



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 01:47 AM EDT

PDB ID : 6W1O / pdb_00006w1o
Title : RT XFEL structure of the dark-stable state of Photosystem II (0F, S1-rich) at 2.08 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.08 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)

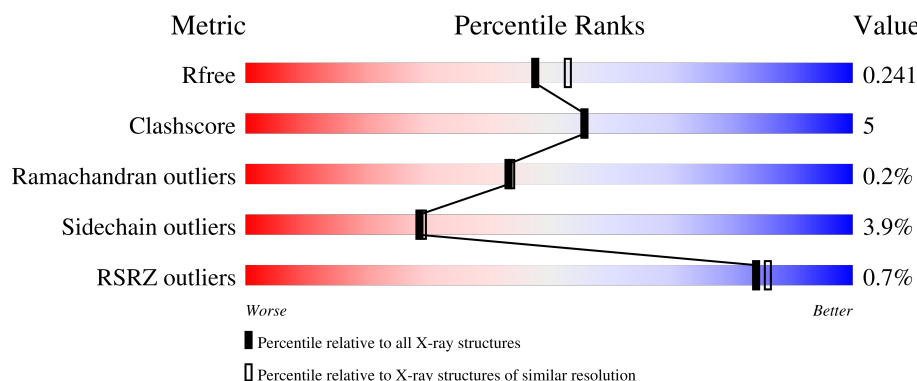
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

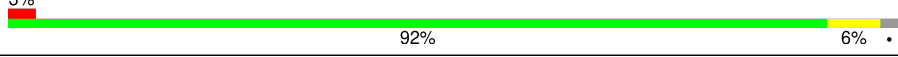
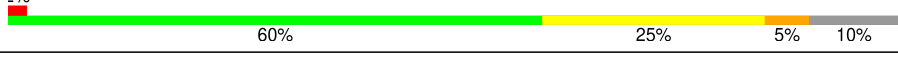
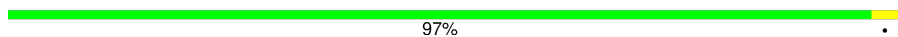
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	334	 88% 12%
1	a	334	 89% 11%

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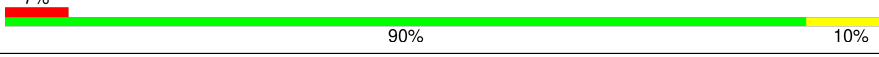
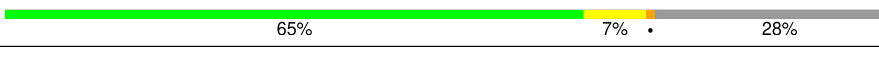
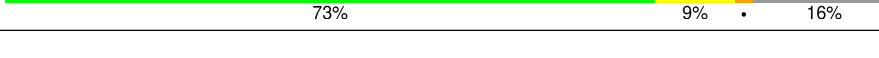
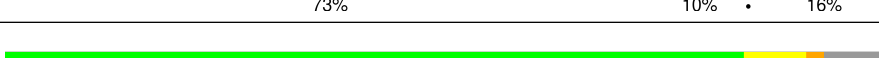
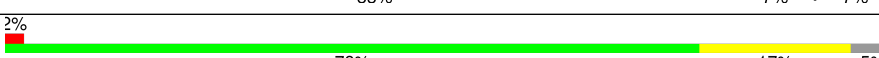
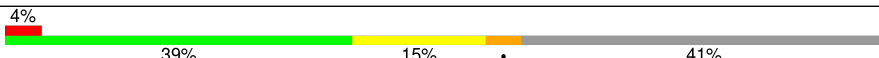
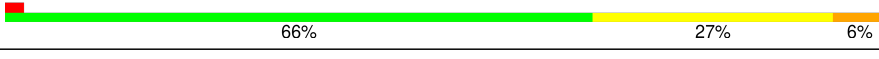
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	B	506	
2	b	506	
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	R	40	

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Mol	Chain	Length	Quality of chain
14	r	40	
15	T	30	
15	t	30	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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
34	HEC	F	102	X	-	-	-
34	HEC	V	201	X	-	-	-
34	HEC	f	101	X	-	-	-
34	HEC	v	201	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 103895 atoms, of which 51610 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6768	2249	3342	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6913	2290	3413	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		

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

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

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

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

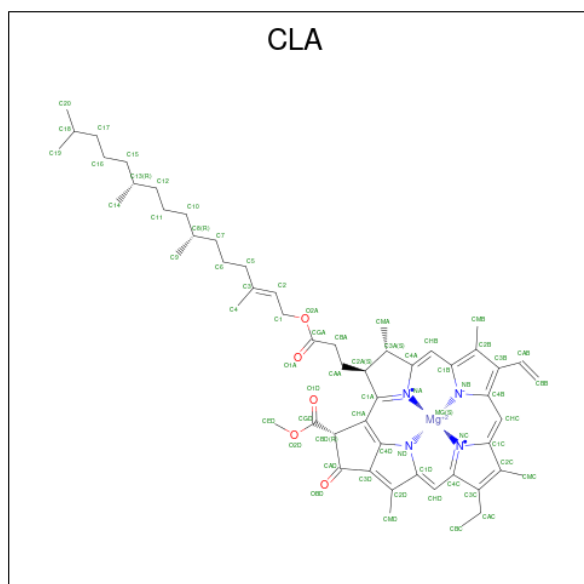
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		

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

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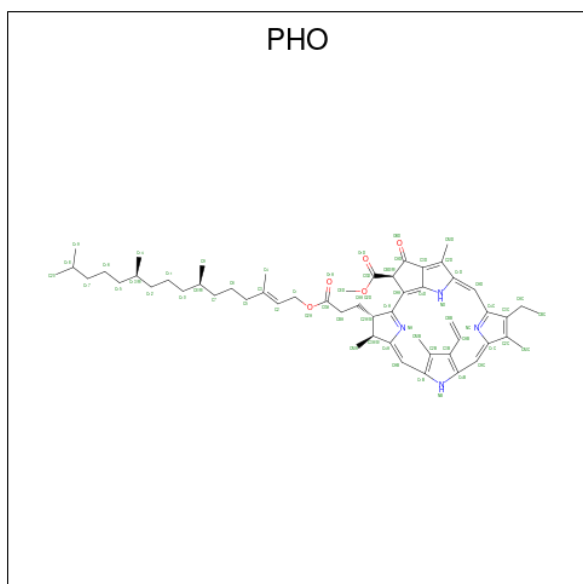
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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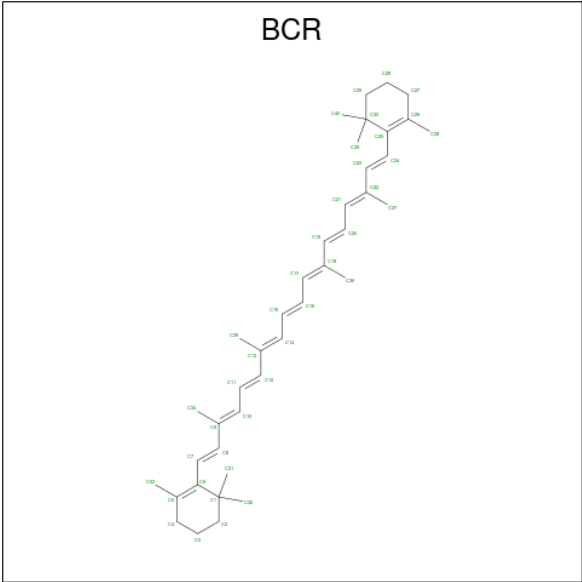
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	C	1	Total	C	H	0	0
			96	40	56		
24	F	1	Total	C	H	0	0
			96	40	56		
24	H	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	T	1	Total	C	H	0	0
			96	40	56		
24	a	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		

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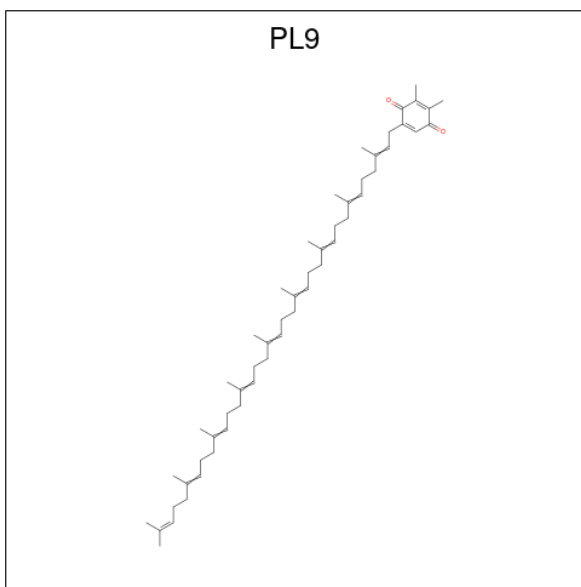
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

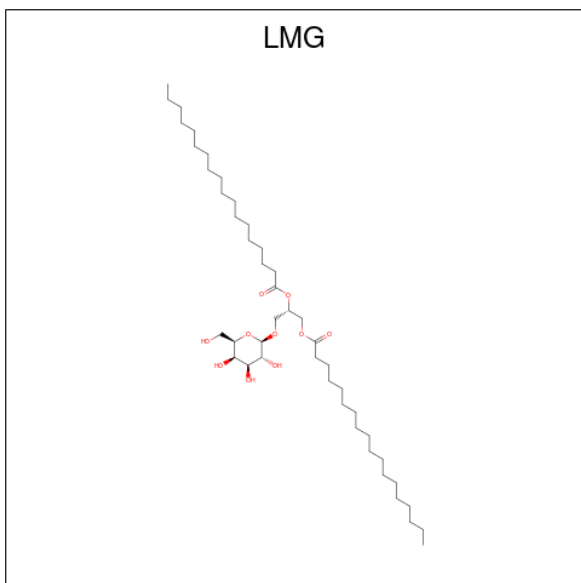
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 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) (labeled as "Ligand of Interest" by depositor).



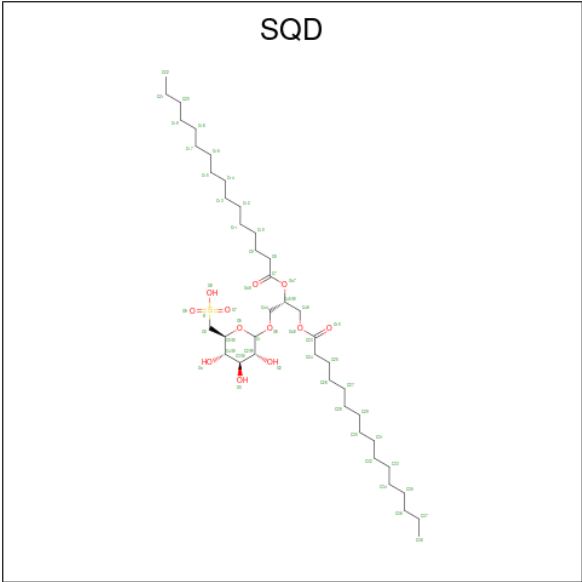
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



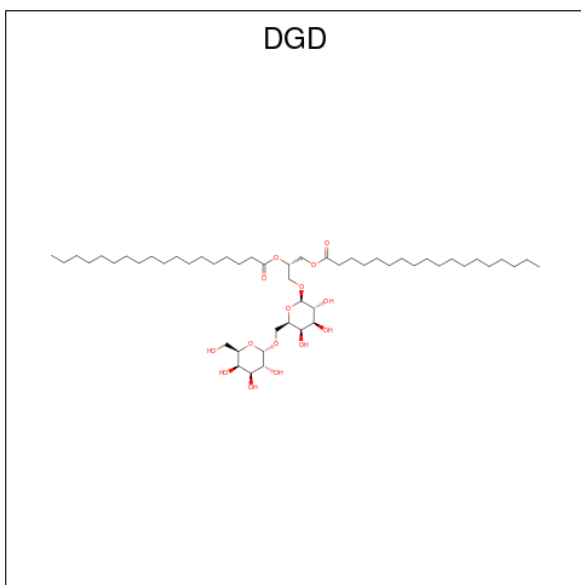
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	Y	1	Total	C	H	O	0	0
			114	38	66	10		
27	a	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



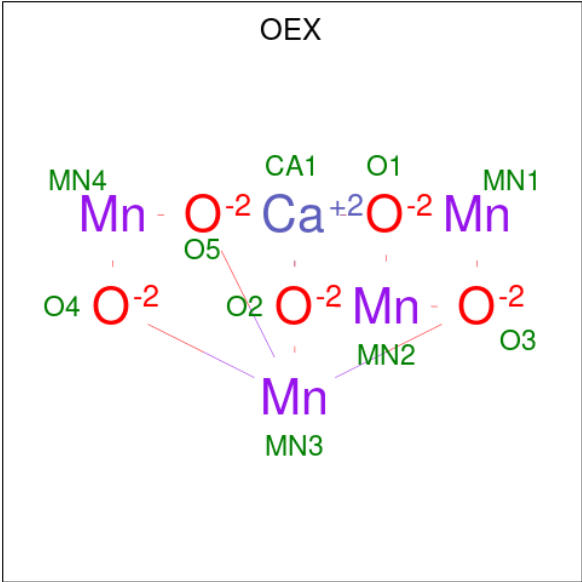
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
28	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



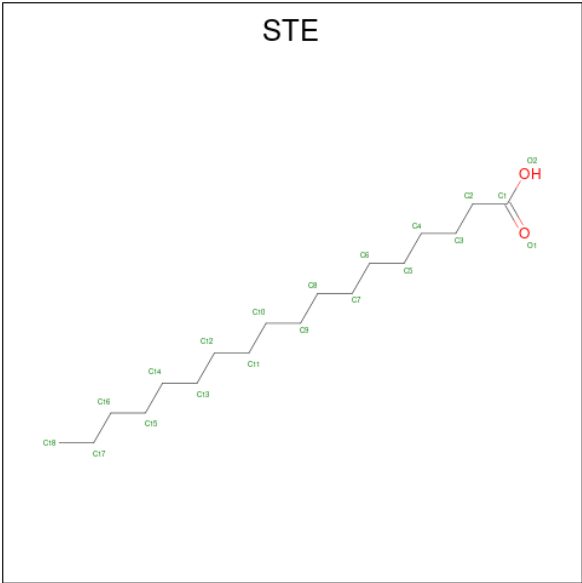
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 31 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			43	15	26	2		

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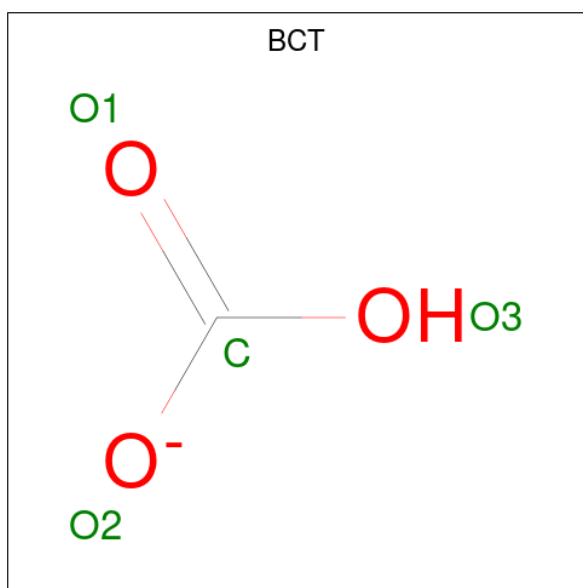
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C H O 34 12 20 2	0	0
31	B	1	Total C H O 28 10 16 2	0	0
31	B	1	Total C H O 46 16 28 2	0	0
31	B	1	Total C H 47 16 31	0	0
31	B	1	Total C H 41 15 26	0	0
31	C	1	Total C H O 28 10 16 2	0	0
31	C	1	Total C H 47 16 31	0	0
31	C	1	Total C H O 28 10 16 2	0	0
31	D	1	Total C H O 55 18 35 2	0	0
31	E	1	Total C H O 28 10 16 2	0	0
31	H	1	Total C H 53 18 35	0	0
31	I	1	Total C H 41 15 26	0	0
31	J	1	Total C H O 28 10 16 2	0	0
31	M	1	Total C H O 37 13 22 2	0	0
31	M	1	Total C H 26 10 16	0	0
31	T	1	Total C H 44 15 29	0	0
31	Z	1	Total C H 20 8 12	0	0
31	a	1	Total C H 26 10 16	0	0
31	a	1	Total C H O 28 10 16 2	0	0
31	b	1	Total C H 47 16 31	0	0
31	b	1	Total C H O 55 18 35 2	0	0

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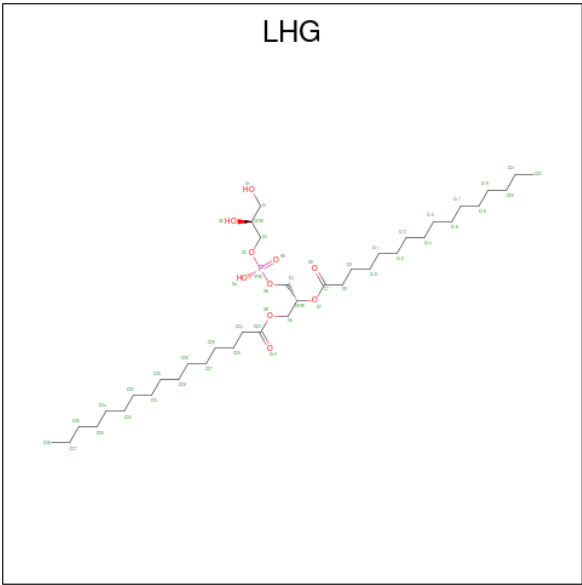
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H 26 10 16	0	0
31	b	1	Total C H 41 14 27	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	c	1	Total C H O 28 10 16 2	0	0
31	c	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 40 14 24 2	0	0
31	d	1	Total C H O 43 15 26 2	0	0
31	d	1	Total C H O 55 18 35 2	0	0
31	j	1	Total C H O 28 10 16 2	0	0
31	m	1	Total C H 53 18 35	0	0
31	m	1	Total C H O 28 10 16 2	0	0

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



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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



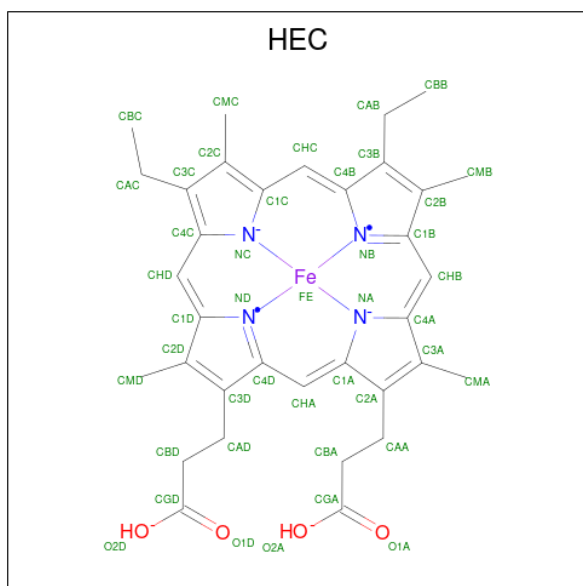
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	1	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	142	Total O 142 142	0	0
35	B	212	Total O 212 212	0	0
35	C	184	Total O 184 184	0	0
35	D	138	Total O 138 138	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	E	36	Total 36	O 36	0	0
35	F	8	Total 8	O 8	0	0
35	H	40	Total 40	O 40	0	0
35	I	24	Total 24	O 24	0	0
35	J	15	Total 15	O 15	0	0
35	K	7	Total 7	O 7	0	0
35	L	9	Total 9	O 9	0	0
35	M	11	Total 11	O 11	0	0
35	O	104	Total 104	O 104	0	0
35	R	4	Total 4	O 4	0	0
35	T	10	Total 10	O 10	0	0
35	U	52	Total 52	O 52	0	0
35	V	59	Total 59	O 59	0	0
35	X	15	Total 15	O 15	0	0
35	Y	5	Total 5	O 5	0	0
35	Z	6	Total 6	O 6	0	0
35	a	116	Total 116	O 116	0	0
35	b	201	Total 201	O 201	0	0
35	c	187	Total 187	O 187	0	0
35	d	115	Total 115	O 115	0	0
35	e	21	Total 21	O 21	0	0

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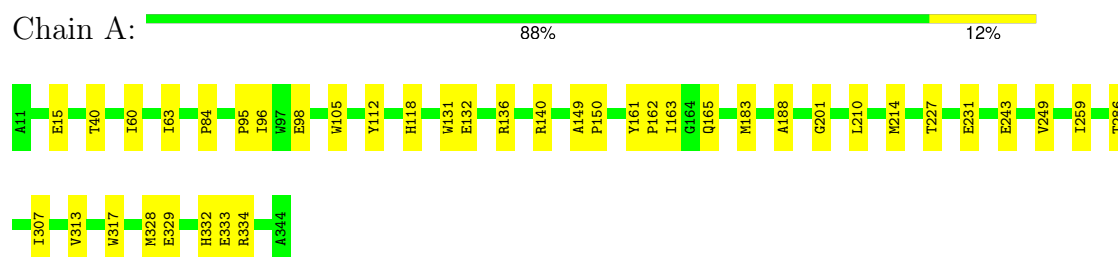
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	f	6	Total 6	O 6	0	0
35	h	31	Total 31	O 31	0	0
35	i	12	Total 12	O 12	0	0
35	j	6	Total 6	O 6	0	0
35	k	7	Total 7	O 7	0	0
35	l	5	Total 5	O 5	0	0
35	m	10	Total 10	O 10	0	0
35	o	86	Total 86	O 86	0	0
35	r	6	Total 6	O 6	0	0
35	t	9	Total 9	O 9	0	0
35	u	53	Total 53	O 53	0	0
35	v	62	Total 62	O 62	0	0
35	x	8	Total 8	O 8	0	0
35	y	4	Total 4	O 4	0	0
35	z	11	Total 11	O 11	0	0

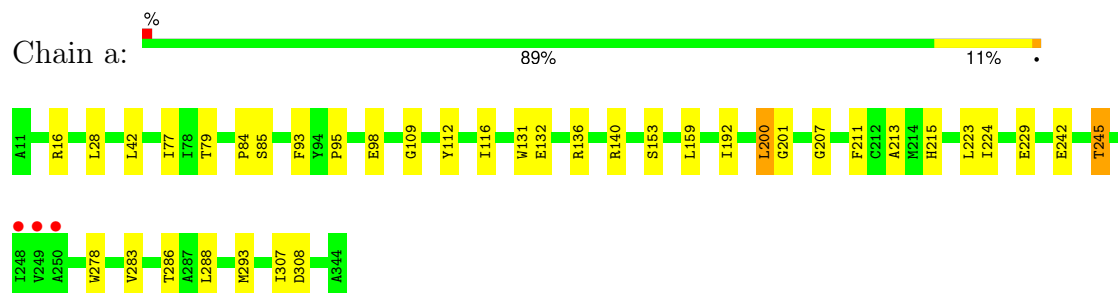
3 Residue-property plots [i](#)

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

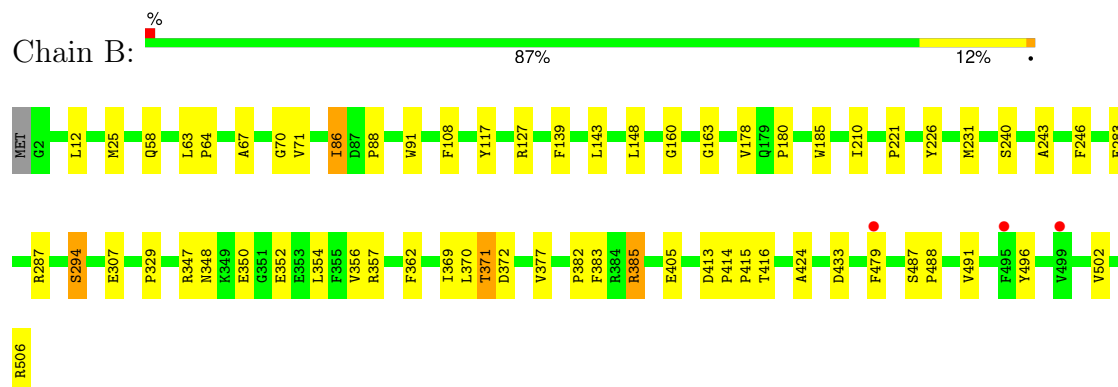
- Molecule 1: Photosystem II protein D1 1



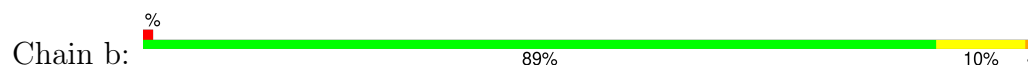
- Molecule 1: Photosystem II protein D1 1

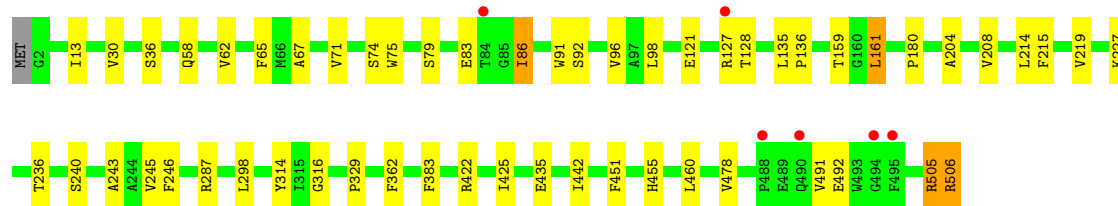


- Molecule 2: Photosystem II CP47 reaction center protein



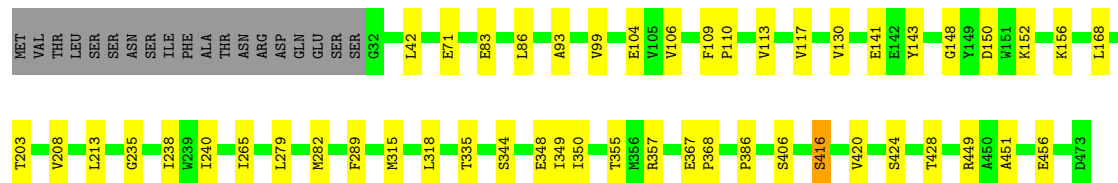
- Molecule 2: Photosystem II CP47 reaction center protein





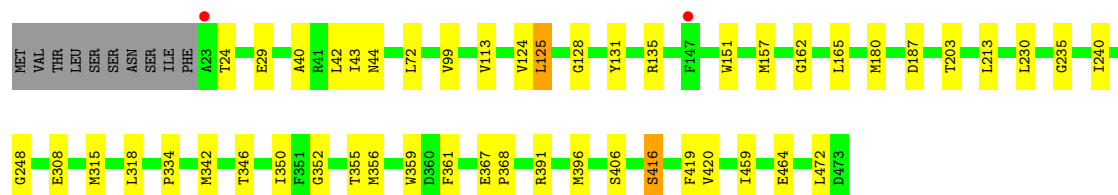
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 85% 11% •



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 10% •



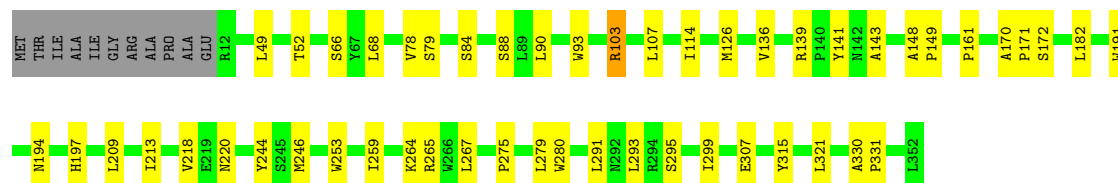
• Molecule 4: Photosystem II D2 protein

Chain D: 87% 9% • •

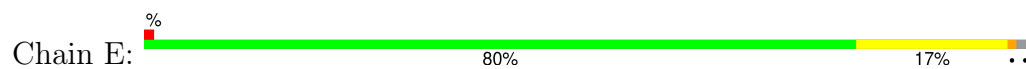


• Molecule 4: Photosystem II D2 protein

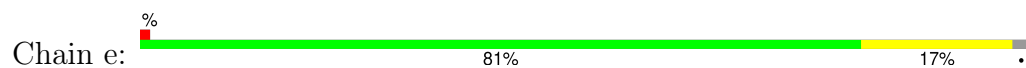
Chain d: 82% 14% •



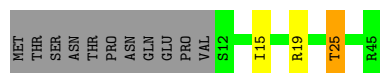
• Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



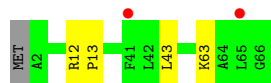
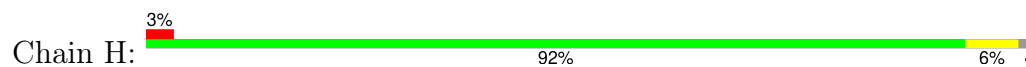
- Molecule 6: Cytochrome b559 subunit beta



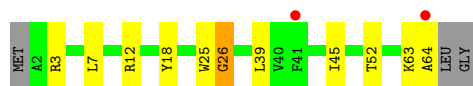
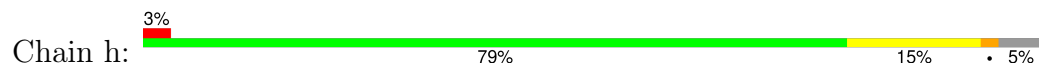
- Molecule 6: Cytochrome b559 subunit beta



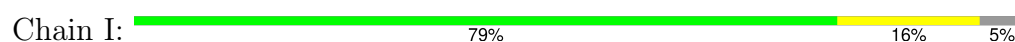
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

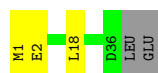


- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  87% 8% 5%



• Molecule 9: Photosystem II reaction center protein J

Chain J:  70% 18% 10%



• Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 60% 25% 5% 10%



• Molecule 10: Photosystem II reaction center protein K

Chain K:  65% 15% 20%

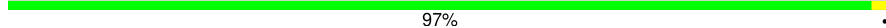


• Molecule 10: Photosystem II reaction center protein K

Chain k:  61% 20% 20%



• Molecule 11: Photosystem II reaction center protein L

Chain L:  97% 1% 2%



• Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 11% 3%



• Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 17% 8%



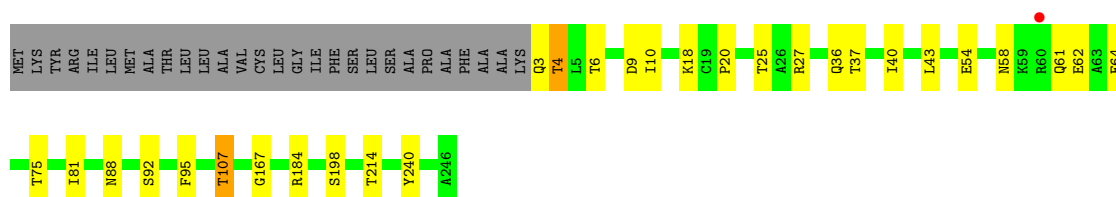
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 14% 11%



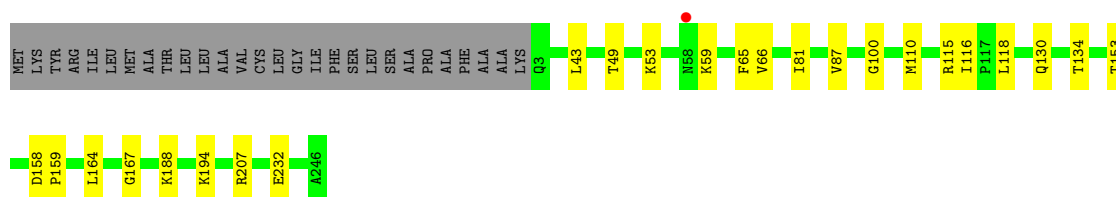
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  79% 10% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  81% 9% 10%



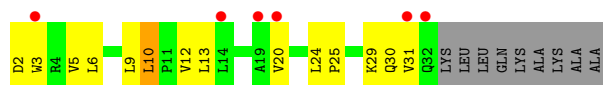
- Molecule 14: Photosystem II protein Y

Chain R:  5% 52% 32% 15%



- Molecule 14: Photosystem II protein Y

Chain r:  15% 42% 32% 22%



- Molecule 15: Photosystem II reaction center protein T

Chain T:  90% 7% •



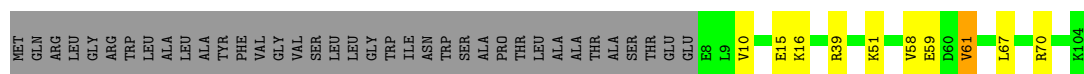
- Molecule 15: Photosystem II reaction center protein T

Chain t:  7% 90% 10%



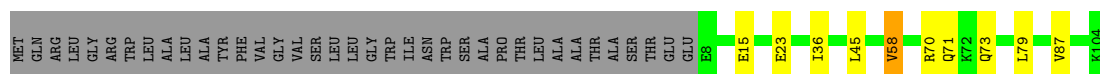
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:  65% 7% • 28%



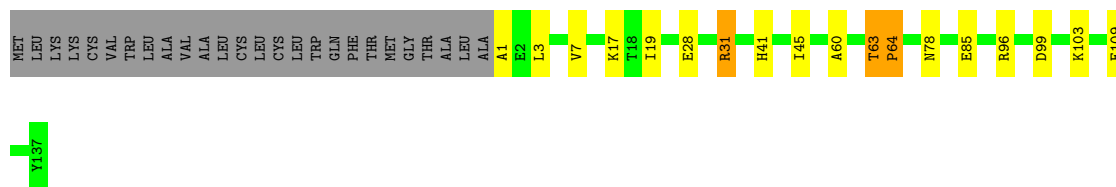
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  65% 7% • 28%



- Molecule 17: Cytochrome c-550

Chain V:  73% 9% • 16%



- Molecule 17: Cytochrome c-550

Chain v:  73% 10% • 16%

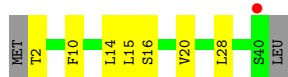
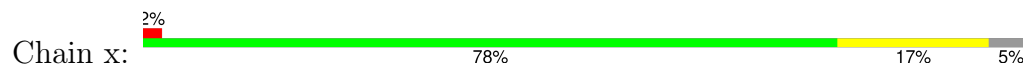


- Molecule 18: Photosystem II reaction center X protein

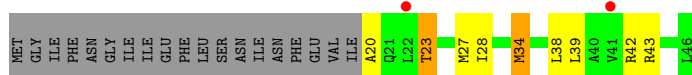
Chain X:  83% 7% • 7%



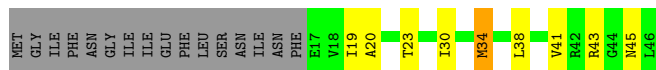
- Molecule 18: Photosystem II reaction center X protein



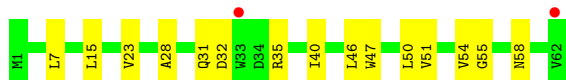
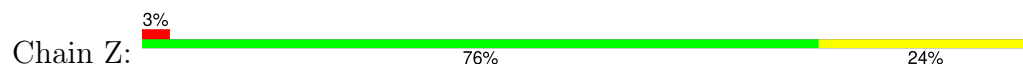
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 221.63Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 2.08 33.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.64-2.08) 85.0 (33.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.181 , 0.240 0.182 , 0.241	Depositor DCC
R_{free} test set	4226 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103895	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: HEC, OEX, FME, BCR, LMG, BCT, LHG, PL9, DGD, PHO, CLA, SQD, STE, FE2, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/2707	0.72	0/3692
1	a	0.61	0/2704	0.71	1/3688 (0.0%)
2	B	0.59	0/4161	0.66	0/5669
2	b	0.59	0/4118	0.67	0/5611
3	C	0.59	0/3547	0.68	0/4830
3	c	0.55	0/3619	0.63	0/4926
4	D	0.62	0/2812	0.70	0/3832
4	d	0.59	0/2821	0.69	0/3844
5	E	0.48	0/688	0.60	0/940
5	e	0.43	0/683	0.61	0/932
6	F	0.50	0/284	0.60	0/387
6	f	0.45	0/284	0.69	0/387
7	H	0.61	0/523	0.67	0/713
7	h	0.51	0/511	0.62	0/697
8	I	0.55	0/293	0.70	0/396
8	i	0.60	0/293	0.67	0/396
9	J	0.46	0/263	0.67	0/356
9	j	0.44	0/263	0.57	0/356
10	K	0.45	0/303	0.60	0/416
10	k	0.45	0/303	0.55	0/416
11	L	0.68	0/311	0.68	0/422
11	l	0.67	0/303	0.63	0/412
12	M	0.66	0/249	0.80	0/341
12	m	0.63	0/244	0.74	0/334
13	O	0.58	0/1904	0.67	0/2585
13	o	0.58	0/1905	0.67	0/2583
14	R	0.42	0/277	0.55	0/380
14	r	0.38	0/246	0.46	0/339
15	T	0.62	0/257	0.72	0/349
15	t	0.56	0/255	0.65	0/346
16	U	0.49	0/785	0.62	0/1064
16	u	0.58	0/785	0.67	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.59	0/1085	0.66	0/1473
17	v	0.51	0/1085	0.62	0/1473
18	X	0.44	0/284	0.61	0/384
18	x	0.35	0/289	0.48	0/391
19	Y	0.42	0/197	0.64	0/264
19	y	0.37	0/219	0.54	0/294
20	Z	0.37	0/490	0.53	0/669
20	z	0.35	0/488	0.49	0/666
All	All	0.57	0/42838	0.66	1/58317 (0.0%)

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
17	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	131	TRP	CA-CB-CG	-5.11	103.89	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	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	2622	2508	2519	26	0
1	a	2619	2499	2510	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4005	3859	3867	43	0
2	b	3978	3822	3836	30	0
3	C	3426	3342	3343	23	0
3	c	3500	3413	3426	28	0
4	D	2717	2613	2621	27	0
4	d	2723	2619	2627	34	0
5	E	666	650	651	12	0
5	e	664	647	648	11	0
6	F	275	281	282	3	0
6	f	275	281	282	10	0
7	H	510	532	532	3	0
7	h	498	518	518	5	0
8	I	296	311	311	3	0
8	i	296	311	311	1	0
9	J	257	268	268	6	0
9	j	257	268	268	10	0
10	K	293	305	305	3	0
10	k	293	305	305	5	0
11	L	304	316	316	1	0
11	l	296	304	304	0	0
12	M	256	269	269	4	0
12	m	251	267	267	2	0
13	O	1870	1828	1830	21	0
13	o	1874	1844	1846	13	0
14	R	271	298	298	5	0
14	r	240	253	250	8	0
15	T	258	261	261	3	0
15	t	256	256	256	2	0
16	U	774	772	773	5	0
16	u	774	772	773	5	0
17	V	1064	1068	1073	11	0
17	v	1064	1068	1073	11	0
18	X	281	312	312	2	0
18	x	286	316	314	3	0
19	Y	196	217	217	6	0
19	y	218	241	241	4	0
20	Z	479	516	516	7	0
20	z	477	509	509	12	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	3	0
22	B	970	1067	1067	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	839	922	922	8	0
22	D	195	216	216	6	0
22	H	65	72	72	2	0
22	a	260	288	288	4	0
22	b	1035	1139	1139	16	0
22	c	839	919	919	12	0
22	d	130	144	144	1	0
23	A	64	74	74	1	0
23	D	64	74	74	1	0
23	a	64	74	74	1	0
23	d	64	74	74	1	0
24	A	40	56	56	1	0
24	B	120	168	168	7	0
24	C	40	56	56	0	0
24	F	40	56	56	5	0
24	H	40	56	56	3	0
24	K	120	168	168	4	0
24	T	40	56	56	4	0
24	a	40	56	56	2	0
24	b	120	168	168	2	0
24	c	80	112	112	6	0
24	d	40	56	56	3	0
24	h	40	56	56	1	0
24	k	80	112	112	2	0
24	t	40	56	56	3	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	2	0
26	D	55	80	80	0	0
26	a	55	80	80	3	0
26	d	55	80	80	1	0
27	A	48	66	66	0	0
27	B	28	40	40	0	0
27	D	84	117	117	4	0
27	M	51	72	72	1	0
27	Y	48	66	66	0	0
27	a	55	86	86	2	0
27	b	106	158	158	1	0
27	c	134	181	181	1	0
27	d	44	58	58	0	0
28	A	91	136	134	3	0
28	B	54	78	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	36	46	45	0	0
28	L	49	65	65	0	0
28	a	90	134	133	1	0
28	f	41	48	48	1	0
29	A	66	96	96	1	0
29	C	186	246	246	1	0
29	H	62	82	82	1	0
29	c	186	245	241	3	0
29	h	62	82	81	0	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	B	104	163	163	2	0
31	C	40	63	63	0	0
31	D	20	35	35	0	0
31	E	12	16	16	0	0
31	H	18	35	35	0	0
31	I	15	26	26	0	0
31	J	12	16	16	0	0
31	M	25	38	38	0	0
31	T	15	29	29	0	0
31	Z	8	12	12	1	0
31	a	22	32	32	1	0
31	b	100	179	179	2	0
31	c	32	51	51	2	0
31	d	53	85	85	1	0
31	j	12	16	16	0	0
31	m	30	51	51	1	0
32	D	4	1	1	0	0
32	d	4	1	1	0	0
33	D	145	215	215	6	0
33	E	49	74	74	1	0
33	L	49	74	74	1	0
33	d	137	199	199	3	0
33	e	42	57	57	1	0
33	l	49	74	74	0	0
34	F	43	30	32	3	0
34	V	43	30	30	2	0
34	f	43	30	32	5	0
34	v	43	30	30	1	0
35	A	142	0	0	3	0
35	B	212	0	0	4	0
35	C	184	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	138	0	0	4	0
35	E	36	0	0	0	0
35	F	8	0	0	0	0
35	H	40	0	0	1	0
35	I	24	0	0	1	0
35	J	15	0	0	2	0
35	K	7	0	0	0	0
35	L	9	0	0	0	0
35	M	11	0	0	1	0
35	O	104	0	0	3	0
35	R	4	0	0	0	0
35	T	10	0	0	1	0
35	U	52	0	0	1	0
35	V	59	0	0	1	0
35	X	15	0	0	0	0
35	Y	5	0	0	0	0
35	Z	6	0	0	0	0
35	a	116	0	0	0	0
35	b	201	0	0	2	0
35	c	187	0	0	2	0
35	d	115	0	0	1	0
35	e	21	0	0	0	0
35	f	6	0	0	0	0
35	h	31	0	0	0	0
35	i	12	0	0	0	0
35	j	6	0	0	2	0
35	k	7	0	0	1	0
35	l	5	0	0	0	0
35	m	10	0	0	1	0
35	o	86	0	0	2	0
35	r	6	0	0	1	0
35	t	9	0	0	0	0
35	u	53	0	0	1	0
35	v	62	0	0	3	0
35	x	8	0	0	0	0
35	y	4	0	0	0	0
35	z	11	0	0	0	0
All	All	52285	51610	51694	478	0

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

All (478) 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)
13:O:27:ARG:NH1	35:O:301:HOH:O	2.09	0.85
3:c:391[B]:ARG:NE	35:c:602:HOH:O	2.15	0.80
5:e:30:LEU:HD11	34:f:101:HEC:HBB3	1.64	0.78
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.66	0.78
9:j:36:LEU:O	35:j:201:HOH:O	2.00	0.76
3:c:44:ASN:O	35:c:601:HOH:O	2.04	0.75
24:T:101:BCR:H321	24:T:101:BCR:HC8	1.70	0.74
34:F:102:HEC:HBC3	34:F:102:HEC:HHD	1.69	0.73
9:J:19:MET:O	9:J:23:VAL:HG23	1.88	0.73
2:B:86:ILE:HD12	2:B:88:PRO:HD3	1.69	0.73
5:e:30:LEU:HD11	34:f:101:HEC:CBB	2.21	0.71
16:U:58:VAL:O	16:U:61:VAL:HG22	1.91	0.70
9:J:15:THR:HG22	9:J:19:MET:HE2	1.71	0.70
20:z:34:ASP:O	20:z:38:GLN:NE2	2.25	0.70
17:V:109:GLU:OE1	35:V:301:HOH:O	2.10	0.69
20:z:1:MET:SD	20:z:1:MET:N	2.66	0.68
9:J:36:LEU:O	35:J:201:HOH:O	2.11	0.68
16:U:39:ARG:NH2	17:V:60:ALA:O	2.26	0.67
16:U:70:ARG:NH2	17:V:85:GLU:OE1	2.27	0.67
9:j:34:ALA:O	35:j:201:HOH:O	2.10	0.67
31:m:102:STE:O2	35:m:201:HOH:O	2.12	0.67
17:v:104:MET:HA	17:v:107:LEU:HD22	1.77	0.67
24:t:101:BCR:HC8	24:t:101:BCR:H311	1.76	0.66
13:o:194:LYS:NZ	35:o:301:HOH:O	2.27	0.66
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.31	0.66
8:I:36:ASP:OD1	35:I:201:HOH:O	2.13	0.66
4:d:126:MET:HE3	4:d:143:ALA:O	1.95	0.66
17:v:57:GLU:OE1	35:v:301:HOH:O	2.15	0.65
3:c:459:ILE:HG21	3:c:464:GLU:HG3	1.79	0.64
9:j:18:GLY:O	9:j:22:ILE:HD12	1.97	0.64
1:a:245:THR:HG22	4:d:265:ARG:NH2	2.13	0.63
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.32	0.63
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.80	0.63
4:d:267:LEU:C	4:d:267:LEU:HD23	2.23	0.63
5:E:68:ASP:O	5:E:72:ALA:HB2	2.00	0.62
6:f:19:ARG:NH2	34:f:101:HEC:O2D	2.32	0.62
7:H:63:LYS:NZ	35:H:201:HOH:O	2.32	0.62
13:O:88:ASN:OD1	13:O:92:SER:OG	2.18	0.61
28:A:412:SQD:H383	22:b:606:CLA:H93	1.82	0.61
10:k:46:ARG:NH2	35:k:201:HOH:O	2.30	0.61
13:O:107:THR:HG22	35:O:342:HOH:O	2.00	0.61
19:Y:23:THR:HG22	19:Y:27:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:405:BCR:H331	24:d:405:BCR:C8	2.30	0.61
3:C:148:GLY:O	3:C:156:LYS:NZ	2.34	0.61
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.82	0.61
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.82	0.61
2:B:371:THR:HG23	2:B:372:ASP:O	2.01	0.60
4:d:79:SER:HA	4:d:172:SER:HB3	1.83	0.60
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.84	0.60
6:f:24:HIS:O	6:f:28:VAL:HG13	2.02	0.59
26:A:409:PL9:H361	6:F:25:THR:HG21	1.85	0.59
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.03	0.59
15:T:15:ALA:HB2	24:T:101:BCR:H14C	1.83	0.59
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.85	0.59
2:B:506:ARG:NH1	35:B:707:HOH:O	2.32	0.58
2:b:127:ARG:NH1	7:h:18:TYR:O	2.35	0.58
2:B:413:ASP:OD1	35:B:701:HOH:O	2.16	0.58
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.39	0.58
14:R:16:ALA:O	14:R:20:VAL:HG23	2.03	0.58
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.85	0.57
20:z:38:GLN:O	20:z:42:LEU:HD22	2.04	0.57
16:U:10:VAL:HG21	16:U:15:GLU:OE2	2.04	0.57
22:b:615:CLA:HHC	22:b:615:CLA:HBB1	1.87	0.56
3:C:143:TYR:CE2	22:C:513:CLA:HED3	2.40	0.56
20:z:32:ASP:N	20:z:32:ASP:OD1	2.37	0.56
22:c:502:CLA:H192	22:c:508:CLA:HBB1	1.87	0.56
22:B:604:CLA:HBD	22:B:605:CLA:H43	1.88	0.56
3:C:203:THR:O	3:C:235:GLY:HA3	2.05	0.56
20:z:10:ALA:O	20:z:14:ILE:HD13	2.06	0.56
24:K:101:BCR:H331	24:K:101:BCR:C8	2.34	0.56
2:b:121:GLU:OE1	7:h:12:ARG:NH1	2.40	0.55
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.55
24:K:102:BCR:H321	24:K:102:BCR:HC8	1.88	0.55
3:C:318:LEU:C	3:C:318:LEU:HD23	2.32	0.55
12:M:6:LEU:HA	35:M:204:HOH:O	2.07	0.55
34:F:102:HEC:HBB2	34:F:102:HEC:HMB3	1.89	0.54
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.40	0.54
5:e:14:ILE:O	5:e:20:TRP:NE1	2.40	0.54
22:H:101:CLA:H92	24:H:102:BCR:H21C	1.89	0.54
3:c:342:MET:SD	3:c:356:MET:HE2	2.48	0.54
9:j:18:GLY:O	9:j:21:VAL:HG12	2.07	0.54
1:A:63:ILE:HB	3:C:335:THR:HG21	1.88	0.54
4:d:49:LEU:HD13	24:d:405:BCR:C15	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D:412:LHG:H152	33:L:102:LHG:H281	1.91	0.53
16:U:16:LYS:NZ	35:U:201:HOH:O	2.11	0.53
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.91	0.53
24:H:102:BCR:H331	24:H:102:BCR:C8	2.39	0.52
4:D:279:LEU:HD22	23:D:401:PHO:HBC3	1.91	0.52
34:F:102:HEC:HHD	34:F:102:HEC:CBC	2.39	0.52
2:b:92:SER:O	2:b:96:VAL:HG23	2.10	0.52
27:b:621:LMG:O10	12:m:4:ASN:ND2	2.40	0.52
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.91	0.52
17:V:63:THR:HG22	17:V:64:PRO:CD	2.40	0.52
13:o:164:LEU:HD13	13:o:188:LYS:O	2.09	0.52
22:C:502:CLA:H61	22:C:512:CLA:H42	1.92	0.52
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.45	0.52
13:O:64:GLU:OE1	13:O:64:GLU:N	2.36	0.52
4:D:272:LEU:C	4:D:272:LEU:HD23	2.35	0.52
1:a:215:HIS:ND1	26:a:409:PL9:O1	2.30	0.52
5:e:26:THR:HB	34:f:101:HEC:HBB2	1.92	0.51
2:B:117:TYR:HA	11:L:1:MET:HE1	1.91	0.51
3:c:42:LEU:HD21	22:c:512:CLA:H2A	1.93	0.51
19:y:41:VAL:C	19:y:43:ARG:H	2.18	0.51
3:c:151:TRP:HA	3:c:157:MET:HE3	1.92	0.51
1:A:201:GLY:HA3	1:A:286:THR:HB	1.93	0.51
24:B:618:BCR:H331	24:B:618:BCR:C8	2.40	0.51
27:D:411:LMG:O4	35:D:501:HOH:O	2.18	0.51
10:k:25:LEU:N	10:k:26:PRO:CD	2.74	0.51
22:B:613:CLA:HBB1	22:B:613:CLA:HMB1	1.93	0.51
4:D:269:PHE:CD2	33:D:412:LHG:HC12	2.45	0.51
10:K:25:LEU:N	10:K:26:PRO:HD2	2.26	0.50
13:o:110:MET:HE2	13:o:116:ILE:CG1	2.42	0.50
5:e:17:VAL:HG23	9:j:7:ARG:HD3	1.94	0.50
27:M:101:LMG:HC71	27:M:101:LMG:O9	2.10	0.50
17:V:63:THR:HG22	17:V:64:PRO:HD2	1.93	0.50
20:Z:51:VAL:O	20:Z:54:VAL:O	2.29	0.50
24:B:619:BCR:H331	24:B:619:BCR:C8	2.41	0.50
22:C:512:CLA:H72	22:C:512:CLA:H41	1.94	0.50
3:c:187:ASP:HB2	3:c:230:LEU:HD12	1.94	0.50
2:B:294:SER:O	2:B:294:SER:OG	2.28	0.49
13:O:27:ARG:O	13:O:27:ARG:HG2	2.11	0.49
34:f:101:HEC:HBC2	34:f:101:HEC:HMC3	1.94	0.49
2:B:91:TRP:HE1	31:B:620:STE:H32	1.78	0.49
3:C:109:PHE:N	3:C:110:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:442:ILE:HD12	4:d:299:ILE:HG12	1.93	0.49
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.95	0.49
3:C:424:SER:O	3:C:428:THR:HG23	2.13	0.49
5:E:53:ASP:O	17:V:1:ALA:N	2.46	0.49
10:K:13:GLU:OE2	10:K:13:GLU:N	2.46	0.49
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.49
3:c:131:TYR:OH	22:c:514:CLA:HED2	2.12	0.49
1:A:183:MET:HE2	22:D:403:CLA:HMC1	1.94	0.49
22:B:606:CLA:H72	24:B:619:BCR:H311	1.94	0.49
24:d:405:BCR:H402	9:j:21:VAL:HG21	1.94	0.49
24:t:101:BCR:H23C	24:t:101:BCR:H382	1.94	0.49
4:D:59:TYR:O	5:E:65:LEU:HD12	2.13	0.49
34:V:201:HEC:HMC1	34:V:201:HEC:HBC3	1.94	0.49
2:b:65:PHE:HE2	22:b:604:CLA:HED2	1.78	0.49
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.49
18:x:16:SER:O	18:x:20:VAL:HG23	2.12	0.49
1:a:200:LEU:HD13	29:c:519:DGD:CCA	2.42	0.48
3:c:318:LEU:C	3:c:318:LEU:HD23	2.38	0.48
13:o:110:MET:HE2	13:o:116:ILE:HG13	1.95	0.48
19:y:34:MET:HE3	19:y:34:MET:HA	1.95	0.48
2:B:348:ASN:HB3	2:B:354:LEU:HD11	1.95	0.48
17:V:41:HIS:HA	17:V:45:ILE:O	2.13	0.48
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.96	0.48
20:Z:23:VAL:HG22	20:Z:40:ILE:HD12	1.95	0.48
2:B:487:SER:OG	2:B:488:PRO:HD2	2.14	0.48
2:B:357:ARG:NE	35:B:708:HOH:O	2.35	0.48
23:A:404:PHO:HMB3	23:A:404:PHO:HBB1	1.95	0.48
13:O:27:ARG:HG3	13:O:27:ARG:HH11	1.78	0.48
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.49	0.48
4:d:170:ALA:HB1	4:d:171:PRO:CD	2.44	0.48
1:a:132:GLU:O	1:a:136:ARG:HG2	2.14	0.47
4:d:194:ASN:HA	4:d:295:SER:OG	2.14	0.47
5:e:8:ARG:NH2	5:e:12:ASP:OD2	2.47	0.47
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.49	0.47
3:C:42:LEU:HD21	22:C:511:CLA:H2A	1.95	0.47
4:D:246:MET:HE2	4:D:246:MET:HA	1.95	0.47
9:J:20:GLY:O	9:J:24:ILE:HG13	2.14	0.47
4:D:198:MET:SD	22:D:404:CLA:HED2	2.55	0.47
33:D:409:LHG:H321	15:T:21:ILE:HD11	1.97	0.47
6:f:37:ILE:HG22	9:j:28:PHE:CE1	2.49	0.47
4:D:12:ARG:NH1	35:D:512:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:308:ASP:OD1	1:a:308:ASP:C	2.58	0.47
1:A:210:LEU:HD23	1:A:214:MET:HG2	1.96	0.47
3:C:113:VAL:O	3:C:117:VAL:HG23	2.14	0.47
24:F:101:BCR:H392	24:F:101:BCR:H23C	1.96	0.47
22:c:506:CLA:HBC2	24:c:516:BCR:H341	1.97	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.44	0.47
15:T:25:GLU:OE2	35:T:201:HOH:O	2.20	0.47
1:a:153:SER:HB3	22:a:402:CLA:H43	1.96	0.47
22:b:605:CLA:HHC	22:b:605:CLA:HBB1	1.97	0.47
22:b:615:CLA:H121	22:b:615:CLA:H91	1.97	0.47
2:B:185:TRP:HB3	22:H:101:CLA:HMA3	1.97	0.47
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.97	0.47
29:A:413:DGD:HD5	2:b:75:TRP:HB3	1.96	0.47
1:a:213:ALA:HB2	4:d:275:PRO:HG2	1.97	0.47
2:b:287:ARG:NH1	35:b:701:HOH:O	2.22	0.47
20:Z:47:TRP:CE3	31:Z:101:STE:H142	2.49	0.47
24:t:101:BCR:H311	24:t:101:BCR:C8	2.43	0.47
3:C:203:THR:HG21	3:C:208:VAL:HG11	1.96	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	1.97	0.46
33:D:412:LHG:H221	12:M:18:PRO:HG3	1.96	0.46
9:J:5:GLY:N	35:J:204:HOH:O	2.48	0.46
1:a:283:VAL:HA	1:a:286:THR:HG22	1.97	0.46
22:b:601:CLA:CHA	22:b:601:CLA:HBA2	2.43	0.46
17:v:87:GLU:CD	17:v:96:ARG:HH12	2.22	0.46
22:c:504:CLA:H203	22:c:511:CLA:HAB	1.98	0.46
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.97	0.46
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.96	0.46
6:f:19:ARG:O	6:f:23:VAL:HG13	2.14	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.50	0.46
2:B:67:ALA:HA	2:B:71:VAL:O	2.15	0.46
2:B:413:ASP:OD1	2:B:416:THR:HB	2.16	0.46
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.51	0.46
24:c:516:BCR:H331	24:c:516:BCR:C8	2.45	0.46
6:f:21:VAL:O	6:f:25:THR:HG23	2.16	0.46
2:B:382:PRO:HG2	2:B:385:ARG:HD2	1.97	0.46
22:b:615:CLA:H143	22:b:616:CLA:HMA2	1.96	0.46
13:O:3:GLN:O	13:O:4:THR:HG23	2.16	0.46
4:d:246:MET:HE3	4:d:264:LYS:CG	2.46	0.46
31:B:627:STE:H62	31:a:413:STE:C1	2.46	0.46
9:j:9:PRO:HG2	9:j:12:ILE:HD12	1.96	0.46
19:y:20:ALA:O	19:y:23:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LEU:N	2:B:64:PRO:HD2	2.30	0.46
13:O:184:ARG:NE	35:O:310:HOH:O	2.48	0.46
19:Y:34:MET:O	19:Y:38:LEU:HG	2.16	0.46
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.96	0.46
1:A:161:TYR:N	1:A:162:PRO:CD	2.79	0.45
6:F:15:ILE:HD13	14:R:23:ILE:HD11	1.98	0.45
26:a:409:PL9:H453	18:x:28:LEU:HD21	1.98	0.45
3:C:71:GLU:HB3	3:C:86:LEU:HD22	1.98	0.45
22:D:405:CLA:H42	7:H:43:LEU:HD11	1.99	0.45
12:M:24:ILE:HG12	12:m:24:ILE:HG13	1.98	0.45
22:B:614:CLA:H141	22:B:614:CLA:H161	1.83	0.45
24:B:617:BCR:H20C	24:B:617:BCR:H361	1.81	0.45
5:E:8:ARG:O	6:F:19:ARG:NH2	2.32	0.45
14:r:24:LEU:N	14:r:25:PRO:HD2	2.30	0.45
22:C:501:CLA:HHC	22:C:501:CLA:HBB1	1.99	0.45
31:c:521:STE:H51	31:c:521:STE:O2	2.16	0.45
10:k:18:PHE:HE2	20:z:13:VAL:HG21	1.81	0.45
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.97	0.45
22:a:402:CLA:H143	23:a:404:PHO:H61	1.99	0.45
28:A:411:SQD:H381	9:J:22:ILE:HD11	1.98	0.45
1:a:286:THR:HG23	22:a:402:CLA:HED3	1.98	0.45
7:h:63:LYS:O	7:h:64:ALA:HB2	2.17	0.45
13:o:115:ARG:NH1	35:o:303:HOH:O	2.39	0.45
35:A:582:HOH:O	13:O:107:THR:HG21	2.17	0.45
14:R:27:ALA:O	14:R:31:VAL:HG23	2.16	0.45
34:V:201:HEC:HBC3	34:V:201:HEC:CMC	2.47	0.45
14:r:2:ASP:HB3	14:r:5:VAL:HG23	1.98	0.45
2:B:347:ARG:HA	2:B:352:GLU:O	2.17	0.45
2:B:377:VAL:HG11	4:D:342:PRO:HG3	1.99	0.45
5:E:65:LEU:O	5:E:67:THR:HG23	2.17	0.45
1:A:334:ARG:HD3	4:D:320:LEU:HD13	1.98	0.45
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.88	0.45
2:b:215:PHE:CE1	2:b:219:VAL:HG21	2.52	0.45
17:v:40:CYS:SG	34:v:201:HEC:HMC1	2.57	0.45
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.52	0.44
2:B:160:GLY:HA2	2:B:163:GLY:O	2.17	0.44
2:B:496:TYR:N	2:B:496:TYR:CD1	2.85	0.44
24:a:406:BCR:C8	24:a:406:BCR:H331	2.47	0.44
20:Z:55:GLY:HA2	20:Z:58:ASN:CB	2.48	0.44
14:r:2:ASP:OD1	14:r:3:TRP:N	2.49	0.44
3:c:203:THR:O	3:c:235:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:460:LEU:HG	4:d:280:TRP:HZ3	1.81	0.44
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.52	0.44
5:e:25:ILE:HD12	5:e:25:ILE:N	2.32	0.44
14:r:29:LYS:O	14:r:31:VAL:N	2.51	0.44
17:v:76:MET:HE1	17:v:112:LEU:HA	2.00	0.44
20:z:3:ILE:O	20:z:7:LEU:HD23	2.17	0.44
3:c:131:TYR:HH	22:c:514:CLA:HED2	1.83	0.44
3:C:168:LEU:HD21	22:C:509:CLA:H61	1.99	0.44
4:D:201:VAL:HG11	22:D:404:CLA:C3D	2.47	0.44
2:b:91:TRP:HE1	31:b:622:STE:H111	1.83	0.44
5:E:9:PRO:O	5:E:13:ILE:HG13	2.18	0.44
22:c:514:CLA:CHC	24:c:515:BCR:H383	2.48	0.44
4:d:246:MET:HE2	4:d:246:MET:HA	2.00	0.44
19:Y:39:LEU:HD21	20:Z:28:ALA:HB3	2.00	0.44
16:u:87:VAL:HG23	35:u:241:HOH:O	2.18	0.44
2:B:221:PRO:HA	22:B:609:CLA:HED3	1.99	0.44
2:B:502:VAL:HG22	2:B:502:VAL:O	2.18	0.44
4:D:295:SER:O	4:D:295:SER:OG	2.27	0.44
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.32	0.44
2:b:135:LEU:N	2:b:136:PRO:CD	2.81	0.44
4:d:209:LEU:HD23	4:d:209:LEU:C	2.43	0.44
1:A:40:THR:O	1:A:118:HIS:HB3	2.18	0.43
13:O:58:ASN:HB3	35:b:705:HOH:O	2.18	0.43
4:d:52:THR:O	4:d:66:SER:HA	2.18	0.43
24:h:101:BCR:H331	24:h:101:BCR:C8	2.48	0.43
1:A:95:PRO:HD2	1:A:98:GLU:HG3	2.00	0.43
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.48	0.43
4:D:85:MET:HE1	5:E:72:ALA:HB2	2.00	0.43
22:a:410:CLA:O1A	22:a:410:CLA:H43	2.18	0.43
3:c:213:LEU:HD13	3:c:213:LEU:HA	1.90	0.43
3:c:391[B]:ARG:HG2	3:c:391[B]:ARG:HH21	1.83	0.43
22:c:505:CLA:H62	22:c:505:CLA:H41	1.90	0.43
13:O:27:ARG:NH1	13:O:27:ARG:HG3	2.34	0.43
22:b:614:CLA:H121	22:b:614:CLA:H91	2.00	0.43
24:k:102:BCR:H20C	24:k:102:BCR:H361	1.89	0.43
22:A:402:CLA:HBB1	22:A:402:CLA:HMB1	1.99	0.43
1:a:207:GLY:O	1:a:211:PHE:CD2	2.72	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.54	0.43
28:A:412:SQD:H383	22:b:606:CLA:C9	2.48	0.43
24:K:102:BCR:H10C	19:Y:28:ILE:HG23	1.99	0.43
13:O:6:THR:HG22	13:O:9:ASP:CG	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:409:PL9:H43	28:f:102:SQD:H291	2.01	0.43
3:c:125:LEU:HD13	24:c:515:BCR:H361	2.00	0.43
3:c:367:GLU:N	3:c:368:PRO:CD	2.82	0.43
14:r:20:VAL:O	14:r:24:LEU:HB2	2.19	0.43
22:A:402:CLA:H203	22:A:402:CLA:H162	1.83	0.43
22:B:608:CLA:H172	22:B:609:CLA:H193	1.99	0.43
22:B:613:CLA:H192	33:D:412:LHG:H201	2.01	0.43
27:D:411:LMG:HC71	35:D:522:HOH:O	2.19	0.43
17:V:99:ASP:N	17:V:99:ASP:OD1	2.51	0.43
4:d:93:TRP:CZ3	31:d:413:STE:H62	2.53	0.43
4:d:191:TRP:CZ2	4:d:197:HIS:HB2	2.53	0.43
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.49	0.43
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.07	0.43
17:v:41:HIS:HA	17:v:45:ILE:O	2.19	0.43
35:A:624:HOH:O	33:E:101:LHG:H281	2.17	0.43
2:B:479[A]:PHE:O	4:D:139:ARG:NH2	2.38	0.43
2:b:478:VAL:O	4:d:139:ARG:HG2	2.18	0.43
3:c:128:GLY:HA3	22:c:514:CLA:C3C	2.48	0.43
22:d:403:CLA:HBC3	22:d:403:CLA:HHD	2.01	0.43
8:i:18:LEU:HD23	8:i:18:LEU:HA	1.83	0.43
14:R:5:VAL:O	14:R:9:LEU:HG	2.19	0.43
2:b:36:SER:OG	24:b:618:BCR:H362	2.19	0.43
3:c:40:ALA:O	3:c:43:ILE:HD12	2.18	0.43
4:d:84:SER:O	5:e:69:ARG:HB2	2.19	0.43
14:r:3:TRP:CD1	14:r:3:TRP:C	2.97	0.43
17:v:90:GLU:HB2	35:v:331:HOH:O	2.18	0.43
1:a:200:LEU:HD13	29:c:519:DGD:HAW2	2.01	0.42
3:c:113:VAL:HG11	31:c:521:STE:H72	2.00	0.42
4:d:141:TYR:OH	33:d:407:LHG:O4	2.28	0.42
1:A:161:TYR:CZ	1:A:165:GLN:HG3	2.54	0.42
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.00	0.42
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.42
4:d:103:ARG:O	4:d:107:LEU:HG	2.19	0.42
7:h:25:TRP:O	7:h:26:GLY:C	2.62	0.42
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.54	0.42
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.42
24:F:101:BCR:H392	24:F:101:BCR:C23	2.49	0.42
1:a:85:SER:HA	1:a:109:GLY:HA3	2.02	0.42
28:a:411:SQD:H361	10:k:34:ALA:HB2	2.02	0.42
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.54	0.42
13:o:53:LYS:NZ	13:o:232:GLU:OE2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:ASP:OD1	2:B:433:ASP:C	2.62	0.42
3:C:150:ASP:OD1	3:C:152:LYS:N	2.45	0.42
22:D:405:CLA:HMB1	22:D:405:CLA:HBB1	2.01	0.42
27:D:407:LMG:H171	24:F:101:BCR:H382	2.02	0.42
13:O:20:PRO:HB2	13:O:240:TYR:CD2	2.55	0.42
1:a:112:TYR:O	1:a:116:ILE:HG12	2.19	0.42
2:b:79:SER:HB3	2:b:86:ILE:HG12	2.02	0.42
22:b:602:CLA:H43	7:h:45:ILE:HG22	2.01	0.42
5:e:27:ILE:HB	5:e:28:PRO:HD3	2.01	0.42
1:A:163:ILE:HD11	29:C:515:DGD:HA32	2.01	0.42
22:A:405:CLA:H41	22:A:405:CLA:H61	1.87	0.42
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.54	0.42
3:C:348:GLU:O	3:C:350:ILE:HG23	2.20	0.42
13:O:36:GLN:HG3	13:O:37:THR:N	2.35	0.42
3:c:180:MET:HE1	27:c:522:LMG:HC92	2.02	0.42
4:d:68:LEU:HA	6:f:40:MET:SD	2.59	0.42
4:d:330:ALA:HB3	4:d:331:PRO:HD3	2.02	0.42
14:r:6:LEU:O	14:r:10:LEU:HD23	2.18	0.42
22:B:605:CLA:HMA1	22:B:606:CLA:H3A	2.01	0.42
3:C:83:GLU:OE1	17:V:103:LYS:NZ	2.52	0.42
3:C:265:ILE:HD11	3:C:449:ARG:HD3	2.01	0.42
1:a:201:GLY:HA3	1:a:286:THR:HB	2.01	0.42
2:b:30:VAL:HG12	22:b:605:CLA:HHD	2.01	0.42
2:b:58:GLN:C	2:b:329:PRO:HB3	2.44	0.42
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.54	0.42
3:c:352:GLY:O	3:c:355:THR:HG22	2.20	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.01	0.42
2:B:369:ILE:C	2:B:370:LEU:HD12	2.45	0.42
28:B:622:SQD:H442	15:t:23:PHE:CD1	2.54	0.42
17:V:28:GLU:OE2	17:V:31:ARG:NH1	2.52	0.42
19:Y:42:ARG:HH12	20:Z:31:GLN:NE2	2.18	0.42
1:a:278:TRP:CD1	1:a:278:TRP:C	2.98	0.42
27:a:415:LMG:O8	27:a:415:LMG:C10	2.67	0.42
6:f:26:LEU:O	6:f:29:PRO:HD2	2.20	0.42
17:v:123:PRO:HG3	35:v:321:HOH:O	2.19	0.42
2:B:414:PRO:N	2:B:415:PRO:HD2	2.35	0.42
2:b:159:THR:O	2:b:180:PRO:HB3	2.19	0.42
2:B:283:GLU:O	2:B:287:ARG:HG3	2.20	0.42
4:D:52:THR:O	4:D:66:SER:HA	2.20	0.42
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.01	0.42
1:a:245:THR:HG22	4:d:265:ARG:HH21	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:405:CLA:H192	18:X:15:LEU:HD11	2.01	0.41
3:c:135:ARG:NH1	20:z:33:TRP:CE2	2.87	0.41
22:c:502:CLA:C3D	22:c:504:CLA:H2	2.50	0.41
24:c:516:BCR:H382	24:c:516:BCR:H23C	2.02	0.41
6:f:28:VAL:N	6:f:29:PRO:CD	2.83	0.41
24:k:102:BCR:H24C	24:k:102:BCR:H371	1.81	0.41
1:A:329:GLU:HG3	35:A:595:HOH:O	2.21	0.41
24:K:101:BCR:H371	24:K:101:BCR:H24C	1.78	0.41
24:T:101:BCR:H24C	24:T:101:BCR:H371	1.90	0.41
1:a:95:PRO:HG2	1:a:98:GLU:HG2	2.00	0.41
2:b:422:ARG:O	2:b:425:ILE:HG12	2.20	0.41
24:B:617:BCR:H371	24:B:617:BCR:H24C	1.88	0.41
3:C:355:THR:C	3:C:357:ARG:N	2.76	0.41
20:Z:31:GLN:NE2	20:Z:32:ASP:HB2	2.35	0.41
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.01	0.41
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.41
24:a:406:BCR:H20C	24:a:406:BCR:H361	1.91	0.41
2:b:204:ALA:O	2:b:208:VAL:HG23	2.19	0.41
20:z:36:SER:HA	20:z:39:LEU:HD23	2.02	0.41
2:B:307:GLU:OE1	13:o:59:LYS:HD3	2.21	0.41
3:C:344:SER:O	13:O:75:THR:HG22	2.20	0.41
5:E:17:VAL:O	5:E:21:VAL:HG23	2.20	0.41
5:E:22[A]:ILE:HD11	5:E:26:THR:HG21	2.02	0.41
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.03	0.41
3:c:419:PHE:HA	29:c:518:DGD:O3E	2.20	0.41
22:c:504:CLA:CHA	22:c:504:CLA:HBA2	2.49	0.41
1:A:332:HIS:O	1:A:333:GLU:C	2.64	0.41
5:E:23:HIS:HB3	5:E:27:ILE:HD12	2.01	0.41
24:b:618:BCR:C8	24:b:618:BCR:H331	2.50	0.41
13:o:53:LYS:HE3	13:o:65:PHE:CE2	2.55	0.41
13:o:158:ASP:HB2	13:o:159:PRO:CD	2.51	0.41
16:u:70:ARG:NH1	16:u:73:GLN:OE1	2.54	0.41
20:z:3:ILE:HG22	20:z:7:LEU:HD23	2.02	0.41
2:B:148:LEU:HD23	2:B:210:ILE:HD11	2.02	0.41
22:B:616:CLA:H91	24:B:619:BCR:H14C	2.02	0.41
8:I:7:THR:O	8:I:11:VAL:HG23	2.21	0.41
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.03	0.41
19:y:34:MET:O	19:y:38:LEU:HG	2.20	0.41
26:A:409:PL9:C30	4:D:45:LEU:HD22	2.50	0.41
27:D:411:LMG:O10	27:D:411:LMG:H132	2.21	0.41
22:b:608:CLA:H141	22:b:608:CLA:H161	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:u:45:LEU:HD21	16:u:71:GLN:HB3	2.03	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.41
2:B:356:VAL:HG21	2:B:424:ALA:HB3	2.02	0.41
2:B:414:PRO:N	2:B:415:PRO:CD	2.84	0.41
4:D:12:ARG:HH21	4:D:17:ILE:HD13	1.86	0.41
4:D:136:VAL:O	4:D:136:VAL:CG1	2.67	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.02	0.41
35:D:581:HOH:O	18:X:6:SER:HA	2.20	0.41
5:E:35:TRP:CD1	5:E:35:TRP:C	2.99	0.41
24:H:102:BCR:H15C	24:H:102:BCR:H351	1.91	0.41
12:M:13:LEU:HA	12:M:13:LEU:HD23	1.90	0.41
2:b:62:VAL:HB	22:b:605:CLA:HED3	2.02	0.41
2:b:67:ALA:HA	2:b:71:VAL:O	2.21	0.41
2:b:298:LEU:HD23	2:b:298:LEU:HA	1.90	0.41
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.56	0.41
22:b:604:CLA:H91	22:b:615:CLA:H42	2.03	0.41
4:d:218:VAL:HG22	4:d:244:TYR:CE1	2.56	0.41
4:d:279:LEU:HD22	23:d:401:PHO:HBC3	2.02	0.41
24:A:406:BCR:H24C	24:A:406:BCR:H371	1.96	0.41
1:a:77:ILE:HD11	26:d:406:PL9:H503	2.02	0.41
2:b:505:ARG:HG3	2:b:506:ARG:N	2.36	0.41
16:u:36:ILE:O	16:u:36:ILE:HG22	2.20	0.41
2:B:357:ARG:NH2	35:B:708:HOH:O	2.48	0.40
22:C:501:CLA:HBD	22:C:501:CLA:HAA1	2.03	0.40
4:D:123:ILE:HD11	29:H:103:DGD:HAH1	2.02	0.40
19:Y:20:ALA:N	19:Y:23:THR:HG1	2.18	0.40
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.56	0.40
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.03	0.40
4:d:170:ALA:HB1	4:d:171:PRO:HD2	2.03	0.40
14:r:2:ASP:N	35:r:101:HOH:O	2.54	0.40
17:v:72:LEU:HD11	17:v:120:LEU:HD21	2.02	0.40
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.51	0.40
2:B:12:LEU:HB2	22:B:612:CLA:HMC2	2.04	0.40
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.56	0.40
3:C:367:GLU:N	3:C:368:PRO:CD	2.84	0.40
3:C:451:ALA:HA	3:C:456:GLU:OE2	2.21	0.40
1:a:140:ARG:HD3	35:d:574:HOH:O	2.21	0.40
5:e:10:PHE:N	33:e:101:LHG:O4	2.53	0.40
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.03	0.40
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.56	0.40
2:B:348:ASN:OD1	2:B:348:ASN:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:ALA:HB1	3:C:99:VAL:HG11	2.03	0.40
33:D:412:LHG:H222	33:D:412:LHG:H191	1.88	0.40
24:F:101:BCR:H23C	24:F:101:BCR:C39	2.51	0.40
24:F:101:BCR:H20C	24:F:101:BCR:H361	1.81	0.40
2:b:159:THR:OG1	2:b:161:LEU:HB2	2.21	0.40
2:b:214:LEU:HD23	2:b:214:LEU:HA	1.96	0.40
22:c:514:CLA:C4B	24:c:515:BCR:H383	2.51	0.40
33:d:408:LHG:H321	15:t:21:ILE:HD11	2.02	0.40
9:j:10:LEU:O	9:j:13:VAL:HG22	2.22	0.40
17:v:3:LEU:HD12	17:v:3:LEU:HA	1.90	0.40
20:z:57:LEU:O	20:z:58:ASN:C	2.65	0.40
1:A:227:THR:HB	1:A:231:GLU:HG3	2.02	0.40
22:C:513:CLA:H61	22:C:513:CLA:H41	1.90	0.40
14:R:20:VAL:O	14:R:24:LEU:HB2	2.21	0.40
24:T:101:BCR:H321	24:T:101:BCR:C8	2.48	0.40
27:a:415:LMG:O9	27:a:415:LMG:O10	2.38	0.40
22:b:606:CLA:C1C	31:b:622:STE:H51	2.51	0.40
22:b:613:CLA:H192	33:d:407:LHG:H212	2.03	0.40
3:c:472:LEU:HA	3:c:472:LEU:HD23	1.87	0.40
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.51	0.40
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.57	0.40
24:B:618:BCR:H24C	24:B:618:BCR:H371	1.96	0.40
13:O:10:ILE:HD13	13:O:10:ILE:HA	1.91	0.40
3:c:350:ILE:HG21	3:c:359:TRP:HB2	2.04	0.40
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.21	0.40
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	36	36
1	a	332/334 (99%)	326 (98%)	6 (2%)	0	100	100
2	B	508/506 (100%)	499 (98%)	9 (2%)	0	100	100
2	b	503/506 (99%)	490 (97%)	13 (3%)	0	100	100
3	C	442/461 (96%)	433 (98%)	8 (2%)	1 (0%)	43	44
3	c	451/461 (98%)	435 (96%)	15 (3%)	1 (0%)	43	44
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	56 (92%)	4 (7%)	1 (2%)	7	4
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%)	30 (88%)	4 (12%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	224 (92%)	18 (7%)	1 (0%)	30	28
13	o	242/272 (89%)	230 (95%)	12 (5%)	0	100	100
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	26 (90%)	2 (7%)	1 (3%)	3	1
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	14
17	v	135/163 (83%)	131 (97%)	4 (3%)	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	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	0
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	3
All	All	5240/5666 (92%)	5072 (97%)	159 (3%)	9 (0%)	43	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	62	GLU
19	Y	43	ARG
14	r	30	GLN
20	z	61	VAL
1	A	259	ILE
7	h	26	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/270 (100%)	268 (99%)	2 (1%)	76	82
1	a	269/270 (100%)	257 (96%)	12 (4%)	24	24
2	B	408/404 (101%)	399 (98%)	9 (2%)	45	51
2	b	402/404 (100%)	386 (96%)	16 (4%)	28	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	346/362 (96%)	334 (96%)	12 (4%)	32	33
3	c	354/362 (98%)	342 (97%)	12 (3%)	32	34
4	D	276/283 (98%)	272 (99%)	4 (1%)	59	66
4	d	277/283 (98%)	269 (97%)	8 (3%)	37	40
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	42
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	42
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	32
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	9
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	13
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	38
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	26
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	7
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	32
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	34
13	o	207/228 (91%)	200 (97%)	7 (3%)	32	34
14	R	28/32 (88%)	23 (82%)	5 (18%)	2	1
14	r	23/32 (72%)	19 (83%)	4 (17%)	2	1
15	T	26/26 (100%)	25 (96%)	1 (4%)	29	30
15	t	25/26 (96%)	25 (100%)	0	100	100
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	22
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	32
17	V	117/138 (85%)	112 (96%)	5 (4%)	26	26
17	v	117/138 (85%)	112 (96%)	5 (4%)	26	26
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	12
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
19	y	22/37 (60%)	18 (82%)	4 (18%)	2	1
20	Z	52/52 (100%)	47 (90%)	5 (10%)	8	5
20	z	51/52 (98%)	43 (84%)	8 (16%)	2	1
All	All	4328/4622 (94%)	4157 (96%)	171 (4%)	28	28

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	243	GLU
2	B	86	ILE
2	B	127	ARG
2	B	240	SER
2	B	294	SER
2	B	350	GLU
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
2	B	405	GLU
3	C	104	GLU
3	C	106	VAL
3	C	130	VAL
3	C	141	GLU
3	C	213	LEU
3	C	238	ILE
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	349	ILE
3	C	386	PRO
3	C	416	SER
4	D	43	LEU
4	D	264	LYS
4	D	272	LEU
4	D	295	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR

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Mol	Chain	Res	Type
8	I	4	LEU
8	I	6	ILE
9	J	24	ILE
10	K	10	LYS
10	K	17	ILE
10	K	27	VAL
12	M	20	VAL
13	O	4	THR
13	O	18	LYS
13	O	25	THR
13	O	54	GLU
13	O	107	THR
13	O	198	SER
13	O	214	THR
14	R	6	LEU
14	R	21	ARG
14	R	26	TYR
14	R	32	GLN
14	R	35	LEU
15	T	25	GLU
16	U	51	LYS
16	U	59	GLU
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	17	LYS
17	V	19	ILE
17	V	31	ARG
18	X	2	THR
18	X	3	ILE
18	X	15	LEU
19	Y	23	THR
19	Y	34	MET
20	Z	7	LEU
20	Z	15	LEU
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU

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Mol	Chain	Res	Type
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	224	ILE
1	a	229	GLU
1	a	242	GLU
1	a	245	THR
1	a	288	LEU
1	a	307	ILE
2	b	13	ILE
2	b	74	SER
2	b	83	GLU
2	b	86	ILE
2	b	98	LEU
2	b	128	THR
2	b	161	LEU
2	b	227	LYS
2	b	236	THR
2	b	240	SER
2	b	245	VAL
2	b	362	PHE
2	b	435	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	315	MET
3	c	346	THR
3	c	396	MET
3	c	416	SER
4	d	90	LEU
4	d	103	ARG
4	d	182	LEU
4	d	259	ILE
4	d	291	LEU

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Mol	Chain	Res	Type
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	66	VAL
5	e	83	LEU
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
7	h	3	ARG
7	h	7	LEU
7	h	39	LEU
7	h	52	THR
8	i	2	GLU
9	j	13	VAL
9	j	22	ILE
10	k	10	LYS
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
13	o	66	VAL
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	207	ARG
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
14	r	13	LEU
16	u	15	GLU
16	u	23	GLU
16	u	58	VAL
17	v	19	ILE
17	v	30	LYS
17	v	45	ILE
17	v	52	LEU

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Mol	Chain	Res	Type
17	v	107	LEU
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	30	ILE
19	y	34	MET
19	y	45	ASN
20	z	1	MET
20	z	7	LEU
20	z	20	VAL
20	z	31	GLN
20	z	38	GLN
20	z	40	ILE
20	z	42	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	315	ASN
1	A	338	ASN
2	B	497	GLN
3	C	44	ASN
3	C	311	GLN
3	C	327	ASN
3	C	385	GLN
3	C	415	ASN
4	D	61	HIS
4	D	186	GLN
11	L	8	GLN
13	O	3	GLN
13	O	36	GLN
13	O	88	ASN
14	R	22	ASN
16	U	37	GLN
20	Z	6	GLN
20	Z	31	GLN
1	a	19	ASN
1	a	165	GLN
1	a	181	ASN
1	a	234	ASN

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Mol	Chain	Res	Type
1	a	296	ASN
2	b	179	GLN
2	b	338	GLN
2	b	409	GLN
3	c	322	GLN
3	c	373	ASN
3	c	378	ASN
3	c	382	ASN
4	d	338	ASN
4	d	350	ASN
5	e	60	GLN
7	h	59	ASN
13	o	124	ASN
13	o	147	ASN
13	o	155	ASN
13	o	231	HIS
14	r	30	GLN
16	u	37	GLN
20	z	6	GLN
20	z	31	GLN
20	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	$\# Z > 2$
12	FME	M	1	12	8,9,10	1.10	1 (12%)	8,9,11	0.80	0
15	FME	T	1	15	8,9,10	1.18	0	8,9,11	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	I	1	8	8,9,10	1.03	0	8,9,11	1.08	0
8	FME	i	1	8	8,9,10	1.23	1 (12%)	8,9,11	1.44	2 (25%)
12	FME	m	1	12	8,9,10	1.15	1 (12%)	8,9,11	0.73	0
15	FME	t	1	15	8,9,10	1.04	0	8,9,11	1.25	1 (12%)

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
12	FME	M	1	12	-	2/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.86	1.42	1.46
12	m	1	FME	CA-N	-2.42	1.43	1.46
12	M	1	FME	CA-N	-2.16	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CB-CA-N	2.52	115.11	110.52
8	i	1	FME	CA-N-CN	-2.41	119.12	122.82
15	t	1	FME	C-CA-N	2.37	114.06	109.50

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
15	T	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
8	I	1	FME	C-CA-CB-CG
12	M	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 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$
31	STE	M	102	-	14,14,19	1.03	1 (7%)	14,14,19	0.69	0
28	SQD	L	101	-	47,49,54	0.93	2 (4%)	57,60,65	2.35	14 (24%)
33	LHG	D	412	-	48,48,48	0.79	1 (2%)	51,54,54	1.34	5 (9%)
22	CLA	c	509	3	68,72,73	1.48	10 (14%)	80,111,113	1.38	9 (11%)
33	LHG	D	410	-	46,46,48	1.06	3 (6%)	49,52,54	1.24	4 (8%)
24	BCR	F	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.30	6 (10%)
22	CLA	b	608	2	69,73,73	1.36	8 (11%)	82,113,113	1.36	8 (9%)
31	STE	a	413	-	9,9,19	0.57	0	8,8,19	0.57	0
22	CLA	H	101	35	69,73,73	1.47	10 (14%)	82,113,113	1.48	7 (8%)
27	LMG	b	623	-	55,55,55	0.88	2 (3%)	63,63,63	1.61	11 (17%)
22	CLA	C	510	3	69,73,73	1.13	7 (10%)	82,113,113	1.24	8 (9%)
23	PHO	D	401	-	58,69,69	1.94	9 (15%)	55,99,99	1.39	6 (10%)
24	BCR	k	101	-	41,41,41	1.08	4 (9%)	56,56,56	1.12	3 (5%)
26	PL9	D	406	-	55,55,55	1.33	7 (12%)	68,69,69	1.60	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	C	514	-	41,41,41	1.23	3 (7%)	56,56,56	1.25	9 (16%)
31	STE	H	104	-	17,17,19	0.42	0	16,16,19	0.89	0
22	CLA	C	503	3	69,73,73	1.38	8 (11%)	82,113,113	1.48	13 (15%)
28	SQD	a	411	-	52,54,54	1.01	4 (7%)	62,65,65	2.15	15 (24%)
22	CLA	A	403	35	69,73,73	1.28	10 (14%)	82,113,113	1.31	12 (14%)
27	LMG	A	410	-	48,48,55	1.01	2 (4%)	56,56,63	1.44	7 (12%)
27	LMG	D	407	-	51,51,55	0.92	2 (3%)	59,59,63	1.38	8 (13%)
31	STE	d	412	-	16,16,19	0.63	0	16,16,19	1.07	1 (6%)
22	CLA	C	506	3	69,73,73	1.84	10 (14%)	82,113,113	1.25	8 (9%)
31	STE	B	626	-	15,15,19	0.48	0	14,14,19	0.71	0
29	DGD	c	519	-	63,63,67	1.21	8 (12%)	77,77,81	1.40	8 (10%)
22	CLA	d	403	4	69,73,73	1.21	8 (11%)	82,113,113	1.18	7 (8%)
22	CLA	a	405	1	69,73,73	1.22	8 (11%)	82,113,113	1.32	8 (9%)
22	CLA	C	504	35	63,67,73	1.33	10 (15%)	74,105,113	1.37	11 (14%)
31	STE	m	102	-	11,11,19	0.76	0	11,11,19	1.32	2 (18%)
33	LHG	D	409	-	48,48,48	0.96	2 (4%)	51,54,54	1.29	6 (11%)
27	LMG	a	415	-	55,55,55	1.44	6 (10%)	63,63,63	1.46	7 (11%)
22	CLA	C	508	3	69,73,73	1.41	8 (11%)	82,113,113	1.40	5 (6%)
33	LHG	e	101	-	41,41,48	0.93	1 (2%)	44,47,54	1.24	4 (9%)
24	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.46	8 (14%)
31	STE	B	624	-	11,11,19	0.96	2 (18%)	11,11,19	1.06	0
28	SQD	a	412	-	35,35,54	1.22	2 (5%)	37,37,65	1.48	4 (10%)
31	STE	C	518	-	11,11,19	0.79	0	11,11,19	0.96	0
28	SQD	A	412	-	38,38,54	1.04	3 (7%)	40,40,65	1.30	4 (10%)
33	LHG	d	409	-	38,38,48	1.02	2 (5%)	41,44,54	1.08	2 (4%)
22	CLA	c	512	3	69,73,73	1.50	8 (11%)	82,113,113	1.43	6 (7%)
22	CLA	D	403	4	69,73,73	1.14	7 (10%)	82,113,113	1.37	12 (14%)
23	PHO	a	404	-	58,69,69	1.94	7 (12%)	55,99,99	1.57	9 (16%)
31	STE	b	620	-	15,15,19	0.46	0	14,14,19	0.82	0
33	LHG	l	101	-	48,48,48	0.62	0	51,54,54	1.16	4 (7%)
22	CLA	b	612	2	69,73,73	1.15	7 (10%)	82,113,113	1.35	13 (15%)
22	CLA	D	404	35	69,73,73	1.37	7 (10%)	82,113,113	1.31	5 (6%)
27	LMG	c	522	-	48,48,55	1.13	5 (10%)	56,56,63	1.19	3 (5%)
31	STE	B	601	-	11,11,19	0.62	0	11,11,19	1.30	1 (9%)
27	LMG	d	410	-	44,44,55	1.16	4 (9%)	52,52,63	1.32	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	K	102	-	41,41,41	1.03	3 (7%)	56,56,56	1.27	5 (8%)
22	CLA	a	402	1	69,73,73	1.41	8 (11%)	82,113,113	1.45	13 (15%)
26	PL9	A	409	-	55,55,55	0.97	1 (1%)	68,69,69	1.55	13 (19%)
22	CLA	A	402	1	69,73,73	1.42	9 (13%)	82,113,113	1.34	6 (7%)
34	HEC	f	101	6,5	50,50,50	1.55	9 (18%)	68,82,82	1.66	13 (19%)
22	CLA	C	502	3	69,73,73	1.27	8 (11%)	82,113,113	1.23	8 (9%)
29	DGD	h	102	-	63,63,67	1.16	11 (17%)	77,77,81	1.37	10 (12%)
22	CLA	c	506	3	69,73,73	1.14	8 (11%)	82,113,113	1.35	8 (9%)
22	CLA	c	504	3	69,73,73	1.22	11 (15%)	82,113,113	1.53	10 (12%)
29	DGD	C	516	-	63,63,67	1.20	10 (15%)	77,77,81	1.38	10 (12%)
31	STE	m	101	-	17,17,19	0.44	0	16,16,19	0.80	0
22	CLA	C	511	3	69,73,73	1.22	9 (13%)	82,113,113	1.20	4 (4%)
24	BCR	d	405	-	41,41,41	1.22	3 (7%)	56,56,56	1.29	6 (10%)
28	SQD	D	408	-	34,36,54	0.94	2 (5%)	42,45,65	1.75	9 (21%)
22	CLA	B	611	2	69,73,73	1.26	7 (10%)	82,113,113	1.50	14 (17%)
33	LHG	L	102	-	48,48,48	0.82	2 (4%)	51,54,54	1.20	2 (3%)
31	STE	b	627	-	19,19,19	0.61	0	19,19,19	1.23	2 (10%)
22	CLA	C	509	3	69,73,73	1.30	13 (18%)	82,113,113	1.26	10 (12%)
24	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.42	9 (16%)
31	STE	c	501	-	11,11,19	0.86	0	11,11,19	1.06	0
24	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.48	14 (25%)
24	BCR	b	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	7 (12%)
22	CLA	B	616	2	64,68,73	1.70	10 (15%)	76,107,113	1.56	10 (13%)
22	CLA	D	405	4	69,73,73	1.38	9 (13%)	82,113,113	1.10	5 (6%)
22	CLA	b	607	35	69,73,73	1.45	9 (13%)	82,113,113	1.32	10 (12%)
22	CLA	B	614	2	69,73,73	1.27	9 (13%)	82,113,113	1.27	10 (12%)
24	BCR	T	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.21	4 (7%)
30	OEX	a	416	1,3,35	0,14,14	-	-	-	-	-
24	BCR	b	617	-	41,41,41	1.14	4 (9%)	56,56,56	1.38	10 (17%)
24	BCR	a	406	-	41,41,41	1.26	3 (7%)	56,56,56	1.24	6 (10%)
23	PHO	d	401	-	58,69,69	2.06	10 (17%)	55,99,99	1.74	10 (18%)
22	CLA	C	505	3	69,73,73	1.31	8 (11%)	82,113,113	1.38	9 (10%)
31	STE	E	102	-	11,11,19	0.98	1 (9%)	11,11,19	0.99	1 (9%)
31	STE	T	102	-	14,14,19	0.44	0	13,13,19	0.86	0
31	STE	Z	101	-	7,7,19	0.44	0	6,6,19	0.57	0
31	STE	C	520	-	11,11,19	0.80	0	11,11,19	1.44	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	B	625	-	17,17,19	0.66	0	17,17,19	1.27	1 (5%)
22	CLA	c	503	3	69,73,73	1.15	8 (11%)	82,113,113	1.35	7 (8%)
26	PL9	a	409	-	55,55,55	1.03	4 (7%)	68,69,69	1.59	10 (14%)
22	CLA	c	513	3	69,73,73	1.26	11 (15%)	82,113,113	1.31	6 (7%)
22	CLA	C	512	3	69,73,73	1.55	9 (13%)	82,113,113	1.28	10 (12%)
22	CLA	B	606	2	69,73,73	1.60	9 (13%)	82,113,113	1.44	7 (8%)
22	CLA	C	513	3	69,73,73	1.21	10 (14%)	82,113,113	1.46	11 (13%)
22	CLA	c	508	35	69,73,73	1.28	6 (8%)	82,113,113	1.26	8 (9%)
22	CLA	B	608	2	69,73,73	1.62	9 (13%)	82,113,113	1.40	10 (12%)
23	PHO	A	404	-	58,69,69	1.92	12 (20%)	55,99,99	1.46	9 (16%)
22	CLA	B	605	2	69,73,73	1.32	9 (13%)	82,113,113	1.58	13 (15%)
22	CLA	b	609	2	69,73,73	1.49	8 (11%)	82,113,113	1.31	11 (13%)
22	CLA	B	613	2	69,73,73	1.52	11 (15%)	82,113,113	1.40	9 (10%)
32	BCT	d	402	21	3,3,3	1.13	0	2,3,3	3.61	2 (100%)
22	CLA	B	612	2	69,73,73	1.11	5 (7%)	82,113,113	1.38	12 (14%)
27	LMG	M	101	-	51,51,55	1.17	3 (5%)	59,59,63	1.49	10 (16%)
33	LHG	d	407	-	48,48,48	1.03	2 (4%)	51,54,54	1.46	5 (9%)
24	BCR	B	617	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	5 (8%)
24	BCR	B	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.47	9 (16%)
24	BCR	k	102	-	41,41,41	0.98	2 (4%)	56,56,56	1.22	4 (7%)
33	LHG	E	101	-	48,48,48	0.88	3 (6%)	51,54,54	1.22	6 (11%)
22	CLA	B	602	2	69,73,73	1.33	6 (8%)	82,113,113	1.36	10 (12%)
22	CLA	b	611	2	69,73,73	1.41	8 (11%)	82,113,113	1.72	11 (13%)
22	CLA	C	507	35	69,73,73	1.39	7 (10%)	82,113,113	1.64	13 (15%)
22	CLA	a	403	35	69,73,73	1.25	9 (13%)	82,113,113	1.44	11 (13%)
31	STE	c	521	-	19,19,19	0.74	1 (5%)	19,19,19	0.92	1 (5%)
24	BCR	c	516	-	41,41,41	1.26	5 (12%)	56,56,56	1.31	6 (10%)
27	LMG	Y	101	-	48,48,55	0.97	2 (4%)	56,56,63	1.35	6 (10%)
22	CLA	b	610	35	69,73,73	1.30	8 (11%)	82,113,113	1.48	17 (20%)
22	CLA	b	615	2	69,73,73	1.82	11 (15%)	82,113,113	1.44	10 (12%)
31	STE	B	620	-	16,16,19	0.99	2 (12%)	16,16,19	0.90	0
22	CLA	d	404	4	69,73,73	1.15	8 (11%)	82,113,113	1.19	10 (12%)
32	BCT	D	402	21	3,3,3	1.14	0	2,3,3	2.97	2 (100%)
22	CLA	b	613	2	69,73,73	1.15	9 (13%)	82,113,113	1.37	11 (13%)
31	STE	b	626	-	13,13,19	0.41	0	12,12,19	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	d	411	-	15,15,19	0.90	1 (6%)	15,15,19	0.95	2 (13%)
22	CLA	b	603	2	69,73,73	1.33	8 (11%)	82,113,113	1.51	13 (15%)
22	CLA	b	606	2	69,73,73	1.48	9 (13%)	82,113,113	1.45	6 (7%)
27	LMG	B	621	-	26,26,55	0.67	0	26,26,63	1.27	2 (7%)
28	SQD	A	411	-	50,52,54	1.11	5 (10%)	60,63,65	1.69	12 (20%)
31	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.73	0
31	STE	b	624	-	19,19,19	0.69	0	19,19,19	1.33	3 (15%)
22	CLA	B	609	2	69,73,73	1.38	7 (10%)	82,113,113	1.31	6 (7%)
34	HEC	F	102	6,5	50,50,50	1.54	5 (10%)	68,82,82	1.33	8 (11%)
22	CLA	c	505	35	64,68,73	1.25	8 (12%)	76,107,113	1.38	11 (14%)
29	DGD	c	518	-	63,63,67	1.14	6 (9%)	77,77,81	1.41	11 (14%)
31	STE	b	622	-	19,19,19	0.72	0	19,19,19	0.90	0
22	CLA	B	615	2	69,73,73	1.47	10 (14%)	82,113,113	1.43	9 (10%)
24	BCR	A	406	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	7 (12%)
31	STE	j	101	-	11,11,19	1.06	1 (9%)	11,11,19	1.41	2 (18%)
24	BCR	h	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	8 (14%)
31	STE	C	519	-	15,15,19	0.60	0	14,14,19	0.50	0
27	LMG	D	411	-	31,31,55	1.12	3 (9%)	33,33,63	1.17	2 (6%)
28	SQD	B	622	-	52,54,54	1.01	3 (5%)	62,65,65	1.83	12 (19%)
31	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.50	2 (18%)
29	DGD	c	517	-	63,63,67	1.37	7 (11%)	77,77,81	1.34	8 (10%)
22	CLA	b	605	2	69,73,73	1.11	7 (10%)	82,113,113	1.51	16 (19%)
29	DGD	C	517	-	63,63,67	1.17	6 (9%)	77,77,81	1.47	12 (15%)
31	STE	d	413	-	19,19,19	0.70	0	19,19,19	0.94	1 (5%)
27	LMG	c	520	-	37,37,55	1.17	4 (10%)	45,45,63	1.28	6 (13%)
29	DGD	H	103	-	63,63,67	1.31	9 (14%)	77,77,81	1.53	14 (18%)
30	OEX	A	414	1,3,35	0,14,14	-	-	-	-	-
31	STE	B	627	-	14,14,19	0.55	0	13,13,19	0.64	0
22	CLA	b	604	2	69,73,73	1.49	9 (13%)	82,113,113	1.62	10 (12%)
22	CLA	c	502	3	69,73,73	1.27	7 (10%)	82,113,113	1.50	6 (7%)
33	LHG	d	408	-	48,48,48	1.01	2 (4%)	51,54,54	1.17	3 (5%)
22	CLA	b	616	2	64,68,73	1.15	5 (7%)	76,107,113	1.64	12 (15%)
29	DGD	A	413	-	67,67,67	1.33	10 (14%)	81,81,81	1.53	13 (16%)
34	HEC	V	201	17	50,50,50	1.41	4 (8%)	68,82,82	1.38	15 (22%)
22	CLA	c	511	3	69,73,73	1.20	8 (11%)	82,113,113	1.45	7 (8%)
24	BCR	H	102	-	41,41,41	0.98	1 (2%)	56,56,56	1.36	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	D	413	-	19,19,19	0.70	0	19,19,19	0.99	0
24	BCR	c	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.18	4 (7%)
22	CLA	B	604	2	69,73,73	1.19	6 (8%)	82,113,113	1.65	14 (17%)
22	CLA	B	607	35	69,73,73	1.16	8 (11%)	82,113,113	1.40	9 (10%)
22	CLA	b	602	2	69,73,73	1.48	9 (13%)	82,113,113	1.33	11 (13%)
34	HEC	v	201	17	50,50,50	1.40	6 (12%)	68,82,82	1.35	7 (10%)
22	CLA	c	514	3	69,73,73	1.52	10 (14%)	82,113,113	1.16	10 (12%)
31	STE	B	623	-	13,13,19	0.64	0	13,13,19	1.31	2 (15%)
22	CLA	b	601	35	69,73,73	1.42	8 (11%)	82,113,113	1.34	9 (10%)
27	LMG	c	523	-	49,49,55	1.06	5 (10%)	57,57,63	1.30	5 (8%)
28	SQD	f	102	-	39,41,54	1.11	4 (10%)	49,52,65	1.79	10 (20%)
22	CLA	B	610	35	69,73,73	1.38	11 (15%)	82,113,113	1.37	14 (17%)
22	CLA	c	507	3	69,73,73	1.32	10 (14%)	82,113,113	1.25	11 (13%)
22	CLA	a	410	35	69,73,73	1.43	7 (10%)	82,113,113	1.40	9 (10%)
22	CLA	c	510	3	69,73,73	1.19	6 (8%)	82,113,113	1.64	9 (10%)
22	CLA	C	501	3	69,73,73	1.52	12 (17%)	82,113,113	1.45	11 (13%)
24	BCR	b	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	9 (16%)
29	DGD	C	515	-	63,63,67	1.46	10 (15%)	77,77,81	1.45	12 (15%)
22	CLA	B	603	2	69,73,73	1.27	6 (8%)	82,113,113	1.43	13 (15%)
31	STE	b	625	-	9,9,19	0.53	0	8,8,19	0.54	0
31	STE	a	414	-	11,11,19	0.84	1 (9%)	11,11,19	1.24	1 (9%)
22	CLA	A	405	1	58,62,73	1.46	10 (17%)	68,99,113	1.42	8 (11%)
27	LMG	b	621	-	51,51,55	1.02	4 (7%)	59,59,63	1.43	10 (16%)
22	CLA	b	614	2	69,73,73	1.17	9 (13%)	82,113,113	1.15	6 (7%)
24	BCR	K	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	7 (12%)
31	STE	I	101	-	14,14,19	0.56	0	13,13,19	0.45	0
26	PL9	d	406	-	55,55,55	1.58	10 (18%)	68,69,69	1.80	15 (22%)

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
31	STE	M	102	-	-	6/12/12/17	-
28	SQD	L	101	-	-	24/44/64/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	D	412	-	-	20/53/53/53	-
22	CLA	c	509	3	-	5/38/114/115	-
33	LHG	D	410	-	-	21/51/51/53	-
24	BCR	F	101	-	-	6/29/63/63	0/2/2/2
22	CLA	b	608	2	-	5/39/115/115	-
31	STE	a	413	-	-	5/7/7/17	-
22	CLA	H	101	35	-	19/39/115/115	-
27	LMG	b	623	-	-	27/50/70/70	0/1/1/1
22	CLA	C	510	3	-	6/39/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
26	PL9	D	406	-	-	12/53/73/73	0/1/1/1
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
31	STE	H	104	-	-	9/15/15/17	-
22	CLA	C	503	3	-	7/39/115/115	-
28	SQD	a	411	-	-	22/49/69/69	0/1/1/1
22	CLA	A	403	35	-	15/39/115/115	-
27	LMG	A	410	-	-	18/43/63/70	0/1/1/1
27	LMG	D	407	-	-	16/46/66/70	0/1/1/1
31	STE	d	412	-	-	7/14/14/17	-
22	CLA	C	506	3	-	7/39/115/115	-
31	STE	B	626	-	-	8/13/13/17	-
29	DGD	c	519	-	-	17/51/91/95	0/2/2/2
22	CLA	d	403	4	-	12/39/115/115	-
22	CLA	a	405	1	-	5/39/115/115	-
22	CLA	C	504	35	-	6/32/108/115	-
31	STE	m	102	-	-	5/9/9/17	-
33	LHG	D	409	-	-	26/53/53/53	-
27	LMG	a	415	-	-	31/50/70/70	0/1/1/1
22	CLA	C	508	3	-	6/39/115/115	-
33	LHG	e	101	-	-	22/46/46/53	-
24	BCR	K	101	-	-	9/29/63/63	0/2/2/2
31	STE	B	624	-	-	5/9/9/17	-
28	SQD	a	412	-	-	15/37/37/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	C	518	-	-	6/9/9/17	-
28	SQD	A	412	-	-	17/39/39/69	-
33	LHG	d	409	-	-	12/43/43/53	-
22	CLA	c	512	3	-	8/39/115/115	-
22	CLA	D	403	4	-	5/39/115/115	-
23	PHO	a	404	-	-	6/37/103/103	0/5/6/6
31	STE	b	620	-	-	7/13/13/17	-
33	LHG	l	101	-	-	17/53/53/53	-
22	CLA	b	612	2	-	5/39/115/115	-
22	CLA	D	404	35	-	8/39/115/115	-
27	LMG	c	522	-	-	25/43/63/70	0/1/1/1
31	STE	B	601	-	-	4/9/9/17	-
27	LMG	d	410	-	-	11/39/59/70	0/1/1/1
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	a	402	1	-	6/39/115/115	-
34	HEC	f	101	6,5	1/1/7/7	9/14/54/54	-
22	CLA	A	402	1	-	3/39/115/115	-
26	PL9	A	409	-	-	22/53/73/73	0/1/1/1
22	CLA	C	502	3	-	9/39/115/115	-
29	DGD	h	102	-	-	18/51/91/95	0/2/2/2
22	CLA	c	506	3	-	8/39/115/115	-
22	CLA	c	504	3	-	10/39/115/115	-
29	DGD	C	516	-	-	22/51/91/95	0/2/2/2
31	STE	m	101	-	-	7/15/15/17	-
22	CLA	C	511	3	-	7/39/115/115	-
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
28	SQD	D	408	-	-	12/28/48/69	0/1/1/1
22	CLA	B	611	2	-	2/39/115/115	-
33	LHG	L	102	-	-	18/53/53/53	-
31	STE	b	627	-	-	9/17/17/17	-
22	CLA	C	509	3	-	10/39/115/115	-
24	BCR	B	618	-	-	8/29/63/63	0/2/2/2
31	STE	c	501	-	-	3/9/9/17	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	618	-	-	5/29/63/63	0/2/2/2
22	CLA	B	616	2	-	12/33/109/115	-
22	CLA	D	405	4	-	6/39/115/115	-
22	CLA	b	607	35	-	13/39/115/115	-
22	CLA	B	614	2	-	8/39/115/115	-
24	BCR	T	101	-	-	14/29/63/63	0/2/2/2
24	BCR	b	617	-	-	8/29/63/63	0/2/2/2
24	BCR	a	406	-	-	3/29/63/63	0/2/2/2
23	PHO	d	401	-	-	5/37/103/103	0/5/6/6
22	CLA	C	505	3	-	10/39/115/115	-
31	STE	E	102	-	-	4/9/9/17	-
31	STE	T	102	-	-	7/12/12/17	-
31	STE	Z	101	-	-	2/5/5/17	-
31	STE	C	520	-	-	2/9/9/17	-
31	STE	B	625	-	-	15/15/15/17	-
22	CLA	c	503	3	-	7/39/115/115	-
26	PL9	a	409	-	-	21/53/73/73	0/1/1/1
22	CLA	c	513	3	-	19/39/115/115	-
22	CLA	C	512	3	-	14/39/115/115	-
22	CLA	B	606	2	-	11/39/115/115	-
22	CLA	C	513	3	-	16/39/115/115	-
22	CLA	c	508	35	-	10/39/115/115	-
22	CLA	B	608	2	-	4/39/115/115	-
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
22	CLA	B	605	2	-	9/39/115/115	-
22	CLA	b	609	2	-	10/39/115/115	-
22	CLA	B	613	2	-	12/39/115/115	-
22	CLA	B	612	2	-	11/39/115/115	-
27	LMG	M	101	-	-	27/46/66/70	0/1/1/1
33	LHG	d	407	-	-	14/53/53/53	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
24	BCR	B	619	-	-	6/29/63/63	0/2/2/2
24	BCR	k	102	-	-	3/29/63/63	0/2/2/2
33	LHG	E	101	-	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	602	2	-	7/39/115/115	-
22	CLA	b	611	2	-	8/39/115/115	-
22	CLA	C	507	35	-	5/39/115/115	-
22	CLA	a	403	35	-	10/39/115/115	-
31	STE	c	521	-	-	11/17/17/17	-
24	BCR	c	516	-	-	5/29/63/63	0/2/2/2
27	LMG	Y	101	-	-	24/43/63/70	0/1/1/1
22	CLA	b	610	35	-	2/39/115/115	-
22	CLA	b	615	2	-	8/39/115/115	-
31	STE	B	620	-	-	9/14/14/17	-
22	CLA	d	404	4	-	3/39/115/115	-
22	CLA	b	613	2	-	7/39/115/115	-
31	STE	b	626	-	-	5/11/11/17	-
31	STE	d	411	-	-	6/13/13/17	-
22	CLA	b	603	2	-	6/39/115/115	-
22	CLA	b	606	2	-	5/39/115/115	-
27	LMG	B	621	-	-	10/22/22/70	-
28	SQD	A	411	-	-	9/47/67/69	0/1/1/1
31	STE	M	103	-	-	3/7/7/17	-
31	STE	b	624	-	-	10/17/17/17	-
22	CLA	B	609	2	-	7/39/115/115	-
34	HEC	F	102	6,5	1/1/7/7	6/14/54/54	-
22	CLA	c	505	35	-	4/33/109/115	-
29	DGD	c	518	-	-	21/51/91/95	0/2/2/2
31	STE	b	622	-	-	8/17/17/17	-
22	CLA	B	615	2	-	10/39/115/115	-
24	BCR	A	406	-	-	9/29/63/63	0/2/2/2
31	STE	j	101	-	-	4/9/9/17	-
24	BCR	h	101	-	-	4/29/63/63	0/2/2/2
31	STE	C	519	-	-	5/13/13/17	-
27	LMG	D	411	-	-	15/33/33/70	-
28	SQD	B	622	-	-	19/49/69/69	0/1/1/1
31	STE	J	101	-	-	5/9/9/17	-
29	DGD	c	517	-	-	23/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	605	2	-	6/39/115/115	-
29	DGD	C	517	-	-	14/51/91/95	0/2/2/2
31	STE	d	413	-	-	11/17/17/17	-
27	LMG	c	520	-	-	10/31/51/70	0/1/1/1
29	DGD	H	103	-	-	17/51/91/95	0/2/2/2
31	STE	B	627	-	-	5/12/12/17	-
22	CLA	b	604	2	-	6/39/115/115	-
22	CLA	c	502	3	-	1/39/115/115	-
33	LHG	d	408	-	-	19/53/53/53	-
22	CLA	b	616	2	-	9/33/109/115	-
29	DGD	A	413	-	-	28/55/95/95	0/2/2/2
34	HEC	V	201	17	1/1/7/7	4/14/54/54	-
22	CLA	c	511	3	-	6/39/115/115	-
24	BCR	H	102	-	-	5/29/63/63	0/2/2/2
31	STE	D	413	-	-	9/17/17/17	-
24	BCR	c	515	-	-	10/29/63/63	0/2/2/2
22	CLA	B	604	2	-	10/39/115/115	-
22	CLA	B	607	35	-	5/39/115/115	-
34	HEC	v	201	17	1/1/7/7	5/14/54/54	-
22	CLA	b	602	2	-	5/39/115/115	-
22	CLA	c	514	3	-	8/39/115/115	-
31	STE	B	623	-	-	3/11/11/17	-
22	CLA	b	601	35	-	16/39/115/115	-
27	LMG	c	523	-	-	23/44/64/70	0/1/1/1
28	SQD	f	102	-	-	15/36/56/69	0/1/1/1
22	CLA	B	610	35	-	5/39/115/115	-
22	CLA	c	507	3	-	13/39/115/115	-
22	CLA	a	410	35	-	4/39/115/115	-
22	CLA	c	510	3	-	15/39/115/115	-
22	CLA	C	501	3	-	3/39/115/115	-
24	BCR	b	619	-	-	8/29/63/63	0/2/2/2
29	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	B	603	2	-	12/39/115/115	-
31	STE	b	625	-	-	6/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	a	414	-	-	2/9/9/17	-
22	CLA	A	405	1	-	3/26/102/115	-
27	LMG	b	621	-	-	15/46/66/70	0/1/1/1
22	CLA	b	614	2	-	15/39/115/115	-
24	BCR	K	103	-	-	6/29/63/63	0/2/2/2
31	STE	I	101	-	-	7/12/12/17	-
26	PL9	d	406	-	-	15/53/73/73	0/1/1/1

