2.02	0.59
26:b:601:CLA:H12	26:b:601:CLA:H71	1.84	0.59
4:D:12:ARG:HB3	4:D:17:ILE:HD11	1.85	0.59
33:c:518:LMG:H312	33:c:518:LMG:H121	1.85	0.58
26:C:504:CLA:H93	32:C:525:DGD:HBT2	1.86	0.58
28:B:618:BCR:H343	37:B:988:HOH:O	2.04	0.58
6:f:14:PRO:HB2	37:f:201:HOH:O	2.03	0.58
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.86	0.58
2:B:149[B]:LEU:HD11	26:B:604:CLA:H112	1.84	0.58
15:U:58:VAL:O	15:U:61:VAL:HG22	2.04	0.57
28:D:404:BCR:H392	28:D:404:BCR:H23C	1.86	0.57
26:B:601:CLA:H122	26:B:601:CLA:H192	1.87	0.57
26:B:615:CLA:H2	26:B:616:CLA:HBB2	1.86	0.57
1:a:231:GLU:HB3	37:a:824:HOH:O	2.05	0.56
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.87	0.56
26:c:511:CLA:H171	19:z:20:VAL:HA	1.88	0.56
19:z:47:TRP:CE3	30:z:101:STE:H61	2.40	0.56
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.86	0.56
13:O:200:ASN:HD22	13:O:214:THR:HG22	1.70	0.56
37:A:786:HOH:O	13:O:107:THR:HG21	2.06	0.56
3:C:114:VAL:HG22	30:C:528:STE:H102	1.88	0.56
4:D:123:ILE:HD11	32:H:102:DGD:HAW2	1.88	0.56
6:f:24:HIS:O	6:f:28:VAL:HG13	2.05	0.55
31:f:101:SQD:H312	18:x:27:VAL:HG11	1.88	0.55
1:A:234:ASN:HD21	34:D:410:LHG:HC11	1.71	0.55
2:B:230:ARG:HH12	33:B:620:LMG:HC1	1.69	0.55
4:d:103:ARG:HH21	5:e:77:GLU:HG3	1.70	0.55
32:A:617:DGD:HE4	2:b:76:SER:HB3	1.88	0.55
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:180:MET:HE1	33:c:523:LMG:HC72	1.89	0.55
2:B:172:TYR:OH	7:H:63:LYS:HE2	2.07	0.55
3:c:42:LEU:HD21	26:c:511:CLA:H2A	1.88	0.55
18:X:25:PHE:O	18:X:29:ILE:HG12	2.07	0.54
1:a:271:LEU:HD21	29:a:612:PL9:HC71	1.88	0.54
2:b:278:SER:C	37:b:701:HOH:O	2.50	0.54
15:u:94:GLY:HA3	37:u:207:HOH:O	2.08	0.54
19:z:5:PHE:HA	19:z:57:LEU:HD23	1.90	0.54
26:c:501:CLA:C3D	26:c:503:CLA:H2	2.38	0.54
34:B:622:LHG:H322	12:M:18:PRO:HB3	1.88	0.53
28:T:101:BCR:H311	28:T:101:BCR:HC8	1.90	0.53
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.90	0.53
19:Z:48:ILE:HD11	30:Z:101:STE:H132	1.91	0.53
19:z:50:LEU:O	19:z:54:VAL:HG23	2.09	0.53
1:a:217:SER:HA	4:d:272:LEU:HD12	1.91	0.53
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.90	0.52
1:a:227:THR:HB	1:a:231:GLU:HG3	1.91	0.52
3:c:97:TRP:HE1	33:c:518:LMG:HC91	1.75	0.52
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.45	0.52
4:d:186:GLN:HB2	26:d:402:CLA:HBC1	1.92	0.52
17:Y:34:MET:HE2	17:Y:38:LEU:HD11	1.90	0.52
30:D:411:STE:H22	18:X:12:ILE:HD13	1.91	0.52
33:c:523:LMG:H292	33:c:523:LMG:H112	1.91	0.52
3:C:420:VAL:HA	37:C:607:HOH:O	2.10	0.52
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.75	0.52
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.51
26:B:610:CLA:H122	26:B:615:CLA:HAA1	1.93	0.51
9:j:15:THR:HG22	9:j:19:MET:HE2	1.92	0.51
3:C:281:MET:HG3	33:C:522:LMG:H392	1.91	0.51
5:e:8:ARG:HG2	5:e:13:ILE:HG13	1.91	0.51
2:B:12:LEU:HB2	26:B:612:CLA:HMC2	1.92	0.51
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.93	0.51
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.93	0.51
2:B:119:ASP:H	11:L:1:MET:HE1	1.76	0.51
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.46	0.51
3:c:56:HIS:HA	3:c:59:LEU:HD12	1.93	0.51
26:D:402:CLA:H192	33:D:407:LMG:H242	1.94	0.50
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.11	0.50
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.94	0.50
1:A:227:THR:HB	1:A:231:GLU:HG3	1.94	0.50
2:B:476:ARG:HG2	37:B:817:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.94	0.50
2:b:36:SER:OG	28:b:618:BCR:H362	2.11	0.50
26:B:613:CLA:H51	34:D:410:LHG:H351	1.93	0.50
3:C:216:SER:HB2	33:C:522:LMG:HC72	1.92	0.50
5:E:68:ASP:O	5:E:72:ALA:HB2	2.12	0.50
5:e:17:VAL:H	9:j:7:ARG:NE	2.10	0.50
17:y:27:MET:O	17:y:30:ILE:HG22	2.12	0.50
3:c:169:GLY:HA3	37:c:603:HOH:O	2.12	0.50
26:C:509:CLA:HBB1	26:C:509:CLA:HMB1	1.94	0.49
16:V:28:GLU:HG2	37:V:366:HOH:O	2.11	0.49
28:t:101:BCR:H23C	28:t:101:BCR:H382	1.94	0.49
26:B:610:CLA:HHC	26:B:610:CLA:HBB1	1.94	0.49
4:D:99:GLY:HA3	30:D:411:STE:H32	1.94	0.49
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.49
35:e:102:HEM:HHC	35:e:102:HEM:HBB2	1.94	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.49
4:D:279:LEU:HD22	27:D:401:PHO:HBC3	1.95	0.49
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.48	0.49
33:B:620:LMG:HC92	33:B:620:LMG:H122	1.94	0.49
30:T:102:STE:H101	30:T:102:STE:H72	1.48	0.48
3:C:203:THR:O	3:C:235:GLY:HA3	2.14	0.48
2:b:264:PRO:HG2	2:b:267:LEU:HD22	1.94	0.48
17:y:20:ALA:HB3	37:y:103:HOH:O	2.13	0.48
17:y:20:ALA:O	17:y:24:MET:HG2	2.13	0.48
5:e:81:GLU:O	5:e:84:LYS:HE2	2.14	0.48
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.95	0.48
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.96	0.48
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.96	0.48
29:a:612:PL9:H461	4:d:39:PRO:HG3	1.96	0.48
3:c:429:SER:HA	32:c:520:DGD:HBW2	1.95	0.48
2:b:65:PHE:HE1	26:b:604:CLA:HED2	1.78	0.47
20:r:24:LEU:O	20:r:28:VAL:HG23	2.13	0.47
13:O:27:ARG:O	13:O:27:ARG:HG2	2.15	0.47
26:b:616:CLA:H91	28:b:619:BCR:H14C	1.97	0.47
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.49	0.47
4:D:93:TRP:HB3	30:D:411:STE:H51	1.96	0.47
30:H:103:STE:H181	37:H:240:HOH:O	2.14	0.47
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.96	0.47
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.95	0.47
2:b:149:LEU:HD11	26:b:604:CLA:H111	1.96	0.47
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:503:CLA:H203	26:c:510:CLA:HAB	1.96	0.47
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.97	0.47
5:e:80:LEU:HA	5:e:83:LEU:HD23	1.96	0.47
6:f:16:PHE:HB2	31:f:101:SQD:H82	1.95	0.47
15:u:70:ARG:NH1	15:u:73:GLN:HE21	2.12	0.47
26:B:613:CLA:H192	34:D:410:LHG:H202	1.96	0.47
26:C:508:CLA:H192	32:C:524:DGD:HAT2	1.97	0.47
26:b:613:CLA:H203	34:d:407:LHG:H211	1.97	0.47
26:b:615:CLA:H2	26:b:616:CLA:CBB	2.44	0.47
26:A:607:CLA:HMB1	26:A:607:CLA:HBB1	1.97	0.47
26:B:614:CLA:H43	31:B:623:SQD:H132	1.96	0.47
29:a:612:PL9:H322	29:a:612:PL9:H301	1.80	0.47
33:D:406:LMG:H111	33:D:406:LMG:H321	1.97	0.47
3:c:127:PHE:HA	26:c:511:CLA:H201	1.97	0.47
4:d:134:ARG:HG2	30:d:406:STE:H41	1.96	0.47
1:A:121:LEU:HD11	26:C:505:CLA:H121	1.97	0.47
16:V:57:GLU:CD	16:V:57:GLU:H	2.23	0.47
26:b:609:CLA:H141	26:b:609:CLA:H161	1.63	0.47
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.97	0.46
5:e:15:THR:OG1	9:j:6:GLY:HA2	2.15	0.46
3:C:462:GLU:HG2	37:C:821:HOH:O	2.15	0.46
26:d:403:CLA:H42	7:h:43:LEU:HD11	1.96	0.46
26:A:608:CLA:H202	26:A:608:CLA:H161	1.79	0.46
32:A:617:DGD:HD5	2:b:75:TRP:HB3	1.98	0.46
2:B:227:LYS:HE3	33:B:620:LMG:O3	2.15	0.46
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.50	0.46
28:T:101:BCR:HC7	37:b:980:HOH:O	2.16	0.46
4:d:192:THR:HG23	26:d:402:CLA:HBC2	1.97	0.46
2:b:445:THR:HA	37:b:702:HOH:O	2.15	0.46
3:c:381:LYS:HG3	37:c:710:HOH:O	2.15	0.46
5:e:18:ARG:H	9:j:7:ARG:NH2	2.13	0.46
32:h:101:DGD:HE5	37:h:216:HOH:O	2.14	0.46
26:C:506:CLA:H91	26:C:506:CLA:H111	1.66	0.46
6:F:22:ALA:C	37:F:201:HOH:O	2.57	0.46
26:c:512:CLA:H202	26:c:512:CLA:H161	1.78	0.46
19:Z:15:LEU:HD23	37:Z:207:HOH:O	2.15	0.46
6:f:36:ALA:O	6:f:40:MET:HG3	2.16	0.46
4:D:186:GLN:HB2	26:D:402:CLA:HBC1	1.98	0.46
4:D:194:ASN:HA	4:D:295:SER:OG	2.15	0.46
19:Z:37:LYS:HZ3	30:Z:101:STE:H51	1.80	0.46
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:610:CLA:H41	26:A:610:CLA:H61	1.69	0.46
32:H:102:DGD:HB21	32:H:102:DGD:HB51	1.83	0.46
34:a:615:LHG:HC81	30:e:104:STE:H31	1.98	0.46
26:B:613:CLA:HBB1	26:B:613:CLA:HMB1	1.96	0.46
4:d:267:LEU:C	4:d:267:LEU:HD23	2.40	0.46
10:k:26:PRO:O	10:k:29:PRO:HD2	2.16	0.46
5:E:10:PHE:HB3	30:E:103:STE:H161	1.98	0.46
26:B:609:CLA:HBC1	30:H:103:STE:H51	1.98	0.45
28:T:101:BCR:H382	28:T:101:BCR:H23C	1.98	0.45
26:c:508:CLA:H152	26:c:508:CLA:H112	1.54	0.45
26:B:605:CLA:HHC	26:B:605:CLA:HBB1	1.98	0.45
26:b:610:CLA:H11	26:b:612:CLA:H191	1.98	0.45
28:b:618:BCR:H371	28:b:618:BCR:H24C	1.80	0.45
26:A:614:CLA:HHC	26:A:614:CLA:HBB1	1.99	0.45
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.99	0.45
2:b:137:LYS:HE2	37:b:746:HOH:O	2.16	0.45
5:e:84:LYS:HE3	5:e:84:LYS:HB2	1.68	0.45
13:o:92:SER:HB3	13:o:131:PRO:HA	1.98	0.45
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.99	0.45
5:E:17:VAL:HG12	37:J:210:HOH:O	2.16	0.45
5:E:18:ARG:O	5:E:18:ARG:HG2	2.17	0.45
1:a:159[A]:LEU:O	1:a:163[A]:ILE:HG12	2.17	0.45
33:a:617:LMG:H301	33:a:617:LMG:H352	1.98	0.45
37:B:1008:HOH:O	33:a:617:LMG:H382	2.16	0.45
30:D:411:STE:H102	18:X:16:SER:HB3	1.99	0.45
9:j:18:GLY:HA3	28:k:101:BCR:H371	1.99	0.45
1:A:271:LEU:HD11	29:A:612:PL9:HC71	1.99	0.45
4:D:61:HIS:HE1	4:D:80:THR:O	2.00	0.45
13:O:133:VAL:C	13:O:135:SER:H	2.24	0.45
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.70	0.45
26:A:607:CLA:H192	26:A:607:CLA:H162	1.71	0.44
2:b:298:LEU:HD23	2:b:298:LEU:HA	1.78	0.44
9:j:18:GLY:O	9:j:21:VAL:HG22	2.17	0.44
1:A:183[B]:MET:HA	26:A:607:CLA:HMD1	2.00	0.44
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.98	0.44
26:A:614:CLA:H141	26:A:614:CLA:H161	1.68	0.44
34:a:615:LHG:HC41	34:a:615:LHG:HC2	1.98	0.44
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.00	0.44
2:B:487:SER:HB3	37:B:925:HOH:O	2.18	0.44
33:D:407:LMG:H141	33:D:407:LMG:H171	1.64	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.47	0.44
13:O:180:GLU:CD	13:O:180:GLU:H	2.26	0.44
33:a:617:LMG:H371	33:a:617:LMG:H342	1.57	0.44
3:c:166:ILE:HA	37:c:603:HOH:O	2.17	0.44
26:c:506:CLA:H142	26:c:506:CLA:H72	1.99	0.44
29:A:612:PL9:H33	4:D:42:TYR:HB2	2.00	0.44
30:C:516:STE:H82	30:C:516:STE:H111	1.72	0.44
33:c:523:LMG:H371	33:c:523:LMG:H402	1.76	0.44
5:e:17:VAL:HB	9:j:7:ARG:HH21	1.82	0.44
31:B:623:SQD:H442	14:t:23:PHE:CD1	2.53	0.44
2:b:281:GLN:HB3	37:b:701:HOH:O	2.18	0.44
30:j:102:STE:H71	30:j:102:STE:H41	1.74	0.44
3:C:315:MET:HE2	3:C:365:TRP:CZ3	2.53	0.44
1:a:286:THR:HG23	26:a:607:CLA:HED3	1.99	0.44
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.00	0.44
26:C:505:CLA:H162	26:C:505:CLA:H193	1.71	0.44
5:E:28:PRO:O	5:E:32:ILE:HG12	2.17	0.44
30:k:103:STE:H22	30:k:103:STE:H52	1.61	0.44
12:m:17:VAL:HB	12:m:18:PRO:HD3	2.00	0.44
2:b:12:LEU:HB2	26:b:612:CLA:HMC2	2.00	0.44
4:d:126:MET:HE3	4:d:143:ALA:O	2.17	0.44
14:t:18:PHE:HB2	28:t:101:BCR:HC8	2.00	0.44
26:A:607:CLA:HBD	26:A:614:CLA:HAC2	1.99	0.43
26:B:614:CLA:H201	30:B:624:STE:H122	1.99	0.43
1:A:227:THR:HB	1:A:231:GLU:CG	2.48	0.43
31:a:614:SQD:H261	31:a:614:SQD:H292	1.51	0.43
26:B:611:CLA:H72	26:B:611:CLA:H112	1.72	0.43
31:B:623:SQD:H382	31:B:623:SQD:H352	1.84	0.43
10:K:26:PRO:O	10:K:29:PRO:HD2	2.19	0.43
31:a:616:SQD:H302	31:a:616:SQD:H331	1.67	0.43
2:b:458:PHE:HB3	26:b:604:CLA:HBC2	2.01	0.43
37:A:783:HOH:O	13:O:107:THR:HG22	2.18	0.43
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.18	0.43
26:B:614:CLA:H161	26:B:614:CLA:H192	1.69	0.43
3:C:36:TRP:CZ3	34:D:409:LHG:HC92	2.54	0.43
5:e:68:ASP:O	5:e:72:ALA:HB2	2.18	0.43
12:m:8:LEU:HD22	14:t:1:FME:HE3	1.99	0.43
20:r:29:LYS:HE2	20:r:29:LYS:HB2	1.77	0.43
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.43
30:T:102:STE:H81	30:T:102:STE:H51	1.44	0.43
20:R:10:LEU:HB3	20:R:11:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:135:ARG:HD3	19:z:27:TYR:CD1	2.53	0.43
30:i:101:STE:H92	30:i:101:STE:H61	1.91	0.43
9:j:7:ARG:H	9:j:7:ARG:HD3	1.84	0.43
29:A:612:PL9:H251	29:A:612:PL9:H271	1.70	0.43
1:a:202:VAL:HG11	26:a:608:CLA:C3D	2.49	0.43
2:b:119:ASP:HB3	37:l:205:HOH:O	2.18	0.43
6:f:19:ARG:O	6:f:23:VAL:HG13	2.18	0.43
19:z:4:LEU:HD23	19:z:57:LEU:HD21	2.00	0.43
26:B:602:CLA:HMB3	37:B:718:HOH:O	2.17	0.43
3:c:95:LEU:HD21	26:c:501:CLA:OBD	2.19	0.43
1:A:183[A]:MET:HA	26:A:607:CLA:HMD1	2.00	0.43
30:A:619:STE:H101	30:A:619:STE:H72	1.59	0.43
26:B:614:CLA:H62	26:B:614:CLA:H41	1.68	0.43
6:f:28:VAL:HG22	6:f:29:PRO:HD3	2.00	0.43
3:C:42:LEU:HD21	26:C:511:CLA:H2A	2.01	0.43
1:a:219:VAL:O	1:a:223:LEU:HD13	2.19	0.43
4:d:307:GLU:HG3	37:d:600:HOH:O	2.19	0.43
10:k:20:PRO:HB3	17:y:21:GLN:HG3	2.00	0.43
13:o:32:ILE:HG13	13:o:93:LEU:HD11	2.01	0.43
26:A:608:CLA:H102	26:A:608:CLA:H61	1.82	0.42
1:a:183[A]:MET:HA	26:a:607:CLA:HMD1	2.00	0.42
28:a:611:BCR:H20C	28:a:611:BCR:H361	1.80	0.42
26:b:603:CLA:H142	26:b:603:CLA:H111	1.76	0.42
26:B:609:CLA:H141	26:B:609:CLA:H161	1.75	0.42
27:D:401:PHO:HBC2	27:D:401:PHO:HHD	2.01	0.42
5:E:35:TRP:HE1	30:E:104:STE:H162	1.83	0.42
26:a:613:CLA:H203	26:a:613:CLA:H162	1.88	0.42
29:A:612:PL9:H422	29:A:612:PL9:H401	1.68	0.42
2:B:299[B]:GLU:HG3	2:B:402:TYR:HD1	1.84	0.42
5:E:18:ARG:C	37:E:201:HOH:O	2.61	0.42
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.01	0.42
2:b:91:TRP:HE1	30:b:621:STE:H62	1.85	0.42
13:o:59:LYS:HB2	13:o:61:GLN:HG2	2.01	0.42
26:B:612:CLA:H193	26:B:613:CLA:CBB	2.50	0.42
26:C:508:CLA:H122	26:C:508:CLA:H161	1.63	0.42
26:b:602:CLA:HBB1	37:b:788:HOH:O	2.18	0.42
26:c:510:CLA:H142	26:c:510:CLA:H111	1.79	0.42
15:u:51:LYS:HB2	15:u:51:LYS:HE2	1.64	0.42
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.90	0.42
2:b:185:TRP:HB3	26:b:601:CLA:HMA3	2.02	0.42
2:b:498:LYS:HE3	4:d:20:ASP:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:404:BCR:H392	28:d:404:BCR:H23C	2.01	0.42
26:B:610:CLA:HHC	26:B:610:CLA:CBB	2.50	0.42
37:a:802:HOH:O	5:e:61:ARG:HA	2.20	0.42
15:u:52:ASN:C	37:u:201:HOH:O	2.63	0.42
28:b:617:BCR:H322	33:m:101:LMG:H111	2.02	0.42
26:c:510:CLA:H61	26:c:510:CLA:H2	1.78	0.42
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.02	0.42
31:a:614:SQD:H301	31:a:614:SQD:H332	1.68	0.42
2:b:86:ILE:H	2:b:86:ILE:HG13	1.60	0.42
3:c:150:ASP:OD2	3:c:152:LYS:HB2	2.20	0.42
10:k:27:VAL:O	10:k:30:VAL:HG13	2.20	0.42
26:B:616:CLA:H61	26:B:616:CLA:H41	1.83	0.42
4:D:103:ARG:HE	5:E:77:GLU:HG3	1.85	0.42
5:E:35:TRP:NE1	30:E:104:STE:H162	2.33	0.42
2:b:373:LYS:HG3	37:b:722:HOH:O	2.19	0.42
26:c:511:CLA:H162	26:c:511:CLA:H141	1.66	0.42
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.86	0.42
3:C:167:VAL:HG13	26:C:512:CLA:H93	2.02	0.42
12:M:27:VAL:HG13	30:m:103:STE:H61	2.00	0.42
2:b:247:PHE:CE2	26:b:602:CLA:H102	2.54	0.42
28:c:514:BCR:H24C	28:c:514:BCR:H371	1.87	0.42
26:A:607:CLA:H191	34:D:408:LHG:H162	2.01	0.41
34:B:622:LHG:H272	34:D:410:LHG:H152	2.02	0.41
37:B:908:HOH:O	7:H:65:LEU:HD22	2.20	0.41
26:C:508:CLA:H18	32:C:524:DGD:HAW2	2.02	0.41
33:a:618:LMG:H342	32:c:519:DGD:HA82	2.02	0.41
30:a:620:STE:H62	30:a:620:STE:H92	1.68	0.41
26:b:608:CLA:H141	26:b:608:CLA:H161	1.89	0.41
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.20	0.41
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.41
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.41
3:C:349:ILE:HD12	13:O:101:ILE:HD13	2.02	0.41
29:D:405:PL9:H412	11:L:29:LEU:HD23	2.02	0.41
1:a:131:TRP:CH2	26:c:505:CLA:HAA2	2.55	0.41
33:b:622:LMG:O9	33:b:622:LMG:H292	2.20	0.41
5:e:8:ARG:HD2	5:e:12:ASP:OD2	2.19	0.41
2:B:67:ALA:HA	2:B:71:VAL:O	2.20	0.41
2:B:149[B]:LEU:CD1	26:B:604:CLA:H112	2.50	0.41
2:B:357:ARG:HD3	37:B:824:HOH:O	2.19	0.41
28:C:514:BCR:H20C	28:C:514:BCR:H361	1.88	0.41
2:b:86:ILE:HA	37:b:925:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:194:ASN:HA	4:d:295:SER:OG	2.20	0.41
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.02	0.41
28:k:102:BCR:H20C	28:k:102:BCR:H361	1.92	0.41
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.55	0.41
1:A:201:GLY:HA3	1:A:286:THR:HB	2.02	0.41
2:B:422:ARG:O	2:B:425:ILE:HG12	2.21	0.41
26:B:603:CLA:HAB	26:B:605:CLA:H162	2.03	0.41
2:b:317:ASN:HA	2:b:330:MET:HE1	2.01	0.41
2:b:491:VAL:HG12	4:d:136:VAL:HG13	2.03	0.41
26:b:609:CLA:C2B	28:x:101:BCR:H323	2.51	0.41
26:c:509:CLA:H3A	26:c:509:CLA:HBA1	1.87	0.41
13:o:228:HIS:HD2	37:o:1501:HOH:O	2.02	0.41
19:z:47:TRP:CE2	30:z:101:STE:H81	2.56	0.41
2:B:227:LYS:HD3	33:D:406:LMG:H291	2.03	0.41
26:B:601:CLA:H41	30:H:103:STE:H183	2.02	0.41
28:B:619:BCR:H20C	28:B:619:BCR:H361	1.82	0.41
26:b:610:CLA:HBB1	28:x:101:BCR:HC22	2.01	0.41
2:B:233:ASN:HD21	2:B:476:ARG:NH2	2.18	0.41
26:C:508:CLA:H161	26:C:508:CLA:H202	1.82	0.41
17:Y:30:ILE:HD12	17:Y:30:ILE:HA	1.85	0.41
20:r:28:VAL:O	20:r:29:LYS:HG3	2.21	0.41
34:E:101:LHG:HC92	34:E:101:LHG:H121	1.94	0.41
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	2.03	0.41
26:b:603:CLA:H62	26:b:603:CLA:H41	1.91	0.41
3:c:135:ARG:HD3	19:z:27:TYR:HD1	1.86	0.41
13:o:178:LYS:HA	13:o:178:LYS:HD3	1.85	0.41
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.56	0.41
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.56	0.41
3:C:363:GLY:O	3:C:367:GLU:HG2	2.20	0.41
28:C:515:BCR:H20C	28:C:515:BCR:H361	1.94	0.41
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.51	0.41
14:T:1:FME:H	30:T:102:STE:C3	2.34	0.41
2:b:224:ARG:NH2	30:d:410:STE:H22	2.36	0.41
2:b:278:SER:HB3	37:b:701:HOH:O	2.20	0.41
37:d:601:HOH:O	30:h:102:STE:H112	2.20	0.41
9:j:10:LEU:O	9:j:13:VAL:HG22	2.20	0.41
16:v:41:HIS:CD2	36:v:201:HEC:NB	2.89	0.41
2:B:193:TYR:O	7:H:65:LEU:HD23	2.21	0.41
30:E:104:STE:H102	30:E:104:STE:H132	1.39	0.41
10:K:25:LEU:HB2	37:K:204:HOH:O	2.21	0.41
33:m:101:LMG:H381	33:m:101:LMG:H411	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:GLU:HG2	37:B:947:HOH:O	2.21	0.40
26:B:614:CLA:H191	30:B:624:STE:H122	2.03	0.40
28:H:101:BCR:H24C	28:H:101:BCR:H371	1.85	0.40
28:x:101:BCR:H20C	28:x:101:BCR:H361	1.81	0.40
28:H:101:BCR:H361	28:H:101:BCR:H20C	1.90	0.40
1:a:200:LEU:HD13	32:c:521:DGD:HAT2	2.02	0.40
3:c:455:PHE:HD2	8:i:33:LYS:HG3	1.86	0.40
26:d:403:CLA:H93	26:d:403:CLA:H61	1.85	0.40
5:e:25:ILE:HD13	20:r:18:TRP:CE2	2.56	0.40
9:j:5:GLY:HA3	9:j:7:ARG:HH11	1.86	0.40
17:y:22:LEU:HA	17:y:25:ILE:HG22	2.03	0.40
3:C:223:TRP:CG	3:C:224:ILE:H	2.39	0.40
30:H:103:STE:H141	30:H:103:STE:H172	1.61	0.40
30:a:619:STE:H22	37:a:843:HOH:O	2.20	0.40
2:b:125:ASP:HB2	2:b:132:ALA:HB3	2.04	0.40
29:d:405:PL9:H421	29:d:405:PL9:H401	1.91	0.40
13:o:59:LYS:H	13:o:59:LYS:HG3	1.45	0.40
12:M:12:ALA:O	12:M:16:LEU:HB2	2.22	0.40
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.51	0.40
26:A:608:CLA:H91	26:D:402:CLA:H172	2.04	0.40
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.22	0.40
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.22	0.40
1:a:183[B]:MET:HA	26:a:607:CLA:HMD1	2.01	0.40
2:b:385:ARG:HG2	13:o:165:ALA:O	2.21	0.40
16:v:19:ILE:HG12	16:v:20:THR:N	2.37	0.40
20:r:3:TRP:O	20:r:7:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/344 (116%)	395 (99%)	4 (1%)	1 (0%)	36	30
1	a	400/344 (116%)	394 (98%)	6 (2%)	0	100	100
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
2	b	504/510 (99%)	495 (98%)	8 (2%)	1 (0%)	43	37
3	C	451/461 (98%)	444 (98%)	6 (1%)	1 (0%)	43	37
3	c	461/461 (100%)	451 (98%)	9 (2%)	1 (0%)	43	37
4	D	348/352 (99%)	338 (97%)	10 (3%)	0	100	100
4	d	349/352 (99%)	341 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	3	0
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	30 (100%)	0	0	100	100
13	O	243/272 (89%)	233 (96%)	9 (4%)	1 (0%)	30	22
13	o	242/272 (89%)	233 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	4
16	V	135/163 (83%)	132 (98%)	2 (2%)	1 (1%)	18	9
16	v	135/163 (83%)	133 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	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%)	2 (3%)	1 (2%)	7	1
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	0	1 (4%)	2	0
All	All	5405/5700 (95%)	5289 (98%)	106 (2%)	10 (0%)	43	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
15	u	53	ALA
13	O	57	LYS
2	b	278	SER
9	J	7	ARG
19	z	2	THR
20	r	28	VAL
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	326/280 (116%)	323 (99%)	3 (1%)	70	67
1	a	325/280 (116%)	317 (98%)	8 (2%)	42	29
2	B	408/407 (100%)	404 (99%)	4 (1%)	68	64
2	b	403/407 (99%)	399 (99%)	4 (1%)	68	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	353/362 (98%)	350 (99%)	3 (1%)	73	71
3	c	362/362 (100%)	352 (97%)	10 (3%)	38	25
4	D	285/283 (101%)	284 (100%)	1 (0%)	84	84
4	d	286/283 (101%)	280 (98%)	6 (2%)	47	37
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	25
5	e	71/73 (97%)	71 (100%)	0	100	100
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	17
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	3
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	40
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%)	23 (96%)	1 (4%)	26	13
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	20
10	k	30/37 (81%)	28 (93%)	2 (7%)	15	4
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	17
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	17
13	O	206/228 (90%)	202 (98%)	4 (2%)	50	40
13	o	207/228 (91%)	204 (99%)	3 (1%)	59	52
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%)	83 (99%)	1 (1%)	63	57
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	44
16	v	117/138 (85%)	116 (99%)	1 (1%)	70	67
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	11
18	X	31/34 (91%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	20
19	Z	52/52 (100%)	52 (100%)	0	100	100
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	18 (82%)	4 (18%)	2	0
All	All	4467/4654 (96%)	4397 (98%)	70 (2%)	57	46

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	205	VAL
2	B	76	SER
2	B	79	SER
2	B	86	ILE
2	B	371	THR
3	C	240	ILE
3	C	289	PHE
3	C	416	SER
4	D	43	LEU
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
10	K	19	ASP
12	M	20	VAL
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	214	THR
15	U	61	VAL
16	V	3	LEU
16	V	7	VAL
1	a	28	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	245	THR
1	a	286	THR

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Mol	Chain	Res	Type
1	a	288	LEU
2	b	63	LEU
2	b	161	LEU
2	b	315	ILE
2	b	362	PHE
3	c	78	GLU
3	c	99	VAL
3	c	124	VAL
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	354[A]	GLU
3	c	354[B]	GLU
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
9	j	7	ARG
10	k	19	ASP
10	k	30	VAL
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	49	THR
13	o	59	LYS
13	o	118	LEU
16	v	52	LEU
17	y	19	ILE
18	x	2	THR
20	r	3	TRP
20	r	9	LEU
20	r	10	LEU
20	r	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	234	ASN
1	A	261	GLN
2	B	282	GLN
2	B	289	GLN
2	B	331	ASN
2	B	394	GLN
2	B	490	GLN
3	C	155	ASN
3	C	201	ASN
3	C	385	GLN
3	C	415	ASN
4	D	61	HIS
4	D	186	GLN
5	E	82	GLN
7	H	59	ASN
13	O	61	GLN
13	O	155	ASN
13	O	200	ASN
13	O	231	HIS
15	U	73	GLN
16	V	34	GLN
18	X	38	GLN
20	R	22	ASN
2	b	338	GLN
2	b	409	GLN
2	b	497	GLN
3	c	311	GLN
3	c	322	GLN
3	c	378	ASN
3	c	415	ASN
4	d	186	GLN
4	d	236	ASN
4	d	255	GLN
5	e	82	GLN
7	h	59	ASN
12	m	5	GLN
12	m	32	GLN
13	o	36	GLN
13	o	61	GLN
13	o	155	ASN
15	u	73	GLN
16	v	25	GLN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.48	0	8,9,11	0.77	0
14	FME	T	1	14	8,9,10	0.48	0	8,9,11	0.99	0
12	FME	m	1	12	8,9,10	0.41	0	8,9,11	0.59	0
8	FME	I	1	8	8,9,10	0.45	0	8,9,11	0.80	0
8	FME	i	1	8	8,9,10	0.51	0	8,9,11	0.68	0
12	FME	M	1	12	8,9,10	0.43	0	8,9,11	0.59	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	2/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 213 ligands modelled in this entry, 6 are monoatomic - leaving 207 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	DGD	c	519	-	63,63,67	0.54	0	77,77,81	0.88	3 (3%)
33	LMG	d	411	-	44,44,55	0.54	0	52,52,63	0.68	0
30	STE	e	103	-	8,8,19	0.36	0	7,7,19	0.70	0
26	CLA	c	503	3	69,73,73	1.39	8 (11%)	82,113,113	1.44	8 (9%)
21	OEY	A	601[B]	3,37,1	0,16,16	-	-	-		
28	BCR	B	619	-	41,41,41	0.39	0	56,56,56	0.79	0
30	STE	B	624	-	17,17,19	0.63	0	17,17,19	1.16	0
26	CLA	b	601	37	69,73,73	1.20	6 (8%)	82,113,113	1.38	5 (6%)
30	STE	C	528	-	15,15,19	0.34	0	14,14,19	0.82	0
28	BCR	A	611	-	41,41,41	0.39	0	56,56,56	0.58	0
26	CLA	c	509	3	69,73,73	1.23	7 (10%)	82,113,113	1.34	7 (8%)
30	STE	A	620	-	10,10,19	0.37	0	9,9,19	0.75	0
29	PL9	D	405	-	55,55,55	0.99	2 (3%)	68,69,69	1.48	14 (20%)
28	BCR	C	521	-	41,41,41	0.36	0	56,56,56	0.89	1 (1%)
31	SQD	A	616	-	41,43,54	1.78	8 (19%)	51,54,65	1.59	8 (15%)
32	DGD	C	525	-	63,63,67	0.59	0	77,77,81	0.79	2 (2%)
26	CLA	b	606	2	69,73,73	1.48	7 (10%)	82,113,113	1.41	7 (8%)
30	STE	A	618	-	7,7,19	0.31	0	6,6,19	0.79	0
34	LHG	B	622	-	48,48,48	0.50	0	51,54,54	0.71	0
33	LMG	c	523	-	48,48,55	0.51	0	56,56,63	0.92	2 (3%)
29	PL9	d	405	-	55,55,55	1.03	2 (3%)	68,69,69	1.62	12 (17%)
28	BCR	B	617	-	41,41,41	0.42	0	56,56,56	0.80	2 (3%)
26	CLA	A	608	37	69,73,73	1.20	6 (8%)	82,113,113	1.21	6 (7%)
26	CLA	c	504	37	64,68,73	1.28	7 (10%)	76,107,113	1.33	9 (11%)
32	DGD	c	520	-	63,63,67	0.55	0	77,77,81	0.77	1 (1%)
35	HEM	F	101	6,5	50,50,50	1.45	4 (8%)	67,82,82	1.20	5 (7%)
26	CLA	b	602	2	69,73,73	1.25	7 (10%)	82,113,113	1.39	12 (14%)
35	HEM	e	102	6,5	50,50,50	1.53	8 (16%)	67,82,82	1.43	8 (11%)
36	HEC	v	201	16	50,50,50	1.69	4 (8%)	68,82,82	1.28	6 (8%)
31	SQD	a	614	-	52,54,54	1.55	7 (13%)	62,65,65	1.95	9 (14%)
25	BCT	A	606	23	3,3,3	0.76	0	2,3,3	2.19	1 (50%)
29	PL9	A	612	-	55,55,55	0.77	1 (1%)	68,69,69	1.49	12 (17%)
26	CLA	C	506	3	69,73,73	1.27	8 (11%)	82,113,113	1.25	7 (8%)
26	CLA	B	615	2	69,73,73	1.42	7 (10%)	82,113,113	1.46	5 (6%)
33	LMG	a	617	-	55,55,55	0.49	0	63,63,63	1.07	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	STE	M	102	-	14,14,19	0.68	0	14,14,19	1.19	1 (7%)
34	LHG	D	408	-	48,48,48	0.58	0	51,54,54	0.59	1 (1%)
33	LMG	C	522	-	48,48,55	0.46	0	56,56,63	0.65	0
28	BCR	d	404	-	41,41,41	0.38	0	56,56,56	1.07	3 (5%)
26	CLA	b	608	2	69,73,73	1.18	6 (8%)	82,113,113	1.41	10 (12%)
32	DGD	C	523	-	63,63,67	0.57	0	77,77,81	0.86	2 (2%)
26	CLA	B	604	2	69,73,73	1.51	7 (10%)	82,113,113	1.47	8 (9%)
33	LMG	M	101	-	51,51,55	0.51	0	59,59,63	0.90	2 (3%)
33	LMG	m	101	-	51,51,55	0.49	0	59,59,63	0.79	2 (3%)
26	CLA	B	606	2	69,73,73	1.39	7 (10%)	82,113,113	1.45	6 (7%)
34	LHG	l	101	-	48,48,48	0.48	0	51,54,54	0.63	0
33	LMG	B	620	-	45,45,55	0.46	0	53,53,63	0.89	5 (9%)
28	BCR	c	515	-	41,41,41	0.38	0	56,56,56	0.76	1 (1%)
30	STE	T	102	-	15,15,19	0.38	0	14,14,19	0.79	0
26	CLA	B	605	2	69,73,73	1.20	7 (10%)	82,113,113	1.29	8 (9%)
30	STE	b	625	-	10,10,19	0.32	0	9,9,19	0.82	0
26	CLA	b	611	2	69,73,73	1.21	8 (11%)	82,113,113	1.37	6 (7%)
26	CLA	c	512	3	69,73,73	1.16	7 (10%)	82,113,113	1.36	5 (6%)
30	STE	I	101	-	16,16,19	0.64	0	16,16,19	1.04	0
22	OEX	a	602[A]	3,37,1	0,14,14	-	-	-		
34	LHG	d	408	-	48,48,48	0.52	0	51,54,54	0.75	2 (3%)
26	CLA	D	403	4	69,73,73	1.22	8 (11%)	82,113,113	1.30	8 (9%)
30	STE	a	619	-	11,11,19	0.76	0	11,11,19	0.98	0
26	CLA	A	614	37	69,73,73	1.27	7 (10%)	82,113,113	1.29	5 (6%)
30	STE	C	520	-	9,9,19	0.36	0	8,8,19	0.75	0
30	STE	H	103	-	17,17,19	0.39	0	16,16,19	0.76	0
26	CLA	c	507	37	69,73,73	1.25	6 (8%)	82,113,113	1.34	7 (8%)
30	STE	e	101	-	8,8,19	0.39	0	7,7,19	0.64	0
30	STE	C	529	-	13,13,19	0.37	0	12,12,19	0.77	0
30	STE	e	104	-	12,12,19	0.64	0	12,12,19	1.37	2 (16%)
34	LHG	E	101	-	48,48,48	0.56	0	51,54,54	0.52	0
30	STE	B	621	-	16,16,19	0.62	0	16,16,19	1.26	0
26	CLA	a	607	1	69,73,73	1.25	10 (14%)	82,113,113	1.34	8 (9%)
31	SQD	a	616	-	52,54,54	1.62	8 (15%)	62,65,65	1.55	10 (16%)
30	STE	C	527	-	11,11,19	0.74	0	11,11,19	1.50	2 (18%)
30	STE	c	517	-	17,17,19	0.34	0	16,16,19	0.81	0
26	CLA	b	603	2	69,73,73	1.23	7 (10%)	82,113,113	1.34	8 (9%)
28	BCR	c	514	-	41,41,41	0.31	0	56,56,56	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	C	517	-	35,35,55	0.52	0	43,43,63	1.41	6 (13%)
26	CLA	C	502	3	69,73,73	1.25	7 (10%)	82,113,113	1.32	6 (7%)
26	CLA	d	402	4	69,73,73	1.17	8 (11%)	82,113,113	1.31	9 (10%)
28	BCR	K	101	-	41,41,41	0.40	0	56,56,56	0.88	0
26	CLA	a	608	37	69,73,73	1.24	7 (10%)	82,113,113	1.27	9 (10%)
26	CLA	a	613	37	69,73,73	1.19	7 (10%)	82,113,113	1.30	10 (12%)
30	STE	E	102	-	11,11,19	0.74	0	11,11,19	1.15	1 (9%)
30	STE	b	623	-	15,15,19	0.60	0	15,15,19	1.28	2 (13%)
30	STE	c	516	-	12,12,19	0.34	0	11,11,19	0.78	0
26	CLA	C	512	3	69,73,73	1.30	9 (13%)	82,113,113	1.26	7 (8%)
26	CLA	b	613	2	69,73,73	1.18	7 (10%)	82,113,113	1.33	9 (10%)
30	STE	C	516	-	13,13,19	0.76	0	13,13,19	0.98	0
25	BCT	a	606	23	3,3,3	0.81	0	2,3,3	2.00	1 (50%)
31	SQD	F	102	-	34,36,54	1.43	4 (11%)	42,45,65	1.42	8 (19%)
26	CLA	a	610	1	69,73,73	1.26	6 (8%)	82,113,113	1.29	7 (8%)
33	LMG	b	622	-	55,55,55	0.47	0	63,63,63	1.13	5 (7%)
30	STE	i	101	-	11,11,19	0.74	0	11,11,19	1.14	0
26	CLA	c	501	3	69,73,73	1.13	6 (8%)	82,113,113	1.39	6 (7%)
26	CLA	B	611	2	69,73,73	1.14	5 (7%)	82,113,113	1.40	6 (7%)
30	STE	C	519	-	6,6,19	0.35	0	5,5,19	0.71	0
26	CLA	D	402	4	69,73,73	1.11	5 (7%)	82,113,113	1.30	8 (9%)
26	CLA	b	615	2	69,73,73	1.37	8 (11%)	82,113,113	1.31	8 (9%)
26	CLA	C	507	37	69,73,73	1.20	7 (10%)	82,113,113	1.37	8 (9%)
31	SQD	f	101	-	39,41,54	1.63	7 (17%)	49,52,65	1.91	10 (20%)
34	LHG	d	409	-	38,38,48	0.56	0	41,44,54	0.55	0
30	STE	A	619	-	16,16,19	0.34	0	15,15,19	0.79	0
30	STE	B	625	-	11,11,19	0.74	0	11,11,19	1.11	0
30	STE	J	101	-	11,11,19	0.68	0	11,11,19	1.17	0
26	CLA	b	609	2	69,73,73	1.28	8 (11%)	82,113,113	1.39	11 (13%)
28	BCR	b	619	-	41,41,41	0.40	0	56,56,56	0.89	1 (1%)
26	CLA	c	502	3	69,73,73	1.19	7 (10%)	82,113,113	1.29	6 (7%)
30	STE	b	624	-	9,9,19	0.34	0	8,8,19	0.76	0
31	SQD	A	615	-	50,52,54	1.56	5 (10%)	60,63,65	1.90	12 (20%)
32	DGD	h	101	-	63,63,67	0.55	0	77,77,81	0.98	6 (7%)
26	CLA	A	607	1	69,73,73	1.34	8 (11%)	82,113,113	1.24	6 (7%)
27	PHO	d	401	-	58,69,69	2.18	9 (15%)	55,99,99	1.81	11 (20%)
28	BCR	D	404	-	41,41,41	0.41	0	56,56,56	1.02	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PHO	a	609	-	58,69,69	2.08	10 (17%)	55,99,99	1.63	7 (12%)
34	LHG	D	409	-	46,46,48	0.57	0	49,52,54	0.54	0
26	CLA	B	612	2	69,73,73	1.13	7 (10%)	82,113,113	1.39	8 (9%)
26	CLA	C	508	3	69,73,73	1.38	9 (13%)	82,113,113	1.36	7 (8%)
26	CLA	B	613	2	69,73,73	1.25	8 (11%)	82,113,113	1.46	6 (7%)
26	CLA	C	511	3	69,73,73	1.28	7 (10%)	82,113,113	1.39	5 (6%)
30	STE	h	102	-	9,9,19	0.36	0	8,8,19	0.72	0
31	SQD	b	620	-	47,49,54	1.62	8 (17%)	57,60,65	1.74	10 (17%)
36	HEC	V	201	16	50,50,50	1.69	6 (12%)	68,82,82	1.40	9 (13%)
26	CLA	B	610	37	69,73,73	1.20	7 (10%)	82,113,113	1.39	8 (9%)
32	DGD	C	524	-	63,63,67	0.55	0	77,77,81	0.75	1 (1%)
26	CLA	d	403	4	69,73,73	1.38	8 (11%)	82,113,113	1.18	9 (10%)
26	CLA	b	614	2	69,73,73	1.27	6 (8%)	82,113,113	1.35	6 (7%)
30	STE	t	102	-	13,13,19	0.60	0	13,13,19	1.32	2 (15%)
28	BCR	T	101	-	41,41,41	0.49	0	56,56,56	0.93	1 (1%)
28	BCR	k	101	-	41,41,41	0.42	0	56,56,56	1.01	3 (5%)
30	STE	C	518	-	4,4,19	0.37	0	3,3,19	0.47	0
26	CLA	c	510	3	69,73,73	1.34	8 (11%)	82,113,113	1.24	6 (7%)
30	STE	m	103	-	17,17,19	0.35	0	16,16,19	0.82	0
26	CLA	C	510	3	69,73,73	1.24	8 (11%)	82,113,113	1.27	7 (8%)
33	LMG	c	518	-	29,29,55	0.42	0	31,31,63	0.59	0
26	CLA	B	614	2	69,73,73	1.33	8 (11%)	82,113,113	1.34	9 (10%)
30	STE	D	411	-	19,19,19	0.59	0	19,19,19	1.21	2 (10%)
30	STE	j	101	-	11,11,19	0.78	0	11,11,19	1.18	1 (9%)
26	CLA	C	513	3	69,73,73	1.28	7 (10%)	82,113,113	1.28	8 (9%)
26	CLA	b	607	37	69,73,73	1.20	6 (8%)	82,113,113	1.26	9 (10%)
26	CLA	C	505	3	69,73,73	1.20	7 (10%)	82,113,113	1.36	12 (14%)
26	CLA	B	601	37	69,73,73	1.32	7 (10%)	82,113,113	1.32	6 (7%)
30	STE	d	410	-	19,19,19	0.57	0	19,19,19	1.00	0
26	CLA	c	506	3	69,73,73	1.26	9 (13%)	82,113,113	1.18	5 (6%)
26	CLA	C	501	3	69,73,73	1.43	8 (11%)	82,113,113	1.36	6 (7%)
28	BCR	C	514	-	41,41,41	0.32	0	56,56,56	0.64	0
26	CLA	B	616	2	64,68,73	1.43	10 (15%)	76,107,113	1.34	6 (7%)
34	LHG	D	410	-	48,48,48	0.56	0	51,54,54	0.69	0
26	CLA	c	511	3	69,73,73	1.54	6 (8%)	82,113,113	1.39	7 (8%)
28	BCR	b	618	-	41,41,41	0.46	0	56,56,56	0.94	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	STE	D	412	-	8,8,19	0.33	0	7,7,19	0.77	0
26	CLA	B	603	2	69,73,73	1.28	6 (8%)	82,113,113	1.37	8 (9%)
33	LMG	a	618	-	49,49,55	0.51	0	57,57,63	0.82	2 (3%)
26	CLA	b	610	37	69,73,73	1.22	6 (8%)	82,113,113	1.30	9 (10%)
27	PHO	A	609	-	58,69,69	1.94	9 (15%)	55,99,99	1.69	9 (16%)
32	DGD	c	521	-	63,63,67	0.53	0	77,77,81	0.68	2 (2%)
30	STE	b	621	-	19,19,19	0.56	0	19,19,19	1.11	0
32	DGD	A	617	-	67,67,67	0.53	0	81,81,81	1.00	6 (7%)
30	STE	d	412	-	19,19,19	0.61	0	19,19,19	1.04	0
30	STE	f	102	-	7,7,19	0.36	0	6,6,19	0.67	0
30	STE	T	103	-	14,14,19	0.31	0	13,13,19	0.95	0
26	CLA	B	608	2	69,73,73	1.20	8 (11%)	82,113,113	1.36	8 (9%)
30	STE	E	104	-	19,19,19	0.59	0	19,19,19	1.14	1 (5%)
28	BCR	B	618	-	41,41,41	0.43	0	56,56,56	0.68	1 (1%)
33	LMG	c	522	-	46,46,55	0.52	0	54,54,63	0.68	0
26	CLA	A	610	1	58,62,73	1.11	3 (5%)	68,99,113	1.39	9 (13%)
26	CLA	c	513	3	69,73,73	1.18	7 (10%)	82,113,113	1.22	7 (8%)
34	LHG	d	407	-	48,48,48	0.54	0	51,54,54	0.61	1 (1%)
26	CLA	b	605	2	69,73,73	1.30	7 (10%)	82,113,113	1.36	9 (10%)
26	CLA	c	505	3	69,73,73	1.19	8 (11%)	82,113,113	1.29	8 (9%)
28	BCR	a	611	-	41,41,41	0.47	0	56,56,56	0.75	1 (1%)
26	CLA	C	503	3	69,73,73	1.53	9 (13%)	82,113,113	1.56	12 (14%)
30	STE	I	102	-	14,14,19	0.70	0	14,14,19	1.10	0
30	STE	d	406	-	19,19,19	0.61	0	19,19,19	1.01	0
30	STE	j	102	-	15,15,19	0.37	0	14,14,19	0.76	0
30	STE	z	101	-	8,8,19	0.38	0	7,7,19	0.61	0
32	DGD	H	102	-	63,63,67	0.54	0	77,77,81	0.93	3 (3%)
28	BCR	C	515	-	41,41,41	0.33	0	56,56,56	0.64	0
30	STE	k	103	-	13,13,19	0.69	0	13,13,19	1.14	0
30	STE	E	103	-	11,11,19	0.33	0	10,10,19	0.77	0
22	OEX	A	602[A]	3,37,1	0,14,14	-	-	-	-	-
26	CLA	B	609	2	69,73,73	1.30	4 (5%)	82,113,113	1.29	7 (8%)
21	OXY	a	601[B]	3,37,1	0,16,16	-	-	-	-	-
27	PHO	D	401	-	58,69,69	2.05	9 (15%)	55,99,99	1.70	10 (18%)
30	STE	t	103	-	9,9,19	0.41	0	8,8,19	0.67	0
31	SQD	B	623	-	52,54,54	1.57	9 (17%)	62,65,65	1.67	12 (19%)
26	CLA	B	602	2	69,73,73	1.19	6 (8%)	82,113,113	1.26	8 (9%)
28	BCR	b	617	-	41,41,41	0.42	0	56,56,56	0.75	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	STE	a	620	-	14,14,19	0.34	0	13,13,19	0.82	0
33	LMG	D	407	-	51,51,55	0.49	0	59,59,63	0.73	1 (1%)
28	BCR	H	101	-	41,41,41	0.40	0	56,56,56	0.96	3 (5%)
28	BCR	k	102	-	41,41,41	0.39	0	56,56,56	0.87	1 (1%)
26	CLA	C	504	37	63,67,73	1.31	8 (12%)	74,105,113	1.27	5 (6%)
30	STE	m	102	-	11,11,19	0.68	0	11,11,19	1.36	2 (18%)
28	BCR	t	101	-	41,41,41	0.48	0	56,56,56	1.05	5 (8%)
33	LMG	C	526	-	48,48,55	0.50	0	56,56,63	0.65	0
30	STE	M	103	-	9,9,19	0.31	0	8,8,19	0.88	0
33	LMG	D	406	-	50,50,55	0.48	0	58,58,63	1.15	5 (8%)
26	CLA	b	612	2	69,73,73	1.13	7 (10%)	82,113,113	1.29	9 (10%)
30	STE	A	613	-	8,8,19	0.34	0	7,7,19	0.71	0
26	CLA	b	604	2	69,73,73	1.21	8 (11%)	82,113,113	1.55	11 (13%)
26	CLA	c	508	3	68,72,73	1.24	8 (11%)	80,111,113	1.24	7 (8%)
29	PL9	a	612	-	55,55,55	0.78	1 (1%)	68,69,69	1.56	11 (16%)
26	CLA	C	509	3	69,73,73	1.18	7 (10%)	82,113,113	1.25	7 (8%)
26	CLA	b	616	2	64,68,73	1.26	7 (10%)	76,107,113	1.49	10 (13%)
28	BCR	x	101	-	41,41,41	0.43	0	56,56,56	0.87	2 (3%)
34	LHG	a	615	-	41,41,48	0.57	0	44,47,54	0.58	0
26	CLA	B	607	37	69,73,73	1.11	6 (8%)	82,113,113	1.26	6 (7%)
30	STE	K	102	-	13,13,19	0.34	0	12,12,19	0.75	0
30	STE	i	102	-	5,5,19	0.37	0	4,4,19	0.53	0
30	STE	Z	101	-	16,16,19	0.36	0	15,15,19	0.73	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
32	DGD	c	519	-	-	17/51/91/95	0/2/2/2
33	LMG	d	411	-	-	11/39/59/70	0/1/1/1
30	STE	e	103	-	-	5/6/6/17	-
26	CLA	c	503	3	-	8/39/115/115	-
28	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	STE	B	624	-	-	11/15/15/17	-
26	CLA	b	601	37	-	10/39/115/115	-
30	STE	C	528	-	-	5/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	A	611	-	-	0/29/63/63	0/2/2/2
26	CLA	c	509	3	-	10/39/115/115	-
30	STE	A	620	-	-	5/8/8/17	-
29	PL9	D	405	-	-	6/53/73/73	0/1/1/1
28	BCR	C	521	-	-	5/29/63/63	0/2/2/2
31	SQD	A	616	-	-	18/38/58/69	0/1/1/1
32	DGD	C	525	-	-	13/51/91/95	0/2/2/2
26	CLA	b	606	2	-	9/39/115/115	-
30	STE	A	618	-	-	3/5/5/17	-
34	LHG	B	622	-	-	19/53/53/53	-
33	LMG	c	523	-	-	14/43/63/70	0/1/1/1
29	PL9	d	405	-	-	9/53/73/73	0/1/1/1
36	HEC	v	201	16	1/1/3/7	4/14/54/54	-
26	CLA	A	608	37	-	6/39/115/115	-
26	CLA	c	504	37	-	5/33/109/115	-
28	BCR	B	617	-	-	4/29/63/63	0/2/2/2
32	DGD	c	520	-	-	18/51/91/95	0/2/2/2
26	CLA	b	602	2	-	4/39/115/115	-
35	HEM	F	101	6,5	-	3/14/54/54	-
35	HEM	e	102	6,5	-	3/14/54/54	-
31	SQD	a	614	-	-	26/49/69/69	0/1/1/1
34	LHG	D	408	-	-	14/53/53/53	-
29	PL9	A	612	-	-	21/53/73/73	0/1/1/1
26	CLA	C	506	3	-	8/39/115/115	-
26	CLA	B	615	2	-	14/39/115/115	-
33	LMG	a	617	-	-	24/50/70/70	0/1/1/1
30	STE	M	102	-	-	8/12/12/17	-
33	LMG	C	522	-	-	19/43/63/70	0/1/1/1
28	BCR	d	404	-	-	2/29/63/63	0/2/2/2
26	CLA	b	608	2	-	4/39/115/115	-
32	DGD	C	523	-	-	20/51/91/95	0/2/2/2
26	CLA	B	604	2	-	10/39/115/115	-
33	LMG	M	101	-	-	22/46/66/70	0/1/1/1
33	LMG	m	101	-	-	17/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	606	2	-	9/39/115/115	-
34	LHG	l	101	-	-	13/53/53/53	-
33	LMG	B	620	-	-	23/40/60/70	0/1/1/1
28	BCR	c	515	-	-	0/29/63/63	0/2/2/2
30	STE	T	102	-	-	10/13/13/17	-
26	CLA	B	605	2	-	9/39/115/115	-
30	STE	b	625	-	-	3/8/8/17	-
26	CLA	b	611	2	-	5/39/115/115	-
26	CLA	c	512	3	-	15/39/115/115	-
30	STE	I	101	-	-	7/14/14/17	-
34	LHG	d	408	-	-	15/53/53/53	-
26	CLA	D	403	4	-	8/39/115/115	-
30	STE	a	619	-	-	4/9/9/17	-
26	CLA	A	614	37	-	5/39/115/115	-
30	STE	C	520	-	-	5/7/7/17	-
30	STE	H	103	-	-	9/15/15/17	-
26	CLA	c	507	37	-	13/39/115/115	-
30	STE	e	101	-	-	2/6/6/17	-
30	STE	C	529	-	-	5/11/11/17	-
30	STE	e	104	-	-	6/10/10/17	-
34	LHG	E	101	-	-	21/53/53/53	-
30	STE	B	621	-	-	7/14/14/17	-
26	CLA	a	607	1	-	5/39/115/115	-
31	SQD	a	616	-	-	18/49/69/69	0/1/1/1
30	STE	C	527	-	-	2/9/9/17	-
30	STE	c	517	-	-	11/15/15/17	-
26	CLA	b	603	2	-	14/39/115/115	-
28	BCR	c	514	-	-	0/29/63/63	0/2/2/2
33	LMG	C	517	-	-	12/30/50/70	0/1/1/1
26	CLA	C	502	3	-	6/39/115/115	-
26	CLA	d	402	4	-	5/39/115/115	-
28	BCR	K	101	-	-	4/29/63/63	0/2/2/2
26	CLA	a	608	37	-	3/39/115/115	-
26	CLA	a	613	37	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	STE	E	102	-	-	2/9/9/17	-
30	STE	b	623	-	-	5/13/13/17	-
30	STE	c	516	-	-	5/10/10/17	-
26	CLA	C	512	3	-	11/39/115/115	-
26	CLA	b	613	2	-	4/39/115/115	-
30	STE	C	516	-	-	6/11/11/17	-
31	SQD	F	102	-	-	17/28/48/69	0/1/1/1
33	LMG	b	622	-	-	23/50/70/70	0/1/1/1
26	CLA	a	610	1	-	10/39/115/115	-
30	STE	i	101	-	-	6/9/9/17	-
26	CLA	c	501	3	-	4/39/115/115	-
26	CLA	B	611	2	-	4/39/115/115	-
30	STE	C	519	-	-	2/4/4/17	-
26	CLA	D	402	4	-	4/39/115/115	-
26	CLA	b	615	2	-	2/39/115/115	-
26	CLA	C	507	37	-	10/39/115/115	-
31	SQD	f	101	-	-	17/36/56/69	0/1/1/1
34	LHG	d	409	-	-	9/43/43/53	-
30	STE	A	619	-	-	10/14/14/17	-
30	STE	B	625	-	-	3/9/9/17	-
30	STE	J	101	-	-	5/9/9/17	-
26	CLA	b	609	2	-	1/39/115/115	-
28	BCR	b	619	-	-	0/29/63/63	0/2/2/2
26	CLA	c	502	3	-	3/39/115/115	-
30	STE	b	624	-	-	5/7/7/17	-
31	SQD	A	615	-	-	18/47/67/69	0/1/1/1
32	DGD	h	101	-	-	10/51/91/95	0/2/2/2
26	CLA	A	607	1	-	6/39/115/115	-
27	PHO	d	401	-	-	4/37/103/103	0/5/6/6
28	BCR	D	404	-	-	2/29/63/63	0/2/2/2
27	PHO	a	609	-	-	1/37/103/103	0/5/6/6
34	LHG	D	409	-	-	11/51/51/53	-
26	CLA	B	612	2	-	12/39/115/115	-
26	CLA	C	508	3	-	6/39/115/115	-
36	HEC	V	201	16	1/1/3/7	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	613	2	-	12/39/115/115	-
26	CLA	C	511	3	-	5/39/115/115	-
30	STE	h	102	-	-	4/7/7/17	-
31	SQD	b	620	-	-	19/44/64/69	0/1/1/1
26	CLA	B	610	37	-	2/39/115/115	-
32	DGD	C	524	-	-	20/51/91/95	0/2/2/2
26	CLA	d	403	4	-	10/39/115/115	-
26	CLA	b	614	2	-	12/39/115/115	-
30	STE	t	102	-	-	2/11/11/17	-
28	BCR	T	101	-	-	7/29/63/63	0/2/2/2
28	BCR	k	101	-	-	8/29/63/63	0/2/2/2
30	STE	C	518	-	-	0/2/2/17	-
26	CLA	c	510	3	-	3/39/115/115	-
30	STE	m	103	-	-	6/15/15/17	-
26	CLA	C	510	3	-	3/39/115/115	-
33	LMG	c	518	-	-	8/31/31/70	-
26	CLA	B	614	2	-	14/39/115/115	-
30	STE	D	411	-	-	4/17/17/17	-
30	STE	j	101	-	-	5/9/9/17	-
26	CLA	C	513	3	-	12/39/115/115	-
26	CLA	b	607	37	-	10/39/115/115	-
26	CLA	C	505	3	-	8/39/115/115	-
26	CLA	B	601	37	-	23/39/115/115	-
30	STE	d	410	-	-	8/17/17/17	-
26	CLA	c	506	3	-	11/39/115/115	-
26	CLA	C	501	3	-	6/39/115/115	-
28	BCR	C	514	-	-	1/29/63/63	0/2/2/2
26	CLA	B	616	2	-	8/33/109/115	-
34	LHG	D	410	-	-	18/53/53/53	-
26	CLA	c	511	3	-	6/39/115/115	-
28	BCR	b	618	-	-	0/29/63/63	0/2/2/2
30	STE	D	412	-	-	3/6/6/17	-
26	CLA	B	603	2	-	5/39/115/115	-
33	LMG	a	618	-	-	21/44/64/70	0/1/1/1
26	CLA	b	610	37	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PHO	A	609	-	-	1/37/103/103	0/5/6/6
32	DGD	c	521	-	-	19/51/91/95	0/2/2/2
30	STE	b	621	-	-	7/17/17/17	-
32	DGD	A	617	-	-	20/55/95/95	0/2/2/2
30	STE	d	412	-	-	9/17/17/17	-
30	STE	f	102	-	-	2/5/5/17	-
30	STE	T	103	-	-	8/12/12/17	-
26	CLA	B	608	2	-	5/39/115/115	-
30	STE	E	104	-	-	14/17/17/17	-
28	BCR	B	618	-	-	0/29/63/63	0/2/2/2
33	LMG	c	522	-	-	15/41/61/70	0/1/1/1
26	CLA	A	610	1	-	2/26/102/115	-
26	CLA	c	513	3	-	13/39/115/115	-
34	LHG	d	407	-	-	20/53/53/53	-
26	CLA	b	605	2	-	4/39/115/115	-
26	CLA	c	505	3	-	11/39/115/115	-
28	BCR	a	611	-	-	1/29/63/63	0/2/2/2
26	CLA	C	503	3	-	3/39/115/115	-
30	STE	I	102	-	-	7/12/12/17	-
30	STE	d	406	-	-	8/17/17/17	-
30	STE	j	102	-	-	9/13/13/17	-
30	STE	z	101	-	-	3/6/6/17	-
32	DGD	H	102	-	-	20/51/91/95	0/2/2/2
28	BCR	C	515	-	-	0/29/63/63	0/2/2/2
30	STE	k	103	-	-	7/11/11/17	-
30	STE	E	103	-	-	3/9/9/17	-
26	CLA	B	609	2	-	2/39/115/115	-
27	PHO	D	401	-	-	1/37/103/103	0/5/6/6
30	STE	t	103	-	-	3/7/7/17	-
31	SQD	B	623	-	-	24/49/69/69	0/1/1/1
26	CLA	B	602	2	-	6/39/115/115	-
28	BCR	b	617	-	-	2/29/63/63	0/2/2/2
30	STE	a	620	-	-	8/12/12/17	-
33	LMG	D	407	-	-	17/46/66/70	0/1/1/1
28	BCR	H	101	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	k	102	-	-	2/29/63/63	0/2/2/2
26	CLA	C	504	37	-	9/32/108/115	-
30	STE	m	102	-	-	4/9/9/17	-
28	BCR	t	101	-	-	6/29/63/63	0/2/2/2
33	LMG	C	526	-	-	8/43/63/70	0/1/1/1
30	STE	M	103	-	-	4/7/7/17	-
33	LMG	D	406	-	-	21/45/65/70	0/1/1/1
26	CLA	b	612	2	-	1/39/115/115	-
30	STE	A	613	-	-	4/6/6/17	-
26	CLA	b	604	2	-	8/39/115/115	-
26	CLA	c	508	3	-	8/38/114/115	-
29	PL9	a	612	-	-	12/53/73/73	0/1/1/1
26	CLA	C	509	3	-	12/39/115/115	-
26	CLA	b	616	2	-	1/33/109/115	-
28	BCR	x	101	-	-	1/29/63/63	0/2/2/2
34	LHG	a	615	-	-	22/46/46/53	-
26	CLA	B	607	37	-	7/39/115/115	-
30	STE	K	102	-	-	6/11/11/17	-
30	STE	i	102	-	-	3/3/3/17	-
30	STE	Z	101	-	-	9/14/14/17	-

All (620) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	401	PHO	C3B-C4B	9.56	1.51	1.41
27	d	401	PHO	C1B-C2B	9.44	1.49	1.39
27	a	609	PHO	C1B-C2B	8.88	1.49	1.39
27	D	401	PHO	C3B-C4B	8.69	1.50	1.41
26	c	511	CLA	MG-NA	8.68	2.26	2.06
27	D	401	PHO	C1B-C2B	8.54	1.48	1.39
26	b	606	CLA	MG-NA	8.28	2.25	2.06
26	B	604	CLA	MG-NA	8.04	2.25	2.06
27	a	609	PHO	C3B-C4B	7.86	1.49	1.41
26	C	503	CLA	MG-NA	7.76	2.24	2.06
36	v	201	HEC	C3D-C2D	7.67	1.53	1.36
27	A	609	PHO	C1B-C2B	7.64	1.47	1.39
27	A	609	PHO	C3B-C4B	7.36	1.49	1.41
36	V	201	HEC	C3D-C2D	7.26	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	606	CLA	MG-NA	6.46	2.21	2.06
26	C	501	CLA	MG-NA	6.19	2.21	2.06
26	c	510	CLA	MG-NA	5.76	2.20	2.06
26	d	403	CLA	MG-ND	-5.74	1.94	2.05
26	B	609	CLA	MG-NA	5.73	2.19	2.06
26	B	601	CLA	MG-NA	5.55	2.19	2.06
26	A	607	CLA	MG-NA	5.51	2.19	2.06
26	B	616	CLA	MG-NA	5.42	2.19	2.06
26	c	503	CLA	MG-NA	5.42	2.19	2.06
26	B	603	CLA	MG-NA	5.33	2.18	2.06
26	b	609	CLA	MG-NA	5.18	2.18	2.06
26	b	605	CLA	MG-NA	5.10	2.18	2.06
35	e	102	HEM	FE-NA	5.09	2.12	1.95
26	B	615	CLA	MG-NA	5.08	2.18	2.06
35	F	101	HEM	FE-NC	4.99	2.11	1.95
26	b	615	CLA	MG-NB	4.97	2.15	2.05
36	V	201	HEC	FE-ND	4.96	2.10	1.94
31	a	614	SQD	O48-C23	4.83	1.47	1.33
26	C	508	CLA	MG-ND	4.82	2.15	2.05
31	a	616	SQD	O48-C23	4.78	1.47	1.33
26	b	603	CLA	MG-NA	4.75	2.17	2.06
27	a	609	PHO	C1D-C2D	4.64	1.44	1.39
26	C	511	CLA	MG-NA	4.64	2.17	2.06
31	A	615	SQD	O48-C23	4.64	1.46	1.33
27	D	401	PHO	C1D-C2D	4.62	1.44	1.39
31	F	102	SQD	O48-C23	4.57	1.46	1.33
31	B	623	SQD	O48-C23	4.56	1.46	1.33
31	A	616	SQD	O48-C23	4.53	1.46	1.33
31	f	101	SQD	O48-C23	4.49	1.46	1.33
27	A	609	PHO	C1D-C2D	4.49	1.44	1.39
36	v	201	HEC	FE-ND	4.47	2.08	1.94
26	B	615	CLA	MG-NC	4.45	2.16	2.06
26	C	508	CLA	MG-NA	4.43	2.16	2.06
31	b	620	SQD	O48-C23	4.43	1.46	1.33
26	A	608	CLA	MG-NA	4.37	2.16	2.06
26	a	613	CLA	MG-NA	4.33	2.16	2.06
26	b	611	CLA	MG-NA	4.28	2.16	2.06
26	a	610	CLA	C1D-ND	4.27	1.43	1.37
26	C	502	CLA	MG-NA	4.17	2.16	2.06
26	b	614	CLA	MG-NA	4.16	2.16	2.06
27	d	401	PHO	C1D-C2D	4.14	1.44	1.39
26	B	604	CLA	C1D-ND	4.13	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	610	CLA	C1D-ND	4.07	1.43	1.37
26	b	614	CLA	C1D-ND	4.07	1.43	1.37
26	C	504	CLA	MG-NA	4.05	2.15	2.06
26	B	614	CLA	C1D-ND	3.98	1.43	1.37
26	B	616	CLA	C1D-ND	3.97	1.43	1.37
26	C	501	CLA	C1D-ND	3.95	1.43	1.37
26	b	604	CLA	C1D-ND	3.94	1.43	1.37
26	D	403	CLA	C1D-ND	3.94	1.43	1.37
26	b	615	CLA	MG-NA	3.93	2.15	2.06
31	A	616	SQD	O5-C1	3.91	1.51	1.41
26	C	510	CLA	C1D-ND	3.89	1.43	1.37
31	A	615	SQD	O47-C45	-3.89	1.37	1.46
26	B	613	CLA	MG-NA	3.89	2.15	2.06
26	c	510	CLA	C1D-ND	3.89	1.43	1.37
26	B	610	CLA	C1D-ND	3.88	1.43	1.37
26	C	505	CLA	MG-NA	3.86	2.15	2.06
26	C	513	CLA	MG-NA	3.85	2.15	2.06
26	b	616	CLA	C1D-ND	3.85	1.42	1.37
26	b	602	CLA	MG-ND	-3.84	1.98	2.05
26	C	507	CLA	MG-NA	3.81	2.15	2.06
26	A	614	CLA	C1D-ND	3.80	1.42	1.37
26	A	614	CLA	MG-NA	3.79	2.15	2.06
26	C	512	CLA	MG-NA	3.74	2.15	2.06
26	C	502	CLA	C1D-ND	3.73	1.42	1.37
26	C	501	CLA	MG-ND	-3.72	1.98	2.05
36	v	201	HEC	FE-NA	3.70	2.07	1.95
26	B	614	CLA	MG-NA	3.70	2.15	2.06
26	c	513	CLA	C1D-ND	3.69	1.42	1.37
26	c	507	CLA	C1D-ND	3.69	1.42	1.37
31	a	616	SQD	O47-C45	-3.68	1.37	1.46
31	a	616	SQD	O5-C1	3.67	1.51	1.41
26	B	614	CLA	C4B-NB	3.66	1.42	1.37
26	B	615	CLA	C4B-NB	3.66	1.42	1.37
35	e	102	HEM	FE-NB	3.65	2.06	1.94
26	B	615	CLA	C1D-ND	3.64	1.42	1.37
26	b	602	CLA	C1D-ND	3.63	1.42	1.37
26	B	602	CLA	C1D-ND	3.62	1.42	1.37
26	c	503	CLA	MG-NB	3.62	2.13	2.05
26	c	509	CLA	C1D-ND	3.61	1.42	1.37
27	d	401	PHO	C4D-CHA	3.61	1.44	1.39
31	B	623	SQD	O47-C45	-3.61	1.38	1.46
26	C	506	CLA	MG-NA	3.59	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	601	CLA	C1D-ND	3.59	1.42	1.37
26	d	403	CLA	C1D-ND	3.58	1.42	1.37
26	C	512	CLA	C1D-ND	3.58	1.42	1.37
31	f	101	SQD	O47-C7	3.58	1.44	1.34
26	c	501	CLA	C1D-ND	3.58	1.42	1.37
31	a	614	SQD	O47-C45	-3.58	1.38	1.46
26	C	506	CLA	C1D-ND	3.57	1.42	1.37
26	B	609	CLA	C1D-ND	3.56	1.42	1.37
26	c	505	CLA	MG-NA	3.56	2.14	2.06
26	b	610	CLA	MG-NB	-3.56	1.98	2.05
26	C	509	CLA	C1D-ND	3.55	1.42	1.37
27	a	609	PHO	C4D-CHA	3.55	1.44	1.39
26	b	607	CLA	MG-NA	3.55	2.14	2.06
26	b	613	CLA	C1D-ND	3.54	1.42	1.37
26	c	506	CLA	C1D-ND	3.54	1.42	1.37
31	b	620	SQD	O47-C7	3.54	1.44	1.34
29	D	405	PL9	C3-C4	-3.53	1.44	1.49
31	A	616	SQD	O47-C45	-3.51	1.38	1.46
26	a	610	CLA	MG-NA	3.50	2.14	2.06
26	c	502	CLA	C1D-ND	3.49	1.42	1.37
26	a	607	CLA	C1D-ND	3.47	1.42	1.37
26	B	611	CLA	C1D-ND	3.47	1.42	1.37
26	A	607	CLA	MG-NB	3.46	2.12	2.05
26	C	513	CLA	C1D-ND	3.46	1.42	1.37
26	B	606	CLA	MG-NB	3.45	2.12	2.05
26	b	612	CLA	C1D-ND	3.45	1.42	1.37
26	A	608	CLA	C1D-ND	3.45	1.42	1.37
26	b	604	CLA	MG-NA	3.44	2.14	2.06
26	B	608	CLA	C1D-ND	3.44	1.42	1.37
35	F	101	HEM	FE-NB	3.42	2.05	1.94
26	C	511	CLA	C1D-ND	3.41	1.42	1.37
26	d	402	CLA	C1D-ND	3.40	1.42	1.37
26	B	603	CLA	C1D-ND	3.40	1.42	1.37
26	B	601	CLA	C1D-ND	3.38	1.42	1.37
26	B	608	CLA	MG-NA	3.38	2.14	2.06
26	c	511	CLA	C1D-ND	3.38	1.42	1.37
26	a	608	CLA	C4B-NB	3.38	1.42	1.37
26	b	613	CLA	C4B-NB	3.37	1.42	1.37
26	A	607	CLA	C1D-ND	3.37	1.42	1.37
31	b	620	SQD	O5-C1	3.37	1.50	1.41
26	b	607	CLA	C1D-ND	3.37	1.42	1.37
26	a	607	CLA	MG-NB	3.36	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	504	CLA	MG-NA	3.36	2.14	2.06
27	A	609	PHO	C4D-CHA	3.36	1.44	1.39
26	C	507	CLA	C1D-ND	3.36	1.42	1.37
31	A	616	SQD	O47-C7	3.35	1.43	1.34
26	b	614	CLA	C4B-NB	3.34	1.42	1.37
26	b	607	CLA	MG-ND	-3.34	1.99	2.05
26	B	610	CLA	MG-NA	3.34	2.14	2.06
31	f	101	SQD	O47-C45	-3.34	1.38	1.46
26	a	610	CLA	MG-ND	-3.33	1.99	2.05
31	a	614	SQD	O47-C7	3.33	1.43	1.34
26	c	507	CLA	MG-NA	3.33	2.14	2.06
26	c	504	CLA	C4B-NB	3.31	1.42	1.37
26	b	613	CLA	MG-NA	3.31	2.14	2.06
26	B	615	CLA	C1B-C2B	3.30	1.50	1.43
26	C	504	CLA	C4B-NB	3.29	1.42	1.37
31	B	623	SQD	O47-C7	3.29	1.43	1.34
26	b	615	CLA	C1D-ND	3.29	1.42	1.37
26	c	503	CLA	C1D-ND	3.29	1.42	1.37
26	b	606	CLA	C1D-ND	3.28	1.42	1.37
26	C	505	CLA	C1D-ND	3.28	1.42	1.37
26	C	501	CLA	C4B-NB	3.28	1.42	1.37
26	d	403	CLA	C4B-NB	3.27	1.42	1.37
26	b	608	CLA	MG-NA	3.27	2.14	2.06
26	c	508	CLA	C1D-ND	3.27	1.42	1.37
36	V	201	HEC	FE-NB	3.25	2.04	1.94
26	c	512	CLA	C1D-ND	3.25	1.42	1.37
26	B	613	CLA	C1D-ND	3.24	1.42	1.37
26	b	603	CLA	C4B-NB	3.23	1.42	1.37
26	A	607	CLA	C1B-C2B	3.23	1.50	1.43
26	a	608	CLA	C1D-ND	3.21	1.42	1.37
26	B	610	CLA	C4B-NB	3.21	1.42	1.37
26	B	611	CLA	C1B-C2B	3.20	1.50	1.43
31	a	616	SQD	O47-C7	3.20	1.43	1.34
26	B	601	CLA	C4B-NB	3.19	1.42	1.37
26	a	613	CLA	C1D-ND	3.19	1.42	1.37
31	A	615	SQD	O5-C1	3.19	1.50	1.41
26	c	503	CLA	C1B-C2B	3.17	1.50	1.43
31	B	623	SQD	O5-C1	3.17	1.50	1.41
26	b	605	CLA	C4B-NB	3.16	1.42	1.37
27	a	609	PHO	C3D-C4D	3.16	1.45	1.41
26	b	609	CLA	C1D-ND	3.16	1.42	1.37
26	C	508	CLA	C1B-C2B	3.16	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	616	SQD	C24-C23	3.15	1.59	1.50
26	c	508	CLA	C4B-NB	3.14	1.42	1.37
26	A	614	CLA	MG-NB	3.14	2.12	2.05
31	A	616	SQD	C24-C23	3.13	1.59	1.50
26	c	502	CLA	MG-NA	3.12	2.13	2.06
26	B	607	CLA	MG-NA	3.12	2.13	2.06
26	a	610	CLA	C4B-NB	3.12	1.42	1.37
26	C	507	CLA	C1B-C2B	3.12	1.50	1.43
26	B	606	CLA	C1D-ND	3.11	1.42	1.37
26	b	601	CLA	C4B-NB	3.11	1.41	1.37
26	B	605	CLA	C1D-ND	3.11	1.41	1.37
26	B	612	CLA	C4B-NB	3.10	1.41	1.37
26	B	605	CLA	MG-ND	3.10	2.11	2.05
26	B	602	CLA	C4B-NB	3.10	1.41	1.37
26	C	502	CLA	C4B-NB	3.09	1.41	1.37
26	b	602	CLA	C4B-NB	3.09	1.41	1.37
26	c	511	CLA	C4B-NB	3.09	1.41	1.37
27	A	609	PHO	C3D-C4D	3.09	1.45	1.41
26	c	509	CLA	C1B-C2B	3.09	1.50	1.43
31	a	614	SQD	C24-C23	3.09	1.59	1.50
26	C	504	CLA	C1D-ND	3.09	1.41	1.37
31	b	620	SQD	O47-C45	-3.09	1.39	1.46
26	a	607	CLA	MG-NA	3.08	2.13	2.06
26	C	512	CLA	MG-NC	3.08	2.13	2.06
31	f	101	SQD	C24-C23	3.08	1.59	1.50
26	c	509	CLA	MG-ND	-3.06	1.99	2.05
26	b	605	CLA	C1B-C2B	3.05	1.50	1.43
31	F	102	SQD	C24-C23	3.05	1.59	1.50
26	b	612	CLA	C4B-NB	3.05	1.41	1.37
26	B	605	CLA	C4B-NB	3.04	1.41	1.37
26	C	503	CLA	MG-ND	3.03	2.11	2.05
26	b	611	CLA	C1B-C2B	3.03	1.50	1.43
26	b	615	CLA	C4B-NB	3.03	1.41	1.37
26	B	606	CLA	C1B-C2B	3.03	1.50	1.43
26	C	513	CLA	C1B-C2B	3.03	1.50	1.43
26	C	503	CLA	C1D-ND	3.03	1.41	1.37
26	b	610	CLA	C4B-NB	3.02	1.41	1.37
26	b	601	CLA	C1B-C2B	3.01	1.50	1.43
26	B	613	CLA	C4B-NB	3.01	1.41	1.37
26	C	507	CLA	C4B-NB	3.01	1.41	1.37
26	c	503	CLA	C4B-NB	3.01	1.41	1.37
26	b	609	CLA	C4B-NB	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	615	SQD	O47-C7	3.00	1.42	1.34
26	b	603	CLA	C1D-ND	3.00	1.41	1.37
26	C	511	CLA	C4B-NB	3.00	1.41	1.37
31	b	620	SQD	C24-C23	3.00	1.59	1.50
26	B	603	CLA	C4B-NB	2.99	1.41	1.37
31	A	615	SQD	C24-C23	2.99	1.59	1.50
26	C	513	CLA	MG-ND	2.98	2.11	2.05
26	B	608	CLA	C4B-NB	2.98	1.41	1.37
26	c	508	CLA	C1B-C2B	2.98	1.50	1.43
26	a	608	CLA	CHC-C1C	2.97	1.44	1.38
26	c	512	CLA	C1B-C2B	2.97	1.50	1.43
26	C	503	CLA	C1B-C2B	2.97	1.50	1.43
26	c	507	CLA	C1B-C2B	2.97	1.50	1.43
31	B	623	SQD	C24-C23	2.96	1.59	1.50
26	C	511	CLA	C1B-C2B	2.96	1.50	1.43
26	D	402	CLA	C1B-C2B	2.96	1.50	1.43
26	c	504	CLA	MG-NB	2.96	2.11	2.05
26	C	510	CLA	C1B-C2B	2.96	1.50	1.43
26	C	506	CLA	C4B-NB	2.95	1.41	1.37
36	V	201	HEC	FE-NC	2.95	2.04	1.95
26	b	615	CLA	C1B-C2B	2.95	1.50	1.43
26	C	510	CLA	C4B-NB	2.94	1.41	1.37
26	c	509	CLA	MG-NC	2.94	2.13	2.06
26	c	505	CLA	C1D-ND	2.94	1.41	1.37
26	c	509	CLA	C4B-NB	2.94	1.41	1.37
26	c	507	CLA	C4B-NB	2.94	1.41	1.37
29	d	405	PL9	C3-C4	-2.94	1.45	1.49
26	a	607	CLA	C1B-C2B	2.94	1.50	1.43
26	B	613	CLA	MG-NC	2.94	2.13	2.06
26	C	502	CLA	C1B-C2B	2.93	1.50	1.43
26	D	403	CLA	C1B-C2B	2.93	1.50	1.43
26	b	611	CLA	C1D-ND	2.92	1.41	1.37
26	B	612	CLA	MG-NA	2.92	2.13	2.06
26	B	603	CLA	C1B-C2B	2.92	1.50	1.43
26	B	614	CLA	MG-ND	-2.92	2.00	2.05
26	C	508	CLA	C4B-NB	2.92	1.41	1.37
26	C	512	CLA	C1B-C2B	2.91	1.50	1.43
35	e	102	HEM	CAC-C3C	2.91	1.55	1.47
26	C	508	CLA	C3B-C4B	2.90	1.51	1.42
26	B	612	CLA	C1B-C2B	2.90	1.49	1.43
26	b	605	CLA	C1D-ND	2.90	1.41	1.37
26	B	605	CLA	C1B-C2B	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	610	CLA	C1B-C2B	2.90	1.49	1.43
26	B	608	CLA	MG-NC	2.90	2.13	2.06
26	b	606	CLA	C1B-C2B	2.89	1.49	1.43
26	a	608	CLA	MG-NB	2.89	2.11	2.05
26	b	608	CLA	C4B-NB	2.89	1.41	1.37
31	a	614	SQD	O5-C1	2.89	1.49	1.41
26	C	505	CLA	C1B-C2B	2.89	1.49	1.43
35	F	101	HEM	CAB-C3B	2.88	1.55	1.47
27	D	401	PHO	C4D-CHA	2.88	1.43	1.39
26	B	613	CLA	C1B-C2B	2.88	1.49	1.43
26	b	610	CLA	C1B-C2B	2.87	1.49	1.43
26	B	605	CLA	C3B-C4B	2.86	1.51	1.42
26	c	506	CLA	MG-NA	2.86	2.13	2.06
26	A	608	CLA	CHC-C1C	2.86	1.44	1.38
26	D	402	CLA	C1D-ND	2.86	1.41	1.37
26	c	506	CLA	C4B-NB	2.85	1.41	1.37
26	C	508	CLA	C1D-ND	2.84	1.41	1.37
26	d	402	CLA	C1B-C2B	2.84	1.49	1.43
26	c	510	CLA	C1B-C2B	2.84	1.49	1.43
26	A	610	CLA	C1D-ND	2.84	1.41	1.37
26	B	612	CLA	C1D-ND	2.84	1.41	1.37
26	c	504	CLA	C1D-ND	2.84	1.41	1.37
26	B	610	CLA	C3B-C4B	2.83	1.51	1.42
26	c	504	CLA	C1B-C2B	2.83	1.49	1.43
26	B	607	CLA	C1B-C2B	2.82	1.49	1.43
26	c	501	CLA	C1B-C2B	2.82	1.49	1.43
26	C	512	CLA	C4B-NB	2.82	1.41	1.37
26	c	510	CLA	C4B-NB	2.81	1.41	1.37
26	b	616	CLA	C1B-C2B	2.81	1.49	1.43
26	b	602	CLA	C1B-C2B	2.81	1.49	1.43
26	D	403	CLA	C4B-NB	2.81	1.41	1.37
26	c	506	CLA	MG-ND	-2.81	2.00	2.05
26	A	608	CLA	C1B-C2B	2.80	1.49	1.43
26	B	616	CLA	C1B-C2B	2.80	1.49	1.43
26	C	509	CLA	C1B-C2B	2.80	1.49	1.43
26	c	502	CLA	C1B-C2B	2.79	1.49	1.43
26	C	503	CLA	C4B-NB	2.79	1.41	1.37
26	A	610	CLA	C4B-NB	2.79	1.41	1.37
26	c	502	CLA	C4B-NB	2.79	1.41	1.37
26	D	402	CLA	MG-NA	2.78	2.12	2.06
35	F	101	HEM	CAC-C3C	2.77	1.54	1.47
26	c	513	CLA	C4B-NB	2.77	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	615	CLA	C3B-C4B	2.77	1.50	1.42
26	C	513	CLA	C4B-NB	2.76	1.41	1.37
35	e	102	HEM	CAB-C3B	2.76	1.54	1.47
26	B	616	CLA	MG-NB	-2.75	2.00	2.05
26	B	604	CLA	C1B-C2B	2.75	1.49	1.43
26	A	608	CLA	C4B-NB	2.75	1.41	1.37
26	A	614	CLA	C1B-C2B	2.73	1.49	1.43
26	c	507	CLA	MG-NB	-2.73	2.00	2.05
26	b	606	CLA	C4B-NB	2.73	1.41	1.37
26	b	608	CLA	C1B-C2B	2.73	1.49	1.43
26	c	505	CLA	CHC-C1C	2.73	1.43	1.38
26	c	506	CLA	C1B-C2B	2.72	1.49	1.43
26	C	512	CLA	C3B-C4B	2.72	1.50	1.42
26	b	608	CLA	CHC-C1C	2.72	1.43	1.38
26	b	604	CLA	C4B-NB	2.71	1.41	1.37
26	B	614	CLA	CHC-C1C	2.71	1.43	1.38
26	C	505	CLA	C4B-NB	2.71	1.41	1.37
26	d	403	CLA	C1B-C2B	2.71	1.49	1.43
26	b	612	CLA	MG-ND	-2.71	2.00	2.05
26	B	614	CLA	MG-NB	2.71	2.11	2.05
26	b	608	CLA	C3B-C4B	2.71	1.50	1.42
26	b	613	CLA	CHC-C1C	2.70	1.43	1.38
26	d	403	CLA	MG-NA	2.70	2.12	2.06
26	b	604	CLA	C1B-C2B	2.70	1.49	1.43
26	B	609	CLA	C1B-C2B	2.70	1.49	1.43
26	A	610	CLA	C1B-C2B	2.69	1.49	1.43
26	b	608	CLA	C1D-ND	2.69	1.41	1.37
26	b	614	CLA	CHC-C1C	2.69	1.43	1.38
26	A	614	CLA	C3B-C4B	2.69	1.50	1.42
26	c	511	CLA	C1B-C2B	2.69	1.49	1.43
26	B	607	CLA	C4B-NB	2.69	1.41	1.37
26	C	504	CLA	C1B-C2B	2.68	1.49	1.43
26	C	510	CLA	CHC-C1C	2.68	1.43	1.38
35	e	102	HEM	FE-ND	2.67	2.03	1.94
26	C	509	CLA	C4B-NB	2.67	1.41	1.37
26	C	501	CLA	C1B-C2B	2.67	1.49	1.43
26	c	513	CLA	C3B-C4B	2.67	1.50	1.42
26	c	508	CLA	CHC-C1C	2.66	1.43	1.38
26	B	602	CLA	C1B-C2B	2.66	1.49	1.43
26	b	616	CLA	MG-NA	2.66	2.12	2.06
26	B	613	CLA	CHC-C1C	2.66	1.43	1.38
26	B	602	CLA	MG-NC	2.66	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	509	CLA	MG-NA	2.66	2.12	2.06
26	b	616	CLA	C4B-NB	2.66	1.41	1.37
26	C	510	CLA	MG-NC	2.66	2.12	2.06
26	c	505	CLA	C1B-C2B	2.66	1.49	1.43
26	B	616	CLA	C4B-NB	2.65	1.41	1.37
26	B	604	CLA	C4B-NB	2.65	1.41	1.37
26	B	609	CLA	C4B-NB	2.65	1.41	1.37
26	B	607	CLA	C1D-ND	2.64	1.41	1.37
31	A	616	SQD	O5-C5	2.64	1.50	1.44
31	F	102	SQD	O5-C1	2.63	1.48	1.41
31	f	101	SQD	O5-C1	2.62	1.48	1.41
26	C	511	CLA	C3B-C4B	2.62	1.50	1.42
26	C	506	CLA	C1B-C2B	2.62	1.49	1.43
26	C	510	CLA	C3B-C4B	2.62	1.50	1.42
26	a	613	CLA	C1B-C2B	2.62	1.49	1.43
27	a	609	PHO	CMB-C2B	-2.61	1.46	1.51
26	c	508	CLA	C3B-C4B	2.61	1.50	1.42
26	C	507	CLA	MG-ND	-2.61	2.00	2.05
26	b	603	CLA	C1B-C2B	2.61	1.49	1.43
26	b	614	CLA	C1B-C2B	2.60	1.49	1.43
26	B	610	CLA	C1B-C2B	2.60	1.49	1.43
26	B	611	CLA	MG-NA	2.60	2.12	2.06
26	c	508	CLA	MG-NB	2.60	2.10	2.05
29	a	612	PL9	C53-C6	-2.59	1.45	1.50
27	A	609	PHO	CMD-C2D	-2.59	1.46	1.51
26	c	505	CLA	C3B-C4B	2.59	1.50	1.42
31	A	616	SQD	O7-S	2.58	1.52	1.45
26	b	611	CLA	C3B-C4B	2.58	1.50	1.42
26	A	607	CLA	C3B-C4B	2.58	1.50	1.42
31	a	616	SQD	O9-S	2.58	1.52	1.45
31	A	616	SQD	O9-S	2.58	1.52	1.45
26	c	513	CLA	C1B-C2B	2.57	1.49	1.43
26	b	613	CLA	C1B-C2B	2.56	1.49	1.43
26	a	608	CLA	C3B-C4B	2.56	1.50	1.42
27	D	401	PHO	CMD-C2D	-2.55	1.46	1.51
26	C	501	CLA	CHC-C1C	2.55	1.43	1.38
26	A	614	CLA	C4B-NB	2.55	1.41	1.37
26	c	505	CLA	MG-ND	2.54	2.10	2.05
27	a	609	PHO	CBD-CGD	-2.54	1.49	1.52
26	C	509	CLA	C3B-C4B	2.54	1.50	1.42
26	A	614	CLA	CHC-C1C	2.53	1.43	1.38
26	B	606	CLA	C4B-NB	2.53	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	608	CLA	C1B-C2B	2.52	1.49	1.43
31	f	101	SQD	O9-S	2.51	1.52	1.45
26	B	611	CLA	C4B-NB	2.51	1.41	1.37
26	c	512	CLA	C4B-NB	2.51	1.41	1.37
26	C	506	CLA	MG-NB	2.51	2.10	2.05
26	b	607	CLA	C1B-C2B	2.51	1.49	1.43
26	b	605	CLA	C3B-C4B	2.51	1.50	1.42
26	c	503	CLA	CHC-C1C	2.50	1.43	1.38
31	a	616	SQD	O7-S	2.49	1.52	1.45
26	B	611	CLA	C3B-C4B	2.49	1.50	1.42
26	a	607	CLA	C4B-NB	2.49	1.41	1.37
26	C	511	CLA	CHC-C1C	2.49	1.43	1.38
26	b	609	CLA	C1B-C2B	2.49	1.49	1.43
26	B	606	CLA	CHC-C1C	2.48	1.43	1.38
26	c	510	CLA	CHC-C1C	2.48	1.43	1.38
26	C	504	CLA	C3B-C4B	2.47	1.49	1.42
26	C	501	CLA	C3B-C4B	2.47	1.49	1.42
26	D	402	CLA	C4B-NB	2.47	1.41	1.37
27	d	401	PHO	C4D-ND	-2.46	1.34	1.38
26	C	508	CLA	CHC-C1C	2.46	1.43	1.38
27	d	401	PHO	C3D-C4D	2.46	1.44	1.41
26	B	601	CLA	C1B-C2B	2.46	1.48	1.43
26	B	614	CLA	C1B-C2B	2.46	1.48	1.43
26	B	603	CLA	CMD-C2D	-2.46	1.45	1.50
26	B	605	CLA	CHC-C1C	2.46	1.43	1.38
36	V	201	HEC	CMB-C2B	2.46	1.55	1.50
26	b	613	CLA	C3B-C4B	2.45	1.49	1.42
26	d	402	CLA	MG-NA	2.45	2.12	2.06
26	B	616	CLA	MG-ND	2.45	2.10	2.05
26	c	506	CLA	CHC-C1C	2.45	1.43	1.38
27	D	401	PHO	CMB-C2B	-2.45	1.46	1.51
27	a	609	PHO	CMC-C2C	-2.44	1.46	1.50
26	c	505	CLA	C4B-NB	2.44	1.41	1.37
26	B	605	CLA	MG-NA	2.44	2.12	2.06
26	c	501	CLA	C4B-NB	2.44	1.41	1.37
26	d	402	CLA	C3B-C4B	2.43	1.49	1.42
26	b	601	CLA	CHC-C1C	2.43	1.43	1.38
26	b	605	CLA	CHC-C1C	2.43	1.43	1.38
26	C	506	CLA	MG-ND	-2.43	2.01	2.05
26	c	506	CLA	C3B-C4B	2.43	1.49	1.42
27	d	401	PHO	CMD-C2D	-2.42	1.46	1.51
26	b	601	CLA	C3B-C4B	2.42	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	608	CLA	C1B-C2B	2.42	1.48	1.43
26	B	602	CLA	MG-NA	2.42	2.12	2.06
26	a	607	CLA	CHC-C1C	2.42	1.43	1.38
26	C	506	CLA	C3B-C4B	2.42	1.49	1.42
26	d	403	CLA	MG-NB	2.42	2.10	2.05
26	A	607	CLA	CHC-C1C	2.42	1.43	1.38
26	a	613	CLA	C4B-NB	2.41	1.41	1.37
26	b	607	CLA	C4B-NB	2.41	1.41	1.37
27	d	401	PHO	CMC-C2C	-2.41	1.46	1.50
26	c	504	CLA	CHC-C1C	2.41	1.43	1.38
26	b	614	CLA	C3B-C4B	2.41	1.49	1.42
26	C	504	CLA	CHC-C1C	2.40	1.43	1.38
26	A	607	CLA	C4B-NB	2.40	1.41	1.37
26	d	403	CLA	C3B-C4B	2.40	1.49	1.42
26	C	503	CLA	CHC-C1C	2.40	1.43	1.38
29	d	405	PL9	C6-C1	-2.40	1.44	1.48
26	c	513	CLA	CHC-C1C	2.40	1.43	1.38
31	b	620	SQD	O9-S	2.40	1.51	1.45
26	c	512	CLA	C3B-C4B	2.39	1.49	1.42
26	c	511	CLA	CHC-C1C	2.39	1.43	1.38
26	d	402	CLA	C4B-NB	2.39	1.41	1.37
26	a	607	CLA	C3B-C4B	2.39	1.49	1.42
26	C	505	CLA	CHC-C1C	2.38	1.43	1.38
26	c	511	CLA	C3B-C4B	2.38	1.49	1.42
26	B	616	CLA	CHC-C1C	2.38	1.43	1.38
26	d	402	CLA	MG-NC	2.38	2.11	2.06
26	b	612	CLA	CMC-C2C	-2.37	1.45	1.50
26	b	609	CLA	MG-ND	2.37	2.10	2.05
26	b	611	CLA	CHC-C1C	2.37	1.43	1.38
31	f	101	SQD	O7-S	2.37	1.51	1.45
26	b	606	CLA	CHC-C1C	2.37	1.43	1.38
31	B	623	SQD	O9-S	2.37	1.51	1.45
26	B	610	CLA	CHC-C1C	2.36	1.43	1.38
26	b	604	CLA	MG-NC	2.35	2.11	2.06
26	B	613	CLA	C3B-C4B	2.35	1.49	1.42
26	b	610	CLA	CMD-C2D	-2.35	1.46	1.50
26	C	506	CLA	CHC-C1C	2.35	1.43	1.38
26	D	403	CLA	MG-NC	2.34	2.11	2.06
26	C	505	CLA	MG-NC	2.33	2.11	2.06
26	B	614	CLA	MG-NC	2.33	2.11	2.06
26	B	615	CLA	CHC-C1C	2.32	1.43	1.38
26	b	612	CLA	CHC-C1C	2.32	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	603	CLA	C3B-C4B	2.32	1.49	1.42
26	c	504	CLA	C3B-C4B	2.32	1.49	1.42
31	b	620	SQD	O5-C5	2.32	1.50	1.44
26	b	612	CLA	C3B-C4B	2.32	1.49	1.42
26	b	604	CLA	C3B-C4B	2.31	1.49	1.42
26	c	503	CLA	MG-NC	2.31	2.11	2.06
26	b	612	CLA	C1B-C2B	2.31	1.48	1.43
27	D	401	PHO	CMC-C2C	-2.31	1.47	1.50
26	c	512	CLA	CHC-C1C	2.31	1.43	1.38
26	c	501	CLA	MG-NC	2.31	2.11	2.06
26	C	502	CLA	C3B-C4B	2.30	1.49	1.42
26	C	507	CLA	CHC-C1C	2.29	1.43	1.38
26	D	403	CLA	MG-ND	-2.29	2.01	2.05
26	b	601	CLA	MG-NA	2.29	2.11	2.06
26	A	608	CLA	C3B-C4B	2.28	1.49	1.42
26	C	513	CLA	C3B-C4B	2.28	1.49	1.42
26	c	508	CLA	MG-NA	2.28	2.11	2.06
26	B	604	CLA	CHC-C1C	2.27	1.43	1.38
26	B	616	CLA	C3B-C4B	2.27	1.49	1.42
26	B	608	CLA	C3B-C4B	2.27	1.49	1.42
26	b	603	CLA	C3B-C4B	2.26	1.49	1.42
26	b	605	CLA	MG-NB	2.26	2.10	2.05
26	B	606	CLA	C3B-C4B	2.26	1.49	1.42
26	C	510	CLA	CMD-C2D	-2.26	1.46	1.50
26	c	502	CLA	C3B-C4B	2.26	1.49	1.42
31	a	616	SQD	O5-C5	2.26	1.49	1.44
26	B	601	CLA	CMC-C2C	-2.25	1.46	1.50
26	B	612	CLA	CHC-C1C	2.25	1.43	1.38
26	C	513	CLA	MG-NB	-2.25	2.01	2.05
26	a	613	CLA	C3B-C4B	2.24	1.49	1.42
26	b	616	CLA	MG-ND	-2.24	2.01	2.05
26	C	502	CLA	CHC-C1C	2.24	1.43	1.38
26	D	402	CLA	C3B-C4B	2.24	1.49	1.42
26	C	504	CLA	CMB-C2B	-2.24	1.46	1.50
26	b	606	CLA	C3B-C4B	2.23	1.49	1.42
31	b	620	SQD	O7-S	2.23	1.51	1.45
26	B	604	CLA	C3B-C4B	2.22	1.49	1.42
26	C	505	CLA	C3B-C4B	2.22	1.49	1.42
26	c	512	CLA	CMD-C2D	-2.21	1.46	1.50
26	B	601	CLA	C3B-C4B	2.21	1.49	1.42
26	C	503	CLA	C3B-C4B	2.21	1.49	1.42
26	b	609	CLA	C3B-C4B	2.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	608	CLA	CHC-C1C	2.21	1.42	1.38
27	D	401	PHO	C4D-ND	-2.21	1.35	1.38
26	c	509	CLA	CHC-C1C	2.20	1.42	1.38
26	b	616	CLA	CMC-C2C	-2.19	1.46	1.50
29	D	405	PL9	C46-C44	-2.19	1.46	1.51
29	A	612	PL9	C53-C6	-2.19	1.46	1.50
26	b	607	CLA	C3B-C4B	2.18	1.49	1.42
27	A	609	PHO	CBD-CGD	-2.18	1.49	1.52
26	C	508	CLA	C1D-C2D	2.17	1.49	1.45
31	F	102	SQD	O9-S	2.16	1.51	1.45
26	b	603	CLA	CMD-C2D	-2.16	1.46	1.50
26	c	503	CLA	C3B-C4B	2.16	1.49	1.42
26	b	611	CLA	C4B-NB	2.16	1.40	1.37
26	B	604	CLA	MG-ND	-2.15	2.01	2.05
31	B	623	SQD	O7-S	2.15	1.51	1.45
26	C	501	CLA	CMD-C2D	-2.15	1.46	1.50
26	B	616	CLA	MG-NC	2.15	2.11	2.06
26	c	510	CLA	CMB-C2B	-2.15	1.46	1.50
26	C	503	CLA	C1D-C2D	2.15	1.49	1.45
26	c	513	CLA	CMB-C2B	-2.15	1.46	1.50
26	c	507	CLA	CMC-C2C	-2.15	1.46	1.50
26	C	503	CLA	MG-NB	2.14	2.10	2.05
26	a	608	CLA	MG-ND	-2.14	2.01	2.05
26	c	510	CLA	C3B-C4B	2.14	1.49	1.42
26	C	512	CLA	CHC-C1C	2.13	1.42	1.38
27	a	609	PHO	CMD-C2D	-2.13	1.47	1.51
36	V	201	HEC	CAC-C3C	2.11	1.56	1.51
26	B	602	CLA	C3B-C4B	2.11	1.48	1.42
26	b	615	CLA	CHC-C1C	2.11	1.42	1.38
27	a	609	PHO	C4D-ND	-2.11	1.35	1.38
35	e	102	HEM	CMC-C2C	2.11	1.55	1.50
26	D	403	CLA	MG-NA	2.11	2.11	2.06
31	a	614	SQD	O7-S	2.11	1.51	1.45
26	c	501	CLA	C3B-C4B	2.10	1.48	1.42
26	b	602	CLA	C3B-C4B	2.10	1.48	1.42
35	e	102	HEM	C2A-C3A	-2.10	1.33	1.38
26	b	604	CLA	CHC-C1C	2.10	1.42	1.38
27	A	609	PHO	CMB-C2B	-2.10	1.47	1.51
26	d	403	CLA	CMD-C2D	-2.09	1.46	1.50
26	C	504	CLA	O2D-CGD	2.09	1.38	1.33
26	C	507	CLA	C3B-C4B	2.09	1.48	1.42
31	a	614	SQD	O9-S	2.08	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	615	CLA	C3B-C4B	2.08	1.48	1.42
26	a	610	CLA	CMC-C2C	-2.08	1.46	1.50
26	b	604	CLA	C3D-C4D	2.07	1.48	1.44
26	b	616	CLA	C3B-C4B	2.07	1.48	1.42
26	b	609	CLA	CHC-C1C	2.07	1.42	1.38
26	b	603	CLA	CHC-C1C	2.07	1.42	1.38
26	c	512	CLA	MG-NB	2.07	2.09	2.05
26	B	607	CLA	C3B-C4B	2.07	1.48	1.42
26	B	612	CLA	C3B-C4B	2.06	1.48	1.42
26	C	502	CLA	CMB-C2B	-2.06	1.46	1.50
26	c	502	CLA	CMD-C2D	-2.06	1.46	1.50
26	b	611	CLA	C1D-C2D	2.06	1.49	1.45
26	b	602	CLA	CHC-C1C	2.06	1.42	1.38
26	d	402	CLA	CMD-C2D	-2.06	1.46	1.50
26	C	511	CLA	CMD-C2D	-2.05	1.46	1.50
26	c	510	CLA	CMD-C2D	-2.05	1.46	1.50
27	d	401	PHO	CMB-C2B	-2.05	1.47	1.51
26	B	607	CLA	CMD-C2D	-2.05	1.46	1.50
26	c	502	CLA	CHC-C1C	2.05	1.42	1.38
26	c	506	CLA	MG-NB	2.05	2.09	2.05
26	c	505	CLA	CMB-C2B	-2.05	1.46	1.50
26	C	508	CLA	CMC-C2C	-2.04	1.46	1.50
26	b	606	CLA	CMD-C2D	-2.04	1.46	1.50
26	B	613	CLA	CMD-C2D	-2.04	1.46	1.50
26	B	608	CLA	C1D-C2D	2.04	1.49	1.45
26	b	613	CLA	CMD-C2D	-2.04	1.46	1.50
26	B	616	CLA	CMC-C2C	-2.04	1.46	1.50
26	b	602	CLA	MG-NC	2.04	2.11	2.06
26	a	607	CLA	C3D-C4D	2.04	1.48	1.44
27	A	609	PHO	C4D-ND	-2.04	1.35	1.38
26	d	402	CLA	CMB-C2B	-2.04	1.46	1.50
26	a	607	CLA	C1D-C2D	2.04	1.49	1.45
26	c	501	CLA	CHC-C1C	2.04	1.42	1.38
26	C	509	CLA	CMD-C2D	-2.04	1.46	1.50
27	D	401	PHO	C3D-C4D	2.04	1.44	1.41
26	b	611	CLA	CMD-C2D	-2.03	1.46	1.50
26	c	509	CLA	C3B-C4B	2.03	1.48	1.42
26	b	615	CLA	CMD-C2D	-2.03	1.46	1.50
26	B	601	CLA	CHC-C1C	2.03	1.42	1.38
26	c	508	CLA	MG-NC	2.03	2.11	2.06
35	e	102	HEM	C3B-C2B	-2.03	1.33	1.37
26	A	607	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	403	CLA	C3B-C4B	2.02	1.48	1.42
26	c	506	CLA	MG-NC	2.02	2.11	2.06
26	a	613	CLA	CHC-C1C	2.02	1.42	1.38
26	a	613	CLA	MG-NC	2.02	2.11	2.06
26	c	513	CLA	MG-NC	2.02	2.11	2.06
26	B	610	CLA	C1D-C2D	2.02	1.49	1.45
26	B	612	CLA	CMC-C2C	-2.01	1.46	1.50
26	a	607	CLA	C3C-C2C	2.01	1.41	1.36
26	C	510	CLA	MG-NA	2.01	2.11	2.06
36	v	201	HEC	CMD-C2D	2.01	1.54	1.50
26	D	403	CLA	CMC-C2C	-2.01	1.46	1.50
26	C	512	CLA	CMD-C2D	-2.01	1.46	1.50
31	B	623	SQD	O5-C5	2.01	1.49	1.44
31	B	623	SQD	C8-C7	2.00	1.56	1.50
26	b	609	CLA	C3D-C4D	2.00	1.48	1.44
26	b	610	CLA	C3B-C4B	2.00	1.48	1.42
26	C	512	CLA	CMB-C2B	-2.00	1.46	1.50
26	C	509	CLA	CMB-C2B	-2.00	1.46	1.50