All (908) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	MG-ND	-9.62	1.86	2.05
23	d	401	PHO	C1B-C2B	9.55	1.50	1.39
23	a	404	PHO	C1B-C2B	8.80	1.49	1.39
22	b	615	CLA	MG-NA	8.66	2.26	2.06
23	D	401	PHO	C1B-C2B	8.33	1.48	1.39
23	d	401	PHO	C3B-C4B	8.16	1.49	1.41
22	B	616	CLA	MG-NA	7.90	2.25	2.06
22	b	606	CLA	MG-NA	7.76	2.24	2.06
22	b	604	CLA	MG-NA	7.64	2.24	2.06
22	C	512	CLA	MG-NB	7.63	2.20	2.05
22	B	608	CLA	MG-NA	7.61	2.24	2.06
22	c	514	CLA	MG-NC	-7.03	1.89	2.06
22	c	512	CLA	MG-NA	7.01	2.22	2.06
23	A	404	PHO	C3B-C4B	6.96	1.48	1.41
23	A	404	PHO	C1B-C2B	6.81	1.47	1.39
23	a	404	PHO	C3B-C4B	6.77	1.48	1.41
23	D	401	PHO	C3B-C4B	6.71	1.48	1.41
22	b	609	CLA	MG-NA	6.44	2.21	2.06
22	b	608	CLA	MG-NA	6.43	2.21	2.06
22	B	613	CLA	MG-ND	-6.40	1.93	2.05
22	D	404	CLA	MG-NA	6.36	2.21	2.06
22	b	601	CLA	MG-NA	6.26	2.21	2.06
22	B	608	CLA	MG-NC	-6.25	1.91	2.06
22	C	508	CLA	MG-NA	6.07	2.20	2.06
22	b	602	CLA	MG-NA	6.06	2.20	2.06
22	a	402	CLA	MG-NA	6.02	2.20	2.06
22	C	507	CLA	MG-NA	6.00	2.20	2.06
22	B	606	CLA	MG-NC	5.96	2.20	2.06
22	b	607	CLA	MG-NB	-5.95	1.94	2.05
22	a	410	CLA	MG-NA	5.92	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	MG-NB	5.88	2.17	2.05
22	C	503	CLA	MG-NA	5.87	2.20	2.06
22	B	603	CLA	MG-ND	5.83	2.17	2.05
22	H	101	CLA	MG-NA	5.72	2.19	2.06
22	C	506	CLA	MG-NA	5.70	2.19	2.06
27	a	415	LMG	C4-C5	5.60	1.65	1.53
22	b	615	CLA	MG-NB	5.58	2.16	2.05
22	B	609	CLA	MG-NA	5.56	2.19	2.06
22	D	405	CLA	MG-NB	-5.52	1.94	2.05
22	B	606	CLA	MG-NB	-5.44	1.95	2.05
22	C	501	CLA	MG-ND	-5.29	1.95	2.05
22	c	514	CLA	MG-NA	5.13	2.18	2.06
22	B	606	CLA	MG-NA	5.01	2.18	2.06
26	d	406	PL9	C6-C1	-4.93	1.40	1.48
22	C	512	CLA	MG-ND	-4.92	1.96	2.05
22	b	610	CLA	C1D-ND	4.86	1.44	1.37
22	b	602	CLA	MG-NC	-4.83	1.94	2.06
22	b	615	CLA	MG-ND	-4.82	1.96	2.05
22	B	604	CLA	MG-NA	4.77	2.17	2.06
27	M	101	LMG	O7-C8	-4.73	1.35	1.46
22	b	607	CLA	MG-NA	4.68	2.17	2.06
22	B	615	CLA	MG-NB	4.63	2.15	2.05
24	C	514	BCR	C1-C6	-4.63	1.47	1.53
24	b	618	BCR	C30-C25	-4.62	1.47	1.53
22	B	615	CLA	MG-NC	4.57	2.17	2.06
24	c	516	BCR	C1-C6	-4.55	1.48	1.53
22	c	509	CLA	MG-NA	4.54	2.17	2.06
29	c	517	DGD	C3G-C2G	4.52	1.64	1.50
22	B	616	CLA	MG-NB	-4.49	1.96	2.05
33	d	408	LHG	O8-C6	-4.49	1.35	1.45
22	B	602	CLA	C1D-ND	4.48	1.43	1.37
23	a	404	PHO	C1D-C2D	4.45	1.44	1.39
29	H	103	DGD	C4E-C5E	4.43	1.62	1.53
22	b	611	CLA	MG-NB	4.41	2.14	2.05
22	A	402	CLA	MG-NB	4.40	2.14	2.05
22	B	614	CLA	MG-ND	-4.39	1.97	2.05
24	T	101	BCR	C1-C6	-4.38	1.48	1.53
34	f	101	HEC	CBB-CAB	-4.38	1.32	1.51
24	a	406	BCR	C1-C6	-4.36	1.48	1.53
22	b	612	CLA	MG-ND	-4.35	1.97	2.05
22	B	610	CLA	C1D-ND	4.35	1.43	1.37
22	b	609	CLA	MG-NB	-4.31	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	506	CLA	MG-NA	4.31	2.16	2.06
34	F	102	HEC	CBC-CAC	-4.31	1.33	1.51
22	b	611	CLA	MG-ND	4.30	2.14	2.05
29	C	517	DGD	O2G-C2G	-4.26	1.36	1.46
23	D	401	PHO	C4D-ND	-4.25	1.32	1.38
34	f	101	HEC	FE-NA	4.24	2.09	1.95
22	C	506	CLA	MG-NB	4.23	2.14	2.05
24	d	405	BCR	C30-C25	-4.19	1.48	1.53
22	b	603	CLA	MG-NB	-4.19	1.97	2.05
26	D	406	PL9	C52-C5	-4.15	1.42	1.50
22	b	603	CLA	MG-NA	4.15	2.16	2.06
29	C	515	DGD	O2G-C2G	-4.14	1.36	1.46
22	b	604	CLA	C4B-NB	4.14	1.43	1.37
22	c	510	CLA	C1D-ND	4.13	1.43	1.37
22	B	610	CLA	MG-NC	-4.13	1.96	2.06
28	a	412	SQD	O47-C7	4.10	1.45	1.34
22	B	613	CLA	MG-NA	4.07	2.15	2.06
29	C	515	DGD	C6E-C5E	4.05	1.65	1.51
22	B	609	CLA	MG-ND	4.05	2.13	2.05
28	a	411	SQD	O48-C23	4.04	1.45	1.33
33	D	410	LHG	P-O6	4.03	1.75	1.59
27	A	410	LMG	O1-C7	-4.03	1.36	1.43
34	F	102	HEC	CBB-CAB	-4.03	1.34	1.51
22	B	611	CLA	MG-NA	4.03	2.15	2.06
34	f	101	HEC	CBC-CAC	-4.03	1.34	1.51
22	B	616	CLA	C1D-ND	4.01	1.43	1.37
34	F	102	HEC	FE-ND	3.98	2.07	1.94
22	C	501	CLA	C1D-ND	3.97	1.43	1.37
22	c	508	CLA	MG-NB	-3.96	1.97	2.05
29	c	517	DGD	O3E-C3E	-3.96	1.33	1.43
34	v	201	HEC	FE-NA	3.96	2.08	1.95
27	d	410	LMG	C4-C5	3.93	1.61	1.53
33	D	409	LHG	O7-C5	-3.92	1.37	1.46
22	C	509	CLA	MG-NB	-3.89	1.98	2.05
29	c	518	DGD	C4D-C3D	3.89	1.62	1.52
29	c	517	DGD	O2G-C2G	-3.88	1.37	1.46
22	c	511	CLA	MG-NA	3.87	2.15	2.06
34	V	201	HEC	CBB-CAB	-3.87	1.35	1.51
22	c	502	CLA	C1D-ND	3.86	1.42	1.37
22	B	605	CLA	MG-NB	3.86	2.13	2.05
22	B	605	CLA	C1D-ND	3.85	1.42	1.37
22	b	603	CLA	CMD-C2D	-3.83	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	BCR	C1-C6	-3.83	1.48	1.53
22	C	502	CLA	MG-NA	3.82	2.15	2.06
22	b	610	CLA	MG-NB	-3.81	1.98	2.05
22	c	502	CLA	MG-ND	-3.80	1.98	2.05
24	K	102	BCR	C30-C25	-3.79	1.48	1.53
27	D	407	LMG	C4-C5	3.78	1.61	1.53
34	v	201	HEC	CBC-CAC	-3.78	1.35	1.51
24	F	101	BCR	C1-C6	-3.78	1.48	1.53
22	C	511	CLA	MG-NA	3.77	2.15	2.06
22	H	101	CLA	C1D-ND	3.77	1.42	1.37
22	b	615	CLA	C4B-NB	3.76	1.42	1.37
22	b	602	CLA	C1D-ND	3.73	1.42	1.37
22	b	615	CLA	CMD-C2D	-3.72	1.43	1.50
22	D	404	CLA	C1D-ND	3.71	1.42	1.37
24	B	619	BCR	C1-C6	-3.71	1.49	1.53
23	A	404	PHO	CBD-CGD	-3.70	1.47	1.52
22	C	501	CLA	MG-NB	3.70	2.13	2.05
34	V	201	HEC	FE-ND	3.69	2.06	1.94
22	C	505	CLA	CHC-C1C	3.69	1.45	1.38
28	a	412	SQD	O48-C23	3.69	1.44	1.33
22	C	504	CLA	C1B-NB	-3.68	1.33	1.37
22	A	402	CLA	MG-ND	-3.68	1.98	2.05
24	b	619	BCR	C30-C25	-3.66	1.49	1.53
22	a	410	CLA	MG-NB	3.65	2.13	2.05
22	D	403	CLA	C1D-ND	3.65	1.42	1.37
24	A	406	BCR	C1-C6	-3.64	1.49	1.53
34	V	201	HEC	FE-NB	3.64	2.06	1.94
22	C	501	CLA	MG-NA	3.64	2.14	2.06
24	K	101	BCR	C30-C25	-3.64	1.49	1.53
29	A	413	DGD	C3E-C2E	3.64	1.61	1.52
33	d	407	LHG	C24-C23	3.63	1.61	1.50
22	b	611	CLA	MG-NA	3.63	2.14	2.06
22	A	405	CLA	C4B-NB	3.63	1.42	1.37
22	B	605	CLA	C1B-C2B	3.62	1.51	1.43
22	a	410	CLA	C1D-ND	3.61	1.42	1.37
24	d	405	BCR	C1-C6	-3.61	1.49	1.53
23	A	404	PHO	CMD-C2D	-3.61	1.44	1.51
22	c	505	CLA	C4B-NB	3.61	1.42	1.37
22	B	607	CLA	MG-ND	-3.60	1.98	2.05
22	B	610	CLA	MG-ND	-3.59	1.98	2.05
27	c	522	LMG	O1-C1	3.59	1.46	1.40
22	d	403	CLA	MG-NA	3.58	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	519	DGD	O2E-C2E	-3.56	1.34	1.43
23	a	404	PHO	C4D-ND	-3.56	1.33	1.38
24	b	617	BCR	C30-C25	-3.55	1.49	1.53
22	A	402	CLA	C1B-C2B	3.54	1.51	1.43
22	c	502	CLA	MG-NA	3.53	2.14	2.06
26	d	406	PL9	C46-C44	-3.53	1.44	1.51
27	D	411	LMG	C9-C8	3.53	1.61	1.50
24	h	101	BCR	C30-C25	-3.52	1.49	1.53
22	c	506	CLA	MG-NC	-3.52	1.97	2.06
22	B	616	CLA	MG-ND	3.51	2.12	2.05
22	A	405	CLA	MG-NC	-3.51	1.97	2.06
22	B	602	CLA	MG-ND	-3.51	1.98	2.05
22	c	505	CLA	MG-NB	-3.50	1.98	2.05
22	c	509	CLA	CHC-C1C	3.49	1.45	1.38
22	c	508	CLA	C1D-ND	3.49	1.42	1.37
22	c	507	CLA	MG-ND	-3.49	1.98	2.05
27	b	621	LMG	O7-C8	-3.48	1.38	1.46
22	B	614	CLA	MG-NA	3.48	2.14	2.06
22	D	405	CLA	C1D-ND	3.47	1.42	1.37
22	C	509	CLA	MG-NA	3.46	2.14	2.06
28	B	622	SQD	O48-C23	3.46	1.43	1.33
22	B	613	CLA	C4B-NB	3.46	1.42	1.37
29	C	515	DGD	C4E-C3E	3.45	1.61	1.52
24	B	617	BCR	C30-C25	-3.45	1.49	1.53
34	V	201	HEC	CBC-CAC	-3.45	1.36	1.51
24	H	102	BCR	C30-C25	-3.44	1.49	1.53
22	D	405	CLA	CMD-C2D	-3.43	1.43	1.50
29	c	519	DGD	O3D-C3D	-3.43	1.34	1.43
22	C	505	CLA	MG-NA	3.43	2.14	2.06
22	B	609	CLA	C1B-C2B	3.43	1.51	1.43
34	v	201	HEC	CBB-CAB	-3.43	1.36	1.51
22	A	405	CLA	MG-NA	3.42	2.14	2.06
22	C	507	CLA	C1D-ND	3.42	1.42	1.37
24	b	619	BCR	C1-C6	-3.42	1.49	1.53
26	D	406	PL9	C7-C3	-3.41	1.46	1.51
22	B	602	CLA	C4B-NB	3.40	1.42	1.37
27	d	410	LMG	O7-C8	-3.40	1.38	1.46
22	C	505	CLA	MG-ND	3.39	2.12	2.05
26	d	406	PL9	C26-C24	-3.39	1.44	1.51
28	B	622	SQD	O47-C7	3.39	1.43	1.34
28	f	102	SQD	O48-C23	3.39	1.43	1.33
24	k	101	BCR	C1-C6	-3.38	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	412	SQD	O48-C23	3.38	1.43	1.33
22	C	502	CLA	MG-NB	-3.38	1.99	2.05
27	a	415	LMG	O8-C9	-3.37	1.37	1.45
22	C	504	CLA	MG-NB	3.36	2.12	2.05
22	b	609	CLA	C1D-ND	3.36	1.42	1.37
23	D	401	PHO	CMB-C2B	-3.36	1.44	1.51
23	d	401	PHO	C4D-ND	-3.34	1.33	1.38
22	b	606	CLA	C1D-ND	3.34	1.42	1.37
22	b	604	CLA	MG-ND	-3.34	1.99	2.05
22	B	610	CLA	CMB-C2B	-3.33	1.43	1.50
22	B	615	CLA	MG-NA	3.33	2.14	2.06
22	C	505	CLA	C4B-NB	3.33	1.42	1.37
22	c	507	CLA	MG-NB	3.32	2.12	2.05
22	C	506	CLA	C4B-NB	3.31	1.42	1.37
22	b	601	CLA	C1B-C2B	3.30	1.50	1.43
22	a	405	CLA	CHC-C4B	-3.29	1.32	1.39
27	Y	101	LMG	O7-C8	-3.29	1.38	1.46
22	C	511	CLA	C1B-C2B	3.29	1.50	1.43
22	b	614	CLA	C1D-ND	3.28	1.42	1.37
22	A	405	CLA	C1D-ND	3.28	1.42	1.37
28	A	411	SQD	O48-C23	3.28	1.42	1.33
22	B	606	CLA	C1D-ND	3.27	1.42	1.37
22	C	513	CLA	C1D-ND	3.27	1.42	1.37
22	A	403	CLA	C3B-C4B	3.26	1.52	1.42
27	c	523	LMG	C4-C5	3.26	1.60	1.53
22	C	508	CLA	C1B-C2B	3.25	1.50	1.43
26	d	406	PL9	C3-C4	-3.22	1.44	1.49
22	B	615	CLA	CMD-C2D	-3.22	1.44	1.50
22	c	513	CLA	C1D-ND	3.22	1.42	1.37
22	C	506	CLA	C1D-ND	3.22	1.42	1.37
24	K	101	BCR	C1-C6	-3.21	1.49	1.53
22	A	402	CLA	C1B-NB	-3.21	1.33	1.37
34	F	102	HEC	FE-NA	3.21	2.05	1.95
33	d	409	LHG	P-O6	3.21	1.71	1.59
22	C	502	CLA	C1B-C2B	3.20	1.50	1.43
22	H	101	CLA	MG-ND	-3.19	1.99	2.05
28	L	101	SQD	O48-C23	3.19	1.42	1.33
22	a	403	CLA	C1D-ND	3.19	1.42	1.37
29	H	103	DGD	C4D-C5D	3.18	1.59	1.53
22	A	403	CLA	C4B-NB	3.18	1.42	1.37
29	A	413	DGD	C4D-C3D	3.18	1.60	1.52
22	a	405	CLA	C1B-C2B	3.17	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	103	DGD	C3E-C2E	3.17	1.60	1.52
29	A	413	DGD	C1E-C2E	3.17	1.61	1.52
22	b	602	CLA	CMD-C2D	-3.17	1.44	1.50
22	c	508	CLA	MG-ND	3.17	2.12	2.05
22	H	101	CLA	C4B-NB	3.17	1.42	1.37
26	d	406	PL9	C25-C24	-3.16	1.43	1.50
22	A	402	CLA	MG-NA	3.15	2.13	2.06
22	b	616	CLA	C1D-ND	3.14	1.42	1.37
22	a	405	CLA	CMC-C2C	-3.14	1.44	1.50
29	A	413	DGD	C4E-C5E	3.14	1.59	1.53
22	d	403	CLA	C1B-C2B	3.13	1.50	1.43
22	c	512	CLA	C1B-C2B	3.13	1.50	1.43
22	c	512	CLA	CHC-C1C	3.13	1.44	1.38
24	B	618	BCR	C30-C25	-3.13	1.49	1.53
24	T	101	BCR	C30-C25	-3.12	1.49	1.53
22	c	507	CLA	CMD-C2D	-3.12	1.44	1.50
22	A	403	CLA	C1D-ND	3.12	1.42	1.37
22	D	405	CLA	C1B-C2B	3.12	1.50	1.43
26	d	406	PL9	C31-C29	-3.11	1.44	1.51
22	H	101	CLA	C1B-C2B	3.11	1.50	1.43
22	b	601	CLA	C1D-ND	3.11	1.41	1.37
24	a	406	BCR	C38-C26	-3.10	1.46	1.50
26	a	409	PL9	C7-C3	3.10	1.55	1.51
22	c	507	CLA	C1D-ND	3.10	1.41	1.37
22	a	403	CLA	MG-NA	3.09	2.13	2.06
28	A	412	SQD	O47-C45	-3.08	1.41	1.47
22	B	613	CLA	C1D-ND	3.08	1.41	1.37
28	f	102	SQD	O47-C7	3.07	1.43	1.34
22	d	404	CLA	C1B-C2B	3.07	1.50	1.43
22	c	513	CLA	MG-NB	3.07	2.11	2.05
22	C	501	CLA	C4B-NB	3.06	1.41	1.37
24	b	617	BCR	C1-C6	-3.06	1.49	1.53
22	c	513	CLA	C1B-C2B	3.06	1.50	1.43
28	D	408	SQD	O48-C23	3.05	1.42	1.33
29	A	413	DGD	O5D-C6D	-3.05	1.38	1.43
24	c	515	BCR	C30-C25	-3.04	1.49	1.53
24	B	617	BCR	C1-C6	-3.03	1.49	1.53
29	A	413	DGD	O1G-C1G	-3.03	1.38	1.45
22	C	505	CLA	MG-NB	-3.02	1.99	2.05
22	C	513	CLA	MG-NA	3.01	2.13	2.06
23	A	404	PHO	C1D-C2D	3.01	1.42	1.39
29	H	103	DGD	C1G-C2G	3.01	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	CMC-C2C	-3.01	1.44	1.50
28	L	101	SQD	O47-C7	3.01	1.42	1.34
22	B	603	CLA	CMD-C2D	-3.01	1.44	1.50
22	A	403	CLA	MG-ND	3.00	2.11	2.05
22	b	605	CLA	MG-ND	3.00	2.11	2.05
29	C	515	DGD	O5D-C1E	2.99	1.45	1.40
22	B	612	CLA	CMC-C2C	-2.99	1.44	1.50
23	a	404	PHO	CBD-CGD	-2.99	1.48	1.52
28	A	412	SQD	O47-C7	2.99	1.42	1.34
22	C	511	CLA	C1D-ND	2.98	1.41	1.37
22	b	607	CLA	MG-ND	-2.98	1.99	2.05
22	C	508	CLA	C3B-C4B	2.97	1.51	1.42
22	B	602	CLA	C1B-C2B	2.97	1.50	1.43
22	c	512	CLA	C4B-NB	2.96	1.41	1.37
22	C	508	CLA	MG-ND	2.96	2.11	2.05
22	b	613	CLA	MG-NA	2.96	2.13	2.06
23	A	404	PHO	CAC-C3C	-2.96	1.46	1.51
22	C	503	CLA	C4B-NB	2.95	1.41	1.37
29	A	413	DGD	O2G-C2G	-2.95	1.39	1.46
22	B	611	CLA	C1B-NB	-2.94	1.34	1.37
27	c	520	LMG	O1-C1	2.93	1.45	1.40
22	C	510	CLA	MG-NC	2.93	2.13	2.06
22	a	402	CLA	C1B-NB	-2.92	1.34	1.37
27	D	411	LMG	C7-C8	2.92	1.58	1.51
22	a	402	CLA	CHC-C1C	2.92	1.44	1.38
22	b	608	CLA	CHC-C1C	2.91	1.44	1.38
24	K	102	BCR	C1-C6	-2.91	1.50	1.53
23	d	401	PHO	CMC-C2C	-2.91	1.46	1.50
24	K	103	BCR	C1-C6	-2.91	1.50	1.53
22	b	609	CLA	C4B-NB	2.90	1.41	1.37
27	c	523	LMG	O1-C7	-2.90	1.38	1.43
22	B	602	CLA	MG-NA	2.90	2.13	2.06
22	B	611	CLA	C1B-C2B	2.89	1.49	1.43
22	b	606	CLA	C1B-C2B	2.89	1.49	1.43
22	D	404	CLA	CHC-C1C	2.89	1.44	1.38
23	D	401	PHO	CAC-C3C	-2.89	1.46	1.51
22	b	613	CLA	MG-ND	-2.89	2.00	2.05
22	C	507	CLA	MG-ND	2.89	2.11	2.05
22	b	607	CLA	CMD-C2D	-2.89	1.44	1.50
22	a	403	CLA	CHC-C1C	2.88	1.44	1.38
22	A	405	CLA	MG-ND	-2.88	2.00	2.05
33	E	101	LHG	P-O6	2.88	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	402	CLA	C4B-NB	2.88	1.41	1.37
22	a	403	CLA	CMB-C2B	-2.88	1.44	1.50
29	c	519	DGD	O4D-C4D	-2.88	1.35	1.43
22	b	613	CLA	C1D-ND	2.87	1.41	1.37
22	c	509	CLA	C1D-ND	2.87	1.41	1.37
22	a	405	CLA	C1D-ND	2.87	1.41	1.37
22	b	605	CLA	C3B-C4B	2.87	1.51	1.42
26	D	406	PL9	C31-C29	-2.87	1.45	1.51
22	c	503	CLA	C1D-ND	2.86	1.41	1.37
22	b	601	CLA	C4B-NB	2.86	1.41	1.37
22	c	513	CLA	MG-NA	2.86	2.13	2.06
22	a	402	CLA	C1B-C2B	2.86	1.49	1.43
22	C	503	CLA	C1B-C2B	2.85	1.49	1.43
24	T	101	BCR	C38-C26	-2.84	1.46	1.50
22	c	507	CLA	CHC-C1C	2.84	1.44	1.38
22	B	606	CLA	C4B-NB	2.84	1.41	1.37
22	c	510	CLA	C1B-C2B	2.84	1.49	1.43
22	c	511	CLA	CMB-C2B	-2.84	1.45	1.50
22	a	402	CLA	CMB-C2B	-2.84	1.45	1.50
22	c	512	CLA	MG-ND	2.84	2.11	2.05
29	C	517	DGD	C6E-C5E	2.84	1.61	1.51
23	A	404	PHO	C3B-C2B	-2.83	1.36	1.40
22	B	615	CLA	C1D-ND	2.83	1.41	1.37
22	a	403	CLA	C4B-NB	2.82	1.41	1.37
22	D	405	CLA	MG-ND	-2.82	2.00	2.05
24	k	102	BCR	C30-C25	-2.82	1.50	1.53
29	c	518	DGD	C3E-C2E	2.82	1.59	1.52
22	b	605	CLA	C1B-C2B	2.82	1.49	1.43
22	B	612	CLA	C1C-NC	-2.81	1.33	1.37
22	a	405	CLA	CMD-C2D	-2.81	1.45	1.50
28	A	411	SQD	O47-C7	2.81	1.42	1.34
22	c	507	CLA	C4B-NB	2.81	1.41	1.37
24	F	101	BCR	C30-C25	-2.81	1.50	1.53
22	C	504	CLA	MG-NC	2.81	2.12	2.06
22	B	608	CLA	C1B-C2B	2.81	1.49	1.43
23	A	404	PHO	C4D-ND	-2.81	1.34	1.38
22	B	608	CLA	C1D-ND	2.80	1.41	1.37
28	A	411	SQD	O2-C2	-2.80	1.36	1.43
22	C	509	CLA	C1D-ND	2.80	1.41	1.37
22	B	607	CLA	MG-NA	2.80	2.12	2.06
33	D	410	LHG	O7-C5	-2.80	1.40	1.46
27	M	101	LMG	C4-C3	2.79	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	MG-NB	2.79	2.11	2.05
22	B	616	CLA	C1B-C2B	2.78	1.49	1.43
22	C	509	CLA	CMB-C2B	-2.78	1.45	1.50
27	b	621	LMG	C4-C3	2.78	1.59	1.52
22	c	508	CLA	C1B-C2B	2.78	1.49	1.43
22	C	509	CLA	MG-NC	-2.78	1.99	2.06
22	b	602	CLA	C1B-C2B	2.77	1.49	1.43
22	C	507	CLA	C1B-C2B	2.77	1.49	1.43
22	b	614	CLA	CMC-C2C	-2.77	1.45	1.50
22	b	611	CLA	C1D-ND	2.77	1.41	1.37
22	d	403	CLA	C4B-NB	2.77	1.41	1.37
24	k	101	BCR	C30-C25	-2.77	1.50	1.53
23	A	404	PHO	CMC-C2C	-2.76	1.46	1.50
22	B	612	CLA	C1B-NB	-2.76	1.34	1.37
23	D	401	PHO	C1D-C2D	2.76	1.42	1.39
26	a	409	PL9	C53-C6	-2.76	1.45	1.50
22	d	404	CLA	C4B-NB	2.75	1.41	1.37
27	c	522	LMG	C4-C3	2.75	1.59	1.52
23	d	401	PHO	C1D-ND	2.75	1.43	1.38
22	b	604	CLA	C1B-C2B	2.75	1.49	1.43
22	B	605	CLA	C3B-C4B	2.74	1.50	1.42
22	b	613	CLA	CMB-C2B	-2.74	1.45	1.50
22	A	405	CLA	MG-NB	-2.73	2.00	2.05
22	b	607	CLA	C1D-ND	2.73	1.41	1.37
33	L	102	LHG	O7-C5	-2.73	1.40	1.46
24	A	406	BCR	C30-C25	-2.73	1.50	1.53
22	C	502	CLA	C3B-C4B	2.73	1.50	1.42
29	C	517	DGD	O3G-C1D	2.73	1.44	1.40
22	b	609	CLA	CMB-C2B	-2.72	1.45	1.50
24	c	516	BCR	C30-C25	-2.72	1.50	1.53
29	C	516	DGD	O2G-C2G	-2.72	1.40	1.46
22	b	616	CLA	C3B-C4B	2.72	1.50	1.42
22	c	509	CLA	C1B-C2B	2.71	1.49	1.43
22	c	508	CLA	CMD-C2D	-2.71	1.45	1.50
22	B	614	CLA	C1D-ND	2.70	1.41	1.37
22	C	511	CLA	C4B-NB	2.70	1.41	1.37
22	b	604	CLA	C1D-ND	2.70	1.41	1.37
22	b	601	CLA	CHC-C1C	2.70	1.43	1.38
22	C	505	CLA	C1B-C2B	2.70	1.49	1.43
22	B	615	CLA	C1B-C2B	2.70	1.49	1.43
33	D	412	LHG	O7-C5	-2.70	1.40	1.46
22	C	510	CLA	CMD-C2D	-2.70	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	103	BCR	C30-C25	-2.69	1.50	1.53
29	c	518	DGD	O1G-C1G	-2.69	1.39	1.45
22	B	604	CLA	C1D-ND	2.69	1.41	1.37
22	c	502	CLA	C4B-NB	2.69	1.41	1.37
22	B	611	CLA	C1D-ND	2.68	1.41	1.37
27	a	415	LMG	C3-C2	2.67	1.59	1.52
22	c	507	CLA	C1B-C2B	2.67	1.49	1.43
22	A	405	CLA	CMD-C2D	-2.66	1.45	1.50
22	b	608	CLA	C1D-ND	2.66	1.41	1.37
22	a	410	CLA	CMB-C2B	-2.66	1.45	1.50
22	c	504	CLA	C1D-ND	2.66	1.41	1.37
29	C	516	DGD	C1E-C2E	2.66	1.60	1.52
22	D	403	CLA	C4B-NB	2.66	1.41	1.37
22	B	616	CLA	CMC-C2C	-2.65	1.45	1.50
22	C	501	CLA	CHC-C1C	2.65	1.43	1.38
27	c	520	LMG	C4-C3	2.65	1.59	1.52
22	b	615	CLA	C1D-ND	2.65	1.41	1.37
22	b	611	CLA	MG-NC	2.64	2.12	2.06
33	d	407	LHG	O7-C5	-2.64	1.40	1.46
22	c	509	CLA	C3B-C4B	2.64	1.50	1.42
29	c	517	DGD	C4D-C3D	2.64	1.59	1.52
29	h	102	DGD	O1G-C1G	-2.64	1.39	1.45
22	C	502	CLA	C4B-NB	2.64	1.41	1.37
23	A	404	PHO	CMB-C2B	-2.64	1.46	1.51
22	c	514	CLA	C1B-C2B	2.64	1.49	1.43
22	b	615	CLA	C3B-C4B	2.64	1.50	1.42
22	b	611	CLA	CHC-C1C	2.63	1.43	1.38
27	c	522	LMG	C3-C2	2.63	1.59	1.52
22	c	512	CLA	C3B-C4B	2.63	1.50	1.42
24	A	406	BCR	C33-C5	-2.63	1.46	1.50
22	C	506	CLA	C1B-NB	-2.63	1.34	1.37
29	A	413	DGD	C4D-C5D	2.62	1.58	1.53
22	B	611	CLA	CMB-C2B	-2.62	1.45	1.50
22	C	501	CLA	C3B-C4B	2.61	1.50	1.42
34	v	201	HEC	CMA-C3A	2.61	1.56	1.50
22	d	403	CLA	CMD-C2D	-2.60	1.45	1.50
22	b	606	CLA	CMB-C2B	-2.60	1.45	1.50
22	c	512	CLA	MG-NC	2.60	2.12	2.06
22	B	605	CLA	C1B-NB	-2.60	1.34	1.37
22	B	608	CLA	C1B-NB	-2.60	1.34	1.37
24	C	514	BCR	C30-C25	-2.60	1.50	1.53
22	C	502	CLA	CHC-C1C	2.60	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	e	101	LHG	P-O6	2.60	1.69	1.59
22	c	513	CLA	CMD-C2D	-2.59	1.45	1.50
24	b	618	BCR	C1-C6	-2.59	1.50	1.53
22	B	603	CLA	CMB-C2B	-2.59	1.45	1.50
22	c	514	CLA	C3B-C4B	2.59	1.50	1.42
27	c	522	LMG	C1-C2	2.59	1.60	1.52
22	C	511	CLA	C3B-C4B	2.59	1.50	1.42
22	C	504	CLA	O2D-CGD	2.58	1.39	1.33
22	B	611	CLA	MG-NC	-2.58	2.00	2.06
22	c	510	CLA	CHC-C1C	2.58	1.43	1.38
29	c	517	DGD	O3D-C3D	-2.57	1.36	1.43
22	b	611	CLA	C1B-NB	-2.57	1.34	1.37
22	a	402	CLA	C1D-ND	2.57	1.41	1.37
22	c	502	CLA	CMD-C2D	-2.57	1.45	1.50
22	B	614	CLA	CMC-C2C	-2.57	1.45	1.50
22	C	506	CLA	CMC-C2C	-2.57	1.45	1.50
22	c	504	CLA	C1B-C2B	2.57	1.49	1.43
22	a	410	CLA	C1B-C2B	2.57	1.49	1.43
23	D	401	PHO	CMD-C2D	-2.57	1.46	1.51
22	b	601	CLA	O2A-CGA	2.57	1.40	1.33
23	d	401	PHO	CAC-C3C	-2.56	1.47	1.51
22	A	403	CLA	CMD-C2D	-2.56	1.45	1.50
22	b	613	CLA	CMD-C2D	-2.56	1.45	1.50
22	b	607	CLA	CMB-C2B	-2.56	1.45	1.50
22	c	510	CLA	MG-ND	2.56	2.10	2.05
22	B	604	CLA	C3B-C4B	2.55	1.50	1.42
22	c	509	CLA	CMD-C2D	-2.55	1.45	1.50
22	b	611	CLA	C1B-C2B	2.55	1.49	1.43
22	B	609	CLA	CMD-C2D	-2.55	1.45	1.50
22	D	404	CLA	CMD-C2D	-2.55	1.45	1.50
29	C	515	DGD	O1G-C1A	2.54	1.40	1.33
22	C	507	CLA	C1B-NB	-2.54	1.34	1.37
27	a	415	LMG	C14-C13	2.54	1.64	1.51
22	B	602	CLA	CMB-C2B	-2.54	1.45	1.50
24	a	406	BCR	C30-C25	-2.54	1.50	1.53
22	C	503	CLA	C3B-C4B	2.54	1.50	1.42
22	b	608	CLA	C3B-C4B	2.54	1.50	1.42
22	C	501	CLA	C1B-C2B	2.54	1.49	1.43
34	f	101	HEC	FE-ND	2.53	2.02	1.94
22	c	514	CLA	CHC-C1C	2.53	1.43	1.38
22	H	101	CLA	C3B-C4B	2.53	1.50	1.42
22	C	508	CLA	C4B-NB	2.51	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	103	DGD	C4E-C3E	2.51	1.58	1.52
22	C	503	CLA	CHC-C1C	2.51	1.43	1.38
29	h	102	DGD	O3E-C3E	-2.51	1.36	1.43
22	C	504	CLA	CMD-C2D	-2.50	1.45	1.50
22	c	513	CLA	C4B-NB	2.50	1.41	1.37
22	d	404	CLA	C3B-C4B	2.50	1.50	1.42
22	c	505	CLA	CMD-C2D	-2.50	1.45	1.50
22	C	501	CLA	C1B-NB	-2.50	1.34	1.37
22	B	615	CLA	CMB-C2B	-2.50	1.45	1.50
22	c	503	CLA	C1B-C2B	2.49	1.49	1.43
22	c	511	CLA	C1D-ND	2.49	1.41	1.37
24	t	101	BCR	C30-C25	-2.49	1.50	1.53
29	h	102	DGD	C4D-C3D	2.49	1.58	1.52
22	C	512	CLA	C1D-ND	2.49	1.41	1.37
27	d	410	LMG	O6-C5	-2.49	1.38	1.44
22	b	610	CLA	C1B-C2B	2.49	1.49	1.43
22	c	502	CLA	C1B-C2B	2.49	1.49	1.43
22	A	403	CLA	C1B-C2B	2.49	1.49	1.43
29	C	516	DGD	C6E-C5E	2.48	1.60	1.51
22	C	510	CLA	C1D-ND	2.48	1.41	1.37
22	C	513	CLA	CMB-C2B	-2.48	1.45	1.50
22	B	613	CLA	C1B-C2B	2.48	1.48	1.43
22	C	512	CLA	C3B-C4B	2.47	1.49	1.42
26	d	406	PL9	C30-C29	-2.47	1.44	1.50
29	H	103	DGD	O6D-C5D	-2.47	1.38	1.44
29	c	517	DGD	C3D-C2D	2.47	1.58	1.52
22	C	513	CLA	C3B-C4B	2.47	1.49	1.42
22	C	504	CLA	C3B-C4B	2.47	1.49	1.42
29	c	518	DGD	O3D-C3D	-2.46	1.36	1.43
22	b	614	CLA	O2D-CGD	2.46	1.39	1.33
29	c	519	DGD	O3G-C3G	-2.45	1.39	1.43
22	C	513	CLA	C1B-C2B	2.45	1.48	1.43
22	D	403	CLA	CMB-C2B	-2.45	1.45	1.50
22	C	513	CLA	CMC-C2C	-2.45	1.45	1.50
33	E	101	LHG	C24-C23	2.44	1.57	1.50
22	c	503	CLA	CMD-C2D	-2.44	1.45	1.50
26	d	406	PL9	C53-C6	-2.44	1.45	1.50
22	c	504	CLA	CMB-C2B	-2.44	1.45	1.50
22	b	606	CLA	CHC-C4B	-2.44	1.34	1.39
22	b	614	CLA	C1B-NB	-2.44	1.34	1.37
22	C	504	CLA	CHC-C1C	2.44	1.43	1.38
22	B	610	CLA	MG-NA	2.43	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	CMD-C2D	-2.43	1.45	1.50
22	B	612	CLA	C3B-C4B	2.43	1.49	1.42
23	A	404	PHO	C4D-CHA	2.43	1.43	1.39
24	c	516	BCR	C33-C5	-2.43	1.47	1.50
22	c	503	CLA	MG-NA	2.43	2.12	2.06
22	C	502	CLA	C1D-ND	2.43	1.41	1.37
22	c	509	CLA	CMB-C2B	-2.42	1.45	1.50
22	B	613	CLA	CHC-C1C	2.42	1.43	1.38
22	b	610	CLA	MG-NC	2.42	2.12	2.06
22	a	403	CLA	CMD-C2D	-2.42	1.45	1.50
34	f	101	HEC	FE-NB	2.42	2.02	1.94
22	b	614	CLA	C4B-NB	2.42	1.41	1.37
22	A	402	CLA	C1D-ND	2.42	1.41	1.37
28	A	411	SQD	O3-C3	-2.42	1.37	1.43
22	B	615	CLA	O2D-CGD	2.41	1.39	1.33
22	C	504	CLA	C4B-NB	2.41	1.41	1.37
22	B	606	CLA	CMC-C2C	-2.41	1.45	1.50
29	C	515	DGD	C4D-C3D	2.41	1.58	1.52
22	B	607	CLA	C1B-NB	-2.41	1.34	1.37
22	c	505	CLA	C1B-NB	-2.41	1.34	1.37
22	d	403	CLA	CHC-C4B	-2.41	1.34	1.39
27	c	523	LMG	O7-C8	-2.40	1.40	1.46
24	b	617	BCR	C33-C5	-2.40	1.47	1.50
22	b	612	CLA	C1D-ND	2.40	1.41	1.37
22	B	606	CLA	CHC-C1C	2.40	1.43	1.38
27	c	523	LMG	C1-C2	2.40	1.59	1.52
22	C	513	CLA	MG-ND	2.40	2.10	2.05
22	c	507	CLA	C3B-C4B	2.39	1.49	1.42
22	C	512	CLA	C4B-NB	2.39	1.41	1.37
22	c	504	CLA	C4B-NB	2.39	1.41	1.37
22	a	405	CLA	C1B-NB	-2.39	1.34	1.37
22	B	605	CLA	CMC-C2C	-2.39	1.45	1.50
27	c	523	LMG	O8-C9	-2.39	1.39	1.45
22	B	606	CLA	CMB-C2B	-2.39	1.45	1.50
22	b	606	CLA	CMD-C2D	-2.38	1.45	1.50
27	b	621	LMG	C4-C5	2.38	1.58	1.53
22	b	616	CLA	CMC-C2C	-2.38	1.45	1.50
33	D	410	LHG	O3-C3	-2.38	1.35	1.44
22	B	607	CLA	C1D-ND	2.38	1.41	1.37
22	C	503	CLA	CMB-C2B	-2.37	1.45	1.50
22	c	504	CLA	C5-C3	-2.37	1.46	1.51
31	j	101	STE	C2-C1	2.37	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	CMC-C2C	-2.37	1.45	1.50
22	b	613	CLA	CAA-C2A	-2.37	1.49	1.54
22	A	405	CLA	C1B-C2B	2.37	1.48	1.43
29	h	102	DGD	C4E-C5E	2.37	1.58	1.53
22	b	604	CLA	C3B-C4B	2.36	1.49	1.42
27	b	621	LMG	C1-C2	2.36	1.59	1.52
22	B	616	CLA	CMD-C2D	-2.36	1.45	1.50
22	c	509	CLA	MG-NC	-2.36	2.00	2.06
29	h	102	DGD	O2D-C2D	-2.36	1.37	1.43
24	T	101	BCR	C27-C26	-2.36	1.46	1.51
22	H	101	CLA	CMC-C2C	-2.36	1.45	1.50
22	C	501	CLA	C1D-C2D	2.35	1.50	1.45
22	C	512	CLA	CHC-C1C	2.35	1.43	1.38
22	B	610	CLA	CMD-C2D	-2.35	1.46	1.50
22	d	404	CLA	MG-ND	-2.34	2.01	2.05
22	c	506	CLA	CHC-C1C	2.34	1.43	1.38
22	b	615	CLA	CMC-C2C	-2.34	1.46	1.50
22	b	615	CLA	CHC-C1C	2.34	1.43	1.38
22	a	403	CLA	C1B-C2B	2.34	1.48	1.43
23	d	401	PHO	C1D-C2D	2.34	1.42	1.39
22	c	502	CLA	CMC-C2C	-2.34	1.46	1.50
22	A	402	CLA	C5-C3	-2.34	1.46	1.51
22	D	403	CLA	C1B-C2B	2.34	1.48	1.43
23	d	401	PHO	CMD-C2D	-2.34	1.46	1.51
22	b	609	CLA	C3B-C4B	2.34	1.49	1.42
22	D	404	CLA	C4B-NB	2.34	1.40	1.37
22	b	612	CLA	CMC-C2C	-2.34	1.46	1.50
22	B	616	CLA	CAC-C3C	-2.34	1.45	1.51
29	c	519	DGD	C2A-C1A	-2.34	1.43	1.50
22	c	505	CLA	CMC-C2C	-2.34	1.46	1.50
22	C	510	CLA	C1B-C2B	2.34	1.48	1.43
28	B	622	SQD	O2-C2	-2.33	1.37	1.43
22	c	507	CLA	C1B-NB	-2.33	1.34	1.37
22	b	616	CLA	MG-NC	-2.33	2.00	2.06
22	b	614	CLA	CHC-C1C	2.33	1.43	1.38
22	c	505	CLA	CMB-C2B	-2.33	1.46	1.50
23	d	401	PHO	CMB-C2B	-2.33	1.47	1.51
26	d	406	PL9	C45-C44	-2.33	1.45	1.50
22	B	607	CLA	CMD-C2D	-2.33	1.46	1.50
22	C	509	CLA	C1B-C2B	2.33	1.48	1.43
22	B	614	CLA	C1B-NB	-2.33	1.34	1.37
22	c	504	CLA	MG-NC	2.33	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	CMB-C2B	-2.33	1.46	1.50
27	b	623	LMG	C4-C5	2.33	1.58	1.53
22	B	613	CLA	CMD-C2D	-2.33	1.46	1.50
22	B	613	CLA	CMC-C2C	-2.32	1.46	1.50
28	A	411	SQD	O47-C45	-2.32	1.41	1.46
22	B	603	CLA	C3B-C4B	2.32	1.49	1.42
22	B	610	CLA	C3D-C4D	2.32	1.49	1.44
22	b	614	CLA	C1A-CHA	-2.31	1.33	1.43
22	B	603	CLA	MG-NB	-2.31	2.01	2.05
22	b	606	CLA	C3B-C4B	2.31	1.49	1.42
24	C	514	BCR	C33-C5	-2.31	1.47	1.50
22	b	608	CLA	C1B-C2B	2.31	1.48	1.43
22	b	609	CLA	O2D-CGD	2.31	1.38	1.33
22	c	505	CLA	C1B-C2B	2.31	1.48	1.43
22	C	511	CLA	CMC-C2C	-2.31	1.46	1.50
22	A	402	CLA	CMB-C2B	-2.31	1.46	1.50
22	d	403	CLA	C1B-NB	-2.31	1.34	1.37
22	b	602	CLA	CHC-C4B	-2.31	1.34	1.39
22	C	501	CLA	CMD-C2D	-2.31	1.46	1.50
23	d	401	PHO	C4D-CHA	2.30	1.43	1.39
31	B	620	STE	C2-C1	2.30	1.55	1.50
27	a	415	LMG	C4-C3	2.30	1.58	1.52
22	C	510	CLA	MG-NA	2.30	2.11	2.06
22	c	511	CLA	C1B-C2B	2.30	1.48	1.43
22	b	605	CLA	C4B-NB	2.30	1.40	1.37
22	b	603	CLA	C1B-C2B	2.30	1.48	1.43
22	C	512	CLA	C1B-C2B	2.29	1.48	1.43
22	c	504	CLA	CHC-C1C	2.29	1.43	1.38
22	A	405	CLA	CHC-C4B	-2.29	1.34	1.39
33	D	409	LHG	C3-C2	2.29	1.58	1.51
22	c	503	CLA	MG-NB	-2.29	2.01	2.05
22	b	615	CLA	C1B-C2B	2.29	1.48	1.43
22	B	613	CLA	O2D-CED	-2.29	1.40	1.45
23	D	401	PHO	O2D-CGD	2.28	1.38	1.33
22	C	504	CLA	C1B-C2B	2.28	1.48	1.43
29	c	518	DGD	C6D-C5D	2.28	1.58	1.51
22	B	615	CLA	C4B-NB	2.28	1.40	1.37
22	c	503	CLA	CMC-C2C	-2.28	1.46	1.50
22	d	403	CLA	CMB-C2B	-2.28	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.28	1.46	1.50
28	a	411	SQD	O47-C7	2.28	1.40	1.34
29	C	516	DGD	C4E-C3E	2.28	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	f	102	SQD	O3-C3	-2.28	1.37	1.43
22	C	511	CLA	CMB-C2B	-2.27	1.46	1.50
29	C	516	DGD	O3D-C3D	-2.27	1.37	1.43
26	D	406	PL9	C27-C28	-2.27	1.43	1.50
22	a	403	CLA	MG-NC	2.27	2.11	2.06
27	Y	101	LMG	C3-C2	2.27	1.58	1.52
22	a	402	CLA	C3B-C4B	2.27	1.49	1.42
22	b	607	CLA	C1B-C2B	2.27	1.48	1.43
22	b	610	CLA	CMD-C2D	-2.27	1.46	1.50
22	b	613	CLA	C1B-C2B	2.27	1.48	1.43
22	B	610	CLA	C3B-C4B	2.27	1.49	1.42
22	b	614	CLA	CMB-C2B	-2.27	1.46	1.50
22	c	514	CLA	C4B-NB	2.26	1.40	1.37
22	B	613	CLA	MG-NC	2.26	2.11	2.06
31	M	102	STE	O1-C1	2.26	1.29	1.22
22	b	613	CLA	C4B-NB	2.26	1.40	1.37
22	D	405	CLA	C3B-C4B	2.26	1.49	1.42
22	c	505	CLA	C3B-C4B	2.26	1.49	1.42
22	B	609	CLA	C3B-C4B	2.26	1.49	1.42
29	c	517	DGD	C4E-C3E	2.26	1.58	1.52
22	c	511	CLA	C1B-NB	-2.25	1.34	1.37
22	B	606	CLA	C1B-C2B	2.25	1.48	1.43
22	C	507	CLA	C3B-C4B	2.25	1.49	1.42
22	c	504	CLA	CMC-C2C	-2.25	1.46	1.50
22	b	608	CLA	C4B-NB	2.25	1.40	1.37
22	c	513	CLA	CMB-C2B	-2.25	1.46	1.50
29	C	517	DGD	C4E-C3E	2.25	1.58	1.52
22	C	503	CLA	CHC-C4B	-2.24	1.34	1.39
22	C	510	CLA	CMC-C2C	-2.24	1.46	1.50
24	c	516	BCR	C36-C18	-2.24	1.46	1.50
22	C	513	CLA	C4B-NB	2.24	1.40	1.37
22	c	514	CLA	CMC-C2C	-2.24	1.46	1.50
22	c	513	CLA	C1B-NB	-2.24	1.34	1.37
22	C	506	CLA	C1B-C2B	2.24	1.48	1.43
22	a	410	CLA	MG-NC	-2.24	2.01	2.06
22	b	601	CLA	C1D-C2D	2.23	1.49	1.45
22	B	614	CLA	CHC-C1C	2.23	1.43	1.38
22	C	512	CLA	MG-NA	2.23	2.11	2.06
22	c	507	CLA	CMC-C2C	-2.23	1.46	1.50
26	a	409	PL9	C18-C19	2.23	1.38	1.33
22	b	603	CLA	CMB-C2B	-2.23	1.46	1.50
27	c	520	LMG	O2-C2	-2.23	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	409	PL9	C3-C4	2.23	1.53	1.49
22	C	501	CLA	CMC-C2C	-2.23	1.46	1.50
22	B	605	CLA	C5-C3	-2.23	1.46	1.51
23	a	404	PHO	C3D-CAD	-2.22	1.43	1.47
29	c	519	DGD	C1D-C2D	2.22	1.59	1.52
22	D	405	CLA	CHC-C4B	-2.22	1.34	1.39
22	b	604	CLA	C3D-C4D	2.22	1.49	1.44
27	a	415	LMG	O7-C10	2.22	1.40	1.34
22	C	509	CLA	CMD-C2D	-2.22	1.46	1.50
24	h	101	BCR	C1-C6	-2.22	1.50	1.53
22	B	612	CLA	MG-NC	2.22	2.11	2.06
29	A	413	DGD	C3G-C2G	2.22	1.57	1.50
22	H	101	CLA	C1D-C2D	2.21	1.49	1.45
22	c	514	CLA	C1D-ND	2.21	1.40	1.37
22	C	504	CLA	C1D-ND	2.21	1.40	1.37
27	b	623	LMG	C4-C3	2.21	1.58	1.52
22	D	403	CLA	CHC-C1C	2.21	1.42	1.38
26	A	409	PL9	C31-C29	-2.21	1.46	1.51
22	B	608	CLA	C1D-C2D	2.21	1.49	1.45
22	b	602	CLA	CAC-C3C	-2.20	1.45	1.51
24	k	102	BCR	C1-C6	-2.20	1.51	1.53
29	C	516	DGD	O3G-C3G	-2.20	1.39	1.43
22	b	612	CLA	C3B-C4B	2.20	1.49	1.42
29	C	517	DGD	O6D-C5D	-2.20	1.39	1.44
24	F	101	BCR	C27-C26	-2.20	1.46	1.51
29	C	517	DGD	C3D-C2D	2.20	1.58	1.52
27	c	522	LMG	O7-C8	-2.19	1.41	1.46
22	c	511	CLA	C3B-C4B	2.19	1.49	1.42
22	D	404	CLA	O2D-CGD	2.19	1.38	1.33
22	c	504	CLA	C3D-C4D	2.19	1.49	1.44
28	a	411	SQD	O3-C3	-2.19	1.37	1.43
22	c	513	CLA	CHC-C1C	2.19	1.42	1.38
22	d	404	CLA	C1D-ND	2.19	1.40	1.37
22	C	510	CLA	O2A-CGA	2.19	1.39	1.33
22	c	512	CLA	C1D-ND	2.19	1.40	1.37
22	B	616	CLA	C1B-NB	-2.18	1.35	1.37
34	f	101	HEC	CMA-C3A	2.18	1.55	1.50
22	D	404	CLA	C1B-C2B	2.18	1.48	1.43
22	C	508	CLA	C1D-C2D	2.18	1.49	1.45
29	c	519	DGD	O4E-C4E	-2.17	1.37	1.43
22	b	605	CLA	CHC-C4B	-2.17	1.34	1.39
22	C	506	CLA	CHC-C1C	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	CMC-C2C	-2.17	1.46	1.50
22	b	601	CLA	C3B-C4B	2.17	1.49	1.42
22	B	614	CLA	C4B-NB	2.17	1.40	1.37
31	d	411	STE	C2-C1	2.17	1.55	1.50
34	v	201	HEC	FE-ND	2.17	2.01	1.94
22	b	602	CLA	CMB-C2B	-2.16	1.46	1.50
22	d	404	CLA	CHC-C4B	-2.16	1.34	1.39
29	A	413	DGD	O3G-C1D	2.16	1.43	1.40
22	C	505	CLA	CMC-C2C	-2.16	1.46	1.50
22	b	606	CLA	CHC-C1C	2.15	1.42	1.38
26	D	406	PL9	C26-C24	-2.15	1.46	1.51
22	c	514	CLA	C1B-NB	-2.15	1.35	1.37
31	a	414	STE	O1-C1	2.15	1.29	1.22
29	C	515	DGD	O1G-C1G	-2.15	1.40	1.45
29	h	102	DGD	C4E-C3E	2.14	1.57	1.52
22	A	403	CLA	CAA-C2A	-2.14	1.50	1.54
22	b	606	CLA	CMC-C2C	-2.14	1.46	1.50
22	B	607	CLA	C1B-C2B	2.14	1.48	1.43
22	c	514	CLA	CMD-C2D	-2.13	1.46	1.50
22	C	513	CLA	CHC-C1C	2.13	1.42	1.38
26	D	406	PL9	C36-C34	2.13	1.55	1.51
22	c	506	CLA	C3B-C4B	2.13	1.48	1.42
22	A	403	CLA	CHC-C1C	2.13	1.42	1.38
22	B	607	CLA	C3B-C4B	2.13	1.48	1.42
26	d	406	PL9	C21-C19	-2.13	1.46	1.51
22	b	613	CLA	CMC-C2C	-2.13	1.46	1.50
34	v	201	HEC	CMD-C2D	2.13	1.55	1.50
22	B	613	CLA	C1C-NC	-2.12	1.34	1.37
28	f	102	SQD	O2-C2	-2.12	1.37	1.43
24	t	101	BCR	C1-C6	-2.12	1.51	1.53
33	L	102	LHG	O8-C23	2.12	1.39	1.33
22	b	610	CLA	C3D-C4D	2.12	1.49	1.44
22	a	403	CLA	C3B-C4B	2.12	1.48	1.42
22	d	403	CLA	C3B-C4B	2.12	1.48	1.42
22	B	609	CLA	C1D-ND	2.11	1.40	1.37
22	B	604	CLA	O2A-CGA	2.11	1.39	1.33
27	d	410	LMG	O1-C7	-2.11	1.40	1.43
22	B	611	CLA	CHC-C1C	2.11	1.42	1.38
22	c	511	CLA	CMC-C2C	-2.11	1.46	1.50
29	C	515	DGD	O3G-C1D	-2.11	1.36	1.40
22	D	405	CLA	CMB-C2B	-2.11	1.46	1.50
29	C	515	DGD	C3E-C2E	2.11	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	610	CLA	CMC-C2C	-2.11	1.46	1.50
22	C	508	CLA	C1D-ND	2.10	1.40	1.37
22	B	610	CLA	C1B-C2B	2.10	1.48	1.43
22	C	511	CLA	CHC-C1C	2.10	1.42	1.38
22	b	608	CLA	C3D-C4D	2.10	1.48	1.44
22	b	604	CLA	CHC-C1C	2.10	1.42	1.38
31	c	521	STE	C2-C1	2.10	1.55	1.50
22	B	604	CLA	C1B-C2B	2.10	1.48	1.43
29	h	102	DGD	C1E-C2E	2.10	1.58	1.52
29	c	518	DGD	O2E-C2E	-2.10	1.37	1.43
22	c	509	CLA	CMC-C2C	-2.10	1.46	1.50
34	F	102	HEC	C3C-C2C	-2.09	1.33	1.38
29	H	103	DGD	C1E-C2E	2.09	1.58	1.52
22	A	405	CLA	CAC-C3C	-2.09	1.45	1.51
22	C	513	CLA	CMD-C2D	-2.09	1.46	1.50
27	c	520	LMG	C7-C8	2.09	1.57	1.50
22	B	607	CLA	CAC-C3C	-2.09	1.45	1.51
22	a	405	CLA	C4B-NB	2.09	1.40	1.37
22	d	404	CLA	MG-NB	-2.09	2.01	2.05
34	f	101	HEC	C3B-C2B	-2.09	1.32	1.36
22	a	405	CLA	C3B-C4B	2.09	1.48	1.42
22	B	609	CLA	O2D-CGD	2.09	1.38	1.33
22	C	509	CLA	O2D-CGD	2.09	1.38	1.33
31	B	620	STE	O1-C1	2.09	1.28	1.22
29	h	102	DGD	O2G-C2G	-2.08	1.41	1.46
22	b	608	CLA	CMA-C3A	-2.08	1.48	1.53
22	C	509	CLA	C4B-NB	2.08	1.40	1.37
22	b	615	CLA	CMB-C2B	-2.08	1.46	1.50
22	D	403	CLA	C3B-C4B	2.08	1.48	1.42
22	B	608	CLA	MG-NB	2.08	2.09	2.05
23	D	401	PHO	CMC-C2C	-2.08	1.47	1.50
27	M	101	LMG	C9-C8	2.08	1.57	1.50
22	B	604	CLA	CMD-C2D	-2.08	1.46	1.50
22	b	603	CLA	C3B-C4B	2.08	1.48	1.42
22	C	503	CLA	CMC-C2C	-2.07	1.46	1.50
22	c	511	CLA	C5-C3	-2.07	1.47	1.51
22	D	403	CLA	C3D-C4D	2.07	1.48	1.44
22	b	610	CLA	C3B-C4B	2.07	1.48	1.42
24	K	102	BCR	C38-C26	-2.07	1.47	1.50
24	B	619	BCR	C30-C25	-2.06	1.51	1.53
34	f	101	HEC	CMC-C2C	2.06	1.55	1.50
22	C	509	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	DGD	O4E-C4E	-2.06	1.37	1.43
29	H	103	DGD	O2D-C2D	-2.06	1.37	1.43
22	H	101	CLA	CMB-C2B	-2.06	1.46	1.50
22	c	503	CLA	O2D-CGD	2.06	1.38	1.33
22	C	509	CLA	C1B-NB	-2.06	1.35	1.37
29	h	102	DGD	O2E-C2E	-2.06	1.37	1.43
22	B	605	CLA	CMD-C2D	-2.06	1.46	1.50
29	c	519	DGD	O6D-C5D	-2.06	1.39	1.44
22	b	609	CLA	C3D-C4D	2.06	1.48	1.44
22	B	608	CLA	C3C-C2C	2.05	1.41	1.36
22	c	510	CLA	C1B-NB	-2.05	1.35	1.37
29	h	102	DGD	O2G-C1B	2.05	1.40	1.34
24	c	516	BCR	C38-C26	-2.05	1.47	1.50
22	B	610	CLA	CMA-C3A	-2.05	1.48	1.53
29	C	516	DGD	C4D-C3D	2.05	1.57	1.52
22	A	403	CLA	C3C-C2C	2.05	1.41	1.36
22	a	410	CLA	C1B-NB	-2.05	1.35	1.37
24	b	617	BCR	C4-C5	-2.05	1.47	1.51
22	c	503	CLA	CHC-C1C	2.05	1.42	1.38
22	H	101	CLA	CHC-C4B	-2.05	1.34	1.39
22	B	603	CLA	C1B-NB	-2.05	1.35	1.37
31	E	102	STE	C2-C1	2.04	1.55	1.50
33	E	101	LHG	O8-C23	2.04	1.39	1.33
34	f	101	HEC	CMB-C2B	2.04	1.55	1.50
22	c	508	CLA	CMC-C2C	-2.04	1.46	1.50
22	b	607	CLA	C1B-NB	-2.04	1.35	1.37
27	D	407	LMG	O6-C5	-2.04	1.39	1.44
22	c	513	CLA	C3B-C4B	2.04	1.48	1.42
24	k	101	BCR	C38-C26	-2.04	1.47	1.50
22	C	505	CLA	C3B-C4B	2.04	1.48	1.42
22	b	612	CLA	CMB-C2B	-2.04	1.46	1.50
33	d	408	LHG	C3-C2	2.04	1.58	1.51
23	A	404	PHO	CHA-CBD	-2.04	1.49	1.51
22	b	607	CLA	C4B-NB	2.03	1.40	1.37
22	C	502	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	603	CLA	C1C-NC	-2.03	1.34	1.37
22	B	614	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	614	CLA	CAB-C3B	-2.03	1.42	1.47
22	c	506	CLA	CMC-C2C	-2.03	1.46	1.50
27	D	411	LMG	O8-C28	2.03	1.39	1.33
22	c	513	CLA	MG-NC	2.03	2.11	2.06
22	D	405	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	C4C-C3C	2.03	1.48	1.45
27	A	410	LMG	C3-C2	2.03	1.57	1.52
29	C	516	DGD	C6D-C5D	2.03	1.57	1.51
22	B	616	CLA	CHC-C4B	-2.03	1.34	1.39
29	H	103	DGD	O5D-C1E	2.03	1.43	1.40
28	a	411	SQD	O2-C2	-2.02	1.37	1.43
22	A	403	CLA	C5-C3	-2.02	1.47	1.51
28	D	408	SQD	O4-C4	-2.02	1.37	1.43
22	B	605	CLA	MG-NA	2.02	2.11	2.06
29	h	102	DGD	O3D-C3D	-2.02	1.37	1.43
22	B	608	CLA	CHC-C4B	-2.02	1.34	1.39
29	C	516	DGD	C1G-C2G	2.02	1.57	1.50
22	b	612	CLA	C1B-NB	-2.02	1.35	1.37
22	b	612	CLA	C4B-NB	2.02	1.40	1.37
22	c	506	CLA	CMB-C2B	-2.02	1.46	1.50
31	B	624	STE	O1-C1	2.02	1.28	1.22
22	c	504	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	402	CLA	C3B-C4B	2.02	1.48	1.42
26	D	406	PL9	C6-C1	-2.02	1.45	1.48
22	d	404	CLA	CMD-C2D	-2.01	1.46	1.50
22	c	506	CLA	MG-ND	2.01	2.09	2.05
24	k	101	BCR	C33-C5	-2.01	1.47	1.50
24	d	405	BCR	C38-C26	-2.01	1.47	1.50
23	a	404	PHO	CMD-C2D	-2.01	1.47	1.51
22	C	509	CLA	O2A-CGA	2.01	1.39	1.33
22	C	507	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	615	CLA	CHC-C1C	2.01	1.42	1.38
22	b	605	CLA	MG-NB	2.01	2.09	2.05
22	C	509	CLA	C3B-C4B	2.01	1.48	1.42
29	C	515	DGD	O6D-C5D	-2.01	1.39	1.44
33	d	409	LHG	P-O3	2.01	1.67	1.59
31	B	624	STE	C2-C1	2.00	1.55	1.50
22	c	510	CLA	CMB-C2B	-2.00	1.46	1.50
22	B	614	CLA	C1B-C2B	2.00	1.47	1.43
22	c	506	CLA	C4B-NB	2.00	1.40	1.37
22	b	602	CLA	C1B-NB	-2.00	1.35	1.37
22	C	511	CLA	CMD-C2D	-2.00	1.46	1.50
22	C	506	CLA	C3D-C4D	2.00	1.48	1.44

All (1286) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	101	SQD	O6-C1-C2	10.63	124.41	108.27
28	a	411	SQD	O6-C1-C2	10.10	123.61	108.27
22	b	604	CLA	C4A-NA-C1A	9.40	110.97	106.68
22	b	611	CLA	C4A-NA-C1A	9.36	110.95	106.68
22	c	510	CLA	C4A-NA-C1A	9.18	110.87	106.68
22	C	507	CLA	C4A-NA-C1A	8.53	110.57	106.68
22	c	512	CLA	C4A-NA-C1A	8.24	110.44	106.68
22	B	604	CLA	C4A-NA-C1A	8.20	110.42	106.68
22	c	504	CLA	C4A-NA-C1A	8.07	110.36	106.68
22	b	606	CLA	C4A-NA-C1A	7.81	110.24	106.68
22	B	616	CLA	C4A-NA-C1A	7.79	110.23	106.68
22	C	508	CLA	C4A-NA-C1A	7.70	110.19	106.68
22	H	101	CLA	C4A-NA-C1A	7.67	110.18	106.68
22	B	605	CLA	C4A-NA-C1A	7.51	110.10	106.68
22	C	511	CLA	C4A-NA-C1A	7.39	110.05	106.68
22	C	513	CLA	C4A-NA-C1A	7.36	110.03	106.68
22	c	502	CLA	C4A-NA-C1A	7.28	110.00	106.68
28	A	411	SQD	O6-C1-C2	6.92	118.78	108.27
22	c	511	CLA	C4A-NA-C1A	6.88	109.82	106.68
22	c	503	CLA	C4A-NA-C1A	6.82	109.79	106.68
22	B	606	CLA	C4A-NA-C1A	6.74	109.75	106.68
22	B	609	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	D	404	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	a	410	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	a	403	CLA	C4A-NA-C1A	6.56	109.67	106.68
26	a	409	PL9	C7-C3-C4	6.54	122.29	116.91
26	d	406	PL9	C7-C3-C4	6.50	122.26	116.91
22	C	503	CLA	C4A-NA-C1A	6.46	109.63	106.68
28	f	102	SQD	O9-S-C6	6.40	116.31	106.76
28	B	622	SQD	O6-C1-C2	6.24	117.75	108.27
22	C	501	CLA	C4A-NA-C1A	6.18	109.50	106.68
22	b	601	CLA	C4A-NA-C1A	6.00	109.42	106.68
22	B	607	CLA	C4A-NA-C1A	5.94	109.39	106.68
22	b	615	CLA	C4A-NA-C1A	5.89	109.37	106.68
22	C	505	CLA	C4A-NA-C1A	5.87	109.36	106.68
28	L	101	SQD	O7-S-C6	5.83	115.45	106.76
22	a	402	CLA	C4A-NA-C1A	5.83	109.34	106.68
22	c	513	CLA	C4A-NA-C1A	5.80	109.32	106.68
22	A	402	CLA	C4A-NA-C1A	5.72	109.29	106.68
22	b	616	CLA	O2D-CGD-O1D	-5.58	112.99	123.85
22	c	502	CLA	O2D-CGD-O1D	-5.57	113.01	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	PHO	C4D-CHA-CBD	-5.55	105.80	108.45
22	D	403	CLA	C4A-NA-C1A	5.54	109.20	106.68
27	b	623	LMG	O1-C1-C2	-5.46	99.98	108.27
22	B	615	CLA	C4A-NA-C1A	5.36	109.12	106.68
22	b	616	CLA	C4A-NA-C1A	5.35	109.12	106.68
34	f	101	HEC	CAB-C3B-C4B	5.35	131.75	124.79
28	a	412	SQD	O47-C7-C8	5.34	123.03	111.48
27	a	415	LMG	C1-C2-C3	-5.31	98.83	110.01
28	D	408	SQD	O9-S-C6	5.30	114.67	106.76
23	D	401	PHO	C2B-C1B-NB	-5.26	105.63	109.43
23	A	404	PHO	C4D-CHA-CBD	-5.22	105.95	108.45
23	d	401	PHO	C4D-CHA-CBD	-5.17	105.97	108.45
22	B	602	CLA	C4A-NA-C1A	5.17	109.04	106.68
22	B	608	CLA	C4A-NA-C1A	5.11	109.01	106.68
23	d	401	PHO	O1D-CGD-CBD	5.06	132.40	124.72
22	A	405	CLA	C4A-NA-C1A	5.06	108.99	106.68
22	b	605	CLA	C4A-NA-C1A	5.04	108.98	106.68
28	a	411	SQD	O9-S-C6	5.00	114.22	106.76
22	b	603	CLA	C4A-NA-C1A	4.98	108.95	106.68
22	c	508	CLA	C4A-NA-C1A	4.98	108.95	106.68
22	a	405	CLA	C4A-NA-C1A	4.96	108.94	106.68
29	H	103	DGD	O3G-C3G-C2G	-4.96	98.76	110.82
22	b	613	CLA	C4A-NA-C1A	4.95	108.94	106.68
28	D	408	SQD	O6-C1-C2	4.90	115.71	108.27
22	b	615	CLA	C3B-C4B-NB	-4.84	106.21	110.53
34	f	101	HEC	CBD-CAD-C3D	-4.80	99.27	112.53
26	A	409	PL9	C7-C3-C4	4.78	120.84	116.91
22	c	502	CLA	O2D-CGD-CBD	4.77	119.56	111.23
22	c	509	CLA	C4A-NA-C1A	4.69	108.82	106.68
22	B	613	CLA	C1-C2-C3	-4.64	118.59	126.20
22	b	602	CLA	C4A-NA-C1A	4.63	108.79	106.68
28	L	101	SQD	C1-C2-C3	-4.61	100.31	110.01
22	b	608	CLA	C4A-NA-C1A	4.55	108.75	106.68
26	D	406	PL9	C7-C3-C4	4.53	120.64	116.91
22	c	505	CLA	C4A-NA-C1A	4.52	108.74	106.68
29	C	517	DGD	O3G-C3G-C2G	-4.49	99.89	110.82
22	B	613	CLA	C4A-NA-C1A	4.46	108.71	106.68
33	E	101	LHG	O4-P-O5	4.46	133.19	112.44
22	C	502	CLA	C4A-NA-C1A	4.45	108.71	106.68
28	f	102	SQD	O6-C1-C2	4.45	115.03	108.27
22	B	615	CLA	C3B-C4B-NB	-4.44	106.56	110.53
22	b	616	CLA	O1D-CGD-CBD	4.44	133.28	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	C4A-NA-C1A	4.41	108.69	106.68
22	B	611	CLA	O2D-CGD-O1D	-4.38	115.31	123.85
33	D	410	LHG	O4-P-O5	4.37	132.78	112.44
29	C	516	DGD	O3G-C3G-C2G	-4.37	100.20	110.82
22	b	611	CLA	O2D-CGD-O1D	-4.37	115.35	123.85
26	a	409	PL9	C7-C3-C2	-4.32	118.29	123.39
22	C	510	CLA	C4A-NA-C1A	4.31	108.65	106.68
22	b	608	CLA	C3B-C4B-NB	-4.31	106.69	110.53
28	f	102	SQD	O9-S-O7	-4.30	99.84	113.82
33	e	101	LHG	O4-P-O5	4.29	132.42	112.44
33	L	102	LHG	O4-P-O5	4.29	132.40	112.44
22	c	506	CLA	O2D-CGD-O1D	-4.29	115.51	123.85
28	B	622	SQD	O47-C7-C8	4.27	120.73	111.48
33	d	407	LHG	O4-P-O5	4.27	132.30	112.44
22	b	603	CLA	O2D-CGD-O1D	-4.26	115.55	123.85
22	B	605	CLA	O2D-CGD-O1D	-4.26	115.55	123.85
22	B	611	CLA	O2D-CGD-CBD	4.25	118.66	111.23
22	B	602	CLA	O2D-CGD-CBD	4.25	118.66	111.23
26	d	406	PL9	C7-C3-C2	-4.23	118.41	123.39
22	a	402	CLA	C3B-C4B-NB	-4.21	106.77	110.53
24	T	101	BCR	C7-C8-C9	-4.20	120.02	126.23
28	A	411	SQD	C1-C2-C3	-4.18	101.21	110.01
22	B	610	CLA	C4A-NA-C1A	4.16	108.58	106.68
32	d	402	BCT	O2-C-O1	4.16	130.31	119.68
27	b	623	LMG	C1-O6-C5	-4.15	105.62	113.72
33	d	408	LHG	O4-P-O5	4.13	131.66	112.44
29	A	413	DGD	O3G-C3G-C2G	-4.13	100.78	110.82
22	A	403	CLA	O2D-CGD-O1D	-4.12	115.83	123.85
24	B	619	BCR	C2-C1-C6	4.10	116.39	110.44
22	b	605	CLA	O2D-CGD-O1D	-4.09	115.88	123.85
23	d	401	PHO	C2B-C1B-NB	-4.09	106.47	109.43
22	c	505	CLA	CMB-C2B-C1B	-4.07	119.22	125.42
22	c	506	CLA	C4A-NA-C1A	4.07	108.54	106.68
23	a	404	PHO	CMB-C2B-C3B	4.05	132.78	124.68
28	a	412	SQD	O48-C23-C24	4.05	124.18	111.83
22	A	405	CLA	O2D-CGD-O1D	-4.05	115.97	123.85
29	C	515	DGD	O6D-C1D-O3G	-4.04	100.50	110.04
22	D	404	CLA	C3B-C4B-NB	-4.03	106.94	110.53
22	H	101	CLA	CAA-CBA-CGA	-4.03	101.78	113.21
29	c	519	DGD	O3G-C3G-C2G	-4.02	101.03	110.82
22	B	612	CLA	C11-C12-C13	-4.02	102.61	115.97
33	d	409	LHG	O4-P-O5	4.01	131.08	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	412	SQD	O47-C7-C8	3.99	120.12	111.48
26	d	406	PL9	C22-C23-C24	-3.98	118.51	127.62
22	B	610	CLA	O2D-CGD-O1D	-3.98	116.10	123.85
33	d	407	LHG	O8-C23-C24	3.97	123.94	111.83
22	A	402	CLA	CHB-C4A-NA	3.97	130.13	124.40
33	l	101	LHG	O4-P-O5	3.96	130.85	112.44
28	B	622	SQD	C1-O5-C5	-3.95	106.00	113.72
24	b	617	BCR	C2-C1-C6	3.95	116.17	110.44
33	D	409	LHG	O4-P-O5	3.94	130.76	112.44
22	b	602	CLA	O2D-CGD-CBD	3.93	118.10	111.23
28	a	411	SQD	O9-S-O7	-3.93	101.04	113.82
34	f	101	HEC	CAB-C3B-C2B	-3.92	120.36	127.56
28	B	622	SQD	O5-C5-C4	3.91	116.75	109.70
33	D	412	LHG	O4-P-O5	3.91	130.63	112.44
22	B	603	CLA	C3B-C4B-NB	-3.89	107.06	110.53
28	a	411	SQD	C1-O5-C5	-3.88	106.14	113.72
22	B	608	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
22	c	506	CLA	C3B-C4B-NB	-3.86	107.08	110.53
22	B	606	CLA	C3B-C4B-NB	-3.84	107.10	110.53
28	L	101	SQD	O2-C2-C1	3.84	119.22	110.08
29	C	515	DGD	O3G-C3G-C2G	-3.81	101.54	110.82
28	B	622	SQD	O7-S-C6	3.81	112.44	106.76
27	a	415	LMG	O6-C1-C2	-3.81	102.55	110.37
24	A	406	BCR	C27-C26-C25	3.80	127.84	122.70
22	b	605	CLA	C1-C2-C3	-3.80	119.97	126.20
22	B	615	CLA	CHC-C4B-NB	3.80	129.75	124.05
33	d	407	LHG	O8-C23-O10	-3.77	114.19	123.63
22	B	613	CLA	C3B-C4B-NB	-3.77	107.16	110.53
22	B	612	CLA	C4A-NA-C1A	3.77	108.40	106.68
31	B	625	STE	C3-C2-C1	-3.77	104.68	114.51
28	f	102	SQD	O5-C5-C4	3.77	116.48	109.70
24	K	101	BCR	C15-C16-C17	-3.76	115.83	123.52
28	L	101	SQD	O48-C23-C24	3.75	123.27	111.83
22	c	510	CLA	CHB-C4A-NA	3.75	129.81	124.40
28	a	411	SQD	O47-C7-O49	-3.73	114.99	123.70
24	K	101	BCR	C2-C1-C6	3.73	115.85	110.44
22	b	604	CLA	C3B-C4B-NB	-3.73	107.20	110.53
29	c	517	DGD	O3G-C3G-C2G	-3.72	101.77	110.82
22	c	512	CLA	C3B-C4B-NB	-3.70	107.22	110.53
22	C	501	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
22	C	503	CLA	C7-C6-C5	-3.68	103.45	113.26
22	B	614	CLA	C3B-C4B-NB	-3.68	107.25	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	PHO	O2D-CGD-O1D	-3.68	116.69	123.85
32	D	402	BCT	O2-C-O1	3.66	129.05	119.68
22	b	607	CLA	C4A-NA-C1A	3.65	108.34	106.68
22	C	512	CLA	CHB-C4A-NA	3.64	129.66	124.40
23	d	401	PHO	C3B-C4B-NB	-3.64	105.09	107.46
22	D	404	CLA	CHB-C4A-NA	3.63	129.64	124.40
28	L	101	SQD	O9-S-O7	-3.62	102.03	113.82
28	a	411	SQD	C1-C2-C3	-3.62	102.39	110.01
22	b	606	CLA	O2D-CGD-CBD	3.61	117.55	111.23
22	D	403	CLA	C6-C5-C3	3.61	122.27	113.47
22	C	501	CLA	C3B-C4B-NB	-3.61	107.31	110.53
22	B	604	CLA	C3B-C4B-NB	-3.60	107.31	110.53
22	C	513	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
24	b	619	BCR	C29-C30-C25	3.59	115.66	110.44
23	a	404	PHO	C1-C2-C3	-3.58	120.32	126.20
26	A	409	PL9	C7-C3-C2	-3.58	119.17	123.39
29	c	518	DGD	O3G-C3G-C2G	-3.57	102.12	110.82
22	b	601	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
22	b	603	CLA	O2D-CGD-CBD	3.56	117.46	111.23
26	D	406	PL9	C36-C34-C33	-3.56	113.17	121.17
24	B	617	BCR	C2-C1-C6	3.54	115.58	110.44
22	B	608	CLA	O2D-CGD-CBD	3.54	117.41	111.23
31	b	624	STE	C3-C2-C1	-3.53	105.30	114.51
28	B	622	SQD	C3-C4-C5	3.52	116.62	110.23
22	c	510	CLA	O2A-CGA-O1A	-3.52	114.81	123.63
22	b	609	CLA	C3B-C4B-NB	-3.52	107.39	110.53
22	C	501	CLA	O2D-CGD-CBD	3.52	117.38	111.23
28	A	411	SQD	C1-O5-C5	-3.52	106.85	113.72
22	C	504	CLA	C4A-NA-C1A	3.51	108.28	106.68
22	H	101	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
24	B	618	BCR	C29-C30-C25	3.51	115.53	110.44
22	C	505	CLA	C3B-C4B-NB	-3.51	107.40	110.53
22	C	509	CLA	C4A-NA-C1A	3.50	108.28	106.68
22	B	613	CLA	C4-C3-C5	3.50	121.31	115.23
22	C	507	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
22	b	611	CLA	O2D-CGD-CBD	3.49	117.34	111.23
22	c	509	CLA	CHB-C4A-NA	3.49	129.44	124.40
26	d	406	PL9	C41-C39-C38	-3.49	113.34	121.17
22	a	410	CLA	C3B-C4B-NB	-3.48	107.42	110.53
22	b	614	CLA	C3B-C4B-NB	-3.48	107.42	110.53
29	C	516	DGD	O2D-C2D-C1D	-3.48	101.78	110.08
22	b	611	CLA	C1D-ND-C4D	3.48	108.75	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	406	PL9	C22-C23-C24	-3.48	119.67	127.62
24	K	101	BCR	C11-C10-C9	-3.47	122.41	127.28
22	B	602	CLA	CHB-C4A-NA	3.47	129.41	124.40
22	B	606	CLA	O2A-CGA-O1A	-3.46	114.97	123.63
22	c	504	CLA	C3B-C4B-NB	-3.46	107.44	110.53
22	b	610	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
22	c	510	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
22	B	615	CLA	O2D-CGD-CBD	3.44	117.25	111.23
22	c	511	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
24	t	101	BCR	C7-C8-C9	-3.44	121.15	126.23
22	b	607	CLA	C4-C3-C5	3.43	121.19	115.23
22	B	603	CLA	CMB-C2B-C1B	-3.43	120.20	125.42
28	A	411	SQD	O47-C7-C8	3.43	118.90	111.48
22	c	511	CLA	C3B-C4B-NB	-3.43	107.47	110.53
22	c	514	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
24	F	101	BCR	C28-C27-C26	-3.41	107.97	114.06
22	b	610	CLA	C4A-NA-C1A	3.41	108.23	106.68
22	B	604	CLA	C1-C2-C3	-3.41	120.61	126.20
23	D	401	PHO	C4D-CHA-CBD	-3.41	106.82	108.45
29	H	103	DGD	O2D-C2D-C1D	-3.40	101.97	110.08
24	h	101	BCR	C27-C26-C25	3.40	127.30	122.70
22	B	614	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
22	H	101	CLA	O2D-CGD-CBD	3.38	117.14	111.23
22	D	405	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
24	K	101	BCR	C33-C5-C6	-3.38	120.80	124.48
22	C	512	CLA	C3B-C4B-NB	-3.37	107.52	110.53
22	b	607	CLA	C6-C7-C8	-3.37	104.75	115.97
22	C	507	CLA	O2D-CGD-CBD	3.37	117.13	111.23
22	C	512	CLA	C4A-NA-C1A	3.37	108.22	106.68
22	b	616	CLA	CHB-C4A-NA	3.37	129.26	124.40
22	C	504	CLA	C3B-C4B-NB	-3.37	107.52	110.53
26	A	409	PL9	C35-C34-C36	3.36	121.07	115.23
22	b	603	CLA	C3B-C4B-NB	-3.35	107.54	110.53
23	A	404	PHO	CMB-C2B-C3B	3.35	131.38	124.68
34	f	101	HEC	CBB-CAB-C3B	3.34	121.48	112.42
22	B	608	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
22	b	612	CLA	C11-C12-C13	-3.34	104.87	115.97
31	C	520	STE	C3-C2-C1	-3.33	105.81	114.51
24	c	516	BCR	C27-C26-C25	3.33	127.20	122.70
22	a	410	CLA	CHB-C4A-NA	3.32	129.19	124.40
26	D	406	PL9	C50-C49-C48	-3.31	112.71	122.66
22	c	509	CLA	C3B-C4B-NB	-3.31	107.58	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	406	PL9	C35-C34-C36	3.30	120.96	115.23
22	B	611	CLA	C14-C13-C15	-3.30	99.52	111.27
22	b	616	CLA	CMB-C2B-C3B	3.29	134.29	126.55
22	c	511	CLA	C6-C5-C3	-3.29	105.46	113.47
22	C	506	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
22	c	513	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
22	C	509	CLA	C1-C2-C3	-3.28	120.83	126.20
27	b	621	LMG	O3-C3-C2	-3.25	102.71	110.38
24	T	101	BCR	C27-C26-C25	3.25	127.09	122.70
28	D	408	SQD	O8-S-C6	3.25	112.24	105.97
24	k	102	BCR	C2-C1-C6	3.25	115.15	110.44
22	C	510	CLA	C3B-C4B-NB	-3.24	107.63	110.53
22	C	506	CLA	O1D-CGD-CBD	3.23	130.90	124.52
28	B	622	SQD	O48-C23-C24	3.23	121.69	111.83
27	M	101	LMG	O6-C1-O1	-3.23	102.41	110.04
34	f	101	HEC	CHB-C1B-NB	3.23	127.90	124.42
22	b	616	CLA	CMB-C2B-C1B	-3.22	120.51	125.42
26	D	406	PL9	C37-C38-C39	-3.22	120.25	127.62
33	D	412	LHG	O8-C23-O10	-3.22	115.58	123.63
22	B	615	CLA	CHB-C4A-NA	3.22	129.04	124.40
22	c	509	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
33	D	412	LHG	O8-C23-C24	3.21	121.63	111.83
24	b	618	BCR	C35-C13-C14	-3.20	117.62	122.82
22	b	609	CLA	CHB-C1B-NB	3.20	128.85	124.05
22	b	604	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
22	b	615	CLA	CHB-C1B-NB	3.19	128.84	124.05
22	a	402	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
29	C	517	DGD	O6D-C1D-O3G	-3.18	102.52	110.04
22	D	405	CLA	C4A-NA-C1A	3.18	108.13	106.68
34	F	102	HEC	CBB-CAB-C3B	3.18	121.03	112.42
22	b	615	CLA	C1-C2-C3	3.17	131.40	126.20
22	A	402	CLA	CAA-CBA-CGA	-3.17	104.20	113.21
23	A	404	PHO	CBC-CAC-C3C	3.17	117.41	112.87
22	D	403	CLA	CHB-C4A-NA	3.17	128.97	124.40
22	a	405	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
22	C	503	CLA	C3B-C4B-NB	-3.15	107.71	110.53
22	b	611	CLA	C3B-C4B-NB	-3.15	107.72	110.53
22	C	506	CLA	C3B-C4B-NB	-3.15	107.72	110.53
23	D	401	PHO	C1-C2-C3	-3.15	121.03	126.20
24	b	617	BCR	C29-C30-C25	3.15	115.02	110.44
29	c	517	DGD	C3D-C4D-C5D	-3.15	104.52	110.23
27	b	623	LMG	O2-C2-C1	-3.15	102.58	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	102	HEC	CBD-CAD-C3D	-3.14	103.84	112.53
22	A	405	CLA	C4-C3-C5	3.14	120.68	115.23
22	b	606	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
22	B	602	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
29	A	413	DGD	O5E-C6E-C5E	-3.12	100.69	111.33
22	b	601	CLA	C3B-C4B-NB	-3.12	107.74	110.53
29	A	413	DGD	C4E-C3E-C2E	-3.12	105.35	110.83
29	c	519	DGD	C3G-C2G-C1G	-3.12	104.52	111.78
28	B	622	SQD	O8-S-C6	3.11	111.98	105.97
22	a	405	CLA	CHB-C4A-NA	3.11	128.89	124.40
22	b	612	CLA	CHB-C4A-NA	3.11	128.89	124.40
29	C	517	DGD	O3E-C3E-C2E	-3.11	103.04	110.38
34	v	201	HEC	CHB-C1B-NB	3.11	127.77	124.42
22	a	405	CLA	O2D-CGD-CBD	3.11	116.66	111.23
27	D	407	LMG	O6-C1-O1	-3.11	102.70	110.04
22	b	601	CLA	CHB-C4A-NA	3.10	128.88	124.40
26	d	406	PL9	C36-C34-C33	-3.10	114.20	121.17
24	a	406	BCR	C27-C26-C25	3.10	126.89	122.70
26	D	406	PL9	C7-C3-C2	-3.10	119.74	123.39
24	d	405	BCR	C38-C26-C25	-3.09	121.11	124.48
22	B	610	CLA	CHB-C4A-NA	3.09	128.86	124.40
22	B	602	CLA	C1-C2-C3	-3.09	121.14	126.20
22	b	614	CLA	CHD-C1D-ND	-3.09	120.46	124.80
28	L	101	SQD	O47-C7-C8	3.09	118.16	111.48
22	b	614	CLA	O2A-CGA-O1A	-3.09	115.91	123.63
22	c	503	CLA	C1-C2-C3	-3.09	121.14	126.20
29	C	517	DGD	O6D-C5D-C6D	-3.09	100.58	106.69
24	F	101	BCR	C7-C8-C9	-3.08	121.67	126.23
29	C	516	DGD	O6E-C1E-O5D	-3.08	102.76	110.04
31	j	101	STE	O2-C1-O1	-3.08	115.41	123.33
29	h	102	DGD	C3D-C4D-C5D	-3.08	104.65	110.23
22	c	504	CLA	C7-C6-C5	-3.08	105.06	113.26
28	a	411	SQD	O5-C1-C2	-3.07	104.06	110.37
22	C	508	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
29	h	102	DGD	O3G-C3G-C2G	-3.07	103.35	110.82
22	c	504	CLA	CHB-C4A-NA	3.07	128.83	124.40
26	A	409	PL9	C22-C23-C24	-3.07	120.61	127.62
24	F	101	BCR	C2-C1-C6	3.06	114.89	110.44
22	B	606	CLA	CHC-C4B-NB	3.06	128.64	124.05
24	H	102	BCR	C2-C1-C6	3.05	114.88	110.44
22	b	603	CLA	C4D-CHA-C1A	3.05	124.89	121.24
34	V	201	HEC	CHB-C4A-NA	3.05	127.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	O2A-CGA-O1A	-3.05	116.01	123.63
22	a	403	CLA	CAC-C3C-C4C	3.04	128.75	124.79
22	b	603	CLA	CHC-C4B-NB	3.04	128.61	124.05
28	L	101	SQD	O5-C1-C2	-3.04	104.13	110.37
24	b	618	BCR	C36-C18-C17	-3.04	117.89	122.82
22	C	512	CLA	O2D-CGD-CBD	3.04	116.54	111.23
22	B	605	CLA	O1D-CGD-CBD	3.03	130.50	124.52
27	d	410	LMG	O6-C1-O1	-3.03	102.88	110.04
27	Y	101	LMG	O1-C1-C2	-3.03	103.67	108.27
27	a	415	LMG	C9-C8-C7	-3.03	104.72	111.78
22	C	513	CLA	C3B-C4B-NB	-3.03	107.83	110.53
22	D	403	CLA	C4-C3-C5	3.03	120.48	115.23
27	b	623	LMG	C8-O7-C10	3.03	125.04	117.80
22	c	513	CLA	CHB-C4A-NA	3.03	128.77	124.40
31	a	414	STE	C3-C2-C1	-3.02	106.62	114.51
22	B	612	CLA	CMB-C2B-C1B	-3.02	120.82	125.42
22	B	612	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
27	c	523	LMG	O6-C1-O1	-3.02	102.91	110.04
22	A	402	CLA	C6-C5-C3	3.02	120.82	113.47
24	c	515	BCR	C24-C23-C22	-3.01	121.78	126.23
28	A	412	SQD	O48-C23-C24	3.00	121.00	111.83
24	F	101	BCR	C24-C23-C22	-3.00	121.79	126.23
34	v	201	HEC	CAB-C3B-C4B	3.00	128.69	124.79
26	D	406	PL9	C35-C34-C36	3.00	120.44	115.23
22	B	608	CLA	CHD-C1D-ND	-3.00	120.58	124.80
27	b	621	LMG	O1-C1-C2	-3.00	103.72	108.27
22	b	607	CLA	CHB-C1B-NB	3.00	128.54	124.05
22	B	608	CLA	CMB-C2B-C3B	2.99	133.59	126.55
28	a	411	SQD	O48-C23-C24	2.99	120.96	111.83
28	A	411	SQD	O8-S-C6	2.99	111.75	105.97
22	B	604	CLA	CHB-C4A-NA	2.99	128.71	124.40
29	h	102	DGD	O6E-C5E-C4E	2.99	115.08	109.70
23	a	404	PHO	CBC-CAC-C3C	-2.99	108.60	112.87
27	a	415	LMG	O6-C5-C4	2.98	115.07	109.70
28	a	411	SQD	O7-S-C6	2.97	111.19	106.76
26	d	406	PL9	C30-C29-C31	-2.97	110.07	115.23
26	a	409	PL9	C35-C34-C36	2.97	120.38	115.23
22	d	403	CLA	C2D-C1D-ND	-2.97	107.19	110.13
22	c	509	CLA	CHD-C1D-ND	-2.97	120.63	124.80
22	C	505	CLA	C1-C2-C3	-2.96	121.34	126.20
26	d	406	PL9	C37-C38-C39	-2.96	120.84	127.62
28	A	411	SQD	O47-C7-O49	-2.96	116.78	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	CAC-C3C-C4C	2.96	128.64	124.79
22	B	613	CLA	CHA-C1A-NA	-2.96	119.69	126.39
22	B	607	CLA	CED-O2D-CGD	2.96	122.63	115.92
24	k	102	BCR	C27-C26-C25	2.96	126.70	122.70
34	F	102	HEC	CBC-CAC-C3C	2.95	120.42	112.42
27	M	101	LMG	C1-O6-C5	-2.95	107.96	113.72
32	d	402	BCT	O3-C-O1	-2.95	112.13	119.68
31	J	101	STE	C3-C2-C1	-2.95	106.81	114.51
29	A	413	DGD	O6E-C5E-C4E	2.95	115.02	109.70
22	C	504	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
22	C	501	CLA	O2A-CGA-O1A	-2.95	116.26	123.63
27	Y	101	LMG	O2-C2-C1	-2.94	103.07	110.08
24	B	617	BCR	C3-C4-C5	-2.94	108.81	114.06
22	c	507	CLA	C3B-C4B-NB	-2.94	107.91	110.53
29	c	519	DGD	C3D-C4D-C5D	-2.94	104.90	110.23
22	b	606	CLA	CHB-C4A-NA	2.94	128.64	124.40
22	c	511	CLA	CHB-C4A-NA	2.94	128.64	124.40
24	B	618	BCR	C2-C1-C6	2.94	114.70	110.44
22	b	609	CLA	C4A-NA-C1A	2.93	108.02	106.68
22	B	611	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
22	B	603	CLA	C2D-C1D-ND	-2.93	107.22	110.13
22	d	403	CLA	O1D-CGD-CBD	2.93	130.30	124.52
22	B	604	CLA	C11-C10-C8	-2.93	106.23	115.97
22	B	606	CLA	CGD-CBD-CAD	-2.93	101.37	110.85
28	a	411	SQD	O2-C2-C1	2.93	117.05	110.08
28	D	408	SQD	O9-S-O7	-2.93	104.31	113.82
22	b	611	CLA	C2D-C1D-ND	-2.92	107.23	110.13
24	t	101	BCR	C2-C1-C6	2.92	114.68	110.44
31	j	101	STE	O2-C1-C2	2.92	123.22	114.00
22	C	513	CLA	O2A-CGA-O1A	-2.92	116.34	123.63
22	a	403	CLA	C3B-C4B-NB	-2.91	107.93	110.53
34	f	101	HEC	CBC-CAC-C3C	2.91	120.32	112.42
24	B	619	BCR	C29-C30-C25	2.91	114.67	110.44
22	b	610	CLA	C6-C5-C3	2.91	120.56	113.47
27	A	410	LMG	O6-C1-O1	-2.91	103.18	110.04
29	c	517	DGD	CBB-CAB-C9B	-2.90	99.69	114.37
27	A	410	LMG	C9-C8-C7	-2.90	105.01	111.78
26	A	409	PL9	C36-C34-C33	-2.90	114.65	121.17
27	b	621	LMG	O6-C1-O1	-2.90	103.18	110.04
26	a	409	PL9	C22-C23-C24	-2.90	120.99	127.62
22	c	506	CLA	C6-C7-C8	-2.89	106.35	115.97
27	d	410	LMG	O2-C2-C1	-2.89	103.19	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	520	LMG	O3-C3-C2	-2.89	103.56	110.38
23	D	401	PHO	CMB-C2B-C3B	2.89	130.46	124.68
24	b	619	BCR	C16-C15-C14	-2.89	117.61	123.52
22	b	605	CLA	C4-C3-C5	2.89	120.24	115.23
24	h	101	BCR	C2-C1-C6	2.88	114.63	110.44
22	b	610	CLA	CAC-C3C-C4C	2.88	128.54	124.79
24	A	406	BCR	C2-C1-C6	2.88	114.62	110.44
22	B	603	CLA	CHD-C1D-C2D	2.88	131.47	125.49
22	c	503	CLA	C3B-C4B-NB	-2.87	107.96	110.53
29	c	519	DGD	O6D-C1D-O3G	-2.87	103.26	110.04
31	m	102	STE	O2-C1-C2	2.87	123.05	114.00
24	K	103	BCR	C15-C16-C17	-2.86	117.66	123.52
28	L	101	SQD	C3-C4-C5	2.86	115.41	110.23
22	c	505	CLA	O2D-CGD-CBD	2.85	116.22	111.23
28	a	411	SQD	O47-C7-C8	2.85	117.65	111.48
24	H	102	BCR	C38-C26-C25	-2.85	121.37	124.48
22	b	610	CLA	CHB-C4A-NA	2.85	128.51	124.40
26	a	409	PL9	O2-C1-C2	-2.85	115.36	121.83
22	b	614	CLA	CHB-C4A-NA	2.84	128.50	124.40
22	b	601	CLA	O2D-CGD-CBD	2.84	116.19	111.23
22	B	611	CLA	CHD-C4C-NC	2.84	128.63	124.23
24	a	406	BCR	C2-C1-C6	2.84	114.56	110.44
24	H	102	BCR	C29-C30-C25	2.84	114.56	110.44
28	L	101	SQD	C45-O47-C7	2.84	124.58	117.80
22	b	601	CLA	CHD-C1D-ND	-2.84	120.81	124.80
22	b	611	CLA	CHB-C4A-NA	2.84	128.49	124.40
22	C	507	CLA	C4-C3-C5	2.83	120.15	115.23
22	b	605	CLA	CHB-C4A-NA	2.83	128.49	124.40
22	B	603	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
22	B	612	CLA	C16-C15-C13	-2.83	106.57	115.97
22	c	507	CLA	C4-C3-C2	-2.83	116.37	123.63
27	d	410	LMG	O1-C1-C2	-2.82	103.99	108.27
34	v	201	HEC	CBD-CAD-C3D	-2.82	104.73	112.53
22	B	612	CLA	CMB-C2B-C3B	2.82	133.18	126.55
22	B	613	CLA	CAC-C3C-C4C	2.82	128.46	124.79
34	f	101	HEC	CAC-C3C-C4C	-2.82	121.04	124.91
22	B	608	CLA	C6-C7-C8	-2.82	106.61	115.97
22	b	609	CLA	CHA-C1A-NA	-2.81	120.02	126.39
22	c	509	CLA	O2A-CGA-O1A	-2.81	116.59	123.63
22	B	610	CLA	O2D-CGD-CBD	2.81	116.15	111.23
22	A	405	CLA	O2D-CGD-CBD	2.81	116.15	111.23
28	a	412	SQD	O48-C23-O10	-2.81	116.61	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	C4A-NA-C1A	2.81	107.96	106.68
22	B	613	CLA	C2A-C1A-CHA	2.80	128.73	123.87
27	b	623	LMG	C3-C4-C5	-2.80	105.15	110.23
22	b	613	CLA	CHB-C4A-NA	2.80	128.44	124.40
29	H	103	DGD	C6D-C5D-C4D	2.80	117.95	112.07
34	F	102	HEC	CBA-CAA-C2A	-2.80	104.80	112.53
29	C	516	DGD	O5D-C6D-C5D	-2.80	103.12	109.42
31	B	623	STE	C3-C2-C1	-2.79	107.22	114.51
22	C	502	CLA	C3B-C4B-NB	-2.79	108.04	110.53
29	H	103	DGD	C1D-C2D-C3D	-2.79	104.14	110.01
24	t	101	BCR	C3-C4-C5	-2.79	109.09	114.06
22	b	615	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
28	f	102	SQD	C1-C2-C3	-2.78	104.16	110.01
22	b	613	CLA	CMB-C2B-C1B	-2.78	121.19	125.42
22	b	613	CLA	C1-C2-C3	-2.78	121.64	126.20
27	c	522	LMG	O7-C10-O9	-2.77	117.23	123.70
22	c	505	CLA	CMB-C2B-C3B	2.77	133.05	126.55
29	C	515	DGD	C2G-O2G-C1B	2.76	124.41	117.80
22	c	507	CLA	CHB-C4A-NA	2.76	128.39	124.40
22	c	511	CLA	C4-C3-C5	2.76	120.03	115.23
22	B	605	CLA	CHB-C4A-NA	2.76	128.39	124.40
22	a	410	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
22	B	607	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
22	c	512	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
23	A	404	PHO	C1-O2A-CGA	2.75	123.32	116.65
22	C	507	CLA	CHD-C1D-ND	-2.75	120.93	124.80
22	B	605	CLA	C4D-CHA-C1A	2.75	124.53	121.24
24	h	101	BCR	C38-C26-C25	-2.75	121.48	124.48
22	C	504	CLA	O2D-CGD-CBD	2.75	116.04	111.23
24	d	405	BCR	C27-C26-C25	2.74	126.41	122.70
31	b	624	STE	O2-C1-C2	2.74	122.66	114.00
22	c	504	CLA	C5-C3-C2	-2.74	115.02	121.17
29	c	518	DGD	O2G-C1B-O1B	-2.73	117.32	123.70
22	b	603	CLA	CHD-C1D-ND	-2.73	120.96	124.80
22	b	602	CLA	CHB-C4A-NA	2.73	128.34	124.40
22	C	504	CLA	C4-C3-C5	2.73	119.96	115.23
22	D	403	CLA	CED-O2D-CGD	2.73	122.10	115.92
22	C	505	CLA	CHB-C1B-NB	2.72	128.13	124.05
22	B	603	CLA	CMB-C2B-C3B	2.72	132.95	126.55
28	L	101	SQD	O5-C5-C4	2.72	114.60	109.70
22	C	511	CLA	CHB-C4A-NA	2.72	128.32	124.40
27	M	101	LMG	C38-C37-C36	-2.72	100.64	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	517	DGD	O6D-C1D-O3G	-2.72	103.63	110.04
24	K	103	BCR	C3-C4-C5	-2.71	109.22	114.06
23	a	404	PHO	C2B-C1B-NB	-2.71	107.47	109.43
22	b	610	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
24	H	102	BCR	C27-C26-C25	2.71	126.36	122.70
22	c	510	CLA	CHD-C1D-ND	-2.70	121.00	124.80
22	B	610	CLA	C1-C2-C3	-2.70	121.77	126.20
22	b	610	CLA	C1-C2-C3	-2.70	121.77	126.20
22	a	403	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
22	C	508	CLA	CHD-C1D-ND	-2.70	121.00	124.80
22	A	403	CLA	O2D-CGD-CBD	2.70	115.95	111.23
22	C	504	CLA	CED-O2D-CGD	2.70	122.03	115.92
22	a	405	CLA	C4-C3-C5	2.70	119.91	115.23
29	A	413	DGD	C3G-C2G-C1G	-2.69	105.50	111.78
28	L	101	SQD	O9-S-C6	2.69	110.78	106.76
22	a	403	CLA	CHB-C4A-NA	2.69	128.28	124.40
29	A	413	DGD	O5D-C6D-C5D	-2.69	103.36	109.42
22	b	611	CLA	C2B-C1B-NB	-2.69	107.54	110.33
33	D	409	LHG	O8-C23-O10	-2.69	116.91	123.63
22	B	609	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
27	b	623	LMG	O7-C10-O9	-2.69	117.42	123.70
29	c	519	DGD	C1D-C2D-C3D	-2.69	104.36	110.01
28	L	101	SQD	O48-C23-O10	-2.68	116.91	123.63
22	B	605	CLA	C7-C6-C5	-2.68	106.11	113.26
22	b	603	CLA	CMA-C3A-C4A	2.68	118.98	111.77
22	B	605	CLA	C16-C15-C13	-2.68	107.05	115.97
33	l	101	LHG	O8-C23-C24	2.68	120.01	111.83
22	B	605	CLA	CHD-C1D-ND	-2.68	121.03	124.80
22	a	403	CLA	O2D-CGD-CBD	2.68	115.91	111.23
29	A	413	DGD	O2D-C2D-C1D	-2.68	103.69	110.08
24	k	101	BCR	C27-C26-C25	2.68	126.32	122.70
22	b	604	CLA	CMB-C2B-C3B	2.68	132.85	126.55
34	f	101	HEC	CHD-C4C-NC	2.68	128.71	123.86
22	b	616	CLA	C4-C3-C5	2.67	119.87	115.23
22	B	609	CLA	CMC-C2C-C1C	2.67	129.21	125.03
22	c	505	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
24	t	101	BCR	C15-C16-C17	-2.67	118.05	123.52
22	a	402	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
29	C	515	DGD	O5D-C6D-C5D	-2.67	103.40	109.42
22	b	608	CLA	CHA-C1A-NA	-2.67	120.35	126.39
22	B	616	CLA	C1-O2A-CGA	2.67	123.11	116.65
29	C	517	DGD	O1G-C1A-C2A	-2.66	103.72	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	403	CLA	C4A-NA-C1A	2.66	107.89	106.68
22	b	607	CLA	C3B-C4B-NB	-2.66	108.16	110.53
24	d	405	BCR	C2-C1-C6	2.66	114.30	110.44
22	C	512	CLA	C1-C2-C3	-2.66	121.84	126.20
22	C	512	CLA	C6-C5-C3	-2.66	106.99	113.47
24	K	101	BCR	C27-C26-C25	2.66	126.30	122.70
22	B	610	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
22	b	613	CLA	C7-C6-C5	-2.66	106.19	113.26
22	c	504	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
29	A	413	DGD	C1D-C2D-C3D	-2.65	104.43	110.01
24	c	516	BCR	C2-C1-C6	2.65	114.29	110.44
27	b	623	LMG	O8-C28-O10	-2.65	117.00	123.63
33	D	409	LHG	C18-C17-C16	-2.65	100.99	114.37
27	b	621	LMG	O7-C10-O9	-2.65	117.52	123.70
26	A	409	PL9	O1-C4-C3	-2.64	117.95	120.73
27	c	522	LMG	O6-C1-O1	-2.64	103.81	110.04
22	b	603	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
22	A	403	CLA	C3B-C4B-NB	-2.64	108.18	110.53
22	c	508	CLA	C4-C3-C5	2.63	119.80	115.23
22	c	505	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
24	K	102	BCR	C27-C26-C25	2.63	126.26	122.70
33	D	409	LHG	O8-C23-C24	2.63	119.85	111.83
27	b	623	LMG	C4-C3-C2	-2.63	106.21	110.83
22	D	405	CLA	CAC-C3C-C4C	2.63	128.21	124.79
22	B	603	CLA	CHD-C4C-NC	2.63	128.30	124.23
22	b	602	CLA	CED-O2D-CGD	2.63	121.87	115.92
29	H	103	DGD	C3E-C4E-C5E	-2.62	105.47	110.23
29	H	103	DGD	C3D-C4D-C5D	-2.62	105.47	110.23
26	d	406	PL9	C20-C19-C21	2.62	119.78	115.23
34	F	102	HEC	O2D-CGD-CBD	2.62	122.29	114.00
22	c	503	CLA	O2A-CGA-O1A	-2.62	117.08	123.63
22	b	604	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	B	602	CLA	CMB-C2B-C1B	-2.62	121.44	125.42
22	d	404	CLA	O2A-CGA-O1A	-2.62	117.09	123.63
24	a	406	BCR	C8-C7-C6	-2.62	120.01	127.00
27	c	522	LMG	O3-C3-C2	-2.61	104.21	110.38
28	D	408	SQD	O48-C23-O10	-2.61	117.11	123.63
24	b	618	BCR	C15-C14-C13	-2.61	123.62	127.28
27	A	410	LMG	C1-O6-C5	-2.60	108.63	113.72
22	b	612	CLA	C3B-C4B-NB	-2.60	108.21	110.53
27	c	523	LMG	O8-C28-O10	-2.60	117.12	123.63
22	B	611	CLA	C11-C12-C13	-2.60	107.33	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	CHC-C4B-NB	2.60	127.95	124.05
24	B	619	BCR	C36-C18-C17	-2.60	118.61	122.82
22	B	615	CLA	C1-O2A-CGA	2.60	122.94	116.65
26	a	409	PL9	O2-C1-C6	2.60	124.61	120.48
22	b	605	CLA	C3B-C4B-NB	-2.59	108.22	110.53
26	d	406	PL9	C40-C39-C38	-2.59	116.97	123.63
23	d	401	PHO	C1-C2-C3	-2.59	121.95	126.20
22	a	403	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
33	e	101	LHG	O8-C23-C24	2.59	119.73	111.83
24	K	101	BCR	C7-C8-C9	-2.59	122.41	126.23
26	A	409	PL9	O2-C1-C2	-2.59	115.94	121.83
27	b	621	LMG	C38-C37-C36	-2.59	101.29	114.37
22	c	514	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	B	614	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
23	D	401	PHO	O2D-CGD-O1D	-2.58	118.82	123.85
24	B	619	BCR	C38-C26-C25	-2.58	121.67	124.48
26	d	406	PL9	C40-C39-C41	2.58	119.71	115.23
24	H	102	BCR	C16-C15-C14	-2.58	118.23	123.52
22	B	616	CLA	CHA-C1A-NA	-2.58	120.54	126.39
24	k	102	BCR	C40-C30-C25	2.58	114.29	110.24
24	K	103	BCR	C16-C15-C14	-2.58	118.24	123.52
22	b	612	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
27	Y	101	LMG	O1-C7-C8	-2.58	104.54	110.82
22	B	603	CLA	C1D-ND-C4D	2.58	108.12	106.31
34	v	201	HEC	CHA-C4D-ND	2.58	127.20	124.42
22	a	402	CLA	C3A-C2A-C1A	2.58	105.20	101.34
22	c	506	CLA	O2D-CGD-CBD	2.58	115.73	111.23
29	c	518	DGD	O2D-C2D-C1D	-2.58	103.94	110.08
24	K	103	BCR	C27-C26-C25	2.57	126.18	122.70
28	a	411	SQD	O10-C23-C24	-2.57	113.72	123.78
22	C	507	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
22	b	612	CLA	CBC-CAC-C3C	2.57	119.39	112.42
24	b	618	BCR	C38-C26-C25	-2.57	121.68	124.48
22	B	604	CLA	C6-C5-C3	-2.57	107.21	113.47
22	b	602	CLA	CHC-C1C-NC	2.56	128.17	124.31
27	Y	101	LMG	O6-C1-O1	-2.56	103.99	110.04
22	c	513	CLA	C3B-C4B-NB	-2.56	108.25	110.53
22	B	614	CLA	CBC-CAC-C3C	-2.56	105.49	112.42
22	d	403	CLA	C6-C5-C3	2.56	119.69	113.47
22	B	603	CLA	C4-C3-C5	2.56	119.66	115.23
22	C	512	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
22	B	604	CLA	C1-O2A-CGA	-2.55	110.47	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	611	CLA	CHD-C1D-ND	-2.55	121.21	124.80
24	b	619	BCR	C2-C1-C6	2.55	114.15	110.44
24	A	406	BCR	C15-C16-C17	-2.55	118.30	123.52
22	c	512	CLA	O2D-CGD-CBD	2.55	115.69	111.23
22	B	616	CLA	O1D-CGD-CBD	2.55	129.55	124.52
31	d	412	STE	O2-C1-C2	2.55	122.04	114.00
22	B	604	CLA	CMB-C2B-C1B	-2.54	121.54	125.42
28	A	411	SQD	O5-C1-O6	2.54	116.05	110.04
27	D	407	LMG	C9-C8-C7	-2.54	105.86	111.78
22	C	512	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
23	d	401	PHO	C4B-NB-C1B	2.54	112.52	108.82
22	B	611	CLA	CHB-C4A-NA	2.54	128.06	124.40
33	d	409	LHG	C26-C25-C24	2.54	122.46	113.13
24	B	619	BCR	C15-C16-C17	-2.54	118.33	123.52
22	c	506	CLA	C11-C10-C8	-2.54	107.54	115.97
22	B	610	CLA	CHC-C1C-NC	2.53	128.13	124.31
22	d	404	CLA	C1-C2-C3	-2.53	122.04	126.20
22	A	403	CLA	CHD-C1D-ND	-2.53	121.24	124.80
22	B	609	CLA	C2C-C1C-NC	2.53	112.64	109.98
31	d	413	STE	C3-C2-C1	-2.53	107.92	114.51
22	C	509	CLA	CHA-C4D-ND	2.52	137.75	132.55
22	a	410	CLA	CHD-C1D-ND	-2.52	121.25	124.80
22	d	403	CLA	C1D-ND-C4D	2.52	108.08	106.31
22	C	503	CLA	O2A-C1-C2	-2.52	98.41	108.11
22	B	606	CLA	CHB-C1B-NB	2.52	127.83	124.05
26	D	406	PL9	C30-C29-C31	-2.52	110.86	115.23
31	b	624	STE	O1-C1-C2	-2.52	115.11	123.09
22	B	610	CLA	CHD-C1D-ND	-2.52	121.26	124.80
24	a	406	BCR	C30-C25-C26	-2.52	119.20	122.64
22	c	514	CLA	CHD-C1D-ND	-2.52	121.26	124.80
22	b	610	CLA	CAA-CBA-CGA	-2.51	106.07	113.21
22	a	410	CLA	C1-O2A-CGA	2.51	122.74	116.65
26	D	406	PL9	C7-C8-C9	-2.51	122.50	126.83
22	C	509	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	b	617	BCR	C3-C4-C5	-2.50	109.59	114.06
29	c	517	DGD	C2G-O2G-C1B	2.50	123.78	117.80
29	c	518	DGD	C3D-C4D-C5D	-2.50	105.70	110.23
22	b	608	CLA	CHB-C1B-NB	2.50	127.80	124.05
22	b	616	CLA	CHD-C1D-ND	-2.50	121.29	124.80
22	C	513	CLA	CHB-C4A-NA	2.49	128.00	124.40
27	D	411	LMG	O8-C28-O10	-2.49	117.40	123.63
24	t	101	BCR	C27-C26-C25	2.49	126.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	CHD-C1D-ND	-2.49	121.30	124.80
34	v	201	HEC	C3C-C4C-NC	-2.49	107.39	110.15
22	b	613	CLA	CHA-C1A-NA	-2.49	120.76	126.39
28	A	411	SQD	O9-S-O7	-2.49	105.74	113.82
22	B	603	CLA	CHD-C1D-ND	-2.49	121.31	124.80
22	b	604	CLA	CHB-C1B-NB	2.48	127.78	124.05
22	a	402	CLA	C2B-C1B-NB	-2.48	107.75	110.33
22	B	615	CLA	C2D-C1D-ND	-2.48	107.67	110.13
34	f	101	HEC	O2D-CGD-CBD	2.48	121.83	114.00
24	b	619	BCR	C11-C10-C9	-2.48	123.80	127.28
22	c	509	CLA	CHC-C1C-NC	2.48	128.04	124.31
29	A	413	DGD	O3G-C1D-C2D	-2.48	104.51	108.27
27	Y	101	LMG	C40-C39-C38	-2.47	101.88	114.37
24	A	406	BCR	C1-C6-C5	-2.47	119.26	122.64
22	C	510	CLA	CMB-C2B-C3B	2.47	132.35	126.55
22	b	607	CLA	CHA-C1A-NA	-2.46	120.81	126.39
28	D	408	SQD	O48-C23-C24	2.46	119.35	111.83
24	b	617	BCR	C27-C26-C25	2.46	126.03	122.70
23	a	404	PHO	OBD-CAD-CBD	-2.46	122.21	125.82
33	d	407	LHG	C11-C10-C9	-2.46	101.93	114.37
22	a	403	CLA	CHC-C1C-NC	2.46	128.01	124.31
22	a	402	CLA	C7-C6-C5	-2.46	106.71	113.26
22	c	510	CLA	CHC-C1C-NC	2.46	128.01	124.31
27	A	410	LMG	C40-C39-C38	-2.46	101.95	114.37
22	B	616	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
29	C	517	DGD	O2D-C2D-C1D	-2.46	104.22	110.08
34	F	102	HEC	C3C-C4C-NC	-2.46	107.43	110.15
28	B	622	SQD	O47-C45-C46	2.45	117.15	108.34
34	V	201	HEC	CHB-C1B-NB	2.45	127.06	124.42
22	C	507	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
24	F	101	BCR	C8-C7-C6	-2.45	120.45	127.00
27	M	101	LMG	C1-C2-C3	-2.45	104.86	110.01
22	b	611	CLA	CHD-C1D-C2D	2.45	130.57	125.49
22	d	404	CLA	CHD-C1D-ND	-2.44	121.36	124.80
22	D	403	CLA	C1-C2-C3	-2.44	122.20	126.20
27	M	101	LMG	O2-C2-C1	-2.44	104.27	110.08
22	a	403	CLA	C4D-CHA-C1A	2.44	124.15	121.24
22	B	612	CLA	C1-C2-C3	-2.44	122.20	126.20
22	c	508	CLA	CHD-C1D-ND	-2.43	121.38	124.80
22	a	410	CLA	C2B-C1B-NB	-2.43	107.80	110.33
22	b	608	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
22	C	501	CLA	CHD-C1D-C2D	2.43	130.54	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	515	DGD	O1G-C1A-C2A	-2.43	104.43	111.83
24	A	406	BCR	C37-C22-C21	-2.43	118.88	122.82
26	D	406	PL9	C42-C43-C44	-2.43	122.07	127.62
24	C	514	BCR	C2-C1-C6	2.43	113.96	110.44
24	B	618	BCR	C15-C16-C17	-2.42	118.56	123.52
22	D	405	CLA	O2D-CGD-CBD	2.42	115.46	111.23
22	B	602	CLA	C3B-C4B-NB	-2.42	108.37	110.53
22	B	612	CLA	CHB-C4A-NA	2.42	127.89	124.40
27	c	520	LMG	C1-O6-C5	-2.42	108.99	113.72
22	b	610	CLA	C3A-C2A-C1A	2.42	104.96	101.34
29	C	516	DGD	O6D-C1D-O3G	-2.42	104.33	110.04
22	c	509	CLA	C11-C10-C8	-2.42	107.93	115.97
22	c	505	CLA	C7-C6-C5	-2.42	106.82	113.26
29	h	102	DGD	O5E-C6E-C5E	-2.42	103.11	111.33
34	F	102	HEC	CHB-C1B-NB	2.42	127.02	124.42
27	D	407	LMG	C31-C30-C29	-2.41	104.25	113.13
24	K	103	BCR	C11-C10-C9	-2.41	123.89	127.28
22	C	501	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	b	603	CLA	C7-C6-C5	-2.41	106.83	113.26
28	D	408	SQD	O5-C5-C4	2.41	114.05	109.70
22	C	502	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
24	h	101	BCR	C35-C13-C14	-2.41	118.91	122.82
22	C	507	CLA	CAA-CBA-CGA	-2.41	106.36	113.21
27	b	623	LMG	O6-C5-C6	2.41	112.42	106.44
27	c	520	LMG	O2-C2-C3	-2.41	104.69	110.38
27	D	407	LMG	O2-C2-C1	-2.41	104.33	110.08
28	A	412	SQD	C45-O47-C7	2.41	121.25	117.78
24	b	617	BCR	C38-C26-C25	-2.41	121.86	124.48
22	C	507	CLA	CMB-C2B-C3B	2.41	132.21	126.55
22	c	507	CLA	CED-O2D-CGD	2.41	121.37	115.92
33	D	410	LHG	O8-C23-O10	-2.40	117.62	123.63
23	d	401	PHO	C3D-C4D-ND	2.40	110.79	107.71
22	A	403	CLA	CHD-C1D-C2D	2.40	130.48	125.49
27	M	101	LMG	C17-C16-C15	-2.40	102.23	114.37
22	A	403	CLA	CHB-C1B-NB	2.40	127.65	124.05
26	A	409	PL9	C20-C19-C21	2.40	119.39	115.23
22	b	605	CLA	CHC-C1C-NC	2.40	127.92	124.31
24	B	618	BCR	C37-C22-C21	-2.40	118.93	122.82
22	C	510	CLA	C11-C10-C8	-2.40	108.00	115.97
22	a	410	CLA	O2D-CGD-CBD	2.40	115.42	111.23
28	D	408	SQD	C1-C2-C3	-2.39	104.98	110.01
27	A	410	LMG	C38-C37-C36	-2.39	102.28	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	516	DGD	C1D-C2D-C3D	-2.39	104.98	110.01
27	B	621	LMG	O7-C10-O9	-2.39	117.18	123.33
34	f	101	HEC	C3C-C4C-NC	-2.39	107.50	110.15
22	B	616	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
34	v	201	HEC	CBA-CAA-C2A	-2.39	105.92	112.53
22	A	403	CLA	C1-C2-C3	-2.39	122.29	126.20
29	C	515	DGD	O2G-C1B-C2B	-2.39	106.32	111.48
22	b	612	CLA	CAC-C3C-C4C	2.39	127.89	124.79
22	c	507	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
22	c	503	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
22	B	605	CLA	C11-C10-C8	-2.38	108.05	115.97
34	F	102	HEC	C1D-C2D-C3D	2.38	109.48	106.98
28	a	412	SQD	O49-C7-C8	-2.38	114.47	123.78
26	a	409	PL9	C12-C13-C14	-2.38	122.18	127.62
24	C	514	BCR	C15-C16-C17	-2.38	118.65	123.52
22	b	615	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
22	b	612	CLA	CMD-C2D-C3D	2.38	133.14	127.69
29	C	517	DGD	CAB-C9B-C8B	-2.38	102.36	114.37
29	A	413	DGD	O1G-C1A-O1A	-2.38	117.69	123.63
29	c	518	DGD	O3G-C1D-C2D	-2.38	104.67	108.27
22	B	608	CLA	CHD-C4C-NC	2.37	127.91	124.23
27	b	621	LMG	C20-C19-C18	-2.37	102.37	114.37
29	C	517	DGD	O3D-C3D-C4D	-2.37	104.78	110.38
26	A	409	PL9	C40-C39-C41	2.37	119.35	115.23
26	D	406	PL9	O2-C1-C2	-2.37	116.44	121.83
22	C	502	CLA	C4D-CHA-C1A	2.37	124.07	121.24
22	B	604	CLA	CHA-C1A-NA	-2.37	121.02	126.39
22	B	604	CLA	CGD-CBD-CAD	-2.37	103.17	110.85
22	b	610	CLA	C4-C3-C5	2.37	119.34	115.23
22	c	510	CLA	C3B-C4B-NB	-2.37	108.42	110.53
22	c	504	CLA	C11-C12-C13	-2.37	108.10	115.97
24	k	101	BCR	C38-C26-C25	-2.37	121.90	124.48
23	a	404	PHO	C3D-C4D-ND	2.37	110.74	107.71
27	D	407	LMG	O8-C28-O10	-2.36	117.71	123.63
22	C	503	CLA	C6-C7-C8	-2.36	108.11	115.97
22	B	614	CLA	C4-C3-C5	2.36	119.33	115.23
23	A	404	PHO	C3B-C4B-NB	-2.36	105.92	107.46
22	b	605	CLA	O1D-CGD-CBD	2.36	129.18	124.52
24	H	102	BCR	C35-C13-C14	-2.36	118.99	122.82
31	J	101	STE	O2-C1-C2	2.36	121.46	114.00
24	d	405	BCR	C24-C23-C22	-2.36	122.75	126.23
28	A	411	SQD	O48-C23-C24	2.36	119.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	V	201	HEC	CHC-C1C-NC	2.36	128.13	123.86
22	b	608	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
22	c	514	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
22	B	607	CLA	CHB-C1B-NB	2.36	127.58	124.05
33	D	412	LHG	C20-C19-C18	-2.35	102.47	114.37
29	c	518	DGD	C3G-O3G-C1D	2.35	118.84	113.80
22	c	514	CLA	C4A-NA-C1A	2.35	107.75	106.68
22	B	607	CLA	C3A-C2A-C1A	2.35	104.86	101.34
22	C	505	CLA	CAA-CBA-CGA	-2.35	106.53	113.21
26	d	406	PL9	C7-C8-C9	-2.35	122.78	126.83
31	d	411	STE	O2-C1-O1	-2.35	117.29	123.33
22	b	603	CLA	CHB-C1B-NB	2.35	127.57	124.05
24	b	619	BCR	C28-C27-C26	-2.35	109.87	114.06
22	c	514	CLA	CHB-C4A-NA	2.35	127.78	124.40
22	C	502	CLA	CHA-C1A-NA	-2.35	121.08	126.39
28	B	622	SQD	C46-C45-C44	-2.35	106.32	111.78
22	B	607	CLA	C1C-C2C-C3C	-2.34	104.51	106.98
27	d	410	LMG	C3-C4-C5	-2.34	105.98	110.23
23	A	404	PHO	C5-C3-C2	2.34	126.43	121.17
22	b	616	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	C	514	BCR	C33-C5-C6	-2.34	121.93	124.48
22	c	510	CLA	CAC-C3C-C4C	2.34	127.84	124.79
22	c	513	CLA	C1-C2-C3	-2.34	122.36	126.20
22	c	503	CLA	CHB-C1B-NB	2.34	127.56	124.05
24	B	619	BCR	C40-C30-C29	-2.34	99.97	108.95
29	C	517	DGD	CBB-CAB-C9B	-2.34	102.56	114.37
22	C	503	CLA	CAA-CBA-CGA	-2.34	106.58	113.21
31	B	623	STE	O2-C1-C2	2.34	121.38	114.00
22	b	603	CLA	CHD-C1D-C2D	2.33	130.34	125.49
22	b	609	CLA	C1-C2-C3	-2.33	122.38	126.20
27	b	621	LMG	O8-C28-O10	-2.33	117.80	123.63
22	C	505	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
22	C	501	CLA	C9-C8-C10	-2.33	102.97	111.27
24	d	405	BCR	C16-C15-C14	-2.33	118.75	123.52
24	b	617	BCR	C8-C7-C6	-2.33	120.77	127.00
22	B	603	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
34	V	201	HEC	C3D-C4D-ND	-2.33	108.10	110.35
29	c	517	DGD	C4A-C3A-C2A	-2.33	104.57	113.13
22	B	614	CLA	CHA-C1A-NA	-2.33	121.12	126.39
33	E	101	LHG	O8-C23-C24	2.33	118.93	111.83
22	C	507	CLA	C4D-CHA-C1A	2.33	124.02	121.24
26	A	409	PL9	C27-C28-C29	-2.33	122.30	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	CED-O2D-CGD	2.32	121.19	115.92
22	C	509	CLA	C3B-C4B-NB	-2.32	108.46	110.53
29	c	518	DGD	O4D-C4D-C3D	2.32	115.85	110.38
22	C	509	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
22	b	605	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	b	619	BCR	C8-C7-C6	-2.32	120.80	127.00
22	B	612	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
22	A	405	CLA	CHB-C4A-NA	2.32	127.74	124.40
24	B	617	BCR	C7-C8-C9	-2.32	122.81	126.23
29	H	103	DGD	C7B-C6B-C5B	-2.32	102.66	114.37
22	c	512	CLA	C4D-CHA-C1A	2.32	124.01	121.24
22	b	612	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
22	C	507	CLA	CHB-C4A-NA	2.31	127.74	124.40
22	c	504	CLA	C4-C3-C5	2.31	119.24	115.23
22	b	610	CLA	C3B-C4B-NB	-2.31	108.47	110.53
22	B	616	CLA	C2A-C1A-CHA	2.31	127.87	123.87
29	c	519	DGD	O3D-C3D-C4D	-2.31	104.94	110.38
22	c	502	CLA	CED-O2D-CGD	-2.31	110.68	115.92
22	C	512	CLA	CAA-CBA-CGA	-2.31	106.66	113.21
29	h	102	DGD	C1D-O6D-C5D	-2.31	109.22	113.72
22	c	508	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
22	D	403	CLA	CMD-C2D-C3D	2.31	132.98	127.69
22	c	502	CLA	C3B-C4B-NB	-2.31	108.47	110.53
22	C	506	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
22	B	602	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
29	H	103	DGD	C1D-O6D-C5D	-2.30	109.22	113.72
24	T	101	BCR	C38-C26-C27	-2.30	108.69	113.60
22	B	605	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
27	c	523	LMG	C1-O6-C5	-2.30	109.22	113.72
29	h	102	DGD	C7B-C6B-C5B	-2.30	102.74	114.37
22	B	611	CLA	C1-C2-C3	-2.30	122.43	126.20
31	b	627	STE	C3-C2-C1	-2.30	108.51	114.51
22	b	602	CLA	CHD-C1D-C2D	2.30	130.27	125.49
22	b	608	CLA	CHB-C4A-NA	2.30	127.72	124.40
24	h	101	BCR	C35-C13-C12	2.30	121.60	118.09
34	V	201	HEC	CBD-CAD-C3D	-2.30	106.18	112.53
33	e	101	LHG	C11-C10-C9	-2.30	102.76	114.37
22	C	505	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	B	601	STE	O2-C1-C2	2.30	121.25	114.00
29	C	515	DGD	C3B-C2B-C1B	-2.29	105.29	113.69
24	c	515	BCR	C15-C14-C13	-2.29	124.06	127.28
29	C	517	DGD	C8B-C7B-C6B	-2.29	102.78	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	PHO	O2A-CGA-O1A	-2.29	117.90	123.63
22	C	503	CLA	CHB-C1B-NB	2.29	127.48	124.05
22	A	405	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
29	h	102	DGD	O3E-C3E-C2E	-2.29	104.98	110.38
27	M	101	LMG	O7-C10-C11	-2.29	106.53	111.48
22	b	604	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
24	K	103	BCR	C2-C1-C6	2.29	113.76	110.44
22	b	606	CLA	C4-C3-C5	2.29	119.20	115.23
22	C	509	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
22	c	508	CLA	C3B-C4B-NB	-2.28	108.49	110.53
22	C	505	CLA	C16-C15-C13	-2.28	108.38	115.97
22	b	605	CLA	C16-C15-C13	-2.28	108.38	115.97
33	d	408	LHG	O8-C23-C24	2.28	118.78	111.83
23	d	401	PHO	CMB-C2B-C3B	2.28	129.23	124.68
24	b	618	BCR	C27-C26-C25	2.28	125.78	122.70
24	B	619	BCR	C28-C27-C26	-2.28	110.00	114.06
24	K	101	BCR	C24-C23-C22	-2.28	122.87	126.23
22	B	602	CLA	C11-C12-C13	-2.27	108.41	115.97
24	H	102	BCR	C1-C6-C5	-2.27	119.53	122.64
22	B	610	CLA	O1A-CGA-CBA	2.27	132.67	123.78
22	c	507	CLA	C4-C3-C5	2.27	119.17	115.23
22	b	605	CLA	C1D-ND-C4D	2.27	107.91	106.31
29	C	517	DGD	C1D-C2D-C3D	-2.27	105.23	110.01
33	L	102	LHG	C12-C11-C10	-2.27	102.90	114.37
29	C	515	DGD	C3D-C4D-C5D	-2.27	106.12	110.23
27	c	520	LMG	C40-C39-C38	-2.27	102.91	114.37
22	b	612	CLA	CHD-C1D-ND	-2.27	121.61	124.80
22	b	616	CLA	C2B-C1B-NB	2.27	112.67	110.33
23	D	401	PHO	O2D-CGD-CBD	2.26	113.43	110.95
33	D	412	LHG	C11-C10-C9	-2.26	102.94	114.37
22	B	615	CLA	C1C-C2C-C3C	-2.26	104.61	106.98
29	H	103	DGD	C4D-C3D-C2D	-2.26	106.87	110.83
22	b	602	CLA	CHA-C4D-ND	2.26	137.21	132.55
22	C	511	CLA	C3B-C4B-NB	-2.26	108.52	110.53
22	C	506	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
22	B	610	CLA	CHC-C1C-C2C	-2.26	120.54	126.95
22	c	507	CLA	C4A-NA-C1A	2.26	107.71	106.68
29	h	102	DGD	O2D-C2D-C1D	-2.25	104.70	110.08
24	t	101	BCR	C11-C10-C9	-2.25	124.12	127.28
22	A	403	CLA	CHB-C4A-NA	2.25	127.65	124.40
22	d	404	CLA	CHB-C4A-NA	2.25	127.65	124.40
22	D	404	CLA	CHC-C4B-NB	2.25	127.42	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	O1D-CGD-CBD	2.25	128.95	124.52
29	H	103	DGD	CAB-C9B-C8B	-2.25	103.01	114.37
29	c	518	DGD	O6D-C1D-O3G	-2.25	104.73	110.04
22	C	503	CLA	CHD-C1D-ND	-2.25	121.64	124.80
28	B	622	SQD	O8-S-O7	-2.24	105.79	111.40
22	b	602	CLA	C2D-C1D-ND	-2.24	107.91	110.13
29	A	413	DGD	CDB-CCB-CBB	-2.24	103.04	114.37
22	a	402	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
24	b	617	BCR	C11-C10-C9	-2.24	124.14	127.28
24	t	101	BCR	C36-C18-C19	2.24	121.50	118.09
31	b	627	STE	O2-C1-C2	2.23	121.06	114.00
22	B	607	CLA	C2C-C1C-NC	2.23	112.33	109.98
22	b	612	CLA	C1-C2-C3	-2.23	122.54	126.20
34	V	201	HEC	CBB-CAB-C3B	2.23	118.47	112.42
22	B	610	CLA	C3B-C4B-NB	-2.23	108.54	110.53
22	a	402	CLA	C4-C3-C5	2.23	119.10	115.23
24	B	618	BCR	C38-C26-C25	-2.23	122.05	124.48
22	b	602	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
24	K	101	BCR	C31-C1-C6	2.23	113.74	110.24
24	A	406	BCR	C36-C18-C17	-2.23	119.21	122.82
24	b	617	BCR	C15-C16-C17	-2.23	118.96	123.52
22	b	606	CLA	CHB-C1B-NB	2.23	127.39	124.05
22	c	514	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
24	c	516	BCR	C7-C8-C9	-2.23	122.94	126.23
34	v	201	HEC	C2A-C1A-NA	-2.23	108.18	110.32
34	V	201	HEC	C3C-C4C-NC	-2.22	107.68	110.15
22	b	602	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
22	a	402	CLA	C17-C16-C15	-2.22	103.32	113.28
24	B	619	BCR	C11-C10-C9	-2.22	124.16	127.28
26	d	406	PL9	O2-C1-C2	-2.22	116.78	121.83
22	C	506	CLA	CHC-C4B-NB	2.22	127.38	124.05
22	b	611	CLA	C2A-C3A-C4A	2.22	105.45	101.87
22	B	609	CLA	CHB-C4A-NA	2.22	127.60	124.40
22	b	609	CLA	C3C-C4C-NC	-2.22	107.59	110.43
22	B	608	CLA	C3B-C4B-NB	-2.22	108.55	110.53
22	c	504	CLA	O1D-CGD-CBD	2.22	128.89	124.52
22	c	507	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
24	B	618	BCR	C35-C13-C14	-2.22	119.23	122.82
22	b	609	CLA	CED-O2D-CGD	2.22	120.94	115.92
33	d	408	LHG	C20-C19-C18	-2.22	103.17	114.37
24	C	514	BCR	C1-C6-C5	-2.21	119.61	122.64
22	b	609	CLA	CHB-C1B-C2B	-2.21	121.00	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	CHB-C1B-NB	2.21	127.37	124.05
34	V	201	HEC	CHD-C4C-NC	2.21	127.87	123.86
33	D	409	LHG	C27-C26-C25	-2.21	103.18	114.37
26	a	409	PL9	C36-C34-C33	-2.21	116.20	121.17
22	H	101	CLA	CAA-C2A-C1A	-2.21	104.72	111.97
22	b	613	CLA	C16-C15-C13	-2.21	108.61	115.97
22	D	403	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
24	K	103	BCR	C7-C8-C9	-2.21	122.96	126.23
27	M	101	LMG	C23-C22-C21	-2.21	103.20	114.37
27	b	621	LMG	C22-C21-C20	-2.21	103.20	114.37
29	C	516	DGD	C1D-O6D-C5D	-2.21	109.41	113.72
22	b	607	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
26	A	409	PL9	C7-C8-C9	-2.20	123.03	126.83
24	k	101	BCR	C1-C6-C5	-2.20	119.62	122.64
29	c	517	DGD	O3D-C3D-C4D	-2.20	105.18	110.38
22	a	402	CLA	CHB-C4A-NA	2.20	127.58	124.40
22	C	504	CLA	CHD-C1D-ND	-2.20	121.71	124.80
22	b	612	CLA	O2D-CGD-CBD	2.20	115.07	111.23
22	C	511	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
24	K	102	BCR	C33-C5-C6	-2.20	122.09	124.48
22	b	609	CLA	C7-C6-C5	-2.20	107.41	113.26
22	a	403	CLA	C1D-ND-C4D	2.20	107.85	106.31
27	d	410	LMG	O7-C10-O9	-2.19	118.58	123.70
22	B	609	CLA	CHC-C4B-NB	2.19	127.34	124.05
29	C	515	DGD	C1D-C2D-C3D	-2.19	105.39	110.01
24	T	101	BCR	C30-C25-C26	-2.19	119.64	122.64
22	B	604	CLA	C2A-C3A-C4A	2.19	105.41	101.87
23	A	404	PHO	OBD-CAD-CBD	-2.19	122.61	125.82
29	h	102	DGD	C1D-C2D-C3D	-2.19	105.40	110.01
22	b	612	CLA	CMB-C2B-C3B	2.19	131.71	126.55
27	b	623	LMG	C40-C39-C38	-2.19	103.30	114.37
22	A	405	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
22	c	513	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
22	d	404	CLA	O1D-CGD-CBD	2.19	128.83	124.52
24	C	514	BCR	C35-C13-C14	-2.19	119.28	122.82
22	B	604	CLA	C2A-C1A-CHA	2.19	127.66	123.87
22	B	613	CLA	CHB-C4A-NA	2.18	127.55	124.40
27	c	523	LMG	C4-C3-C2	-2.18	107.00	110.83
22	C	509	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
22	c	509	CLA	CHD-C1D-C2D	2.18	130.03	125.49
27	A	410	LMG	C3-C4-C5	-2.18	106.27	110.23
29	H	103	DGD	O6D-C1D-O3G	-2.18	104.88	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	CHB-C4A-NA	2.18	127.55	124.40
27	c	523	LMG	O5-C6-C5	-2.18	103.90	111.33
34	V	201	HEC	O2D-CGD-CBD	2.18	120.89	114.00
24	b	619	BCR	C30-C25-C26	-2.18	119.66	122.64
22	B	616	CLA	C1D-ND-C4D	2.18	107.84	106.31
22	B	614	CLA	O1D-CGD-CBD	2.18	128.82	124.52
22	c	504	CLA	C2B-C1B-NB	-2.18	108.07	110.33
28	L	101	SQD	O47-C45-C46	2.18	116.16	108.34
22	C	506	CLA	CHA-C1A-NA	-2.18	121.46	126.39
26	A	409	PL9	O2-C1-C6	2.18	123.94	120.48
28	A	412	SQD	O47-C45-C46	2.18	111.22	106.21
29	H	103	DGD	C9A-C8A-C7A	-2.18	103.36	114.37
22	A	403	CLA	CHB-C1B-C2B	-2.18	121.11	127.43
22	b	605	CLA	CHD-C1D-C2D	2.18	130.01	125.49
28	f	102	SQD	O47-C7-O49	-2.18	118.62	123.70
22	C	504	CLA	CHC-C1C-NC	2.18	127.59	124.31
26	d	406	PL9	O1-C4-C3	-2.18	118.44	120.73
22	B	614	CLA	CHB-C1B-NB	2.17	127.31	124.05
29	C	515	DGD	C5B-C4B-C3B	-2.17	103.38	114.37
24	A	406	BCR	C4-C5-C6	2.17	125.64	122.70
29	H	103	DGD	C7A-C6A-C5A	-2.17	103.40	114.37
24	c	516	BCR	C40-C30-C39	-2.17	102.42	108.63
28	f	102	SQD	O47-C7-C8	2.17	118.90	110.93
33	l	101	LHG	C11-C10-C9	-2.17	103.41	114.37
22	C	513	CLA	C3A-C2A-C1A	2.17	104.59	101.34
22	C	501	CLA	C3D-C4D-ND	2.17	113.51	109.99
22	a	402	CLA	C2A-C1A-CHA	2.17	127.63	123.87
24	B	618	BCR	C15-C14-C13	-2.17	124.24	127.28
24	h	101	BCR	C16-C15-C14	-2.16	119.09	123.52
22	c	508	CLA	CED-O2D-CGD	2.16	120.82	115.92
22	b	612	CLA	C1D-ND-C4D	-2.16	104.79	106.31
22	c	508	CLA	CMB-C2B-C3B	2.16	131.64	126.55
22	b	616	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
22	c	507	CLA	CHD-C4C-NC	2.16	127.58	124.23
24	t	101	BCR	C34-C9-C10	-2.16	119.31	122.82
22	B	612	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	C	514	BCR	C29-C30-C25	2.16	113.58	110.44
33	E	101	LHG	C26-C25-C24	2.16	121.06	113.13
31	E	102	STE	O2-C1-C2	2.16	120.82	114.00
22	b	614	CLA	CMB-C2B-C3B	2.16	131.62	126.55
22	B	603	CLA	CMA-C3A-C4A	2.16	117.57	111.77
28	a	411	SQD	O4-C4-C3	-2.16	105.29	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C1D-CHD-C4C	-2.16	121.44	126.02
22	B	605	CLA	C4D-C3D-CAD	-2.16	105.77	108.11
27	Y	101	LMG	C3-C4-C5	-2.16	106.32	110.23
22	b	607	CLA	C2C-C1C-NC	2.15	112.24	109.98
22	A	403	CLA	C1D-ND-C4D	2.15	107.82	106.31
22	b	610	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	c	516	BCR	C1-C6-C5	-2.15	119.70	122.64
22	d	404	CLA	CBC-CAC-C3C	-2.15	106.59	112.42
22	c	505	CLA	C3B-C4B-NB	-2.15	108.61	110.53
22	b	605	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
24	h	101	BCR	C1-C6-C5	-2.15	119.70	122.64
22	c	506	CLA	O1D-CGD-CBD	2.15	128.75	124.52
22	B	613	CLA	CED-O2D-CGD	2.14	120.78	115.92
33	D	410	LHG	O8-C6-C5	-2.14	102.22	108.40
29	c	518	DGD	CDB-CCB-CBB	-2.14	103.53	114.37
24	k	102	BCR	C16-C15-C14	-2.14	119.14	123.52
22	d	403	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
22	B	604	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
23	d	401	PHO	CAA-CBA-CGA	-2.14	107.13	113.21
29	A	413	DGD	O5D-C1E-C2E	2.14	111.52	108.27
22	d	403	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
22	B	610	CLA	C4D-CHA-C1A	2.14	123.80	121.24
22	D	405	CLA	CHB-C4A-NA	2.14	127.49	124.40
22	a	405	CLA	CHD-C4C-NC	2.14	127.55	124.23
22	d	403	CLA	CHA-C4D-ND	2.14	136.96	132.55
22	C	513	CLA	C4-C3-C5	2.14	118.94	115.23
29	h	102	DGD	C1E-O6E-C5E	2.14	117.89	113.72
34	V	201	HEC	CAB-C3B-C4B	2.13	127.57	124.79
27	b	621	LMG	O1-C7-C8	-2.13	105.63	110.82
22	b	614	CLA	C1-C2-C3	-2.13	122.70	126.20
27	b	623	LMG	C1-C2-C3	-2.13	105.52	110.01
24	K	102	BCR	C16-C15-C14	-2.13	119.16	123.52
22	b	615	CLA	CHB-C4A-NA	2.13	127.47	124.40
34	V	201	HEC	CBC-CAC-C3C	2.13	118.19	112.42
22	d	404	CLA	CMB-C2B-C3B	2.13	131.56	126.55
22	b	605	CLA	C1-O2A-CGA	-2.13	111.50	116.65
22	B	608	CLA	CMA-C3A-C2A	-2.13	105.76	113.98
22	B	602	CLA	C2A-C1A-CHA	2.13	127.56	123.87
22	C	510	CLA	CHA-C1A-NA	-2.13	121.58	126.39
24	b	617	BCR	C37-C22-C21	-2.12	119.37	122.82
22	C	510	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
22	b	604	CLA	CHB-C4A-NA	2.12	127.47	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	PHO	OBD-CAD-C3D	2.12	131.20	127.89
26	A	409	PL9	C30-C29-C31	-2.12	111.54	115.23
33	E	101	LHG	C11-C10-C9	-2.12	103.64	114.37
22	C	501	CLA	OBD-CAD-C3D	2.12	133.38	128.42
22	c	503	CLA	CHD-C1D-ND	-2.12	121.82	124.80
24	t	101	BCR	C1-C6-C5	-2.12	119.74	122.64
22	B	612	CLA	CHD-C1D-ND	-2.12	121.82	124.80
26	a	409	PL9	C27-C28-C29	-2.12	122.77	127.62
22	c	506	CLA	CMD-C2D-C3D	2.12	132.55	127.69
29	c	519	DGD	CAB-C9B-C8B	-2.12	103.65	114.37
22	b	602	CLA	CHD-C1D-ND	-2.12	121.82	124.80
22	C	512	CLA	CHA-C1A-NA	-2.12	121.59	126.39
27	a	415	LMG	C1-O6-C5	-2.12	109.58	113.72
24	c	516	BCR	C15-C16-C17	-2.12	119.18	123.52
22	b	604	CLA	C1-C2-C3	-2.12	122.73	126.20
22	C	503	CLA	C1-C2-C3	2.12	129.66	126.20
22	C	502	CLA	C2A-C1A-CHA	2.12	127.54	123.87
34	V	201	HEC	CAD-CBD-CGD	-2.12	108.05	113.67
22	c	514	CLA	CMB-C2B-C3B	2.11	131.52	126.55
24	B	618	BCR	C40-C30-C25	2.11	113.56	110.24
33	e	101	LHG	C20-C19-C18	-2.11	103.68	114.37
29	C	515	DGD	CCB-CBB-CAB	-2.11	103.69	114.37
22	c	507	CLA	CMB-C2B-C3B	2.11	131.52	126.55
24	C	514	BCR	C27-C26-C25	2.11	125.56	122.70
26	D	406	PL9	O2-C1-C6	2.11	123.84	120.48
22	b	610	CLA	C2A-C1A-CHA	2.11	127.53	123.87
27	M	101	LMG	O3-C3-C2	-2.11	105.40	110.38
22	C	505	CLA	C4-C3-C2	-2.11	118.21	123.63
24	a	406	BCR	C24-C23-C22	-2.11	123.11	126.23
22	C	513	CLA	O1D-CGD-CBD	2.11	128.68	124.52
22	C	501	CLA	C2D-C1D-ND	-2.11	108.04	110.13
27	a	415	LMG	O1-C1-C2	2.11	111.47	108.27
22	B	616	CLA	C4D-C3D-CAD	-2.11	105.82	108.11
27	B	621	LMG	O9-C10-C11	2.11	129.78	123.09
33	E	101	LHG	C20-C19-C18	-2.11	103.72	114.37
22	B	605	CLA	CHD-C1D-C2D	2.10	129.86	125.49
33	E	101	LHG	C18-C17-C16	-2.10	103.73	114.37
28	f	102	SQD	C45-O47-C7	2.10	122.83	117.80
24	B	618	BCR	C3-C4-C5	-2.10	110.31	114.06
22	H	101	CLA	C4-C3-C5	2.10	118.88	115.23
22	B	615	CLA	C2B-C1B-NB	-2.10	108.15	110.33
34	f	101	HEC	CAC-C3C-C2C	2.10	130.21	126.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	BCR	C38-C26-C27	-2.10	109.12	113.60
22	b	616	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
22	b	613	CLA	C2A-C1A-CHA	2.10	127.51	123.87
34	f	101	HEC	CBA-CAA-C2A	-2.10	106.73	112.53
22	C	502	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
26	D	406	PL9	C8-C7-C3	2.10	117.45	112.03
22	b	601	CLA	C11-C12-C13	-2.10	108.99	115.97
27	b	621	LMG	C1-O6-C5	-2.10	109.62	113.72
31	c	521	STE	O2-C1-C2	2.10	120.62	114.00
27	D	411	LMG	O7-C10-O9	-2.10	118.81	123.70
31	d	411	STE	O2-C1-C2	2.09	120.62	114.00
22	c	511	CLA	O2D-CGD-CBD	2.09	114.89	111.23
22	C	508	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
28	f	102	SQD	O5-C1-O6	2.09	114.99	110.04
24	t	101	BCR	C2-C3-C4	-2.09	106.67	111.28
22	H	101	CLA	CHA-C4D-ND	2.09	136.87	132.55
24	B	617	BCR	C37-C22-C23	2.09	121.28	118.09
22	b	601	CLA	CBA-CAA-C2A	2.09	120.02	113.79
24	b	619	BCR	C38-C26-C25	-2.09	122.20	124.48
22	a	402	CLA	CMB-C2B-C3B	2.09	131.47	126.55
22	c	505	CLA	CHB-C4A-NA	2.09	127.42	124.40
28	A	411	SQD	O7-S-C6	2.09	109.88	106.76
29	c	519	DGD	CDB-CCB-CBB	-2.09	103.80	114.37
22	c	512	CLA	CHD-C1D-ND	-2.09	121.87	124.80
22	b	605	CLA	O2D-CGD-CBD	2.09	114.88	111.23
22	B	607	CLA	C3B-C4B-NB	-2.09	108.67	110.53
33	D	409	LHG	C20-C19-C18	-2.09	103.83	114.37
22	b	610	CLA	C2C-C1C-NC	2.09	112.17	109.98
22	b	608	CLA	C2A-C3A-C4A	2.09	105.24	101.87
33	d	407	LHG	C25-C24-C23	2.08	121.33	113.69
22	c	502	CLA	CHB-C4A-NA	2.08	127.41	124.40
22	b	607	CLA	CHC-C4B-NB	2.08	127.18	124.05
22	b	615	CLA	CHA-C4D-ND	2.08	136.85	132.55
23	A	404	PHO	OBD-CAD-C3D	2.08	131.14	127.89
27	A	410	LMG	C1-C2-C3	-2.08	105.63	110.01
29	C	517	DGD	CDB-CCB-CBB	-2.08	103.84	114.37
26	a	409	PL9	C40-C39-C41	2.08	118.84	115.23
24	C	514	BCR	C34-C9-C10	-2.08	119.45	122.82
29	A	413	DGD	C5B-C4B-C3B	-2.08	103.85	114.37
24	h	101	BCR	C16-C17-C18	-2.08	124.36	127.28
22	D	403	CLA	C3B-C4B-NB	-2.08	108.67	110.53
22	C	507	CLA	C1-C2-C3	-2.08	122.79	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4D-CHA-C1A	2.08	123.72	121.24
22	b	607	CLA	C4D-CHA-C1A	2.08	123.72	121.24
29	C	516	DGD	C4E-C3E-C2E	-2.08	107.19	110.83
22	B	611	CLA	C15-C13-C12	2.08	122.58	112.07
22	b	603	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
22	c	514	CLA	O1D-CGD-CBD	2.07	128.61	124.52
22	c	510	CLA	O2D-CGD-CBD	2.07	114.86	111.23
22	a	405	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	B	607	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
27	c	520	LMG	O6-C1-O1	-2.07	105.15	110.04
28	B	622	SQD	C1-C2-C3	-2.07	105.65	110.01
24	b	617	BCR	C36-C18-C17	-2.07	119.46	122.82
27	D	407	LMG	O3-C3-C2	-2.07	105.50	110.38
22	B	606	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
22	a	405	CLA	CHC-C1C-NC	2.07	127.43	124.31
22	a	410	CLA	C2A-C1A-CHA	2.07	127.46	123.87
24	b	618	BCR	C30-C25-C26	-2.07	119.81	122.64
28	D	408	SQD	C44-O6-C1	2.07	117.21	113.68
23	A	404	PHO	C3D-C4D-ND	2.07	110.36	107.71
22	B	604	CLA	CMB-C2B-C3B	2.07	131.41	126.55
29	C	516	DGD	C8B-C7B-C6B	-2.06	103.93	114.37
24	K	102	BCR	C36-C18-C17	-2.06	119.47	122.82
22	b	610	CLA	O2D-CGD-CBD	2.06	114.84	111.23
22	b	613	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
29	C	515	DGD	C9B-C8B-C7B	-2.06	103.94	114.37
28	A	411	SQD	O5-C1-C2	-2.06	106.14	110.37
24	t	101	BCR	C39-C30-C25	2.06	113.47	110.24
27	D	407	LMG	O1-C1-C2	-2.06	105.14	108.27
22	b	609	CLA	CHA-C4D-ND	2.06	136.80	132.55
29	C	516	DGD	O3G-C1D-C2D	-2.06	105.15	108.27
22	c	514	CLA	CHD-C4C-NC	2.06	127.42	124.23
22	C	503	CLA	C3A-C2A-C1A	2.06	104.42	101.34
24	t	101	BCR	C30-C25-C26	-2.06	119.82	122.64
22	c	505	CLA	CHB-C1B-NB	2.06	127.14	124.05
29	c	518	DGD	C6D-O5D-C1E	2.05	118.20	113.80
33	l	101	LHG	C20-C19-C18	-2.05	103.98	114.37
28	a	411	SQD	O5-C5-C4	2.05	113.40	109.70
22	c	507	CLA	CHA-C1A-NA	-2.05	121.74	126.39
24	t	101	BCR	C38-C26-C27	-2.05	109.22	113.60
22	b	609	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
22	c	505	CLA	CMC-C2C-C1C	2.05	128.24	125.03
22	C	504	CLA	CHC-C1C-C2C	-2.05	121.12	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	BCR	C15-C14-C13	-2.05	124.40	127.28
22	B	611	CLA	C3D-C4D-ND	2.05	113.32	109.99
32	D	402	BCT	O3-C-O1	-2.05	114.43	119.68
22	b	613	CLA	CMB-C2B-C3B	2.05	131.37	126.55
22	A	403	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	C	509	CLA	CMB-C2B-C3B	2.05	131.37	126.55
24	t	101	BCR	C16-C15-C14	-2.05	119.33	123.52
22	C	508	CLA	CHB-C4A-NA	2.05	127.35	124.40
34	V	201	HEC	C1D-ND-C4D	2.05	107.63	105.21
22	b	611	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
22	d	404	CLA	CHD-C1D-C2D	2.05	129.74	125.49
26	D	406	PL9	C20-C19-C21	2.05	118.78	115.23
26	d	406	PL9	C8-C7-C3	2.05	117.32	112.03
22	C	504	CLA	CHA-C1A-NA	-2.05	121.76	126.39
22	d	404	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
24	B	619	BCR	C37-C22-C21	-2.04	119.51	122.82
29	c	518	DGD	C8B-C7B-C6B	-2.04	104.05	114.37
22	D	403	CLA	C1D-ND-C4D	-2.04	104.88	106.31
22	b	605	CLA	O1A-CGA-CBA	2.04	131.75	123.78
24	b	619	BCR	C15-C16-C17	-2.04	119.35	123.52
29	c	517	DGD	O3E-C3E-C2E	-2.04	105.58	110.38
22	B	612	CLA	C4C-C3C-C2C	-2.04	103.93	106.89
33	D	410	LHG	C6-C5-C4	2.04	116.53	111.78
22	a	403	CLA	C2D-C1D-ND	-2.03	108.11	110.13
34	V	201	HEC	CHC-C4B-C3B	2.03	128.98	125.23
29	H	103	DGD	C8B-C7B-C6B	-2.03	104.08	114.37
27	D	407	LMG	C38-C37-C36	-2.03	104.09	114.37
22	A	402	CLA	C1D-ND-C4D	-2.03	104.89	106.31
24	c	515	BCR	C27-C26-C25	2.03	125.45	122.70
22	B	611	CLA	C4A-NA-C1A	2.03	107.61	106.68
34	f	101	HEC	O1A-CGA-CBA	-2.03	116.65	123.09
22	b	604	CLA	C2A-C1A-CHA	2.03	127.39	123.87
28	A	411	SQD	O5-C5-C4	2.03	113.36	109.70
22	A	405	CLA	CMB-C2B-C3B	2.03	131.32	126.55
22	B	611	CLA	OBD-CAD-C3D	2.03	133.16	128.42
24	d	405	BCR	C21-C20-C19	-2.03	117.32	123.20
22	b	610	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
22	C	510	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
22	c	508	CLA	CHB-C4A-NA	2.03	127.32	124.40
24	B	617	BCR	C15-C16-C17	-2.03	119.37	123.52
22	C	513	CLA	CHC-C1C-NC	2.03	127.36	124.31
22	b	610	CLA	C3B-C2B-C1B	-2.02	104.78	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	CHB-C4A-NA	2.02	127.32	124.40
24	K	102	BCR	C38-C26-C25	-2.02	122.28	124.48
22	b	615	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
22	B	610	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
22	D	404	CLA	C3B-C2B-C1B	-2.02	104.79	107.17
22	B	611	CLA	C3B-C4B-NB	-2.02	108.73	110.53
28	a	411	SQD	O8-S-O9	-2.02	106.35	111.40
22	C	507	CLA	CHA-C4D-ND	2.02	136.71	132.55
22	C	502	CLA	CED-O2D-CGD	2.02	120.49	115.92
24	c	515	BCR	C33-C5-C6	-2.02	122.28	124.48
34	V	201	HEC	C4B-NB-C1B	2.02	107.59	105.21
22	d	404	CLA	C4A-NA-C1A	2.01	107.60	106.68
24	b	618	BCR	C35-C13-C12	2.01	121.17	118.09
22	b	615	CLA	CHA-C1A-NA	-2.01	121.83	126.39
22	b	601	CLA	CHD-C1D-C2D	2.01	129.68	125.49
22	B	605	CLA	C6-C5-C3	2.01	118.37	113.47
27	M	101	LMG	C32-C31-C30	-2.01	104.20	114.37
22	C	513	CLA	C2A-C1A-CHA	2.01	127.35	123.87
28	f	102	SQD	O5-C1-C2	-2.01	106.24	110.37
24	F	101	BCR	C15-C16-C17	-2.01	119.41	123.52
22	D	403	CLA	O1D-CGD-CBD	2.01	128.47	124.52
27	a	415	LMG	O5-C6-C5	-2.01	104.50	111.33
31	m	102	STE	O2-C1-O1	-2.00	118.18	123.33
22	A	402	CLA	CHD-C1D-ND	-2.00	121.98	124.80
22	D	403	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
22	C	503	CLA	CHA-C1A-NA	-2.00	121.86	126.39
27	c	520	LMG	O8-C28-O10	-2.00	118.62	123.63

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	F	102	HEC	NA
34	V	201	HEC	NA
34	f	101	HEC	NA
34	v	201	HEC	NA

All (1812) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C2-C3-C5-C6
22	A	405	CLA	C4-C3-C5-C6
22	B	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C11-C10-C8-C9
22	a	403	CLA	C2B-C3B-CAB-CBB
22	a	403	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	C12-C13-C15-C16
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	CBD-CGD-O2D-CED
24	A	406	BCR	C11-C12-C13-C14
24	A	406	BCR	C20-C21-C22-C37
24	B	617	BCR	C35-C13-C14-C15
24	B	618	BCR	C20-C21-C22-C37
24	C	514	BCR	C16-C17-C18-C19
24	F	101	BCR	C23-C24-C25-C26
24	F	101	BCR	C23-C24-C25-C30
24	H	102	BCR	C11-C12-C13-C14
24	H	102	BCR	C11-C12-C13-C35
24	K	101	BCR	C16-C17-C18-C19
24	K	101	BCR	C16-C17-C18-C36
24	K	102	BCR	C1-C6-C7-C8
24	K	102	BCR	C5-C6-C7-C8
24	K	102	BCR	C21-C22-C23-C24
24	K	102	BCR	C37-C22-C23-C24
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C12-C13-C14-C15
24	T	101	BCR	C16-C17-C18-C36
24	T	101	BCR	C17-C18-C19-C20
24	T	101	BCR	C20-C21-C22-C37
24	b	617	BCR	C20-C21-C22-C37
24	b	619	BCR	C16-C17-C18-C36
24	b	619	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
24	c	515	BCR	C22-C23-C24-C25
24	c	516	BCR	C36-C18-C19-C20
24	k	101	BCR	C35-C13-C14-C15
24	k	101	BCR	C17-C18-C19-C20
24	k	101	BCR	C36-C18-C19-C20
24	k	101	BCR	C37-C22-C23-C24
24	k	102	BCR	C35-C13-C14-C15
26	A	409	PL9	C32-C33-C34-C35
26	A	409	PL9	C32-C33-C34-C36
26	A	409	PL9	C37-C38-C39-C40
26	A	409	PL9	C37-C38-C39-C41
26	D	406	PL9	C32-C33-C34-C36
26	a	409	PL9	C12-C13-C14-C16
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C32-C33-C34-C36
26	a	409	PL9	C42-C43-C44-C45
26	d	406	PL9	C32-C33-C34-C36
26	d	406	PL9	C37-C38-C39-C41
26	d	406	PL9	C42-C43-C44-C45
26	d	406	PL9	C42-C43-C44-C46
27	A	410	LMG	O9-C10-O7-C8
27	c	522	LMG	O6-C1-O1-C7
27	c	523	LMG	O6-C1-O1-C7
28	A	412	SQD	C46-C45-O47-C7
28	B	622	SQD	C2-C1-O6-C44
28	B	622	SQD	O5-C1-O6-C44
28	B	622	SQD	O6-C44-C45-O47
28	B	622	SQD	O49-C7-O47-C45
28	B	622	SQD	C8-C7-O47-C45
28	D	408	SQD	C45-C44-O6-C1
28	D	408	SQD	C5-C6-S-O8
28	L	101	SQD	C8-C7-O47-C45
28	L	101	SQD	O10-C23-O48-C46
28	L	101	SQD	C24-C23-O48-C46
28	a	412	SQD	C8-C7-O47-C45
28	a	412	SQD	O10-C23-O48-C46
28	a	412	SQD	C24-C23-O48-C46
28	f	102	SQD	O5-C1-O6-C44
28	f	102	SQD	O49-C7-O47-C45
29	A	413	DGD	C2B-C1B-O2G-C2G
29	A	413	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
33	D	409	LHG	O2-C2-C3-O3
33	D	409	LHG	C3-O3-P-O4
33	D	409	LHG	C3-O3-P-O6
33	D	409	LHG	C4-O6-P-O4
33	D	410	LHG	C1-C2-C3-O3
33	D	410	LHG	C3-O3-P-O4
33	D	410	LHG	C3-O3-P-O6
33	D	412	LHG	O1-C1-C2-C3
33	E	101	LHG	O1-C1-C2-O2
33	E	101	LHG	O1-C1-C2-C3
33	E	101	LHG	C4-O6-P-O4
33	L	102	LHG	C3-O3-P-O4
33	L	102	LHG	C4-O6-P-O3
33	L	102	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C3-O3-P-O4
33	d	408	LHG	C4-O6-P-O3
33	d	408	LHG	C4-O6-P-O4
33	d	408	LHG	C4-O6-P-O5
33	e	101	LHG	O1-C1-C2-C3
33	e	101	LHG	C1-C2-C3-O3
33	e	101	LHG	C3-O3-P-O5
33	e	101	LHG	C3-O3-P-O6
33	e	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
34	V	201	HEC	C2C-C3C-CAC-CBC
34	f	101	HEC	C2B-C3B-CAB-CBB
34	f	101	HEC	C4B-C3B-CAB-CBB
34	F	102	HEC	C4B-C3B-CAB-CBB
34	f	101	HEC	C2C-C3C-CAC-CBC
22	c	510	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
23	d	401	PHO	CBD-CGD-O2D-CED
27	M	101	LMG	O10-C28-O8-C9
27	c	523	LMG	O10-C28-O8-C9
28	f	102	SQD	O10-C23-O48-C46
33	e	101	LHG	O10-C23-O8-C6
34	F	102	HEC	C2B-C3B-CAB-CBB
34	F	102	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	a	409	PL9	C47-C48-C49-C50
26	a	409	PL9	C47-C48-C49-C51
26	d	406	PL9	C47-C48-C49-C51
22	d	403	CLA	C3-C5-C6-C7
22	b	601	CLA	O1D-CGD-O2D-CED
28	D	408	SQD	C24-C23-O48-C46
28	D	408	SQD	O10-C23-O48-C46
34	f	101	HEC	C4C-C3C-CAC-CBC
27	D	411	LMG	O9-C10-O7-C8
28	a	412	SQD	O49-C7-O47-C45
22	b	614	CLA	C3-C5-C6-C7
27	M	101	LMG	C29-C28-O8-C9
27	c	523	LMG	C29-C28-O8-C9
33	e	101	LHG	C24-C23-O8-C6
34	F	102	HEC	C4C-C3C-CAC-CBC
27	c	520	LMG	C11-C10-O7-C8
22	d	403	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	C11-C10-O7-C8
28	f	102	SQD	C8-C7-O47-C45
22	B	614	CLA	C4-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
22	c	508	CLA	C4-C3-C5-C6
26	A	409	PL9	C35-C34-C36-C37
22	b	607	CLA	C2-C3-C5-C6
22	c	508	CLA	C2-C3-C5-C6
26	A	409	PL9	C23-C24-C26-C27
22	c	514	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	C2A-CAA-CBA-CGA
22	A	403	CLA	C3-C5-C6-C7
22	C	513	CLA	CBA-CGA-O2A-C1
27	a	415	LMG	C29-C28-O8-C9
26	A	409	PL9	C12-C13-C14-C15
34	V	201	HEC	C4C-C3C-CAC-CBC
26	A	409	PL9	C22-C23-C24-C26
22	b	613	CLA	CBD-CGD-O2D-CED
29	h	102	DGD	O6E-C5E-C6E-O5E
27	c	522	LMG	O10-C28-O8-C9
22	c	512	CLA	O1D-CGD-O2D-CED
26	d	406	PL9	C47-C48-C49-C50
22	C	513	CLA	C3-C5-C6-C7
34	v	201	HEC	C2C-C3C-CAC-CBC
33	D	410	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
23	d	401	PHO	O1D-CGD-O2D-CED
27	Y	101	LMG	C29-C28-O8-C9
29	A	413	DGD	C2A-C1A-O1G-C1G
27	c	520	LMG	O9-C10-O7-C8
27	c	522	LMG	O6-C5-C6-O5
29	C	515	DGD	O6E-C5E-C6E-O5E
33	D	409	LHG	C23-C24-C25-C26
22	C	511	CLA	CBD-CGD-O2D-CED
28	f	102	SQD	C24-C23-O48-C46
22	C	513	CLA	C4-C3-C5-C6
22	B	614	CLA	C2-C3-C5-C6
26	a	409	PL9	C33-C34-C36-C37
26	d	406	PL9	C38-C39-C41-C42
22	C	513	CLA	O1A-CGA-O2A-C1
27	a	415	LMG	O10-C28-O8-C9
27	b	621	LMG	O9-C10-O7-C8
28	L	101	SQD	O49-C7-O47-C45
27	M	101	LMG	O6-C5-C6-O5
26	A	409	PL9	C9-C11-C12-C13
26	A	409	PL9	C14-C16-C17-C18
26	a	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C34-C36-C37-C38
26	a	409	PL9	C44-C46-C47-C48
26	d	406	PL9	C34-C36-C37-C38
29	h	102	DGD	C4E-C5E-C6E-O5E
22	c	507	CLA	CBD-CGD-O2D-CED
34	f	101	HEC	C2A-CAA-CBA-CGA
26	A	409	PL9	C47-C48-C49-C50
27	b	623	LMG	O6-C1-O1-C7
29	A	413	DGD	O6E-C5E-C6E-O5E
29	H	103	DGD	C4E-C5E-C6E-O5E
27	c	522	LMG	C29-C28-O8-C9
22	B	613	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CBD-CGD-O2D-CED
33	l	101	LHG	C7-C8-C9-C10
26	A	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C42-C43-C44-C46
27	Y	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C47-C48-C49-C51
26	D	406	PL9	C47-C48-C49-C51
27	a	415	LMG	C4-C5-C6-O5
22	c	507	CLA	CBA-CGA-O2A-C1
28	B	622	SQD	C24-C23-O48-C46
29	c	519	DGD	C2A-C1A-O1G-C1G
27	A	410	LMG	O6-C5-C6-O5
22	c	503	CLA	CBD-CGD-O2D-CED
33	E	101	LHG	C24-C25-C26-C27
27	M	101	LMG	C4-C5-C6-O5
29	A	413	DGD	C4E-C5E-C6E-O5E
22	C	513	CLA	C2-C3-C5-C6
22	A	405	CLA	C3-C5-C6-C7
22	A	403	CLA	C14-C13-C15-C16
22	B	606	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	513	CLA	C6-C7-C8-C9
22	H	101	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C10-C8-C9
22	c	510	CLA	C6-C7-C8-C9
22	c	510	CLA	C11-C12-C13-C14
22	c	511	CLA	C11-C10-C8-C9
23	A	404	PHO	C14-C13-C15-C16
27	b	623	LMG	C2-C1-O1-C7
29	c	519	DGD	O1A-C1A-O1G-C1G
22	b	613	CLA	O1D-CGD-O2D-CED
24	A	406	BCR	C7-C8-C9-C34
24	A	406	BCR	C37-C22-C23-C24
24	B	617	BCR	C7-C8-C9-C34
24	B	618	BCR	C37-C22-C23-C24
24	C	514	BCR	C36-C18-C19-C20
24	K	103	BCR	C7-C8-C9-C34
24	T	101	BCR	C11-C12-C13-C35
24	T	101	BCR	C36-C18-C19-C20
24	a	406	BCR	C36-C18-C19-C20
24	a	406	BCR	C37-C22-C23-C24
24	b	617	BCR	C36-C18-C19-C20
24	b	619	BCR	C11-C12-C13-C35
24	c	515	BCR	C11-C12-C13-C35
24	d	405	BCR	C37-C22-C23-C24
24	k	101	BCR	C7-C8-C9-C34
24	c	515	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	d	405	BCR	C21-C22-C23-C24
27	A	410	LMG	C28-C29-C30-C31
27	b	623	LMG	O10-C28-O8-C9
31	B	627	STE	C5-C6-C7-C8
27	b	623	LMG	O9-C10-O7-C8
28	a	411	SQD	O6-C44-C45-O47
26	a	409	PL9	C12-C13-C14-C15
31	B	626	STE	C11-C12-C13-C14
22	C	509	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
22	c	512	CLA	C15-C16-C17-C18
29	H	103	DGD	O6E-C5E-C6E-O5E
22	b	601	CLA	C3-C5-C6-C7
33	e	101	LHG	C23-C24-C25-C26
22	a	405	CLA	C10-C11-C12-C13
22	C	508	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C15
22	C	507	CLA	C4-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
22	b	604	CLA	C10-C11-C12-C13
27	M	101	LMG	C10-C11-C12-C13
28	A	411	SQD	C7-C8-C9-C10
28	B	622	SQD	C23-C24-C25-C26
31	B	601	STE	C1-C2-C3-C4
26	A	409	PL9	C19-C21-C22-C23
26	A	409	PL9	C24-C26-C27-C28
26	A	409	PL9	C34-C36-C37-C38
26	A	409	PL9	C44-C46-C47-C48
27	A	410	LMG	C4-C5-C6-O5
27	D	411	LMG	C10-C11-C12-C13
22	c	507	CLA	O1A-CGA-O2A-C1
22	c	513	CLA	CBD-CGD-O2D-CED
22	d	403	CLA	O1D-CGD-O2D-CED
22	A	402	CLA	C15-C16-C17-C18
22	B	609	CLA	C13-C15-C16-C17
22	C	504	CLA	C8-C10-C11-C12
22	D	403	CLA	C15-C16-C17-C18
24	B	618	BCR	C18-C19-C20-C21
22	B	605	CLA	C15-C16-C17-C18
22	a	403	CLA	C8-C10-C11-C12
22	b	603	CLA	C5-C6-C7-C8
22	b	608	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	d	410	LMG	C28-C29-C30-C31
28	L	101	SQD	C23-C24-C25-C26
31	C	518	STE	C1-C2-C3-C4
29	C	516	DGD	O6E-C1E-O5D-C6D
28	A	412	SQD	C44-C45-O47-C7
31	C	520	STE	C4-C5-C6-C7
33	d	409	LHG	C24-C25-C26-C27
22	A	403	CLA	C13-C15-C16-C17
22	B	603	CLA	C8-C10-C11-C12
22	B	606	CLA	C15-C16-C17-C18
22	B	612	CLA	C13-C15-C16-C17
22	B	615	CLA	C5-C6-C7-C8
22	C	505	CLA	C5-C6-C7-C8
22	C	513	CLA	C15-C16-C17-C18
22	D	404	CLA	C13-C15-C16-C17
22	D	405	CLA	C13-C15-C16-C17
22	b	606	CLA	C15-C16-C17-C18
22	b	607	CLA	C10-C11-C12-C13
22	b	611	CLA	C8-C10-C11-C12
22	b	616	CLA	C10-C11-C12-C13
22	c	504	CLA	C8-C10-C11-C12
22	c	506	CLA	C13-C15-C16-C17
22	c	506	CLA	C15-C16-C17-C18
22	c	510	CLA	C10-C11-C12-C13
33	d	407	LHG	O2-C2-C3-O3
22	c	504	CLA	CBD-CGD-O2D-CED
27	D	407	LMG	C10-C11-C12-C13
29	c	517	DGD	C1B-C2B-C3B-C4B
22	B	614	CLA	C13-C15-C16-C17
22	C	505	CLA	C10-C11-C12-C13
22	C	512	CLA	C10-C11-C12-C13
22	C	513	CLA	C5-C6-C7-C8
22	B	606	CLA	C13-C15-C16-C17
22	B	607	CLA	C13-C15-C16-C17
22	B	607	CLA	C15-C16-C17-C18
22	C	511	CLA	C8-C10-C11-C12
22	b	605	CLA	C15-C16-C17-C18
22	b	606	CLA	C10-C11-C12-C13
22	b	614	CLA	C5-C6-C7-C8
22	d	404	CLA	CBD-CGD-O2D-CED
29	c	518	DGD	C1A-C2A-C3A-C4A
22	a	405	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C5-C6-C7-C8
22	B	608	CLA	C3-C5-C6-C7
22	B	616	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	C13-C15-C16-C17
29	C	515	DGD	C4E-C5E-C6E-O5E
33	D	409	LHG	C1-C2-C3-O3
33	E	101	LHG	C1-C2-C3-O3
33	d	407	LHG	C1-C2-C3-O3
22	B	603	CLA	C13-C15-C16-C17
22	B	606	CLA	C8-C10-C11-C12
22	C	502	CLA	C13-C15-C16-C17
22	C	506	CLA	C8-C10-C11-C12
22	C	506	CLA	C13-C15-C16-C17
22	a	405	CLA	C5-C6-C7-C8
22	C	513	CLA	CBD-CGD-O2D-CED
22	D	403	CLA	C3-C5-C6-C7
27	c	522	LMG	C10-C11-C12-C13
31	j	101	STE	C1-C2-C3-C4
22	b	615	CLA	C5-C6-C7-C8
33	E	101	LHG	C27-C28-C29-C30
22	b	616	CLA	C8-C10-C11-C12
22	B	604	CLA	CBA-CGA-O2A-C1
22	b	616	CLA	C2-C3-C5-C6
22	b	602	CLA	C15-C16-C17-C18
22	b	605	CLA	C10-C11-C12-C13
27	a	415	LMG	O6-C5-C6-O5
28	D	408	SQD	C2-C1-O6-C44
29	C	516	DGD	C2E-C1E-O5D-C6D
29	c	518	DGD	C2E-C1E-O5D-C6D
34	v	201	HEC	C4C-C3C-CAC-CBC
22	B	615	CLA	C16-C17-C18-C20
22	C	502	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
24	A	406	BCR	C11-C10-C9-C34
24	A	406	BCR	C35-C13-C14-C15
24	B	618	BCR	C35-C13-C14-C15
24	B	619	BCR	C11-C10-C9-C34
24	B	619	BCR	C20-C21-C22-C37
24	C	514	BCR	C16-C17-C18-C36
24	F	101	BCR	C35-C13-C14-C15
24	F	101	BCR	C20-C21-C22-C37
24	K	103	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	K	103	BCR	C35-C13-C14-C15
24	T	101	BCR	C35-C13-C14-C15
24	b	617	BCR	C35-C13-C14-C15
24	b	618	BCR	C35-C13-C14-C15
24	b	618	BCR	C16-C17-C18-C36
24	b	619	BCR	C35-C13-C14-C15
24	c	515	BCR	C35-C13-C14-C15
24	c	516	BCR	C16-C17-C18-C36
24	c	516	BCR	C20-C21-C22-C37
24	d	405	BCR	C35-C13-C14-C15
24	t	101	BCR	C11-C10-C9-C34
24	t	101	BCR	C35-C13-C14-C15
24	t	101	BCR	C16-C17-C18-C36
29	C	515	DGD	C1B-C2B-C3B-C4B
24	b	619	BCR	C7-C8-C9-C34
22	c	513	CLA	C13-C15-C16-C17
33	d	407	LHG	O1-C1-C2-C3
33	d	409	LHG	O1-C1-C2-C3
27	b	623	LMG	C9-C8-O7-C10
28	L	101	SQD	C46-C45-O47-C7
27	a	415	LMG	C12-C13-C14-C15
22	B	616	CLA	C11-C12-C13-C15
22	c	504	CLA	C16-C17-C18-C20
22	c	507	CLA	O1D-CGD-O2D-CED
22	b	602	CLA	C3-C5-C6-C7
24	B	617	BCR	C11-C10-C9-C8
24	B	617	BCR	C12-C13-C14-C15
24	B	619	BCR	C12-C13-C14-C15
24	C	514	BCR	C12-C13-C14-C15
24	K	101	BCR	C11-C10-C9-C8
24	T	101	BCR	C16-C17-C18-C19
24	b	617	BCR	C20-C21-C22-C23
24	h	101	BCR	C11-C10-C9-C8
24	k	101	BCR	C12-C13-C14-C15
29	c	518	DGD	O6E-C1E-O5D-C6D
27	c	522	LMG	C4-C5-C6-O5
22	C	507	CLA	C2-C3-C5-C6
22	B	613	CLA	O1D-CGD-O2D-CED
28	a	411	SQD	C24-C23-O48-C46
22	c	503	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	C16-C17-C18-C19
22	a	402	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	C16-C17-C18-C19
22	c	513	CLA	C16-C17-C18-C20
22	b	603	CLA	C8-C10-C11-C12
29	C	515	DGD	C3B-C4B-C5B-C6B
29	c	519	DGD	C5B-C6B-C7B-C8B
31	C	518	STE	C4-C5-C6-C7
31	c	521	STE	C9-C10-C11-C12
33	E	101	LHG	C32-C33-C34-C35
27	b	621	LMG	C16-C17-C18-C19
27	c	520	LMG	C36-C37-C38-C39
28	L	101	SQD	C26-C27-C28-C29
28	a	411	SQD	C18-C19-C20-C21
29	C	515	DGD	C5B-C6B-C7B-C8B
29	C	517	DGD	C8A-C9A-CAA-CBA
29	h	102	DGD	C6B-C7B-C8B-C9B
33	E	101	LHG	C18-C19-C20-C21
33	d	407	LHG	C28-C29-C30-C31
33	d	408	LHG	C13-C14-C15-C16
22	C	511	CLA	O1D-CGD-O2D-CED
22	b	616	CLA	O1D-CGD-O2D-CED
31	B	624	STE	C1-C2-C3-C4
27	b	623	LMG	C32-C33-C34-C35
29	c	517	DGD	C4A-C5A-C6A-C7A
31	c	521	STE	C7-C8-C9-C10
33	d	407	LHG	C17-C18-C19-C20
33	l	101	LHG	C17-C18-C19-C20
27	M	101	LMG	C37-C38-C39-C40
29	c	519	DGD	C4A-C5A-C6A-C7A
31	B	623	STE	C11-C10-C9-C8
31	B	627	STE	C9-C10-C11-C12
31	H	104	STE	C4-C5-C6-C7
33	D	410	LHG	C29-C30-C31-C32
33	D	412	LHG	O1-C1-C2-O2
33	e	101	LHG	O1-C1-C2-O2
28	a	411	SQD	C9-C10-C11-C12
29	c	517	DGD	C6B-C7B-C8B-C9B
29	h	102	DGD	C6A-C7A-C8A-C9A
33	d	408	LHG	C26-C27-C28-C29
22	b	609	CLA	C4B-C3B-CAB-CBB
31	d	412	STE	C5-C6-C7-C8
22	B	609	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
28	a	411	SQD	C34-C35-C36-C37
29	C	516	DGD	C7A-C8A-C9A-CAA
31	Z	101	STE	C11-C12-C13-C14
22	C	512	CLA	C13-C15-C16-C17
22	b	615	CLA	C15-C16-C17-C18
22	c	507	CLA	C13-C15-C16-C17
27	D	411	LMG	C11-C10-O7-C8
27	D	407	LMG	C15-C16-C17-C18
27	a	415	LMG	C36-C37-C38-C39
31	B	625	STE	C11-C12-C13-C14
27	c	523	LMG	C15-C16-C17-C18
29	h	102	DGD	C2B-C3B-C4B-C5B
31	E	102	STE	C6-C7-C8-C9
33	d	408	LHG	C29-C30-C31-C32
27	M	101	LMG	C28-C29-C30-C31
33	d	407	LHG	C23-C24-C25-C26
22	H	101	CLA	CBA-CGA-O2A-C1
27	A	410	LMG	C31-C32-C33-C34
29	c	519	DGD	CCB-CDB-CEB-CFB
31	B	624	STE	C6-C7-C8-C9
31	b	620	STE	C6-C7-C8-C9
33	d	408	LHG	C28-C29-C30-C31
22	H	101	CLA	C3A-C2A-CAA-CBA
22	b	601	CLA	C3A-C2A-CAA-CBA
22	c	513	CLA	C3A-C2A-CAA-CBA
27	c	522	LMG	C31-C32-C33-C34
31	d	412	STE	C11-C12-C13-C14
33	D	410	LHG	C25-C26-C27-C28
33	E	101	LHG	C12-C13-C14-C15
22	B	602	CLA	C13-C15-C16-C17
22	b	612	CLA	C13-C15-C16-C17
22	b	615	CLA	C8-C10-C11-C12
22	d	404	CLA	O1D-CGD-O2D-CED
29	C	517	DGD	C9A-CAA-CBA-CCA
31	B	626	STE	C5-C6-C7-C8
31	b	622	STE	C6-C7-C8-C9
27	a	415	LMG	C13-C14-C15-C16
31	d	411	STE	C2-C3-C4-C5
31	m	101	STE	C9-C10-C11-C12
29	c	518	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
33	L	102	LHG	C14-C15-C16-C17
27	A	410	LMG	C12-C13-C14-C15
27	a	415	LMG	C14-C15-C16-C17
28	A	412	SQD	C15-C16-C17-C18
29	C	516	DGD	C3A-C4A-C5A-C6A
31	B	625	STE	C2-C3-C4-C5
31	I	101	STE	C7-C8-C9-C10
31	M	102	STE	C11-C10-C9-C8
33	D	409	LHG	C29-C30-C31-C32
33	L	102	LHG	C30-C31-C32-C33
27	b	623	LMG	C28-C29-C30-C31
28	f	102	SQD	C23-C24-C25-C26
22	B	613	CLA	C8-C10-C11-C12
27	M	101	LMG	C32-C33-C34-C35
27	b	621	LMG	C33-C34-C35-C36
28	A	411	SQD	C10-C11-C12-C13
28	a	412	SQD	C14-C15-C16-C17
28	f	102	SQD	C33-C34-C35-C36
29	h	102	DGD	C3A-C4A-C5A-C6A
31	B	620	STE	C10-C11-C12-C13
31	T	102	STE	C10-C11-C12-C13
31	m	101	STE	C10-C11-C12-C13
33	D	410	LHG	C13-C14-C15-C16
33	L	102	LHG	C12-C13-C14-C15
27	Y	101	LMG	O6-C5-C6-O5
27	A	410	LMG	C35-C36-C37-C38
27	c	522	LMG	C14-C15-C16-C17
28	a	412	SQD	C15-C16-C17-C18
29	A	413	DGD	C5B-C6B-C7B-C8B
29	A	413	DGD	C8B-C9B-CAB-CBB
29	c	517	DGD	C3B-C4B-C5B-C6B
31	B	601	STE	C5-C6-C7-C8
31	d	412	STE	C3-C4-C5-C6
33	D	409	LHG	C34-C35-C36-C37
27	A	410	LMG	C16-C17-C18-C19
31	d	413	STE	C10-C11-C12-C13
33	E	101	LHG	C30-C31-C32-C33
22	c	513	CLA	O1D-CGD-O2D-CED
28	a	411	SQD	C15-C16-C17-C18
31	D	413	STE	C4-C5-C6-C7
31	M	102	STE	C6-C7-C8-C9
31	d	411	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	D	409	LHG	C31-C32-C33-C34
26	D	406	PL9	C32-C33-C34-C35
26	d	406	PL9	C32-C33-C34-C35
28	B	622	SQD	O10-C23-O48-C46
22	b	609	CLA	C2B-C3B-CAB-CBB
24	A	406	BCR	C23-C24-C25-C26
24	A	406	BCR	C23-C24-C25-C30
24	H	102	BCR	C23-C24-C25-C26
24	H	102	BCR	C23-C24-C25-C30
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	k	101	BCR	C1-C6-C7-C8
24	k	101	BCR	C5-C6-C7-C8
27	c	522	LMG	C39-C40-C41-C42
28	f	102	SQD	C28-C29-C30-C31
29	C	516	DGD	C5A-C6A-C7A-C8A
29	H	103	DGD	C6B-C7B-C8B-C9B
33	D	410	LHG	C9-C10-C11-C12
27	b	621	LMG	C11-C10-O7-C8
27	D	411	LMG	C34-C35-C36-C37
29	C	515	DGD	C4B-C5B-C6B-C7B
31	T	102	STE	C7-C8-C9-C10
33	e	101	LHG	C27-C28-C29-C30
27	M	101	LMG	C35-C36-C37-C38
27	c	522	LMG	C30-C31-C32-C33
28	B	622	SQD	C33-C34-C35-C36
33	d	407	LHG	C16-C17-C18-C19
28	L	101	SQD	C24-C25-C26-C27
31	B	626	STE	C4-C5-C6-C7
31	b	620	STE	C9-C10-C11-C12
31	d	413	STE	C9-C10-C11-C12
22	B	604	CLA	O1A-CGA-O2A-C1
27	Y	101	LMG	O10-C28-O8-C9
33	L	102	LHG	O10-C23-O8-C6
27	c	520	LMG	C39-C40-C41-C42
27	d	410	LMG	C38-C39-C40-C41
28	B	622	SQD	C11-C12-C13-C14
29	c	517	DGD	C4B-C5B-C6B-C7B
31	c	521	STE	C6-C7-C8-C9
27	Y	101	LMG	O9-C10-O7-C8
27	D	407	LMG	C17-C18-C19-C20
29	h	102	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
33	l	101	LHG	C32-C33-C34-C35
24	K	101	BCR	C18-C19-C20-C21
24	K	102	BCR	C10-C11-C12-C13
24	d	405	BCR	C10-C11-C12-C13
27	b	623	LMG	C19-C20-C21-C22
29	C	516	DGD	CCA-CDA-CEA-CFA
31	D	413	STE	C9-C10-C11-C12
33	D	410	LHG	C34-C35-C36-C37
22	b	607	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C10-C8-C9
27	D	407	LMG	C12-C13-C14-C15
27	Y	101	LMG	C36-C37-C38-C39
28	B	622	SQD	C17-C18-C19-C20
28	a	412	SQD	C11-C12-C13-C14
29	C	516	DGD	C4A-C5A-C6A-C7A
29	C	517	DGD	CBA-CCA-CDA-CEA
31	a	414	STE	C4-C5-C6-C7
33	l	101	LHG	C29-C30-C31-C32
22	b	602	CLA	C8-C10-C11-C12
27	D	407	LMG	C30-C31-C32-C33
27	c	523	LMG	C17-C18-C19-C20
31	H	104	STE	C6-C7-C8-C9
31	M	102	STE	C7-C8-C9-C10
31	b	627	STE	C10-C11-C12-C13
33	d	408	LHG	C34-C35-C36-C37
24	B	617	BCR	C6-C7-C8-C9
24	d	405	BCR	C22-C23-C24-C25
27	M	101	LMG	C33-C34-C35-C36
27	c	523	LMG	C2-C1-O1-C7
28	f	102	SQD	C2-C1-O6-C44
22	C	512	CLA	CBD-CGD-O2D-CED
27	b	623	LMG	C18-C19-C20-C21
29	C	516	DGD	C6A-C7A-C8A-C9A
33	e	101	LHG	C16-C17-C18-C19
27	b	621	LMG	C37-C38-C39-C40
27	c	520	LMG	C33-C34-C35-C36
27	c	523	LMG	C31-C32-C33-C34
28	f	102	SQD	C24-C25-C26-C27
29	A	413	DGD	C4B-C5B-C6B-C7B
31	b	624	STE	C3-C4-C5-C6
31	m	102	STE	C3-C4-C5-C6
33	d	408	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	CBA-CGA-O2A-C1
27	b	621	LMG	C29-C28-O8-C9
22	D	404	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
22	d	403	CLA	C16-C17-C18-C19
27	M	101	LMG	C11-C10-O7-C8
27	b	623	LMG	C11-C10-O7-C8
33	D	409	LHG	C8-C7-O7-C5
27	Y	101	LMG	C13-C14-C15-C16
33	d	409	LHG	C27-C28-C29-C30
27	c	522	LMG	O9-C10-O7-C8
27	D	407	LMG	C35-C36-C37-C38
28	a	412	SQD	C24-C25-C26-C27
29	A	413	DGD	CAA-CBA-CCA-CDA
29	C	516	DGD	C8B-C9B-CAB-CBB
31	b	627	STE	C13-C14-C15-C16
33	D	409	LHG	C14-C15-C16-C17
22	c	511	CLA	CBD-CGD-O2D-CED
24	F	101	BCR	C37-C22-C23-C24
29	H	103	DGD	C7B-C8B-C9B-CAB
31	b	622	STE	C5-C6-C7-C8
24	h	101	BCR	C11-C12-C13-C14
27	a	415	LMG	C8-C7-O1-C1
29	c	518	DGD	C8B-C9B-CAB-CBB
33	L	102	LHG	C26-C27-C28-C29
22	B	616	CLA	C11-C12-C13-C14
22	b	611	CLA	C16-C17-C18-C19
27	d	410	LMG	C36-C37-C38-C39
28	D	408	SQD	C32-C33-C34-C35
29	c	519	DGD	C9A-CAA-CBA-CCA
29	c	519	DGD	CBA-CCA-CDA-CEA
22	C	510	CLA	C4-C3-C5-C6
26	D	406	PL9	C30-C29-C31-C32
26	a	409	PL9	C15-C14-C16-C17
31	d	413	STE	C1-C2-C3-C4
27	Y	101	LMG	C17-C18-C19-C20
31	I	101	STE	C10-C11-C12-C13
31	b	627	STE	C5-C6-C7-C8
33	D	409	LHG	C28-C29-C30-C31
33	E	101	LHG	C13-C14-C15-C16
22	A	402	CLA	C2C-C3C-CAC-CBC
29	c	519	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
28	D	408	SQD	C27-C28-C29-C30
31	m	101	STE	C4-C5-C6-C7
22	C	503	CLA	C5-C6-C7-C8
27	A	410	LMG	C33-C34-C35-C36
31	d	413	STE	C4-C5-C6-C7
31	J	101	STE	C1-C2-C3-C4
31	c	521	STE	C1-C2-C3-C4
22	B	615	CLA	C16-C17-C18-C19
22	H	101	CLA	C16-C17-C18-C20
27	a	415	LMG	C38-C39-C40-C41
33	d	409	LHG	C26-C27-C28-C29
22	H	101	CLA	O1A-CGA-O2A-C1
29	c	518	DGD	C7A-C8A-C9A-CAA
31	c	521	STE	C11-C12-C13-C14
29	H	103	DGD	C1A-C2A-C3A-C4A
22	B	613	CLA	C5-C6-C7-C8
22	C	501	CLA	O1D-CGD-O2D-CED
28	a	411	SQD	C12-C13-C14-C15
29	H	103	DGD	C7A-C8A-C9A-CAA
22	B	614	CLA	CBD-CGD-O2D-CED
27	a	415	LMG	O7-C8-C9-O8
29	A	413	DGD	O2G-C2G-C3G-O3G
28	L	101	SQD	C13-C14-C15-C16
33	e	101	LHG	C11-C10-C9-C8
29	c	518	DGD	CAA-CBA-CCA-CDA
31	C	519	STE	C4-C5-C6-C7
31	b	622	STE	C13-C14-C15-C16
31	d	411	STE	C6-C7-C8-C9
31	d	413	STE	C12-C13-C14-C15
33	E	101	LHG	C16-C17-C18-C19
29	C	515	DGD	C6A-C7A-C8A-C9A
31	b	622	STE	C14-C15-C16-C17
33	l	101	LHG	C13-C14-C15-C16
22	B	612	CLA	CBD-CGD-O2D-CED
29	A	413	DGD	CBB-CCB-CDB-CEB
29	C	517	DGD	C5A-C6A-C7A-C8A
29	c	517	DGD	CBB-CCB-CDB-CEB
33	D	412	LHG	C32-C33-C34-C35
22	c	504	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
22	H	101	CLA	C5-C6-C7-C8
27	b	623	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
27	c	522	LMG	C38-C39-C40-C41
28	A	411	SQD	C26-C27-C28-C29
31	b	622	STE	C12-C13-C14-C15
31	c	521	STE	C3-C4-C5-C6
29	c	517	DGD	O6E-C5E-C6E-O5E
31	H	104	STE	C2-C3-C4-C5
22	C	510	CLA	C2-C3-C5-C6
28	A	411	SQD	C24-C25-C26-C27
28	D	408	SQD	C25-C26-C27-C28
29	c	518	DGD	CBB-CCB-CDB-CEB
22	b	603	CLA	CBD-CGD-O2D-CED
27	Y	101	LMG	C35-C36-C37-C38
28	A	412	SQD	C13-C14-C15-C16
28	a	411	SQD	C24-C25-C26-C27
31	M	102	STE	C9-C10-C11-C12
33	d	407	LHG	C11-C10-C9-C8
27	M	101	LMG	C34-C35-C36-C37
27	c	523	LMG	C32-C33-C34-C35
22	c	504	CLA	O1D-CGD-O2D-CED
29	C	517	DGD	C4A-C5A-C6A-C7A
29	h	102	DGD	C3B-C4B-C5B-C6B
33	l	101	LHG	C34-C35-C36-C37
22	b	607	CLA	C8-C10-C11-C12
22	c	504	CLA	C5-C6-C7-C8
33	d	407	LHG	O1-C1-C2-O2
22	B	607	CLA	C3-C5-C6-C7
27	Y	101	LMG	C37-C38-C39-C40
31	B	625	STE	C7-C8-C9-C10
22	C	503	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C1A-C2A-CAA-CBA
22	c	509	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	C1A-C2A-CAA-CBA
33	D	412	LHG	C29-C30-C31-C32
33	E	101	LHG	C28-C29-C30-C31
33	L	102	LHG	C32-C33-C34-C35
27	a	415	LMG	C41-C42-C43-C44
29	C	517	DGD	C6B-C7B-C8B-C9B
33	D	412	LHG	C28-C29-C30-C31
22	c	513	CLA	O1A-CGA-O2A-C1
27	D	407	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
27	c	523	LMG	O9-C10-O7-C8
22	A	403	CLA	C12-C13-C15-C16
22	B	611	CLA	C11-C10-C8-C7
22	B	613	CLA	C12-C13-C15-C16
22	C	505	CLA	C12-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	C	513	CLA	C6-C7-C8-C10
22	D	404	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C10-C8-C7
22	c	509	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
31	d	413	STE	C11-C12-C13-C14
33	D	410	LHG	C32-C33-C34-C35
22	b	611	CLA	C16-C17-C18-C20
27	b	623	LMG	O6-C5-C6-O5
22	C	513	CLA	O1D-CGD-O2D-CED
33	E	101	LHG	C23-C24-C25-C26
33	d	409	LHG	C23-C24-C25-C26
31	B	620	STE	C11-C12-C13-C14
33	L	102	LHG	C13-C14-C15-C16
27	a	415	LMG	C39-C40-C41-C42
22	C	509	CLA	C5-C6-C7-C8
22	C	512	CLA	C8-C10-C11-C12
27	c	523	LMG	C11-C10-O7-C8
22	B	613	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	D	404	CLA	C11-C12-C13-C14
22	H	101	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	609	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	508	CLA	C11-C12-C13-C14
22	c	513	CLA	C6-C7-C8-C9
28	B	622	SQD	C9-C10-C11-C12
28	f	102	SQD	C32-C33-C34-C35
29	C	516	DGD	CCB-CDB-CEB-CFB
31	E	102	STE	C5-C6-C7-C8
24	C	514	BCR	C13-C14-C15-C16
27	B	621	LMG	C29-C30-C31-C32
31	T	102	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	D	411	LMG	C29-C28-O8-C9
33	D	412	LHG	C11-C12-C13-C14
27	c	520	LMG	O6-C5-C6-O5
26	d	406	PL9	C44-C46-C47-C48
27	M	101	LMG	C7-C8-C9-O8
27	c	523	LMG	O1-C7-C8-C9
28	B	622	SQD	O6-C44-C45-C46
28	a	411	SQD	O6-C44-C45-C46
29	A	413	DGD	C1G-C2G-C3G-O3G
33	e	101	LHG	C4-C5-C6-O8
27	B	621	LMG	C16-C17-C18-C19
33	E	101	LHG	C29-C30-C31-C32
27	Y	101	LMG	C15-C16-C17-C18
27	b	623	LMG	C15-C16-C17-C18
27	c	520	LMG	C38-C39-C40-C41
31	b	620	STE	C5-C6-C7-C8
22	b	613	CLA	C10-C11-C12-C13
27	M	101	LMG	C16-C17-C18-C19
27	c	520	LMG	C34-C35-C36-C37
29	C	515	DGD	CCB-CDB-CEB-CFB
31	b	626	STE	C6-C7-C8-C9
22	b	610	CLA	C2C-C3C-CAC-CBC
22	d	403	CLA	C2C-C3C-CAC-CBC
29	H	103	DGD	CCA-CDA-CEA-CFA
33	D	412	LHG	C27-C28-C29-C30
22	b	616	CLA	C5-C6-C7-C8
28	L	101	SQD	C10-C11-C12-C13
31	b	620	STE	C11-C10-C9-C8
31	M	102	STE	C1-C2-C3-C4
31	B	625	STE	C11-C10-C9-C8
26	D	406	PL9	C13-C14-C16-C17
26	d	406	PL9	C43-C44-C46-C47
27	c	523	LMG	C38-C39-C40-C41
22	C	507	CLA	C5-C6-C7-C8
22	H	101	CLA	C16-C17-C18-C19
33	d	409	LHG	C34-C35-C36-C37
27	d	410	LMG	O6-C5-C6-O5
22	b	601	CLA	C10-C11-C12-C13
22	C	502	CLA	CBD-CGD-O2D-CED
29	C	517	DGD	C3B-C4B-C5B-C6B
27	M	101	LMG	C12-C13-C14-C15
29	A	413	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
29	H	103	DGD	CBB-CCB-CDB-CEB
31	d	413	STE	C3-C4-C5-C6
29	h	102	DGD	C2A-C3A-C4A-C5A
29	A	413	DGD	O6D-C5D-C6D-O5D
24	c	515	BCR	C18-C19-C20-C21
22	C	513	CLA	C8-C10-C11-C12
27	c	522	LMG	C15-C16-C17-C18
27	d	410	LMG	C30-C31-C32-C33
28	A	411	SQD	C16-C17-C18-C19
29	A	413	DGD	C4A-C5A-C6A-C7A
29	C	517	DGD	C4B-C5B-C6B-C7B
29	H	103	DGD	C3A-C4A-C5A-C6A
29	c	518	DGD	C7B-C8B-C9B-CAB
31	T	102	STE	C11-C10-C9-C8
31	T	102	STE	C12-C13-C14-C15
31	j	101	STE	C3-C4-C5-C6
31	m	101	STE	C14-C15-C16-C17
33	L	102	LHG	C17-C18-C19-C20
24	K	101	BCR	C15-C16-C17-C18
22	b	607	CLA	C16-C17-C18-C19
24	H	102	BCR	C11-C10-C9-C8
24	b	617	BCR	C11-C10-C9-C8
28	L	101	SQD	O5-C1-O6-C44
31	H	104	STE	C14-C15-C16-C17
27	D	411	LMG	C11-C12-C13-C14
27	b	623	LMG	C40-C41-C42-C43
29	A	413	DGD	CDB-CEB-CFB-CGB
29	h	102	DGD	CDB-CEB-CFB-CGB
27	D	407	LMG	C38-C39-C40-C41
29	c	519	DGD	C3A-C4A-C5A-C6A
33	D	410	LHG	C16-C17-C18-C19
22	C	505	CLA	C2-C3-C5-C6
26	d	406	PL9	C33-C34-C36-C37
31	B	625	STE	C13-C14-C15-C16
31	b	626	STE	C10-C11-C12-C13
33	d	407	LHG	C29-C30-C31-C32
33	l	101	LHG	C14-C15-C16-C17
22	A	403	CLA	C16-C17-C18-C20
27	c	523	LMG	C18-C19-C20-C21
28	a	412	SQD	C17-C18-C19-C20
29	c	517	DGD	C9B-CAB-CBB-CCB
31	C	518	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	b	627	STE	C2-C3-C4-C5
33	d	408	LHG	C19-C20-C21-C22
29	C	515	DGD	O6D-C5D-C6D-O5D
27	c	522	LMG	C40-C41-C42-C43
31	D	413	STE	C5-C6-C7-C8
31	H	104	STE	C11-C10-C9-C8
33	e	101	LHG	C11-C12-C13-C14
33	e	101	LHG	C12-C13-C14-C15
33	l	101	LHG	C27-C28-C29-C30
28	L	101	SQD	O6-C44-C45-O47
33	e	101	LHG	C28-C29-C30-C31
33	d	409	LHG	C35-C36-C37-C38
31	T	102	STE	C4-C5-C6-C7
28	L	101	SQD	C16-C17-C18-C19
33	L	102	LHG	C11-C12-C13-C14
27	d	410	LMG	C40-C41-C42-C43
31	b	626	STE	C5-C6-C7-C8
29	A	413	DGD	O1A-C1A-O1G-C1G
22	a	405	CLA	CBA-CGA-O2A-C1
28	a	412	SQD	C31-C32-C33-C34
33	d	409	LHG	C33-C34-C35-C36
27	c	522	LMG	C33-C34-C35-C36
31	B	601	STE	C4-C5-C6-C7
33	D	409	LHG	C17-C18-C19-C20
24	K	101	BCR	C14-C15-C16-C17
28	B	622	SQD	C13-C14-C15-C16
28	L	101	SQD	C27-C28-C29-C30
31	I	101	STE	C4-C5-C6-C7
33	L	102	LHG	C18-C19-C20-C21
22	b	614	CLA	C8-C10-C11-C12
22	c	510	CLA	C5-C6-C7-C8
22	b	601	CLA	C16-C17-C18-C20
22	b	607	CLA	C16-C17-C18-C20
26	d	406	PL9	C45-C44-C46-C47
28	L	101	SQD	C19-C20-C21-C22
31	b	626	STE	C11-C10-C9-C8
27	b	623	LMG	C29-C28-O8-C9
31	b	625	STE	C7-C8-C9-C10
27	D	411	LMG	C36-C37-C38-C39
33	D	409	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
22	A	403	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C11-C12-C13-C14
22	C	504	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	D	403	CLA	C11-C10-C8-C9
22	b	601	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	b	613	CLA	C6-C7-C8-C9
22	b	614	CLA	C6-C7-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	505	CLA	C11-C10-C8-C9
22	c	508	CLA	C14-C13-C15-C16
22	c	509	CLA	C14-C13-C15-C16
22	c	514	CLA	C11-C12-C13-C14
22	d	403	CLA	C6-C7-C8-C9
28	A	411	SQD	C11-C10-C9-C8
29	C	517	DGD	CAB-CBB-CCB-CDB
29	h	102	DGD	C4A-C5A-C6A-C7A
31	m	102	STE	C5-C6-C7-C8
22	b	613	CLA	C13-C15-C16-C17
29	h	102	DGD	O1A-C1A-O1G-C1G
22	A	403	CLA	C4B-C3B-CAB-CBB
22	C	503	CLA	C4B-C3B-CAB-CBB
22	c	513	CLA	C4B-C3B-CAB-CBB
27	b	621	LMG	C30-C31-C32-C33
31	B	620	STE	C9-C10-C11-C12
31	B	626	STE	C6-C7-C8-C9
31	d	413	STE	C2-C3-C4-C5
29	h	102	DGD	O2G-C1B-C2B-C3B
29	c	517	DGD	CAB-CBB-CCB-CDB
28	a	411	SQD	C29-C30-C31-C32
27	c	523	LMG	C33-C34-C35-C36
31	b	627	STE	C6-C7-C8-C9
33	D	409	LHG	C7-C8-C9-C10
29	C	516	DGD	CDA-CEA-CFA-CGA
29	C	516	DGD	CDB-CEB-CFB-CGB
28	f	102	SQD	C26-C27-C28-C29
29	c	518	DGD	C5B-C6B-C7B-C8B
29	H	103	DGD	O2G-C1B-C2B-C3B
22	A	403	CLA	C11-C10-C8-C7
22	B	615	CLA	C11-C12-C13-C15
22	C	504	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	H	101	CLA	C11-C10-C8-C7
22	a	403	CLA	C11-C10-C8-C7
22	b	601	CLA	C6-C7-C8-C10
22	b	607	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C12-C13-C15
22	b	609	CLA	C12-C13-C15-C16
22	b	615	CLA	C12-C13-C15-C16
22	c	505	CLA	C11-C10-C8-C7
22	c	507	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C12-C13-C15
22	c	510	CLA	C6-C7-C8-C10
22	c	514	CLA	C11-C12-C13-C15
22	B	605	CLA	C10-C11-C12-C13
22	H	101	CLA	C8-C10-C11-C12
22	b	609	CLA	C15-C16-C17-C18
29	c	519	DGD	CDA-CEA-CFA-CGA
31	M	103	STE	C1-C2-C3-C4
27	M	101	LMG	C40-C41-C42-C43
29	c	519	DGD	CBB-CCB-CDB-CEB
31	d	411	STE	C11-C10-C9-C8
22	C	502	CLA	C16-C17-C18-C19
27	b	621	LMG	C32-C33-C34-C35
27	b	623	LMG	C12-C13-C14-C15
27	b	623	LMG	C35-C36-C37-C38
29	c	518	DGD	C9B-CAB-CBB-CCB
22	C	505	CLA	C4-C3-C5-C6
22	B	612	CLA	C10-C11-C12-C13
29	c	517	DGD	O6D-C5D-C6D-O5D
29	c	517	DGD	CAA-CBA-CCA-CDA
31	I	101	STE	C12-C13-C14-C15
27	c	523	LMG	C29-C30-C31-C32
27	Y	101	LMG	C29-C30-C31-C32
31	j	101	STE	C2-C3-C4-C5
33	d	408	LHG	C12-C13-C14-C15
33	e	101	LHG	C14-C15-C16-C17
27	a	415	LMG	C42-C43-C44-C45
22	b	604	CLA	C15-C16-C17-C18
22	c	504	CLA	C15-C16-C17-C18
27	a	415	LMG	C18-C19-C20-C21
31	m	102	STE	C6-C7-C8-C9
33	D	412	LHG	C9-C10-C11-C12
31	b	624	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	C	516	DGD	CBB-CCB-CDB-CEB
29	H	103	DGD	C3B-C4B-C5B-C6B
33	D	412	LHG	C24-C25-C26-C27
27	Y	101	LMG	C18-C19-C20-C21
27	c	523	LMG	C12-C13-C14-C15
31	H	104	STE	C9-C10-C11-C12
31	d	412	STE	C2-C3-C4-C5
33	D	410	LHG	C30-C31-C32-C33
27	Y	101	LMG	O1-C7-C8-C9
27	b	623	LMG	O1-C7-C8-C9
28	a	412	SQD	C44-C45-C46-O48
22	D	405	CLA	CBD-CGD-O2D-CED
27	D	407	LMG	C36-C37-C38-C39
28	A	412	SQD	C18-C19-C20-C21
22	c	508	CLA	C10-C11-C12-C13
31	I	101	STE	C2-C3-C4-C5
31	b	624	STE	C12-C13-C14-C15
27	Y	101	LMG	C32-C33-C34-C35
28	A	412	SQD	C16-C17-C18-C19
33	E	101	LHG	C11-C10-C9-C8
22	b	609	CLA	C4-C3-C5-C6
31	c	501	STE	C6-C7-C8-C9
28	a	411	SQD	C16-C17-C18-C19
29	H	103	DGD	CBA-CCA-CDA-CEA
28	A	412	SQD	O47-C45-C46-O48
27	D	407	LMG	C19-C20-C21-C22
22	B	602	CLA	C16-C17-C18-C20
29	H	103	DGD	CDB-CEB-CFB-CGB
27	a	415	LMG	C29-C30-C31-C32
29	c	518	DGD	C4A-C5A-C6A-C7A
22	C	512	CLA	O1D-CGD-O2D-CED
24	B	617	BCR	C1-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C30
24	b	618	BCR	C23-C24-C25-C30
24	c	515	BCR	C1-C6-C7-C8
27	a	415	LMG	C16-C17-C18-C19
29	H	103	DGD	CCB-CDB-CEB-CFB
22	c	513	CLA	C8-C10-C11-C12
29	c	518	DGD	CDB-CEB-CFB-CGB
27	B	621	LMG	C30-C31-C32-C33
31	C	519	STE	C5-C6-C7-C8
22	B	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	C8-C10-C11-C12
27	a	415	LMG	C21-C22-C23-C24
27	a	415	LMG	C37-C38-C39-C40
28	B	622	SQD	C16-C17-C18-C19
31	c	501	STE	C2-C3-C4-C5
28	a	411	SQD	C30-C31-C32-C33
33	D	410	LHG	C27-C28-C29-C30
22	b	601	CLA	C16-C17-C18-C19
22	b	601	CLA	C2A-CAA-CBA-CGA
27	c	523	LMG	O1-C7-C8-O7
28	a	411	SQD	O47-C45-C46-O48
27	Y	101	LMG	C14-C15-C16-C17
31	b	627	STE	C14-C15-C16-C17
31	d	413	STE	C6-C7-C8-C9
33	e	101	LHG	O9-C7-O7-C5
27	D	407	LMG	C37-C38-C39-C40
27	b	623	LMG	C29-C30-C31-C32
28	A	412	SQD	C32-C33-C34-C35
29	C	515	DGD	CDA-CEA-CFA-CGA
27	D	407	LMG	C20-C21-C22-C23
31	B	620	STE	C3-C4-C5-C6
31	b	620	STE	C12-C13-C14-C15
29	C	515	DGD	C4D-C5D-C6D-O5D
22	B	602	CLA	C16-C17-C18-C19
22	D	404	CLA	C16-C17-C18-C19
31	b	625	STE	C4-C5-C6-C7
31	c	501	STE	C5-C6-C7-C8
33	l	101	LHG	C25-C26-C27-C28
33	d	407	LHG	C7-C8-C9-C10
22	B	616	CLA	O1D-CGD-O2D-CED
31	a	413	STE	C2-C3-C4-C5
33	D	412	LHG	C25-C26-C27-C28
22	B	604	CLA	C14-C13-C15-C16
22	C	509	CLA	C14-C13-C15-C16
22	a	403	CLA	C14-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C9
31	a	413	STE	C1-C2-C3-C4
22	c	511	CLA	O1D-CGD-O2D-CED
31	D	413	STE	C10-C11-C12-C13
24	c	515	BCR	C14-C15-C16-C17
24	k	101	BCR	C14-C15-C16-C17
29	c	519	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	D	409	LHG	C24-C25-C26-C27
27	c	522	LMG	C17-C18-C19-C20
27	a	415	LMG	C30-C31-C32-C33
29	h	102	DGD	CAB-CBB-CCB-CDB
29	A	413	DGD	C8A-C9A-CAA-CBA
33	L	102	LHG	C31-C32-C33-C34
33	d	409	LHG	O1-C1-C2-O2
22	C	512	CLA	C3-C5-C6-C7
24	C	514	BCR	C15-C16-C17-C18
24	T	101	BCR	C13-C14-C15-C16
33	D	409	LHG	C35-C36-C37-C38
22	b	609	CLA	C2-C3-C5-C6
22	A	403	CLA	C16-C17-C18-C19
22	c	510	CLA	C16-C17-C18-C20
27	Y	101	LMG	C33-C34-C35-C36
27	D	411	LMG	C28-C29-C30-C31
28	A	412	SQD	C9-C10-C11-C12
22	B	604	CLA	C13-C15-C16-C17
22	B	614	CLA	C8-C10-C11-C12
27	M	101	LMG	C31-C32-C33-C34
24	K	101	BCR	C11-C10-C9-C34
24	K	102	BCR	C35-C13-C14-C15
24	c	515	BCR	C20-C21-C22-C37
24	h	101	BCR	C20-C21-C22-C37
24	k	102	BCR	C20-C21-C22-C37
33	D	409	LHG	O10-C23-O8-C6
31	b	620	STE	C15-C16-C17-C18
28	L	101	SQD	C29-C30-C31-C32
33	D	409	LHG	C30-C31-C32-C33
22	C	508	CLA	C16-C17-C18-C19
24	B	618	BCR	C7-C8-C9-C34
24	b	617	BCR	C11-C12-C13-C35
27	a	415	LMG	C32-C33-C34-C35
22	B	604	CLA	C12-C13-C15-C16
22	B	606	CLA	C11-C12-C13-C15
22	B	609	CLA	C11-C12-C13-C15
22	C	509	CLA	C12-C13-C15-C16
22	C	512	CLA	C12-C13-C15-C16
22	H	101	CLA	C12-C13-C15-C16
22	a	403	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	a	404	PHO	C6-C7-C8-C10
29	h	102	DGD	CCA-CDA-CEA-CFA
33	D	412	LHG	C15-C16-C17-C18
33	d	408	LHG	C25-C26-C27-C28
26	a	409	PL9	C32-C33-C34-C35
24	K	103	BCR	C7-C8-C9-C10
24	b	617	BCR	C21-C22-C23-C24
22	c	512	CLA	CBA-CGA-O2A-C1
31	C	519	STE	C9-C10-C11-C12
29	C	516	DGD	C2G-C3G-O3G-C1D
29	c	518	DGD	C5D-C6D-O5D-C1E
27	d	410	LMG	O9-C10-O7-C8
29	A	413	DGD	CEA-CFA-CGA-CHA
22	a	405	CLA	O1A-CGA-O2A-C1
27	c	522	LMG	C29-C30-C31-C32
31	J	101	STE	C2-C3-C4-C5
22	B	612	CLA	C3-C5-C6-C7
27	b	623	LMG	C30-C31-C32-C33
27	d	410	LMG	C14-C15-C16-C17
27	a	415	LMG	C9-C8-O7-C10
27	c	523	LMG	C9-C8-O7-C10
27	D	411	LMG	C16-C17-C18-C19
27	D	411	LMG	C32-C33-C34-C35
29	A	413	DGD	C7A-C8A-C9A-CAA
29	c	517	DGD	C7B-C8B-C9B-CAB
31	d	412	STE	C10-C11-C12-C13
27	c	523	LMG	C11-C12-C13-C14
28	a	411	SQD	C17-C18-C19-C20
24	t	101	BCR	C16-C17-C18-C19
27	a	415	LMG	C34-C35-C36-C37
31	m	101	STE	C2-C3-C4-C5
29	c	517	DGD	C4D-C5D-C6D-O5D
33	E	101	LHG	C4-C5-C6-O8
27	B	621	LMG	C28-C29-C30-C31
27	M	101	LMG	C29-C30-C31-C32
27	a	415	LMG	C23-C24-C25-C26
27	c	523	LMG	C20-C21-C22-C23
29	A	413	DGD	C6B-C7B-C8B-C9B
22	H	101	CLA	C4-C3-C5-C6
22	B	603	CLA	C2-C3-C5-C6
26	A	409	PL9	C33-C34-C36-C37
26	A	409	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
26	a	409	PL9	C13-C14-C16-C17
28	L	101	SQD	C18-C19-C20-C21
29	A	413	DGD	C2A-C3A-C4A-C5A
28	A	411	SQD	O6-C44-C45-O47
29	C	515	DGD	O1G-C1G-C2G-O2G
29	c	517	DGD	O1G-C1G-C2G-O2G
33	D	409	LHG	O7-C5-C6-O8
33	E	101	LHG	O7-C5-C6-O8
22	B	602	CLA	C11-C12-C13-C14
22	B	613	CLA	C11-C12-C13-C14
22	c	508	CLA	C6-C7-C8-C9
22	c	512	CLA	C14-C13-C15-C16
27	c	522	LMG	C11-C12-C13-C14
28	L	101	SQD	C12-C13-C14-C15
29	C	516	DGD	CBA-CCA-CDA-CEA
31	a	413	STE	C4-C5-C6-C7
28	a	412	SQD	C29-C30-C31-C32
31	b	626	STE	C11-C12-C13-C14
33	d	408	LHG	C9-C10-C11-C12
33	d	409	LHG	C32-C33-C34-C35
27	D	411	LMG	C14-C15-C16-C17
27	c	523	LMG	C37-C38-C39-C40
31	T	102	STE	C11-C12-C13-C14
31	b	620	STE	C10-C11-C12-C13
31	m	101	STE	C12-C13-C14-C15
33	D	412	LHG	C14-C15-C16-C17
27	M	101	LMG	C18-C19-C20-C21
29	C	515	DGD	C9B-CAB-CBB-CCB
31	B	626	STE	C11-C10-C9-C8
28	f	102	SQD	C29-C30-C31-C32
22	C	509	CLA	C10-C11-C12-C13
22	B	605	CLA	C3-C5-C6-C7
22	B	616	CLA	C2-C1-O2A-CGA
22	c	510	CLA	C16-C17-C18-C19
28	B	622	SQD	C45-C46-O48-C23
28	D	408	SQD	O6-C44-C45-C46
29	A	413	DGD	C6A-C7A-C8A-C9A
31	Z	101	STE	C13-C14-C15-C16
22	B	603	CLA	C16-C17-C18-C20
22	C	508	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C19
27	B	621	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	c	519	DGD	C9B-CAB-CBB-CCB
22	C	509	CLA	C3-C5-C6-C7
28	A	412	SQD	C35-C36-C37-C38
27	d	410	LMG	C32-C33-C34-C35
27	c	522	LMG	C34-C35-C36-C37
22	a	410	CLA	C4C-C3C-CAC-CBC
22	D	404	CLA	C15-C16-C17-C18
22	B	607	CLA	O1D-CGD-O2D-CED
22	B	616	CLA	C3-C5-C6-C7
24	c	516	BCR	C37-C22-C23-C24
29	A	413	DGD	C4D-C5D-C6D-O5D
22	b	601	CLA	C4B-C3B-CAB-CBB
23	a	404	PHO	C4-C3-C5-C6
27	D	407	LMG	C39-C40-C41-C42
29	c	517	DGD	C5A-C6A-C7A-C8A
27	B	621	LMG	C33-C34-C35-C36
28	f	102	SQD	C25-C26-C27-C28
33	D	409	LHG	C12-C13-C14-C15
33	l	101	LHG	O6-C4-C5-C6
31	D	413	STE	C2-C3-C4-C5
33	d	407	LHG	C10-C11-C12-C13
22	B	607	CLA	CBD-CGD-O2D-CED
29	c	517	DGD	O1B-C1B-O2G-C2G
28	D	408	SQD	C5-C6-S-O7
33	L	102	LHG	C33-C34-C35-C36
22	B	605	CLA	C11-C10-C8-C7
22	B	616	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C12-C13-C15
22	b	614	CLA	C12-C13-C15-C16
22	c	506	CLA	C12-C13-C15-C16
22	c	511	CLA	C11-C10-C8-C7
22	c	514	CLA	C11-C10-C8-C7
22	B	610	CLA	C16-C17-C18-C19
22	B	609	CLA	O1A-CGA-O2A-C1
28	a	411	SQD	C25-C26-C27-C28
31	b	627	STE	C12-C13-C14-C15
33	D	410	LHG	C14-C15-C16-C17
33	D	410	LHG	C11-C12-C13-C14
29	C	517	DGD	O1A-C1A-O1G-C1G
33	d	408	LHG	C10-C11-C12-C13
29	c	518	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
22	d	404	CLA	C16-C17-C18-C19
27	b	621	LMG	C38-C39-C40-C41
28	a	411	SQD	C11-C12-C13-C14
31	B	620	STE	C12-C13-C14-C15
22	a	410	CLA	C2C-C3C-CAC-CBC
22	C	512	CLA	C14-C13-C15-C16
22	H	101	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C14
22	c	506	CLA	C6-C7-C8-C9
22	c	507	CLA	C6-C7-C8-C9
23	a	404	PHO	C6-C7-C8-C9
24	B	618	BCR	C15-C16-C17-C18
24	c	515	BCR	C9-C10-C11-C12
24	k	101	BCR	C19-C20-C21-C22
22	B	603	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	C19-C20-C21-C22
27	D	411	LMG	C37-C38-C39-C40
22	c	504	CLA	CBA-CGA-O2A-C1
33	D	410	LHG	C11-C10-C9-C8
28	A	411	SQD	C32-C33-C34-C35
33	D	412	LHG	C26-C27-C28-C29
27	Y	101	LMG	O1-C7-C8-O7
27	b	623	LMG	O1-C7-C8-O7
33	e	101	LHG	O7-C5-C6-O8
31	B	625	STE	C4-C5-C6-C7
33	D	412	LHG	C33-C34-C35-C36
27	a	415	LMG	C7-C8-C9-O8
29	C	515	DGD	C1G-C2G-C3G-O3G
33	D	409	LHG	C4-C5-C6-O8
22	H	101	CLA	C2-C3-C5-C6
31	d	411	STE	C7-C8-C9-C10
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	O1D-CGD-O2D-CED
22	a	402	CLA	C2C-C3C-CAC-CBC
34	f	101	HEC	C3A-C2A-CAA-CBA
27	Y	101	LMG	O6-C1-O1-C7
22	B	603	CLA	C16-C17-C18-C19
29	c	518	DGD	C5A-C6A-C7A-C8A
22	b	606	CLA	O1A-CGA-O2A-C1
31	b	624	STE	C7-C8-C9-C10
27	D	411	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	B	627	STE	C7-C8-C9-C10
22	B	616	CLA	CHA-CBD-CGD-O1D
22	B	616	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
33	D	409	LHG	C4-O6-P-O3
33	D	410	LHG	C3-O3-P-O5
33	E	101	LHG	C3-O3-P-O4
33	E	101	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O4
33	e	101	LHG	C4-O6-P-O5
31	I	101	STE	C1-C2-C3-C4
27	M	101	LMG	C22-C23-C24-C25
22	c	505	CLA	C4-C3-C5-C6
26	A	409	PL9	C20-C19-C21-C22
22	A	403	CLA	C2B-C3B-CAB-CBB
22	H	101	CLA	C2B-C3B-CAB-CBB
28	f	102	SQD	O47-C7-C8-C9
29	c	519	DGD	C3B-C4B-C5B-C6B
33	E	101	LHG	C7-C8-C9-C10
24	B	618	BCR	C36-C18-C19-C20
31	c	521	STE	C15-C16-C17-C18
27	D	407	LMG	C21-C22-C23-C24
22	D	405	CLA	O1D-CGD-O2D-CED
33	D	412	LHG	C18-C19-C20-C21
31	b	625	STE	C2-C3-C4-C5
33	E	101	LHG	C10-C11-C12-C13
26	A	409	PL9	C4-C3-C7-C8
26	a	409	PL9	C4-C3-C7-C8
28	a	411	SQD	C7-C8-C9-C10
27	d	410	LMG	C15-C16-C17-C18
28	B	622	SQD	C34-C35-C36-C37
22	b	609	CLA	O1D-CGD-O2D-CED
27	D	411	LMG	C9-C8-O7-C10
22	c	510	CLA	CAA-CBA-CGA-O2A
27	c	522	LMG	C36-C37-C38-C39
31	m	101	STE	C13-C14-C15-C16
31	B	626	STE	C7-C8-C9-C10
22	b	614	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C4C-C3C-CAC-CBC
22	b	606	CLA	CBA-CGA-O2A-C1
31	b	627	STE	C15-C16-C17-C18
22	A	403	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C12-C13-C14
22	B	605	CLA	C11-C10-C8-C9
22	B	606	CLA	C11-C12-C13-C14
22	b	604	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C12-C13-C15
22	B	606	CLA	C6-C7-C8-C10
22	C	506	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
34	f	101	HEC	C1A-C2A-CAA-CBA
24	c	516	BCR	C20-C21-C22-C23
33	l	101	LHG	O6-C4-C5-O7
29	A	413	DGD	CBA-CCA-CDA-CEA
31	B	625	STE	C12-C13-C14-C15
28	A	412	SQD	C19-C20-C21-C22
33	d	409	LHG	C9-C10-C11-C12
33	L	102	LHG	C27-C28-C29-C30
22	C	505	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	C10-C11-C12-C13
31	C	518	STE	C7-C8-C9-C10
22	B	603	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
29	C	515	DGD	O1G-C1A-C2A-C3A
22	B	609	CLA	CBA-CGA-O2A-C1
33	D	412	LHG	C19-C20-C21-C22
33	D	412	LHG	C7-C8-C9-C10
22	B	604	CLA	C15-C16-C17-C18
33	d	409	LHG	C2-C3-O3-P
27	M	101	LMG	O7-C8-C9-O8
27	c	522	LMG	O1-C7-C8-O7
28	a	412	SQD	O47-C45-C46-O48
31	M	103	STE	C3-C4-C5-C6
27	A	410	LMG	C38-C39-C40-C41
28	D	408	SQD	C28-C29-C30-C31
29	c	517	DGD	CCB-CDB-CEB-CFB
31	D	413	STE	C6-C7-C8-C9
29	c	517	DGD	O1G-C1A-C2A-C3A
22	B	603	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	a	413	STE	C7-C8-C9-C10
29	c	519	DGD	O6D-C5D-C6D-O5D
22	c	512	CLA	O1A-CGA-O2A-C1
31	c	521	STE	C11-C10-C9-C8
33	D	412	LHG	O9-C7-O7-C5
22	b	614	CLA	C4-C3-C5-C6
26	D	406	PL9	C45-C44-C46-C47
31	E	102	STE	C7-C8-C9-C10
24	B	619	BCR	C11-C12-C13-C35
22	b	612	CLA	C16-C17-C18-C20
31	D	413	STE	C12-C13-C14-C15
33	l	101	LHG	C15-C16-C17-C18
22	A	403	CLA	CBA-CGA-O2A-C1
31	b	624	STE	C2-C3-C4-C5
27	M	101	LMG	C8-C7-O1-C1
22	B	611	CLA	C13-C15-C16-C17
27	D	407	LMG	C16-C17-C18-C19
29	h	102	DGD	CBA-CCA-CDA-CEA
22	b	610	CLA	C2A-CAA-CBA-CGA
27	a	415	LMG	C31-C32-C33-C34
23	a	404	PHO	C2-C3-C5-C6
31	b	624	STE	C15-C16-C17-C18
27	a	415	LMG	O8-C28-C29-C30
22	B	614	CLA	C14-C13-C15-C16
22	B	616	CLA	C6-C7-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C10-C8-C9
29	c	517	DGD	C7A-C8A-C9A-CAA
33	D	412	LHG	C24-C23-O8-C6
29	A	413	DGD	C5A-C6A-C7A-C8A
22	B	610	CLA	O1D-CGD-O2D-CED
28	A	412	SQD	C11-C10-C9-C8
22	C	510	CLA	C16-C17-C18-C20
22	C	511	CLA	CBA-CGA-O2A-C1
22	B	613	CLA	C15-C16-C17-C18
22	c	504	CLA	C10-C11-C12-C13
31	b	625	STE	C1-C2-C3-C4
22	c	513	CLA	C4-C3-C5-C6
28	a	411	SQD	C14-C15-C16-C17
27	a	415	LMG	C35-C36-C37-C38
33	E	101	LHG	C31-C32-C33-C34
31	B	626	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
28	a	411	SQD	C11-C10-C9-C8
22	B	612	CLA	O1D-CGD-O2D-CED
27	c	520	LMG	C32-C33-C34-C35
31	H	104	STE	C10-C11-C12-C13
22	b	602	CLA	C11-C12-C13-C15
22	c	506	CLA	C6-C7-C8-C10
22	b	609	CLA	CBD-CGD-O2D-CED
31	a	413	STE	C6-C7-C8-C9
22	C	511	CLA	O1A-CGA-O2A-C1
22	c	504	CLA	O1A-CGA-O2A-C1
27	Y	101	LMG	C31-C32-C33-C34
29	A	413	DGD	CAB-CBB-CCB-CDB
27	Y	101	LMG	C4-C5-C6-O5
33	l	101	LHG	C11-C12-C13-C14
27	A	410	LMG	C13-C14-C15-C16
24	K	101	BCR	C35-C13-C14-C15
24	b	617	BCR	C16-C17-C18-C36
22	c	508	CLA	C5-C6-C7-C8
23	d	401	PHO	C2C-C3C-CAC-CBC
22	B	606	CLA	C10-C11-C12-C13
28	B	622	SQD	C11-C10-C9-C8
22	C	506	CLA	C2-C1-O2A-CGA
24	T	101	BCR	C9-C10-C11-C12
24	b	619	BCR	C9-C10-C11-C12
24	K	103	BCR	C11-C12-C13-C35
24	b	618	BCR	C37-C22-C23-C24
34	V	201	HEC	CAD-CBD-CGD-O1D
22	b	614	CLA	C13-C15-C16-C17
31	B	624	STE	O1-C1-C2-C3
29	c	517	DGD	O1G-C1G-C2G-C3G
22	b	604	CLA	C3-C5-C6-C7
27	B	621	LMG	C36-C37-C38-C39
27	c	523	LMG	C35-C36-C37-C38
28	a	411	SQD	C33-C34-C35-C36
29	C	517	DGD	CDA-CEA-CFA-CGA
22	B	605	CLA	C6-C7-C8-C9
22	B	610	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	a	410	CLA	C14-C13-C15-C16
22	b	601	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	D	401	PHO	C6-C7-C8-C9
29	C	517	DGD	C7A-C8A-C9A-CAA
31	C	520	STE	C5-C6-C7-C8
31	b	624	STE	C1-C2-C3-C4
29	C	517	DGD	C8B-C9B-CAB-CBB
31	B	627	STE	C11-C12-C13-C14
22	d	403	CLA	C4C-C3C-CAC-CBC
27	A	410	LMG	C15-C16-C17-C18
31	B	625	STE	O2-C1-C2-C3
27	M	101	LMG	C9-C8-O7-C10
29	C	517	DGD	O6D-C5D-C6D-O5D
29	c	519	DGD	C2B-C3B-C4B-C5B
22	B	610	CLA	CBD-CGD-O2D-CED
26	D	406	PL9	C33-C34-C36-C37
27	c	520	LMG	C30-C31-C32-C33
31	B	625	STE	C10-C11-C12-C13
31	B	624	STE	O2-C1-C2-C3
34	f	101	HEC	CAA-CBA-CGA-O1A
27	a	415	LMG	C11-C12-C13-C14
29	c	518	DGD	CCB-CDB-CEB-CFB
22	B	610	CLA	C16-C17-C18-C20
22	B	605	CLA	C2B-C3B-CAB-CBB
22	B	615	CLA	C2B-C3B-CAB-CBB
22	C	503	CLA	C2B-C3B-CAB-CBB
22	b	601	CLA	C2B-C3B-CAB-CBB
22	c	513	CLA	C2B-C3B-CAB-CBB
22	d	403	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C5-C6-C7-C8
24	b	618	BCR	C23-C24-C25-C26
24	c	515	BCR	C5-C6-C7-C8
27	D	411	LMG	O10-C28-O8-C9
33	E	101	LHG	C2-C3-O3-P
26	A	409	PL9	C40-C39-C41-C42
31	E	102	STE	C4-C5-C6-C7
33	D	410	LHG	O6-C4-C5-C6
33	E	101	LHG	O6-C4-C5-C6
33	d	408	LHG	O6-C4-C5-C6
22	c	513	CLA	C2-C3-C5-C6
28	a	412	SQD	C30-C31-C32-C33
34	F	102	HEC	CAD-CBD-CGD-O1D
22	A	403	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	B	615	CLA	C6-C7-C8-C10
22	b	604	CLA	C12-C13-C15-C16
22	c	510	CLA	C11-C12-C13-C15
27	b	623	LMG	C31-C32-C33-C34
22	C	509	CLA	C16-C17-C18-C19
22	c	502	CLA	C2A-CAA-CBA-CGA
27	B	621	LMG	O10-C28-C29-C30
33	d	407	LHG	C31-C32-C33-C34
22	b	611	CLA	C15-C16-C17-C18
27	b	621	LMG	C18-C19-C20-C21
31	b	624	STE	O2-C1-C2-C3
31	d	412	STE	O1-C1-C2-C3
29	C	515	DGD	C2A-C3A-C4A-C5A
29	C	515	DGD	CBA-CCA-CDA-CEA
24	K	103	BCR	C37-C22-C23-C24
31	a	414	STE	C5-C6-C7-C8
22	b	603	CLA	C4-C3-C5-C6
26	D	406	PL9	C43-C44-C46-C47
26	a	409	PL9	C28-C29-C31-C32
34	V	201	HEC	CAD-CBD-CGD-O2D
28	a	411	SQD	C32-C33-C34-C35
29	C	516	DGD	O1A-C1A-O1G-C1G
31	b	622	STE	O2-C1-C2-C3
31	b	624	STE	O1-C1-C2-C3
22	C	508	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C12-C13-C14
22	c	513	CLA	C14-C13-C15-C16
27	M	101	LMG	C36-C37-C38-C39
26	D	406	PL9	C16-C17-C18-C19
31	B	620	STE	O1-C1-C2-C3
34	f	101	HEC	CAA-CBA-CGA-O2A
22	c	511	CLA	C15-C16-C17-C18
24	b	619	BCR	C6-C7-C8-C9
27	B	621	LMG	O8-C28-C29-C30
31	c	521	STE	O1-C1-C2-C3
22	C	504	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
22	c	505	CLA	C2-C3-C5-C6
26	d	406	PL9	C28-C29-C31-C32
31	B	625	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C13-C15-C16-C17
31	B	625	STE	O1-C1-C2-C3
28	L	101	SQD	C14-C15-C16-C17
31	j	101	STE	C7-C8-C9-C10
33	L	102	LHG	C29-C30-C31-C32
31	c	521	STE	O2-C1-C2-C3
22	A	403	CLA	O1A-CGA-O2A-C1
27	c	522	LMG	C35-C36-C37-C38
31	B	620	STE	O2-C1-C2-C3
27	b	621	LMG	C39-C40-C41-C42
22	b	612	CLA	C10-C11-C12-C13
33	D	410	LHG	O6-C4-C5-O7
26	a	409	PL9	C35-C34-C36-C37
33	E	101	LHG	C34-C35-C36-C37
33	D	410	LHG	C17-C18-C19-C20
22	d	403	CLA	C4B-C3B-CAB-CBB
31	B	625	STE	C9-C10-C11-C12
31	d	412	STE	O2-C1-C2-C3
28	B	622	SQD	C35-C36-C37-C38
29	c	518	DGD	C9A-CAA-CBA-CCA
29	c	518	DGD	CAB-CBB-CCB-CDB
28	A	412	SQD	C24-C25-C26-C27
23	d	401	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
24	d	405	BCR	C16-C17-C18-C36
27	a	415	LMG	C33-C34-C35-C36
31	c	521	STE	C10-C11-C12-C13
31	B	624	STE	C4-C5-C6-C7
26	D	406	PL9	C15-C14-C16-C17
26	d	406	PL9	C15-C14-C16-C17
27	A	410	LMG	O7-C8-C9-O8
28	L	101	SQD	O47-C45-C46-O48
31	b	622	STE	O1-C1-C2-C3
29	H	103	DGD	C9B-CAB-CBB-CCB
28	D	408	SQD	O5-C1-O6-C44
22	B	608	CLA	C6-C7-C8-C10
22	a	402	CLA	C12-C13-C15-C16
22	b	611	CLA	C6-C7-C8-C10
23	A	404	PHO	C2C-C3C-CAC-CBC
31	b	627	STE	C4-C5-C6-C7
24	K	101	BCR	C9-C10-C11-C12
22	C	511	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	a	402	CLA	C14-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C9
22	c	506	CLA	C14-C13-C15-C16
22	c	507	CLA	C14-C13-C15-C16
27	b	621	LMG	C8-C7-O1-C1
27	b	623	LMG	C8-C7-O1-C1
29	c	517	DGD	C5D-C6D-O5D-C1E
34	v	201	HEC	CAD-CBD-CGD-O2D
22	B	613	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C2-C1-O2A-CGA
22	A	403	CLA	C3A-C2A-CAA-CBA
31	J	101	STE	O2-C1-C2-C3
34	F	102	HEC	CAD-CBD-CGD-O2D
27	b	623	LMG	C17-C18-C19-C20
31	B	623	STE	C3-C4-C5-C6
29	C	515	DGD	O1A-C1A-O1G-C1G
22	c	514	CLA	C13-C15-C16-C17
29	H	103	DGD	CAB-CBB-CCB-CDB
31	b	625	STE	C5-C6-C7-C8
33	E	101	LHG	C19-C20-C21-C22
31	C	519	STE	C14-C15-C16-C17
31	B	623	STE	C9-C10-C11-C12
31	B	625	STE	C6-C7-C8-C9
29	c	517	DGD	C5B-C6B-C7B-C8B
26	D	406	PL9	C28-C29-C31-C32
27	c	523	LMG	C36-C37-C38-C39
29	C	516	DGD	C5B-C6B-C7B-C8B
26	a	409	PL9	C11-C12-C13-C14
31	m	102	STE	C4-C5-C6-C7
27	A	410	LMG	C7-C8-C9-O8
27	M	101	LMG	O1-C7-C8-C9
22	B	616	CLA	C10-C11-C12-C13
22	D	405	CLA	C3-C5-C6-C7
27	M	101	LMG	C21-C22-C23-C24
34	v	201	HEC	CAD-CBD-CGD-O1D
22	B	612	CLA	CAA-CBA-CGA-O2A
27	d	410	LMG	O7-C10-C11-C12
29	C	515	DGD	O2G-C2G-C3G-O3G
28	a	412	SQD	C16-C17-C18-C19
22	D	405	CLA	C10-C11-C12-C13
22	B	604	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C11-C12-C13-C14
22	c	503	CLA	C11-C12-C13-C14
22	c	514	CLA	C11-C10-C8-C9
31	J	101	STE	C4-C5-C6-C7
31	b	624	STE	C14-C15-C16-C17
28	a	411	SQD	O47-C7-C8-C9
31	J	101	STE	O1-C1-C2-C3
31	B	625	STE	C3-C4-C5-C6
22	B	606	CLA	C11-C10-C8-C7
22	B	615	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	C	506	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	C	513	CLA	C11-C10-C8-C7
22	b	612	CLA	C12-C13-C15-C16
22	b	616	CLA	C11-C10-C8-C7
22	c	513	CLA	C12-C13-C15-C16
29	C	516	DGD	C8A-C9A-CAA-CBA
33	D	410	LHG	C24-C25-C26-C27
22	b	607	CLA	C2B-C3B-CAB-CBB
24	k	102	BCR	C5-C6-C7-C8
27	a	415	LMG	C11-C10-O7-C8
28	L	101	SQD	C11-C10-C9-C8
29	C	516	DGD	C2B-C3B-C4B-C5B
22	B	612	CLA	C2-C1-O2A-CGA
22	D	403	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA
31	B	620	STE	C7-C8-C9-C10
22	a	402	CLA	C4C-C3C-CAC-CBC
29	C	515	DGD	O6E-C1E-O5D-C6D
31	b	625	STE	C3-C4-C5-C6
22	H	101	CLA	C15-C16-C17-C18
33	D	409	LHG	C18-C19-C20-C21
22	B	603	CLA	C2A-CAA-CBA-CGA
27	c	522	LMG	C42-C43-C44-C45
22	C	509	CLA	C16-C17-C18-C20
27	M	101	LMG	C30-C31-C32-C33
29	h	102	DGD	O1B-C1B-C2B-C3B
22	c	509	CLA	C4-C3-C5-C6
23	A	404	PHO	C10-C11-C12-C13
22	b	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	h	101	BCR	C11-C10-C9-C34
33	d	408	LHG	C30-C31-C32-C33
31	B	627	STE	C12-C13-C14-C15
31	m	102	STE	C1-C2-C3-C4
22	b	603	CLA	C13-C15-C16-C17
22	B	609	CLA	C14-C13-C15-C16
22	b	604	CLA	C6-C7-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	D	404	CLA	C2C-C3C-CAC-CBC
28	A	412	SQD	O48-C23-C24-C25
28	L	101	SQD	O6-C44-C45-C46
29	C	515	DGD	O1G-C1G-C2G-C3G
29	h	102	DGD	C1G-C2G-C3G-O3G
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C4B-C3B-CAB-CBB
22	B	615	CLA	C4B-C3B-CAB-CBB
22	H	101	CLA	C4B-C3B-CAB-CBB
22	b	605	CLA	C4-C3-C5-C6
29	A	413	DGD	O6D-C1D-O3G-C3G
29	C	516	DGD	O6D-C1D-O3G-C3G
27	A	410	LMG	O1-C7-C8-O7
31	B	620	STE	C4-C5-C6-C7
33	E	101	LHG	C15-C16-C17-C18
24	T	101	BCR	C11-C12-C13-C14
24	a	406	BCR	C21-C22-C23-C24
27	b	623	LMG	O7-C10-C11-C12
28	A	411	SQD	O47-C7-C8-C9
29	C	515	DGD	O2G-C1B-C2B-C3B
22	b	613	CLA	C16-C17-C18-C19
22	B	613	CLA	CAA-CBA-CGA-O2A
27	b	623	LMG	C16-C17-C18-C19
22	B	608	CLA	C13-C15-C16-C17
27	D	407	LMG	C18-C19-C20-C21
28	A	412	SQD	C31-C32-C33-C34
22	B	603	CLA	C12-C13-C15-C16
22	B	613	CLA	C6-C7-C8-C10
22	C	505	CLA	C11-C12-C13-C15
22	H	101	CLA	C11-C12-C13-C15
22	b	602	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
23	a	404	PHO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	B	626	STE	C10-C11-C12-C13
31	B	601	STE	C3-C4-C5-C6
22	b	601	CLA	O2A-C1-C2-C3
23	a	404	PHO	O2A-C1-C2-C3
31	b	622	STE	C11-C10-C9-C8
31	D	413	STE	O2-C1-C2-C3
33	l	101	LHG	O7-C7-C8-C9
31	M	103	STE	C7-C8-C9-C10
27	b	621	LMG	C36-C37-C38-C39
22	c	509	CLA	O1D-CGD-O2D-CED
28	A	412	SQD	O49-C7-O47-C45
34	v	201	HEC	C2B-C3B-CAB-CBB
22	B	603	CLA	C15-C16-C17-C18
26	D	406	PL9	C34-C36-C37-C38
22	a	410	CLA	C15-C16-C17-C18
22	B	602	CLA	C3A-C2A-CAA-CBA
33	D	409	LHG	C19-C20-C21-C22
31	d	411	STE	C1-C2-C3-C4
31	C	519	STE	C11-C10-C9-C8
24	B	619	BCR	C16-C17-C18-C19
29	c	518	DGD	O1A-C1A-C2A-C3A
33	D	412	LHG	C16-C17-C18-C19
33	L	102	LHG	C28-C29-C30-C31
22	B	606	CLA	C5-C6-C7-C8
31	B	625	STE	C1-C2-C3-C4
31	C	518	STE	O1-C1-C2-C3
22	c	503	CLA	C2C-C3C-CAC-CBC
22	B	608	CLA	C16-C17-C18-C19
22	B	603	CLA	O1D-CGD-O2D-CED
22	a	403	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	C6-C7-C8-C9
22	B	615	CLA	C6-C7-C8-C9
22	C	502	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
22	C	508	CLA	C14-C13-C15-C16
22	D	405	CLA	C6-C7-C8-C9
22	a	403	CLA	C6-C7-C8-C9
29	H	103	DGD	C4A-C5A-C6A-C7A
22	c	510	CLA	CAA-CBA-CGA-O1A
31	H	104	STE	C3-C4-C5-C6
27	b	623	LMG	O10-C28-C29-C30
29	c	519	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
27	c	522	LMG	C32-C33-C34-C35
31	d	413	STE	O2-C1-C2-C3
27	Y	101	LMG	C34-C35-C36-C37
22	C	513	CLA	C13-C15-C16-C17
22	b	615	CLA	C13-C15-C16-C17
24	b	619	BCR	C7-C8-C9-C10
22	B	612	CLA	CAA-CBA-CGA-O1A
22	D	404	CLA	C4C-C3C-CAC-CBC
24	A	406	BCR	C18-C19-C20-C21
24	B	619	BCR	C10-C11-C12-C13
28	L	101	SQD	C45-C44-O6-C1
29	C	516	DGD	C5D-C6D-O5D-C1E
27	Y	101	LMG	C2-C1-O1-C7
22	D	403	CLA	C10-C11-C12-C13
28	L	101	SQD	C44-C45-C46-O48
22	C	503	CLA	C8-C10-C11-C12
29	c	517	DGD	O2G-C1B-C2B-C3B
31	H	104	STE	C11-C12-C13-C14
31	C	518	STE	O2-C1-C2-C3
31	D	413	STE	O1-C1-C2-C3
22	C	501	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
27	c	522	LMG	C11-C10-O7-C8
27	A	410	LMG	C14-C15-C16-C17
33	d	407	LHG	O8-C23-C24-C25
33	D	409	LHG	O10-C23-C24-C25
22	B	612	CLA	O1A-CGA-O2A-C1
27	b	621	LMG	C40-C41-C42-C43
24	F	101	BCR	C22-C23-C24-C25
31	d	413	STE	O1-C1-C2-C3
22	a	403	CLA	C16-C17-C18-C20
27	B	621	LMG	C14-C15-C16-C17
31	M	102	STE	O2-C1-C2-C3
22	b	611	CLA	C10-C11-C12-C13
22	C	511	CLA	C6-C7-C8-C10
27	Y	101	LMG	O8-C28-C29-C30
27	b	621	LMG	O8-C28-C29-C30
29	C	516	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
31	I	101	STE	C6-C7-C8-C9
28	A	412	SQD	O10-C23-C24-C25
29	c	518	DGD	O6D-C5D-C6D-O5D