All (839) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	615	CLA	C4A-NA-C1A	9.44	110.98	106.68
26	C	511	CLA	C4A-NA-C1A	8.30	110.47	106.68
26	C	503	CLA	C4A-NA-C1A	8.27	110.45	106.68
26	b	606	CLA	C4A-NA-C1A	8.24	110.44	106.68
26	B	606	CLA	C4A-NA-C1A	8.01	110.33	106.68
26	c	501	CLA	C4A-NA-C1A	7.90	110.28	106.68
26	B	604	CLA	C4A-NA-C1A	7.87	110.27	106.68
27	A	609	PHO	C4D-CHA-CBD	-7.86	104.68	108.45
26	b	601	CLA	C4A-NA-C1A	7.76	110.22	106.68
26	c	503	CLA	C4A-NA-C1A	7.66	110.17	106.68
31	a	614	SQD	O6-C1-C2	7.43	119.56	108.27
26	C	507	CLA	C4A-NA-C1A	7.33	110.02	106.68
26	B	613	CLA	C4A-NA-C1A	7.27	109.99	106.68
26	c	509	CLA	C4A-NA-C1A	7.24	109.98	106.68
26	c	511	CLA	C4A-NA-C1A	7.21	109.97	106.68
26	b	604	CLA	C4A-NA-C1A	7.10	109.92	106.68
27	a	609	PHO	C4D-CHA-CBD	-6.90	105.14	108.45
26	B	601	CLA	C4A-NA-C1A	6.86	109.81	106.68
26	c	502	CLA	C4A-NA-C1A	6.86	109.81	106.68
26	C	508	CLA	C4A-NA-C1A	6.80	109.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	507	CLA	C4A-NA-C1A	6.79	109.78	106.68
31	A	615	SQD	O6-C1-C2	6.78	118.57	108.27
26	B	611	CLA	C4A-NA-C1A	6.76	109.76	106.68
26	b	614	CLA	C4A-NA-C1A	6.75	109.76	106.68
26	B	612	CLA	C4A-NA-C1A	6.72	109.75	106.68
26	c	512	CLA	C4A-NA-C1A	6.65	109.71	106.68
31	a	614	SQD	C1-O5-C5	-6.63	100.77	113.72
26	C	502	CLA	C4A-NA-C1A	6.62	109.70	106.68
26	b	611	CLA	C4A-NA-C1A	6.52	109.65	106.68
26	B	609	CLA	C4A-NA-C1A	6.48	109.64	106.68
26	d	402	CLA	C4A-NA-C1A	6.46	109.63	106.68
29	a	612	PL9	C7-C3-C4	6.43	122.20	116.91
27	d	401	PHO	C4D-CHA-CBD	-6.41	105.38	108.45
26	C	510	CLA	C4A-NA-C1A	6.36	109.58	106.68
26	b	616	CLA	C4A-NA-C1A	6.31	109.56	106.68
26	B	616	CLA	C4A-NA-C1A	6.30	109.55	106.68
26	B	607	CLA	C4A-NA-C1A	6.29	109.55	106.68
26	C	501	CLA	C4A-NA-C1A	6.28	109.55	106.68
26	b	609	CLA	C4A-NA-C1A	6.21	109.51	106.68
26	B	608	CLA	C4A-NA-C1A	6.12	109.47	106.68
26	a	607	CLA	C4A-NA-C1A	6.12	109.47	106.68
26	A	614	CLA	C4A-NA-C1A	5.97	109.40	106.68
26	c	510	CLA	C4A-NA-C1A	5.96	109.40	106.68
26	c	505	CLA	C4A-NA-C1A	5.93	109.38	106.68
26	b	615	CLA	C4A-NA-C1A	5.88	109.36	106.68
26	c	504	CLA	C4A-NA-C1A	5.88	109.36	106.68
26	C	513	CLA	C4A-NA-C1A	5.78	109.31	106.68
26	D	402	CLA	C4A-NA-C1A	5.77	109.31	106.68
31	A	615	SQD	C1-O5-C5	-5.75	102.49	113.72
26	C	509	CLA	C4A-NA-C1A	5.74	109.30	106.68
26	B	610	CLA	C4A-NA-C1A	5.71	109.28	106.68
26	C	505	CLA	C4A-NA-C1A	5.71	109.28	106.68
26	C	512	CLA	C4A-NA-C1A	5.71	109.28	106.68
26	b	605	CLA	C4A-NA-C1A	5.70	109.28	106.68
26	B	603	CLA	C4A-NA-C1A	5.69	109.27	106.68
26	a	610	CLA	C4A-NA-C1A	5.64	109.25	106.68
26	b	608	CLA	C4A-NA-C1A	5.63	109.25	106.68
26	C	504	CLA	C4A-NA-C1A	5.59	109.23	106.68
26	b	610	CLA	C4A-NA-C1A	5.53	109.20	106.68
26	b	602	CLA	C4A-NA-C1A	5.50	109.19	106.68
26	B	614	CLA	C4A-NA-C1A	5.39	109.14	106.68
36	V	201	HEC	C1D-ND-C4D	5.34	111.53	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	612	PL9	C7-C3-C4	5.33	121.30	116.91
31	f	101	SQD	C1-O5-C5	-5.27	103.42	113.72
26	A	610	CLA	C4A-NA-C1A	5.26	109.08	106.68
26	B	613	CLA	C1-C2-C3	-5.22	117.64	126.20
26	c	513	CLA	C4A-NA-C1A	5.20	109.05	106.68
26	c	506	CLA	C4A-NA-C1A	5.17	109.04	106.68
26	c	508	CLA	C4A-NA-C1A	5.16	109.03	106.68
31	f	101	SQD	O9-S-C6	5.15	114.44	106.76
26	D	403	CLA	C4A-NA-C1A	5.11	109.01	106.68
26	C	506	CLA	C4A-NA-C1A	5.10	109.01	106.68
29	d	405	PL9	C7-C3-C4	5.09	121.11	116.91
26	a	608	CLA	C4A-NA-C1A	5.05	108.98	106.68
26	a	613	CLA	C4A-NA-C1A	5.00	108.96	106.68
26	B	605	CLA	C4A-NA-C1A	4.99	108.96	106.68
36	v	201	HEC	C1D-ND-C4D	4.98	111.11	105.21
26	b	613	CLA	C4A-NA-C1A	4.91	108.92	106.68
33	b	622	LMG	C8-O7-C10	4.88	129.49	117.80
26	A	607	CLA	C4A-NA-C1A	4.87	108.90	106.68
26	b	607	CLA	C4A-NA-C1A	4.86	108.89	106.68
31	A	615	SQD	C1-C2-C3	-4.75	100.01	110.01
26	b	603	CLA	C4A-NA-C1A	4.70	108.82	106.68
26	b	616	CLA	O2D-CGD-O1D	-4.70	114.71	123.85
31	b	620	SQD	O6-C1-C2	4.68	115.38	108.27
27	a	609	PHO	CMA-C3A-C4A	-4.61	104.68	114.61
31	f	101	SQD	O9-S-O7	-4.61	98.84	113.82
27	A	609	PHO	CMA-C3A-C4A	-4.59	104.72	114.61
29	a	612	PL9	C7-C3-C2	-4.59	117.98	123.39
31	b	620	SQD	O47-C7-C8	4.53	121.28	111.48
26	b	603	CLA	O2D-CGD-O1D	-4.52	115.05	123.85
31	a	616	SQD	O7-S-C6	4.49	113.47	106.76
33	C	517	LMG	C4-C3-C2	4.49	118.71	110.83
31	f	101	SQD	O6-C1-C2	4.44	115.02	108.27
27	D	401	PHO	C4D-CHA-CBD	-4.44	106.33	108.45
27	d	401	PHO	O1D-CGD-CBD	4.42	131.43	124.72
33	D	406	LMG	O6-C5-C4	4.41	117.65	109.70
26	A	608	CLA	C4A-NA-C1A	4.41	108.69	106.68
26	b	604	CLA	C1-C2-C3	-4.40	118.98	126.20
31	a	614	SQD	C1-C2-C3	-4.23	101.11	110.01
26	B	610	CLA	O2D-CGD-O1D	-4.20	115.68	123.85
26	C	501	CLA	O2D-CGD-O1D	-4.19	115.69	123.85
31	B	623	SQD	O9-S-O7	-4.17	100.27	113.82
27	D	401	PHO	C1-C2-C3	-4.16	119.38	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	401	PHO	C1-C2-C3	-4.14	119.41	126.20
31	a	616	SQD	O9-S-O7	-4.12	100.42	113.82
33	a	617	LMG	C1-C2-C3	-4.12	101.34	110.01
33	c	523	LMG	C4-C3-C2	4.12	118.05	110.83
31	B	623	SQD	O6-C1-C2	4.11	114.52	108.27
27	D	401	PHO	CBC-CAC-C3C	4.09	118.73	112.87
33	C	517	LMG	C8-O7-C10	4.08	127.57	117.80
31	A	615	SQD	O47-C7-C8	4.07	120.28	111.48
26	B	611	CLA	O2D-CGD-O1D	-4.06	115.95	123.85
26	B	602	CLA	C4A-NA-C1A	4.05	108.53	106.68
31	A	616	SQD	O7-S-C6	4.01	112.75	106.76
26	b	611	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
31	A	616	SQD	O5-C5-C4	3.94	116.80	109.70
26	b	602	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
31	A	616	SQD	O47-C7-C8	3.92	119.96	111.48
31	a	616	SQD	O47-C7-C8	3.89	119.89	111.48
29	d	405	PL9	C40-C39-C41	3.89	121.97	115.23
31	B	623	SQD	C1-O5-C5	-3.88	106.14	113.72
31	b	620	SQD	C1-C2-C3	-3.87	101.88	110.01
27	D	401	PHO	CMA-C3A-C4A	-3.85	106.31	114.61
26	b	615	CLA	C3B-C4B-NB	-3.84	107.10	110.53
26	c	501	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
26	C	501	CLA	C3B-C4B-NB	-3.83	107.11	110.53
28	d	404	BCR	C38-C26-C25	-3.83	120.31	124.48
26	C	502	CLA	O2D-CGD-O1D	-3.82	116.40	123.85
26	b	613	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
26	b	614	CLA	C1-C2-C3	-3.78	120.00	126.20
33	a	617	LMG	O1-C1-C2	3.77	113.99	108.27
26	B	610	CLA	C3B-C4B-NB	-3.76	107.17	110.53
26	B	602	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
26	C	513	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
29	D	405	PL9	C7-C3-C4	3.74	119.99	116.91
26	b	610	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
26	b	601	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
26	B	608	CLA	O2D-CGD-O1D	-3.71	116.64	123.85
26	b	608	CLA	C3B-C4B-NB	-3.70	107.23	110.53
31	b	620	SQD	O9-S-O7	-3.69	101.84	113.82
26	c	511	CLA	C3B-C4B-NB	-3.67	107.25	110.53
26	d	403	CLA	C4A-NA-C1A	3.65	108.34	106.68
26	c	505	CLA	C3B-C4B-NB	-3.64	107.28	110.53
31	a	614	SQD	O48-C23-C24	3.63	122.92	111.83
35	e	102	HEM	CBD-CAD-C3D	-3.61	102.54	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	612	CLA	C1-C2-C3	-3.60	120.30	126.20
31	a	614	SQD	O47-C7-C8	3.59	119.25	111.48
26	c	509	CLA	O2A-CGA-O1A	-3.59	114.66	123.63
26	B	603	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
31	a	616	SQD	C3-C4-C5	3.55	116.67	110.23
29	A	612	PL9	C7-C3-C2	-3.55	119.20	123.39
26	B	611	CLA	O2D-CGD-CBD	3.55	117.43	111.23
28	k	102	BCR	C7-C8-C9	-3.53	121.02	126.23
26	d	402	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
33	M	101	LMG	O1-C1-C2	3.51	113.60	108.27
26	b	612	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
26	B	614	CLA	C3B-C4B-NB	-3.50	107.41	110.53
27	d	401	PHO	CMA-C3A-C4A	-3.49	107.09	114.61
28	b	618	BCR	C2-C1-C6	3.48	115.49	110.44
27	d	401	PHO	O2D-CGD-O1D	-3.47	117.09	123.85
27	D	401	PHO	O1D-CGD-CBD	3.47	129.99	124.72
26	C	508	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
26	B	614	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
26	B	614	CLA	C1-C2-C3	-3.46	120.53	126.20
26	b	616	CLA	O2D-CGD-CBD	3.46	117.27	111.23
26	A	614	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
31	F	102	SQD	O8-S-C6	3.43	112.60	105.97
26	a	607	CLA	C3B-C4B-NB	-3.43	107.47	110.53
29	d	405	PL9	C7-C3-C2	-3.43	119.34	123.39
31	B	623	SQD	O47-C7-C8	3.42	118.89	111.48
31	b	620	SQD	O9-S-C6	3.42	111.87	106.76
31	B	623	SQD	O48-C23-C24	3.42	122.25	111.83
27	d	401	PHO	CBC-CAC-C3C	3.42	117.77	112.87
26	c	512	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
26	b	608	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
27	D	401	PHO	CMB-C2B-C3B	3.39	131.45	124.68
26	A	610	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
35	F	101	HEM	CBD-CAD-C3D	-3.38	103.20	112.53
26	c	505	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
26	B	605	CLA	C3B-C4B-NB	-3.36	107.53	110.53
26	b	603	CLA	C3B-C4B-NB	-3.36	107.53	110.53
31	A	616	SQD	O9-S-O7	-3.34	102.95	113.82
27	A	609	PHO	CMB-C2B-C3B	3.34	131.35	124.68
29	d	405	PL9	C37-C38-C39	-3.32	120.02	127.62
26	C	506	CLA	C3B-C4B-NB	-3.32	107.57	110.53
26	b	611	CLA	C3B-C4B-NB	-3.32	107.57	110.53
26	b	605	CLA	C1-C2-C3	-3.31	120.77	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	615	CLA	CHB-C4A-NA	3.31	129.18	124.40
26	B	608	CLA	C3B-C4B-NB	-3.30	107.58	110.53
26	a	608	CLA	C3B-C4B-NB	-3.30	107.58	110.53
26	B	615	CLA	C3B-C4B-NB	-3.30	107.58	110.53
26	D	402	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
26	c	512	CLA	CHB-C4A-NA	3.29	129.15	124.40
26	A	608	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
26	b	612	CLA	C4A-NA-C1A	3.28	108.18	106.68
26	b	605	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
26	b	614	CLA	C3B-C4B-NB	-3.28	107.60	110.53
26	a	610	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
26	B	606	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
26	a	608	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
27	D	401	PHO	O2D-CGD-O1D	-3.27	117.48	123.85
26	B	610	CLA	C1-C2-C3	-3.26	120.85	126.20
26	A	614	CLA	C3B-C4B-NB	-3.25	107.63	110.53
26	B	601	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
26	B	616	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
26	C	505	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
26	b	605	CLA	C3B-C4B-NB	-3.24	107.64	110.53
31	B	623	SQD	O9-S-C6	3.23	111.58	106.76
26	A	608	CLA	C3B-C4B-NB	-3.23	107.65	110.53
29	D	405	PL9	C27-C28-C29	-3.22	120.25	127.62
26	D	402	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
31	a	614	SQD	O8-S-C6	3.22	112.19	105.97
26	B	612	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
26	C	507	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
26	c	506	CLA	C3B-C4B-NB	-3.21	107.66	110.53
29	A	612	PL9	C22-C23-C24	-3.21	120.28	127.62
26	c	501	CLA	O2D-CGD-CBD	3.21	116.84	111.23
28	b	619	BCR	C29-C30-C25	3.20	115.09	110.44
26	B	603	CLA	O2D-CGD-CBD	3.20	116.82	111.23
26	C	501	CLA	O2D-CGD-CBD	3.20	116.82	111.23
26	B	605	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
26	B	613	CLA	C3B-C4B-NB	-3.19	107.68	110.53
26	b	606	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
26	d	403	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
26	b	608	CLA	CHB-C4A-NA	3.17	128.98	124.40
26	A	607	CLA	O2A-CGA-O1A	-3.17	115.70	123.63
26	c	511	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
27	a	609	PHO	CMB-C2B-C3B	3.15	130.98	124.68
26	B	602	CLA	O2D-CGD-CBD	3.15	116.73	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	601	CLA	C3B-C4B-NB	-3.15	107.72	110.53
26	B	603	CLA	O2A-CGA-O1A	-3.14	115.78	123.63
26	D	403	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
26	c	508	CLA	C3B-C4B-NB	-3.13	107.74	110.53
26	b	606	CLA	O2D-CGD-CBD	3.13	116.70	111.23
26	b	608	CLA	O2D-CGD-CBD	3.13	116.69	111.23
31	B	623	SQD	C3-C4-C5	3.12	115.89	110.23
26	a	613	CLA	C3B-C4B-NB	-3.12	107.75	110.53
26	a	607	CLA	O2A-CGA-O1A	-3.12	115.83	123.63
26	b	603	CLA	O2D-CGD-CBD	3.12	116.68	111.23
26	B	610	CLA	CHB-C4A-NA	3.11	128.88	124.40
29	d	405	PL9	C27-C28-C29	-3.11	120.52	127.62
26	c	512	CLA	C1-C2-C3	-3.10	121.11	126.20
33	C	517	LMG	O6-C5-C4	3.09	115.27	109.70
26	a	610	CLA	C1-C2-C3	-3.09	121.14	126.20
26	C	504	CLA	C3B-C4B-NB	-3.09	107.77	110.53
33	b	622	LMG	C3-C4-C5	-3.08	104.64	110.23
26	b	612	CLA	C3B-C4B-NB	-3.08	107.78	110.53
26	b	601	CLA	CHB-C4A-NA	3.08	128.84	124.40
26	b	611	CLA	O2D-CGD-CBD	3.08	116.61	111.23
31	A	616	SQD	O48-C23-C24	3.07	121.18	111.83
33	b	622	LMG	C1-O6-C5	-3.06	107.74	113.72
26	b	613	CLA	C3B-C4B-NB	-3.06	107.80	110.53
26	B	610	CLA	O2A-CGA-O1A	-3.06	115.98	123.63
27	a	609	PHO	C2B-C1B-NB	-3.06	107.22	109.43
26	b	613	CLA	CMB-C2B-C1B	-3.06	120.77	125.42
26	c	507	CLA	C3B-C4B-NB	-3.05	107.80	110.53
29	D	405	PL9	C42-C43-C44	-3.05	120.64	127.62
26	B	612	CLA	CHB-C4A-NA	3.02	128.76	124.40
26	A	614	CLA	O2D-CGD-CBD	3.02	116.50	111.23
26	c	513	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
33	D	406	LMG	C1-C2-C3	-3.01	103.67	110.01
26	C	507	CLA	CHB-C4A-NA	3.01	128.74	124.40
36	V	201	HEC	CBD-CAD-C3D	-3.01	104.22	112.53
26	b	604	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
29	a	612	PL9	C37-C38-C39	-3.00	120.76	127.62
26	b	604	CLA	O2D-CGD-CBD	2.99	116.47	111.23
26	C	512	CLA	C3B-C4B-NB	-2.99	107.86	110.53
26	B	606	CLA	C3B-C4B-NB	-2.99	107.86	110.53
26	c	506	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
31	B	623	SQD	O7-S-C6	2.99	111.22	106.76
26	c	512	CLA	C3B-C4B-NB	-2.99	107.86	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	513	CLA	O2D-CGD-CBD	2.97	116.42	111.23
31	A	615	SQD	O9-S-O7	-2.97	104.17	113.82
26	C	510	CLA	C3B-C4B-NB	-2.96	107.89	110.53
26	b	606	CLA	C3B-C4B-NB	-2.96	107.89	110.53
26	b	609	CLA	C3B-C4B-NB	-2.95	107.90	110.53
26	B	611	CLA	C1-C2-C3	-2.94	121.37	126.20
26	a	610	CLA	O2D-CGD-CBD	2.93	116.36	111.23
26	a	607	CLA	CHB-C4A-NA	2.93	128.63	124.40
26	B	608	CLA	O2D-CGD-CBD	2.93	116.35	111.23
27	a	609	PHO	OBD-CAD-C3D	2.93	132.46	127.89
26	b	610	CLA	CHB-C4A-NA	2.93	128.62	124.40
26	C	506	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	C	508	CLA	C3B-C4B-NB	-2.92	107.92	110.53
26	b	614	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
31	a	614	SQD	O5-C1-C2	-2.91	104.38	110.37
33	D	406	LMG	O6-C1-C2	-2.91	104.39	110.37
26	A	610	CLA	O2D-CGD-CBD	2.91	116.32	111.23
29	d	405	PL9	C42-C43-C44	-2.90	120.98	127.62
31	a	614	SQD	O9-S-O7	-2.90	104.38	113.82
27	d	401	PHO	C2B-C1B-NB	-2.90	107.33	109.43
35	e	102	HEM	C3B-C2B-C1B	2.90	108.59	106.41
26	C	503	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
31	b	620	SQD	O7-S-C6	2.89	111.07	106.76
26	D	403	CLA	C1-C2-C3	-2.89	121.47	126.20
29	D	405	PL9	C7-C8-C9	-2.88	121.86	126.83
26	b	609	CLA	CMB-C2B-C1B	-2.87	121.04	125.42
31	F	102	SQD	O9-S-C6	2.87	111.04	106.76
26	b	602	CLA	O2D-CGD-CBD	2.86	116.23	111.23
26	c	507	CLA	CHB-C4A-NA	2.86	128.53	124.40
30	C	527	STE	C3-C2-C1	-2.85	107.07	114.51
27	d	401	PHO	CMB-C2B-C3B	2.85	130.38	124.68
26	B	608	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
26	c	504	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
31	A	615	SQD	O9-S-C6	2.85	111.01	106.76
26	A	610	CLA	C1-C2-C3	-2.85	121.53	126.20
28	k	101	BCR	C2-C1-C6	2.84	114.57	110.44
26	D	403	CLA	O2D-CGD-CBD	2.83	116.18	111.23
26	A	610	CLA	C3B-C4B-NB	-2.83	108.00	110.53
26	b	616	CLA	C1-C2-C3	-2.82	121.57	126.20
26	C	503	CLA	C7-C6-C5	-2.82	105.75	113.26
26	c	508	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
26	b	612	CLA	O2A-CGA-O1A	-2.81	116.59	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	402	CLA	CHB-C4A-NA	2.81	128.46	124.40
35	F	101	HEM	CBA-CAA-C2A	-2.81	104.76	112.53
26	a	613	CLA	C1-C2-C3	-2.81	121.59	126.20
26	b	602	CLA	CHB-C4A-NA	2.81	128.45	124.40
27	d	401	PHO	CAA-C2A-C3A	-2.80	105.44	113.00
26	c	513	CLA	C3B-C4B-NB	-2.79	108.03	110.53
31	f	101	SQD	O5-C1-C2	-2.79	104.64	110.37
26	a	608	CLA	CHB-C4A-NA	2.78	128.42	124.40
26	b	607	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	B	614	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
26	B	605	CLA	O1D-CGD-CBD	2.77	129.98	124.52
26	b	612	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
26	b	616	CLA	CHB-C4A-NA	2.77	128.39	124.40
26	B	601	CLA	C3B-C4B-NB	-2.77	108.06	110.53
26	B	604	CLA	C3B-C4B-NB	-2.77	108.06	110.53
26	B	616	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
31	A	615	SQD	C45-O47-C7	-2.76	111.19	117.80
26	c	510	CLA	C3B-C4B-NB	-2.76	108.07	110.53
31	A	615	SQD	O7-S-C6	2.76	110.87	106.76
31	f	101	SQD	O48-C23-C24	2.76	120.24	111.83
26	c	507	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
26	a	610	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
26	b	612	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	a	613	CLA	O2D-CGD-CBD	2.74	116.02	111.23
29	d	405	PL9	C22-C23-C24	-2.74	121.36	127.62
26	C	503	CLA	C3B-C4B-NB	-2.74	108.09	110.53
32	A	617	DGD	O3G-C3G-C2G	2.73	117.47	110.82
26	B	610	CLA	O2D-CGD-CBD	2.73	116.01	111.23
35	e	102	HEM	C3B-C4B-NB	-2.73	107.51	109.47
28	H	101	BCR	C16-C17-C18	-2.73	123.45	127.28
29	D	405	PL9	C37-C38-C39	-2.73	121.37	127.62
36	v	201	HEC	CBD-CAD-C3D	-2.73	104.98	112.53
26	a	608	CLA	O2D-CGD-CBD	2.73	116.00	111.23
26	B	611	CLA	CHB-C4A-NA	2.73	128.33	124.40
26	a	613	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
26	B	612	CLA	C1-C2-C3	-2.72	121.74	126.20
26	c	502	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
31	b	620	SQD	O5-C5-C4	2.72	114.60	109.70
26	C	512	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
26	B	604	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
26	b	604	CLA	CHB-C4A-NA	2.72	128.32	124.40
26	b	609	CLA	O1D-CGD-CBD	2.71	129.87	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	607	CLA	CHB-C4A-NA	2.71	128.32	124.40
26	c	503	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	C	502	CLA	C3B-C4B-NB	-2.71	108.11	110.53
28	d	404	BCR	C30-C25-C26	-2.71	118.93	122.64
26	C	505	CLA	O2D-CGD-CBD	2.71	115.97	111.23
29	D	405	PL9	C7-C3-C2	-2.71	120.20	123.39
26	b	613	CLA	CHB-C4A-NA	2.70	128.30	124.40
26	C	511	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
26	b	603	CLA	CHC-C4B-NB	2.70	128.09	124.05
26	A	610	CLA	CHB-C4A-NA	2.69	128.28	124.40
35	e	102	HEM	CBA-CAA-C2A	-2.69	105.10	112.53
29	D	405	PL9	O1-C4-C3	-2.68	117.90	120.73
26	C	508	CLA	CHD-C1D-ND	-2.68	121.03	124.80
26	C	507	CLA	C3B-C4B-NB	-2.68	108.14	110.53
31	F	102	SQD	O9-S-O7	-2.68	105.11	113.82
28	H	101	BCR	C29-C30-C25	2.68	114.33	110.44
26	b	610	CLA	C3B-C4B-NB	-2.68	108.14	110.53
32	C	523	DGD	C6D-O5D-C1E	2.68	119.54	113.80
29	A	612	PL9	C40-C39-C41	2.67	119.87	115.23
26	C	509	CLA	CHB-C4A-NA	2.67	128.26	124.40
26	C	512	CLA	CHB-C4A-NA	2.67	128.25	124.40
35	e	102	HEM	CHB-C1B-NB	2.67	127.67	124.37
30	C	527	STE	O2-C1-C2	2.67	122.42	114.00
26	b	607	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
27	a	609	PHO	OBD-CAD-CBD	-2.66	121.92	125.82
26	B	602	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
29	a	612	PL9	O2-C1-C2	-2.66	115.78	121.83
28	k	101	BCR	C20-C21-C22	2.66	131.01	127.28
26	b	604	CLA	C3B-C4B-NB	-2.66	108.16	110.53
29	A	612	PL9	O2-C1-C2	-2.66	115.79	121.83
32	A	617	DGD	C4E-C3E-C2E	-2.65	106.17	110.83
26	A	607	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
26	B	609	CLA	C3B-C4B-NB	-2.65	108.17	110.53
31	B	623	SQD	O5-C5-C4	2.65	114.47	109.70
26	B	614	CLA	O2D-CGD-CBD	2.65	115.86	111.23
26	c	503	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
26	A	610	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
29	d	405	PL9	C32-C33-C34	-2.64	121.58	127.62
26	c	509	CLA	CHB-C4A-NA	2.64	128.21	124.40
32	h	101	DGD	C6D-C5D-C4D	2.64	117.60	112.07
26	B	604	CLA	C1-O2A-CGA	-2.63	110.28	116.65
26	c	504	CLA	CMB-C2B-C1B	-2.63	121.41	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	616	SQD	C4-C3-C2	2.63	115.44	110.83
31	b	620	SQD	O48-C23-C24	2.63	119.85	111.83
26	a	608	CLA	O2A-CGA-O1A	-2.62	117.06	123.63
30	t	102	STE	C3-C2-C1	-2.62	107.67	114.51
26	c	503	CLA	C7-C6-C5	-2.62	106.28	113.26
26	C	510	CLA	CMB-C2B-C1B	-2.62	121.44	125.42
31	f	101	SQD	O47-C7-C8	2.62	120.54	110.93
26	b	616	CLA	C3B-C4B-NB	-2.61	108.20	110.53
26	b	604	CLA	C6-C7-C8	-2.61	107.28	115.97
26	C	504	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	d	402	CLA	CHB-C4A-NA	2.61	128.16	124.40
31	a	616	SQD	O48-C23-C24	2.61	119.78	111.83
26	c	513	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
33	B	620	LMG	C4-C3-C2	2.60	115.40	110.83
30	e	104	STE	C3-C2-C1	-2.60	107.72	114.51
28	k	101	BCR	C23-C22-C21	-2.60	114.92	119.01
26	c	502	CLA	C1-C2-C3	-2.59	121.95	126.20
32	H	102	DGD	C3G-O3G-C1D	2.59	119.35	113.80
32	A	617	DGD	O5D-C1E-C2E	2.59	112.21	108.27
26	B	604	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
29	a	612	PL9	C22-C23-C24	-2.59	121.70	127.62
26	B	606	CLA	CHB-C4A-NA	2.59	128.13	124.40
26	C	511	CLA	C3B-C4B-NB	-2.58	108.22	110.53
25	A	606	BCT	O2-C-O1	2.58	126.28	119.68
26	B	616	CLA	C1-C2-C3	-2.58	121.97	126.20
32	A	617	DGD	C2G-O2G-C1B	2.58	123.96	117.80
26	c	502	CLA	C3B-C4B-NB	-2.57	108.23	110.53
29	d	405	PL9	C7-C8-C9	-2.57	122.40	126.83
29	d	405	PL9	C8-C7-C3	2.57	118.67	112.03
26	A	607	CLA	C3B-C4B-NB	-2.57	108.24	110.53
26	B	611	CLA	C3B-C4B-NB	-2.57	108.24	110.53
26	C	511	CLA	CHB-C4A-NA	2.56	128.09	124.40
32	c	519	DGD	C3D-C4D-C5D	-2.56	105.60	110.23
31	a	616	SQD	O9-S-C6	2.55	110.57	106.76
26	B	608	CLA	CMB-C2B-C3B	2.55	132.55	126.55
26	c	513	CLA	CHB-C4A-NA	2.55	128.08	124.40
26	D	403	CLA	CHB-C4A-NA	2.55	128.08	124.40
26	C	501	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
33	m	101	LMG	O1-C7-C8	-2.54	104.63	110.82
32	C	524	DGD	C3E-C4E-C5E	-2.54	105.62	110.23
26	C	502	CLA	O1D-CGD-CBD	2.54	129.53	124.52
26	C	503	CLA	C1D-ND-C4D	2.54	108.10	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	505	CLA	C3B-C4B-NB	-2.54	108.26	110.53
28	x	101	BCR	C29-C30-C25	2.54	114.13	110.44
26	c	504	CLA	CHD-C1D-ND	-2.54	121.23	124.80
26	b	605	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
35	e	102	HEM	CAB-C3B-C2B	-2.54	120.18	128.43
26	C	513	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
33	a	618	LMG	C3-C4-C5	-2.54	105.63	110.23
26	B	604	CLA	O2D-CGD-CBD	2.54	115.67	111.23
26	C	506	CLA	CHB-C4A-NA	2.54	128.06	124.40
36	V	201	HEC	CMD-C2D-C1D	2.54	129.00	125.03
26	B	605	CLA	CHD-C1D-ND	-2.53	121.24	124.80
26	a	613	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
26	B	610	CLA	CHD-C1D-ND	-2.53	121.24	124.80
31	A	615	SQD	O8-S-C6	2.53	110.86	105.97
26	A	614	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	b	614	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	c	504	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	C	509	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
26	b	604	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
26	B	603	CLA	C3B-C4B-NB	-2.52	108.28	110.53
33	B	620	LMG	O3-C3-C2	-2.52	104.43	110.38
32	h	101	DGD	C1E-O6E-C5E	2.52	118.65	113.72
33	C	517	LMG	C3-C4-C5	2.52	114.80	110.23
26	B	605	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
26	b	609	CLA	O2A-CGA-O1A	-2.52	117.34	123.63
26	b	612	CLA	O1D-CGD-CBD	2.51	129.47	124.52
26	c	509	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
27	D	401	PHO	C2B-C1B-NB	-2.51	107.62	109.43
26	d	403	CLA	CHB-C4A-NA	2.51	128.02	124.40
26	B	601	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
26	b	610	CLA	CAA-CBA-CGA	-2.50	106.10	113.21
31	A	615	SQD	C44-O6-C1	-2.50	108.43	113.80
26	b	613	CLA	C1-C2-C3	-2.50	122.10	126.20
26	C	510	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
26	b	611	CLA	C1-C2-C3	-2.50	122.10	126.20
26	b	601	CLA	O2D-CGD-CBD	2.50	115.60	111.23
31	F	102	SQD	O5-C5-C4	2.50	114.20	109.70
26	B	612	CLA	O1D-CGD-CBD	2.50	129.44	124.52
26	c	508	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
26	c	510	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
28	c	515	BCR	C2-C1-C6	2.49	114.06	110.44
26	b	612	CLA	CMB-C2B-C3B	2.49	132.41	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	612	PL9	C40-C39-C41	2.49	119.55	115.23
26	B	615	CLA	CHC-C4B-NB	2.49	127.78	124.05
26	d	402	CLA	C4-C3-C5	2.49	119.55	115.23
26	b	610	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
36	V	201	HEC	CHA-C4D-ND	2.48	127.10	124.42
26	B	612	CLA	C3B-C4B-NB	-2.48	108.31	110.53
26	B	613	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
26	A	607	CLA	O1D-CGD-CBD	2.48	129.41	124.52
26	B	612	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
31	f	101	SQD	O7-S-C6	2.48	110.46	106.76
26	c	501	CLA	CHB-C4A-NA	2.48	127.98	124.40
33	a	617	LMG	O3-C3-C4	2.48	116.22	110.38
32	H	102	DGD	C1E-O6E-C5E	2.47	118.55	113.72
28	b	618	BCR	C15-C14-C13	-2.47	123.81	127.28
25	a	606	BCT	O2-C-O1	2.47	126.00	119.68
26	a	607	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
31	A	615	SQD	O48-C23-C24	2.46	119.35	111.83
29	d	405	PL9	C12-C13-C14	-2.46	121.99	127.62
26	B	614	CLA	CHB-C4A-NA	2.46	127.95	124.40
33	D	406	LMG	C3-C4-C5	2.46	114.69	110.23
26	c	505	CLA	O2D-CGD-CBD	2.46	115.53	111.23
26	c	504	CLA	C3B-C4B-NB	-2.46	108.34	110.53
26	C	503	CLA	CHB-C4A-NA	2.46	127.94	124.40
26	c	510	CLA	CHB-C4A-NA	2.45	127.94	124.40
26	c	511	CLA	CHB-C1B-NB	2.45	127.73	124.05
26	C	504	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
26	B	602	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
26	c	508	CLA	O2D-CGD-CBD	2.44	115.50	111.23
36	V	201	HEC	C2A-C1A-NA	-2.44	107.97	110.32
31	F	102	SQD	O48-C23-C24	2.44	119.28	111.83
26	a	613	CLA	CMB-C2B-C3B	2.44	132.29	126.55
26	B	609	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
26	C	510	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	C	505	CLA	CAC-C3C-C4C	2.44	127.96	124.79
26	B	602	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	b	609	CLA	CMB-C2B-C3B	2.43	132.27	126.55
32	h	101	DGD	O3D-C3D-C2D	-2.43	104.65	110.38
26	B	602	CLA	C3B-C4B-NB	-2.43	108.36	110.53
29	a	612	PL9	O1-C4-C3	-2.43	118.17	120.73
29	d	405	PL9	C20-C19-C21	2.42	119.43	115.23
33	c	523	LMG	C8-O7-C10	2.42	123.59	117.80
26	b	613	CLA	CMB-C2B-C3B	2.42	132.25	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	513	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
26	d	403	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
27	d	401	PHO	C3B-C4B-NB	-2.42	105.89	107.46
26	b	608	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
26	C	513	CLA	CHD-C1D-ND	-2.41	121.41	124.80
26	a	607	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
35	F	101	HEM	CHC-C1C-NC	2.41	127.08	124.45
30	M	102	STE	C3-C2-C1	-2.41	108.22	114.51
26	b	610	CLA	O1D-CGD-CBD	2.41	129.27	124.52
26	b	609	CLA	C1-C2-C3	-2.41	122.25	126.20
29	A	612	PL9	C36-C34-C33	-2.41	115.76	121.17
29	D	405	PL9	C40-C39-C41	2.41	119.41	115.23
31	F	102	SQD	C1-C2-C3	-2.40	104.95	110.01
26	c	510	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
26	b	602	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
30	e	104	STE	O2-C1-C2	2.40	121.58	114.00
29	A	612	PL9	C7-C8-C9	-2.40	122.70	126.83
26	c	511	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
26	C	505	CLA	C1-C2-C3	-2.39	122.28	126.20
33	a	617	LMG	C8-O7-C10	2.39	123.52	117.80
28	d	404	BCR	C27-C26-C25	-2.39	119.48	122.70
26	b	610	CLA	C1-C2-C3	-2.38	122.29	126.20
26	c	503	CLA	C1-C2-C3	-2.38	122.30	126.20
26	c	506	CLA	O1D-CGD-CBD	2.38	129.20	124.52
26	b	604	CLA	C11-C12-C13	-2.38	108.07	115.97
31	B	623	SQD	O8-S-C6	2.37	110.56	105.97
27	A	609	PHO	CAA-C2A-C3A	-2.37	106.59	113.00
26	A	608	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
26	b	603	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
33	C	517	LMG	C7-O1-C1	2.37	118.87	113.80
26	b	611	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	d	401	PHO	CMA-C3A-C2A	-2.36	105.00	114.13
26	b	616	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
26	d	402	CLA	O2D-CGD-CBD	2.36	115.36	111.23
26	a	608	CLA	C1-C2-C3	-2.36	122.33	126.20
26	C	503	CLA	C4D-CHA-C1A	2.36	124.06	121.24
31	b	620	SQD	O2-C2-C1	2.36	115.70	110.08
30	D	411	STE	C3-C2-C1	-2.36	108.35	114.51
31	A	616	SQD	C1-O5-C5	2.36	118.33	113.72
26	c	508	CLA	CHB-C4A-NA	2.36	127.80	124.40
26	d	403	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
33	b	622	LMG	O7-C8-C9	2.35	116.79	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	505	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
33	M	101	LMG	C1-C2-C3	-2.35	105.06	110.01
32	c	520	DGD	C3G-O3G-C1D	2.35	118.84	113.80
26	B	607	CLA	CHB-C4A-NA	2.35	127.79	124.40
26	C	506	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
36	v	201	HEC	CHA-C4D-ND	2.35	126.95	124.42
26	b	602	CLA	C3B-C4B-NB	-2.35	108.44	110.53
26	C	510	CLA	CMB-C2B-C3B	2.35	132.07	126.55
26	c	507	CLA	CHC-C4B-NB	2.34	127.57	124.05
26	d	402	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
26	c	501	CLA	C3B-C4B-NB	-2.34	108.44	110.53
36	v	201	HEC	CBA-CAA-C2A	-2.34	106.06	112.53
26	B	607	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
26	b	614	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
26	C	511	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
26	B	603	CLA	CHC-C4B-NB	2.34	127.56	124.05
26	b	613	CLA	O1D-CGD-CBD	2.34	129.13	124.52
32	h	101	DGD	C3D-C4D-C5D	-2.33	106.00	110.23
36	V	201	HEC	CAD-CBD-CGD	-2.33	107.47	113.67
29	A	612	PL9	O2-C1-C6	2.33	124.19	120.48
26	B	604	CLA	CHA-C4D-ND	2.33	137.36	132.55
26	c	502	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
32	C	523	DGD	C3D-C4D-C5D	-2.33	106.01	110.23
26	D	403	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
26	c	509	CLA	C3B-C4B-NB	-2.33	108.45	110.53
30	b	623	STE	O2-C1-C2	2.33	121.35	114.00
30	m	102	STE	C3-C2-C1	-2.33	108.44	114.51
26	B	606	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
26	a	613	CLA	CHB-C4A-NA	2.32	127.75	124.40
26	C	513	CLA	C3B-C4B-NB	-2.32	108.46	110.53
26	D	402	CLA	O2D-CGD-CBD	2.32	115.28	111.23
26	a	613	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
26	C	513	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	A	612	PL9	C20-C19-C21	2.32	119.25	115.23
26	a	607	CLA	CMB-C2B-C3B	2.31	132.00	126.55
29	a	612	PL9	C32-C33-C34	-2.31	122.33	127.62
26	D	402	CLA	C1-C2-C3	-2.31	122.41	126.20
26	B	609	CLA	CHC-C4B-NB	2.31	127.52	124.05
31	F	102	SQD	O6-C1-C2	2.31	111.78	108.27
26	B	612	CLA	C11-C12-C13	-2.31	108.28	115.97
28	D	404	BCR	C7-C8-C9	-2.31	122.82	126.23
26	B	616	CLA	C3B-C4B-NB	-2.31	108.47	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	405	PL9	C50-C49-C48	-2.31	115.74	122.66
26	d	403	CLA	O2D-CGD-CBD	2.30	115.26	111.23
26	C	509	CLA	C1-C2-C3	-2.30	122.42	126.20
33	C	517	LMG	O4-C4-C5	2.30	114.99	109.32
26	b	605	CLA	CHB-C1B-NB	2.30	127.50	124.05
30	b	623	STE	C3-C2-C1	-2.30	108.51	114.51
26	C	506	CLA	C1-C2-C3	-2.30	122.44	126.20
26	c	510	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
28	B	618	BCR	C2-C1-C6	2.29	113.77	110.44
30	t	102	STE	O2-C1-C2	2.29	121.25	114.00
26	b	605	CLA	CHD-C1D-ND	-2.29	121.58	124.80
36	v	201	HEC	CHB-C1B-NB	2.29	126.89	124.42
26	C	508	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
26	C	503	CLA	CHD-C1D-C2D	2.29	130.25	125.49
31	a	616	SQD	O5-C5-C4	2.29	113.82	109.70
36	V	201	HEC	CBA-CAA-C2A	-2.29	106.21	112.53
32	h	101	DGD	C6D-O5D-C1E	2.28	118.69	113.80
26	A	608	CLA	CHB-C4A-NA	2.28	127.69	124.40
31	a	616	SQD	O6-C1-C2	2.28	111.73	108.27
26	B	601	CLA	O2D-CGD-CBD	2.27	115.20	111.23
26	c	509	CLA	C16-C15-C13	-2.27	108.41	115.97
33	B	620	LMG	O1-C1-C2	2.27	111.72	108.27
26	b	602	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
27	D	401	PHO	CAA-C2A-C3A	-2.27	106.86	113.00
31	B	623	SQD	C1-C2-C3	-2.27	105.23	110.01
26	c	503	CLA	O1D-CGD-CBD	2.27	128.99	124.52
32	c	519	DGD	O1G-C1A-C2A	2.26	118.74	111.83
28	b	617	BCR	C11-C10-C9	-2.26	124.11	127.28
31	b	620	SQD	O8-S-C6	2.26	110.33	105.97
26	C	508	CLA	CHD-C1D-C2D	2.25	130.17	125.49
26	B	615	CLA	CHB-C4A-NA	2.25	127.65	124.40
30	m	102	STE	O2-C1-C2	2.25	121.11	114.00
26	a	610	CLA	CHB-C4A-NA	2.25	127.65	124.40
26	c	511	CLA	O2D-CGD-CBD	2.25	115.16	111.23
29	D	405	PL9	C22-C23-C24	-2.25	122.48	127.62
26	C	507	CLA	O2D-CGD-CBD	2.25	115.16	111.23
28	t	101	BCR	C11-C10-C9	-2.25	124.13	127.28
26	b	609	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
26	c	504	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
27	A	609	PHO	CMA-C3A-C2A	-2.24	105.48	114.13
26	B	604	CLA	CHB-C4A-NA	2.24	127.63	124.40
26	B	608	CLA	CHB-C4A-NA	2.24	127.63	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	403	CLA	C6-C7-C8	-2.24	108.53	115.97
32	c	519	DGD	C3G-O3G-C1D	2.24	118.59	113.80
26	B	607	CLA	C3B-C4B-NB	-2.23	108.53	110.53
33	a	617	LMG	O6-C1-C2	-2.23	105.78	110.37
26	b	602	CLA	C1-C2-C3	-2.23	122.54	126.20
26	C	509	CLA	C3B-C4B-NB	-2.23	108.54	110.53
35	F	101	HEM	C4D-ND-C1D	2.23	107.85	105.21
29	a	612	PL9	O2-C1-C6	2.23	124.03	120.48
30	E	104	STE	O2-C1-C2	2.23	121.04	114.00
26	C	502	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
35	e	102	HEM	CHC-C1C-NC	2.23	126.88	124.45
29	A	612	PL9	C35-C34-C36	2.22	119.09	115.23
26	b	615	CLA	C11-C12-C13	-2.22	108.58	115.97
26	d	403	CLA	CMB-C2B-C3B	2.22	131.78	126.55
34	d	408	LHG	C5-O7-C7	2.22	123.11	117.80
26	d	402	CLA	C3B-C4B-NB	-2.22	108.55	110.53
27	A	609	PHO	OBD-CAD-C3D	2.21	131.35	127.89
30	j	101	STE	O2-C1-C2	2.21	120.99	114.00
28	t	101	BCR	C2-C1-C6	2.21	113.65	110.44
26	a	613	CLA	CHC-C4B-NB	2.21	127.36	124.05
26	B	602	CLA	CMB-C2B-C3B	2.20	131.73	126.55
26	b	608	CLA	CMB-C2B-C3B	2.20	131.73	126.55
26	B	603	CLA	CHB-C1B-NB	2.20	127.35	124.05
28	t	101	BCR	C31-C1-C6	2.20	113.69	110.24
26	b	616	CLA	CHC-C4B-NB	2.20	127.34	124.05
26	b	616	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
33	D	406	LMG	C4-C3-C2	2.19	114.68	110.83
29	D	405	PL9	C32-C33-C34	-2.19	122.61	127.62
26	c	506	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	c	508	CLA	CHD-C1D-ND	-2.19	121.72	124.80
26	b	608	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
26	c	503	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	b	607	CLA	CHB-C4A-NA	2.18	127.55	124.40
26	c	507	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
26	b	616	CLA	CMB-C2B-C3B	2.18	131.68	126.55
27	A	609	PHO	C2B-C1B-NB	-2.18	107.85	109.43
26	C	503	CLA	CHD-C1D-ND	-2.18	121.74	124.80
31	f	101	SQD	C1-C2-C3	-2.17	105.44	110.01
26	C	505	CLA	CHB-C4A-NA	2.17	127.53	124.40
34	D	408	LHG	O4-P-O5	2.17	122.55	112.44
28	B	617	BCR	C16-C17-C18	2.17	130.32	127.28
26	B	614	CLA	CMB-C2B-C1B	-2.17	122.11	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	606	CLA	CHB-C1B-NB	2.17	127.30	124.05
26	C	505	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
26	C	505	CLA	C2D-C1D-ND	-2.17	107.98	110.13
26	b	606	CLA	CHB-C4A-NA	2.17	127.53	124.40
26	b	609	CLA	CHB-C4A-NA	2.17	127.53	124.40
26	a	607	CLA	O1D-CGD-CBD	2.17	128.79	124.52
26	D	402	CLA	C3B-C4B-NB	-2.17	108.60	110.53
26	C	504	CLA	O2D-CGD-O1D	-2.16	119.63	123.85
26	B	614	CLA	CED-O2D-CGD	2.16	120.82	115.92
28	H	101	BCR	C2-C1-C6	2.16	113.58	110.44
27	A	609	PHO	O2A-CGA-O1A	-2.16	118.22	123.63
26	C	507	CLA	CHC-C4B-NB	2.16	127.29	124.05
26	A	610	CLA	CHC-C4B-NB	2.16	127.29	124.05
26	c	513	CLA	CMB-C2B-C3B	2.16	131.62	126.55
26	b	607	CLA	CHB-C1B-NB	2.16	127.28	124.05
26	b	609	CLA	C7-C6-C5	-2.15	107.52	113.26
26	C	503	CLA	C2D-C1D-ND	-2.15	108.00	110.13
31	F	102	SQD	C1-O5-C5	-2.15	109.52	113.72
26	A	608	CLA	O2D-CGD-CBD	2.15	114.99	111.23
26	b	603	CLA	CHB-C1B-NB	2.15	127.28	124.05
26	c	505	CLA	C11-C10-C8	-2.15	108.82	115.97
32	c	521	DGD	C3G-O3G-C1D	2.15	118.40	113.80
28	C	521	BCR	C2-C1-C6	2.15	113.56	110.44
26	B	613	CLA	CHB-C4A-NA	2.15	127.50	124.40
26	d	402	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
26	b	608	CLA	C6-C7-C8	-2.14	108.84	115.97
31	B	623	SQD	C45-O47-C7	-2.14	112.67	117.80
31	f	101	SQD	C46-C45-C44	-2.14	106.80	111.78
26	b	615	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
26	B	607	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
26	B	609	CLA	CED-O2D-CGD	2.14	120.76	115.92
28	x	101	BCR	C16-C17-C18	-2.13	124.28	127.28
29	D	405	PL9	C36-C34-C33	-2.13	116.38	121.17
26	C	507	CLA	C2A-C1A-CHA	2.13	127.57	123.87
26	B	603	CLA	CHB-C4A-NA	2.13	127.48	124.40
26	C	502	CLA	CHB-C4A-NA	2.13	127.48	124.40
26	B	601	CLA	CHB-C1B-NB	2.13	127.25	124.05
34	d	407	LHG	O4-P-O5	2.13	122.36	112.44
26	a	608	CLA	CHB-C1B-NB	2.13	127.24	124.05
31	a	614	SQD	O9-S-C6	2.13	109.93	106.76
26	b	615	CLA	CHD-C1D-ND	-2.13	121.81	124.80
28	t	101	BCR	C15-C16-C17	-2.13	119.17	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	606	CLA	O2D-CGD-CBD	2.13	114.95	111.23
26	B	607	CLA	CHC-C4B-NB	2.13	127.24	124.05
32	A	617	DGD	C3G-C2G-C1G	-2.13	106.83	111.78
27	a	609	PHO	CMA-C3A-C2A	-2.13	105.92	114.13
26	C	512	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
26	C	510	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
32	c	521	DGD	C6D-O5D-C1E	2.12	118.35	113.80
32	C	525	DGD	O6D-C1D-O3G	-2.12	105.03	110.04
26	a	610	CLA	CHC-C4B-NB	2.12	127.23	124.05
26	D	403	CLA	CMB-C2B-C3B	2.12	131.53	126.55
26	C	509	CLA	C16-C15-C13	-2.12	108.93	115.97
26	B	616	CLA	O2D-CGD-CBD	2.12	114.93	111.23
31	A	616	SQD	O9-S-C6	2.11	109.91	106.76
26	b	608	CLA	C6-C5-C3	-2.11	108.32	113.47
31	A	615	SQD	O47-C7-O49	-2.11	118.77	123.70
28	B	617	BCR	C29-C30-C25	2.11	113.50	110.44
31	a	616	SQD	C9-C8-C7	-2.11	105.97	113.69
26	D	402	CLA	C4-C3-C5	2.11	118.88	115.23
26	B	613	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
26	d	403	CLA	CHA-C1A-NA	-2.10	121.63	126.39
26	b	607	CLA	C1-C2-C3	-2.10	122.75	126.20
36	v	201	HEC	C2A-C1A-NA	-2.10	108.29	110.32
26	c	504	CLA	O2D-CGD-CBD	2.10	114.91	111.23
28	b	618	BCR	C33-C5-C6	2.10	126.78	124.48
26	b	607	CLA	CMB-C2B-C3B	2.10	131.49	126.55
26	B	615	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
33	B	620	LMG	C8-O7-C10	2.10	122.82	117.80
30	E	102	STE	C3-C2-C1	-2.09	109.04	114.51
26	C	509	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
26	b	609	CLA	CHC-C4B-NB	2.09	127.19	124.05
33	b	622	LMG	O3-C3-C4	2.09	115.31	110.38
33	B	620	LMG	O4-C4-C5	2.09	114.47	109.32
26	c	509	CLA	CHC-C4B-NB	2.09	127.18	124.05
29	a	612	PL9	C7-C8-C9	-2.09	123.23	126.83
26	b	607	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
27	A	609	PHO	O2D-CGD-CBD	2.09	113.24	110.95
33	a	617	LMG	O7-C8-C9	2.09	115.83	108.34
26	b	602	CLA	CMB-C2B-C3B	2.09	131.46	126.55
27	D	401	PHO	C3D-C4D-ND	2.09	110.38	107.71
29	D	405	PL9	C12-C13-C14	-2.08	122.85	127.62
26	c	501	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
26	c	503	CLA	C4-C3-C5	2.08	118.84	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	405	PL9	C8-C7-C3	2.08	117.41	112.03
26	b	605	CLA	O1D-CGD-CBD	2.08	128.62	124.52
26	C	503	CLA	O1D-CGD-CBD	2.08	128.62	124.52
26	C	513	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
26	b	606	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	B	609	CLA	CHB-C4A-NA	2.07	127.39	124.40
28	T	101	BCR	C38-C26-C27	-2.07	109.18	113.60
33	a	618	LMG	O3-C3-C4	2.07	115.26	110.38
32	C	525	DGD	O3E-C3E-C2E	-2.07	105.50	110.38
28	D	404	BCR	C23-C22-C21	-2.07	115.76	119.01
26	C	505	CLA	C1D-ND-C4D	2.07	107.76	106.31
28	t	101	BCR	C12-C13-C14	-2.06	115.76	119.01
26	C	512	CLA	O2D-CGD-CBD	2.06	114.83	111.23
26	B	605	CLA	CHD-C4C-NC	2.06	127.43	124.23
29	A	612	PL9	C12-C13-C14	-2.06	122.91	127.62
31	A	616	SQD	O6-C1-C2	2.06	111.40	108.27
26	C	508	CLA	CHB-C4A-NA	2.06	127.37	124.40
26	c	505	CLA	C1-C2-C3	-2.06	122.82	126.20
26	a	608	CLA	CHD-C1D-ND	-2.06	121.91	124.80
32	A	617	DGD	O4E-C4E-C5E	2.06	114.39	109.32
26	b	603	CLA	C16-C15-C13	-2.06	109.13	115.97
26	c	502	CLA	CHB-C4A-NA	2.05	127.36	124.40
36	V	201	HEC	C4B-NB-C1B	2.05	107.64	105.21
26	C	506	CLA	CHA-C1A-NA	-2.05	121.74	126.39
26	C	501	CLA	CHB-C1B-NB	2.05	127.13	124.05
26	b	615	CLA	C1-C2-C3	-2.05	122.83	126.20
26	B	609	CLA	CHA-C1A-NA	-2.05	121.75	126.39
26	b	605	CLA	C4-C3-C5	2.05	118.78	115.23
33	m	101	LMG	C7-O1-C1	2.05	118.18	113.80
26	C	503	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
26	C	512	CLA	C6-C5-C3	-2.05	108.48	113.47
26	b	602	CLA	C6-C5-C3	-2.05	108.48	113.47
35	F	101	HEM	CHD-C4C-C3C	2.04	128.65	125.21
26	c	504	CLA	CMB-C2B-C3B	2.04	131.35	126.55
26	b	602	CLA	C11-C12-C13	-2.04	109.18	115.97
26	B	608	CLA	CHB-C1B-NB	2.04	127.11	124.05
26	b	607	CLA	CHD-C1D-ND	-2.04	121.93	124.80
26	d	402	CLA	CMB-C2B-C3B	2.04	131.34	126.55
28	a	611	BCR	C33-C5-C4	-2.04	109.25	113.60
26	d	403	CLA	C3B-C4B-NB	-2.04	108.71	110.53
30	D	411	STE	O2-C1-C2	2.03	120.42	114.00
26	b	613	CLA	C16-C15-C13	-2.03	109.22	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	H	102	DGD	C3D-C4D-C5D	-2.03	106.55	110.23
32	h	101	DGD	O3D-C3D-C4D	2.03	115.15	110.38
26	B	605	CLA	C1-C2-C3	-2.02	122.88	126.20
26	b	604	CLA	C6-C5-C3	-2.02	108.54	113.47
26	b	610	CLA	CHC-C4B-NB	2.02	127.08	124.05
35	e	102	HEM	C1B-NB-C4B	2.02	107.60	105.21
26	c	505	CLA	CHB-C4A-NA	2.02	127.31	124.40
34	d	408	LHG	O4-P-O5	2.02	121.84	112.44
26	c	511	CLA	CHA-C1A-NA	-2.02	121.83	126.39
26	C	507	CLA	C1-C2-C3	-2.01	122.90	126.20
29	a	612	PL9	C35-C34-C36	2.01	118.72	115.23
29	A	612	PL9	C42-C43-C44	-2.01	123.02	127.62
36	V	201	HEC	C3D-C4D-ND	-2.01	108.41	110.35
26	b	602	CLA	C11-C10-C8	-2.01	109.28	115.97
26	c	505	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
26	C	505	CLA	CHA-C1A-NA	-2.01	121.84	126.39
26	b	615	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
26	c	507	CLA	O2D-CGD-CBD	2.00	114.73	111.23
26	b	604	CLA	C2A-C1A-CHA	2.00	127.34	123.87
26	A	610	CLA	CHD-C1D-ND	-2.00	121.98	124.80
33	D	407	LMG	O3-C3-C2	-2.00	105.66	110.38

All (2) chirality outliers are listed below:

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

All (1669) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	601	CLA	C1A-C2A-CAA-CBA
26	B	601	CLA	CBA-CGA-O2A-C1
26	B	601	CLA	O1A-CGA-O2A-C1
26	B	614	CLA	CAD-CBD-CGD-O1D
26	B	614	CLA	CAD-CBD-CGD-O2D
26	C	504	CLA	C2B-C3B-CAB-CBB
26	C	504	CLA	C4B-C3B-CAB-CBB
26	C	507	CLA	CHA-CBD-CGD-O1D
26	C	507	CLA	CHA-CBD-CGD-O2D
26	C	512	CLA	C11-C10-C8-C9
26	b	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	b	614	CLA	CAD-CBD-CGD-O2D
26	b	614	CLA	C6-C7-C8-C9
26	c	507	CLA	CHA-CBD-CGD-O1D
26	c	507	CLA	CHA-CBD-CGD-O2D
26	c	507	CLA	C2-C3-C5-C6
26	c	507	CLA	C4-C3-C5-C6
26	c	512	CLA	C2B-C3B-CAB-CBB
26	c	512	CLA	C4B-C3B-CAB-CBB
26	c	512	CLA	C6-C7-C8-C9
28	B	617	BCR	C17-C18-C19-C20
28	C	521	BCR	C1-C6-C7-C8
28	C	521	BCR	C21-C22-C23-C24
28	K	101	BCR	C7-C8-C9-C10
28	K	101	BCR	C17-C18-C19-C20
28	T	101	BCR	C7-C8-C9-C10
28	d	404	BCR	C23-C24-C25-C30
28	k	101	BCR	C5-C6-C7-C8
28	k	101	BCR	C17-C18-C19-C20
28	k	101	BCR	C36-C18-C19-C20
28	k	102	BCR	C7-C8-C9-C10
28	k	102	BCR	C7-C8-C9-C34
29	A	612	PL9	C27-C28-C29-C30
29	A	612	PL9	C27-C28-C29-C31
29	A	612	PL9	C37-C38-C39-C41
29	a	612	PL9	C22-C23-C24-C26
29	a	612	PL9	C24-C26-C27-C28
29	d	405	PL9	C32-C33-C34-C36
29	d	405	PL9	C40-C39-C41-C42
29	d	405	PL9	C42-C43-C44-C45
31	A	616	SQD	O6-C44-C45-O47
31	A	616	SQD	C5-C6-S-O7
31	A	616	SQD	C5-C6-S-O8
31	A	616	SQD	C5-C6-S-O9
31	B	623	SQD	C2-C1-O6-C44
31	B	623	SQD	O5-C1-O6-C44
31	B	623	SQD	O6-C44-C45-O47
31	B	623	SQD	O49-C7-O47-C45
31	B	623	SQD	O5-C5-C6-S
31	F	102	SQD	C45-C44-O6-C1
31	a	614	SQD	O6-C44-C45-O47
31	a	614	SQD	C5-C6-S-O7
31	a	614	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
31	a	616	SQD	O6-C44-C45-O47
31	a	616	SQD	O5-C5-C6-S
31	b	620	SQD	O5-C1-O6-C44
31	b	620	SQD	C46-C45-O47-C7
31	b	620	SQD	C8-C7-O47-C45
33	C	517	LMG	C2-C1-O1-C7
33	C	522	LMG	O6-C1-O1-C7
33	C	522	LMG	C11-C10-O7-C8
33	M	101	LMG	C11-C10-O7-C8
33	a	617	LMG	O6-C1-O1-C7
33	c	518	LMG	C11-C10-O7-C8
33	c	523	LMG	C11-C10-O7-C8
34	B	622	LHG	C4-O6-P-O3
34	B	622	LHG	C4-O6-P-O4
34	B	622	LHG	C4-O6-P-O5
34	D	408	LHG	O2-C2-C3-O3
34	D	408	LHG	C3-O3-P-O4
34	D	408	LHG	C3-O3-P-O6
34	D	410	LHG	O1-C1-C2-C3
34	D	410	LHG	C3-O3-P-O4
34	E	101	LHG	C3-O3-P-O5
34	E	101	LHG	C3-O3-P-O6
34	E	101	LHG	C4-O6-P-O4
34	a	615	LHG	C3-O3-P-O5
34	a	615	LHG	C3-O3-P-O6
34	d	407	LHG	O1-C1-C2-C3
34	d	408	LHG	C3-O3-P-O4
34	d	408	LHG	C3-O3-P-O6
34	d	408	LHG	C4-O6-P-O4
34	l	101	LHG	C4-O6-P-O3
34	l	101	LHG	C4-O6-P-O4
34	l	101	LHG	C4-O6-P-O5
26	b	601	CLA	O1D-CGD-O2D-CED
26	b	601	CLA	CBD-CGD-O2D-CED
33	M	101	LMG	O10-C28-O8-C9
29	a	612	PL9	C47-C48-C49-C50
29	a	612	PL9	C47-C48-C49-C51
26	c	513	CLA	CBD-CGD-O2D-CED
31	F	102	SQD	O10-C23-O48-C46
33	B	620	LMG	O10-C28-O8-C9
31	b	620	SQD	O49-C7-O47-C45
33	C	522	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	M	101	LMG	O9-C10-O7-C8
33	c	518	LMG	O9-C10-O7-C8
33	c	523	LMG	O9-C10-O7-C8
26	b	614	CLA	C3-C5-C6-C7
33	B	620	LMG	C29-C28-O8-C9
33	M	101	LMG	C29-C28-O8-C9
27	d	401	PHO	CBD-CGD-O2D-CED
31	B	623	SQD	C8-C7-O47-C45
26	A	610	CLA	C4-C3-C5-C6
26	B	614	CLA	C4-C3-C5-C6
26	C	504	CLA	C4-C3-C5-C6
26	a	610	CLA	C4-C3-C5-C6
26	b	603	CLA	C4-C3-C5-C6
26	B	614	CLA	C2-C3-C5-C6
26	C	504	CLA	C2-C3-C5-C6
26	a	610	CLA	C2-C3-C5-C6
29	A	612	PL9	C28-C29-C31-C32
29	A	612	PL9	C38-C39-C41-C42
29	d	405	PL9	C38-C39-C41-C42
31	f	101	SQD	O10-C23-O48-C46
26	B	616	CLA	CBA-CGA-O2A-C1
31	B	623	SQD	C24-C23-O48-C46
31	F	102	SQD	C24-C23-O48-C46
31	f	101	SQD	C24-C23-O48-C46
26	B	616	CLA	O1A-CGA-O2A-C1
26	b	601	CLA	O1A-CGA-O2A-C1
31	B	623	SQD	O10-C23-O48-C46
33	b	622	LMG	O10-C28-O8-C9
30	T	102	STE	C5-C6-C7-C8
26	B	615	CLA	C3-C5-C6-C7
26	b	601	CLA	CBA-CGA-O2A-C1
33	C	517	LMG	C29-C28-O8-C9
32	H	102	DGD	O6E-C5E-C6E-O5E
26	c	511	CLA	CBD-CGD-O2D-CED
26	C	513	CLA	CBD-CGD-O2D-CED
33	b	622	LMG	C29-C28-O8-C9
26	B	603	CLA	C4-C3-C5-C6
26	b	605	CLA	C4-C3-C5-C6
29	A	612	PL9	C25-C24-C26-C27
29	A	612	PL9	C40-C39-C41-C42
26	A	610	CLA	C2-C3-C5-C6
26	b	605	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	C	517	LMG	O10-C28-O8-C9
32	A	617	DGD	O6E-C5E-C6E-O5E
32	C	523	DGD	O6E-C5E-C6E-O5E
29	A	612	PL9	C19-C21-C22-C23
29	A	612	PL9	C29-C31-C32-C33
29	a	612	PL9	C44-C46-C47-C48
34	l	101	LHG	C7-C8-C9-C10
29	A	612	PL9	C47-C48-C49-C51
31	f	101	SQD	O5-C1-O6-C44
33	B	620	LMG	O6-C1-O1-C7
33	D	406	LMG	O6-C1-O1-C7
33	M	101	LMG	O6-C1-O1-C7
33	a	618	LMG	O6-C1-O1-C7
33	b	622	LMG	O6-C1-O1-C7
26	B	615	CLA	CBD-CGD-O2D-CED
30	d	410	STE	C1-C2-C3-C4
29	A	612	PL9	C37-C38-C39-C40
30	T	102	STE	C7-C8-C9-C10
33	b	622	LMG	O6-C5-C6-O5
29	D	405	PL9	C47-C48-C49-C51
26	c	506	CLA	CBA-CGA-O2A-C1
26	c	512	CLA	CBA-CGA-O2A-C1
33	a	617	LMG	C29-C28-O8-C9
30	E	104	STE	C10-C11-C12-C13
34	d	409	LHG	C24-C25-C26-C27
30	C	527	STE	C2-C3-C4-C5
26	c	513	CLA	O1D-CGD-O2D-CED
33	m	101	LMG	C38-C39-C40-C41
33	b	622	LMG	C4-C5-C6-O5
26	B	605	CLA	C4-C3-C5-C6
26	B	603	CLA	C2-C3-C5-C6
26	B	605	CLA	C2-C3-C5-C6
26	b	603	CLA	C2-C3-C5-C6
29	A	612	PL9	C33-C34-C36-C37
26	B	602	CLA	C6-C7-C8-C9
26	B	606	CLA	C14-C13-C15-C16
26	B	613	CLA	C11-C12-C13-C14
26	B	614	CLA	C6-C7-C8-C9
26	B	615	CLA	C6-C7-C8-C9
26	C	509	CLA	C11-C10-C8-C9
26	b	601	CLA	C11-C10-C8-C9
26	b	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	b	606	CLA	C14-C13-C15-C16
26	b	607	CLA	C11-C10-C8-C9
26	b	610	CLA	C14-C13-C15-C16
26	c	512	CLA	C11-C12-C13-C14
31	f	101	SQD	C2-C1-O6-C44
33	B	620	LMG	C2-C1-O1-C7
33	D	406	LMG	C2-C1-O1-C7
33	M	101	LMG	C2-C1-O1-C7
33	a	618	LMG	C2-C1-O1-C7
33	b	622	LMG	C2-C1-O1-C7
32	c	519	DGD	C1B-C2B-C3B-C4B
31	F	102	SQD	O6-C44-C45-C46
33	a	617	LMG	O10-C28-O8-C9
28	B	617	BCR	C36-C18-C19-C20
28	C	521	BCR	C37-C22-C23-C24
28	K	101	BCR	C7-C8-C9-C34
28	K	101	BCR	C36-C18-C19-C20
28	T	101	BCR	C7-C8-C9-C34
33	a	618	LMG	C10-C11-C12-C13
26	c	506	CLA	O1A-CGA-O2A-C1
26	C	501	CLA	CBD-CGD-O2D-CED
32	A	617	DGD	O2G-C2G-C3G-O3G
26	B	609	CLA	C13-C15-C16-C17
34	D	409	LHG	C11-C12-C13-C14
27	d	401	PHO	O1D-CGD-O2D-CED
26	B	605	CLA	C13-C15-C16-C17
26	B	614	CLA	C8-C10-C11-C12
26	a	608	CLA	C15-C16-C17-C18
26	b	606	CLA	C15-C16-C17-C18
26	b	607	CLA	C5-C6-C7-C8
26	b	611	CLA	C12-C13-C15-C16
26	c	508	CLA	C11-C12-C13-C15
29	A	612	PL9	C9-C11-C12-C13
29	A	612	PL9	C24-C26-C27-C28
29	A	612	PL9	C34-C36-C37-C38
29	A	612	PL9	C39-C41-C42-C43
26	C	512	CLA	C3-C5-C6-C7
26	A	614	CLA	C13-C15-C16-C17
31	a	616	SQD	C34-C35-C36-C37
31	a	614	SQD	C23-C24-C25-C26
33	D	407	LMG	C10-C11-C12-C13
34	a	615	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	c	512	CLA	O1A-CGA-O2A-C1
26	B	601	CLA	C5-C6-C7-C8
26	b	614	CLA	C5-C6-C7-C8
33	c	522	LMG	O6-C5-C6-O5
32	H	102	DGD	C4E-C5E-C6E-O5E
26	c	508	CLA	C8-C10-C11-C12
26	c	508	CLA	C13-C15-C16-C17
30	B	624	STE	C1-C2-C3-C4
33	D	406	LMG	C10-C11-C12-C13
33	M	101	LMG	C28-C29-C30-C31
33	c	518	LMG	C28-C29-C30-C31
33	c	522	LMG	C28-C29-C30-C31
32	C	525	DGD	C8A-C9A-CAA-CBA
31	a	614	SQD	C12-C13-C14-C15
31	a	614	SQD	C30-C31-C32-C33
26	A	607	CLA	C15-C16-C17-C18
26	A	614	CLA	C15-C16-C17-C18
26	B	603	CLA	C8-C10-C11-C12
26	B	603	CLA	C15-C16-C17-C18
26	B	613	CLA	C8-C10-C11-C12
26	C	506	CLA	C8-C10-C11-C12
26	C	510	CLA	C10-C11-C12-C13
26	C	512	CLA	C10-C11-C12-C13
26	a	607	CLA	C15-C16-C17-C18
26	b	613	CLA	C10-C11-C12-C13
26	c	503	CLA	C8-C10-C11-C12
26	c	509	CLA	C10-C11-C12-C13
26	a	607	CLA	C2C-C3C-CAC-CBC
30	i	101	STE	C6-C7-C8-C9
32	A	617	DGD	CCA-CDA-CEA-CFA
34	a	615	LHG	C7-C8-C9-C10
34	d	409	LHG	C23-C24-C25-C26
26	B	611	CLA	C15-C16-C17-C18
26	C	506	CLA	C13-C15-C16-C17
26	B	615	CLA	C5-C6-C7-C8
26	C	503	CLA	C5-C6-C7-C8
26	C	509	CLA	C13-C15-C16-C17
31	a	614	SQD	C26-C27-C28-C29
32	c	521	DGD	CAB-CBB-CCB-CDB
26	B	611	CLA	C8-C10-C11-C12
33	m	101	LMG	C29-C28-O8-C9
33	B	620	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	b	607	CLA	C8-C10-C11-C12
26	b	615	CLA	C13-C15-C16-C17
26	B	607	CLA	C3-C5-C6-C7
34	D	410	LHG	C11-C12-C13-C14
36	V	201	HEC	C2C-C3C-CAC-CBC
33	B	620	LMG	O9-C10-O7-C8
34	D	408	LHG	C1-C2-C3-O3
26	B	606	CLA	C2A-CAA-CBA-CGA
26	b	606	CLA	C2A-CAA-CBA-CGA
32	c	519	DGD	C7A-C8A-C9A-CAA
34	D	409	LHG	C15-C16-C17-C18
26	A	608	CLA	C15-C16-C17-C18
26	B	616	CLA	C10-C11-C12-C13
26	b	614	CLA	C13-C15-C16-C17
26	c	503	CLA	C15-C16-C17-C18
26	c	506	CLA	C13-C15-C16-C17
26	c	509	CLA	C13-C15-C16-C17
26	c	513	CLA	C13-C15-C16-C17
27	D	401	PHO	C2C-C3C-CAC-CBC
26	c	511	CLA	O1D-CGD-O2D-CED
26	b	610	CLA	C15-C16-C17-C18
26	c	507	CLA	C5-C6-C7-C8
26	C	509	CLA	C8-C10-C11-C12
26	b	611	CLA	C8-C10-C11-C12
26	b	614	CLA	C15-C16-C17-C18
26	c	505	CLA	C10-C11-C12-C13
26	c	508	CLA	C10-C11-C12-C13
26	C	505	CLA	C15-C16-C17-C18
30	A	620	STE	C13-C14-C15-C16
33	M	101	LMG	C10-C11-C12-C13
26	D	403	CLA	C10-C11-C12-C13
32	C	524	DGD	C8A-C9A-CAA-CBA
33	B	620	LMG	C28-C29-C30-C31
33	a	617	LMG	C15-C16-C17-C18
26	c	505	CLA	C8-C10-C11-C12
32	C	523	DGD	C2A-C3A-C4A-C5A
34	d	409	LHG	O1-C1-C2-C3
33	b	622	LMG	C9-C8-O7-C10
32	c	521	DGD	CCB-CDB-CEB-CFB
33	a	617	LMG	C34-C35-C36-C37
29	D	405	PL9	C47-C48-C49-C50
26	B	616	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	C	509	CLA	C16-C17-C18-C19
26	D	403	CLA	C16-C17-C18-C20
31	B	623	SQD	C29-C30-C31-C32
26	C	513	CLA	O1D-CGD-O2D-CED
26	B	616	CLA	C5-C6-C7-C8
30	A	619	STE	C7-C8-C9-C10
30	E	104	STE	C11-C10-C9-C8
26	B	601	CLA	C16-C17-C18-C20
26	B	605	CLA	C16-C17-C18-C20
26	B	612	CLA	C16-C17-C18-C20
26	B	616	CLA	C11-C12-C13-C14
26	C	510	CLA	C16-C17-C18-C19
26	D	403	CLA	C16-C17-C18-C19
26	b	603	CLA	C10-C11-C12-C13
30	a	620	STE	C11-C12-C13-C14
31	a	616	SQD	C9-C10-C11-C12
32	H	102	DGD	C7A-C8A-C9A-CAA
30	H	103	STE	C7-C8-C9-C10
30	M	102	STE	C6-C7-C8-C9
30	b	623	STE	C7-C8-C9-C10
30	e	103	STE	C14-C15-C16-C17
33	C	522	LMG	C32-C33-C34-C35
33	a	617	LMG	C32-C33-C34-C35
33	a	618	LMG	C19-C20-C21-C22
34	E	101	LHG	C30-C31-C32-C33
34	a	615	LHG	C27-C28-C29-C30
34	d	409	LHG	C30-C31-C32-C33
30	c	517	STE	C6-C7-C8-C9
32	A	617	DGD	C2B-C3B-C4B-C5B
32	c	521	DGD	C5B-C6B-C7B-C8B
33	M	101	LMG	C18-C19-C20-C21
34	l	101	LHG	C34-C35-C36-C37
30	H	103	STE	C6-C7-C8-C9
30	I	101	STE	C2-C3-C4-C5
30	c	517	STE	C10-C11-C12-C13
30	h	102	STE	C12-C13-C14-C15
30	k	103	STE	C3-C4-C5-C6
30	k	103	STE	C5-C6-C7-C8
31	b	620	SQD	C26-C27-C28-C29
31	f	101	SQD	C27-C28-C29-C30
32	A	617	DGD	C6B-C7B-C8B-C9B
32	c	521	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
33	D	406	LMG	C13-C14-C15-C16
33	D	406	LMG	C16-C17-C18-C19
33	D	407	LMG	C39-C40-C41-C42
34	D	410	LHG	O1-C1-C2-O2
30	C	528	STE	C5-C6-C7-C8
30	t	102	STE	C6-C7-C8-C9
31	a	614	SQD	C10-C11-C12-C13
33	d	411	LMG	C37-C38-C39-C40
34	D	408	LHG	C15-C16-C17-C18
34	D	410	LHG	C29-C30-C31-C32
30	m	102	STE	C1-C2-C3-C4
31	F	102	SQD	C23-C24-C25-C26
30	H	103	STE	C14-C15-C16-C17
33	C	526	LMG	C11-C12-C13-C14
33	M	101	LMG	C39-C40-C41-C42
26	B	601	CLA	C16-C17-C18-C19
26	B	612	CLA	C16-C17-C18-C19
26	C	509	CLA	C16-C17-C18-C20
33	m	101	LMG	O10-C28-O8-C9
30	i	101	STE	C5-C6-C7-C8
31	A	615	SQD	C11-C12-C13-C14
31	A	616	SQD	C15-C16-C17-C18
31	B	623	SQD	C13-C14-C15-C16
33	C	517	LMG	C16-C17-C18-C19
26	B	604	CLA	C10-C11-C12-C13
30	B	624	STE	C5-C6-C7-C8
32	c	521	DGD	CCA-CDA-CEA-CFA
33	c	523	LMG	C40-C41-C42-C43
26	B	606	CLA	C12-C13-C15-C16
30	A	613	STE	C2-C3-C4-C5
30	d	412	STE	C7-C8-C9-C10
30	E	104	STE	C1-C2-C3-C4
26	b	601	CLA	C5-C6-C7-C8
30	K	102	STE	C9-C10-C11-C12
30	c	516	STE	C5-C6-C7-C8
30	c	517	STE	C9-C10-C11-C12
30	c	517	STE	C12-C13-C14-C15
30	e	101	STE	C13-C14-C15-C16
31	A	616	SQD	C10-C11-C12-C13
32	c	519	DGD	CAB-CBB-CCB-CDB
32	h	101	DGD	C2B-C3B-C4B-C5B
33	B	620	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	C	522	LMG	C16-C17-C18-C19
33	C	522	LMG	C31-C32-C33-C34
33	a	617	LMG	C31-C32-C33-C34
34	B	622	LHG	C25-C26-C27-C28
30	K	102	STE	C7-C8-C9-C10
32	A	617	DGD	C9A-CAA-CBA-CCA
33	M	101	LMG	C37-C38-C39-C40
33	c	522	LMG	C38-C39-C40-C41
33	d	411	LMG	C32-C33-C34-C35
30	a	620	STE	C11-C10-C9-C8
31	a	616	SQD	C18-C19-C20-C21
26	B	605	CLA	C16-C17-C18-C19
26	C	507	CLA	C16-C17-C18-C19
26	C	510	CLA	C16-C17-C18-C20
30	H	103	STE	C2-C3-C4-C5
30	T	102	STE	C6-C7-C8-C9
30	e	104	STE	C3-C4-C5-C6
32	h	101	DGD	C7A-C8A-C9A-CAA
33	M	101	LMG	C15-C16-C17-C18
30	m	103	STE	C6-C7-C8-C9
32	A	617	DGD	C2A-C3A-C4A-C5A
34	d	408	LHG	C13-C14-C15-C16
33	c	523	LMG	O6-C5-C6-O5
31	b	620	SQD	C44-C45-C46-O48
33	m	101	LMG	C7-C8-C9-O8
30	E	104	STE	C9-C10-C11-C12
30	a	620	STE	C6-C7-C8-C9
30	z	101	STE	C2-C3-C4-C5
31	a	614	SQD	C11-C10-C9-C8
31	a	614	SQD	C11-C12-C13-C14
31	f	101	SQD	C25-C26-C27-C28
31	f	101	SQD	C32-C33-C34-C35
32	c	520	DGD	C9A-CAA-CBA-CCA
32	h	101	DGD	C7B-C8B-C9B-CAB
26	B	602	CLA	C13-C15-C16-C17
26	c	512	CLA	C13-C15-C16-C17
30	H	103	STE	C11-C10-C9-C8
30	K	102	STE	C12-C13-C14-C15
30	M	102	STE	C7-C8-C9-C10
30	c	517	STE	C7-C8-C9-C10
30	c	517	STE	C11-C10-C9-C8
30	d	406	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	j	102	STE	C5-C6-C7-C8
30	m	103	STE	C4-C5-C6-C7
33	b	622	LMG	C12-C13-C14-C15
34	E	101	LHG	C14-C15-C16-C17
30	e	103	STE	C13-C14-C15-C16
33	M	101	LMG	C36-C37-C38-C39
30	B	624	STE	C2-C3-C4-C5
30	d	412	STE	C3-C4-C5-C6
31	A	616	SQD	C11-C12-C13-C14
32	c	519	DGD	CAA-CBA-CCA-CDA
32	c	520	DGD	C3B-C4B-C5B-C6B
36	V	201	HEC	C4C-C3C-CAC-CBC
26	B	615	CLA	O1D-CGD-O2D-CED
30	B	624	STE	C9-C10-C11-C12
30	T	102	STE	C13-C14-C15-C16
30	a	619	STE	C4-C5-C6-C7
33	a	617	LMG	C29-C30-C31-C32
33	m	101	LMG	C29-C30-C31-C32
34	D	408	LHG	C11-C10-C9-C8
28	B	617	BCR	C1-C6-C7-C8
28	C	521	BCR	C5-C6-C7-C8
28	T	101	BCR	C1-C6-C7-C8
28	T	101	BCR	C23-C24-C25-C26
28	d	404	BCR	C23-C24-C25-C26
28	k	101	BCR	C1-C6-C7-C8
28	t	101	BCR	C1-C6-C7-C8
28	t	101	BCR	C23-C24-C25-C26
30	J	101	STE	C5-C6-C7-C8
30	a	620	STE	C9-C10-C11-C12
32	H	102	DGD	C4B-C5B-C6B-C7B
32	c	521	DGD	C4A-C5A-C6A-C7A
32	c	521	DGD	C4B-C5B-C6B-C7B
26	c	501	CLA	CBD-CGD-O2D-CED
31	f	101	SQD	C8-C7-O47-C45
26	c	513	CLA	C8-C10-C11-C12
33	C	526	LMG	C35-C36-C37-C38
30	B	624	STE	C6-C7-C8-C9
30	C	529	STE	C11-C12-C13-C14
30	T	102	STE	C14-C15-C16-C17
34	B	622	LHG	C17-C18-C19-C20
30	T	103	STE	C11-C12-C13-C14
33	D	406	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	B	624	STE	C4-C5-C6-C7
31	a	616	SQD	C31-C32-C33-C34
34	D	409	LHG	C34-C35-C36-C37
29	d	405	PL9	C20-C19-C21-C22
30	D	411	STE	C9-C10-C11-C12
30	b	625	STE	C13-C14-C15-C16
31	B	623	SQD	C25-C26-C27-C28
32	C	524	DGD	C6A-C7A-C8A-C9A
33	B	620	LMG	C29-C30-C31-C32
29	A	612	PL9	C32-C33-C34-C36
29	a	612	PL9	C17-C18-C19-C21
26	b	607	CLA	C10-C11-C12-C13
29	D	405	PL9	C33-C34-C36-C37
26	b	610	CLA	C16-C17-C18-C19
30	A	618	STE	C13-C14-C15-C16
30	C	520	STE	C6-C7-C8-C9
30	z	101	STE	C4-C5-C6-C7
31	A	615	SQD	C25-C26-C27-C28
32	C	525	DGD	C5A-C6A-C7A-C8A
33	b	622	LMG	C15-C16-C17-C18
33	b	622	LMG	C29-C30-C31-C32
34	a	615	LHG	C24-C23-O8-C6
26	C	505	CLA	C11-C12-C13-C14
30	H	103	STE	C10-C11-C12-C13
30	a	619	STE	C6-C7-C8-C9
31	a	614	SQD	C18-C19-C20-C21
32	C	525	DGD	CBA-CCA-CDA-CEA
33	D	406	LMG	C32-C33-C34-C35
33	a	618	LMG	C14-C15-C16-C17
33	c	518	LMG	C12-C13-C14-C15
34	D	410	LHG	C13-C14-C15-C16
34	E	101	LHG	C25-C26-C27-C28
33	D	407	LMG	C15-C16-C17-C18
33	D	407	LMG	C18-C19-C20-C21
33	c	523	LMG	C39-C40-C41-C42
33	d	411	LMG	C38-C39-C40-C41
30	A	619	STE	C11-C10-C9-C8
30	T	103	STE	C9-C10-C11-C12
33	B	620	LMG	C32-C33-C34-C35
33	M	101	LMG	C12-C13-C14-C15
33	b	622	LMG	C21-C22-C23-C24
30	A	619	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
30	A	619	STE	C5-C6-C7-C8
30	e	104	STE	C5-C6-C7-C8
32	C	523	DGD	C6A-C7A-C8A-C9A
33	C	522	LMG	C35-C36-C37-C38
27	d	401	PHO	C2C-C3C-CAC-CBC
30	B	621	STE	C5-C6-C7-C8
30	I	102	STE	C6-C7-C8-C9
30	Z	101	STE	C11-C12-C13-C14
30	d	412	STE	C6-C7-C8-C9
30	j	101	STE	C5-C6-C7-C8
31	b	620	SQD	C28-C29-C30-C31
30	I	101	STE	C9-C10-C11-C12
30	t	102	STE	C11-C10-C9-C8
32	C	524	DGD	CCA-CDA-CEA-CFA
32	C	524	DGD	C9B-CAB-CBB-CCB
34	D	410	LHG	C24-C25-C26-C27
28	T	101	BCR	C13-C14-C15-C16
26	B	614	CLA	C16-C17-C18-C20
33	m	101	LMG	C11-C10-O7-C8
30	b	625	STE	C15-C16-C17-C18
26	c	511	CLA	C15-C16-C17-C18
30	T	102	STE	C4-C5-C6-C7
30	d	410	STE	C3-C4-C5-C6
32	H	102	DGD	C3B-C4B-C5B-C6B
33	a	618	LMG	C35-C36-C37-C38
34	a	615	LHG	C12-C13-C14-C15
26	C	504	CLA	C11-C12-C13-C14
26	c	503	CLA	C10-C11-C12-C13
30	B	621	STE	C1-C2-C3-C4
32	c	520	DGD	C6A-C7A-C8A-C9A
26	c	509	CLA	C3-C5-C6-C7
32	C	524	DGD	C2G-C3G-O3G-C1D
32	c	520	DGD	C2G-C3G-O3G-C1D
30	J	101	STE	C6-C7-C8-C9
30	c	516	STE	C7-C8-C9-C10
33	C	522	LMG	C33-C34-C35-C36
33	a	618	LMG	C37-C38-C39-C40
34	D	410	LHG	C28-C29-C30-C31
26	C	507	CLA	C16-C17-C18-C20
30	k	103	STE	C11-C10-C9-C8
32	c	520	DGD	CAA-CBA-CCA-CDA
32	c	520	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
34	d	408	LHG	C30-C31-C32-C33
29	D	405	PL9	C45-C44-C46-C47
30	B	621	STE	C9-C10-C11-C12
30	b	624	STE	C6-C7-C8-C9
30	m	103	STE	C9-C10-C11-C12
26	B	614	CLA	C15-C16-C17-C18
34	D	410	LHG	C27-C28-C29-C30
26	b	604	CLA	C3-C5-C6-C7
26	b	615	CLA	C5-C6-C7-C8
30	a	620	STE	C5-C6-C7-C8
31	F	102	SQD	C30-C31-C32-C33
33	c	523	LMG	C38-C39-C40-C41
33	d	411	LMG	C28-C29-C30-C31
30	j	101	STE	C2-C3-C4-C5
26	B	615	CLA	C15-C16-C17-C18
26	C	509	CLA	C10-C11-C12-C13
26	B	606	CLA	C16-C17-C18-C19
33	D	406	LMG	C31-C32-C33-C34
32	C	523	DGD	C9A-CAA-CBA-CCA
33	c	522	LMG	C12-C13-C14-C15
26	B	609	CLA	C15-C16-C17-C18
30	K	102	STE	C6-C7-C8-C9
30	K	102	STE	C13-C14-C15-C16
31	b	620	SQD	C16-C17-C18-C19
32	C	524	DGD	C5A-C6A-C7A-C8A
32	h	101	DGD	C5B-C6B-C7B-C8B
34	l	101	LHG	C11-C10-C9-C8
31	f	101	SQD	O6-C44-C45-O47
33	D	406	LMG	O7-C8-C9-O8
30	m	102	STE	C2-C3-C4-C5
31	A	616	SQD	C11-C10-C9-C8
30	c	517	STE	C13-C14-C15-C16
30	k	103	STE	C6-C7-C8-C9
33	B	620	LMG	C31-C32-C33-C34
26	d	403	CLA	C8-C10-C11-C12
33	d	411	LMG	O6-C5-C6-O5
30	Z	101	STE	C6-C7-C8-C9
30	j	101	STE	C4-C5-C6-C7
31	B	623	SQD	C10-C11-C12-C13
32	C	524	DGD	C4B-C5B-C6B-C7B
33	b	622	LMG	C31-C32-C33-C34
33	c	522	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
32	A	617	DGD	CFA-CGA-CHA-CIA
30	I	102	STE	C11-C10-C9-C8
30	i	101	STE	C4-C5-C6-C7
32	c	521	DGD	C7A-C8A-C9A-CAA
34	D	408	LHG	C12-C13-C14-C15
26	B	606	CLA	C13-C15-C16-C17
31	A	615	SQD	C9-C10-C11-C12
31	a	614	SQD	C13-C14-C15-C16
33	M	101	LMG	C20-C21-C22-C23
31	f	101	SQD	O49-C7-O47-C45
34	d	407	LHG	C1-C2-C3-O3
30	M	102	STE	C5-C6-C7-C8
32	c	520	DGD	C7B-C8B-C9B-CAB
33	B	620	LMG	C33-C34-C35-C36
33	M	101	LMG	C13-C14-C15-C16
34	a	615	LHG	C11-C12-C13-C14
34	d	409	LHG	C32-C33-C34-C35
30	I	102	STE	C2-C3-C4-C5
33	b	622	LMG	C13-C14-C15-C16
26	B	612	CLA	C10-C11-C12-C13
30	j	102	STE	C7-C8-C9-C10
30	m	102	STE	C6-C7-C8-C9
34	l	101	LHG	C27-C28-C29-C30
34	d	407	LHG	O1-C1-C2-O2
31	a	614	SQD	C25-C26-C27-C28
32	H	102	DGD	CAA-CBA-CCA-CDA
26	c	508	CLA	C1A-C2A-CAA-CBA
26	c	511	CLA	C1A-C2A-CAA-CBA
26	c	513	CLA	C1A-C2A-CAA-CBA
32	c	519	DGD	O6E-C5E-C6E-O5E
30	E	104	STE	C4-C5-C6-C7
31	a	616	SQD	C27-C28-C29-C30
34	d	407	LHG	C25-C26-C27-C28
30	T	103	STE	C14-C15-C16-C17
33	b	622	LMG	C16-C17-C18-C19
26	C	512	CLA	C8-C10-C11-C12
30	E	104	STE	C5-C6-C7-C8
30	I	102	STE	C5-C6-C7-C8
34	d	407	LHG	C28-C29-C30-C31
26	C	509	CLA	C3-C5-C6-C7
26	B	601	CLA	C6-C7-C8-C10
26	B	604	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	B	613	CLA	C12-C13-C15-C16
26	B	614	CLA	C12-C13-C15-C16
26	C	504	CLA	C11-C10-C8-C7
26	C	508	CLA	C12-C13-C15-C16
26	C	512	CLA	C11-C10-C8-C7
26	D	402	CLA	C12-C13-C15-C16
26	a	610	CLA	C6-C7-C8-C10
26	b	603	CLA	C6-C7-C8-C10
26	b	604	CLA	C12-C13-C15-C16
26	b	606	CLA	C6-C7-C8-C10
26	b	607	CLA	C6-C7-C8-C10
26	c	503	CLA	C6-C7-C8-C10
26	c	506	CLA	C11-C10-C8-C7
26	c	506	CLA	C11-C12-C13-C15
26	c	513	CLA	C12-C13-C15-C16
30	J	101	STE	C2-C3-C4-C5
30	b	621	STE	C11-C10-C9-C8
31	B	623	SQD	C33-C34-C35-C36
34	d	409	LHG	C25-C26-C27-C28
26	A	607	CLA	C16-C17-C18-C20
26	B	606	CLA	C16-C17-C18-C20
26	d	402	CLA	C16-C17-C18-C19
34	a	615	LHG	O10-C23-O8-C6
34	d	407	LHG	C16-C17-C18-C19
32	C	524	DGD	C5B-C6B-C7B-C8B
33	b	622	LMG	C22-C23-C24-C25
33	b	622	LMG	C36-C37-C38-C39
32	A	617	DGD	C2B-C1B-O2G-C2G
33	a	617	LMG	C11-C10-O7-C8
26	B	601	CLA	C6-C7-C8-C9
26	B	604	CLA	C14-C13-C15-C16
26	B	613	CLA	C14-C13-C15-C16
26	B	614	CLA	C14-C13-C15-C16
26	a	610	CLA	C11-C12-C13-C14
26	c	506	CLA	C11-C12-C13-C14
26	c	513	CLA	C11-C12-C13-C14
31	a	614	SQD	C9-C10-C11-C12
32	C	524	DGD	C8B-C9B-CAB-CBB
33	d	411	LMG	C30-C31-C32-C33
31	F	102	SQD	C27-C28-C29-C30
33	D	407	LMG	O6-C5-C6-O5
30	A	619	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	I	101	STE	C4-C5-C6-C7
31	A	616	SQD	O6-C44-C45-C46
31	B	623	SQD	O6-C44-C45-C46
32	A	617	DGD	C1G-C2G-C3G-O3G
33	B	620	LMG	C7-C8-C9-O8
33	C	517	LMG	C7-C8-C9-O8
33	b	622	LMG	O1-C7-C8-C9
30	b	621	STE	C3-C4-C5-C6
26	c	504	CLA	C8-C10-C11-C12
32	C	525	DGD	C6A-C7A-C8A-C9A
33	a	617	LMG	O6-C5-C6-O5
30	D	411	STE	C7-C8-C9-C10
30	c	516	STE	C6-C7-C8-C9
34	D	410	LHG	C9-C10-C11-C12
32	c	521	DGD	C6B-C7B-C8B-C9B
33	a	618	LMG	C38-C39-C40-C41
34	a	615	LHG	C25-C26-C27-C28
26	B	613	CLA	C13-C15-C16-C17
30	j	102	STE	C4-C5-C6-C7
32	C	523	DGD	C6B-C7B-C8B-C9B
26	B	613	CLA	C10-C11-C12-C13
26	b	605	CLA	C5-C6-C7-C8
26	c	506	CLA	C8-C10-C11-C12
28	t	101	BCR	C11-C12-C13-C35
26	c	503	CLA	C16-C17-C18-C20
34	d	408	LHG	C11-C12-C13-C14
26	b	603	CLA	C13-C15-C16-C17
26	b	613	CLA	C13-C15-C16-C17
30	T	103	STE	C13-C14-C15-C16
30	d	406	STE	C4-C5-C6-C7
31	A	615	SQD	C33-C34-C35-C36
33	B	620	LMG	O6-C5-C6-O5
32	A	617	DGD	C9B-CAB-CBB-CCB
32	c	519	DGD	C3B-C4B-C5B-C6B
33	B	620	LMG	C30-C31-C32-C33
30	A	620	STE	C12-C13-C14-C15
30	H	103	STE	C11-C12-C13-C14
32	H	102	DGD	C2B-C3B-C4B-C5B
34	B	622	LHG	C10-C11-C12-C13
33	C	517	LMG	C10-C11-C12-C13
30	b	621	STE	C12-C13-C14-C15
30	e	103	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	A	615	SQD	C12-C13-C14-C15
31	a	616	SQD	C11-C10-C9-C8
34	E	101	LHG	C32-C33-C34-C35
33	D	406	LMG	C29-C28-O8-C9
30	Z	101	STE	C2-C3-C4-C5
32	H	102	DGD	CDA-CEA-CFA-CGA
33	C	522	LMG	C40-C41-C42-C43
30	B	624	STE	C12-C13-C14-C15
33	C	517	LMG	C14-C15-C16-C17
34	E	101	LHG	C33-C34-C35-C36
30	C	528	STE	C4-C5-C6-C7
33	C	522	LMG	C17-C18-C19-C20
33	c	522	LMG	C36-C37-C38-C39
26	d	402	CLA	C16-C17-C18-C20
30	A	619	STE	C2-C3-C4-C5
32	c	520	DGD	CAB-CBB-CCB-CDB
34	D	409	LHG	C24-C25-C26-C27
32	C	523	DGD	C4E-C5E-C6E-O5E
30	A	619	STE	C11-C12-C13-C14
30	d	412	STE	C5-C6-C7-C8
33	B	620	LMG	C15-C16-C17-C18
26	c	510	CLA	C10-C11-C12-C13
30	E	103	STE	C9-C10-C11-C12
33	a	618	LMG	C29-C28-O8-C9
33	C	526	LMG	C32-C33-C34-C35
34	d	409	LHG	C27-C28-C29-C30
30	C	529	STE	C15-C16-C17-C18
32	C	523	DGD	CDA-CEA-CFA-CGA
30	A	620	STE	C14-C15-C16-C17
30	b	621	STE	C14-C15-C16-C17
31	a	616	SQD	C30-C31-C32-C33
31	b	620	SQD	C25-C26-C27-C28
33	D	407	LMG	C17-C18-C19-C20
33	a	618	LMG	C16-C17-C18-C19
34	d	408	LHG	C35-C36-C37-C38
32	c	521	DGD	C7B-C8B-C9B-CAB
33	a	618	LMG	C31-C32-C33-C34
34	B	622	LHG	C29-C30-C31-C32
36	v	201	HEC	C2C-C3C-CAC-CBC
30	A	620	STE	C10-C11-C12-C13
30	M	103	STE	C6-C7-C8-C9
31	a	614	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
33	B	620	LMG	C34-C35-C36-C37
33	a	618	LMG	O1-C7-C8-O7
31	A	615	SQD	C13-C14-C15-C16
33	a	618	LMG	C17-C18-C19-C20
34	B	622	LHG	C11-C12-C13-C14
34	D	409	LHG	C27-C28-C29-C30
30	B	621	STE	C12-C13-C14-C15
30	b	624	STE	C7-C8-C9-C10
30	b	625	STE	C11-C10-C9-C8
30	D	411	STE	C4-C5-C6-C7
30	T	102	STE	C12-C13-C14-C15
32	H	102	DGD	C8B-C9B-CAB-CBB
30	K	102	STE	C5-C6-C7-C8
32	H	102	DGD	O2G-C1B-C2B-C3B
26	C	506	CLA	C3-C5-C6-C7
33	D	406	LMG	C34-C35-C36-C37
32	c	519	DGD	O6D-C5D-C6D-O5D
26	B	603	CLA	C10-C11-C12-C13
26	C	509	CLA	C5-C6-C7-C8
30	f	102	STE	C14-C15-C16-C17
31	b	620	SQD	C10-C11-C12-C13
32	C	524	DGD	CBB-CCB-CDB-CEB
29	a	612	PL9	C39-C41-C42-C43
33	D	407	LMG	C11-C12-C13-C14
34	B	622	LHG	C31-C32-C33-C34
34	d	407	LHG	C18-C19-C20-C21
30	c	517	STE	C1-C2-C3-C4
30	i	102	STE	C9-C10-C11-C12
31	B	623	SQD	C24-C25-C26-C27
31	a	614	SQD	C8-C7-O47-C45
29	a	612	PL9	C32-C33-C34-C35
30	I	101	STE	C5-C6-C7-C8
33	a	617	LMG	C35-C36-C37-C38
30	d	410	STE	C5-C6-C7-C8
34	d	407	LHG	C9-C10-C11-C12
30	b	623	STE	C11-C12-C13-C14
33	m	101	LMG	C22-C23-C24-C25
26	a	607	CLA	C4C-C3C-CAC-CBC
33	C	522	LMG	C14-C15-C16-C17
26	C	508	CLA	C15-C16-C17-C18
26	a	610	CLA	C5-C6-C7-C8
29	a	612	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
34	d	407	LHG	C19-C20-C21-C22
26	c	505	CLA	C2-C3-C5-C6
26	B	607	CLA	CBA-CGA-O2A-C1
26	a	610	CLA	C15-C16-C17-C18
26	b	604	CLA	C13-C15-C16-C17
30	j	102	STE	C6-C7-C8-C9
31	A	615	SQD	C11-C10-C9-C8
31	B	623	SQD	C9-C10-C11-C12
33	C	522	LMG	C39-C40-C41-C42
34	d	408	LHG	O1-C1-C2-O2
26	A	608	CLA	C11-C12-C13-C14
26	B	602	CLA	C11-C12-C13-C14
26	B	604	CLA	C11-C12-C13-C14
26	B	605	CLA	C6-C7-C8-C9
26	B	615	CLA	C11-C10-C8-C9
26	B	615	CLA	C11-C12-C13-C14
26	C	504	CLA	C11-C10-C8-C9
26	C	506	CLA	C11-C10-C8-C9
26	D	403	CLA	C6-C7-C8-C9
26	b	603	CLA	C6-C7-C8-C9
26	b	604	CLA	C14-C13-C15-C16
26	b	607	CLA	C6-C7-C8-C9
26	b	607	CLA	C11-C12-C13-C14
26	c	506	CLA	C11-C10-C8-C9
26	c	508	CLA	C11-C12-C13-C14
26	c	509	CLA	C11-C12-C13-C14
26	c	513	CLA	C14-C13-C15-C16
32	h	101	DGD	C6B-C7B-C8B-C9B
33	D	407	LMG	C14-C15-C16-C17
33	M	101	LMG	C32-C33-C34-C35
34	a	615	LHG	C15-C16-C17-C18
26	b	606	CLA	C4B-C3B-CAB-CBB
32	C	525	DGD	CCB-CDB-CEB-CFB
34	d	407	LHG	C26-C27-C28-C29
30	m	103	STE	C1-C2-C3-C4
30	e	104	STE	C2-C3-C4-C5
34	d	408	LHG	C15-C16-C17-C18
26	C	501	CLA	O1D-CGD-O2D-CED
34	d	407	LHG	C11-C12-C13-C14
26	b	616	CLA	C3-C5-C6-C7
30	i	101	STE	C3-C4-C5-C6
33	c	523	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	C31-C32-C33-C34
34	B	622	LHG	C13-C14-C15-C16
30	A	620	STE	C11-C10-C9-C8
30	j	102	STE	C15-C16-C17-C18
26	B	602	CLA	C11-C12-C13-C15
26	B	604	CLA	C12-C13-C15-C16
26	B	612	CLA	C12-C13-C15-C16
26	B	613	CLA	C11-C12-C13-C15
26	B	615	CLA	C6-C7-C8-C10
26	B	615	CLA	C11-C12-C13-C15
26	C	509	CLA	C11-C10-C8-C7
26	C	509	CLA	C12-C13-C15-C16
26	C	513	CLA	C12-C13-C15-C16
26	D	403	CLA	C6-C7-C8-C10
26	a	610	CLA	C12-C13-C15-C16
26	b	606	CLA	C12-C13-C15-C16
26	b	607	CLA	C11-C12-C13-C15
26	b	614	CLA	C6-C7-C8-C10
26	c	505	CLA	C6-C7-C8-C10
26	c	512	CLA	C6-C7-C8-C10
31	b	620	SQD	C11-C12-C13-C14
29	d	405	PL9	C47-C48-C49-C50
34	B	622	LHG	C5-C6-O8-C23
30	C	516	STE	C1-C2-C3-C4
30	A	613	STE	C4-C5-C6-C7
30	m	103	STE	C2-C3-C4-C5
30	I	102	STE	C9-C10-C11-C12
33	M	101	LMG	C33-C34-C35-C36
32	C	523	DGD	C4B-C5B-C6B-C7B
26	B	601	CLA	C3A-C2A-CAA-CBA
26	b	602	CLA	C13-C15-C16-C17
33	m	101	LMG	C10-C11-C12-C13
32	c	521	DGD	CBB-CCB-CDB-CEB
26	a	613	CLA	C13-C15-C16-C17
32	A	617	DGD	C4E-C5E-C6E-O5E
34	D	408	LHG	C16-C17-C18-C19
28	t	101	BCR	C13-C14-C15-C16
28	x	101	BCR	C9-C10-C11-C12
33	D	406	LMG	O10-C28-O8-C9
34	D	409	LHG	C29-C30-C31-C32
34	a	615	LHG	C28-C29-C30-C31
32	A	617	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
32	C	524	DGD	CCB-CDB-CEB-CFB
34	D	410	LHG	C31-C32-C33-C34
34	a	615	LHG	C14-C15-C16-C17
33	b	622	LMG	C11-C12-C13-C14
33	c	523	LMG	C15-C16-C17-C18
34	D	408	LHG	C33-C34-C35-C36
34	d	408	LHG	C12-C13-C14-C15
31	a	614	SQD	O6-C44-C45-C46
31	a	616	SQD	O6-C44-C45-C46
31	f	101	SQD	O6-C44-C45-C46
32	A	617	DGD	O1G-C1G-C2G-C3G
34	B	622	LHG	C11-C10-C9-C8
26	A	607	CLA	C16-C17-C18-C19
26	C	507	CLA	C5-C6-C7-C8
30	b	623	STE	C9-C10-C11-C12
32	H	102	DGD	C6B-C7B-C8B-C9B
32	c	519	DGD	C8B-C9B-CAB-CBB
33	D	406	LMG	C29-C30-C31-C32
34	a	615	LHG	C16-C17-C18-C19
31	A	615	SQD	C30-C31-C32-C33
32	H	102	DGD	CBA-CCA-CDA-CEA
26	b	614	CLA	C4-C3-C5-C6
26	c	505	CLA	C4-C3-C5-C6
30	H	103	STE	C1-C2-C3-C4
30	E	104	STE	C11-C12-C13-C14
32	h	101	DGD	CDB-CEB-CFB-CGB
34	B	622	LHG	C35-C36-C37-C38
34	d	407	LHG	C10-C11-C12-C13
26	B	614	CLA	C16-C17-C18-C19
33	m	101	LMG	O9-C10-O7-C8
26	b	609	CLA	C13-C15-C16-C17
34	a	615	LHG	O6-C4-C5-O7
32	C	523	DGD	O6D-C5D-C6D-O5D
30	i	102	STE	C11-C10-C9-C8
29	A	612	PL9	C47-C48-C49-C50
28	b	617	BCR	C1-C6-C7-C8
34	d	407	LHG	O2-C2-C3-O3
34	d	409	LHG	C2-C3-O3-P
34	l	101	LHG	C26-C27-C28-C29
32	A	617	DGD	CCB-CDB-CEB-CFB
32	H	102	DGD	C5B-C6B-C7B-C8B
33	a	617	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	d	403	CLA	C5-C6-C7-C8
31	b	620	SQD	C13-C14-C15-C16
33	C	526	LMG	C18-C19-C20-C21
31	A	615	SQD	O6-C44-C45-O47
31	f	101	SQD	O47-C45-C46-O48
32	A	617	DGD	O1G-C1G-C2G-O2G
33	B	620	LMG	O7-C8-C9-O8
33	c	523	LMG	O7-C8-C9-O8
34	a	615	LHG	O7-C5-C6-O8
30	c	516	STE	C2-C3-C4-C5
29	a	612	PL9	C4-C3-C7-C8
32	c	521	DGD	C1A-C2A-C3A-C4A
34	d	407	LHG	C7-C8-C9-C10
34	D	410	LHG	C17-C18-C19-C20
34	d	407	LHG	C24-C25-C26-C27
29	D	405	PL9	C43-C44-C46-C47
29	a	612	PL9	C43-C44-C46-C47
32	c	521	DGD	CDA-CEA-CFA-CGA
30	M	102	STE	C4-C5-C6-C7
30	k	103	STE	C4-C5-C6-C7
33	a	618	LMG	C18-C19-C20-C21
30	B	621	STE	C3-C4-C5-C6
32	C	523	DGD	C3B-C4B-C5B-C6B
32	c	519	DGD	C6B-C7B-C8B-C9B
30	j	101	STE	C7-C8-C9-C10
26	B	612	CLA	C14-C13-C15-C16
26	a	610	CLA	C6-C7-C8-C9
26	a	610	CLA	C14-C13-C15-C16
26	c	505	CLA	C11-C12-C13-C14
33	D	406	LMG	C17-C18-C19-C20
30	j	102	STE	C11-C10-C9-C8
26	c	503	CLA	C16-C17-C18-C19
30	T	103	STE	C6-C7-C8-C9
32	C	524	DGD	C3A-C4A-C5A-C6A
26	b	604	CLA	C5-C6-C7-C8
33	a	618	LMG	O10-C28-O8-C9
30	c	516	STE	C9-C10-C11-C12
33	c	523	LMG	C32-C33-C34-C35
32	c	519	DGD	C3A-C4A-C5A-C6A
34	a	615	LHG	O1-C1-C2-O2
32	c	521	DGD	C2A-C1A-O1G-C1G
30	C	529	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	C40-C41-C42-C43
30	j	102	STE	C10-C11-C12-C13
34	E	101	LHG	C8-C7-O7-C5
30	T	103	STE	C5-C6-C7-C8
30	C	528	STE	C12-C13-C14-C15
31	A	616	SQD	C9-C10-C11-C12
26	b	604	CLA	C15-C16-C17-C18
32	h	101	DGD	O6E-C5E-C6E-O5E
31	b	620	SQD	C24-C25-C26-C27
33	D	407	LMG	C30-C31-C32-C33
34	d	407	LHG	C17-C18-C19-C20
26	B	608	CLA	C3-C5-C6-C7
32	C	523	DGD	C5A-C6A-C7A-C8A
32	C	524	DGD	C3B-C4B-C5B-C6B
26	b	610	CLA	C16-C17-C18-C20
32	c	520	DGD	CCB-CDB-CEB-CFB
30	A	619	STE	C4-C5-C6-C7
33	C	526	LMG	C17-C18-C19-C20
26	C	507	CLA	C11-C10-C8-C7
26	C	512	CLA	C11-C12-C13-C15
26	C	513	CLA	C11-C10-C8-C7
26	b	603	CLA	C11-C10-C8-C7
26	b	603	CLA	C11-C12-C13-C15
26	b	604	CLA	C11-C12-C13-C15
26	c	505	CLA	C11-C12-C13-C15
26	c	507	CLA	C12-C13-C15-C16
26	c	508	CLA	C12-C13-C15-C16
26	c	512	CLA	C11-C12-C13-C15
26	d	402	CLA	C11-C12-C13-C15
26	d	403	CLA	C11-C12-C13-C15
34	D	410	LHG	C23-C24-C25-C26
30	Z	101	STE	C11-C10-C9-C8
33	C	522	LMG	C12-C13-C14-C15
32	C	524	DGD	CDB-CEB-CFB-CGB
34	E	101	LHG	C19-C20-C21-C22
28	t	101	BCR	C11-C12-C13-C14
33	C	526	LMG	C29-C28-O8-C9
30	C	520	STE	C5-C6-C7-C8
33	M	101	LMG	C11-C12-C13-C14
34	l	101	LHG	C13-C14-C15-C16
26	B	607	CLA	O1A-CGA-O2A-C1
36	v	201	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
32	C	524	DGD	C5D-C6D-O5D-C1E
32	c	520	DGD	C5D-C6D-O5D-C1E
31	F	102	SQD	C25-C26-C27-C28
26	D	402	CLA	C16-C17-C18-C20
33	a	617	LMG	O9-C10-O7-C8
33	C	517	LMG	C7-C8-O7-C10
32	C	525	DGD	C3A-C4A-C5A-C6A
33	c	523	LMG	C12-C13-C14-C15
26	b	601	CLA	C16-C17-C18-C20
30	T	102	STE	C3-C4-C5-C6
30	E	104	STE	C7-C8-C9-C10
30	h	102	STE	C10-C11-C12-C13
30	M	103	STE	C1-C2-C3-C4
26	b	605	CLA	C8-C10-C11-C12
30	B	625	STE	C2-C3-C4-C5
31	A	615	SQD	C27-C28-C29-C30
26	B	612	CLA	C13-C15-C16-C17
31	A	616	SQD	C16-C17-C18-C19
32	H	102	DGD	CCB-CDB-CEB-CFB
33	D	407	LMG	C40-C41-C42-C43
31	F	102	SQD	O5-C1-O6-C44
30	B	624	STE	C7-C8-C9-C10
31	A	615	SQD	O6-C44-C45-C46
31	f	101	SQD	C44-C45-C46-O48
33	D	406	LMG	C7-C8-C9-O8
33	a	617	LMG	C7-C8-C9-O8
34	a	615	LHG	C4-C5-C6-O8
35	F	101	HEM	C4C-C3C-CAC-CBC
35	e	102	HEM	C4C-C3C-CAC-CBC
26	B	606	CLA	C5-C6-C7-C8
26	B	608	CLA	C15-C16-C17-C18
26	C	505	CLA	C13-C15-C16-C17
32	C	523	DGD	C4D-C5D-C6D-O5D
26	C	513	CLA	C4-C3-C5-C6
32	h	101	DGD	O2G-C1B-C2B-C3B
30	Z	101	STE	C5-C6-C7-C8
26	a	613	CLA	C15-C16-C17-C18
33	c	523	LMG	C37-C38-C39-C40
31	F	102	SQD	C32-C33-C34-C35
31	b	620	SQD	C18-C19-C20-C21
31	a	614	SQD	O47-C45-C46-O48
33	a	617	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
33	a	618	LMG	O7-C8-C9-O8
33	m	101	LMG	O7-C8-C9-O8
26	b	614	CLA	C8-C10-C11-C12
26	C	503	CLA	C11-C10-C8-C9
26	C	513	CLA	C11-C10-C8-C9
26	b	604	CLA	C11-C12-C13-C14
26	c	505	CLA	C6-C7-C8-C9
26	c	507	CLA	C14-C13-C15-C16
32	C	523	DGD	C8B-C9B-CAB-CBB
31	a	614	SQD	O49-C7-O47-C45
34	E	101	LHG	O9-C7-O7-C5
30	Z	101	STE	C13-C14-C15-C16
30	C	516	STE	C11-C10-C9-C8
30	d	410	STE	C11-C12-C13-C14
31	A	615	SQD	C32-C33-C34-C35
31	f	101	SQD	C26-C27-C28-C29
32	A	617	DGD	C7B-C8B-C9B-CAB
33	D	406	LMG	C37-C38-C39-C40
34	D	408	LHG	C25-C26-C27-C28
34	D	410	LHG	C12-C13-C14-C15
26	B	605	CLA	C8-C10-C11-C12
31	f	101	SQD	C24-C25-C26-C27
33	M	101	LMG	C21-C22-C23-C24
30	e	104	STE	C1-C2-C3-C4
30	e	103	STE	C12-C13-C14-C15
31	a	614	SQD	C32-C33-C34-C35
30	a	620	STE	C12-C13-C14-C15
34	D	409	LHG	C32-C33-C34-C35
32	A	617	DGD	CDB-CEB-CFB-CGB
32	H	102	DGD	C7B-C8B-C9B-CAB
30	j	101	STE	C1-C2-C3-C4
34	d	408	LHG	C29-C30-C31-C32
30	D	412	STE	C11-C12-C13-C14
32	h	101	DGD	CAA-CBA-CCA-CDA
26	B	607	CLA	C16-C17-C18-C20
26	C	502	CLA	C16-C17-C18-C20
26	b	602	CLA	C16-C17-C18-C20
30	a	619	STE	C3-C4-C5-C6
31	a	616	SQD	C17-C18-C19-C20
31	a	616	SQD	C24-C25-C26-C27
34	D	410	LHG	C25-C26-C27-C28
32	c	521	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
32	c	520	DGD	C9B-CAB-CBB-CCB
33	D	406	LMG	C11-C12-C13-C14
26	c	501	CLA	O1D-CGD-O2D-CED
27	A	609	PHO	C2C-C3C-CAC-CBC
26	B	615	CLA	C10-C11-C12-C13
26	B	606	CLA	O1D-CGD-O2D-CED
34	l	101	LHG	C16-C17-C18-C19
30	t	103	STE	C7-C8-C9-C10
26	D	402	CLA	C16-C17-C18-C19
26	c	506	CLA	C16-C17-C18-C20
31	B	623	SQD	C45-C46-O48-C23
32	c	519	DGD	C4D-C5D-C6D-O5D
26	B	601	CLA	C4B-C3B-CAB-CBB
26	C	501	CLA	C4B-C3B-CAB-CBB
26	a	608	CLA	C4B-C3B-CAB-CBB
26	b	601	CLA	C4B-C3B-CAB-CBB
26	c	503	CLA	C1A-C2A-CAA-CBA
28	k	101	BCR	C21-C22-C23-C24
30	E	102	STE	C3-C4-C5-C6
32	c	520	DGD	CBA-CCA-CDA-CEA
33	D	407	LMG	C20-C21-C22-C23
33	b	622	LMG	C17-C18-C19-C20
33	C	517	LMG	C11-C12-C13-C14
30	I	102	STE	C7-C8-C9-C10
32	c	521	DGD	C8A-C9A-CAA-CBA
31	a	616	SQD	C10-C11-C12-C13
34	a	615	LHG	O6-C4-C5-C6
32	C	523	DGD	CCA-CDA-CEA-CFA
34	d	407	LHG	C32-C33-C34-C35
31	A	616	SQD	C8-C7-O47-C45
32	C	525	DGD	CBB-CCB-CDB-CEB
34	B	622	LHG	C30-C31-C32-C33
31	a	614	SQD	C5-C6-S-O9
31	a	616	SQD	C5-C6-S-O7
30	h	102	STE	C9-C10-C11-C12
34	d	408	LHG	C9-C10-C11-C12
26	B	602	CLA	C6-C7-C8-C10
26	B	605	CLA	C11-C10-C8-C7
26	B	608	CLA	C6-C7-C8-C10
26	B	614	CLA	C6-C7-C8-C10
26	B	616	CLA	C6-C7-C8-C10
26	C	505	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
26	C	508	CLA	C11-C10-C8-C7
26	C	512	CLA	C12-C13-C15-C16
26	c	512	CLA	C12-C13-C15-C16
30	M	102	STE	C10-C11-C12-C13
32	C	525	DGD	C7B-C8B-C9B-CAB
34	d	409	LHG	C31-C32-C33-C34
26	c	507	CLA	C16-C17-C18-C20
34	d	408	LHG	C32-C33-C34-C35
33	d	411	LMG	C15-C16-C17-C18
31	A	615	SQD	C29-C30-C31-C32
34	l	101	LHG	C29-C30-C31-C32
33	C	526	LMG	O10-C28-O8-C9
33	B	620	LMG	C20-C21-C22-C23
30	t	103	STE	C4-C5-C6-C7
32	H	102	DGD	CAB-CBB-CCB-CDB
33	c	522	LMG	C37-C38-C39-C40
34	B	622	LHG	C28-C29-C30-C31
26	c	507	CLA	C8-C10-C11-C12
30	T	103	STE	C4-C5-C6-C7
26	b	610	CLA	C2A-CAA-CBA-CGA
26	C	509	CLA	C14-C13-C15-C16
26	C	512	CLA	C11-C12-C13-C14
26	b	611	CLA	C14-C13-C15-C16
31	A	615	SQD	C31-C32-C33-C34
26	B	601	CLA	C8-C10-C11-C12
30	M	103	STE	C4-C5-C6-C7
26	A	608	CLA	C13-C15-C16-C17
26	C	513	CLA	C8-C10-C11-C12
30	d	412	STE	C10-C11-C12-C13
31	A	616	SQD	O5-C5-C6-S
34	B	622	LHG	C16-C17-C18-C19
30	T	103	STE	C7-C8-C9-C10
30	B	624	STE	C13-C14-C15-C16
31	b	620	SQD	O47-C45-C46-O48
33	C	517	LMG	O7-C8-C9-O8
33	C	522	LMG	O7-C8-C9-O8
33	b	622	LMG	O1-C7-C8-O7
32	A	617	DGD	CAA-CBA-CCA-CDA
31	F	102	SQD	C2-C1-O6-C44
26	c	505	CLA	C15-C16-C17-C18
30	k	103	STE	C2-C3-C4-C5
30	E	104	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	j	102	STE	C13-C14-C15-C16
33	D	406	LMG	O1-C7-C8-C9
33	a	618	LMG	O1-C7-C8-C9
33	a	618	LMG	C7-C8-C9-O8
33	c	518	LMG	C7-C8-C9-O8
33	c	523	LMG	C7-C8-C9-O8
32	C	523	DGD	C3A-C4A-C5A-C6A
31	B	623	SQD	C11-C12-C13-C14
30	C	528	STE	C3-C4-C5-C6
26	B	607	CLA	CAD-CBD-CGD-O2D
26	C	502	CLA	CAD-CBD-CGD-O2D
26	c	502	CLA	CAD-CBD-CGD-O2D
26	c	504	CLA	CAD-CBD-CGD-O2D
30	E	104	STE	C3-C4-C5-C6
26	b	603	CLA	C16-C17-C18-C20
30	C	519	STE	C4-C5-C6-C7
34	D	410	LHG	C11-C10-C9-C8
26	c	512	CLA	C15-C16-C17-C18
30	a	619	STE	C7-C8-C9-C10
30	E	102	STE	C5-C6-C7-C8
33	B	620	LMG	C13-C14-C15-C16
26	B	601	CLA	CAD-CBD-CGD-O1D
26	B	607	CLA	CAD-CBD-CGD-O1D
26	C	502	CLA	CAD-CBD-CGD-O1D
26	C	504	CLA	CAD-CBD-CGD-O1D
26	c	502	CLA	CAD-CBD-CGD-O1D
26	c	504	CLA	CAD-CBD-CGD-O1D
26	c	509	CLA	CHA-CBD-CGD-O1D
26	c	509	CLA	CHA-CBD-CGD-O2D
27	d	401	PHO	CHA-CBD-CGD-O2D
28	H	101	BCR	C9-C10-C11-C12
34	D	410	LHG	C3-O3-P-O6
34	E	101	LHG	C4-O6-P-O3
34	a	615	LHG	C3-O3-P-O4
34	d	408	LHG	C4-O6-P-O3
34	d	408	LHG	C4-O6-P-O5
26	c	513	CLA	C3-C5-C6-C7
34	B	622	LHG	C24-C25-C26-C27
30	A	619	STE	C10-C11-C12-C13
30	C	529	STE	C13-C14-C15-C16
26	C	503	CLA	C10-C11-C12-C13
26	b	601	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	b	620	SQD	O48-C23-C24-C25
34	D	409	LHG	C2-C3-O3-P
34	a	615	LHG	C2-C3-O3-P
30	e	104	STE	C4-C5-C6-C7
32	C	524	DGD	CAA-CBA-CCA-CDA
34	E	101	LHG	C34-C35-C36-C37
26	B	610	CLA	C16-C17-C18-C19
33	C	517	LMG	C28-C29-C30-C31
32	C	525	DGD	C2B-C3B-C4B-C5B
30	b	623	STE	C5-C6-C7-C8
33	a	617	LMG	C38-C39-C40-C41
29	A	612	PL9	C4-C3-C7-C8
30	b	621	STE	C4-C5-C6-C7
26	c	507	CLA	C16-C17-C18-C19
33	C	522	LMG	C9-C8-O7-C10
32	C	525	DGD	C9A-CAA-CBA-CCA
34	D	408	LHG	C11-C12-C13-C14
33	a	617	LMG	C30-C31-C32-C33
30	e	103	STE	C10-C11-C12-C13
28	C	514	BCR	C13-C14-C15-C16
26	B	601	CLA	C14-C13-C15-C16
26	C	505	CLA	C6-C7-C8-C9
26	C	508	CLA	C11-C10-C8-C9
26	c	508	CLA	C14-C13-C15-C16
26	B	601	CLA	C12-C13-C15-C16
30	A	619	STE	C6-C7-C8-C9
31	A	615	SQD	C16-C17-C18-C19
33	d	411	LMG	C33-C34-C35-C36
31	A	616	SQD	O49-C7-O47-C45
30	C	520	STE	C9-C10-C11-C12
26	c	511	CLA	CBA-CGA-O2A-C1
31	F	102	SQD	C24-C25-C26-C27
32	c	520	DGD	C2E-C1E-O5D-C6D
33	d	411	LMG	C39-C40-C41-C42
31	A	615	SQD	C10-C11-C12-C13
30	d	406	STE	C13-C14-C15-C16
30	z	101	STE	C3-C4-C5-C6
31	a	616	SQD	C33-C34-C35-C36
33	c	518	LMG	O7-C8-C9-O8
30	A	613	STE	C5-C6-C7-C8
32	C	523	DGD	C4A-C5A-C6A-C7A
33	a	617	LMG	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
26	d	403	CLA	C16-C17-C18-C19
30	C	520	STE	C11-C10-C9-C8
32	c	520	DGD	C3A-C4A-C5A-C6A
26	c	511	CLA	O1A-CGA-O2A-C1
26	c	509	CLA	CAA-CBA-CGA-O2A
26	C	506	CLA	C15-C16-C17-C18
26	B	601	CLA	CBD-CGD-O2D-CED
34	d	407	LHG	C12-C13-C14-C15
26	b	603	CLA	C16-C17-C18-C19
33	D	406	LMG	C35-C36-C37-C38
30	C	516	STE	C9-C10-C11-C12
30	A	618	STE	C14-C15-C16-C17
30	A	613	STE	C3-C4-C5-C6
28	k	101	BCR	C15-C16-C17-C18
33	m	101	LMG	C11-C12-C13-C14
34	B	622	LHG	C7-C8-C9-C10
32	C	525	DGD	CAA-CBA-CCA-CDA
32	c	521	DGD	CBA-CCA-CDA-CEA
26	C	506	CLA	C4-C3-C5-C6
26	c	512	CLA	C4-C3-C5-C6
33	C	517	LMG	C17-C18-C19-C20
31	F	102	SQD	C31-C32-C33-C34
30	f	102	STE	C13-C14-C15-C16
31	F	102	SQD	C33-C34-C35-C36
34	D	410	LHG	C1-C2-C3-O3
26	C	508	CLA	C16-C17-C18-C20
31	A	615	SQD	C23-C24-C25-C26
33	D	407	LMG	C28-C29-C30-C31
26	B	608	CLA	C6-C7-C8-C9
26	B	616	CLA	C6-C7-C8-C9
26	C	505	CLA	C14-C13-C15-C16
26	C	513	CLA	C14-C13-C15-C16
26	b	603	CLA	C11-C10-C8-C9
31	a	614	SQD	C16-C17-C18-C19
33	M	101	LMG	C30-C31-C32-C33
30	d	406	STE	C11-C10-C9-C8
34	d	407	LHG	C33-C34-C35-C36
31	f	101	SQD	C23-C24-C25-C26
26	b	608	CLA	C13-C15-C16-C17
29	d	405	PL9	C47-C48-C49-C51
34	D	409	LHG	C16-C17-C18-C19
30	b	624	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
32	H	102	DGD	C8A-C9A-CAA-CBA
26	A	608	CLA	C6-C7-C8-C10
26	B	613	CLA	C11-C10-C8-C7
26	C	505	CLA	C12-C13-C15-C16
26	C	511	CLA	C6-C7-C8-C10
26	c	505	CLA	C5-C6-C7-C8
26	c	505	CLA	C13-C15-C16-C17
30	C	516	STE	C5-C6-C7-C8
30	b	621	STE	C9-C10-C11-C12
34	l	101	LHG	C17-C18-C19-C20
30	D	412	STE	C10-C11-C12-C13
30	b	623	STE	C3-C4-C5-C6
30	t	103	STE	C1-C2-C3-C4
34	D	408	LHG	C18-C19-C20-C21
33	c	518	LMG	O8-C28-C29-C30
26	a	607	CLA	C16-C17-C18-C19
26	d	403	CLA	C16-C17-C18-C20
29	d	405	PL9	C45-C44-C46-C47
32	C	525	DGD	O6D-C5D-C6D-O5D
26	C	506	CLA	C2-C3-C5-C6
29	D	405	PL9	C32-C33-C34-C36
33	D	407	LMG	C19-C20-C21-C22
33	D	407	LMG	C35-C36-C37-C38
30	E	104	STE	C12-C13-C14-C15
30	I	101	STE	C3-C4-C5-C6
31	b	620	SQD	C11-C10-C9-C8
28	k	101	BCR	C37-C22-C23-C24
26	B	614	CLA	C13-C15-C16-C17
30	B	624	STE	C11-C10-C9-C8
26	C	513	CLA	C13-C15-C16-C17
26	B	601	CLA	C4-C3-C5-C6
26	c	509	CLA	C4-C3-C5-C6
30	Z	101	STE	C10-C11-C12-C13
26	B	601	CLA	C2A-CAA-CBA-CGA
30	d	412	STE	O2-C1-C2-C3
31	A	616	SQD	C17-C18-C19-C20
31	B	623	SQD	C17-C18-C19-C20
32	c	520	DGD	CBB-CCB-CDB-CEB
33	D	407	LMG	C36-C37-C38-C39
30	d	410	STE	O2-C1-C2-C3
26	A	614	CLA	C14-C13-C15-C16
26	B	604	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	B	605	CLA	C11-C10-C8-C9
26	C	502	CLA	C6-C7-C8-C9
26	C	507	CLA	C11-C10-C8-C9
26	C	511	CLA	C6-C7-C8-C9
26	C	512	CLA	C14-C13-C15-C16
26	c	507	CLA	C6-C7-C8-C9
31	f	101	SQD	C46-C45-O47-C7
33	a	617	LMG	C7-C8-O7-C10
33	a	617	LMG	C9-C8-O7-C10
31	B	623	SQD	C28-C29-C30-C31
33	m	101	LMG	C39-C40-C41-C42
31	F	102	SQD	O48-C23-C24-C25
26	c	509	CLA	C2-C3-C5-C6
26	c	512	CLA	C2-C3-C5-C6
34	D	408	LHG	C34-C35-C36-C37
30	d	412	STE	O1-C1-C2-C3
26	C	501	CLA	C2A-CAA-CBA-CGA
26	B	601	CLA	O1D-CGD-O2D-CED
33	D	407	LMG	C33-C34-C35-C36
26	b	601	CLA	C16-C17-C18-C19
26	c	506	CLA	C16-C17-C18-C19
30	E	104	STE	O2-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O1D
30	T	102	STE	C10-C11-C12-C13
34	E	101	LHG	C10-C11-C12-C13
26	B	601	CLA	C2B-C3B-CAB-CBB
26	C	501	CLA	C2B-C3B-CAB-CBB
28	B	617	BCR	C5-C6-C7-C8
28	C	521	BCR	C23-C24-C25-C30
28	b	617	BCR	C5-C6-C7-C8
28	t	101	BCR	C5-C6-C7-C8
30	E	104	STE	O1-C1-C2-C3
26	B	615	CLA	C13-C15-C16-C17
33	c	522	LMG	C34-C35-C36-C37
26	C	511	CLA	C8-C10-C11-C12
31	A	616	SQD	C12-C13-C14-C15
32	H	102	DGD	O1B-C1B-C2B-C3B
31	b	620	SQD	C15-C16-C17-C18
30	D	412	STE	C14-C15-C16-C17
35	e	102	HEM	CAD-CBD-CGD-O1D
26	B	604	CLA	C11-C10-C8-C7
26	B	611	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	C	506	CLA	C12-C13-C15-C16
26	b	602	CLA	C11-C10-C8-C7
26	b	606	CLA	C11-C10-C8-C7
26	b	610	CLA	C12-C13-C15-C16
26	c	507	CLA	C11-C10-C8-C7
26	A	614	CLA	C16-C17-C18-C19
26	B	610	CLA	C2A-CAA-CBA-CGA
34	D	409	LHG	C17-C18-C19-C20
30	d	410	STE	O1-C1-C2-C3
30	B	621	STE	C10-C11-C12-C13
33	C	526	LMG	C33-C34-C35-C36
30	I	101	STE	O2-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O2D
33	c	522	LMG	C33-C34-C35-C36
30	I	101	STE	O1-C1-C2-C3
26	B	601	CLA	C2-C3-C5-C6
26	b	614	CLA	C2-C3-C5-C6
32	h	101	DGD	CCA-CDA-CEA-CFA
26	A	607	CLA	C2C-C3C-CAC-CBC
36	V	201	HEC	CAD-CBD-CGD-O1D
32	c	519	DGD	CDA-CEA-CFA-CGA
30	b	621	STE	C7-C8-C9-C10
30	C	528	STE	C7-C8-C9-C10
26	B	602	CLA	C15-C16-C17-C18
26	B	611	CLA	C16-C17-C18-C20
26	C	502	CLA	C16-C17-C18-C19
30	a	620	STE	C4-C5-C6-C7
33	b	622	LMG	C24-C25-C26-C27
30	d	406	STE	C15-C16-C17-C18
30	m	102	STE	C5-C6-C7-C8
29	A	612	PL9	C15-C14-C16-C17
26	C	513	CLA	C2-C3-C5-C6
29	a	612	PL9	C28-C29-C31-C32
31	a	616	SQD	C32-C33-C34-C35
26	b	610	CLA	C8-C10-C11-C12
26	c	503	CLA	C5-C6-C7-C8
26	c	506	CLA	C10-C11-C12-C13
32	C	524	DGD	CDA-CEA-CFA-CGA
31	a	614	SQD	C44-C45-C46-O48
34	E	101	LHG	C4-C5-C6-O8
30	C	516	STE	O2-C1-C2-C3
35	e	102	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	j	102	STE	C9-C10-C11-C12
26	c	501	CLA	C2A-CAA-CBA-CGA
26	c	504	CLA	C10-C11-C12-C13
33	c	522	LMG	C31-C32-C33-C34
30	J	101	STE	O2-C1-C2-C3
31	a	616	SQD	C7-C8-C9-C10
30	B	625	STE	O2-C1-C2-C3
30	i	101	STE	O2-C1-C2-C3
31	B	623	SQD	C34-C35-C36-C37
26	a	613	CLA	C2C-C3C-CAC-CBC
34	l	101	LHG	C15-C16-C17-C18
31	A	616	SQD	C14-C15-C16-C17
26	B	604	CLA	O1A-CGA-O2A-C1
26	C	508	CLA	C16-C17-C18-C19
32	c	519	DGD	CDB-CEB-CFB-CGB
30	C	529	STE	C11-C10-C9-C8
30	C	520	STE	C3-C4-C5-C6
35	F	101	HEM	CAD-CBD-CGD-O2D
31	B	623	SQD	C15-C16-C17-C18
26	c	513	CLA	C16-C17-C18-C19
30	d	412	STE	C9-C10-C11-C12
33	m	101	LMG	C32-C33-C34-C35
36	v	201	HEC	CAD-CBD-CGD-O2D
33	c	522	LMG	C29-C30-C31-C32
33	c	522	LMG	C35-C36-C37-C38
33	d	411	LMG	C11-C12-C13-C14
26	d	403	CLA	C10-C11-C12-C13
30	Z	101	STE	C7-C8-C9-C10
30	T	102	STE	C9-C10-C11-C12
33	D	407	LMG	C12-C13-C14-C15
30	C	516	STE	O1-C1-C2-C3
30	d	406	STE	O1-C1-C2-C3
36	v	201	HEC	CAD-CBD-CGD-O1D
26	d	403	CLA	C14-C13-C15-C16
30	H	103	STE	C9-C10-C11-C12
26	D	402	CLA	C2-C1-O2A-CGA
26	a	607	CLA	C16-C17-C18-C20
26	b	611	CLA	C16-C17-C18-C20
30	M	103	STE	C7-C8-C9-C10
32	C	523	DGD	CDB-CEB-CFB-CGB
30	C	519	STE	C3-C4-C5-C6
30	M	102	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
26	b	608	CLA	C4C-C3C-CAC-CBC
32	H	102	DGD	C1A-C2A-C3A-C4A
31	F	102	SQD	C29-C30-C31-C32
26	b	607	CLA	C16-C17-C18-C20
26	B	604	CLA	CBA-CGA-O2A-C1
26	C	512	CLA	O2A-C1-C2-C3
33	d	411	LMG	C34-C35-C36-C37
30	e	101	STE	C12-C13-C14-C15
33	a	618	LMG	C13-C14-C15-C16
30	J	101	STE	O1-C1-C2-C3
30	i	101	STE	O1-C1-C2-C3
30	B	624	STE	C10-C11-C12-C13
30	e	104	STE	C6-C7-C8-C9
26	B	614	CLA	C2A-CAA-CBA-CGA
31	F	102	SQD	C44-C45-C46-O48
30	c	517	STE	C5-C6-C7-C8
34	E	101	LHG	C24-C23-O8-C6
26	c	512	CLA	C10-C11-C12-C13
26	b	602	CLA	C16-C17-C18-C19
30	d	412	STE	C11-C10-C9-C8
30	B	625	STE	O1-C1-C2-C3
30	k	103	STE	C9-C10-C11-C12
32	H	102	DGD	C9B-CAB-CBB-CCB
32	c	519	DGD	CBA-CCA-CDA-CEA
32	c	520	DGD	O6E-C1E-O5D-C6D
33	m	101	LMG	C35-C36-C37-C38
33	C	522	LMG	C7-C8-C9-O8
30	M	102	STE	O1-C1-C2-C3
30	D	411	STE	C1-C2-C3-C4
33	a	618	LMG	C29-C30-C31-C32
34	E	101	LHG	C24-C25-C26-C27
30	E	103	STE	C10-C11-C12-C13
26	b	608	CLA	C2C-C3C-CAC-CBC
30	B	621	STE	C2-C3-C4-C5
30	c	517	STE	C14-C15-C16-C17
32	C	523	DGD	C9B-CAB-CBB-CCB
32	c	520	DGD	C5A-C6A-C7A-C8A
33	a	617	LMG	C18-C19-C20-C21
34	D	408	LHG	C13-C14-C15-C16
32	c	521	DGD	O6D-C5D-C6D-O5D
30	h	102	STE	C11-C12-C13-C14
34	E	101	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	O10-C23-O8-C6
30	Z	101	STE	C9-C10-C11-C12
26	C	501	CLA	C14-C13-C15-C16
26	d	403	CLA	C11-C12-C13-C14
26	B	612	CLA	CAA-CBA-CGA-O2A
32	c	521	DGD	C9B-CAB-CBB-CCB
33	C	522	LMG	C37-C38-C39-C40
30	d	406	STE	O2-C1-C2-C3
26	a	613	CLA	C4C-C3C-CAC-CBC
26	B	608	CLA	C16-C17-C18-C19
26	C	507	CLA	C11-C12-C13-C15
26	a	608	CLA	C12-C13-C15-C16
26	b	603	CLA	C12-C13-C15-C16
26	b	607	CLA	C11-C10-C8-C7
26	c	513	CLA	C11-C10-C8-C7
26	d	403	CLA	C12-C13-C15-C16
33	D	406	LMG	O6-C5-C6-O5
26	A	607	CLA	C2B-C3B-CAB-CBB
26	B	612	CLA	C2B-C3B-CAB-CBB
26	C	502	CLA	C2B-C3B-CAB-CBB
26	D	403	CLA	C2B-C3B-CAB-CBB
26	b	606	CLA	C2B-C3B-CAB-CBB
26	d	403	CLA	C2B-C3B-CAB-CBB
28	D	404	BCR	C23-C24-C25-C26
28	T	101	BCR	C5-C6-C7-C8
28	a	611	BCR	C5-C6-C7-C8
26	B	613	CLA	C2-C1-O2A-CGA
31	a	616	SQD	C16-C17-C18-C19
33	c	523	LMG	C16-C17-C18-C19
26	c	504	CLA	O1D-CGD-O2D-CED
32	C	524	DGD	O6E-C1E-O5D-C6D
34	a	615	LHG	C17-C18-C19-C20
26	A	614	CLA	C16-C17-C18-C20
29	A	612	PL9	C45-C44-C46-C47
31	a	614	SQD	O47-C7-C8-C9
32	A	617	DGD	CEA-CFA-CGA-CHA
33	c	522	LMG	C11-C12-C13-C14
33	a	617	LMG	C41-C42-C43-C44
26	B	613	CLA	CAA-CBA-CGA-O2A
30	E	104	STE	C13-C14-C15-C16
30	c	517	STE	C11-C12-C13-C14
33	M	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
30	b	624	STE	C4-C5-C6-C7
33	B	620	LMG	O7-C10-C11-C12
31	B	623	SQD	O47-C7-C8-C9
33	c	522	LMG	C13-C14-C15-C16
26	C	507	CLA	C11-C12-C13-C14
26	c	512	CLA	C14-C13-C15-C16
26	c	510	CLA	CAA-CBA-CGA-O2A
30	C	527	STE	C5-C6-C7-C8
33	a	617	LMG	C21-C22-C23-C24
36	V	201	HEC	C2B-C3B-CAB-CBB
26	C	513	CLA	C1A-C2A-CAA-CBA
30	d	410	STE	C10-C11-C12-C13
26	C	507	CLA	C4-C3-C5-C6
26	c	513	CLA	C4-C3-C5-C6
32	C	523	DGD	O6E-C1E-O5D-C6D
32	c	519	DGD	O6E-C1E-O5D-C6D
28	D	404	BCR	C7-C8-C9-C10
28	T	101	BCR	C15-C16-C17-C18
28	k	101	BCR	C19-C20-C21-C22
33	a	618	LMG	C15-C16-C17-C18
26	A	608	CLA	C16-C17-C18-C20
30	E	103	STE	C11-C10-C9-C8
26	B	606	CLA	CBD-CGD-O2D-CED
33	c	522	LMG	C14-C15-C16-C17
26	B	613	CLA	C5-C6-C7-C8
33	b	622	LMG	C23-C24-C25-C26
34	E	101	LHG	C27-C28-C29-C30
26	d	402	CLA	C2-C1-O2A-CGA
26	A	608	CLA	C12-C13-C15-C16
26	B	601	CLA	C11-C12-C13-C15
26	B	615	CLA	C12-C13-C15-C16
26	b	608	CLA	C11-C12-C13-C15
29	d	405	PL9	C43-C44-C46-C47
27	a	609	PHO	O2A-C1-C2-C3
33	B	620	LMG	C9-C8-O7-C10
26	c	509	CLA	CBD-CGD-O2D-CED
30	a	620	STE	C2-C3-C4-C5
30	d	406	STE	C7-C8-C9-C10
32	C	525	DGD	C4A-C5A-C6A-C7A
26	b	614	CLA	C2A-CAA-CBA-CGA
26	B	607	CLA	C16-C17-C18-C19
34	E	101	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	a	610	CLA	C13-C15-C16-C17
26	C	512	CLA	C4-C3-C5-C6
31	a	614	SQD	O49-C7-C8-C9
30	d	410	STE	C9-C10-C11-C12
26	B	612	CLA	C8-C10-C11-C12
26	b	611	CLA	C13-C15-C16-C17
31	b	620	SQD	C27-C28-C29-C30
32	c	519	DGD	C5B-C6B-C7B-C8B
33	B	620	LMG	O9-C10-C11-C12
26	B	612	CLA	CBA-CGA-O2A-C1
32	C	524	DGD	C1B-C2B-C3B-C4B
26	b	603	CLA	C2A-CAA-CBA-CGA
30	M	102	STE	O2-C1-C2-C3
26	b	606	CLA	C11-C10-C8-C9
26	c	502	CLA	C11-C12-C13-C14
26	c	507	CLA	C11-C10-C8-C9
26	d	402	CLA	C11-C12-C13-C14
26	B	612	CLA	CAA-CBA-CGA-O1A
30	m	103	STE	C11-C10-C9-C8
30	I	102	STE	C4-C5-C6-C7
26	b	612	CLA	CAA-CBA-CGA-O2A
26	b	613	CLA	CAA-CBA-CGA-O2A
26	D	403	CLA	O1D-CGD-O2D-CED
26	C	511	CLA	O1A-CGA-O2A-C1
30	A	618	STE	C12-C13-C14-C15
26	B	601	CLA	C13-C15-C16-C17
26	B	613	CLA	CAA-CBA-CGA-O1A
31	B	623	SQD	O49-C7-C8-C9
33	D	406	LMG	C8-C7-O1-C1
33	b	622	LMG	C8-C7-O1-C1
33	m	101	LMG	C8-C7-O1-C1
32	C	524	DGD	C2A-C3A-C4A-C5A
26	D	403	CLA	CBD-CGD-O2D-CED
30	i	102	STE	C7-C8-C9-C10
31	A	616	SQD	O47-C7-C8-C9
33	C	522	LMG	C34-C35-C36-C37
26	B	601	CLA	CAD-CBD-CGD-O2D
26	C	504	CLA	CAD-CBD-CGD-O2D
26	C	509	CLA	CAD-CBD-CGD-O2D
26	c	501	CLA	CAD-CBD-CGD-O2D
26	B	604	CLA	C2C-C3C-CAC-CBC
26	C	513	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	A	607	CLA	C4C-C3C-CAC-CBC
26	B	612	CLA	O1A-CGA-O2A-C1
31	A	615	SQD	C15-C16-C17-C18
30	b	624	STE	C1-C2-C3-C4
34	d	407	LHG	C27-C28-C29-C30
26	b	613	CLA	CAA-CBA-CGA-O1A
33	c	518	LMG	O1-C7-C8-C9
26	B	615	CLA	C16-C17-C18-C20
26	c	513	CLA	C16-C17-C18-C20
33	C	522	LMG	C11-C12-C13-C14
31	a	614	SQD	C35-C36-C37-C38
32	c	520	DGD	CDB-CEB-CFB-CGB
34	B	622	LHG	C18-C19-C20-C21
26	C	511	CLA	CBA-CGA-O2A-C1
32	C	523	DGD	O2G-C1B-C2B-C3B
33	a	617	LMG	O7-C10-C11-C12
34	D	409	LHG	C9-C10-C11-C12
26	C	505	CLA	C16-C17-C18-C19
32	c	519	DGD	O1G-C1A-C2A-C3A
26	c	510	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

141 monomers are involved in 230 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	c	519	DGD	1	0
26	c	503	CLA	2	0
21	A	601[B]	OEY	1	0
28	B	619	BCR	1	0
30	B	624	STE	3	0
26	b	601	CLA	3	0
30	C	528	STE	2	0
26	c	509	CLA	1	0
30	A	620	STE	2	0
29	D	405	PL9	1	0
28	C	521	BCR	2	0
32	C	525	DGD	1	0
26	b	606	CLA	1	0
34	B	622	LHG	2	0
33	c	523	LMG	3	0
29	d	405	PL9	1	0
26	A	608	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	c	520	DGD	1	0
35	F	101	HEM	1	0
26	b	602	CLA	3	0
35	e	102	HEM	2	0
36	v	201	HEC	1	0
31	a	614	SQD	3	0
29	A	612	PL9	6	0
26	C	506	CLA	2	0
26	B	615	CLA	2	0
33	a	617	LMG	5	0
34	D	408	LHG	1	0
33	C	522	LMG	2	0
28	d	404	BCR	1	0
26	b	608	CLA	1	0
26	B	604	CLA	3	0
33	M	101	LMG	2	0
33	m	101	LMG	3	0
33	B	620	LMG	5	0
30	T	102	STE	3	0
26	B	605	CLA	3	0
30	b	625	STE	1	0
26	c	512	CLA	1	0
30	a	619	STE	1	0
26	A	614	CLA	3	0
30	H	103	STE	4	0
26	c	507	CLA	1	0
30	C	529	STE	1	0
30	e	104	STE	1	0
34	E	101	LHG	1	0
26	a	607	CLA	3	0
31	a	616	SQD	1	0
26	b	603	CLA	2	0
28	c	514	BCR	1	0
26	C	502	CLA	1	0
26	d	402	CLA	2	0
26	a	608	CLA	1	0
26	a	613	CLA	1	0
26	C	512	CLA	2	0
26	b	613	CLA	1	0
30	C	516	STE	1	0
26	a	610	CLA	1	0
33	b	622	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	i	101	STE	1	0
26	c	501	CLA	3	0
26	B	611	CLA	1	0
26	D	402	CLA	3	0
26	b	615	CLA	2	0
26	C	507	CLA	1	0
31	f	101	SQD	2	0
30	A	619	STE	3	0
26	b	609	CLA	2	0
28	b	619	BCR	1	0
32	h	101	DGD	1	0
26	A	607	CLA	6	0
28	D	404	BCR	1	0
34	D	409	LHG	2	0
26	B	612	CLA	2	0
26	C	508	CLA	4	0
26	B	613	CLA	4	0
26	C	511	CLA	1	0
30	h	102	STE	1	0
26	B	610	CLA	3	0
32	C	524	DGD	2	0
26	d	403	CLA	2	0
28	T	101	BCR	3	0
28	k	101	BCR	1	0
26	c	510	CLA	3	0
30	m	103	STE	1	0
33	c	518	LMG	2	0
26	B	614	CLA	7	0
30	D	411	STE	4	0
26	C	513	CLA	1	0
26	C	505	CLA	2	0
26	B	601	CLA	2	0
30	d	410	STE	2	0
26	c	506	CLA	1	0
28	C	514	BCR	1	0
26	B	616	CLA	2	0
34	D	410	LHG	4	0
26	c	511	CLA	4	0
28	b	618	BCR	2	0
26	B	603	CLA	1	0
33	a	618	LMG	1	0
26	b	610	CLA	2	0

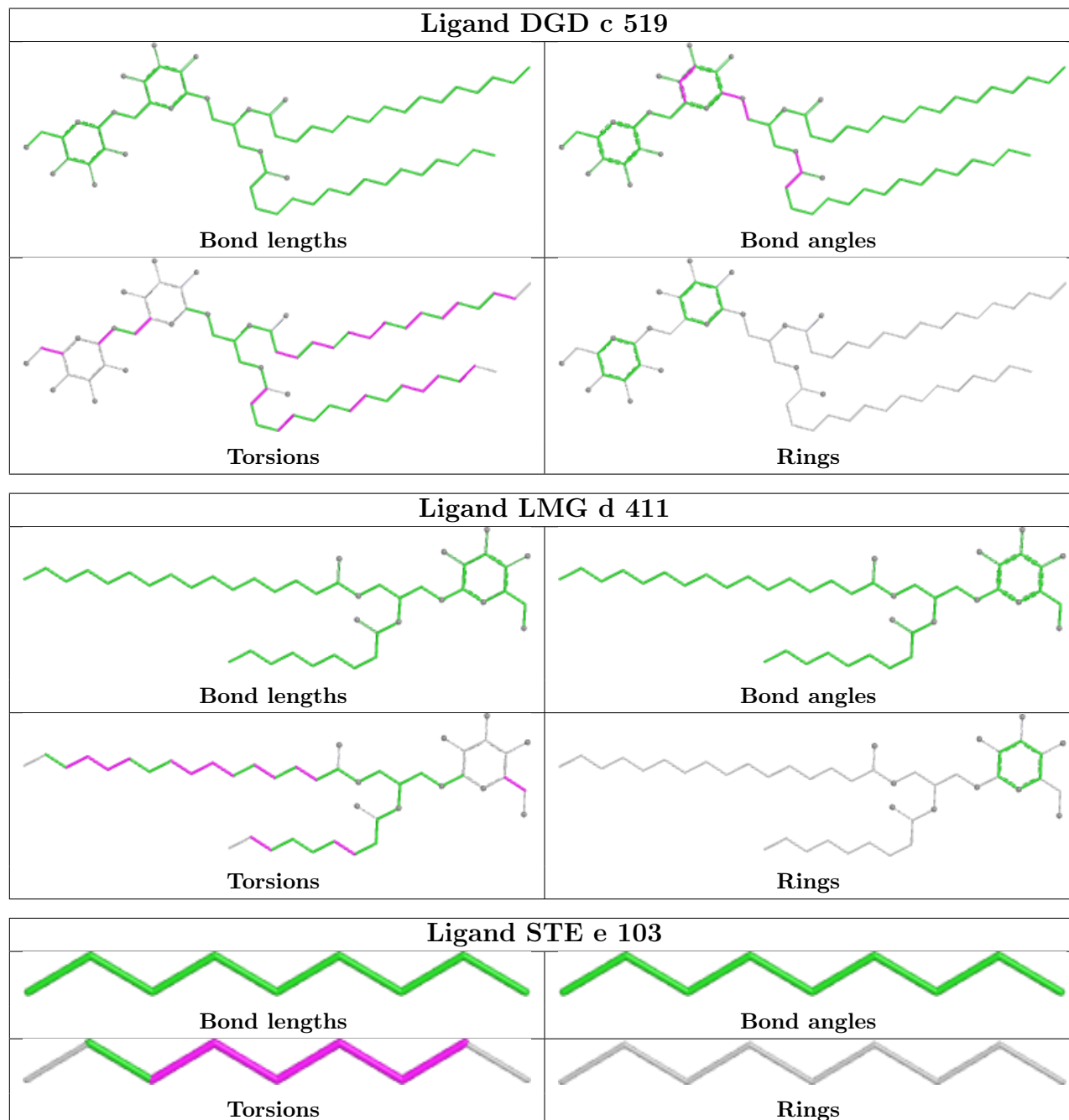
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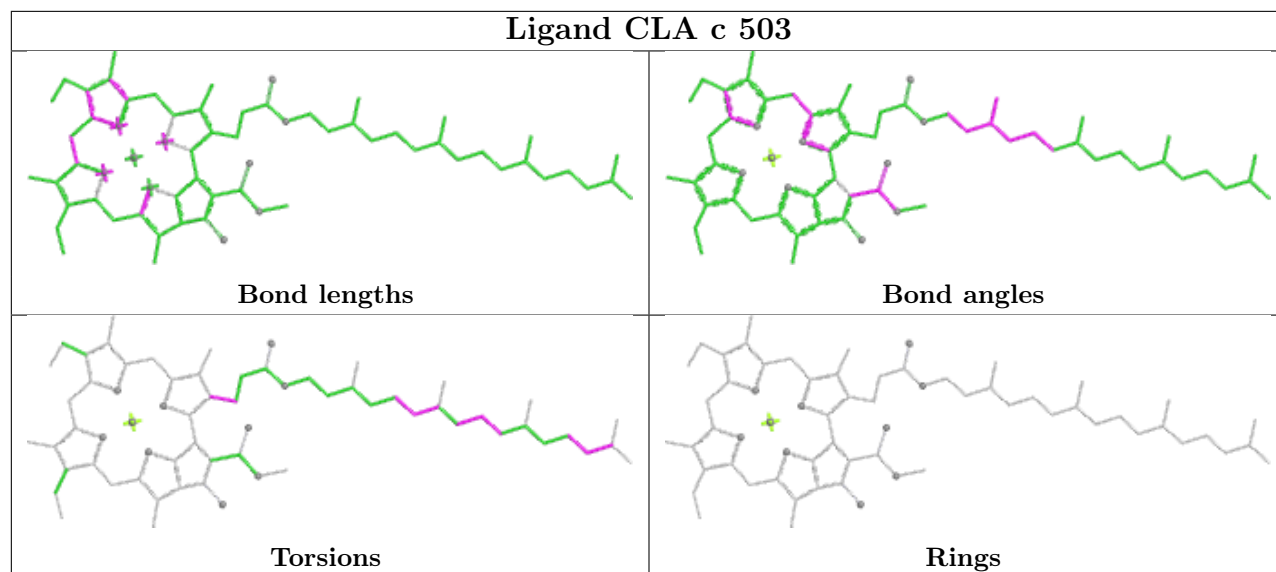
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	c	521	DGD	1	0
30	b	621	STE	1	0
32	A	617	DGD	2	0
30	T	103	STE	1	0
30	E	104	STE	3	0
28	B	618	BCR	1	0
26	A	610	CLA	1	0
34	d	407	LHG	1	0
26	c	505	CLA	1	0
28	a	611	BCR	1	0
30	I	102	STE	1	0
30	d	406	STE	1	0
30	j	102	STE	1	0
30	z	101	STE	2	0
32	H	102	DGD	2	0
28	C	515	BCR	2	0
30	k	103	STE	2	0
30	E	103	STE	2	0
26	B	609	CLA	2	0
27	D	401	PHO	2	0
31	B	623	SQD	4	0
26	B	602	CLA	1	0
28	b	617	BCR	1	0
30	a	620	STE	1	0
33	D	407	LMG	2	0
28	H	101	BCR	2	0
28	k	102	BCR	1	0
26	C	504	CLA	1	0
28	t	101	BCR	3	0
33	C	526	LMG	1	0
33	D	406	LMG	4	0
26	b	612	CLA	2	0
26	b	604	CLA	3	0
26	c	508	CLA	1	0
29	a	612	PL9	3	0
26	C	509	CLA	1	0
26	b	616	CLA	3	0
28	x	101	BCR	3	0
34	a	615	LHG	2	0
30	Z	101	STE	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

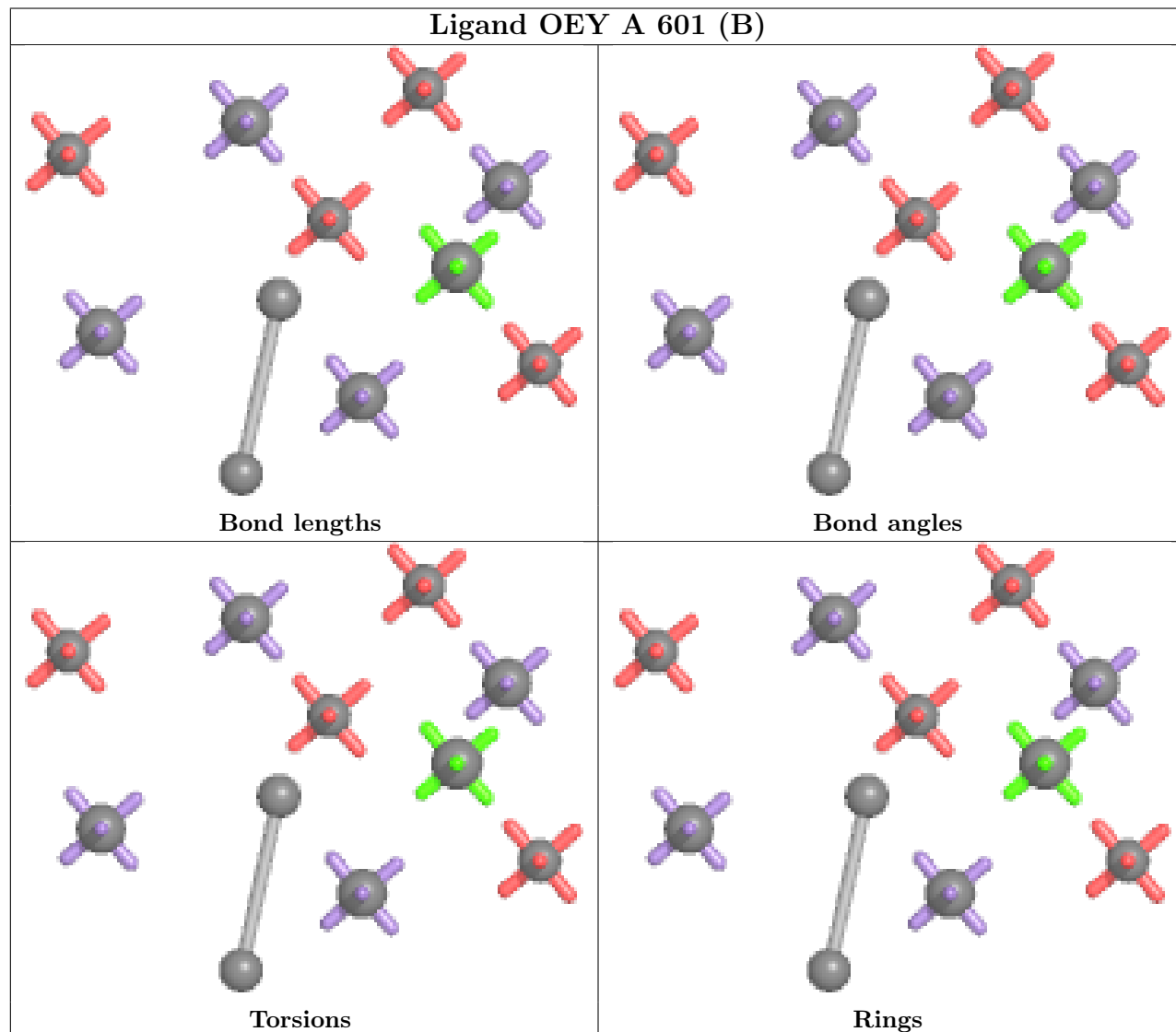
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

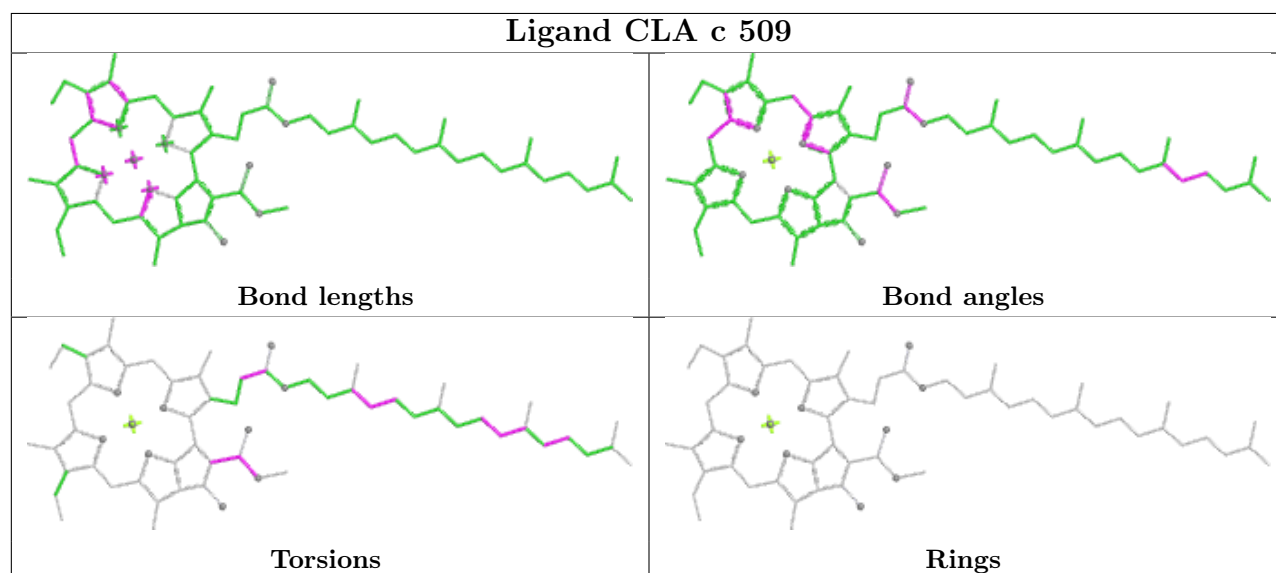
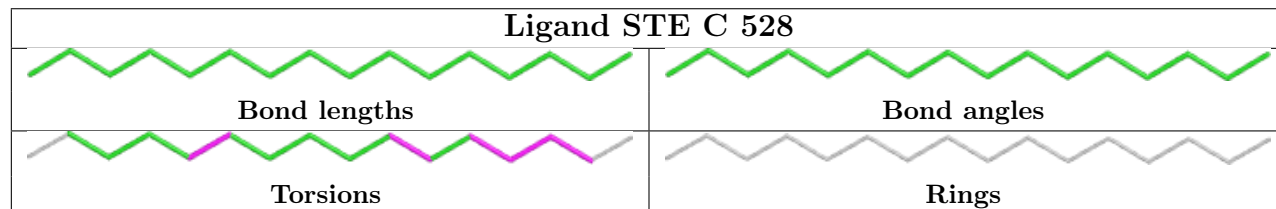
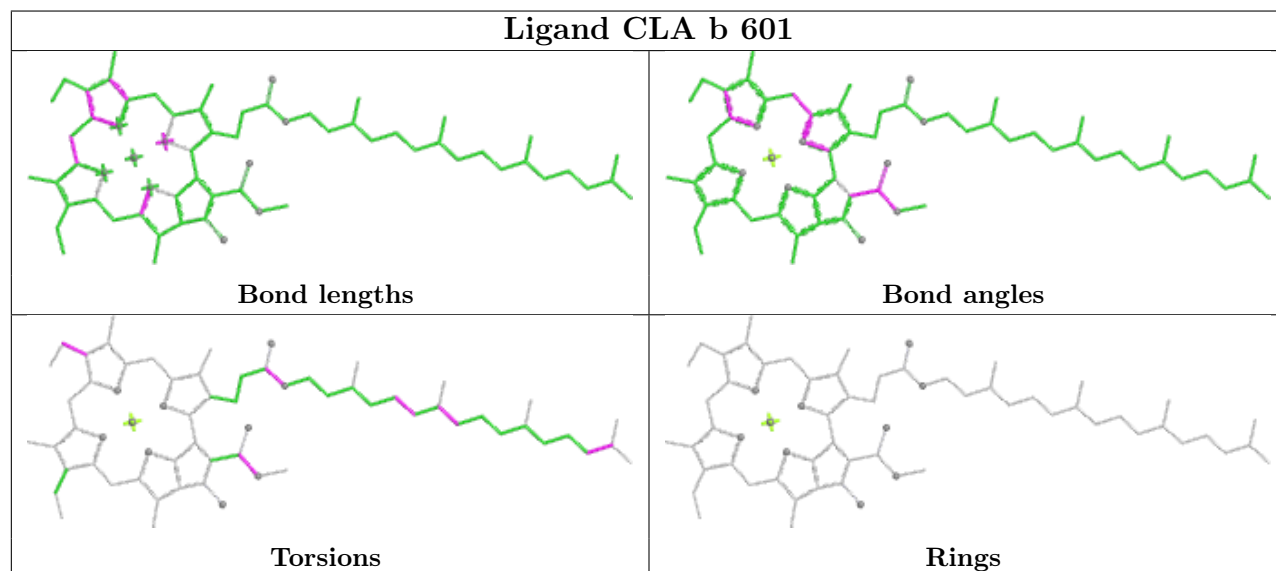
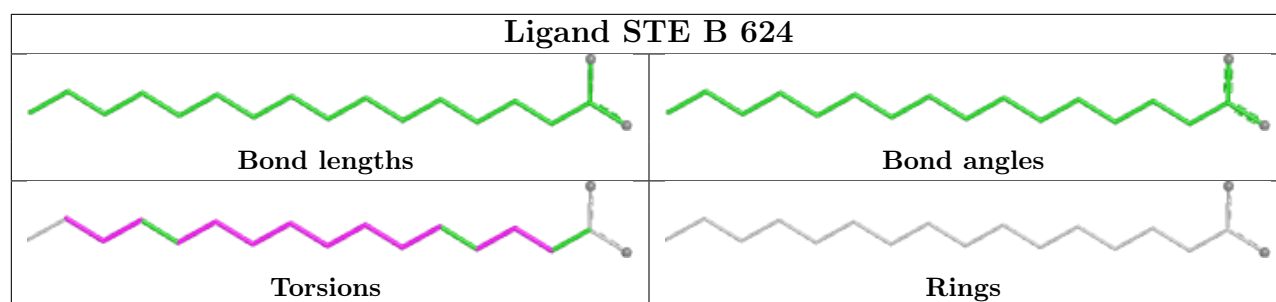


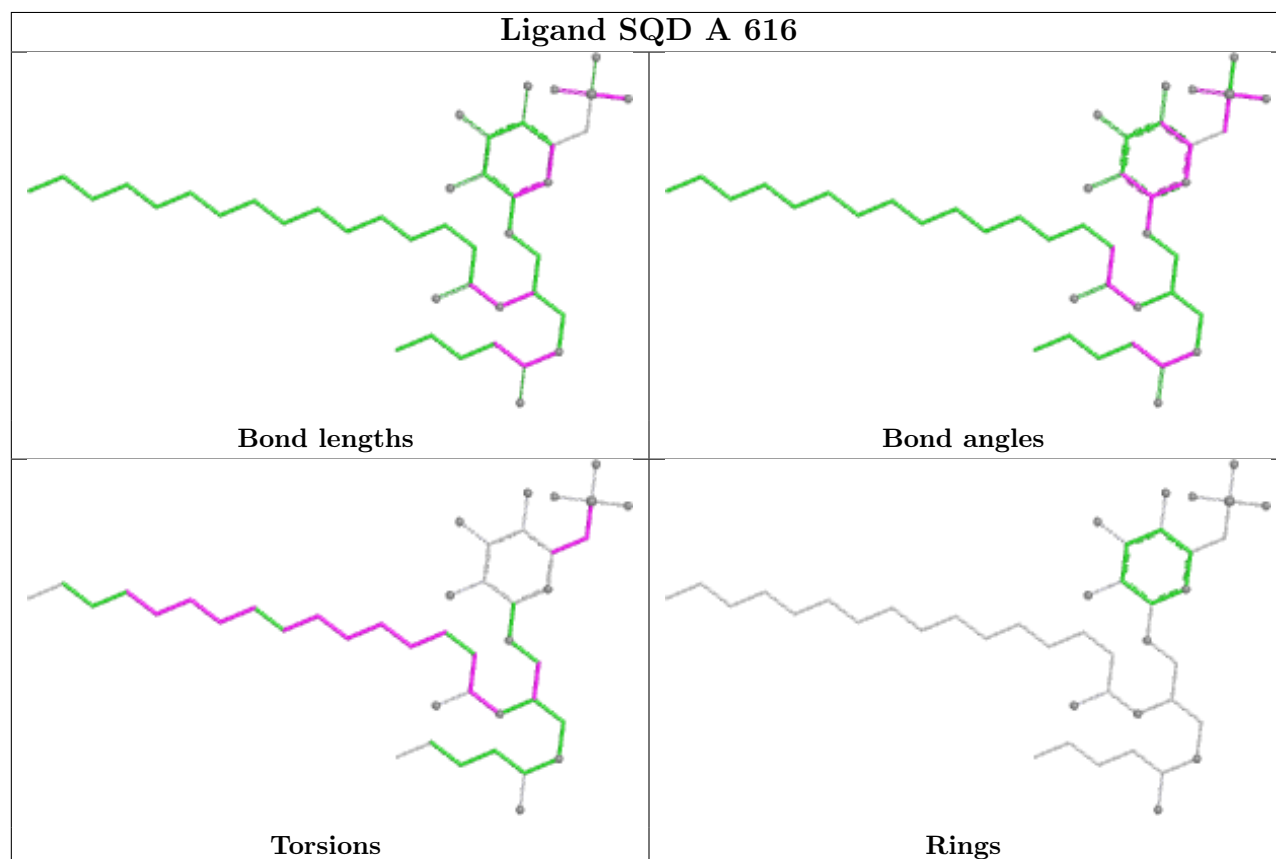
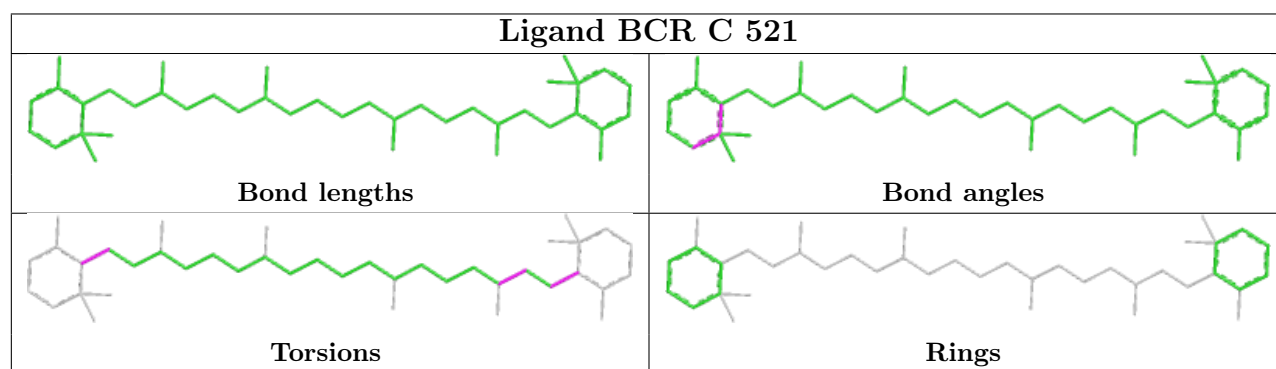
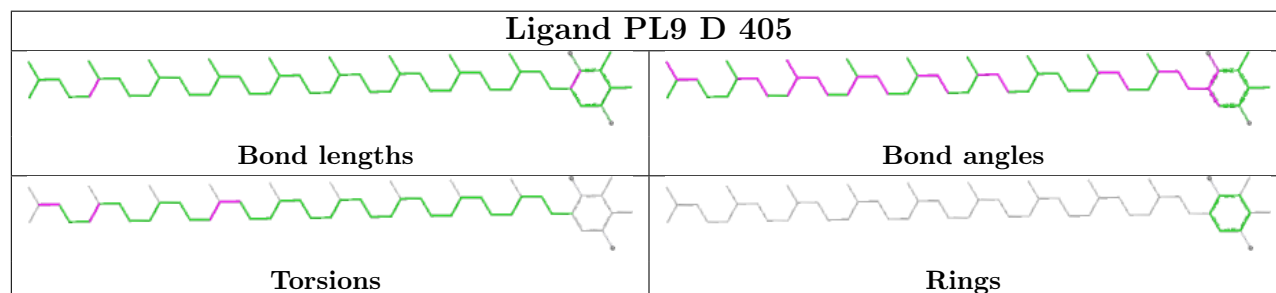
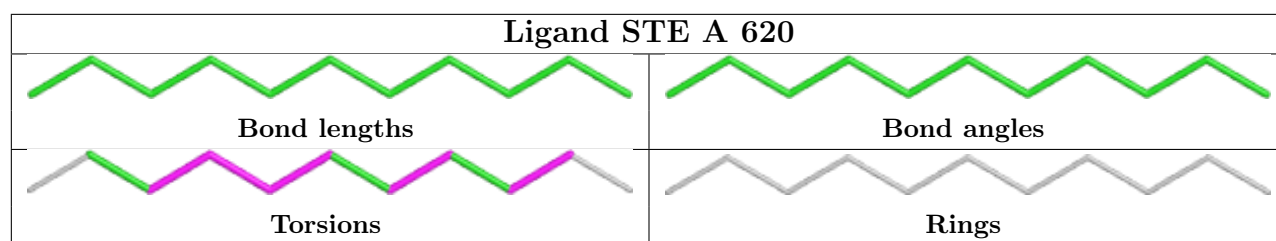
Ligand CLA c 503

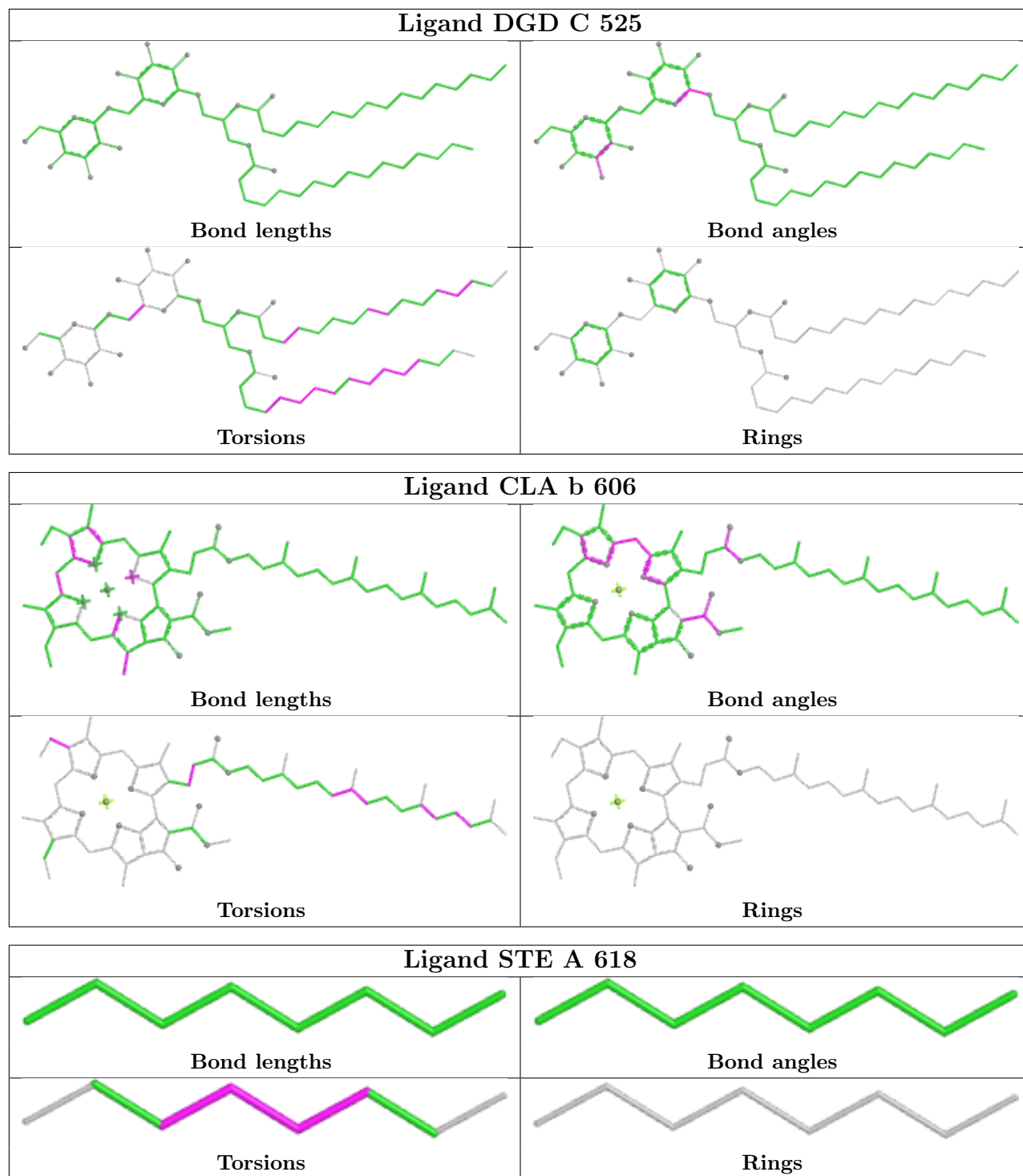


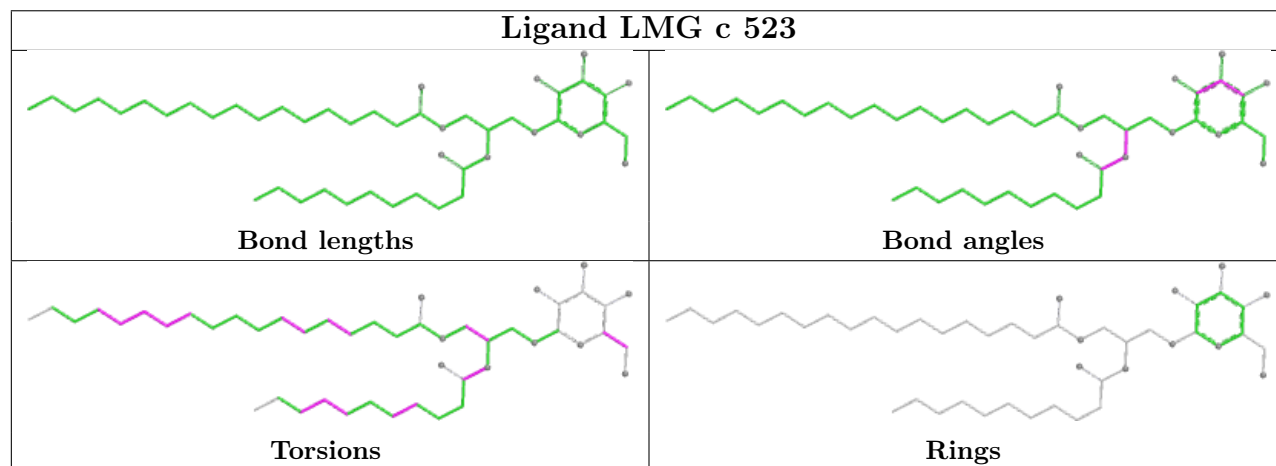
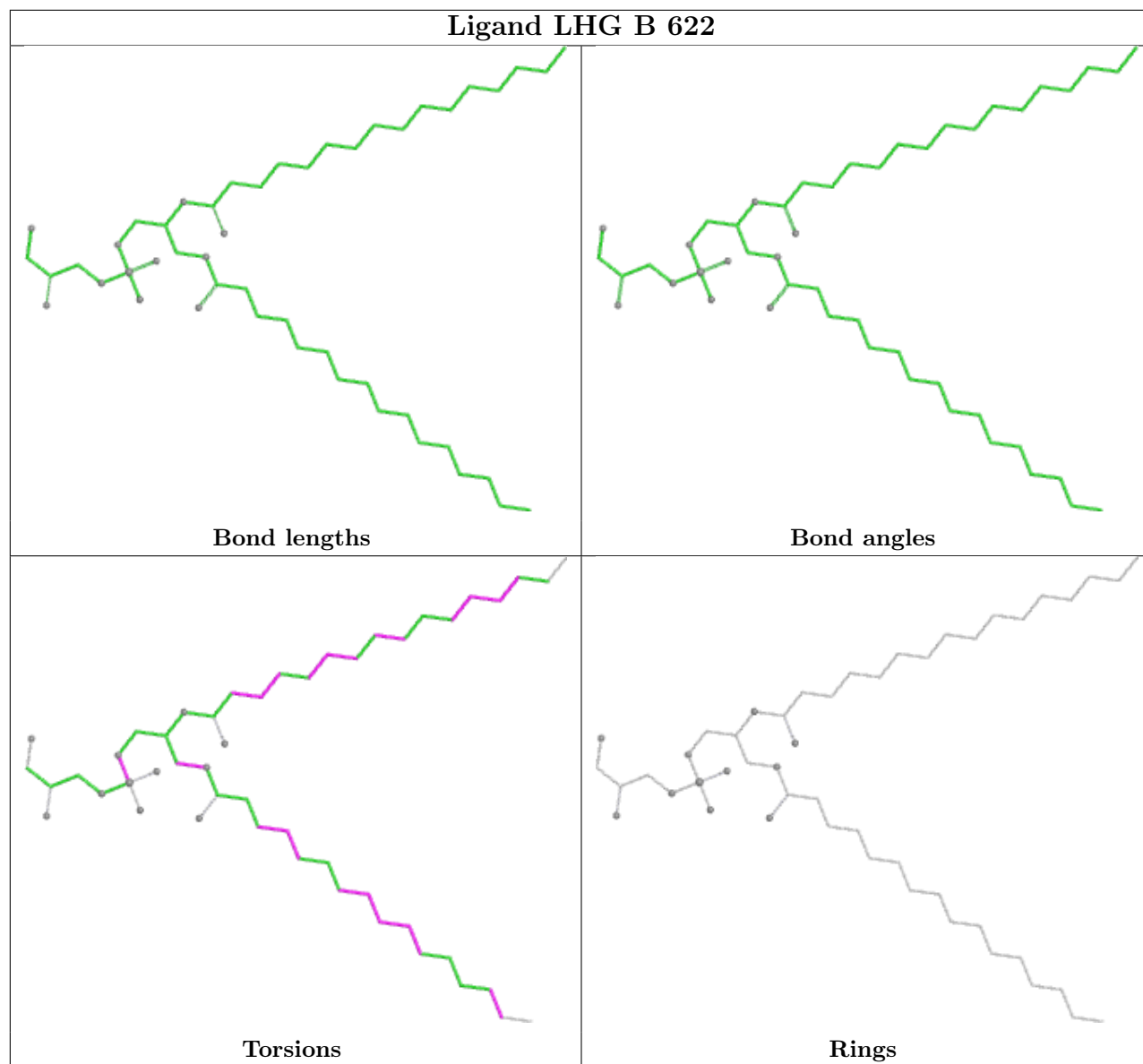
Ligand OEY A 601 (B)

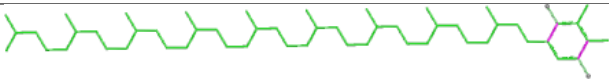
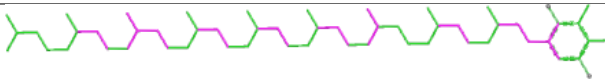
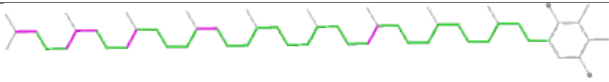
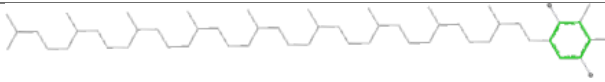


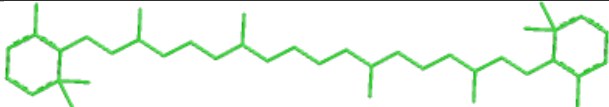
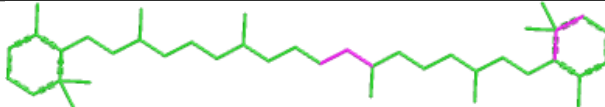
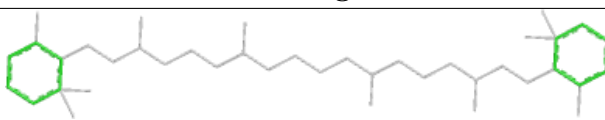


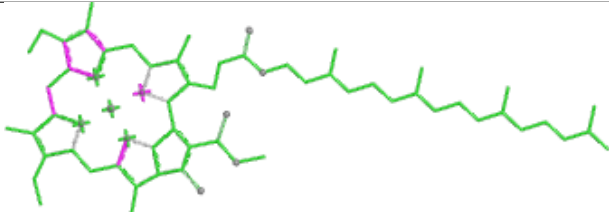
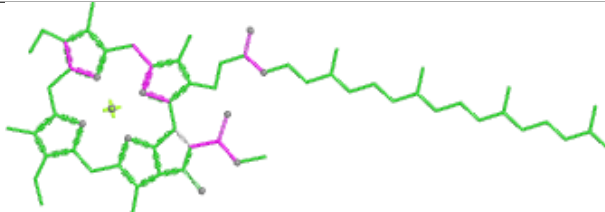
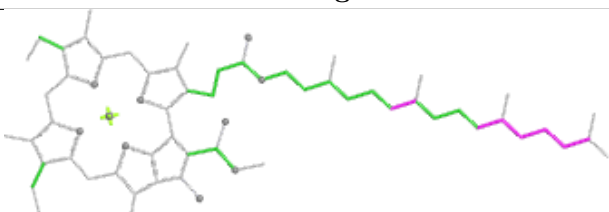
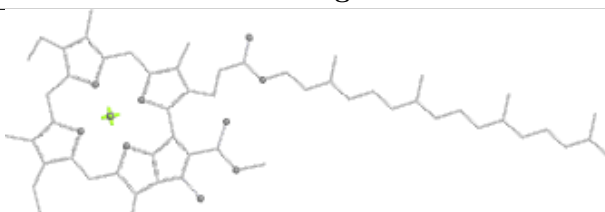




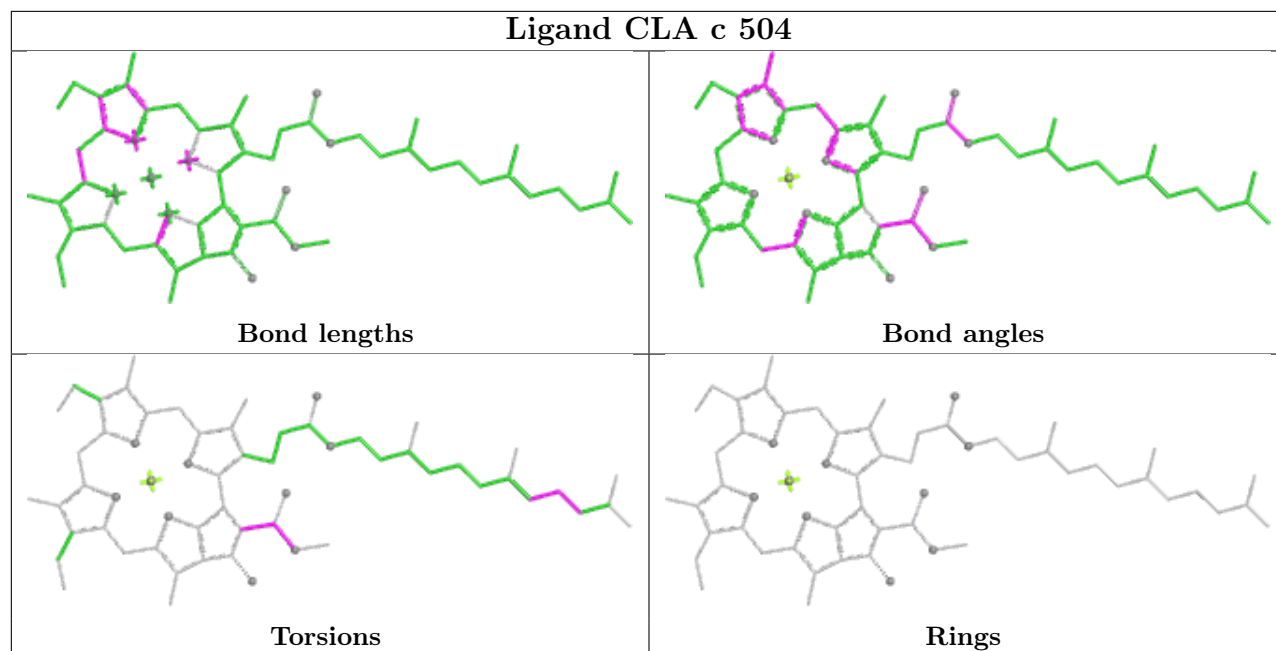


Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

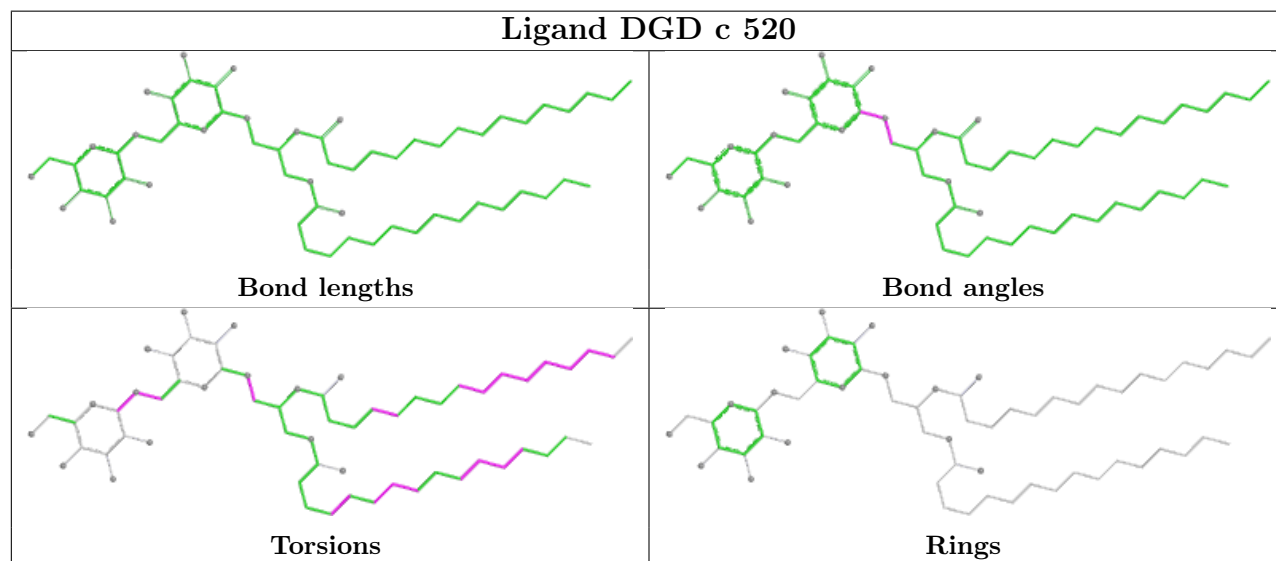
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

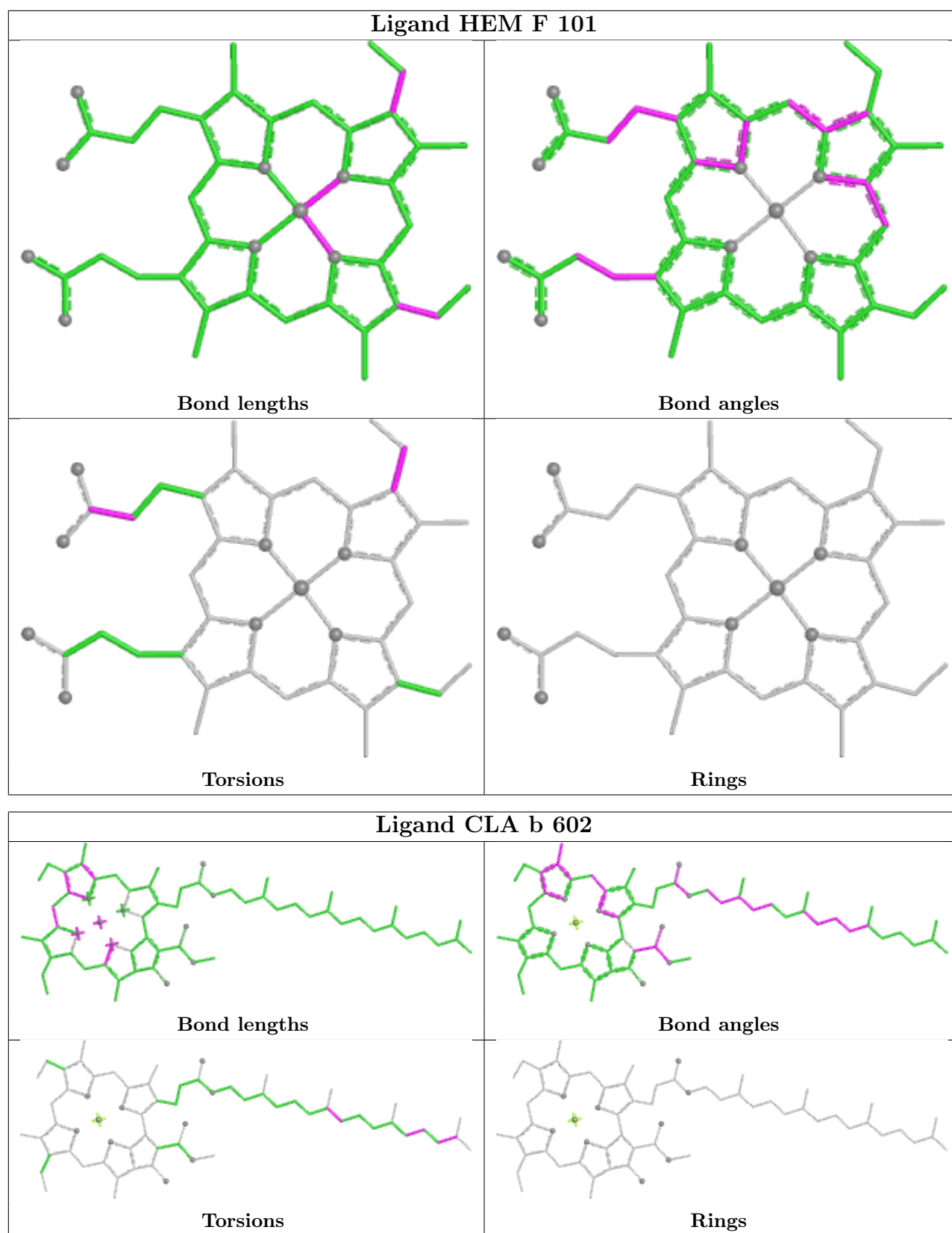
Ligand CLA A 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

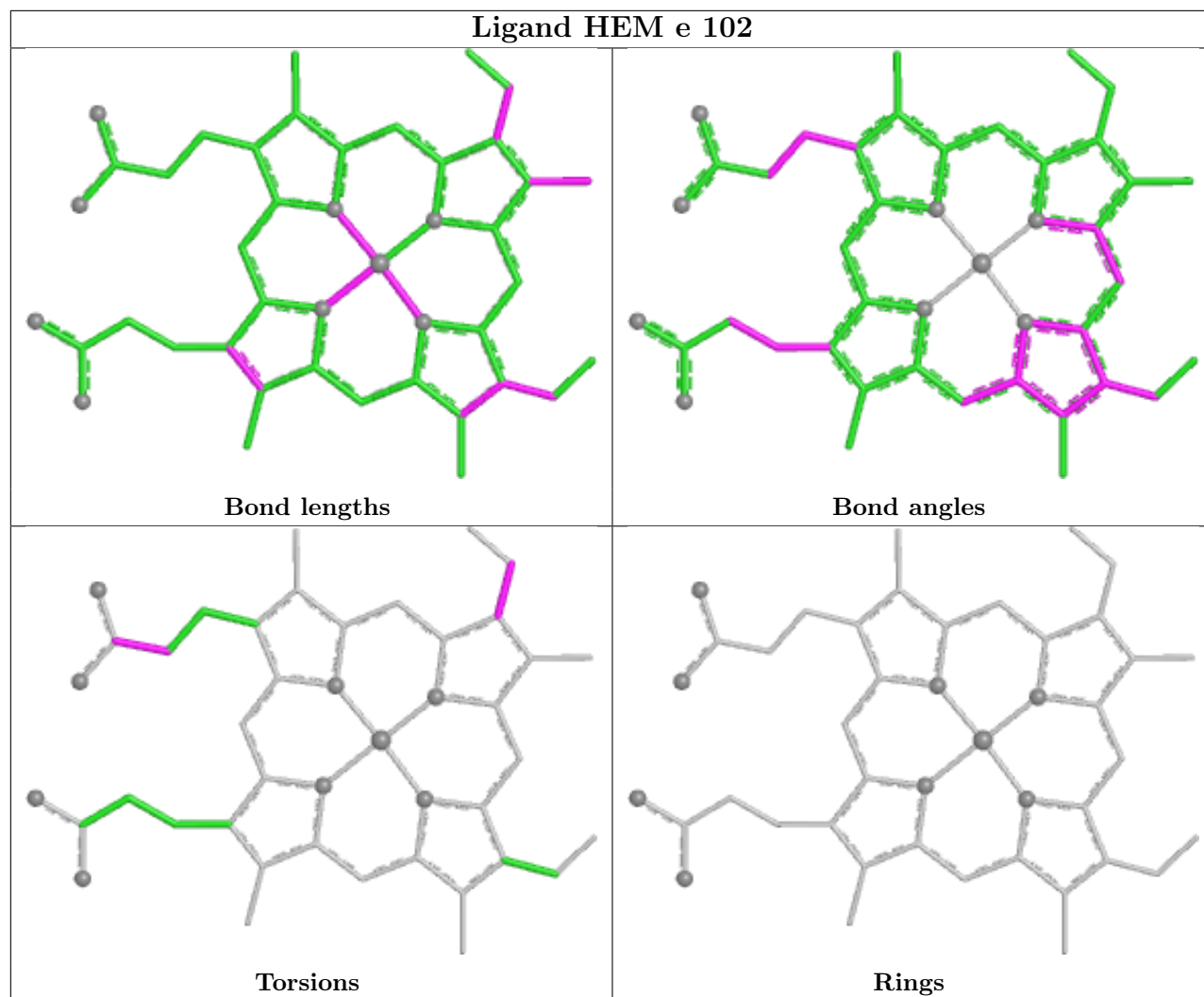
Ligand CLA c 504



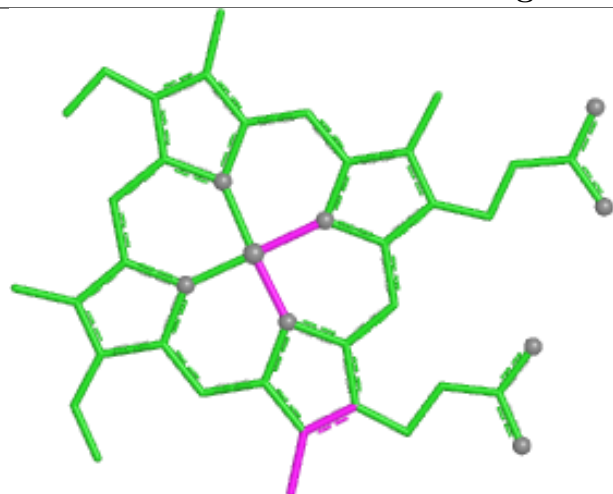
Ligand DGD c 520



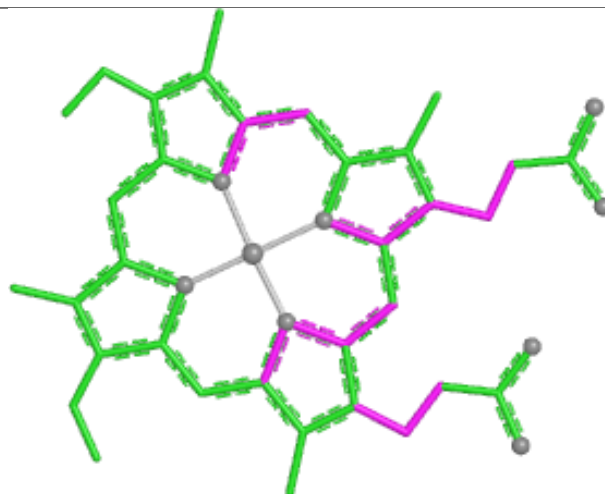




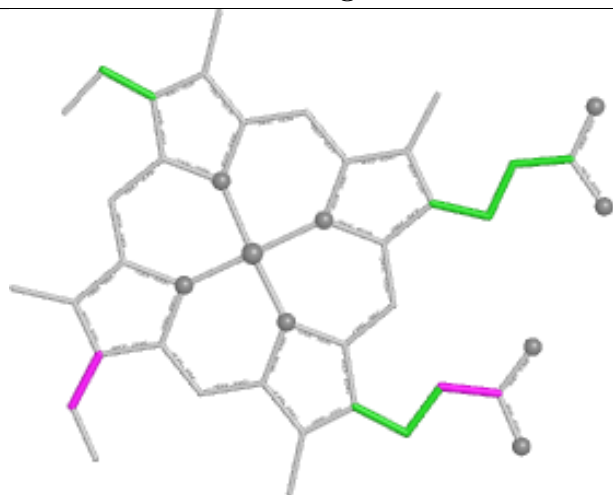
Ligand HEC v 201



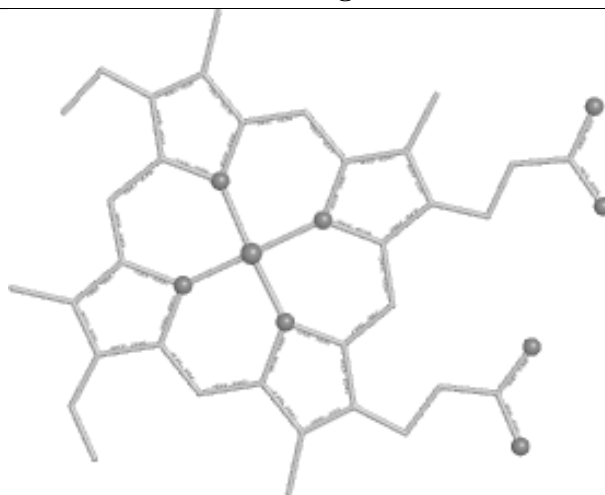
Bond lengths



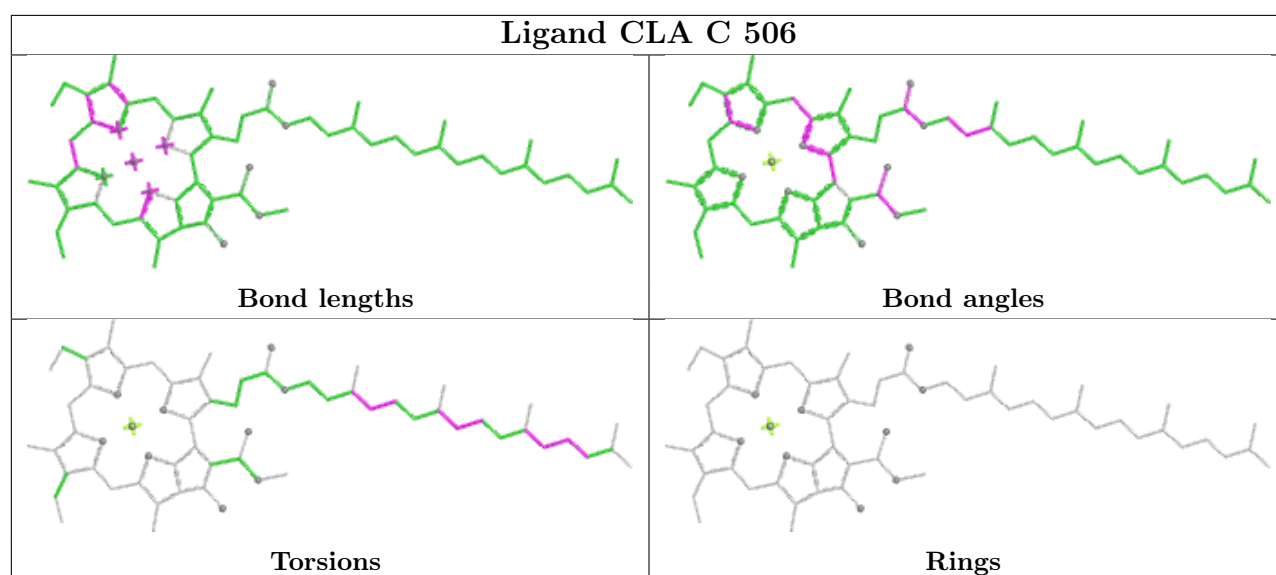
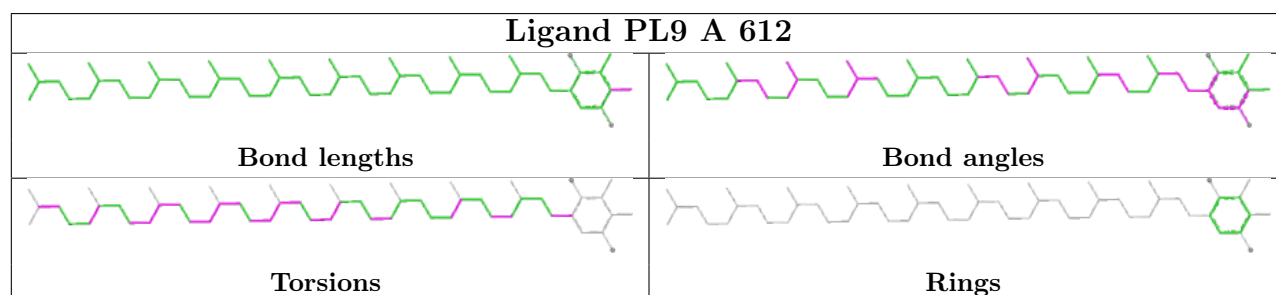
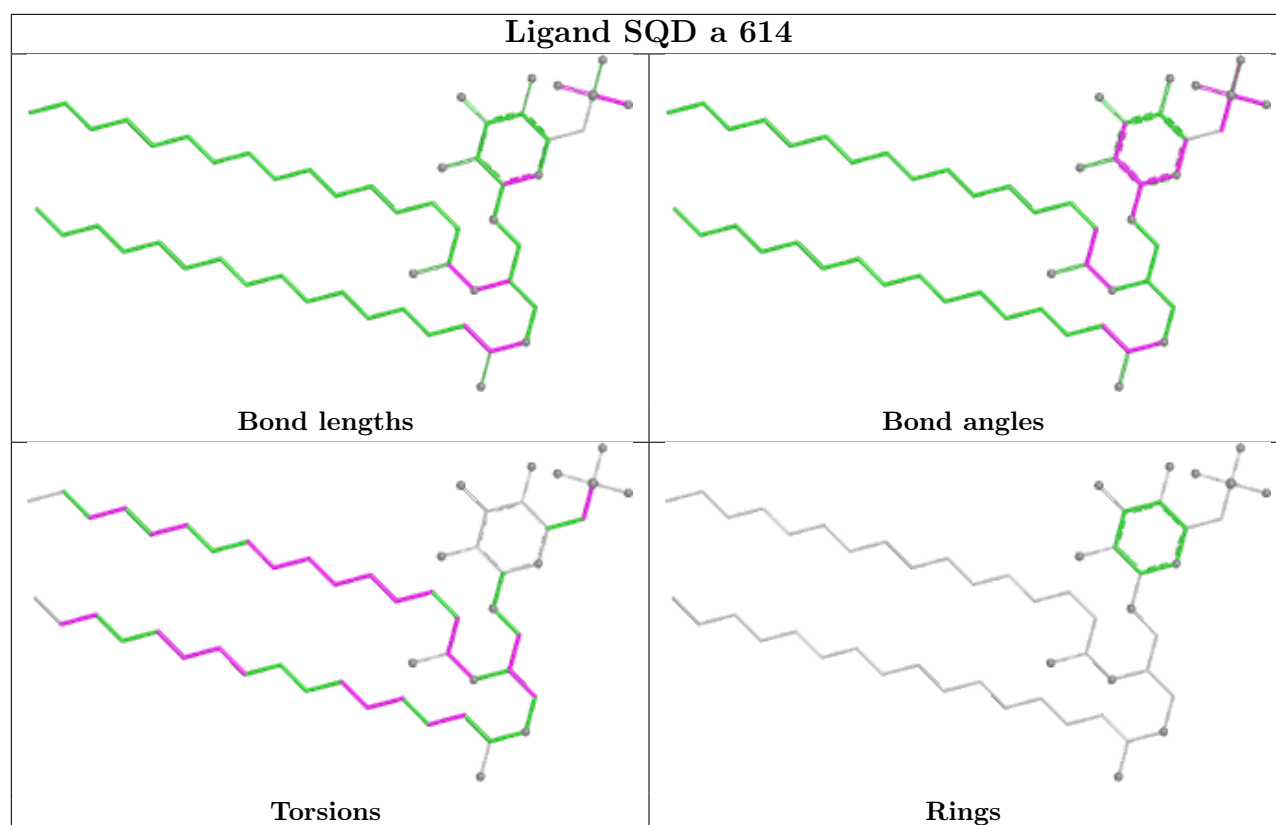
Bond angles

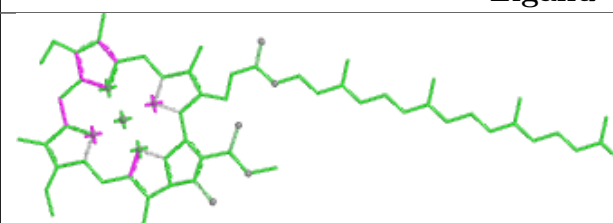
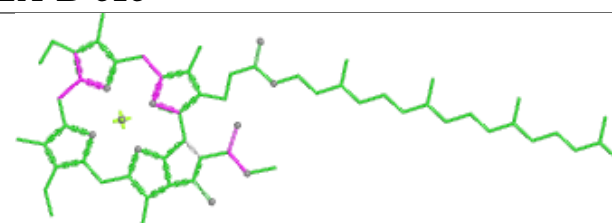
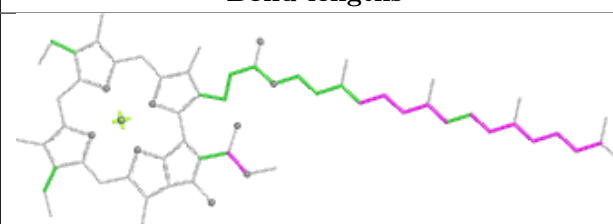
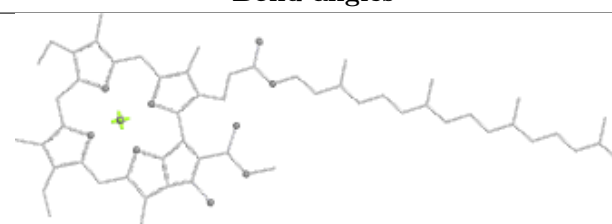


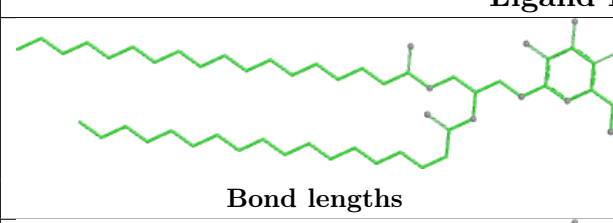
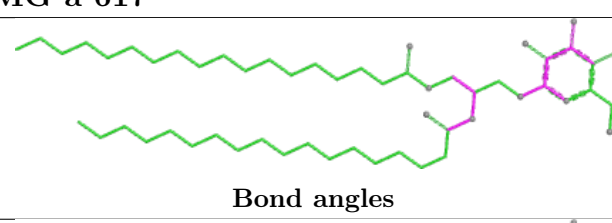
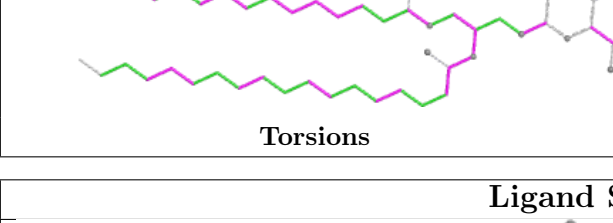
Torsions

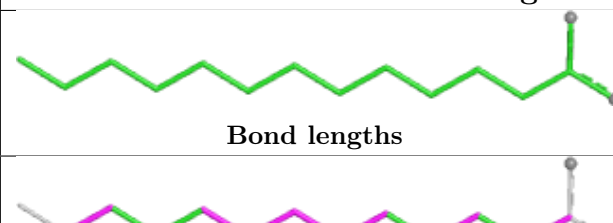
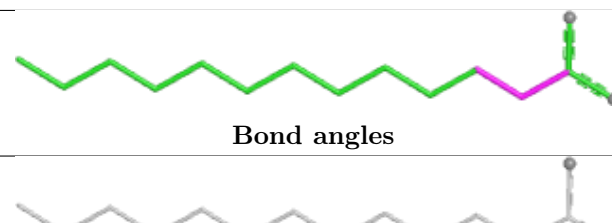
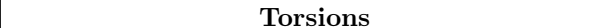


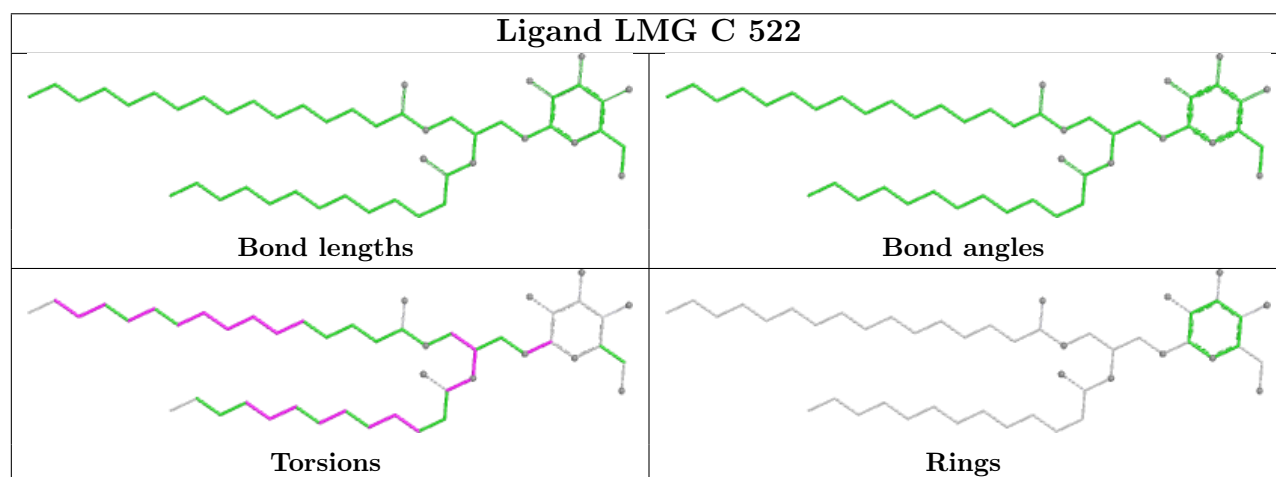
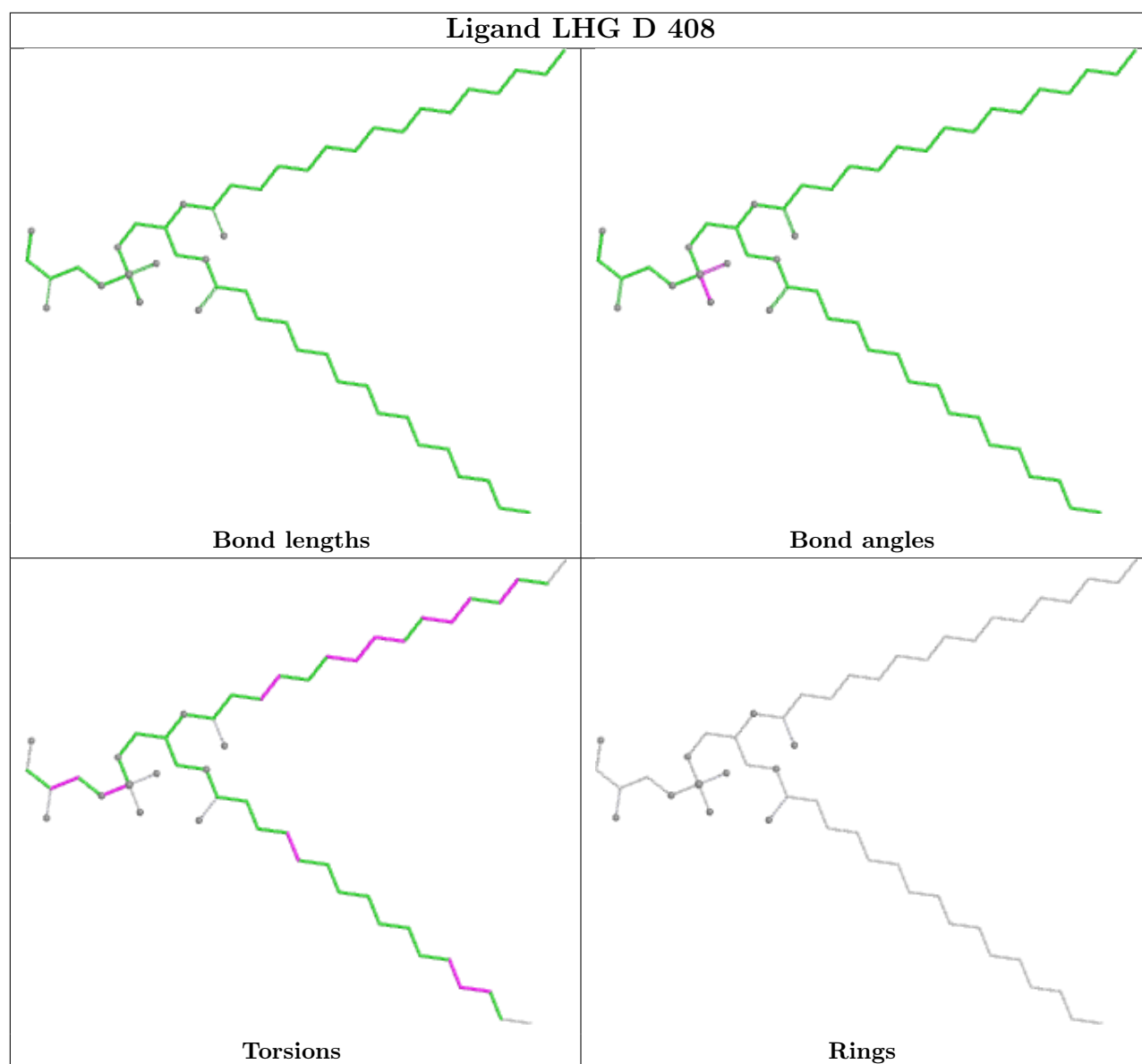
Rings

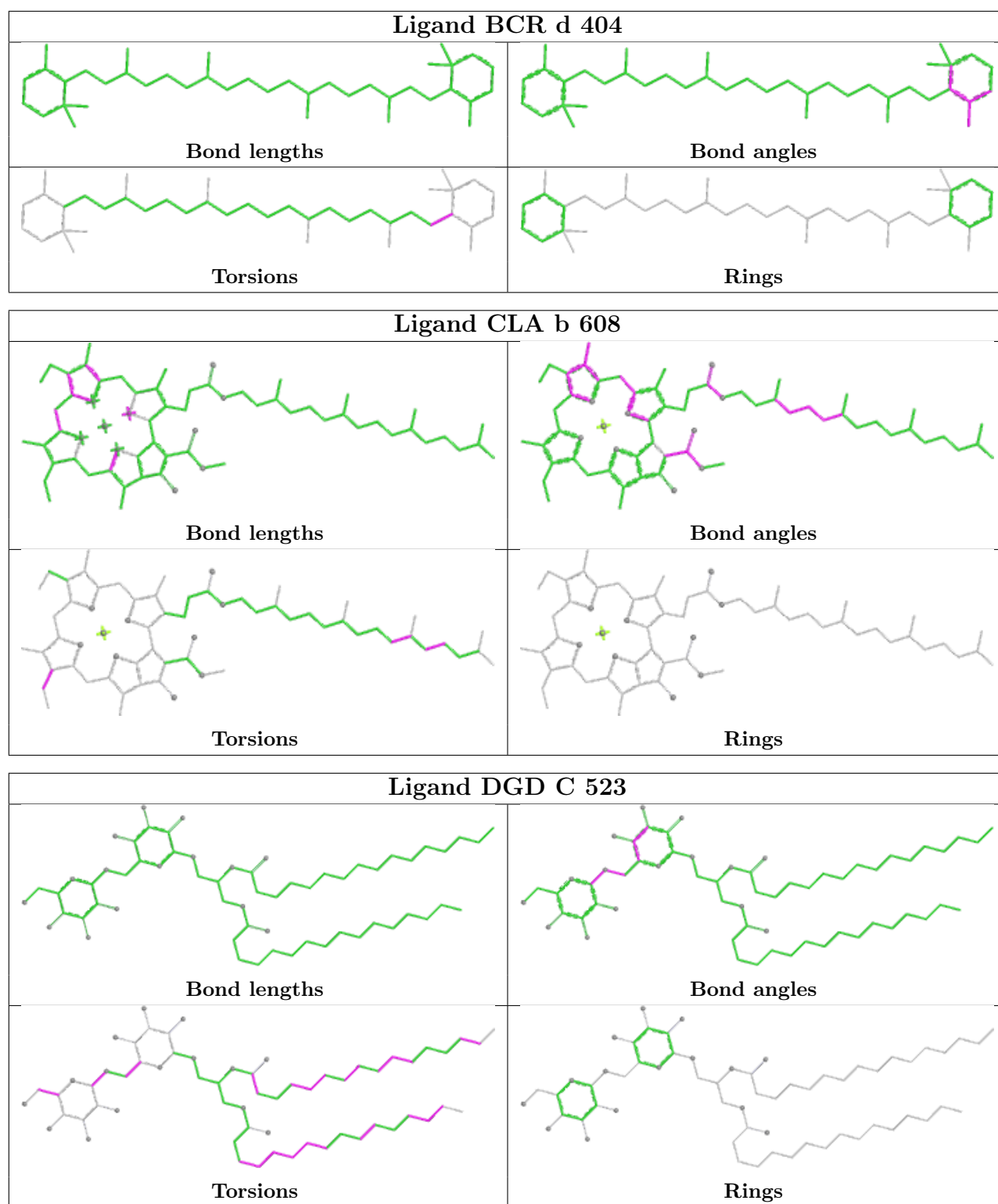


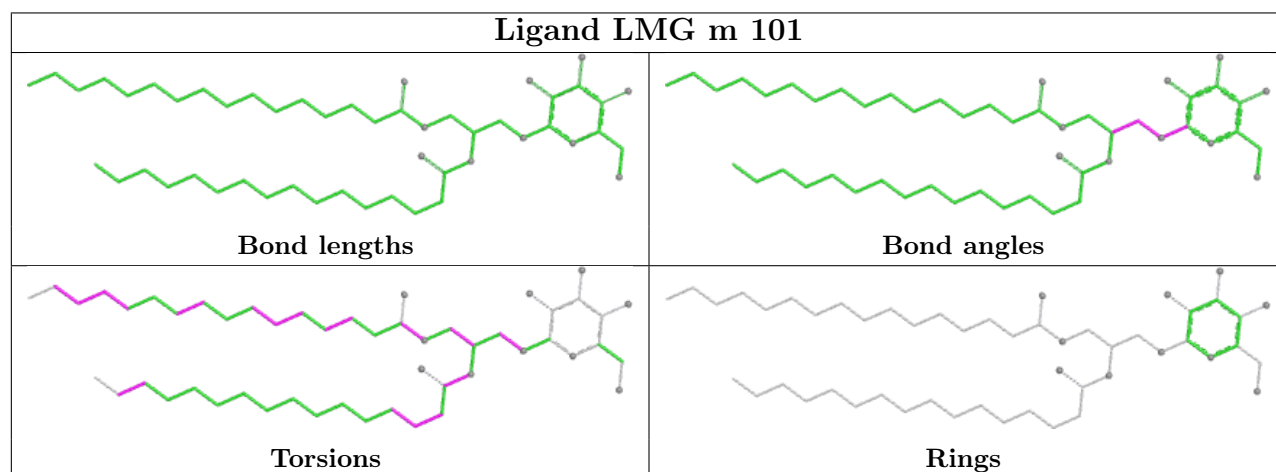
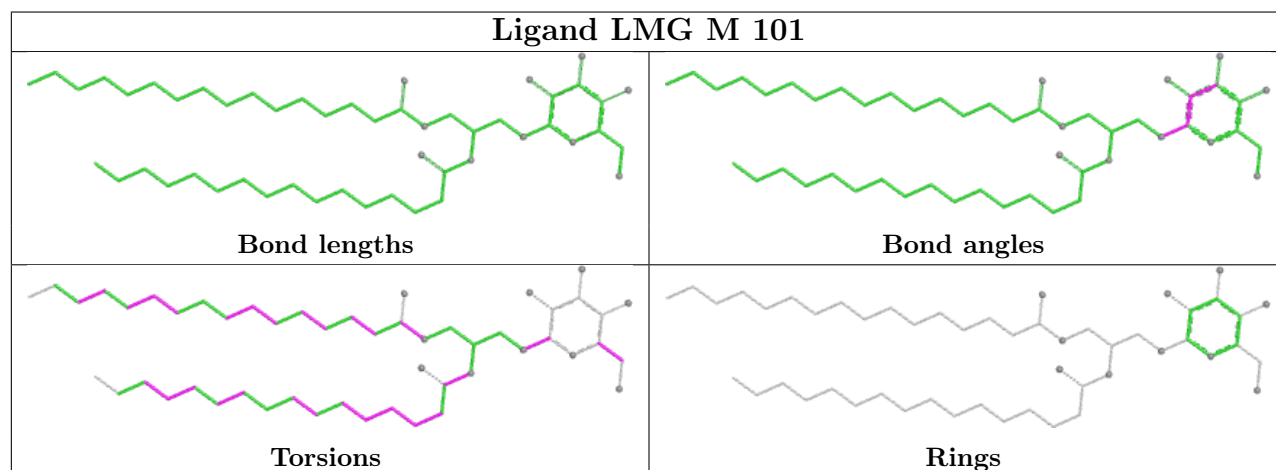
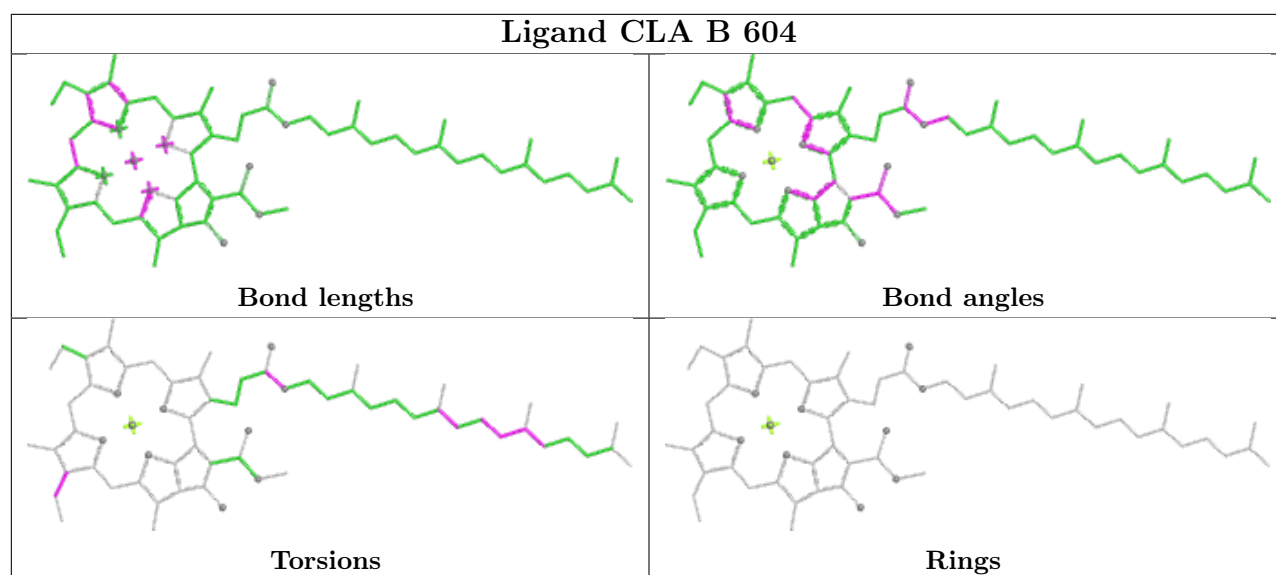
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

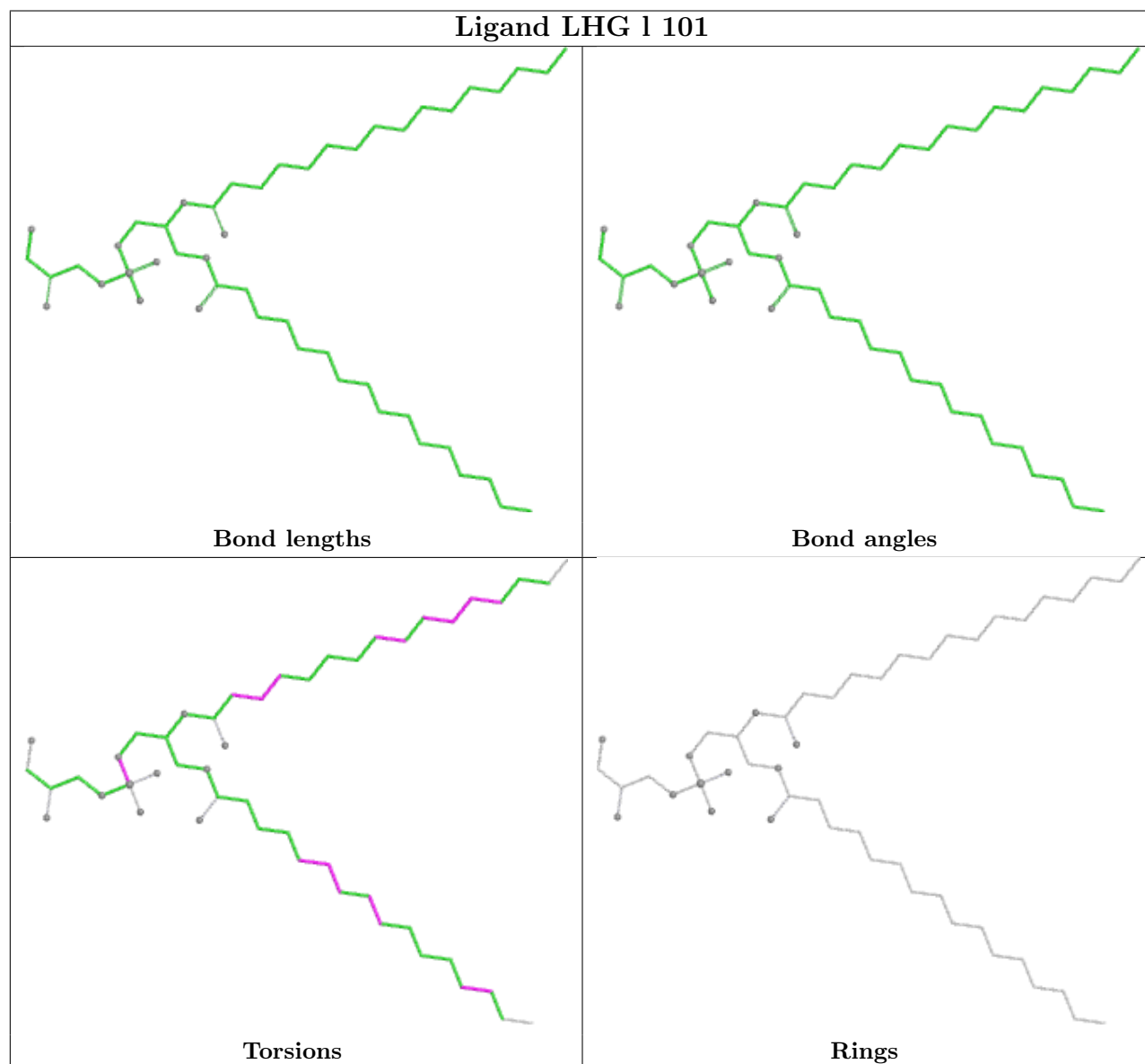
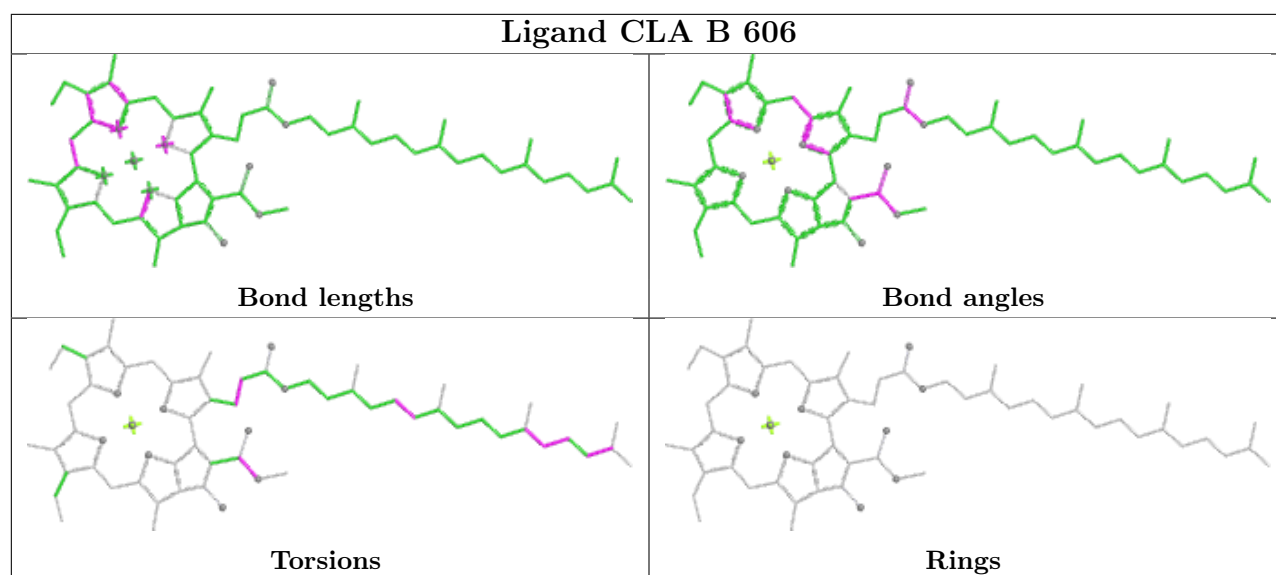
Ligand LMG a 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