There are no ring outliers.

101 monomers are involved in 153 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	D	412	LHG	5	0
24	F	101	BCR	5	0
22	b	608	CLA	1	0
31	a	413	STE	1	0
22	H	101	CLA	2	0
23	D	401	PHO	1	0
28	a	411	SQD	1	0
27	D	407	LMG	1	0
29	c	519	DGD	2	0
22	d	403	CLA	1	0
31	m	102	STE	1	0
33	D	409	LHG	1	0
27	a	415	LMG	2	0
33	e	101	LHG	1	0
24	K	101	BCR	2	0
28	A	412	SQD	2	0
22	c	512	CLA	1	0
22	D	403	CLA	1	0
23	a	404	PHO	1	0
22	D	404	CLA	2	0
27	c	522	LMG	1	0
24	K	102	BCR	2	0
22	a	402	CLA	3	0
26	A	409	PL9	2	0
22	A	402	CLA	2	0
34	f	101	HEC	5	0
22	C	502	CLA	1	0
22	c	506	CLA	1	0
22	c	504	CLA	3	0
22	C	511	CLA	1	0
24	d	405	BCR	3	0
33	L	102	LHG	1	0
22	C	509	CLA	1	0
24	B	618	BCR	2	0

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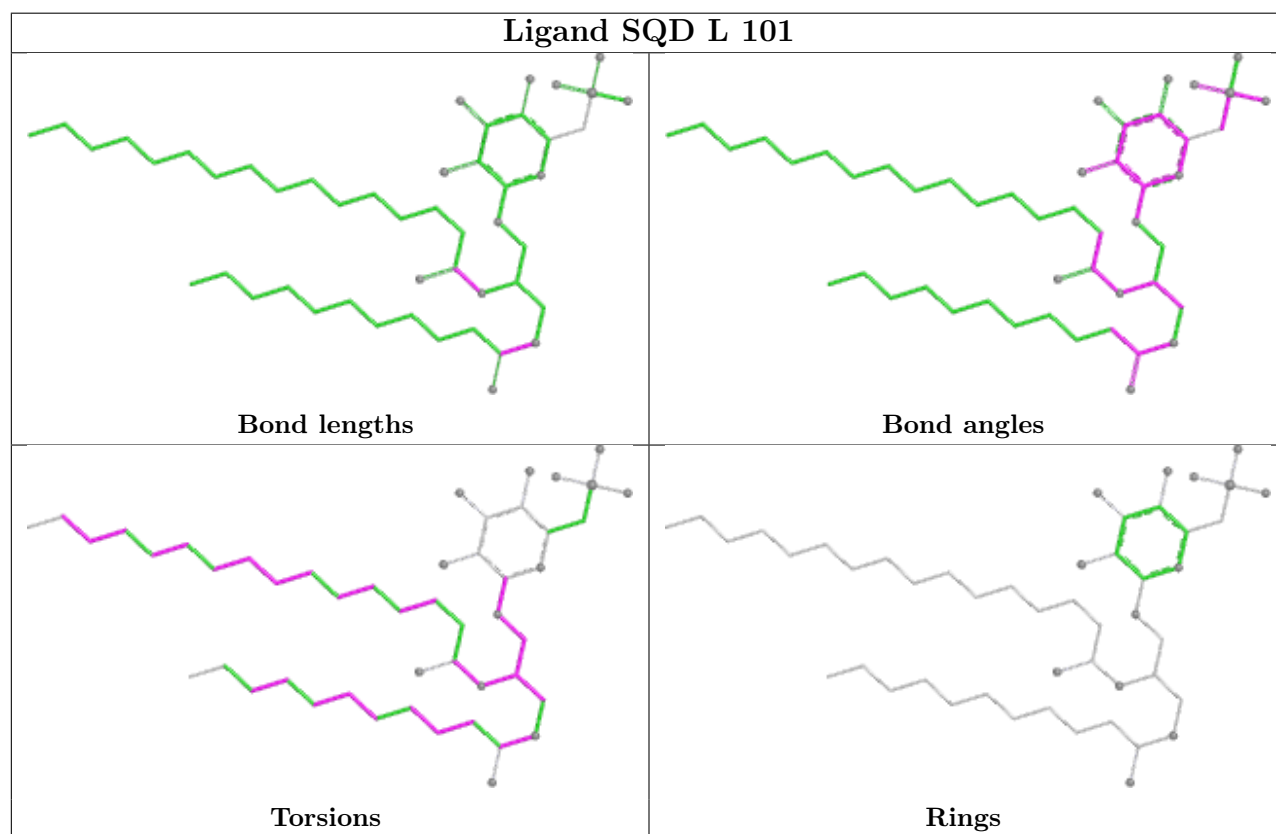
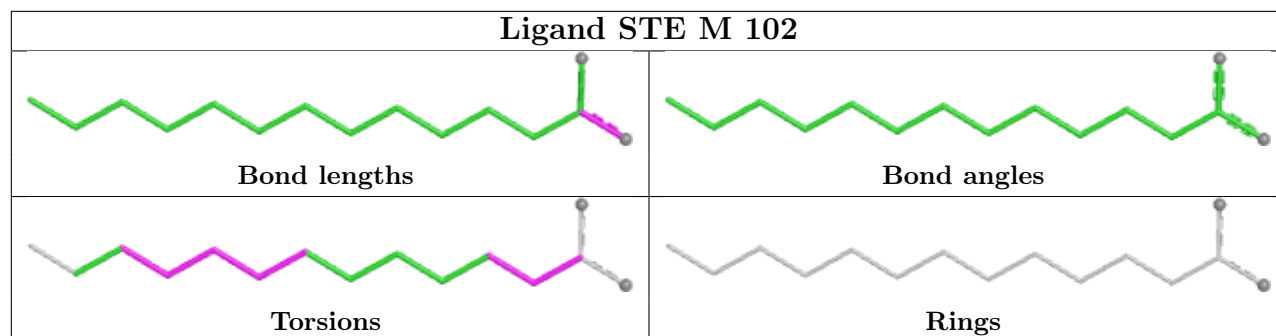
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	t	101	BCR	3	0
24	b	618	BCR	2	0
22	B	616	CLA	1	0
22	D	405	CLA	3	0
22	B	614	CLA	1	0
24	T	101	BCR	4	0
24	a	406	BCR	2	0
23	d	401	PHO	1	0
31	Z	101	STE	1	0
26	a	409	PL9	3	0
22	C	512	CLA	2	0
22	B	606	CLA	2	0
22	C	513	CLA	2	0
22	c	508	CLA	1	0
22	B	608	CLA	1	0
23	A	404	PHO	1	0
22	B	605	CLA	2	0
22	B	613	CLA	2	0
22	B	612	CLA	1	0
27	M	101	LMG	1	0
33	d	407	LHG	2	0
24	B	617	BCR	2	0
24	B	619	BCR	3	0
24	k	102	BCR	2	0
33	E	101	LHG	1	0
31	c	521	STE	2	0
24	c	516	BCR	3	0
22	b	615	CLA	4	0
31	B	620	STE	1	0
22	b	613	CLA	1	0
22	b	606	CLA	3	0
28	A	411	SQD	1	0
22	B	609	CLA	2	0
34	F	102	HEC	3	0
22	c	505	CLA	1	0
29	c	518	DGD	1	0
31	b	622	STE	2	0
24	A	406	BCR	1	0
24	h	101	BCR	1	0
27	D	411	LMG	3	0
28	B	622	SQD	1	0
22	b	605	CLA	3	0

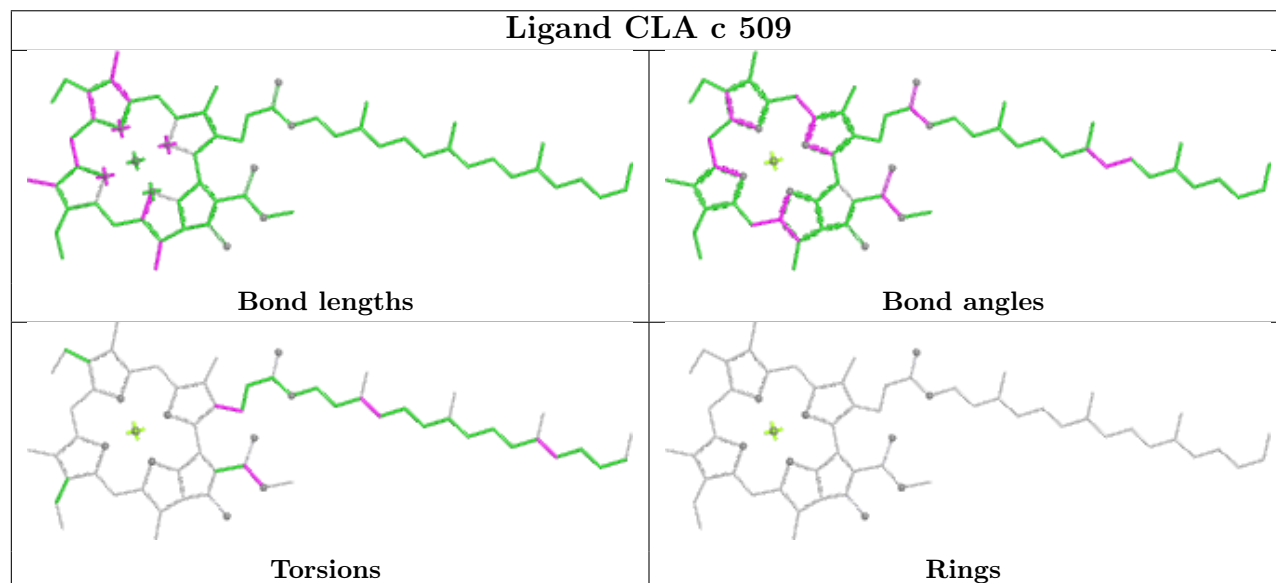
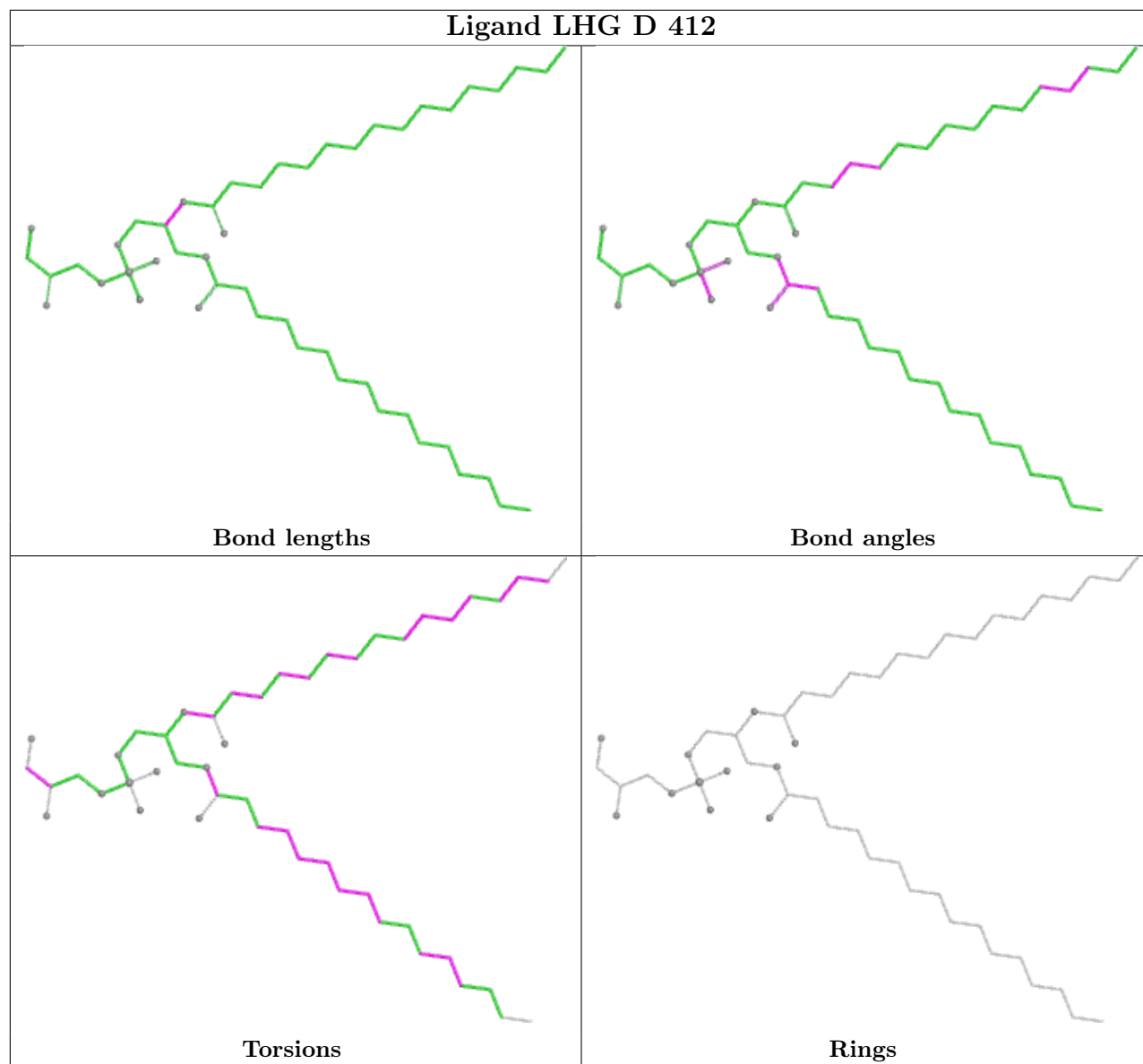
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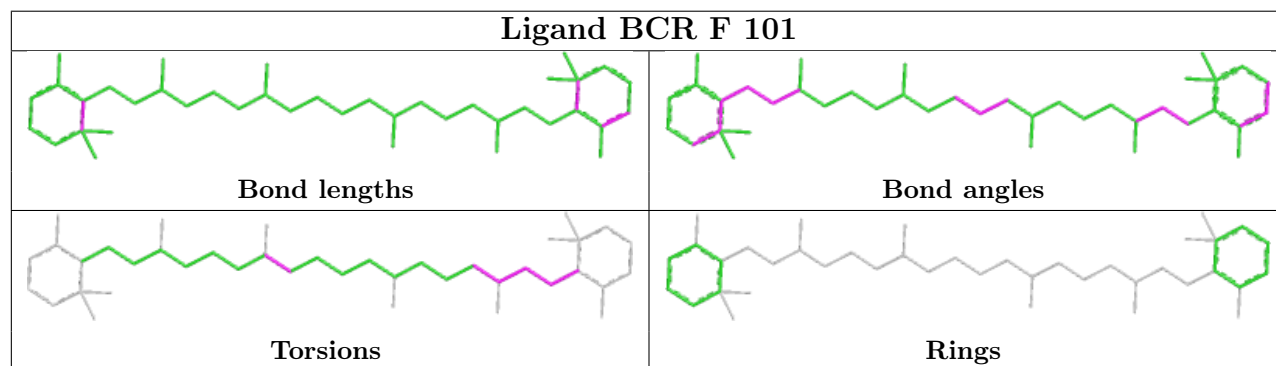
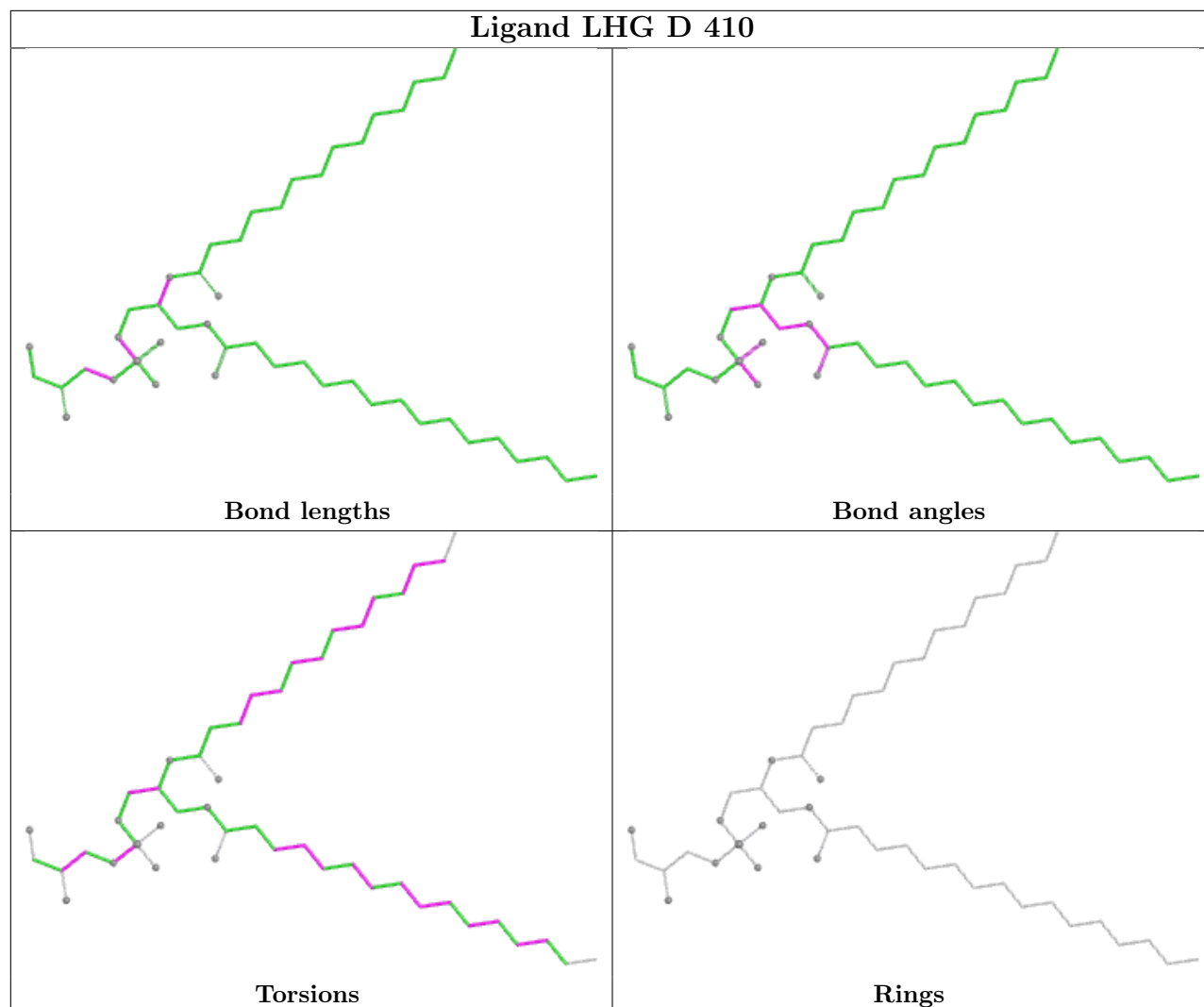
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	d	413	STE	1	0
29	H	103	DGD	1	0
31	B	627	STE	1	0
22	b	604	CLA	2	0
22	c	502	CLA	2	0
33	d	408	LHG	1	0
22	b	616	CLA	1	0
29	A	413	DGD	1	0
34	V	201	HEC	2	0
22	c	511	CLA	1	0
24	H	102	BCR	3	0
24	c	515	BCR	3	0
22	B	604	CLA	1	0
22	b	602	CLA	1	0
34	v	201	HEC	1	0
22	c	514	CLA	5	0
22	b	601	CLA	1	0
28	f	102	SQD	1	0
22	a	410	CLA	1	0
22	C	501	CLA	2	0
29	C	515	DGD	1	0
22	A	405	CLA	1	0
27	b	621	LMG	1	0
22	b	614	CLA	1	0
26	d	406	PL9	1	0

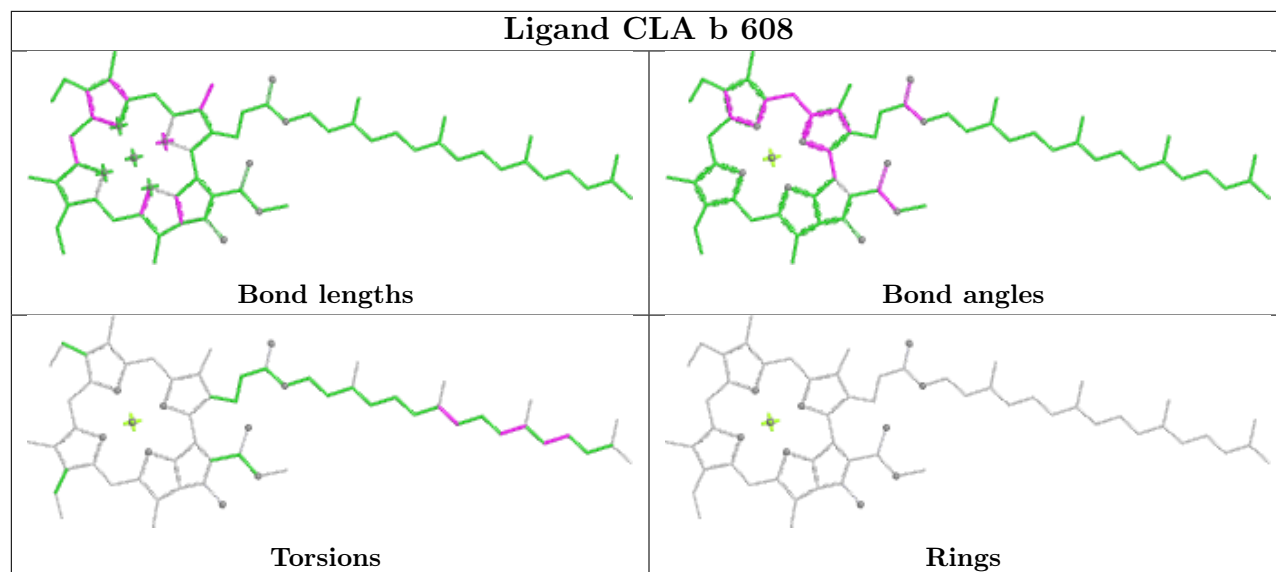
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



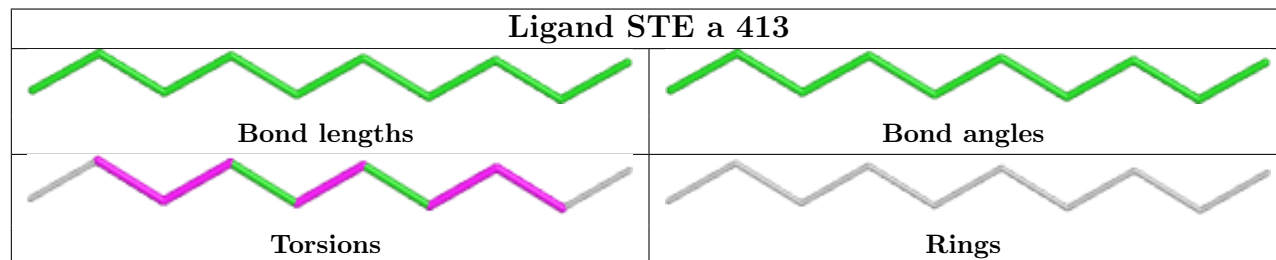




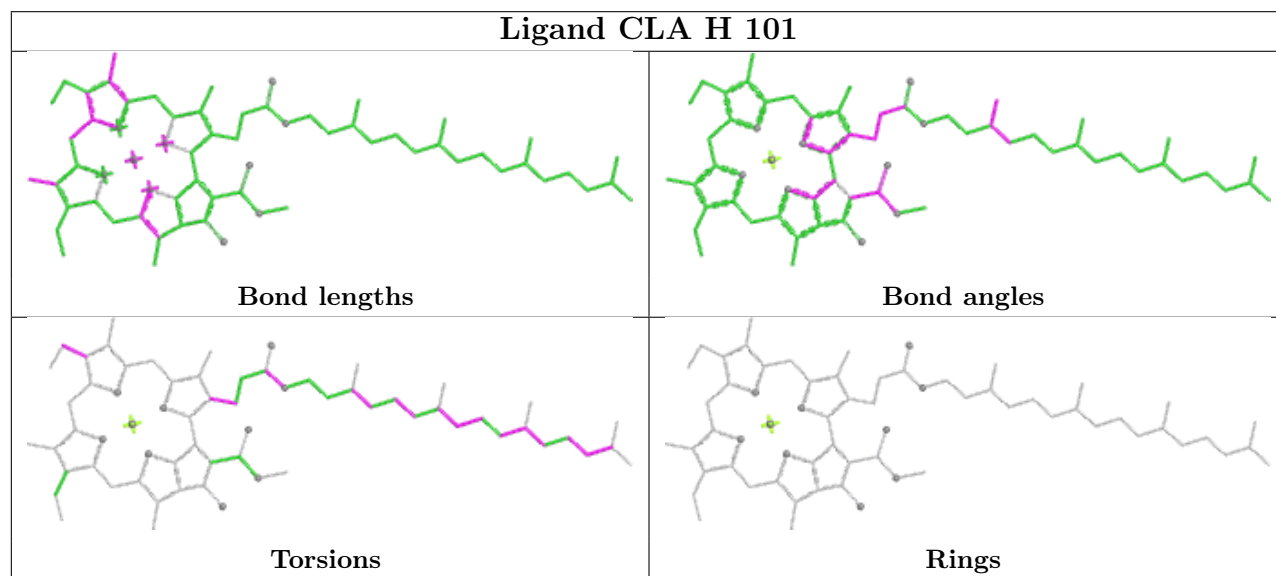
Ligand CLA b 608

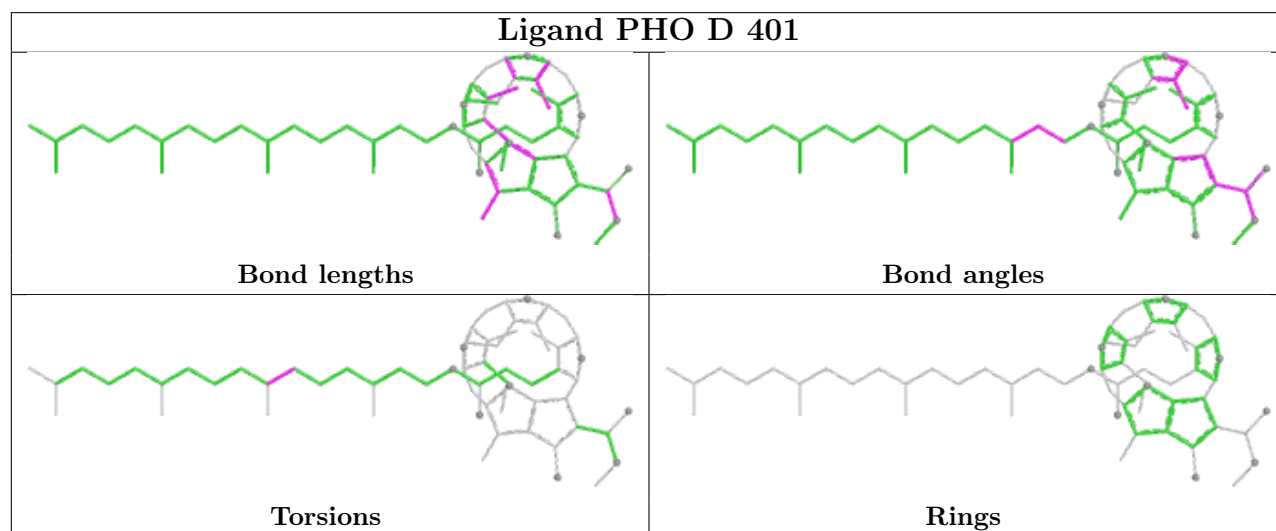
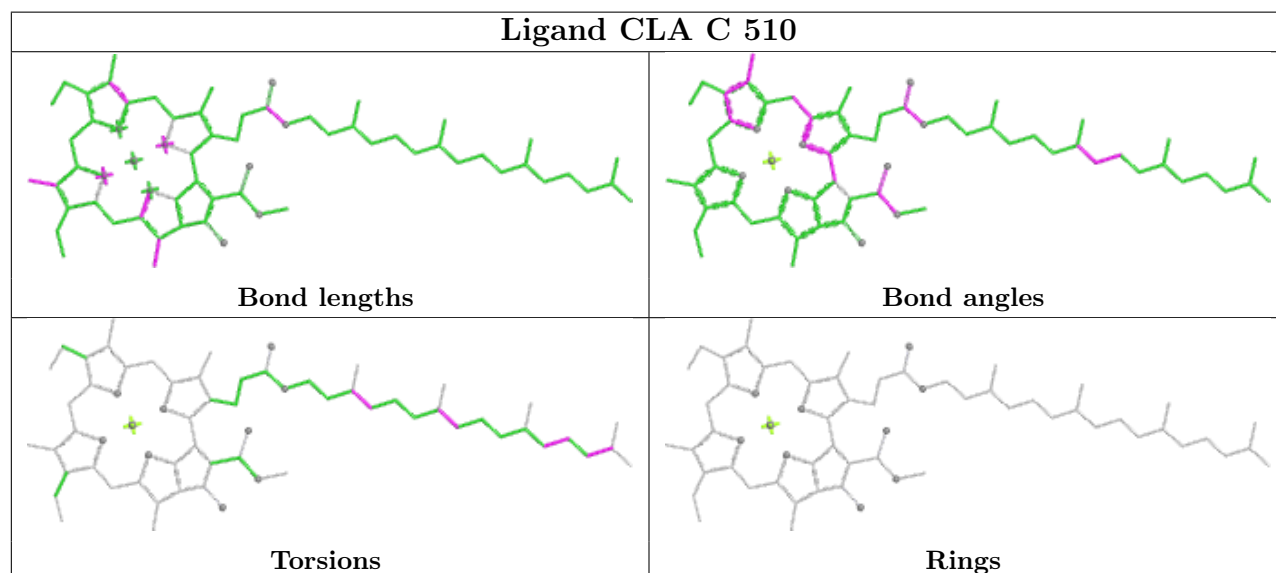
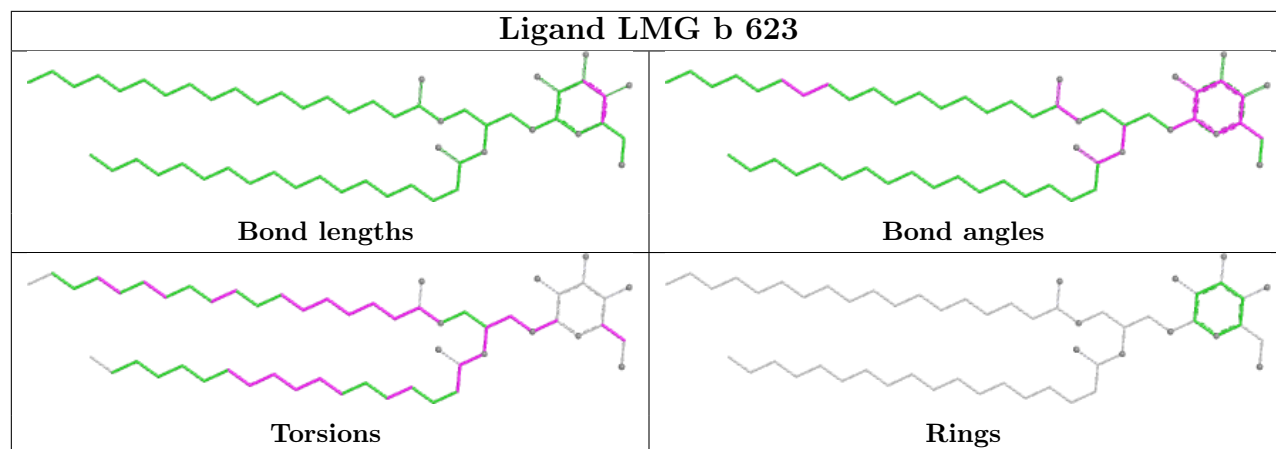


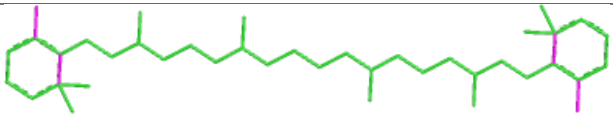
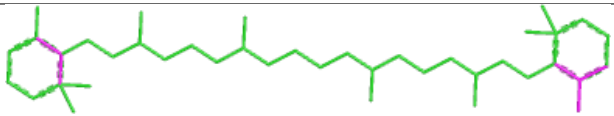
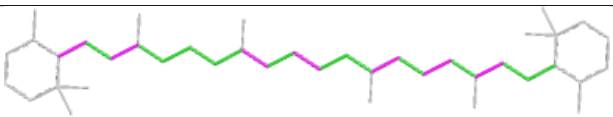
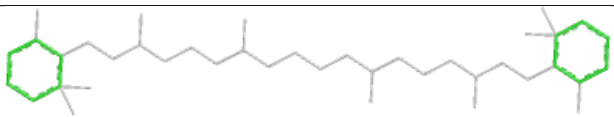
Ligand STE a 413



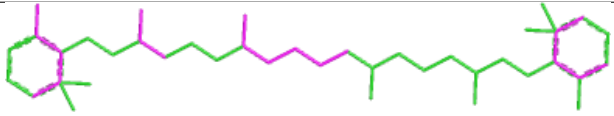
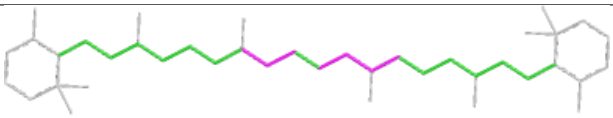
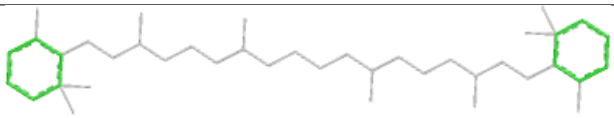
Ligand CLA H 101





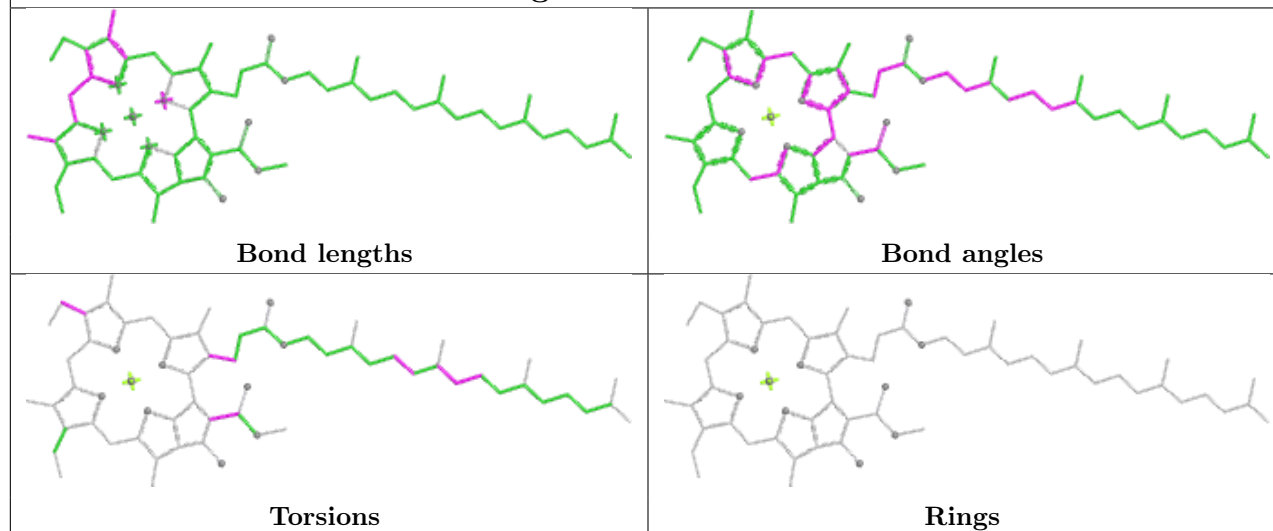
Ligand BCR k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

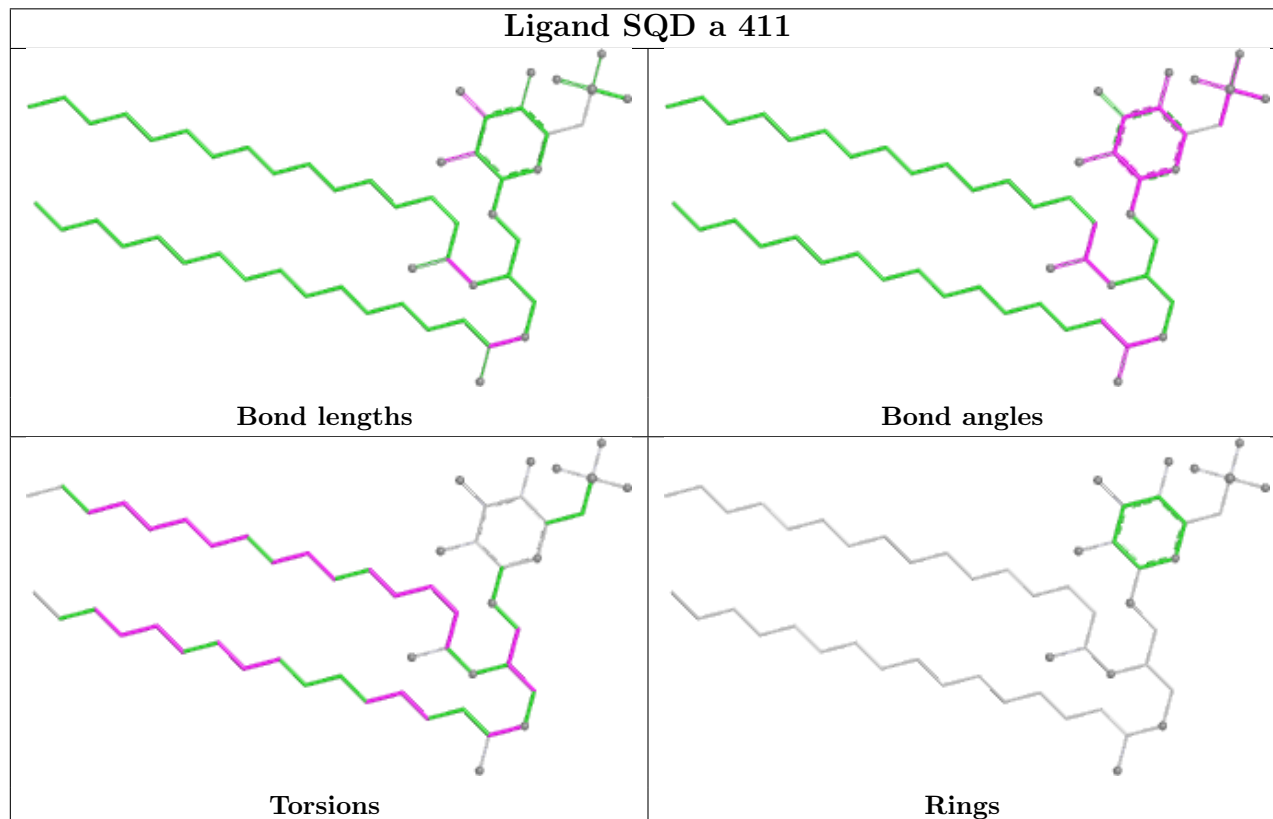
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

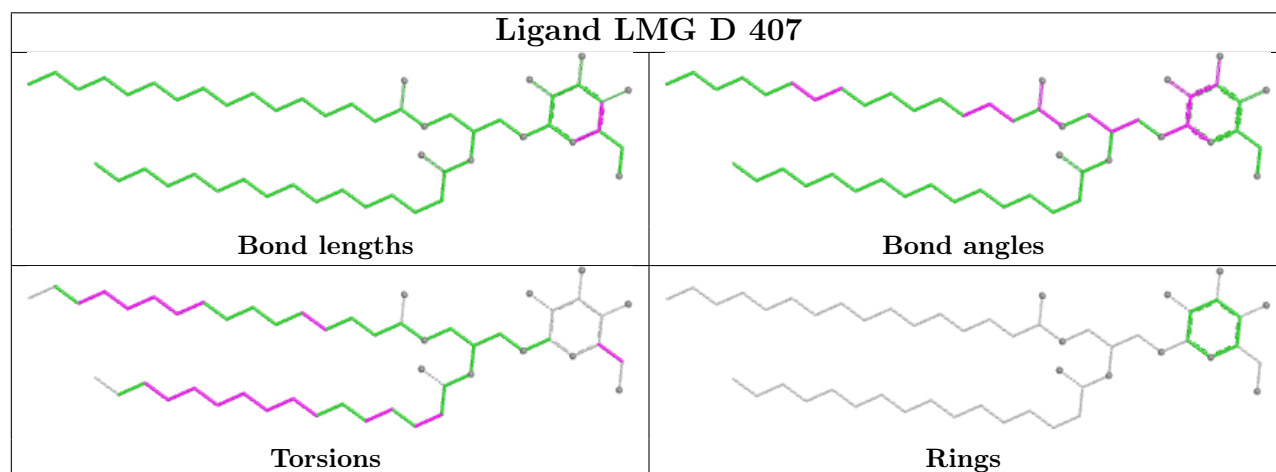
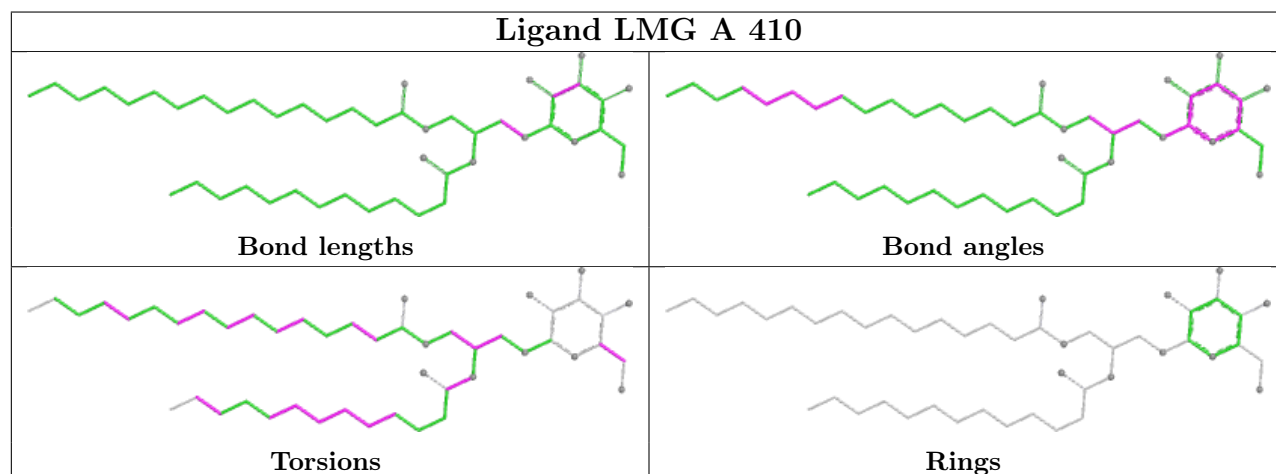
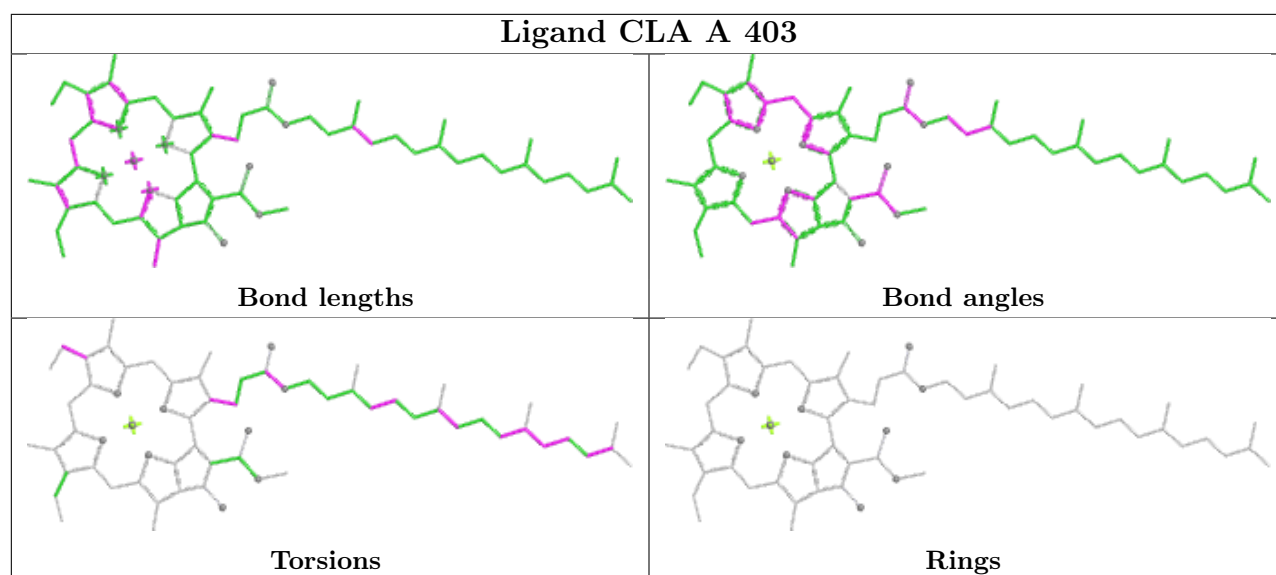
Ligand STE H 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

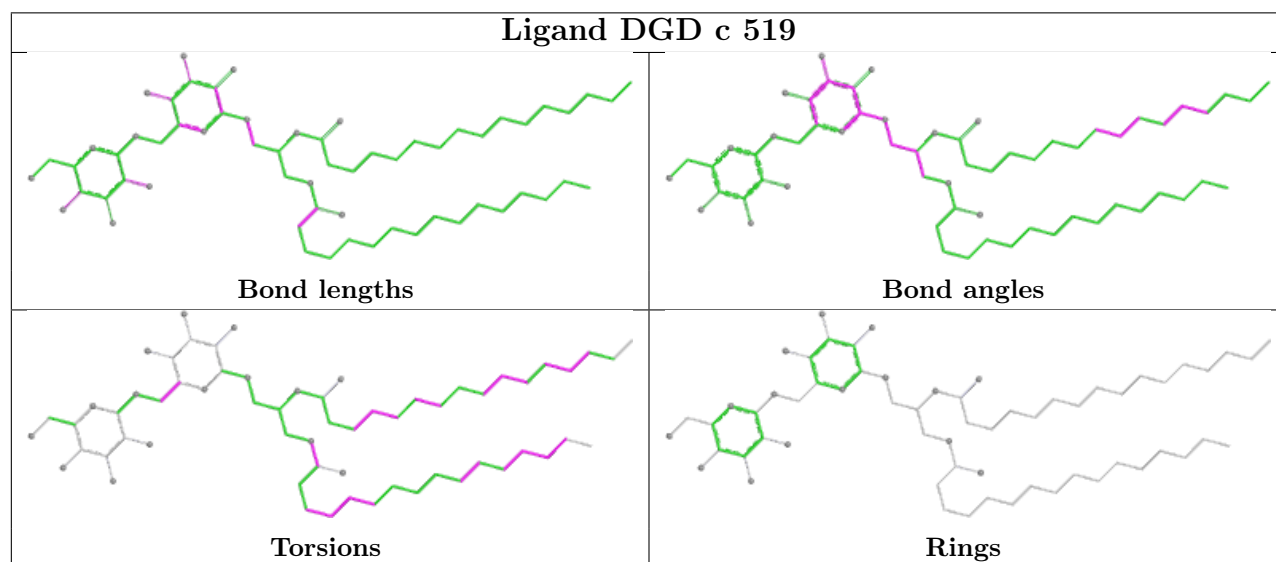
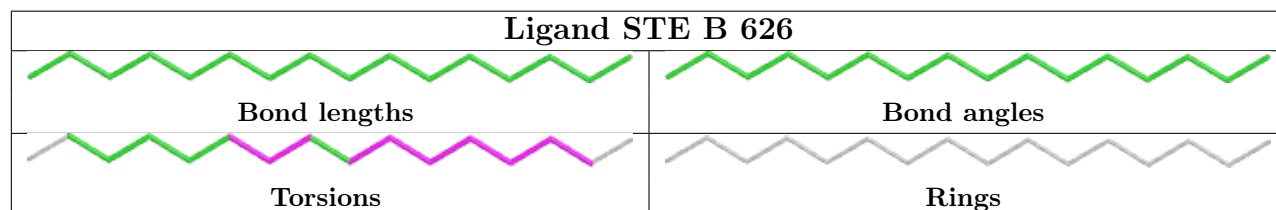
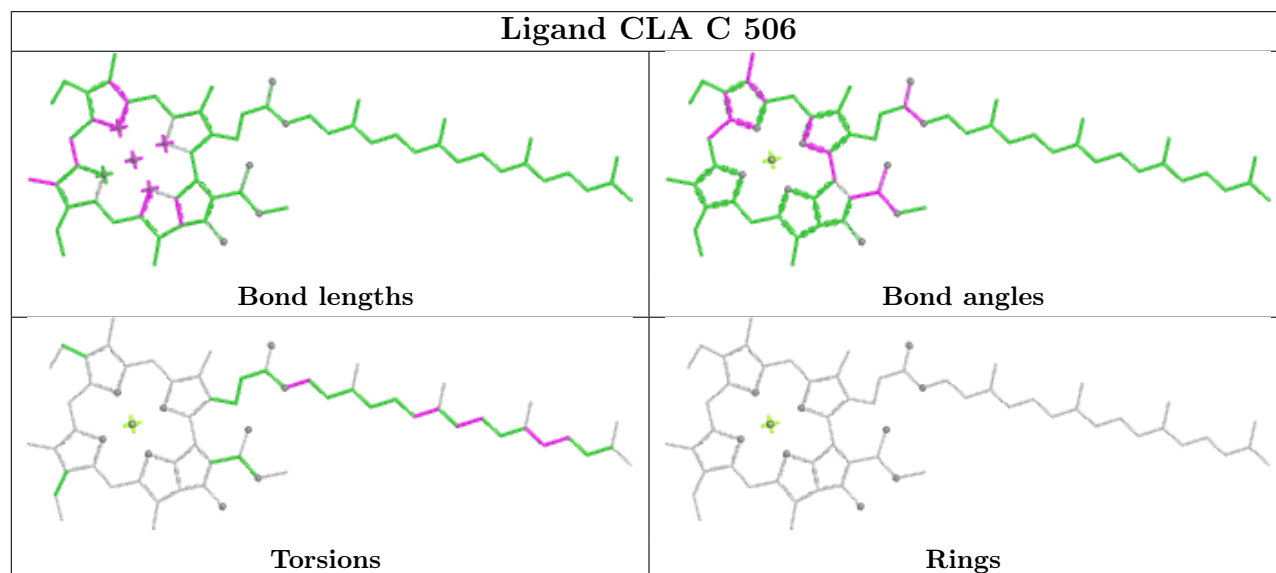
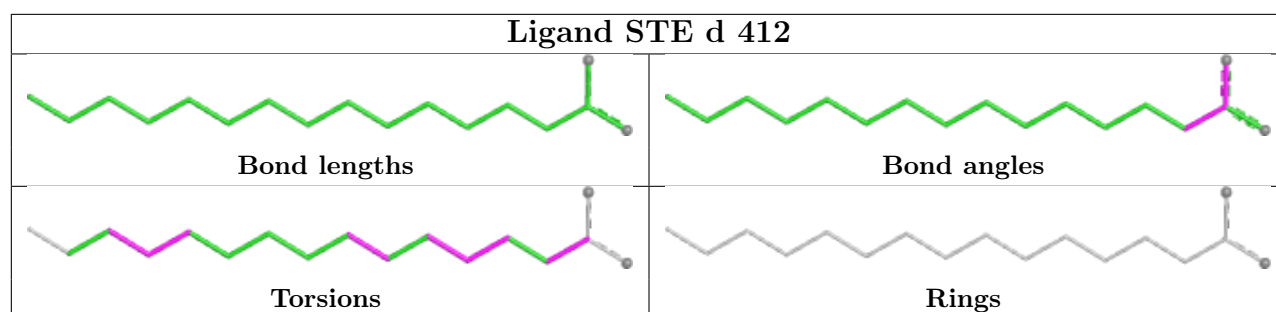
Ligand CLA C 503



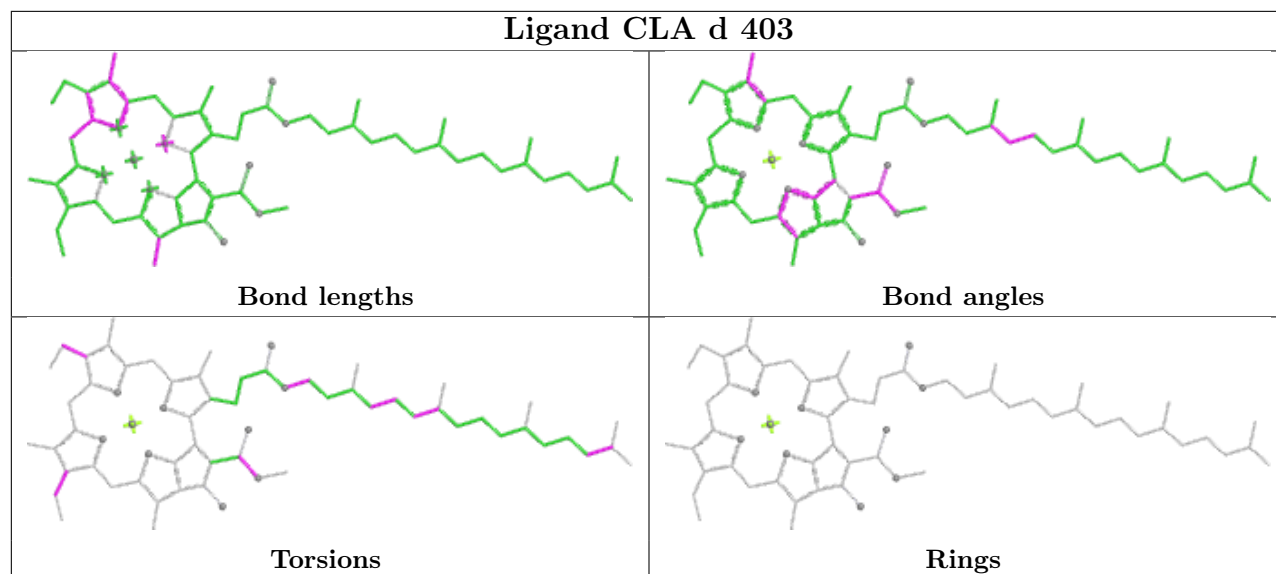
Ligand SQD a 411



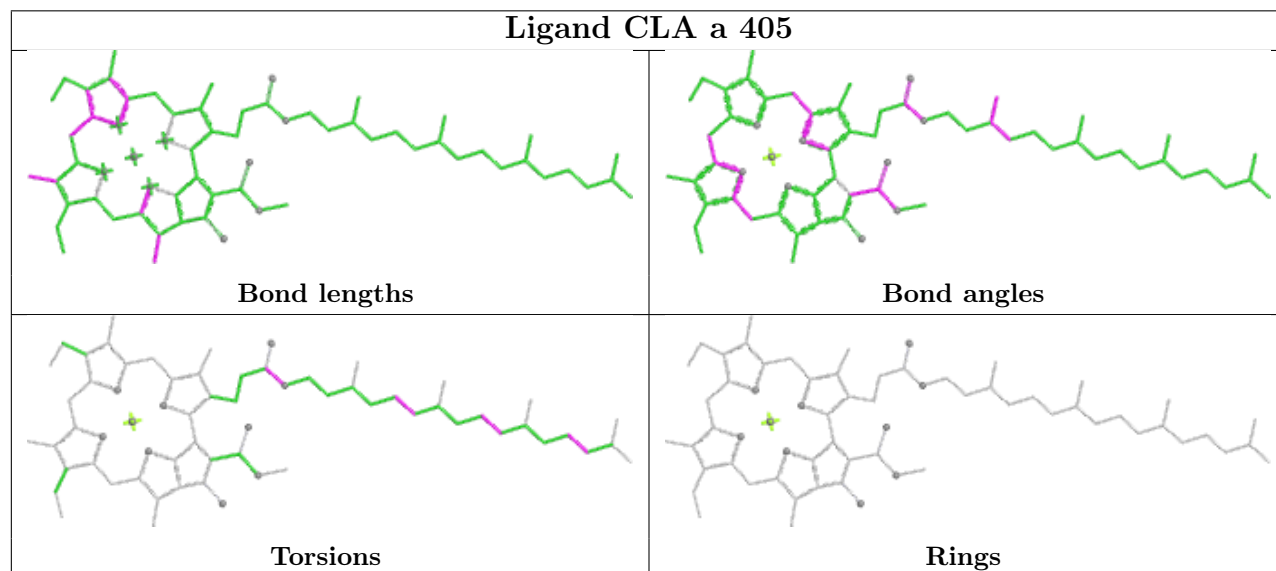




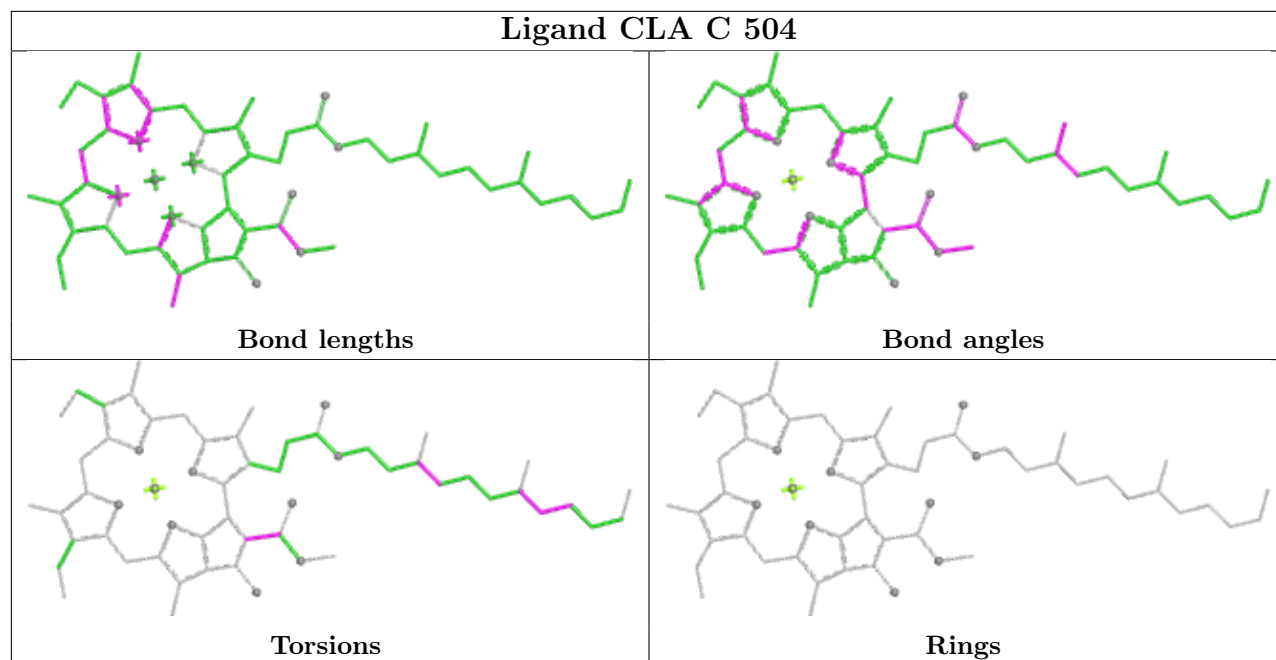
Ligand CLA d 403



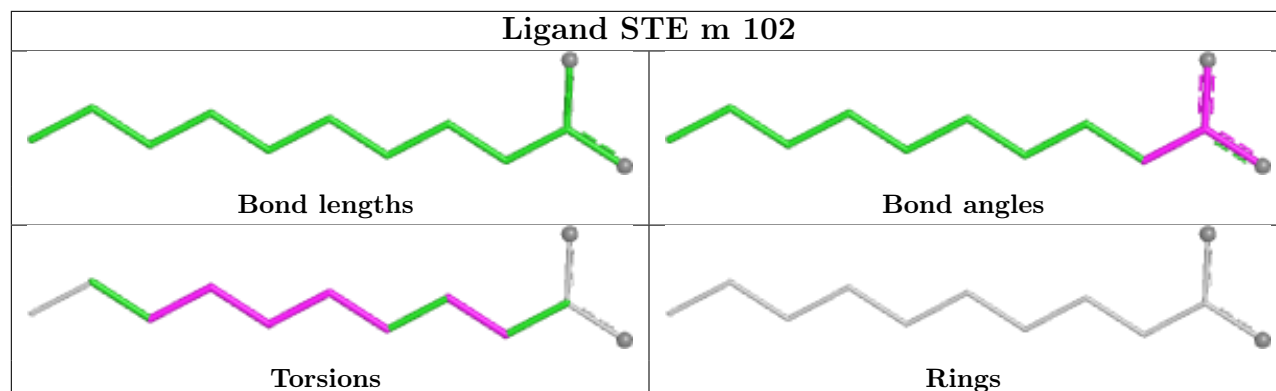
Ligand CLA a 405

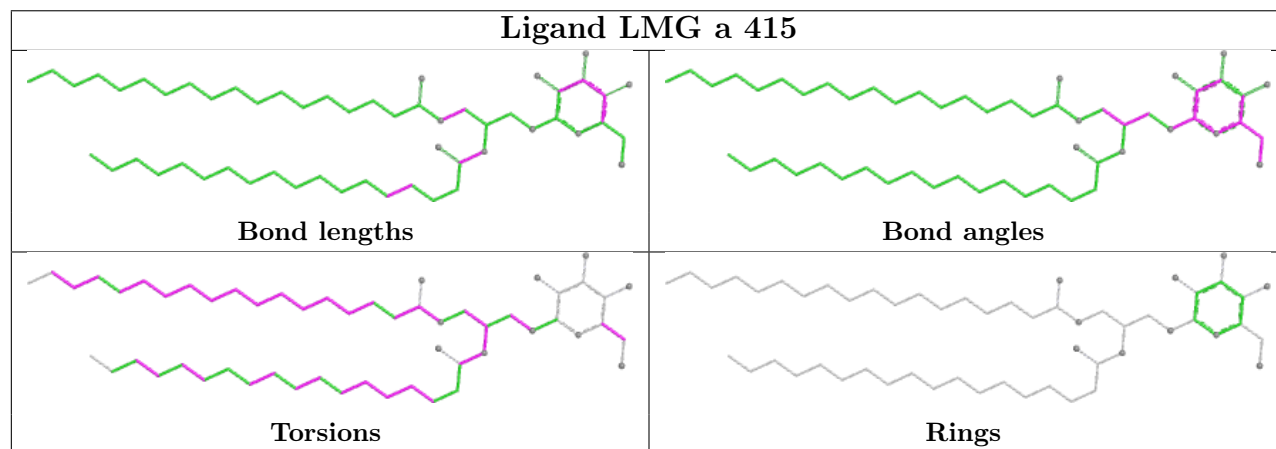
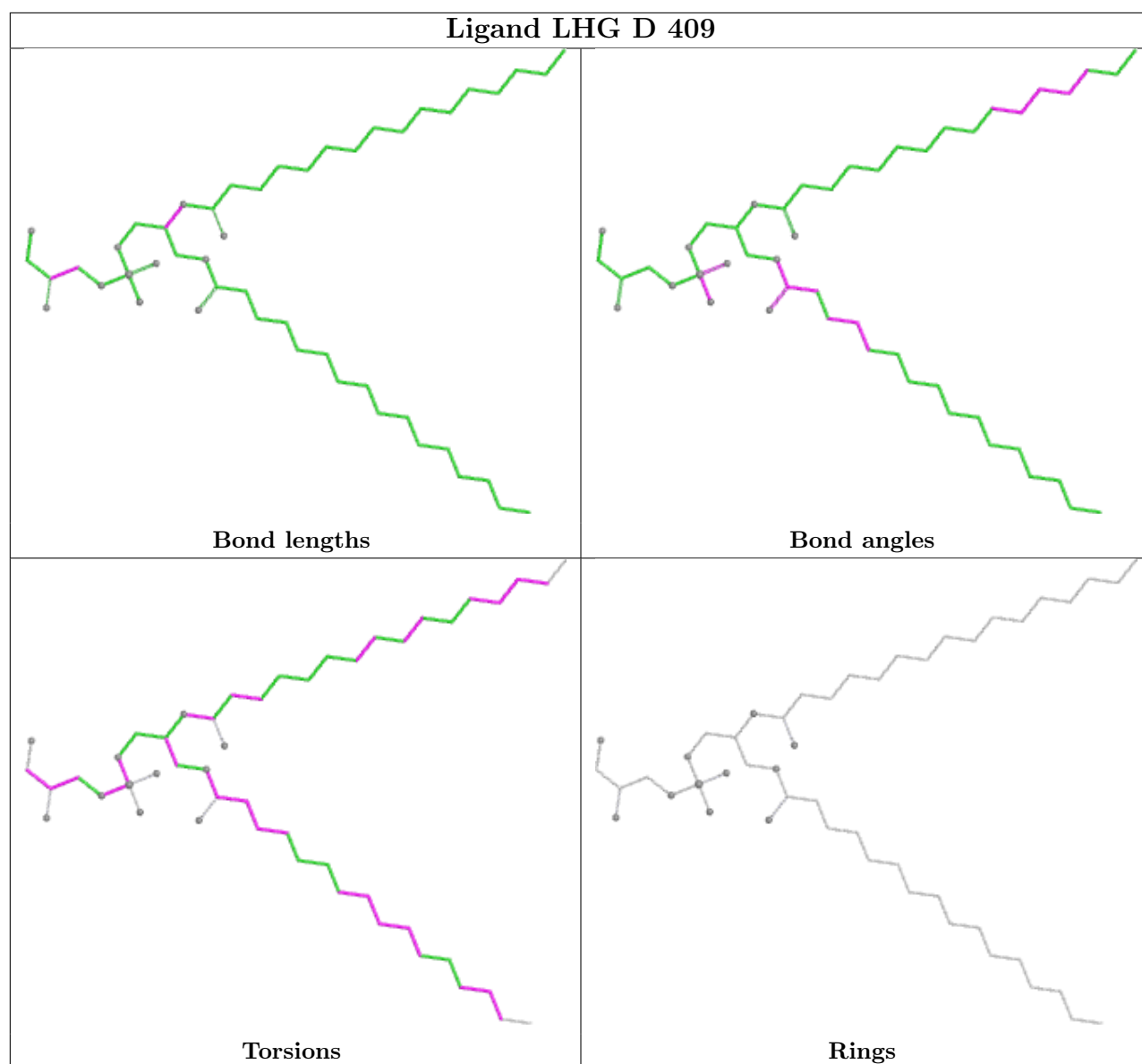


Ligand CLA C 504

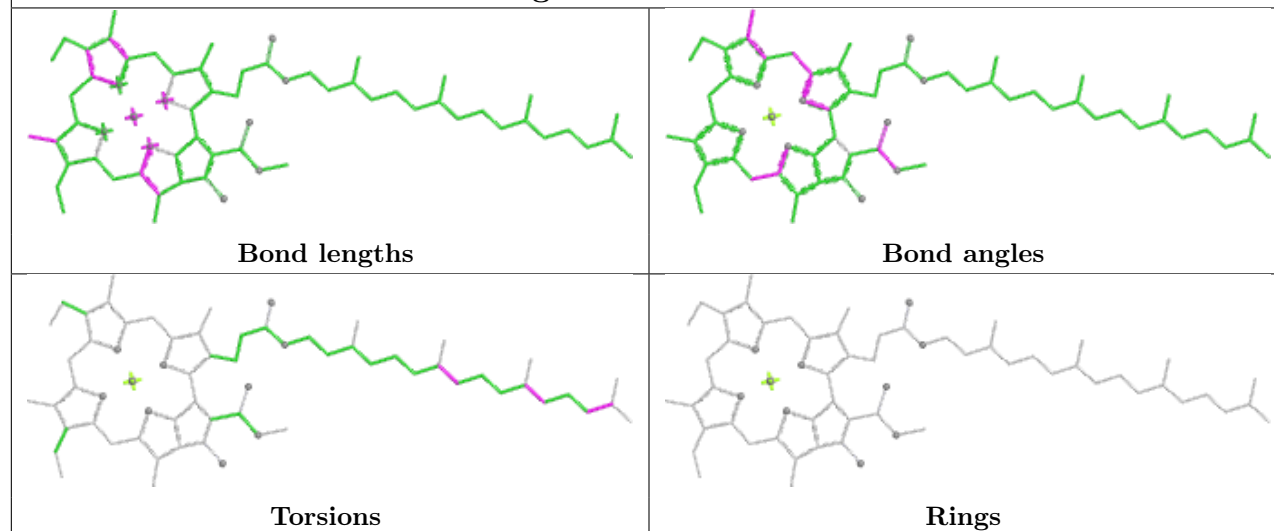


Ligand STE m 102

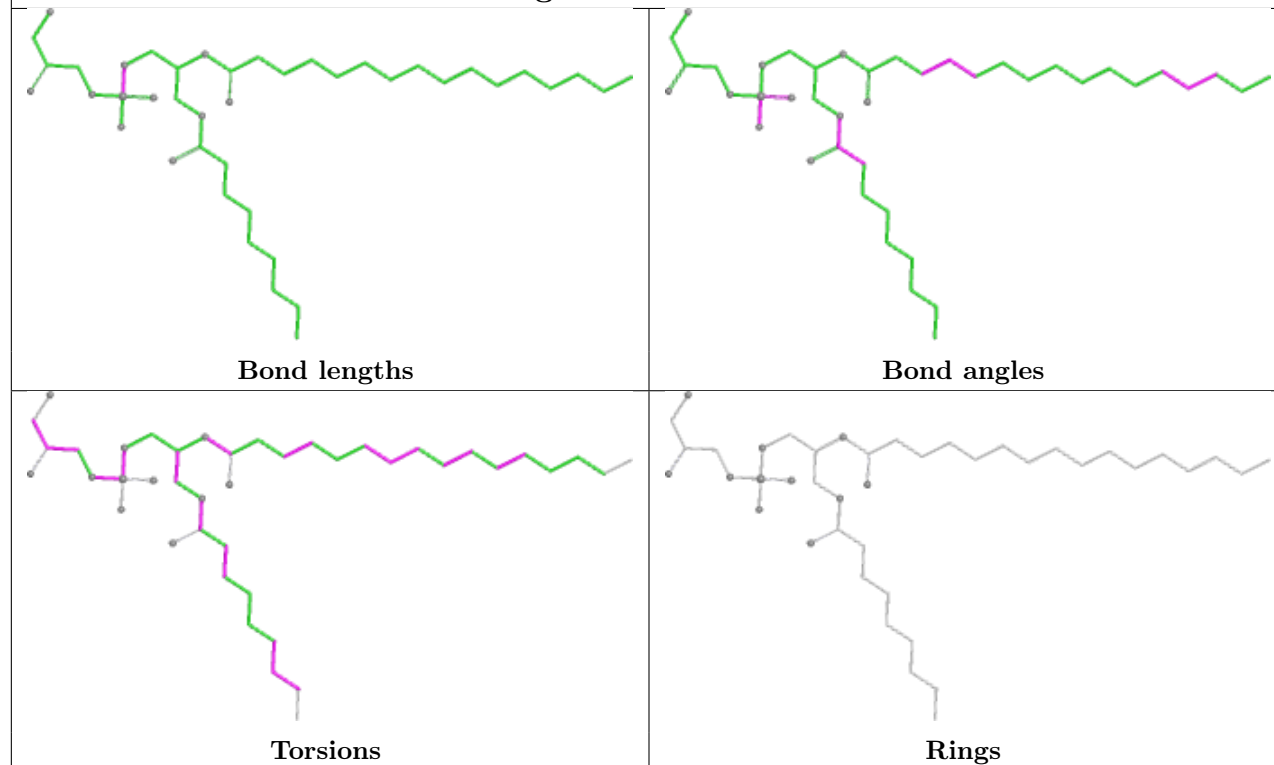




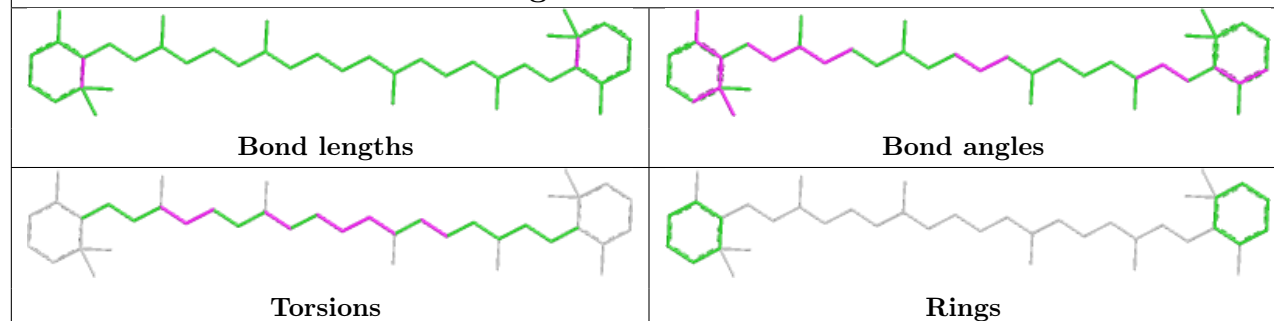
Ligand CLA C 508

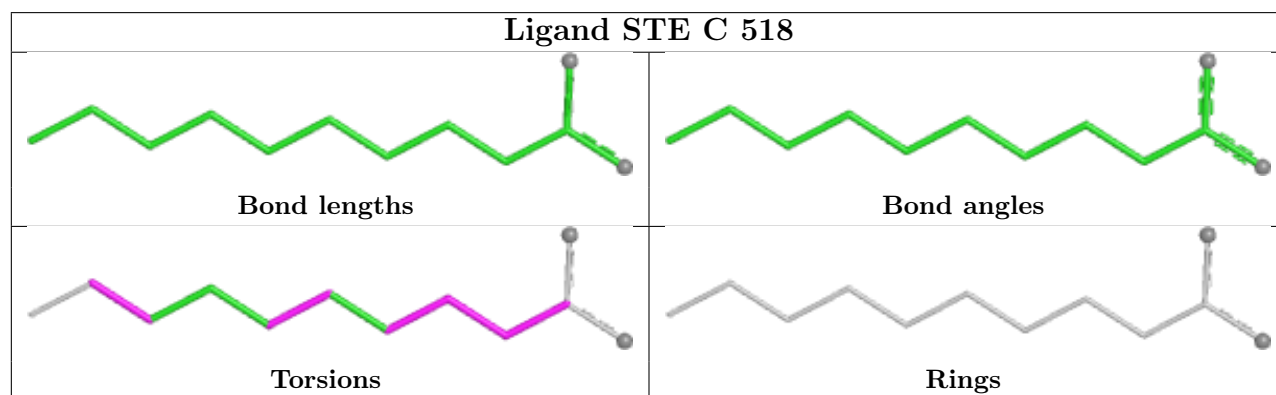
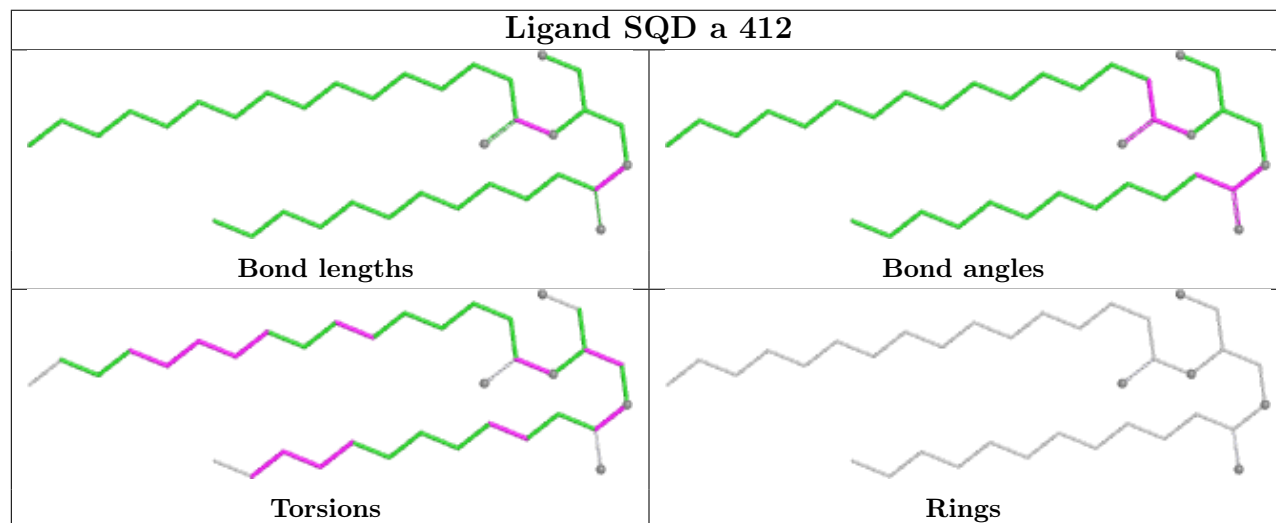
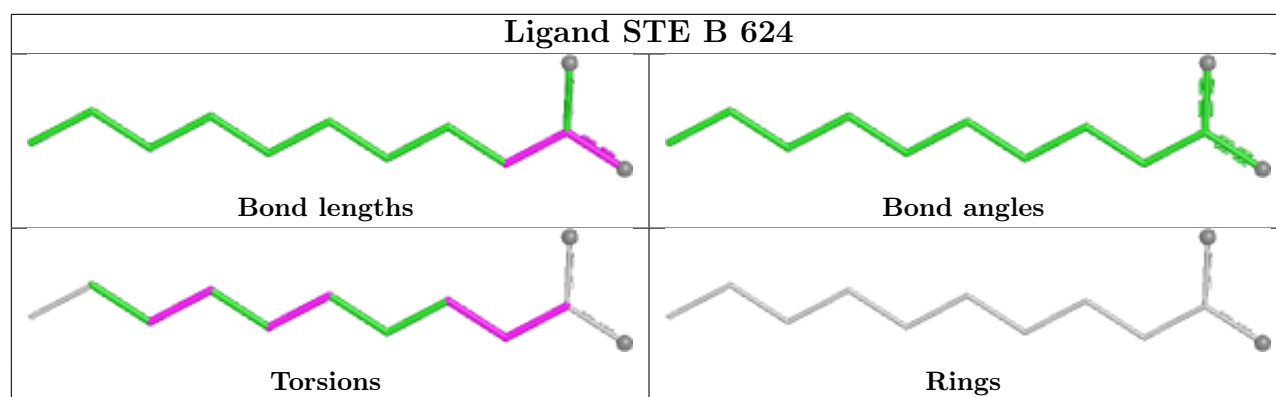