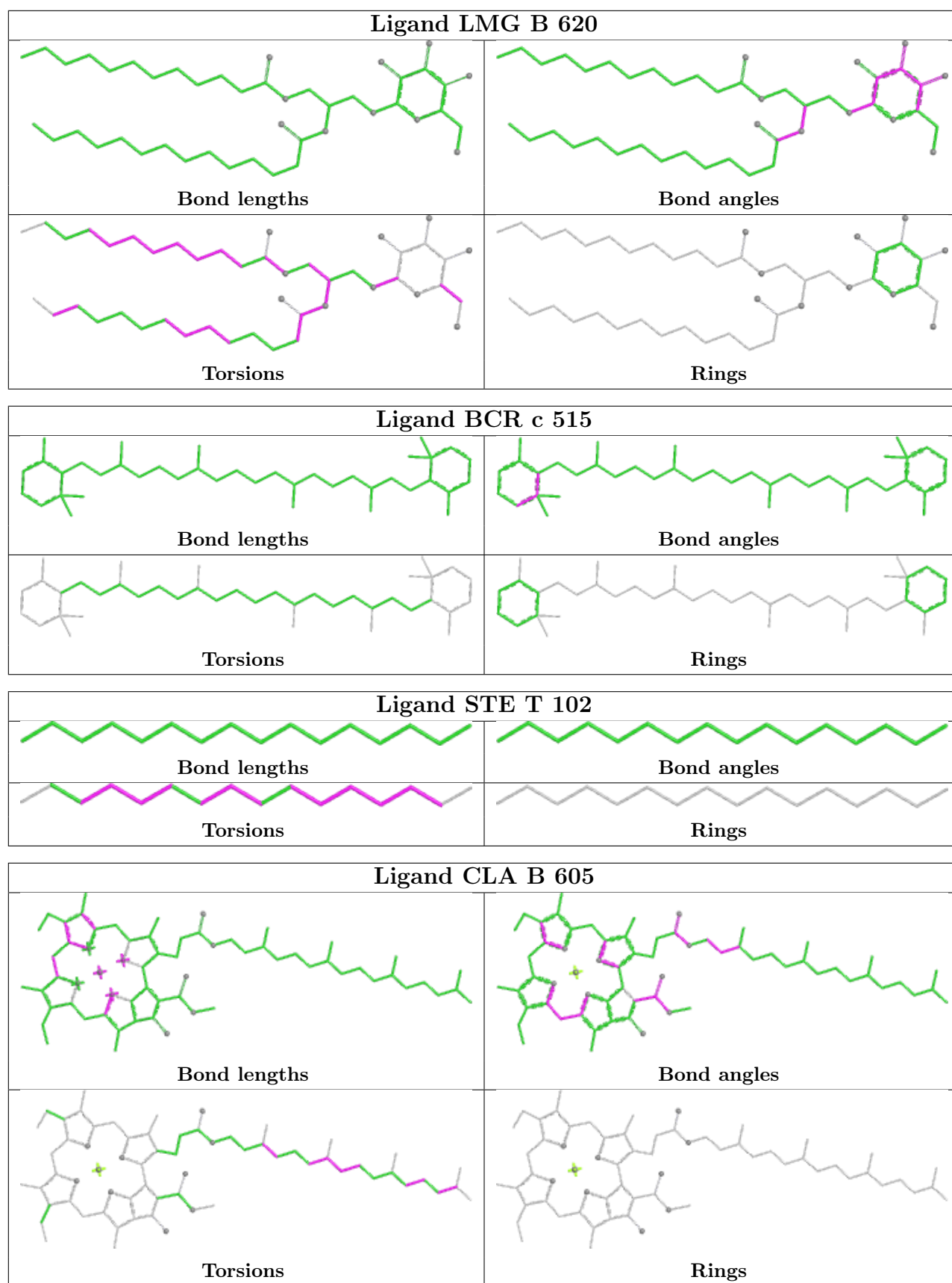
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Bond lengths	Bond angles
	
Torsions	Rings

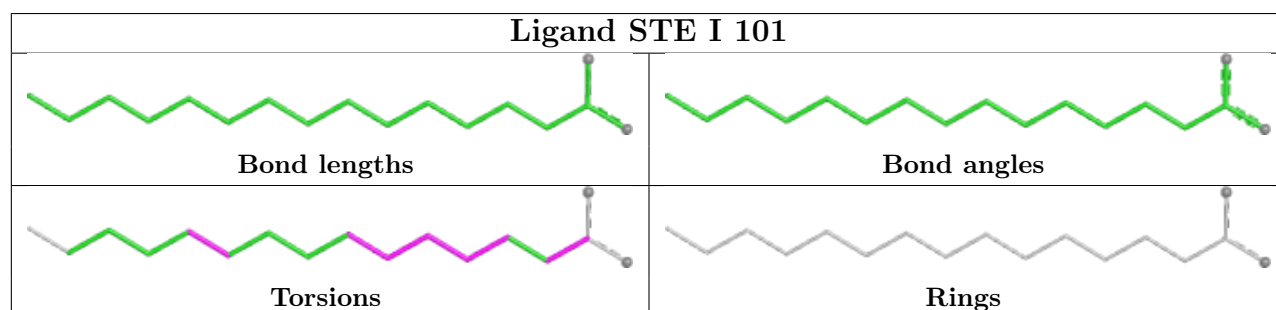
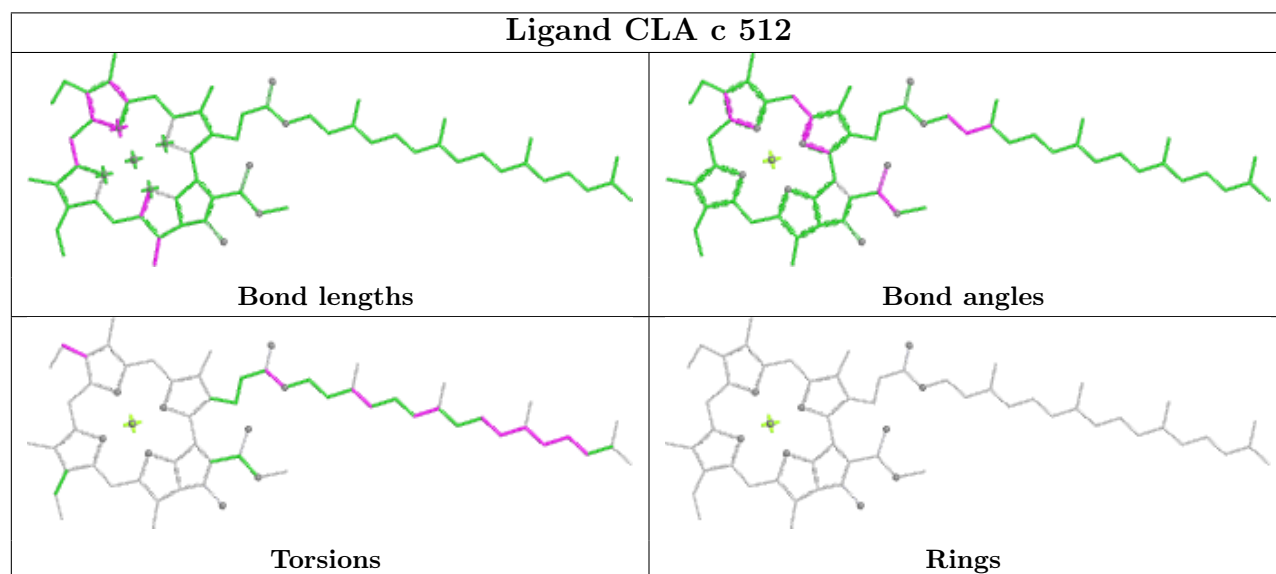
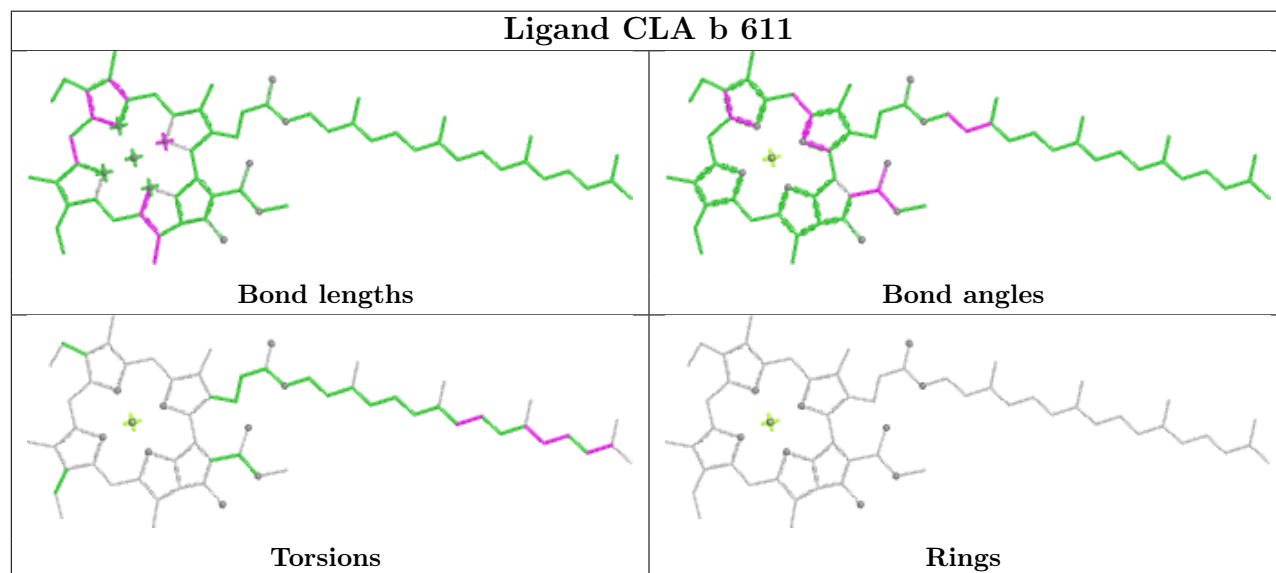
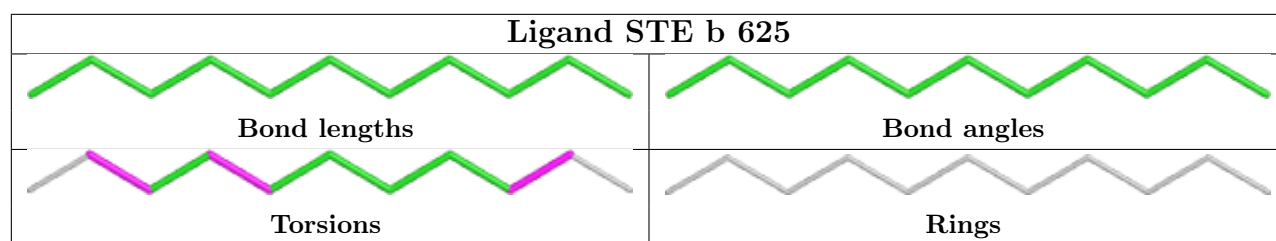


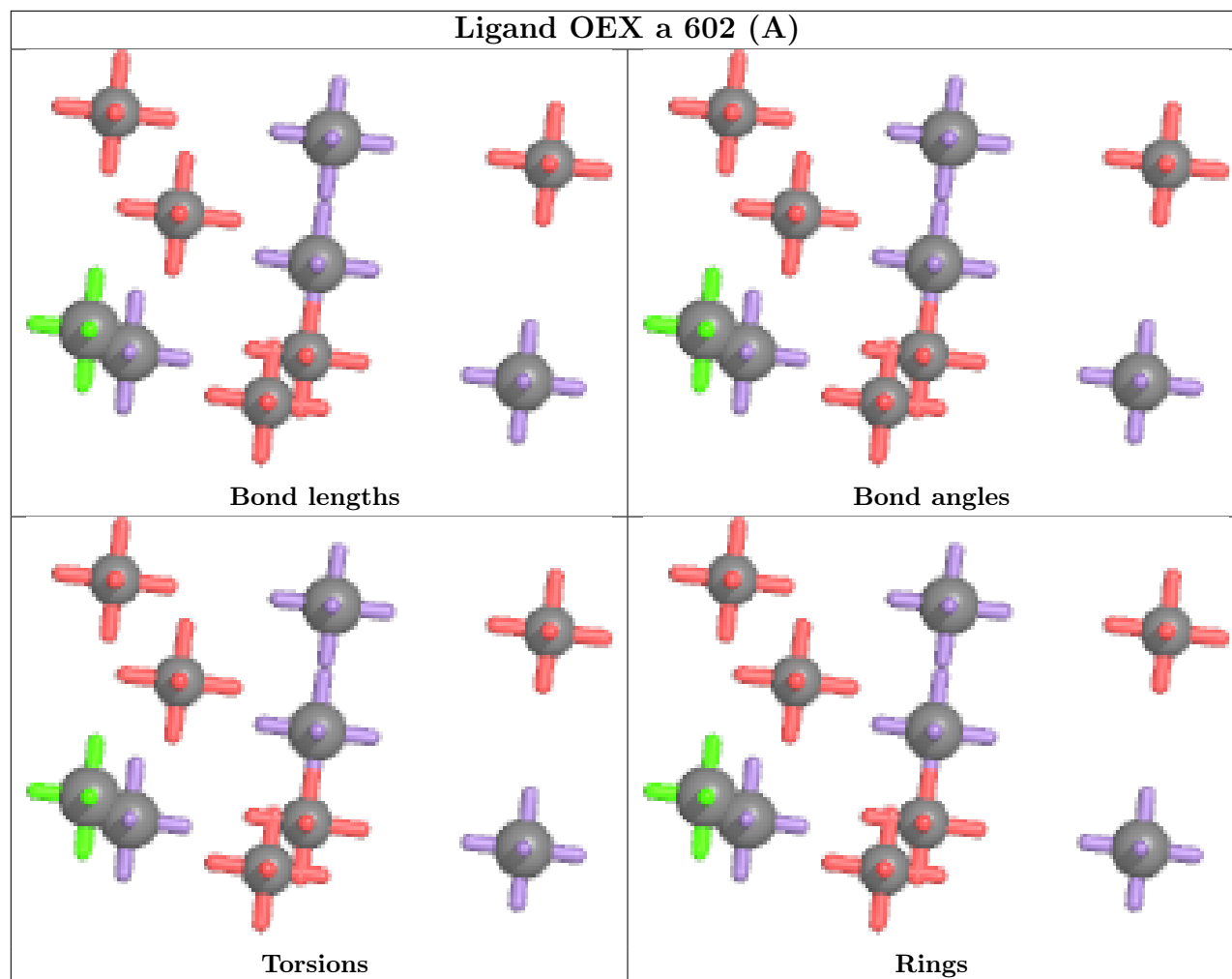


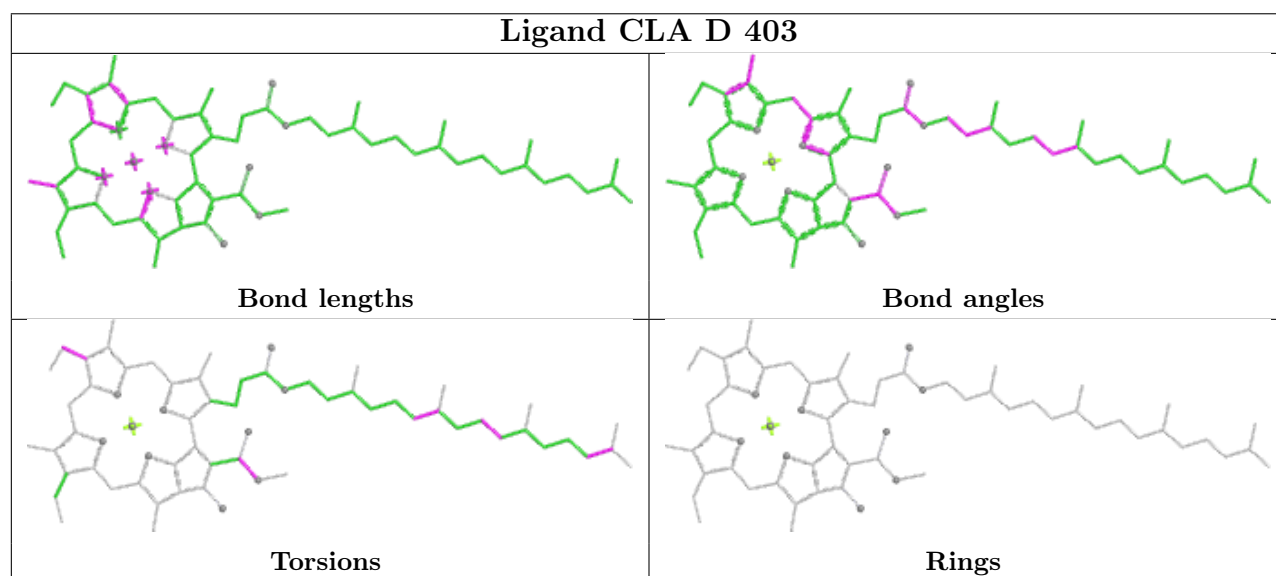
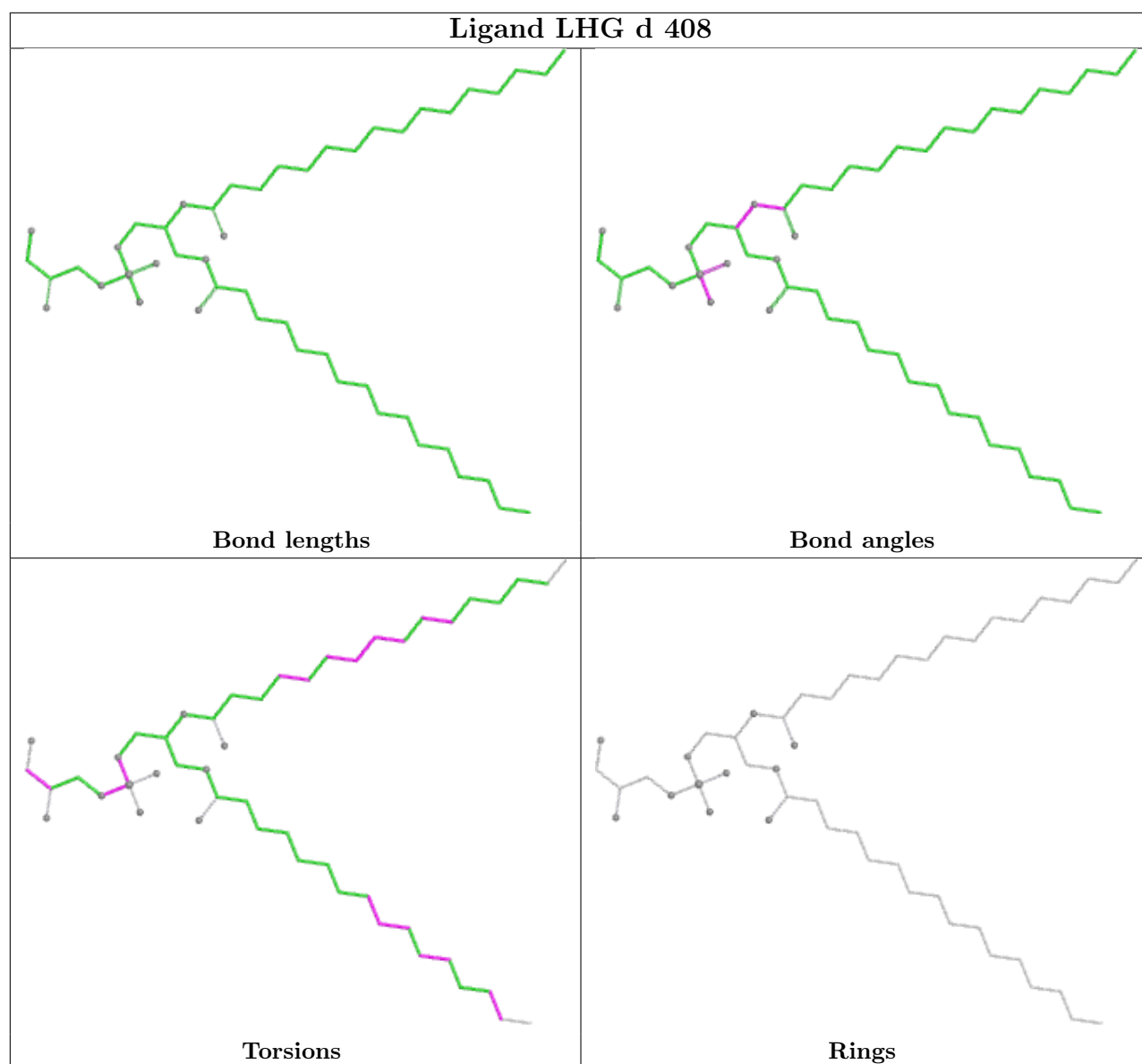


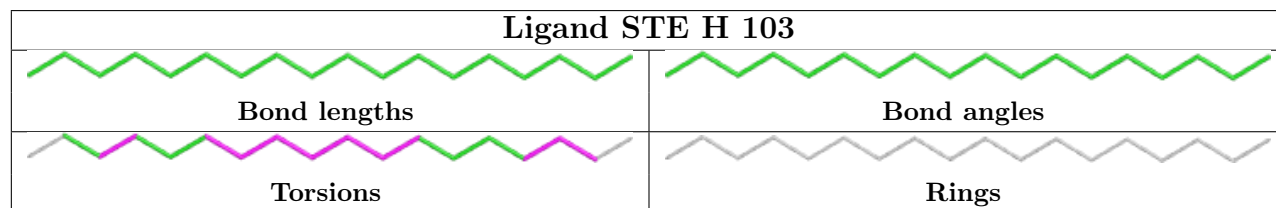
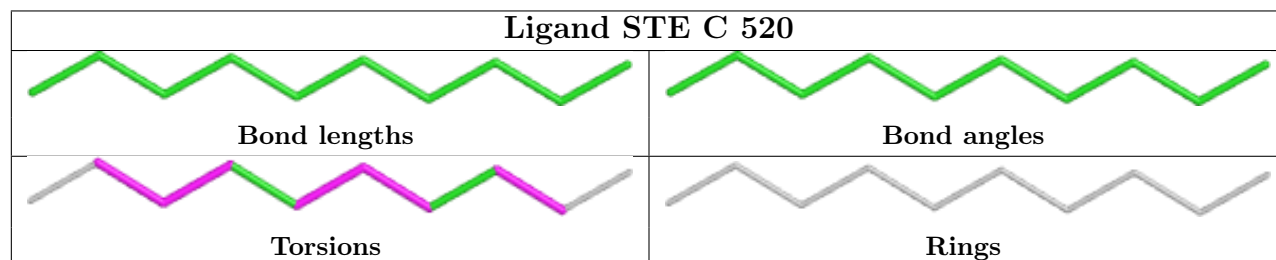
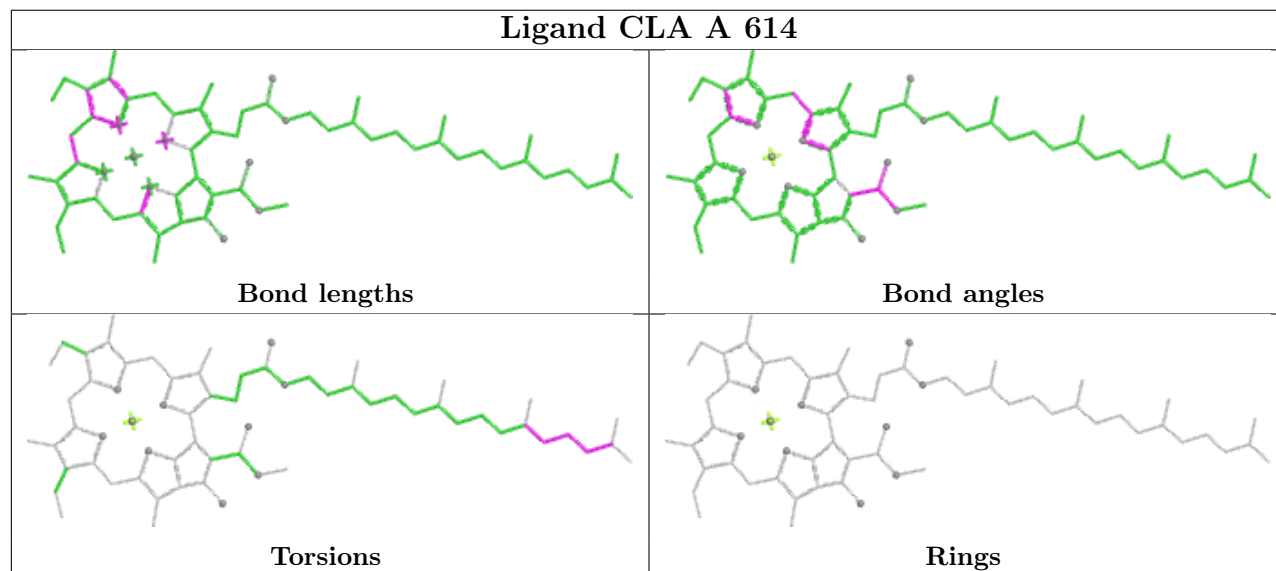
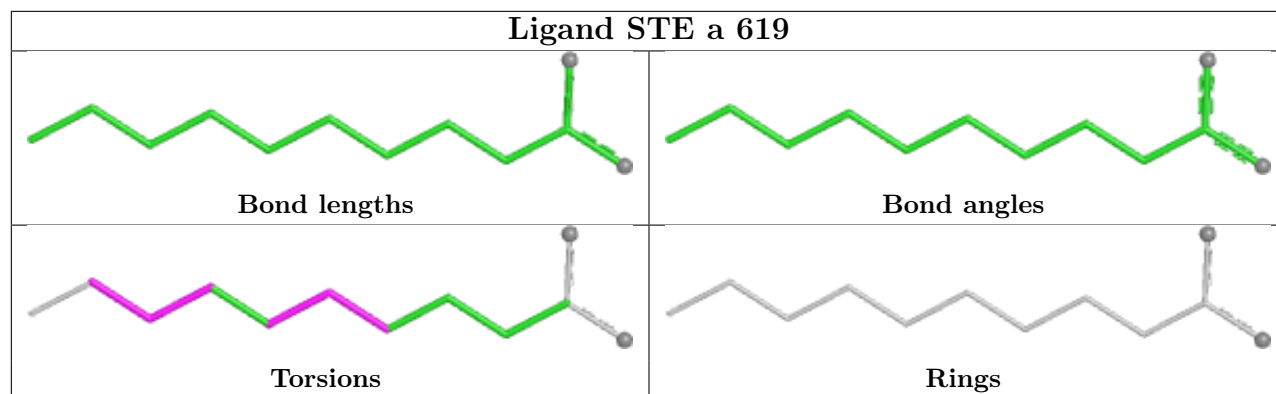


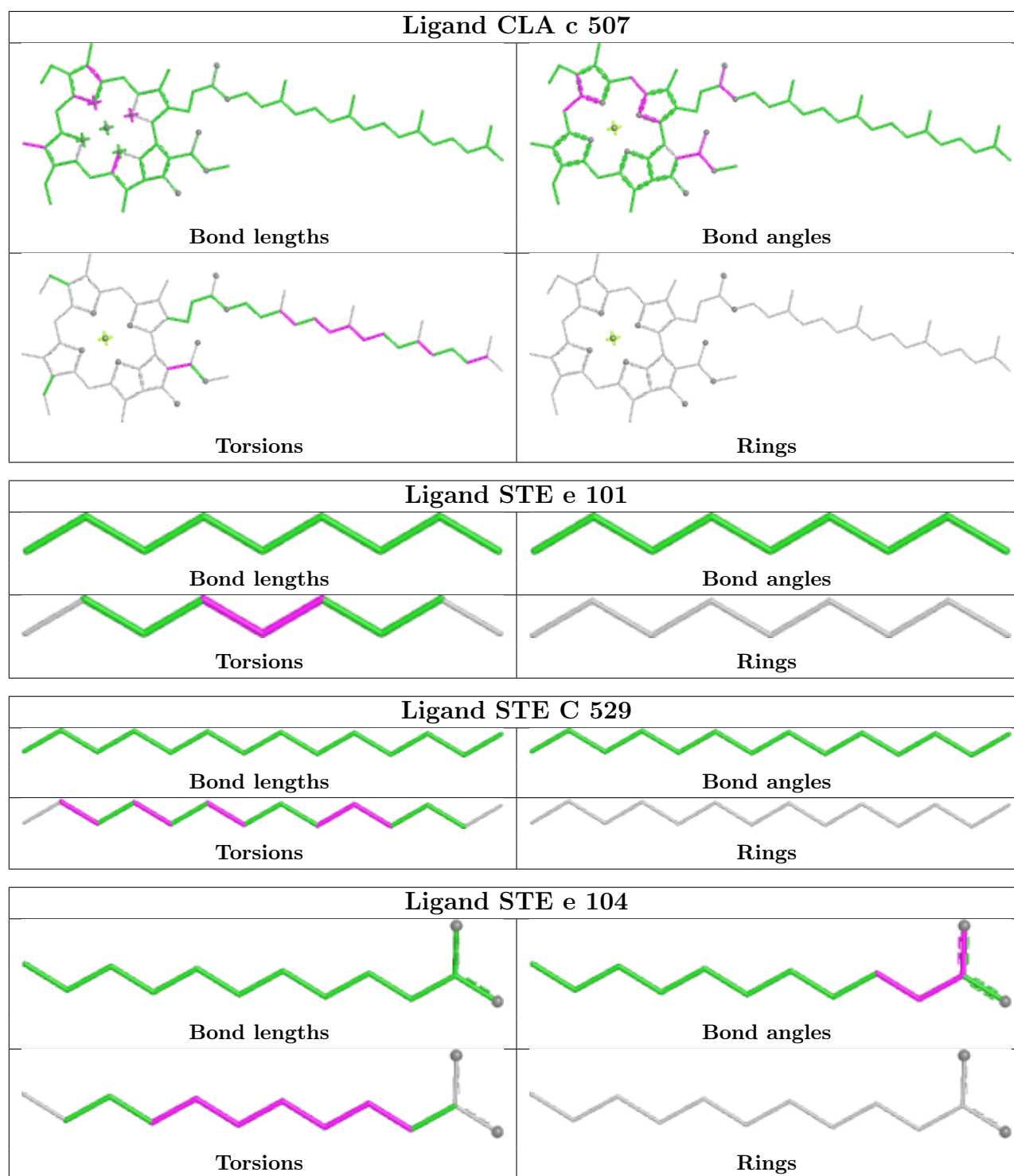


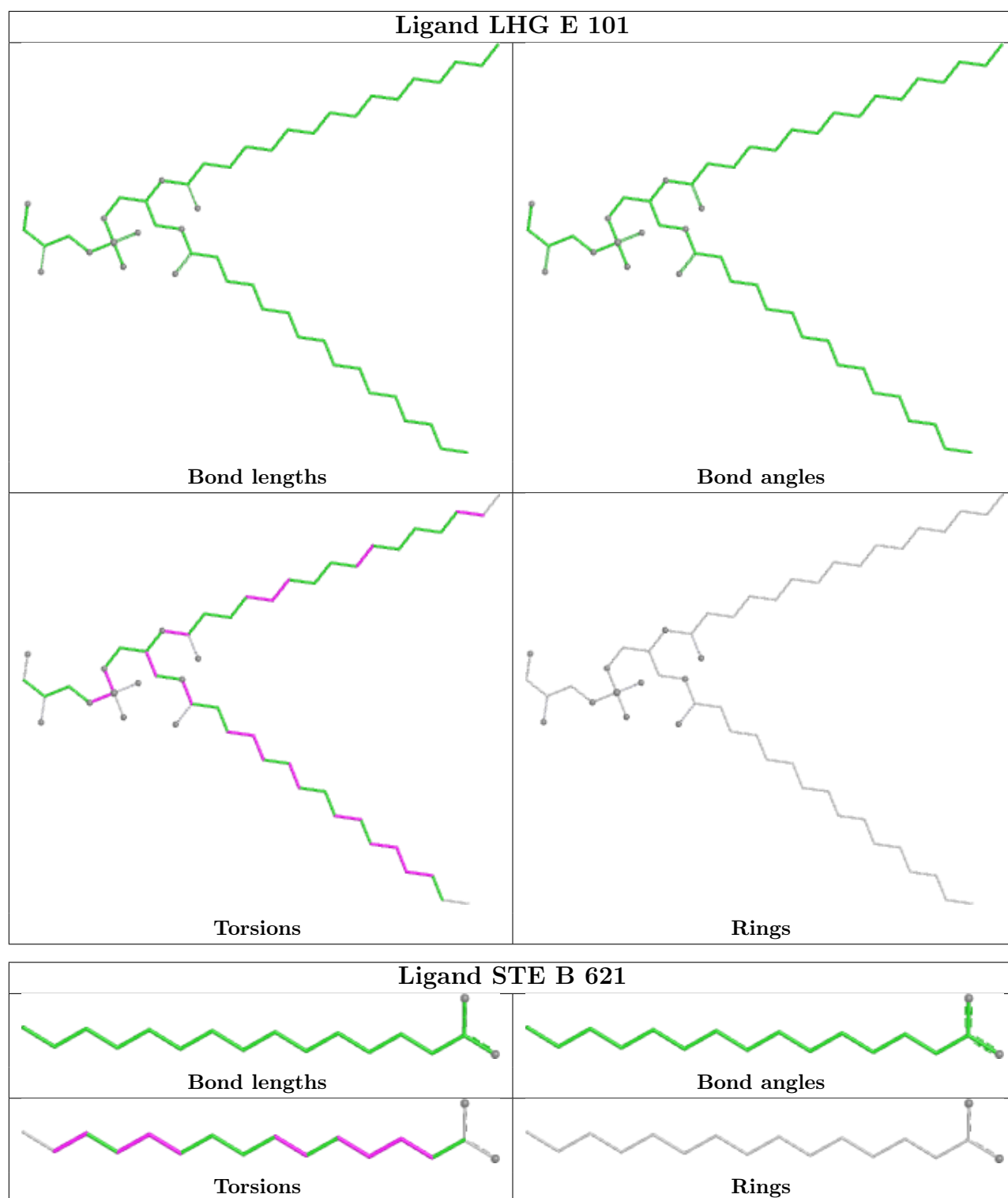




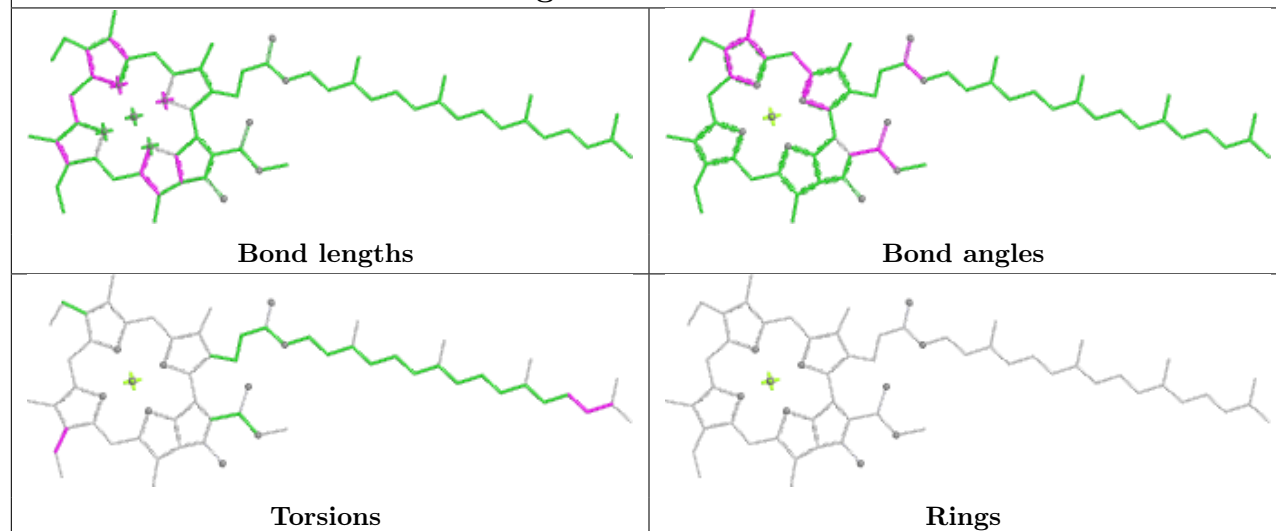




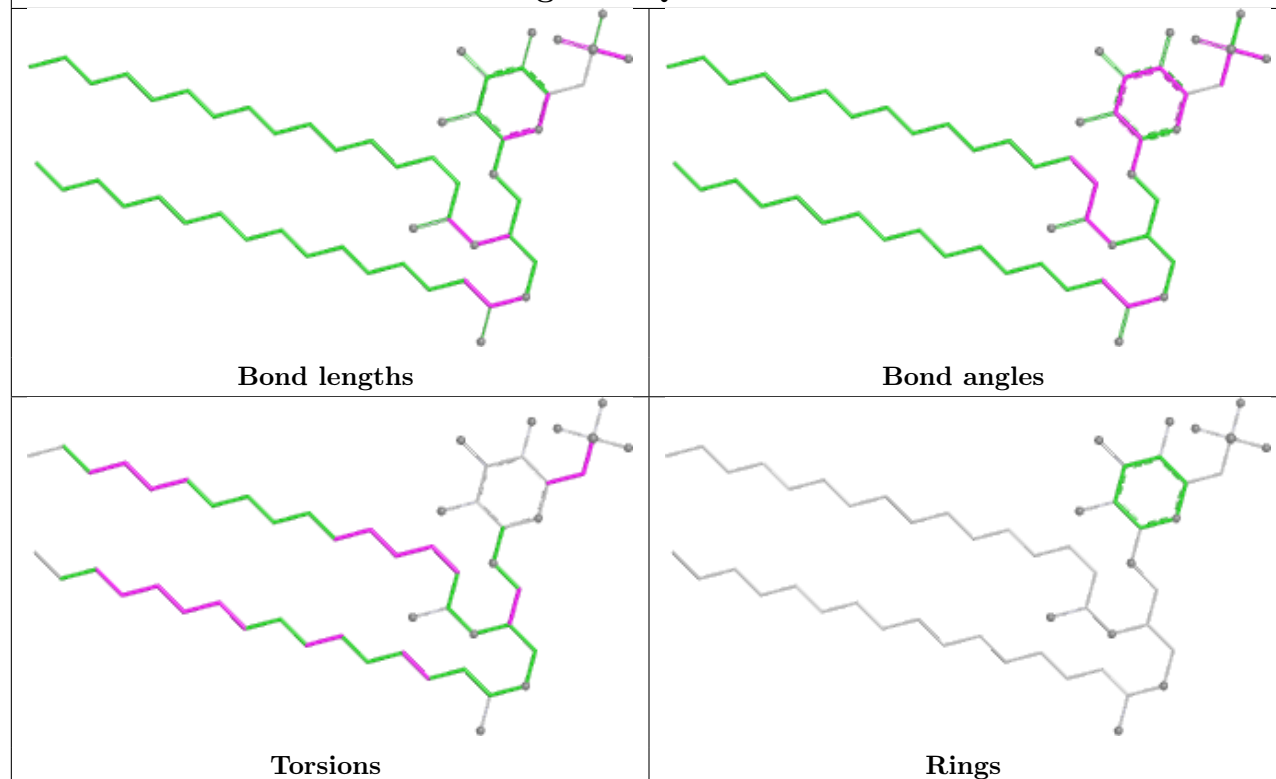


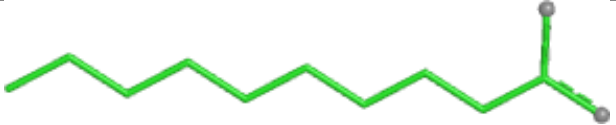
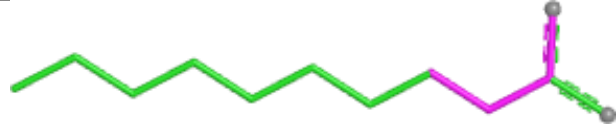
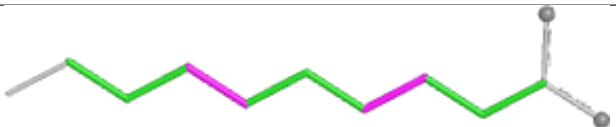
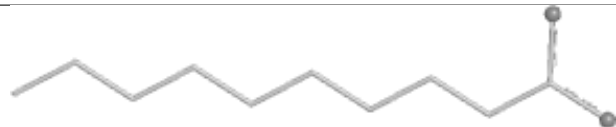


Ligand CLA a 607

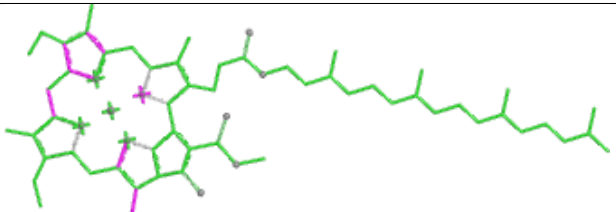
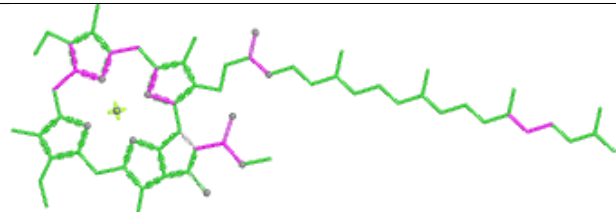
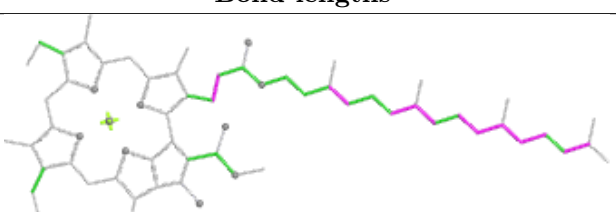
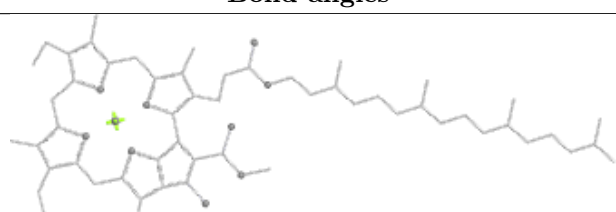


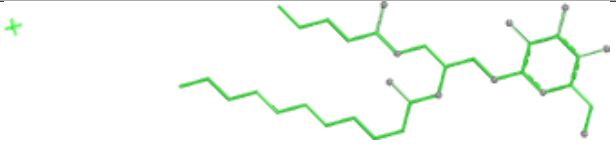
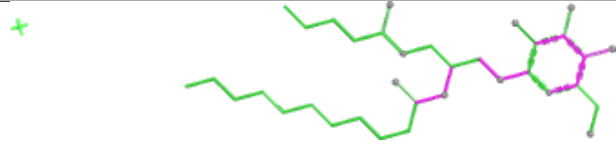
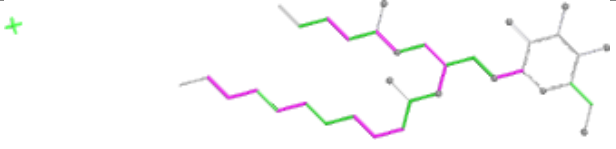
Ligand SQD a 616

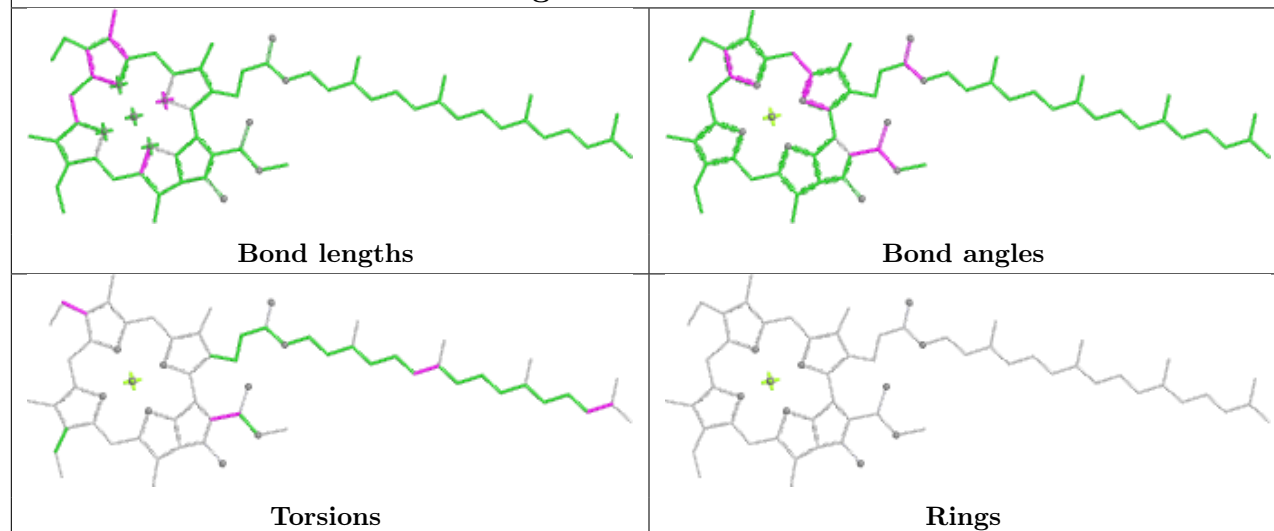
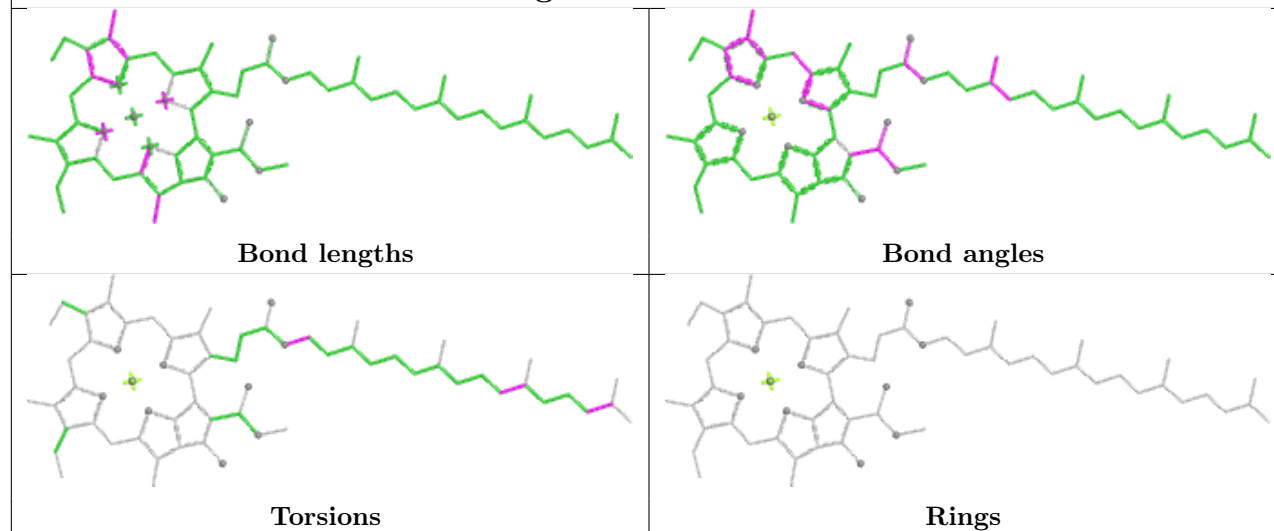
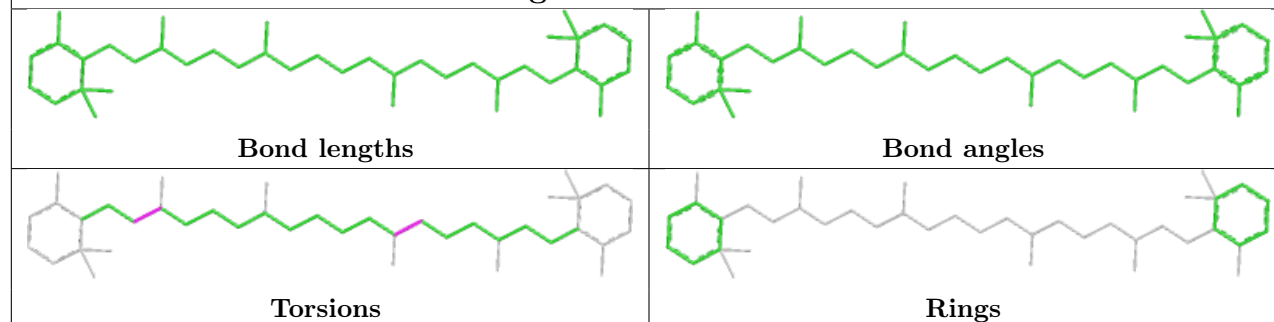


Ligand STE C 527	
 Bond lengths	 Bond angles
 Torsions	 Rings

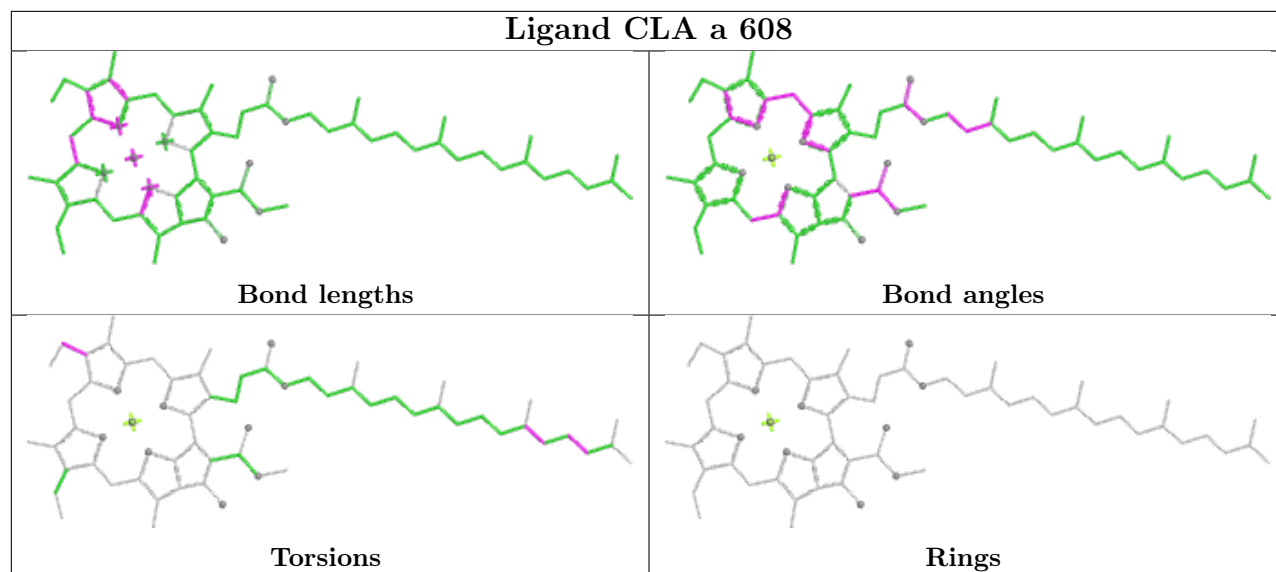
Ligand STE c 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

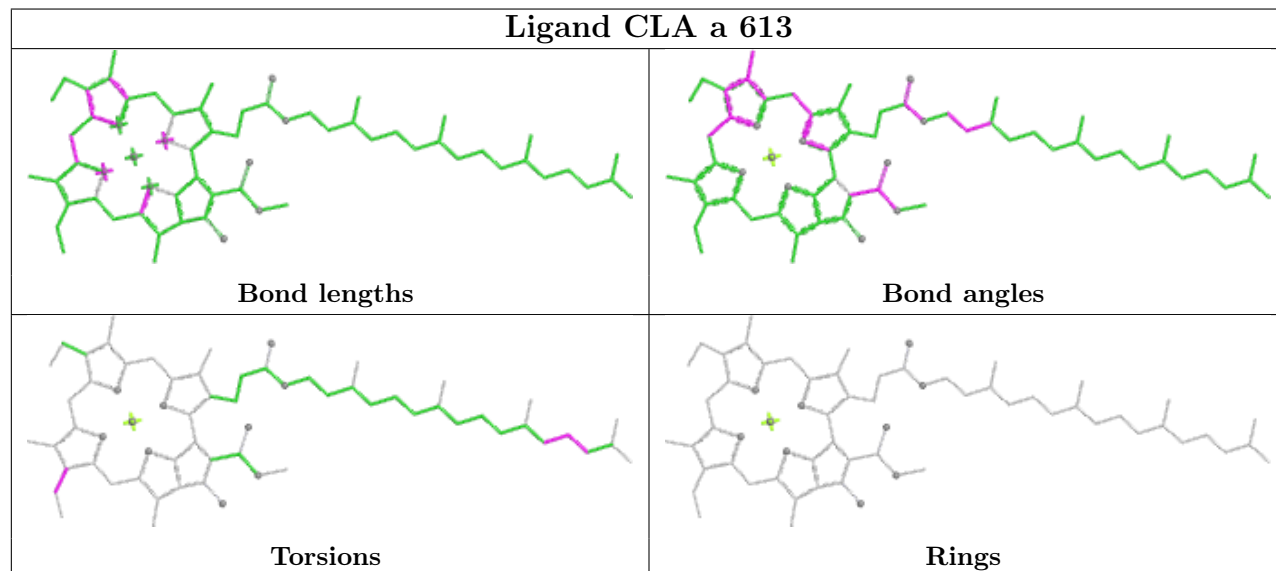
Ligand LMG C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 502**Ligand CLA d 402****Ligand BCR K 101**

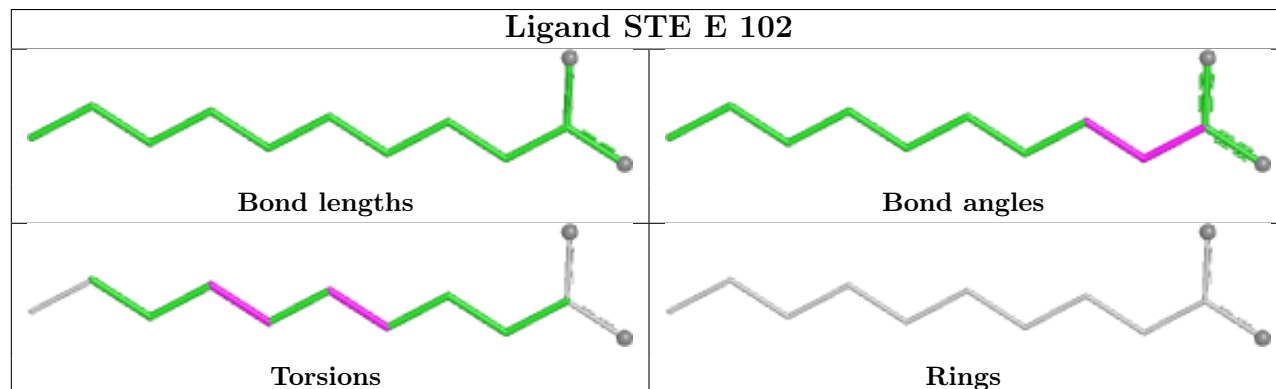
Ligand CLA a 608

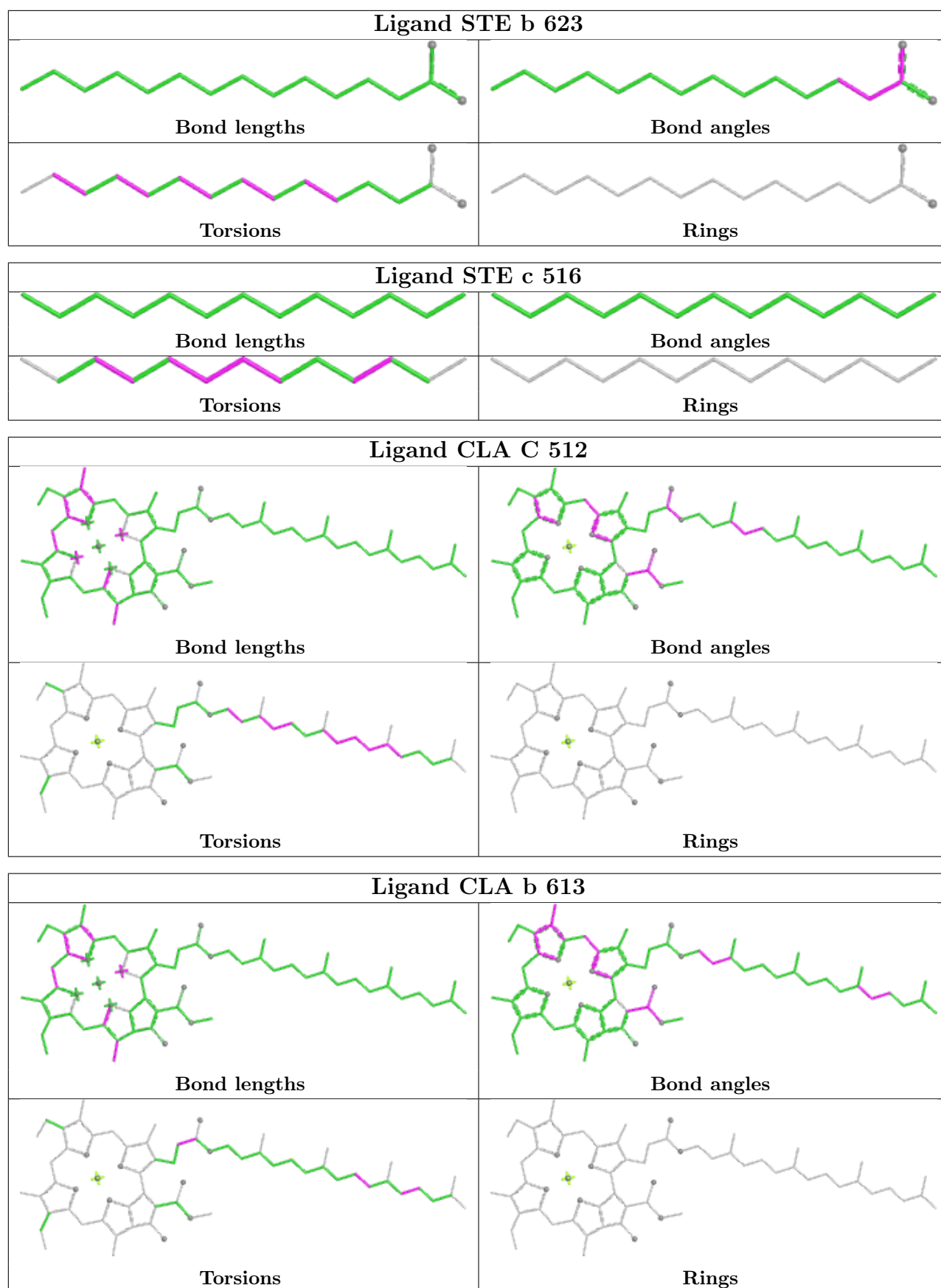


Ligand CLA a 613

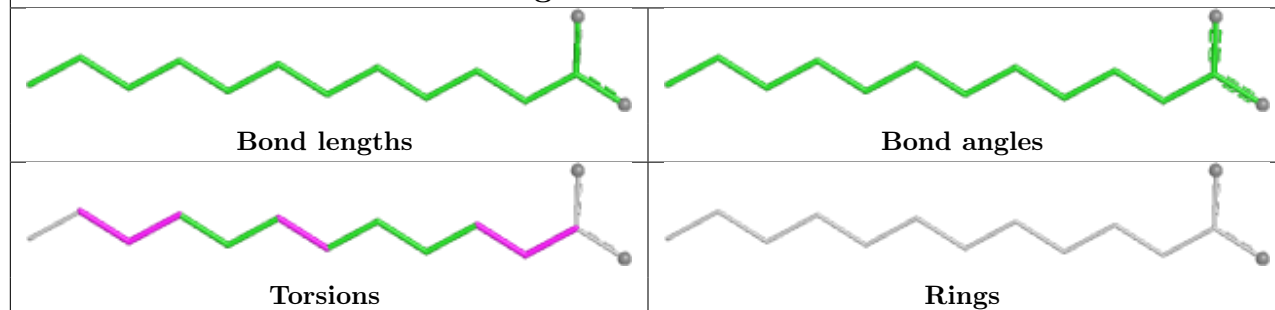


Ligand STE E 102

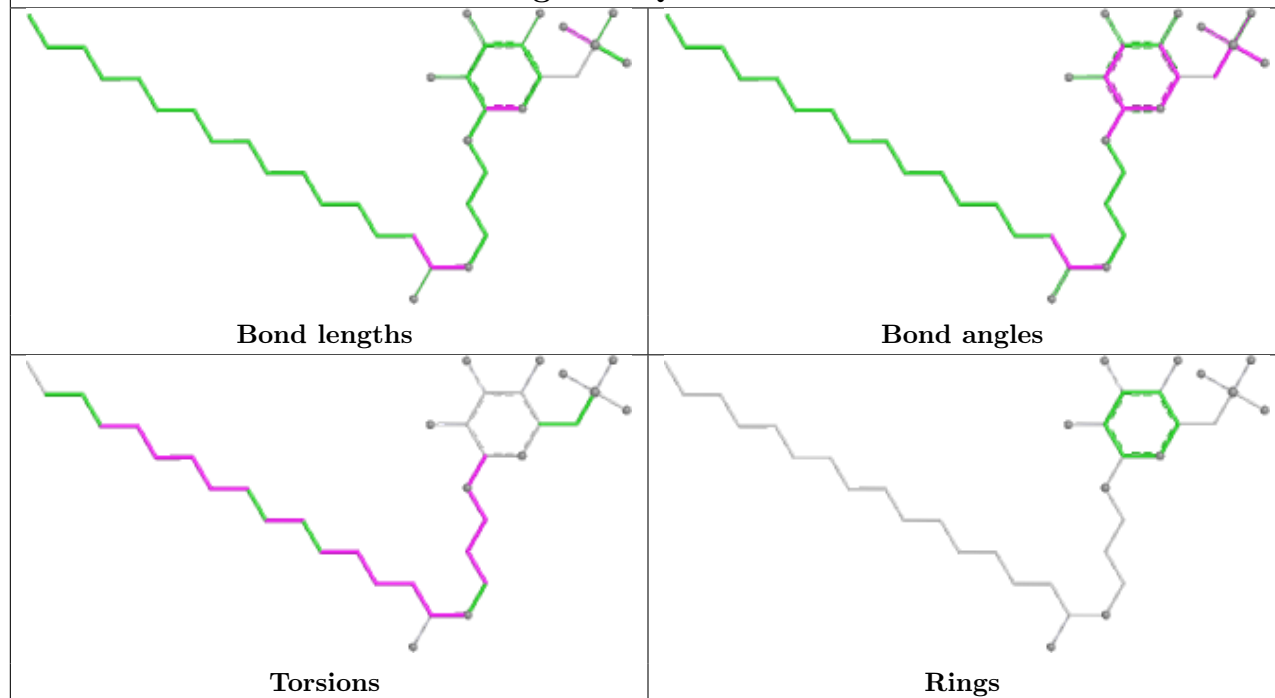




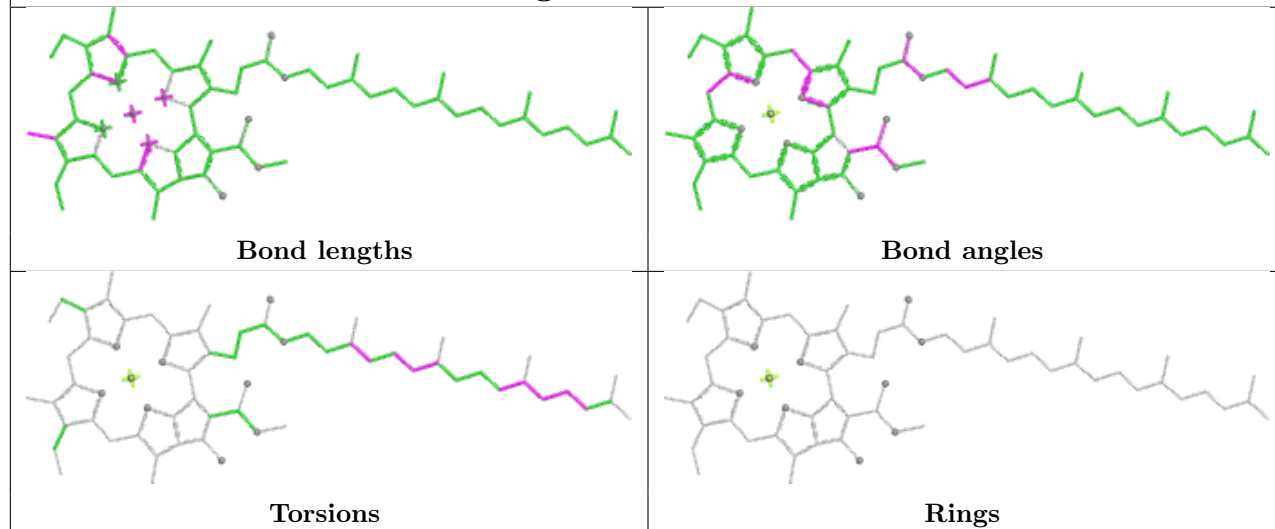
Ligand STE C 516

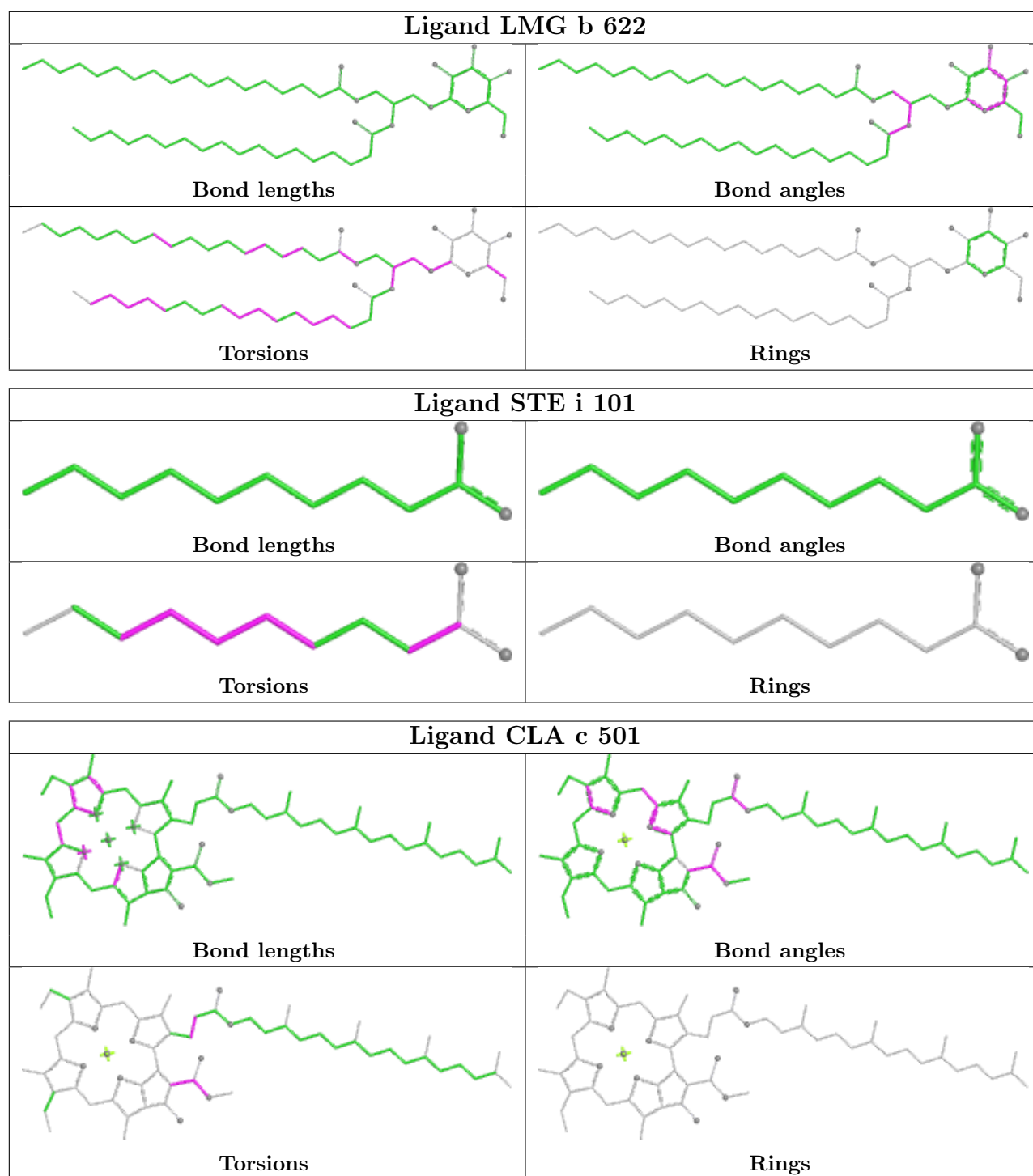


Ligand SQD F 102

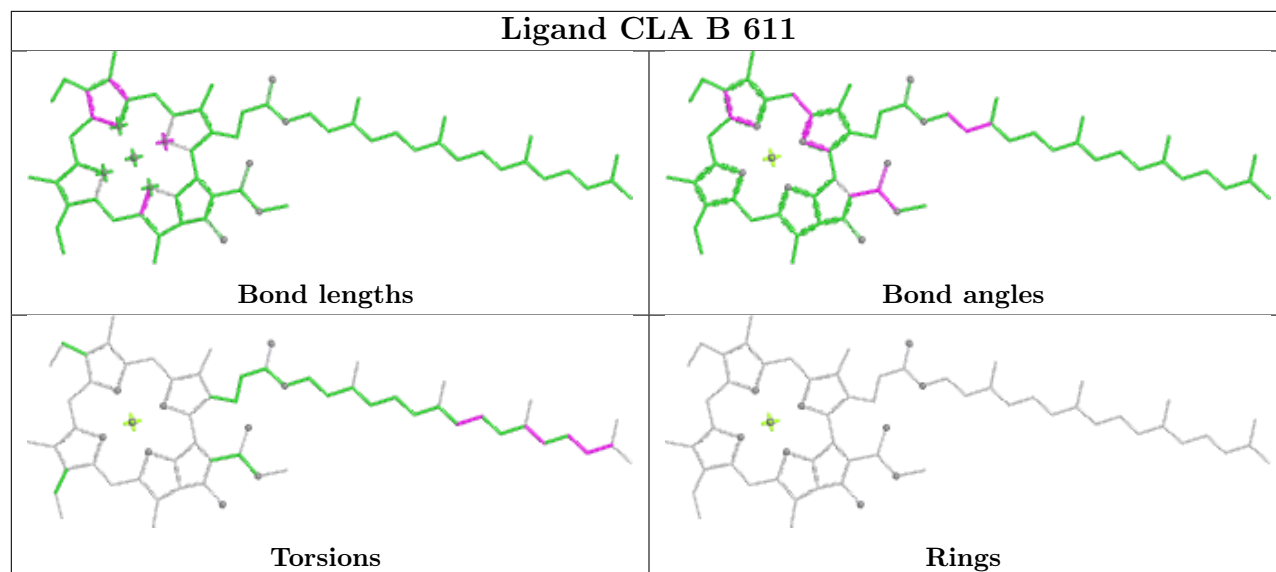


Ligand CLA a 610

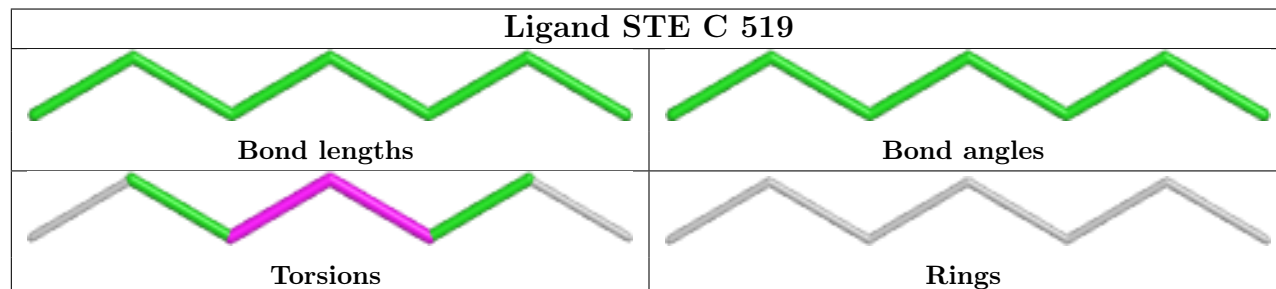




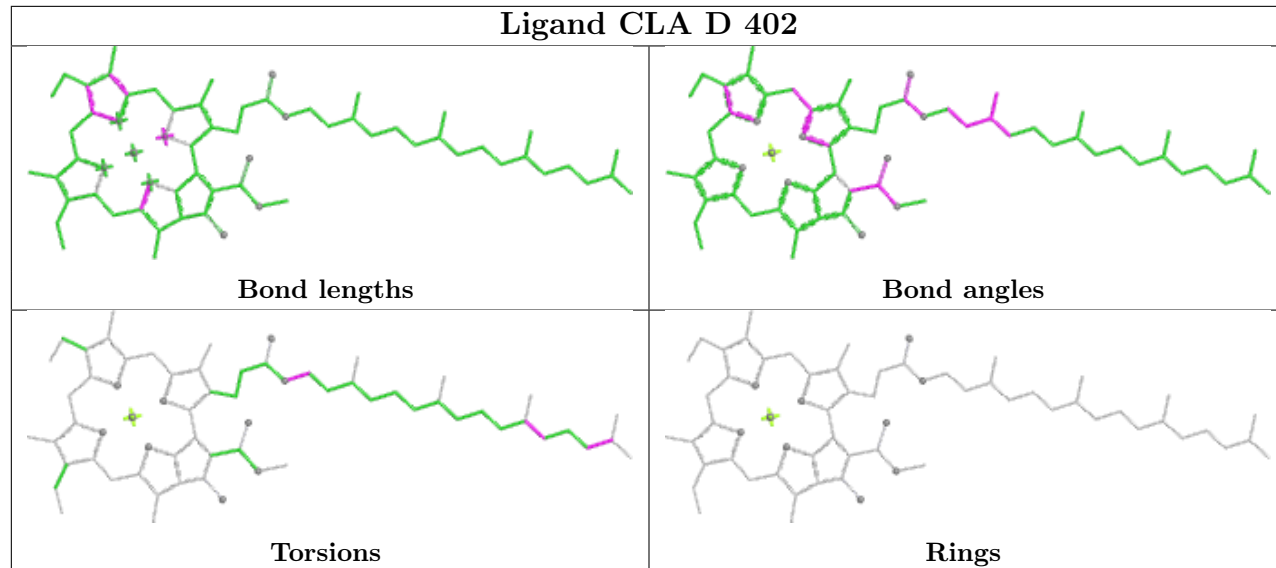
Ligand CLA B 611



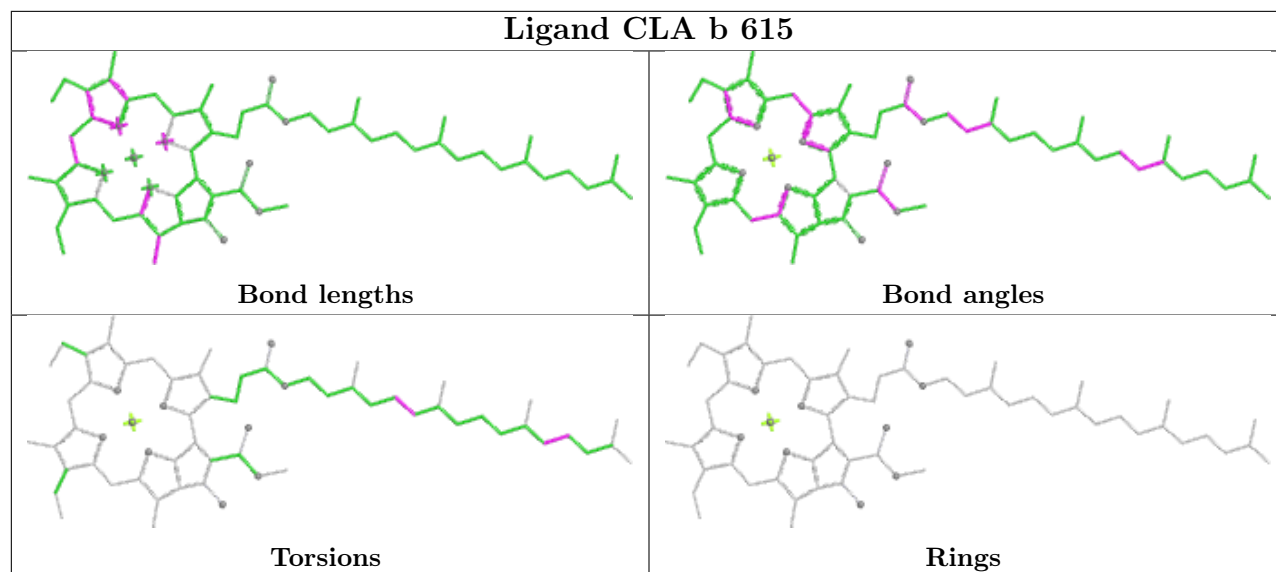
Ligand STE C 519



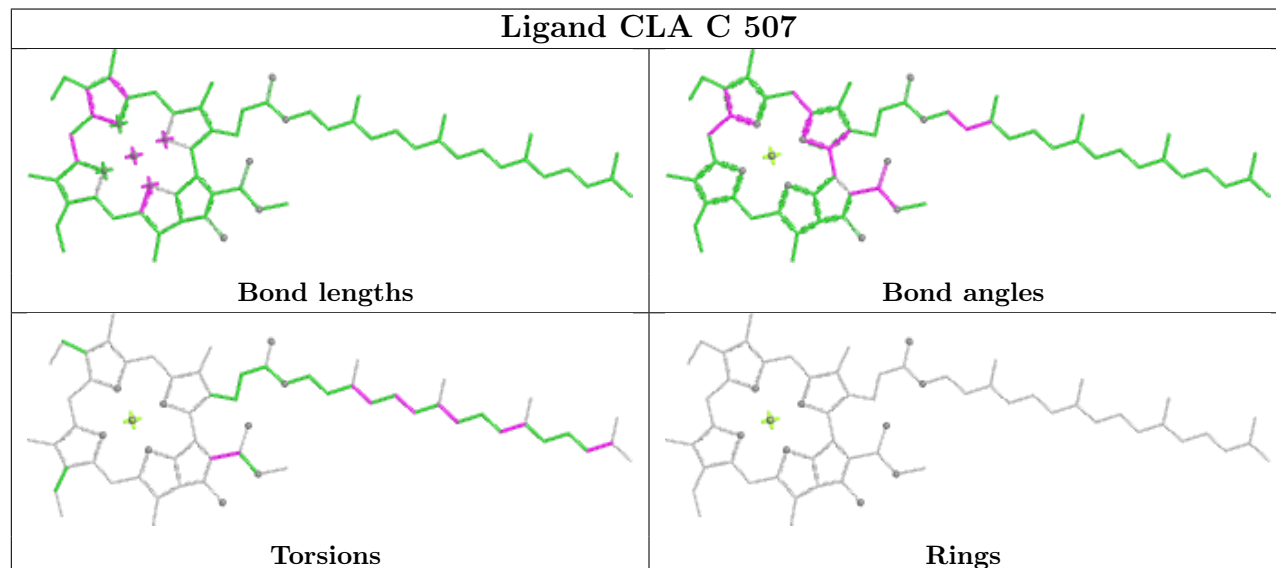
Ligand CLA D 402

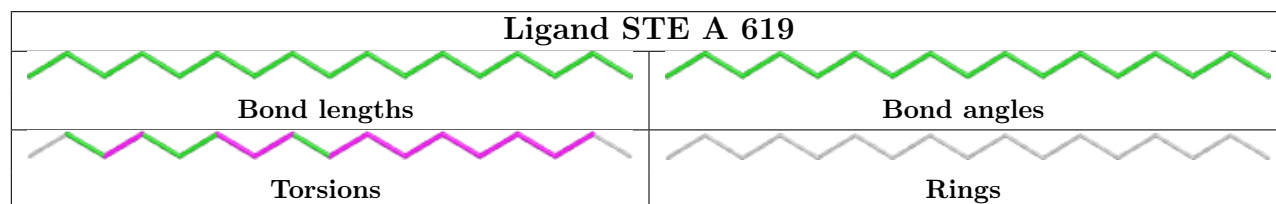
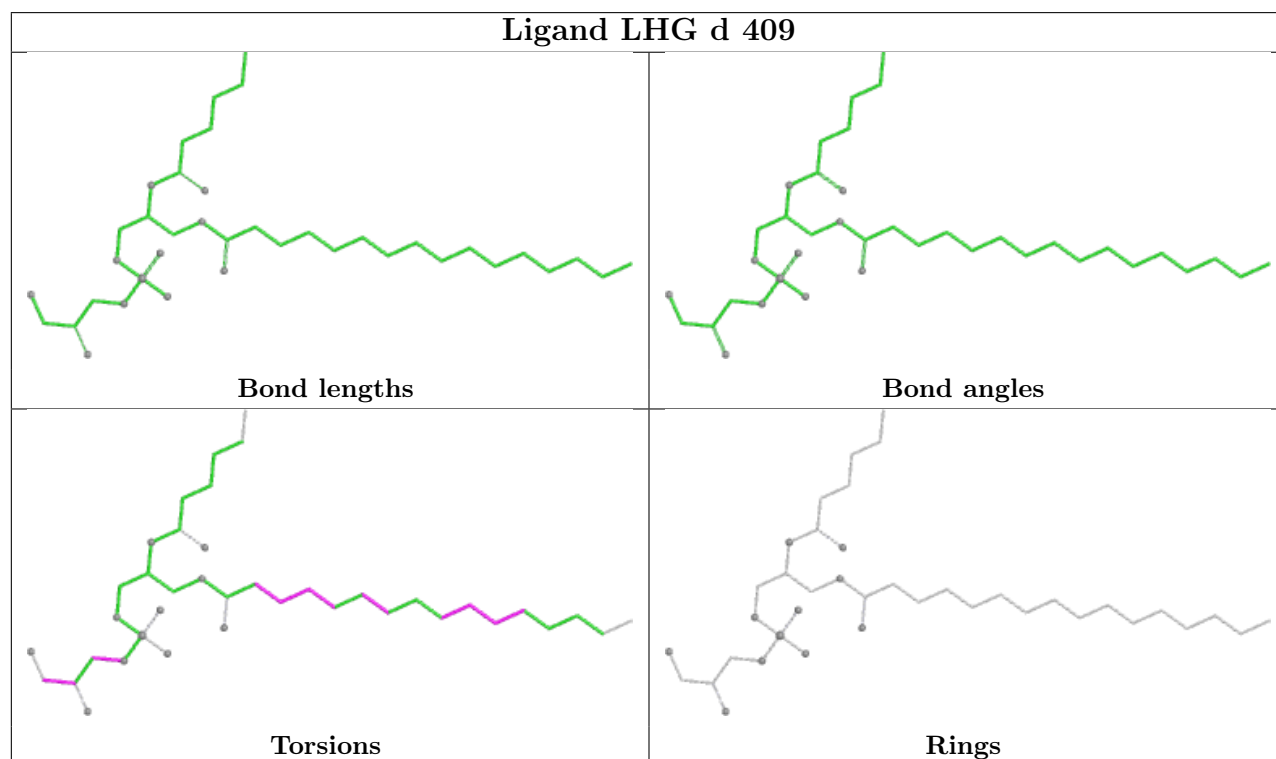
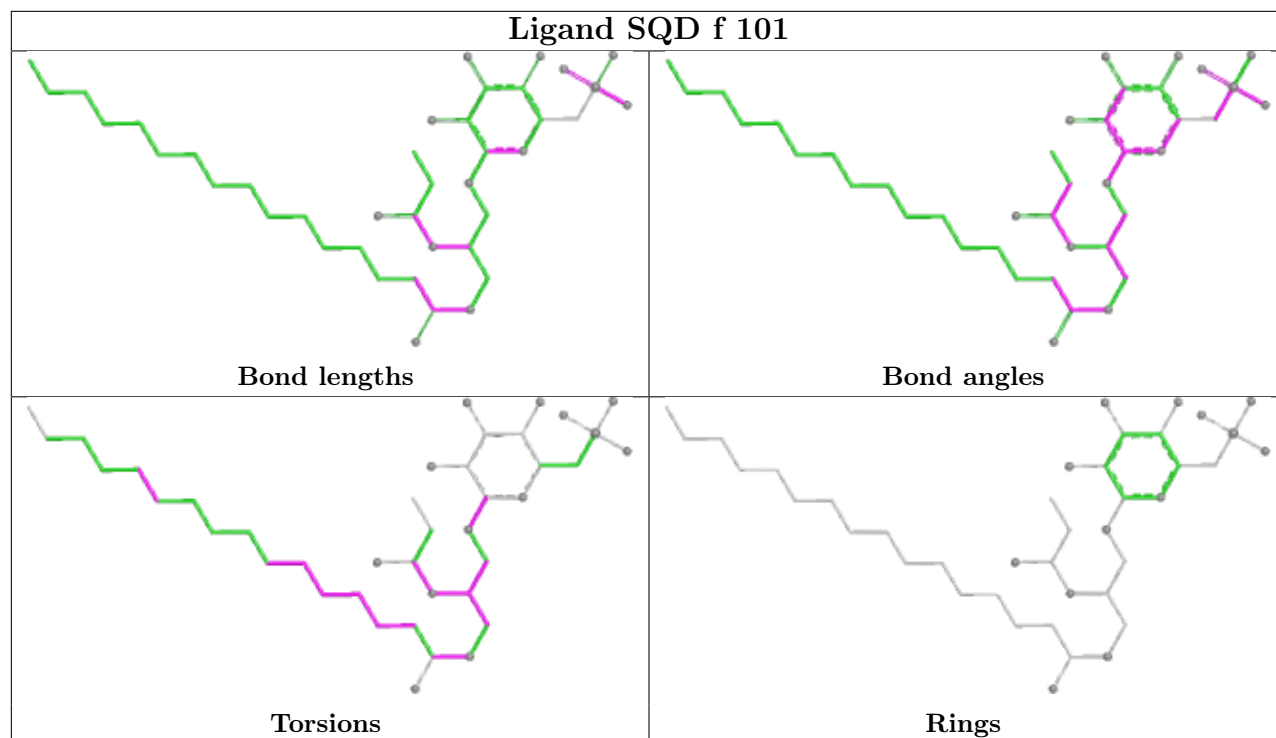


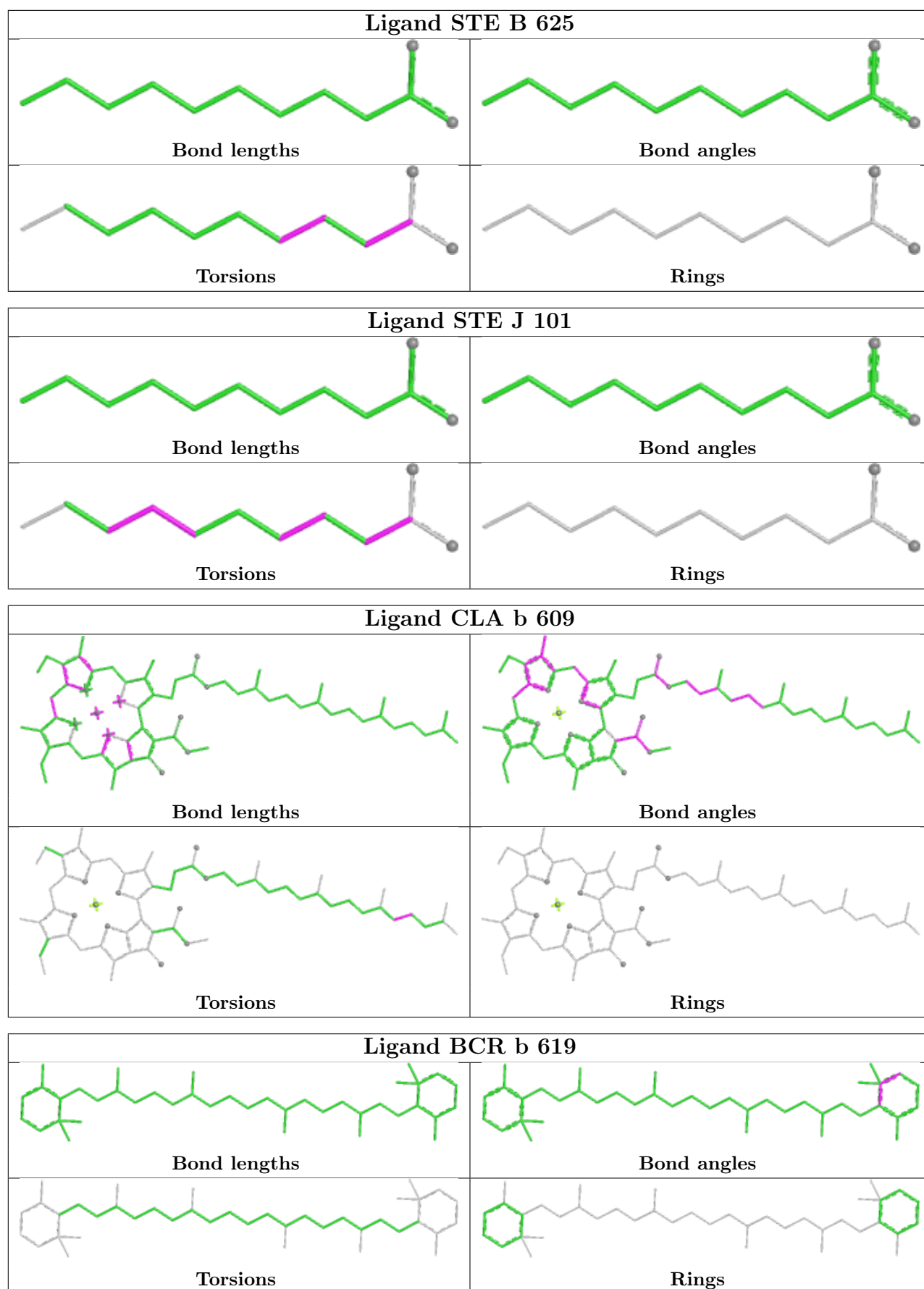
Ligand CLA b 615



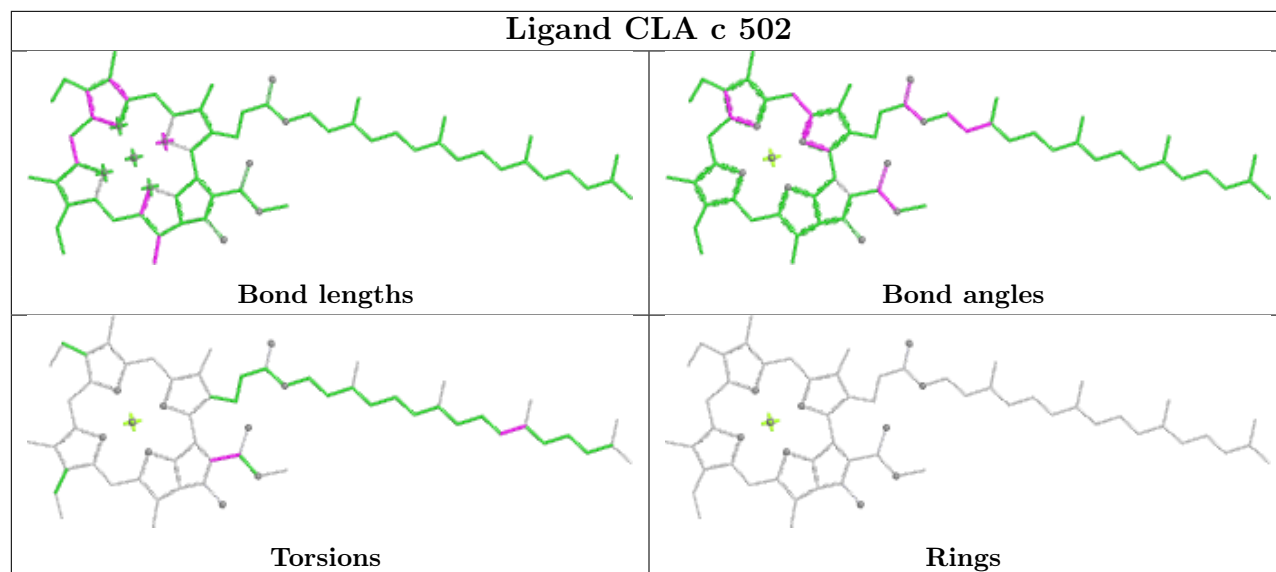
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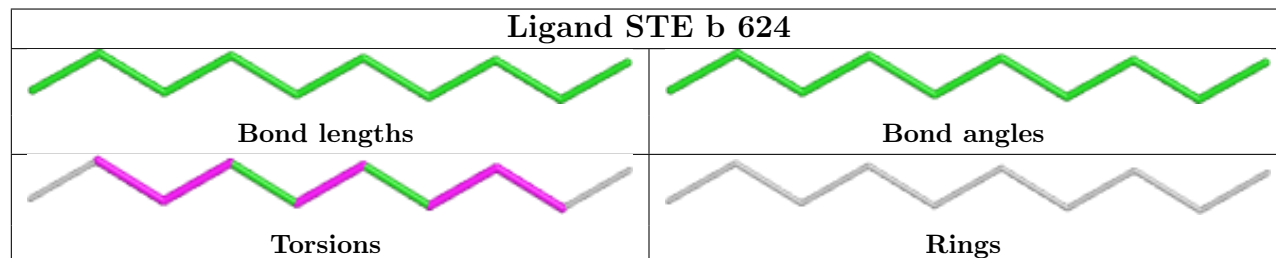




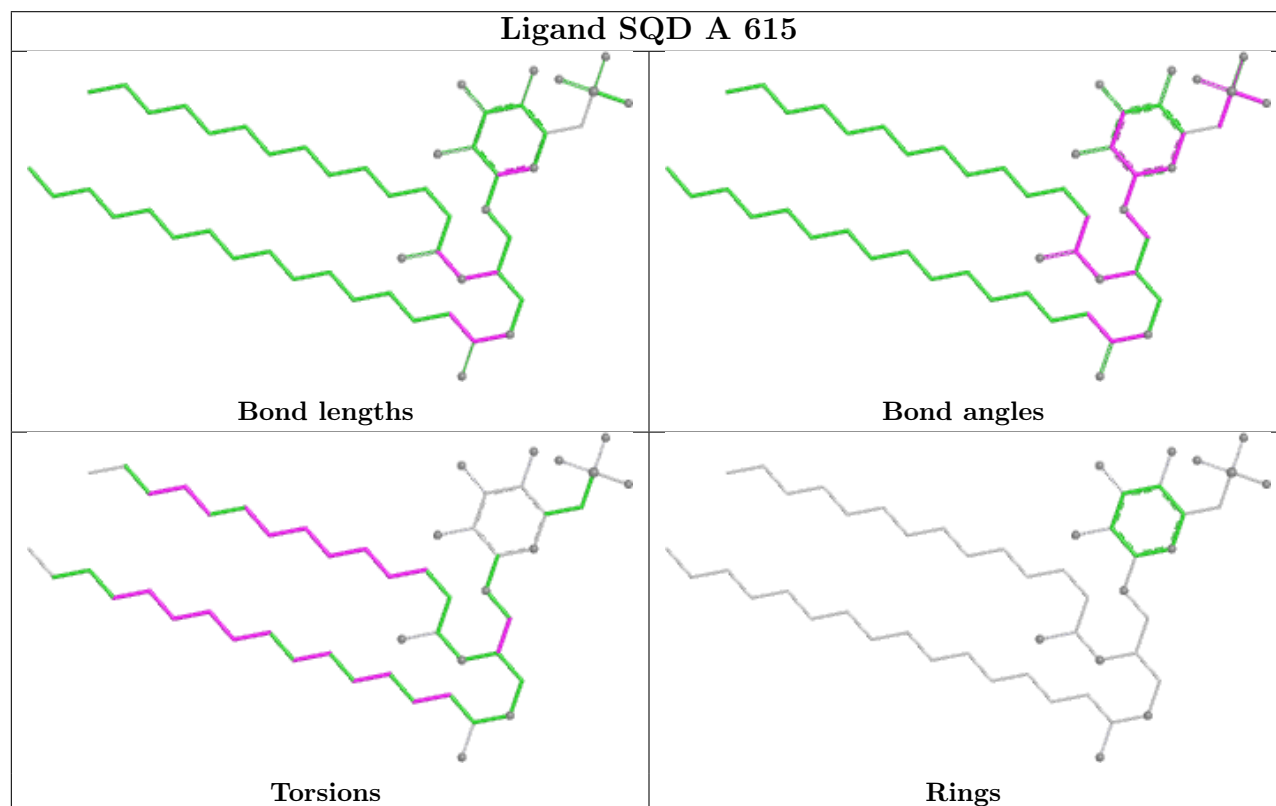
Ligand CLA c 502

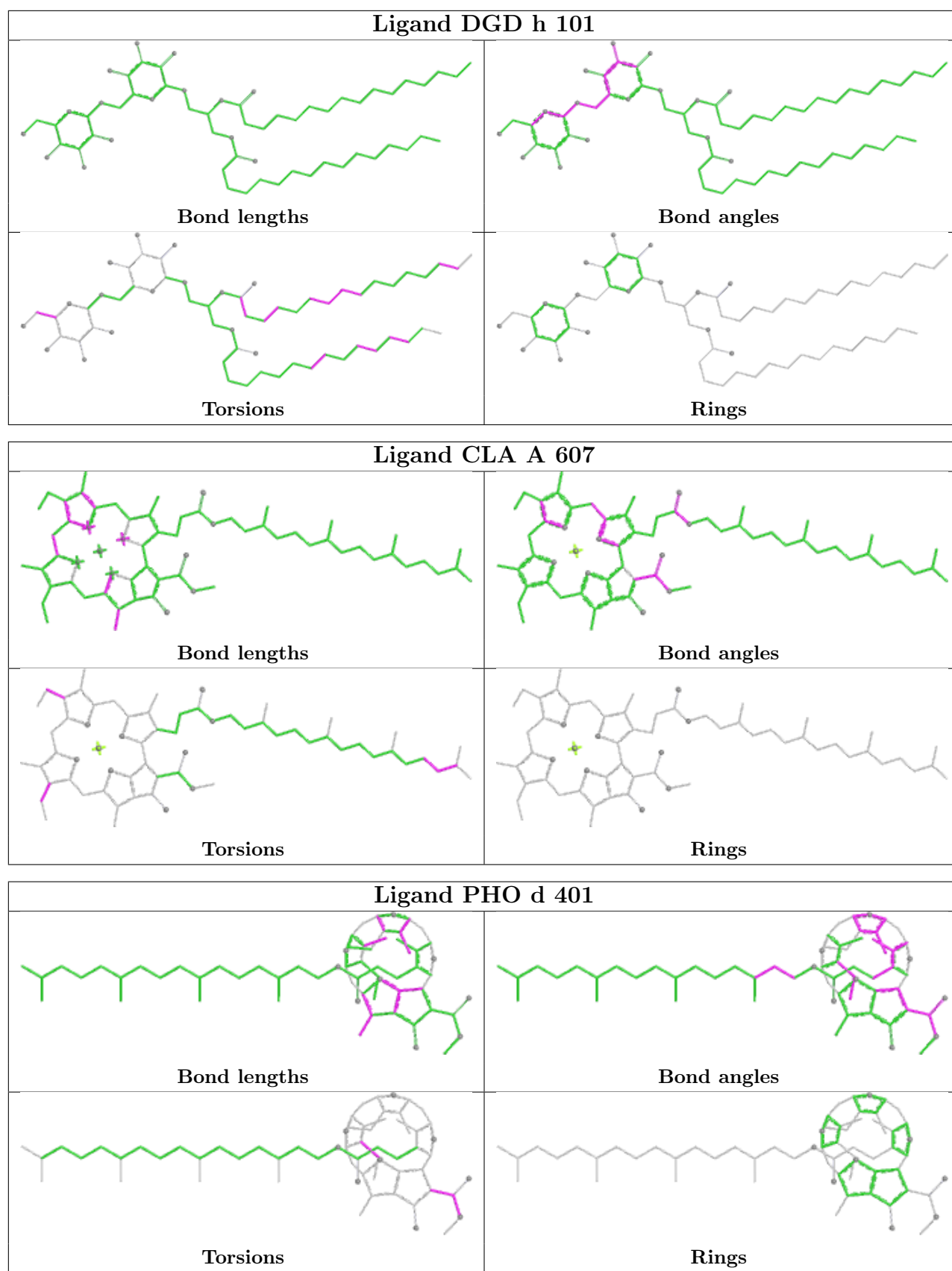


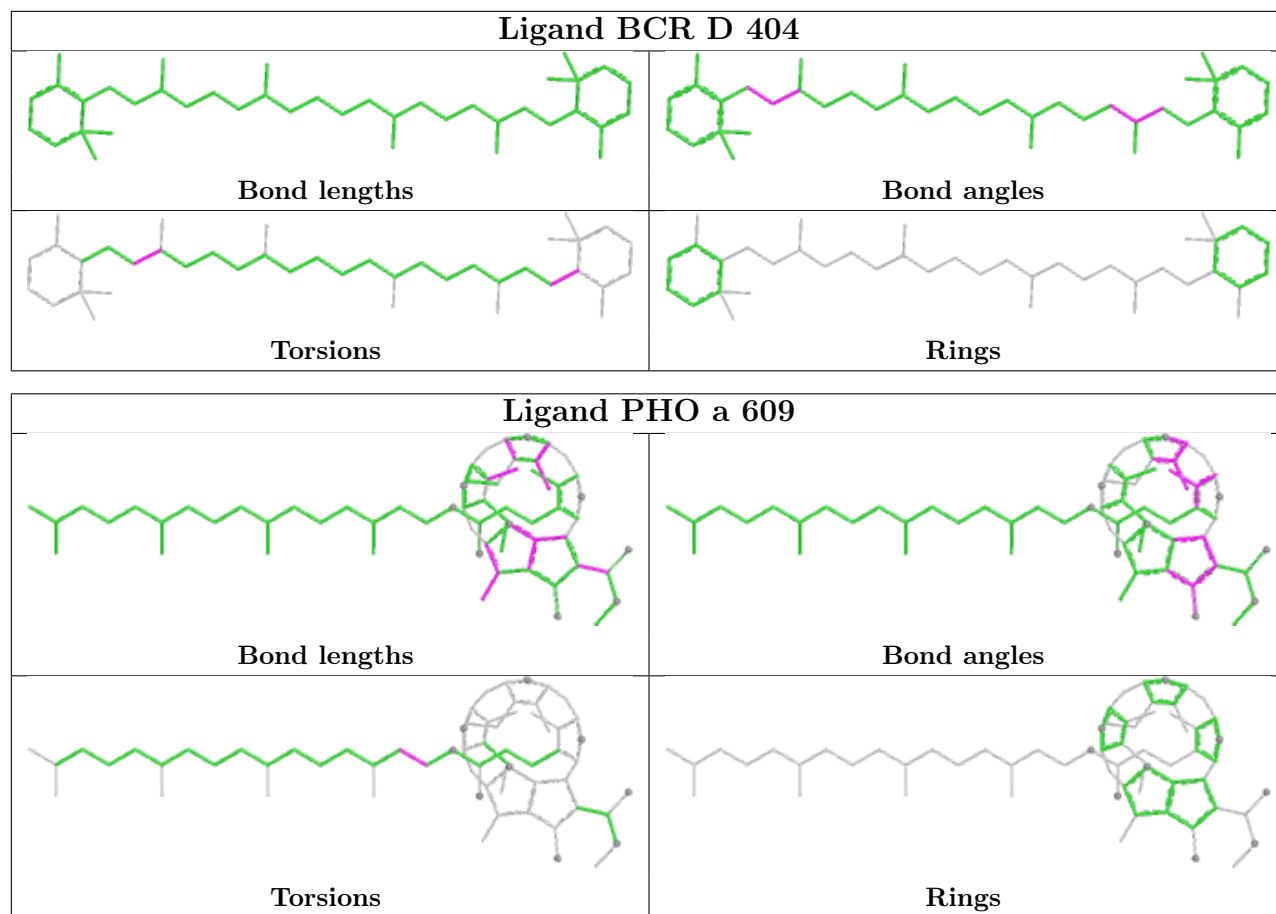
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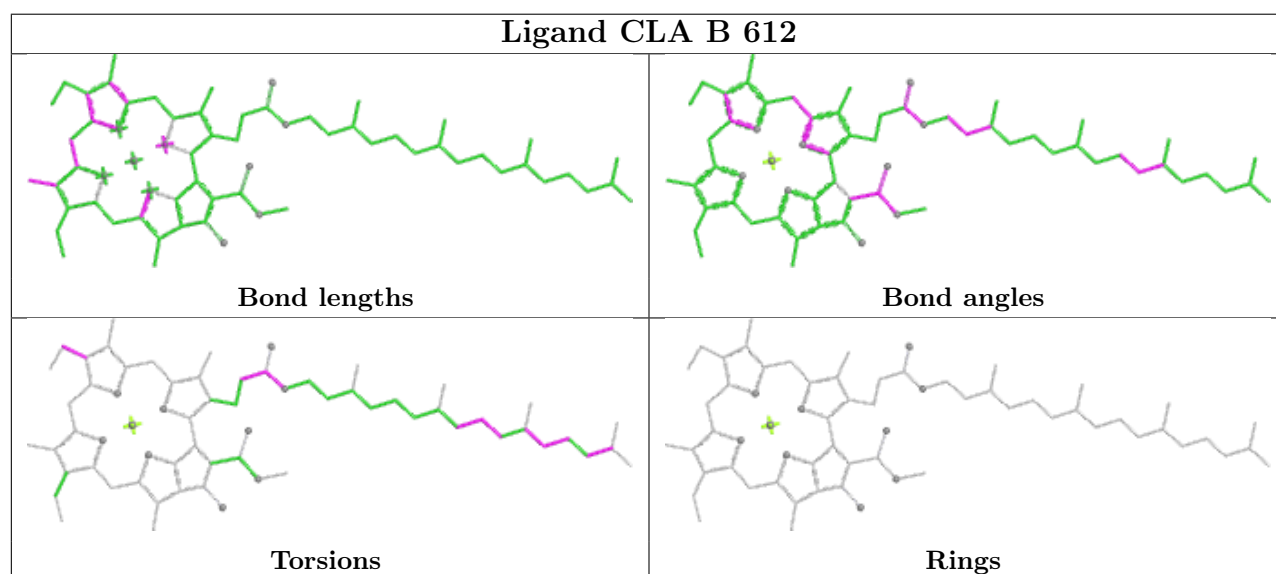
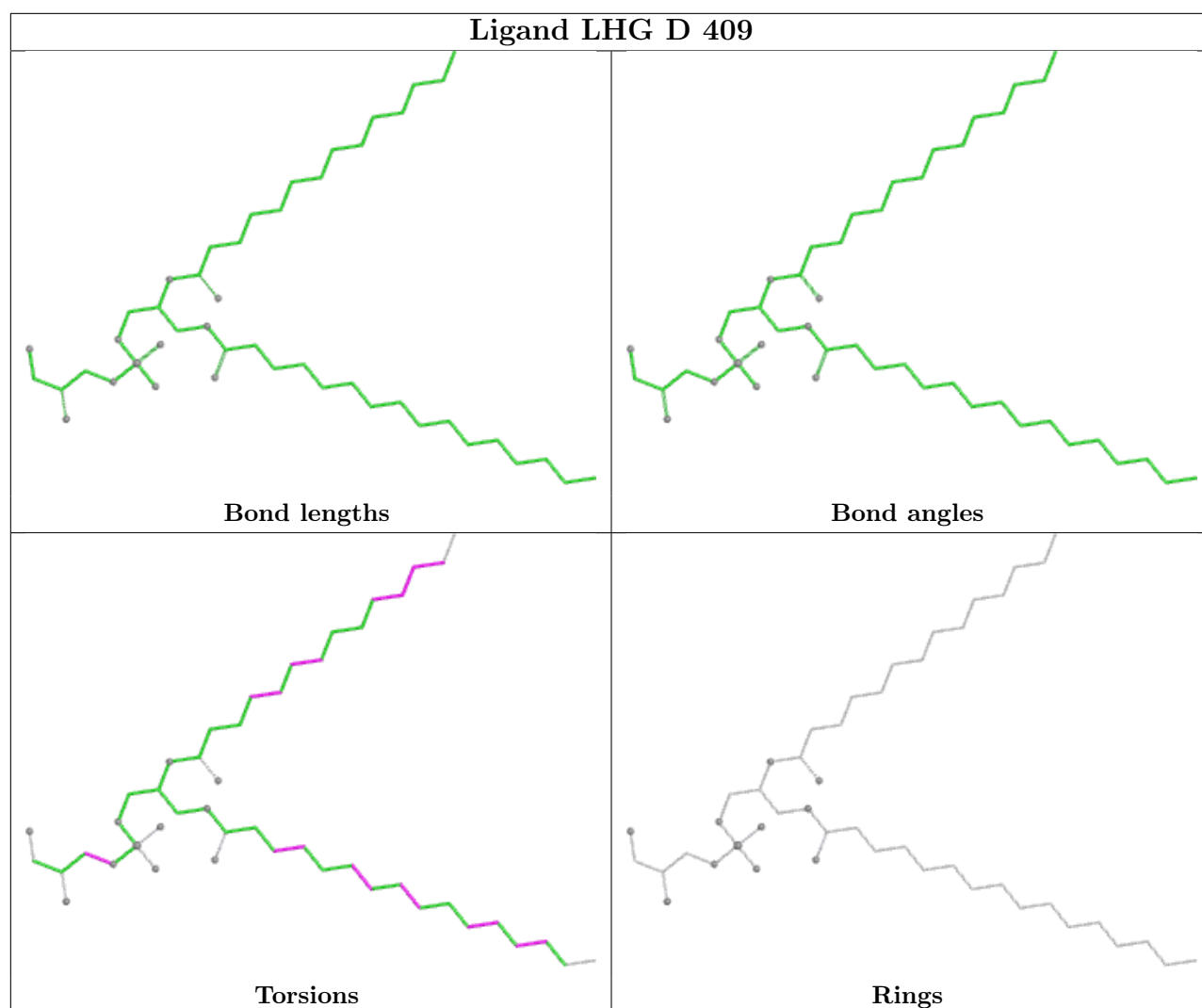


Ligand SQD A 615

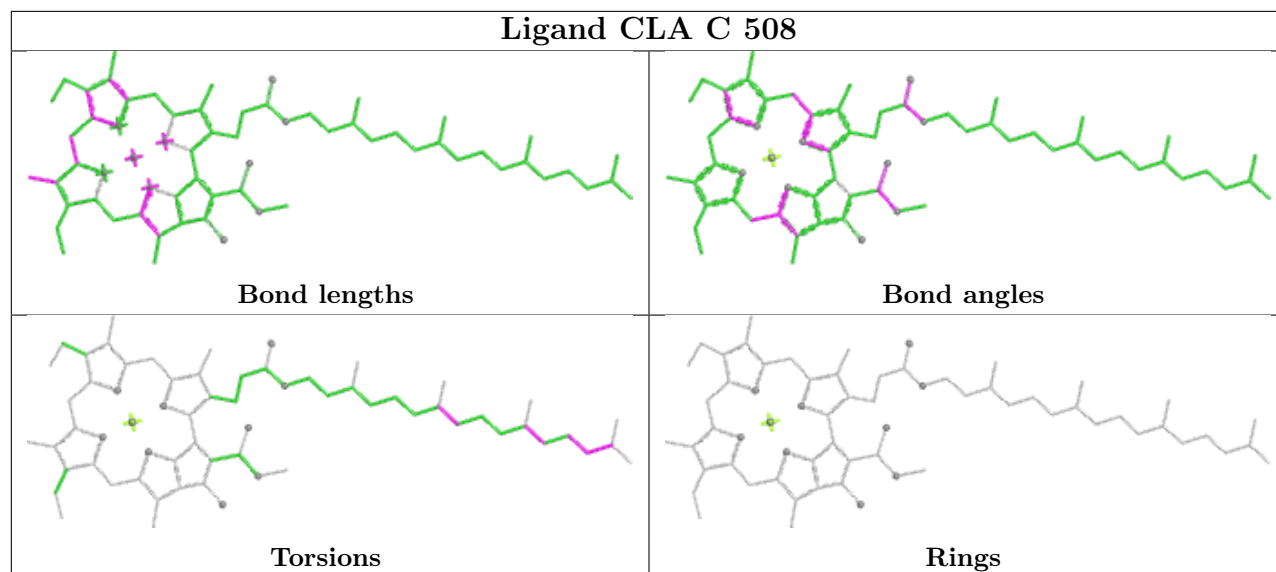




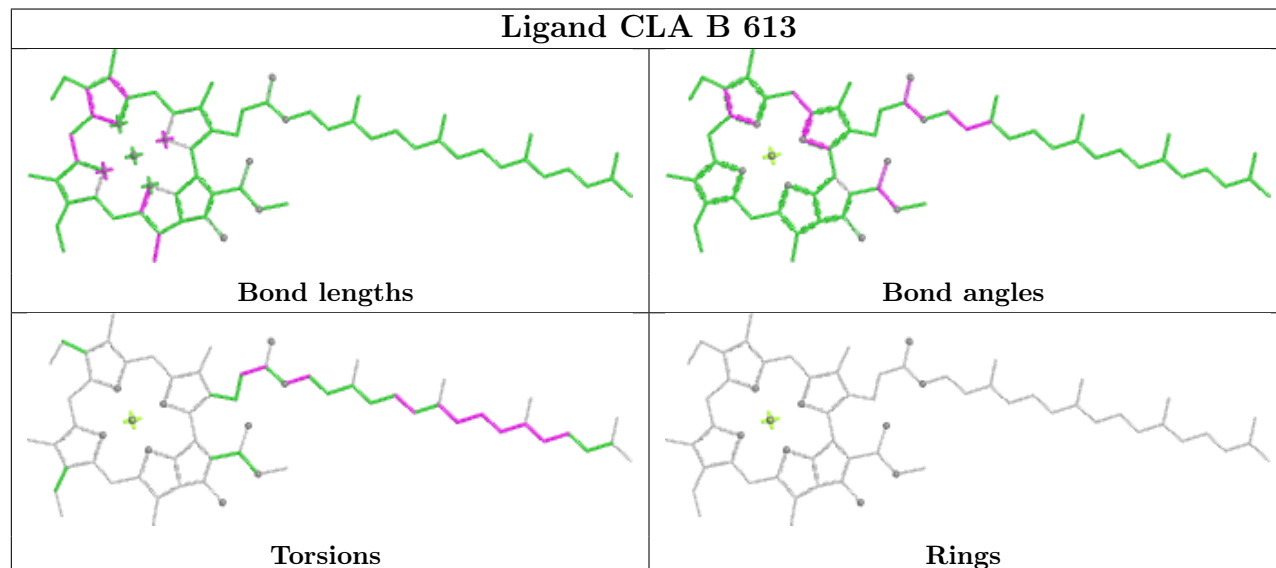




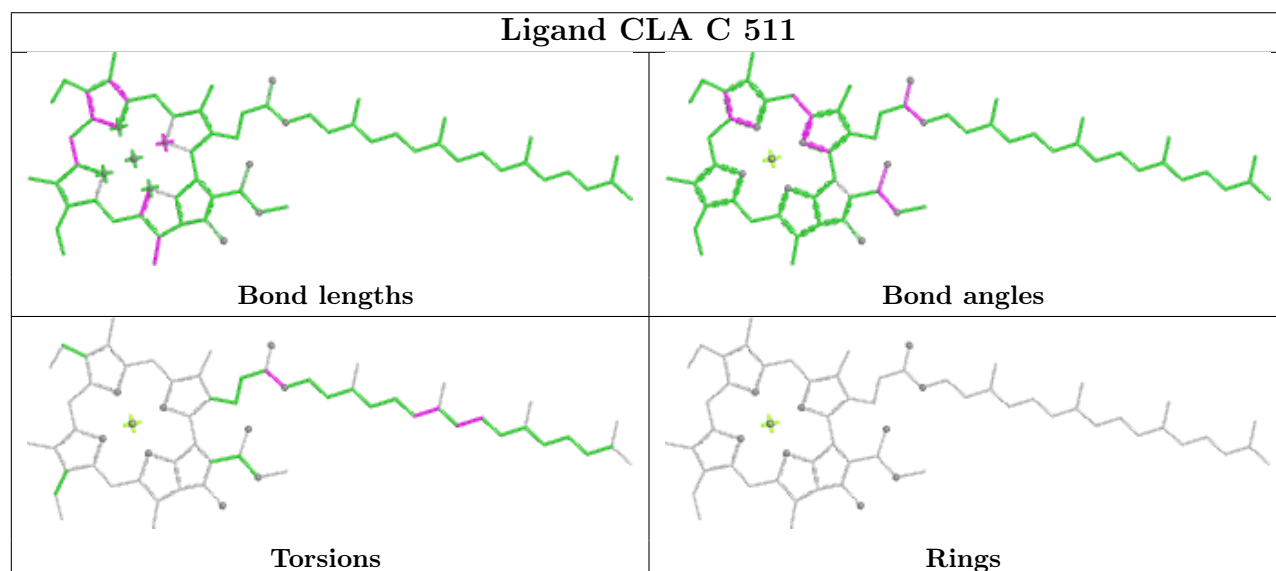
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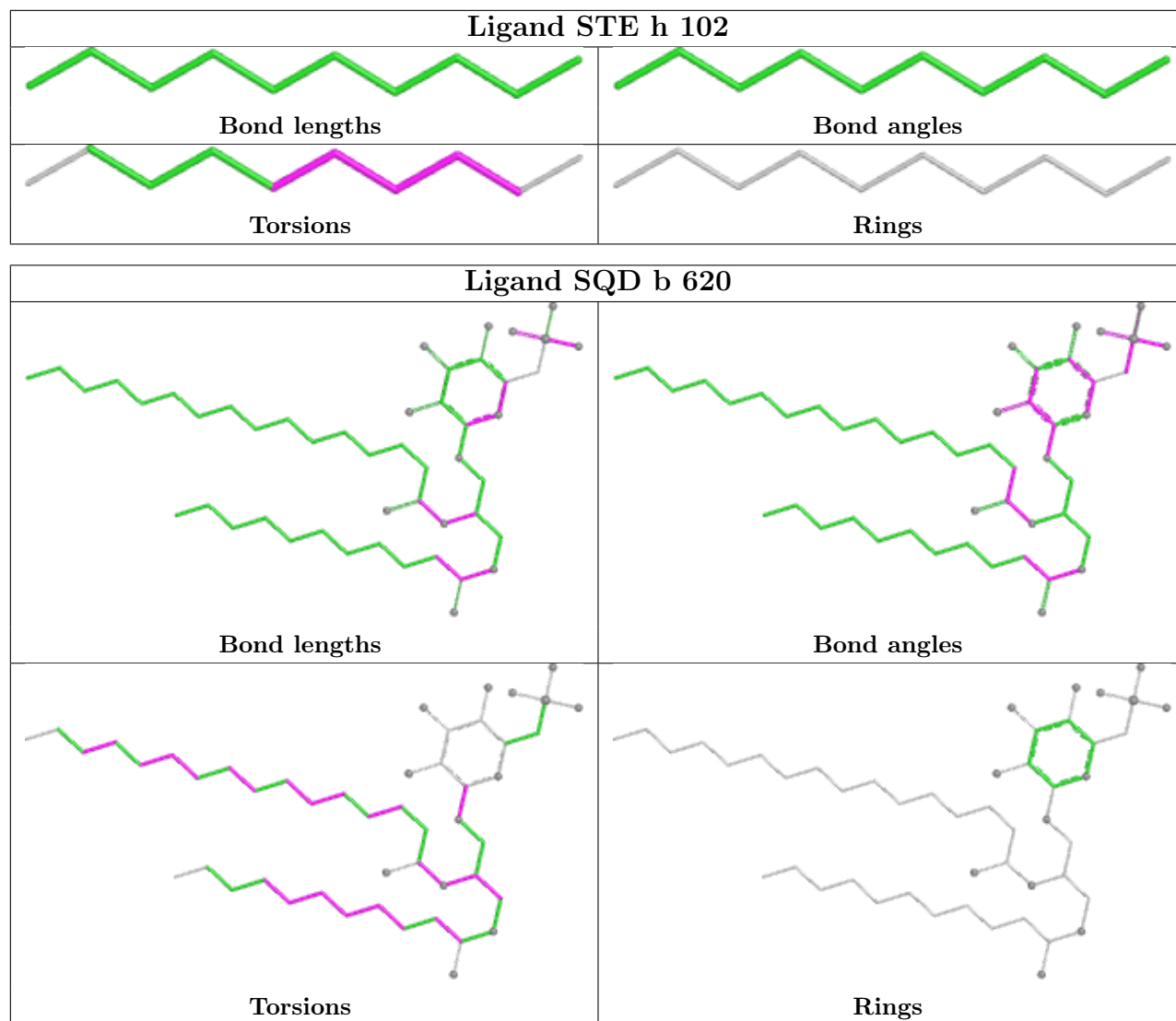


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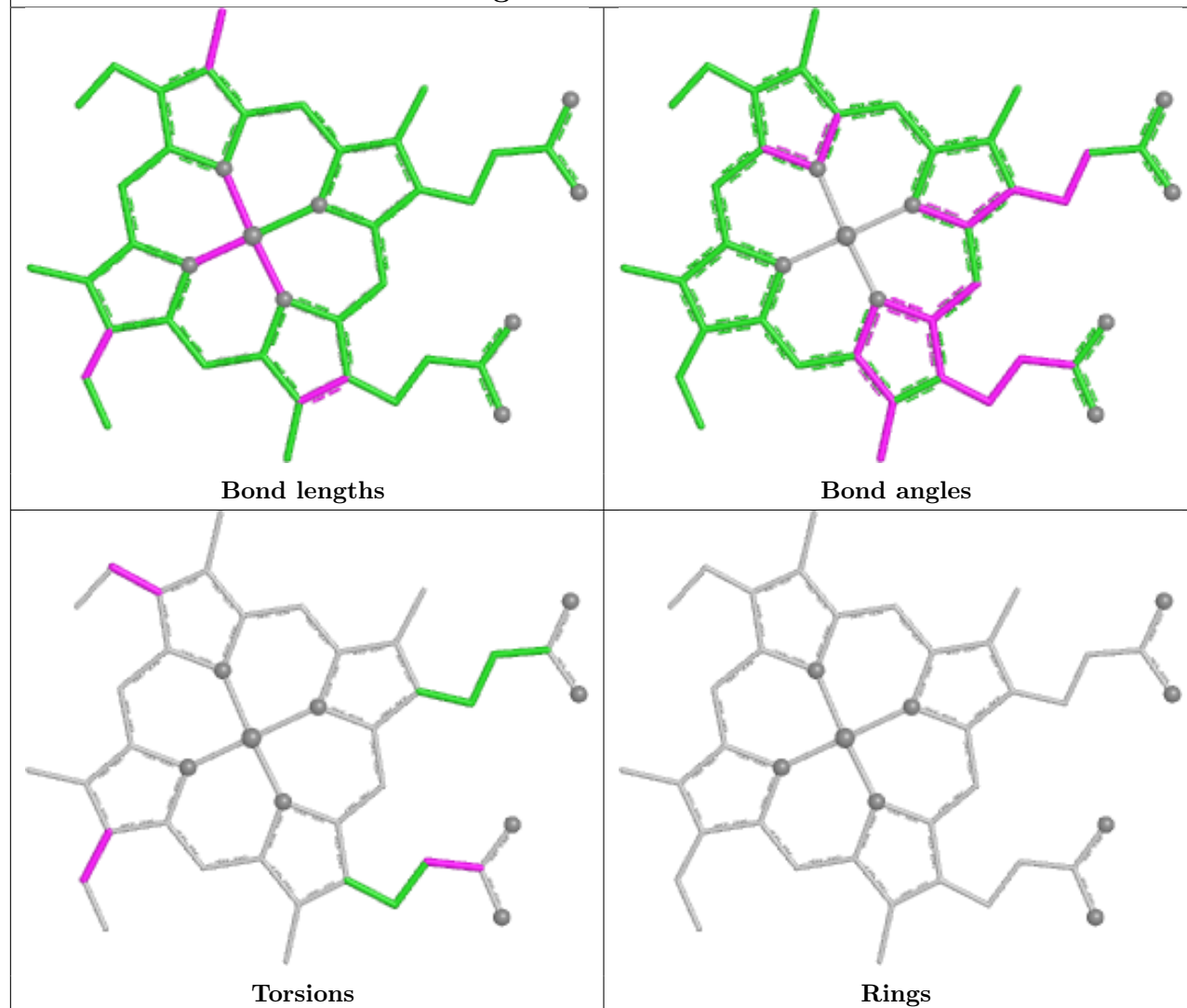


Ligand CLA C 511

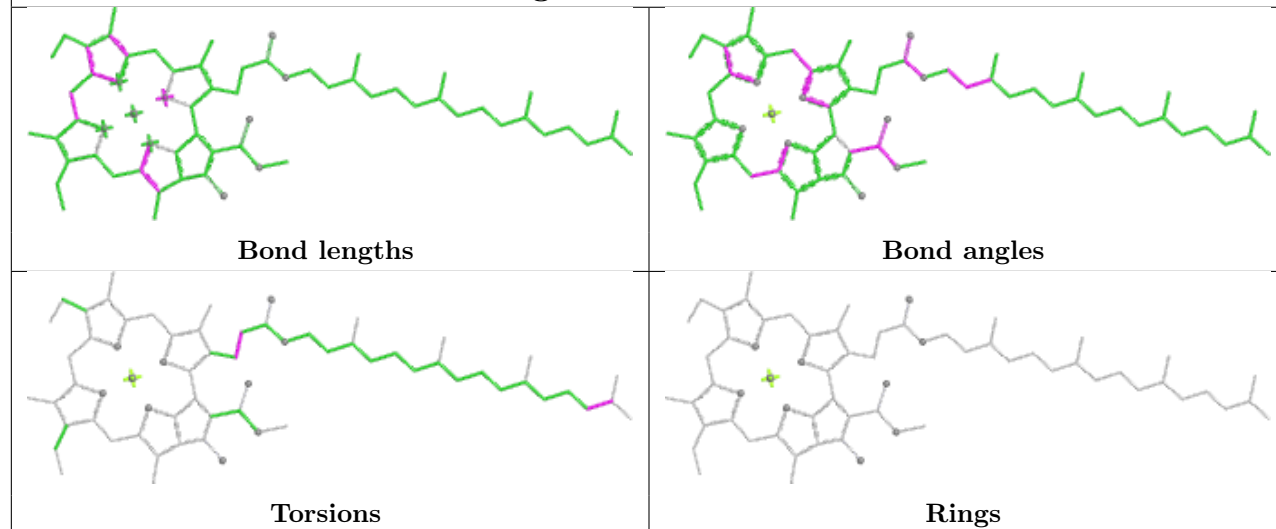


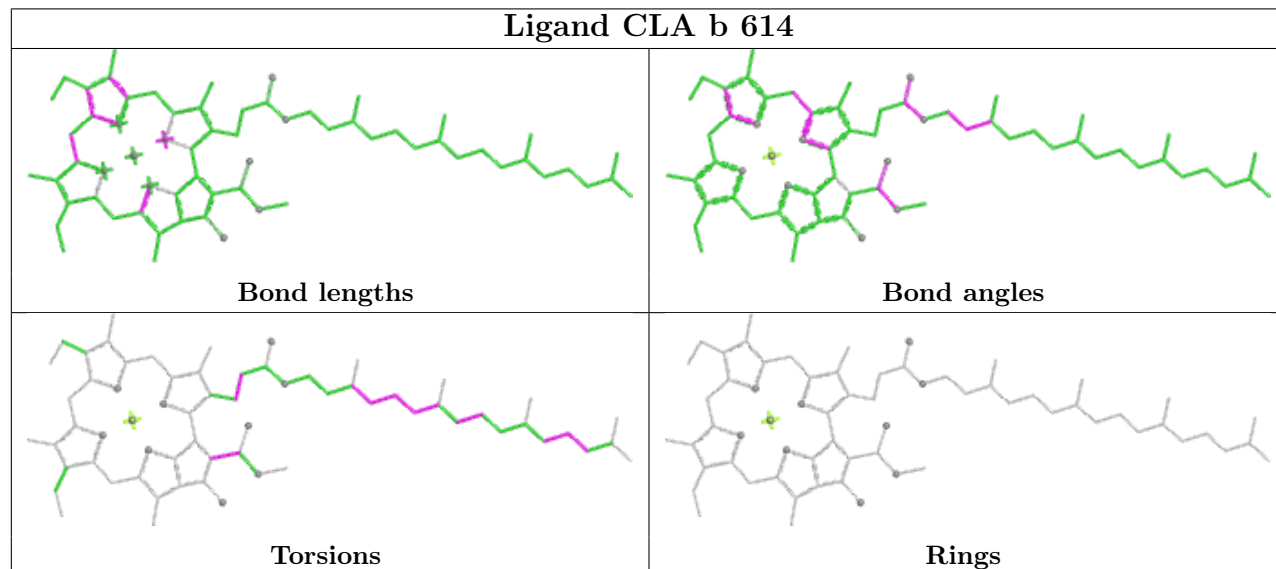
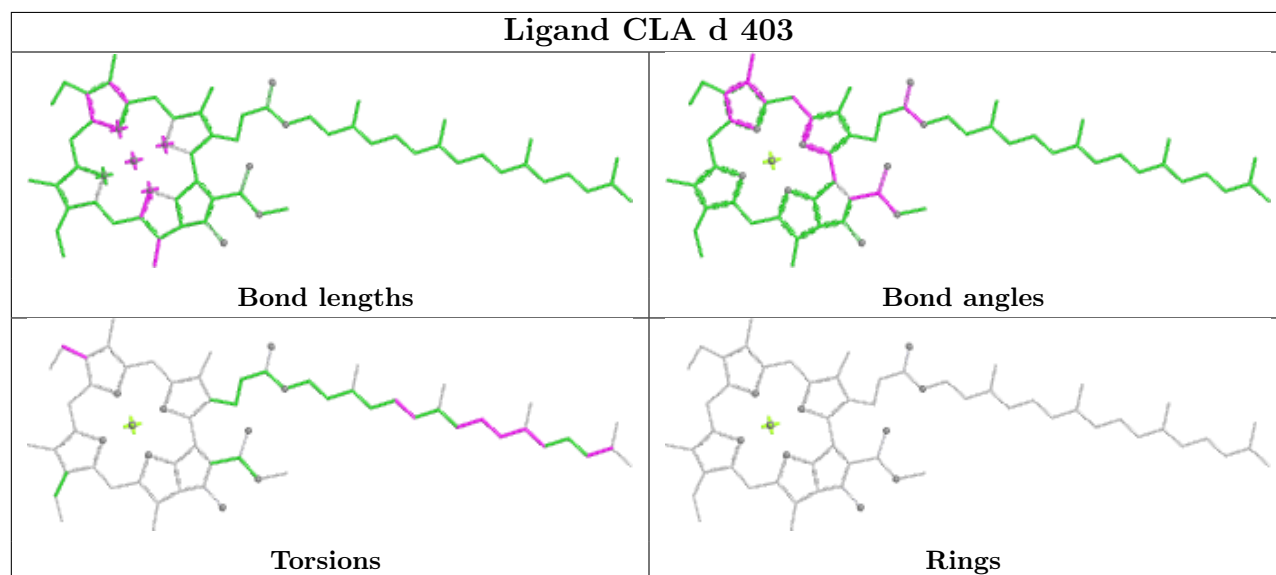
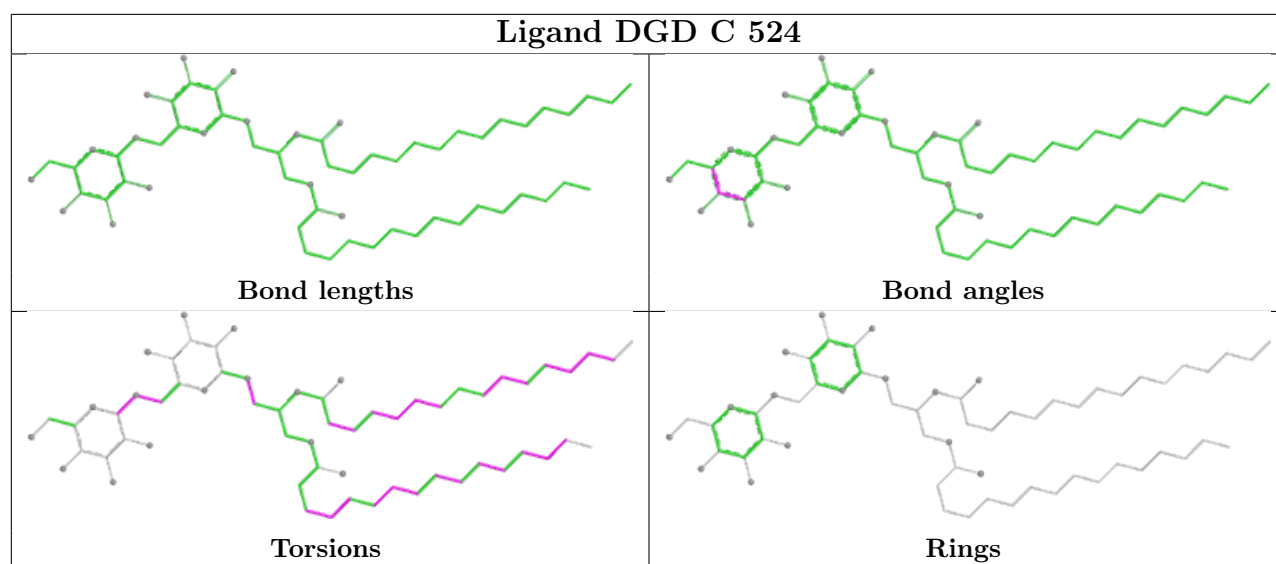


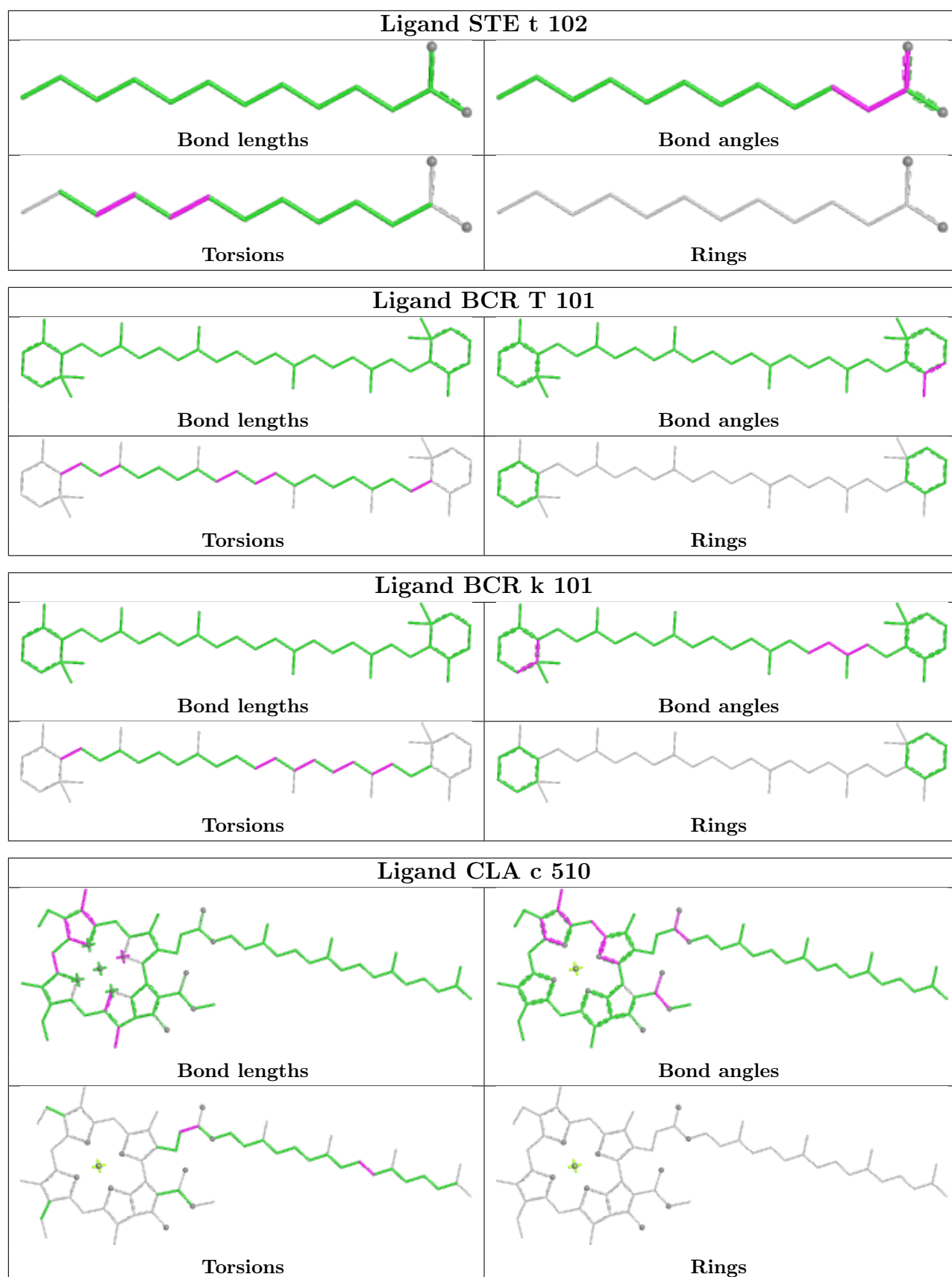
Ligand HEC V 201

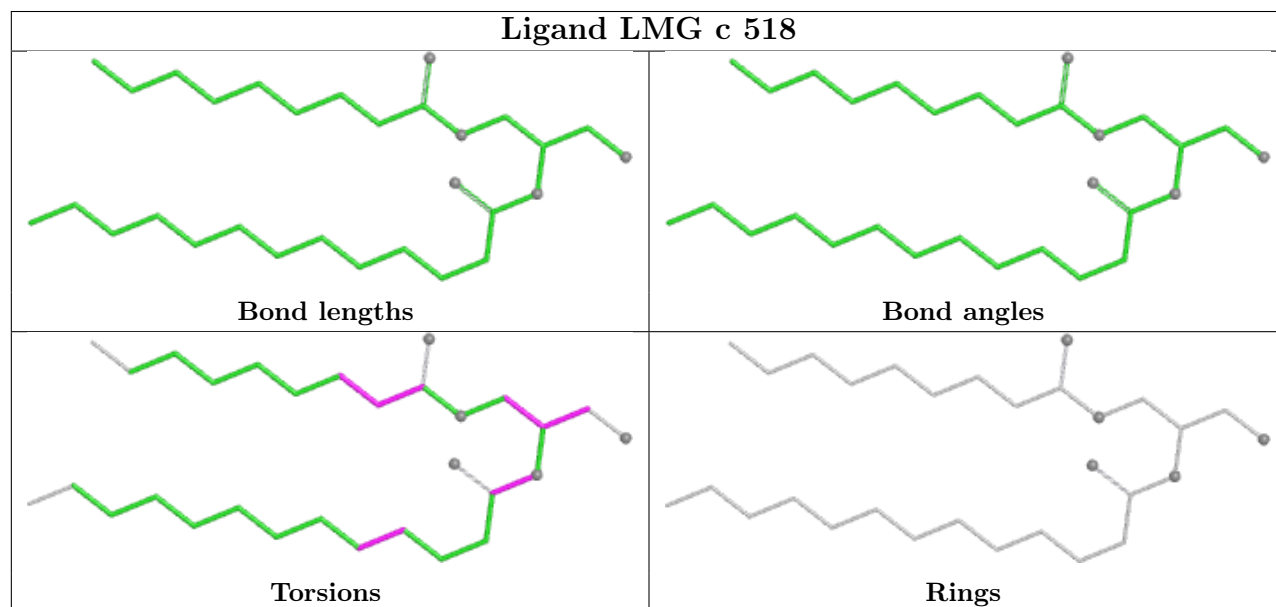
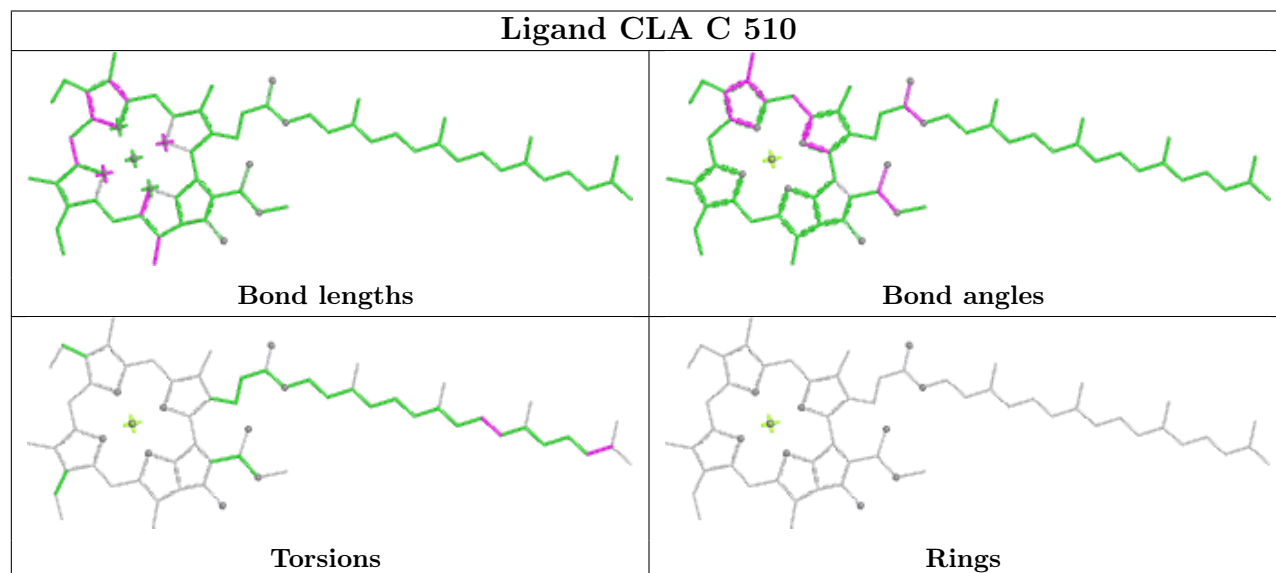
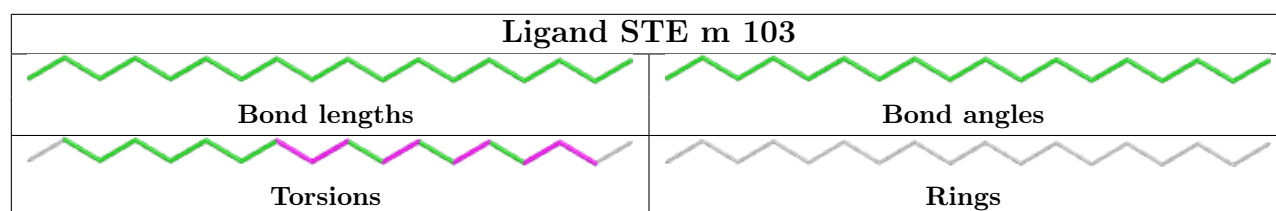


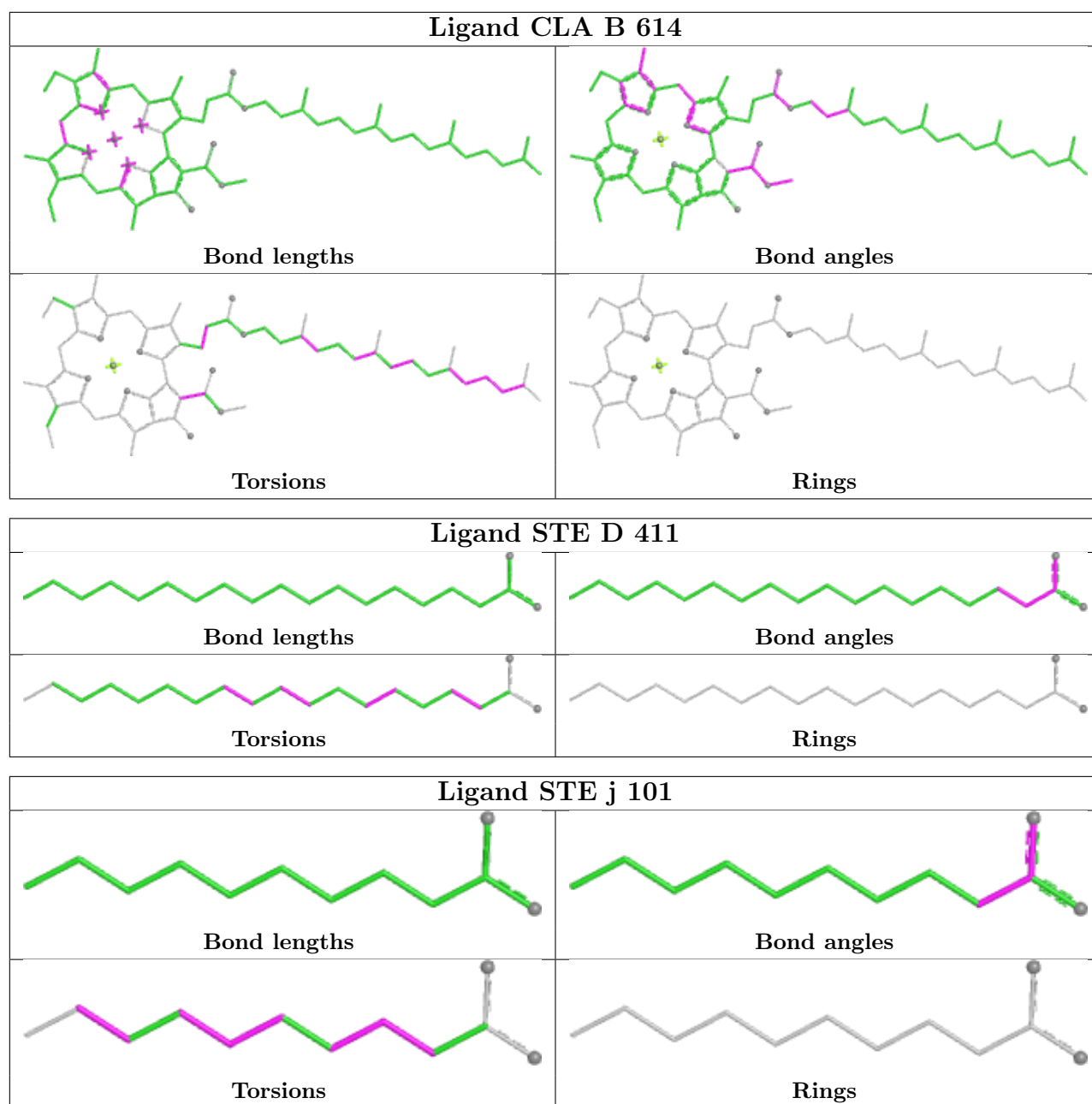
Ligand CLA B 610

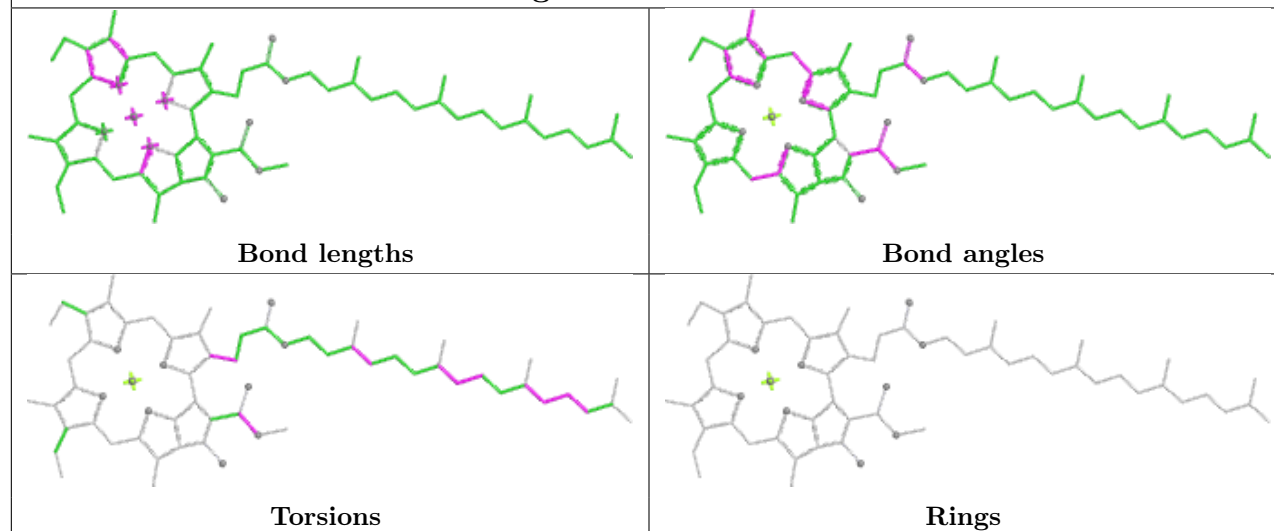
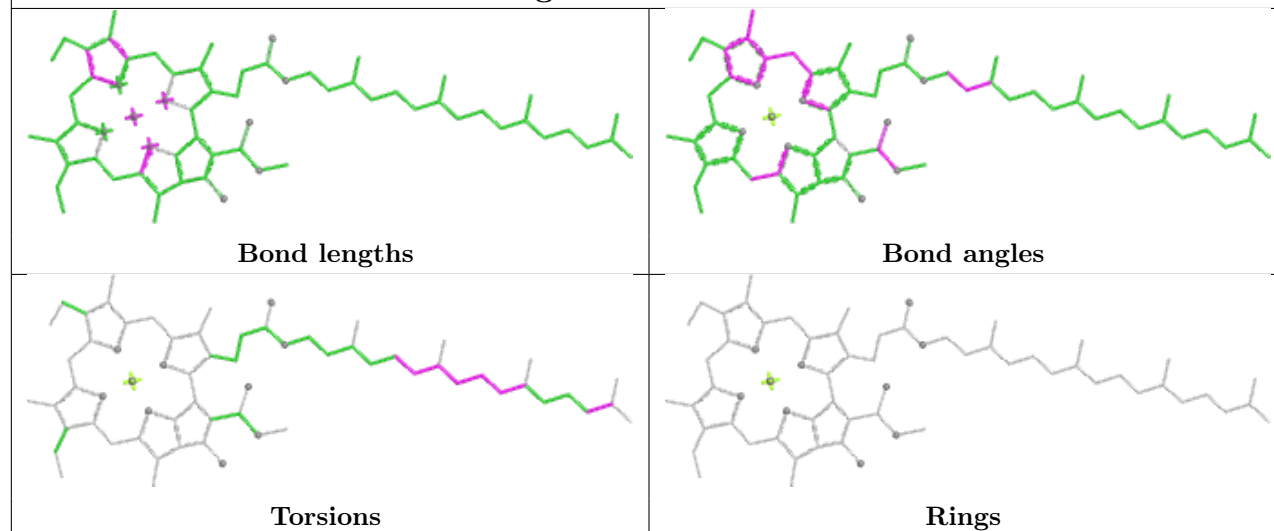
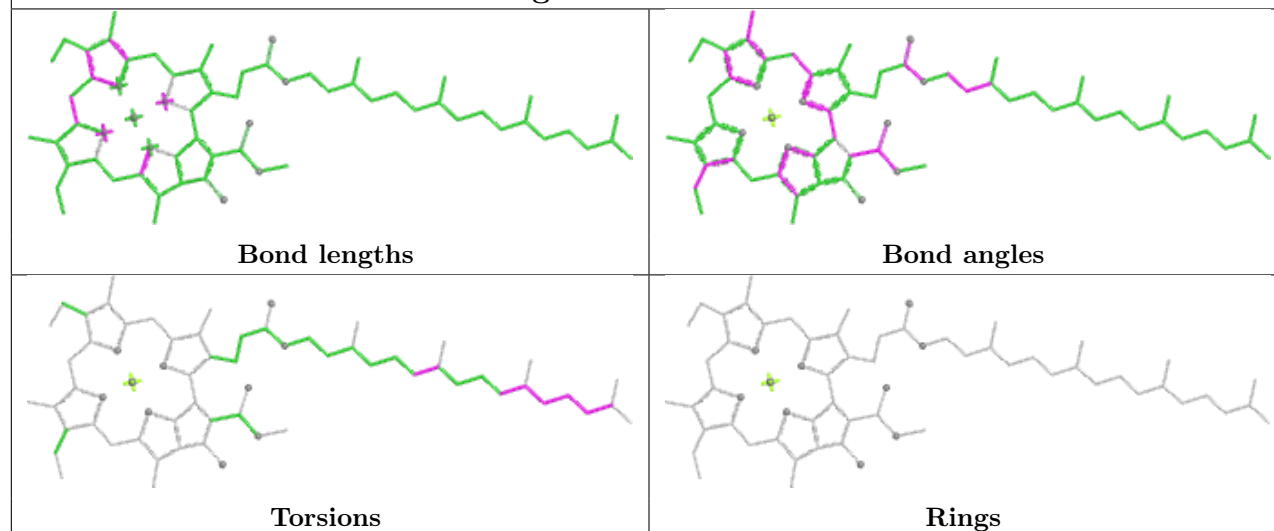


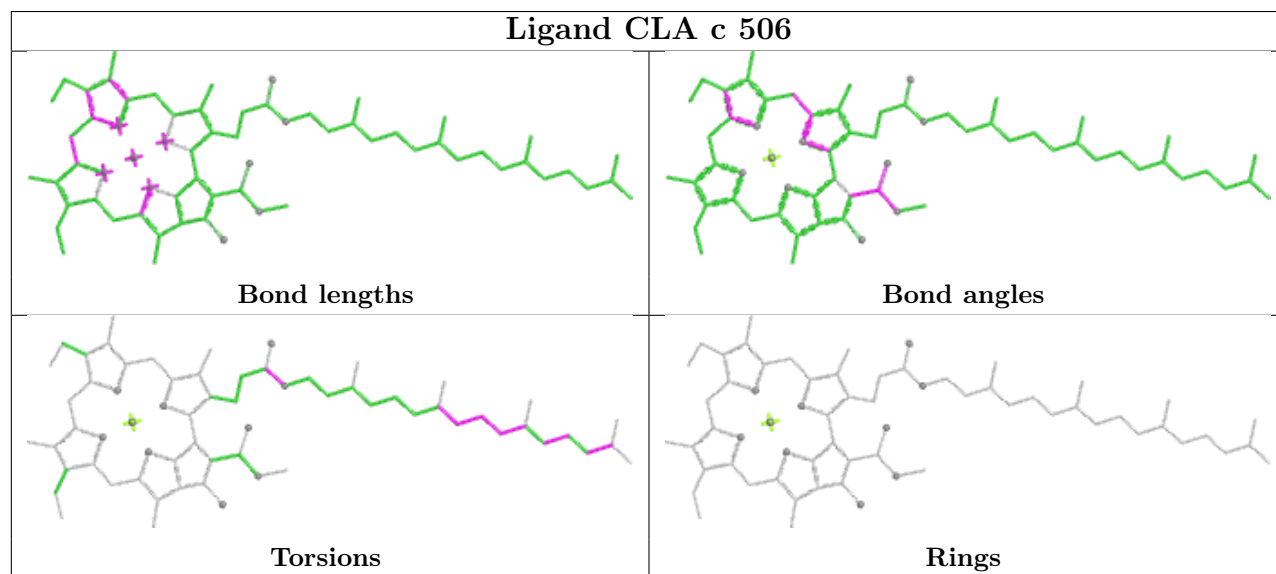
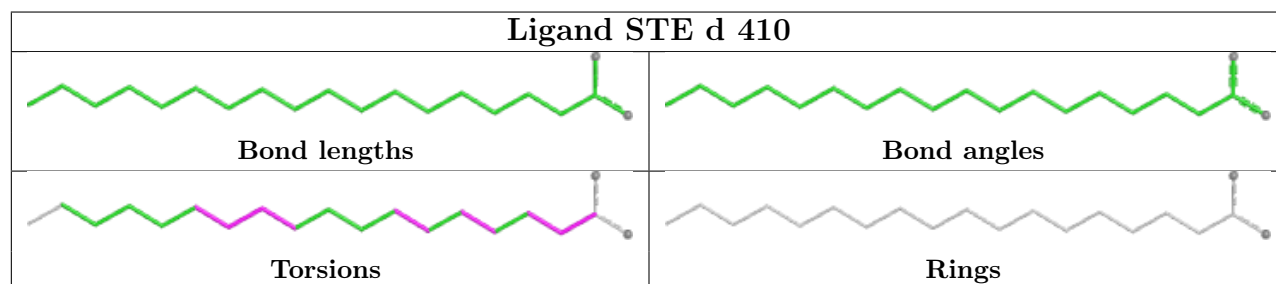
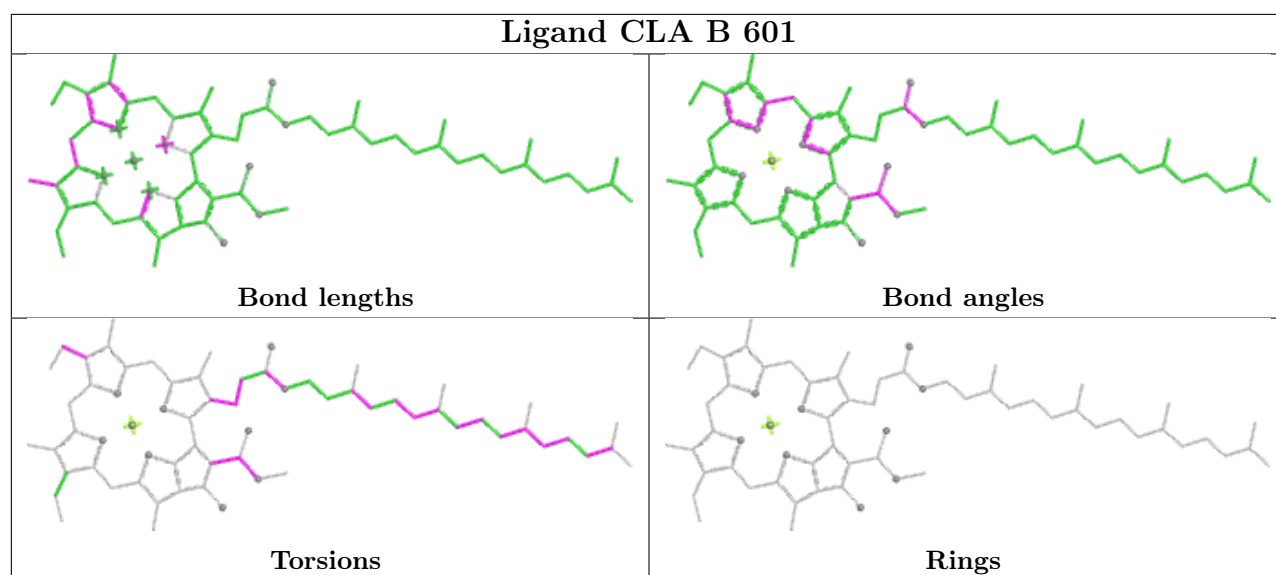


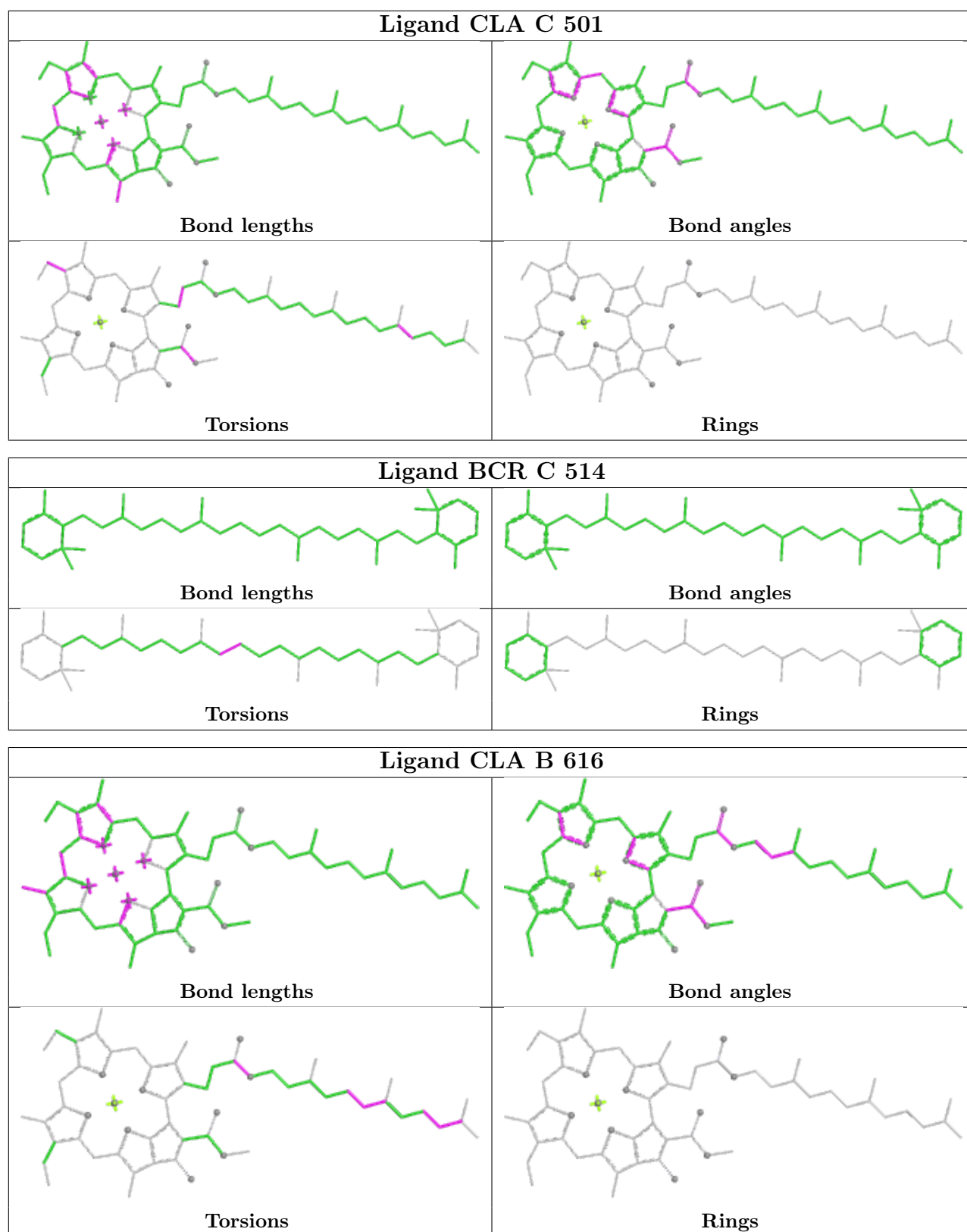


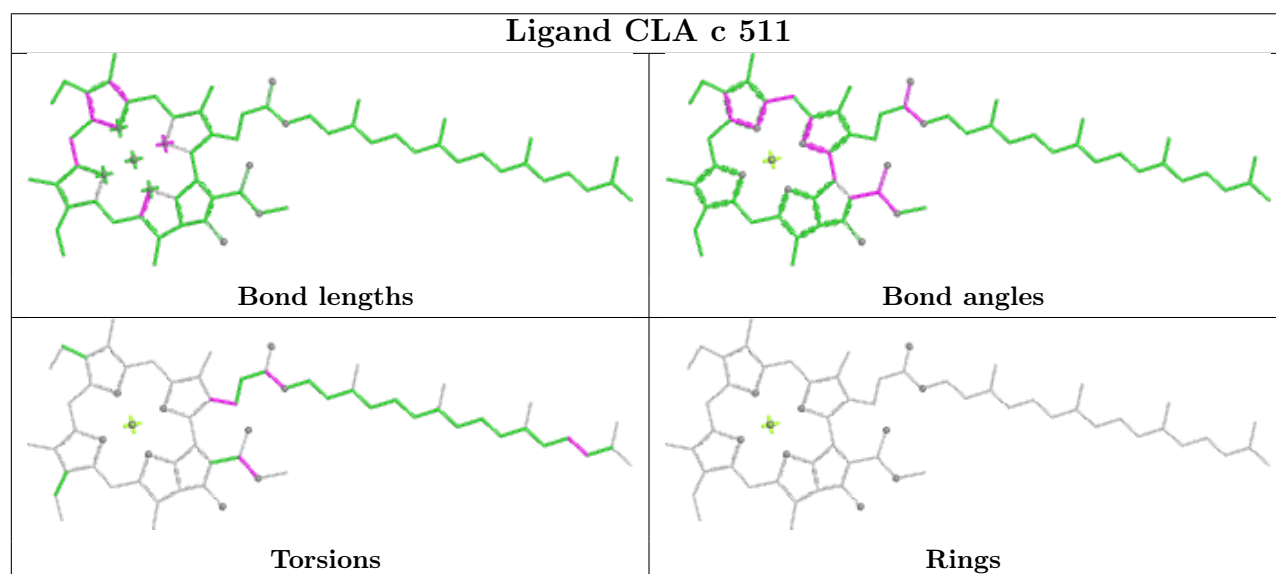
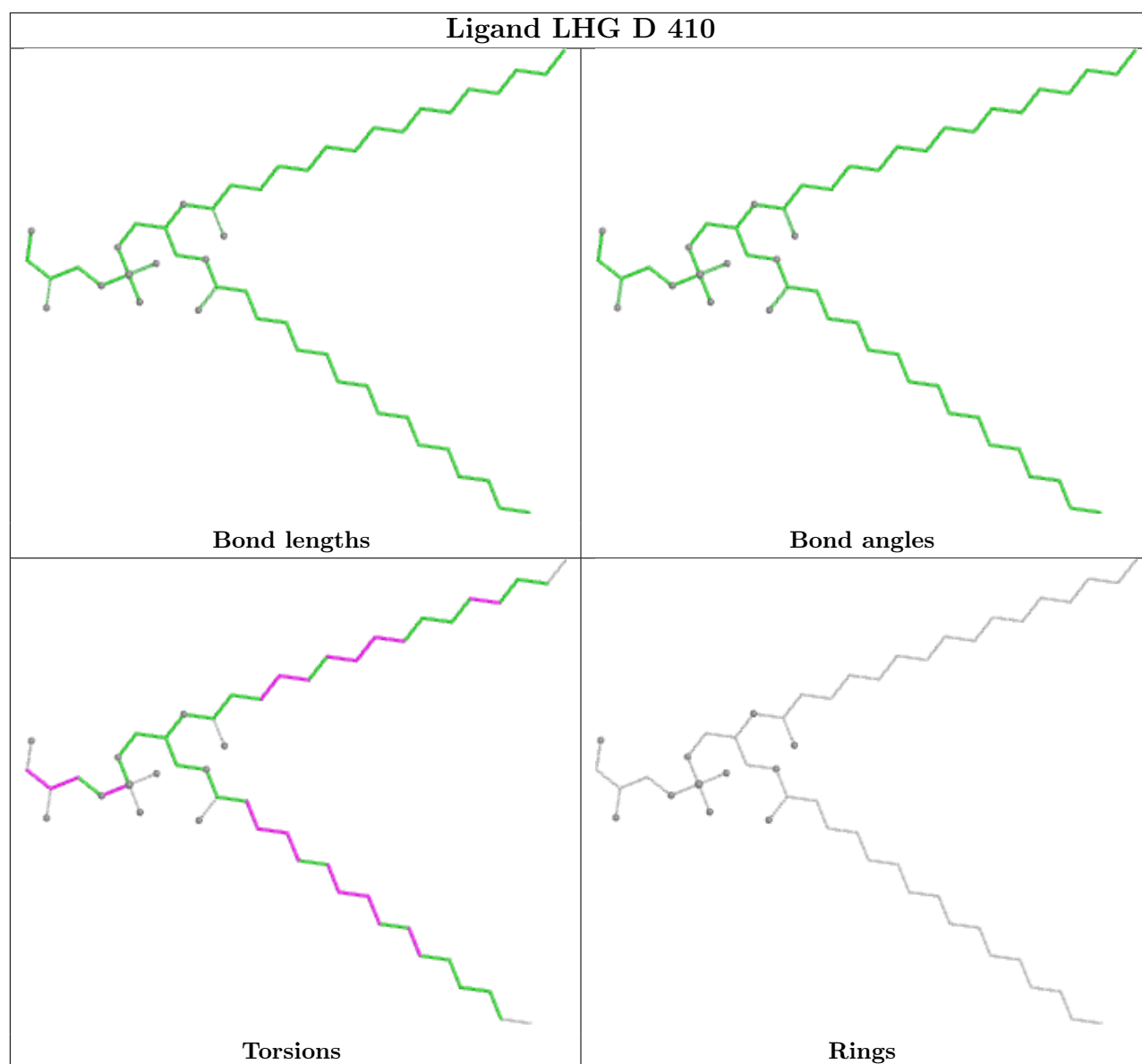


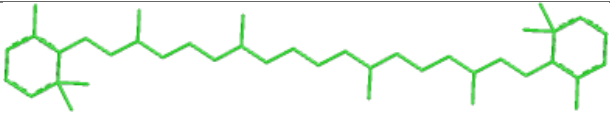
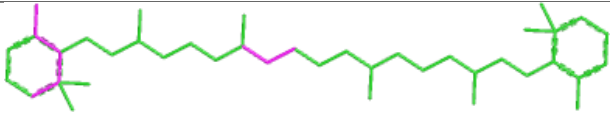
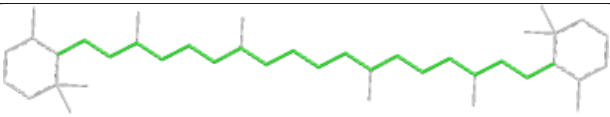
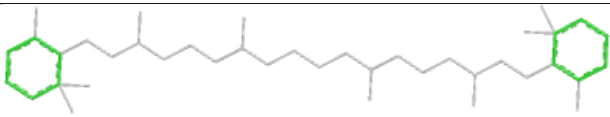
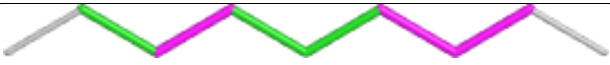
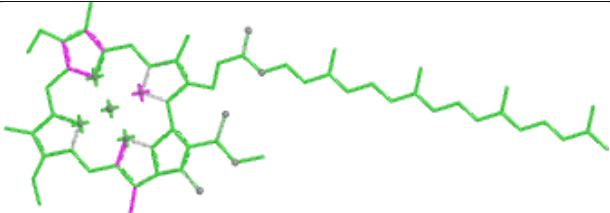
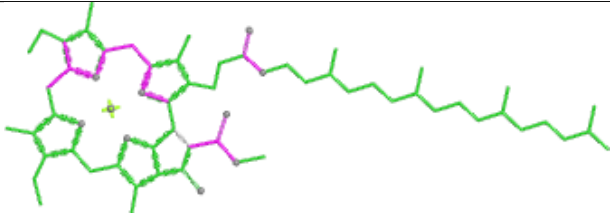
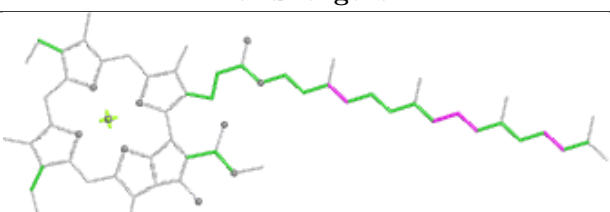
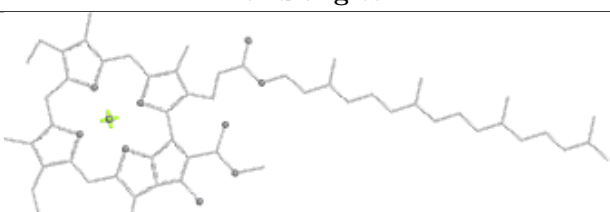
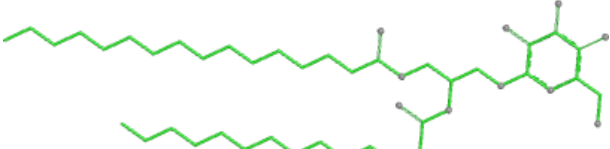
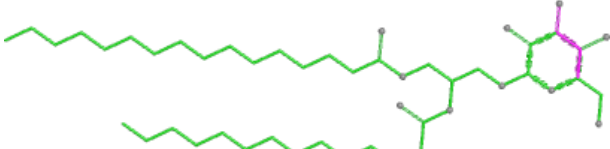
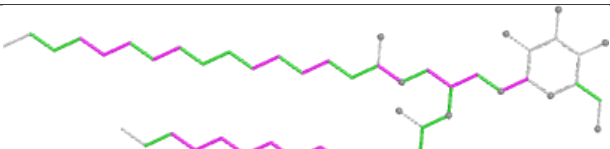
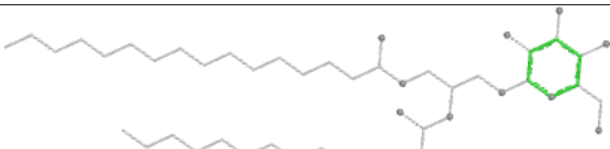


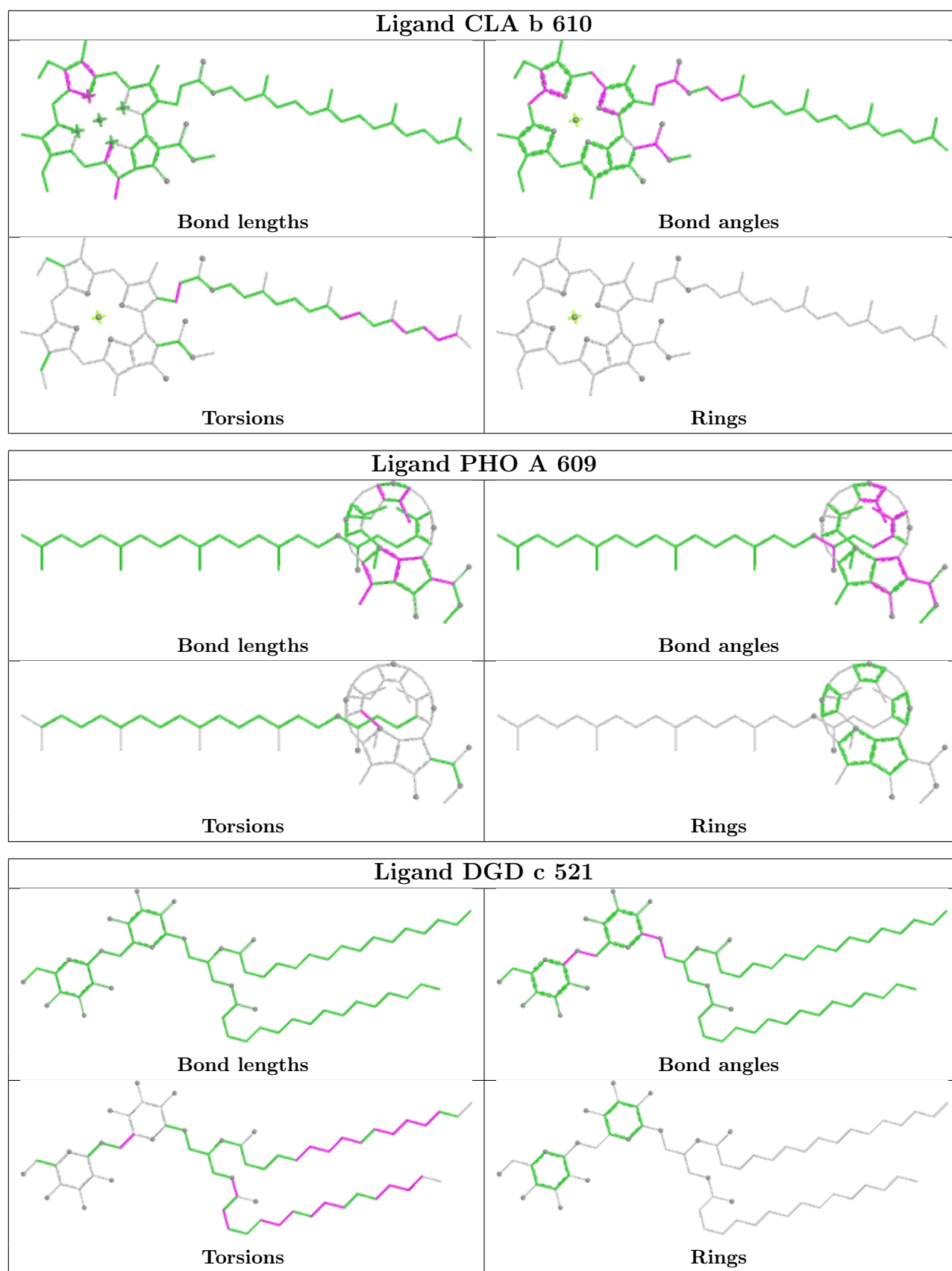
Ligand CLA C 513**Ligand CLA b 607****Ligand CLA C 505**

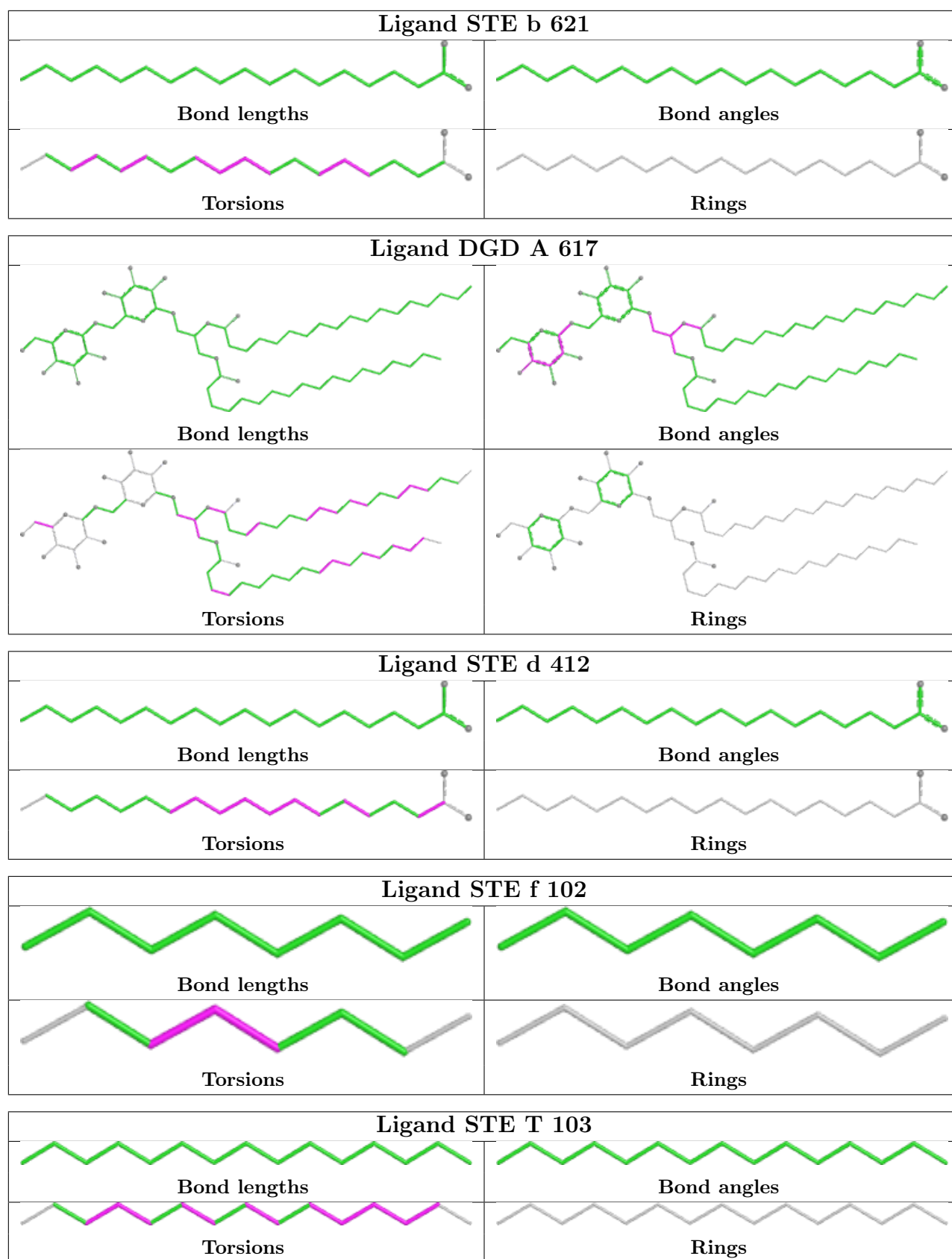


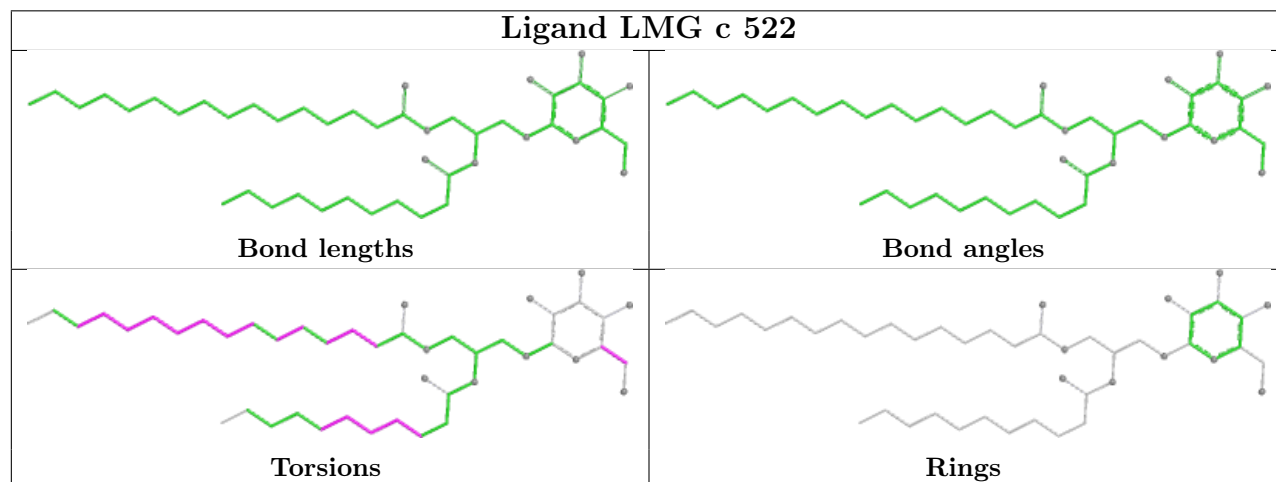
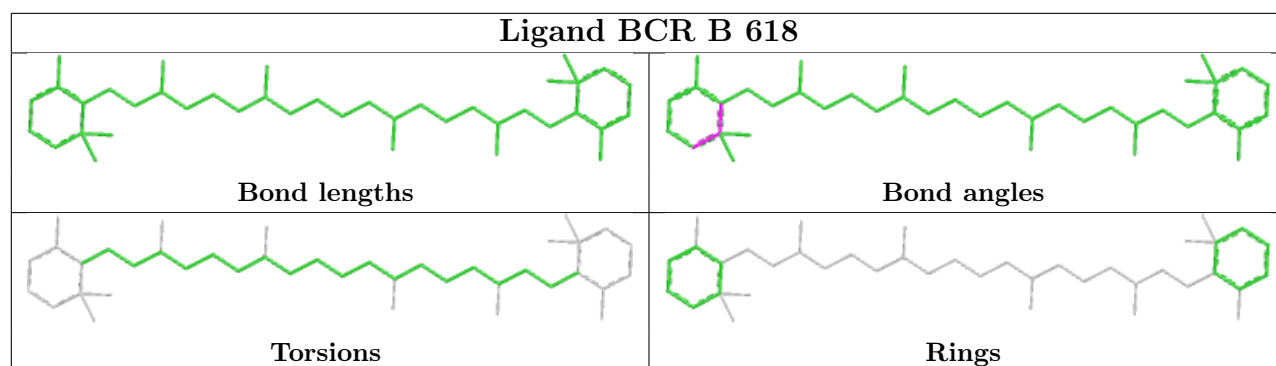
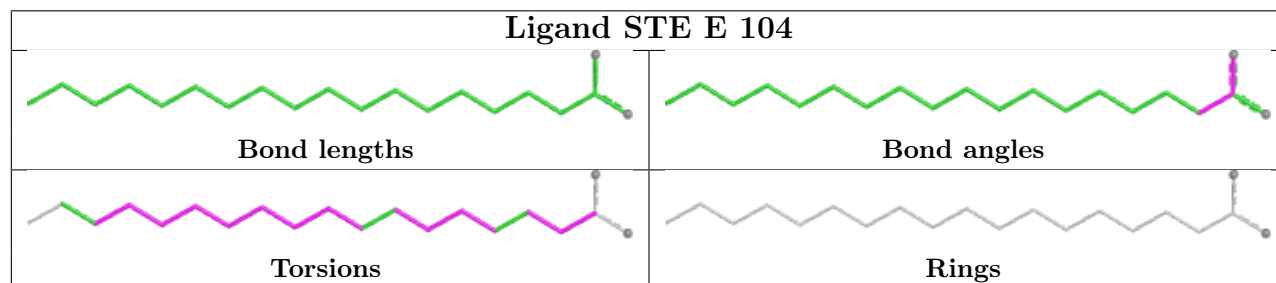
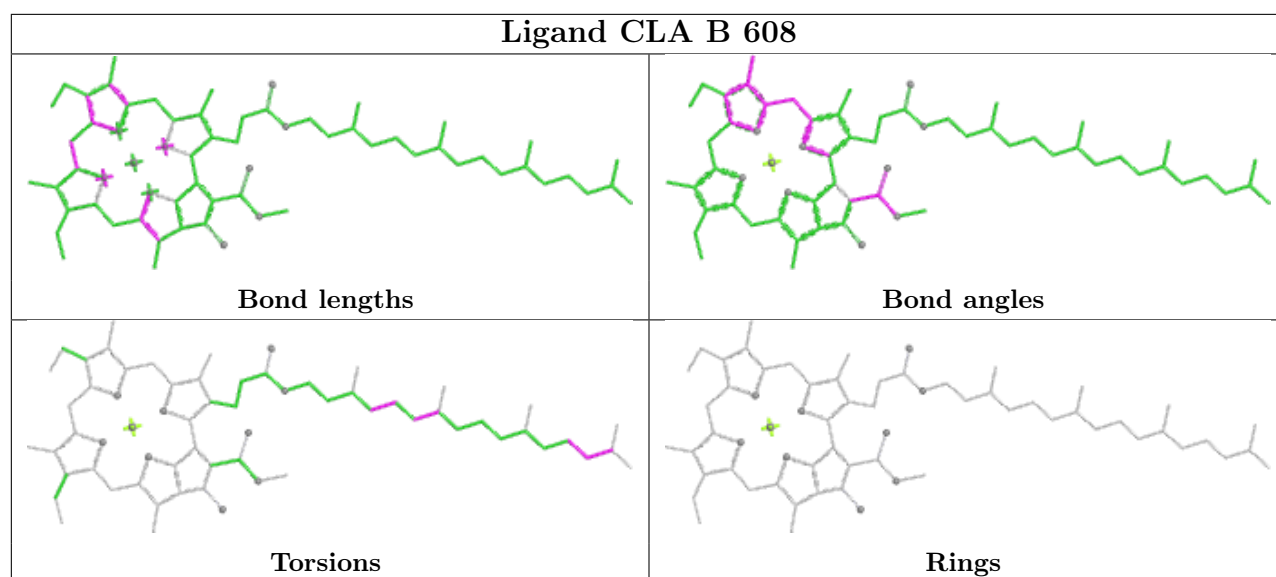




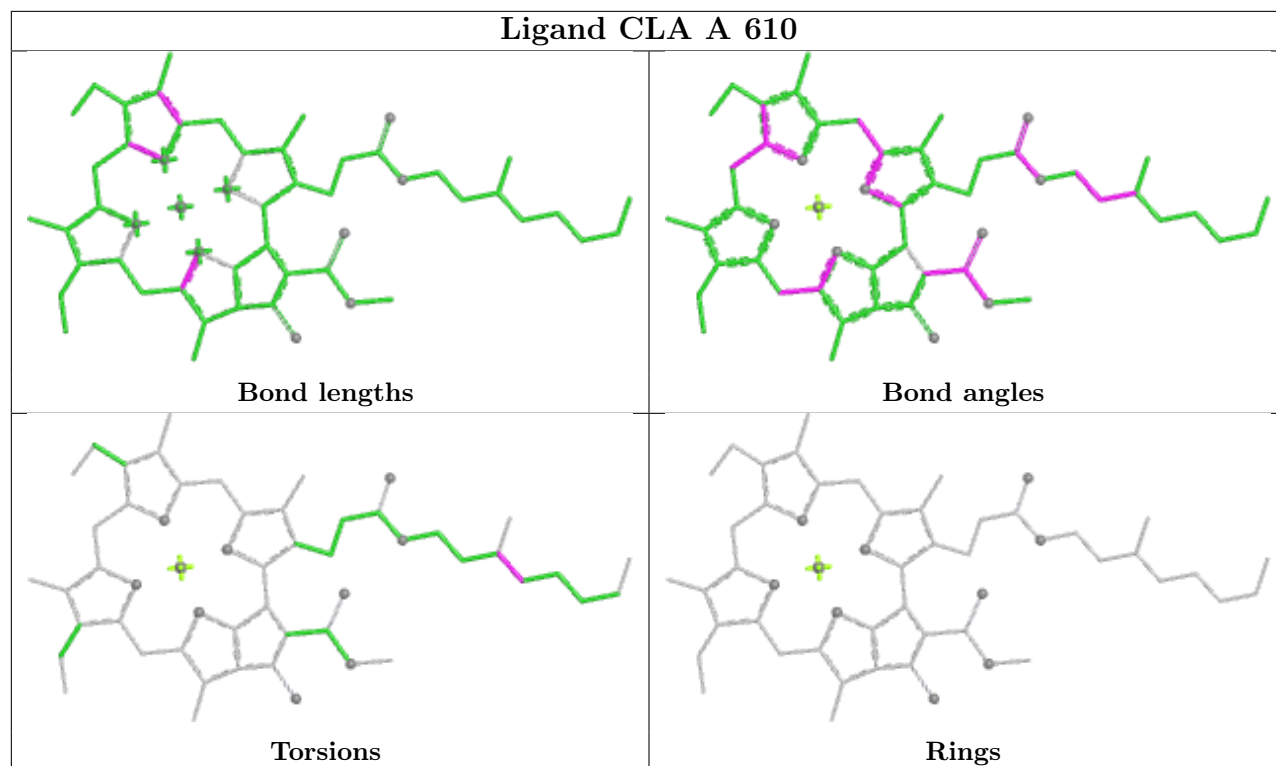
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE D 412	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 618	
 Bond lengths	 Bond angles
 Torsions	 Rings



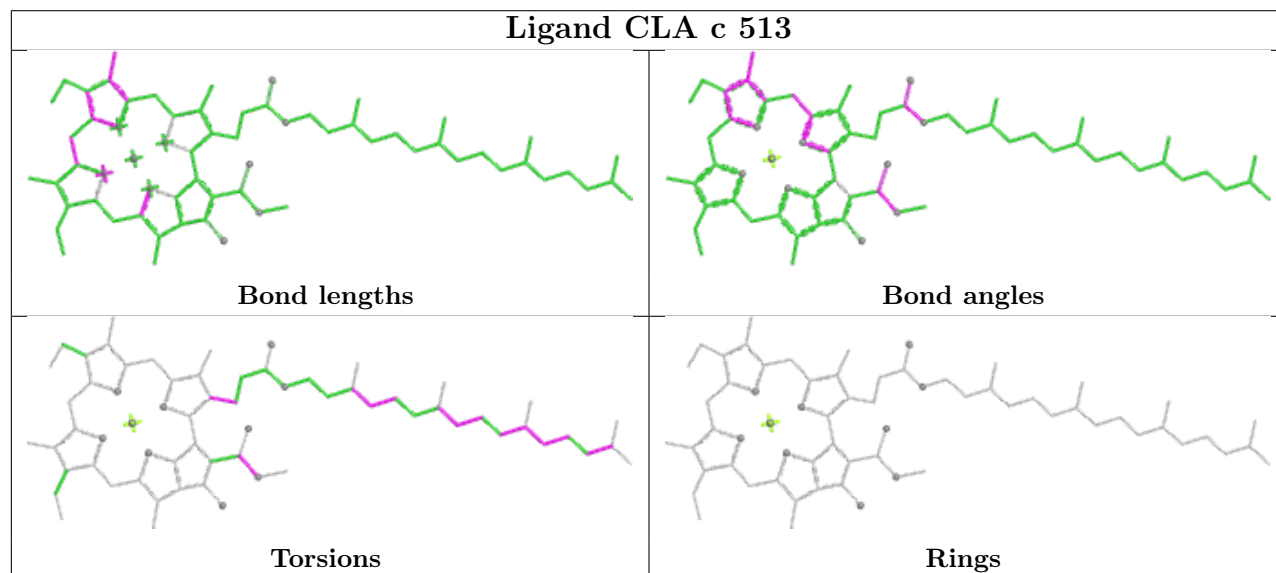


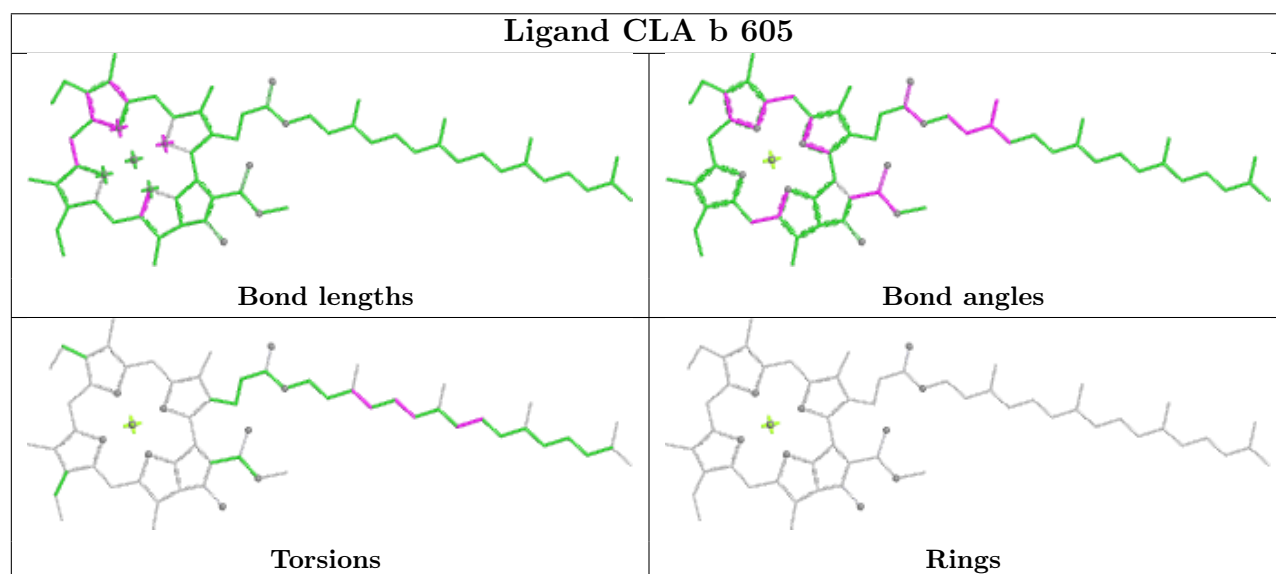
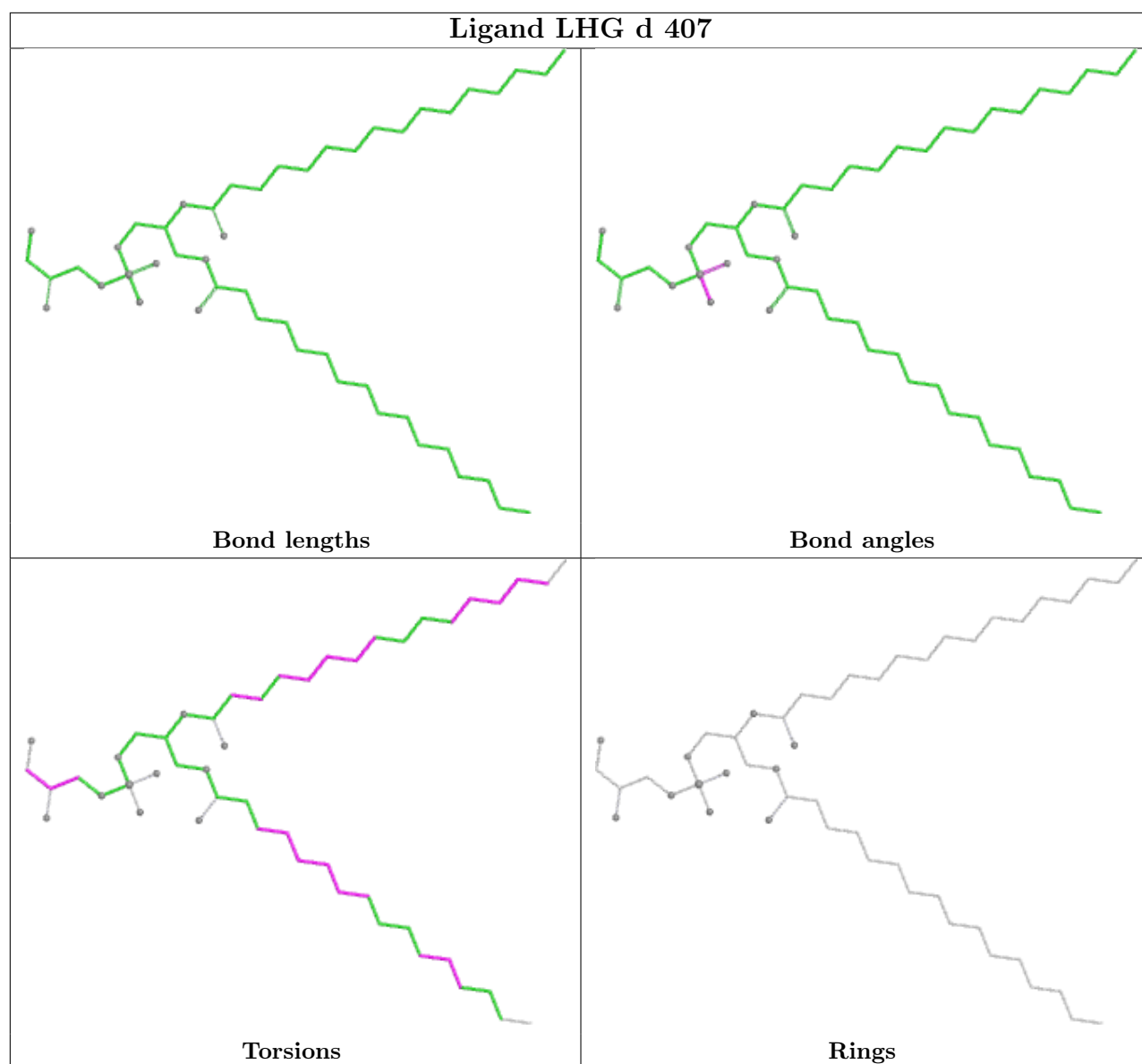


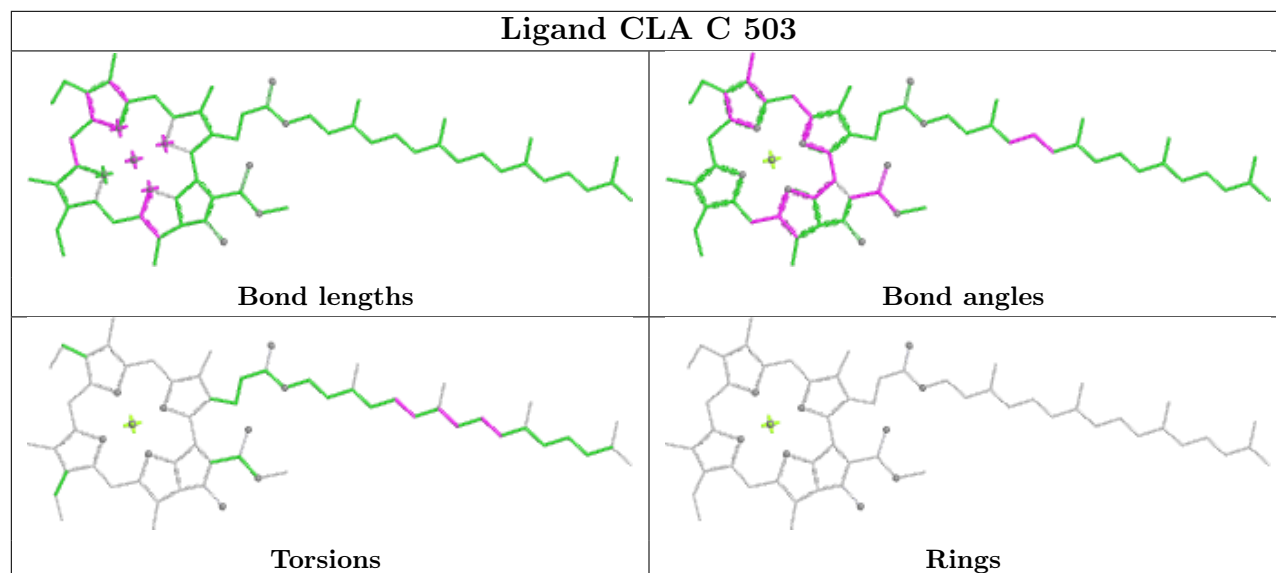
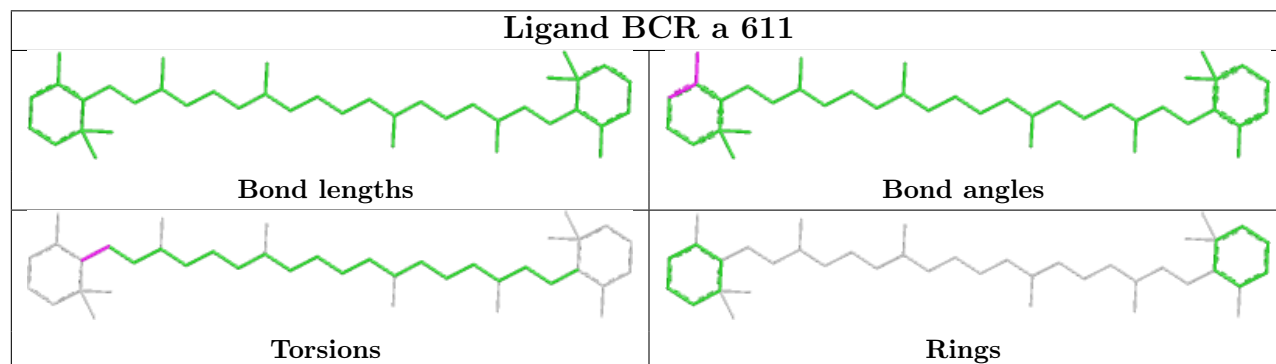
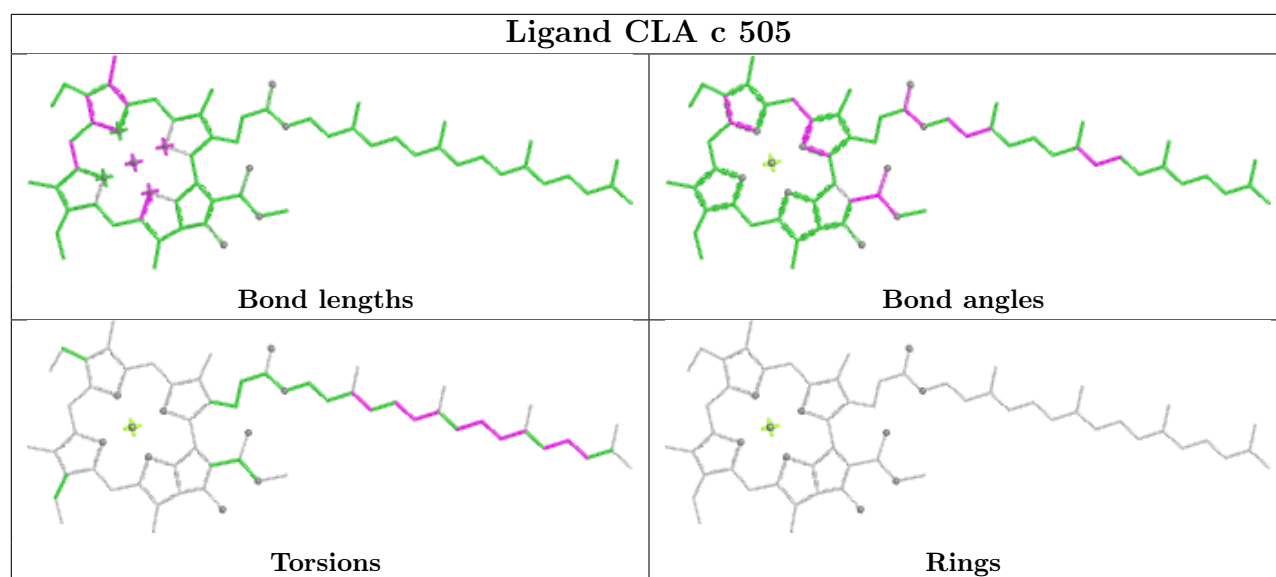
Ligand CLA A 610

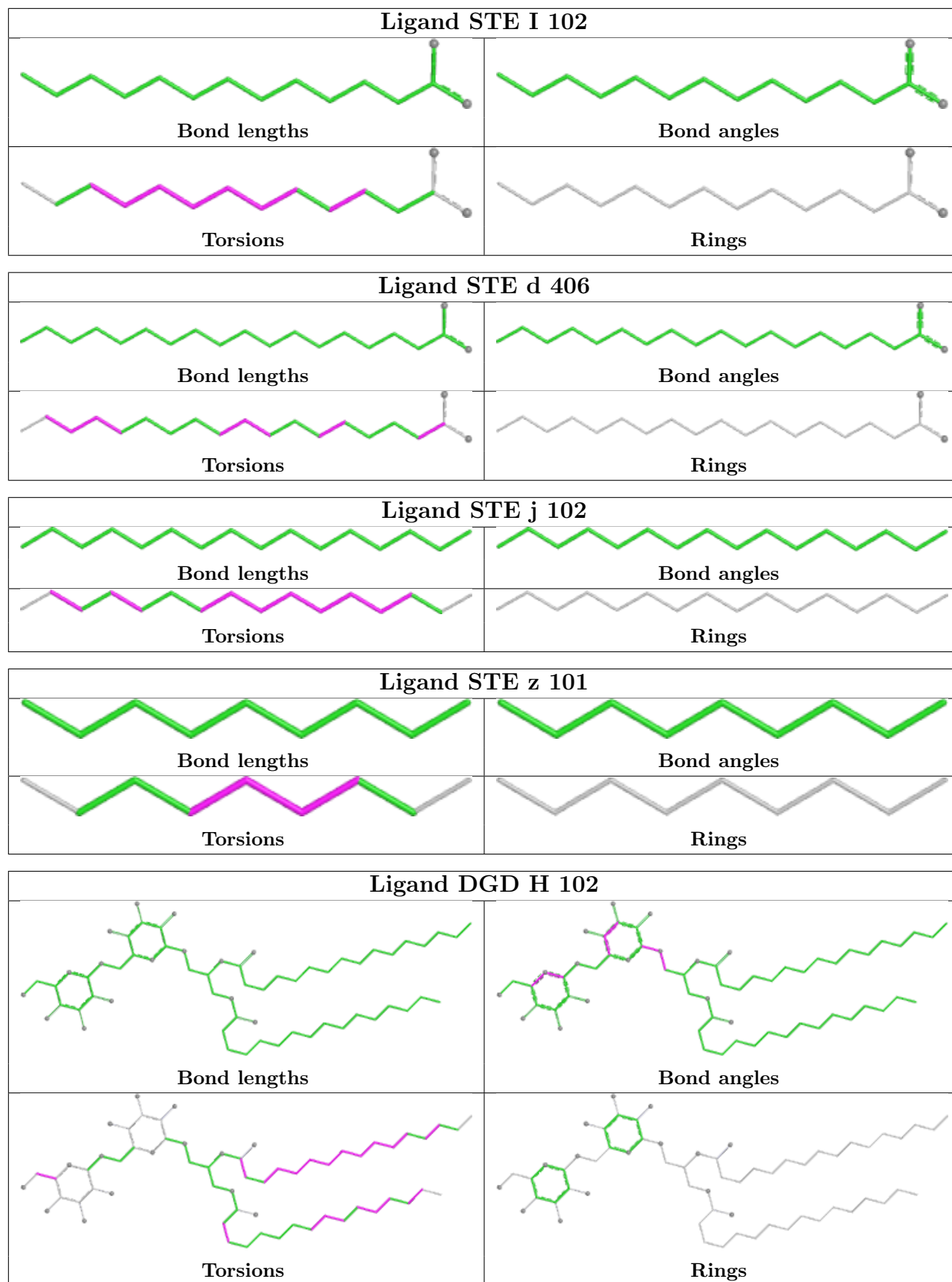


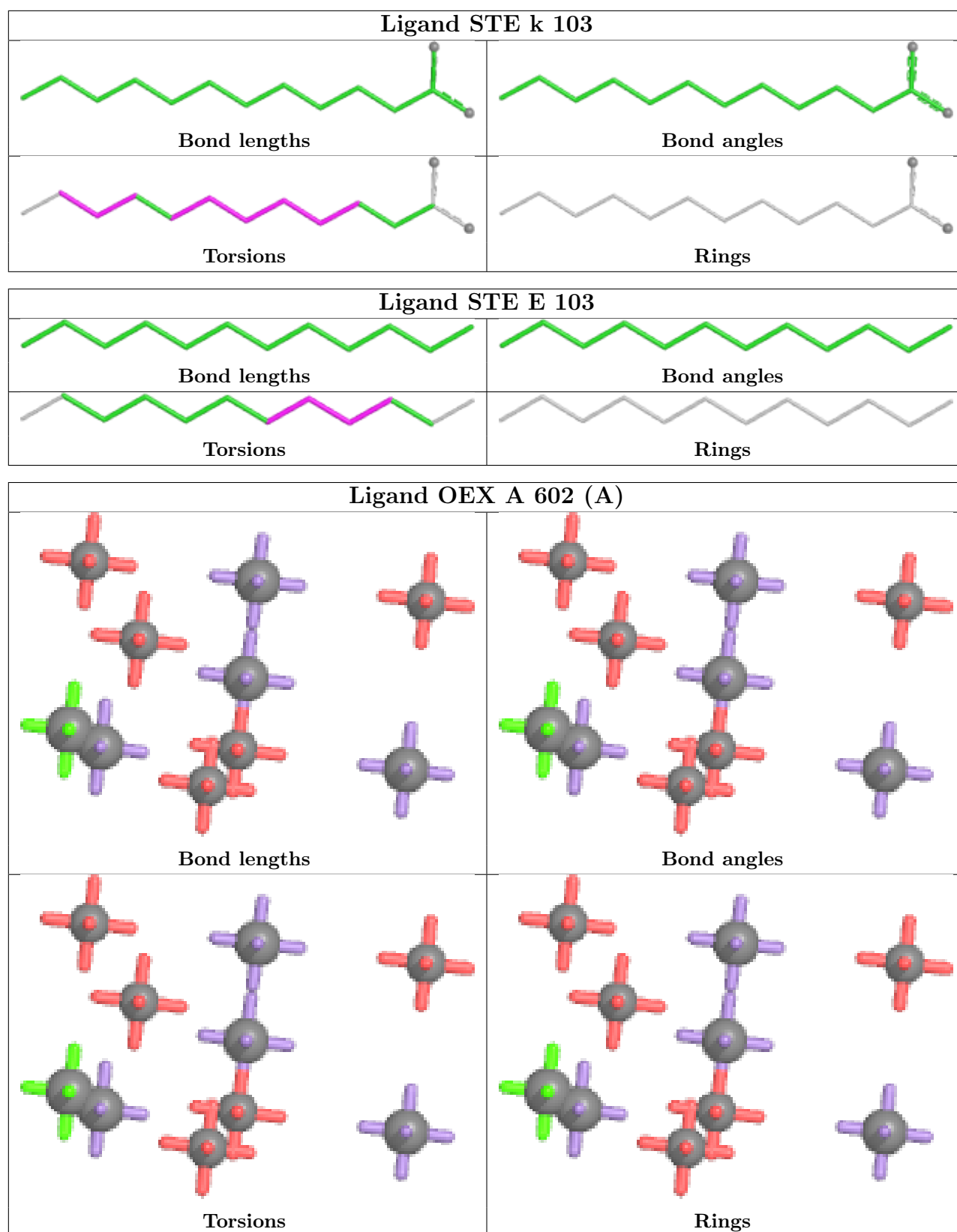
Ligand CLA c 513

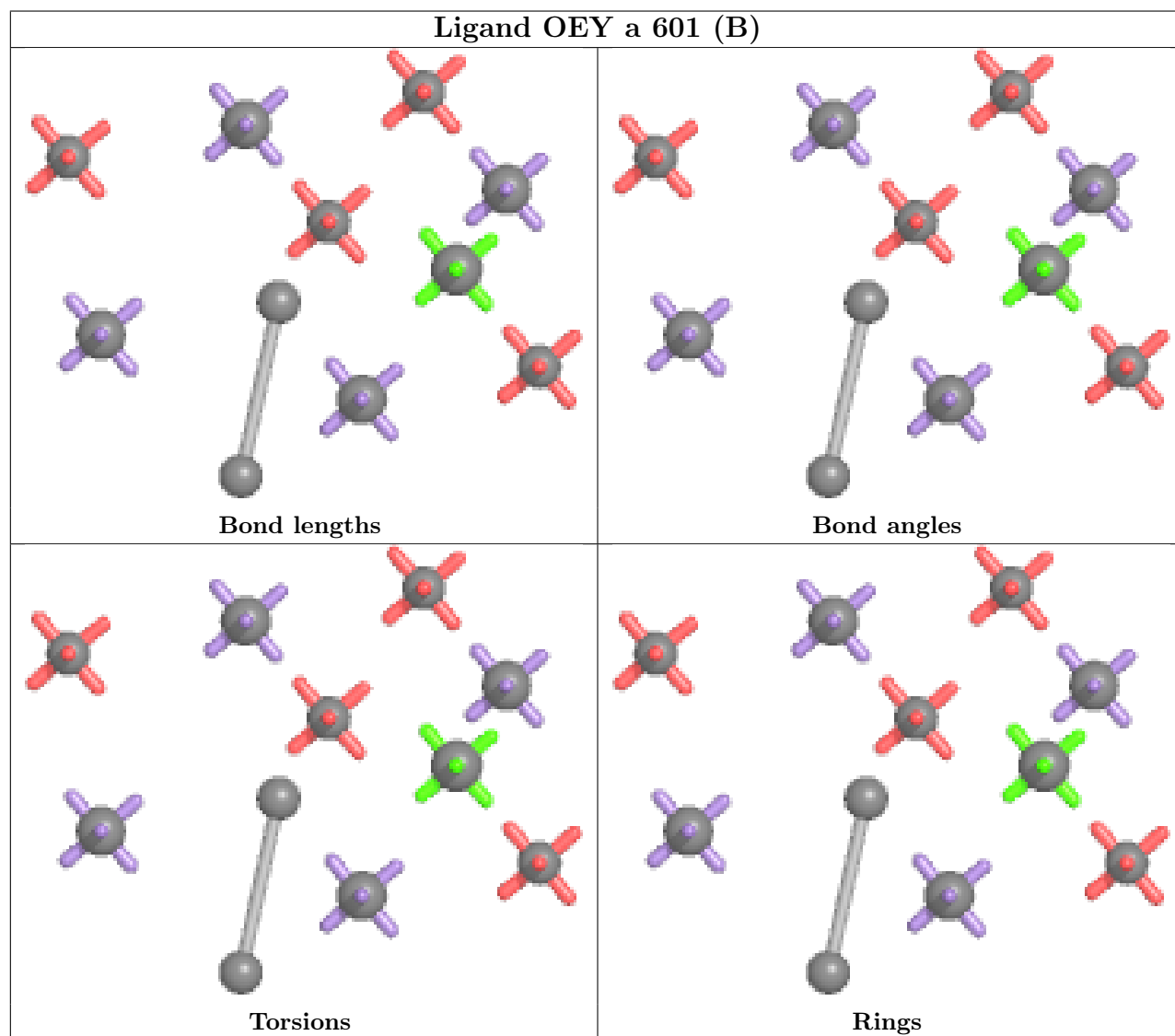
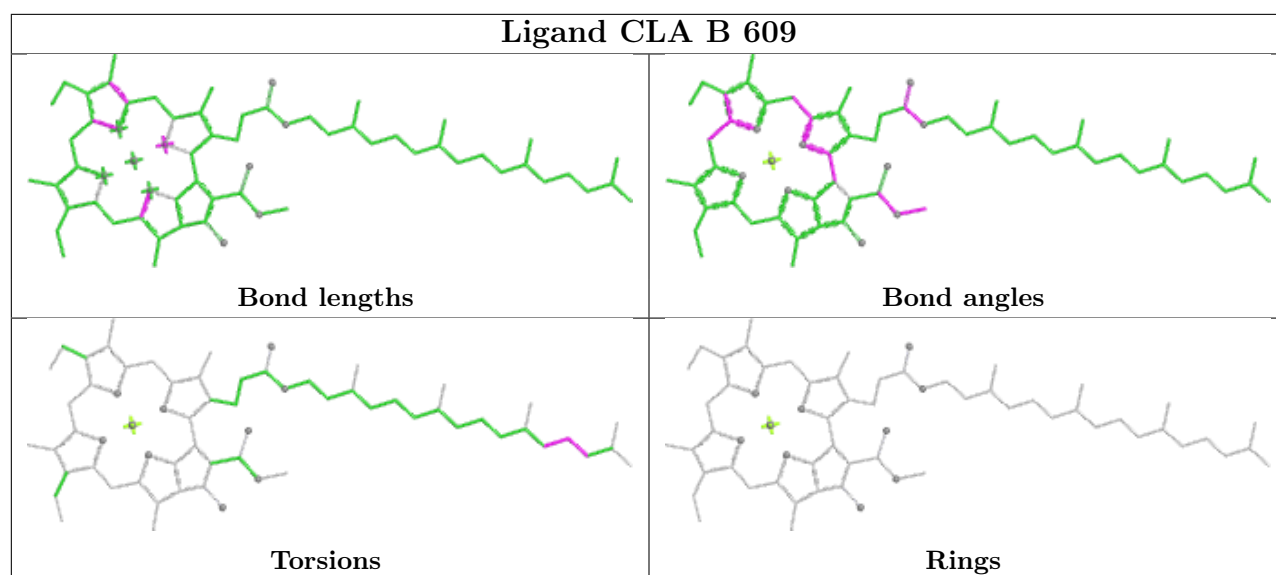


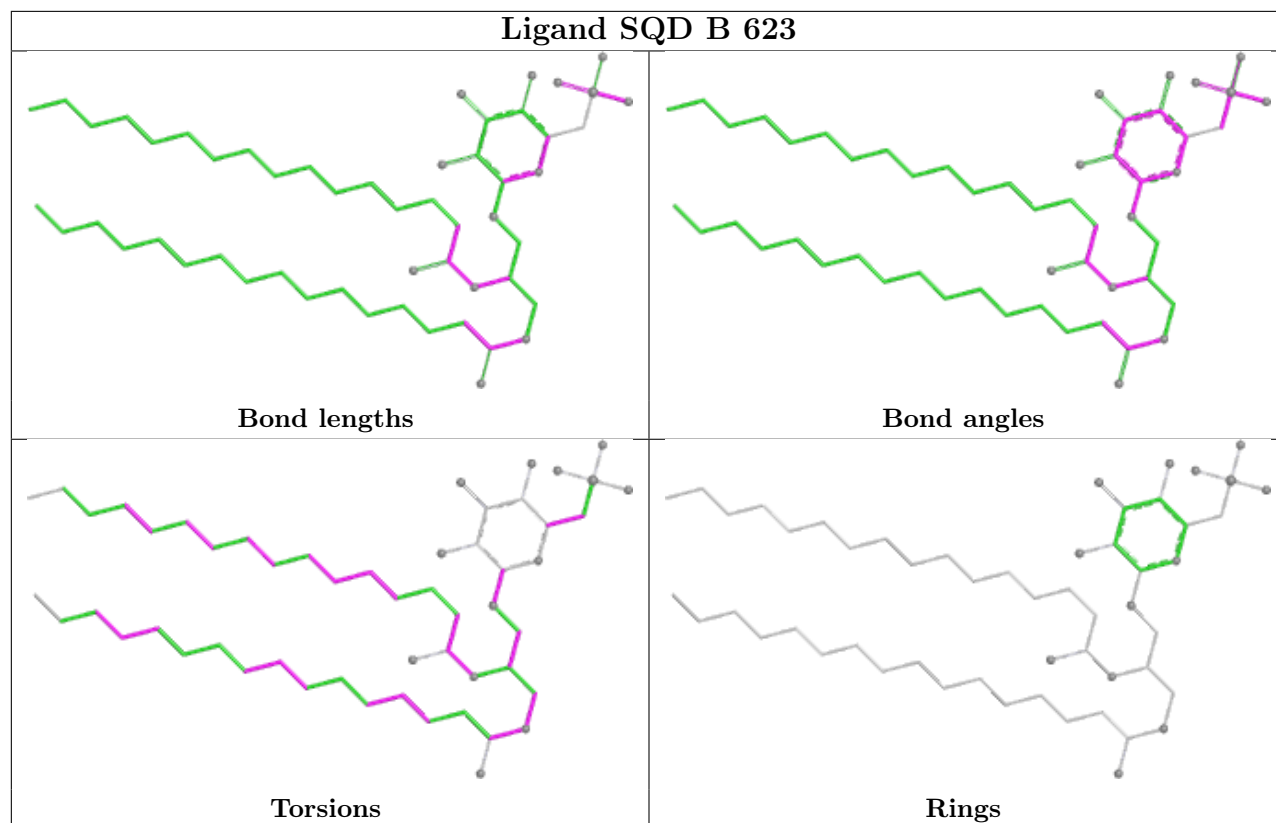
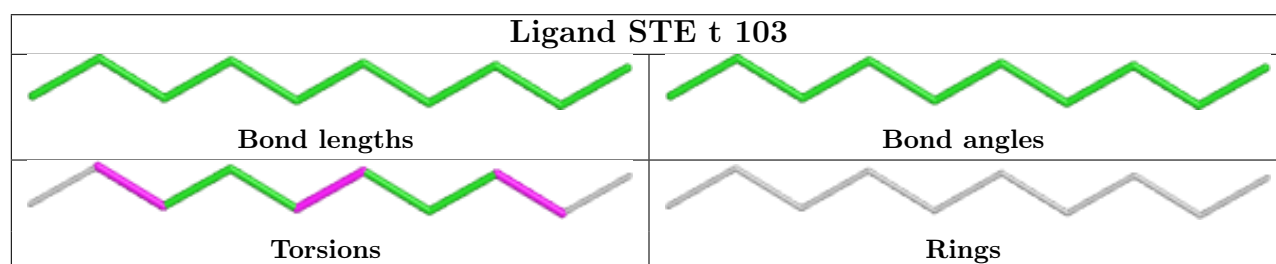
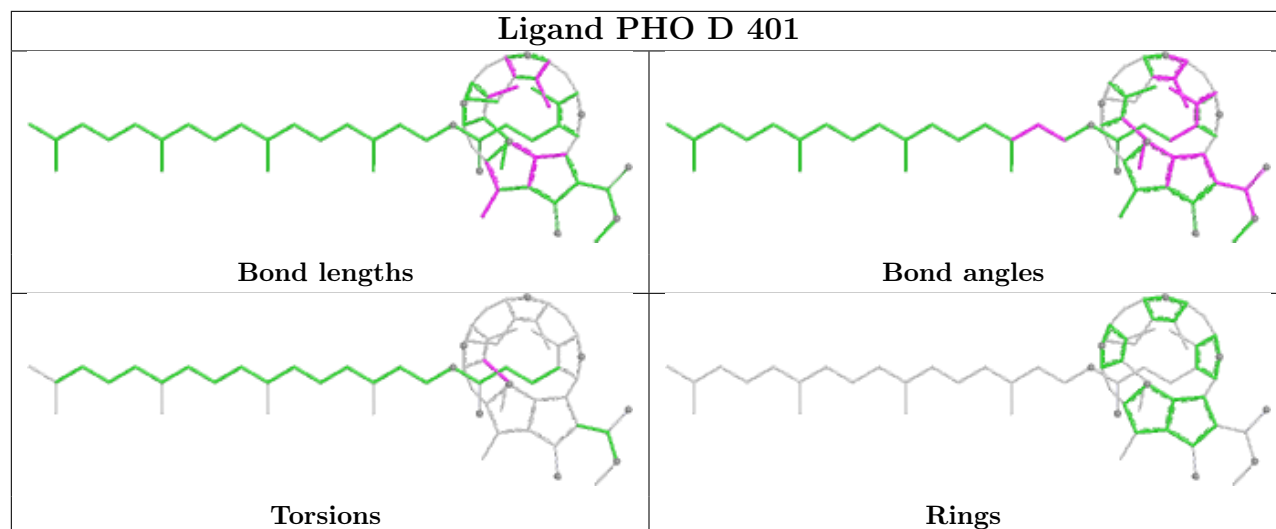


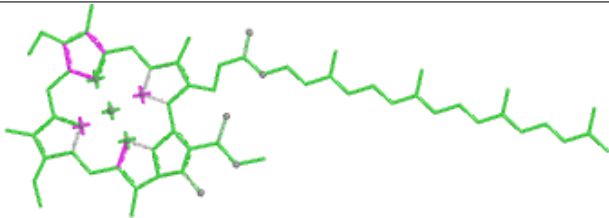
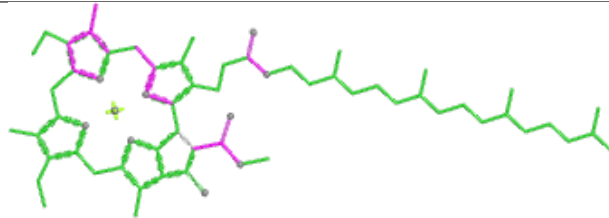
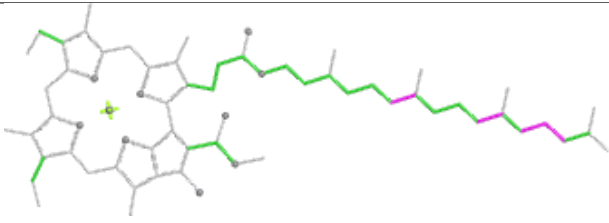
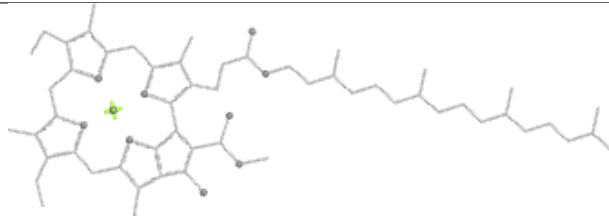