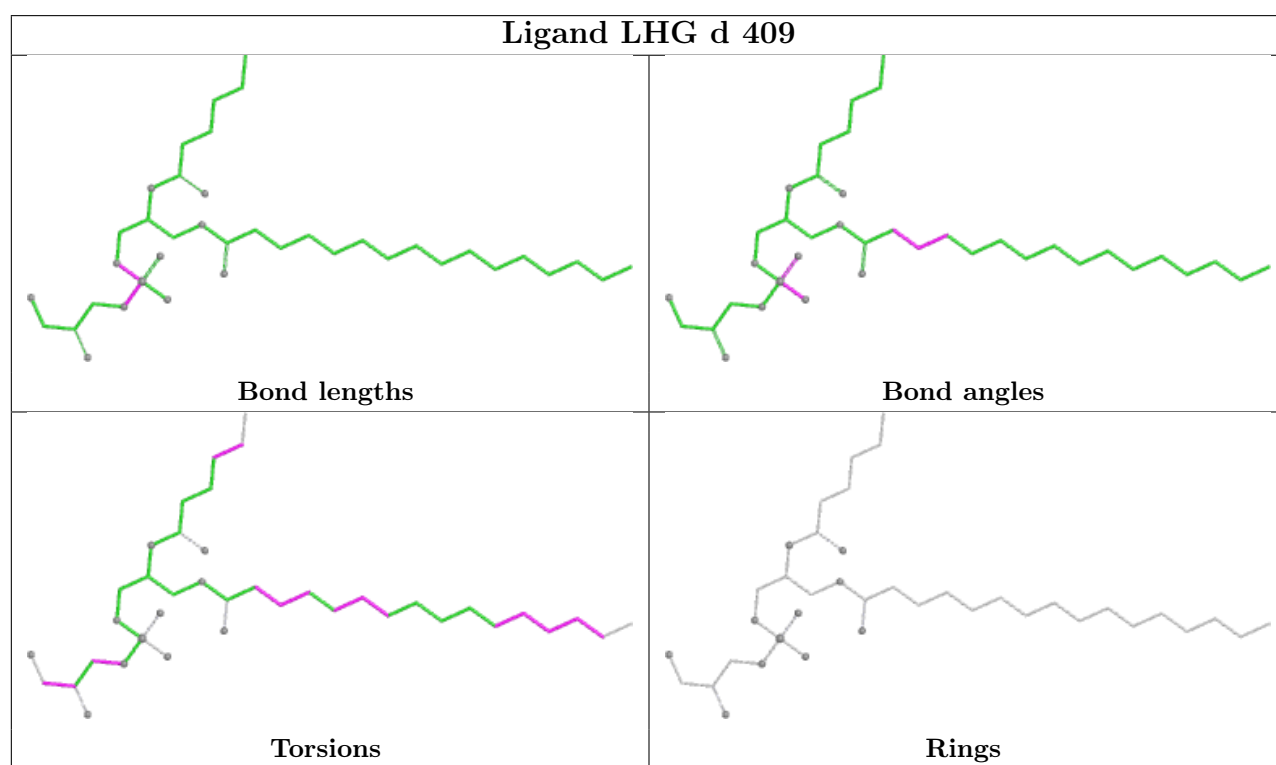
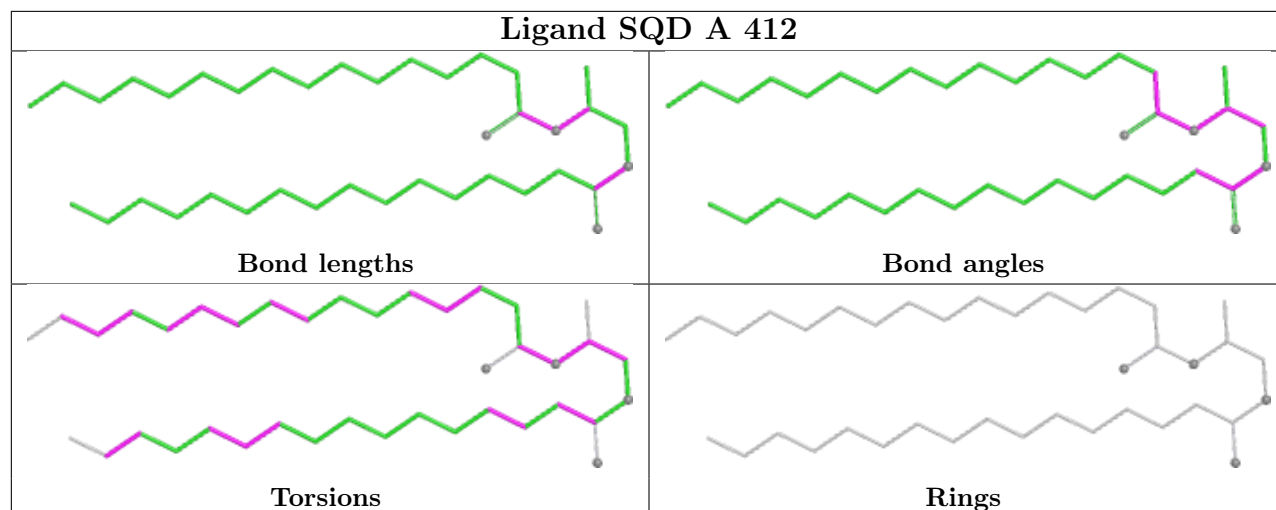
Ligand LHG e 101



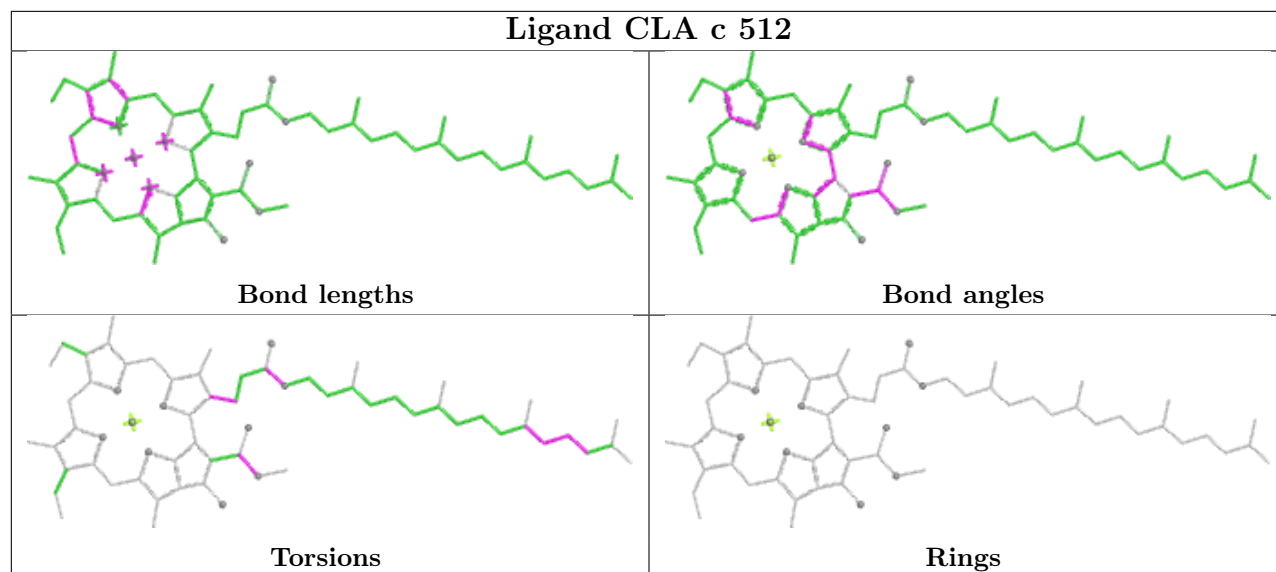
Ligand BCR K 101



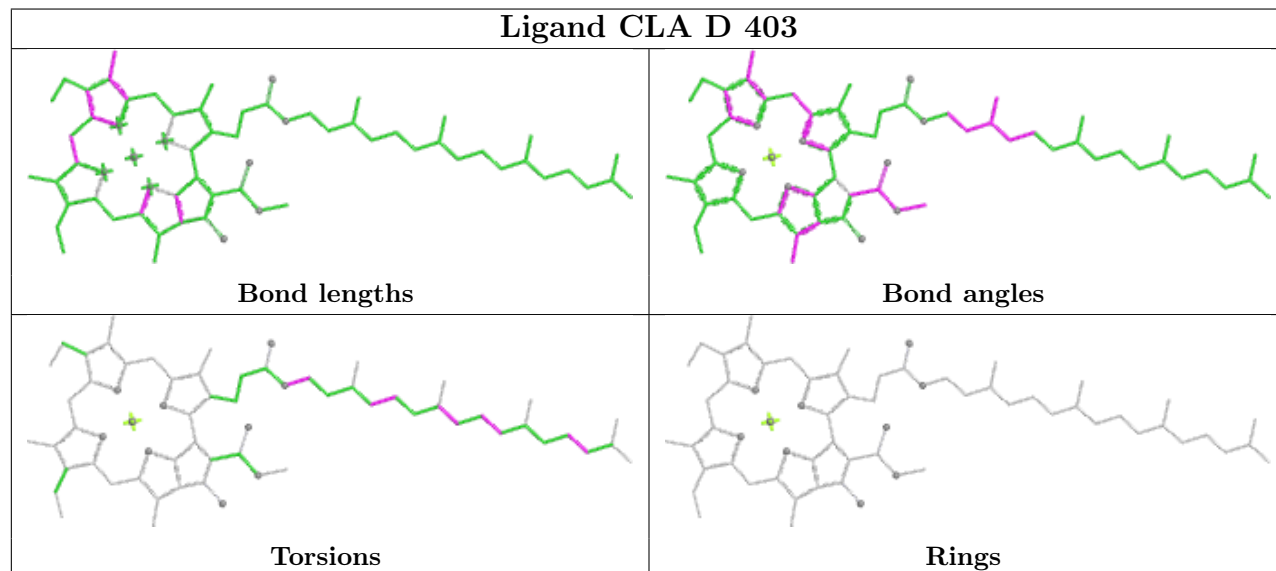




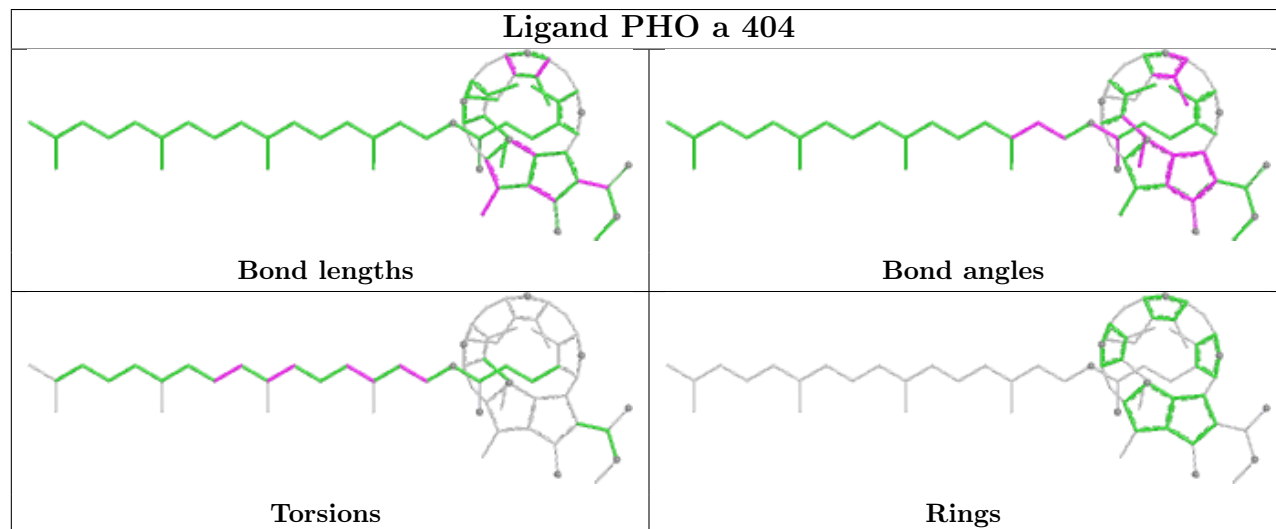
Ligand CLA c 512

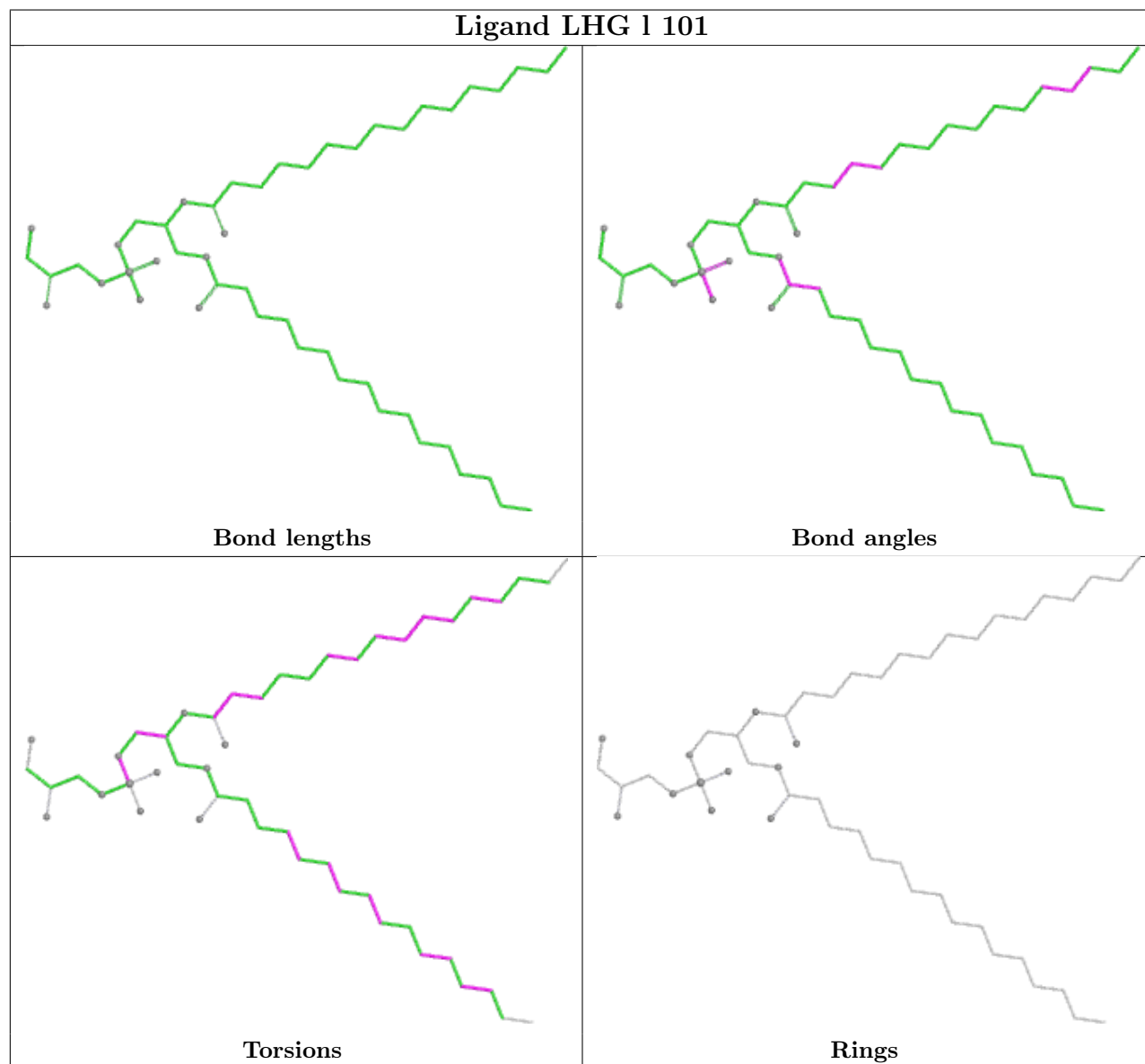
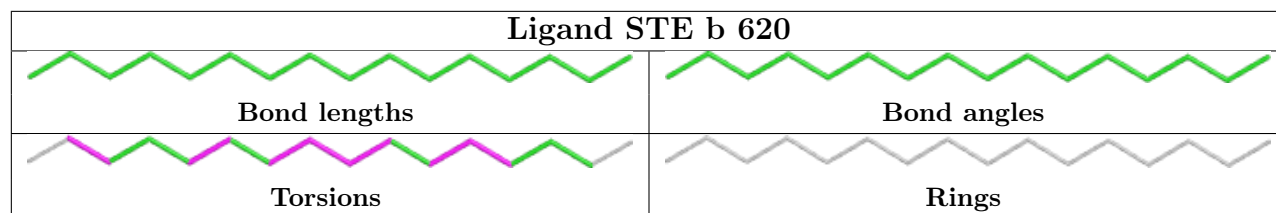


Ligand CLA D 403

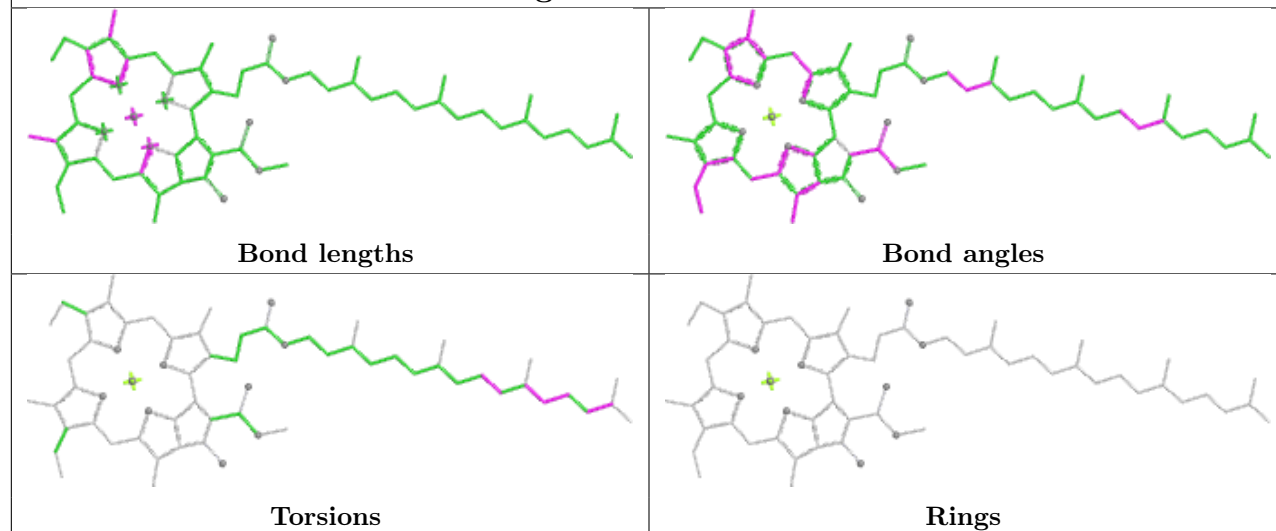


Ligand PHO a 404

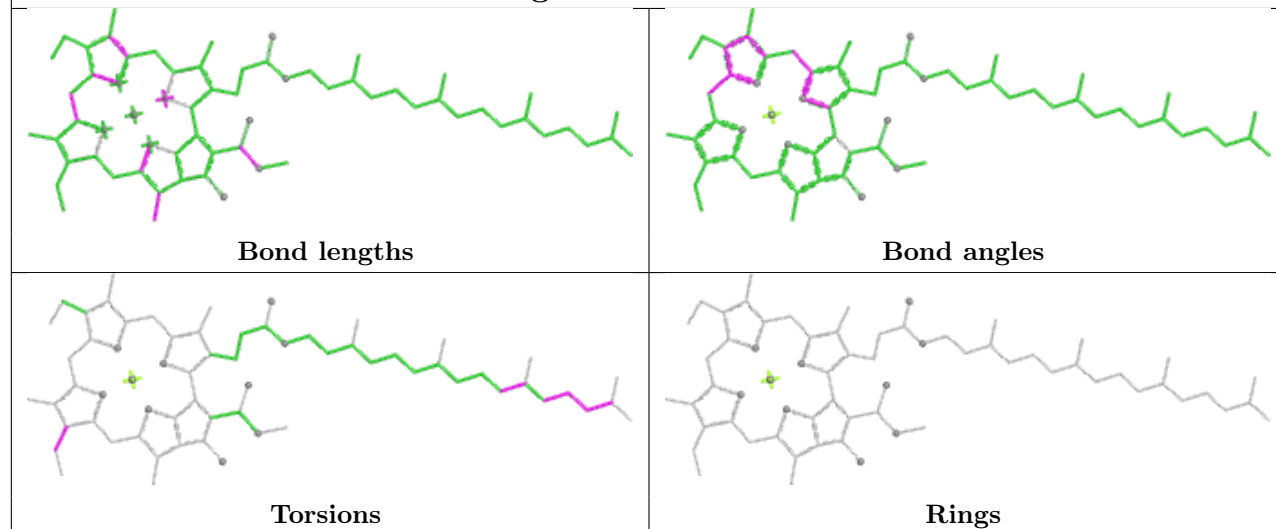




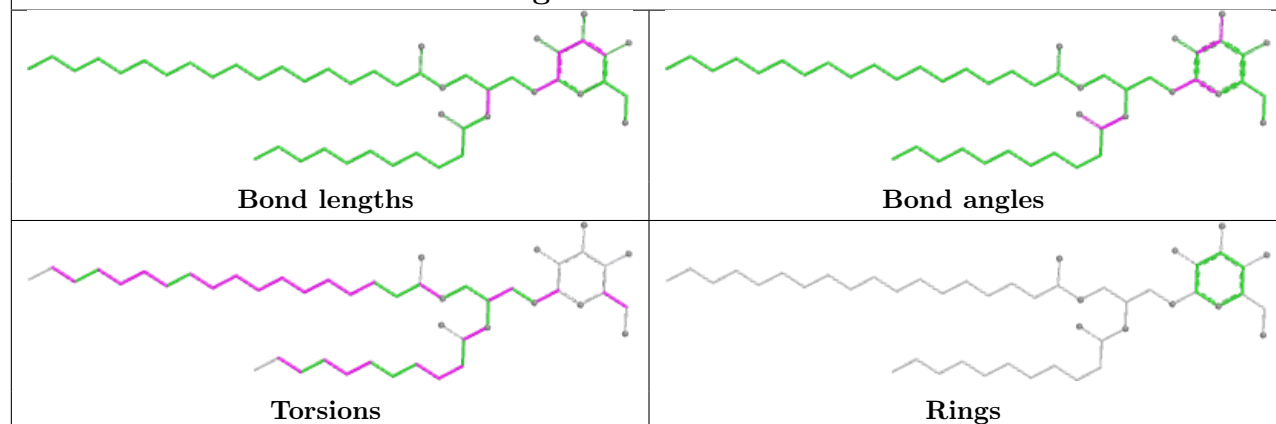
Ligand CLA b 612

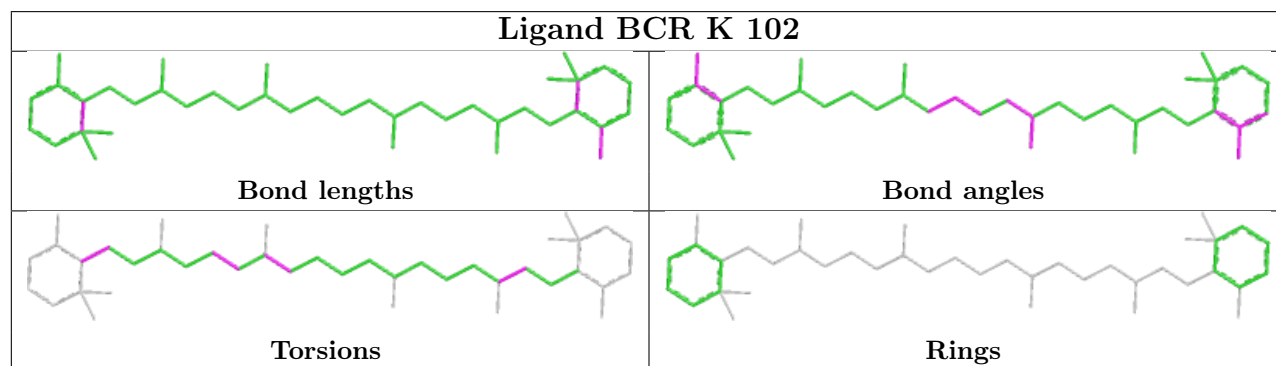
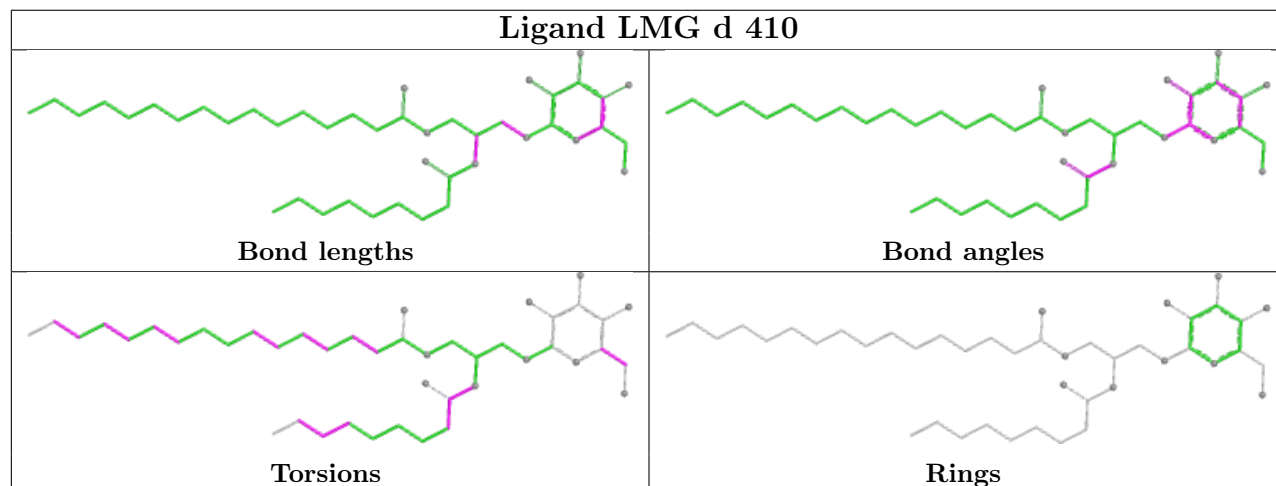
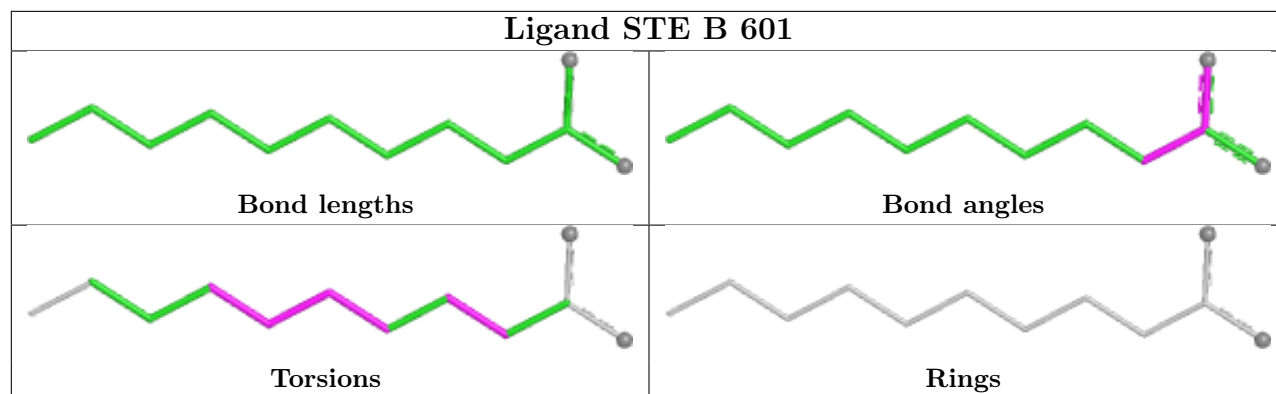


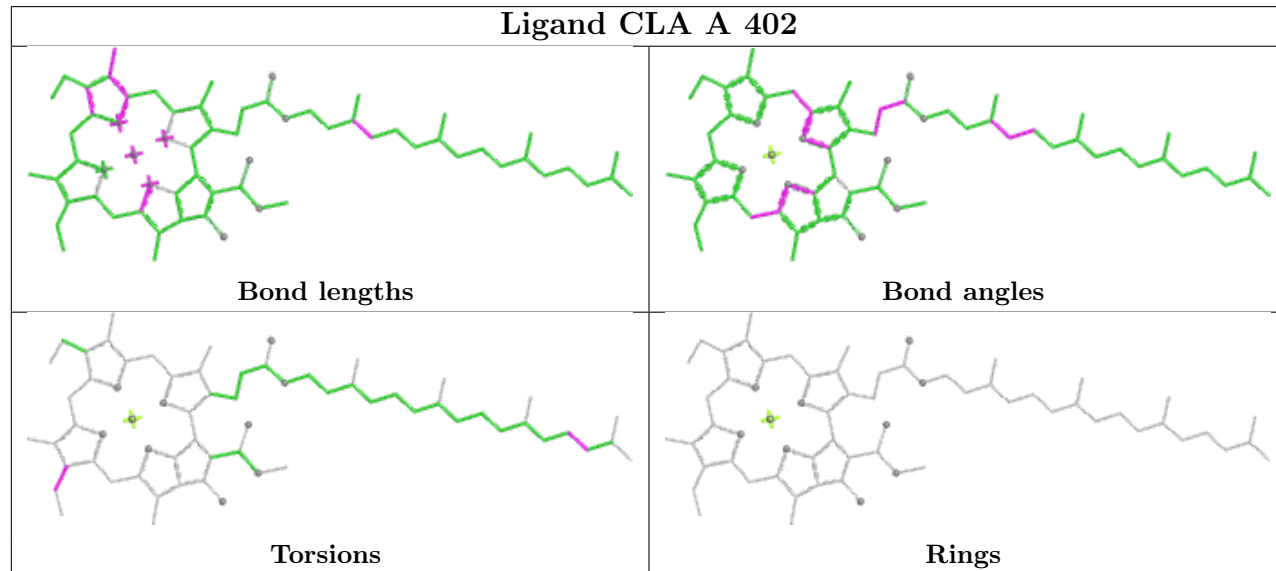
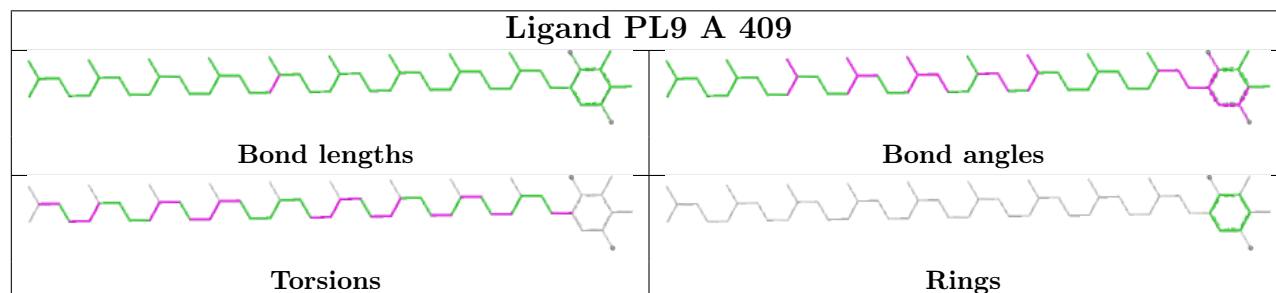
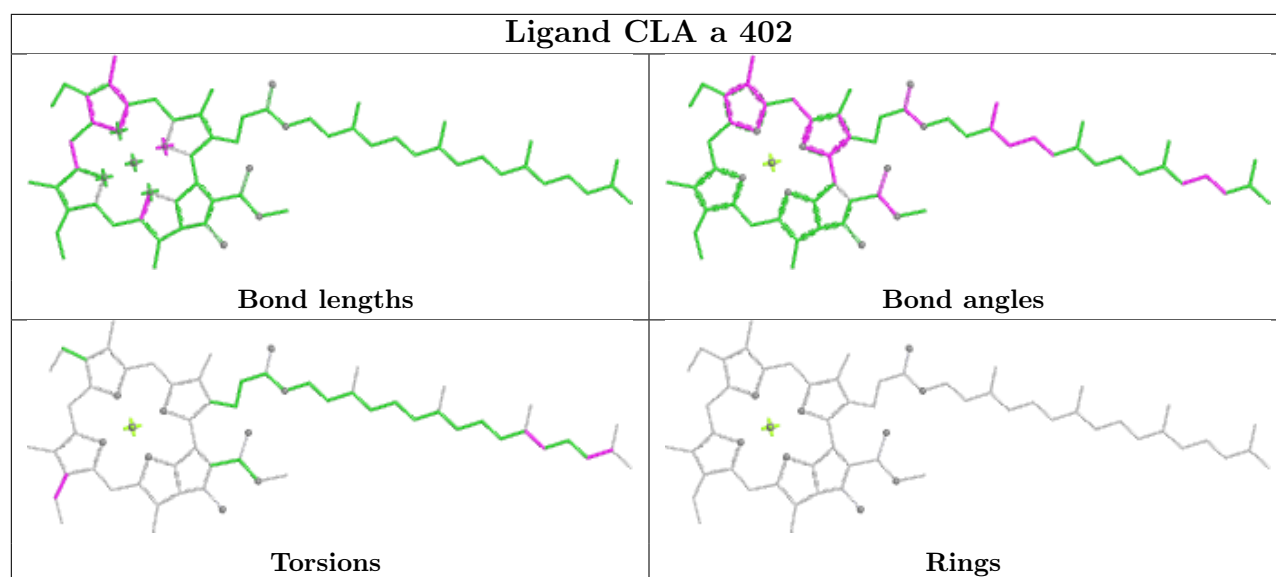
Ligand CLA D 404



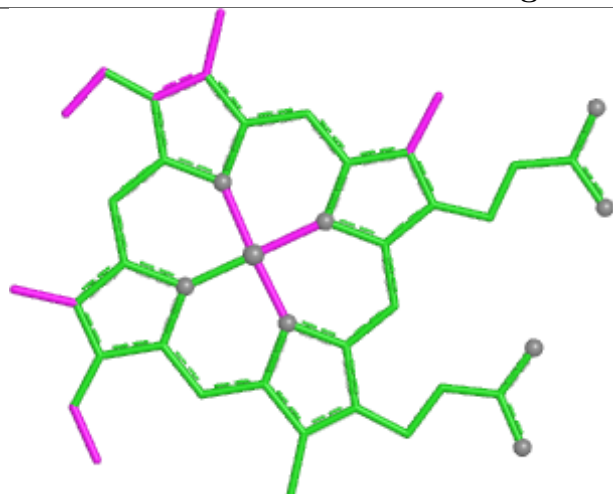
Ligand LMG c 522



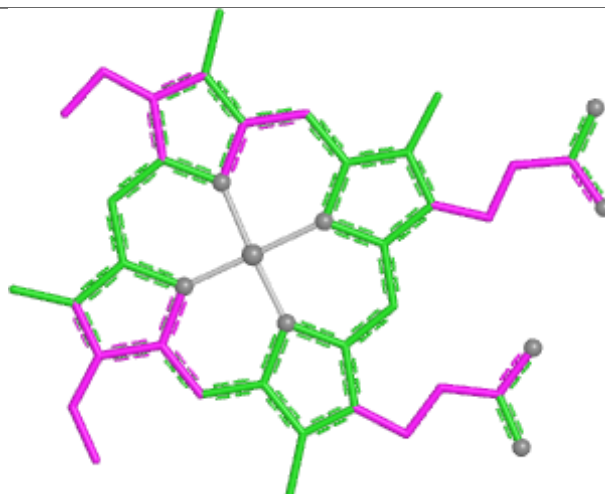




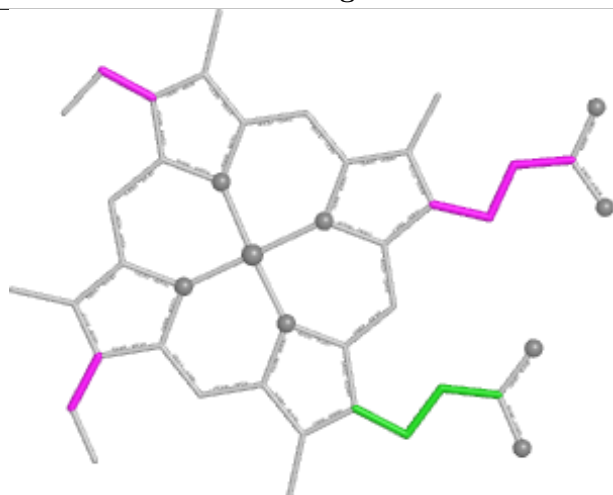
Ligand HEC f 101



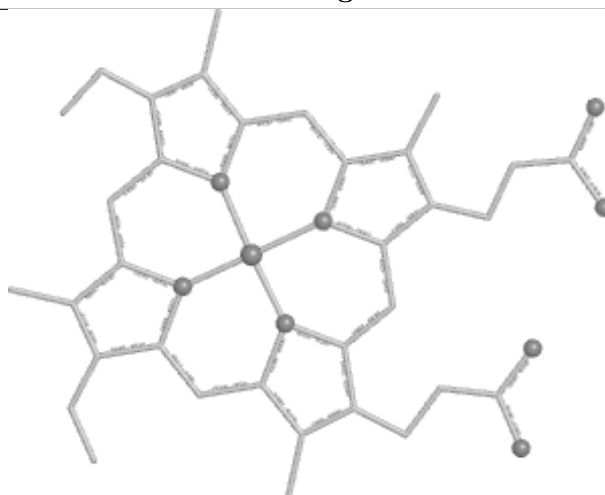
Bond lengths



Bond angles

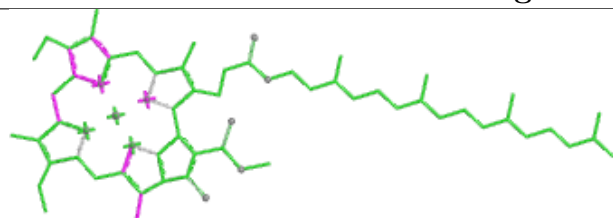


Torsions

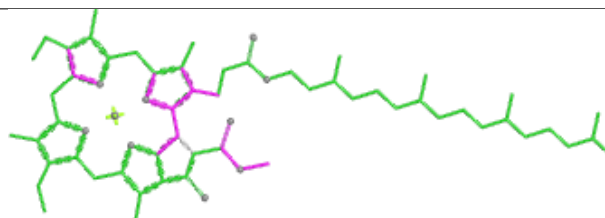


Rings

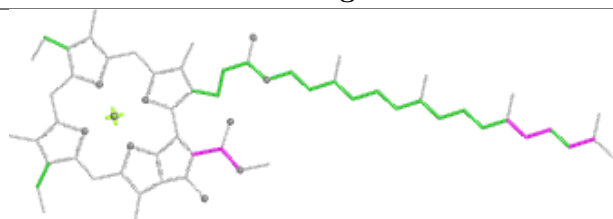
Ligand CLA C 502



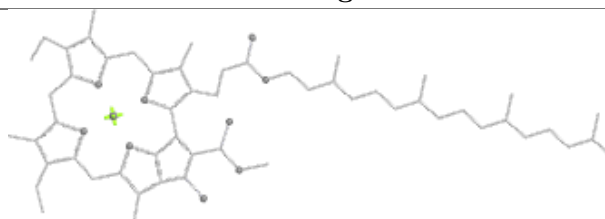
Bond lengths



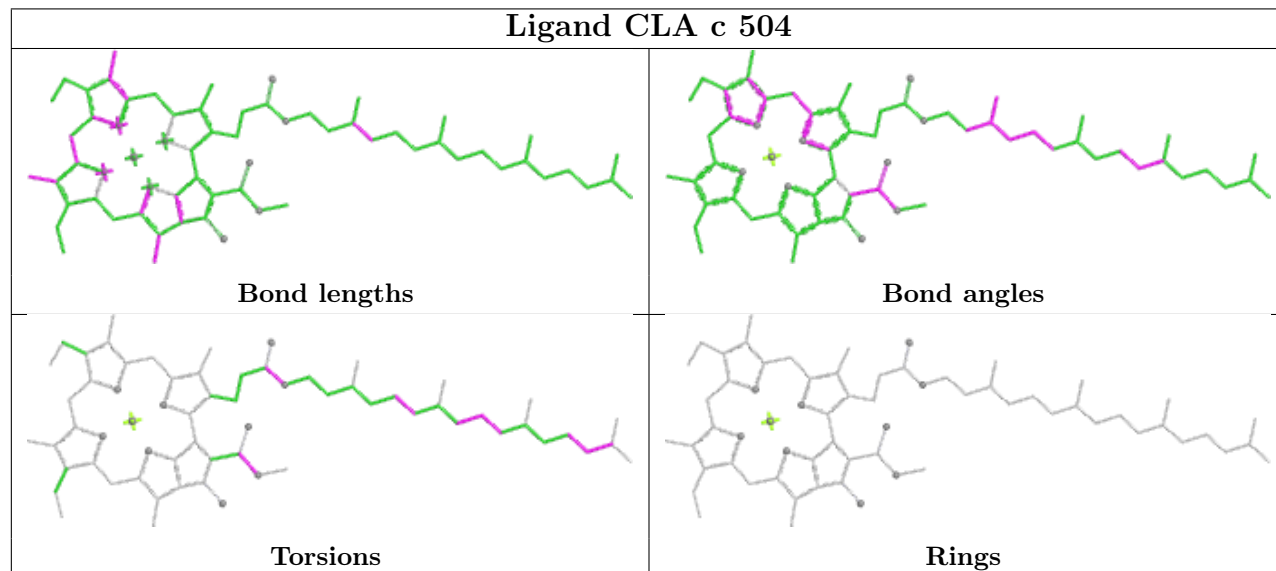
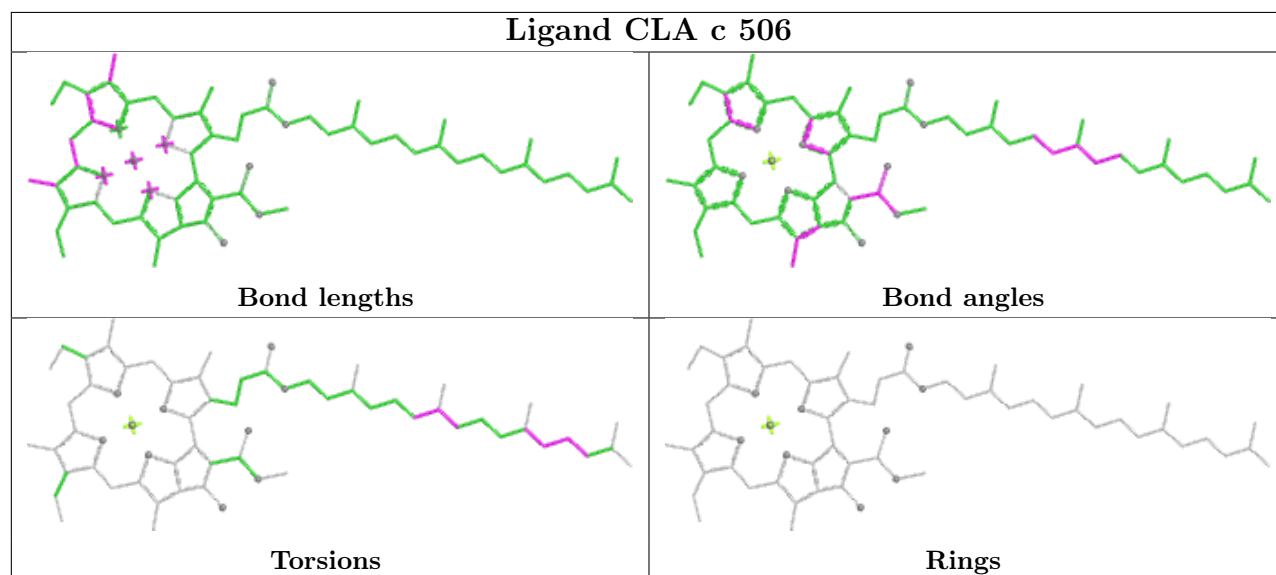
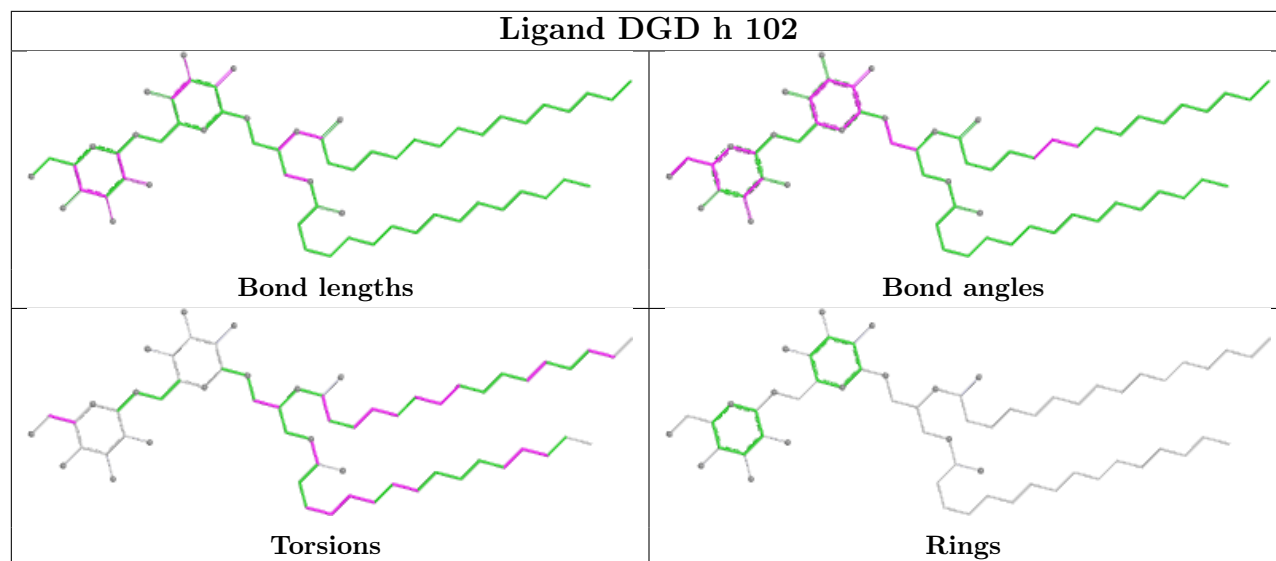
Bond angles

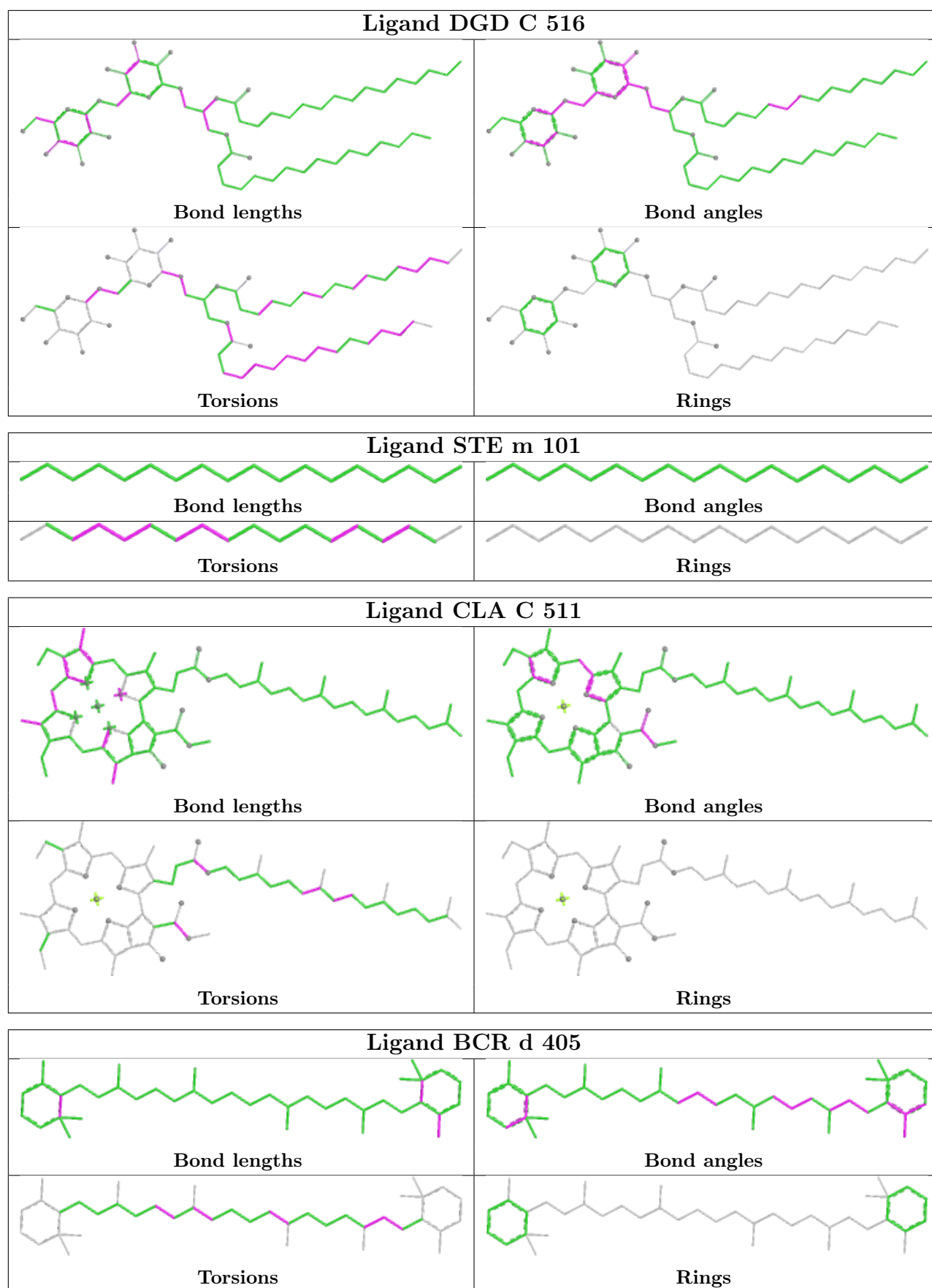


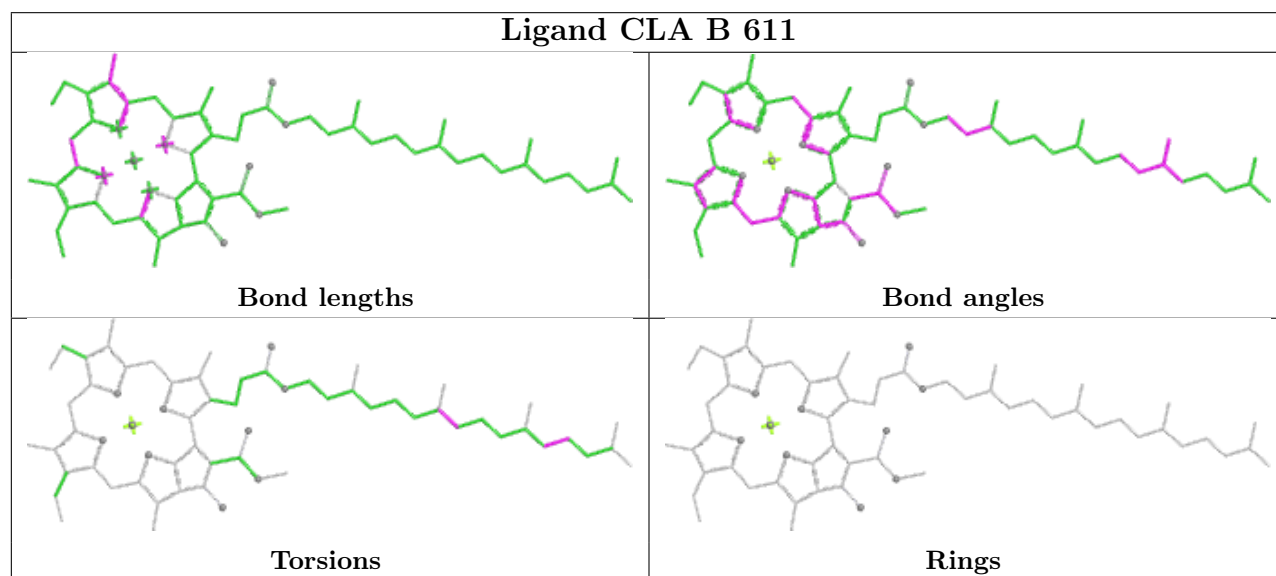
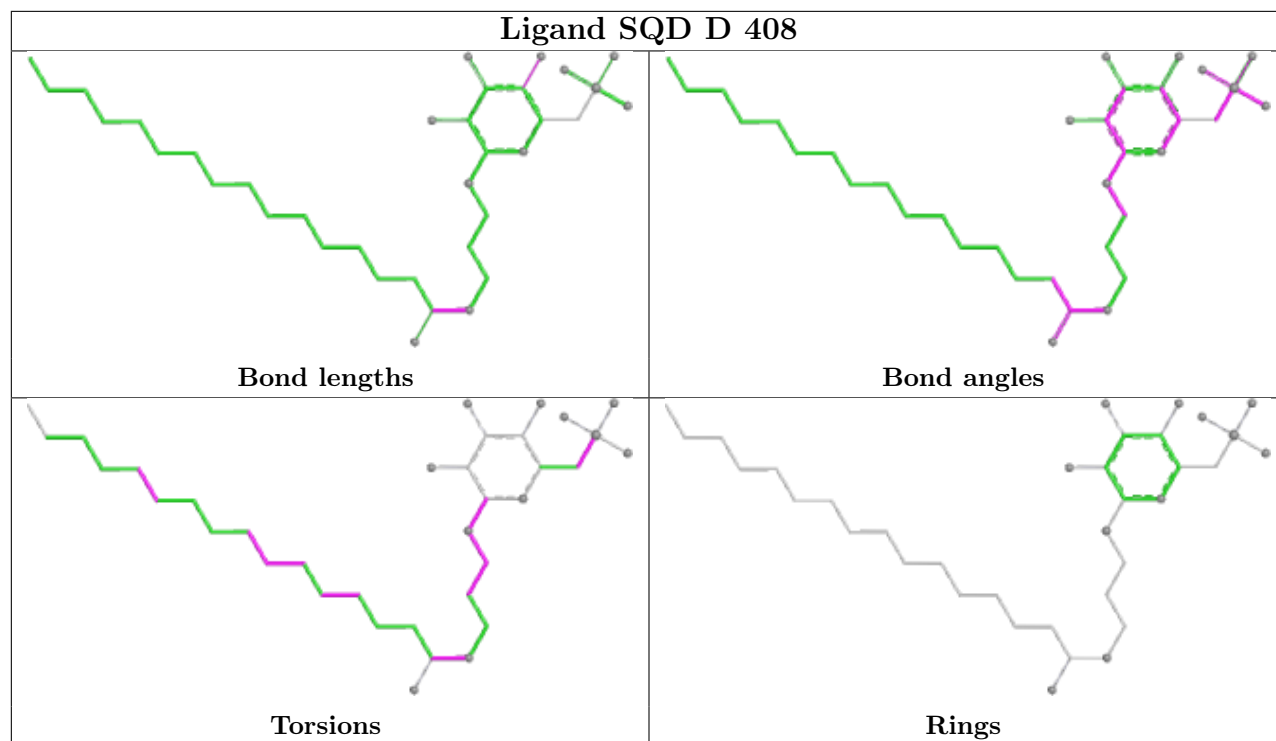
Torsions

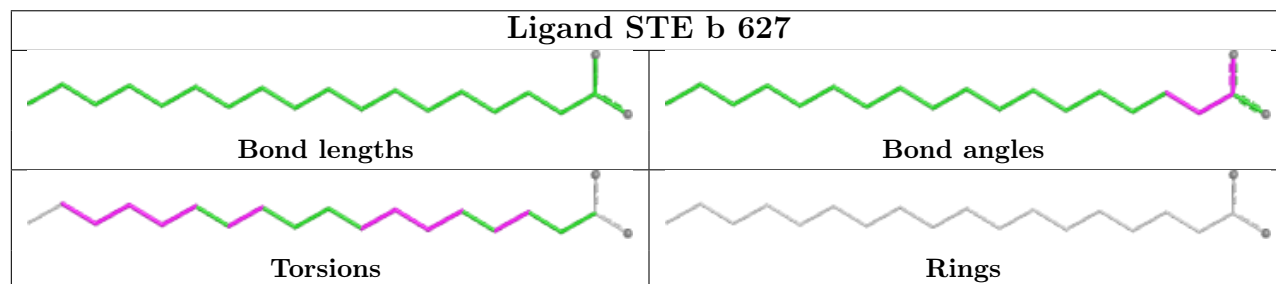
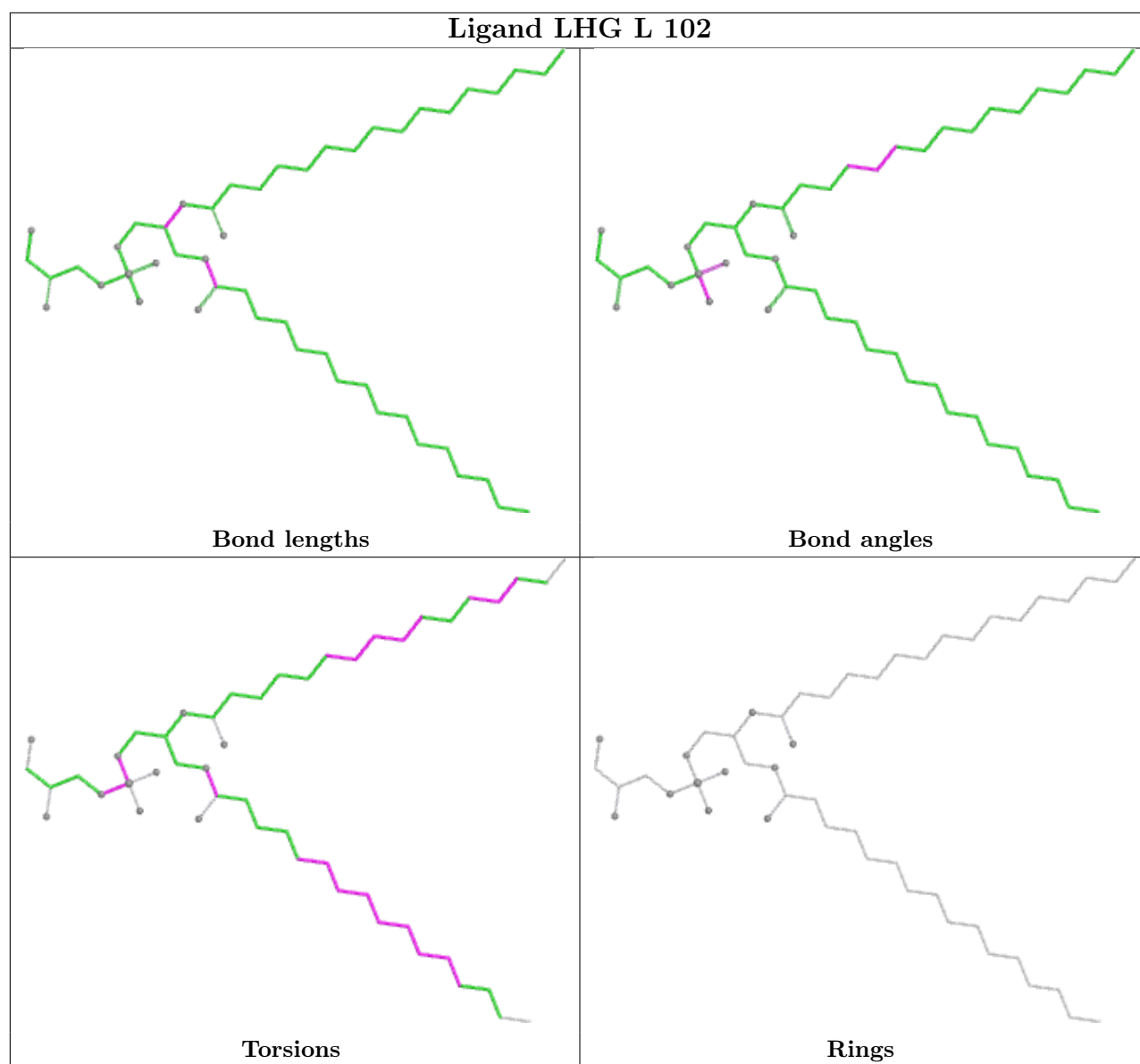


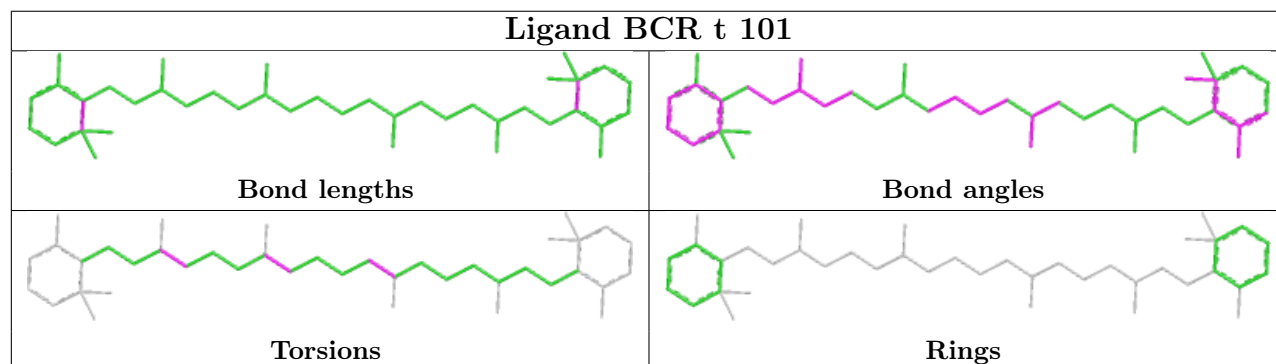
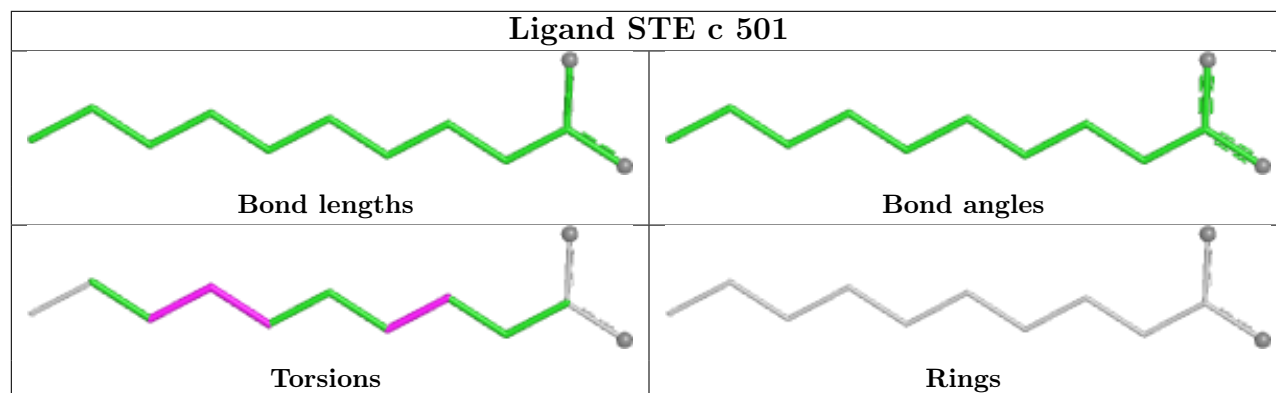
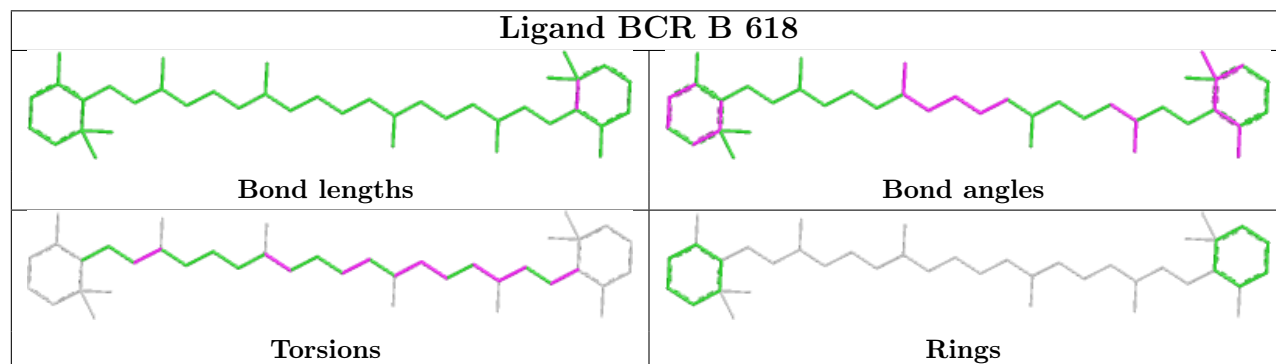
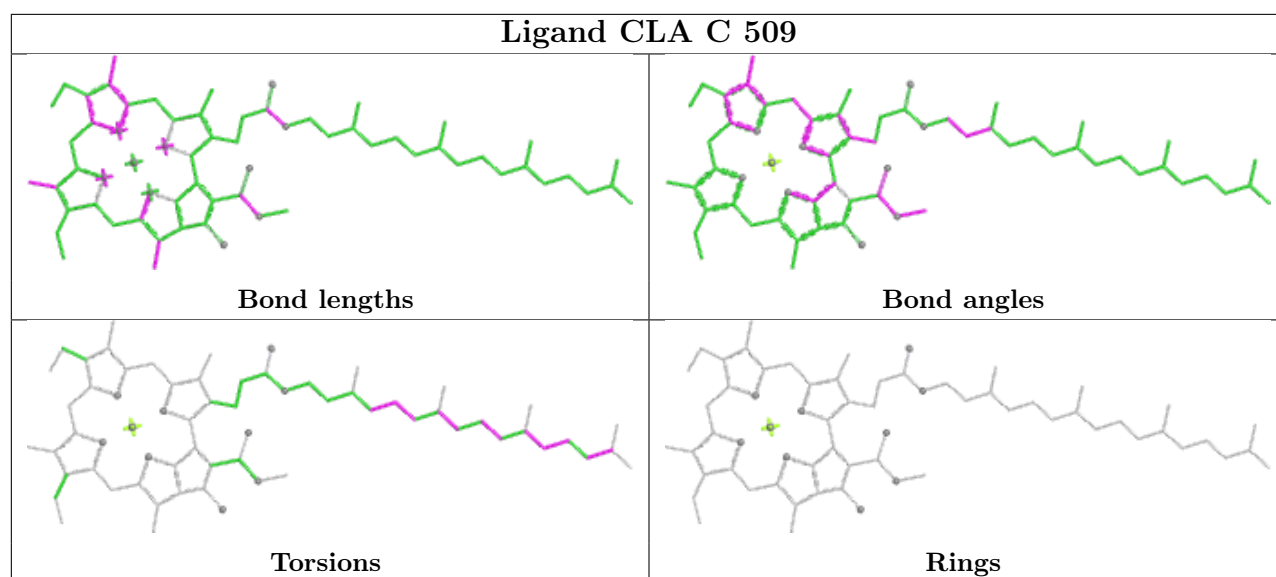
Rings



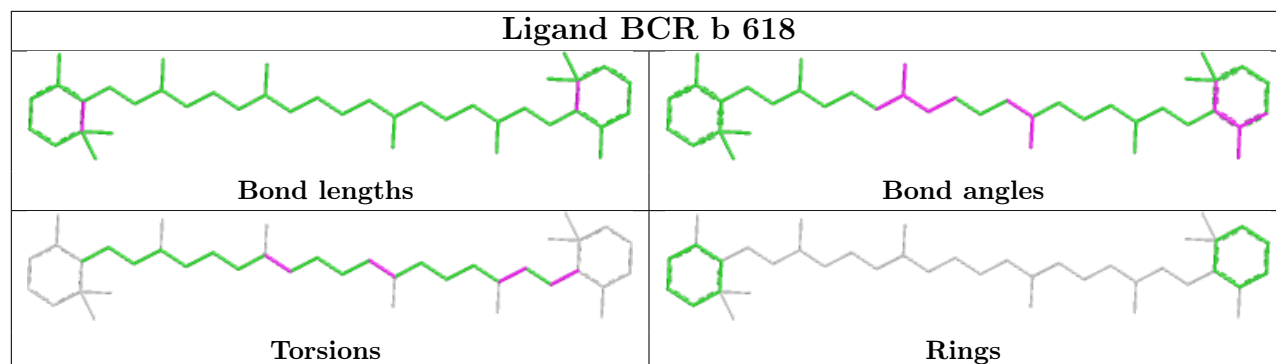




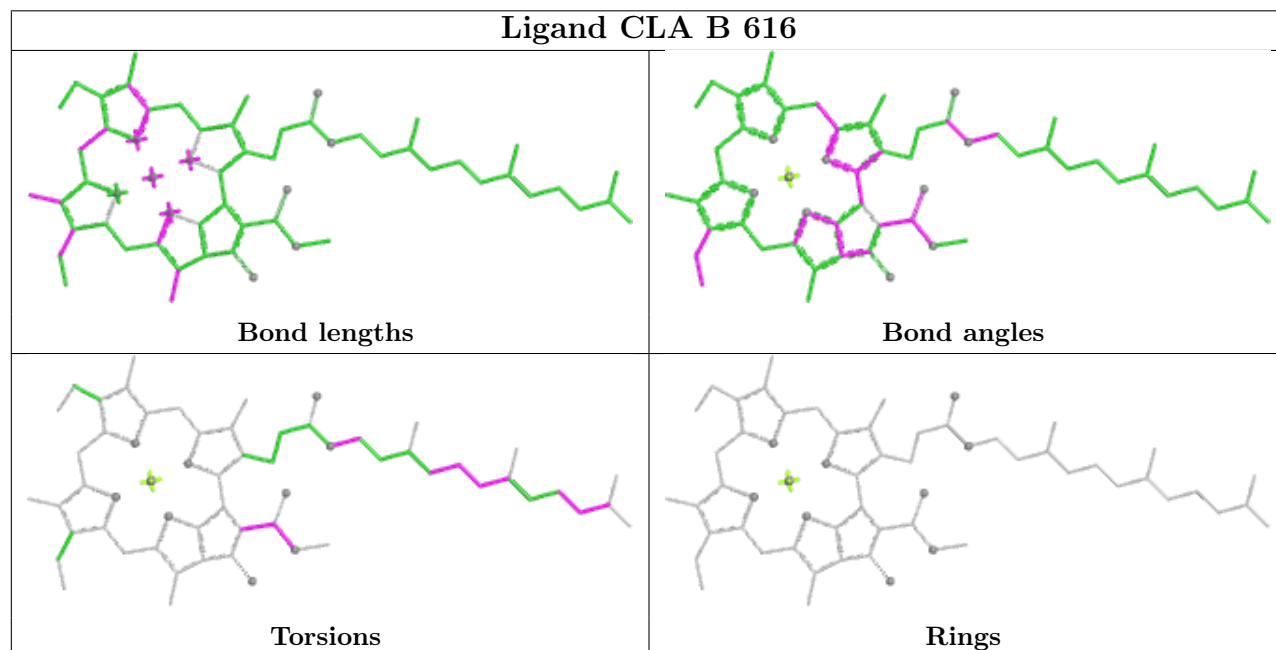




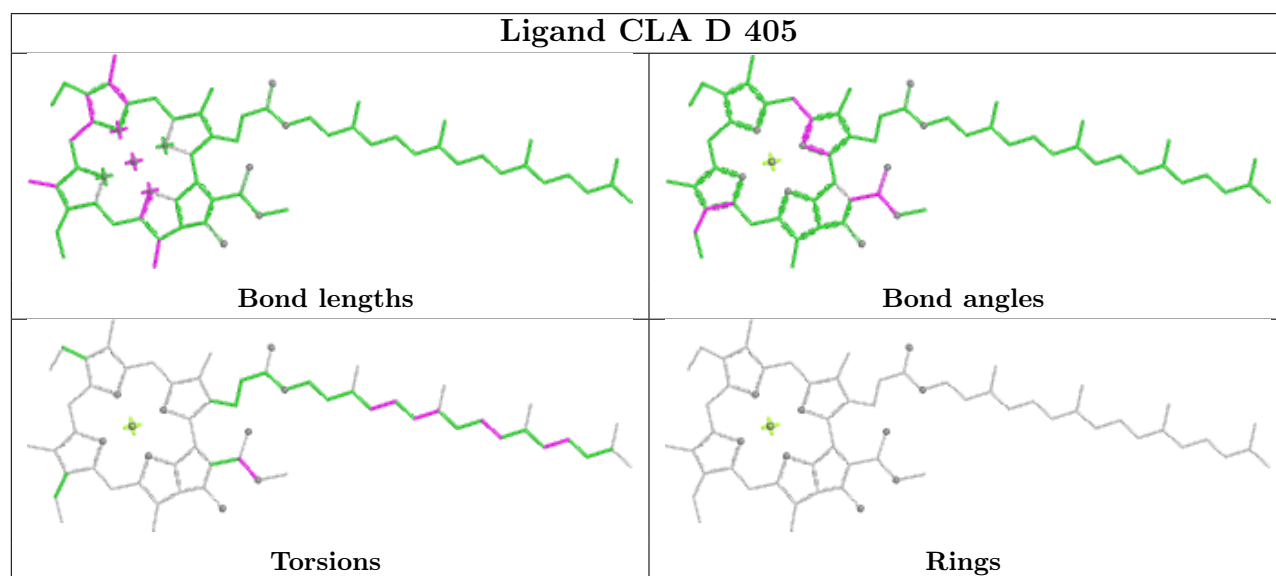
Ligand BCR b 618

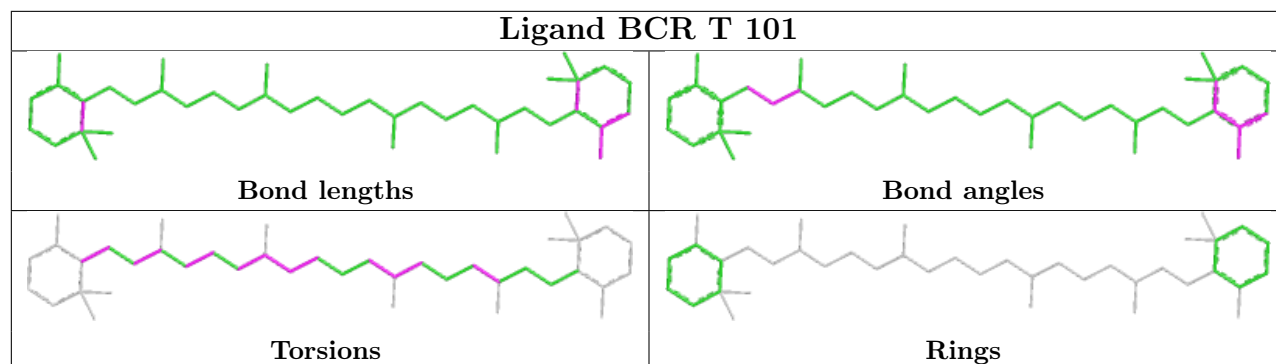
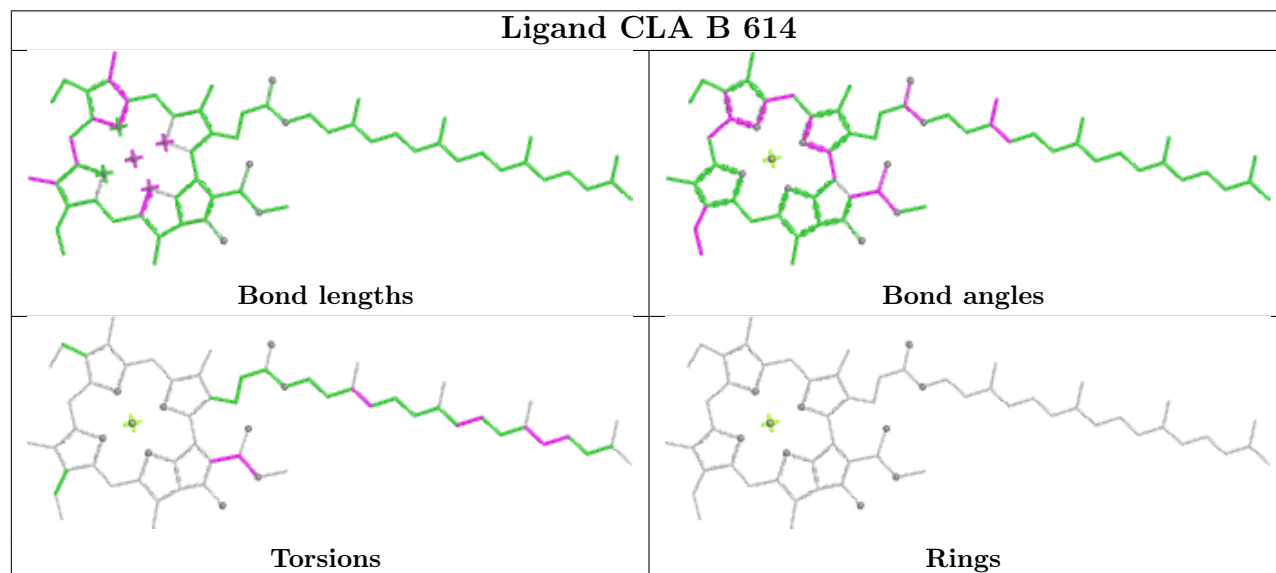
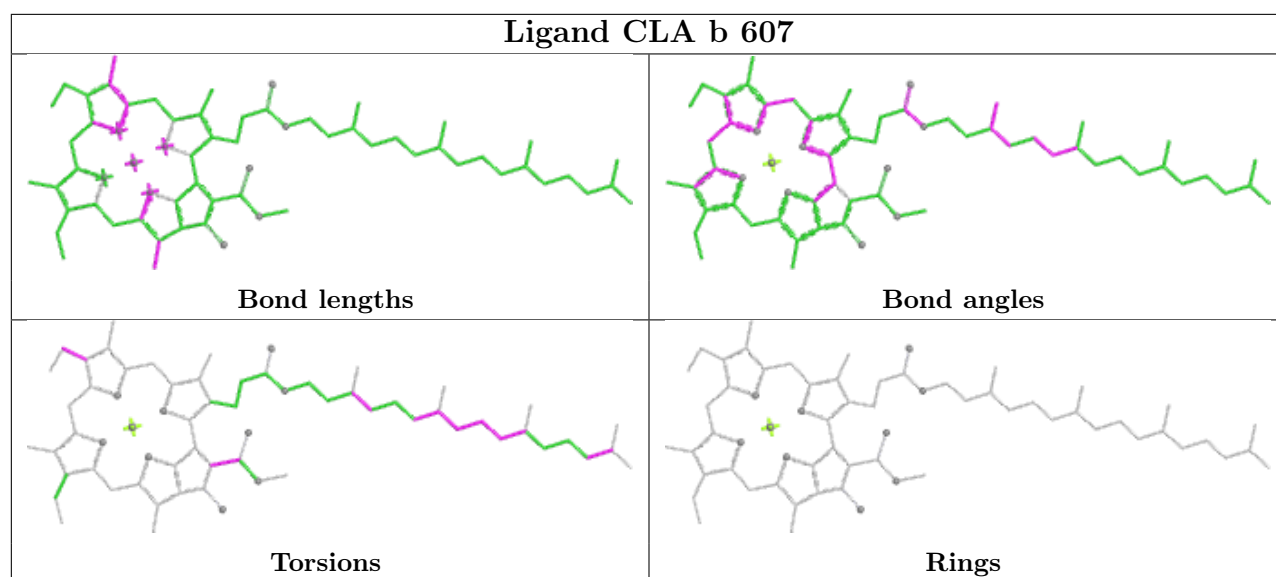


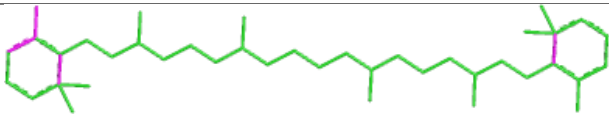
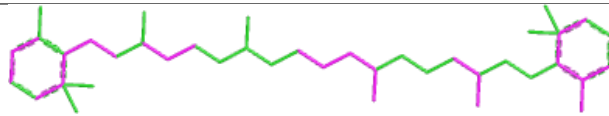
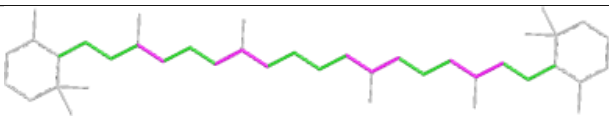
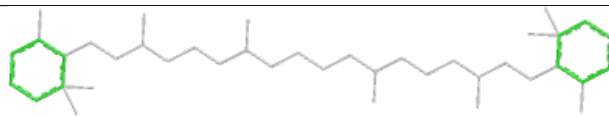
Ligand CLA B 616

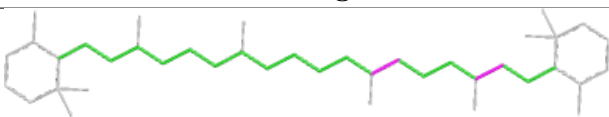
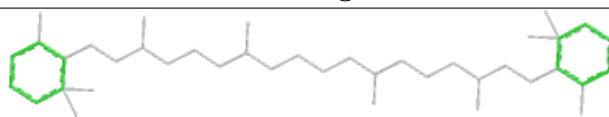


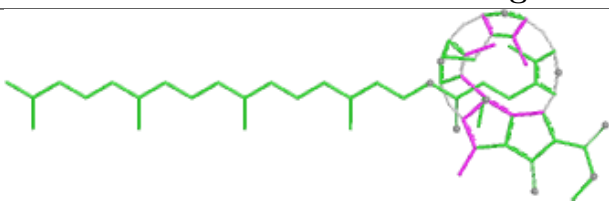
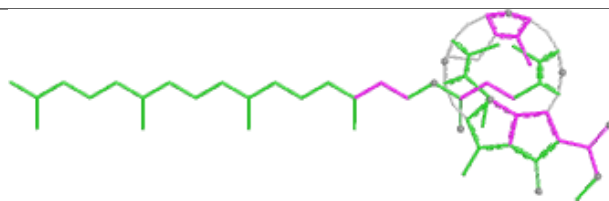
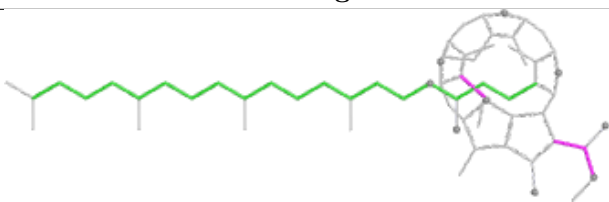
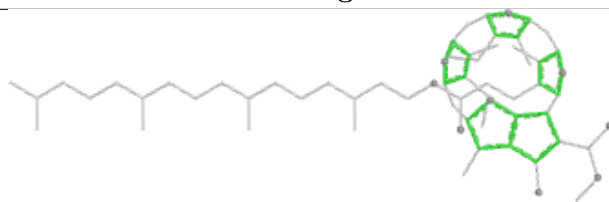
Ligand CLA D 405

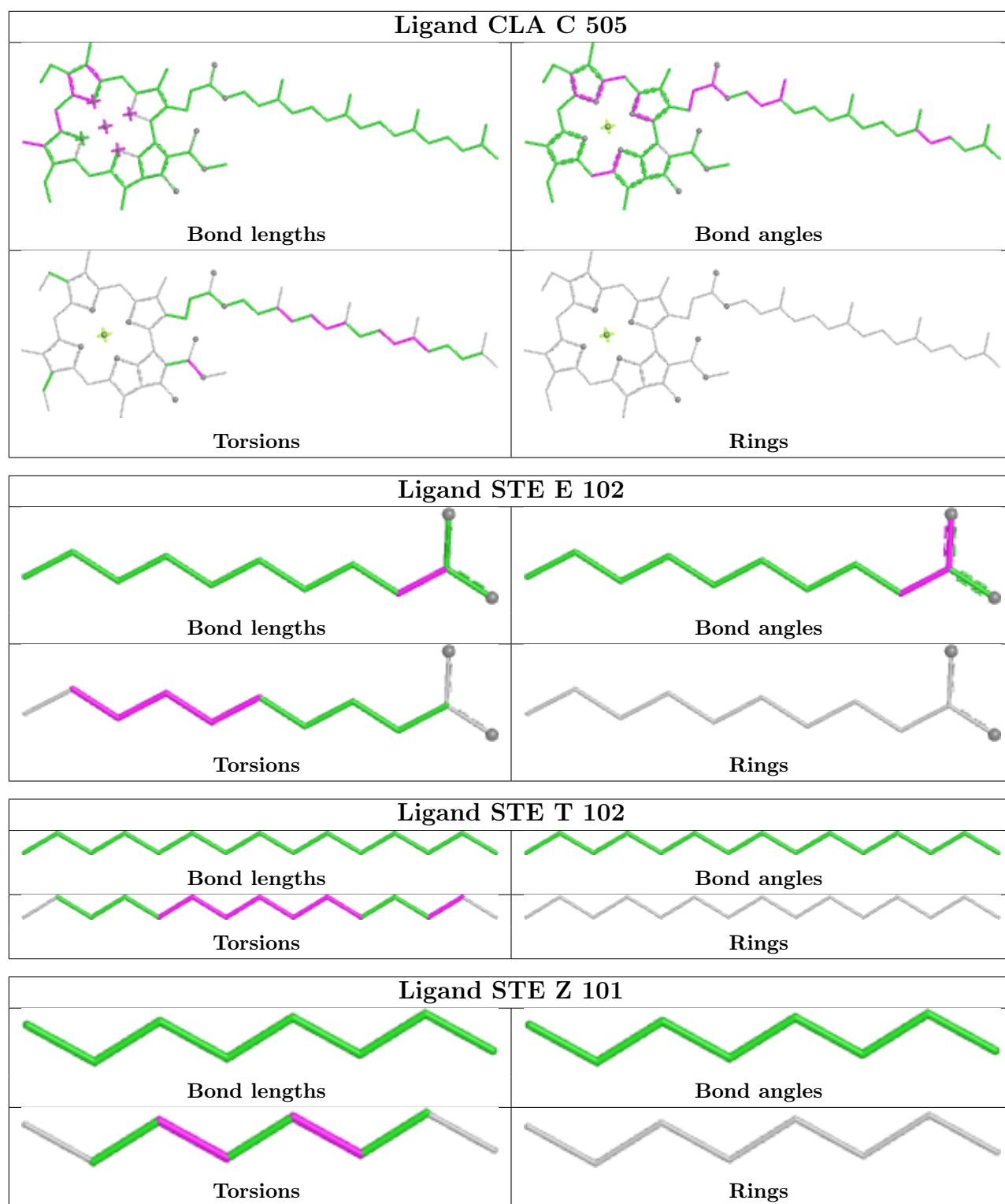


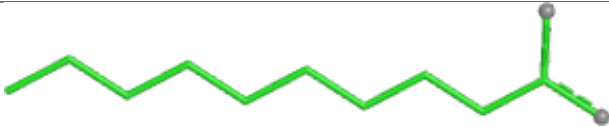
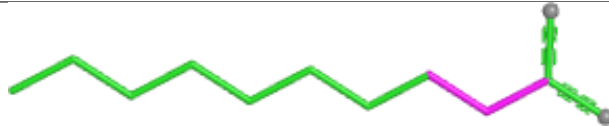
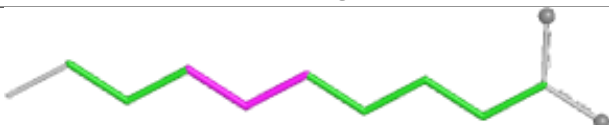
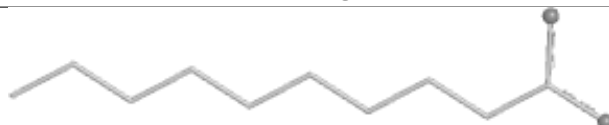


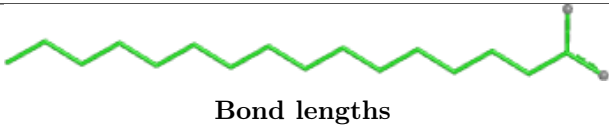
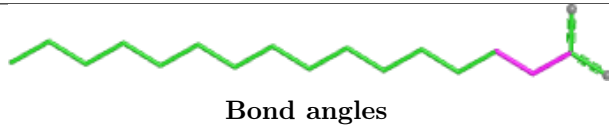
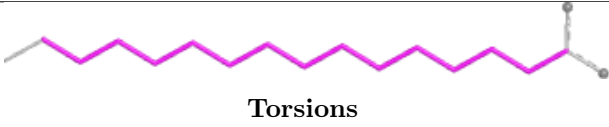
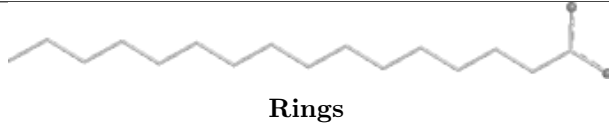
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

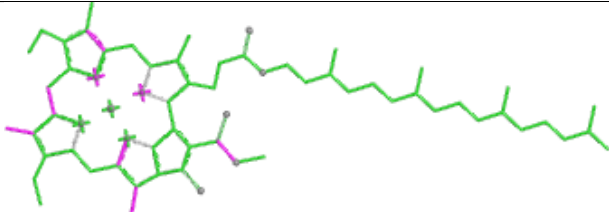
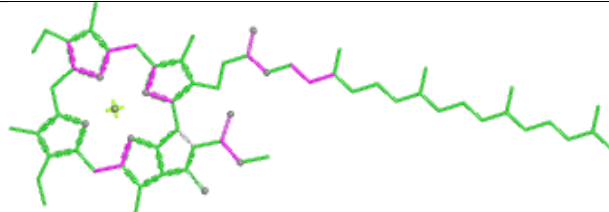
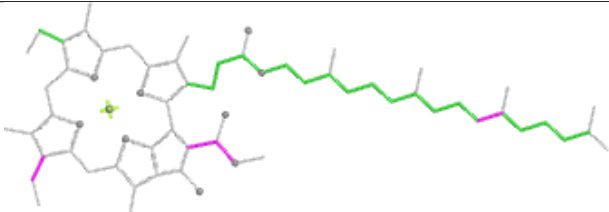
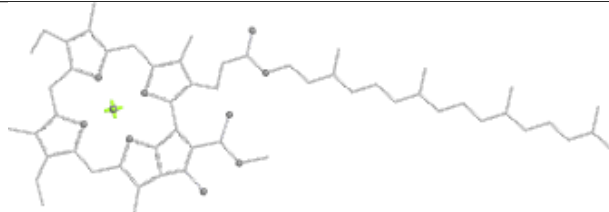
Ligand BCR a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

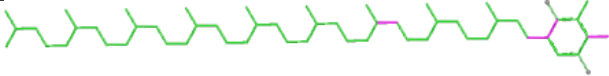
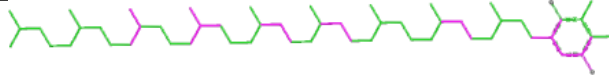
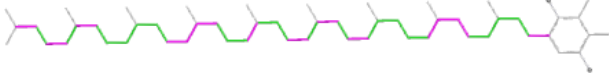
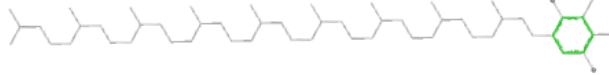
Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings



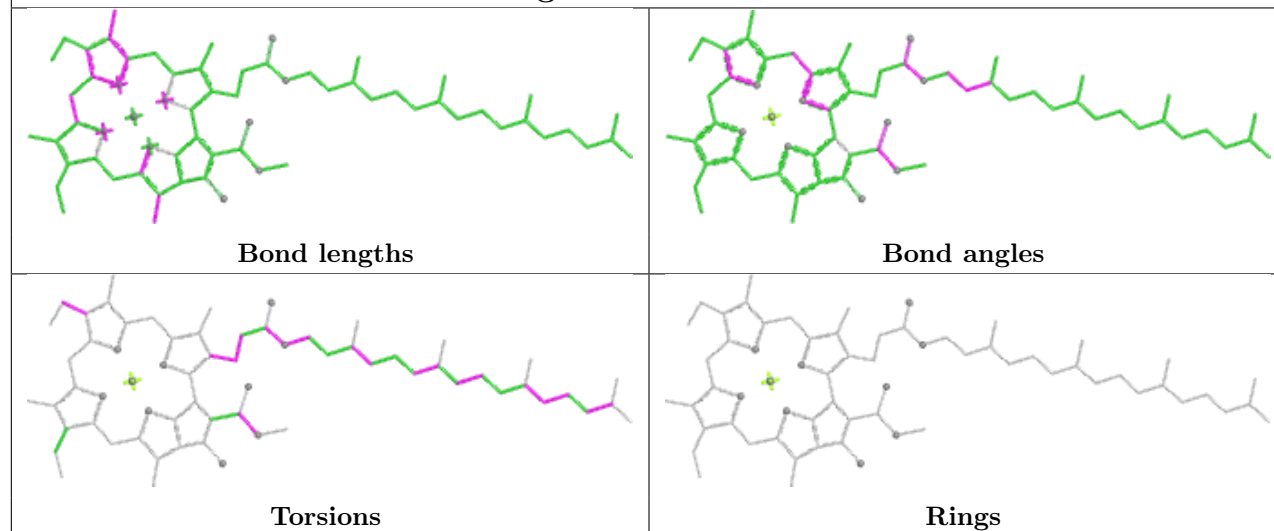
Ligand STE C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

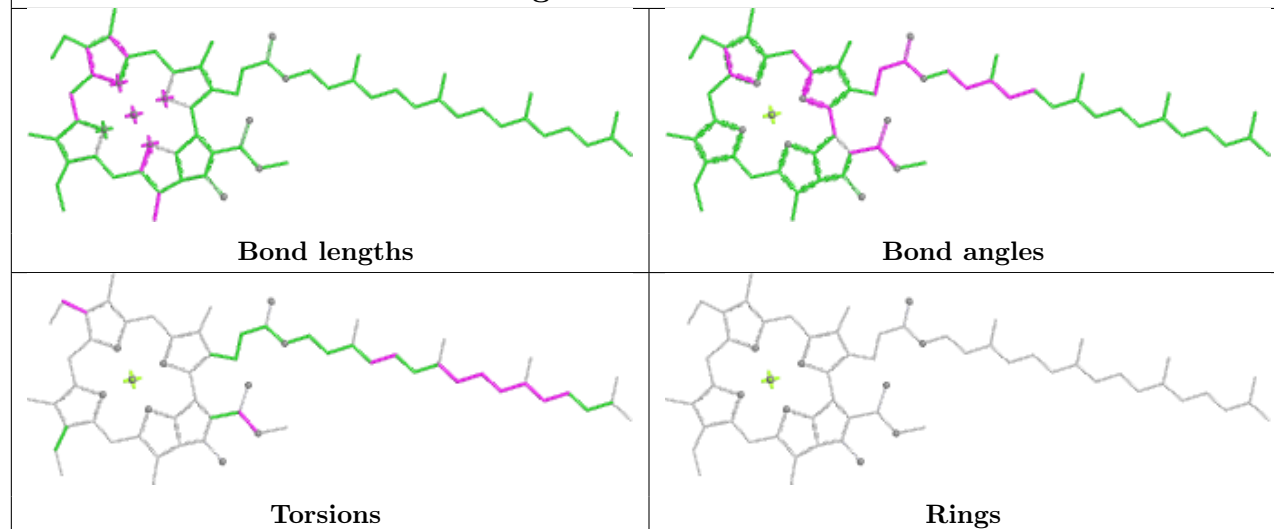
Ligand CLA c 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

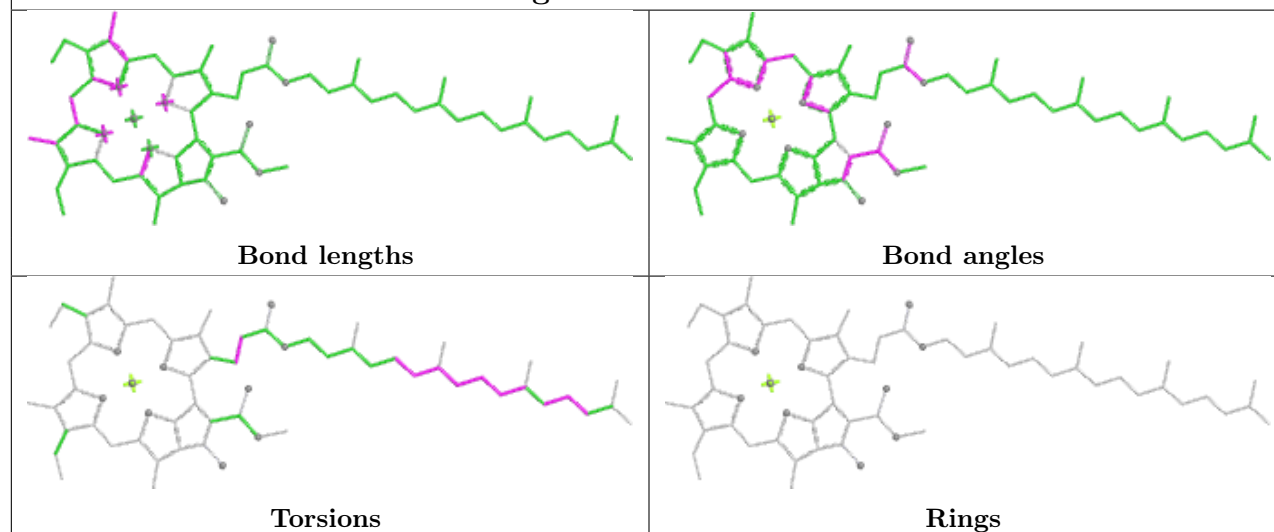
Ligand CLA c 513

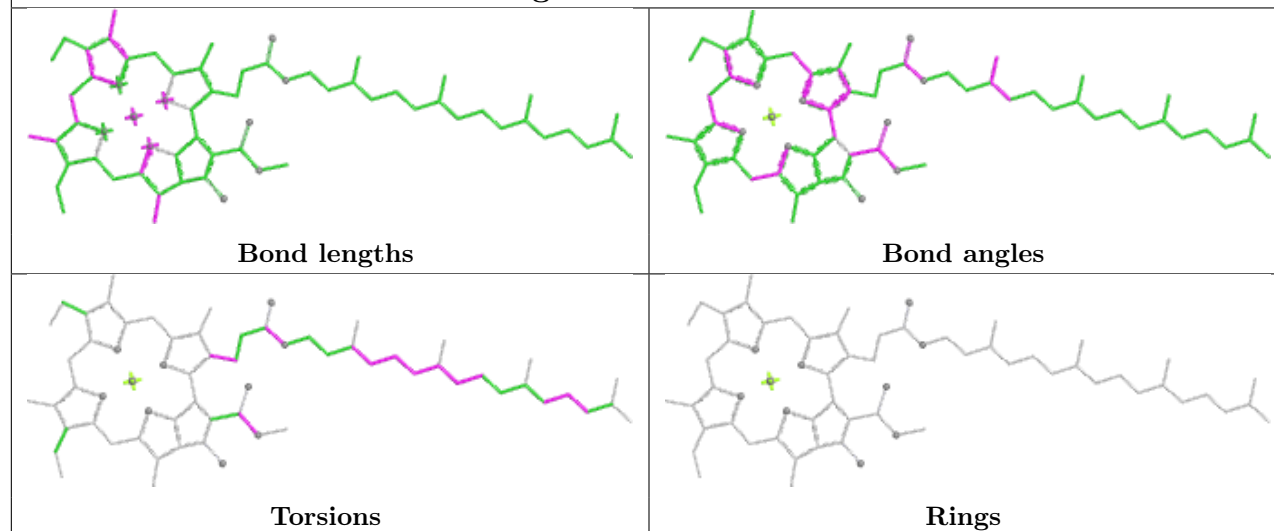
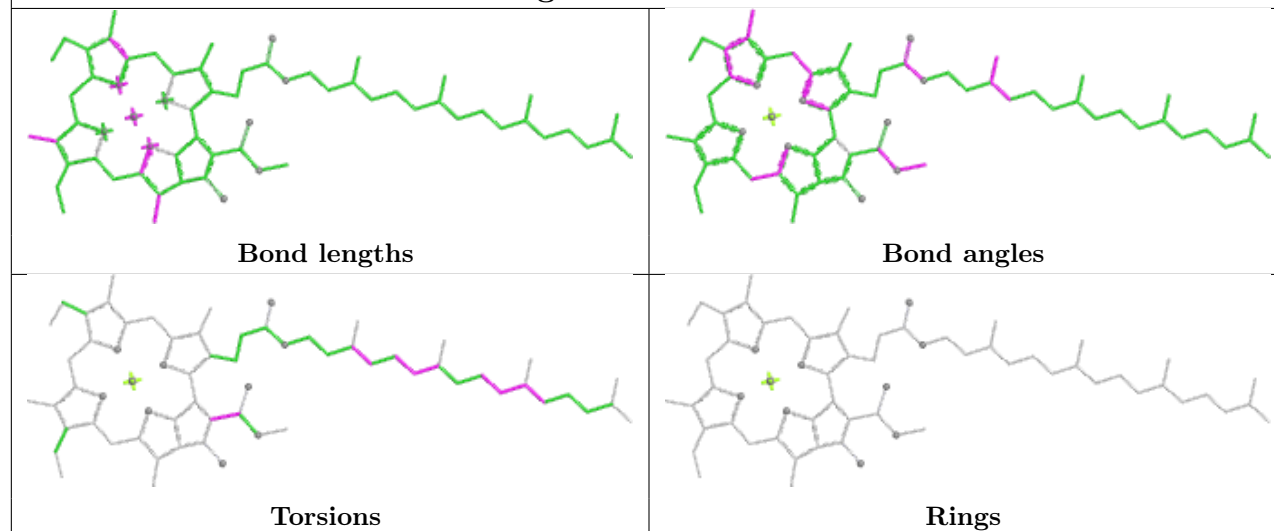
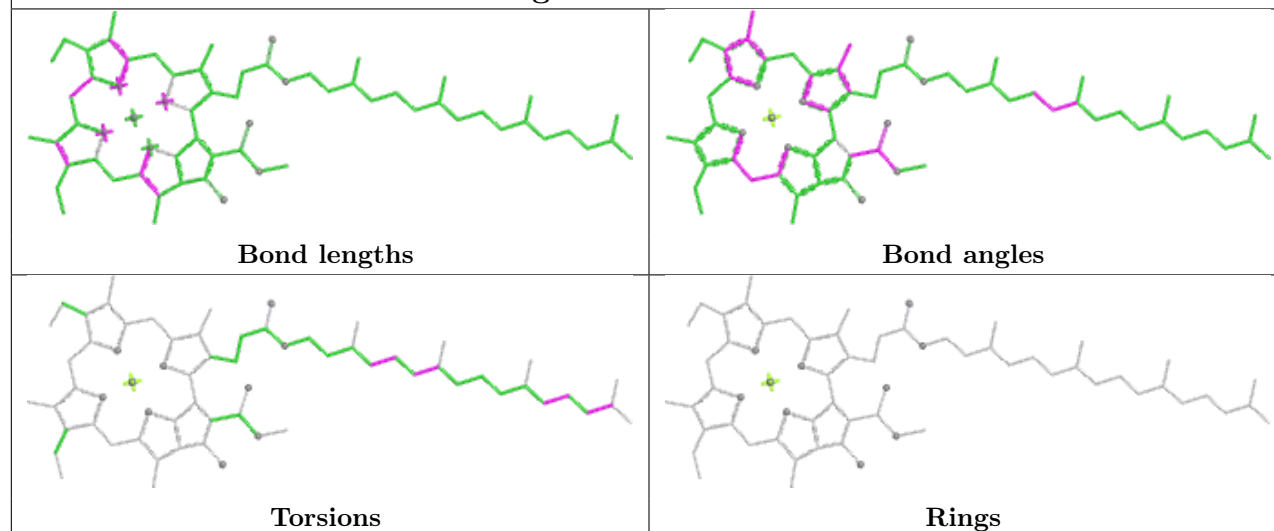


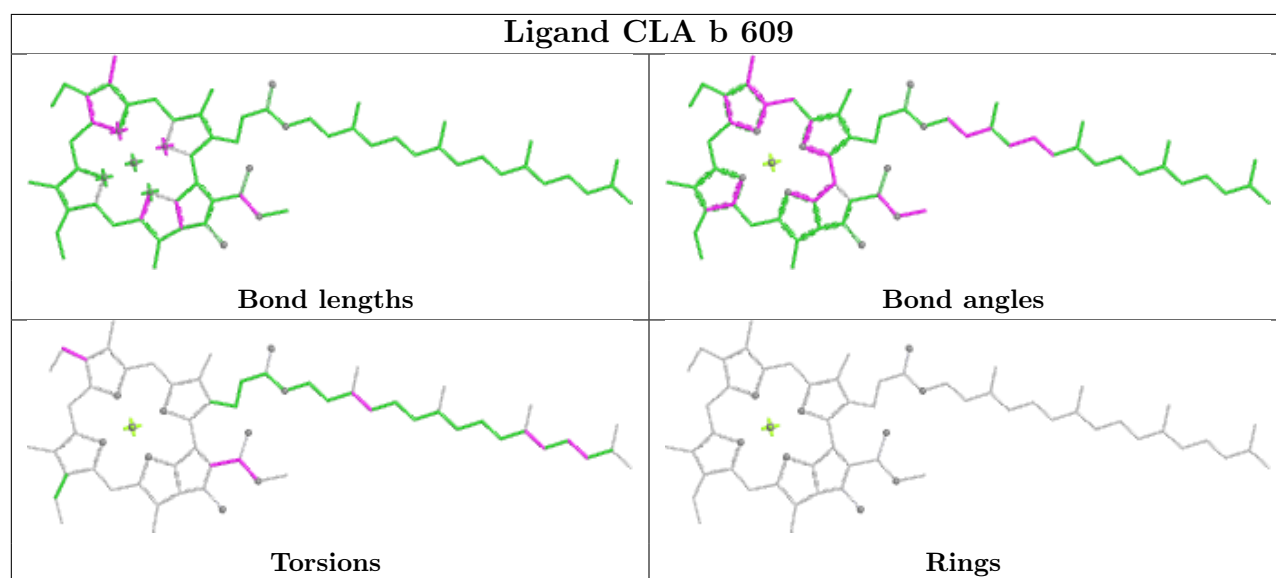
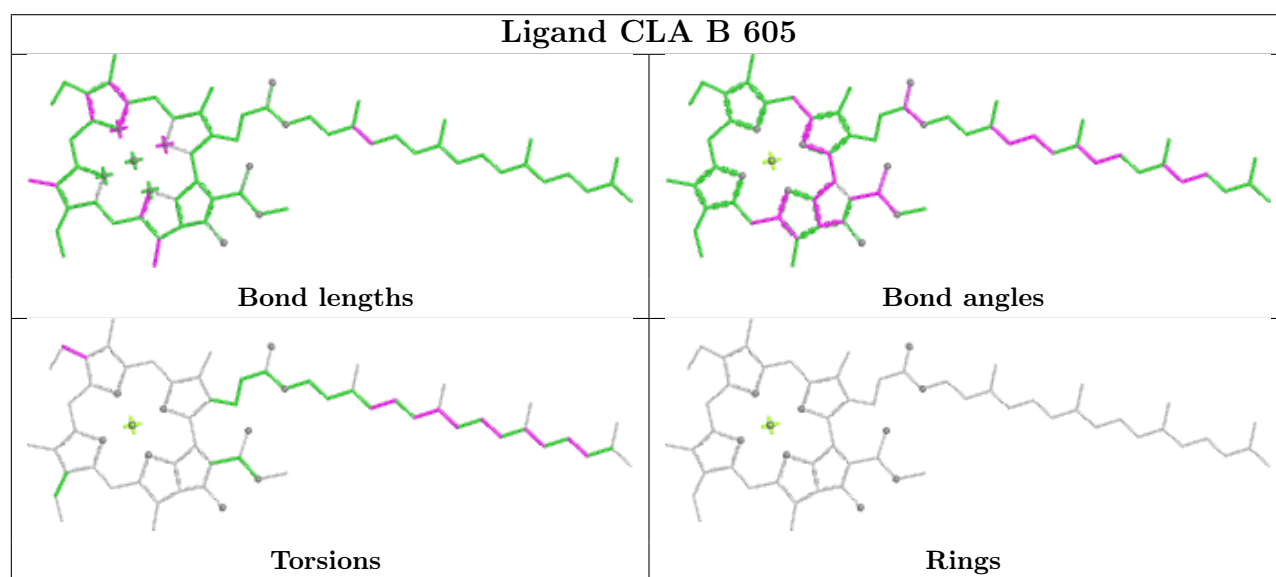
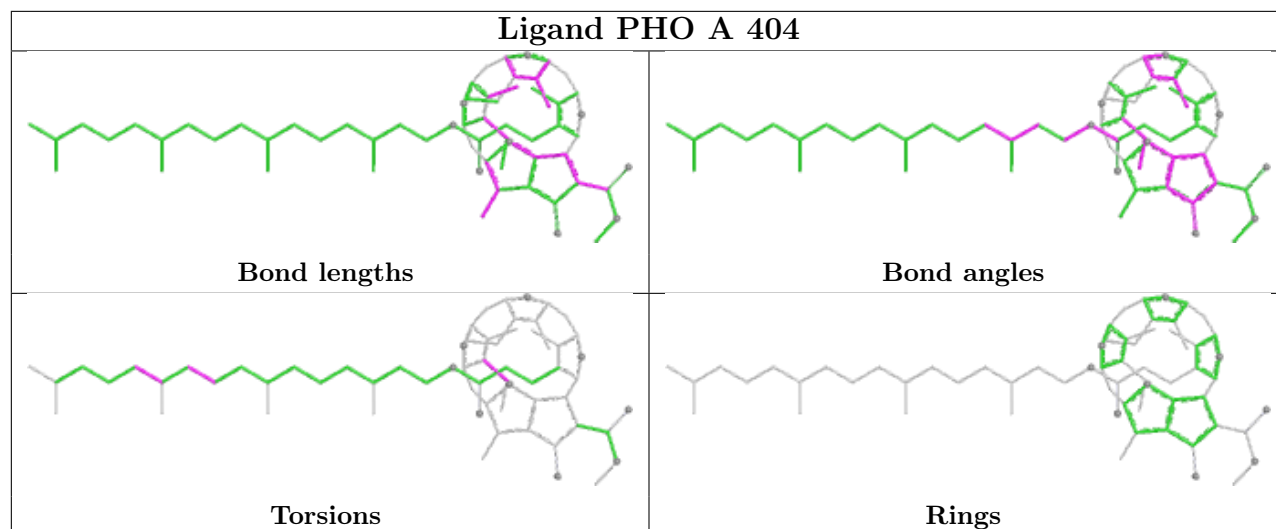
Ligand CLA C 512