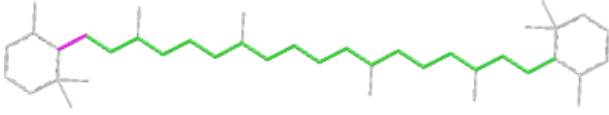
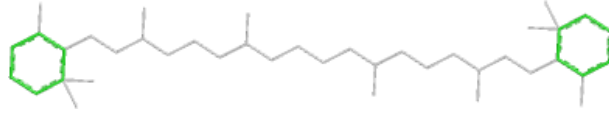


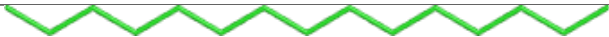
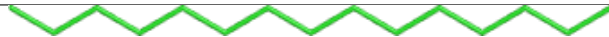


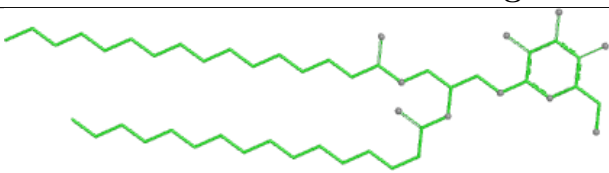
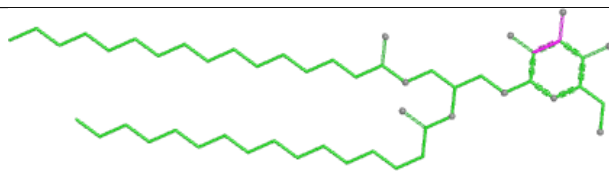
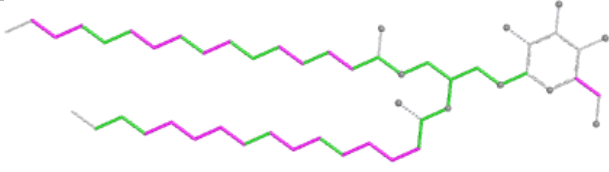
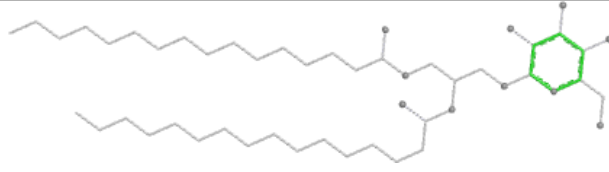


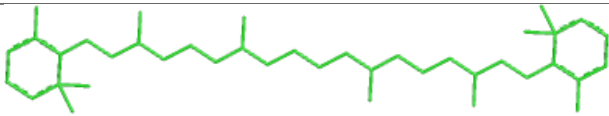
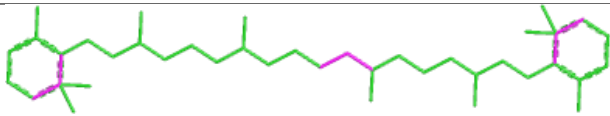
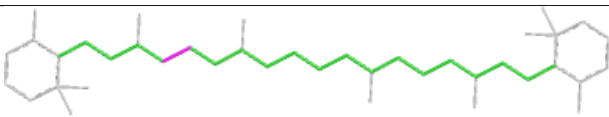
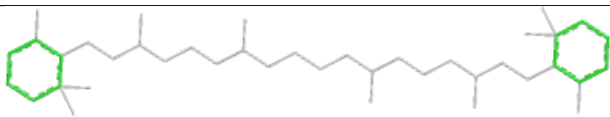


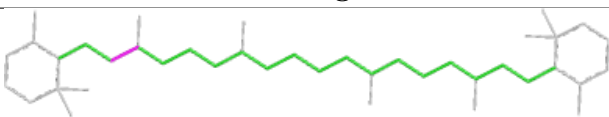
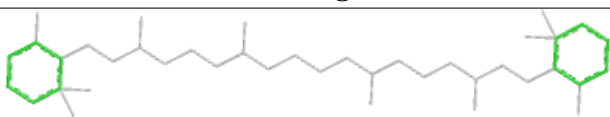
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

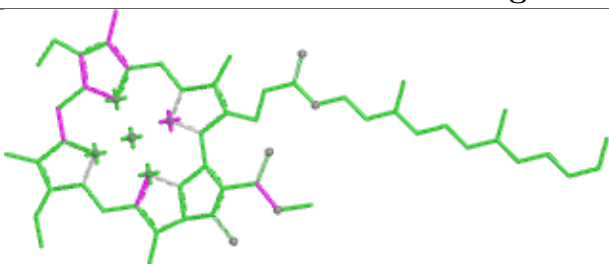
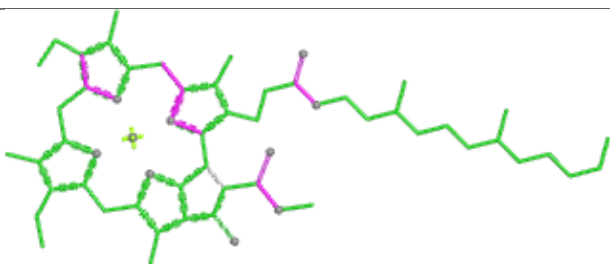
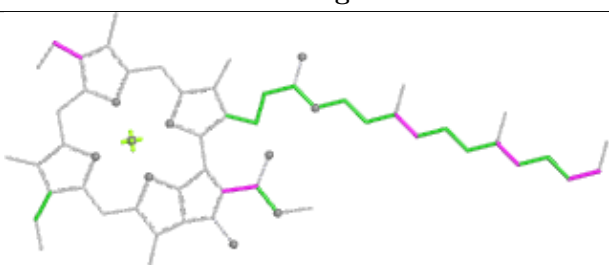
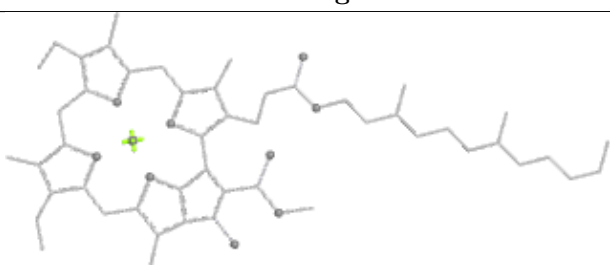
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

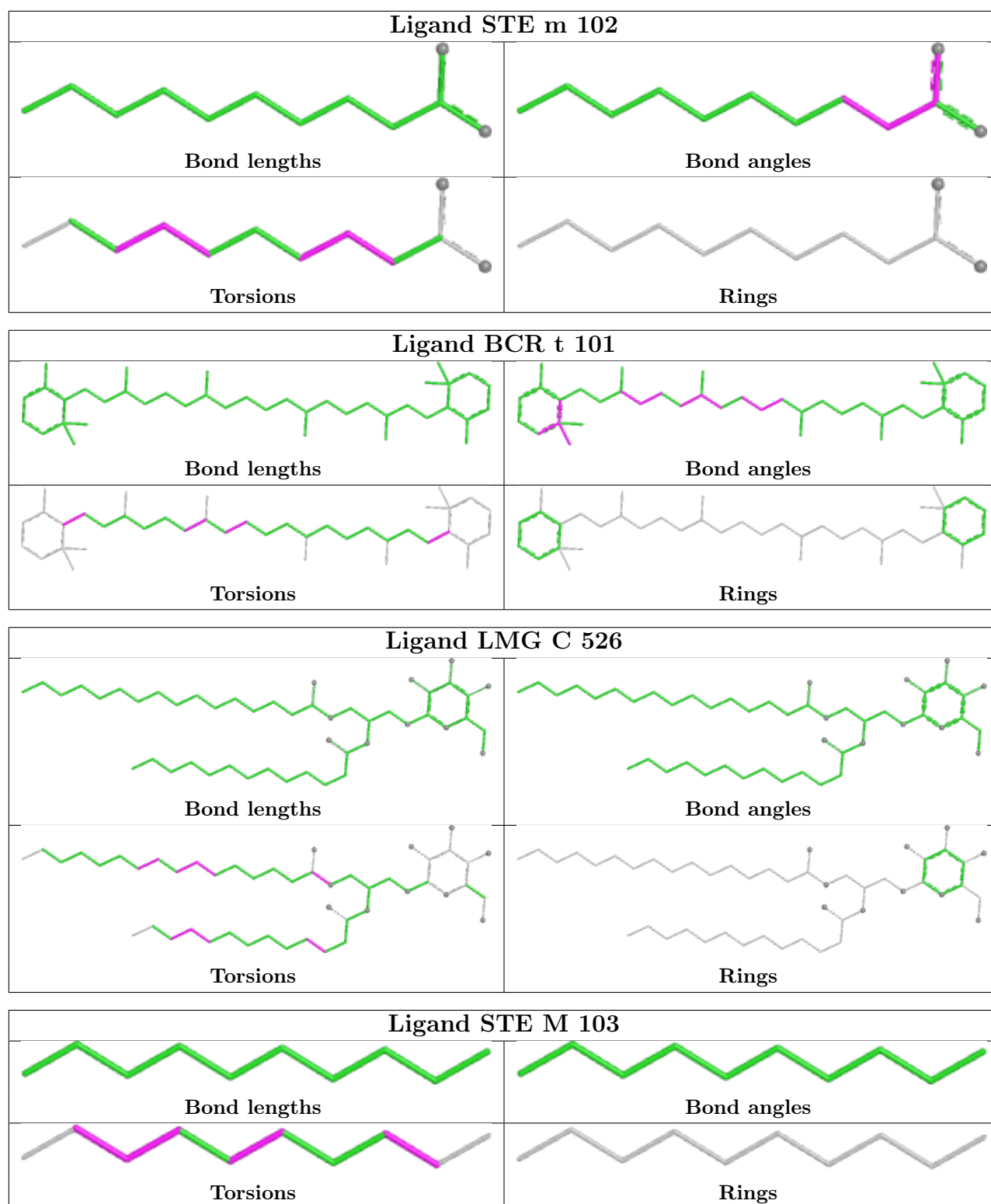
Ligand STE a 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

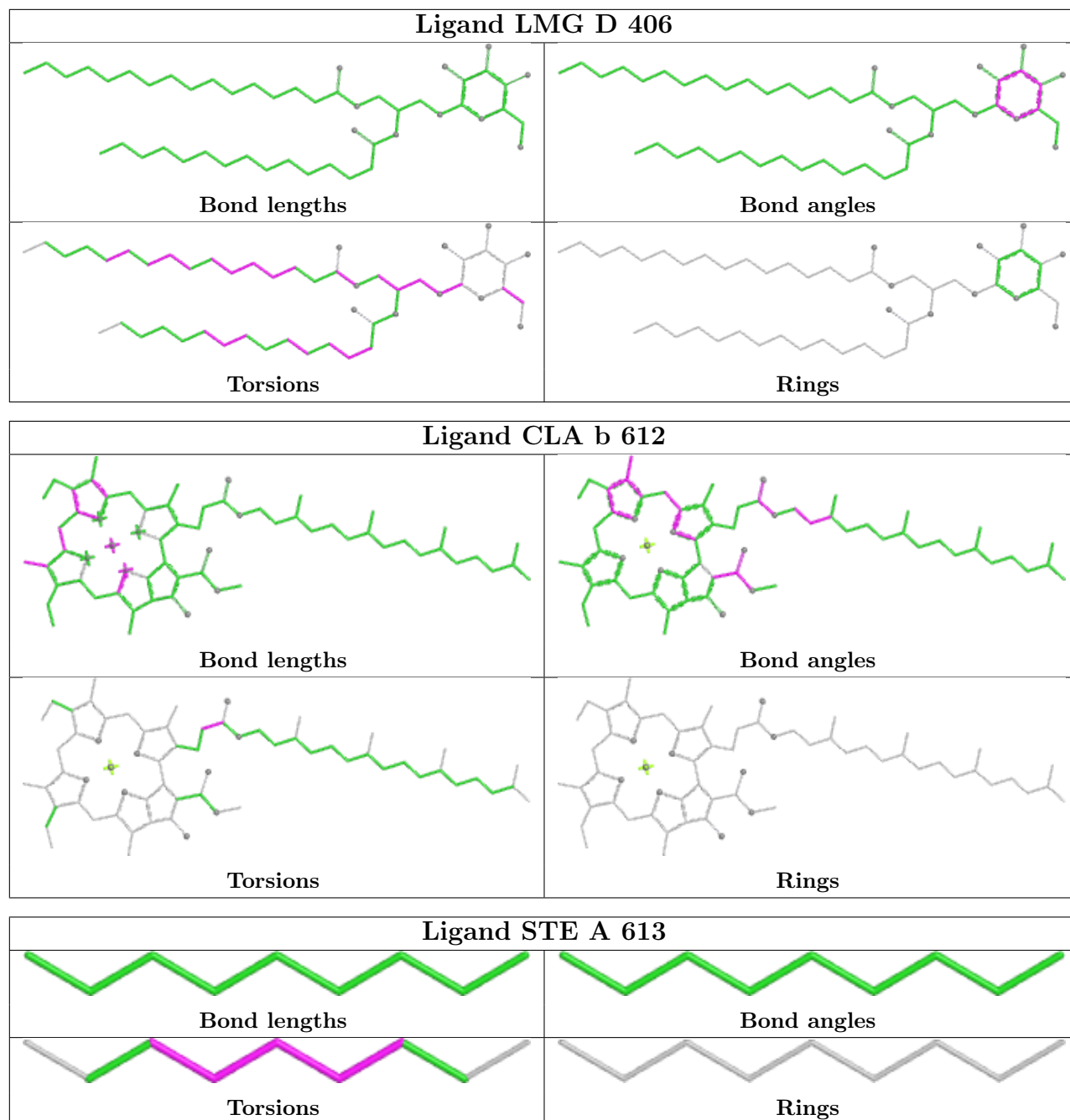
Ligand LMG D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

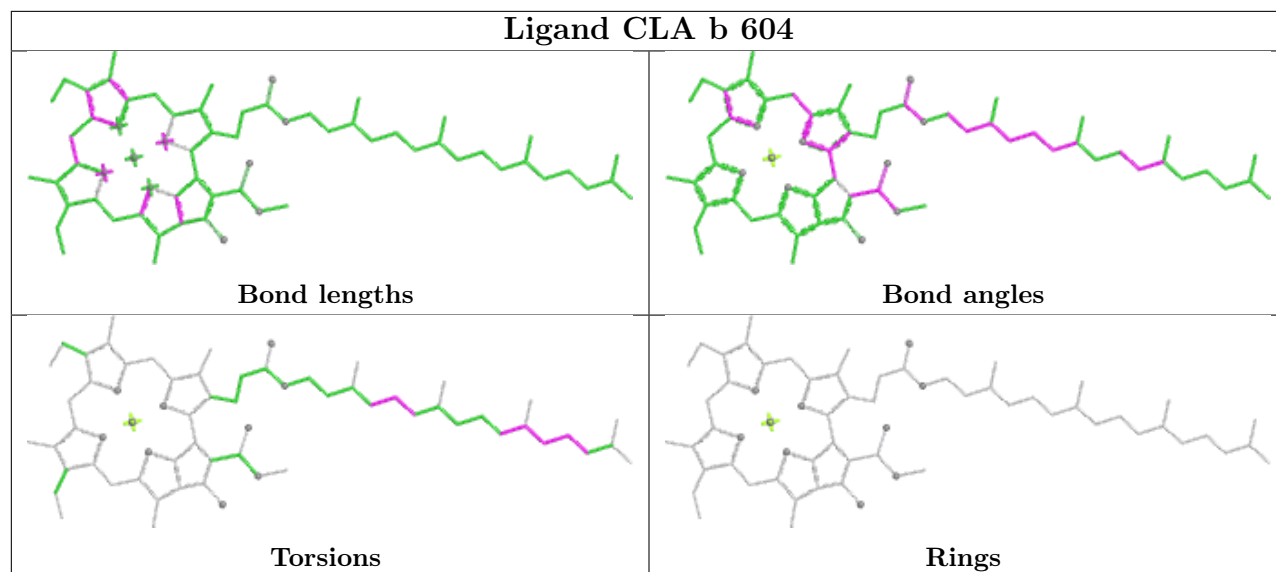
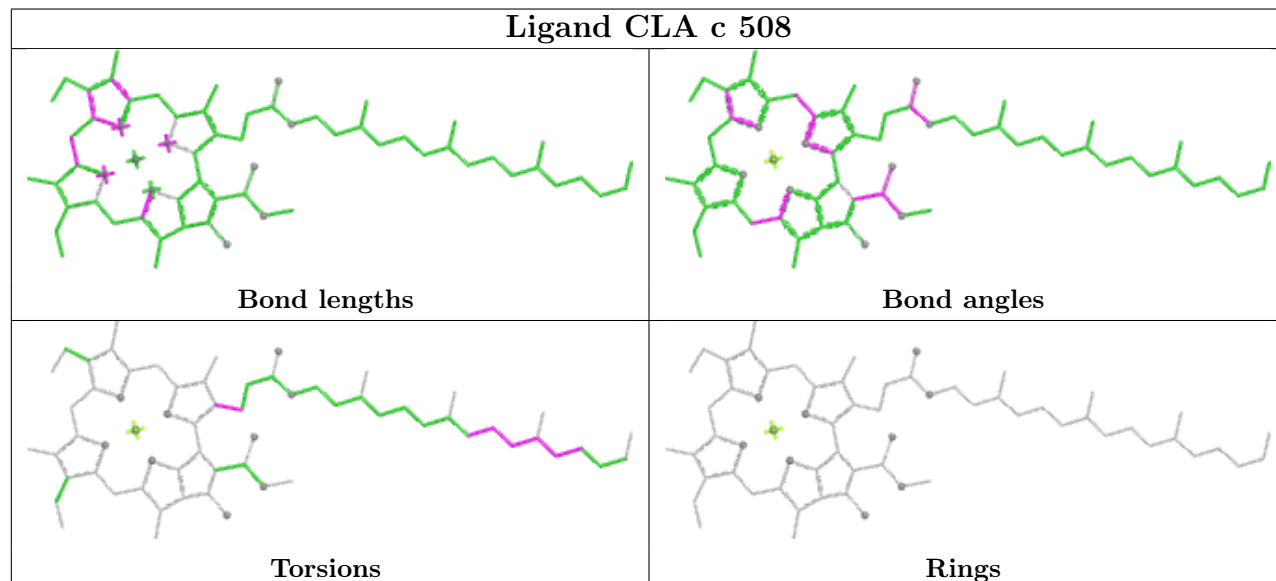
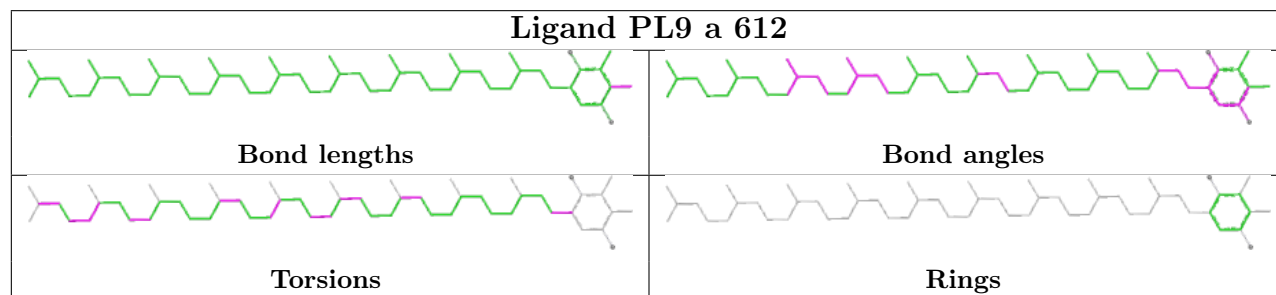
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

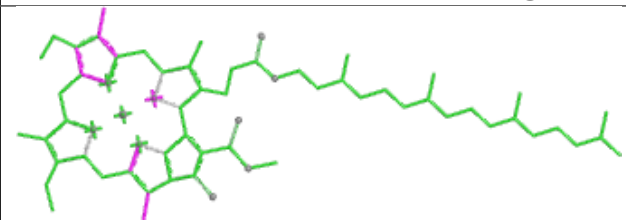
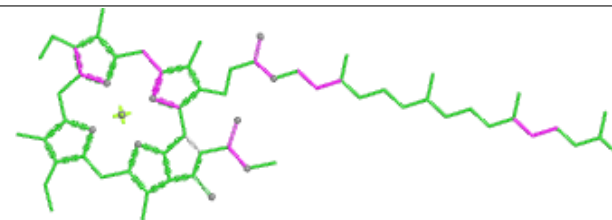
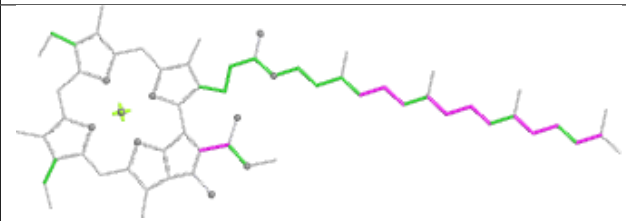
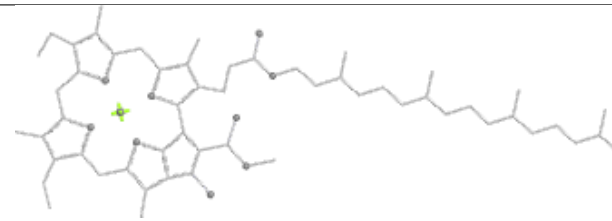
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

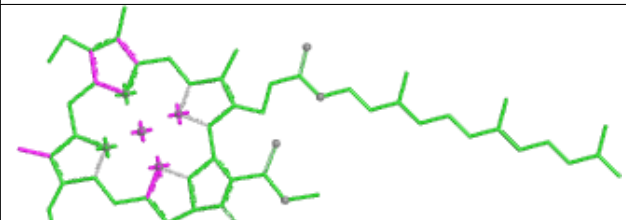
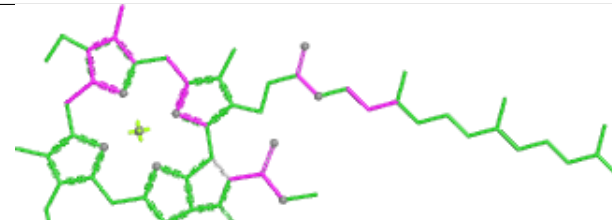
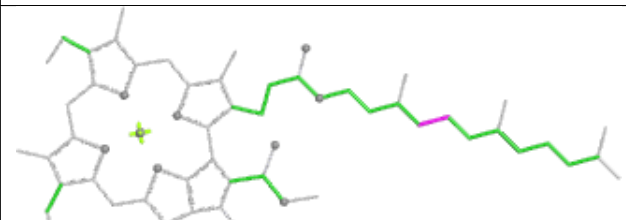
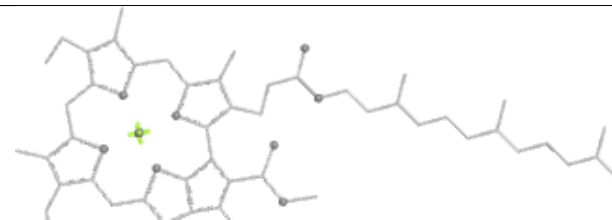
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

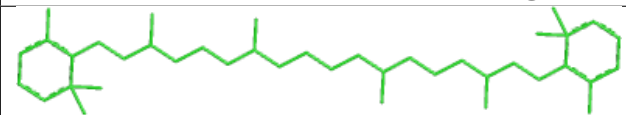
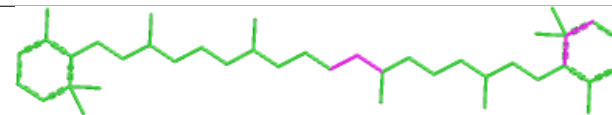
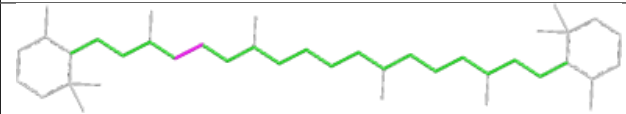
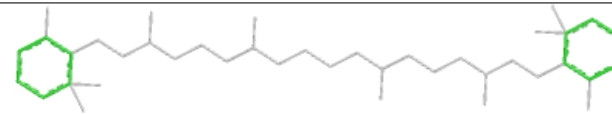


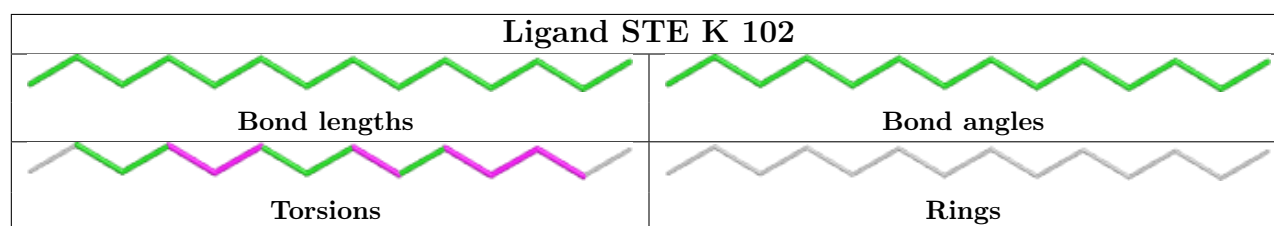
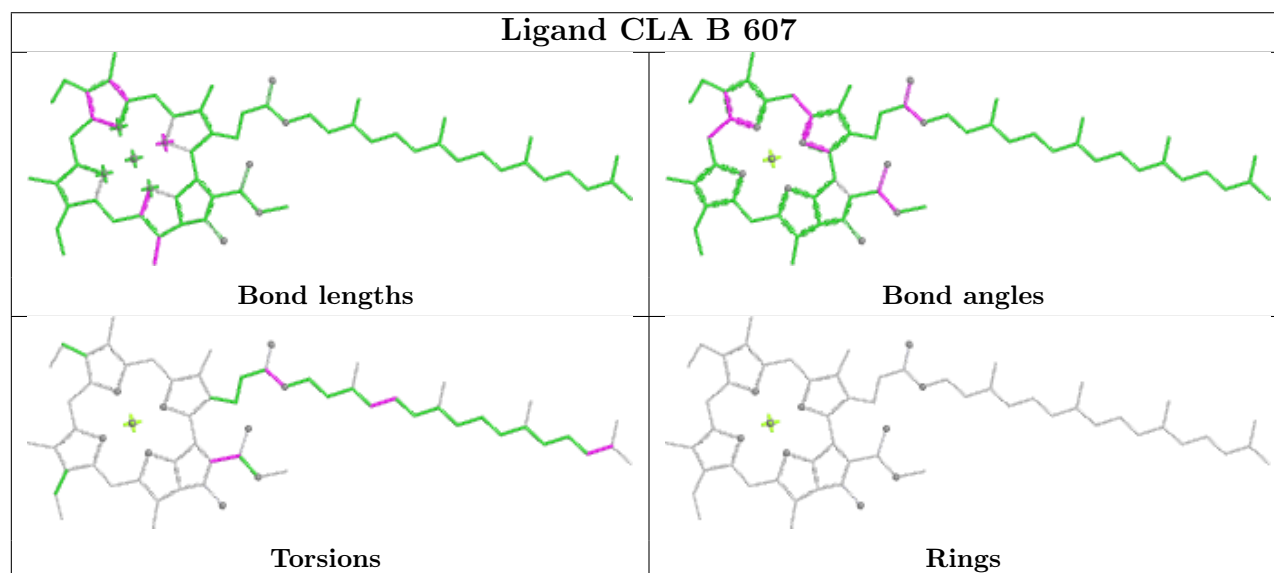
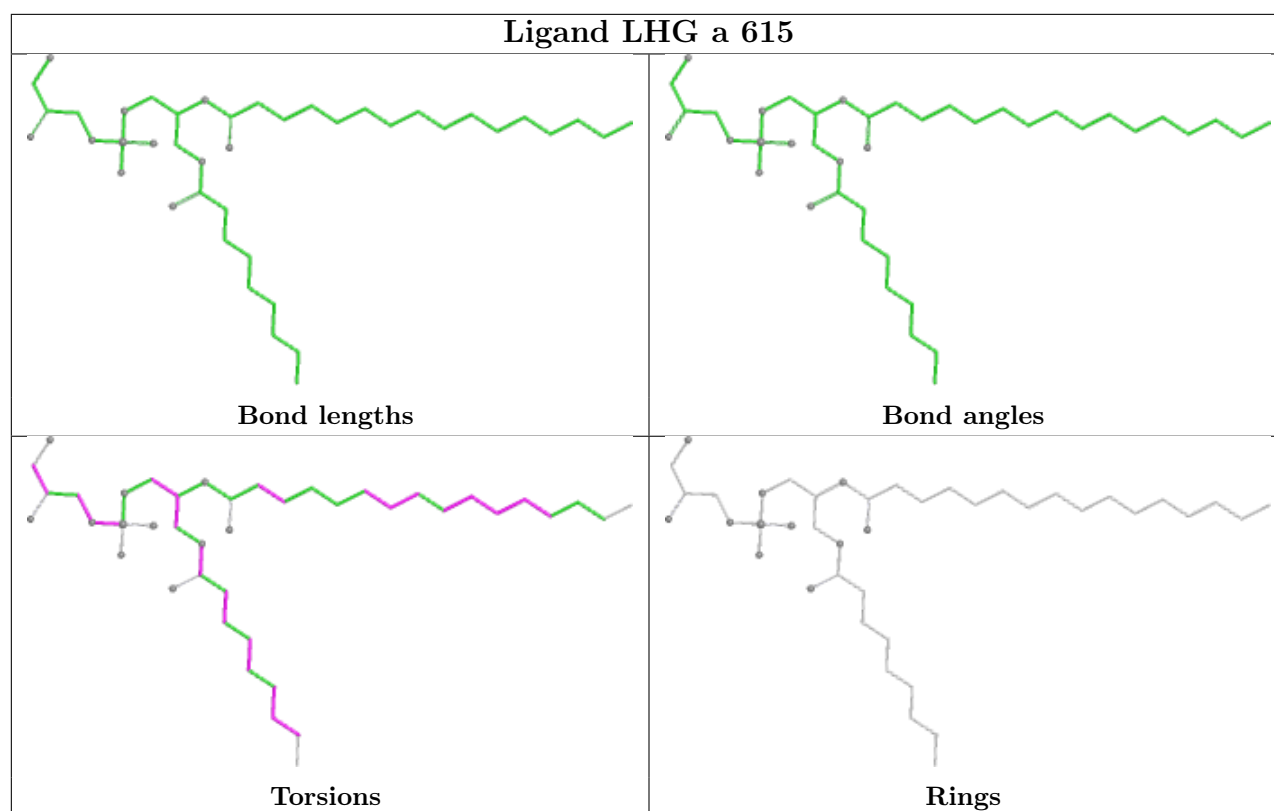


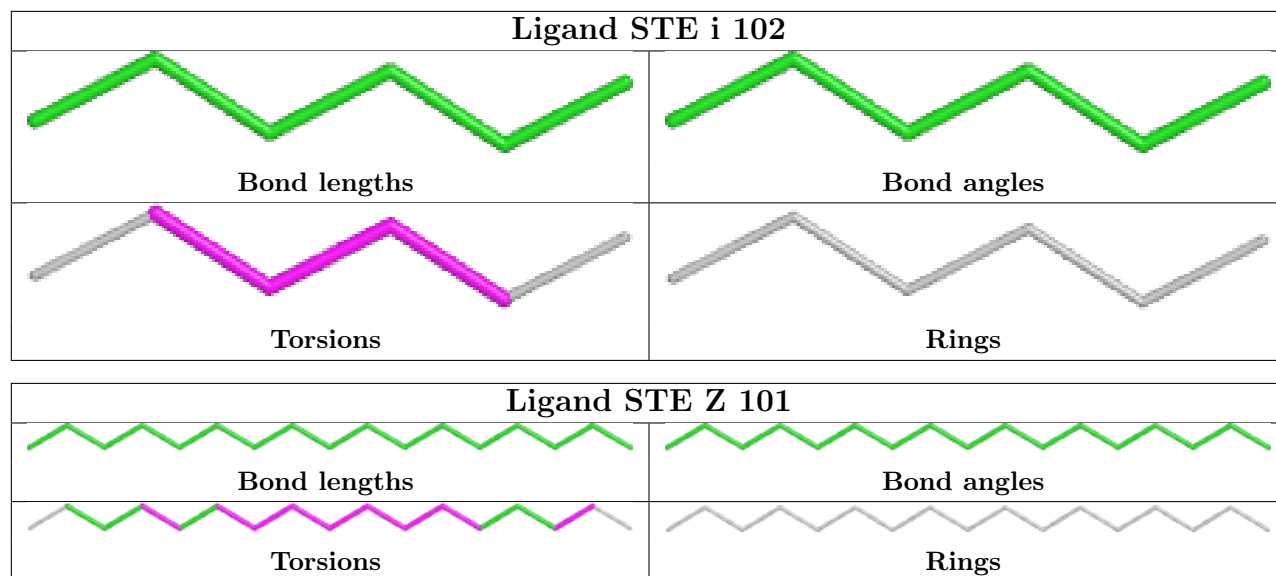
Ligand CLA b 604**Ligand CLA c 508****Ligand PL9 a 612**

Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.41	1 (0%) 90 93	11, 26, 44, 76	69 (20%)
1	a	334/344 (97%)	-0.33	1 (0%) 90 93	10, 28, 52, 76	69 (20%)
2	B	505/510 (99%)	-0.26	5 (0%) 79 84	16, 30, 56, 87	5 (0%)
2	b	505/510 (99%)	-0.12	5 (0%) 79 84	24, 34, 63, 95	1 (0%)
3	C	442/461 (95%)	-0.22	0 100 100	12, 33, 48, 70	11 (2%)
3	c	451/461 (97%)	-0.06	4 (0%) 81 85	12, 37, 55, 83	12 (2%)
4	D	341/352 (96%)	-0.44	0 100 100	12, 28, 43, 70	10 (2%)
4	d	341/352 (96%)	-0.27	0 100 100	12, 32, 51, 70	11 (3%)
5	E	82/84 (97%)	0.41	1 (1%) 76 81	30, 46, 62, 81	1 (1%)
5	e	82/84 (97%)	0.53	2 (2%) 59 67	37, 54, 68, 83	0
6	F	34/45 (75%)	0.13	1 (2%) 53 60	33, 40, 53, 77	0
6	f	34/45 (75%)	0.35	1 (2%) 53 60	38, 46, 68, 86	0
7	H	65/66 (98%)	0.00	1 (1%) 72 78	28, 36, 53, 68	0
7	h	63/66 (95%)	0.28	2 (3%) 50 56	33, 44, 58, 61	0
8	I	35/38 (92%)	-0.17	0 100 100	29, 36, 59, 76	0
8	i	35/38 (92%)	-0.02	1 (2%) 53 60	29, 38, 67, 86	0
9	J	36/40 (90%)	0.29	1 (2%) 55 62	32, 44, 75, 86	0
9	j	36/40 (90%)	0.47	4 (11%) 10 11	36, 51, 78, 83	0
10	K	37/46 (80%)	0.35	0 100 100	38, 47, 64, 72	0
10	k	37/46 (80%)	0.34	0 100 100	43, 50, 66, 77	0
11	L	37/37 (100%)	-0.38	0 100 100	24, 27, 57, 65	0
11	l	36/37 (97%)	-0.45	1 (2%) 55 62	24, 28, 63, 74	0
12	M	32/36 (88%)	-0.24	0 100 100	25, 30, 53, 73	0
12	m	31/36 (86%)	-0.24	0 100 100	26, 31, 49, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.05	4 (1%) 70 77	24, 39, 74, 119	1 (0%)
13	o	244/272 (89%)	0.11	6 (2%) 58 66	23, 39, 75, 120	0
14	T	29/32 (90%)	-0.36	1 (3%) 48 54	24, 29, 51, 68	0
14	t	29/32 (90%)	-0.27	1 (3%) 48 54	24, 30, 61, 76	0
15	U	97/134 (72%)	0.01	0 100 100	29, 40, 63, 89	0
15	u	97/134 (72%)	-0.09	1 (1%) 79 84	29, 38, 54, 84	0
16	V	137/163 (84%)	-0.18	0 100 100	27, 37, 52, 68	0
16	v	137/163 (84%)	0.13	0 100 100	30, 43, 62, 79	0
17	Y	27/46 (58%)	1.31	5 (18%) 3 3	46, 66, 91, 93	0
17	y	30/46 (65%)	0.91	2 (6%) 24 27	55, 66, 77, 92	0
18	X	38/41 (92%)	0.16	1 (2%) 57 64	35, 44, 61, 69	0
18	x	39/41 (95%)	0.44	2 (5%) 33 38	42, 52, 74, 95	0
19	Z	62/62 (100%)	1.04	4 (6%) 25 28	51, 62, 100, 108	0
19	z	62/62 (100%)	1.06	5 (8%) 18 20	55, 66, 109, 118	0
20	R	28/41 (68%)	0.87	1 (3%) 46 52	53, 62, 72, 80	0
20	r	28/41 (68%)	1.34	5 (17%) 3 4	59, 73, 89, 90	0
All	All	5293/5700 (92%)	-0.08	69 (1%) 75 80	10, 35, 66, 120	190 (3%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	6.4
3	c	24	THR	4.9
19	z	33	TRP	4.1
17	Y	25	ILE	3.9
19	Z	62	VAL	3.8
3	c	23	ALA	3.8
7	h	64	ALA	3.7
19	Z	33	TRP	3.6
14	t	30	THR	3.4
9	j	5	GLY	3.3
7	h	6	TRP	3.1
13	o	59	LYS	3.1
13	O	56	PRO	3.1
2	b	495	PHE	3.0
5	e	79	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	b	499	VAL	2.9
20	r	14	LEU	2.9
13	o	63	ALA	2.8
20	r	27	ALA	2.8
19	z	40	ILE	2.8
2	B	495	PHE	2.8
17	Y	22	LEU	2.8
17	Y	20	ALA	2.7
5	E	79	PHE	2.7
13	o	56	PRO	2.6
9	j	6	GLY	2.6
5	e	3	GLY	2.6
1	a	11	ALA	2.6
13	O	133	VAL	2.6
15	u	53	ALA	2.6
3	c	134	ILE	2.5
19	z	3	ILE	2.5
13	O	60	ARG	2.5
20	r	20	VAL	2.5
9	J	5	GLY	2.4
2	B	505	ARG	2.4
19	Z	40	ILE	2.4
2	b	488	PRO	2.4
20	r	28	VAL	2.4
17	y	34	MET	2.4
8	i	36	ASP	2.3
2	b	127	ARG	2.3
7	H	65	LEU	2.3
18	X	2	THR	2.3
13	o	132	ASN	2.3
19	z	62	VAL	2.2
2	B	489	GLU	2.2
17	Y	23	THR	2.2
17	y	29	GLY	2.2
1	A	11	ALA	2.2
18	x	37	VAL	2.2
14	T	30	THR	2.1
2	B	487	SER	2.1
6	F	12	SER	2.1
13	O	59	LYS	2.1
18	x	40	SER	2.1
9	j	7	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
13	o	57	LYS	2.1
6	f	13	TYR	2.1
11	l	2	GLU	2.1
19	Z	7	LEU	2.1
2	B	479[A]	PHE	2.0
9	j	8	ILE	2.0
19	z	41	PHE	2.0
17	Y	24	MET	2.0
20	r	3	TRP	2.0
3	c	135	ARG	2.0
2	b	496	TYR	2.0
20	R	28	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	0.91	0.09	30,35,52,59	0
14	FME	T	1	10/11	0.93	0.08	28,33,51,62	0
8	FME	I	1	10/11	0.95	0.07	38,41,48,48	0
12	FME	M	1	10/11	0.95	0.09	35,43,59,60	0
12	FME	m	1	10/11	0.96	0.08	30,42,61,67	0
8	FME	i	1	10/11	0.97	0.08	33,42,46,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	STE	C	529	14/20	0.58	0.20	56,71,82,83	0
30	STE	i	101	12/20	0.58	0.16	67,81,92,93	0
30	STE	C	520	10/20	0.62	0.19	49,62,65,69	0
30	STE	E	104	20/20	0.68	0.18	51,66,72,74	0
30	STE	A	620	11/20	0.70	0.19	54,61,73,76	0
30	STE	I	101	17/20	0.72	0.16	52,59,66,67	0
30	STE	j	102	16/20	0.72	0.18	55,67,81,82	0
33	LMG	D	406	50/55	0.72	0.18	36,61,85,91	0
30	STE	H	103	18/20	0.73	0.18	54,62,69,70	0
30	STE	K	102	14/20	0.73	0.16	55,64,74,75	0
30	STE	e	101	9/20	0.73	0.24	62,74,80,80	0
30	STE	A	619	17/20	0.74	0.15	53,59,67,67	0
30	STE	i	102	6/20	0.74	0.20	52,66,69,70	0
29	PL9	a	612	55/55	0.75	0.17	43,59,70,75	0
30	STE	e	103	9/20	0.75	0.18	54,61,70,74	0
30	STE	c	517	18/20	0.75	0.17	64,71,81,85	0
34	LHG	a	615	42/49	0.75	0.16	51,77,87,102	0
30	STE	C	519	7/20	0.76	0.18	50,55,58,62	0
30	STE	E	103	12/20	0.76	0.17	59,67,92,95	0
30	STE	C	516	14/20	0.76	0.16	53,60,63,71	0
30	STE	a	619	12/20	0.76	0.14	52,60,75,76	0
33	LMG	b	622	55/55	0.77	0.17	51,61,76,78	0
33	LMG	a	617	55/55	0.77	0.16	36,55,67,73	0
30	STE	C	518	5/20	0.78	0.17	50,56,60,61	0
30	STE	f	102	8/20	0.78	0.20	53,58,65,69	0
30	STE	h	102	10/20	0.78	0.18	59,66,74,76	0
33	LMG	c	518	30/55	0.78	0.15	41,73,82,83	0
34	LHG	E	101	49/49	0.78	0.15	42,64,87,97	0
32	DGD	A	617	66/66	0.78	0.15	45,55,76,79	0
29	PL9	A	612	55/55	0.79	0.17	35,57,71,75	0
30	STE	k	103	14/20	0.79	0.13	59,62,75,76	0
30	STE	e	104	13/20	0.79	0.17	66,70,79,81	0
30	STE	A	613	9/20	0.80	0.17	53,57,66,66	0
30	STE	B	625	12/20	0.80	0.14	43,55,66,67	0
30	STE	T	102	16/20	0.80	0.20	36,49,79,80	0
30	STE	t	103	10/20	0.80	0.16	44,54,62,62	0
30	STE	Z	101	17/20	0.80	0.19	50,69,83,84	0
33	LMG	C	517	36/55	0.80	0.14	44,54,62,68	0
30	STE	z	101	9/20	0.81	0.20	56,57,62,63	0
33	LMG	c	523	48/55	0.81	0.15	49,62,80,82	0
31	SQD	a	616	54/54	0.82	0.13	38,56,83,92	0
30	STE	a	620	15/20	0.82	0.19	42,52,65,65	0
30	STE	C	527	12/20	0.83	0.15	36,43,49,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	STE	J	101	12/20	0.83	0.13	46,49,61,65	0
30	STE	d	410	20/20	0.83	0.13	45,58,73,76	0
30	STE	T	103	15/20	0.84	0.16	47,52,72,78	0
30	STE	B	624	18/20	0.84	0.12	44,49,78,78	0
30	STE	E	102	12/20	0.84	0.14	56,67,76,77	0
30	STE	I	102	15/20	0.84	0.14	43,48,63,63	0
30	STE	j	101	12/20	0.84	0.13	48,55,60,65	0
33	LMG	B	620	45/55	0.84	0.14	34,54,77,84	0
30	STE	b	623	16/20	0.84	0.15	43,53,60,63	0
31	SQD	A	616	43/54	0.85	0.11	39,51,78,85	0
30	STE	m	102	12/20	0.85	0.13	43,50,72,72	0
30	STE	b	625	11/20	0.85	0.15	50,53,59,59	0
30	STE	c	516	13/20	0.85	0.15	57,64,69,70	0
33	LMG	C	522	48/55	0.86	0.12	37,53,66,69	0
30	STE	A	618	8/20	0.86	0.15	46,52,56,57	0
30	STE	B	621	17/20	0.86	0.12	35,45,64,66	0
30	STE	d	412	20/20	0.86	0.13	37,47,63,70	0
30	STE	b	621	20/20	0.87	0.11	39,49,64,64	0
33	LMG	m	101	51/55	0.87	0.11	35,46,57,61	0
33	LMG	C	526	48/55	0.87	0.13	39,60,75,76	0
33	LMG	c	522	46/55	0.87	0.12	40,58,67,68	0
31	SQD	B	623	54/54	0.88	0.11	34,55,68,72	0
30	STE	C	528	16/20	0.88	0.12	38,44,58,58	0
31	SQD	b	620	49/54	0.88	0.11	38,52,68,74	0
30	STE	b	624	10/20	0.88	0.12	46,51,69,73	0
33	LMG	M	101	51/55	0.88	0.11	31,48,56,62	0
30	STE	D	411	20/20	0.88	0.12	35,41,64,72	0
33	LMG	a	618	49/55	0.88	0.11	35,54,68,70	0
28	BCR	C	521	40/40	0.89	0.10	36,46,59,59	0
26	CLA	b	601	65/65	0.89	0.11	37,54,77,83	0
30	STE	t	102	14/20	0.89	0.11	37,45,57,58	0
31	SQD	f	101	41/54	0.89	0.12	49,66,75,86	0
30	STE	d	406	20/20	0.90	0.11	37,45,67,71	0
31	SQD	a	614	54/54	0.90	0.11	40,57,69,70	0
30	STE	D	412	9/20	0.90	0.13	50,54,61,64	0
30	STE	M	102	15/20	0.91	0.10	38,44,60,69	0
26	CLA	C	513	65/65	0.91	0.10	40,51,74,77	0
30	STE	m	103	18/20	0.91	0.11	33,41,60,61	0
28	BCR	c	514	40/40	0.91	0.10	45,53,59,62	0
28	BCR	k	101	40/40	0.91	0.10	44,52,58,61	0
28	BCR	k	102	40/40	0.91	0.11	42,47,56,60	0
26	CLA	B	601	65/65	0.91	0.10	26,42,71,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	STE	M	103	10/20	0.92	0.11	40,43,50,50	0
32	DGD	C	524	62/66	0.92	0.10	31,41,83,92	0
32	DGD	h	101	62/66	0.92	0.09	31,41,48,55	0
26	CLA	c	512	65/65	0.92	0.09	40,48,70,73	0
31	SQD	F	102	36/54	0.92	0.11	42,62,71,72	0
26	CLA	c	513	65/65	0.92	0.11	41,53,77,81	0
28	BCR	d	404	40/40	0.92	0.10	37,43,70,74	0
28	BCR	C	514	40/40	0.92	0.10	39,48,54,58	0
31	SQD	A	615	52/54	0.92	0.10	29,49,73,78	0
33	LMG	D	407	51/55	0.93	0.10	29,42,70,73	0
28	BCR	D	404	40/40	0.93	0.09	30,39,71,79	0
28	BCR	T	101	40/40	0.93	0.07	23,34,43,45	0
32	DGD	H	102	62/66	0.93	0.09	26,36,44,49	0
32	DGD	c	520	62/66	0.93	0.09	32,41,70,76	0
26	CLA	C	512	65/65	0.93	0.09	35,44,68,76	0
26	CLA	C	503	65/65	0.93	0.08	29,36,41,46	0
28	BCR	B	618	40/40	0.93	0.08	25,35,42,46	0
26	CLA	C	511	65/65	0.93	0.09	35,42,54,57	0
34	LHG	D	410	49/49	0.93	0.10	26,39,56,57	0
28	BCR	x	101	40/40	0.93	0.09	33,41,52,52	0
26	CLA	c	503	65/65	0.93	0.08	32,38,44,46	0
28	BCR	b	618	40/40	0.94	0.07	25,35,44,46	0
28	BCR	b	619	40/40	0.94	0.07	28,40,54,54	0
26	CLA	b	606	65/65	0.94	0.08	26,33,58,62	0
28	BCR	c	515	40/40	0.94	0.09	30,42,48,52	0
26	CLA	b	616	60/65	0.94	0.09	27,37,75,82	0
28	BCR	A	611	40/40	0.94	0.07	25,32,36,37	0
28	BCR	H	101	40/40	0.94	0.08	28,35,48,53	0
32	DGD	c	521	62/66	0.94	0.08	27,42,65,76	0
28	BCR	t	101	40/40	0.94	0.07	28,34,42,43	0
28	BCR	K	101	40/40	0.94	0.09	35,42,53,61	0
26	CLA	B	606	65/65	0.94	0.08	23,29,57,64	0
28	BCR	b	617	40/40	0.94	0.07	26,35,42,44	0
29	PL9	d	405	55/55	0.94	0.07	23,30,35,37	0
34	LHG	d	407	49/49	0.94	0.10	32,43,58,62	0
27	PHO	d	401	64/64	0.95	0.07	26,33,38,42	0
32	DGD	C	525	62/66	0.95	0.08	27,38,64,82	0
26	CLA	C	509	65/65	0.95	0.08	27,34,52,55	0
29	PL9	D	405	55/55	0.95	0.06	21,28,35,36	0
28	BCR	B	617	40/40	0.95	0.06	23,34,41,43	0
26	CLA	C	510	65/65	0.95	0.07	28,35,48,57	0
28	BCR	B	619	40/40	0.95	0.07	26,37,49,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	b	610	65/65	0.95	0.07	26,32,40,45	0
28	BCR	C	515	40/40	0.95	0.08	25,35,45,47	0
26	CLA	C	504	59/65	0.95	0.07	28,34,68,73	0
26	CLA	C	506	65/65	0.95	0.09	26,35,68,72	0
26	CLA	c	504	60/65	0.95	0.08	25,38,64,69	0
26	CLA	c	505	65/65	0.95	0.08	27,36,54,57	0
26	CLA	c	506	65/65	0.95	0.09	31,39,74,79	0
28	BCR	a	611	40/40	0.95	0.06	22,30,38,41	0
26	CLA	c	508	64/65	0.95	0.08	31,38,80,90	0
26	CLA	c	509	65/65	0.95	0.09	31,39,52,56	0
26	CLA	c	510	65/65	0.95	0.07	31,39,51,60	0
26	CLA	c	511	65/65	0.95	0.09	35,46,57,61	0
33	LMG	d	411	44/55	0.95	0.09	34,42,65,70	0
26	CLA	C	508	65/65	0.95	0.08	26,33,80,90	0
34	LHG	D	409	47/49	0.95	0.10	26,36,66,71	0
26	CLA	a	607	65/65	0.95	0.07	19,26,37,49	0
26	CLA	d	403	65/65	0.95	0.08	29,35,67,71	0
27	PHO	A	609	64/64	0.95	0.06	19,26,29,32	0
27	PHO	D	401	64/64	0.95	0.06	24,28,33,37	0
34	LHG	d	409	39/49	0.95	0.09	31,38,57,59	0
34	LHG	l	101	49/49	0.95	0.08	29,39,47,55	0
32	DGD	C	523	62/66	0.96	0.08	23,35,63,69	0
26	CLA	b	614	65/65	0.96	0.07	25,33,60,66	0
26	CLA	b	615	65/65	0.96	0.07	26,33,52,62	0
26	CLA	C	507	65/65	0.96	0.07	25,33,45,55	0
32	DGD	c	519	62/66	0.96	0.09	25,33,62,69	0
26	CLA	c	501	65/65	0.96	0.07	27,33,44,48	0
26	CLA	c	502	65/65	0.96	0.07	28,35,48,54	0
26	CLA	B	610	65/65	0.96	0.06	20,27,35,37	0
26	CLA	B	612	65/65	0.96	0.06	20,26,35,43	0
26	CLA	B	614	65/65	0.96	0.08	23,28,60,65	0
26	CLA	B	616	60/65	0.96	0.08	23,30,75,85	0
26	CLA	c	507	65/65	0.96	0.07	30,37,46,52	0
26	CLA	C	501	65/65	0.96	0.06	23,29,40,43	0
26	CLA	C	502	65/65	0.96	0.07	27,33,46,53	0
26	CLA	B	604	65/65	0.96	0.07	21,25,60,62	0
26	CLA	a	608	65/65	0.96	0.08	23,32,79,84	0
26	CLA	a	610	65/65	0.96	0.08	20,26,66,72	0
26	CLA	a	613	65/65	0.96	0.06	18,27,40,44	0
26	CLA	d	402	65/65	0.96	0.07	21,26,46,56	0
26	CLA	B	602	65/65	0.96	0.06	22,28,47,53	0
26	CLA	b	602	65/65	0.96	0.07	28,34,48,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	b	603	65/65	0.96	0.07	23,29,51,55	0
27	PHO	a	609	64/64	0.96	0.06	21,26,32,35	0
34	LHG	B	622	49/49	0.96	0.08	26,36,46,57	0
26	CLA	C	505	65/65	0.96	0.07	24,31,52,59	0
26	CLA	b	607	65/65	0.96	0.07	21,29,53,63	0
26	CLA	b	608	65/65	0.96	0.06	26,34,46,48	0
26	CLA	b	609	65/65	0.96	0.07	28,37,50,56	0
26	CLA	B	608	65/65	0.96	0.06	20,27,43,53	0
34	LHG	d	408	49/49	0.96	0.08	27,36,46,53	0
26	CLA	b	611	65/65	0.96	0.06	22,29,44,47	0
26	CLA	b	613	65/65	0.96	0.07	21,28,60,67	0
26	CLA	b	605	65/65	0.97	0.06	23,30,41,46	0
26	CLA	B	613	65/65	0.97	0.06	19,26,60,66	0
26	CLA	B	603	65/65	0.97	0.06	20,26,45,49	0
26	CLA	B	615	65/65	0.97	0.06	22,29,52,59	0
26	CLA	A	608	65/65	0.97	0.08	21,28,77,84	0
26	CLA	B	605	65/65	0.97	0.05	19,25,37,44	0
26	CLA	D	402	65/65	0.97	0.06	19,24,42,47	0
26	CLA	b	612	65/65	0.97	0.06	21,29,37,46	0
26	CLA	D	403	65/65	0.97	0.07	24,30,95,105	0
34	LHG	D	408	49/49	0.97	0.07	25,34,44,45	0
26	CLA	A	610	54/65	0.97	0.06	20,25,53,55	0
26	CLA	B	607	65/65	0.97	0.06	19,26,50,58	0
26	CLA	A	614	65/65	0.97	0.05	19,24,38,48	0
26	CLA	B	609	65/65	0.97	0.06	24,30,45,54	0
25	BCT	A	606	4/4	0.97	0.06	25,28,30,34	0
26	CLA	B	611	65/65	0.97	0.06	20,25,42,44	0
26	CLA	A	607	65/65	0.97	0.05	17,24,38,47	0
26	CLA	b	604	65/65	0.97	0.07	23,28,59,74	0
35	HEM	F	101	43/43	0.97	0.08	35,41,49,55	0
35	HEM	e	102	43/43	0.97	0.08	43,49,59,68	0
25	BCT	a	606	4/4	0.98	0.05	34,36,41,47	0
36	HEC	v	201	43/43	0.98	0.06	27,32,37,43	0
23	FE2	a	603	1/1	0.99	0.01	34,34,34,34	0
24	CL	A	604	1/1	0.99	0.03	25,25,25,25	0
24	CL	A	605	1/1	0.99	0.09	26,26,26,26	0
24	CL	a	604	1/1	0.99	0.05	26,26,26,26	0
24	CL	a	605	1/1	0.99	0.06	29,29,29,29	0
21	OEY	A	601[B]	11/11	0.99	0.03	21,24,28,29	11
21	OEY	a	601[B]	11/11	0.99	0.03	23,26,29,30	11
22	OEX	A	602[A]	10/10	0.99	0.03	23,24,27,28	10
36	HEC	V	201	43/43	0.99	0.05	24,28,37,39	0

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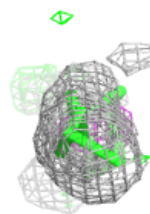
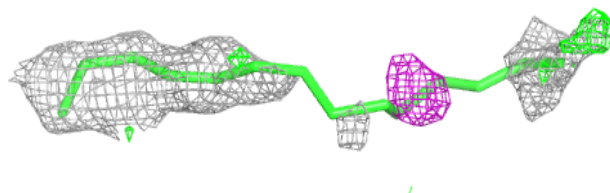
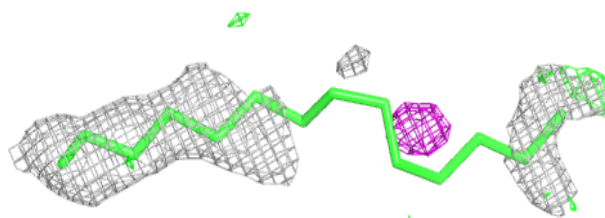
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	OEX	a	602[A]	10/10	0.99	0.03	22,25,28,29	10
23	FE2	A	603	1/1	1.00	0.01	27,27,27,27	0

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.

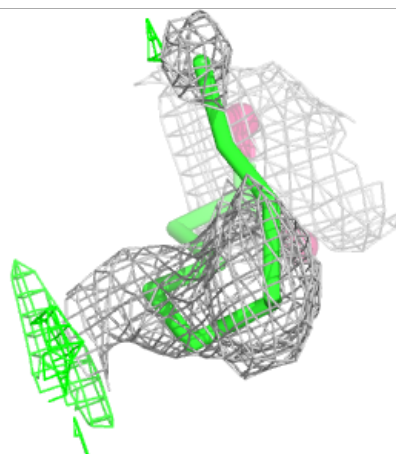
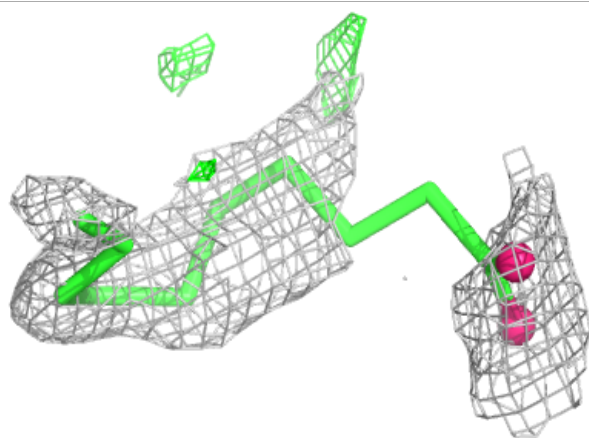
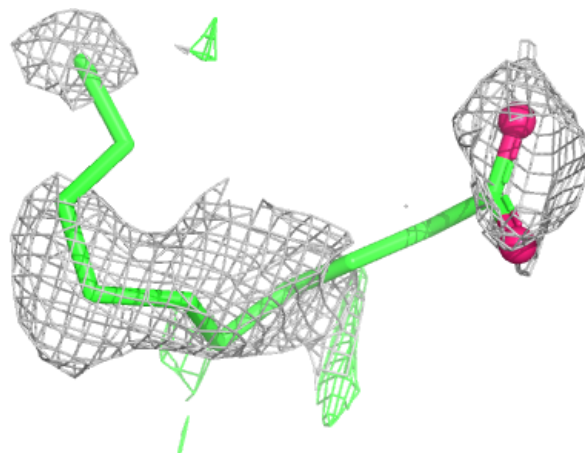
Electron density around STE C 529:

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



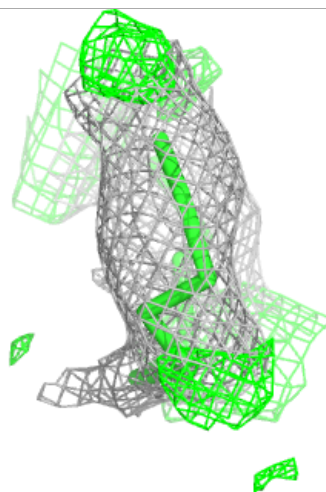
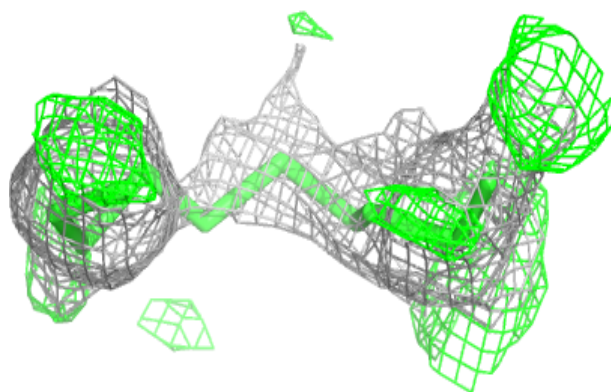
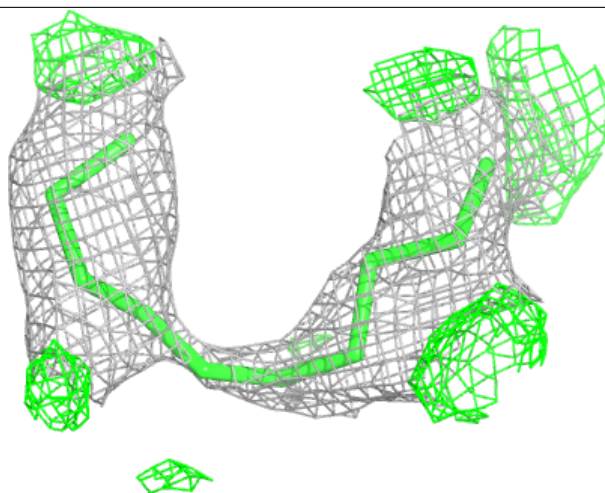
Electron density around STE i 101:

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



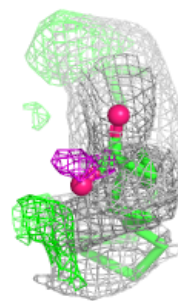
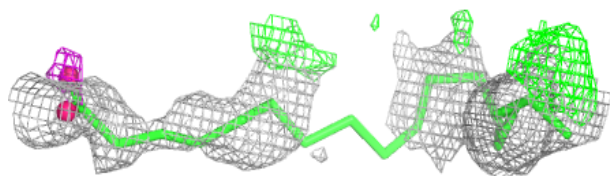
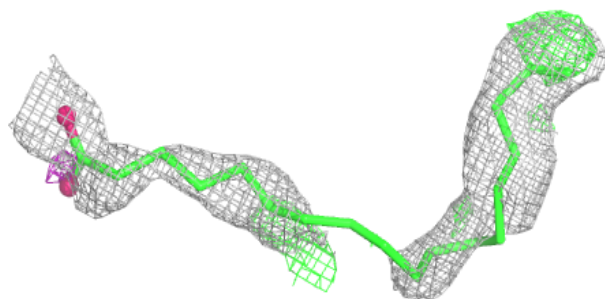
Electron density around STE C 520:

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

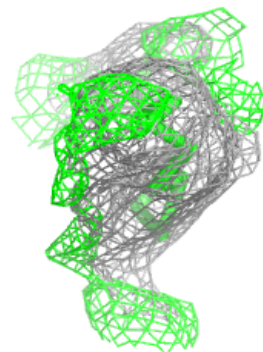
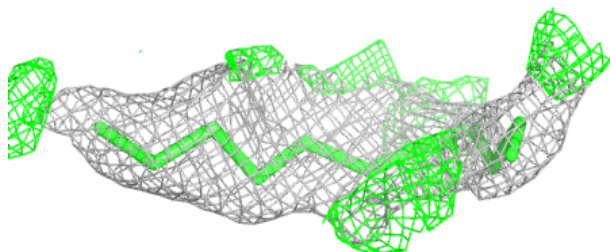
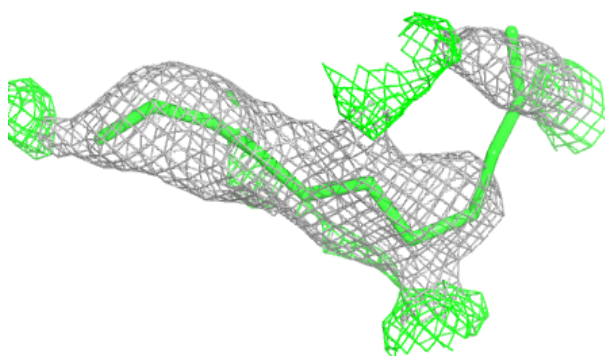


Electron density around STE E 104:

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

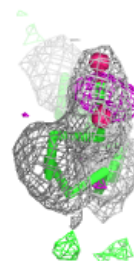
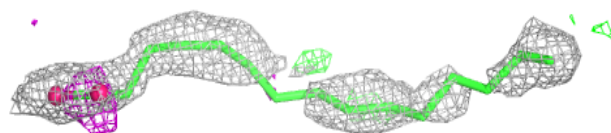
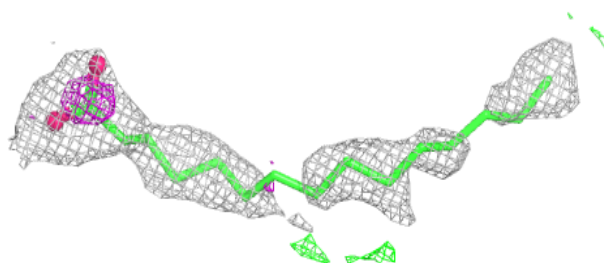
**Electron density around STE A 620:**

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

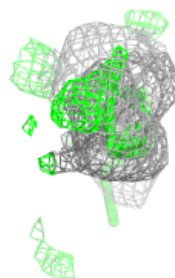
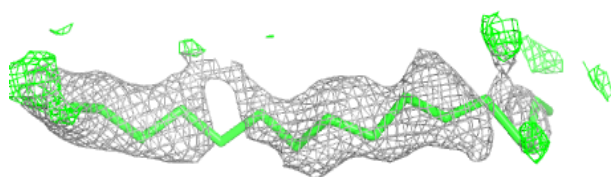
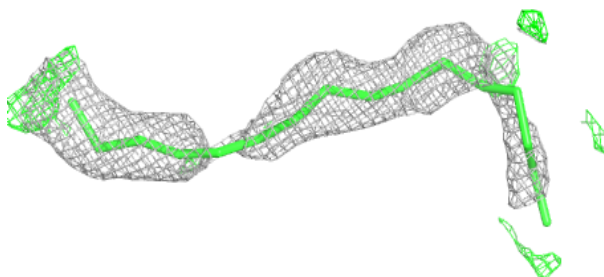


Electron density around STE I 101:

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

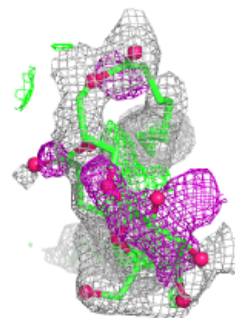
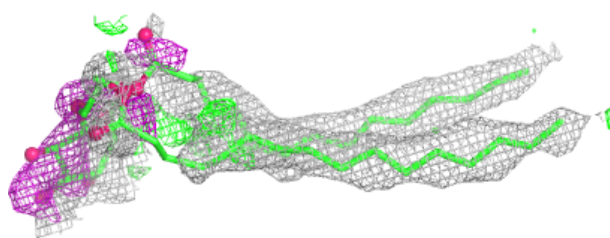
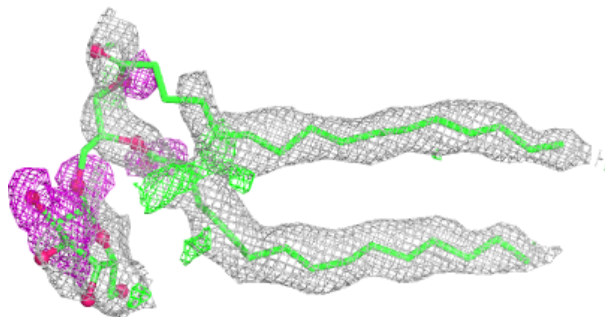
**Electron density around STE j 102:**

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

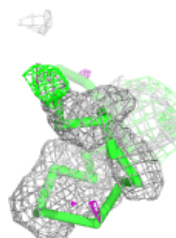
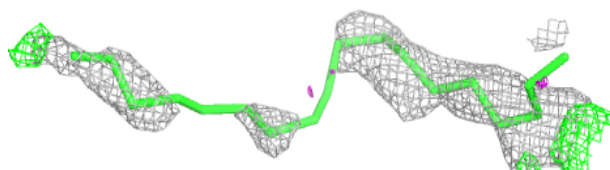
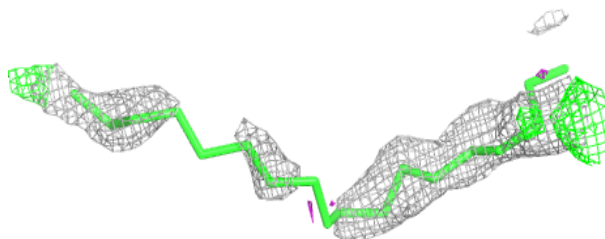


Electron density around LMG D 406:

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

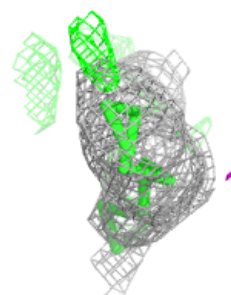
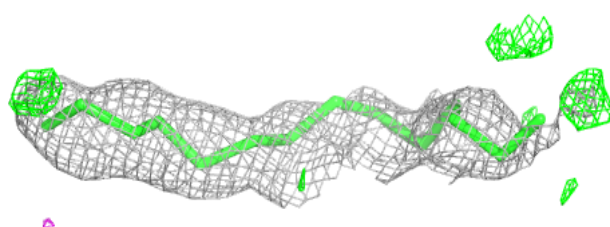
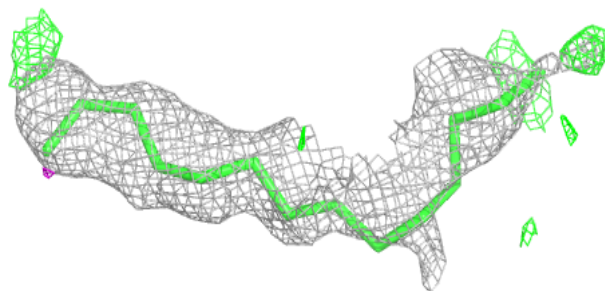
**Electron density around STE H 103:**

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

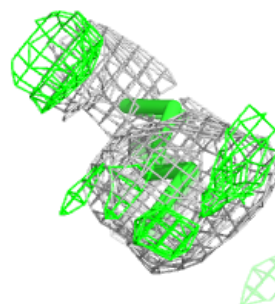
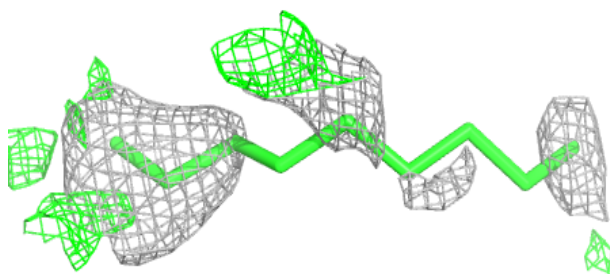
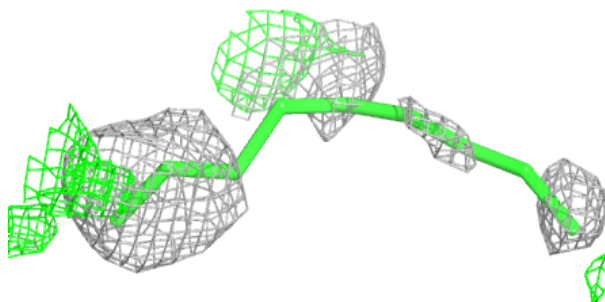


Electron density around STE K 102:

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

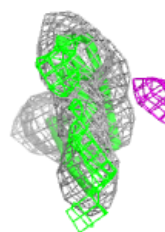
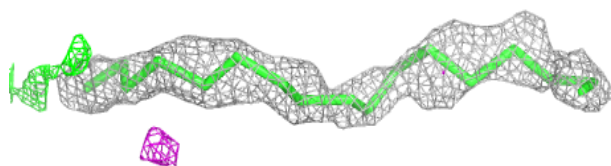
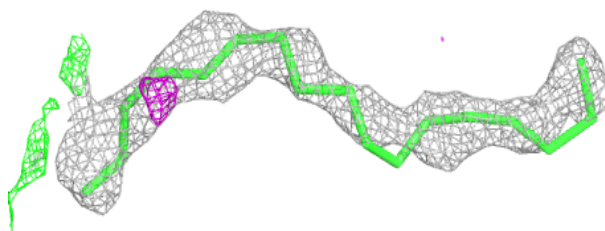
**Electron density around STE e 101:**

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

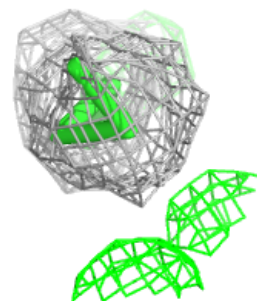
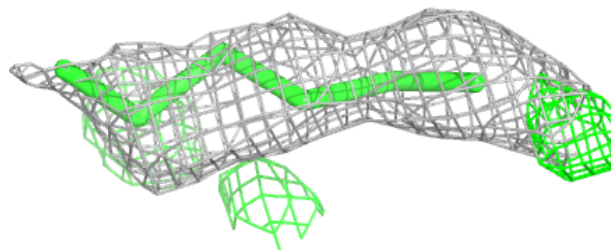
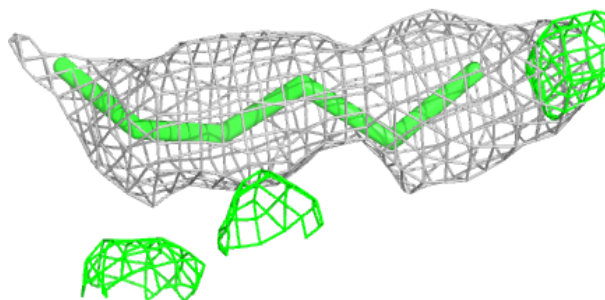


Electron density around STE A 619:

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

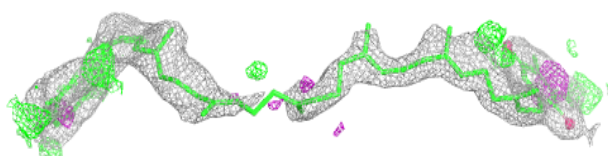
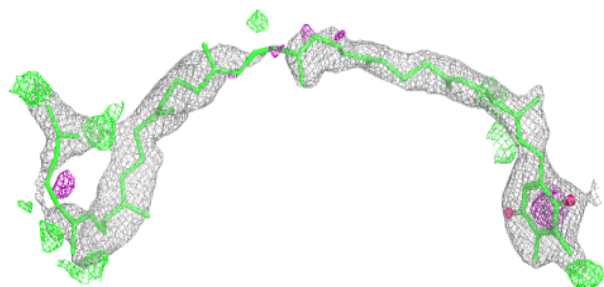
**Electron density around STE i 102:**

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

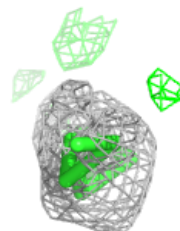
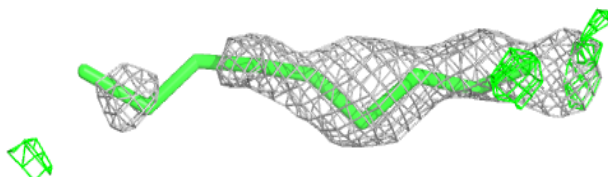
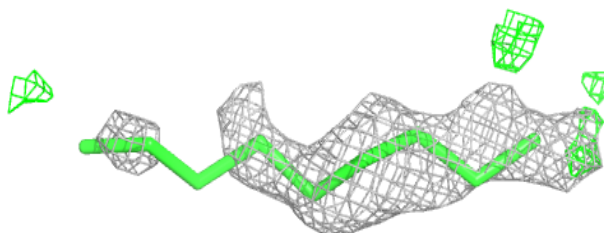


Electron density around PL9 a 612:

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

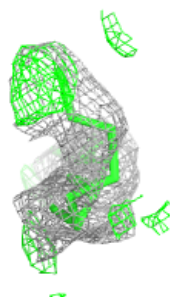
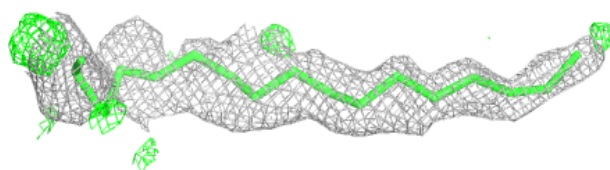
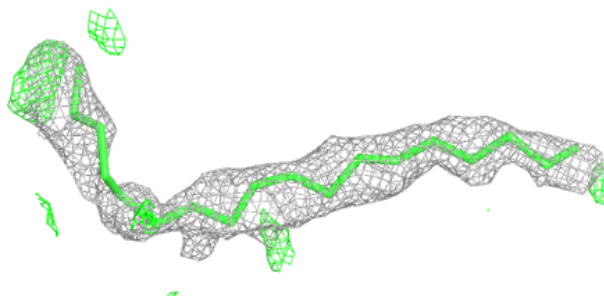
**Electron density around STE e 103:**

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

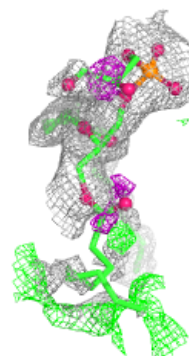
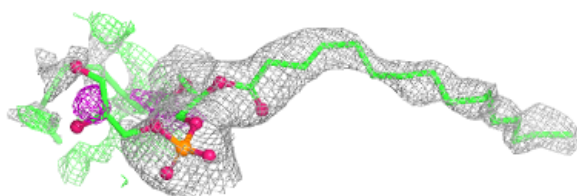
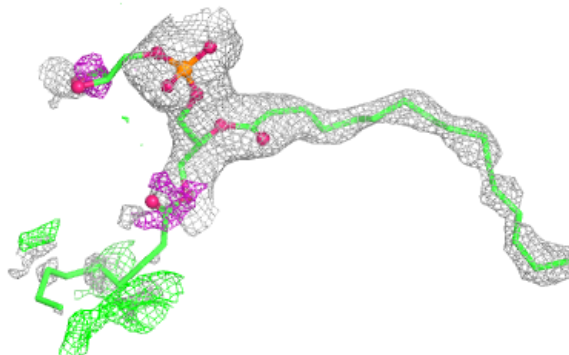


Electron density around STE c 517:

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

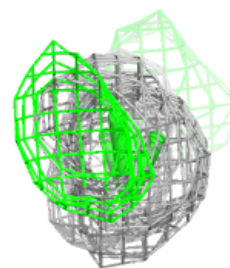
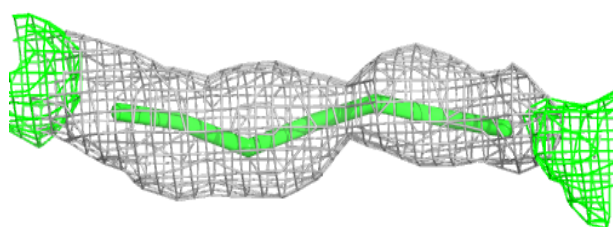
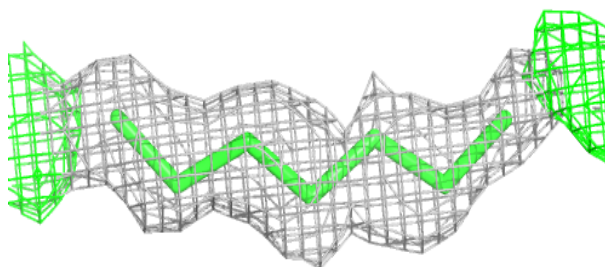
**Electron density around LHG a 615:**

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

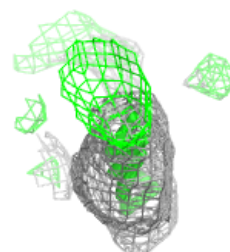
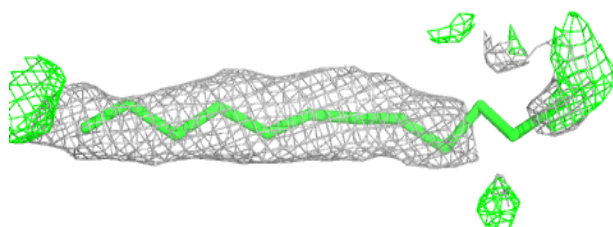
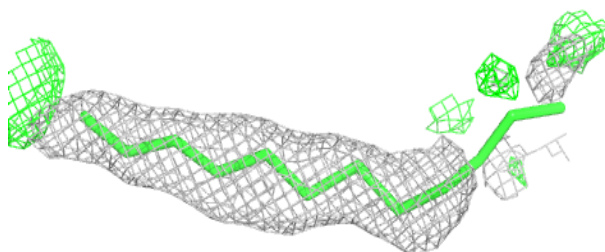


Electron density around STE C 519:

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

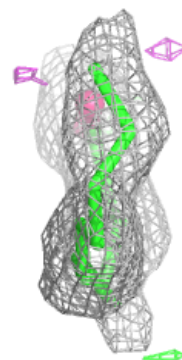
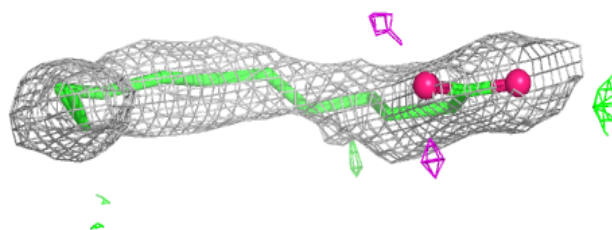
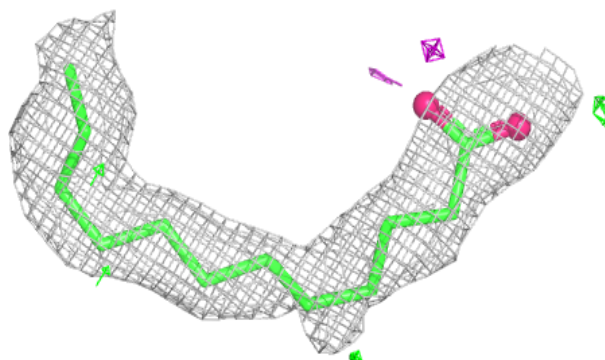
**Electron density around STE E 103:**

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

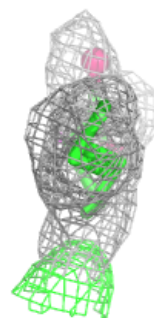
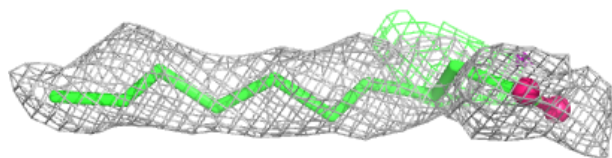
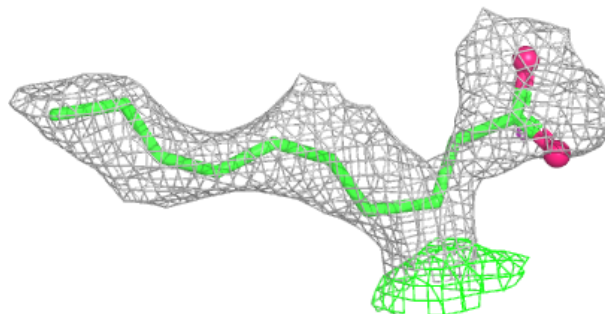


Electron density around STE C 516:

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

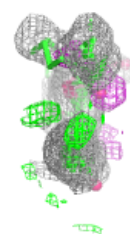
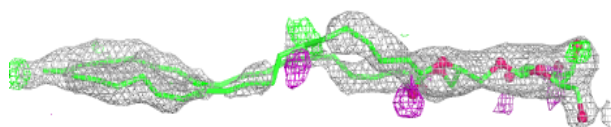
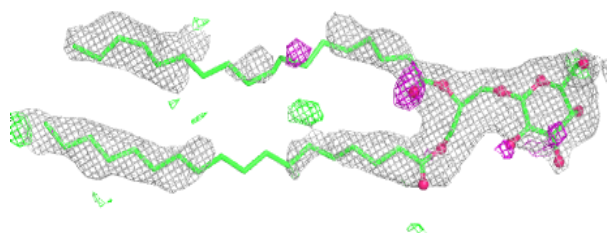
**Electron density around STE a 619:**

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



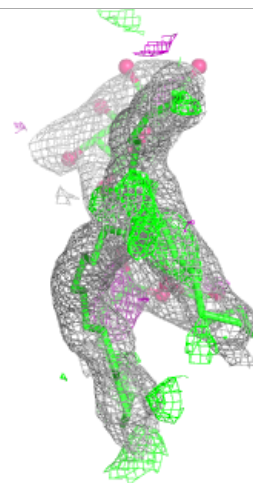
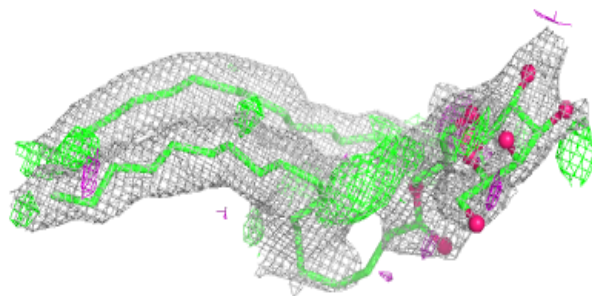
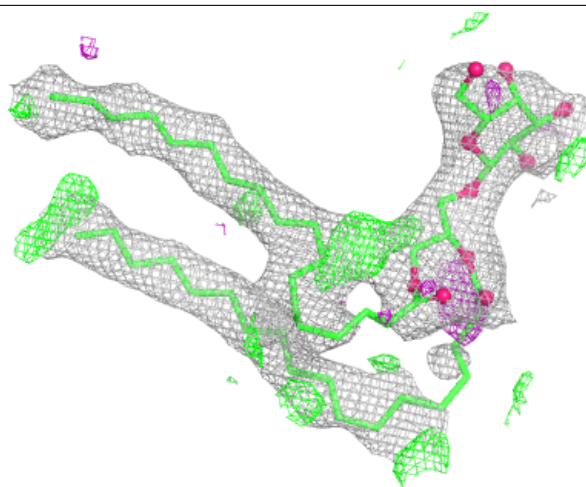
Electron density around LMG b 622:

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



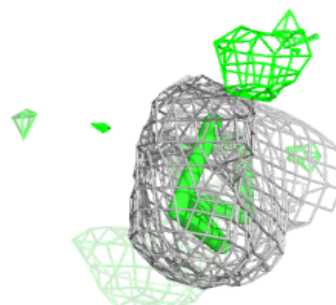
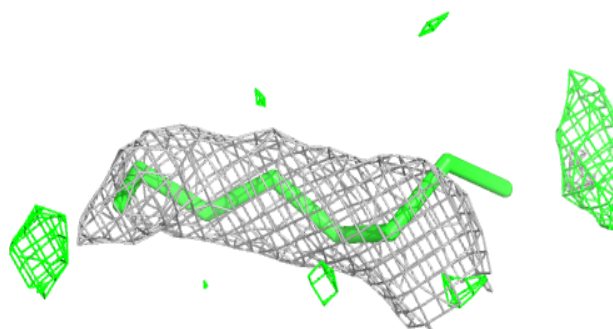
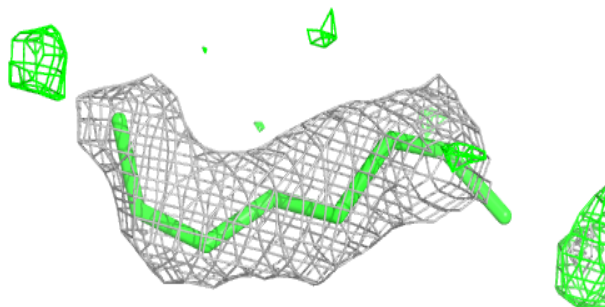
Electron density around LMG a 617:

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

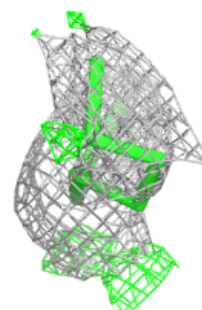
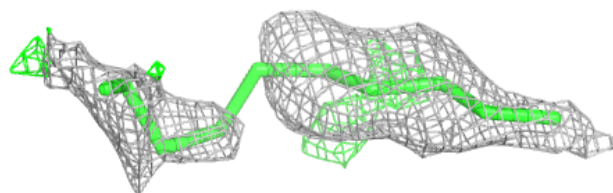
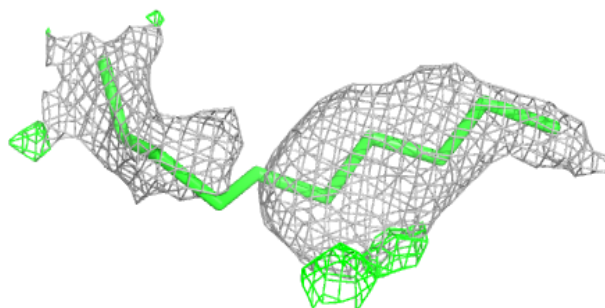


Electron density around STE f 102:

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

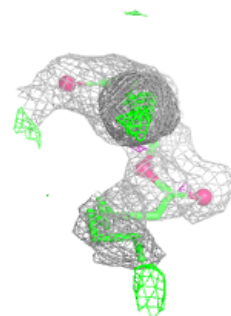
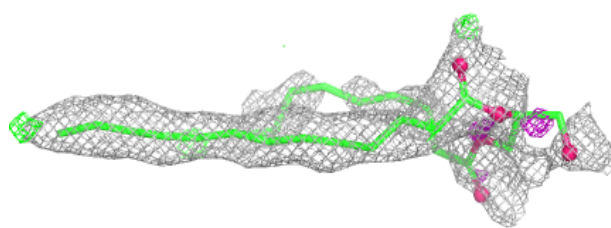
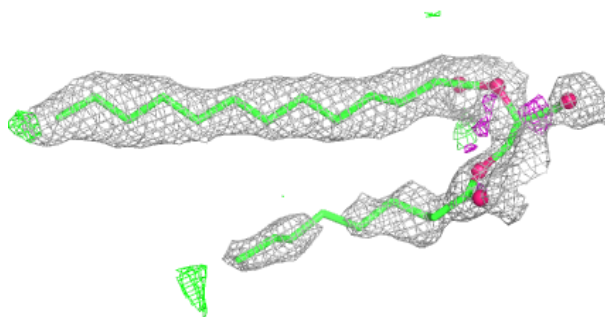
**Electron density around STE h 102:**

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



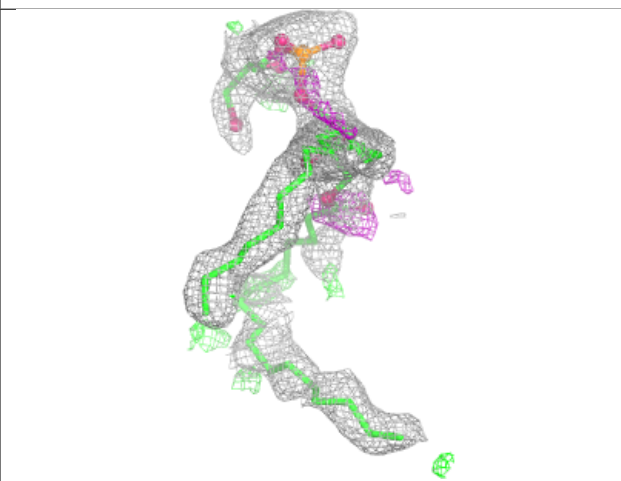
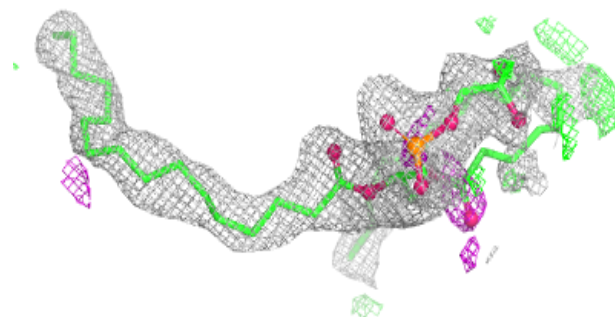
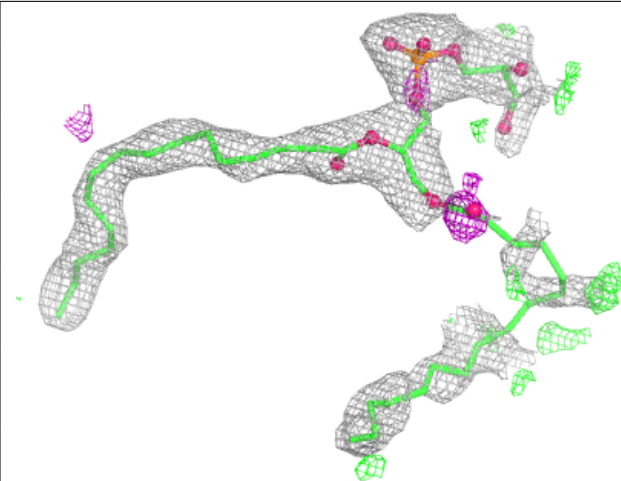
Electron density around LMG c 518:

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



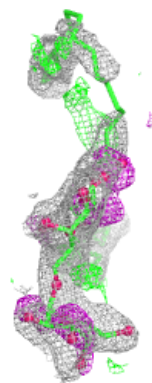
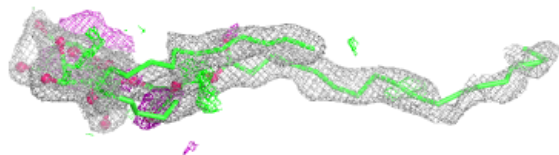
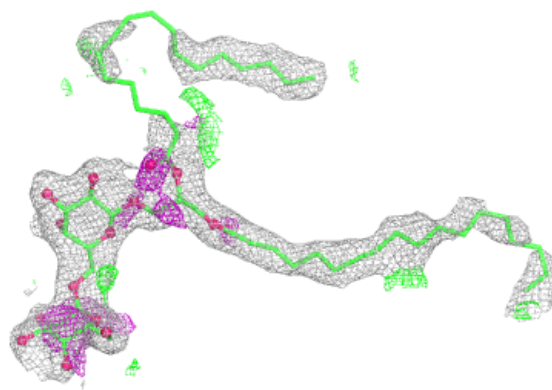
Electron density around LHG E 101:

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

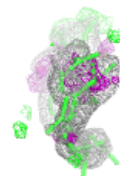
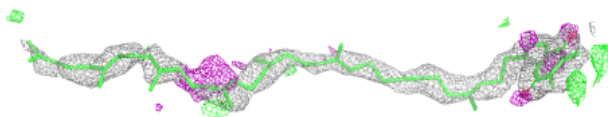
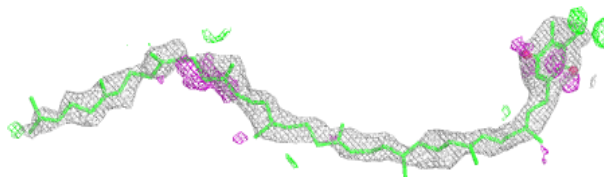


Electron density around DGD A 617:

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

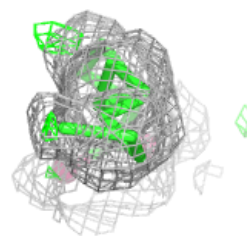
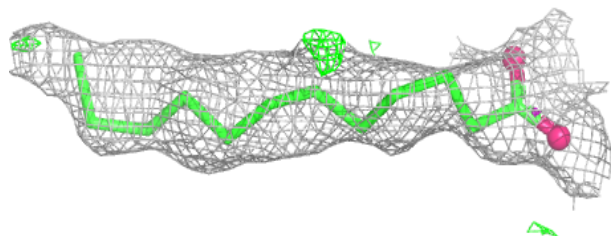
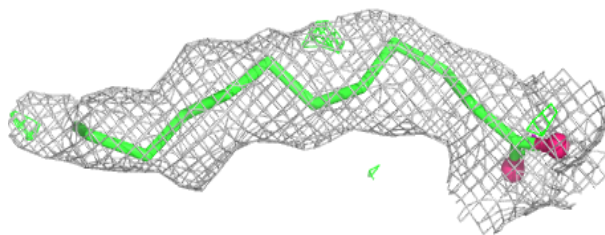
**Electron density around PL9 A 612:**

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

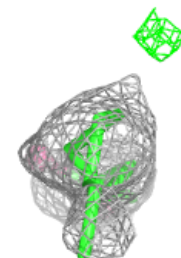
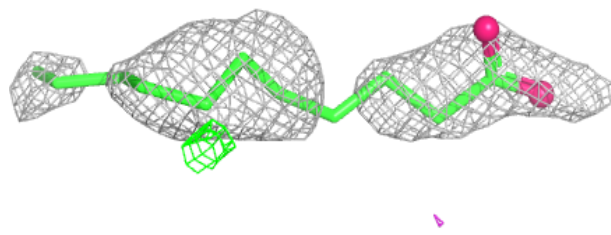
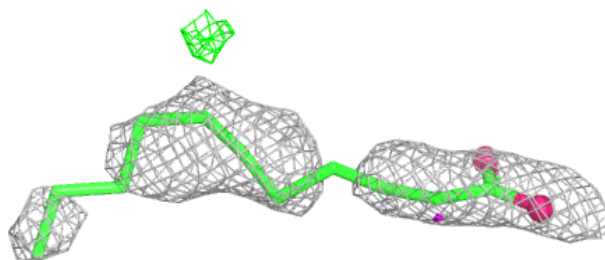


Electron density around STE k 103:

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

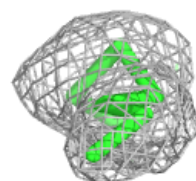
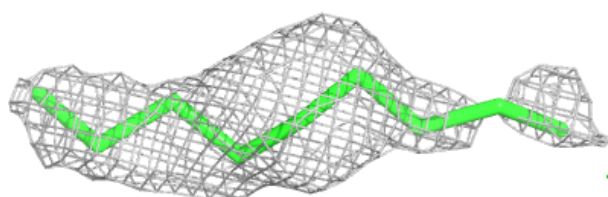
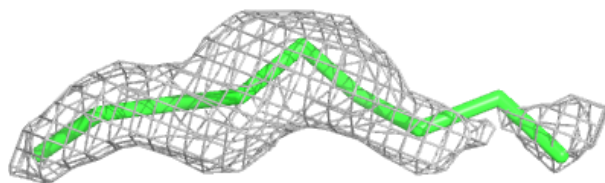
**Electron density around STE e 104:**

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

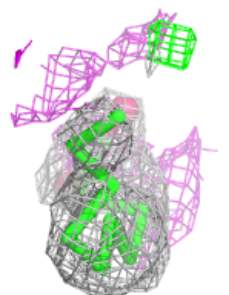
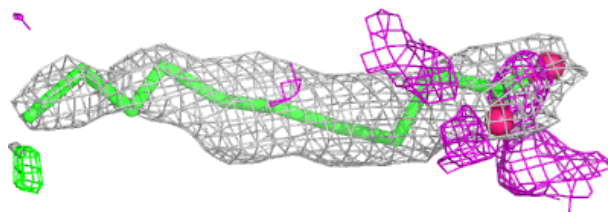
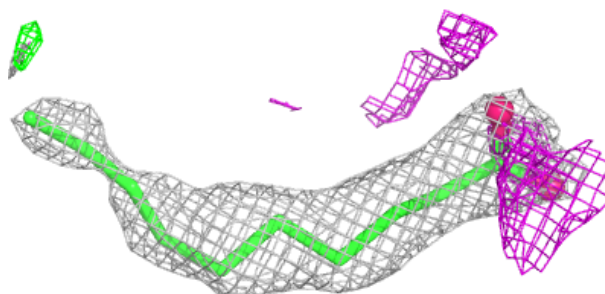


Electron density around STE A 613:

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

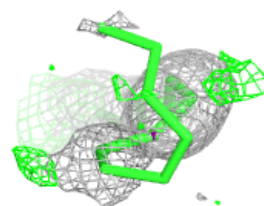
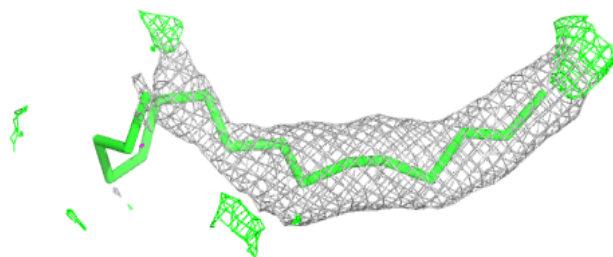
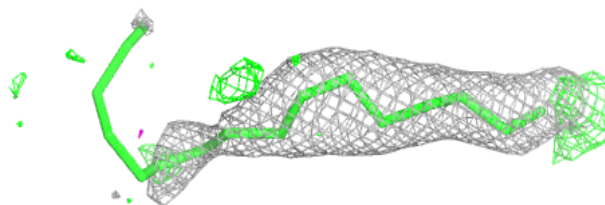
**Electron density around STE B 625:**

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

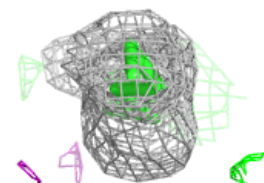
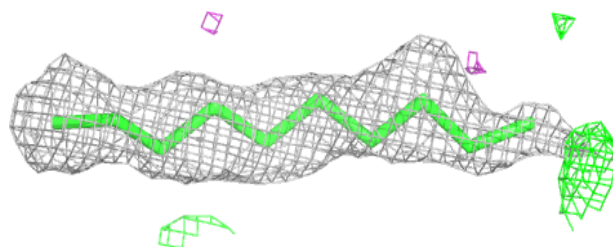
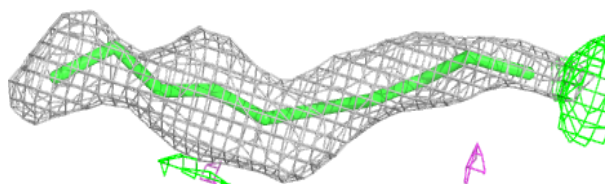


Electron density around STE T 102:

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

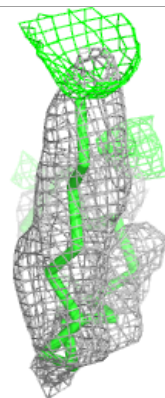
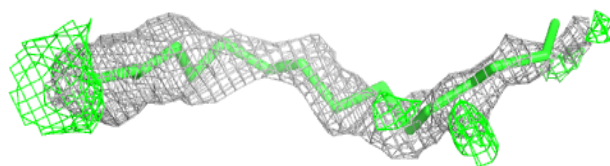
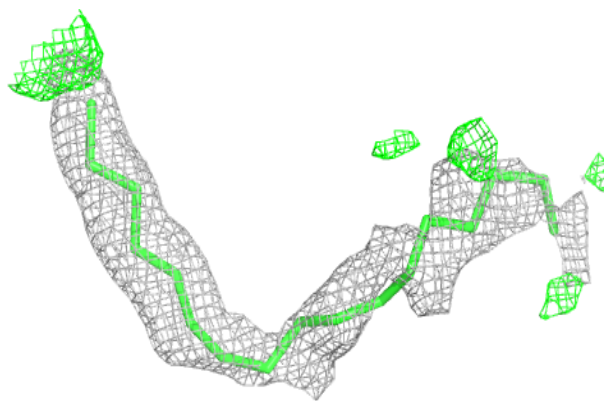
**Electron density around STE t 103:**

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

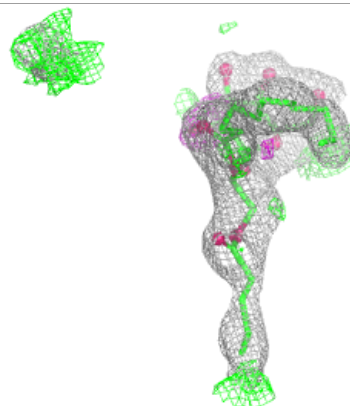
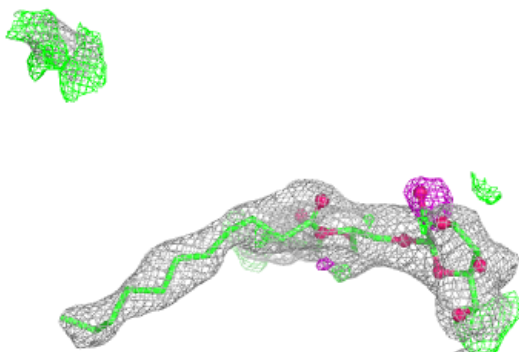
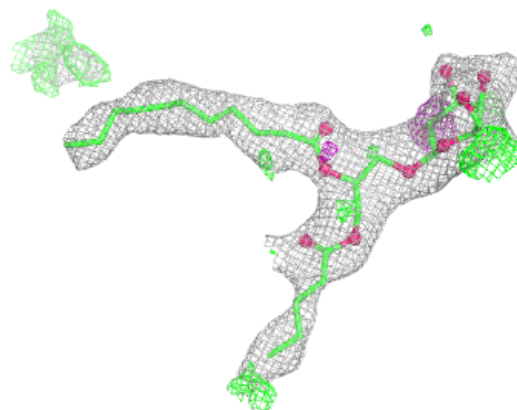


Electron density around STE Z 101:

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

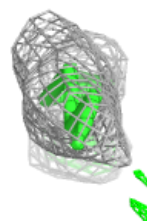
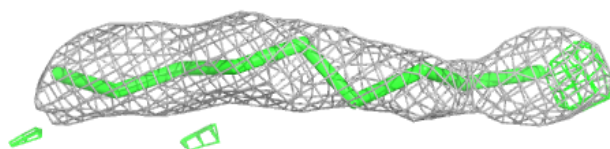
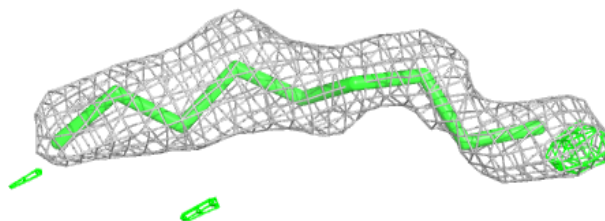
**Electron density around LMG C 517:**

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

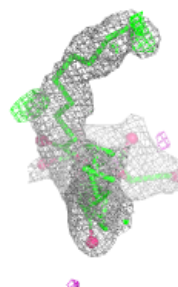
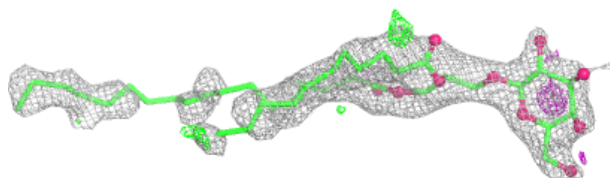
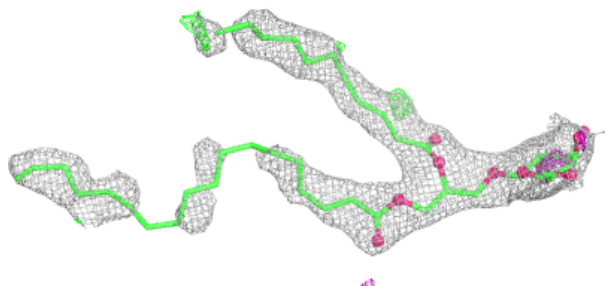


Electron density around STE z 101:

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

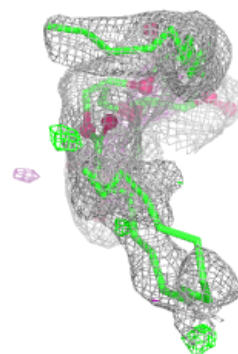
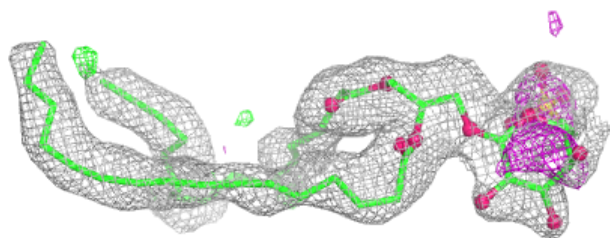
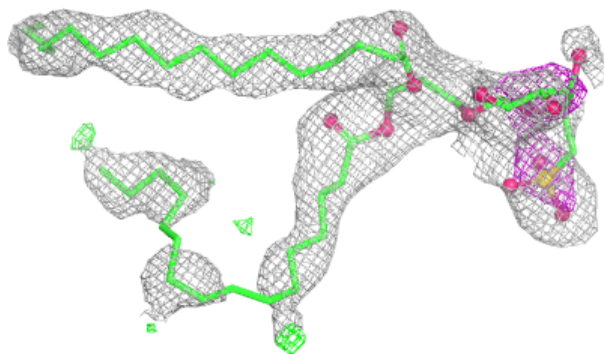
**Electron density around LMG c 523:**

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

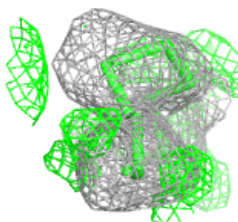
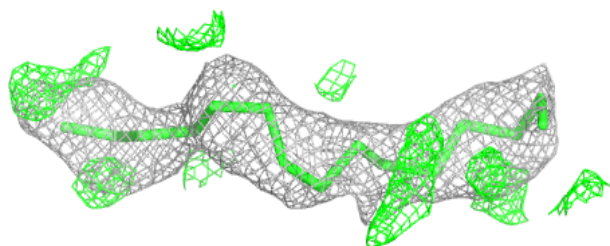
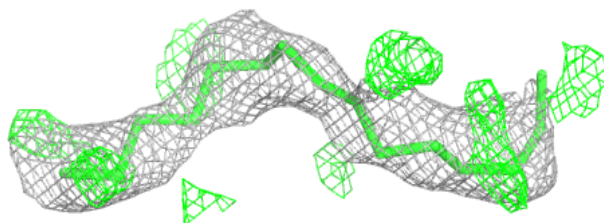


Electron density around SQD a 616:

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

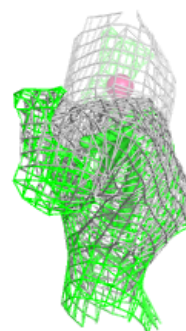
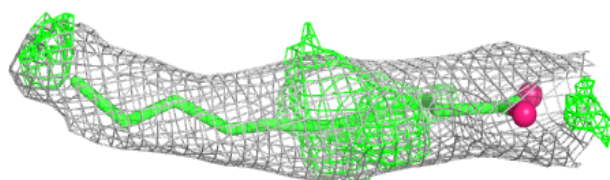
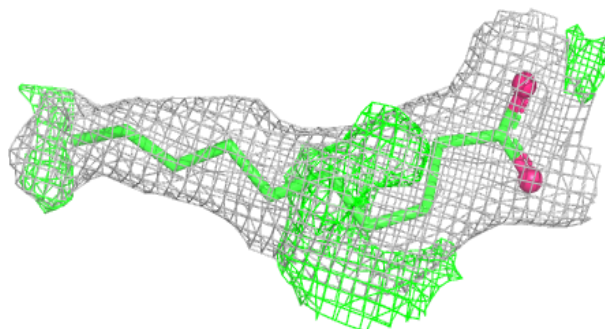
**Electron density around STE a 620:**

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

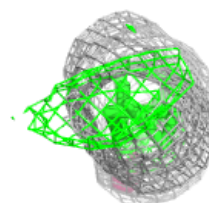
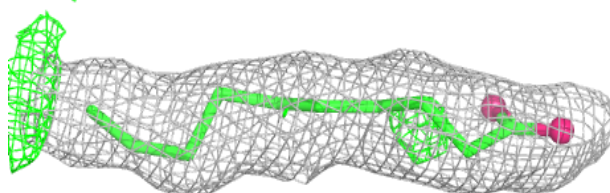
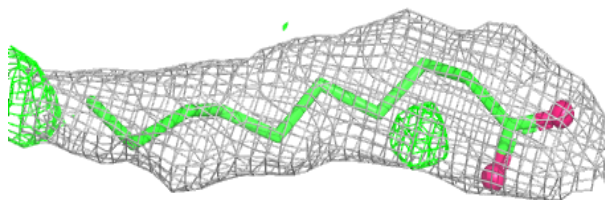


Electron density around STE C 527:

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

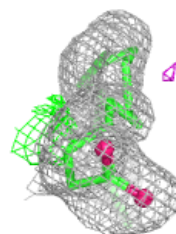
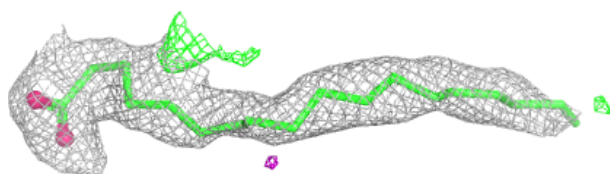
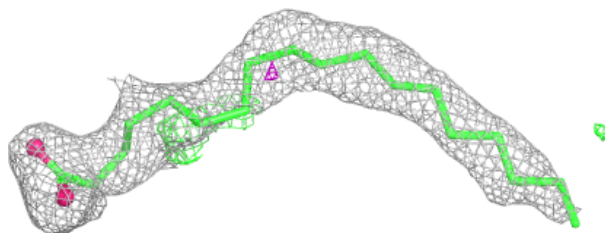
**Electron density around STE J 101:**

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

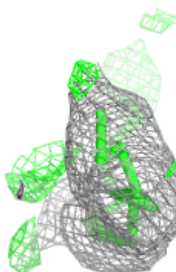
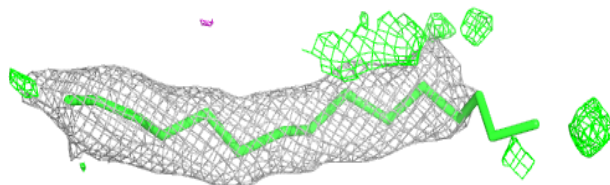
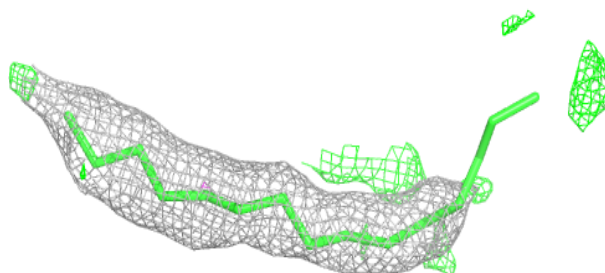


Electron density around STE d 410:

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

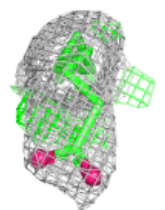
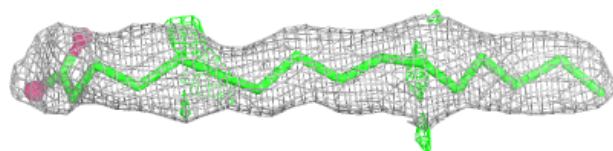
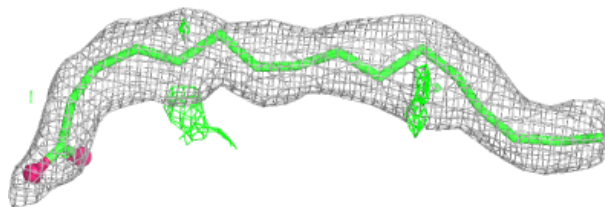
**Electron density around STE T 103:**

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

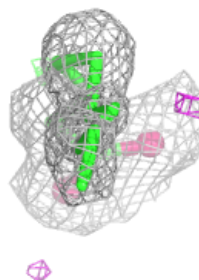
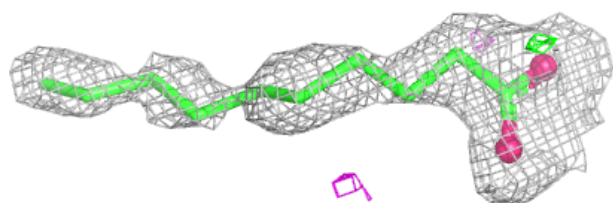
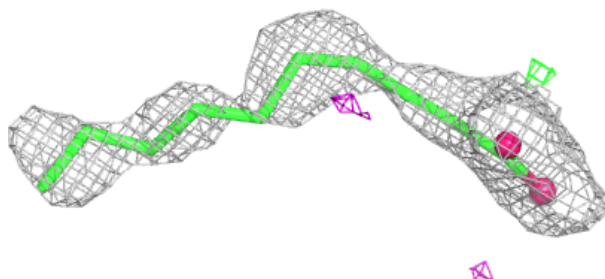


Electron density around STE B 624:

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

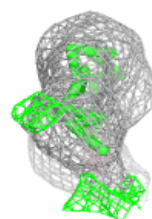
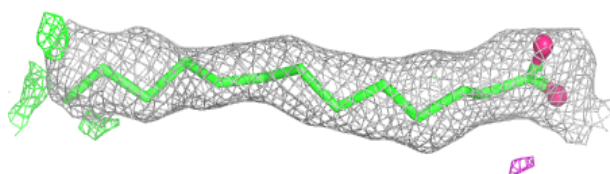
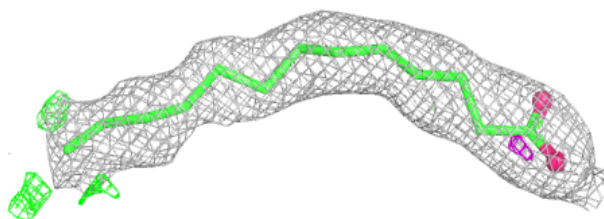
**Electron density around STE E 102:**

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

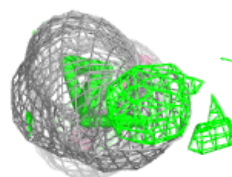
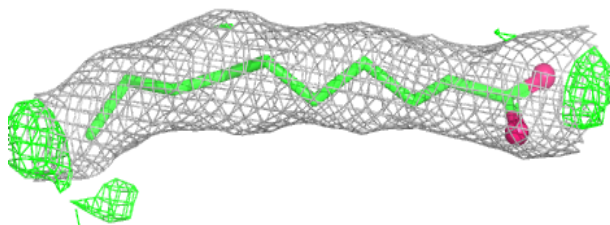
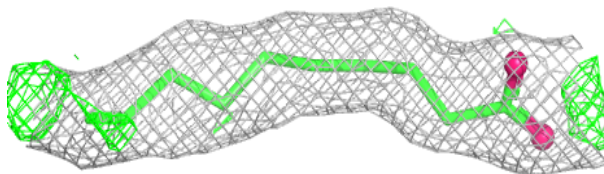


Electron density around STE I 102:

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

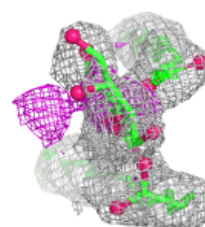
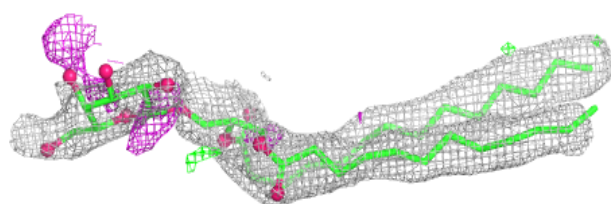
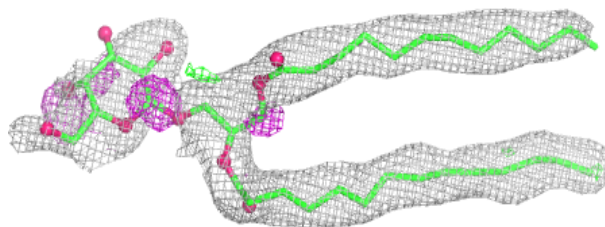
**Electron density around STE j 101:**

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

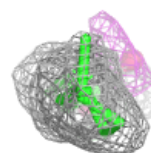
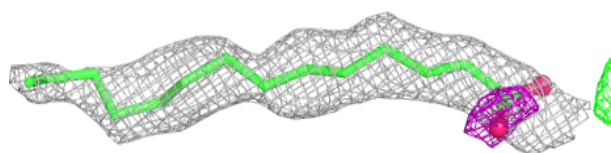
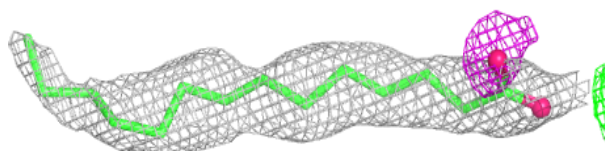


Electron density around LMG B 620:

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

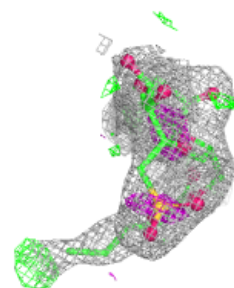
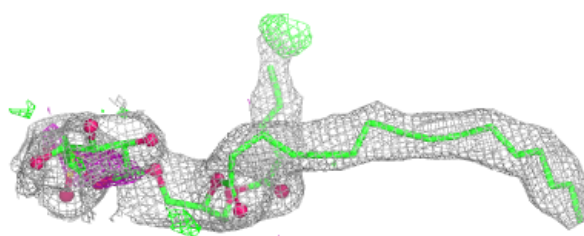
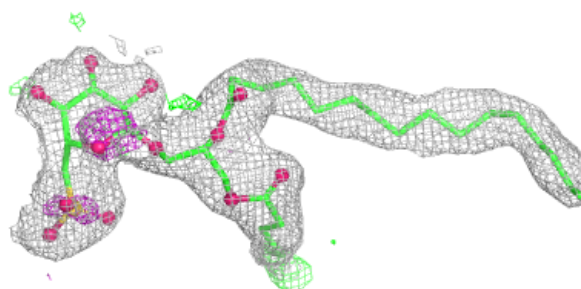
**Electron density around STE b 623:**

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

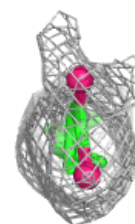
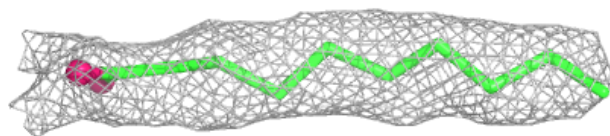
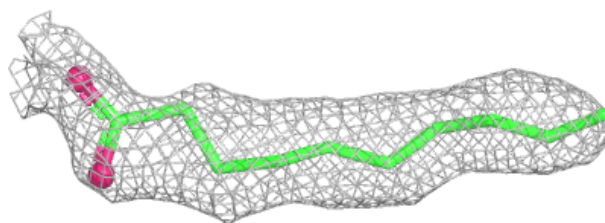


Electron density around SQD A 616:

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

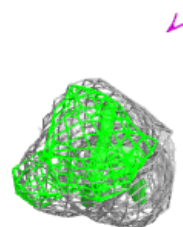
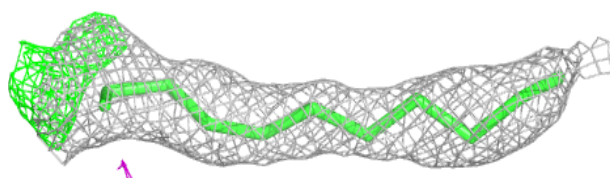
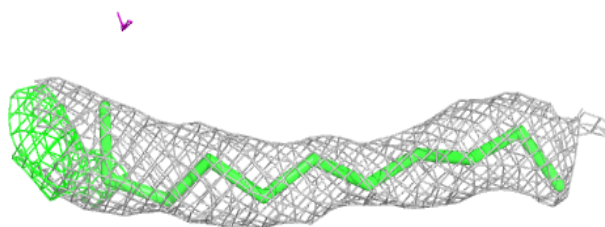
**Electron density around STE m 102:**

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

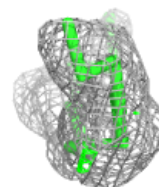
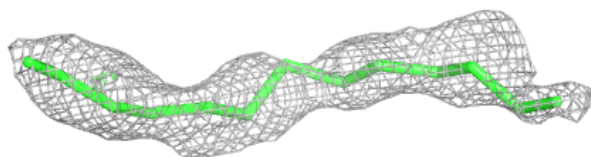
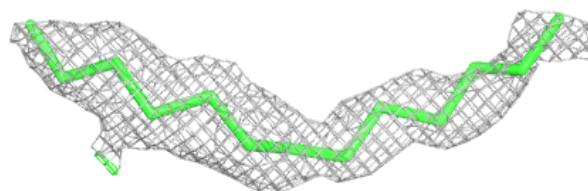


Electron density around STE b 625:

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

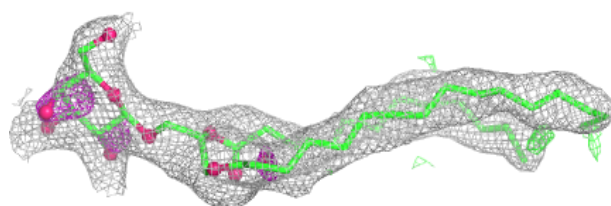
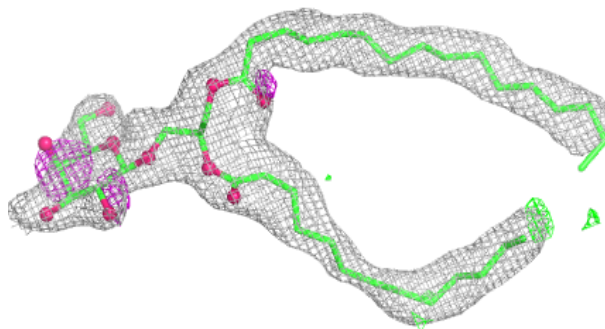
**Electron density around STE c 516:**

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

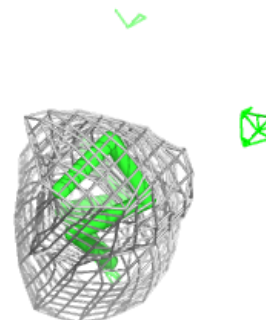
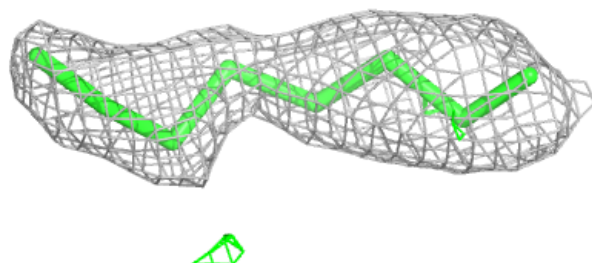
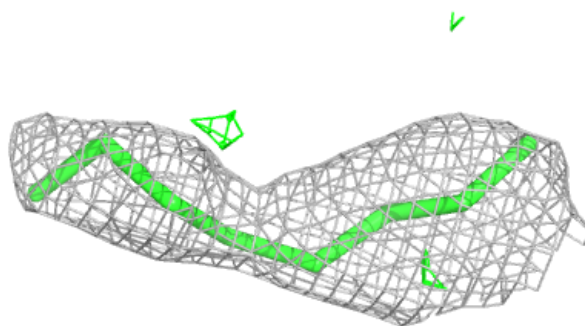


Electron density around LMG C 522:

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

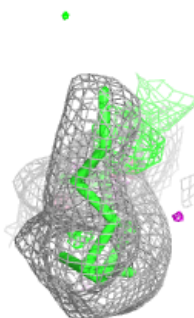
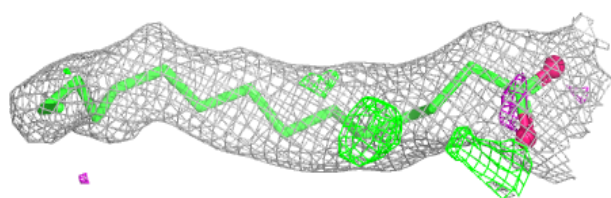
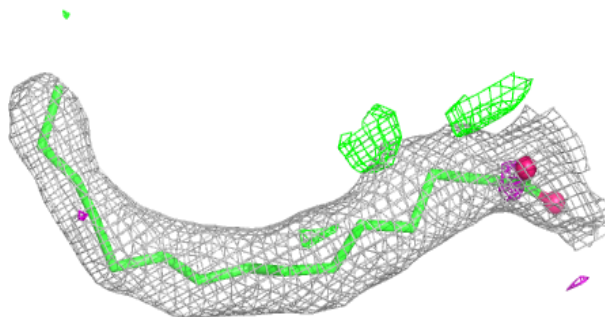
**Electron density around STE A 618:**

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

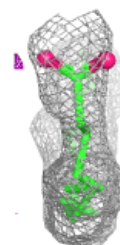
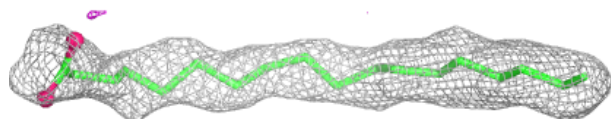
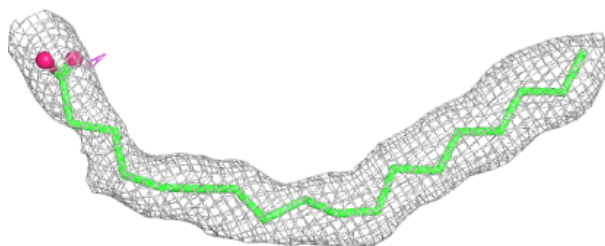


Electron density around STE B 621:

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

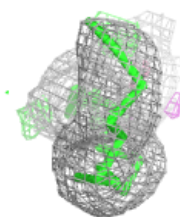
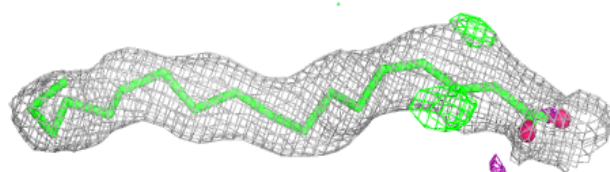
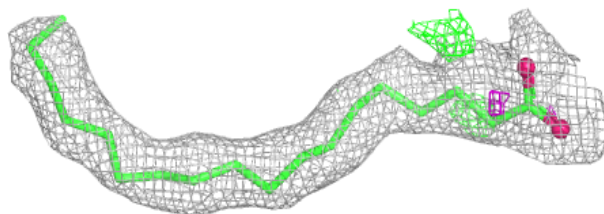
**Electron density around STE d 412:**

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

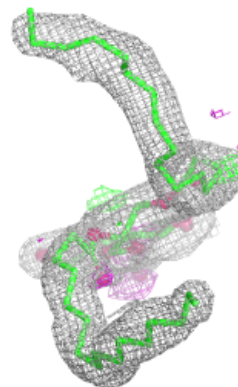
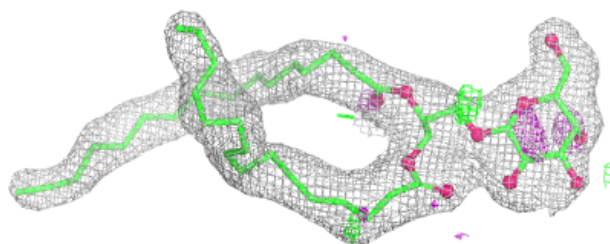
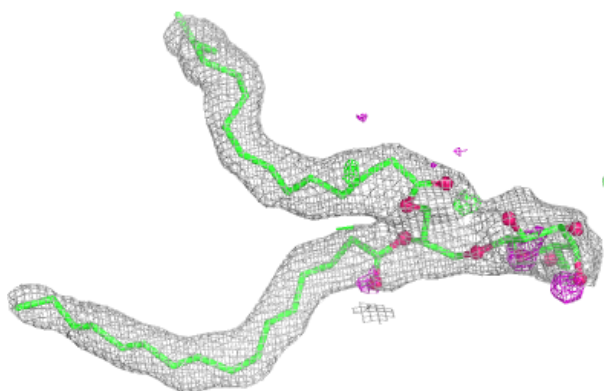


Electron density around STE b 621:

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

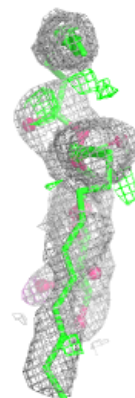
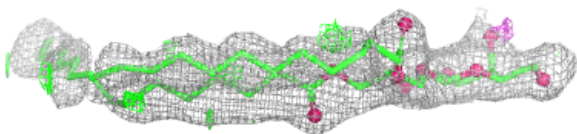
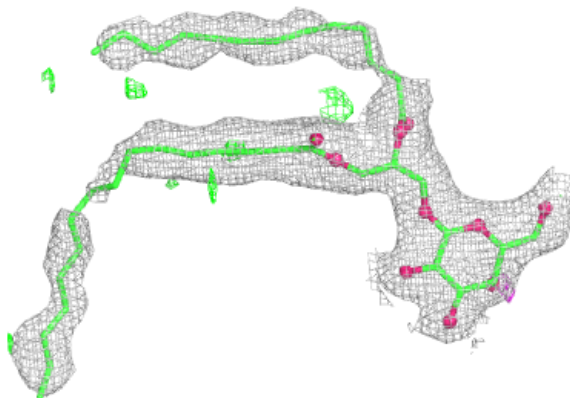
**Electron density around LMG m 101:**

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

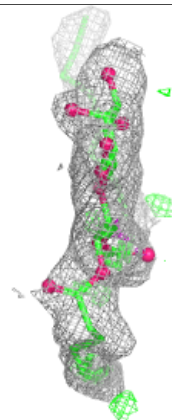
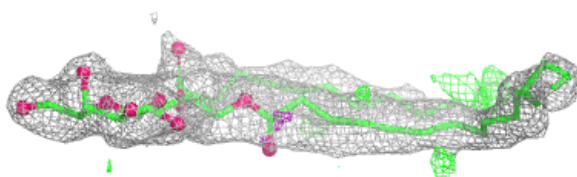
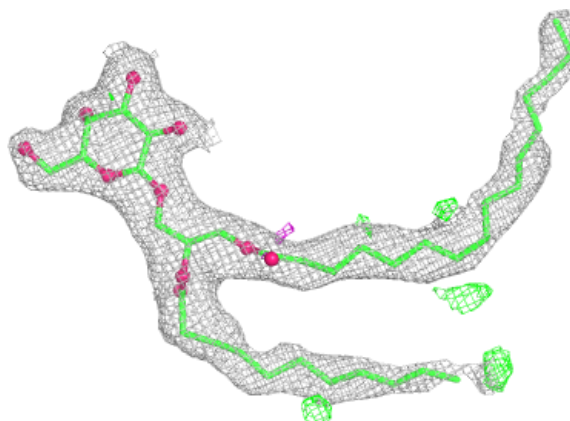


Electron density around LMG C 526:

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

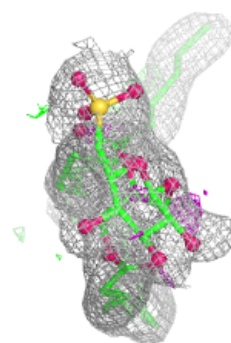
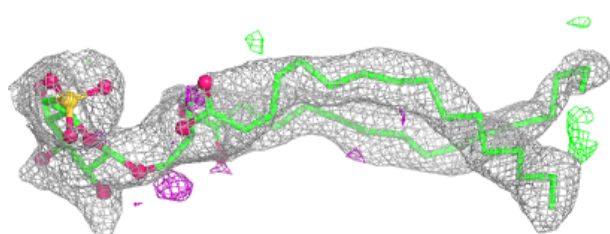
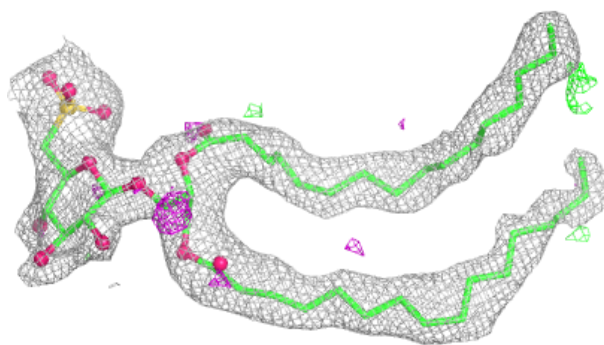
**Electron density around LMG c 522:**

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

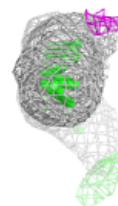
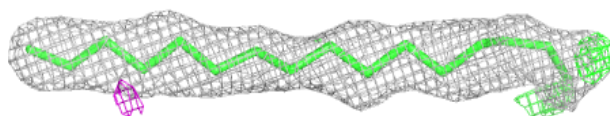
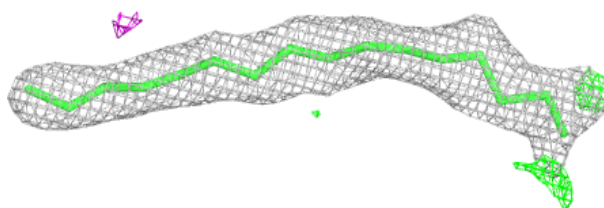


Electron density around SQD B 623:

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

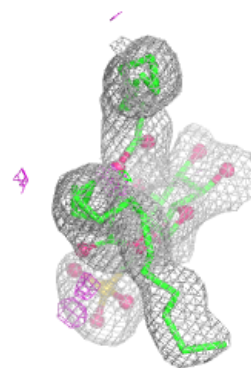
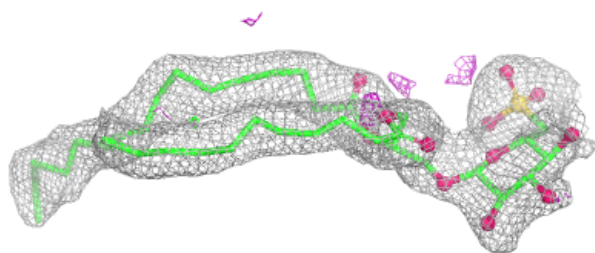
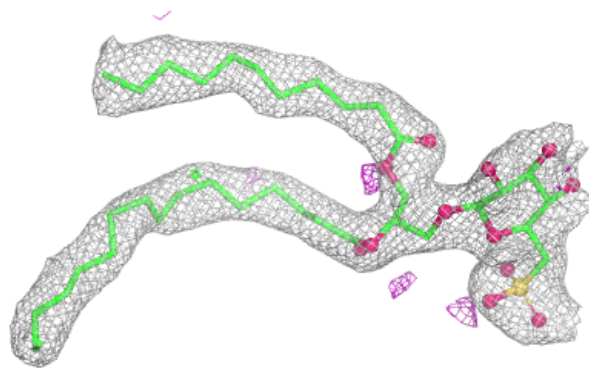
**Electron density around STE C 528:**

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

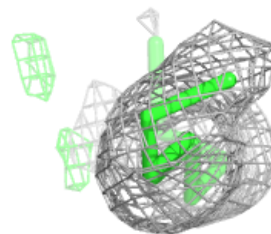
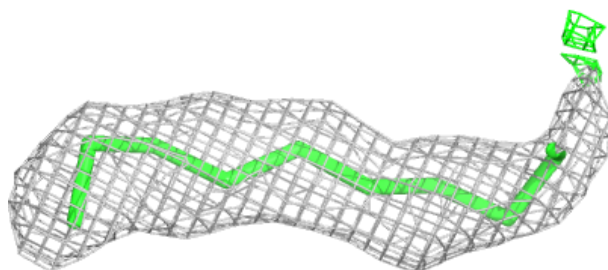
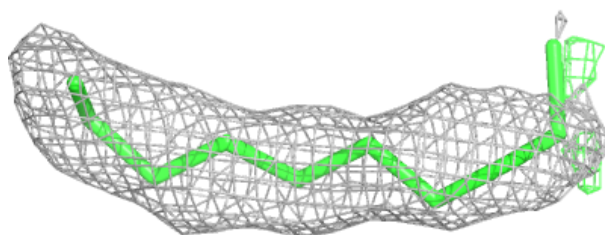


Electron density around SQD b 620:

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

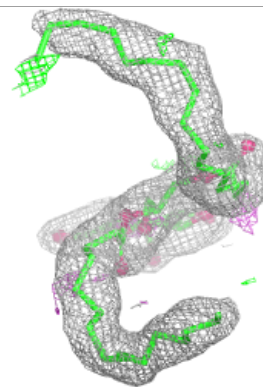
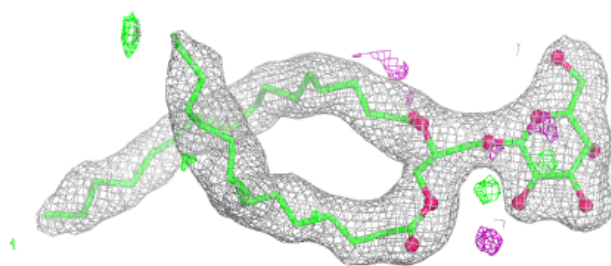
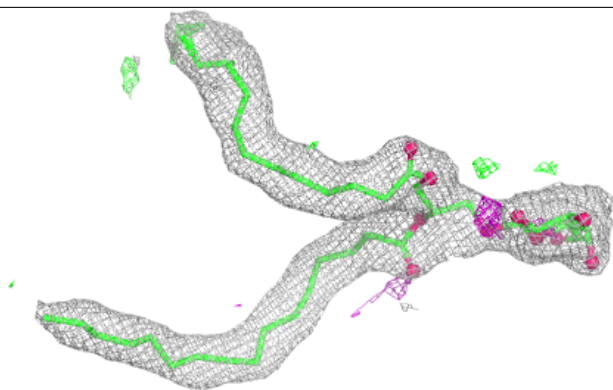
**Electron density around STE b 624:**

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

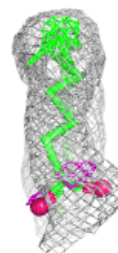
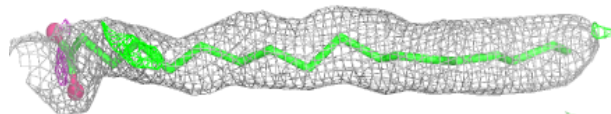
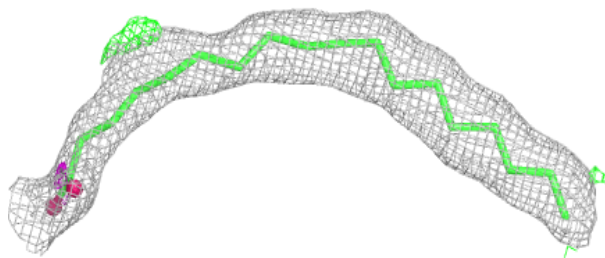


Electron density around LMG M 101:

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

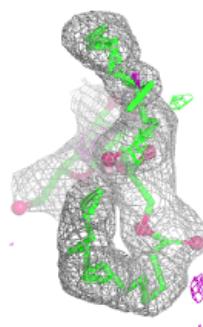
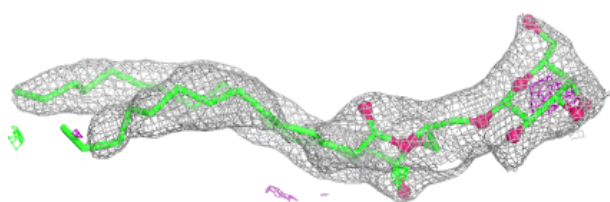
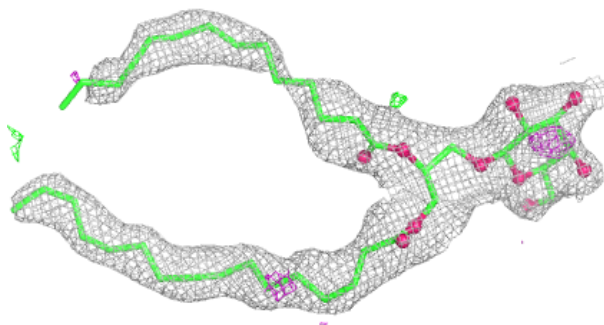
**Electron density around STE D 411:**

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

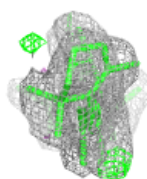
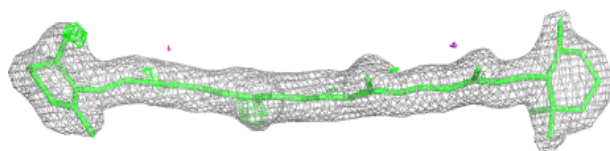
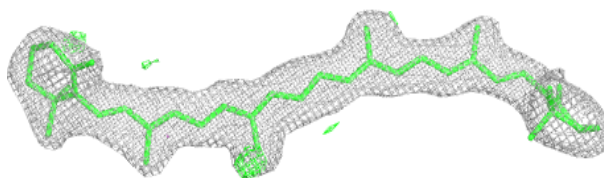


Electron density around LMG a 618:

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

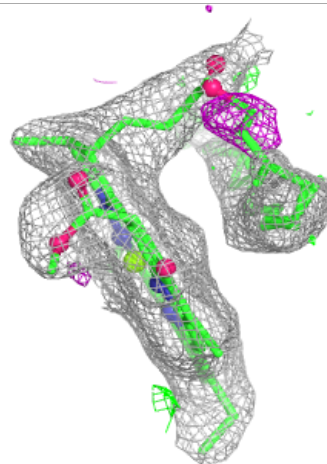
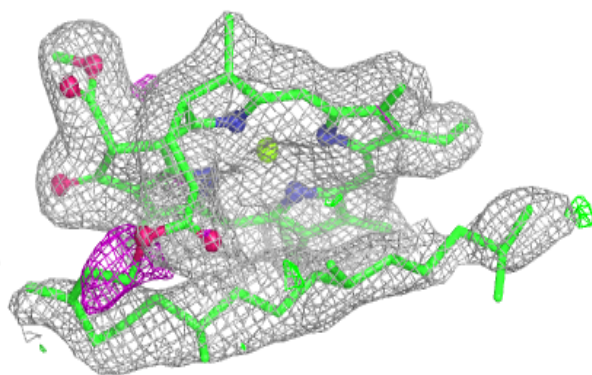
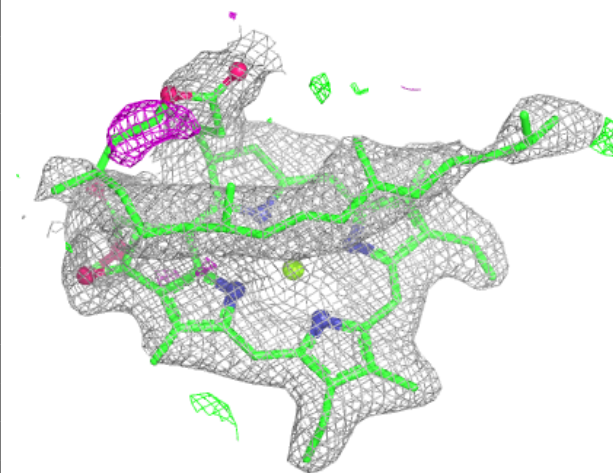
**Electron density around BCR C 521:**

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



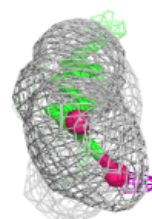
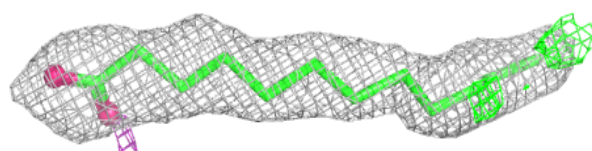
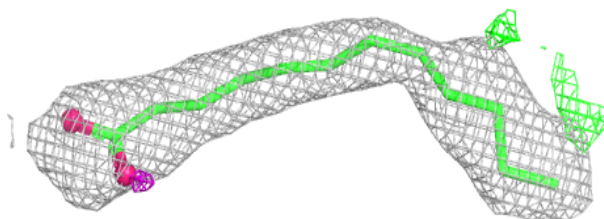
Electron density around CLA b 601:

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

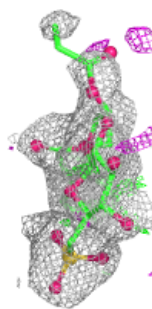
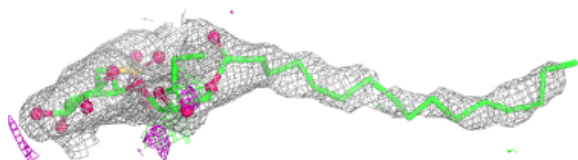
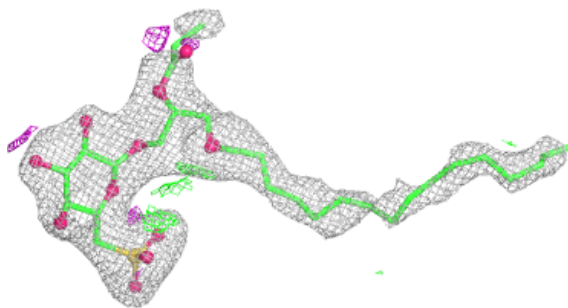


Electron density around STE t 102:

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

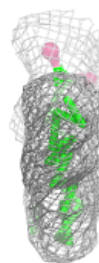
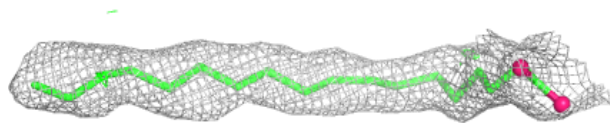
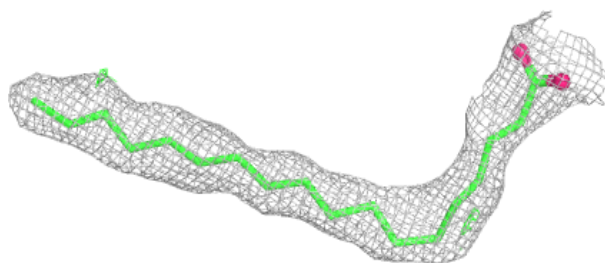
**Electron density around SQD f 101:**

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



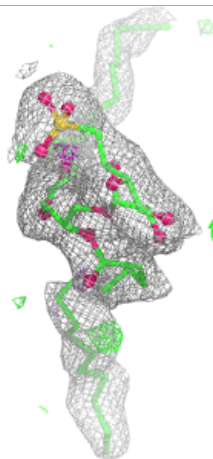
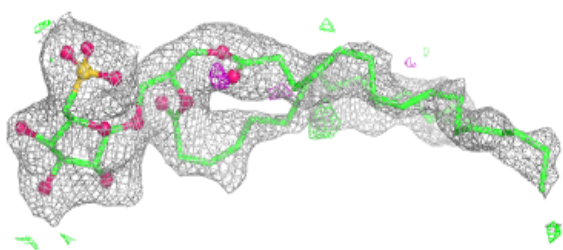
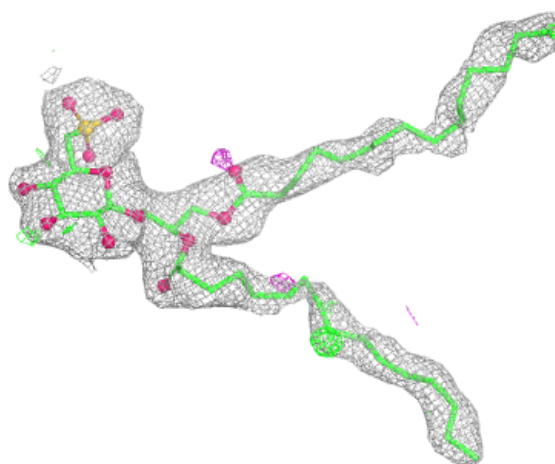
Electron density around STE d 406:

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



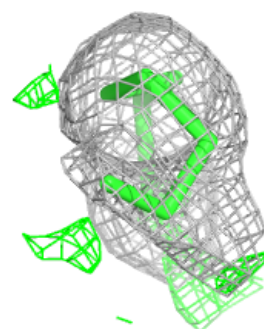
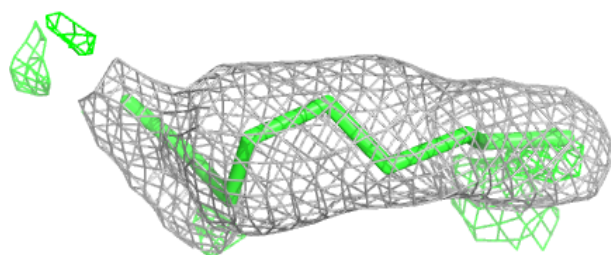
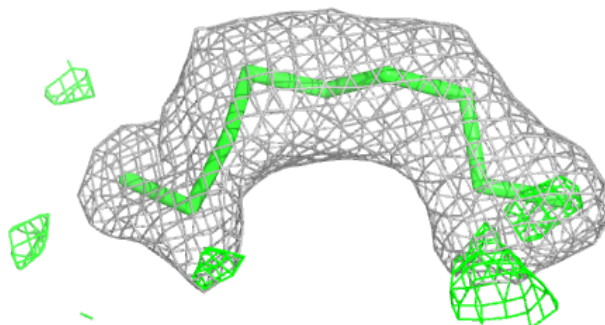
Electron density around SQD a 614:

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

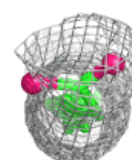
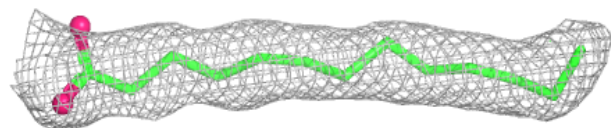
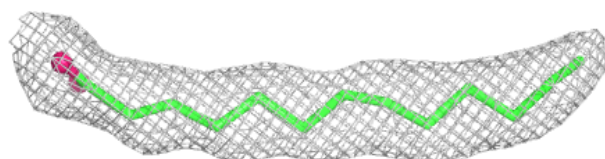


Electron density around STE D 412:

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

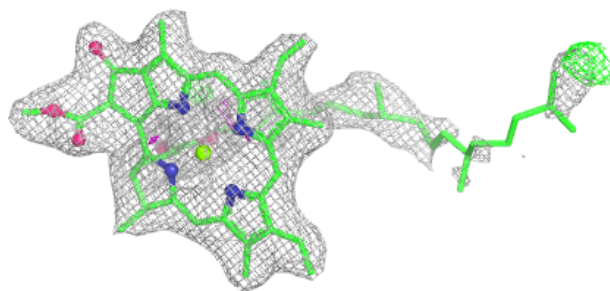
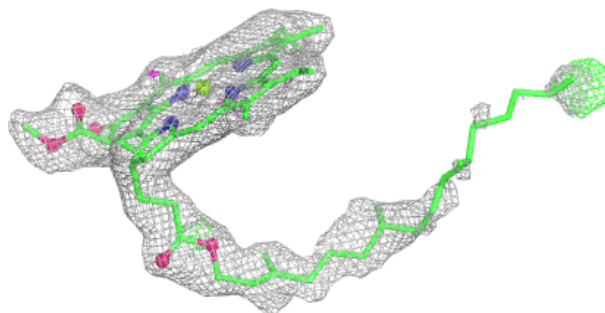
**Electron density around STE M 102:**

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

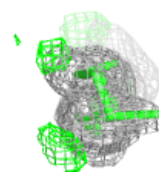
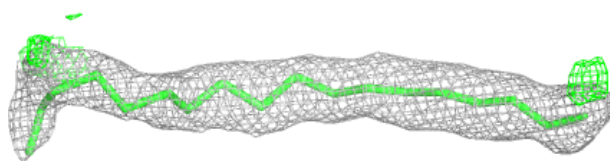
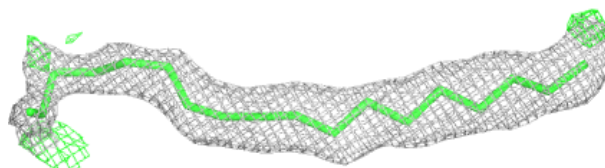


Electron density around CLA C 513:

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

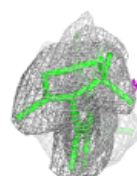
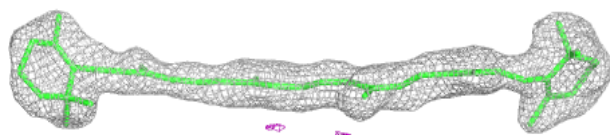
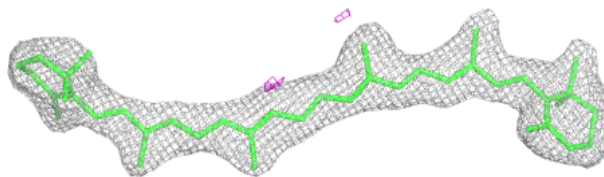
**Electron density around STE m 103:**

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

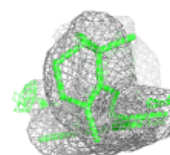
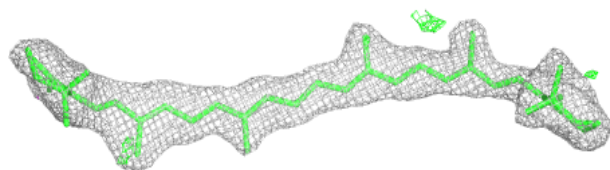
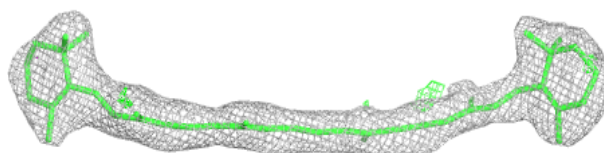


Electron density around BCR k 101:

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

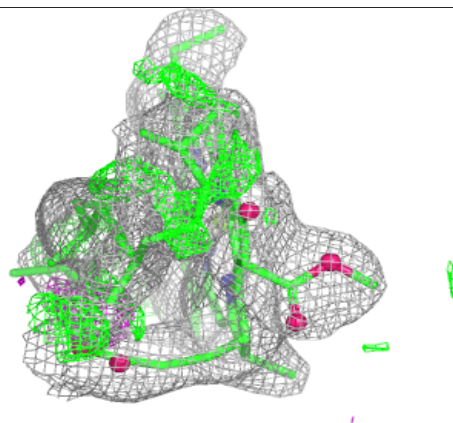
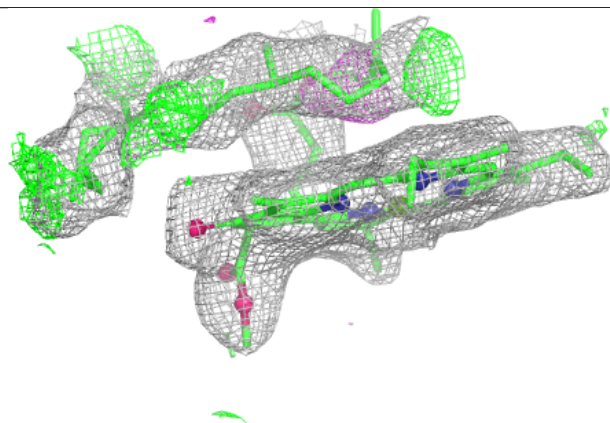
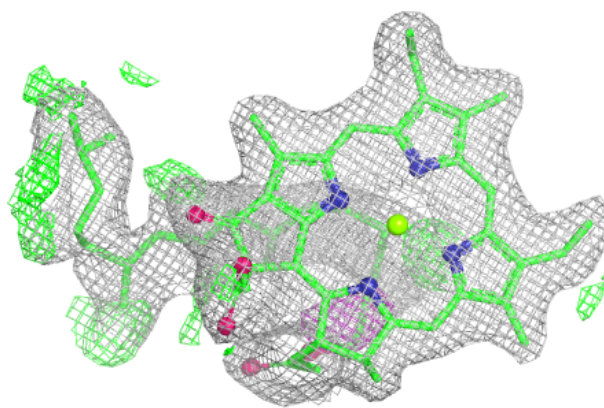
**Electron density around BCR k 102:**

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

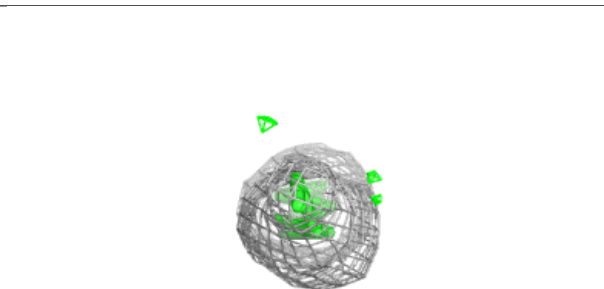
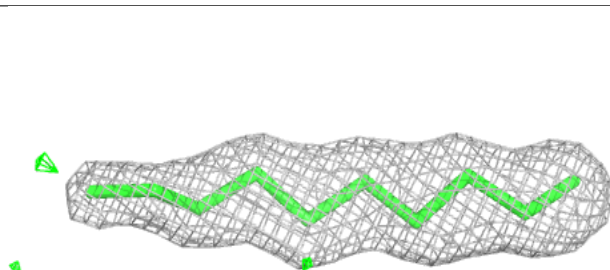
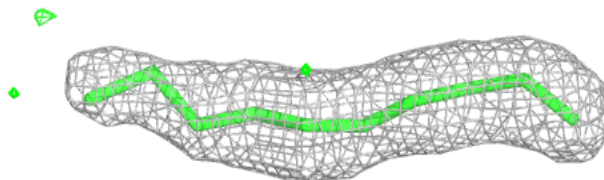


Electron density around CLA B 601:

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

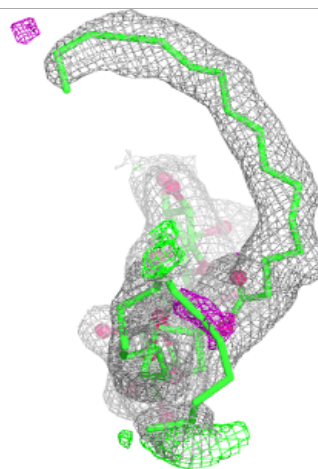
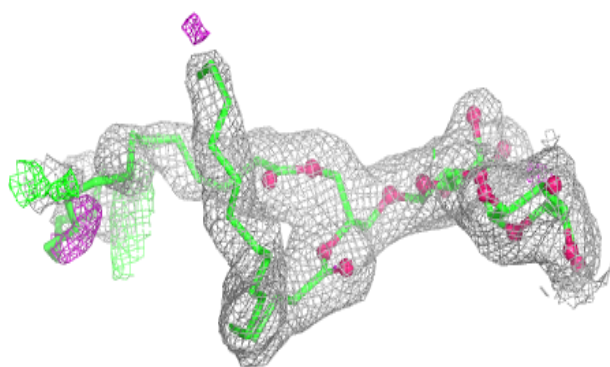
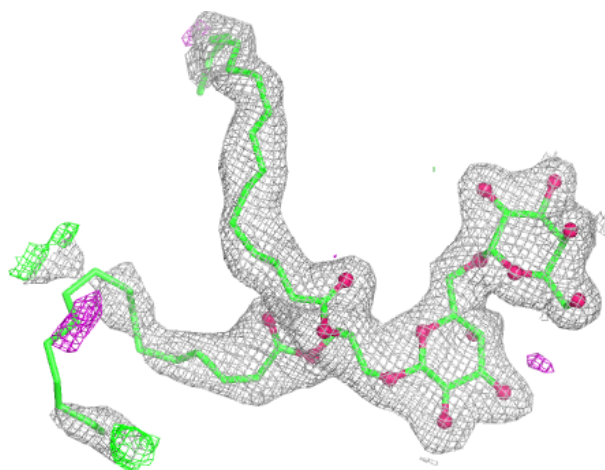
**Electron density around STE M 103:**

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



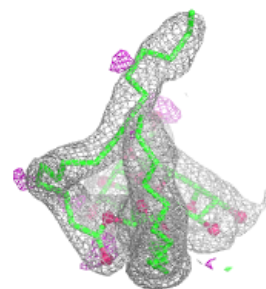
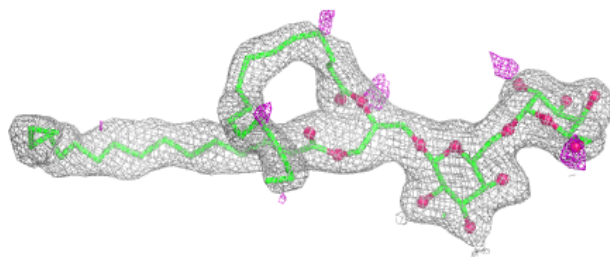
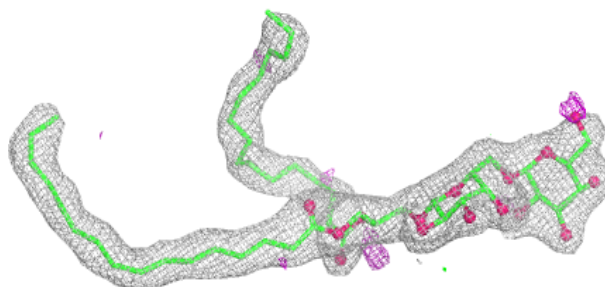
Electron density around DGD C 524:

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



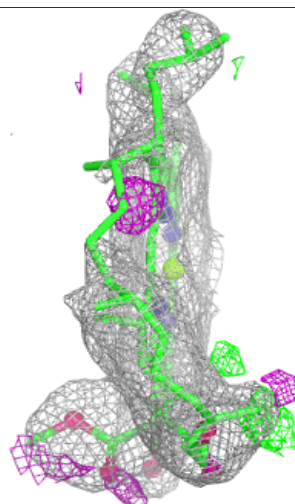
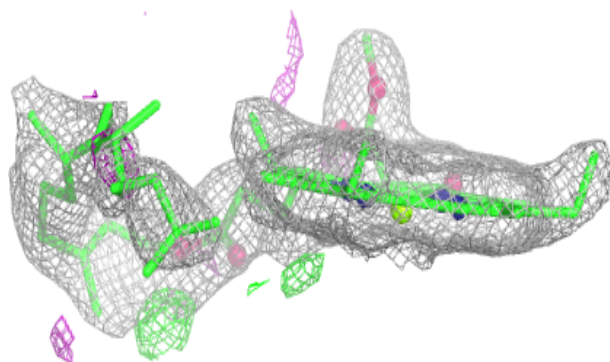
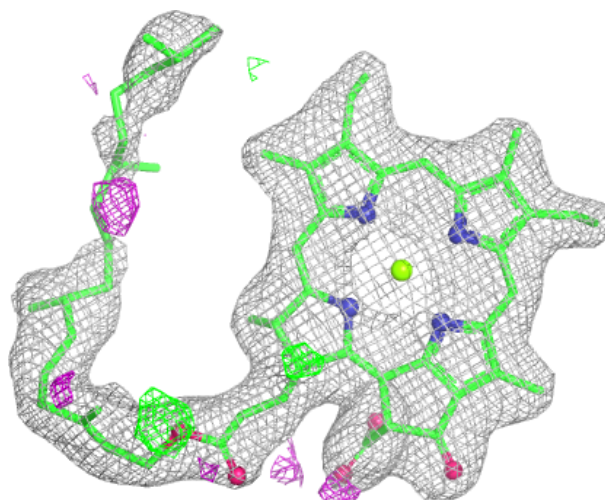
Electron density around DGD h 101:

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



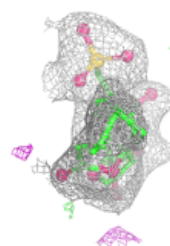
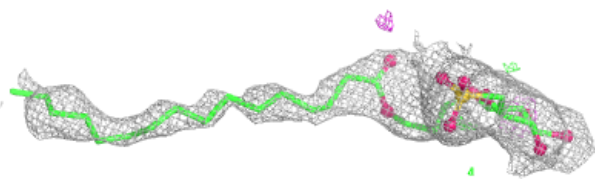
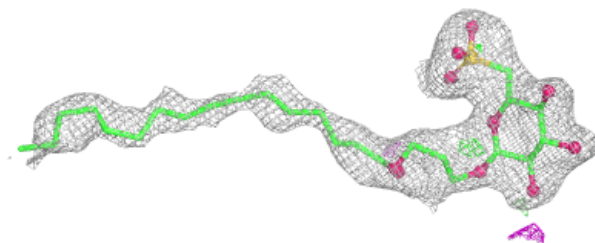
Electron density around CLA c 512:

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

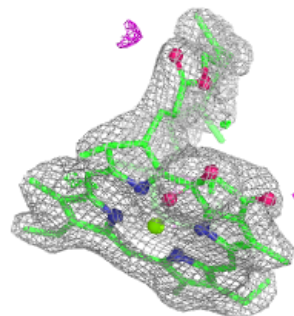
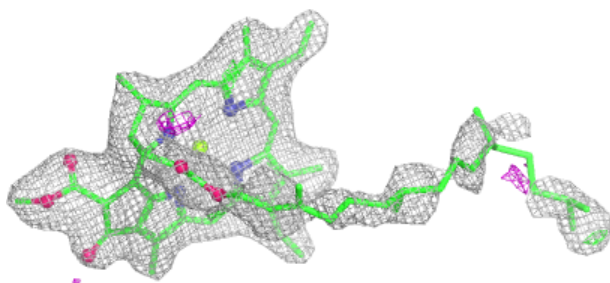
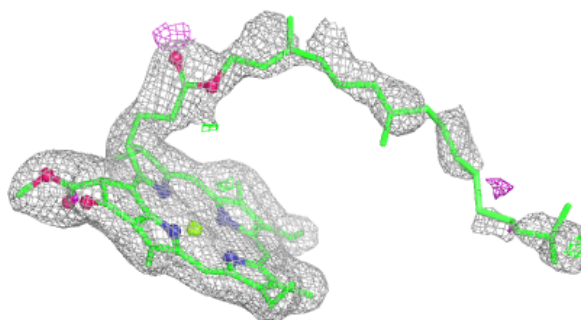


Electron density around SQD F 102:

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

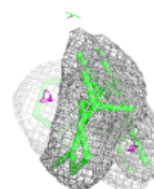
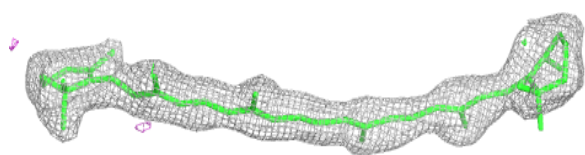
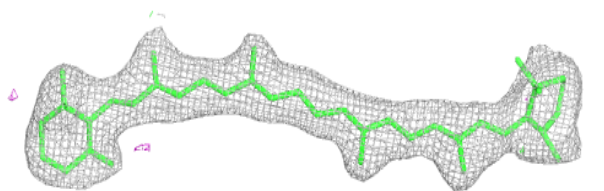
**Electron density around CLA c 513:**

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



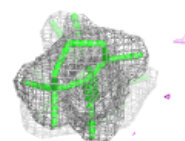
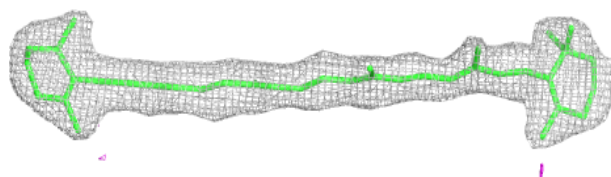
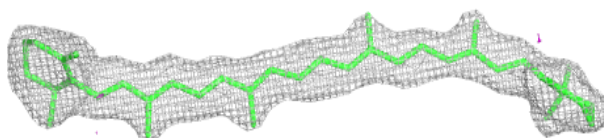
Electron density around BCR d 404:

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



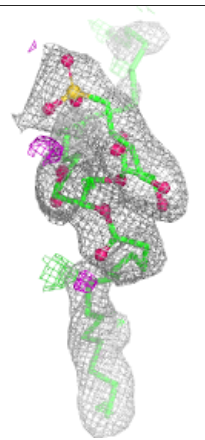
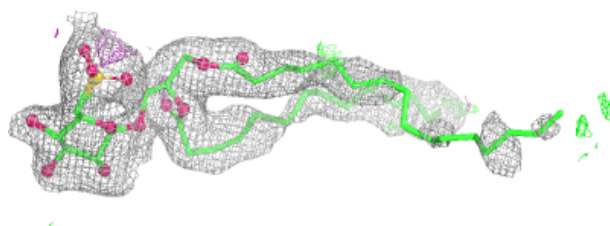
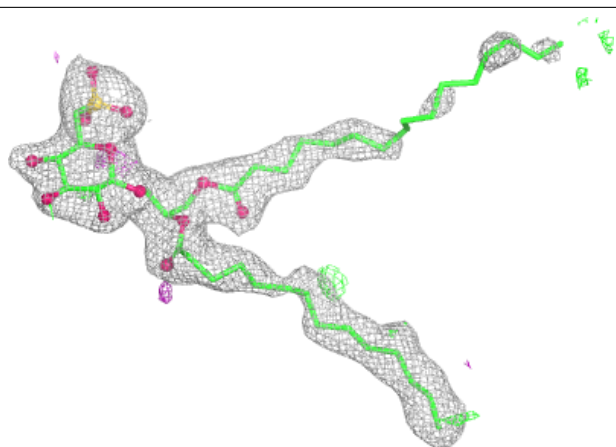
Electron density around BCR C 514:

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

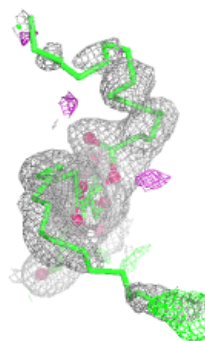
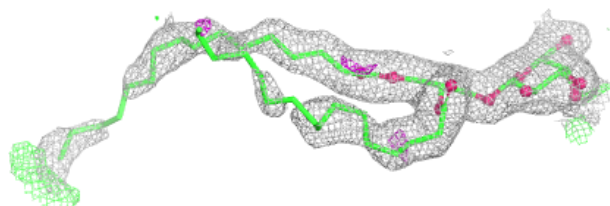
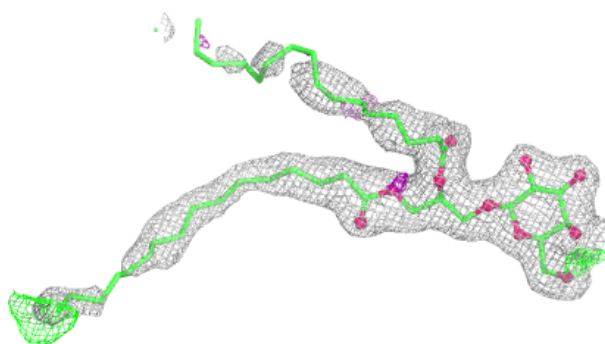


Electron density around SQD A 615:

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

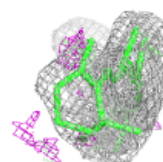
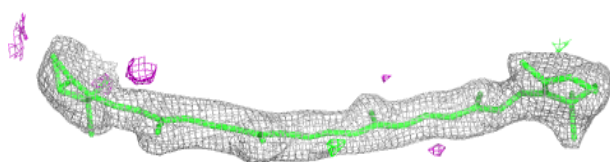
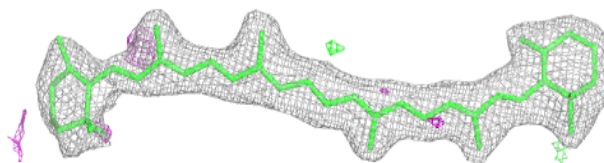
**Electron density around LMG D 407:**

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

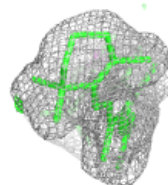
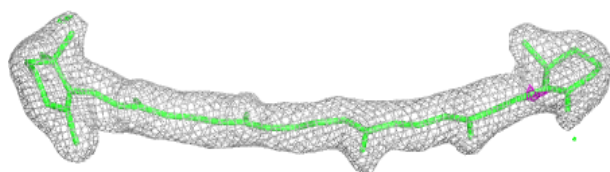
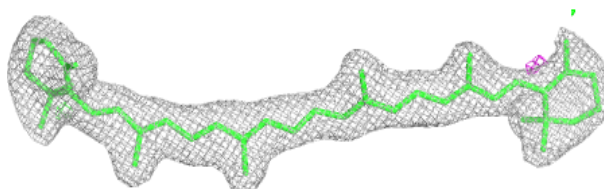


Electron density around BCR D 404:

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

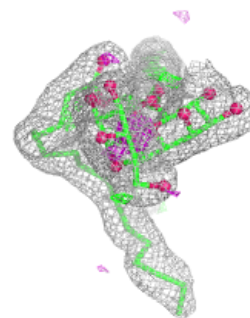
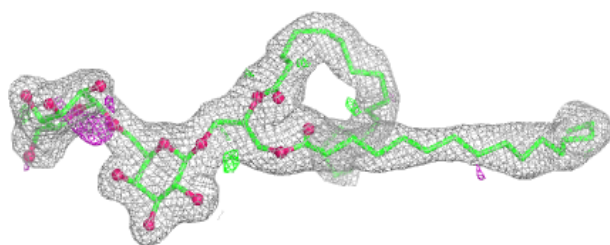
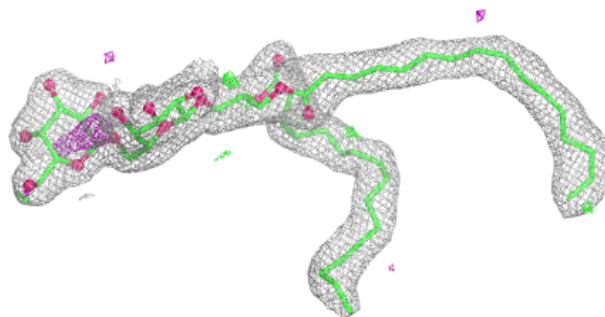
**Electron density around BCR T 101:**

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

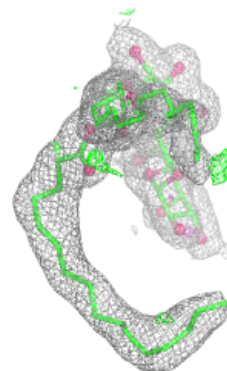
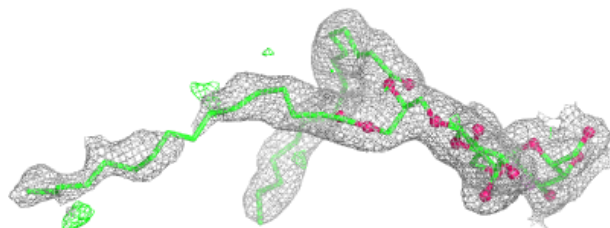
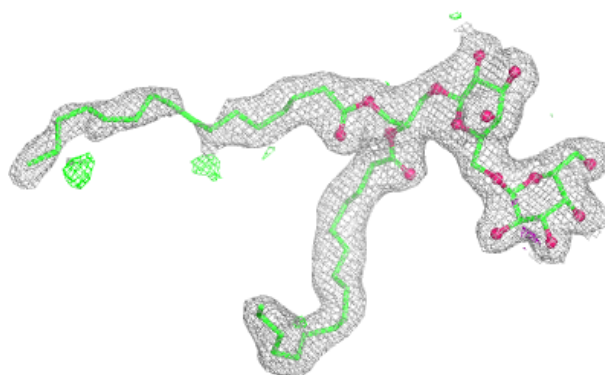


Electron density around DGD H 102:

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

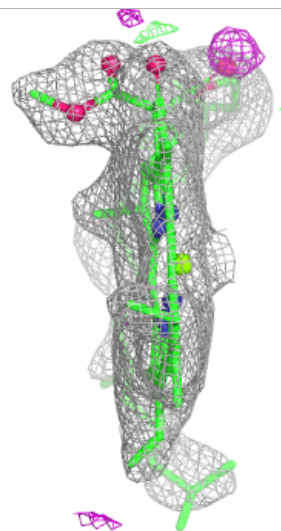
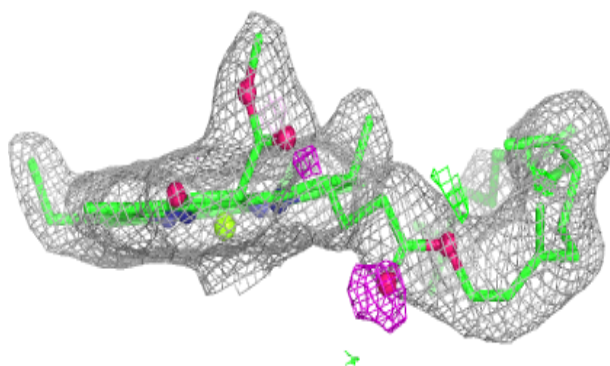
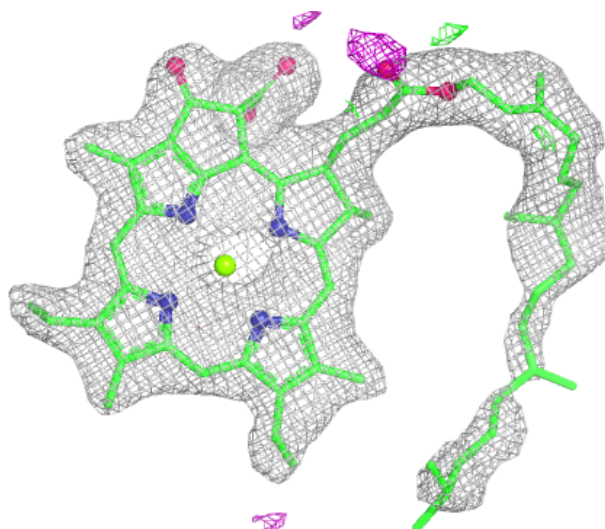
**Electron density around DGD c 520:**

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



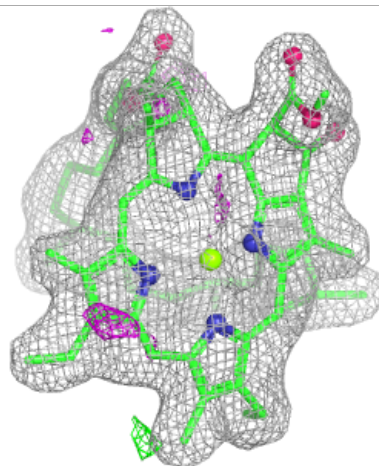
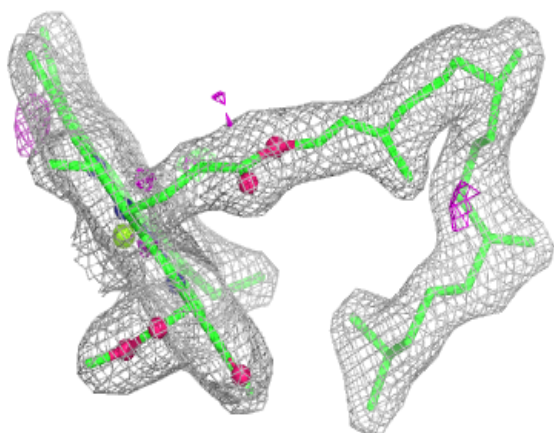
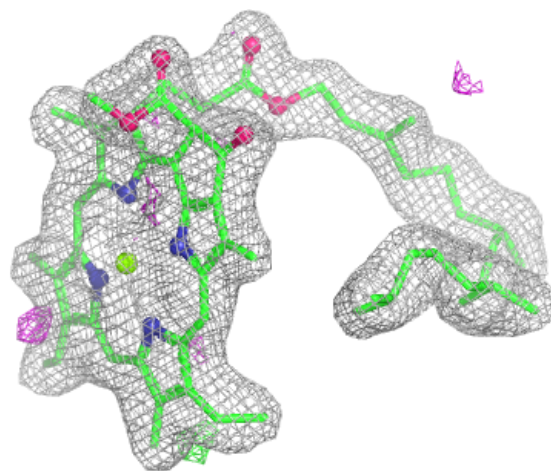
Electron density around CLA C 512:

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



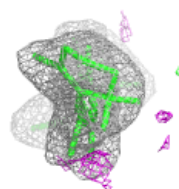
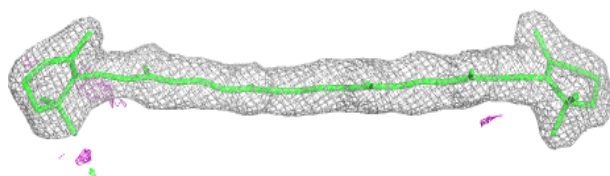
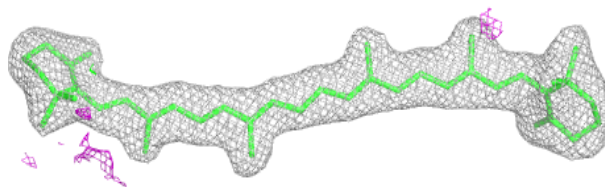
Electron density around CLA C 503:

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

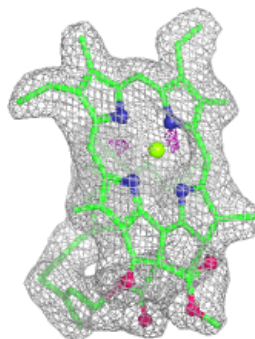
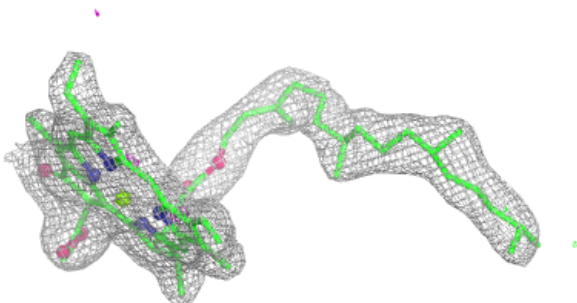
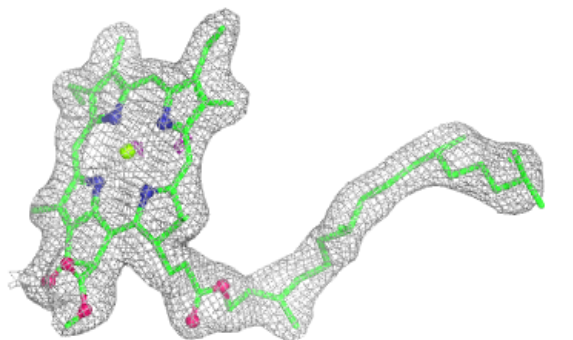


Electron density around BCR B 618:

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

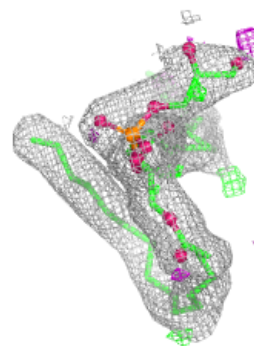
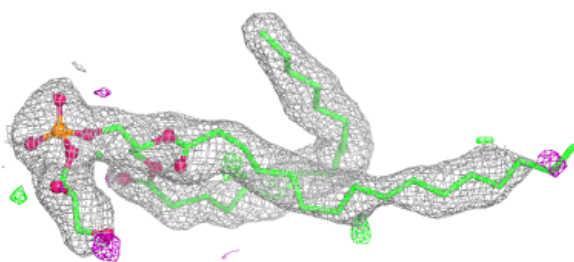
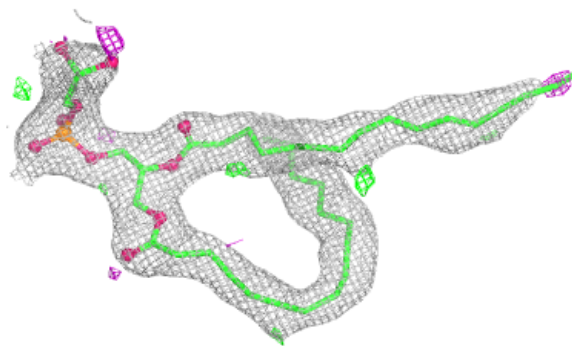
**Electron density around CLA C 511:**

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

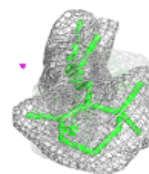
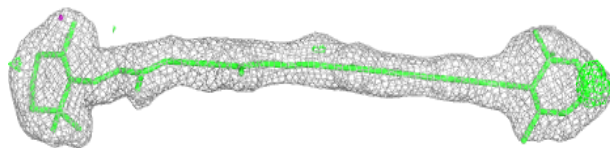
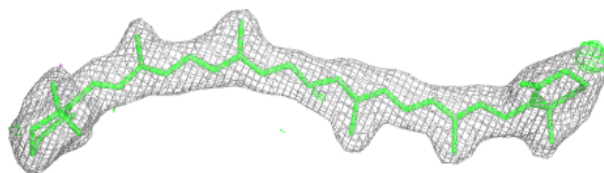


Electron density around LHG D 410:

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

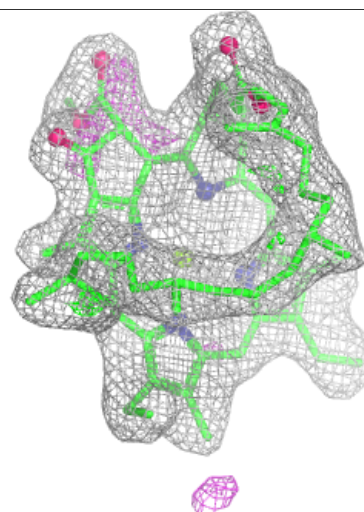
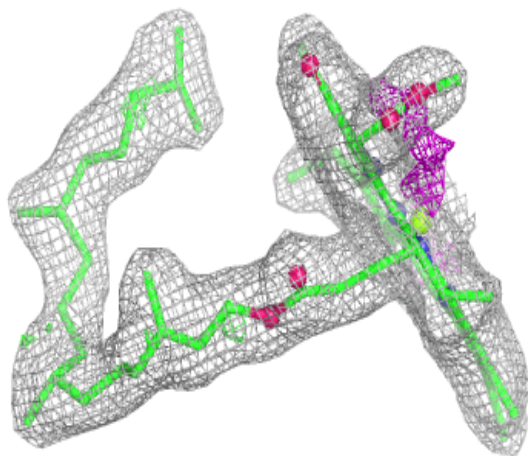
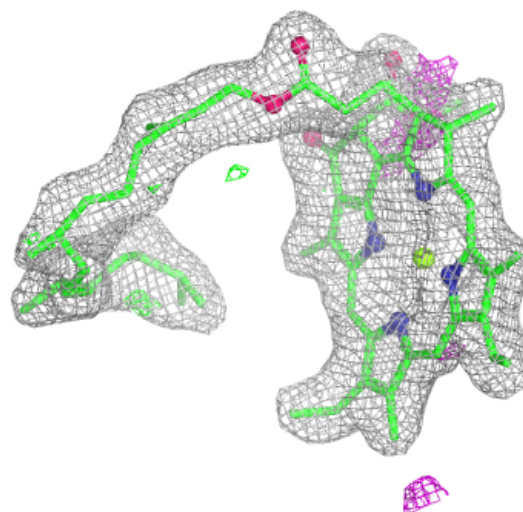
**Electron density around BCR x 101:**

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



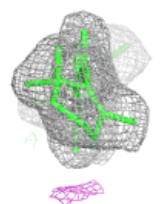
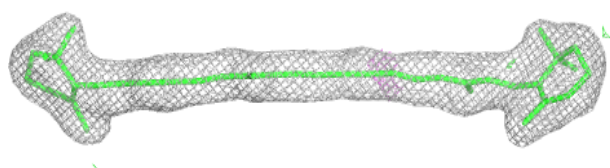
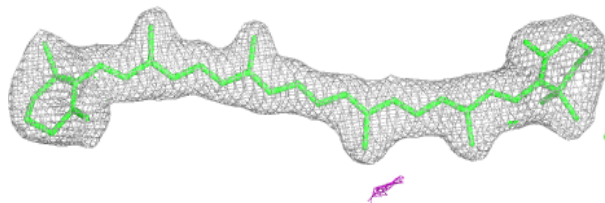
Electron density around CLA c 503:

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

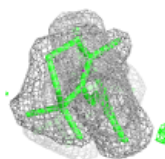
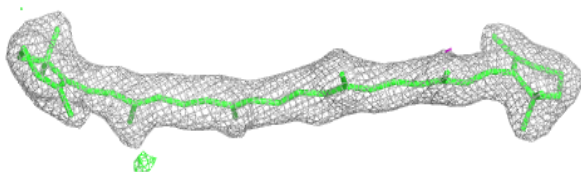
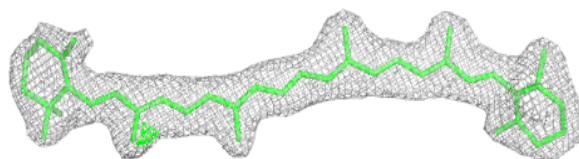


Electron density around BCR b 618:

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

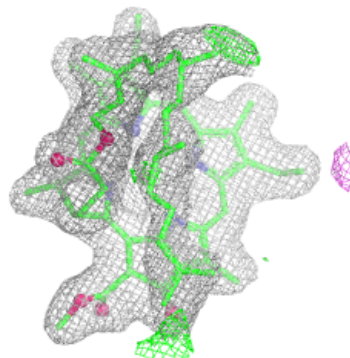
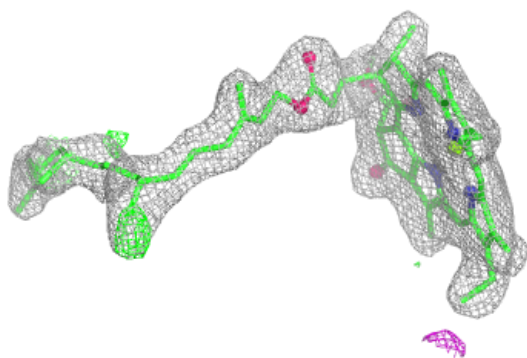
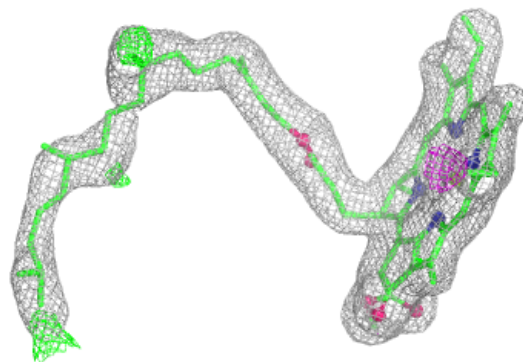
**Electron density around BCR b 619:**

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

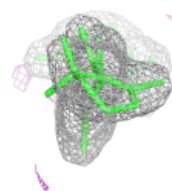
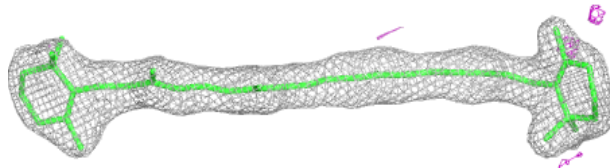
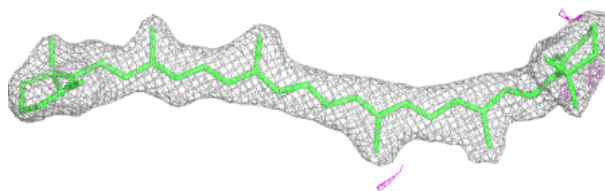


Electron density around CLA b 606:

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

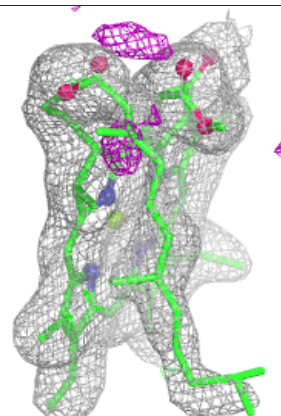
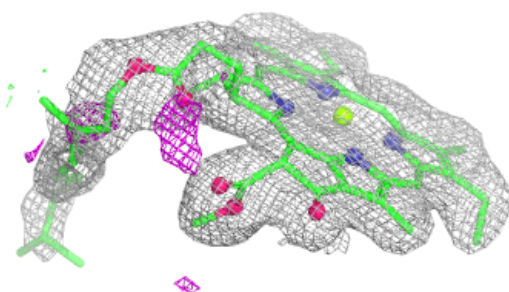
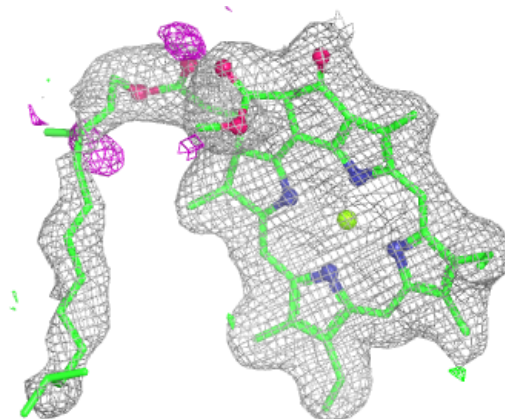
**Electron density around BCR c 515:**

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

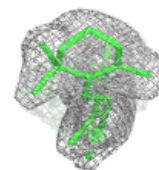
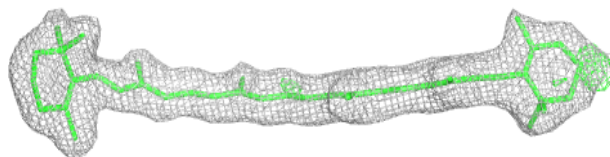
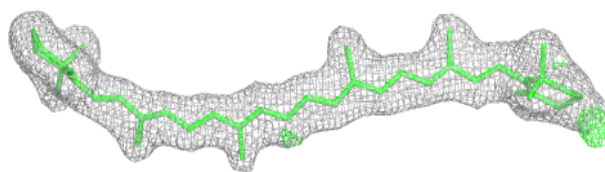


Electron density around CLA b 616:

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

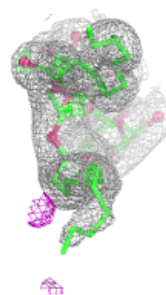
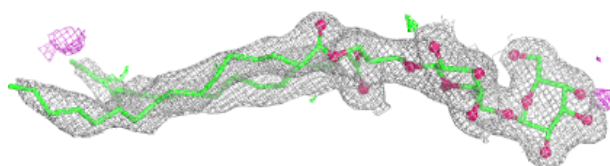
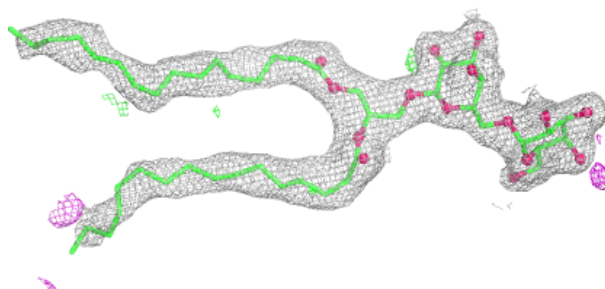
**Electron density around BCR H 101:**

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

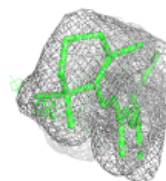
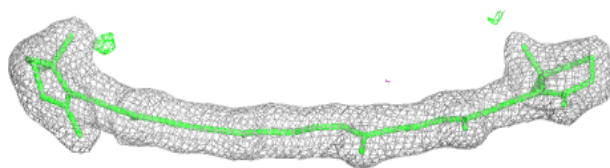
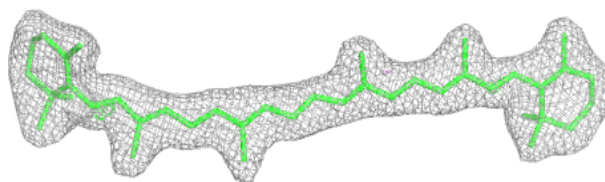


Electron density around DGD c 521:

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

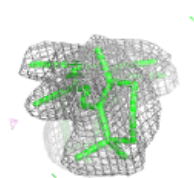
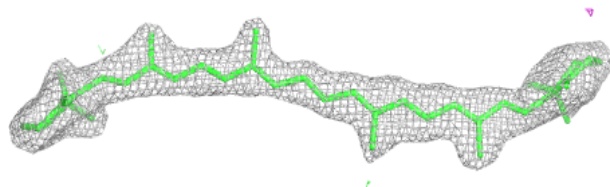
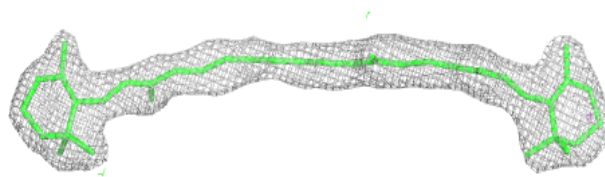
**Electron density around BCR t 101:**

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



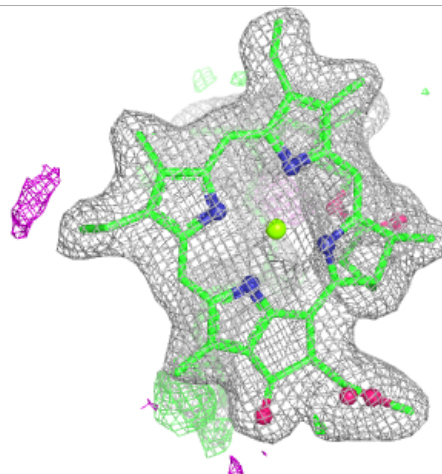
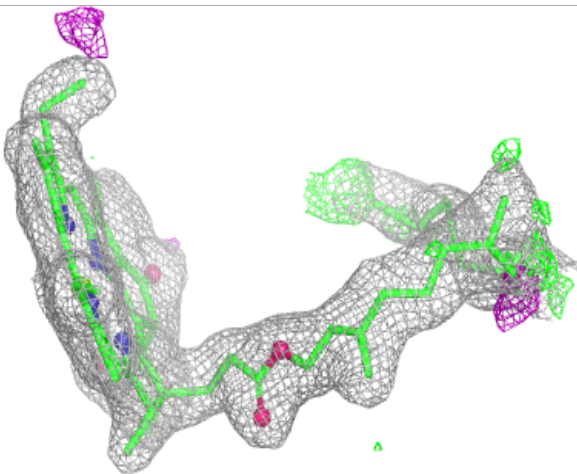
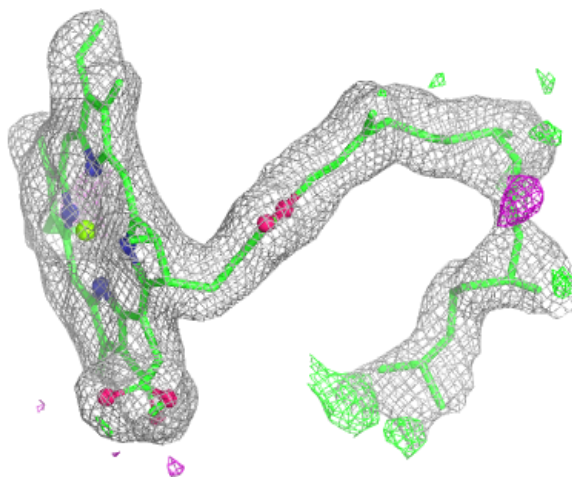
Electron density around BCR K 101:

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



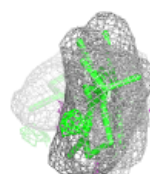
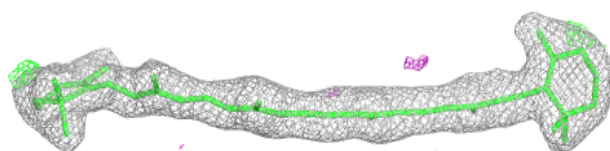
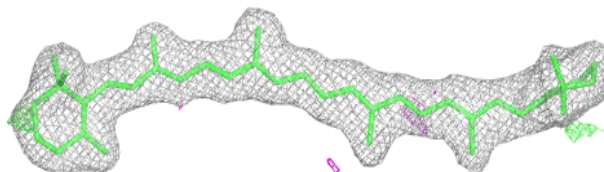
Electron density around CLA B 606:

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

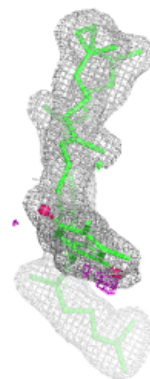
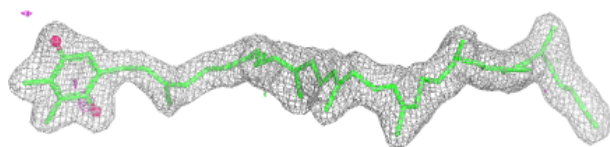
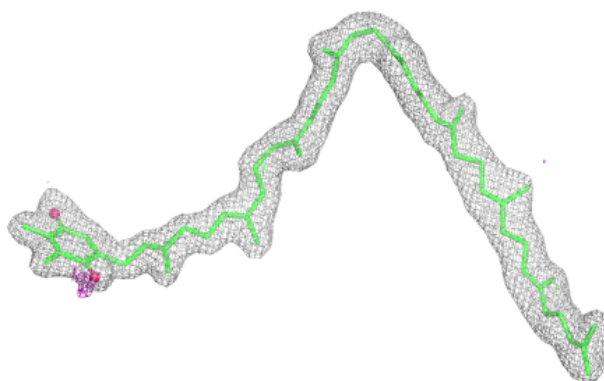


Electron density around BCR b 617:

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

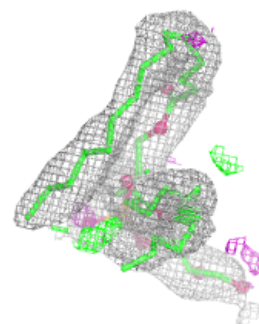
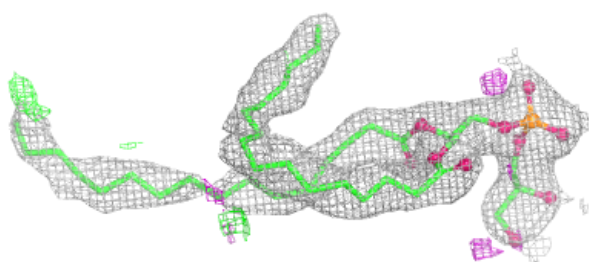
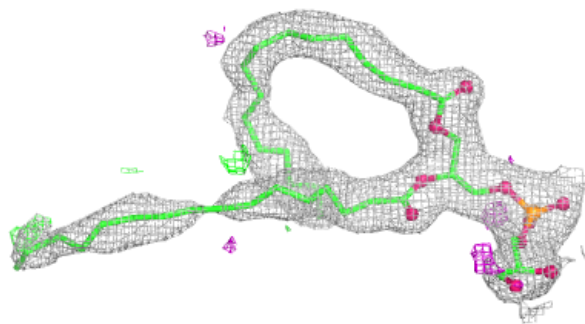
**Electron density around PL9 d 405:**

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

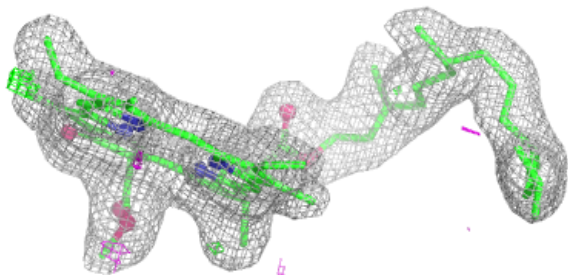
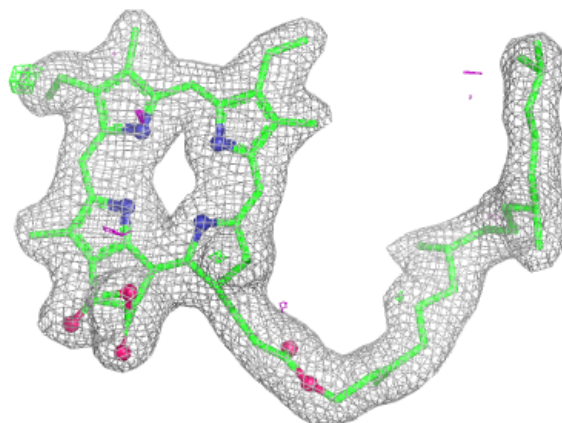


Electron density around LHG d 407:

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

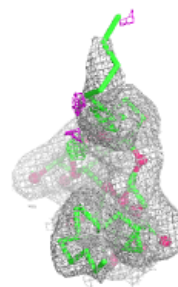
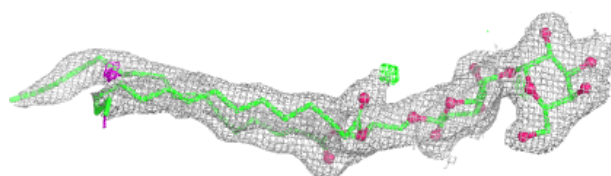
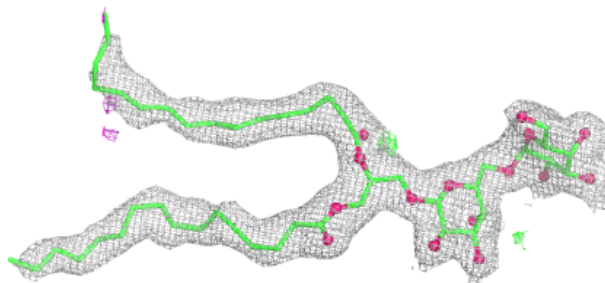
**Electron density around PHO d 401:**

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



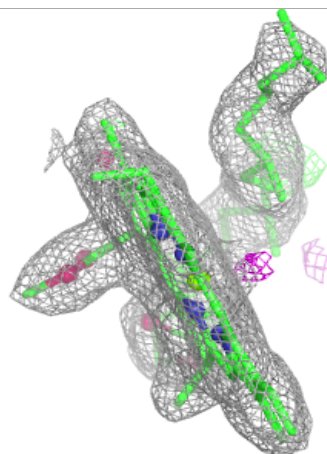
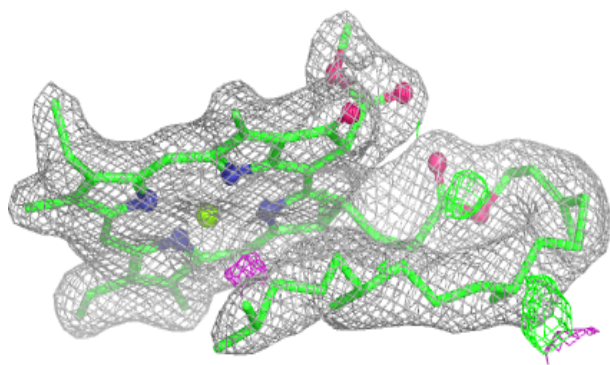
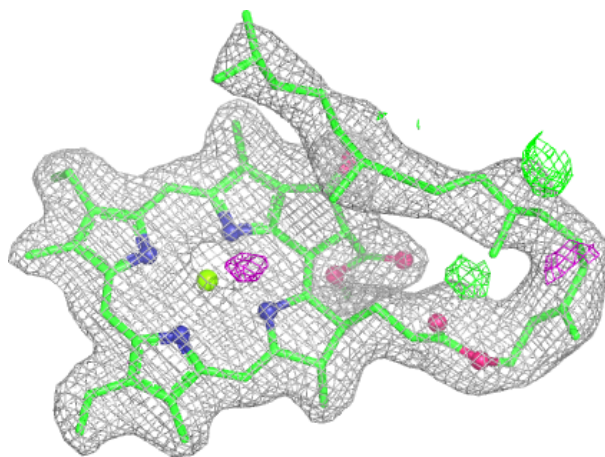
Electron density around DGD C 525:

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



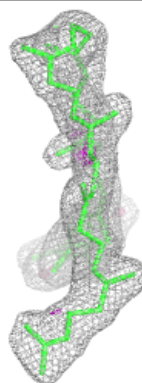
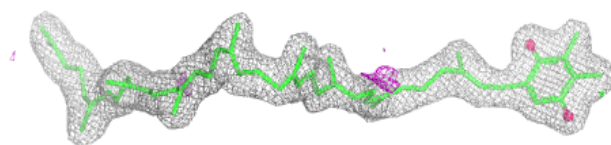
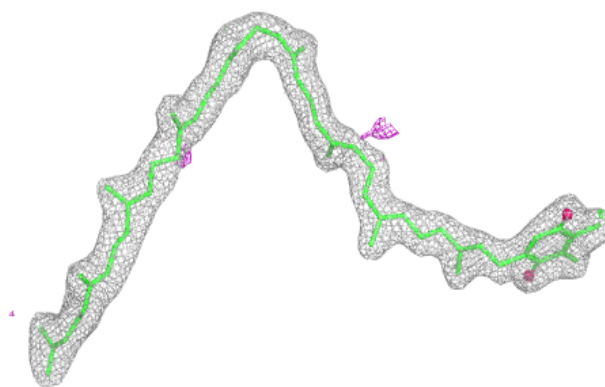
Electron density around CLA C 509:

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

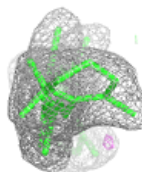
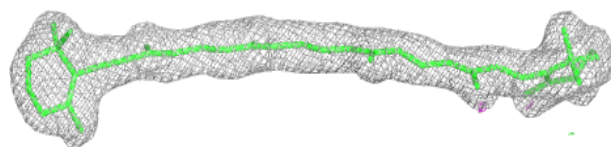
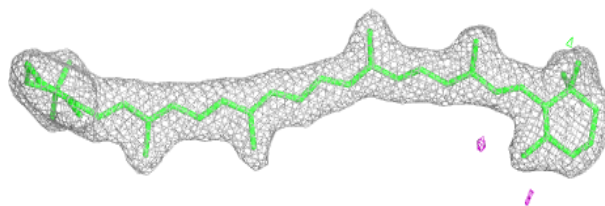


Electron density around PL9 D 405:

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

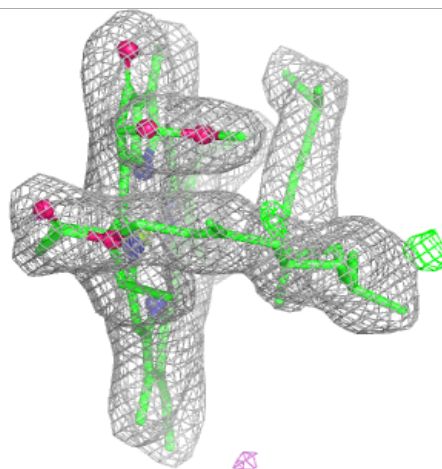
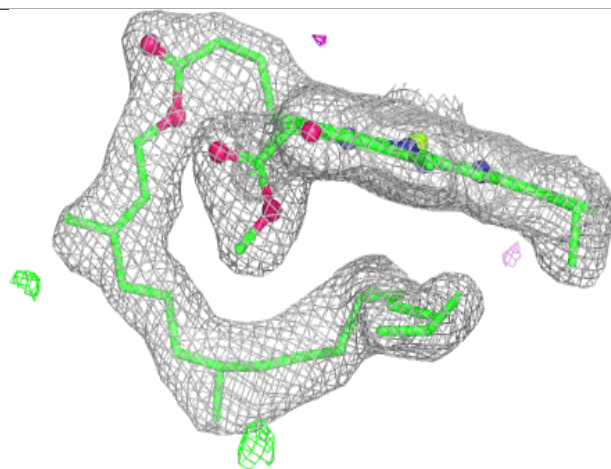
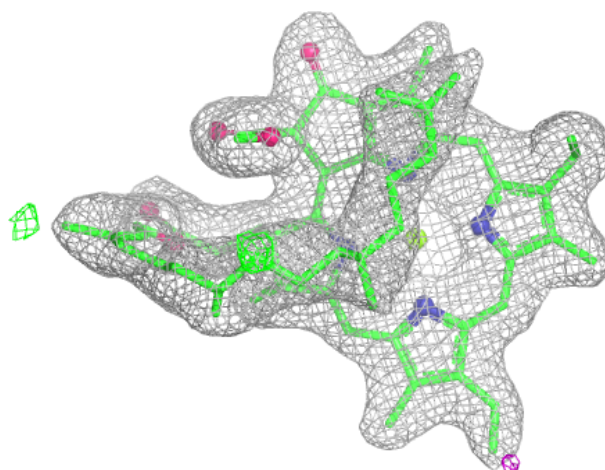
**Electron density around BCR B 617:**

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



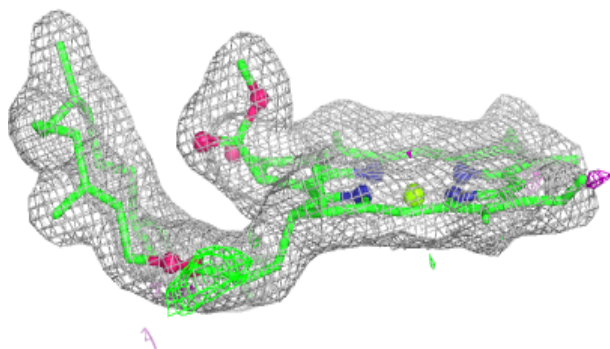
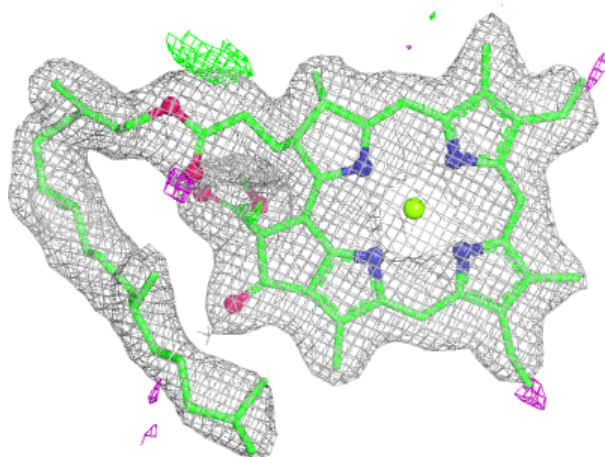
Electron density around CLA C 510:

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



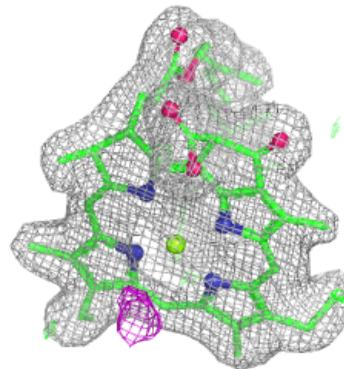
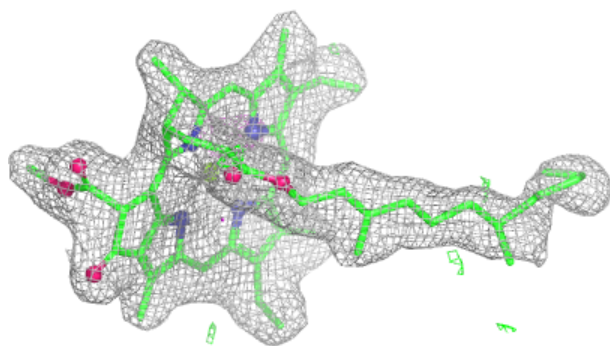
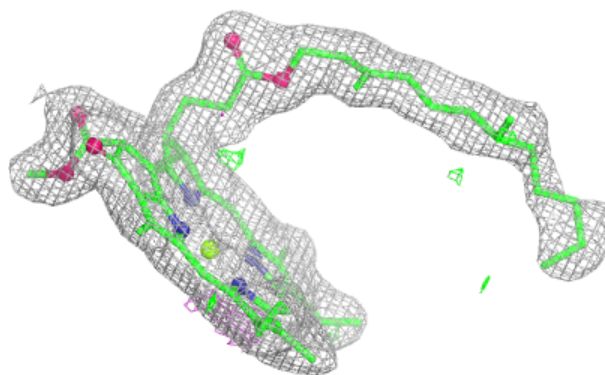
Electron density around CLA b 610:

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

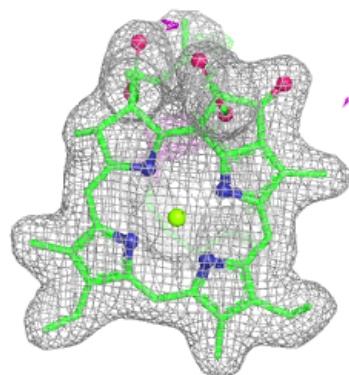
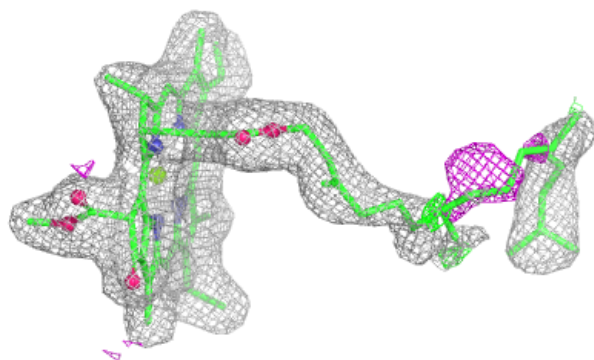
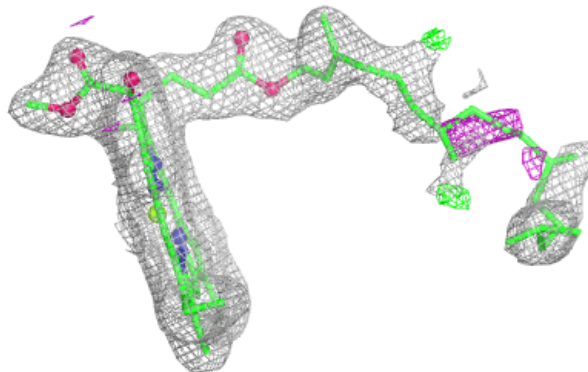


Electron density around CLA C 504:

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

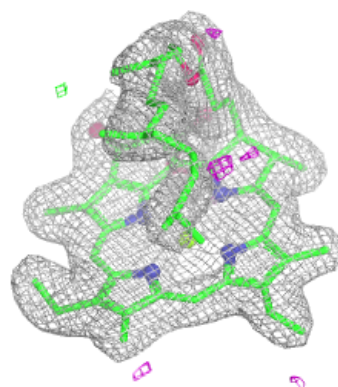
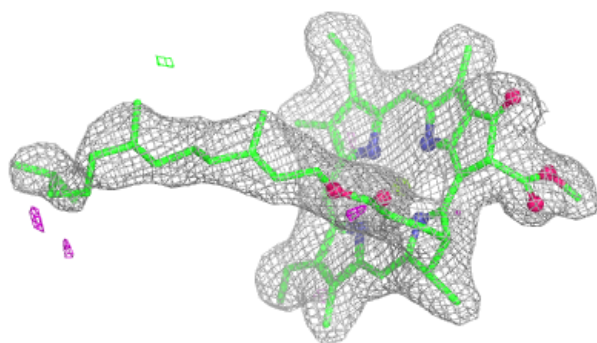
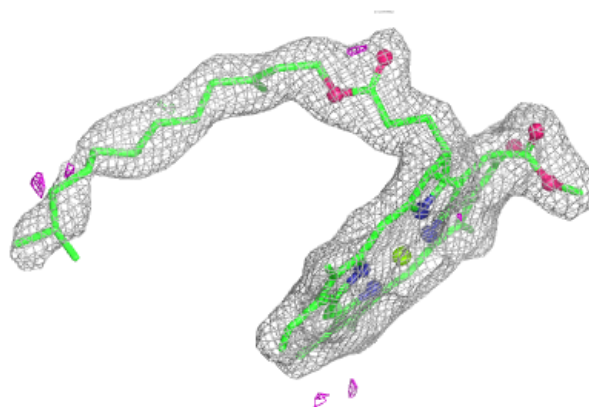
**Electron density around CLA C 506:**

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

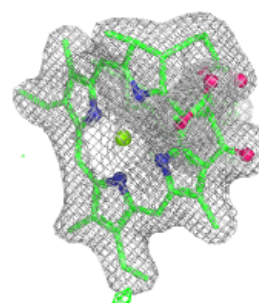
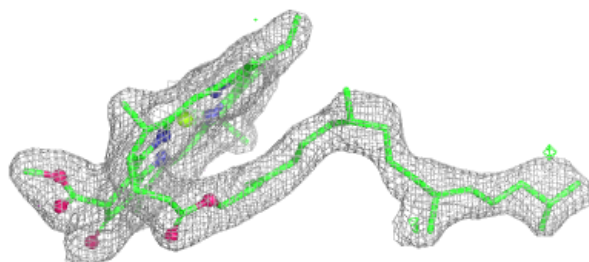
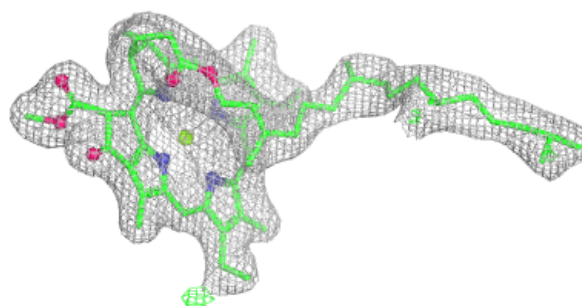


Electron density around CLA c 504:

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

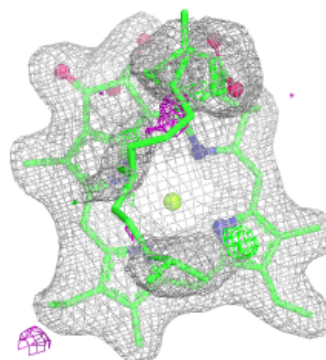
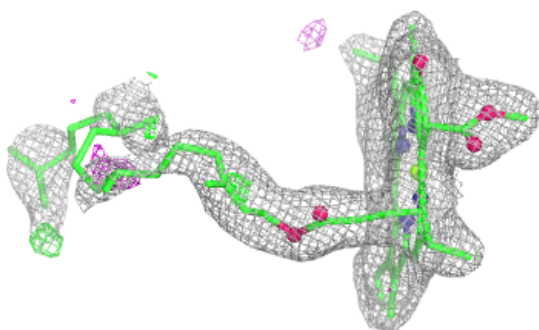
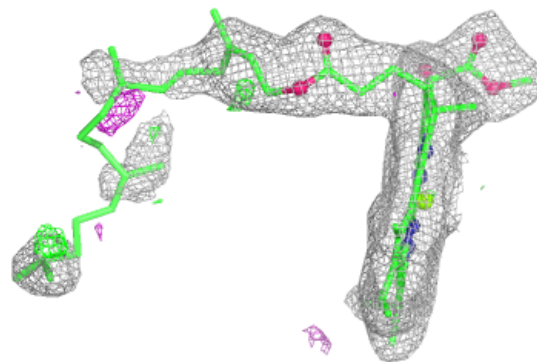
**Electron density around CLA c 505:**

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

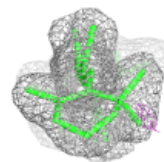
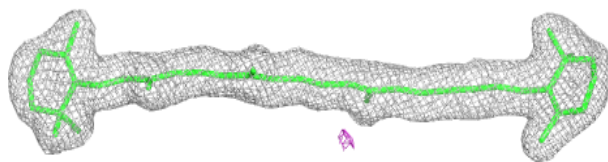
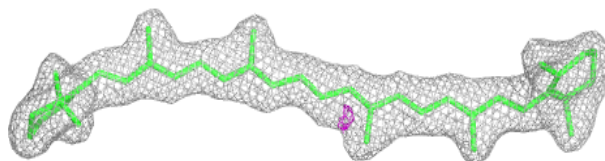


Electron density around CLA c 506:

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

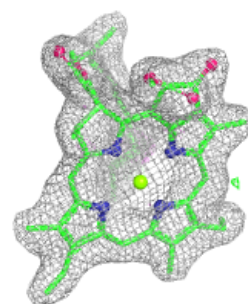
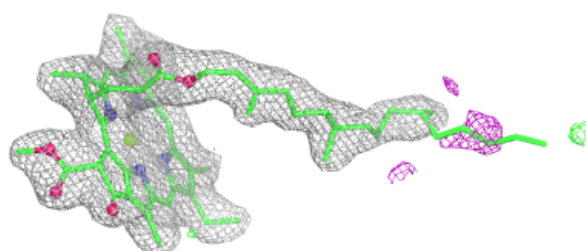
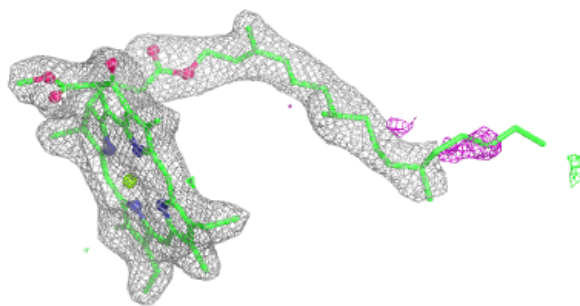
**Electron density around BCR a 611:**