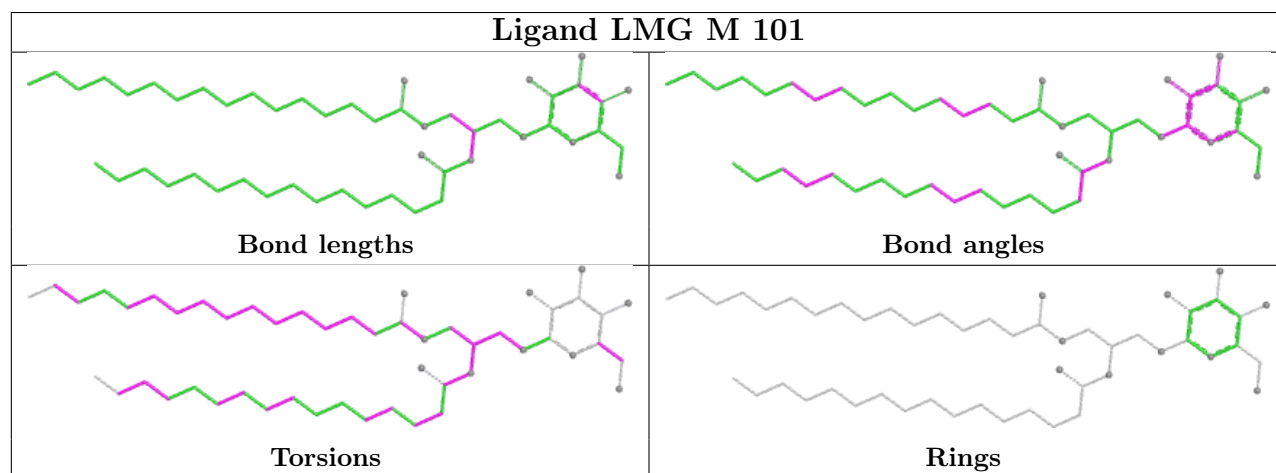
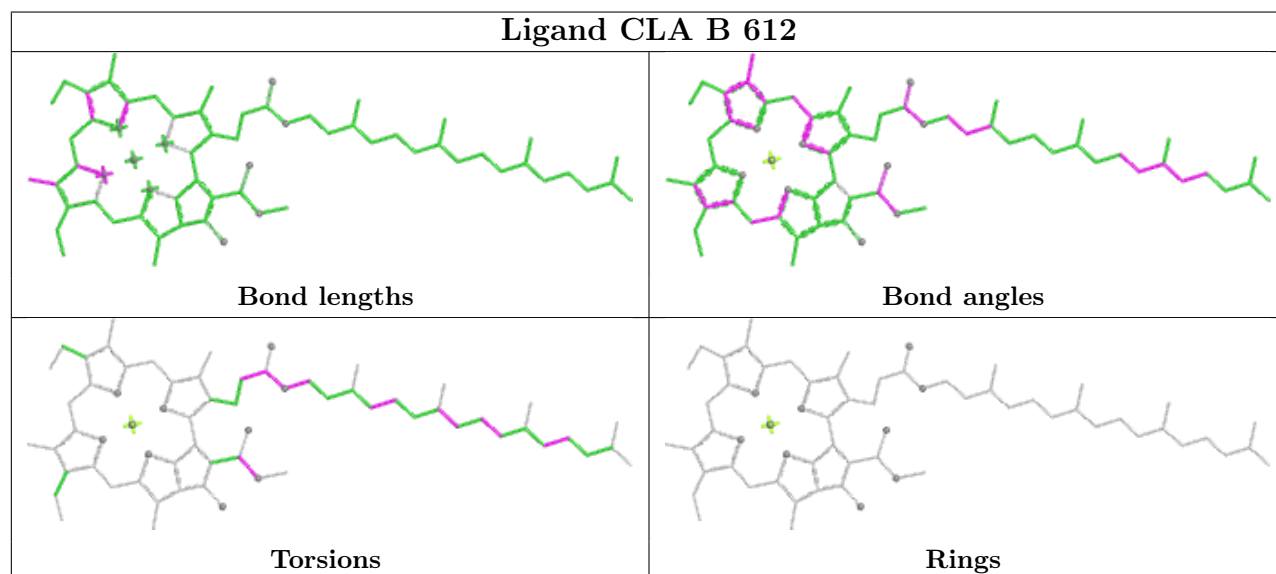
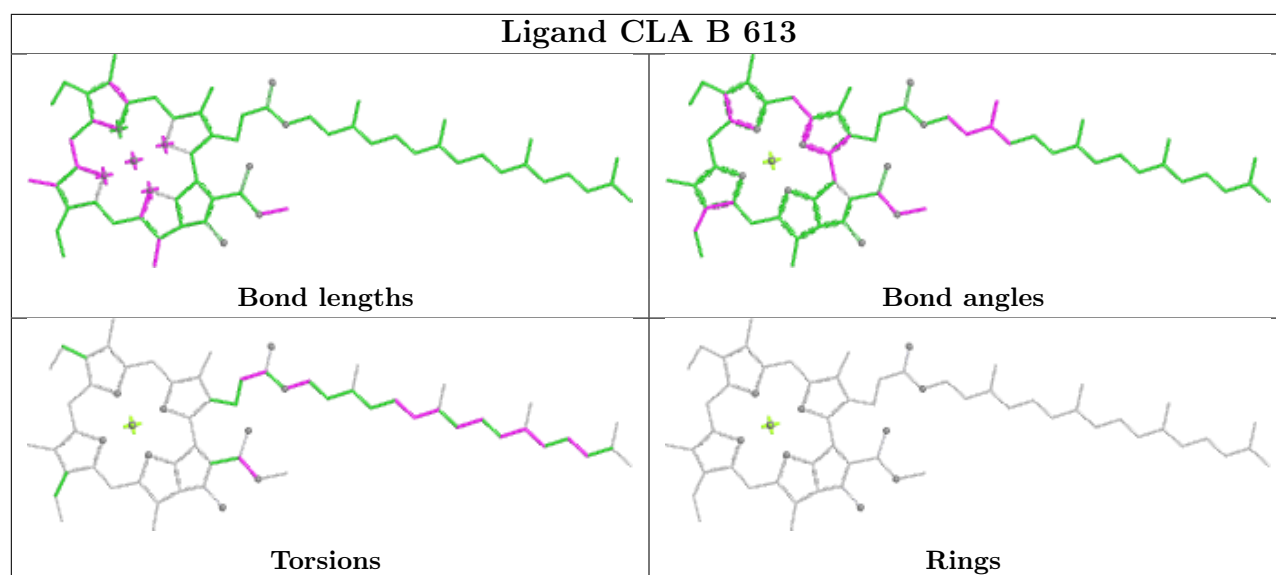


Ligand CLA B 606

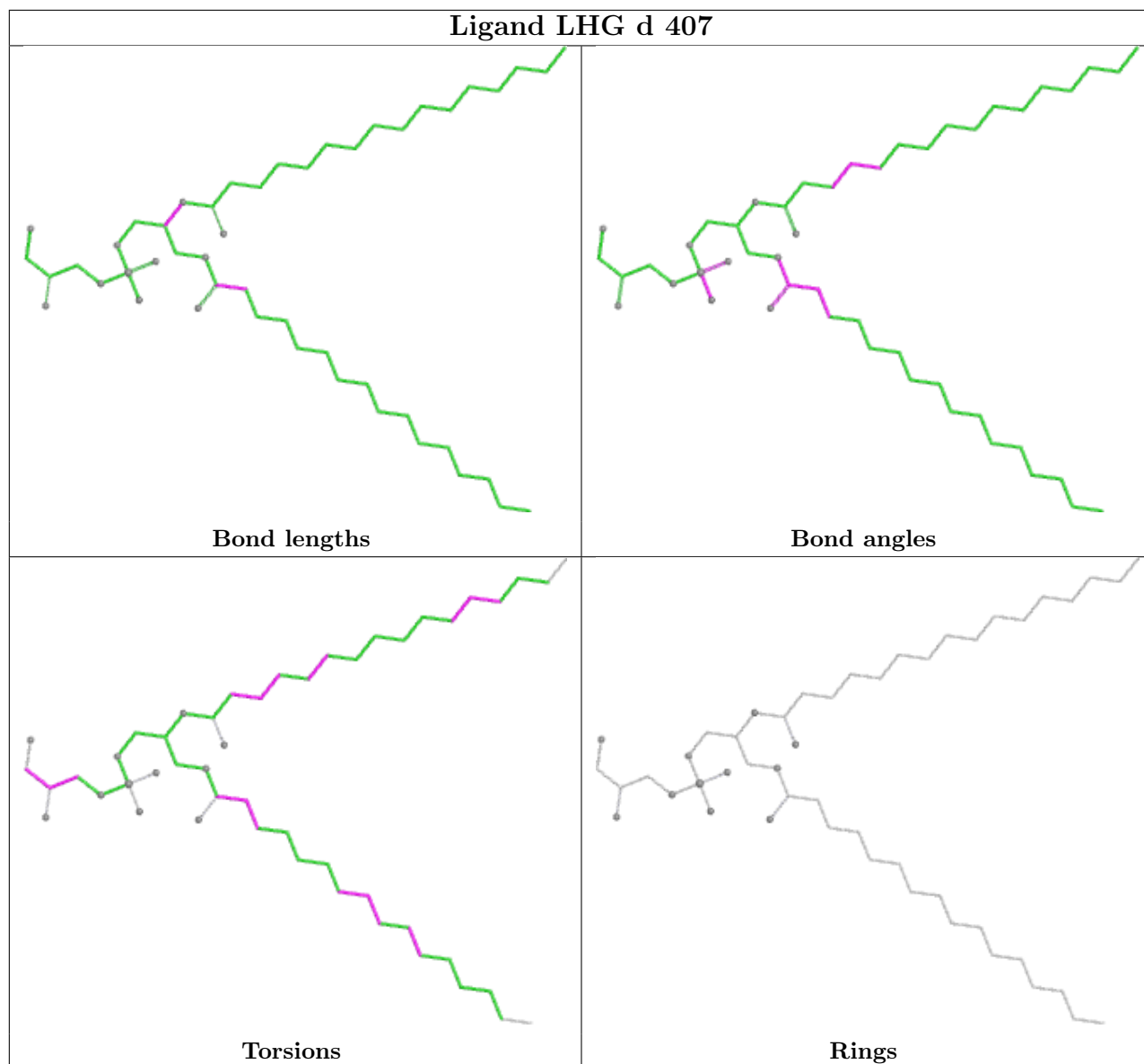


Ligand CLA C 513**Ligand CLA c 508****Ligand CLA B 608**

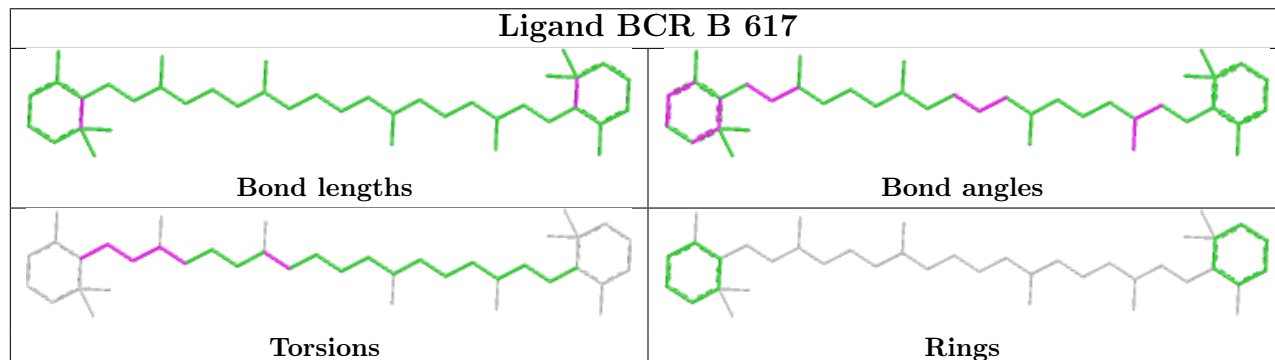


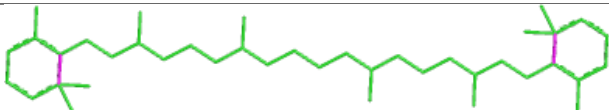
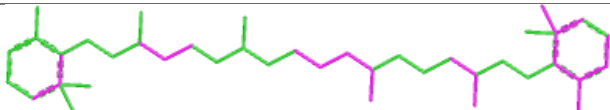
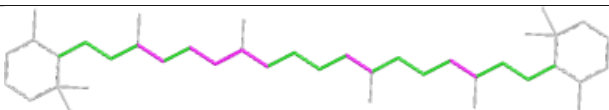
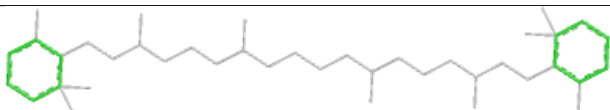
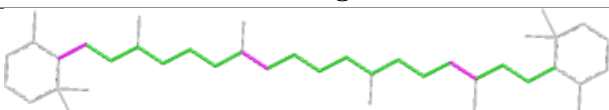
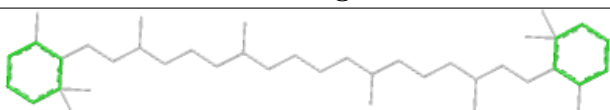


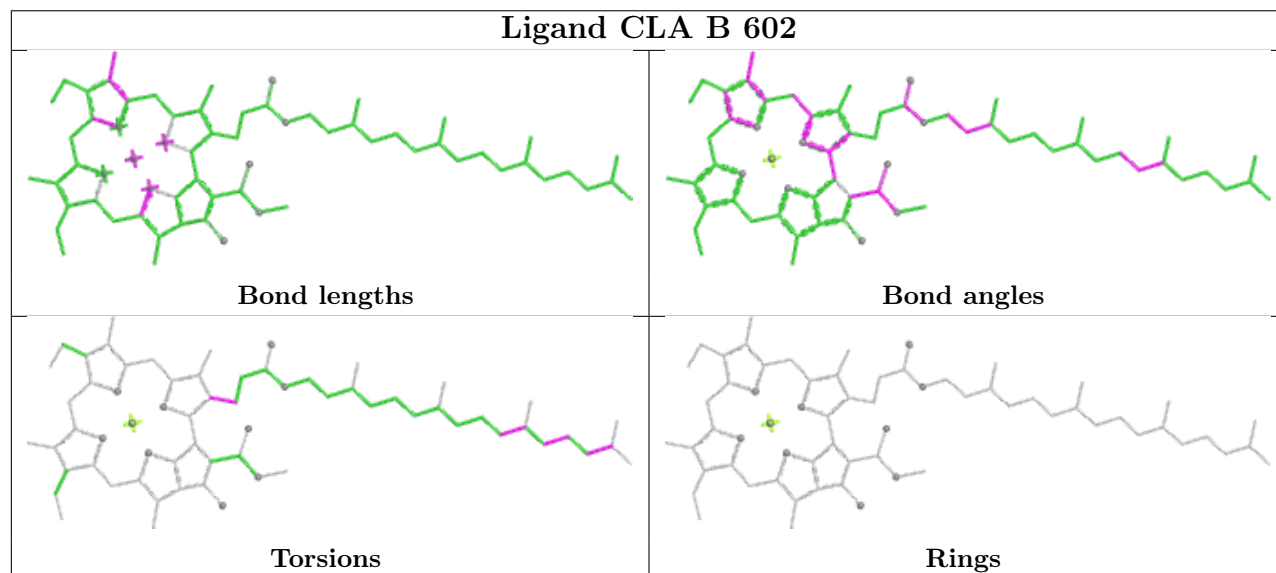
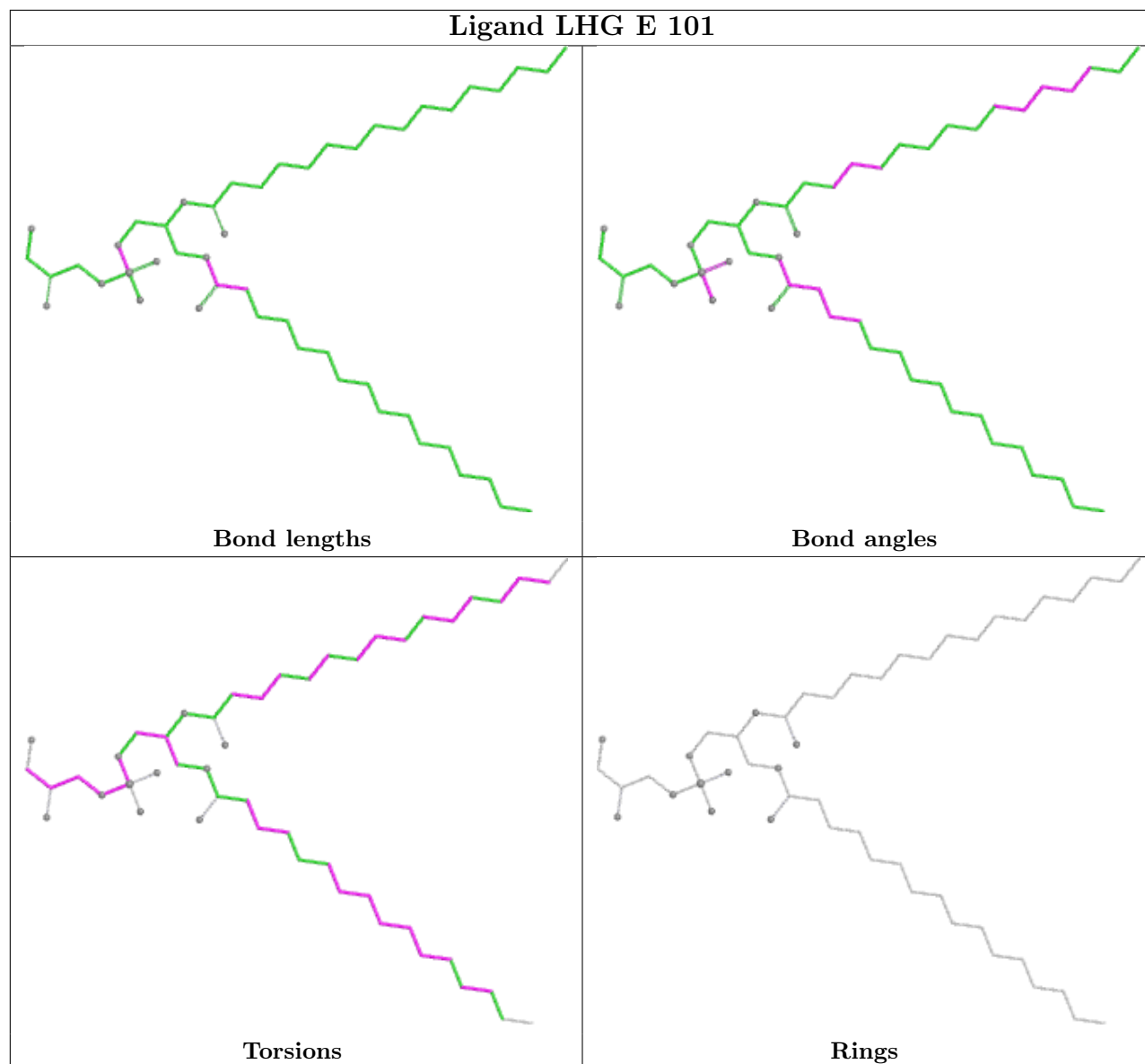
Ligand LHG d 407



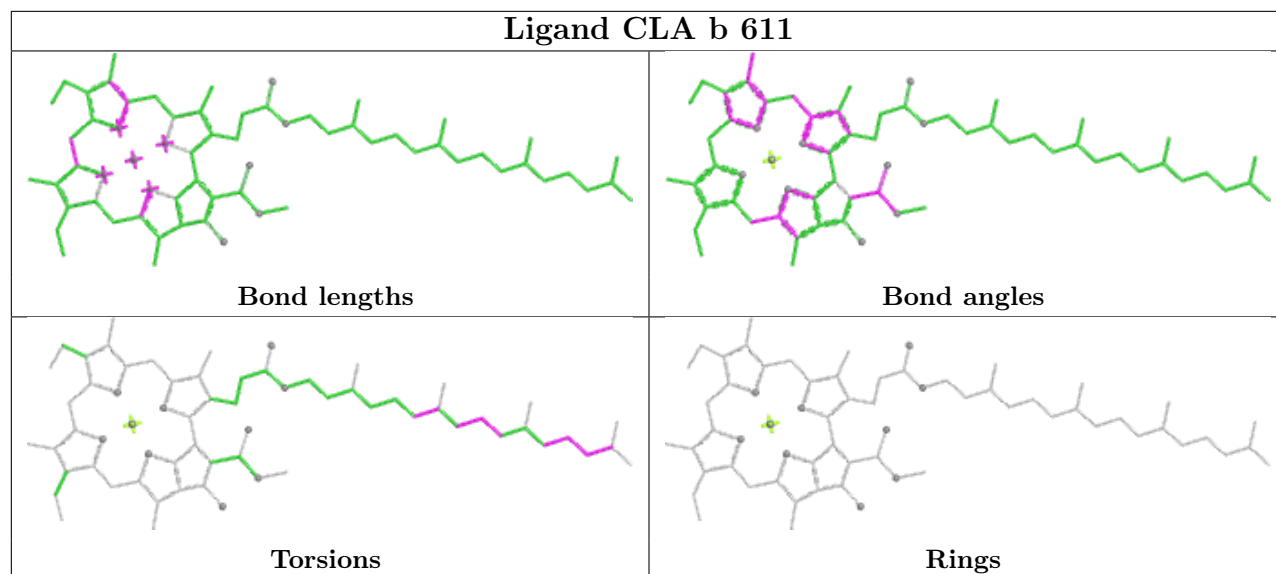
Ligand BCR B 617



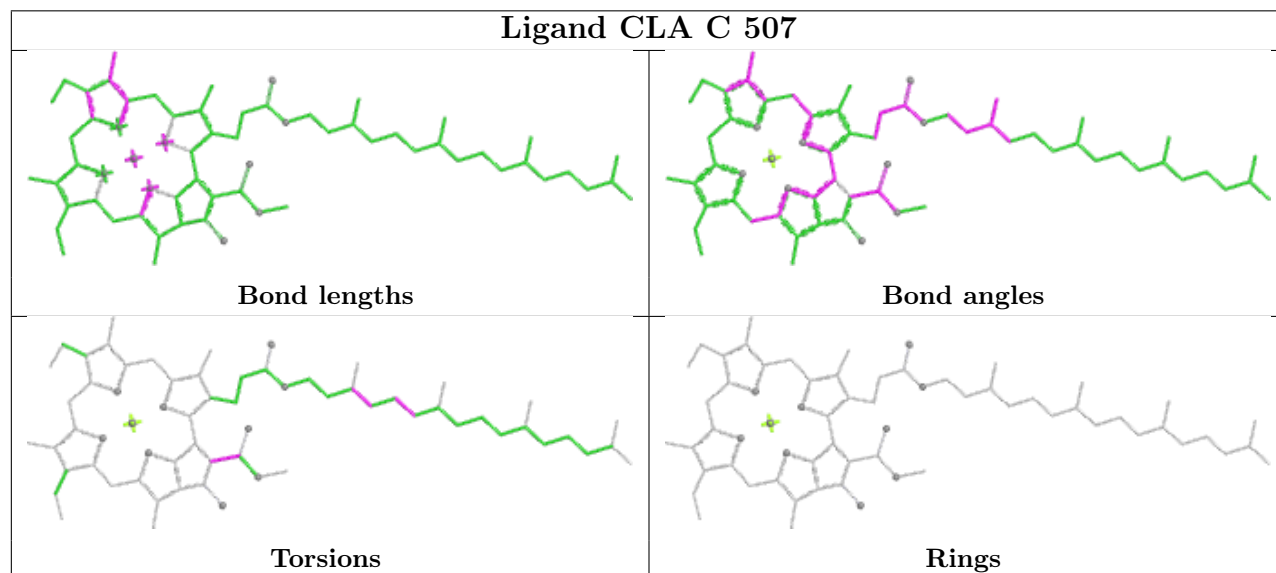
Ligand BCR B 619	
	Bond lengths
	Bond angles
	Torsions
	Rings
Ligand BCR k 102	
	Bond lengths
	Bond angles
	Torsions
	Rings



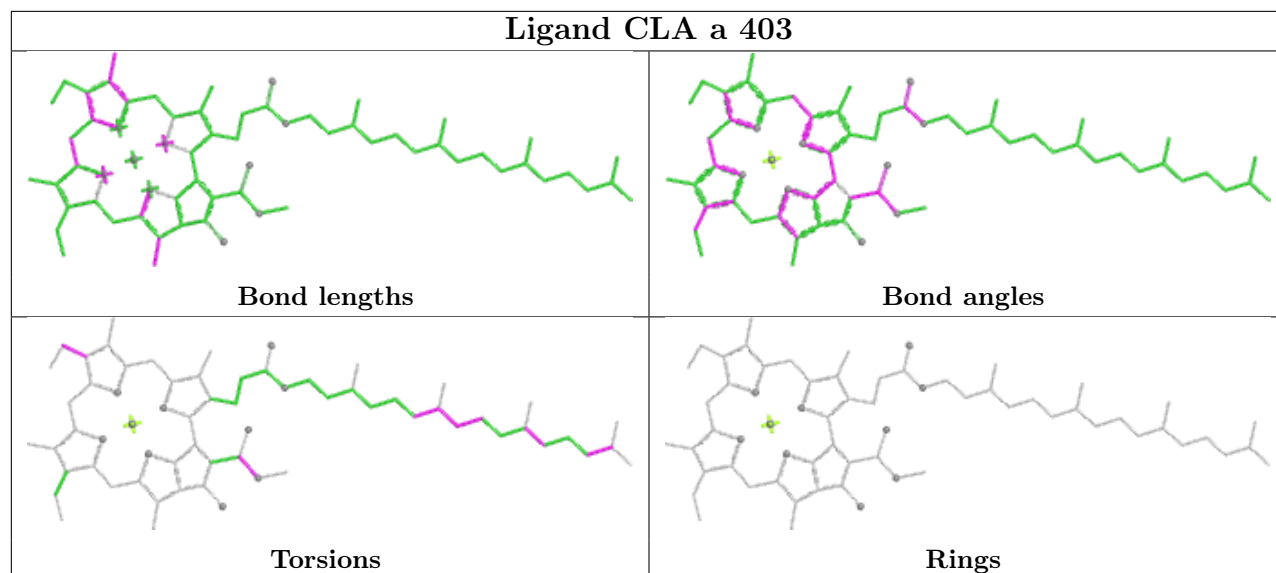
Ligand CLA b 611

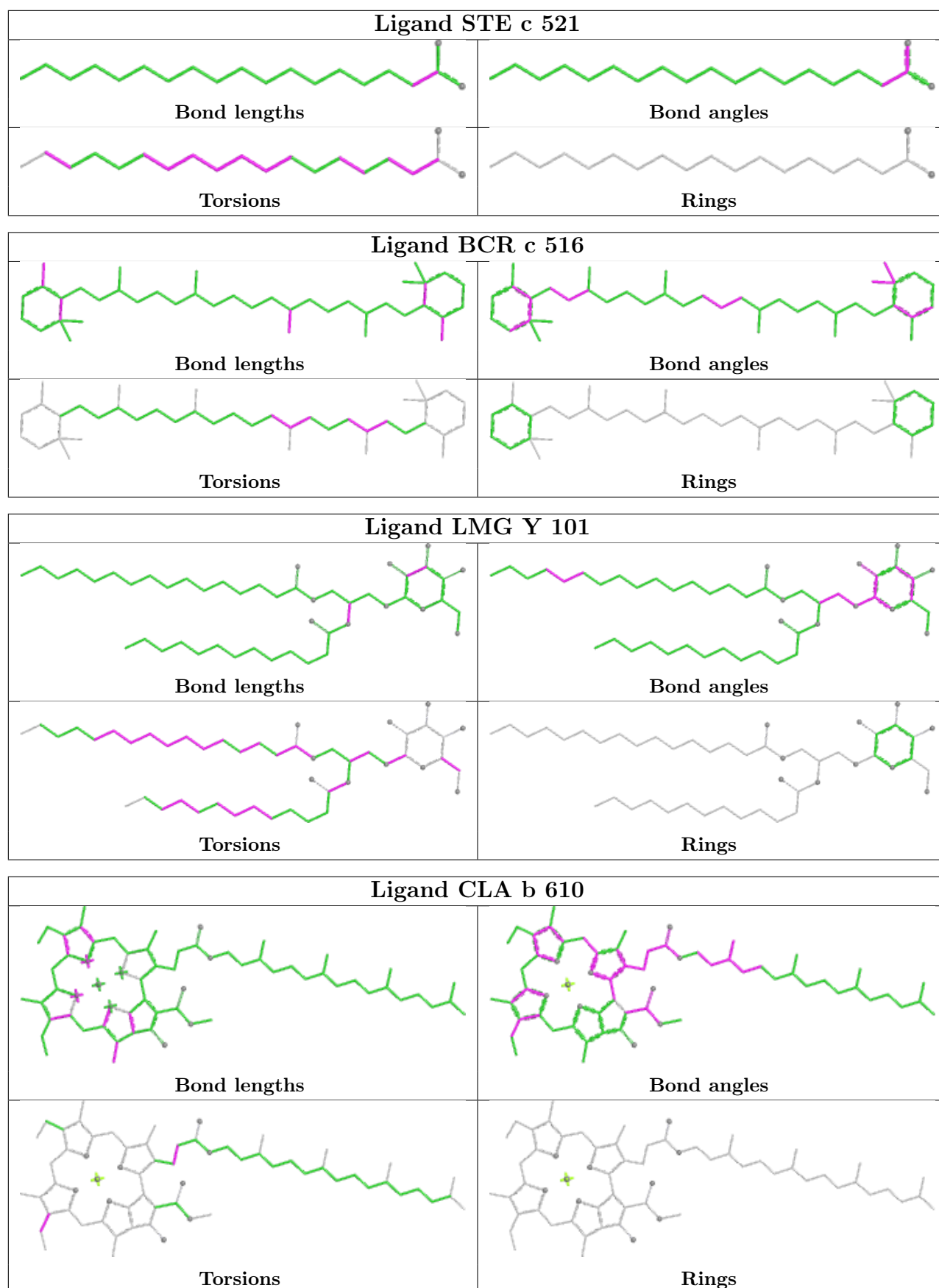


Ligand CLA C 507

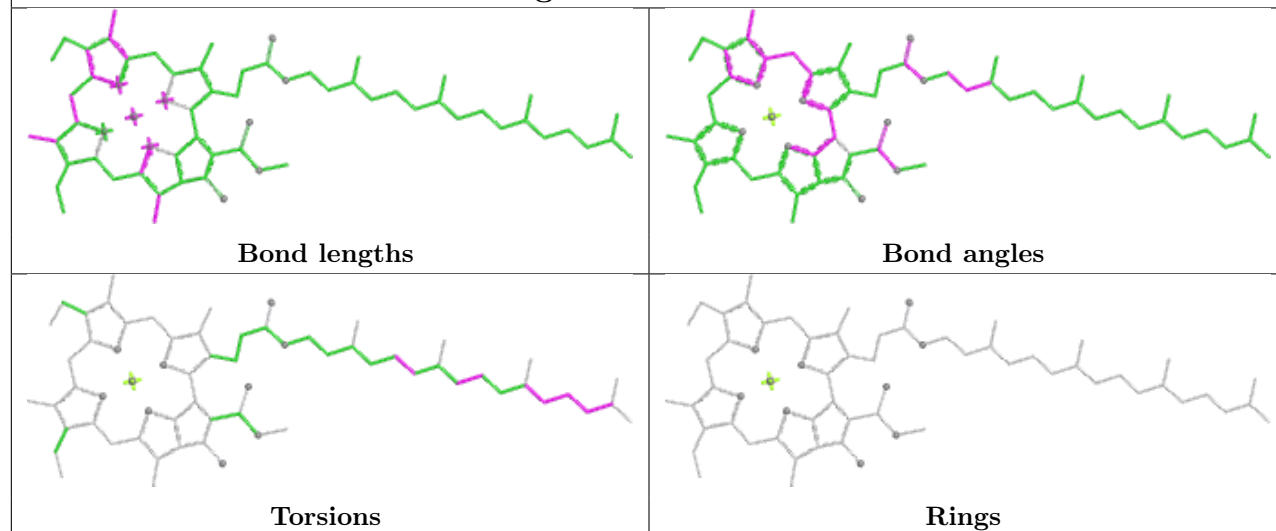


Ligand CLA a 403

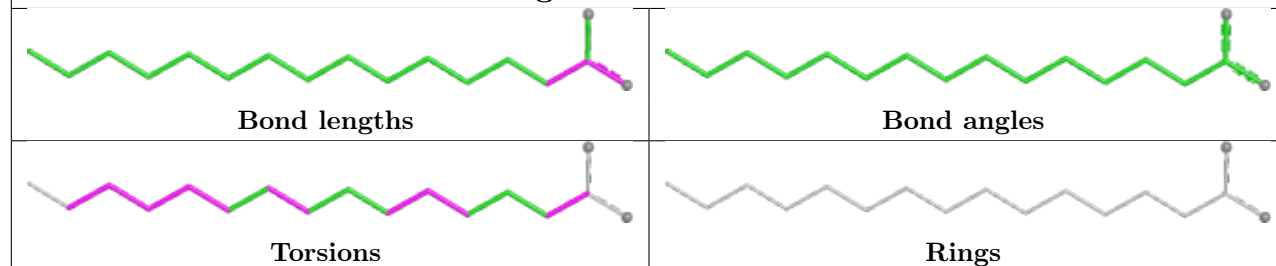




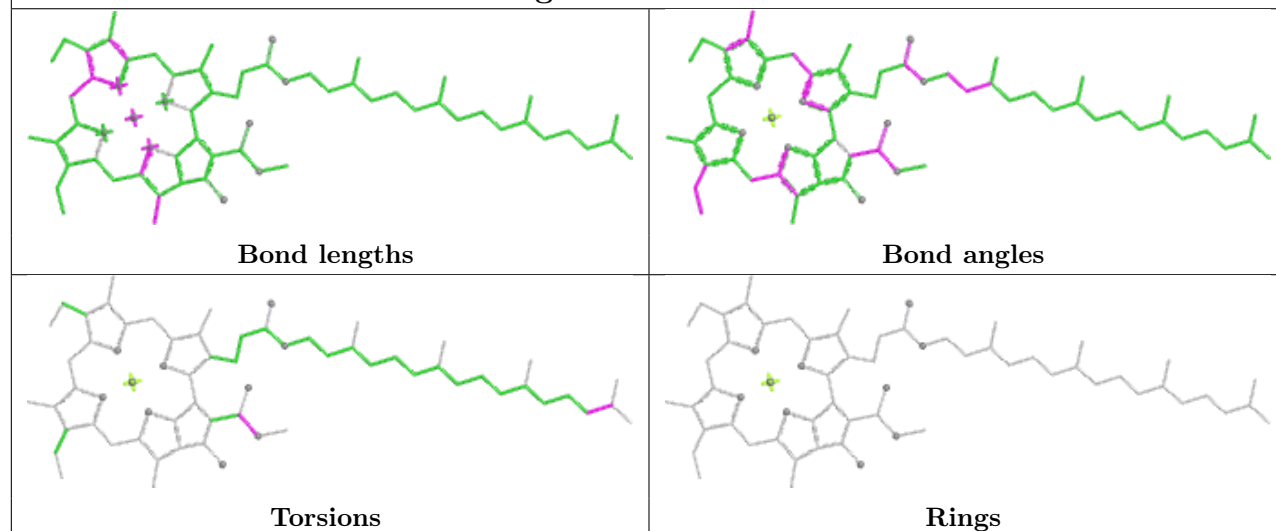
Ligand CLA b 615

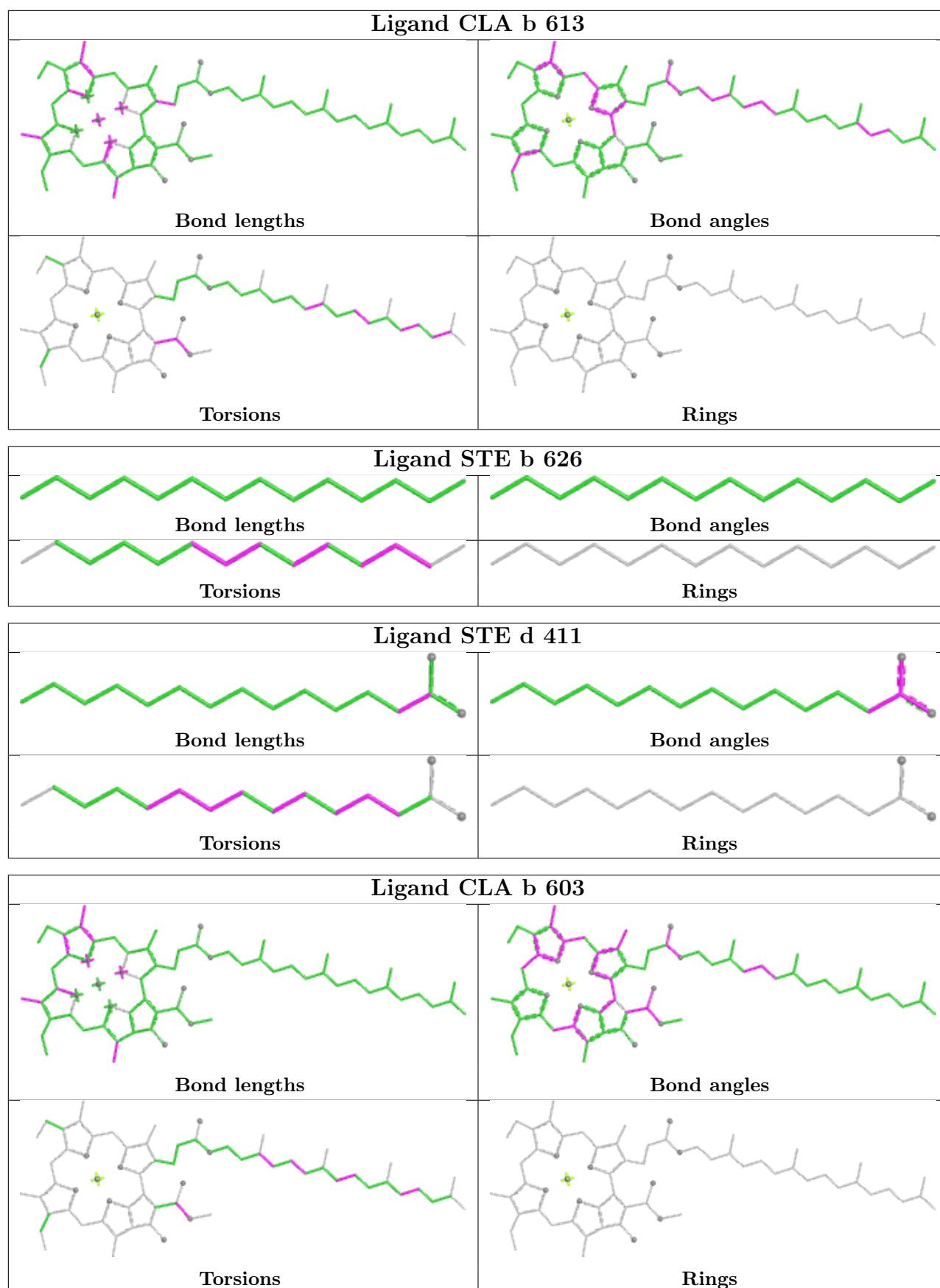


Ligand STE B 620

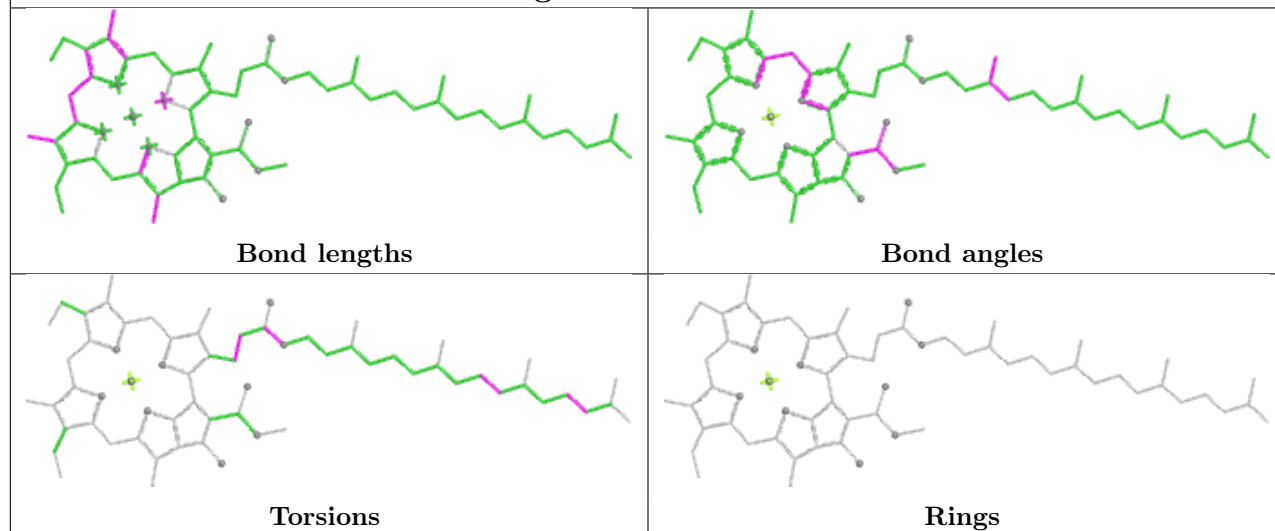


Ligand CLA d 404

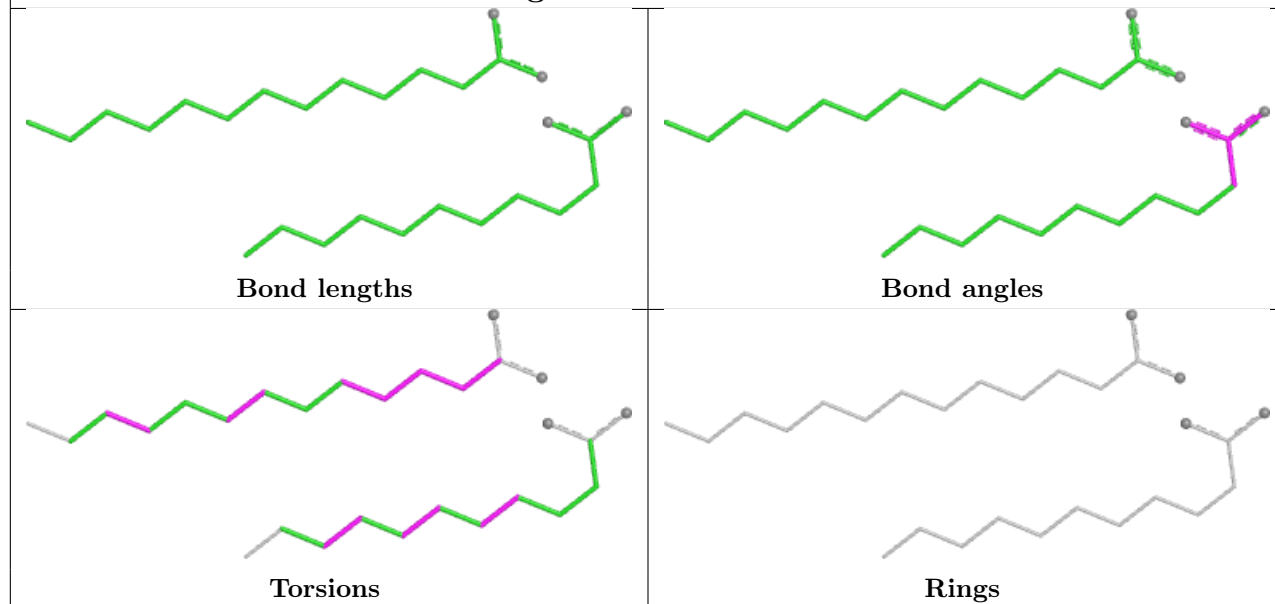


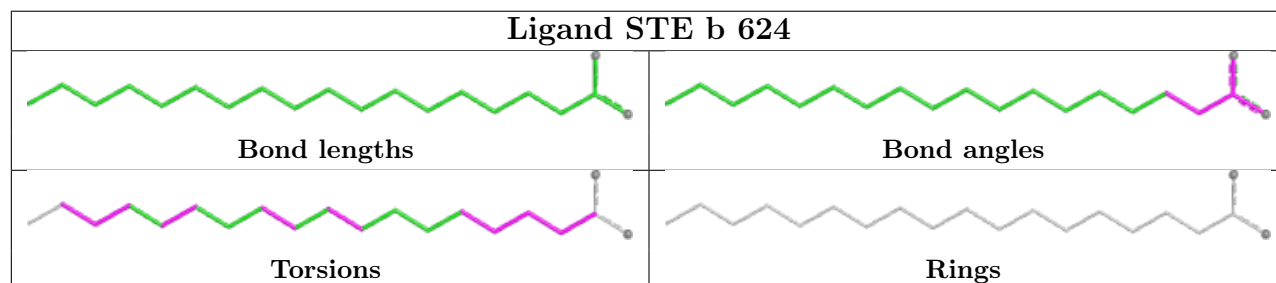
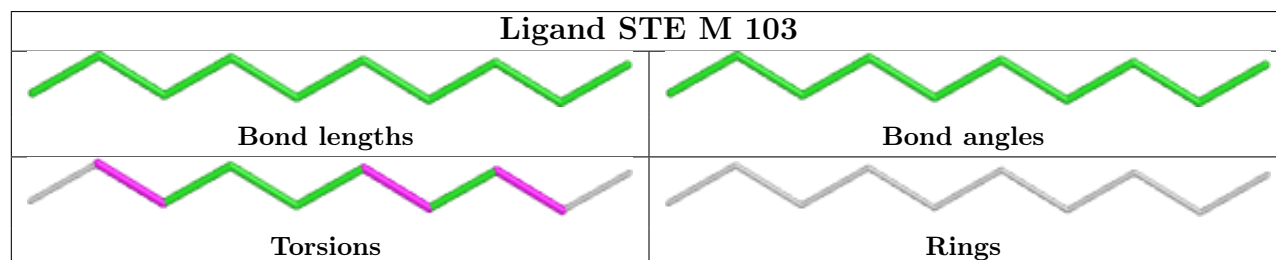
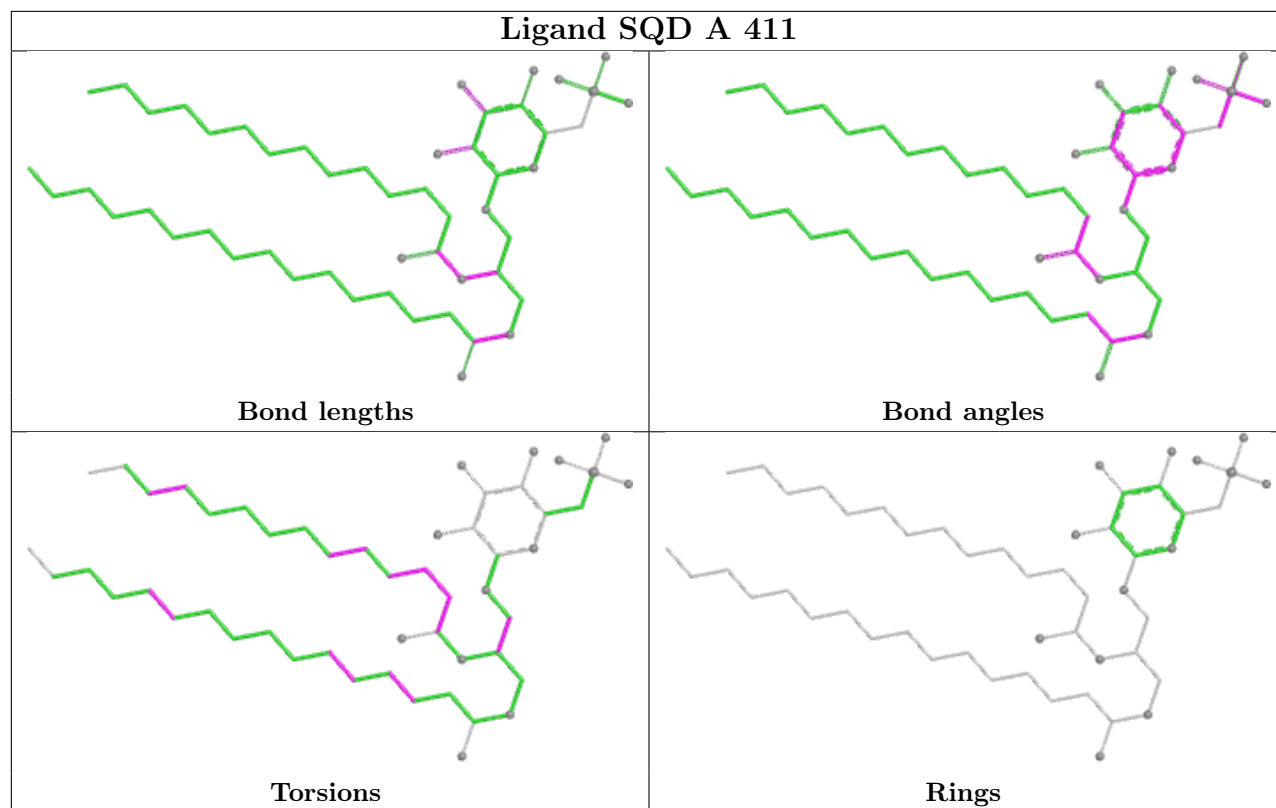


Ligand CLA b 606

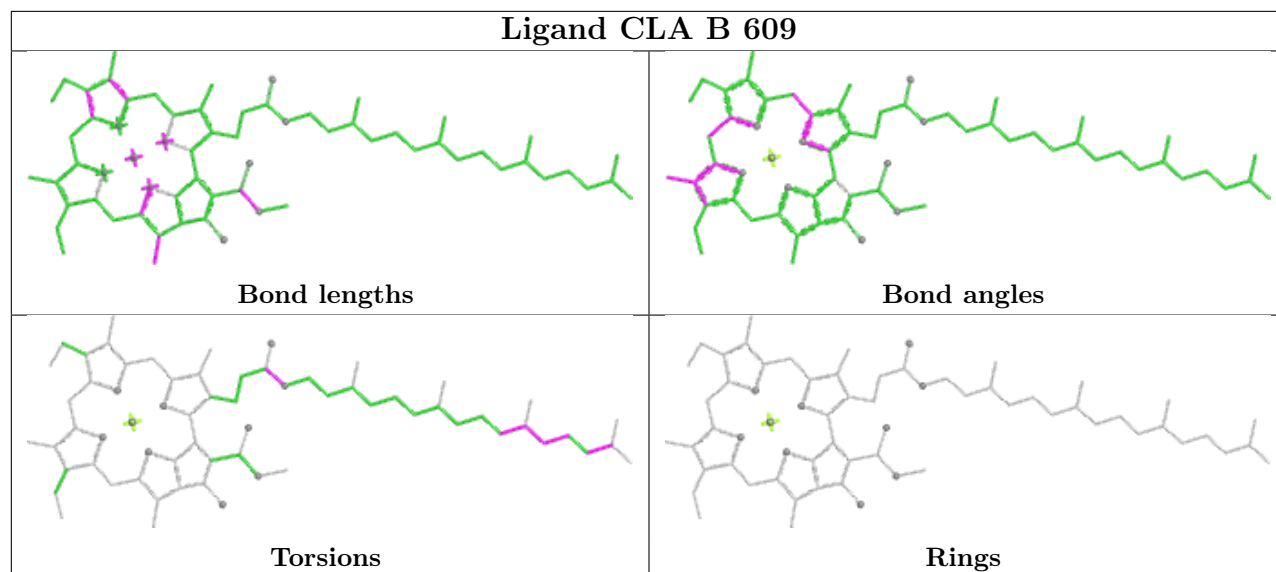


Ligand LMG B 621

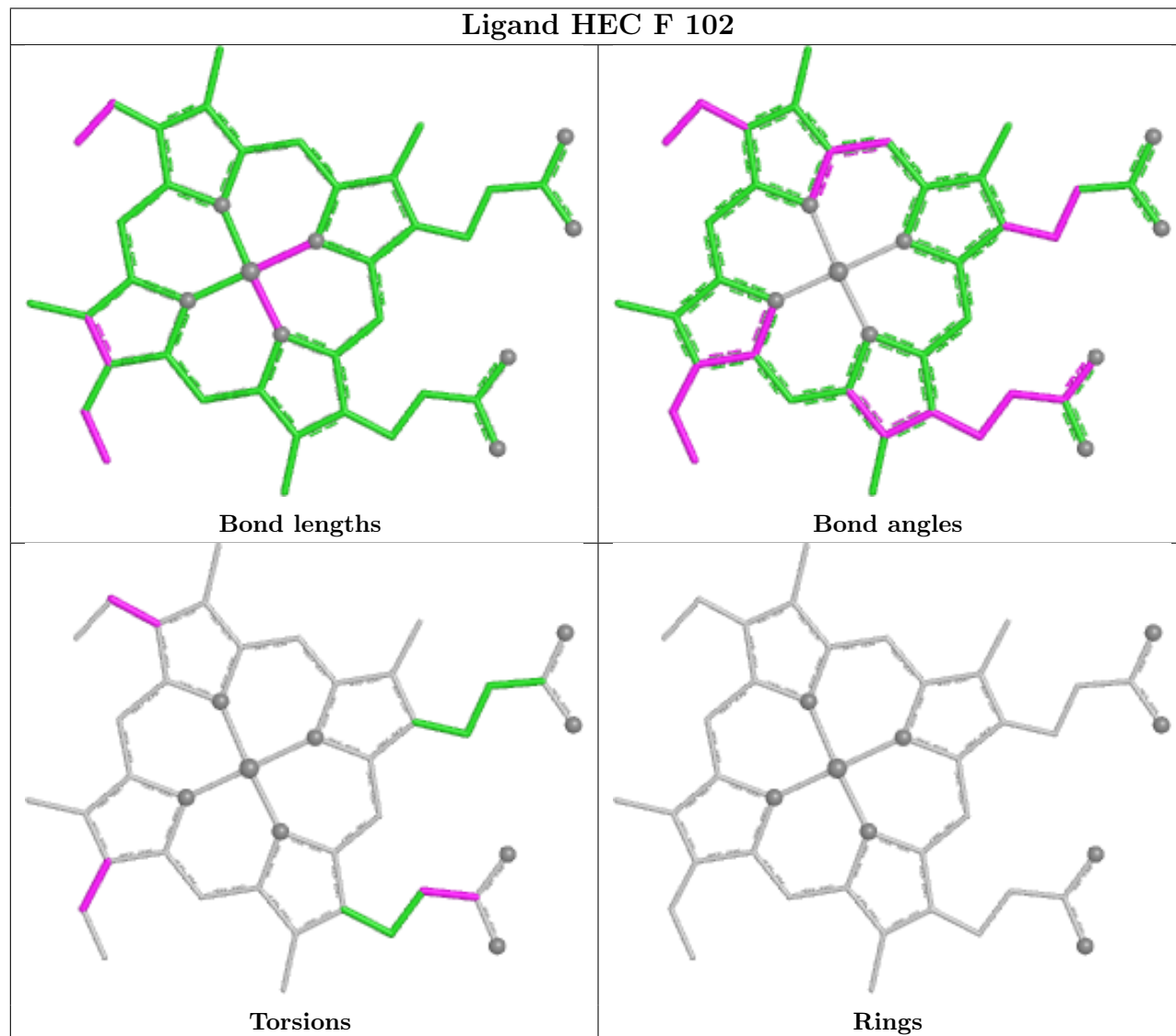


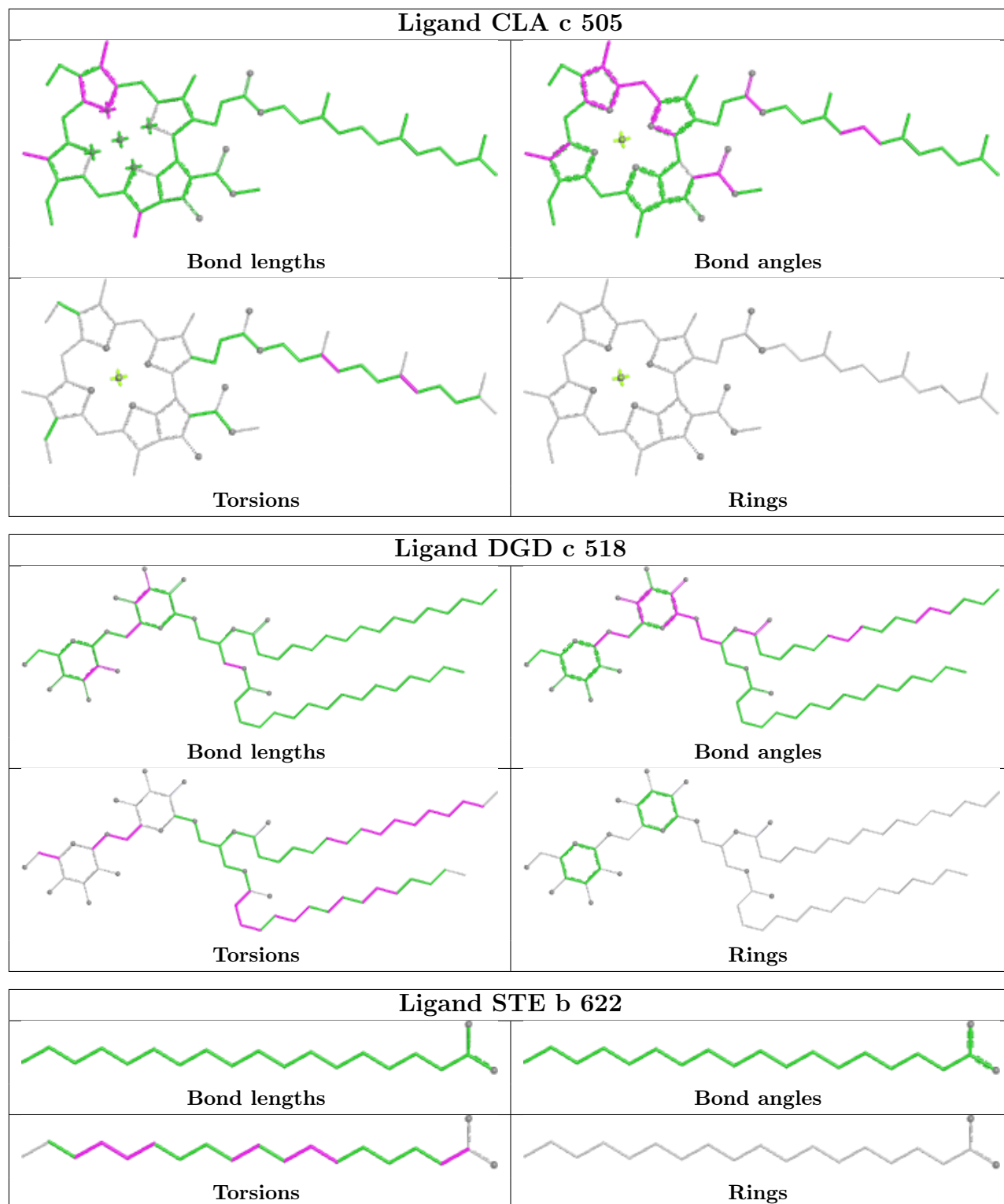


Ligand CLA B 609

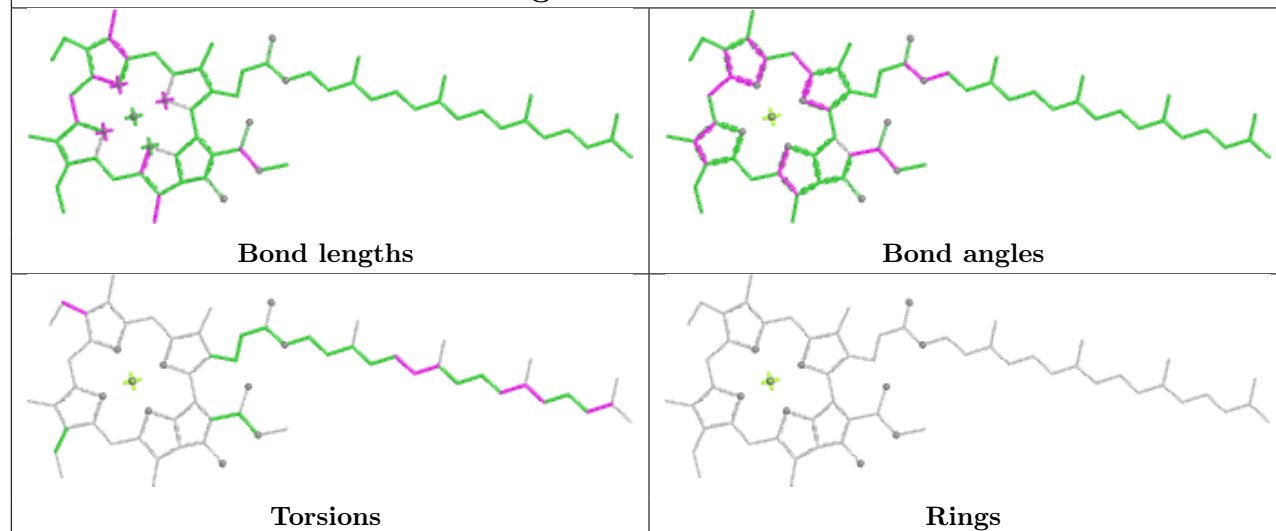


Ligand HEC F 102

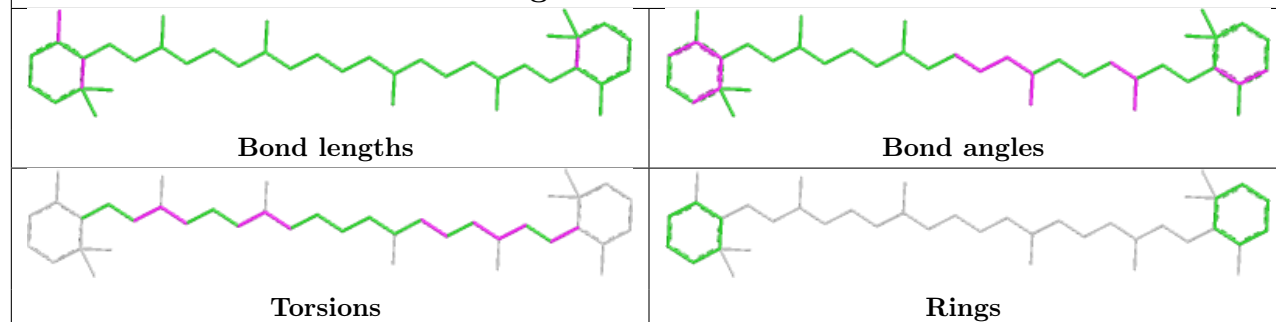




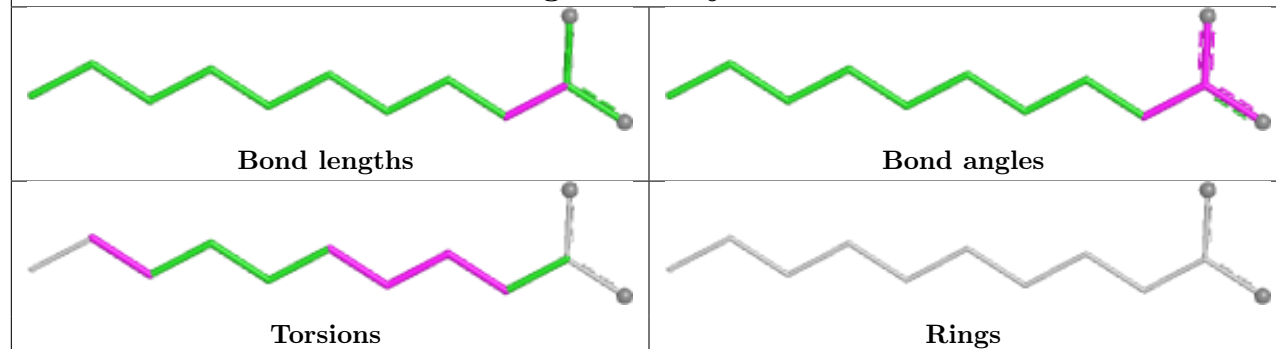
Ligand CLA B 615



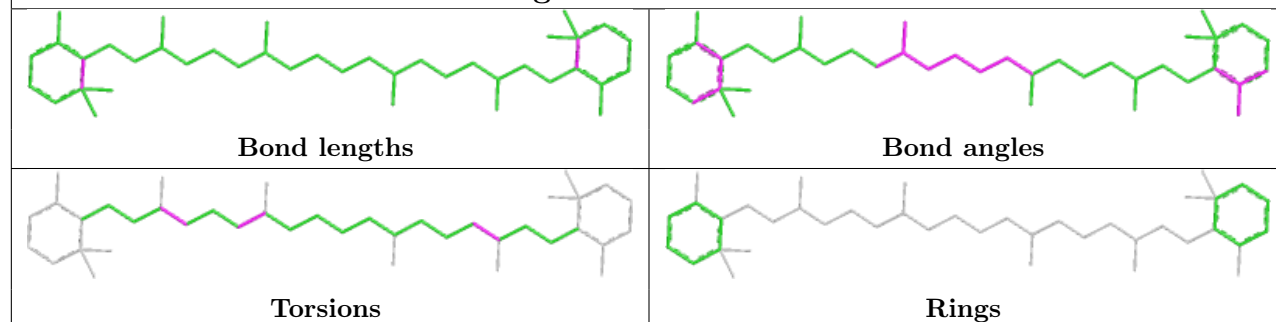
Ligand BCR A 406

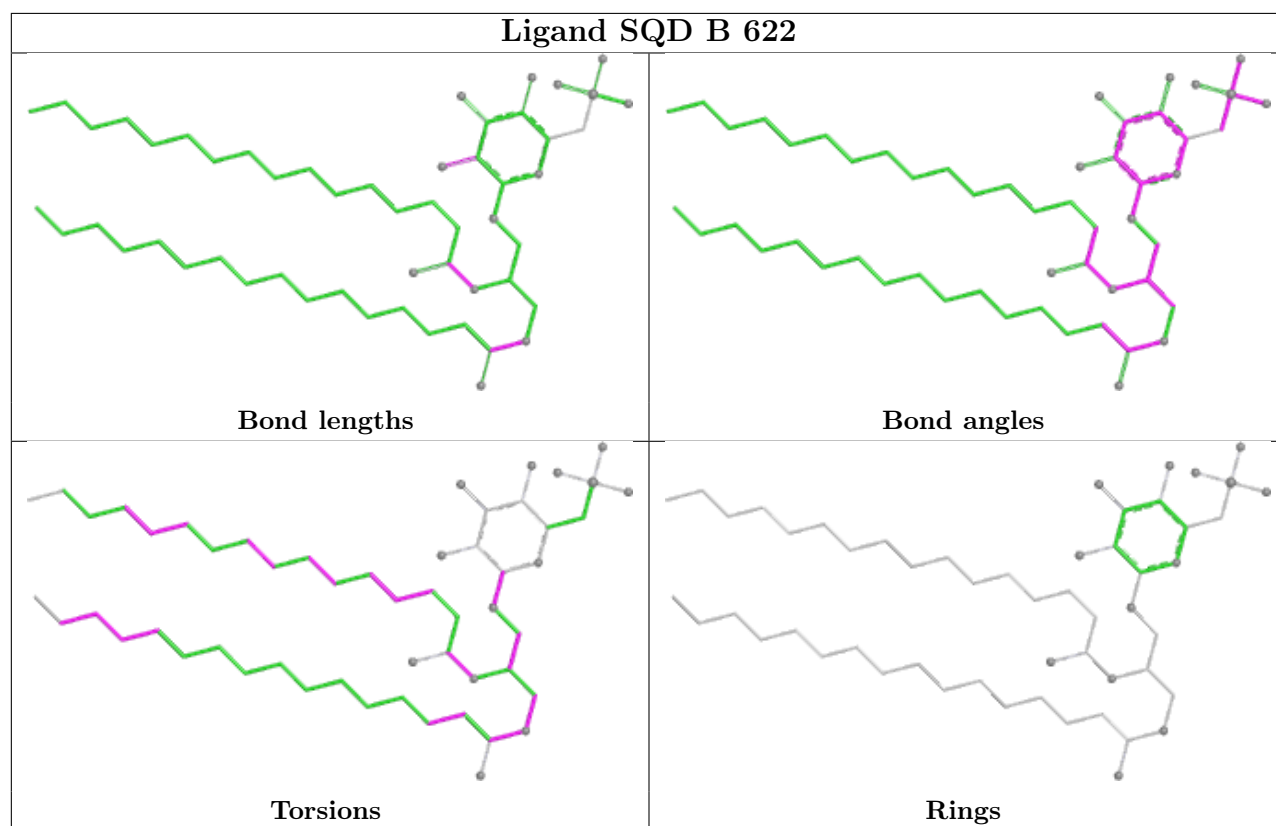
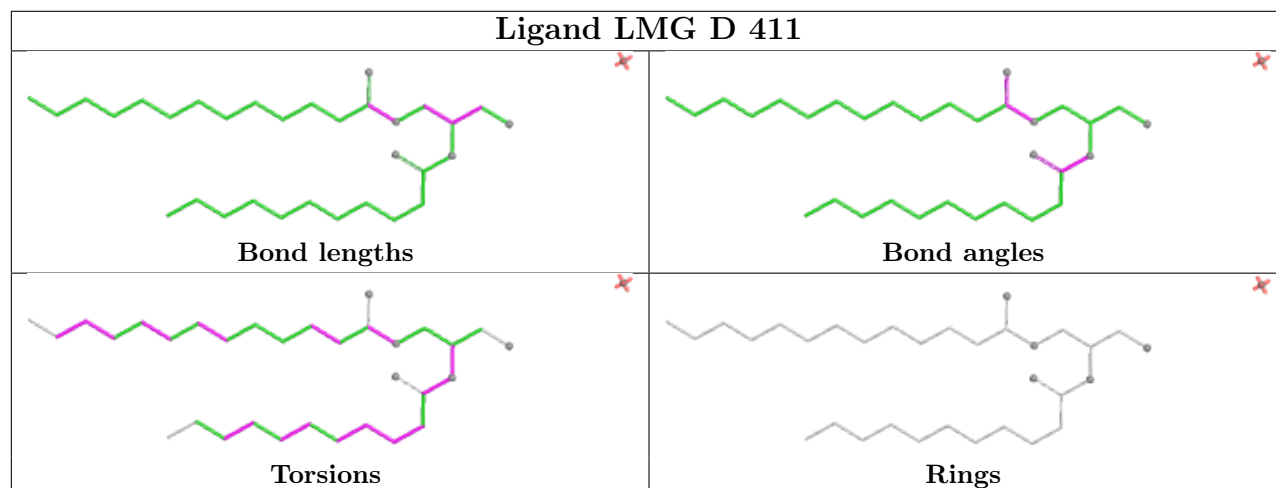
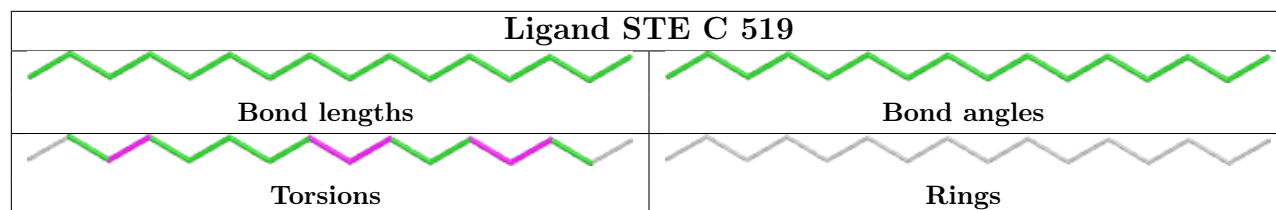


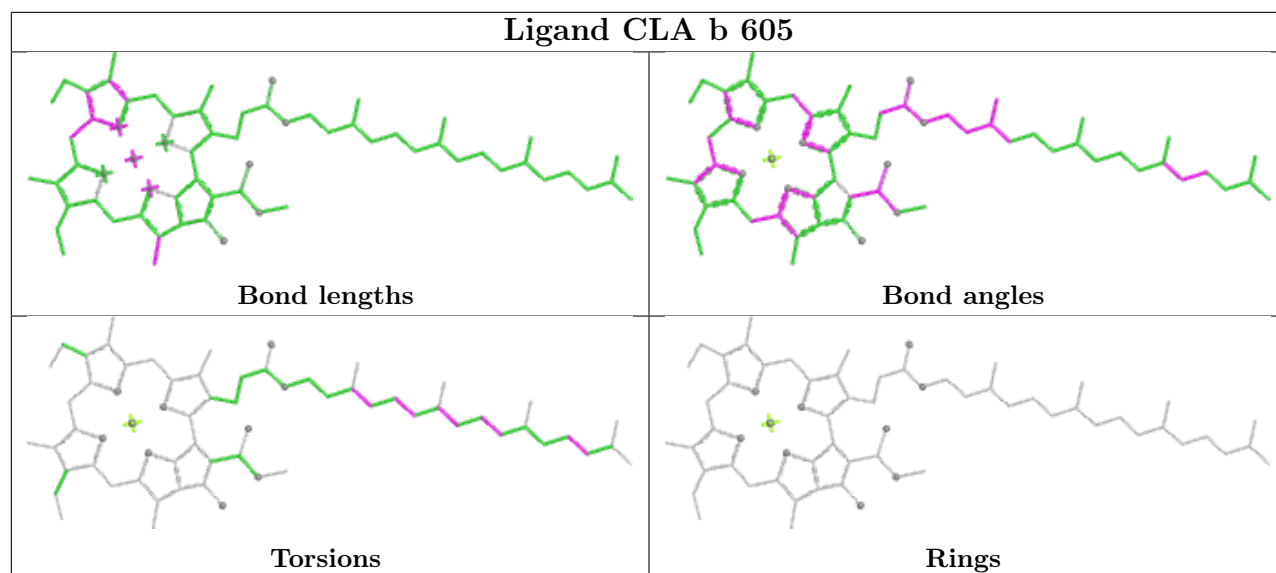
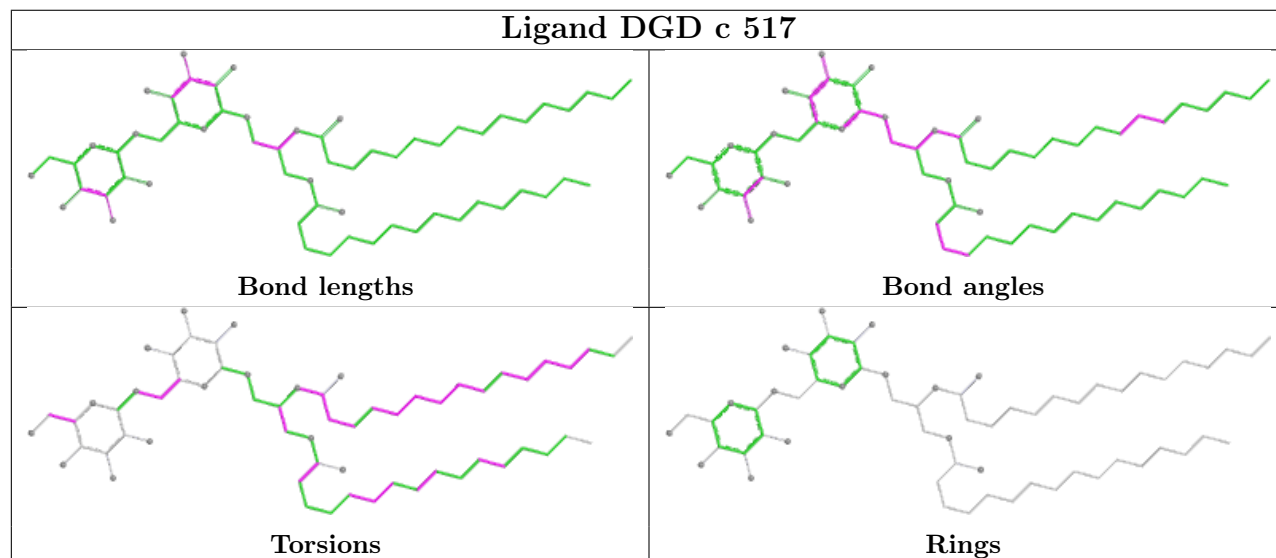
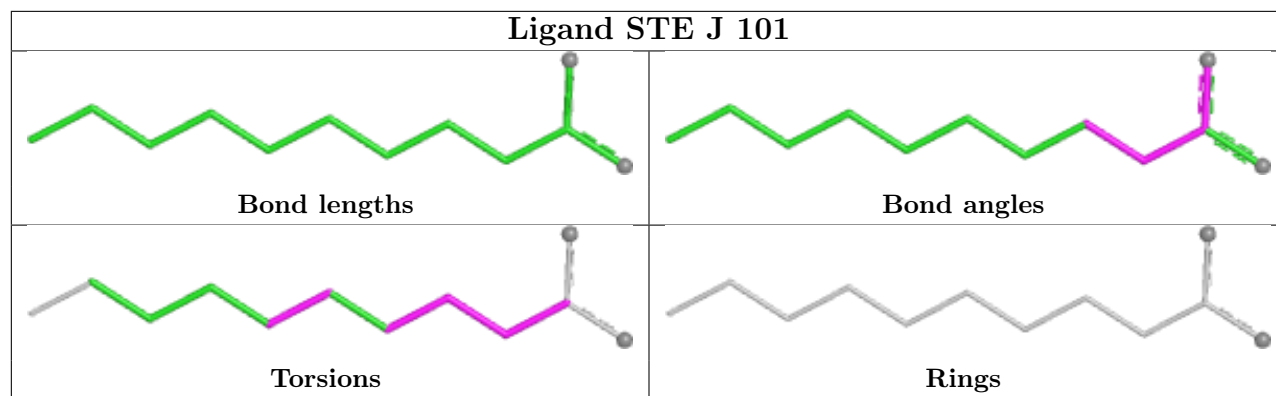
Ligand STE j 101

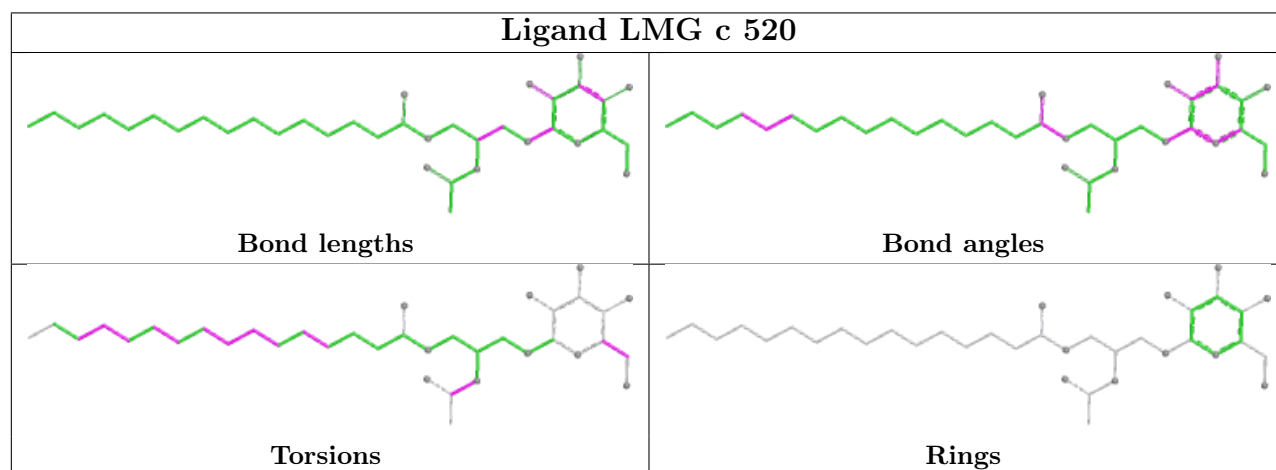
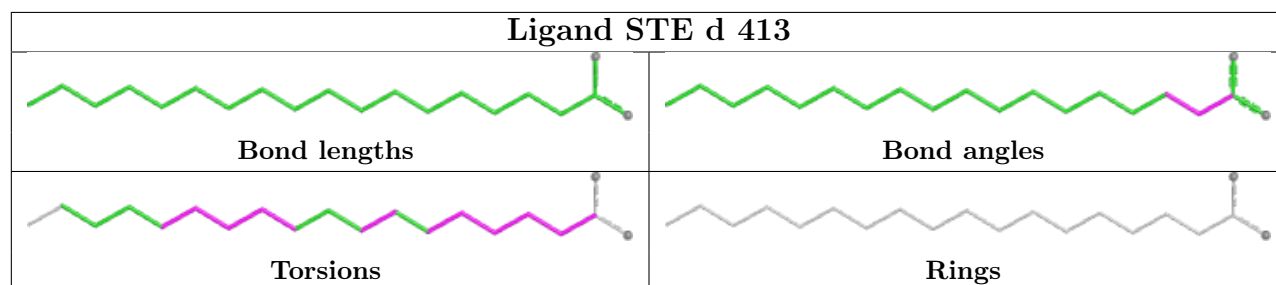
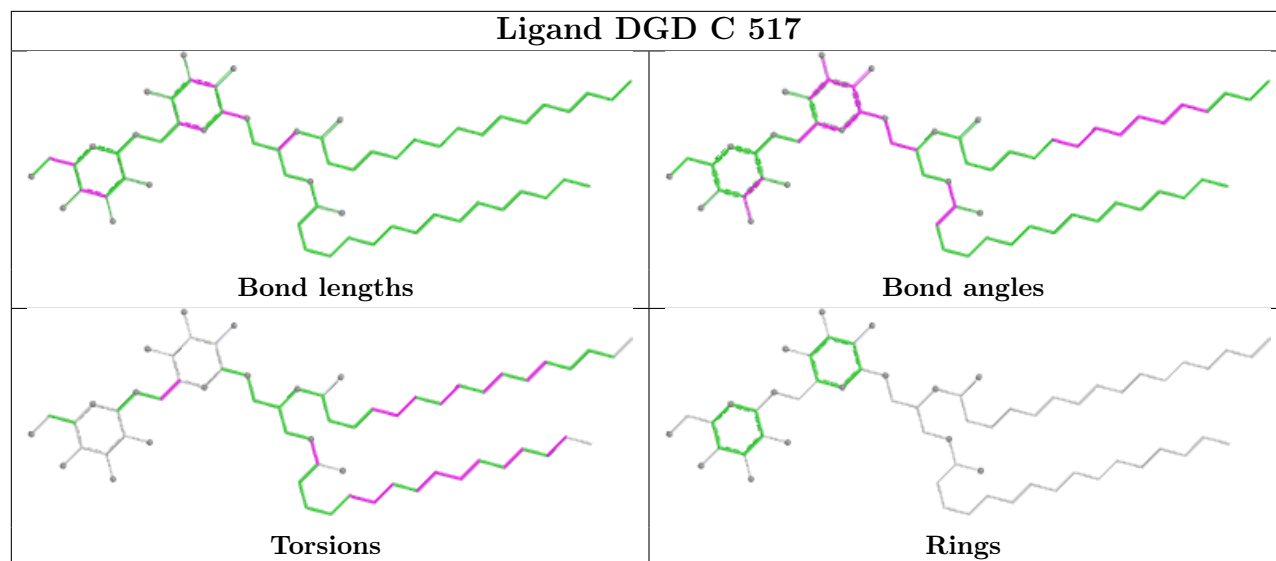


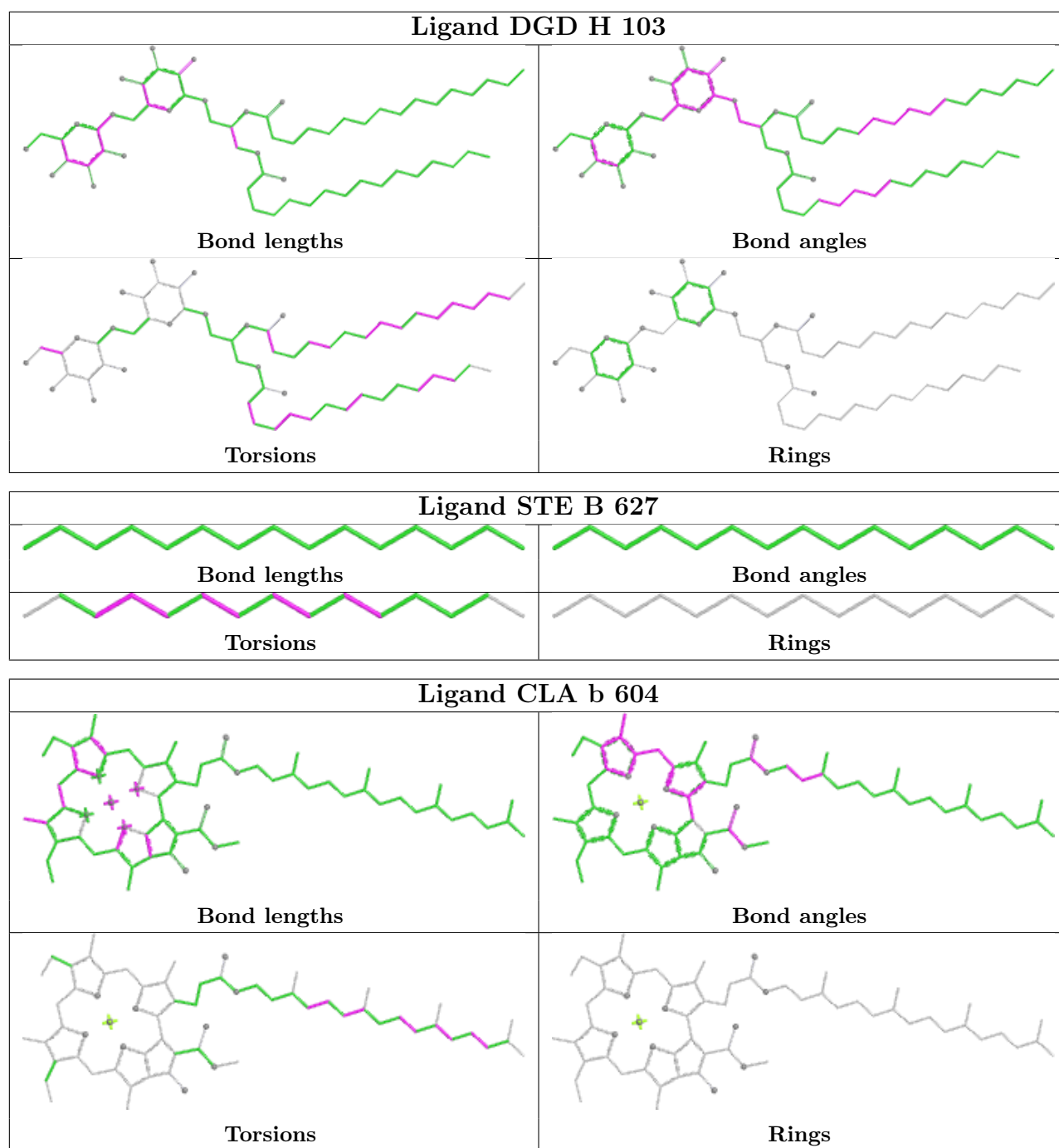
Ligand BCR h 101

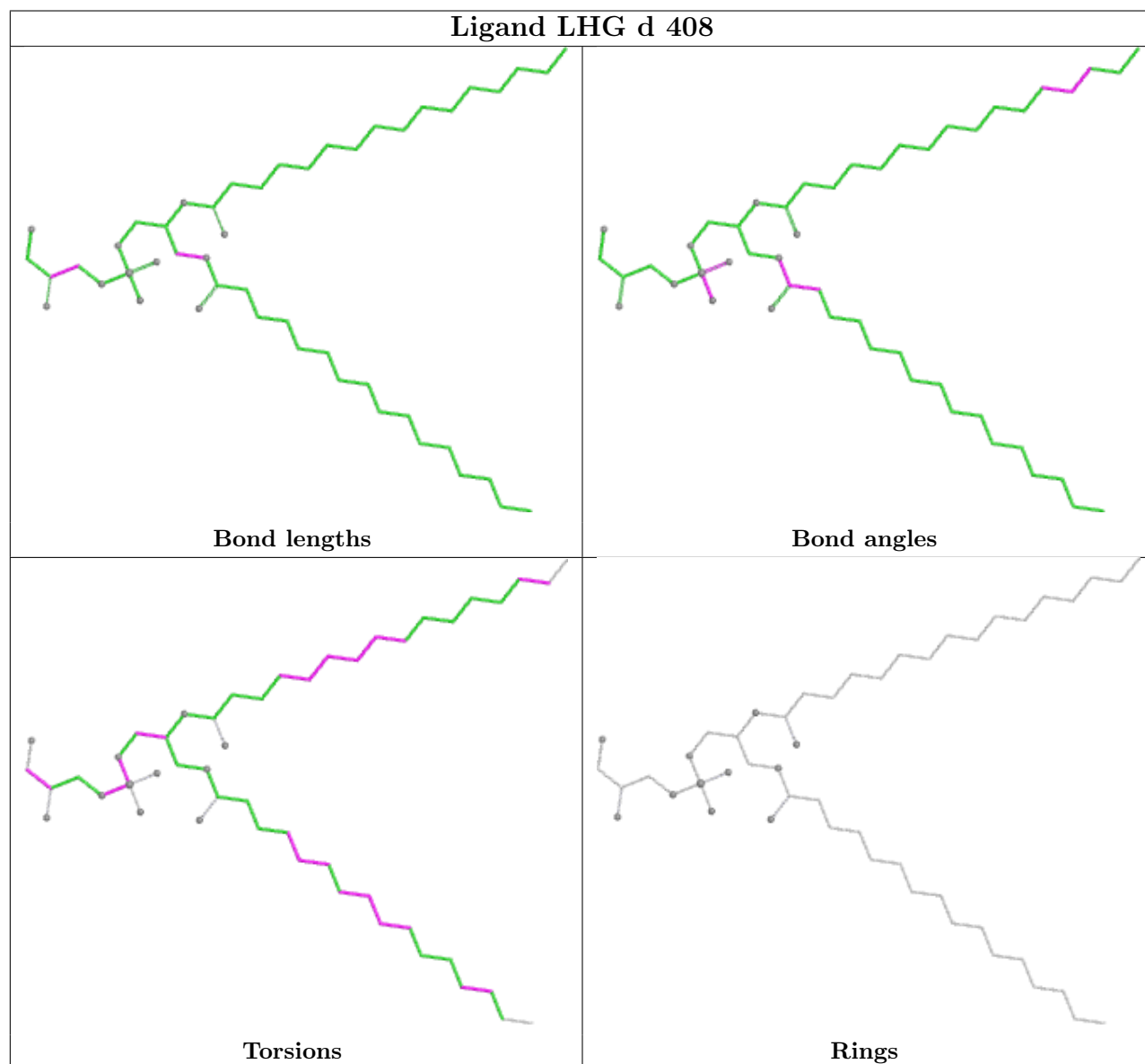
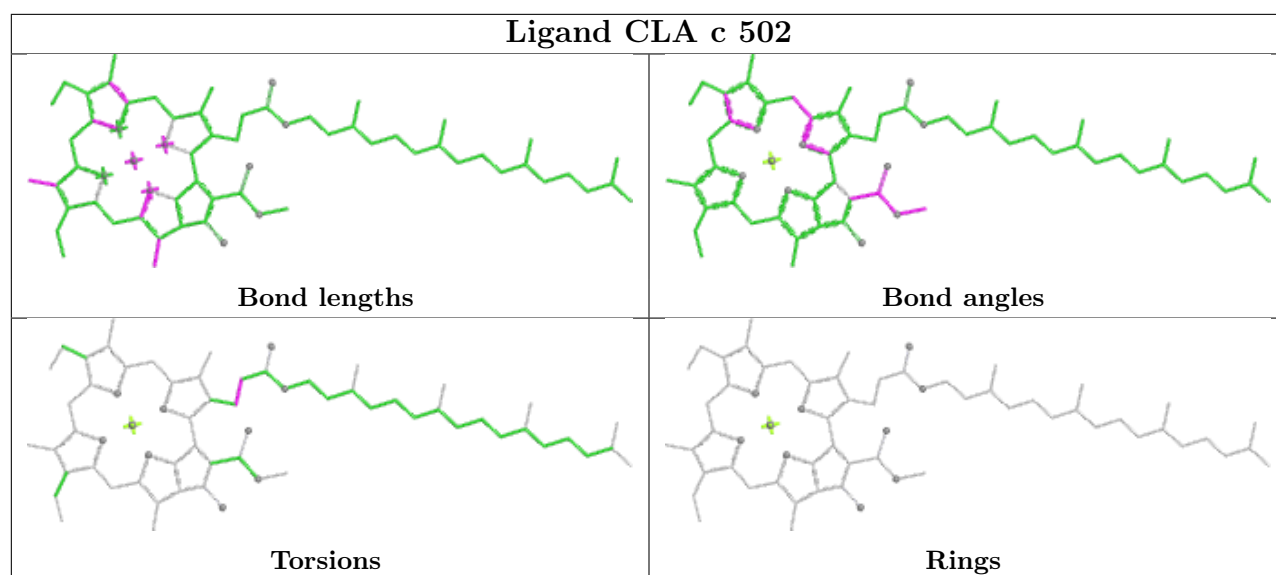


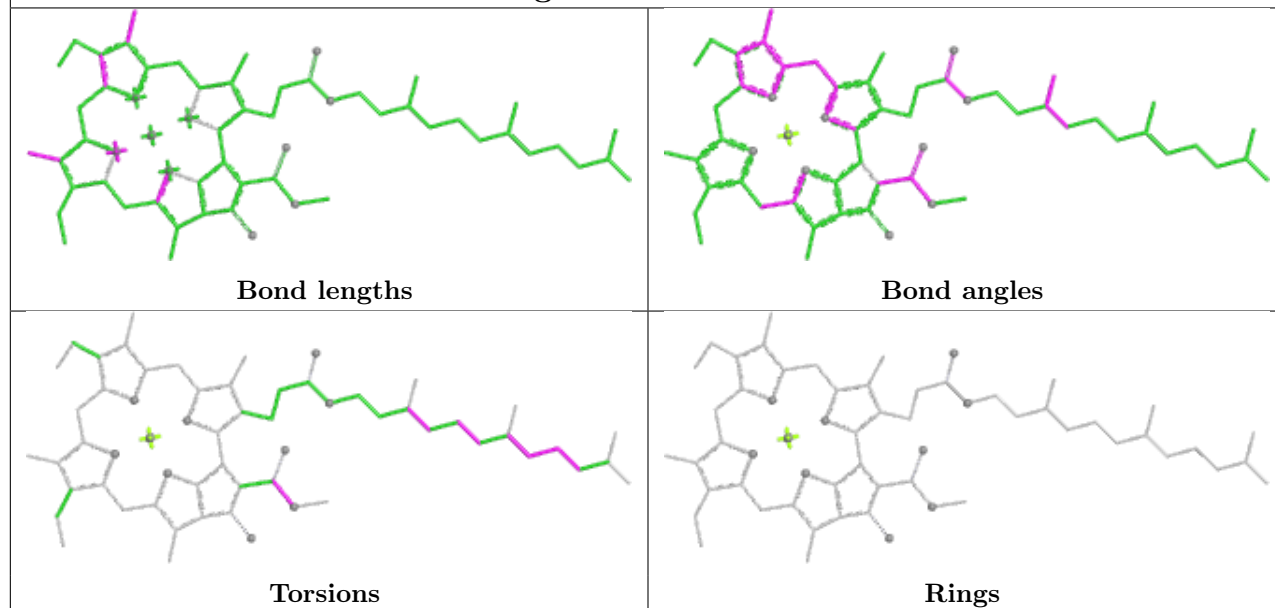
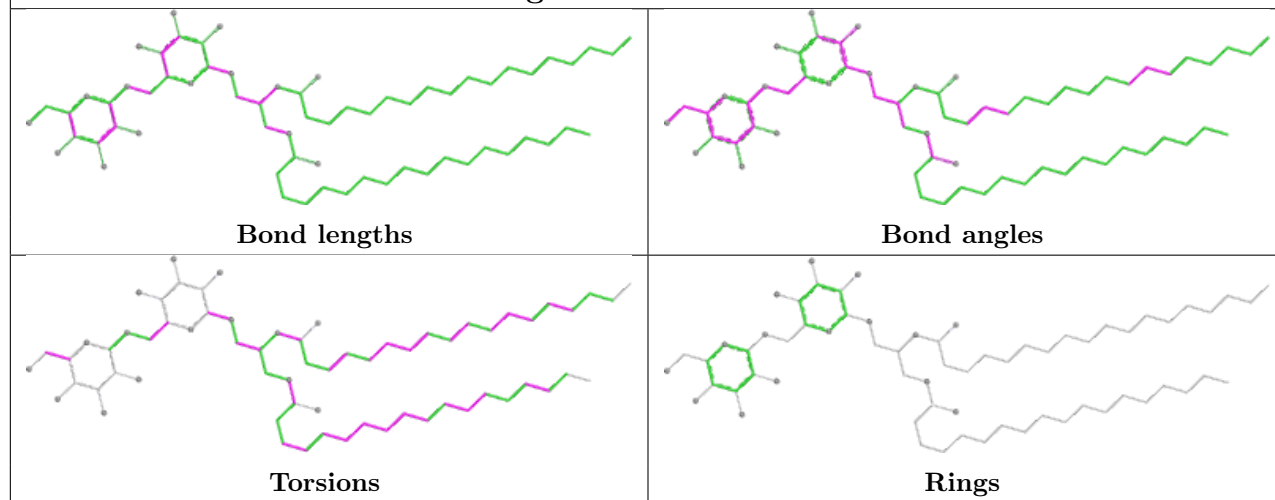




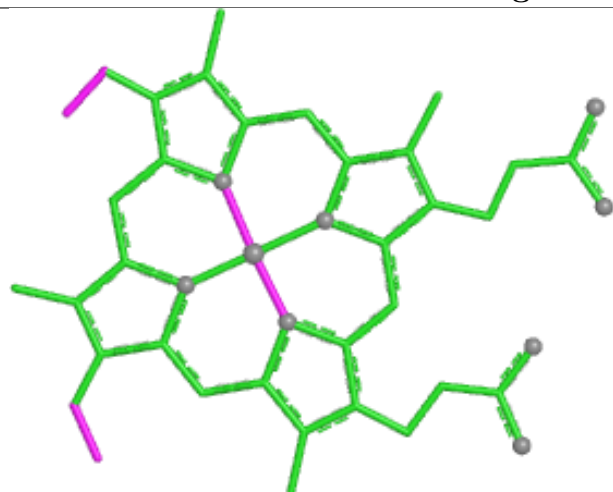




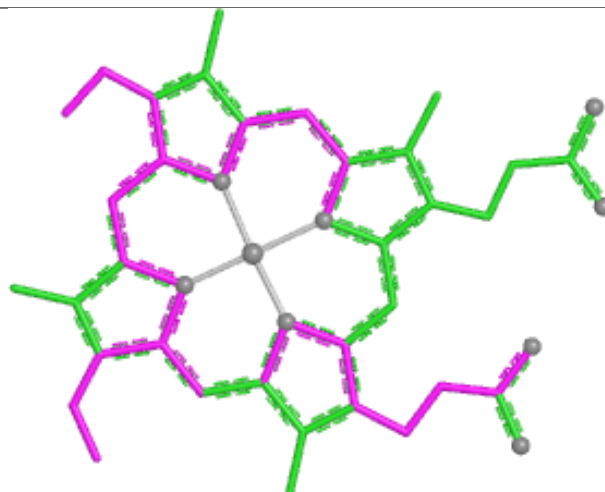


Ligand CLA b 616**Ligand DGD A 413**

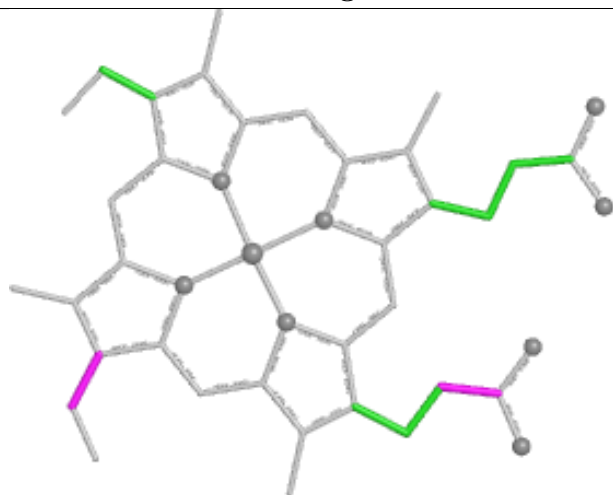
Ligand HEC V 201



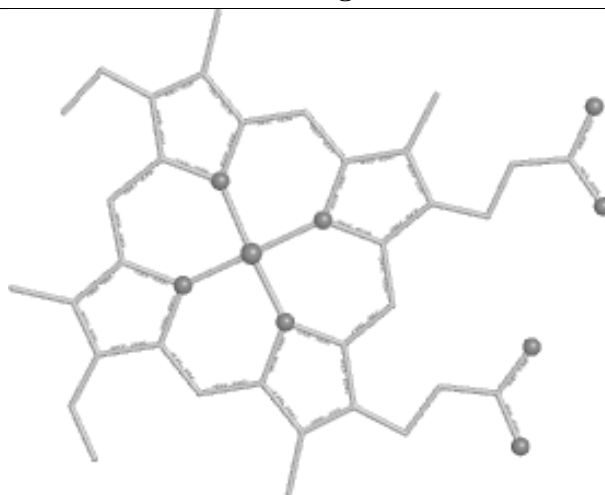
Bond lengths



Bond angles

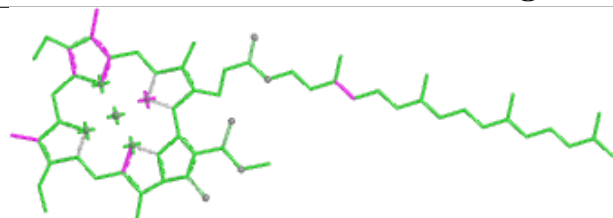


Torsions

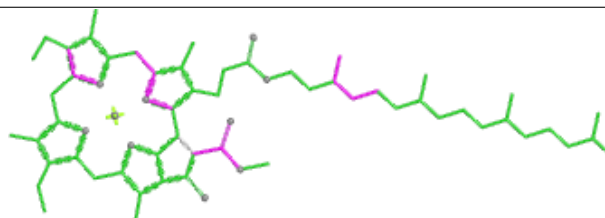


Rings

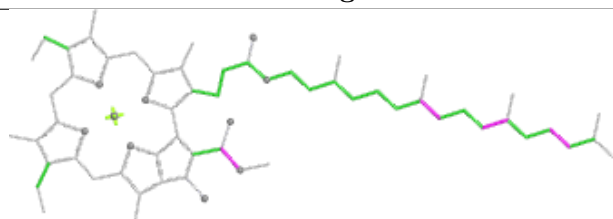
Ligand CLA c 511



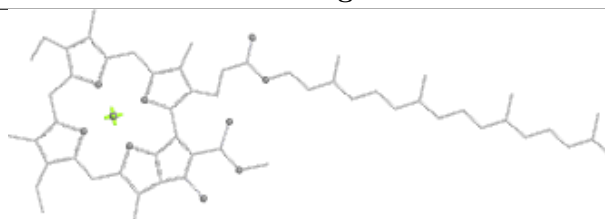
Bond lengths



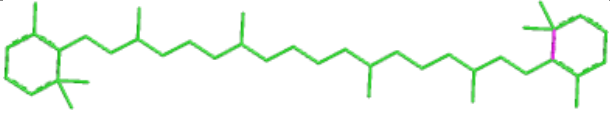
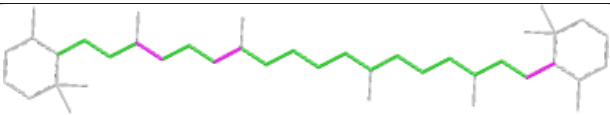
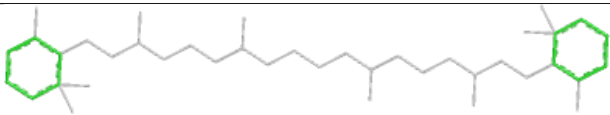
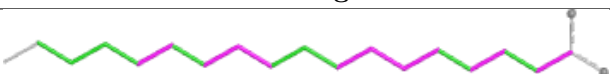
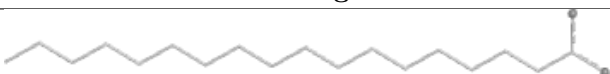
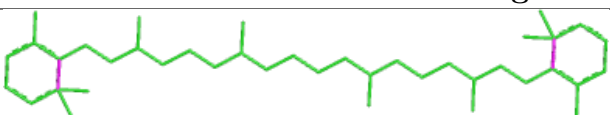
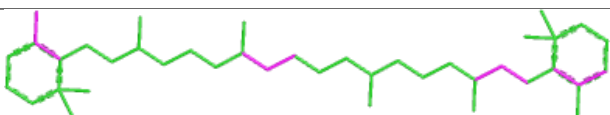
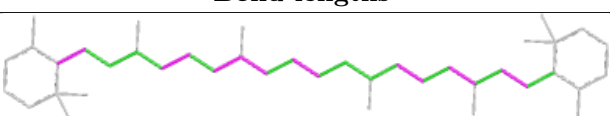
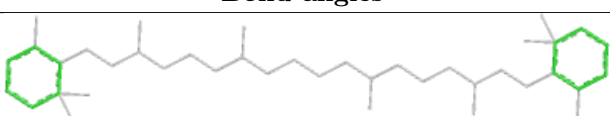
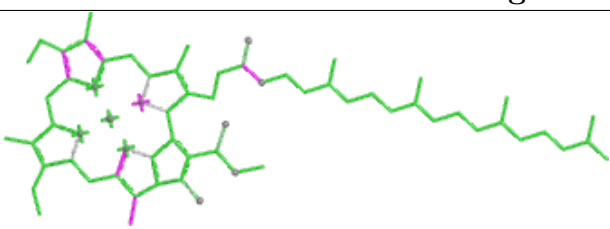
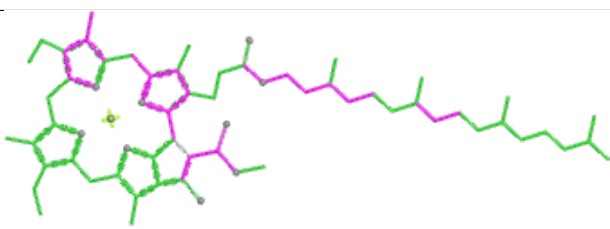
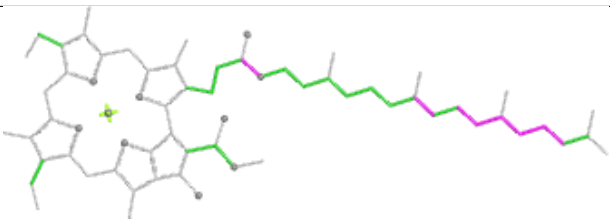
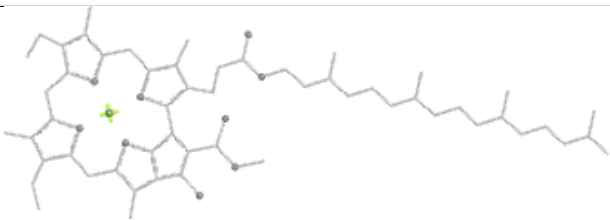
Bond angles