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



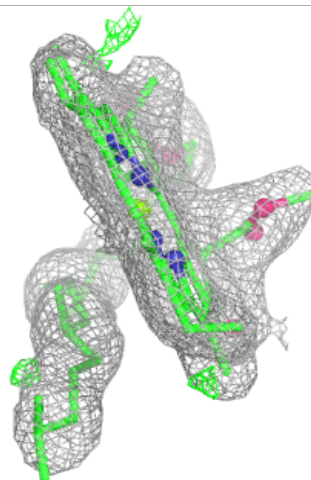
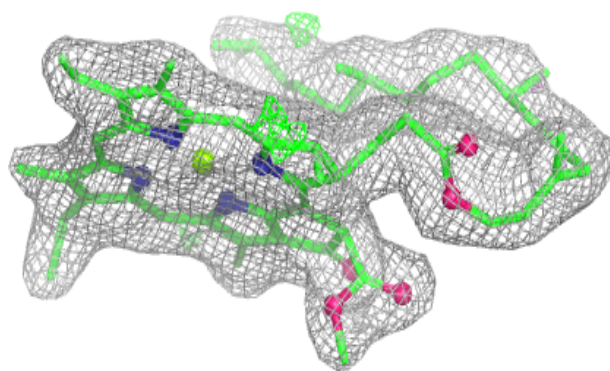
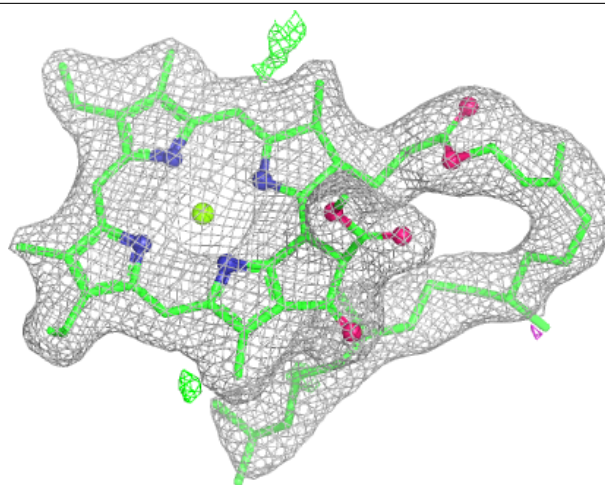
Electron density around CLA c 508:

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



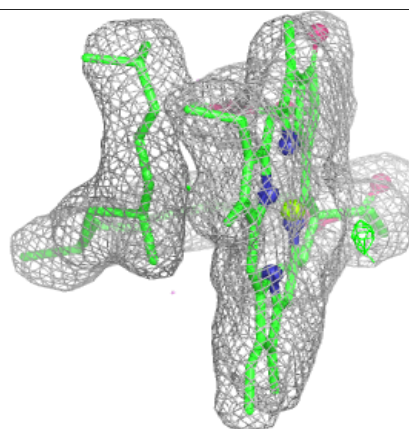
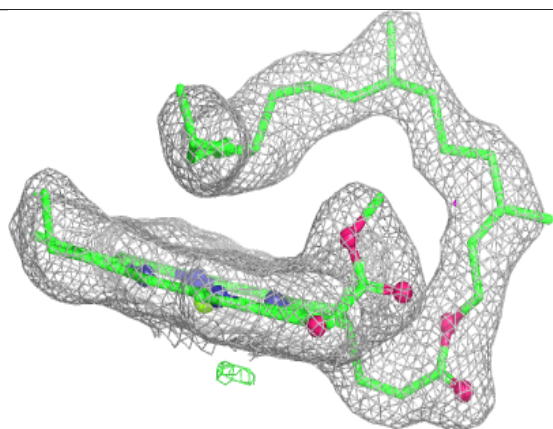
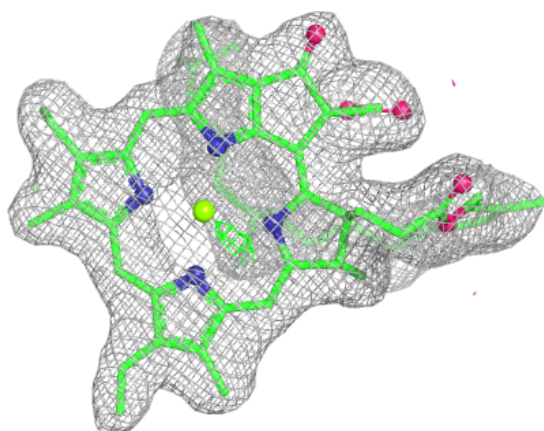
Electron density around CLA c 509:

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

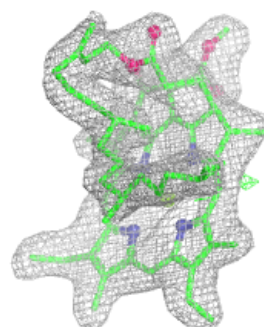
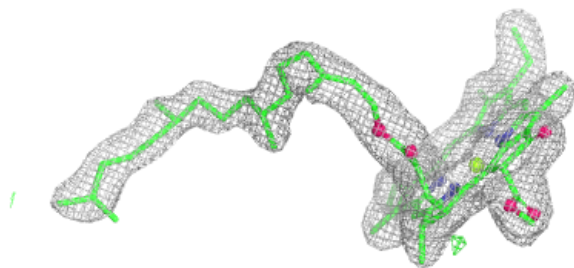
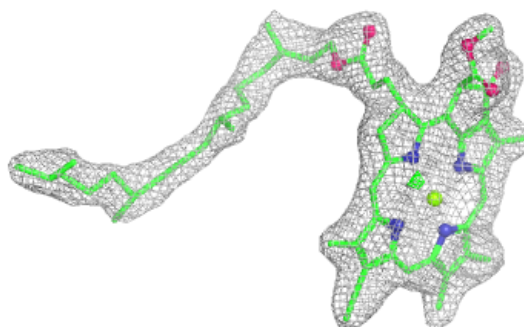


Electron density around CLA c 510:

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

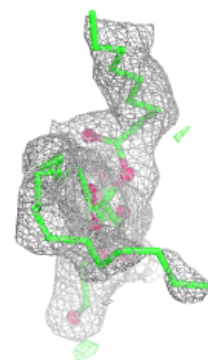
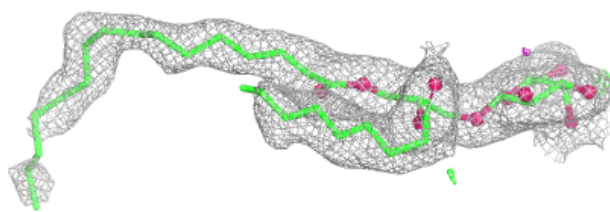
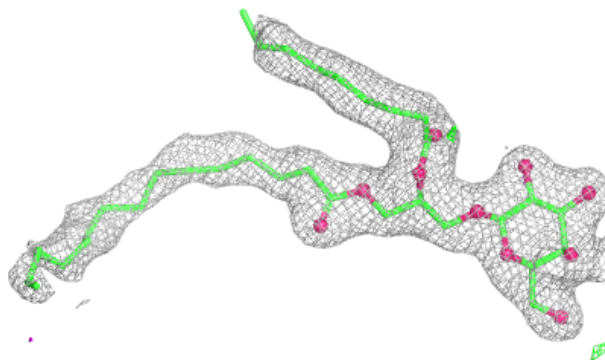
**Electron density around CLA c 511:**

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

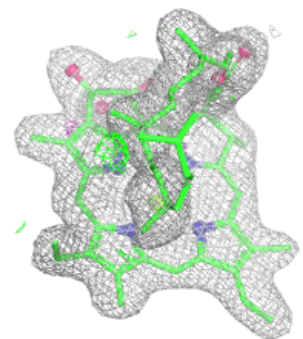
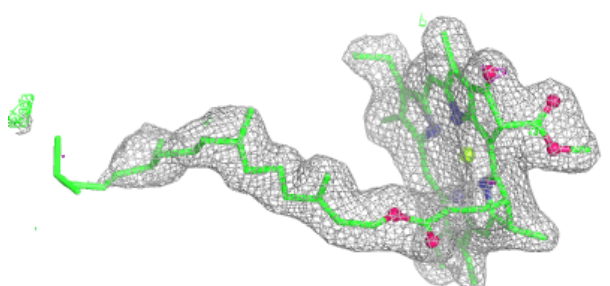
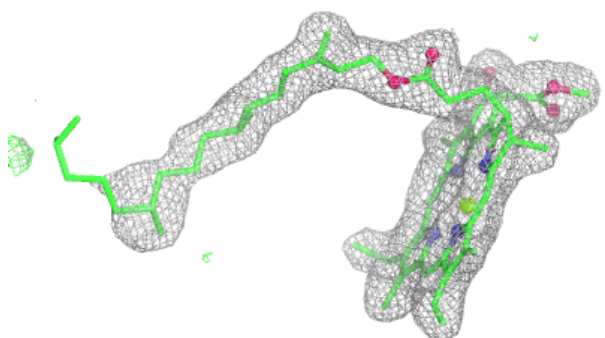


Electron density around LMG d 411:

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

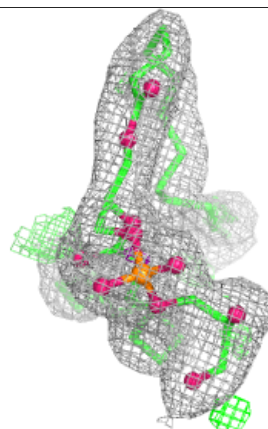
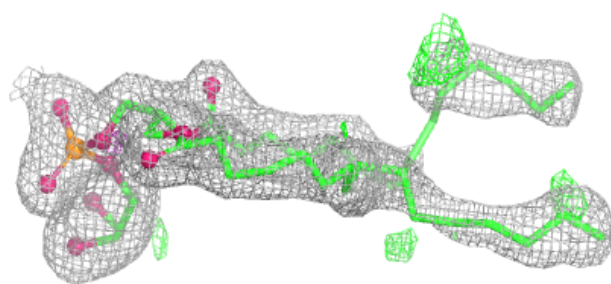
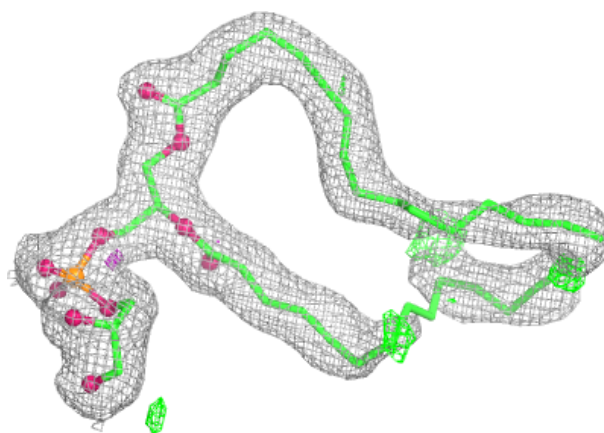
**Electron density around CLA C 508:**

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

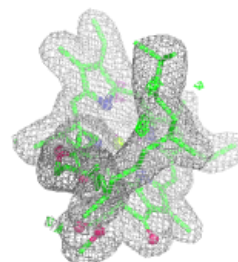
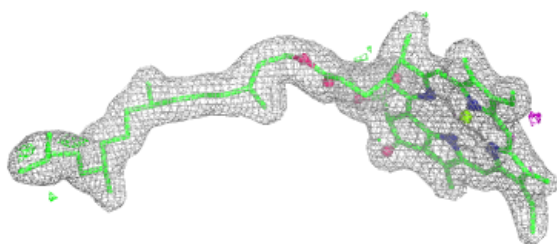
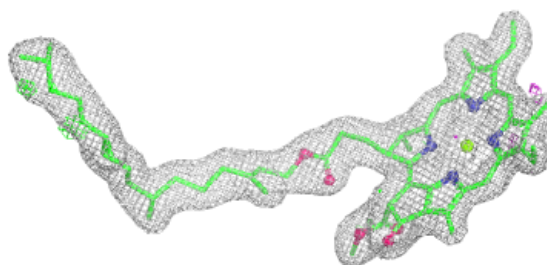


Electron density around LHG D 409:

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

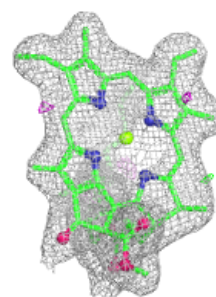
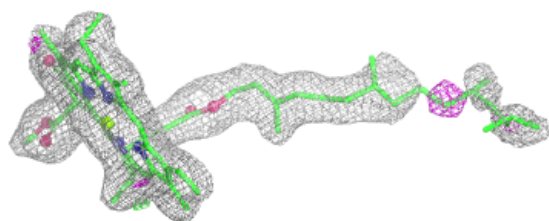
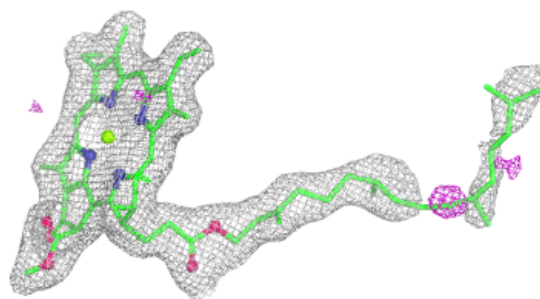
**Electron density around CLA a 607:**

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

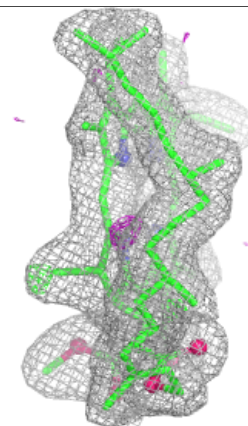
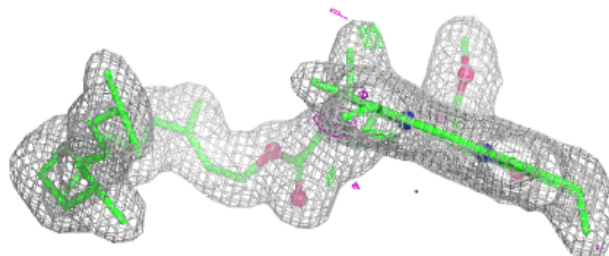
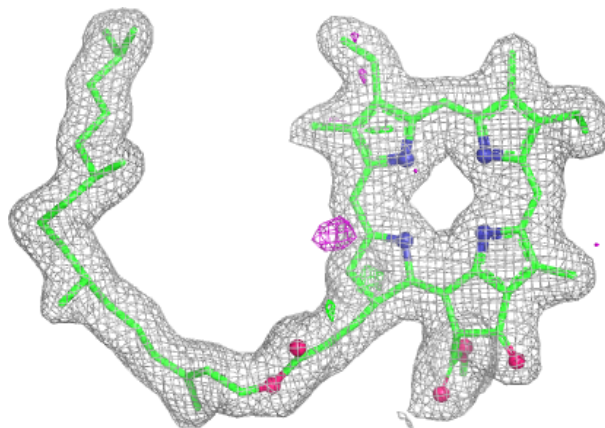


Electron density around CLA d 403:

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

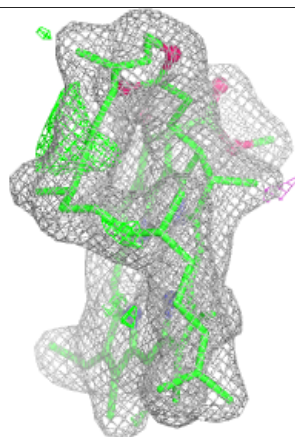
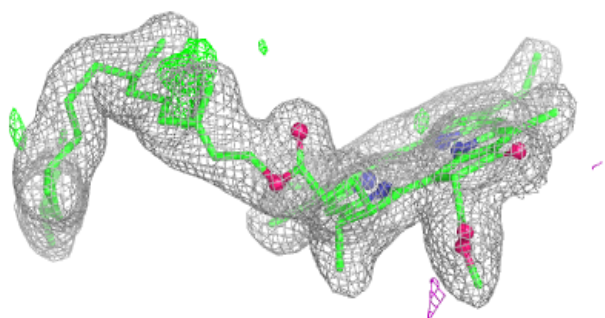
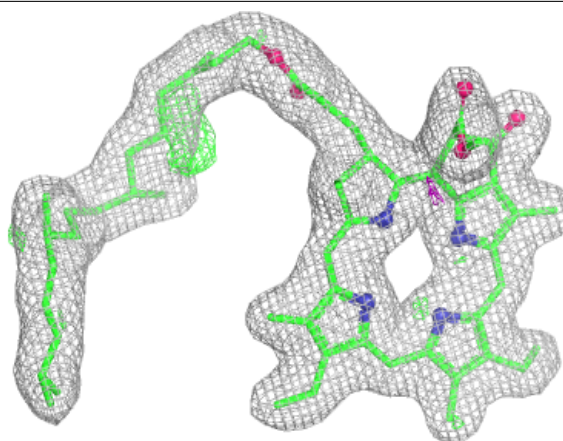
**Electron density around PHO A 609:**

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



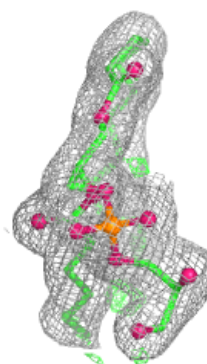
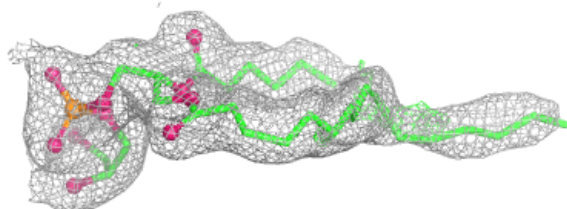
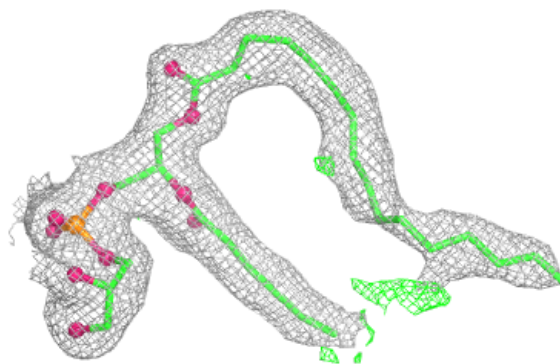
Electron density around PHO D 401:

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



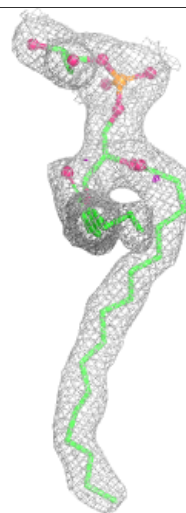
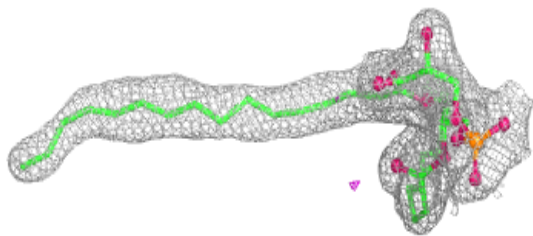
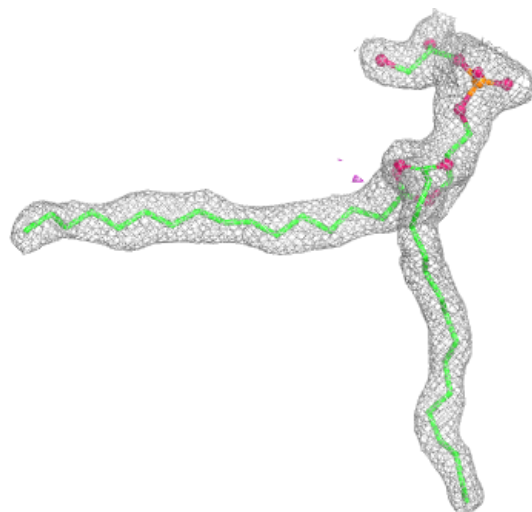
Electron density around LHG d 409:

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



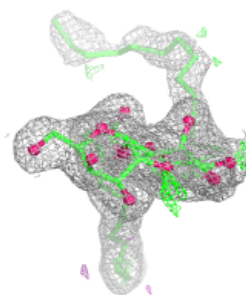
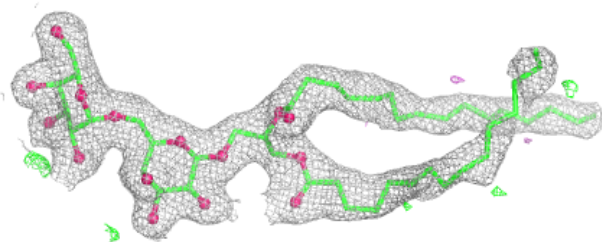
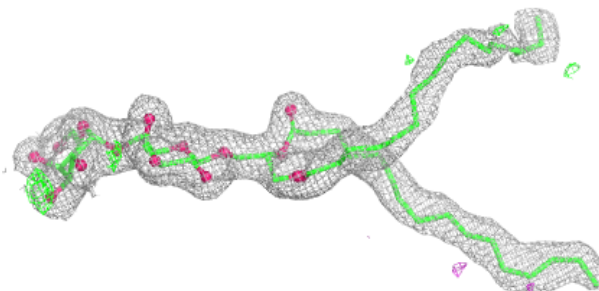
Electron density around LHG 1 101:

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

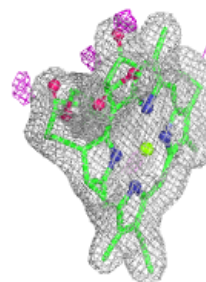
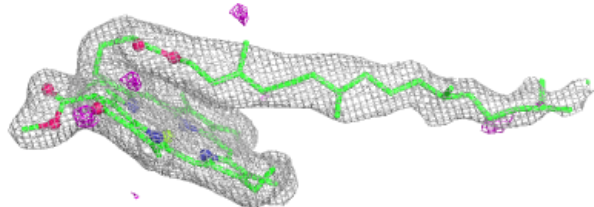
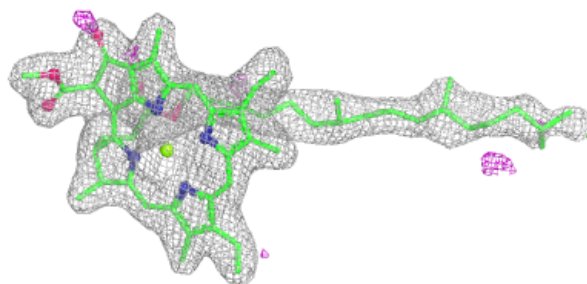


Electron density around DGD C 523:

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

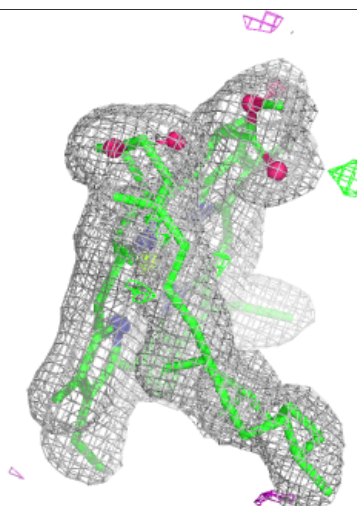
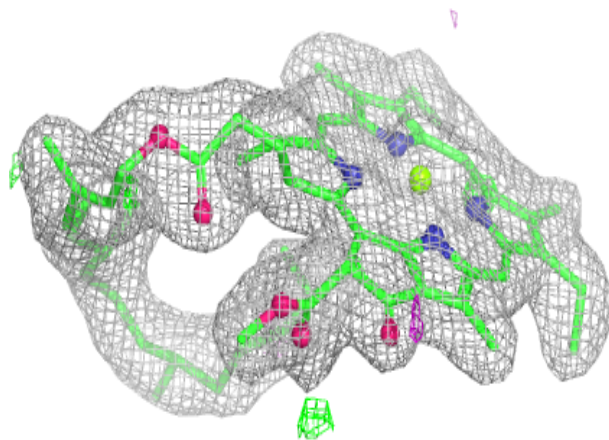
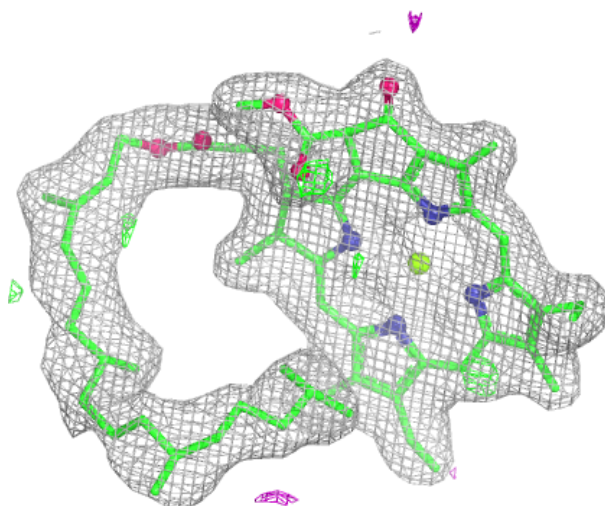
**Electron density around CLA b 614:**

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



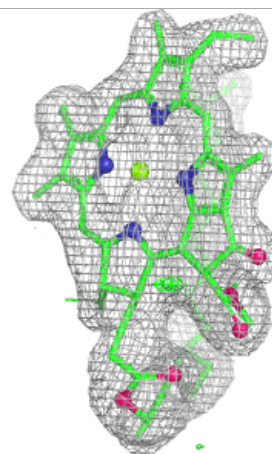
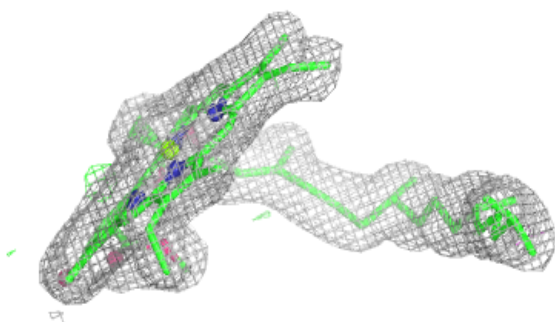
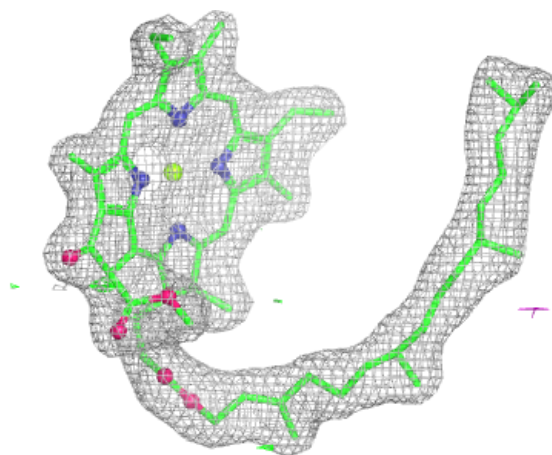
Electron density around CLA b 615:

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



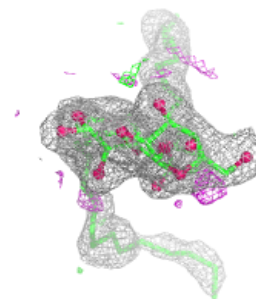
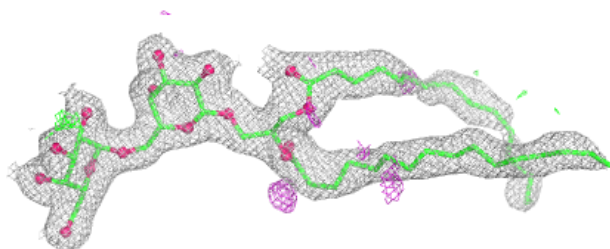
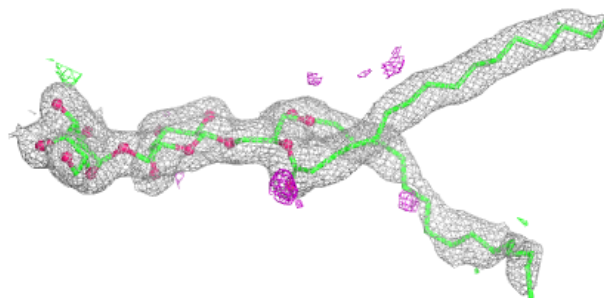
Electron density around CLA C 507:

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

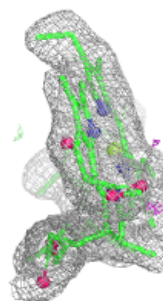
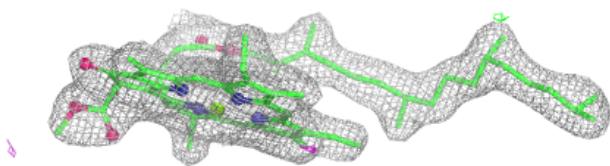
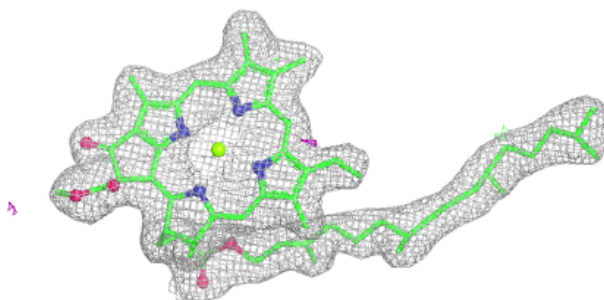


Electron density around DGD c 519:

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

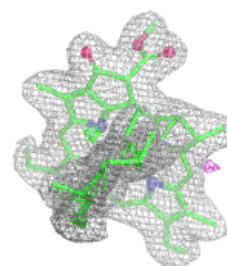
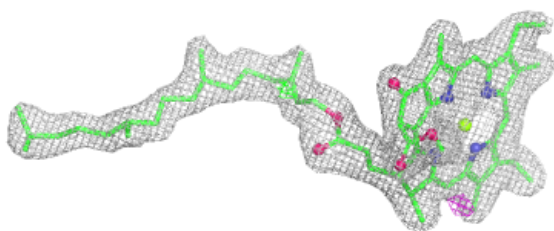
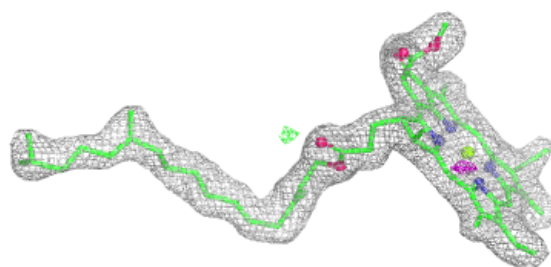
**Electron density around CLA c 501:**

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



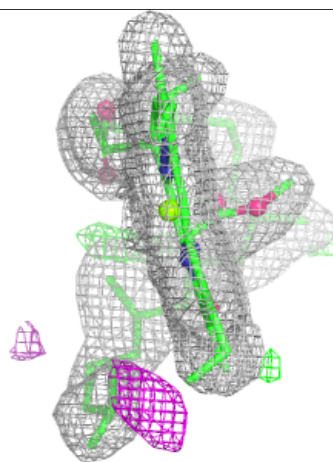
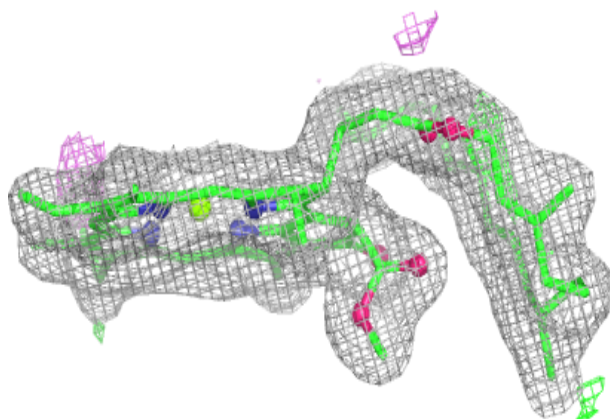
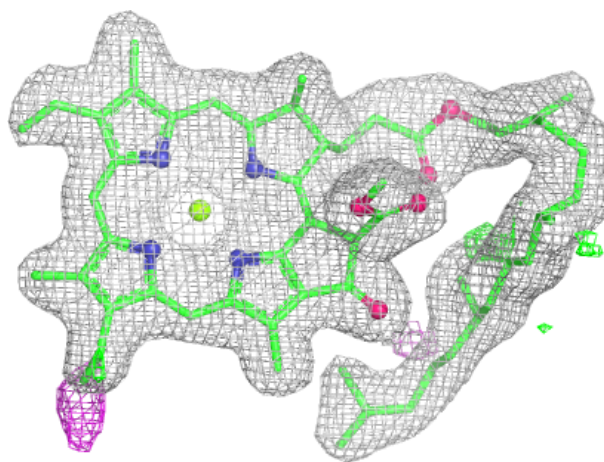
Electron density around CLA c 502:

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



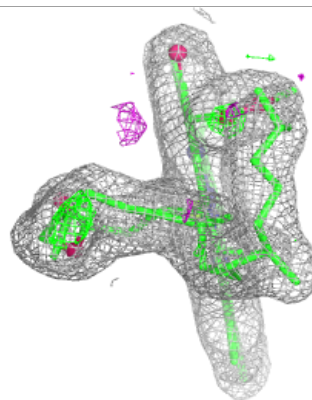
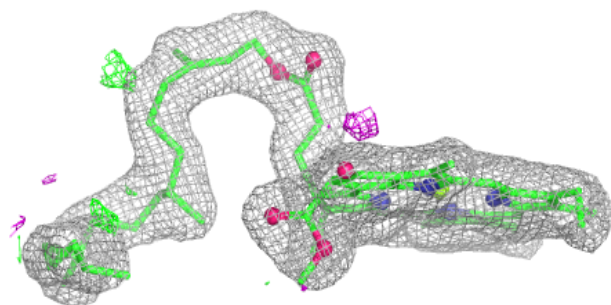
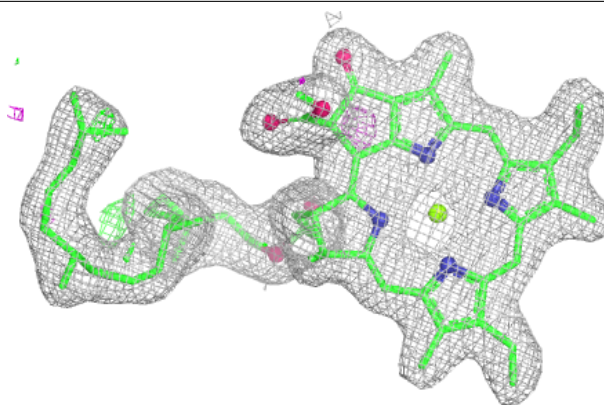
Electron density around CLA B 610:

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

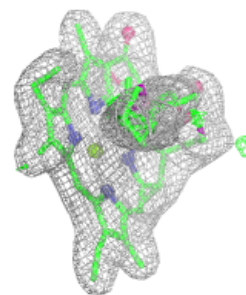
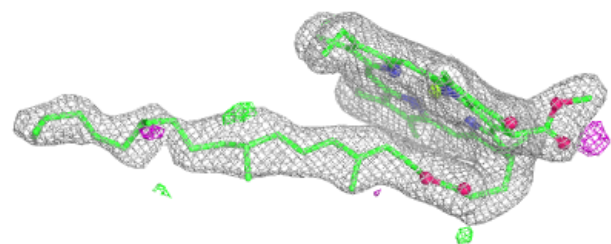
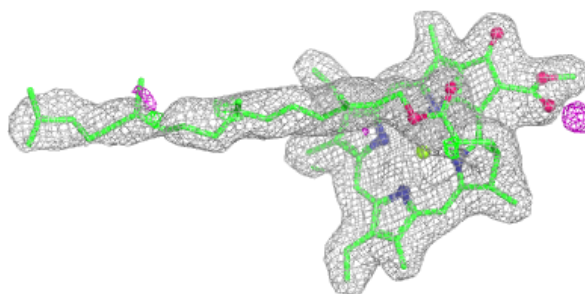


Electron density around CLA B 612:

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

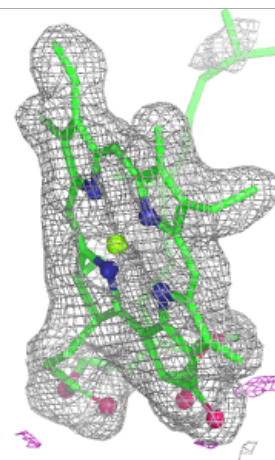
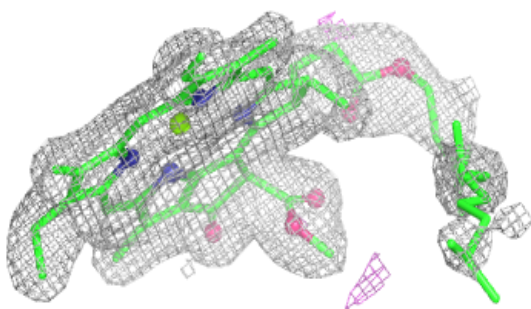
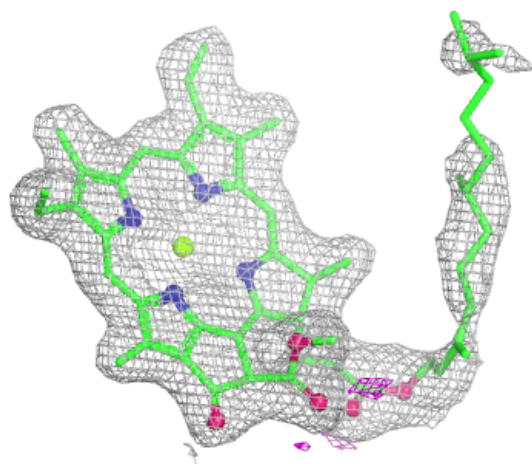
**Electron density around CLA B 614:**

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



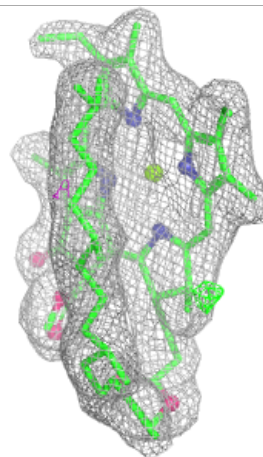
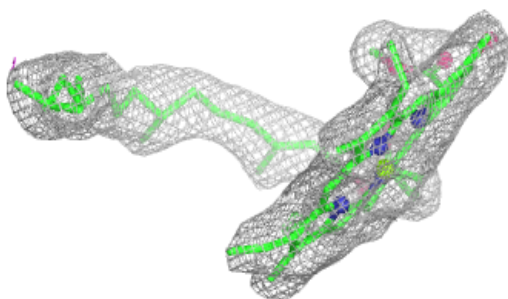
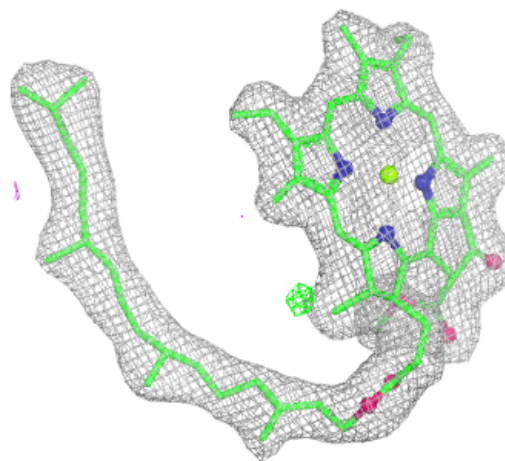
Electron density around CLA B 616:

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



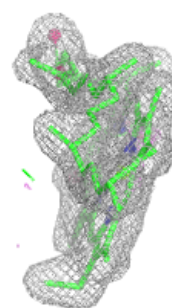
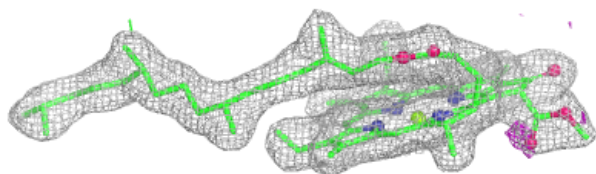
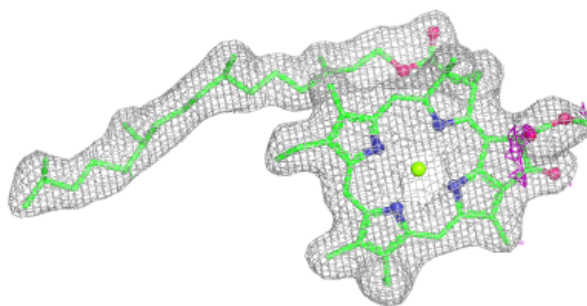
Electron density around CLA c 507:

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

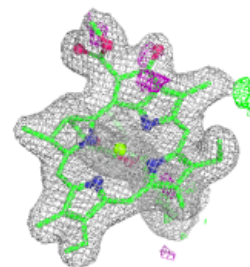
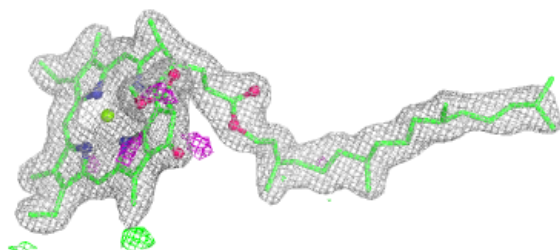
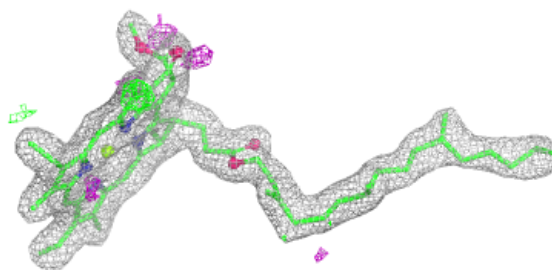


Electron density around CLA C 501:

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

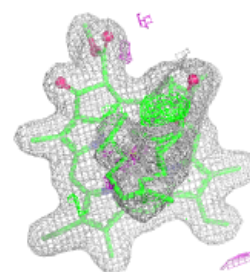
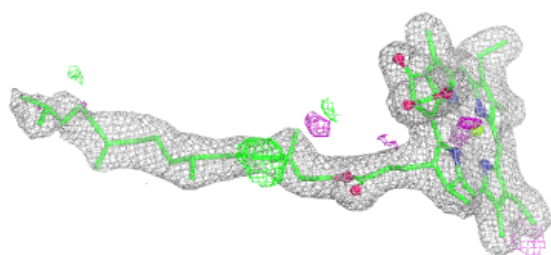
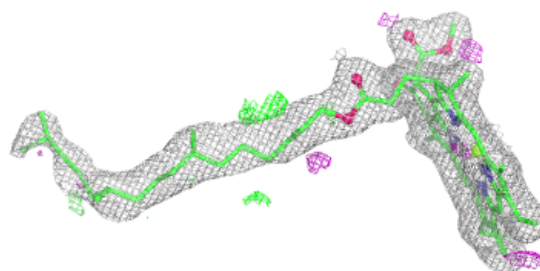
**Electron density around CLA C 502:**

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

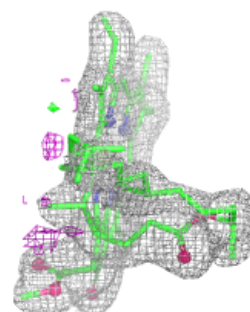
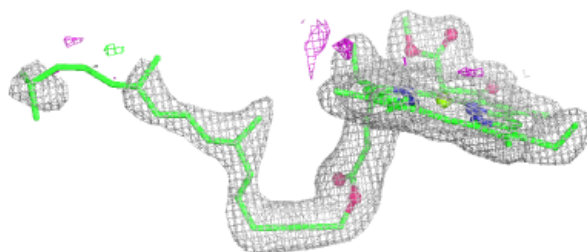
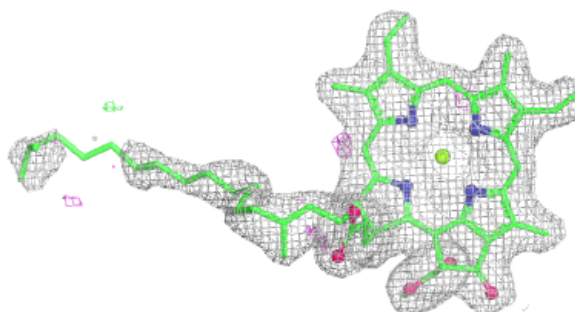


Electron density around CLA B 604:

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

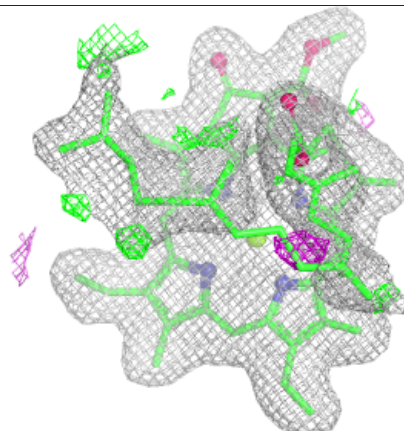
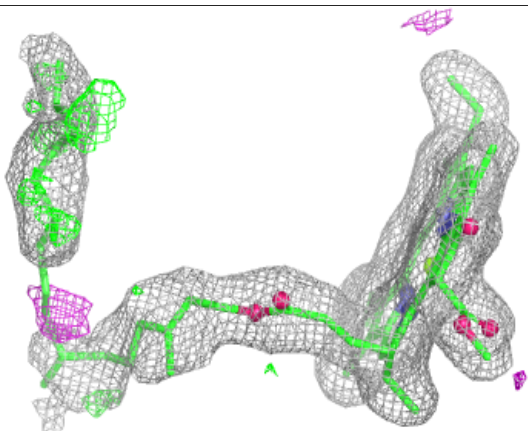
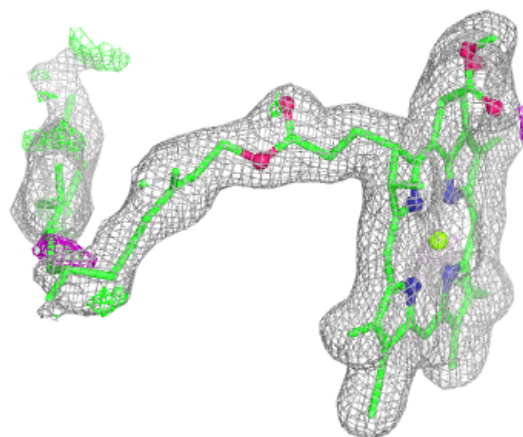
**Electron density around CLA a 608:**

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

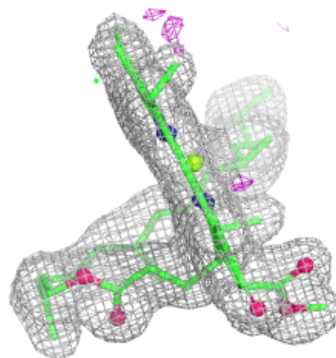
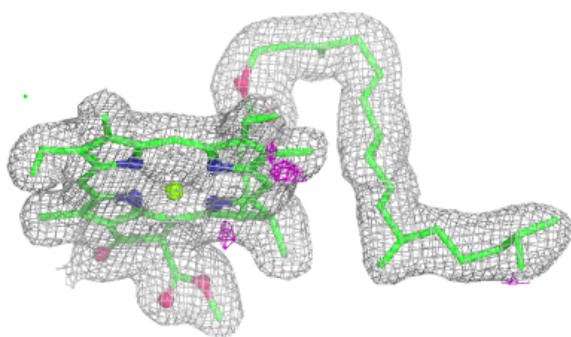
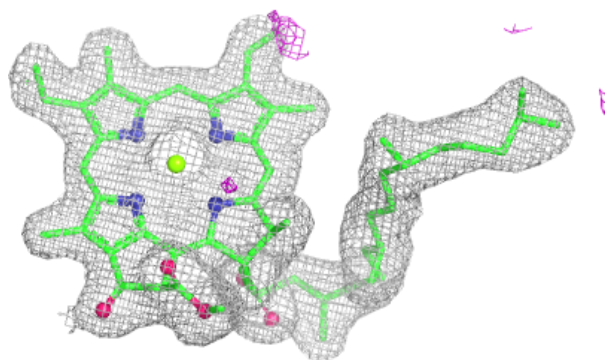


Electron density around CLA a 610:

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

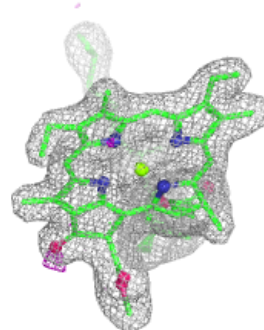
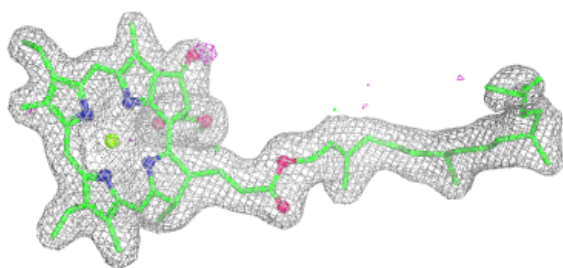
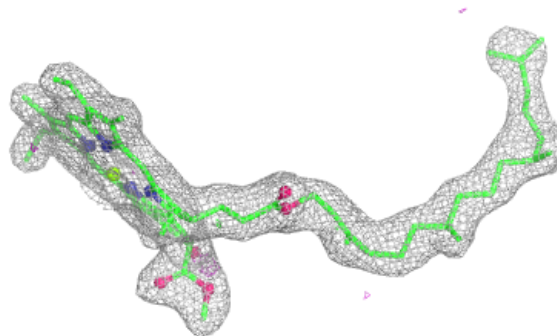
**Electron density around CLA a 613:**

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

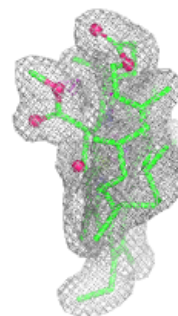
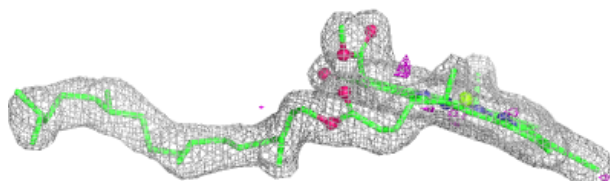
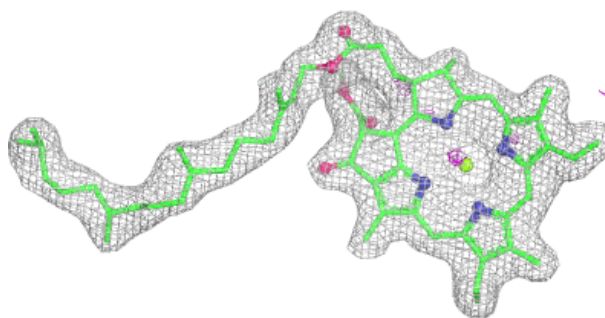


Electron density around CLA d 402:

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

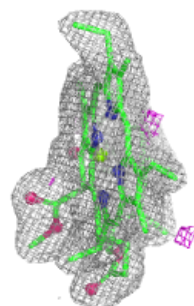
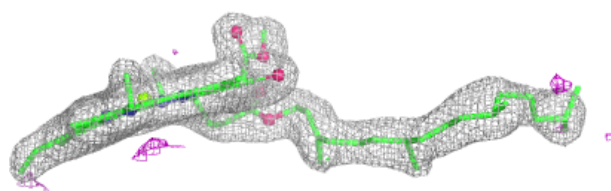
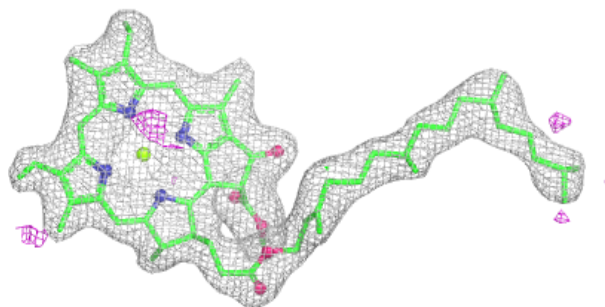
**Electron density around CLA B 602:**

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

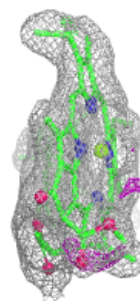
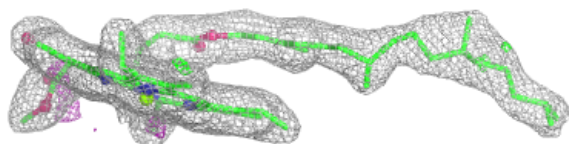
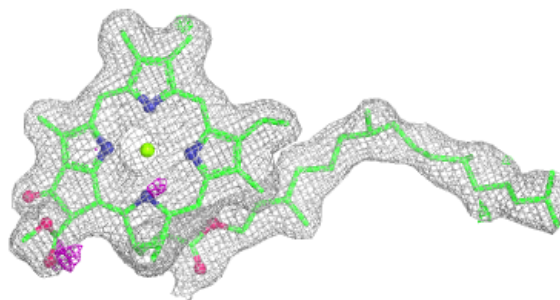


Electron density around CLA b 602:

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

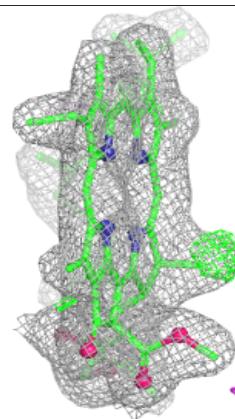
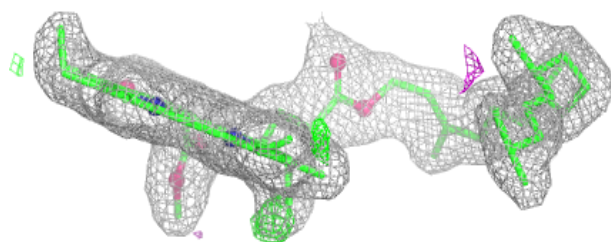
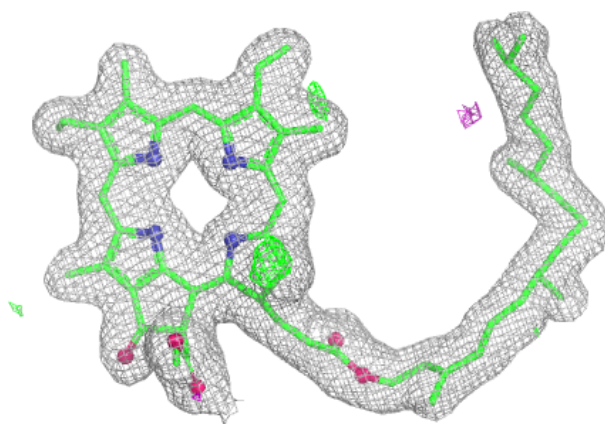
**Electron density around CLA b 603:**

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



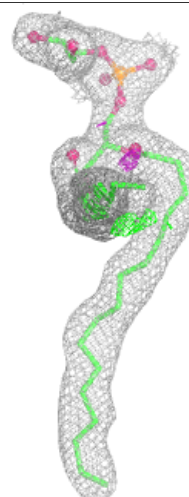
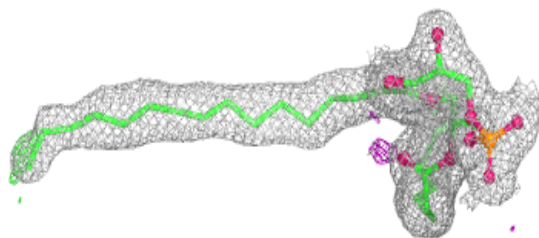
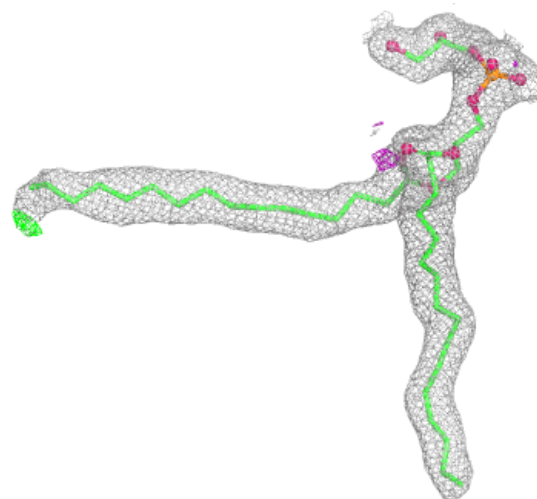
Electron density around PHO a 609:

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



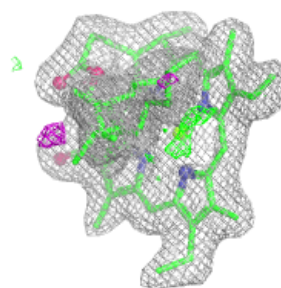
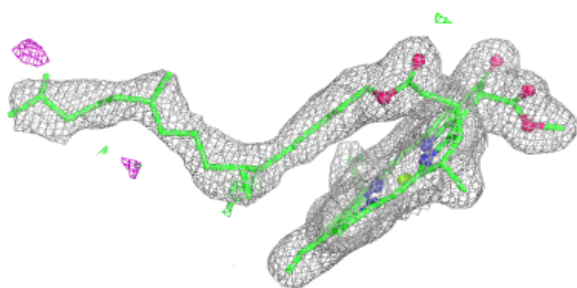
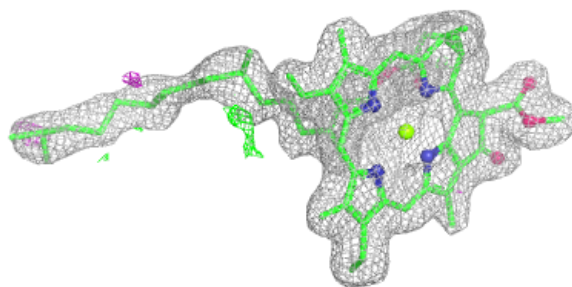
Electron density around LHG B 622:

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

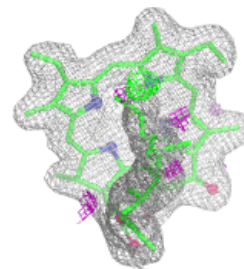
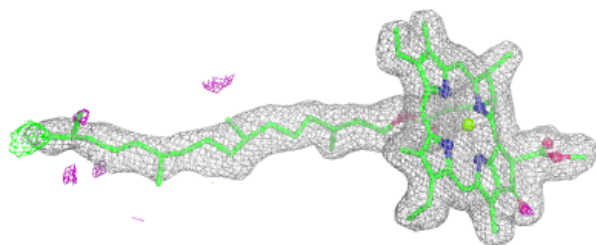
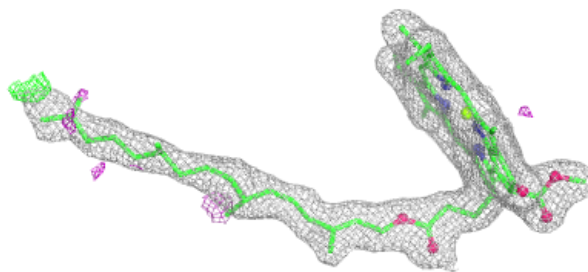


Electron density around CLA C 505:

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

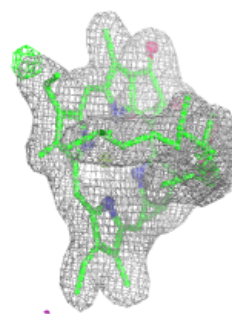
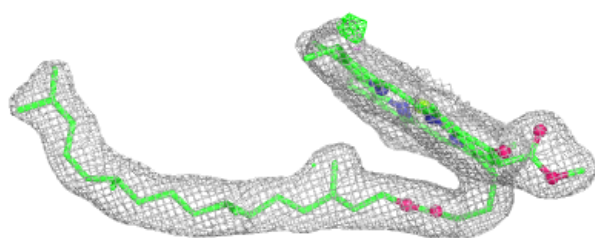
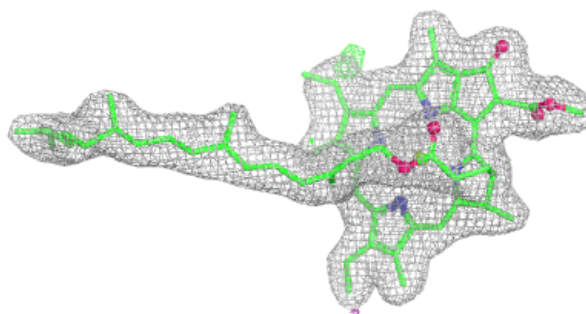
**Electron density around CLA b 607:**

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

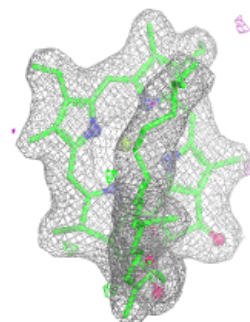
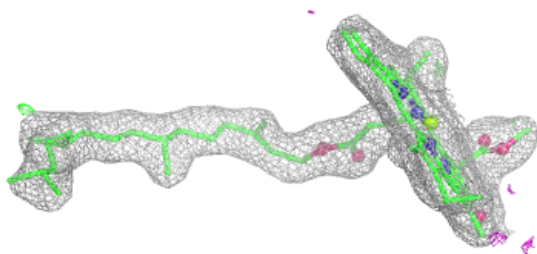
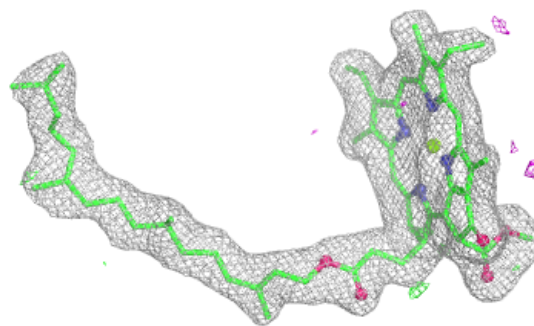


Electron density around CLA b 608:

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

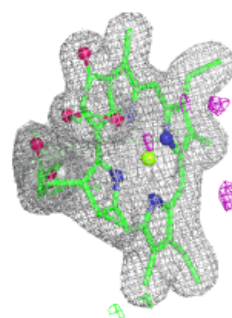
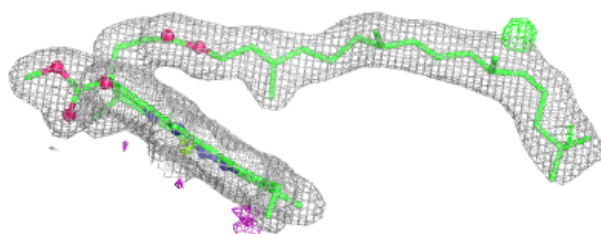
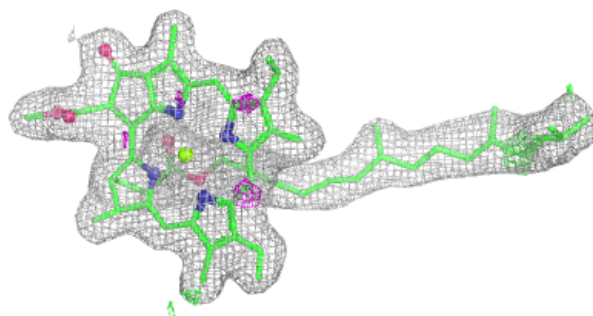
**Electron density around CLA b 609:**

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

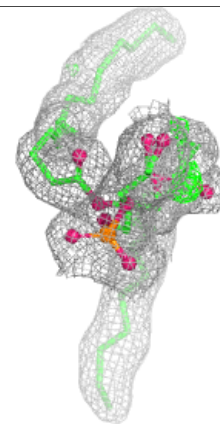
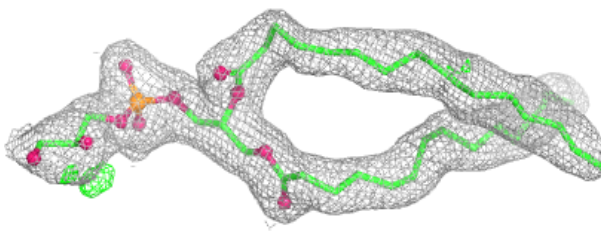
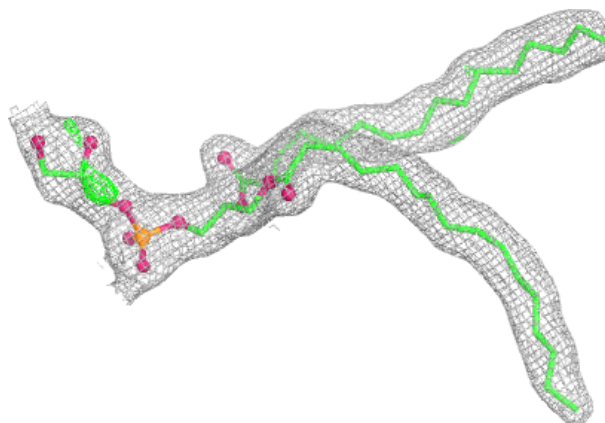


Electron density around CLA B 608:

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

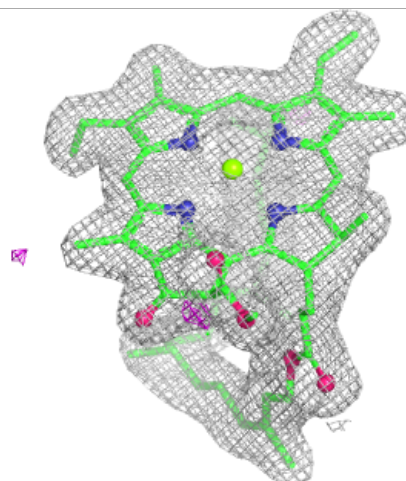
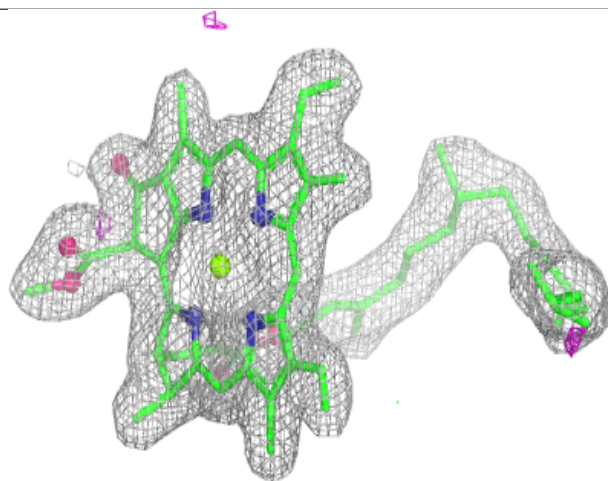
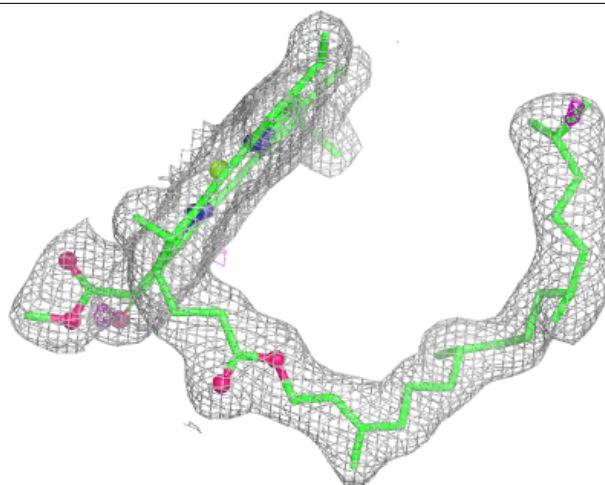
**Electron density around LHG d 408:**

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



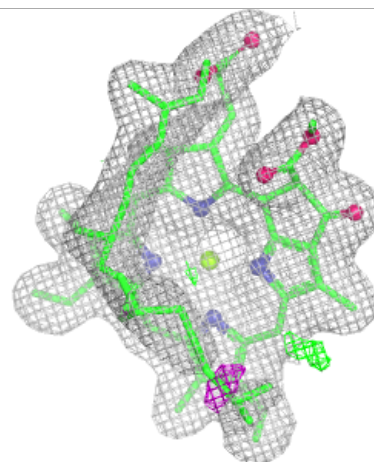
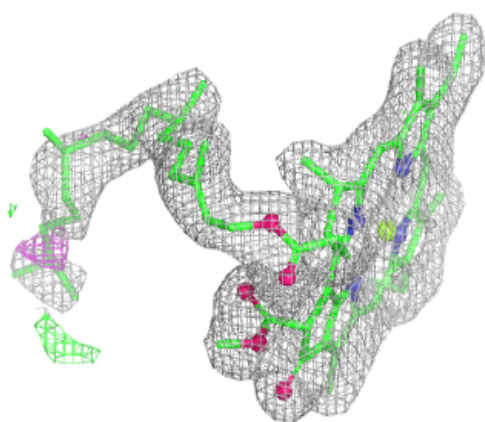
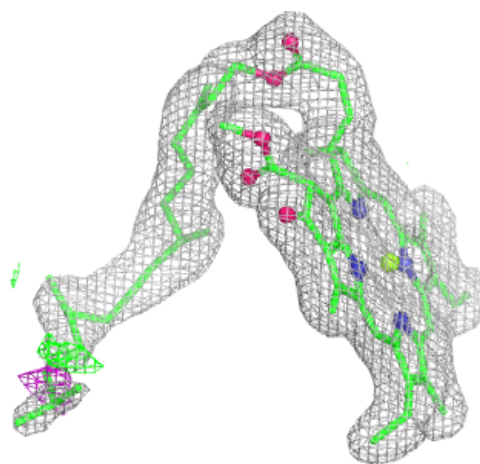
Electron density around CLA b 611:

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



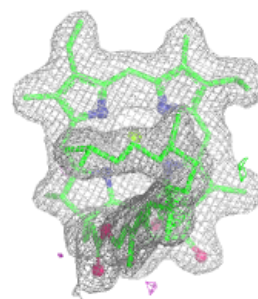
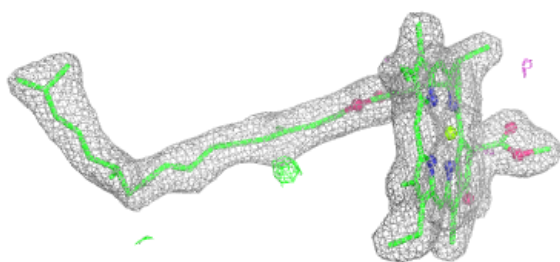
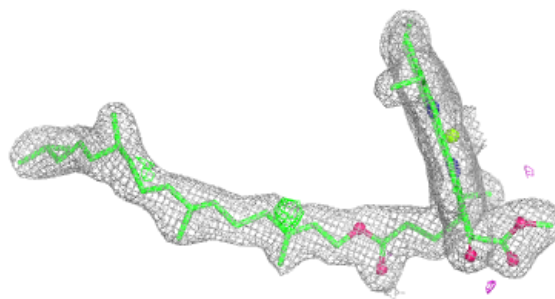
Electron density around CLA b 613:

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



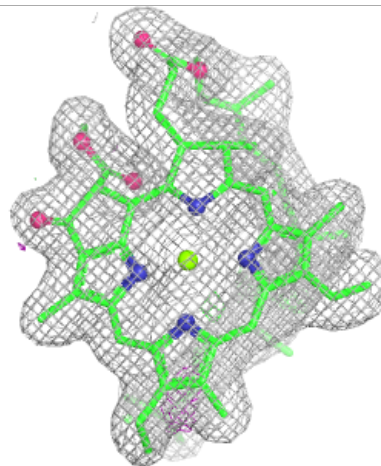
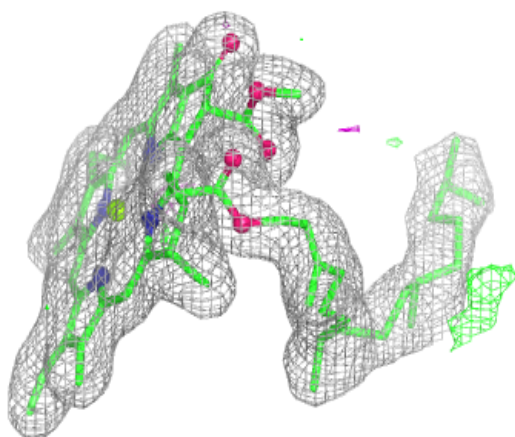
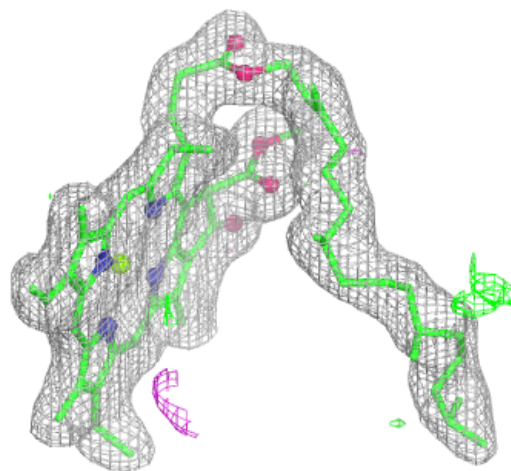
Electron density around CLA b 605:

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



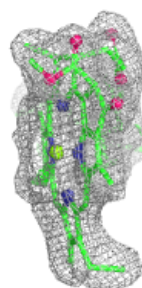
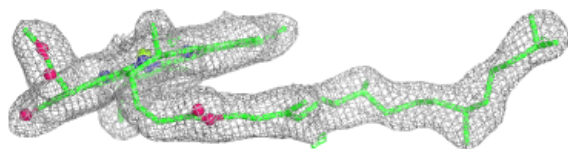
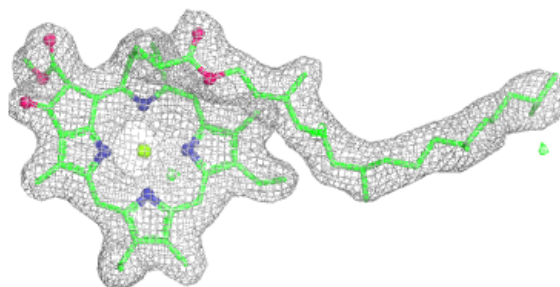
Electron density around CLA B 613:

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



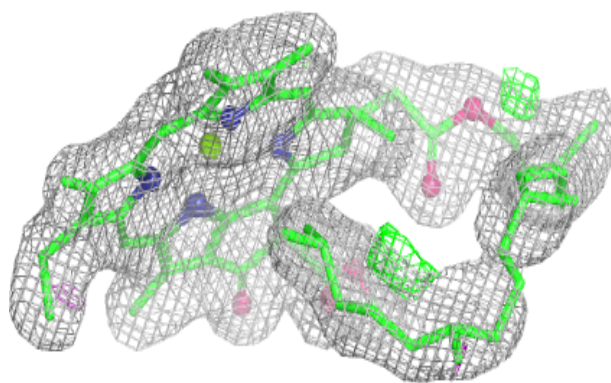
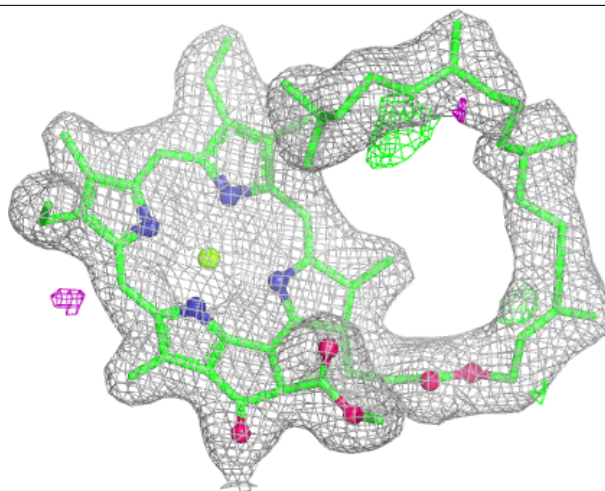
Electron density around CLA B 603:

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



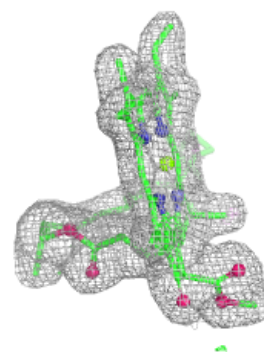
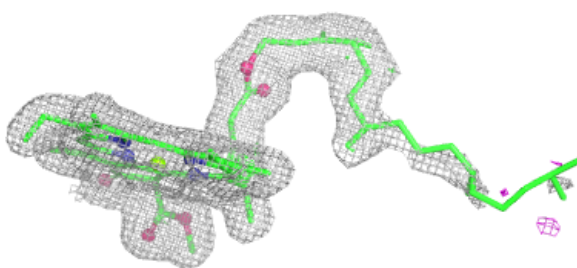
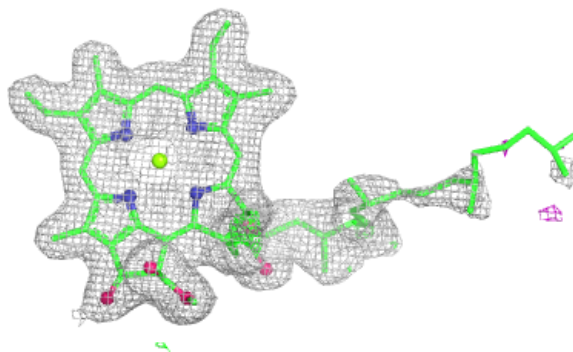
Electron density around CLA B 615:

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

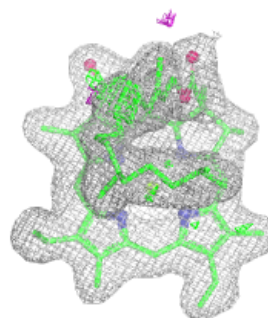
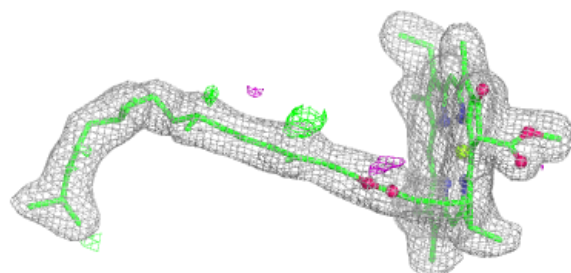
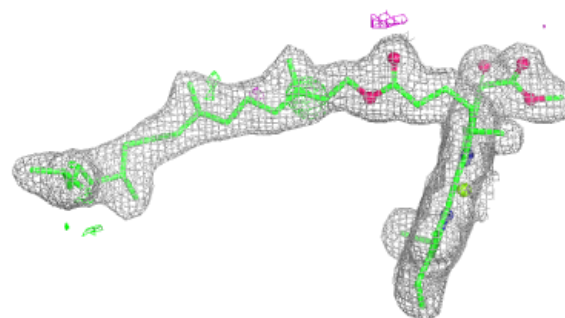


Electron density around CLA A 608:

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

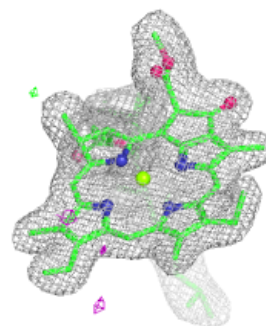
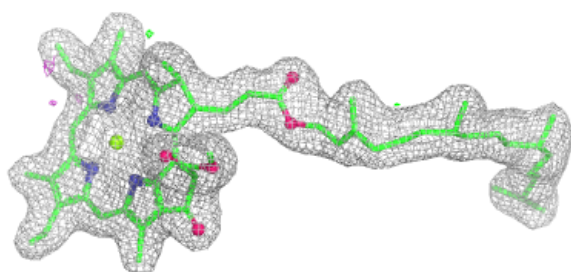
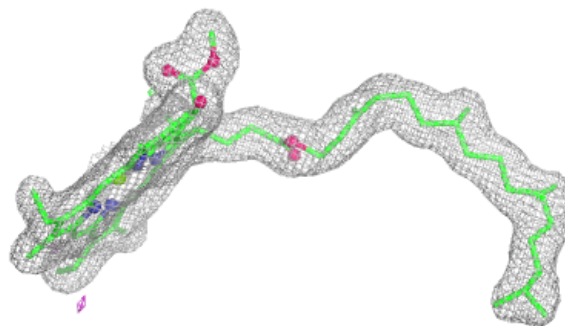
**Electron density around CLA B 605:**

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

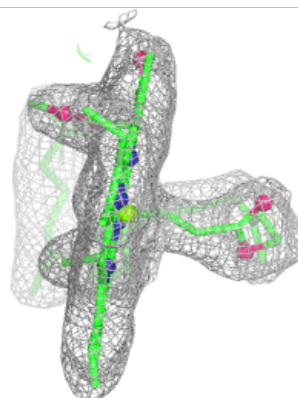
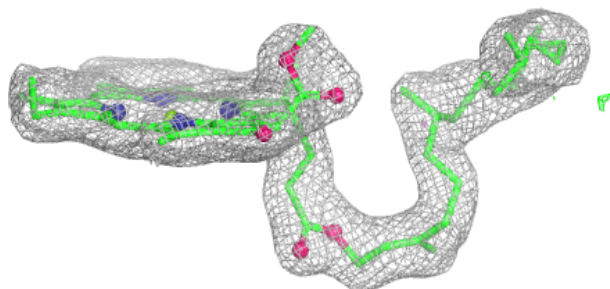
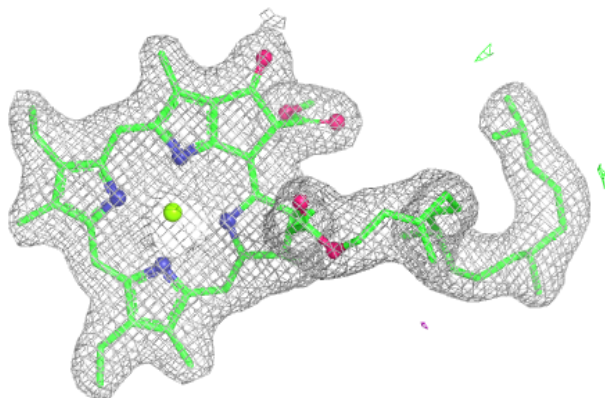


Electron density around CLA D 402:

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

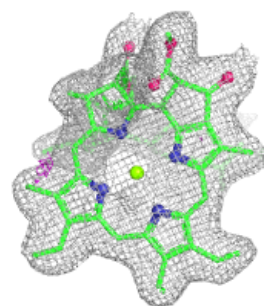
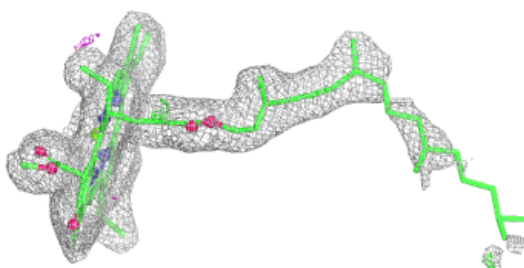
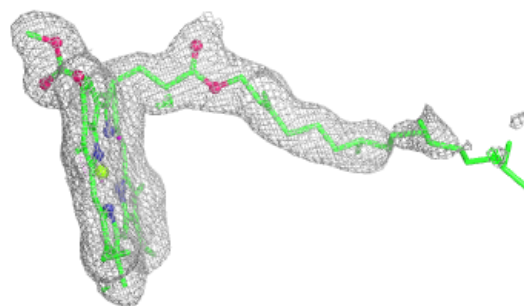
**Electron density around CLA b 612:**

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



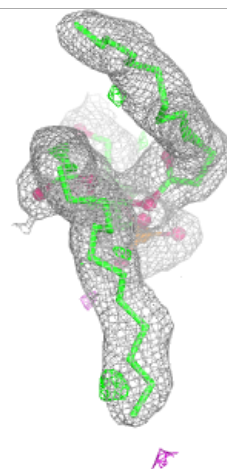
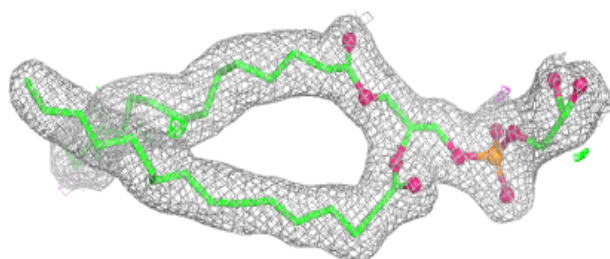
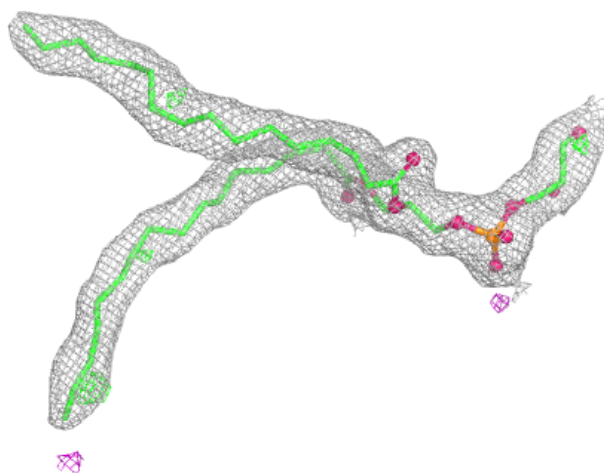
Electron density around CLA D 403:

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



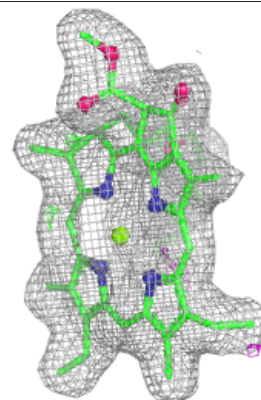
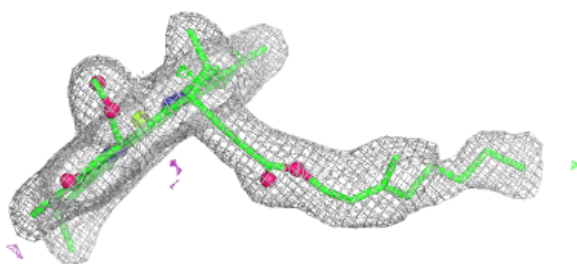
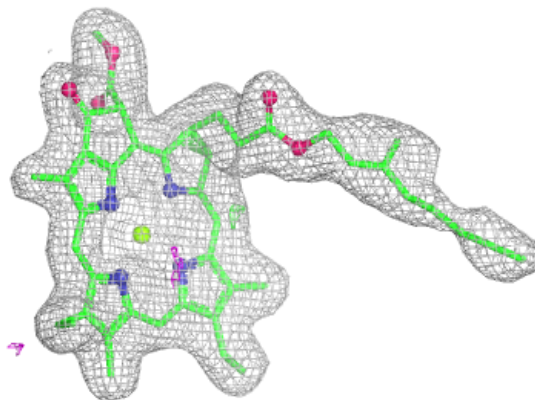
Electron density around LHG D 408:

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

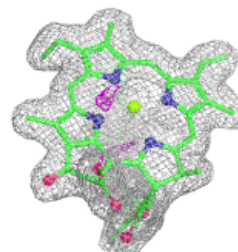
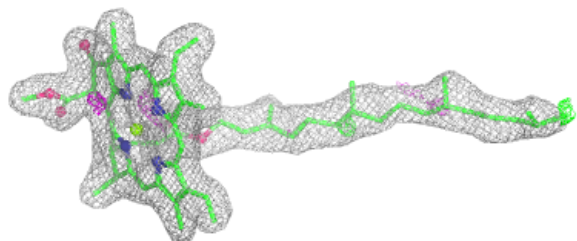
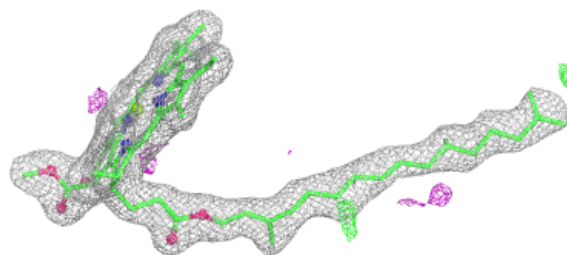


Electron density around CLA A 610:

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

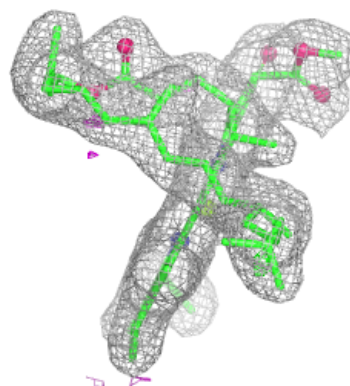
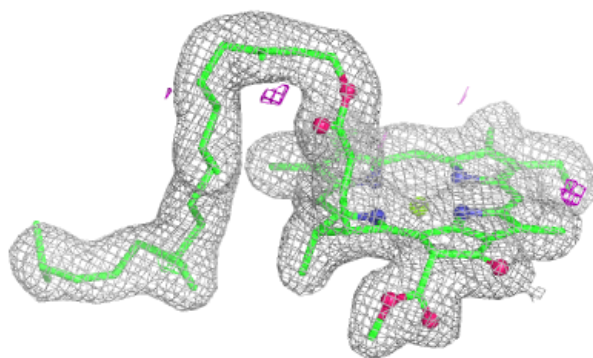
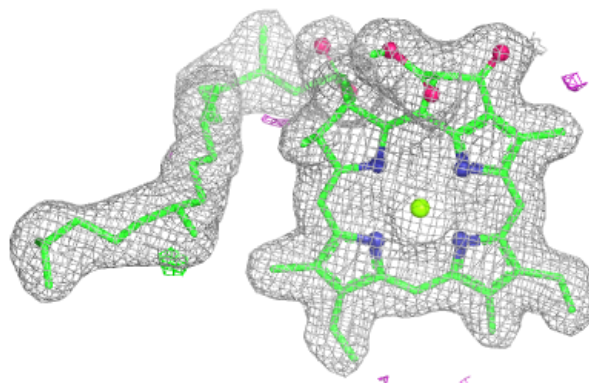
**Electron density around CLA B 607:**

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

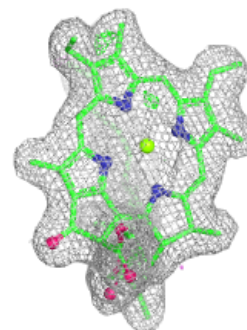
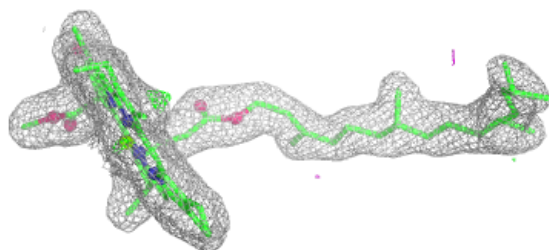
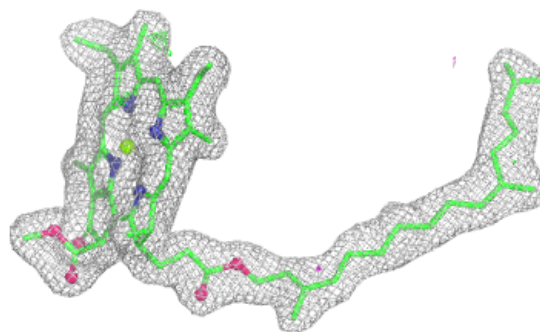


Electron density around CLA A 614:

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

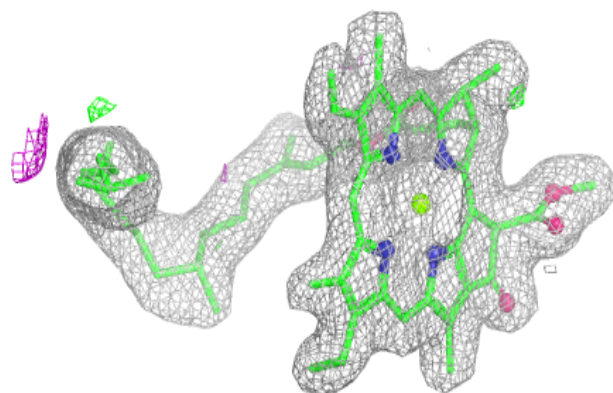
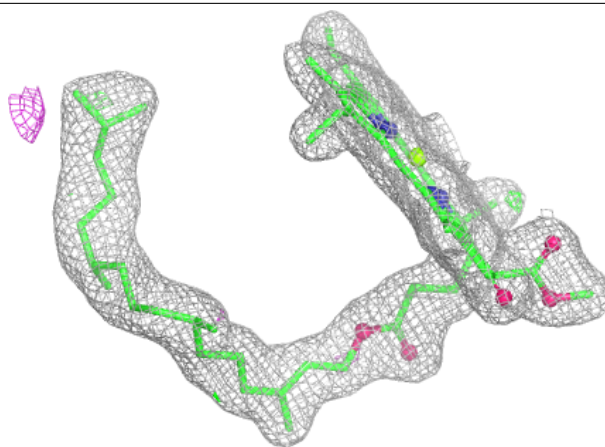
**Electron density around CLA B 609:**

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



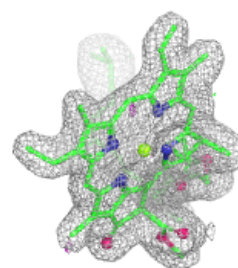
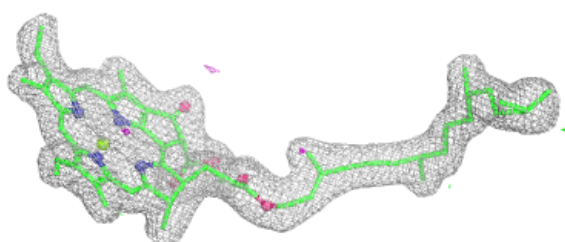
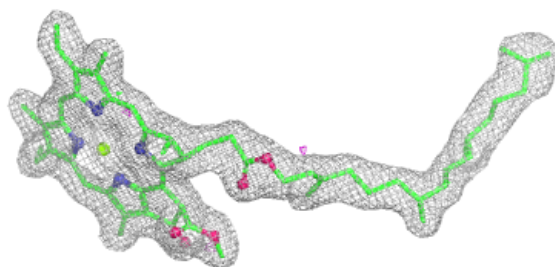
Electron density around CLA B 611:

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

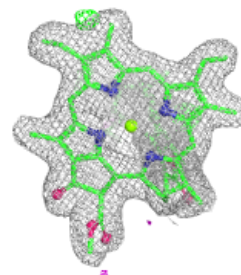
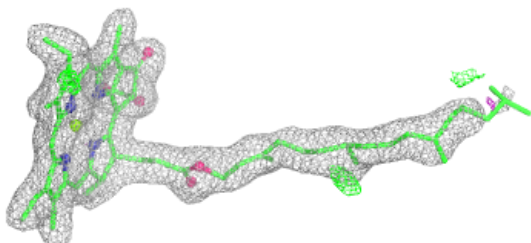
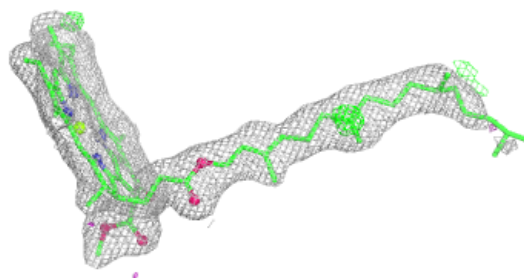


Electron density around CLA A 607:

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

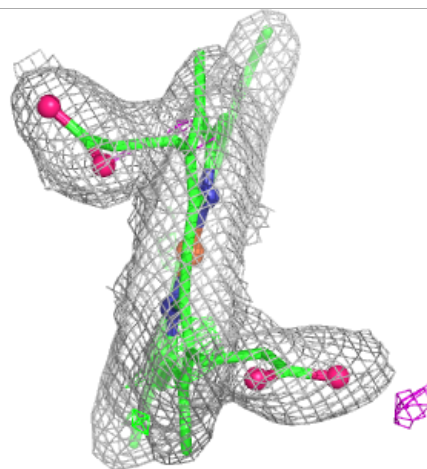
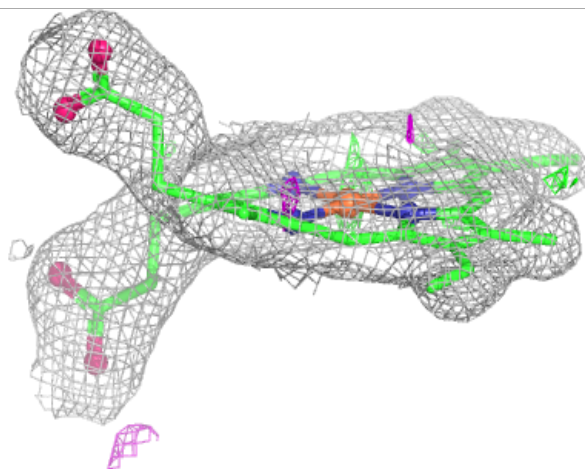
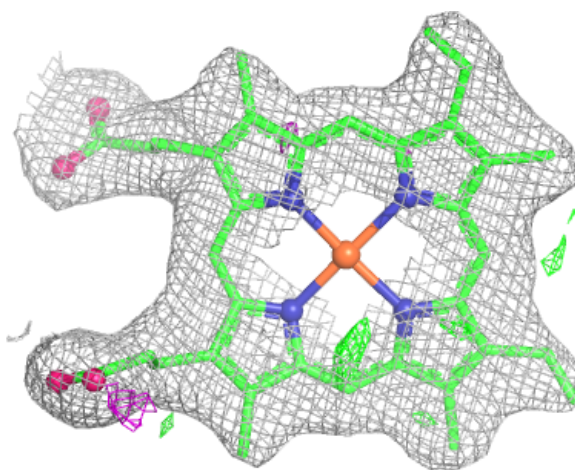
**Electron density around CLA b 604:**

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



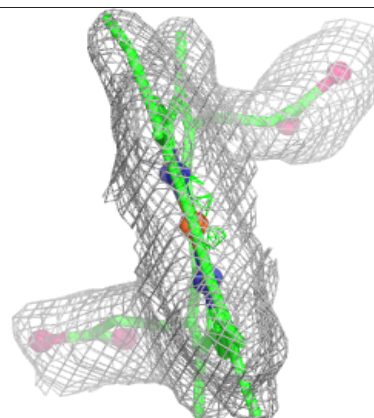
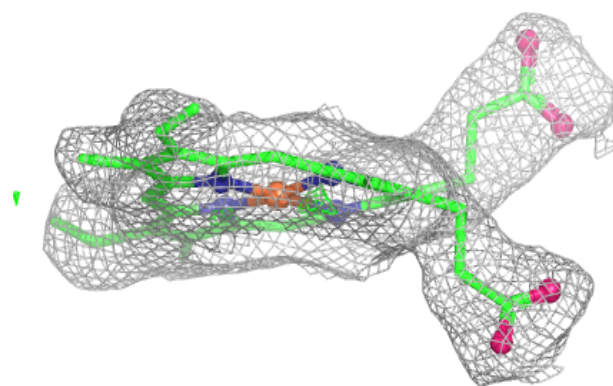
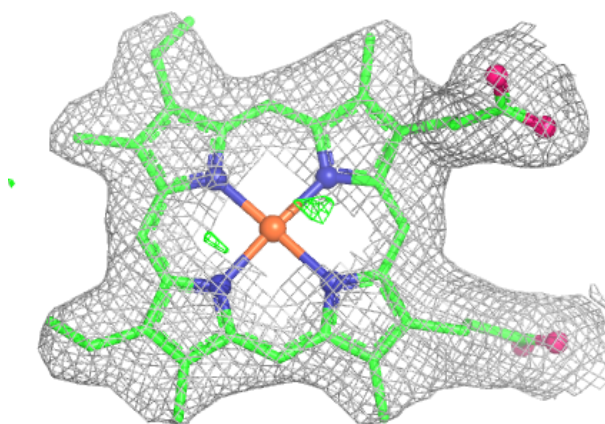
Electron density around HEM F 101:

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



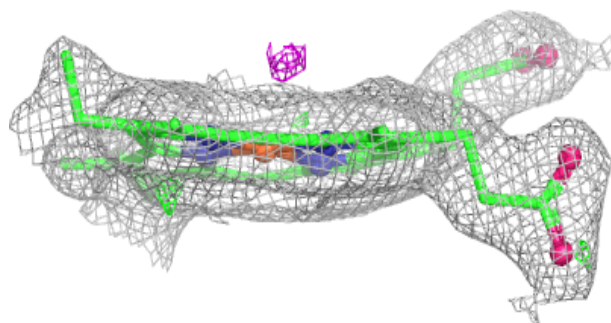
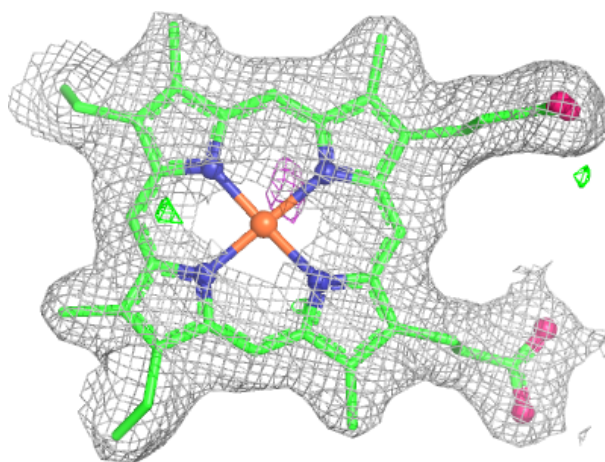
Electron density around HEM e 102:

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



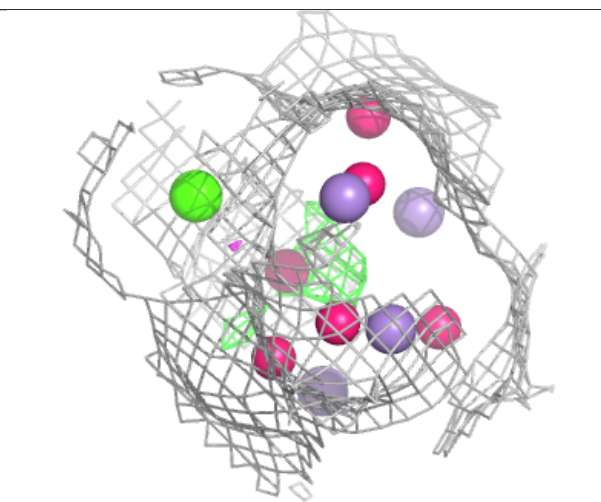
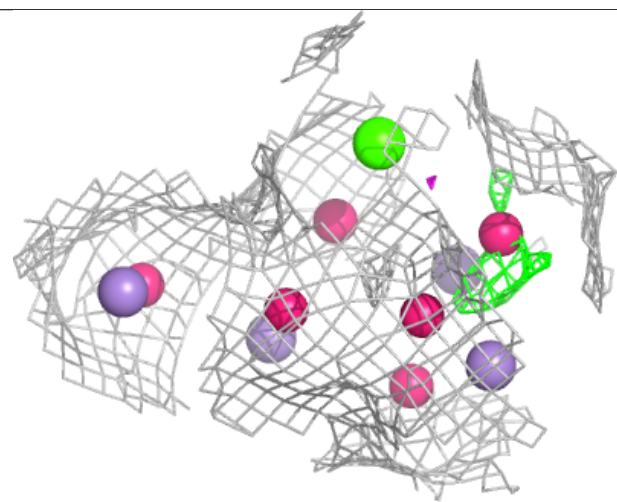
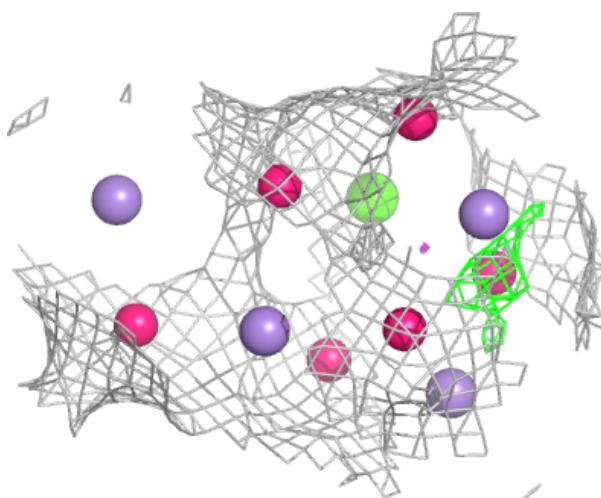
Electron density around HEC v 201:

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



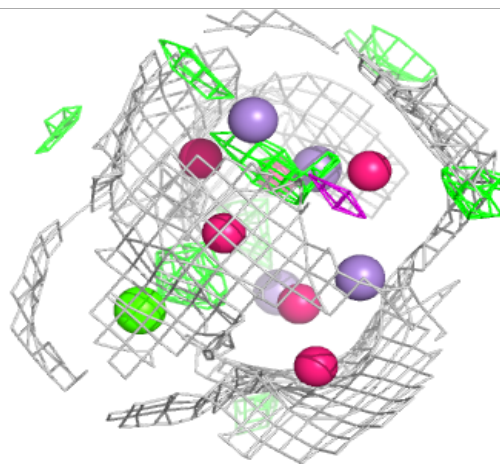
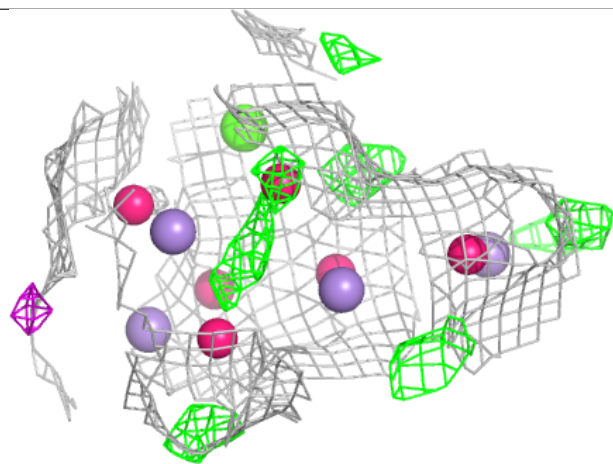
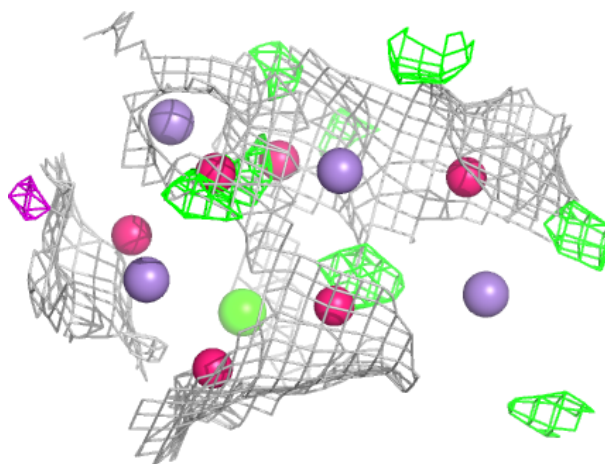
Electron density around OEY A 601 (B):

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



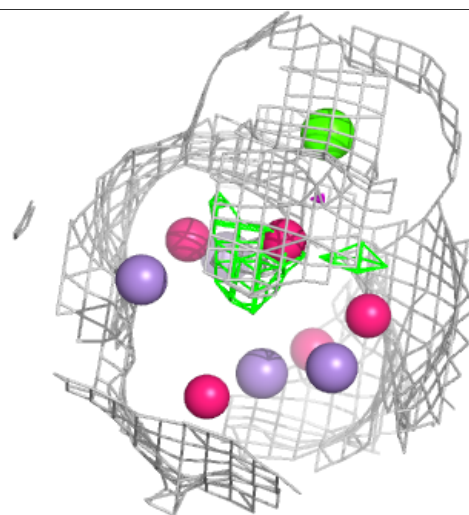
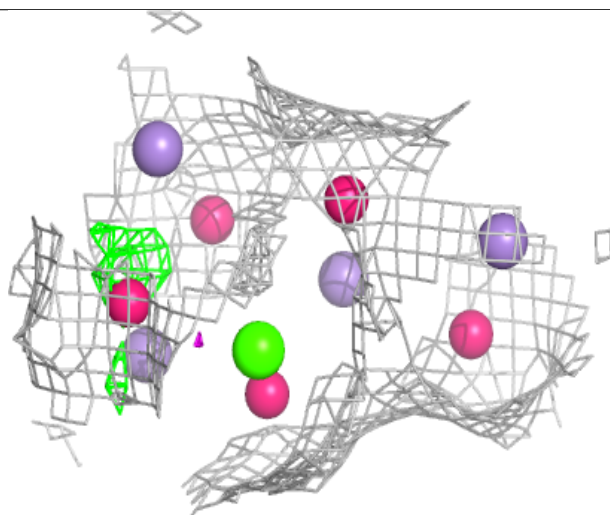
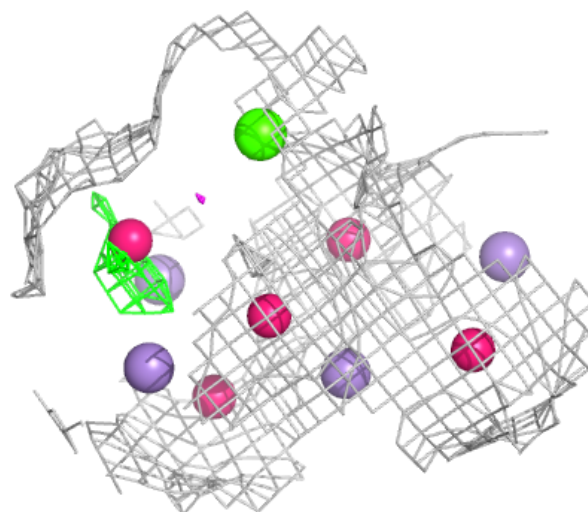
Electron density around OEY a 601 (B):

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



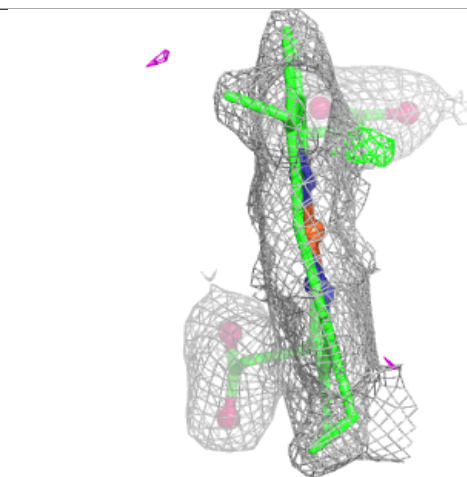
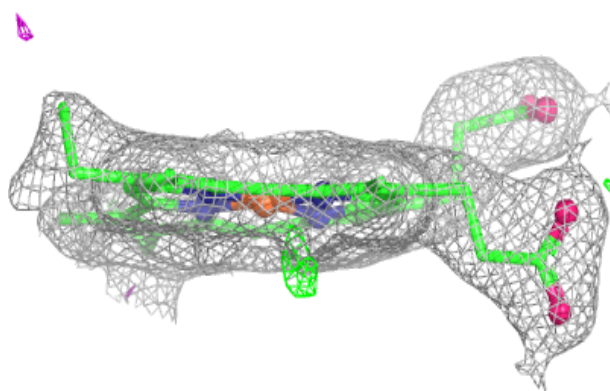
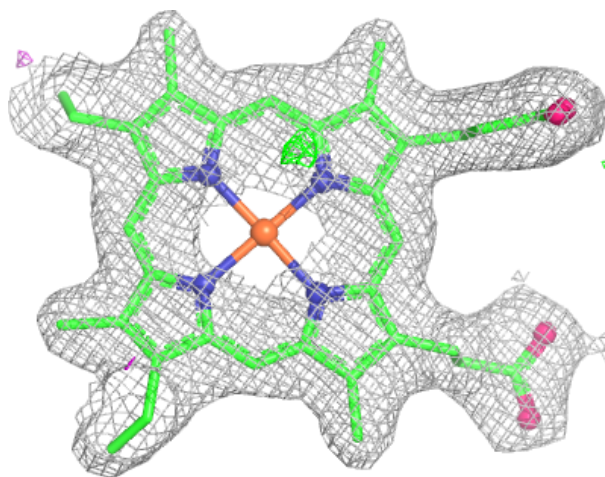
Electron density around OEX A 602 (A):

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



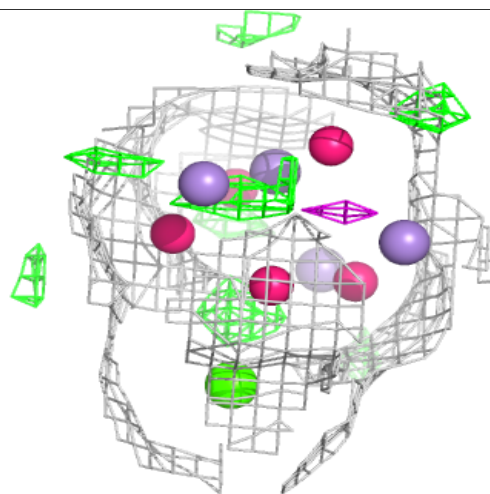
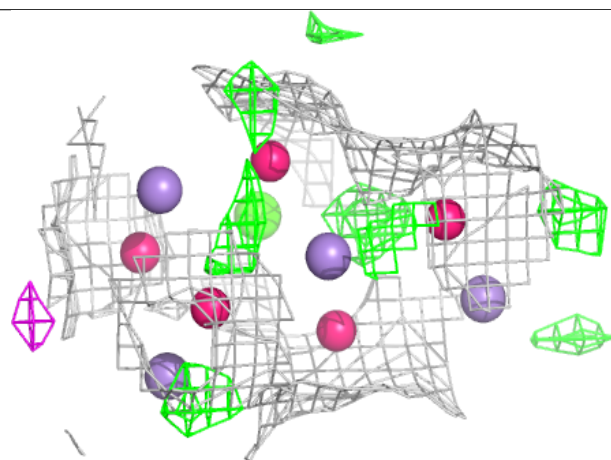
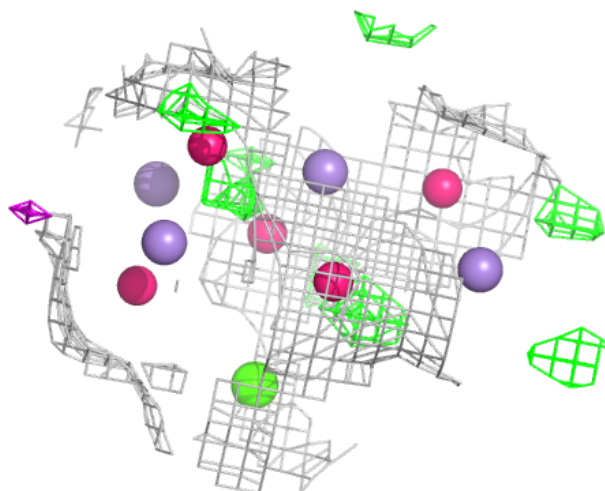
Electron density around HEC V 201:

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



Electron density around OEX a 602 (A):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.