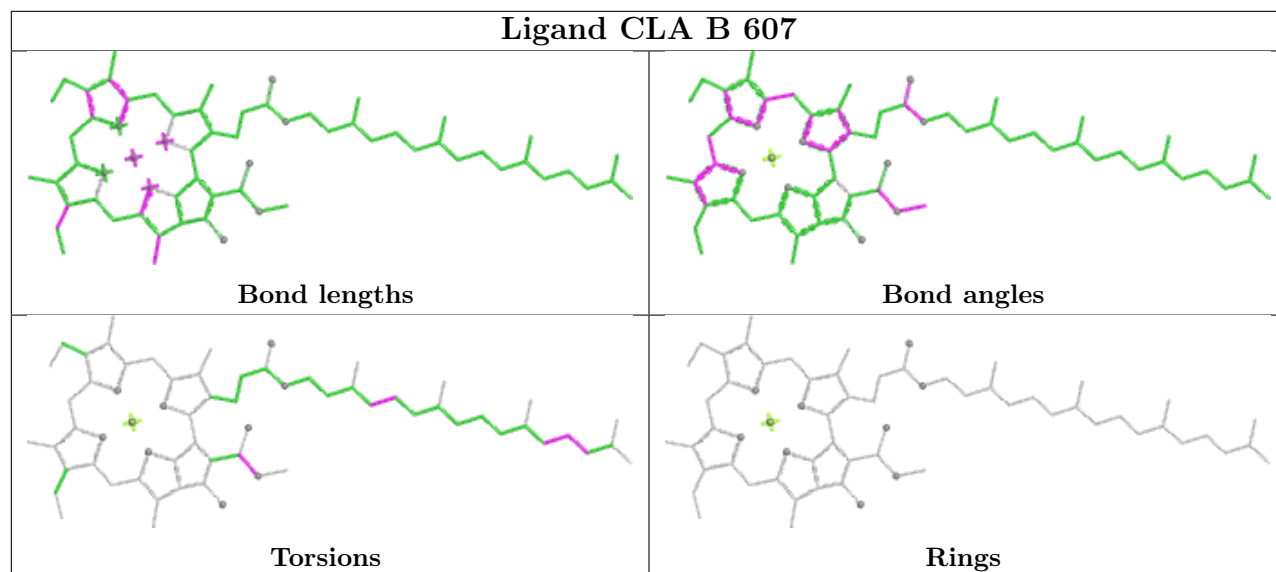
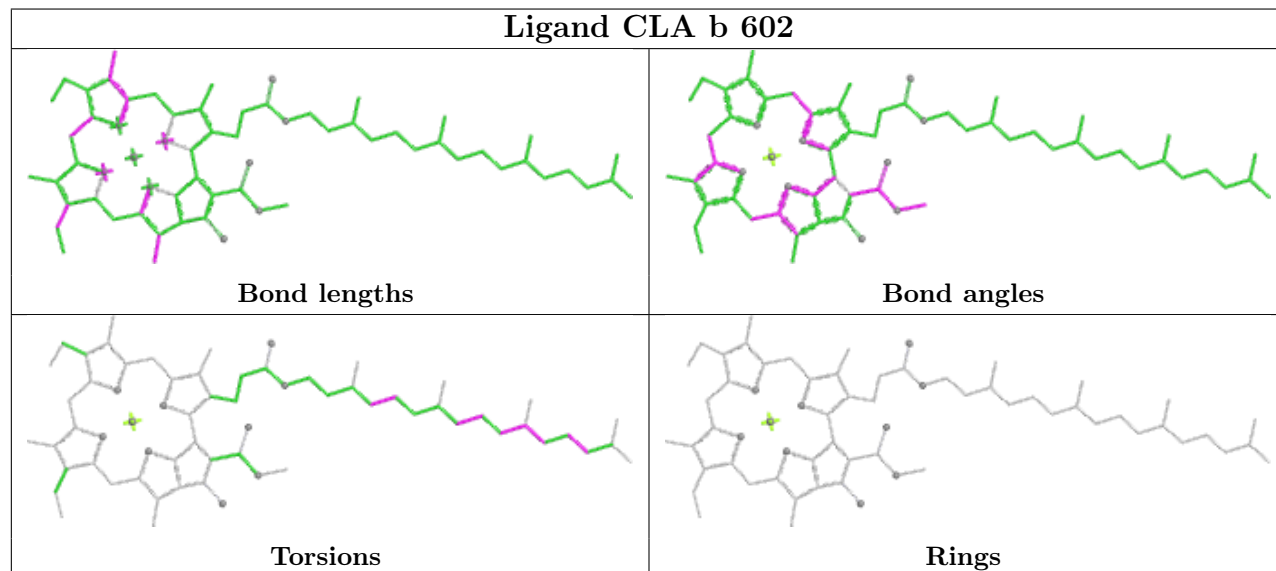


Torsions

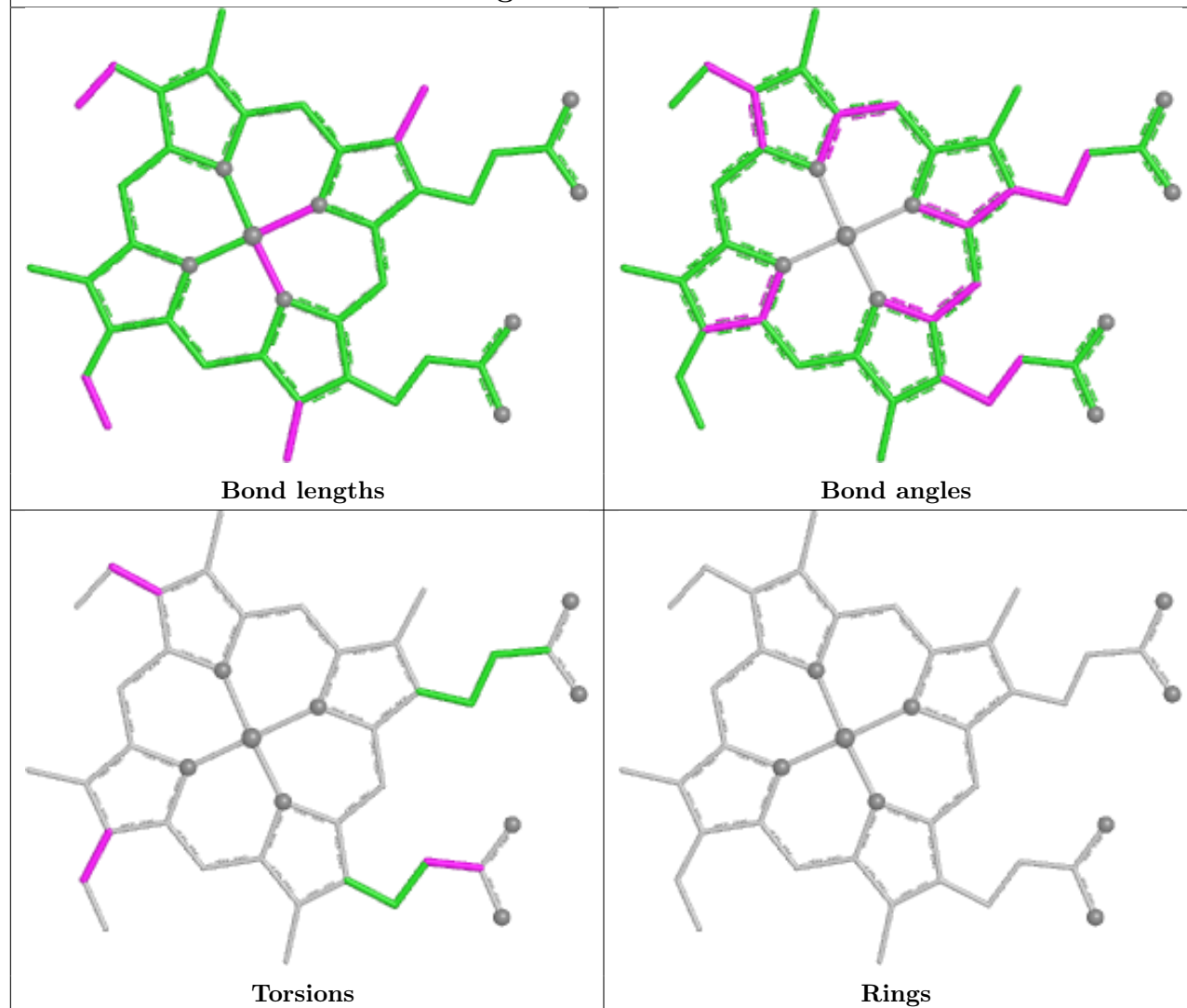


Rings

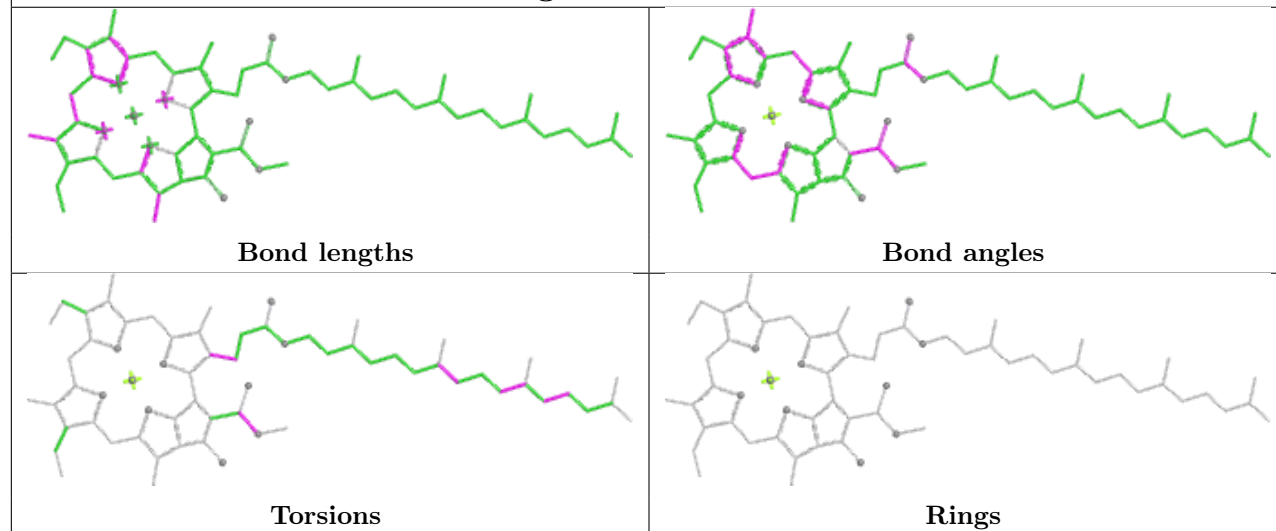
Ligand BCR H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE D 413	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 607**Ligand CLA b 602**

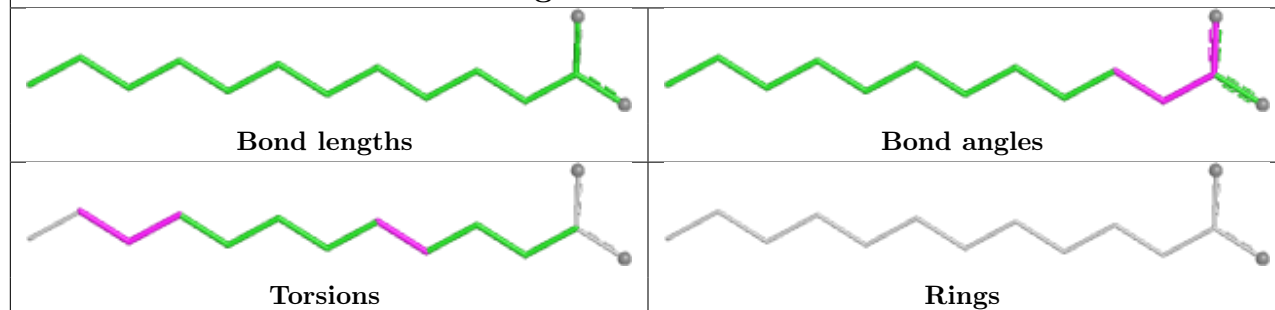
Ligand HEC v 201



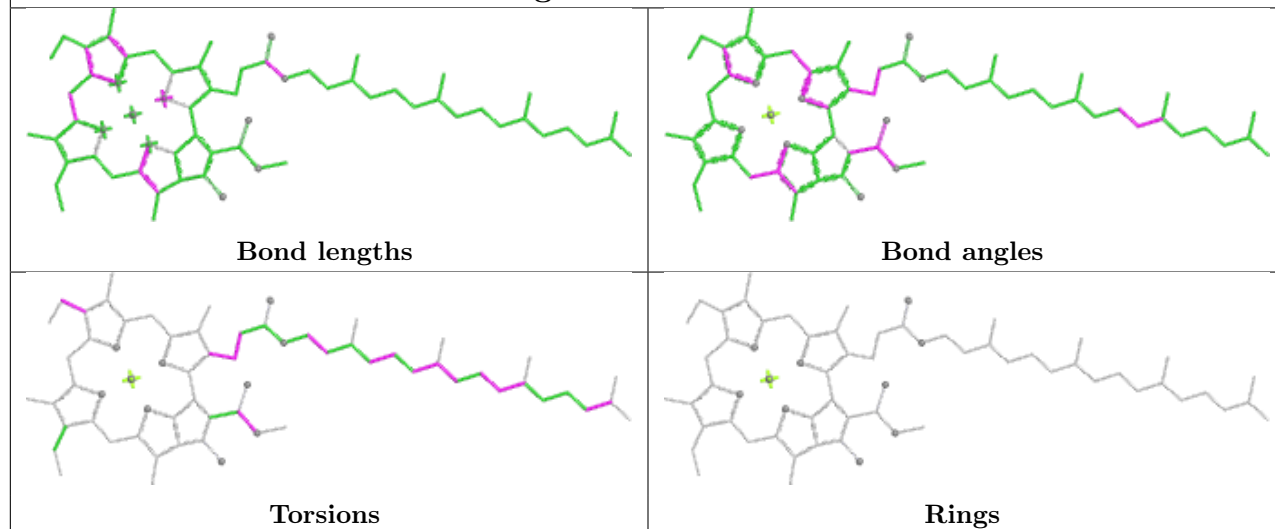
Ligand CLA c 514



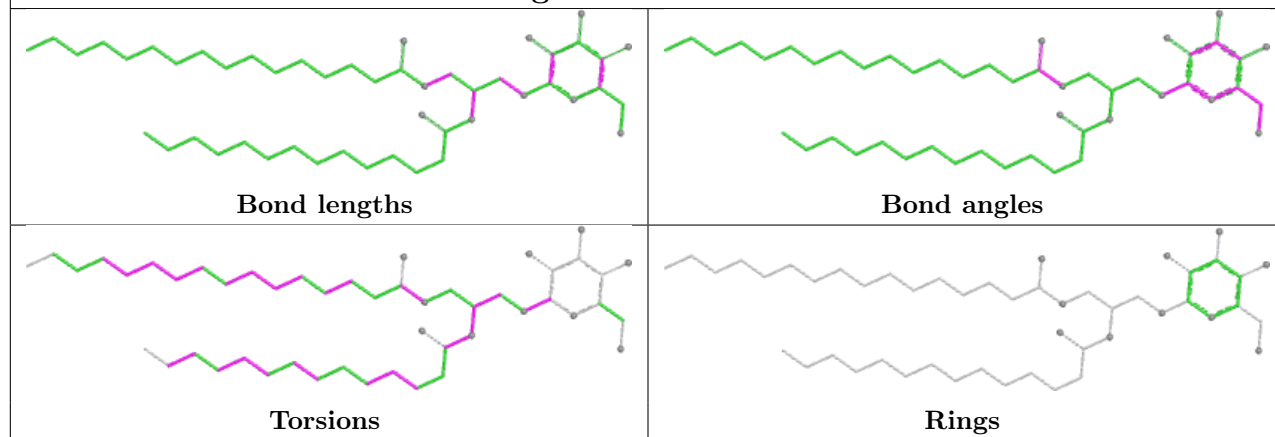
Ligand STE B 623

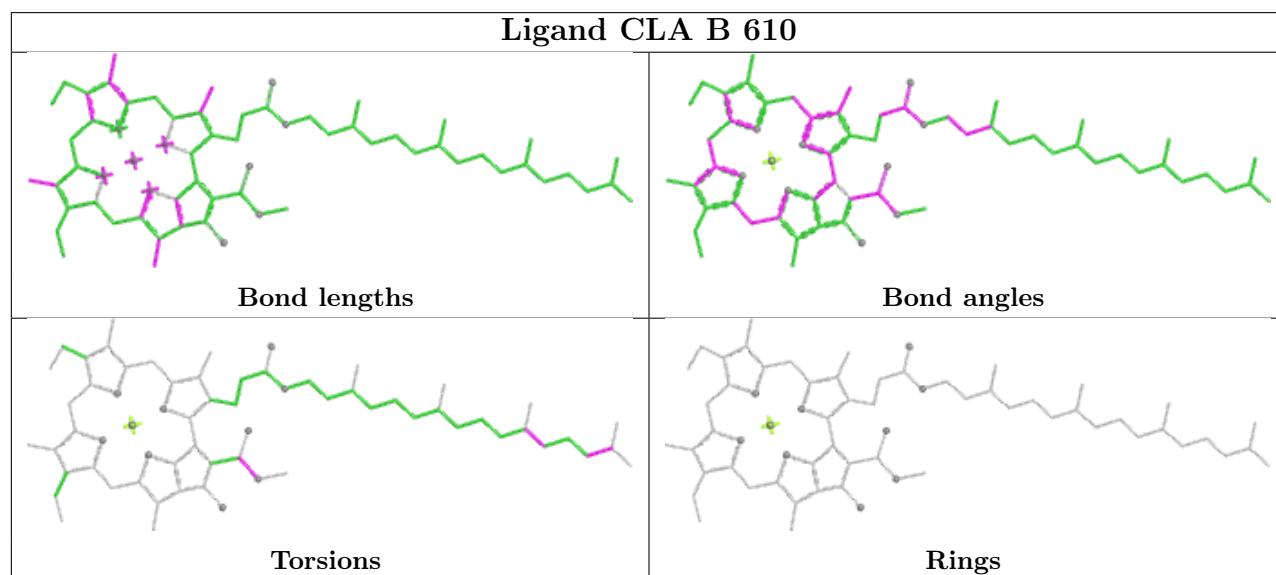
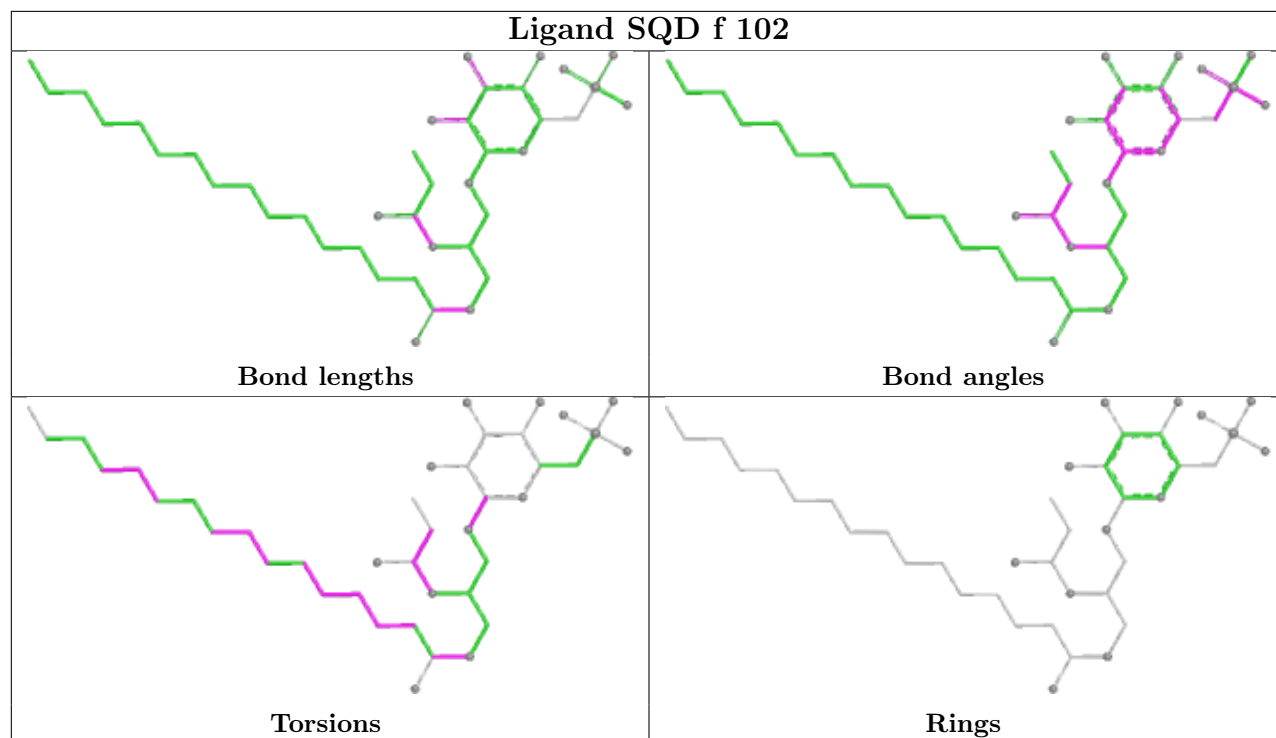


Ligand CLA b 601

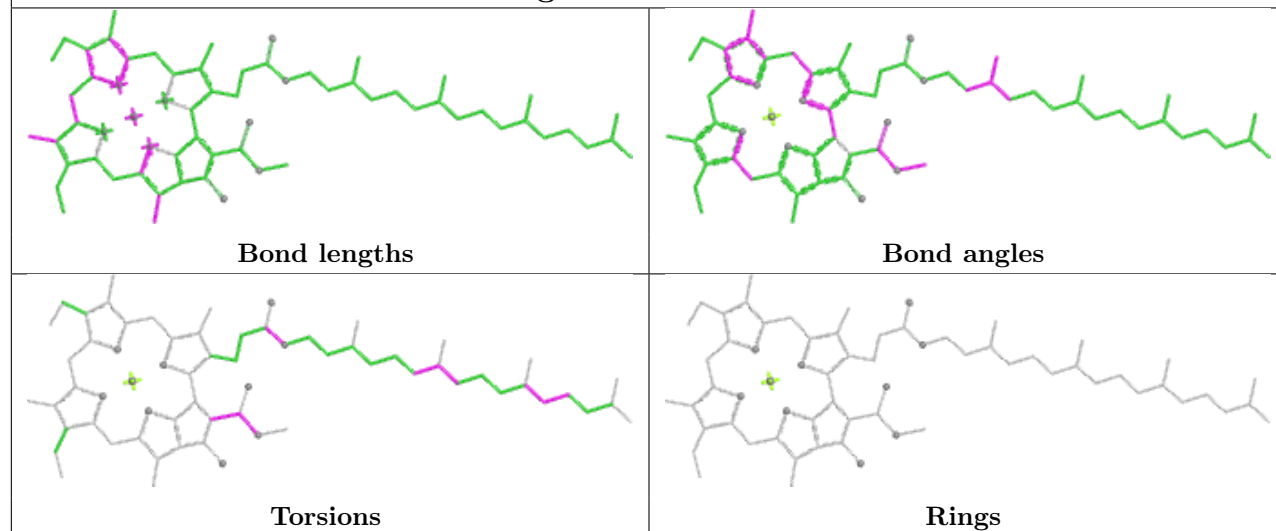


Ligand LMG c 523

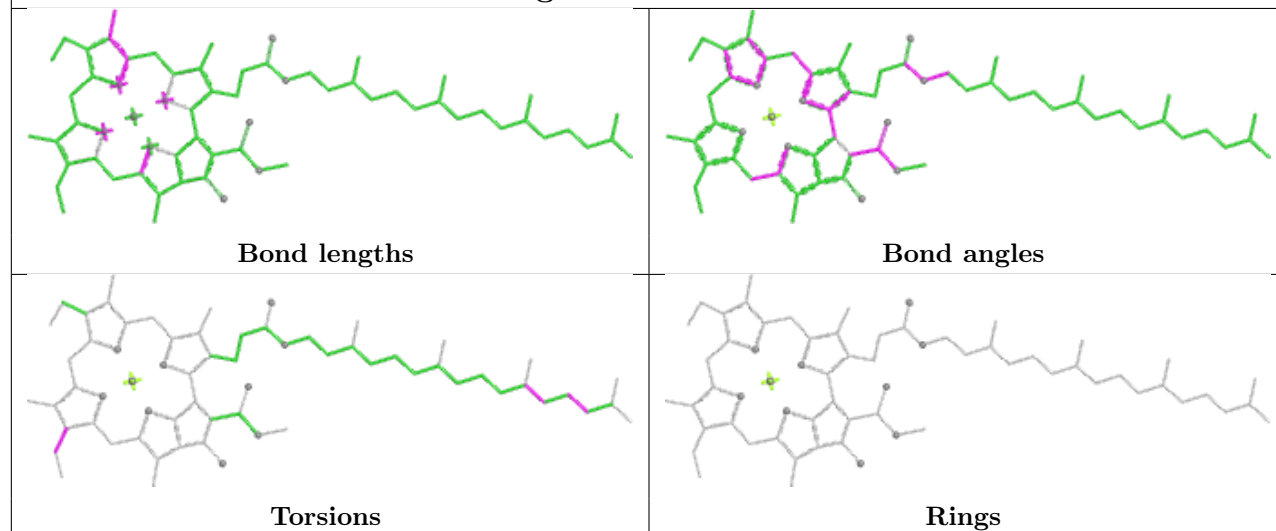




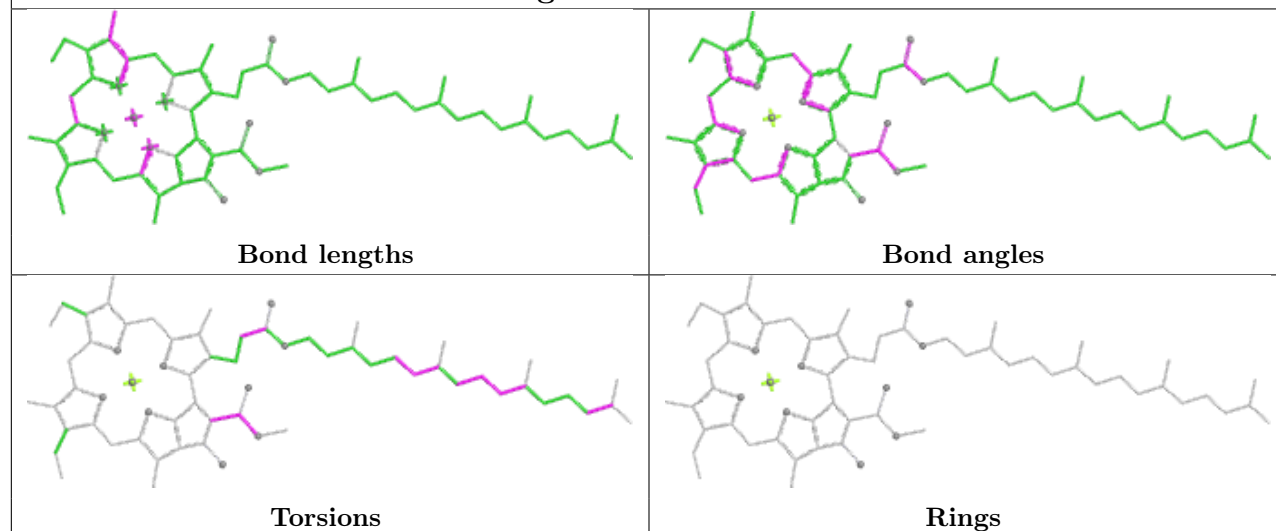
Ligand CLA c 507

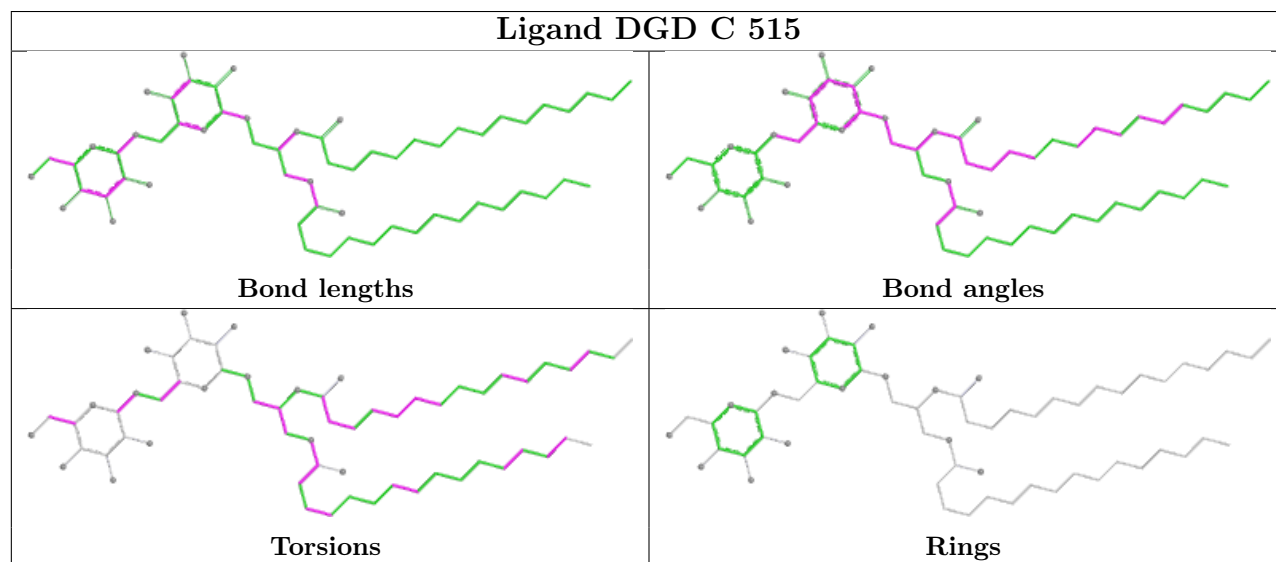
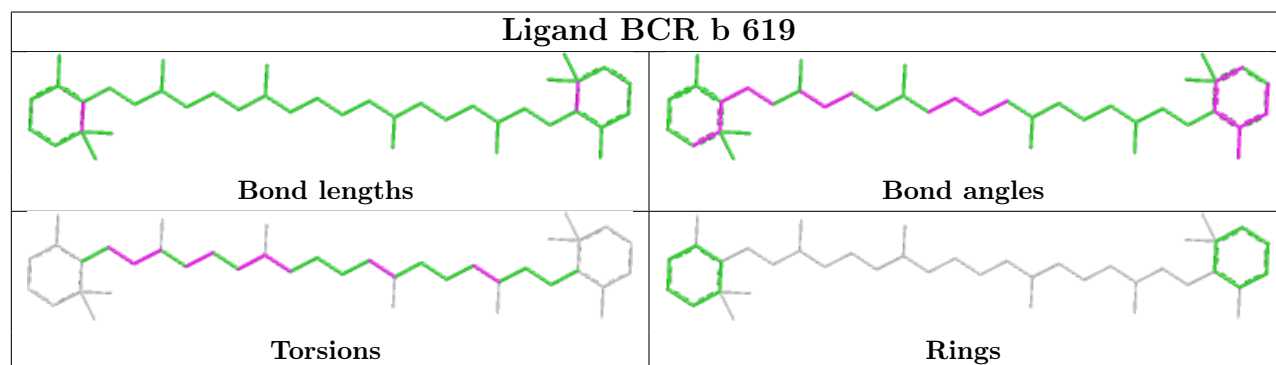
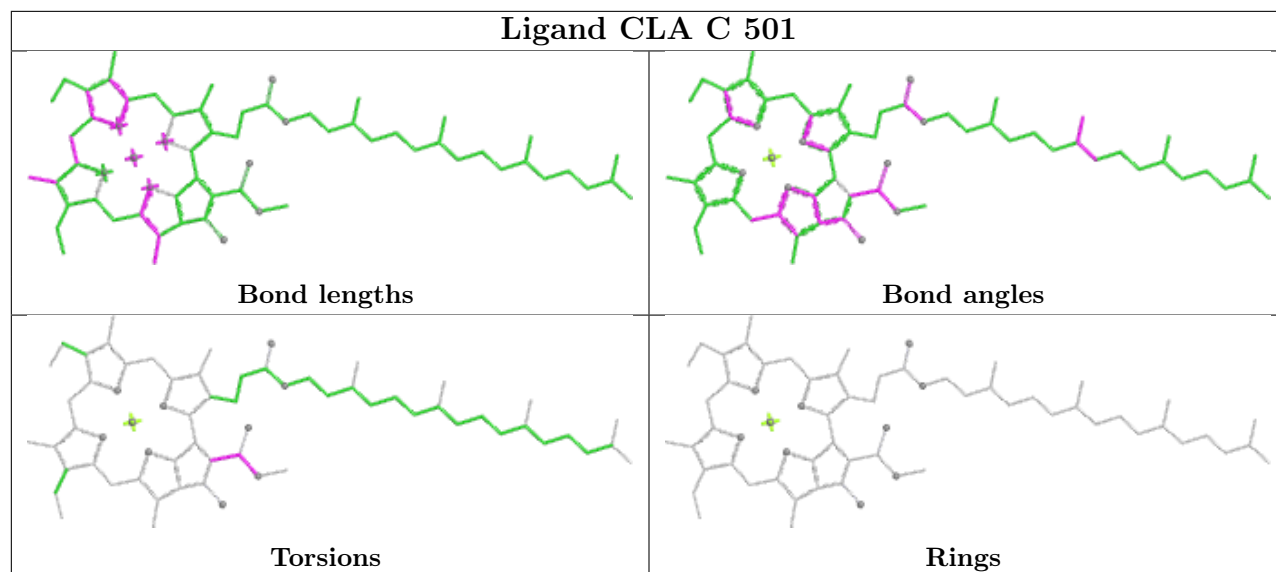


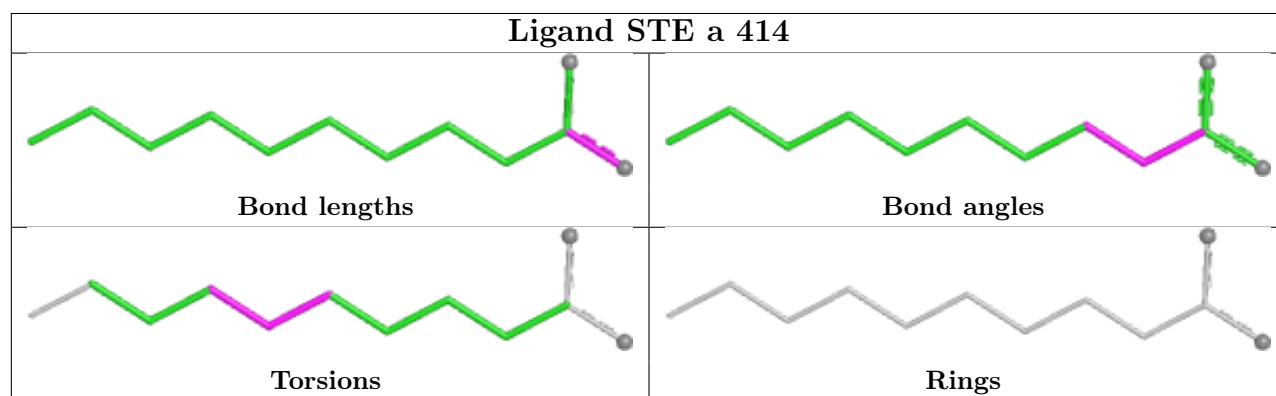
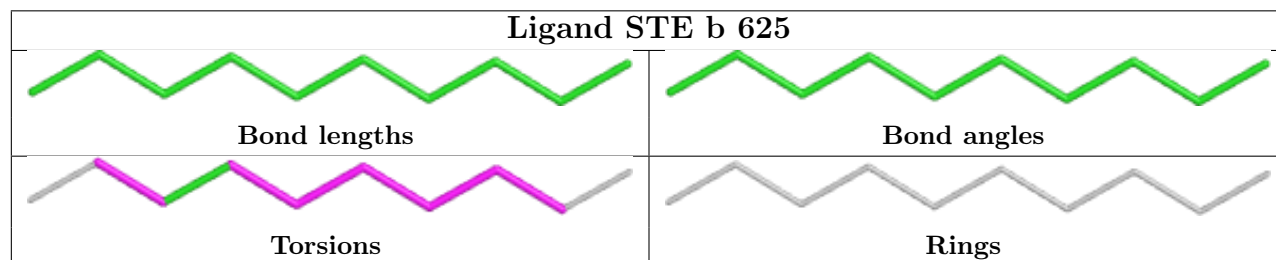
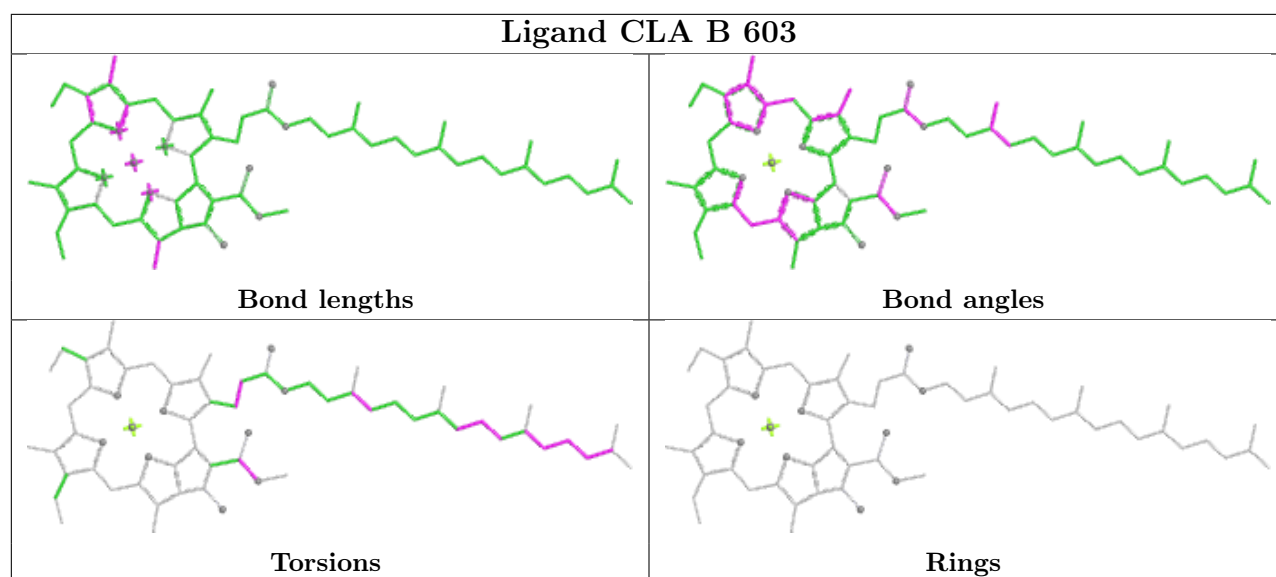
Ligand CLA a 410

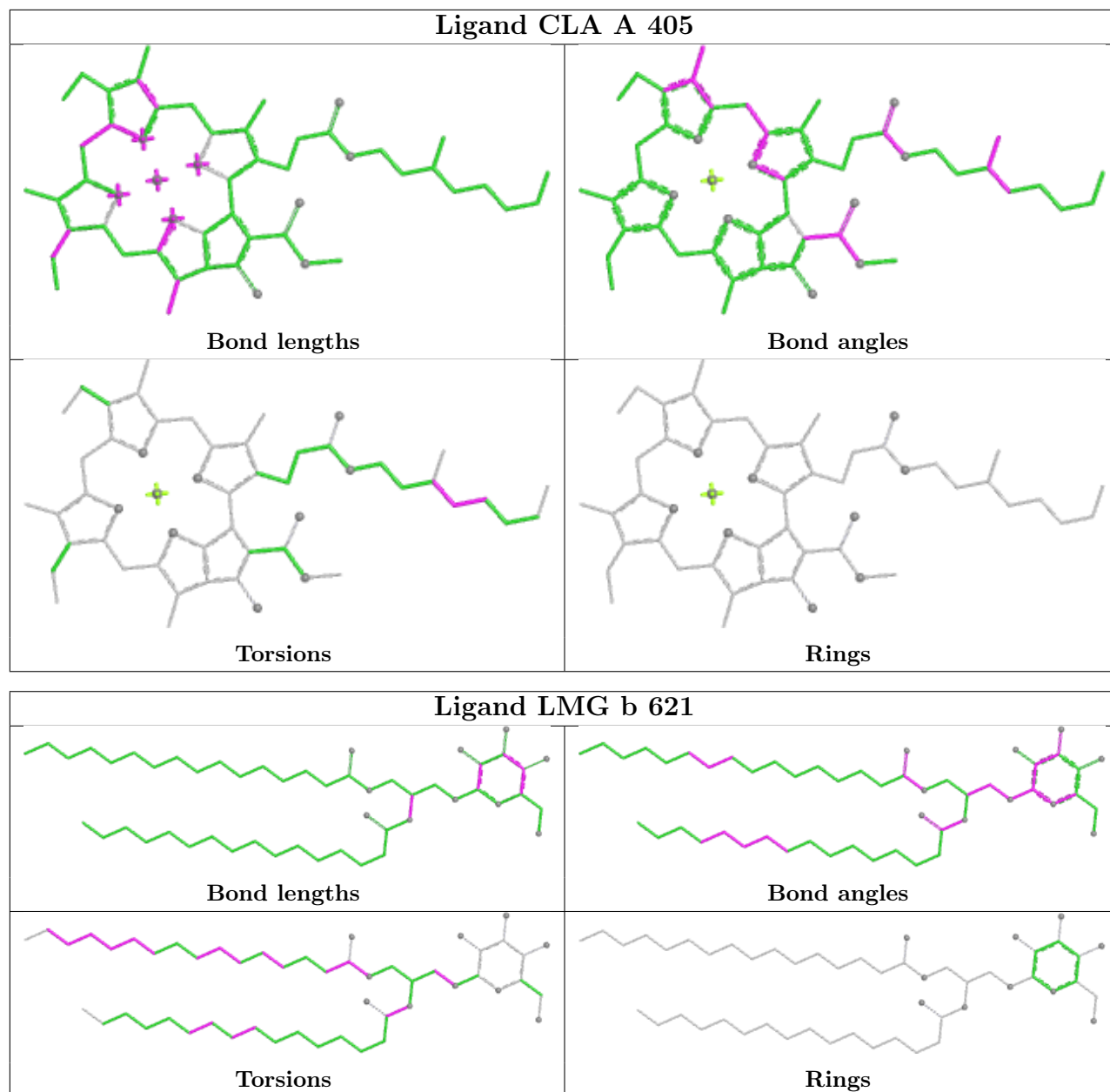


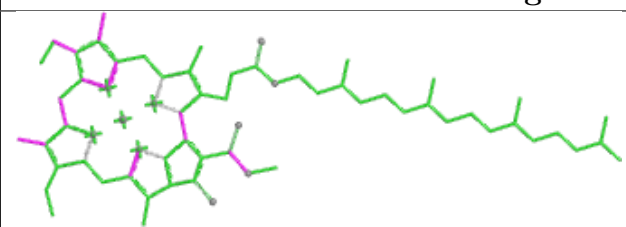
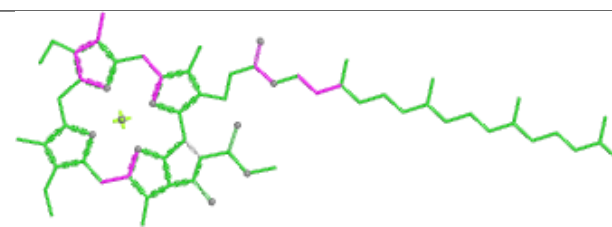
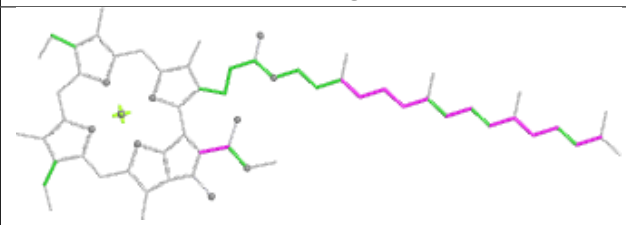
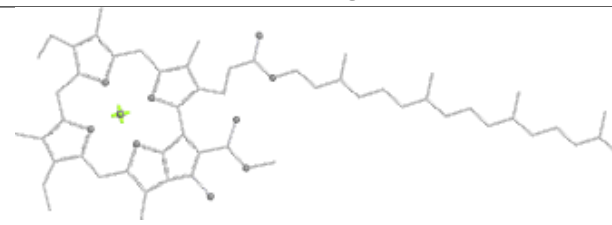
Ligand CLA c 510

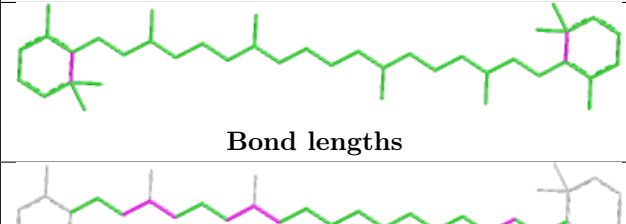
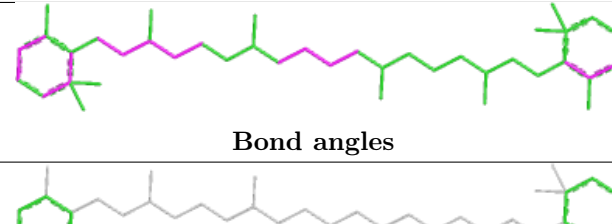
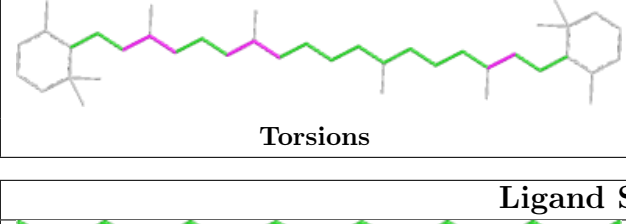
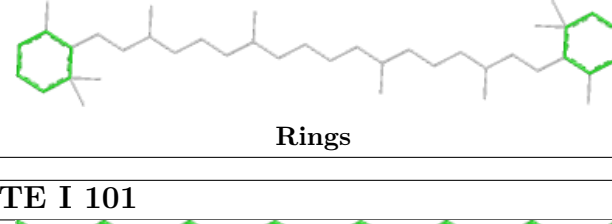


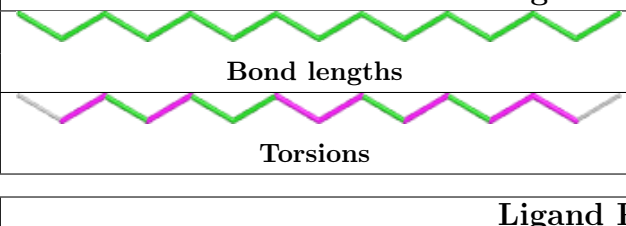
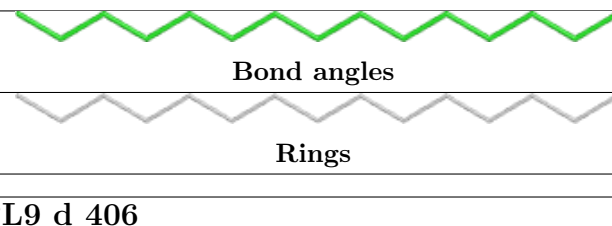
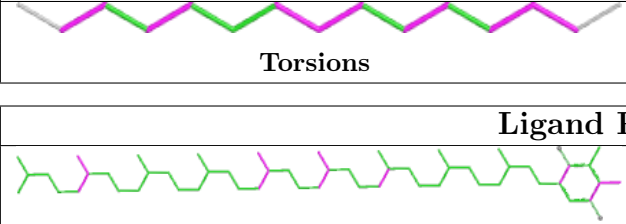
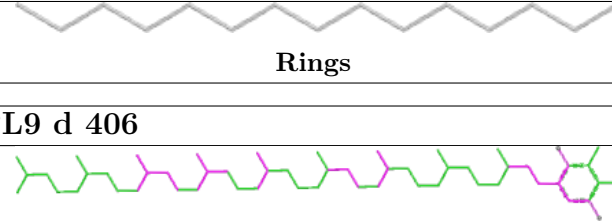


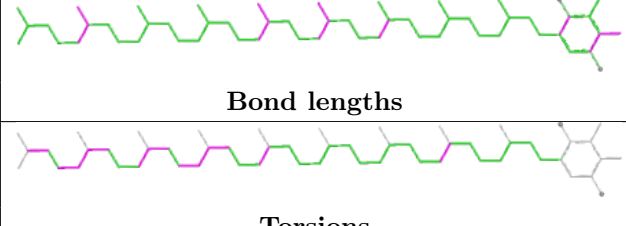
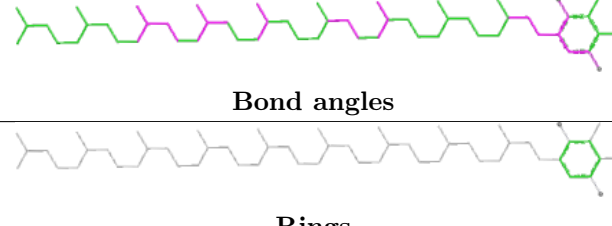
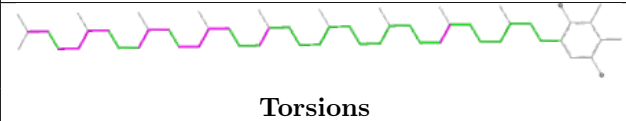
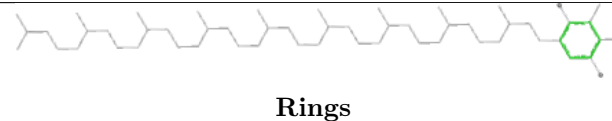




Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.61	0 100 100	22, 30, 53, 81	0
1	a	334/334 (100%)	-0.51	3 (0%) 81 83	23, 33, 62, 80	0
2	B	505/506 (99%)	-0.46	3 (0%) 85 87	18, 35, 66, 99	4 (0%)
2	b	505/506 (99%)	-0.32	6 (1%) 76 78	23, 39, 75, 113	0
3	C	442/461 (95%)	-0.42	0 100 100	16, 38, 57, 84	1 (0%)
3	c	451/461 (97%)	-0.29	2 (0%) 88 90	20, 42, 66, 95	2 (0%)
4	D	341/352 (96%)	-0.60	0 100 100	21, 32, 52, 89	0
4	d	341/352 (96%)	-0.45	0 100 100	23, 36, 59, 85	1 (0%)
5	E	82/84 (97%)	0.17	1 (1%) 76 78	31, 54, 74, 82	1 (1%)
5	e	82/84 (97%)	0.22	1 (1%) 76 78	42, 63, 81, 91	0
6	F	34/45 (75%)	-0.11	0 100 100	38, 46, 70, 95	0
6	f	34/45 (75%)	0.13	0 100 100	45, 52, 83, 93	0
7	H	65/66 (98%)	-0.21	2 (3%) 51 53	33, 44, 63, 74	0
7	h	63/66 (95%)	0.04	2 (3%) 50 52	43, 54, 64, 82	0
8	I	35/38 (92%)	-0.36	0 100 100	31, 41, 72, 87	0
8	i	35/38 (92%)	-0.22	0 100 100	33, 43, 81, 85	0
9	J	36/40 (90%)	-0.06	0 100 100	37, 52, 80, 96	0
9	j	36/40 (90%)	0.08	1 (2%) 55 57	41, 56, 84, 101	0
10	K	37/46 (80%)	-0.05	0 100 100	45, 56, 75, 81	0
10	k	37/46 (80%)	0.16	0 100 100	51, 60, 72, 79	0
11	L	37/37 (100%)	-0.64	0 100 100	26, 33, 66, 71	0
11	l	36/37 (97%)	-0.57	0 100 100	26, 33, 76, 87	0
12	M	32/36 (88%)	-0.51	0 100 100	28, 36, 57, 72	0
12	m	31/36 (86%)	-0.50	0 100 100	29, 37, 53, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.29	1 (0%) 88 90	26, 43, 85, 134	1 (0%)
13	o	244/272 (89%)	-0.26	1 (0%) 88 90	25, 42, 80, 113	0
14	R	34/40 (85%)	0.84	2 (5%) 28 29	66, 80, 102, 111	0
14	r	31/40 (77%)	1.46	6 (19%) 3 3	73, 100, 118, 130	0
15	T	29/30 (96%)	-0.64	0 100 100	27, 33, 65, 80	0
15	t	29/30 (96%)	-0.39	2 (6%) 23 24	26, 34, 80, 96	0
16	U	97/134 (72%)	-0.25	0 100 100	32, 46, 70, 92	0
16	u	97/134 (72%)	-0.36	0 100 100	31, 42, 57, 82	0
17	V	137/163 (84%)	-0.38	0 100 100	31, 43, 60, 79	0
17	v	137/163 (84%)	-0.12	0 100 100	33, 49, 71, 88	0
18	X	38/41 (92%)	-0.14	0 100 100	42, 55, 78, 84	0
18	x	39/41 (95%)	0.19	1 (2%) 57 60	50, 65, 94, 109	0
19	Y	27/46 (58%)	0.81	2 (7%) 20 22	54, 78, 93, 103	0
19	y	30/46 (65%)	0.61	0 100 100	63, 77, 92, 99	0
20	Z	62/62 (100%)	0.61	2 (3%) 50 52	57, 74, 120, 131	0
20	z	62/62 (100%)	0.58	1 (1%) 70 73	59, 75, 112, 130	0
All	All	5302/5666 (93%)	-0.30	39 (0%) 84 86	16, 40, 78, 134	10 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.3
14	R	35	LEU	4.2
15	t	30	THR	3.9
14	r	32	GLN	3.7
20	Z	62	VAL	3.0
7	H	41	PHE	3.0
2	B	479[A]	PHE	2.9
9	j	6	GLY	2.8
7	h	64	ALA	2.8
20	z	33	TRP	2.8
18	x	40	SER	2.7
2	b	494	GLY	2.7
3	c	147	PHE	2.7
5	e	79	PHE	2.7
2	b	495	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
14	r	14	LEU	2.6
19	Y	41	VAL	2.6
2	b	488	PRO	2.6
14	r	19	ALA	2.6
7	h	41	PHE	2.5
2	B	495	PHE	2.5
2	B	499	VAL	2.5
2	b	490	GLN	2.4
14	r	31	VAL	2.4
20	Z	33	TRP	2.4
13	O	60	ARG	2.3
14	r	20	VAL	2.3
1	a	249	VAL	2.3
14	r	3	TRP	2.3
19	Y	22	LEU	2.2
14	R	7	VAL	2.2
3	c	23	ALA	2.1
2	b	127	ARG	2.1
1	a	248	ILE	2.1
15	t	29	ILE	2.1
1	a	250	ALA	2.1
5	E	74	GLN	2.1
2	b	84	THR	2.1
7	H	65	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.94	0.09	40,53,69,79	0
8	FME	I	1	10/11	0.95	0.07	40,48,64,66	0
15	FME	T	1	10/11	0.95	0.08	29,44,67,67	0
12	FME	m	1	10/11	0.96	0.07	33,47,65,76	0
8	FME	i	1	10/11	0.96	0.09	40,50,65,66	0
15	FME	t	1	10/11	0.96	0.07	28,43,73,73	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	STE	E	102	12/20	0.74	0.17	46,78,92,94	0
31	STE	b	625	10/20	0.74	0.17	44,53,61,73	0
31	STE	I	101	15/20	0.77	0.17	37,55,73,76	0
33	LHG	E	101	49/49	0.77	0.14	50,83,110,126	0
31	STE	b	624	20/20	0.79	0.15	41,60,75,89	0
31	STE	b	627	20/20	0.80	0.14	38,64,84,90	0
33	LHG	e	101	42/49	0.80	0.14	65,87,116,127	0
31	STE	H	104	18/20	0.81	0.16	44,73,89,94	0
31	STE	B	627	15/20	0.81	0.19	36,61,74,77	0
31	STE	j	101	12/20	0.81	0.13	42,56,74,75	0
31	STE	a	414	12/20	0.81	0.13	40,65,71,75	0
26	PL9	a	409	55/55	0.81	0.17	47,74,93,96	0
31	STE	m	102	12/20	0.82	0.17	46,61,76,76	0
27	LMG	b	623	55/55	0.82	0.15	42,70,95,101	0
26	PL9	A	409	55/55	0.82	0.16	47,68,94,97	0
27	LMG	c	522	48/55	0.83	0.14	46,80,104,108	0
27	LMG	a	415	55/55	0.83	0.13	34,58,80,92	0
31	STE	C	519	16/20	0.83	0.13	42,58,73,77	0
31	STE	a	413	10/20	0.83	0.13	38,61,67,68	0
31	STE	B	626	16/20	0.84	0.13	35,58,78,79	0
31	STE	c	501	12/20	0.84	0.12	54,68,87,89	0
29	DGD	A	413	66/66	0.85	0.11	44,62,78,99	0
31	STE	T	102	15/20	0.85	0.14	44,59,83,85	0
27	LMG	D	411	33/55	0.85	0.13	34,56,84,89	0
28	SQD	a	412	36/54	0.85	0.13	29,63,90,97	0
31	STE	d	411	16/20	0.86	0.14	45,62,78,83	0
22	CLA	b	601	65/65	0.86	0.12	43,68,89,92	0
31	STE	m	101	18/20	0.86	0.12	34,51,78,79	0
31	STE	b	626	14/20	0.86	0.14	51,65,84,88	0
31	STE	B	620	17/20	0.86	0.11	32,50,63,71	0
27	LMG	Y	101	48/55	0.86	0.12	34,68,86,99	0
31	STE	b	622	20/20	0.87	0.10	36,54,79,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	SQD	f	102	41/54	0.87	0.13	55,91,113,119	0
31	STE	b	620	16/20	0.87	0.12	35,46,64,71	0
31	STE	C	518	12/20	0.88	0.10	41,55,62,66	0
27	LMG	c	520	37/55	0.88	0.11	40,67,80,83	0
31	STE	B	625	18/20	0.88	0.11	40,58,76,83	0
27	LMG	A	410	48/55	0.88	0.10	38,57,72,87	0
28	SQD	A	412	39/54	0.88	0.11	42,61,90,93	0
31	STE	c	521	20/20	0.88	0.11	37,55,93,103	0
24	BCR	K	101	40/40	0.89	0.12	40,58,75,82	0
31	STE	B	601	12/20	0.89	0.13	51,67,78,86	0
28	SQD	B	622	54/54	0.89	0.10	37,61,91,101	0
31	STE	d	413	20/20	0.89	0.10	42,57,76,84	0
28	SQD	L	101	49/54	0.89	0.09	38,60,89,107	0
22	CLA	H	101	65/65	0.89	0.11	33,63,91,110	0
31	STE	J	101	12/20	0.89	0.12	45,59,69,77	0
27	LMG	c	523	49/55	0.89	0.10	30,56,82,98	0
31	STE	Z	101	8/20	0.89	0.16	50,61,70,70	0
31	STE	M	102	15/20	0.90	0.11	32,48,69,74	0
31	STE	M	103	10/20	0.90	0.11	34,47,64,70	0
27	LMG	b	621	51/55	0.90	0.10	32,53,76,97	0
31	STE	B	623	14/20	0.90	0.10	36,47,56,62	0
31	STE	B	624	12/20	0.90	0.10	32,48,63,76	0
31	STE	d	412	17/20	0.90	0.11	41,56,67,74	0
31	STE	C	520	12/20	0.91	0.09	34,46,57,58	0
31	STE	D	413	20/20	0.91	0.10	34,54,71,79	0
24	BCR	h	101	40/40	0.91	0.09	35,54,73,79	0
27	LMG	B	621	28/55	0.91	0.11	35,51,65,73	0
24	BCR	k	101	40/40	0.91	0.10	42,60,81,85	0
24	BCR	K	102	40/40	0.91	0.09	33,53,68,74	0
24	BCR	c	515	40/40	0.91	0.10	41,62,76,77	0
22	CLA	c	513	65/65	0.92	0.10	38,56,91,106	0
27	LMG	M	101	51/55	0.92	0.08	31,48,72,90	0
22	CLA	C	513	65/65	0.92	0.10	38,64,97,109	0
29	DGD	C	516	62/66	0.92	0.09	34,51,97,119	0
29	DGD	h	102	62/66	0.92	0.09	29,48,65,68	0
28	SQD	D	408	36/54	0.92	0.11	46,75,89,100	0
24	BCR	d	405	40/40	0.92	0.10	28,54,85,95	0
24	BCR	C	514	40/40	0.93	0.08	23,38,55,63	0
28	SQD	a	411	54/54	0.93	0.10	39,62,94,96	0
24	BCR	F	101	40/40	0.93	0.09	21,44,82,90	0
24	BCR	H	102	40/40	0.93	0.08	30,50,66,75	0
22	CLA	c	514	65/65	0.93	0.10	39,67,109,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	k	102	40/40	0.93	0.10	40,55,67,68	0
29	DGD	H	103	62/66	0.93	0.08	29,46,61,73	0
24	BCR	B	618	40/40	0.93	0.07	23,39,50,52	0
24	BCR	T	101	40/40	0.93	0.07	23,39,52,52	0
29	DGD	c	518	62/66	0.94	0.08	33,50,90,96	0
27	LMG	d	410	44/55	0.94	0.09	31,51,89,104	0
28	SQD	A	411	52/54	0.94	0.09	34,59,84,88	0
27	LMG	D	407	51/55	0.94	0.09	27,56,86,93	0
24	BCR	c	516	40/40	0.94	0.09	22,44,60,72	0
24	BCR	B	619	40/40	0.94	0.07	25,42,61,72	0
22	CLA	c	512	65/65	0.94	0.09	39,52,65,74	0
24	BCR	K	103	40/40	0.94	0.10	36,54,67,69	0
24	BCR	A	406	40/40	0.94	0.07	23,35,43,47	0
24	BCR	b	617	40/40	0.94	0.07	25,41,54,59	0
24	BCR	b	618	40/40	0.94	0.07	22,38,51,52	0
33	LHG	D	410	47/49	0.94	0.09	24,46,82,99	0
24	BCR	b	619	40/40	0.94	0.08	31,47,63,67	0
33	LHG	d	407	49/49	0.94	0.10	33,49,76,80	0
33	LHG	d	409	39/49	0.94	0.09	29,45,72,80	0
22	CLA	C	512	65/65	0.94	0.09	35,55,82,95	0
22	CLA	C	510	65/65	0.95	0.07	27,46,62,66	0
22	CLA	d	404	65/65	0.95	0.09	32,49,89,106	0
24	BCR	t	101	40/40	0.95	0.06	23,38,51,52	0
23	PHO	d	401	64/64	0.95	0.07	20,37,47,61	0
26	PL9	D	406	55/55	0.95	0.06	21,34,49,54	0
29	DGD	C	515	62/66	0.95	0.09	21,40,73,87	0
22	CLA	C	511	65/65	0.95	0.07	27,49,66,77	0
29	DGD	C	517	62/66	0.95	0.08	26,46,77,87	0
24	BCR	B	617	40/40	0.95	0.06	24,38,59,60	0
22	CLA	B	615	65/65	0.95	0.07	21,38,60,69	0
29	DGD	c	519	62/66	0.95	0.08	28,54,83,91	0
22	CLA	C	503	65/65	0.95	0.07	32,42,51,61	0
22	CLA	C	504	59/65	0.95	0.07	27,41,81,83	0
22	CLA	C	505	65/65	0.95	0.08	19,39,71,77	0
22	CLA	b	606	65/65	0.95	0.07	22,37,73,77	0
22	CLA	b	609	65/65	0.95	0.07	27,43,64,74	0
22	CLA	b	610	65/65	0.95	0.08	23,36,50,56	0
22	CLA	b	616	60/65	0.95	0.08	24,42,86,88	0
22	CLA	c	503	65/65	0.95	0.07	29,41,62,66	0
22	CLA	c	504	65/65	0.95	0.07	28,41,54,58	0
22	CLA	c	506	65/65	0.95	0.08	24,40,64,70	0
22	CLA	c	507	65/65	0.95	0.09	29,48,102,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	c	509	64/65	0.95	0.08	27,46,86,103	0
22	CLA	c	510	65/65	0.95	0.08	33,47,70,77	0
22	CLA	C	506	65/65	0.95	0.09	28,45,83,99	0
22	CLA	C	508	65/65	0.95	0.07	25,42,97,107	0
22	CLA	C	501	65/65	0.96	0.06	19,36,51,56	0
22	CLA	a	402	65/65	0.96	0.06	19,29,46,56	0
22	CLA	d	403	65/65	0.96	0.06	19,34,54,65	0
22	CLA	a	403	65/65	0.96	0.08	25,40,97,106	0
23	PHO	A	404	64/64	0.96	0.06	18,28,40,48	0
23	PHO	D	401	64/64	0.96	0.06	21,32,44,48	0
23	PHO	a	404	64/64	0.96	0.06	19,29,40,44	0
22	CLA	a	405	65/65	0.96	0.08	18,35,82,91	0
22	CLA	a	410	65/65	0.96	0.06	17,29,48,54	0
22	CLA	C	502	65/65	0.96	0.06	26,42,52,53	0
22	CLA	b	602	65/65	0.96	0.08	26,44,65,72	0
22	CLA	b	603	65/65	0.96	0.06	18,36,65,76	0
22	CLA	B	605	65/65	0.96	0.07	19,31,47,52	0
22	CLA	b	608	65/65	0.96	0.07	25,42,60,69	0
22	CLA	B	606	65/65	0.96	0.07	23,36,69,86	0
22	CLA	B	608	65/65	0.96	0.06	20,34,56,61	0
22	CLA	b	611	65/65	0.96	0.06	19,34,53,61	0
22	CLA	b	612	65/65	0.96	0.07	15,33,48,57	0
22	CLA	b	614	65/65	0.96	0.07	21,38,78,86	0
24	BCR	a	406	40/40	0.96	0.06	19,32,50,55	0
22	CLA	b	615	65/65	0.96	0.07	24,39,59,63	0
22	CLA	B	609	65/65	0.96	0.07	24,39,57,69	0
22	CLA	c	502	65/65	0.96	0.06	26,41,53,57	0
22	CLA	C	507	65/65	0.96	0.06	20,40,56,66	0
22	CLA	B	610	65/65	0.96	0.07	18,33,46,50	0
22	CLA	c	505	60/65	0.96	0.07	32,45,76,89	0
29	DGD	c	517	62/66	0.96	0.08	24,42,84,94	0
22	CLA	C	509	65/65	0.96	0.08	25,46,62,69	0
22	CLA	B	611	65/65	0.96	0.06	19,30,46,50	0
22	CLA	c	508	65/65	0.96	0.07	28,44,59,63	0
32	BCT	d	402	4/4	0.96	0.08	31,35,44,53	0
22	CLA	B	612	65/65	0.96	0.07	19,31,47,56	0
33	LHG	D	412	49/49	0.96	0.07	30,44,65,76	0
22	CLA	B	604	65/65	0.96	0.07	19,32,79,84	0
33	LHG	L	102	49/49	0.96	0.07	26,41,53,60	0
22	CLA	c	511	65/65	0.96	0.07	29,47,64,68	0
22	CLA	B	616	60/65	0.96	0.09	25,39,94,110	0
26	PL9	d	406	55/55	0.96	0.06	22,33,42,53	0

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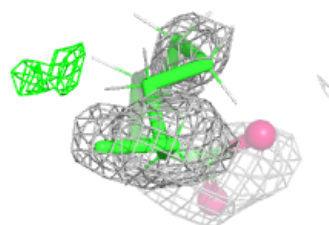
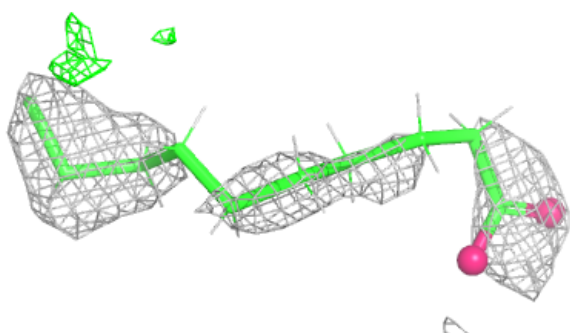
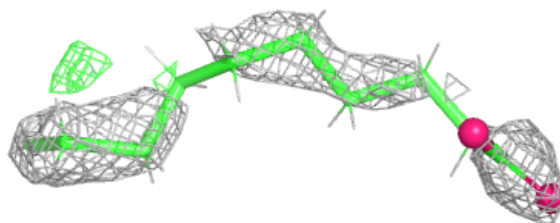
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LHG	l	101	49/49	0.96	0.06	26,45,55,64	0
22	CLA	A	403	65/65	0.97	0.08	21,34,97,110	0
22	CLA	B	602	65/65	0.97	0.06	20,36,55,66	0
22	CLA	B	607	65/65	0.97	0.06	14,34,62,66	0
22	CLA	b	613	65/65	0.97	0.07	17,34,73,87	0
22	CLA	B	613	65/65	0.97	0.06	17,31,71,73	0
22	CLA	B	614	65/65	0.97	0.07	20,36,75,87	0
33	LHG	D	409	49/49	0.97	0.06	26,41,53,56	0
22	CLA	B	603	65/65	0.97	0.07	15,32,63,67	0
22	CLA	D	403	65/65	0.97	0.06	15,29,52,61	0
22	CLA	b	604	65/65	0.97	0.07	20,33,81,91	0
22	CLA	b	605	65/65	0.97	0.06	21,34,49,53	0
22	CLA	D	404	65/65	0.97	0.06	19,28,52,62	0
33	LHG	d	408	49/49	0.97	0.06	23,42,57,68	0
22	CLA	b	607	65/65	0.97	0.07	18,35,69,78	0
22	CLA	D	405	65/65	0.97	0.07	22,42,107,119	0
22	CLA	A	402	65/65	0.97	0.06	16,26,46,49	0
34	HEC	F	102	43/43	0.97	0.08	37,48,64,66	0
34	HEC	f	101	43/43	0.97	0.08	42,58,81,84	0
32	BCT	D	402	4/4	0.98	0.07	22,26,32,36	0
34	HEC	V	201	43/43	0.98	0.06	19,35,43,44	0
22	CLA	A	405	54/65	0.98	0.06	18,31,66,72	0
34	HEC	v	201	43/43	0.98	0.06	27,37,50,51	0
21	FE2	a	401	1/1	0.99	0.02	34,34,34,34	0
25	CL	A	407	1/1	0.99	0.03	29,29,29,29	0
25	CL	a	407	1/1	0.99	0.03	28,28,28,28	0
30	OEX	A	414	10/10	0.99	0.02	22,26,28,29	0
30	OEX	a	416	10/10	0.99	0.03	23,26,30,31	0
25	CL	a	408	1/1	0.99	0.07	28,28,28,28	0
21	FE2	A	401	1/1	0.99	0.02	26,26,26,26	0
25	CL	A	408	1/1	1.00	0.02	30,30,30,30	0

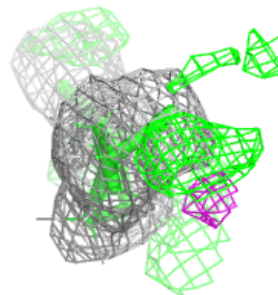
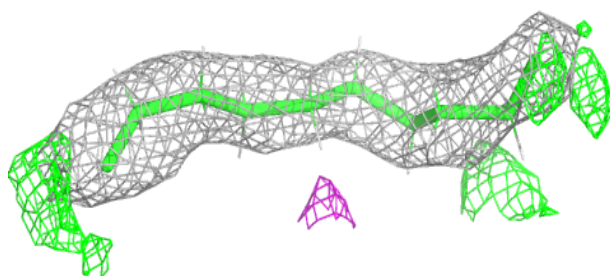
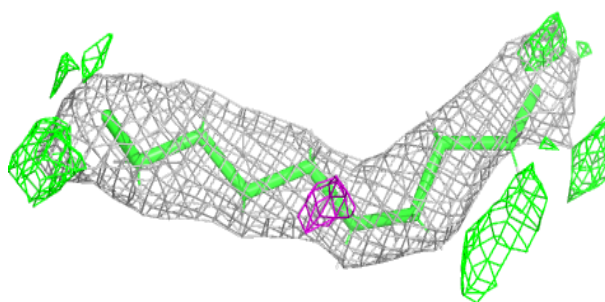
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE E 102:

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

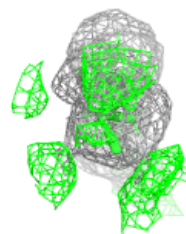
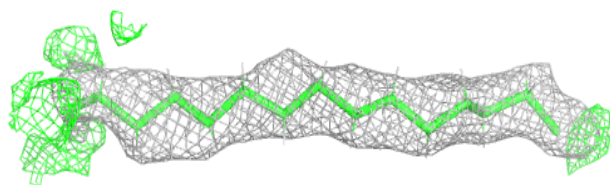
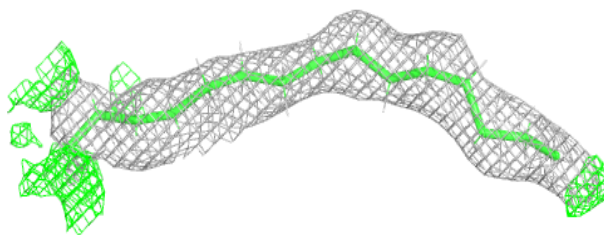
**Electron density around STE b 625:**

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



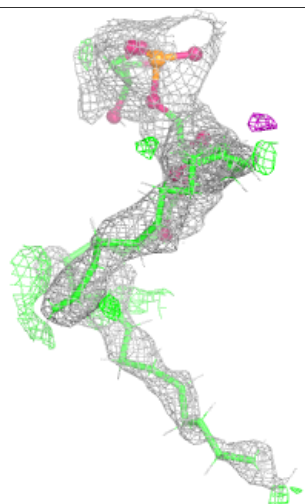
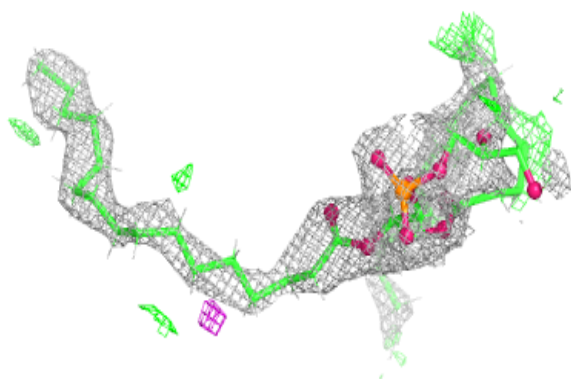
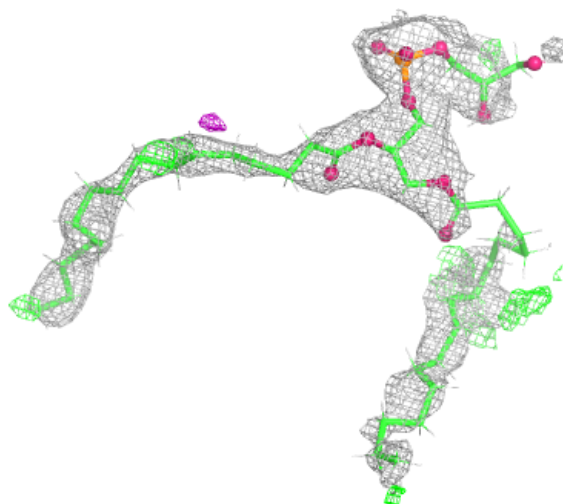
Electron density around STE I 101:

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



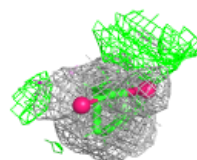
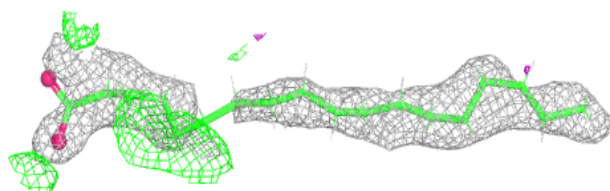
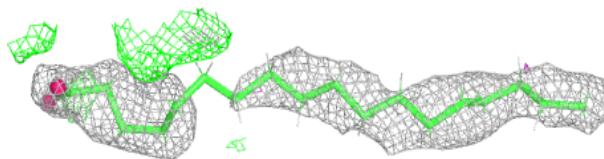
Electron density around LHG E 101:

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

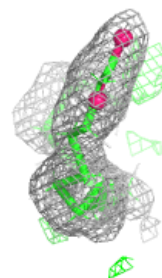
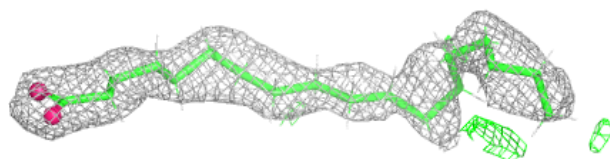
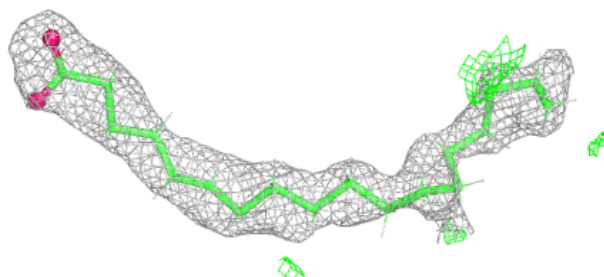


Electron density around STE b 624:

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

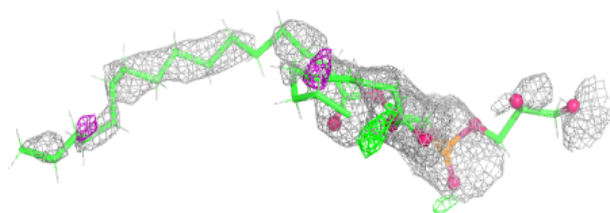
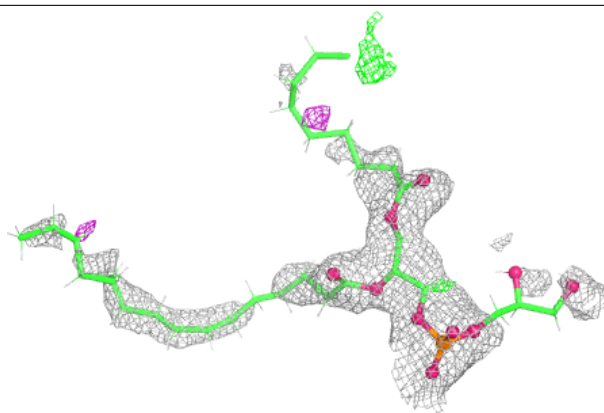
**Electron density around STE b 627:**

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

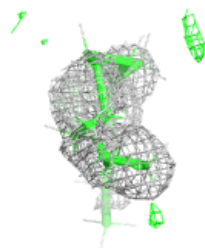
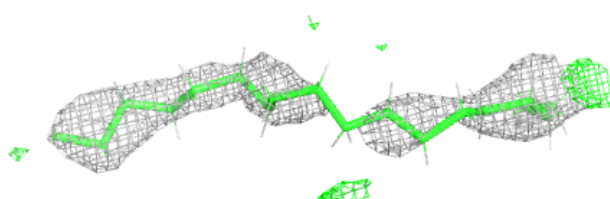
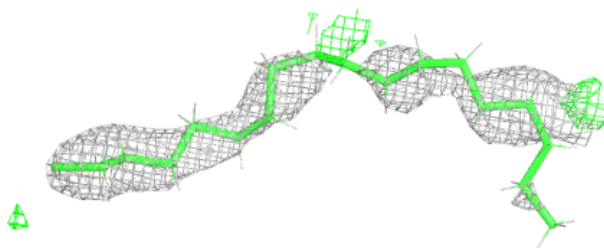


Electron density around LHG e 101:

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

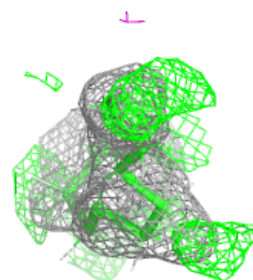
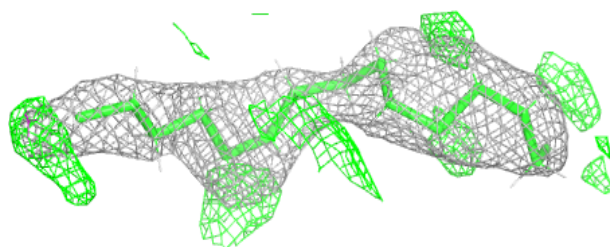
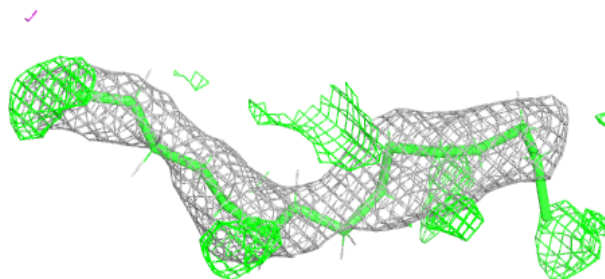
**Electron density around STE H 104:**

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

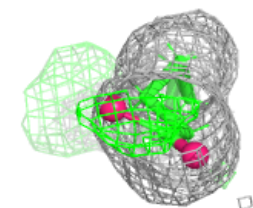
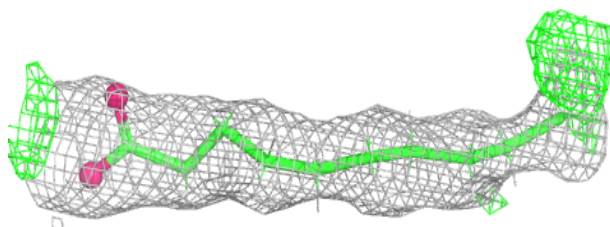
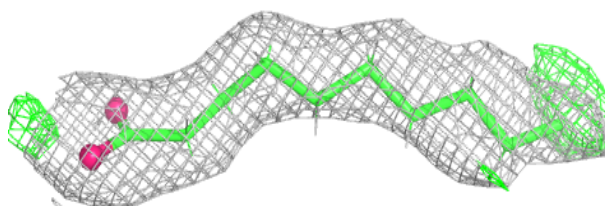


Electron density around STE B 627:

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

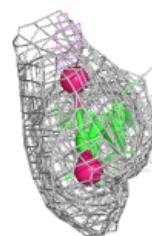
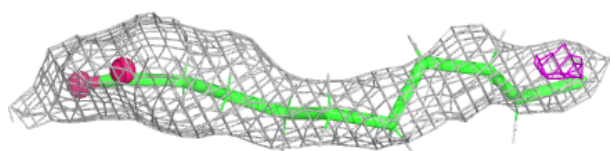
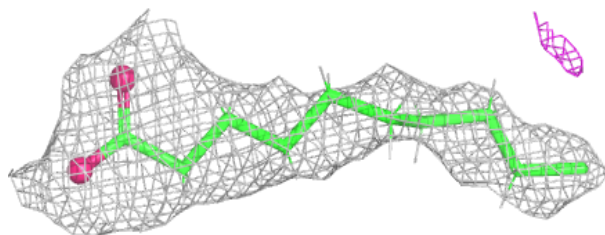
**Electron density around STE j 101:**

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

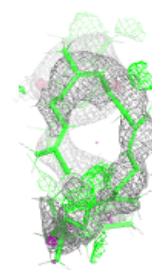
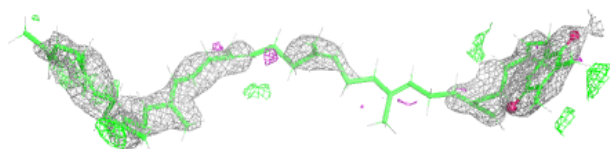
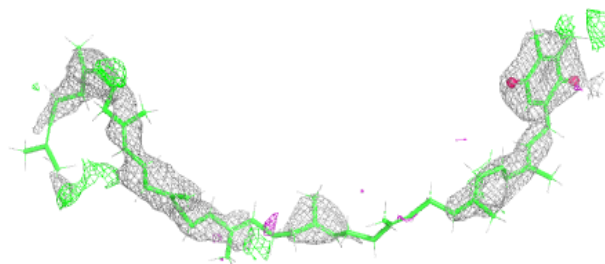


Electron density around STE a 414:

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

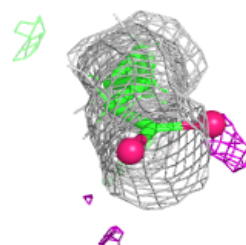
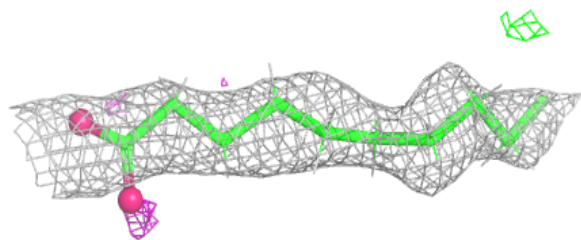
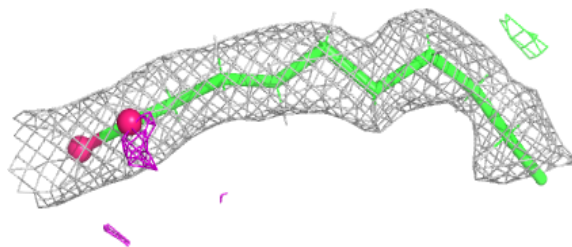
**Electron density around PL9 a 409:**

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

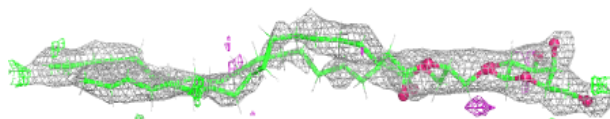
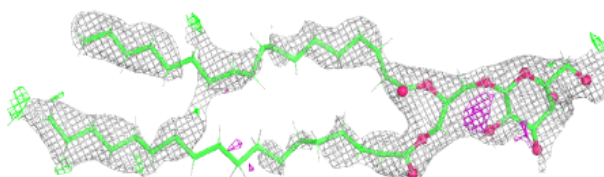


Electron density around STE m 102:

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

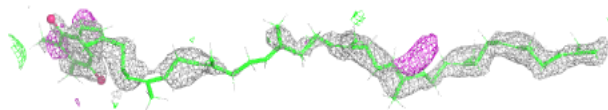
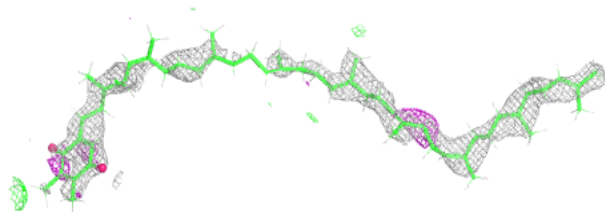
**Electron density around LMG b 623:**

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

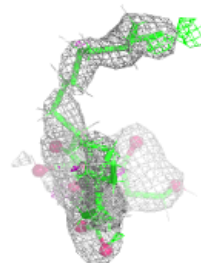
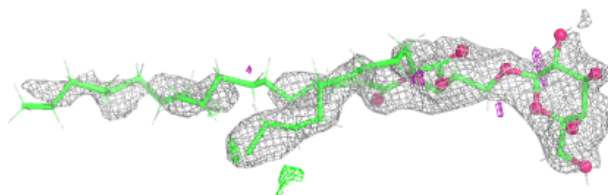
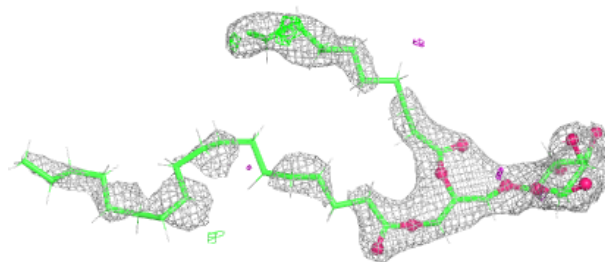


Electron density around PL9 A 409:

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

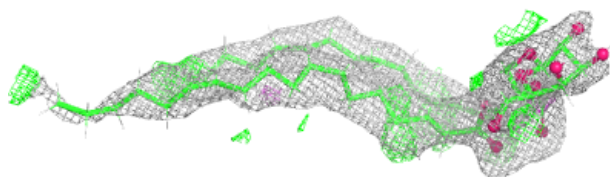
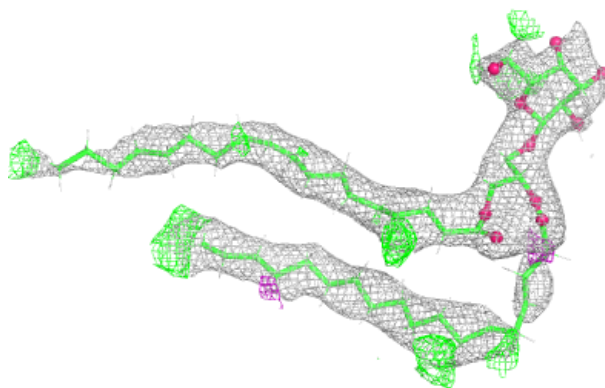
**Electron density around LMG c 522:**

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

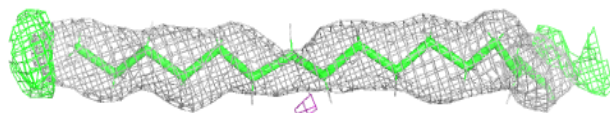
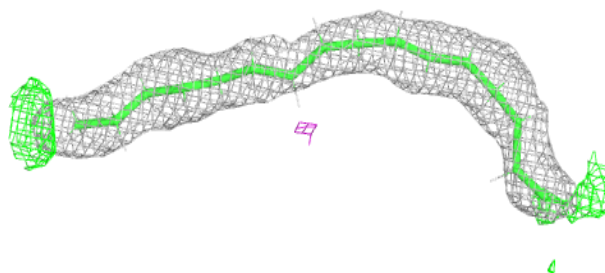


Electron density around LMG a 415:

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

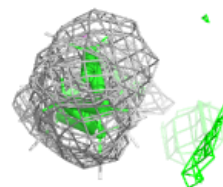
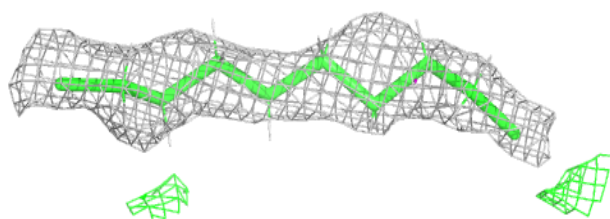
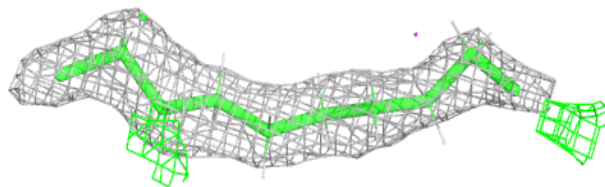
**Electron density around STE C 519:**

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

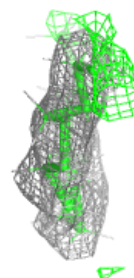
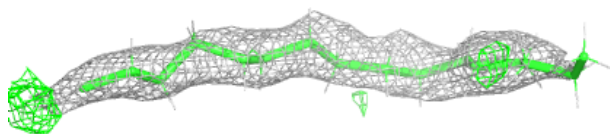
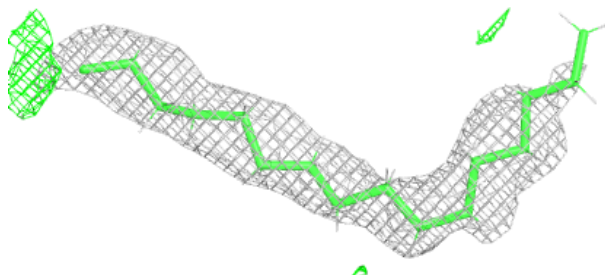


Electron density around STE a 413:

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

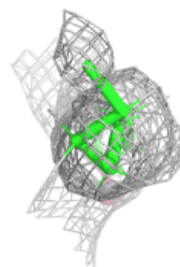
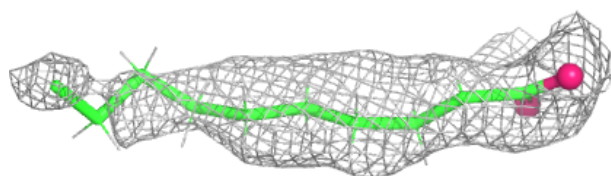
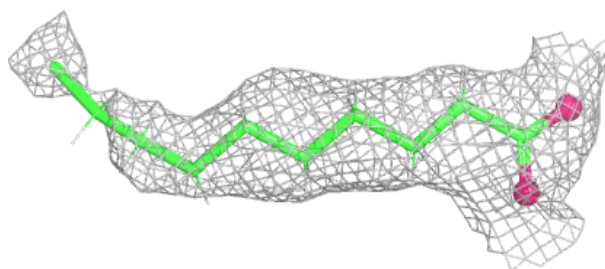
**Electron density around STE B 626:**

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

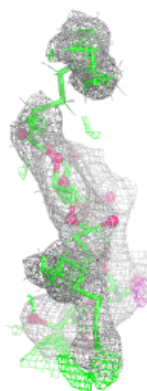
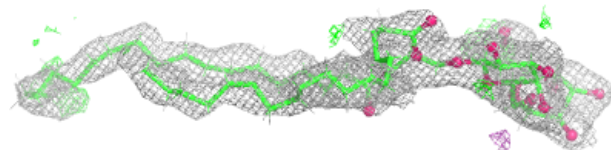
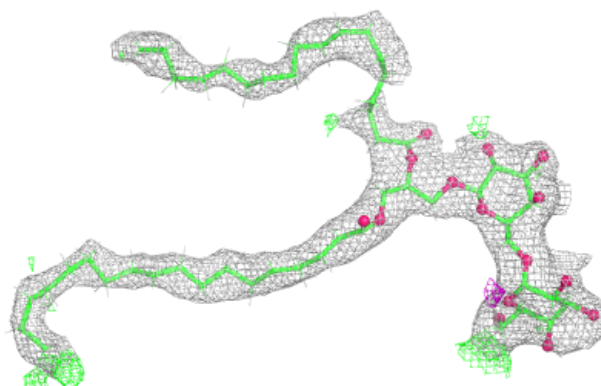


Electron density around STE c 501:

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

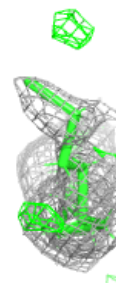
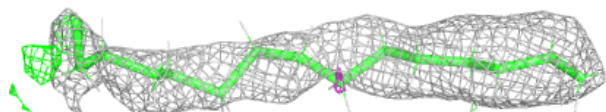
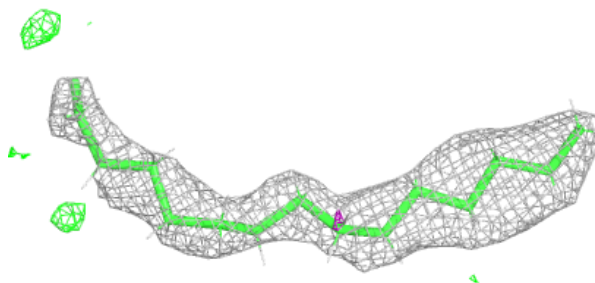
**Electron density around DGD A 413:**

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

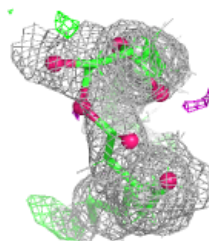
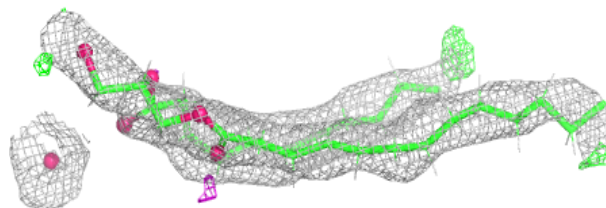
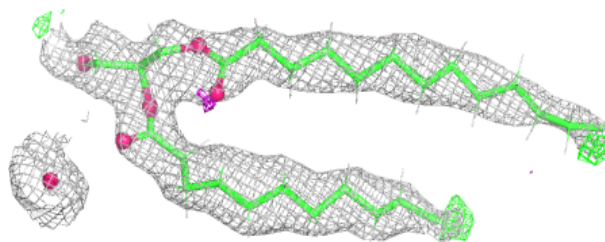


Electron density around STE T 102:

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

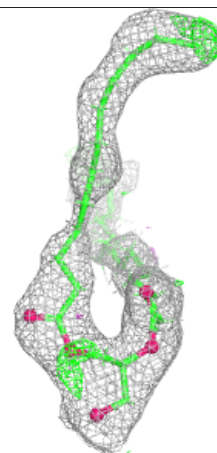
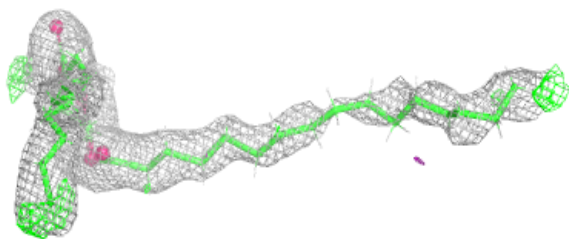
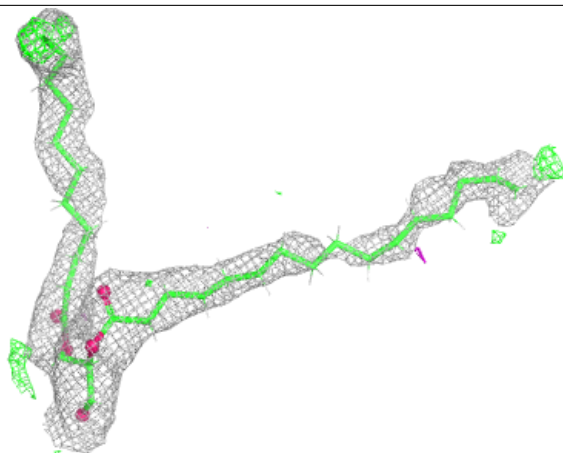
**Electron density around LMG D 411:**

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

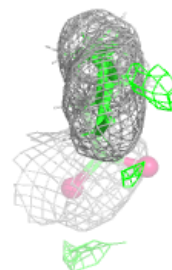
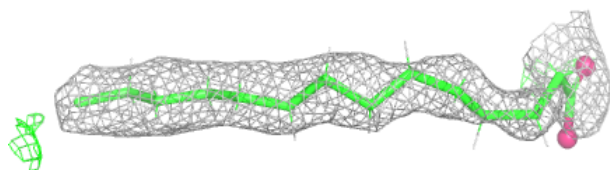
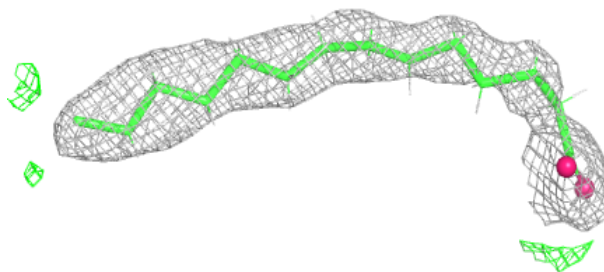


Electron density around SQD a 412:

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

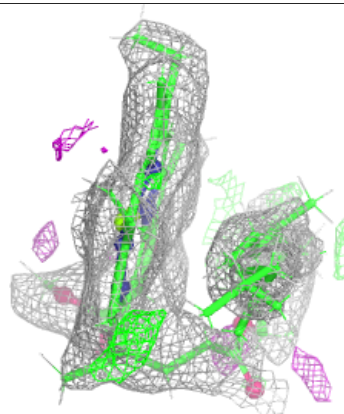
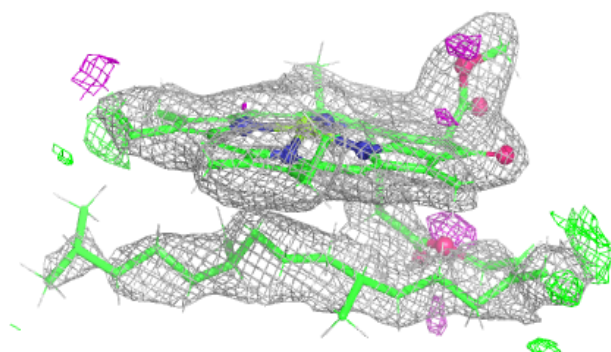
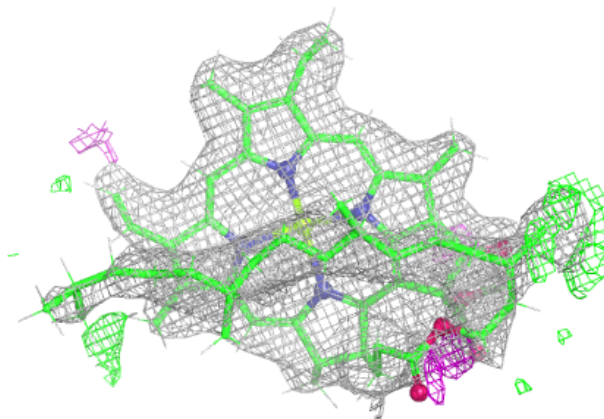
**Electron density around STE d 411:**

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

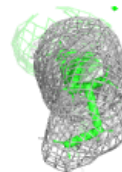
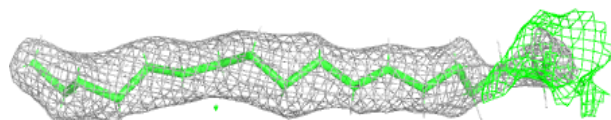
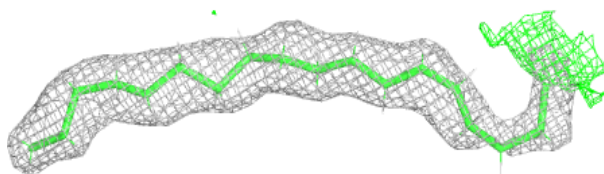


Electron density around CLA b 601:

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

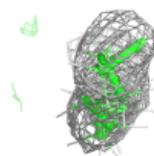
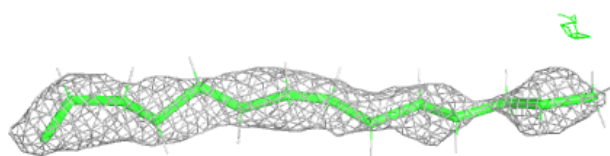
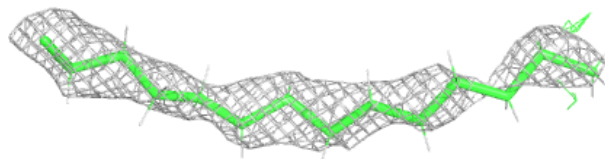
**Electron density around STE m 101:**

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

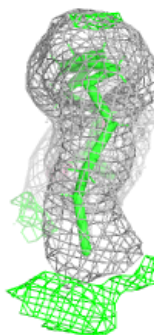
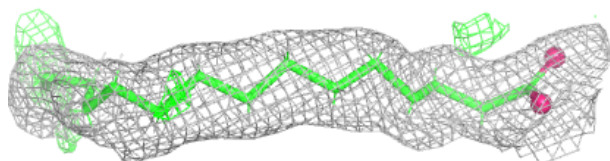
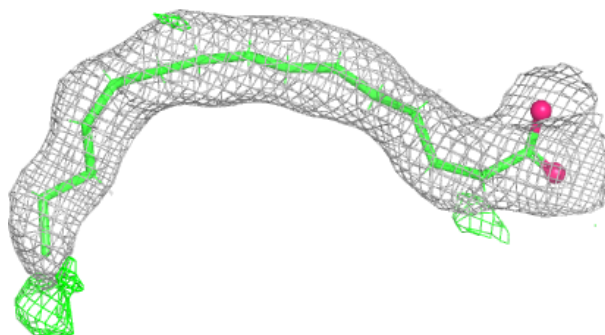


Electron density around STE b 626:

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

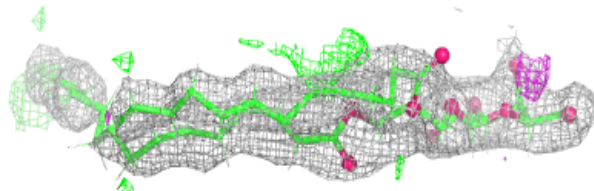
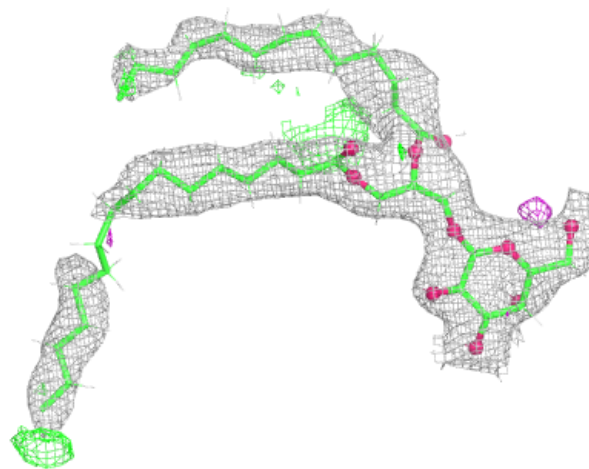
**Electron density around STE B 620:**

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



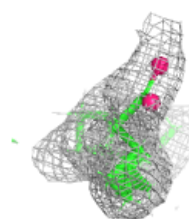
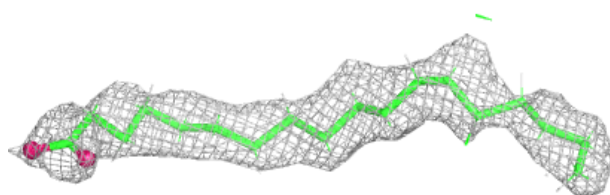
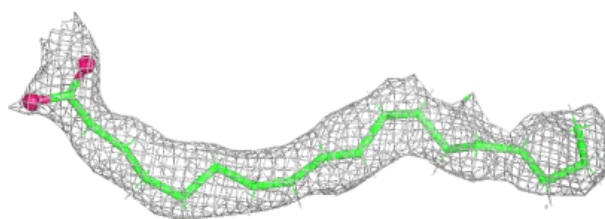
Electron density around LMG Y 101:

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

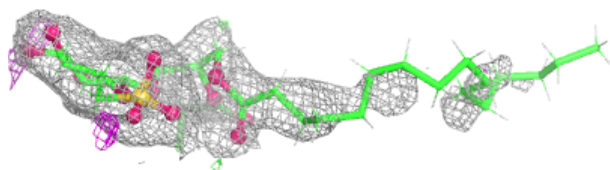
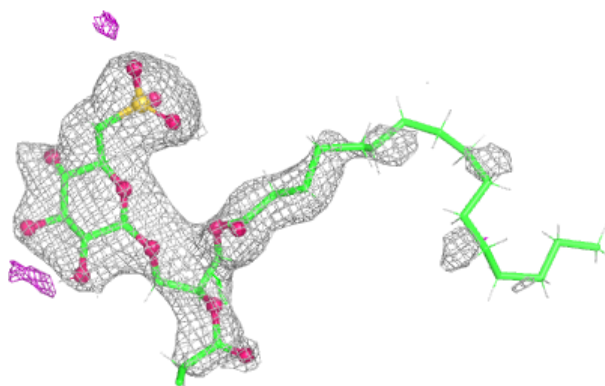


Electron density around STE b 622:

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

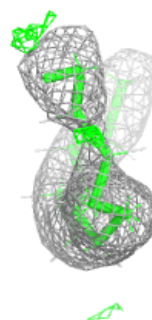
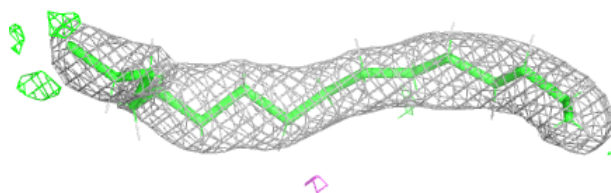
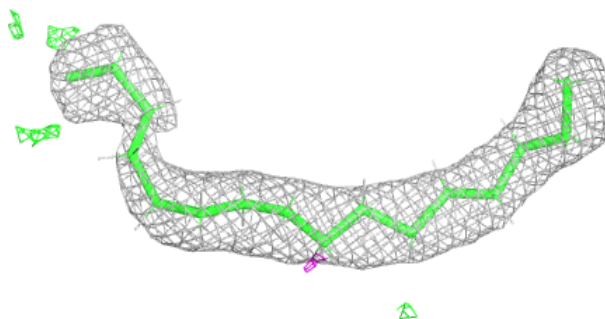
**Electron density around SQD f 102:**

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

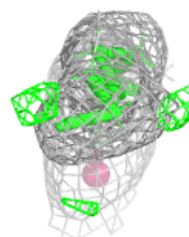
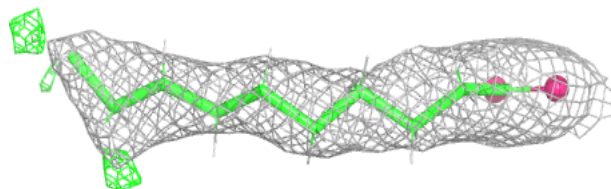
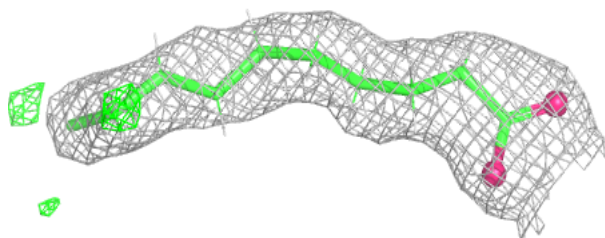


Electron density around STE b 620:

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

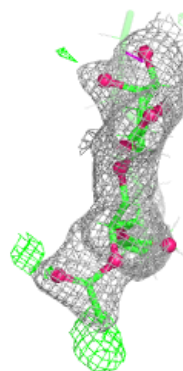
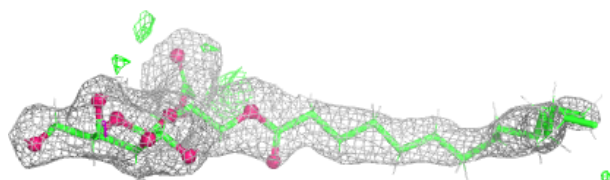
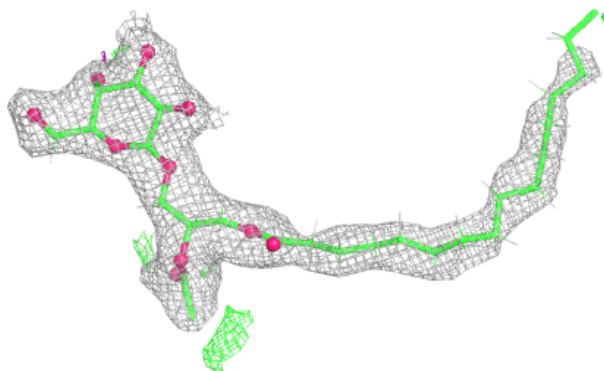
**Electron density around STE C 518:**

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

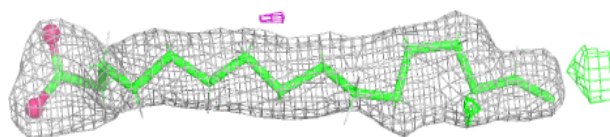
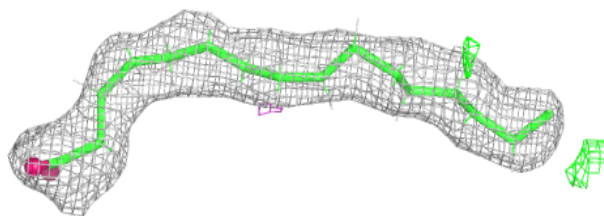


Electron density around LMG c 520:

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

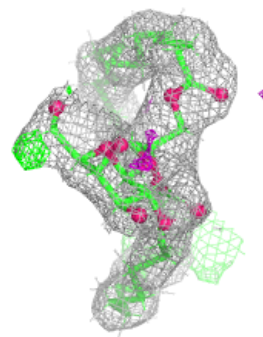
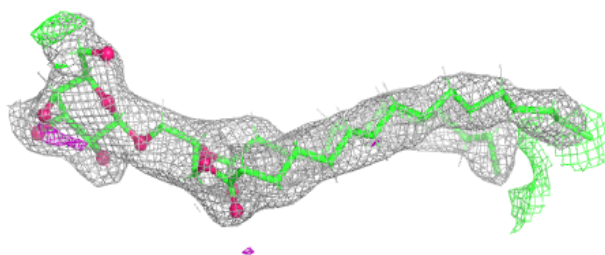
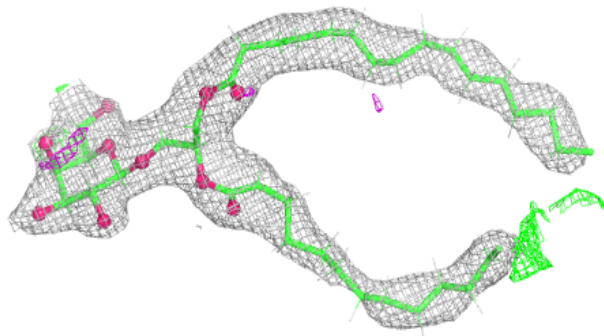
**Electron density around STE B 625:**

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



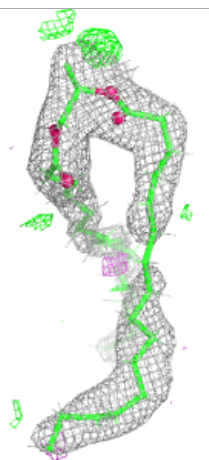
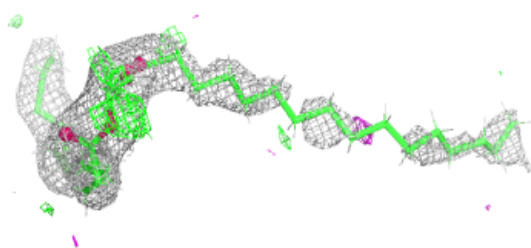
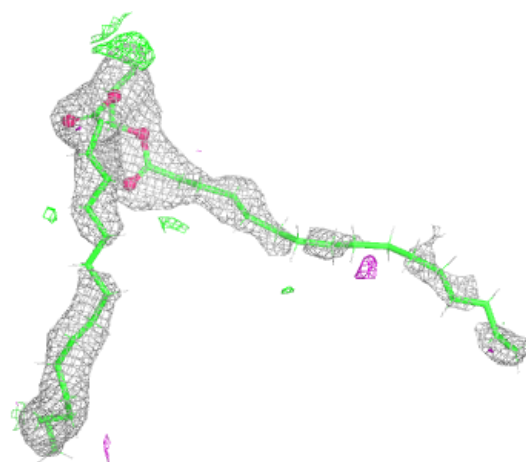
Electron density around LMG A 410:

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



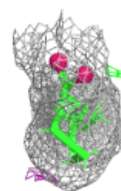
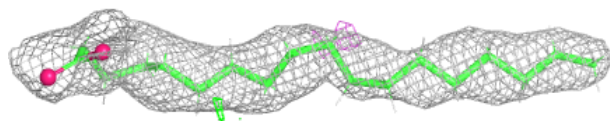
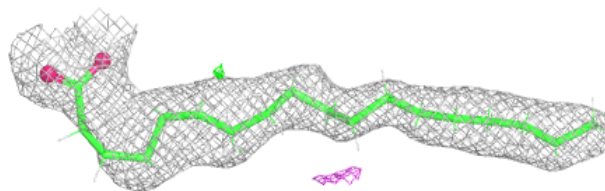
Electron density around SQD A 412:

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

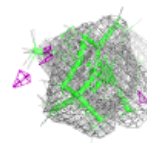
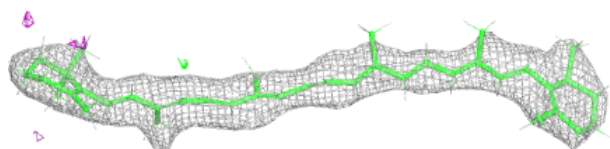
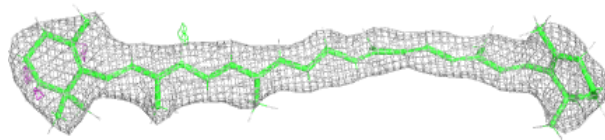


Electron density around STE c 521:

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

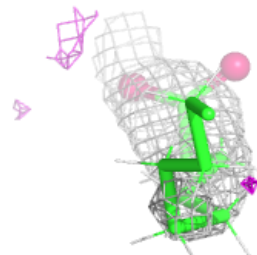
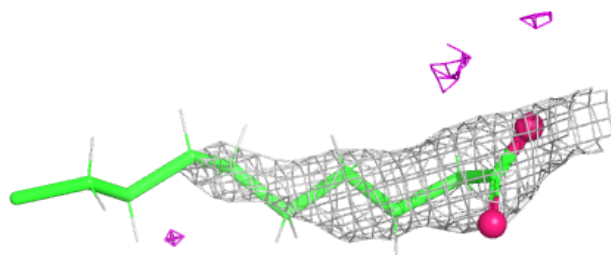
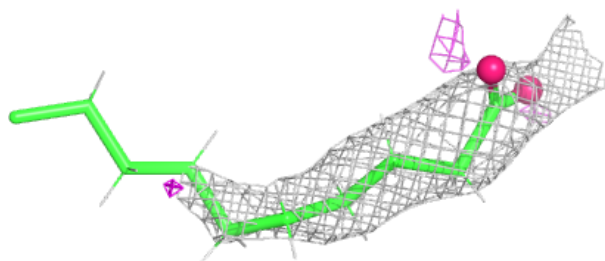
**Electron density around BCR K 101:**

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

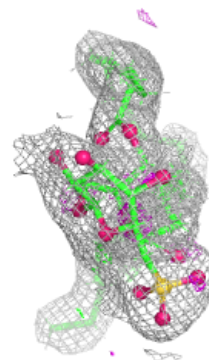
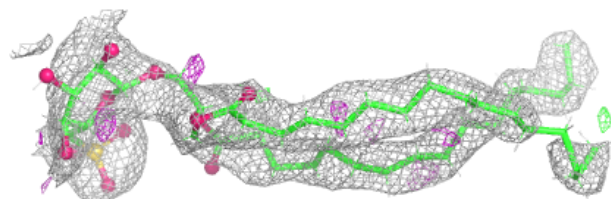
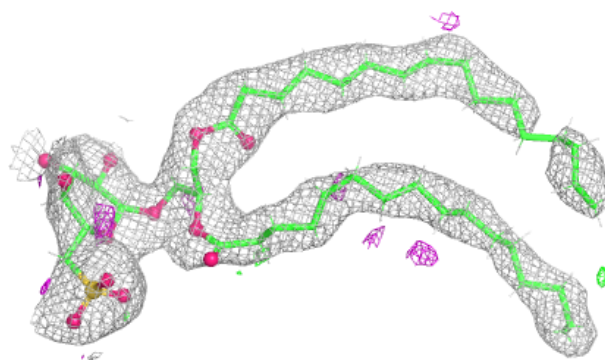


Electron density around STE B 601:

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

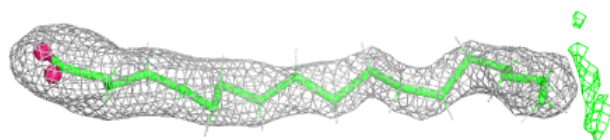
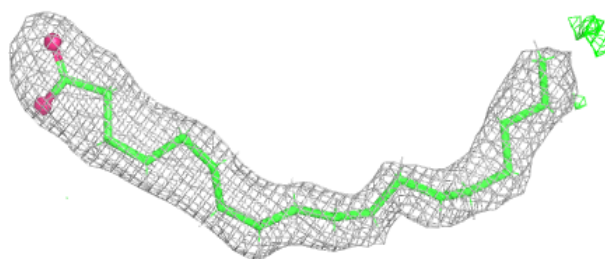
**Electron density around SQD B 622:**

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

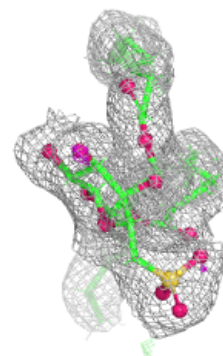
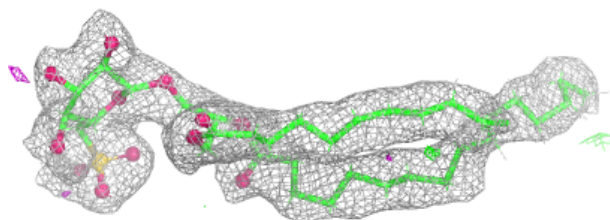
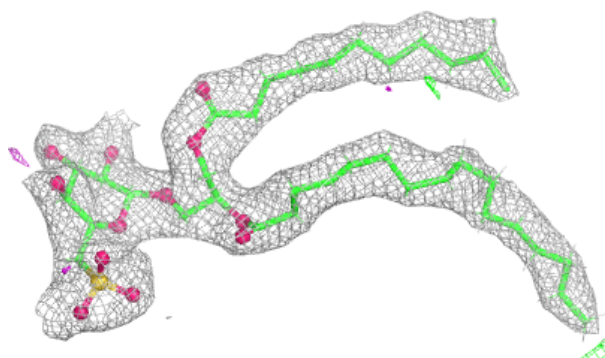


Electron density around STE d 413:

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

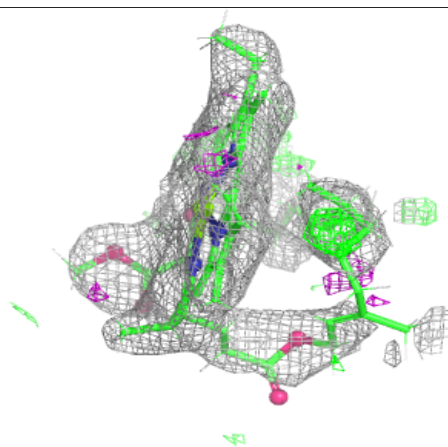
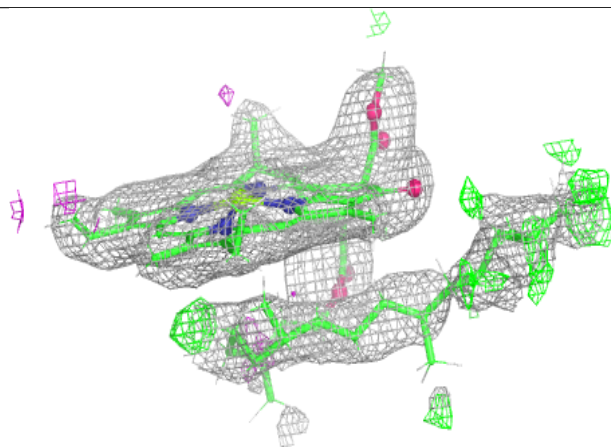
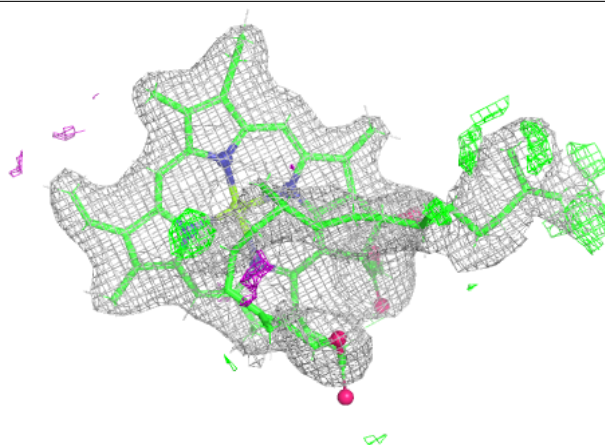
**Electron density around SQD L 101:**

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

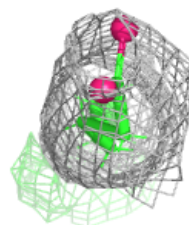
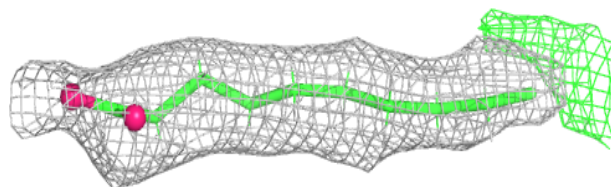
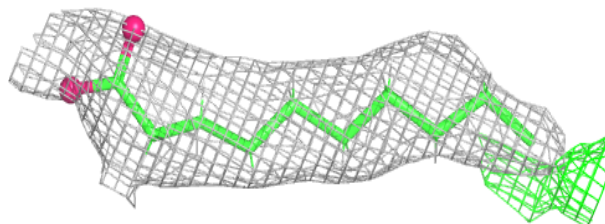


Electron density around CLA H 101:

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

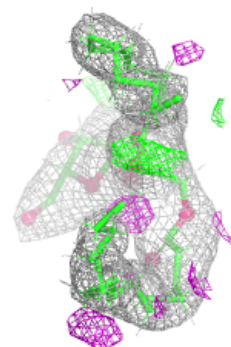
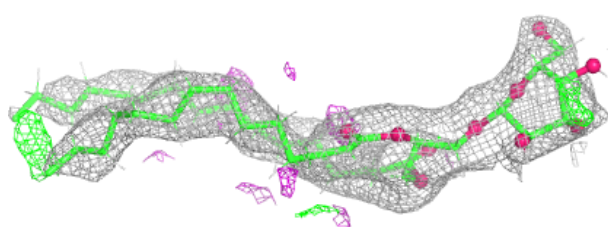
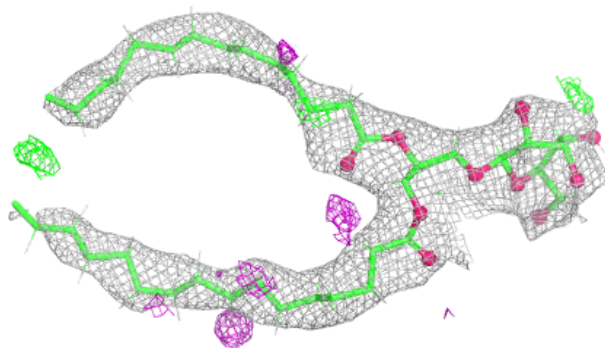
**Electron density around STE J 101:**

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

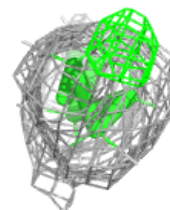
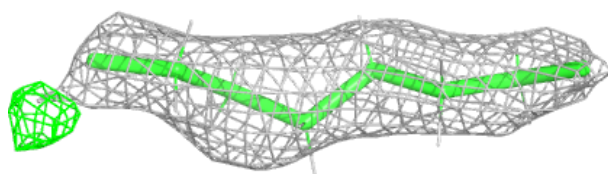
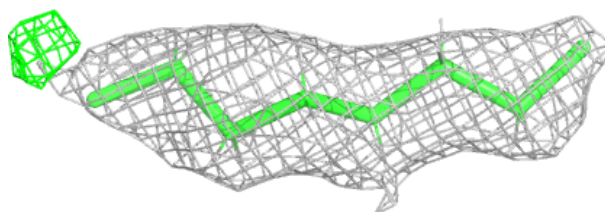


Electron density around LMG c 523:

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

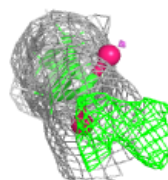
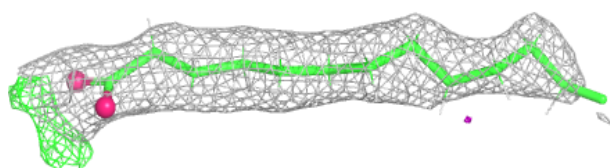
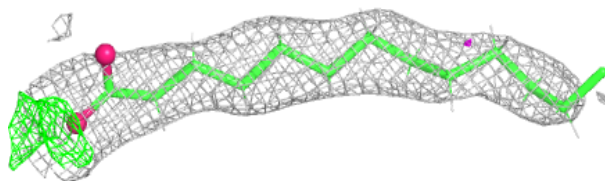
**Electron density around STE Z 101:**

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

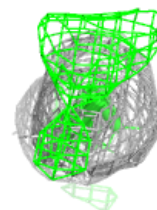
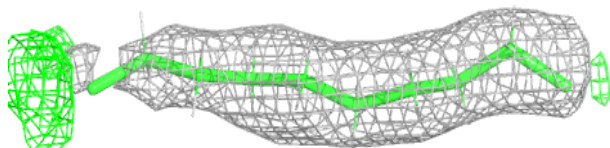
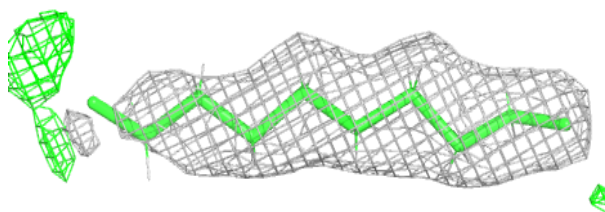


Electron density around STE M 102:

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

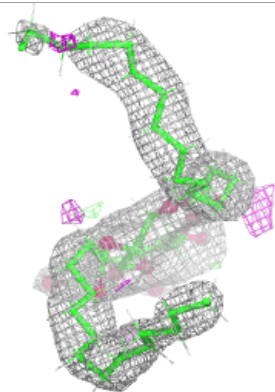
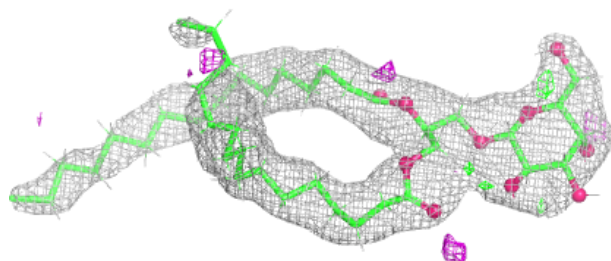
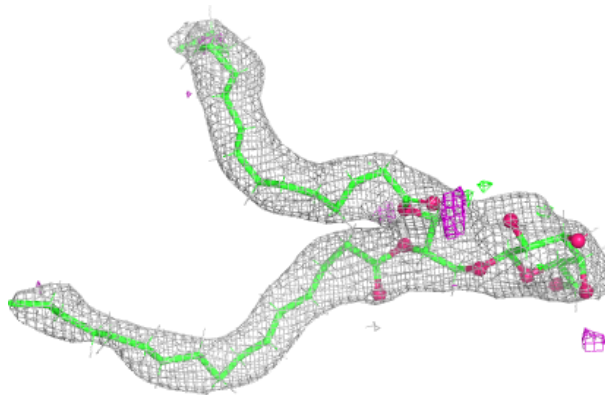
**Electron density around STE M 103:**

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

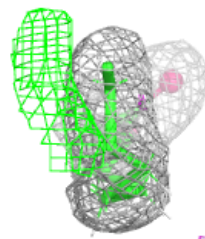
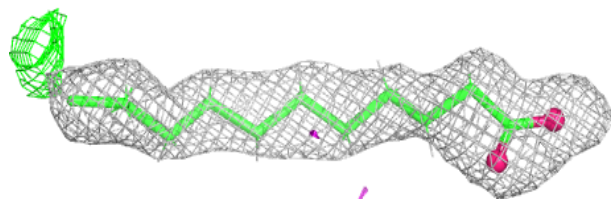
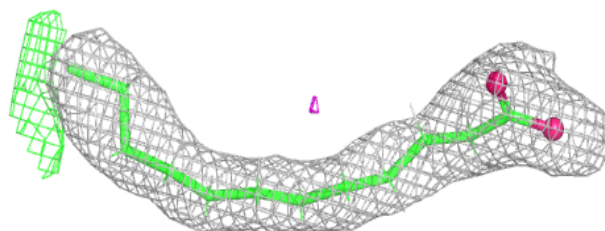


Electron density around LMG b 621:

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

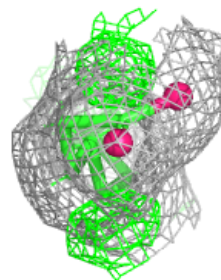
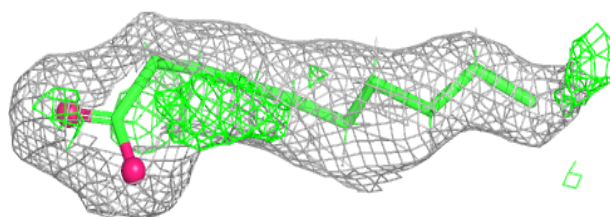
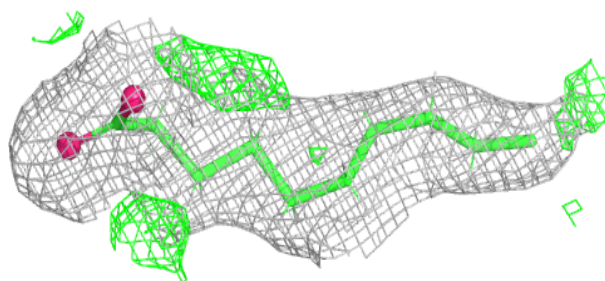
**Electron density around STE B 623:**

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

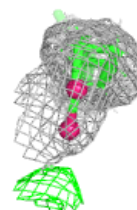
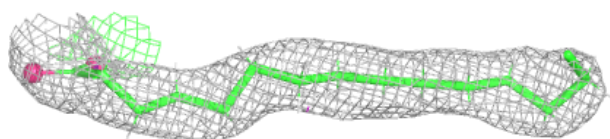
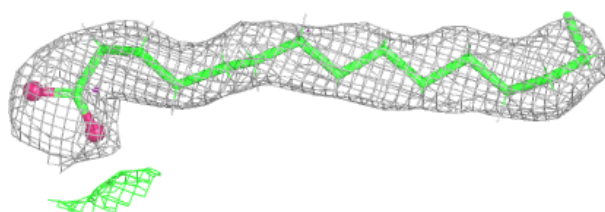


Electron density around STE B 624:

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

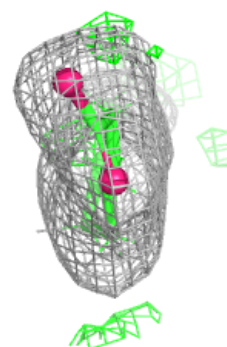
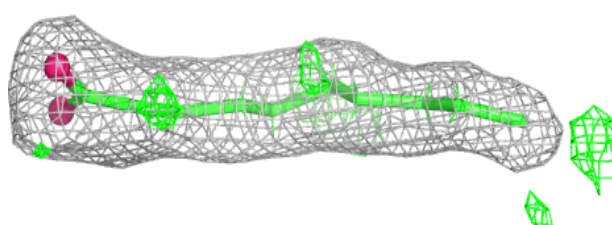
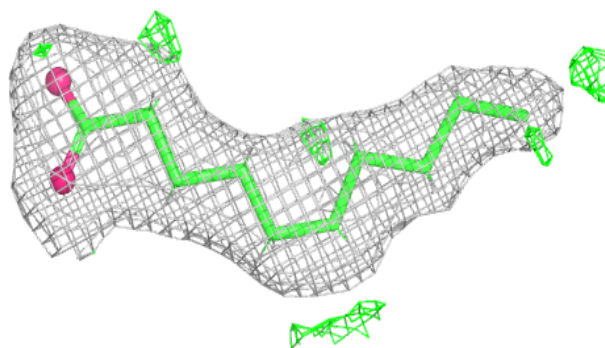
**Electron density around STE d 412:**

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

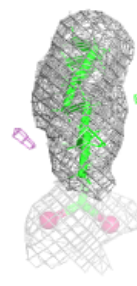
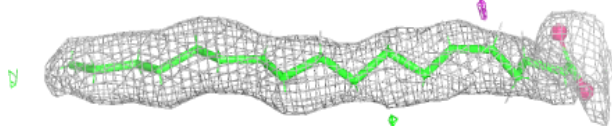
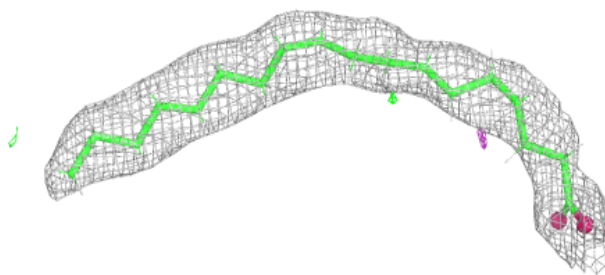


Electron density around STE C 520:

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

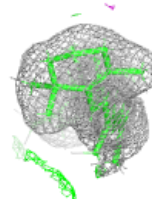
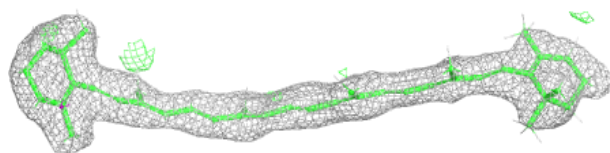
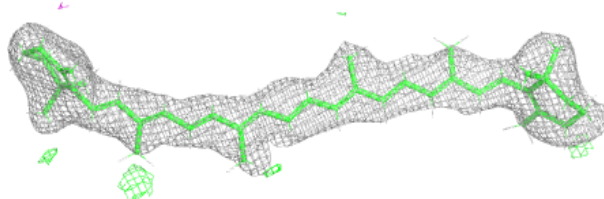
**Electron density around STE D 413:**

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

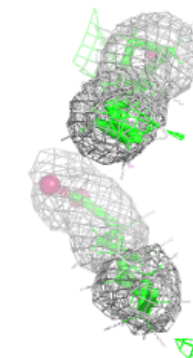
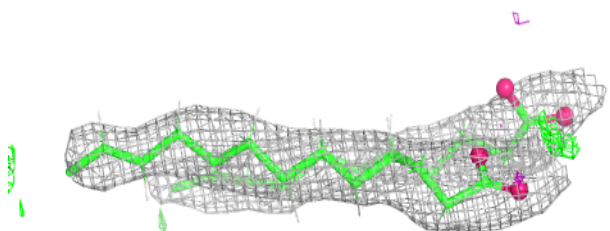
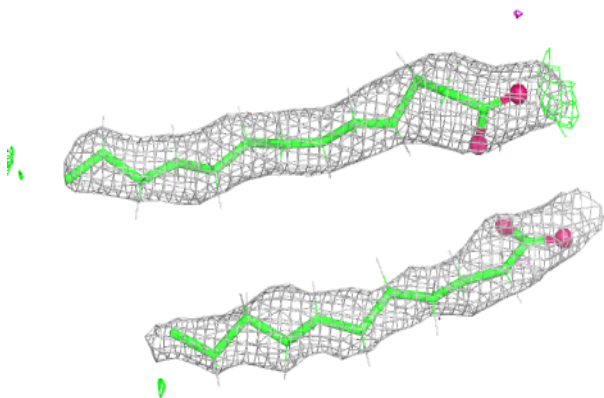


Electron density around BCR h 101:

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

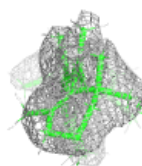
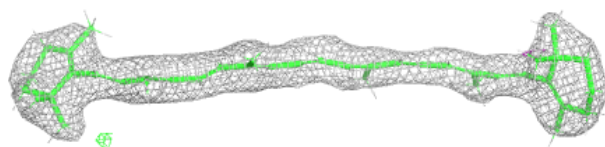
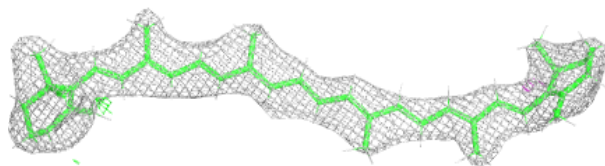
**Electron density around LMG B 621:**

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

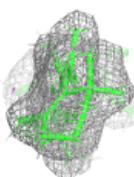
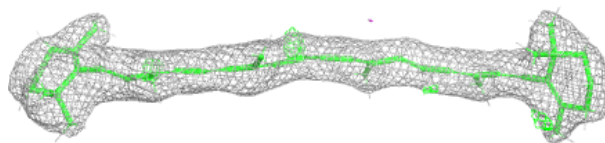


Electron density around BCR k 101:

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

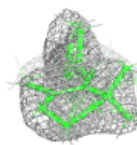
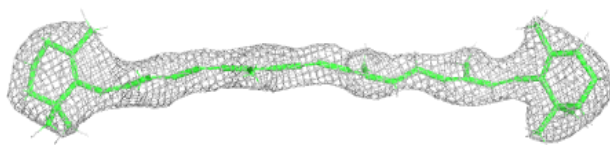
**Electron density around BCR K 102:**

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



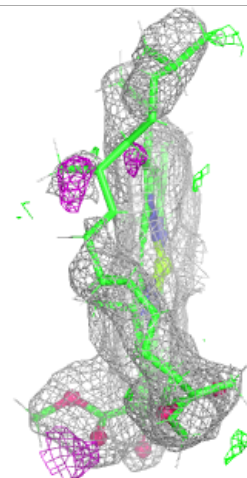
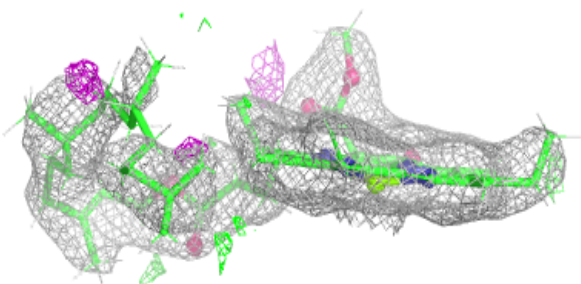
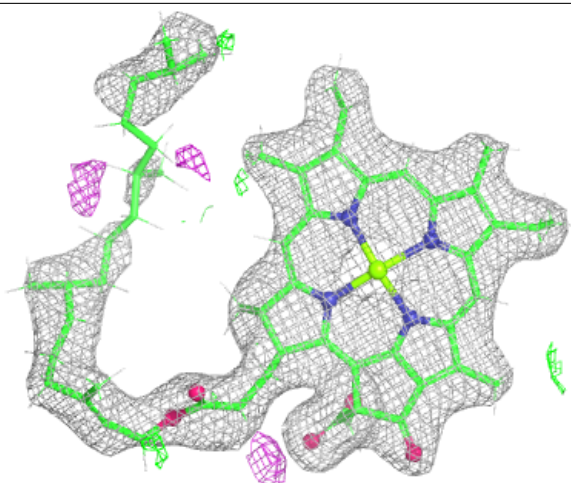
Electron density around BCR c 515:

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



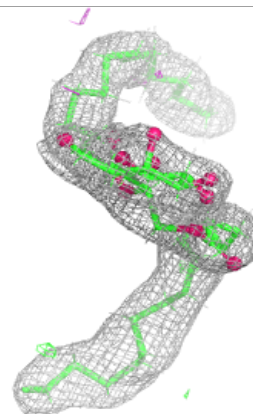
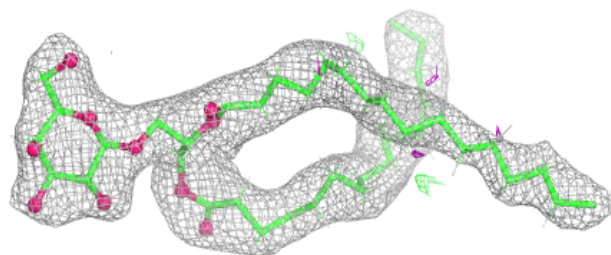
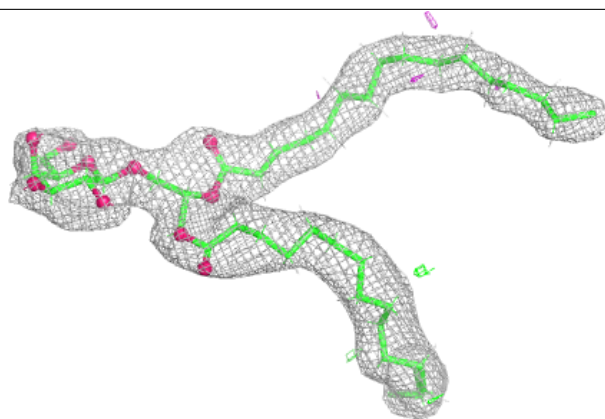
Electron density around CLA c 513:

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

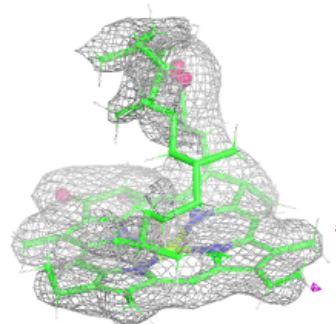
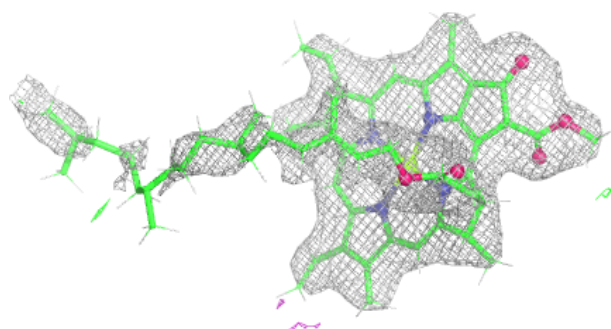
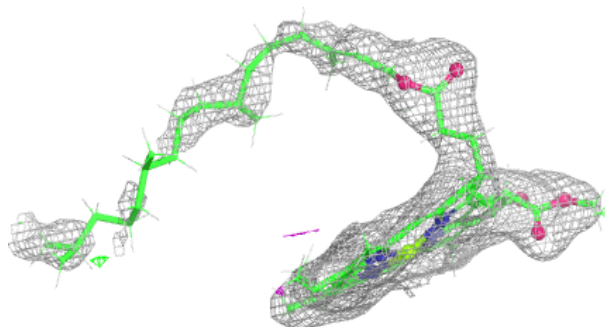


Electron density around LMG M 101:

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

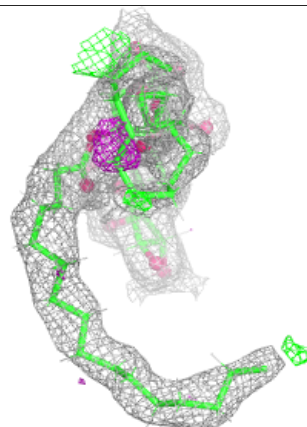
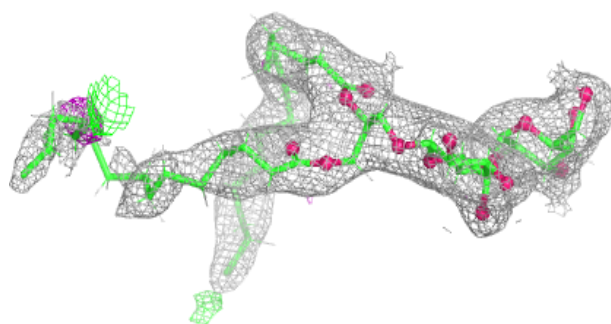
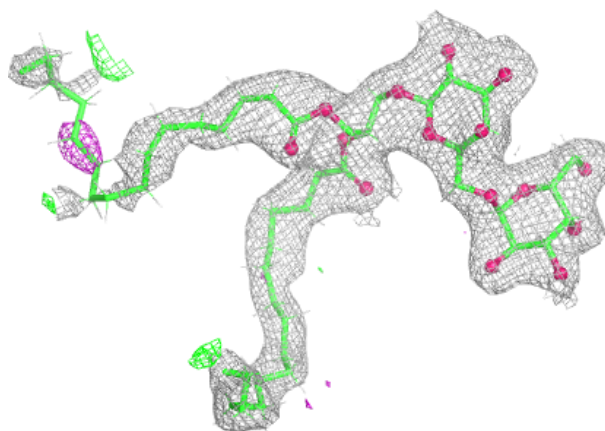
**Electron density around CLA C 513:**

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

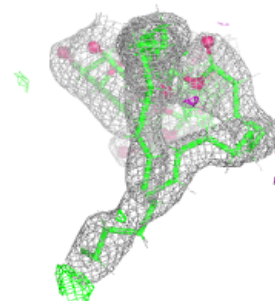
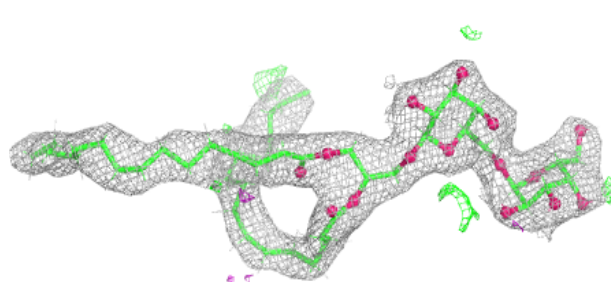
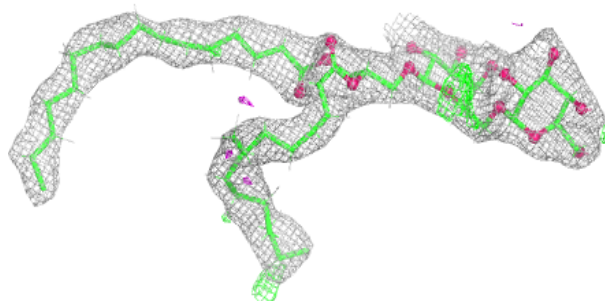


Electron density around DGD C 516:

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

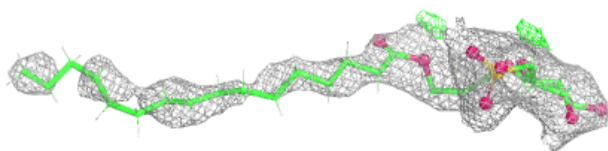
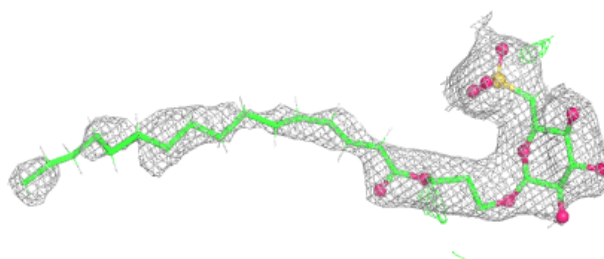
**Electron density around DGD h 102:**

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

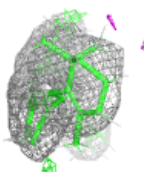
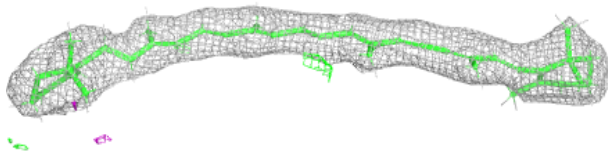


Electron density around SQD D 408:

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

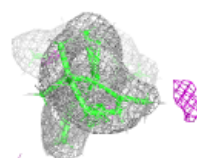
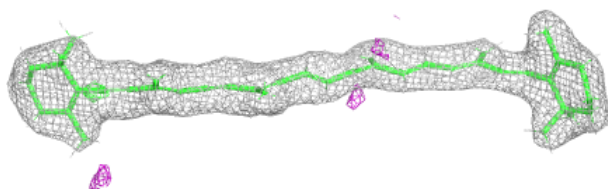
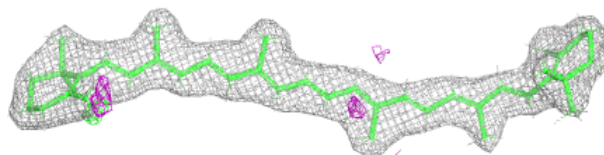
**Electron density around BCR d 405:**

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



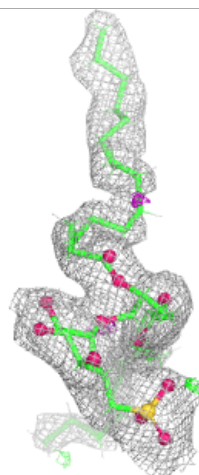
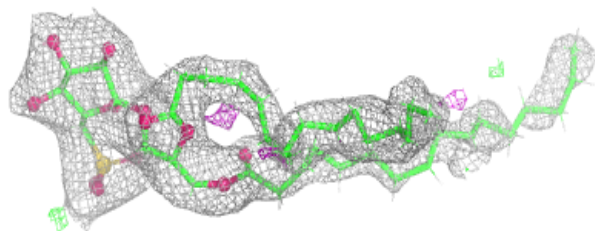
Electron density around BCR C 514:

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



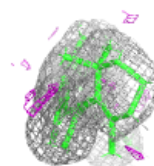
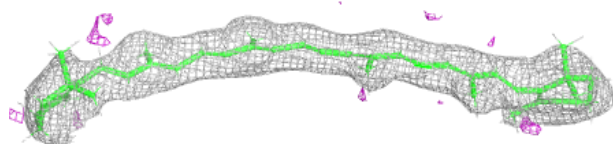
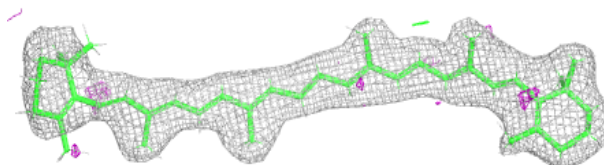
Electron density around SQD a 411:

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

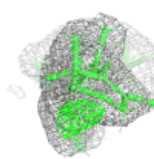
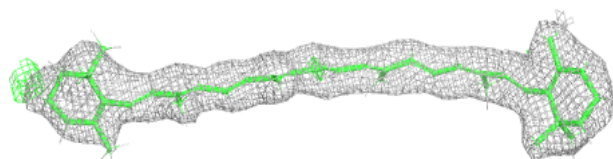
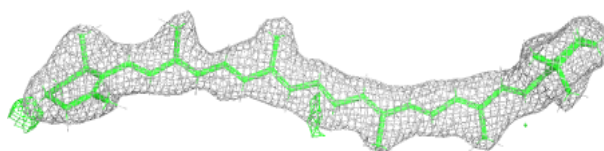


Electron density around BCR F 101:

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

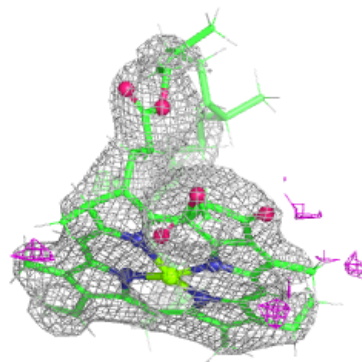
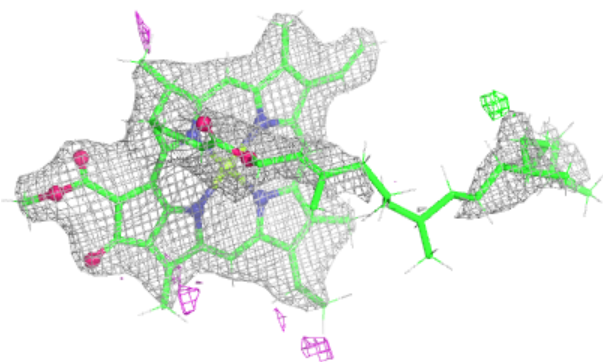
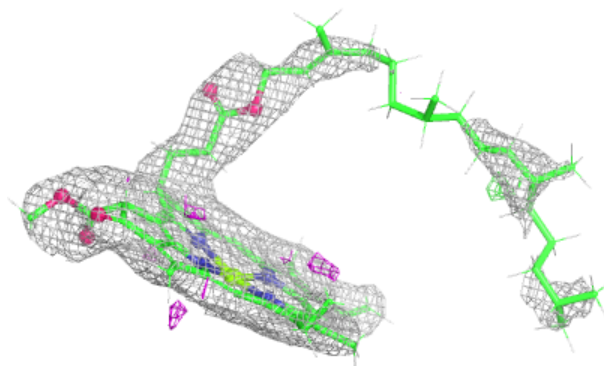
**Electron density around BCR H 102:**

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

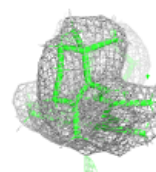
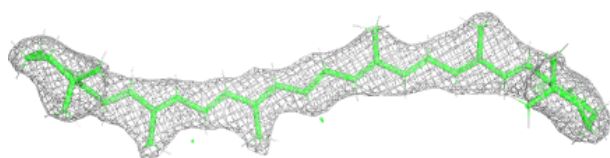
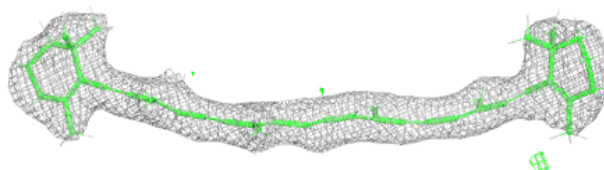


Electron density around CLA c 514:

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

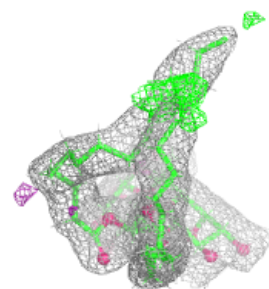
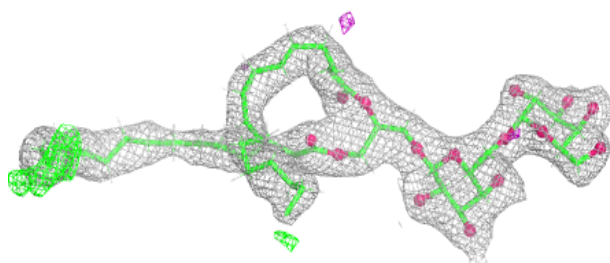
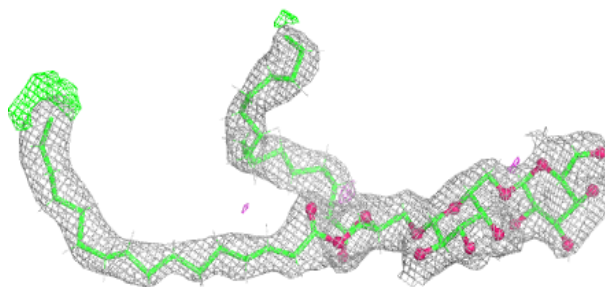
**Electron density around BCR k 102:**

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

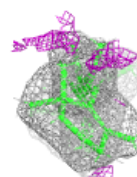
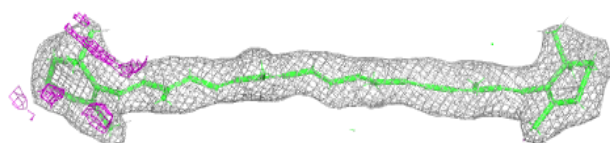
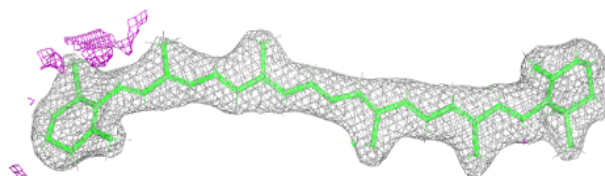


Electron density around DGD H 103:

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

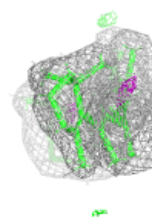
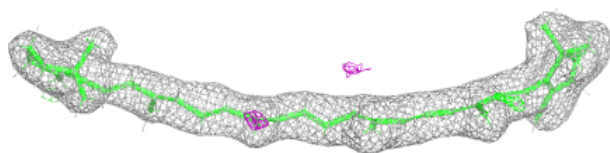
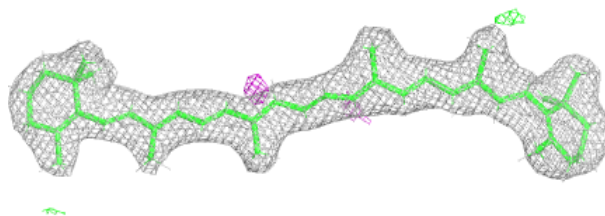
**Electron density around BCR B 618:**

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

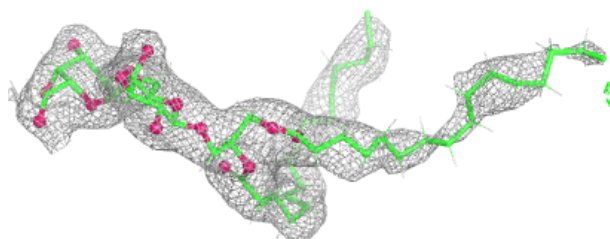
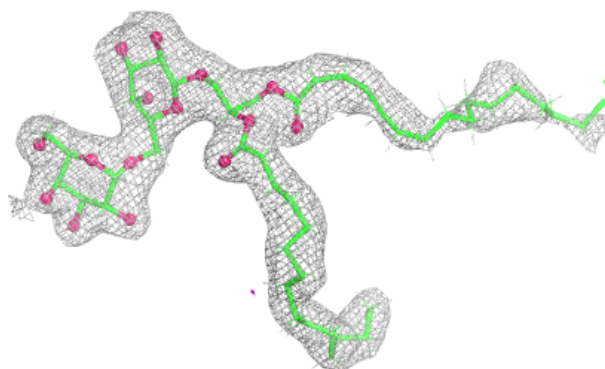


Electron density around BCR T 101:

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

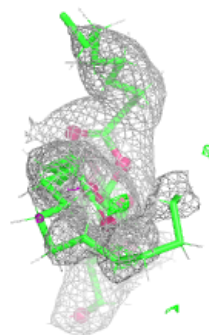
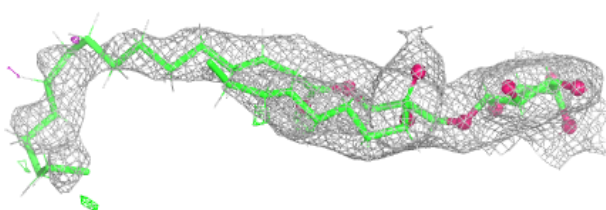
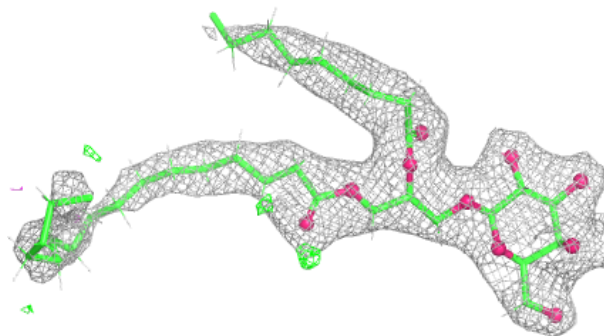
**Electron density around DGD c 518:**

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

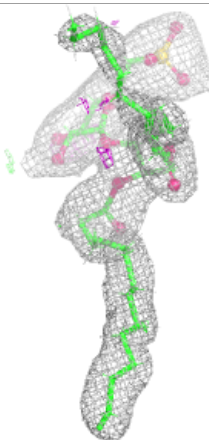
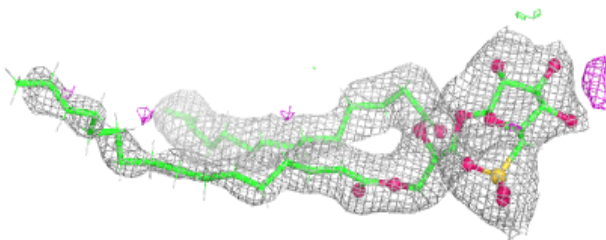
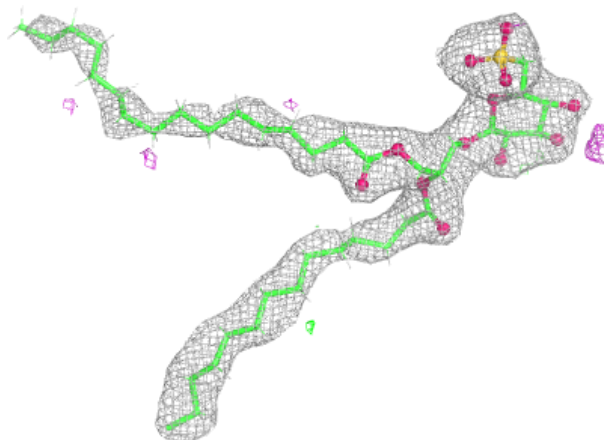


Electron density around LMG d 410:

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

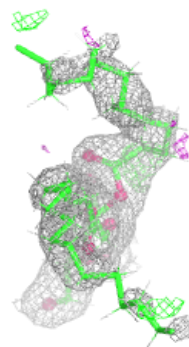
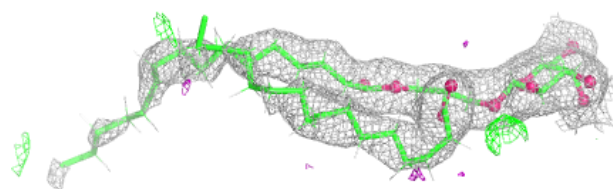
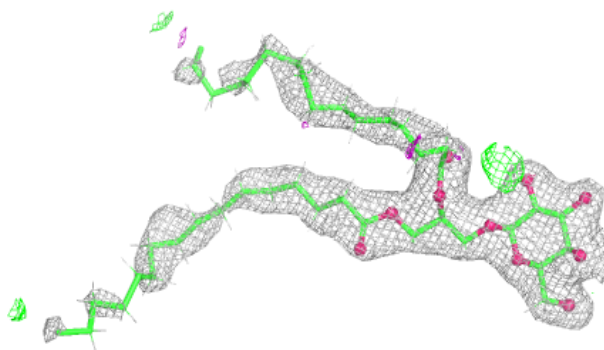
**Electron density around SQD A 411:**

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

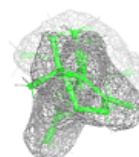
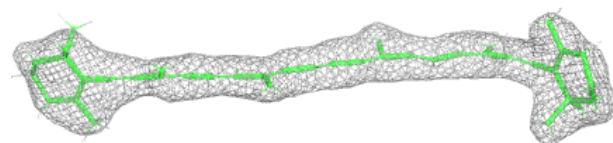
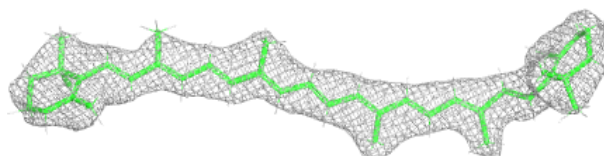


Electron density around LMG D 407:

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

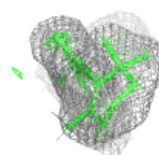
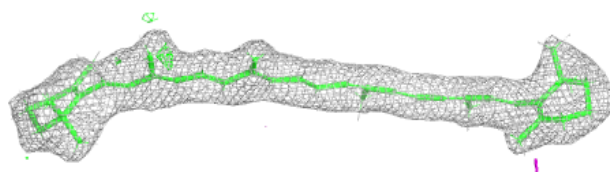
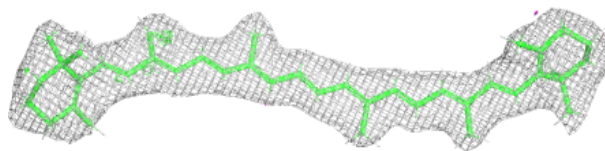
**Electron density around BCR c 516:**

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

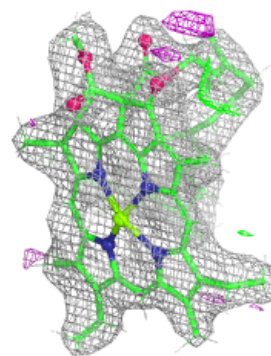
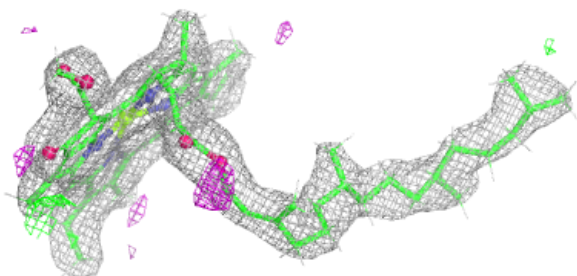
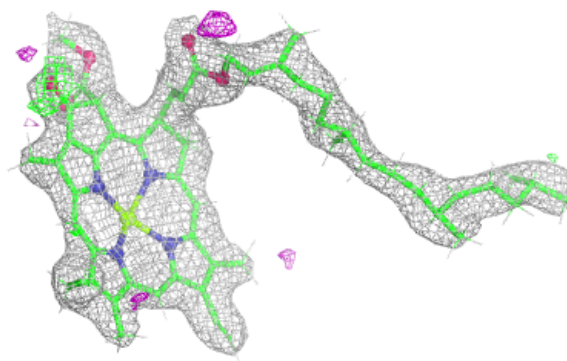


Electron density around BCR B 619:

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

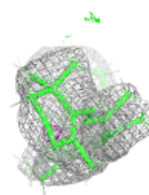
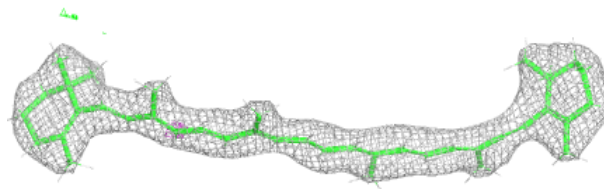
**Electron density around CLA c 512:**

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

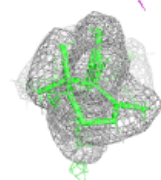
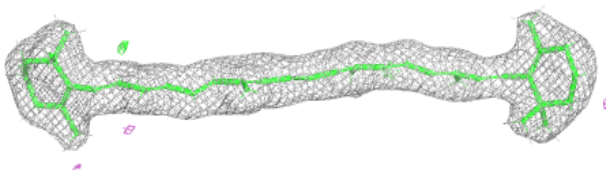
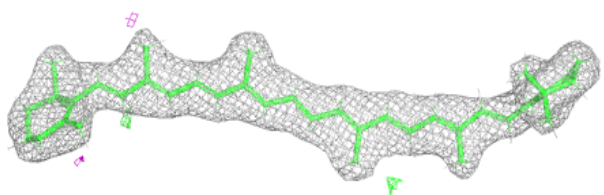


Electron density around BCR K 103:

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

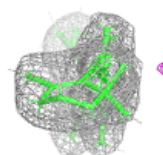
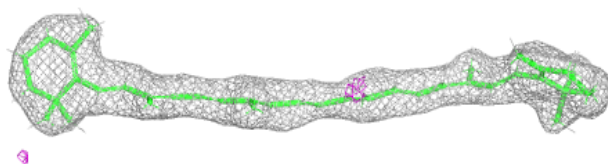
**Electron density around BCR A 406:**

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

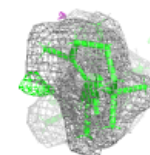
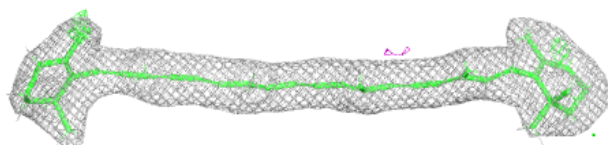
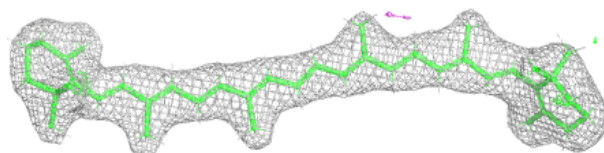


Electron density around BCR b 617:

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

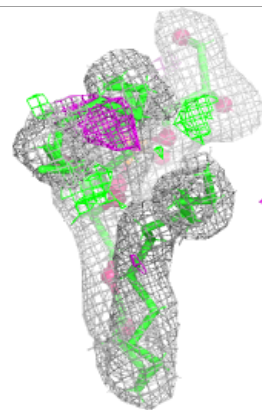
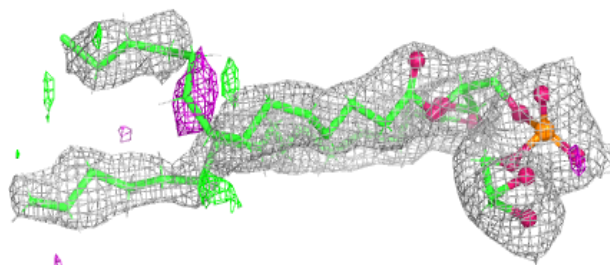
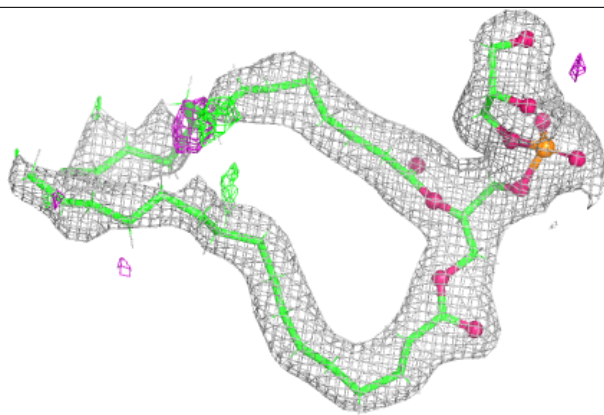
**Electron density around BCR b 618:**

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

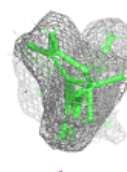
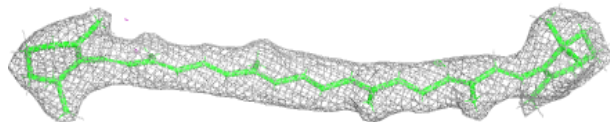
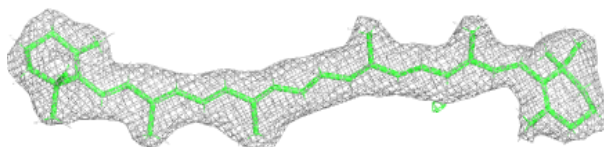


Electron density around LHG D 410:

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

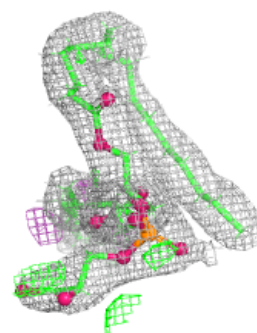
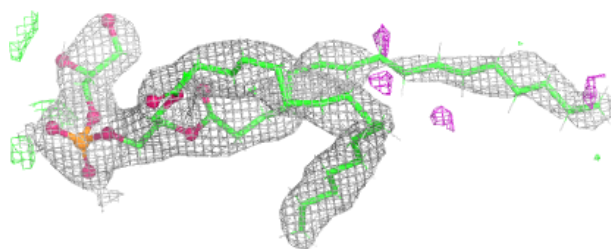
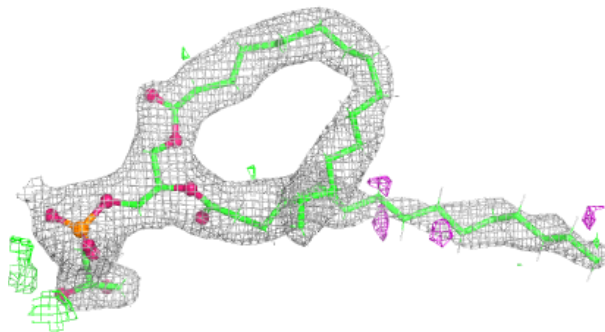
**Electron density around BCR b 619:**

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

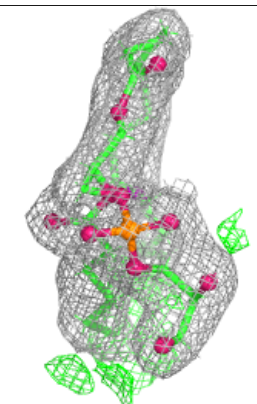
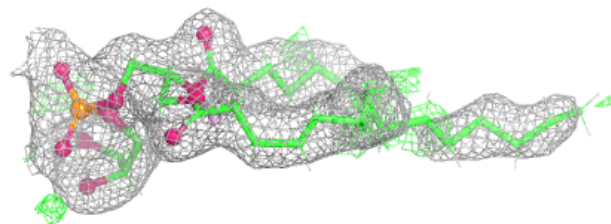
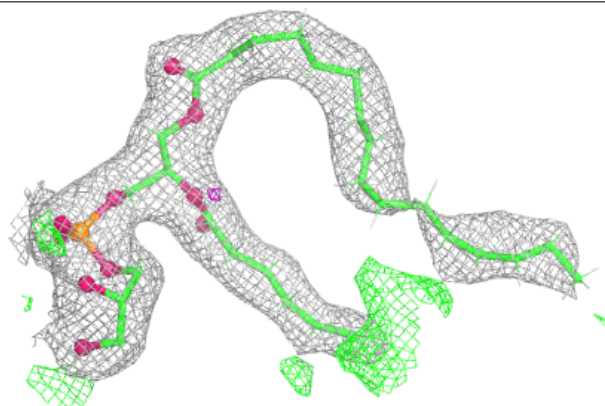


Electron density around LHG d 407:

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

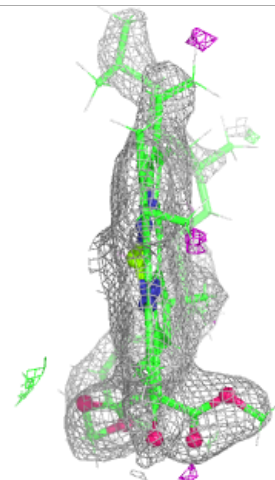
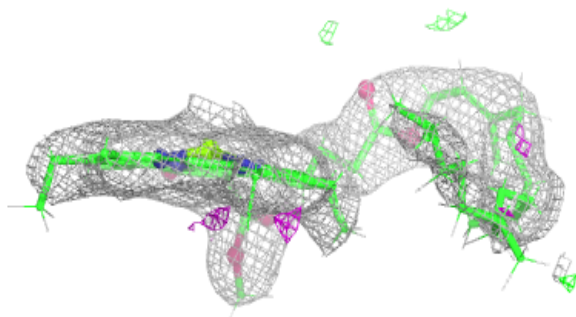
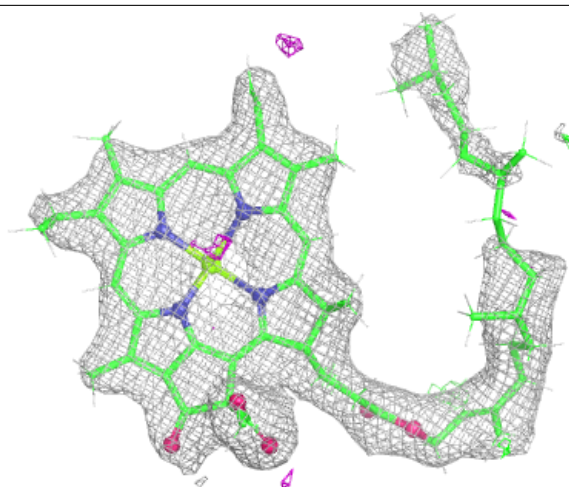
**Electron density around LHG d 409:**

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



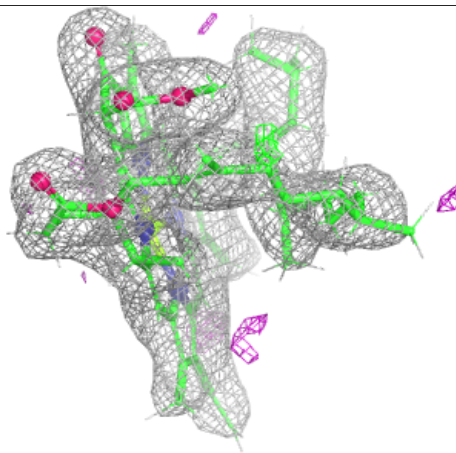
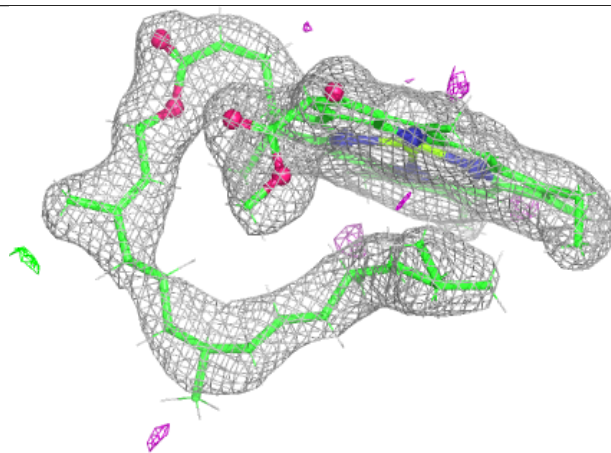
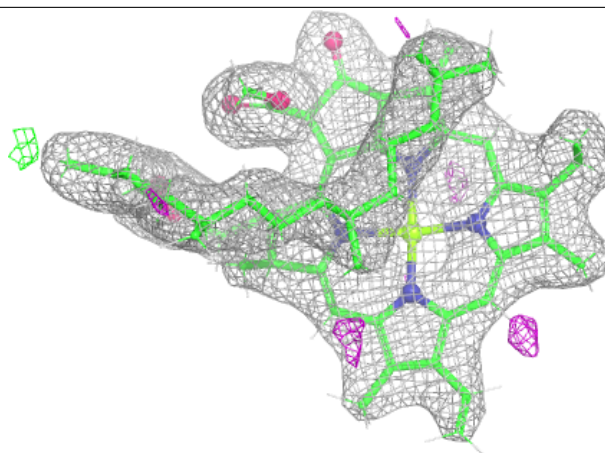
Electron density around CLA C 512:

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



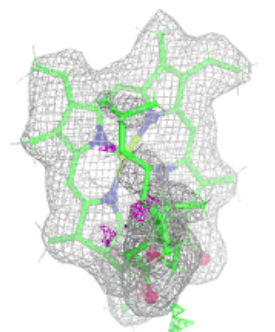
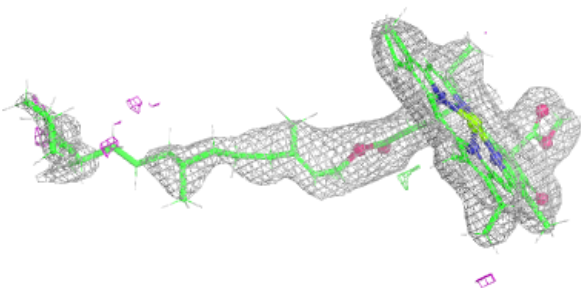
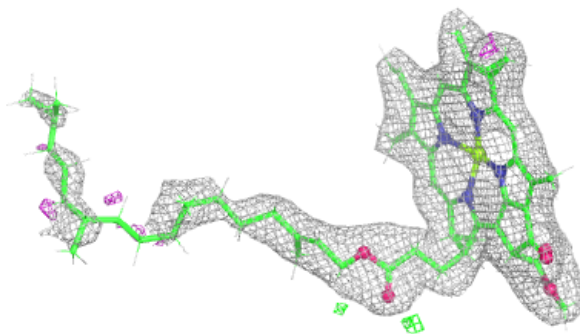
Electron density around CLA C 510:

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

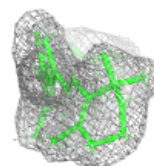
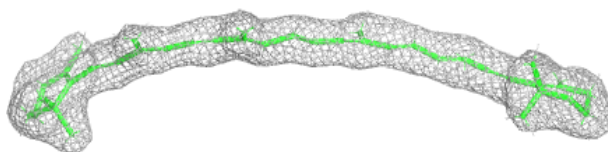
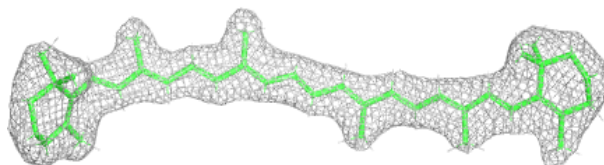


Electron density around CLA d 404:

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

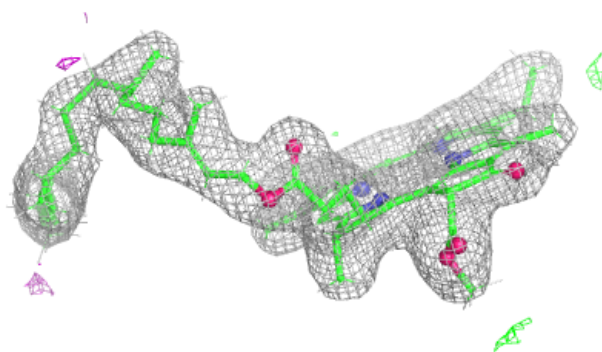
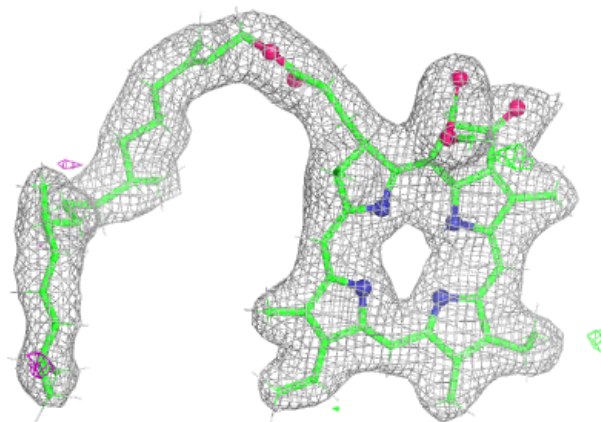
**Electron density around BCR t 101:**

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

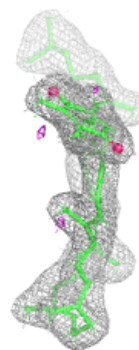
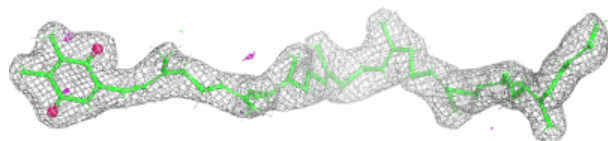
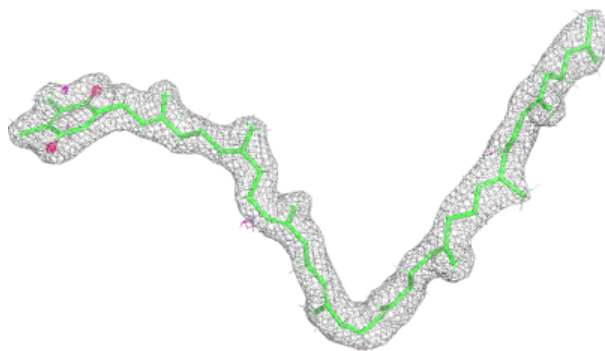


Electron density around PHO d 401:

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

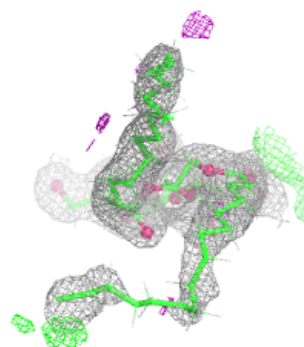
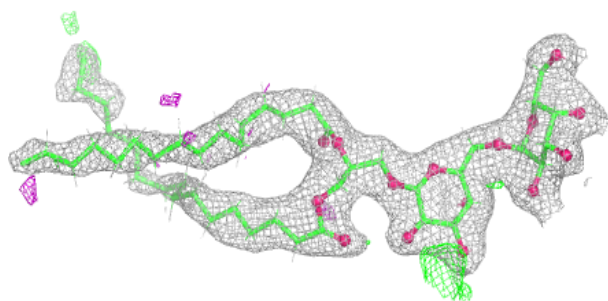
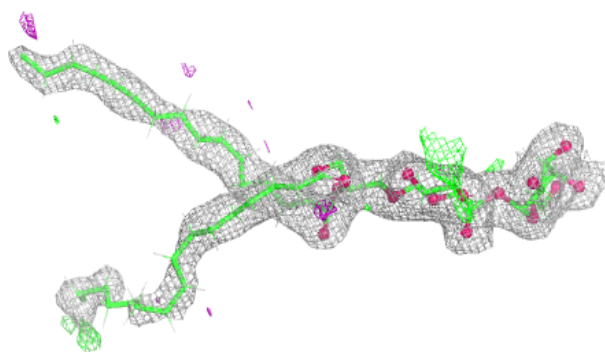
**Electron density around PL9 D 406:**

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

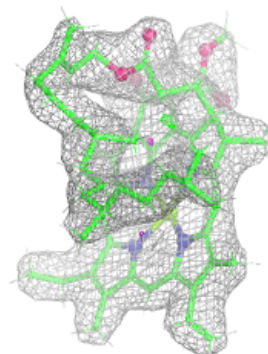
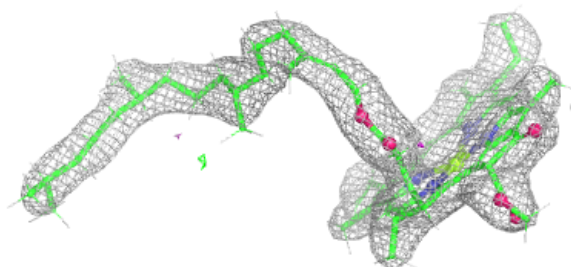
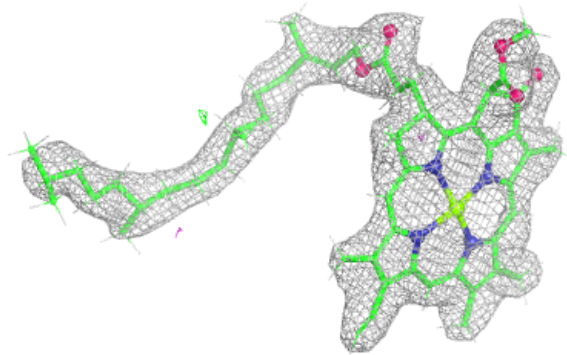


Electron density around DGD C 515:

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

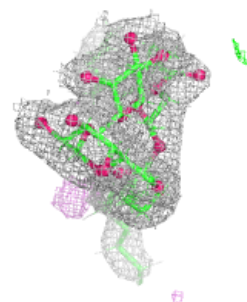
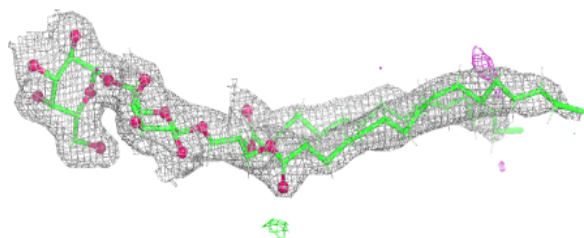
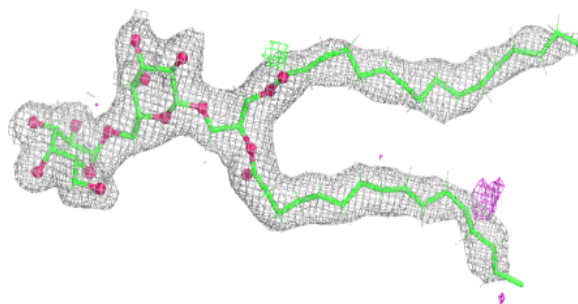
**Electron density around CLA C 511:**

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

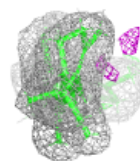
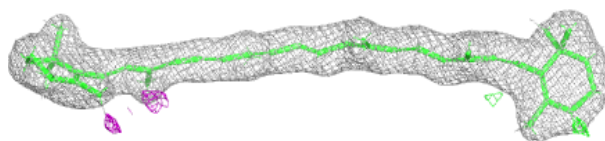
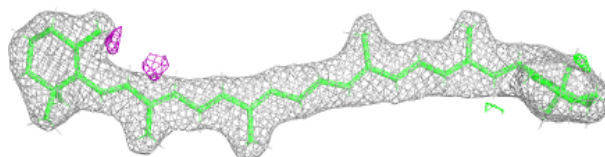


Electron density around DGD C 517:

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

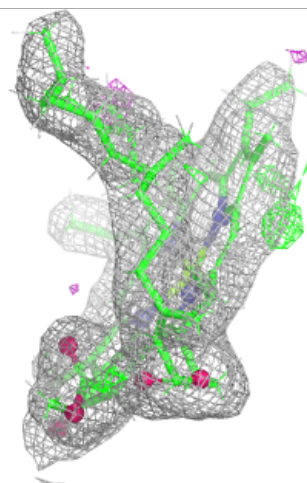
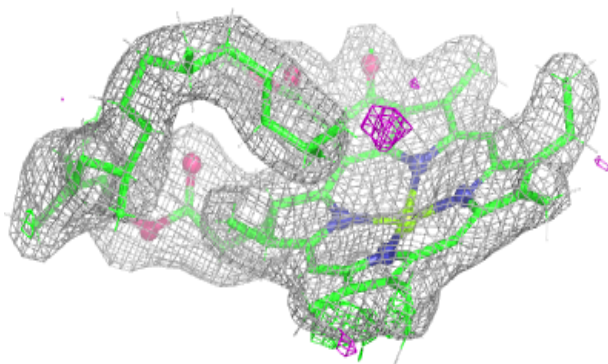
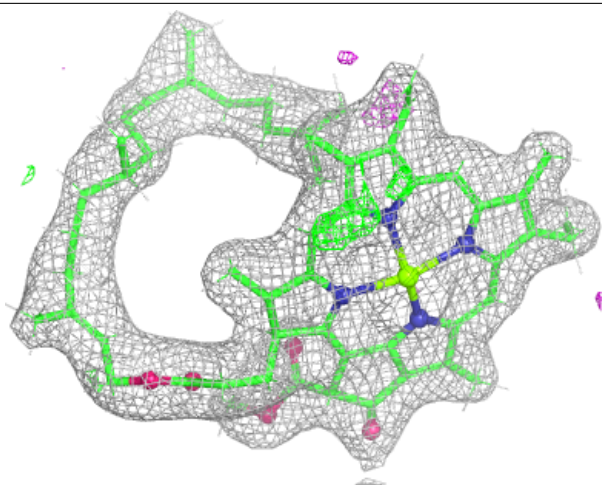
**Electron density around BCR B 617:**

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



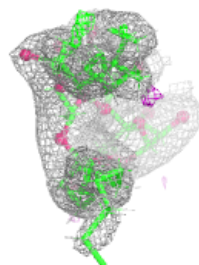
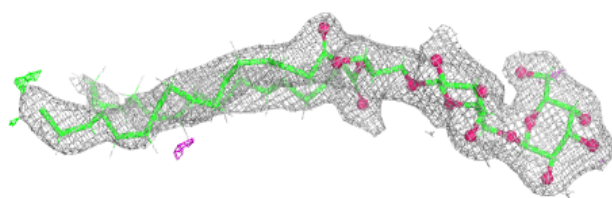
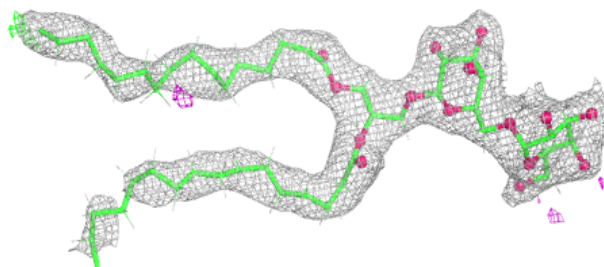
Electron density around CLA B 615:

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

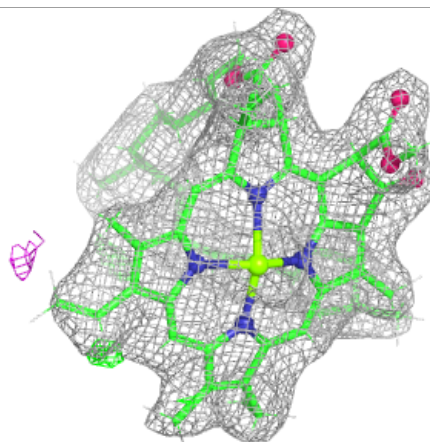
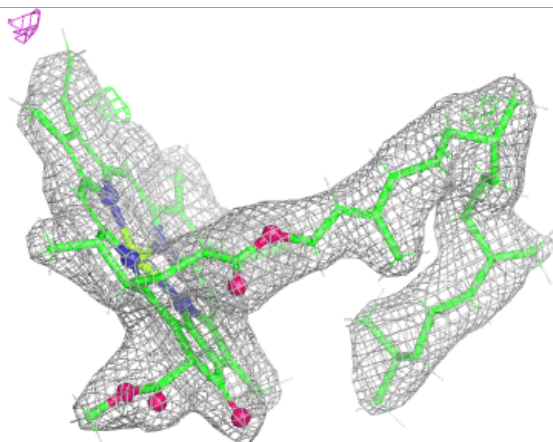
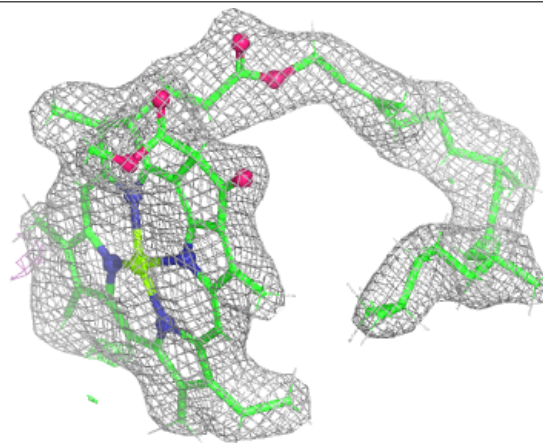


Electron density around DGD c 519:

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

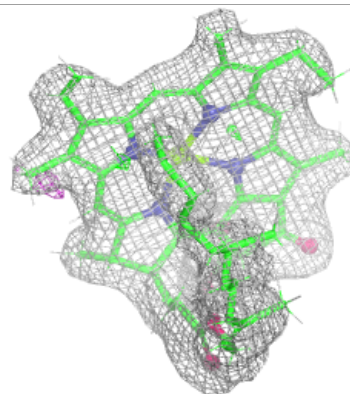
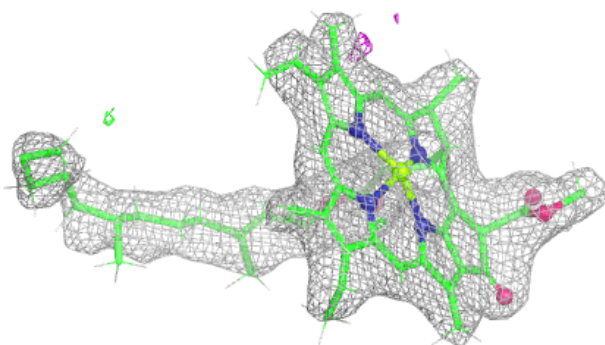
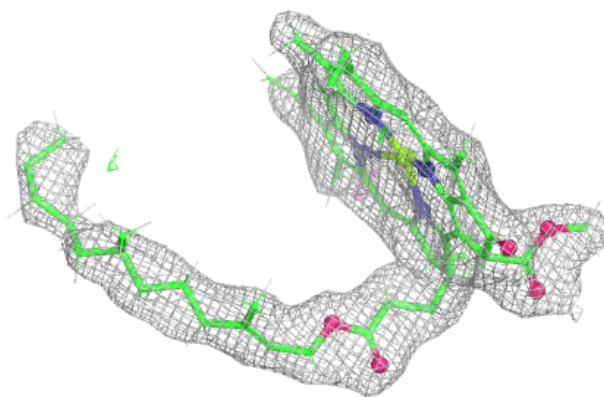
**Electron density around CLA C 503:**

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

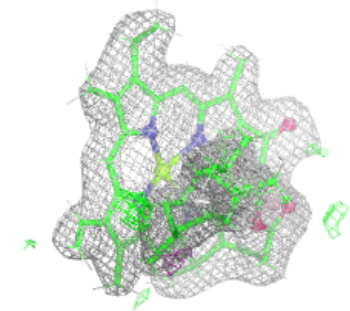
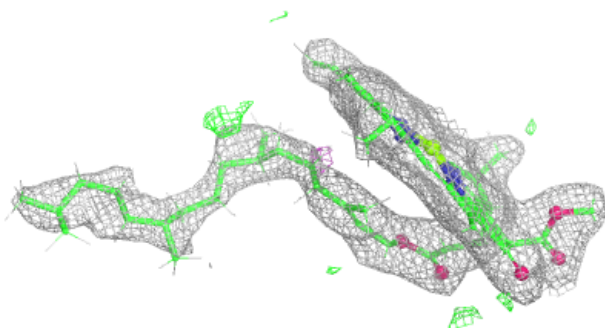
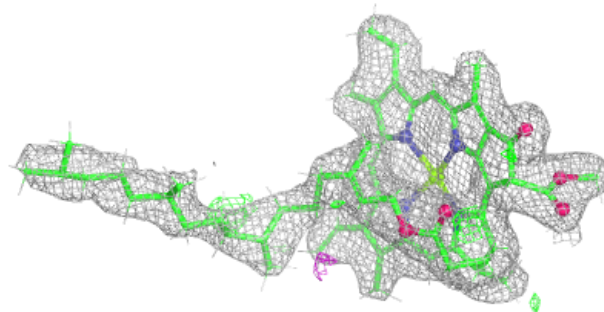


Electron density around CLA C 504:

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

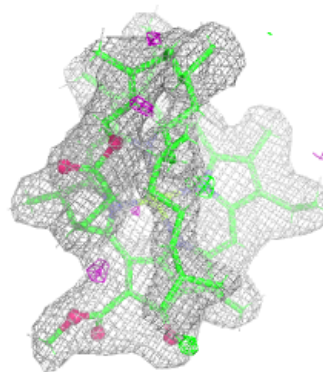
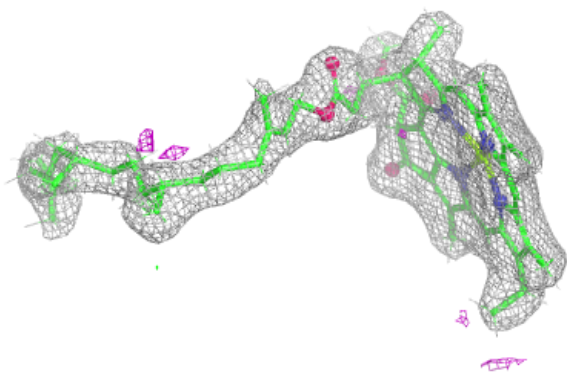
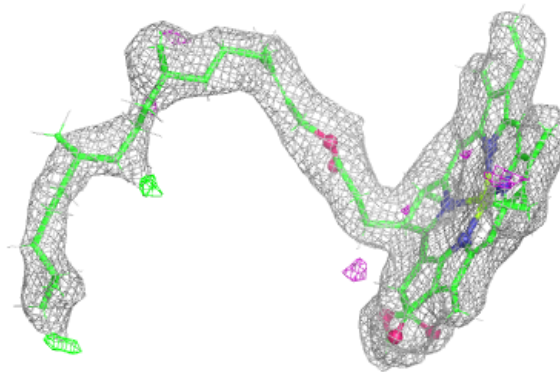
**Electron density around CLA C 505:**

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

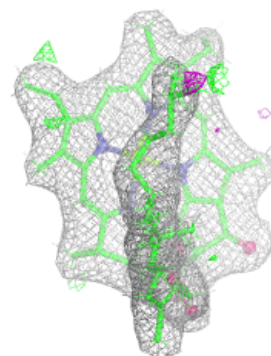
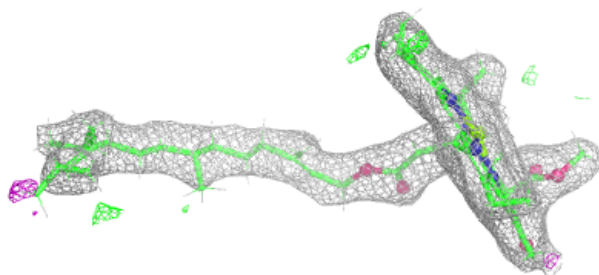
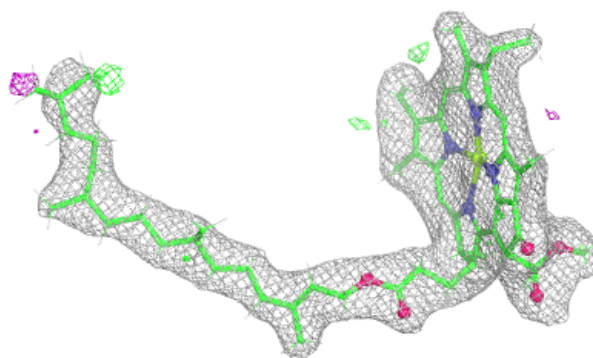


Electron density around CLA b 606:

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

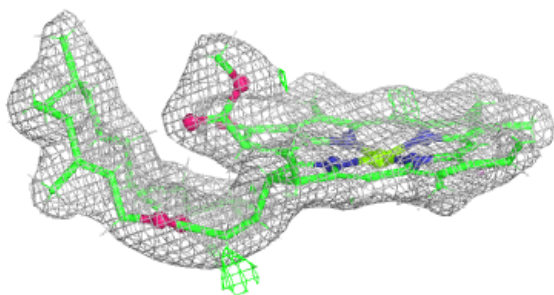
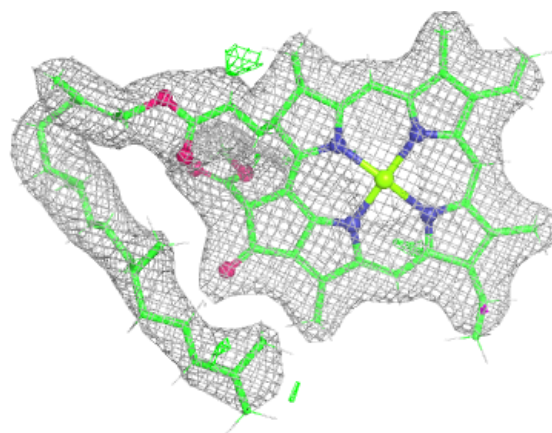
**Electron density around CLA b 609:**

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



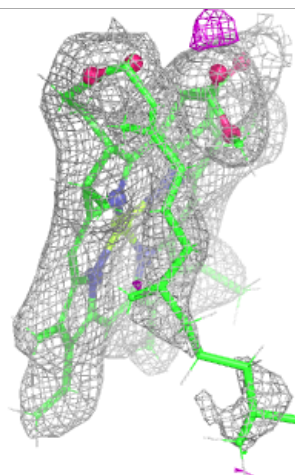
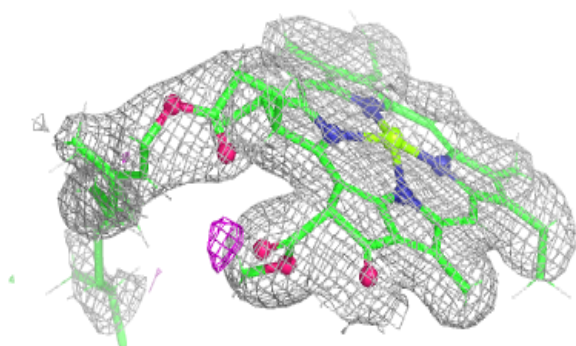
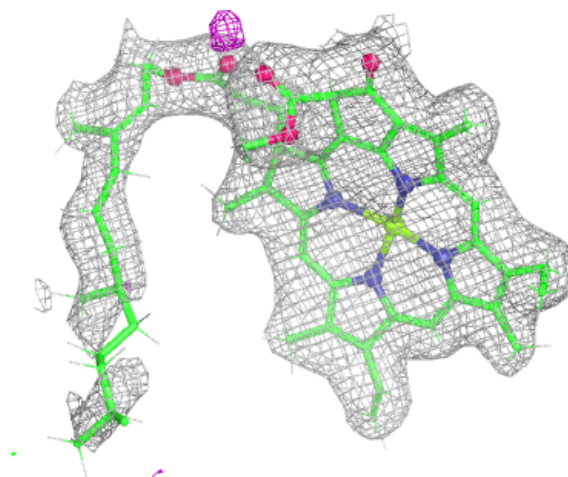
Electron density around CLA b 610:

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



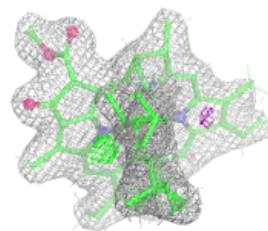
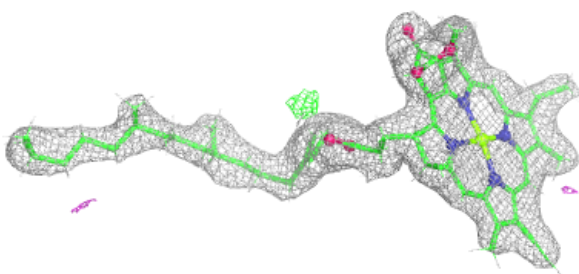
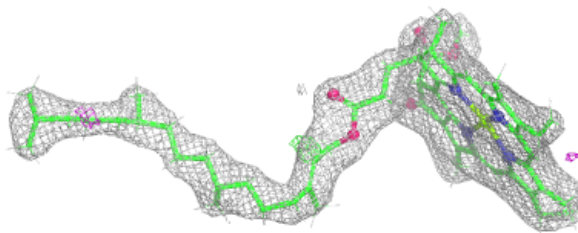
Electron density around CLA b 616:

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



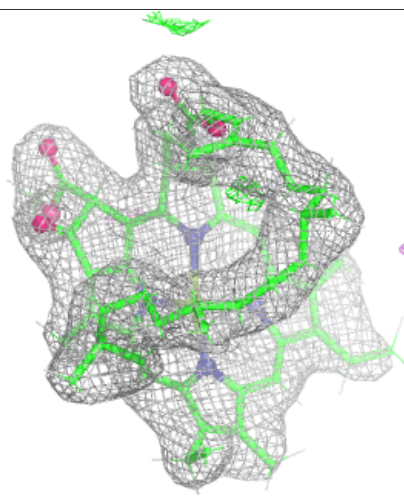
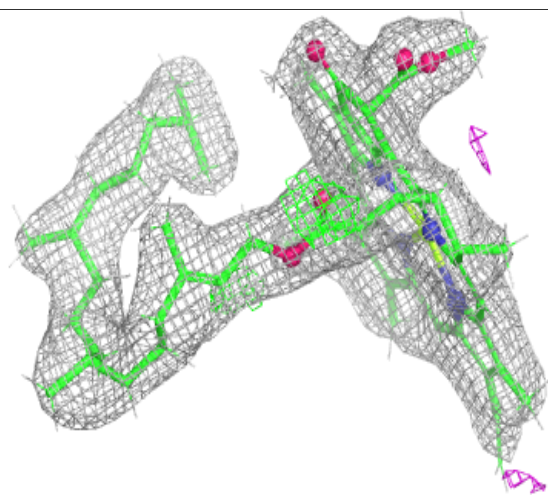
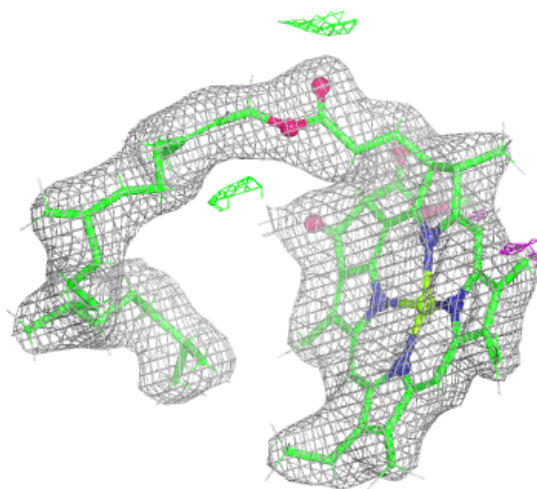
Electron density around CLA c 503:

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



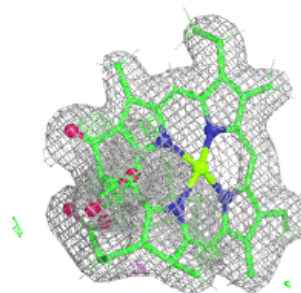
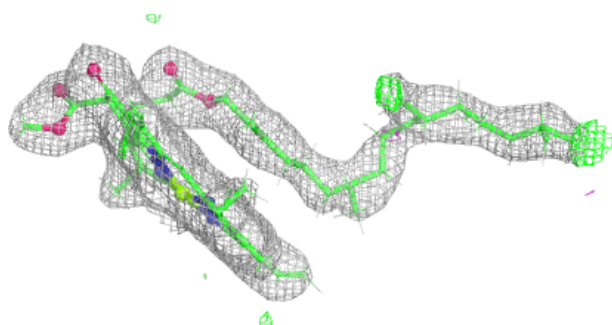
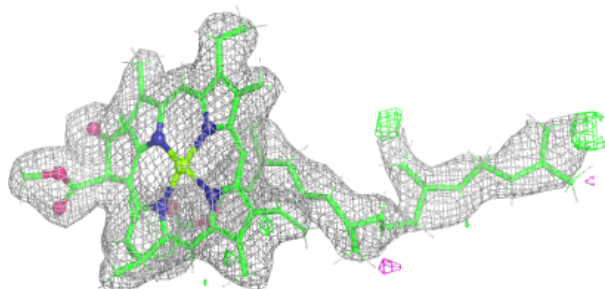
Electron density around CLA c 504:

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

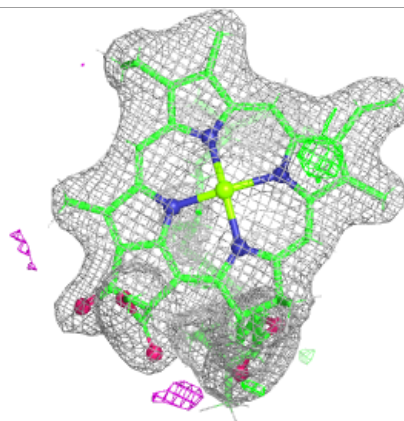
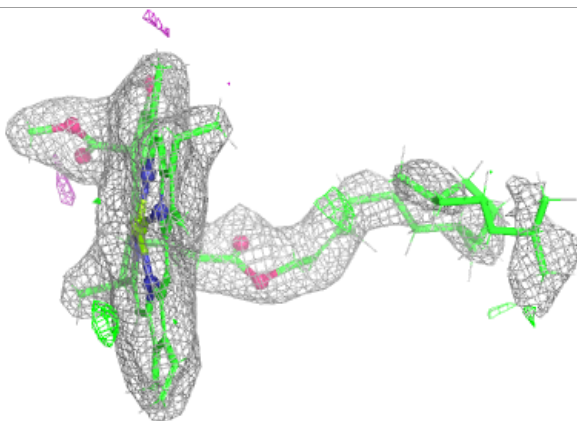
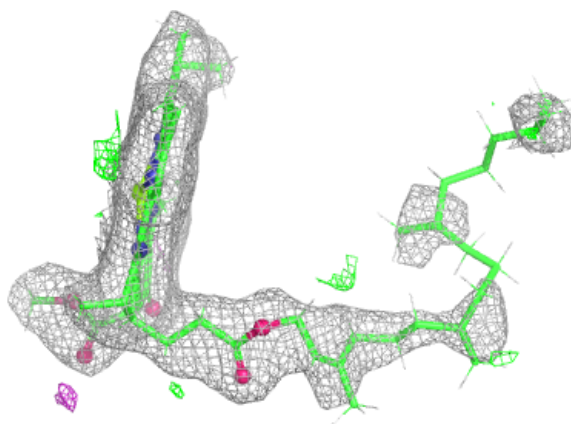


Electron density around CLA c 506:

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

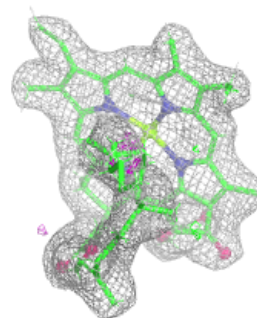
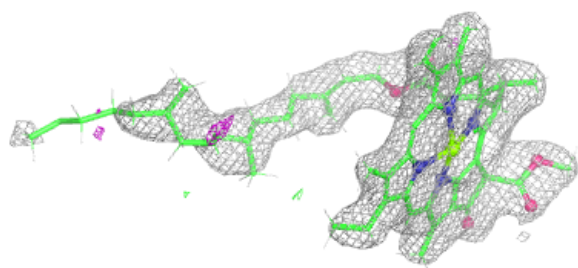
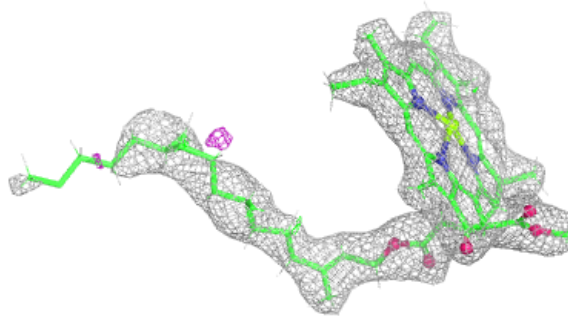
**Electron density around CLA c 507:**

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



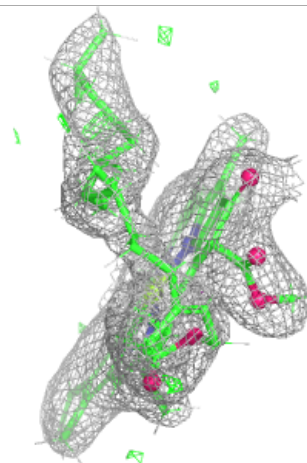
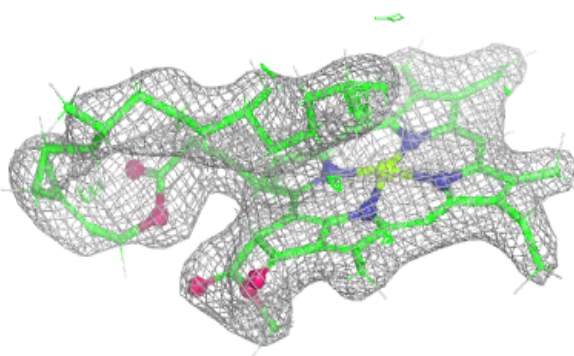
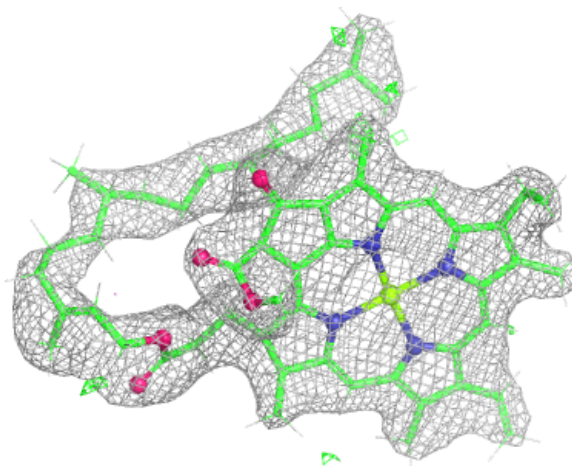
Electron density around CLA c 509:

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



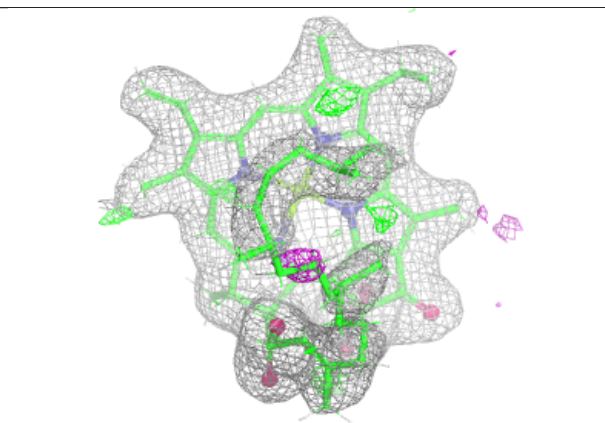
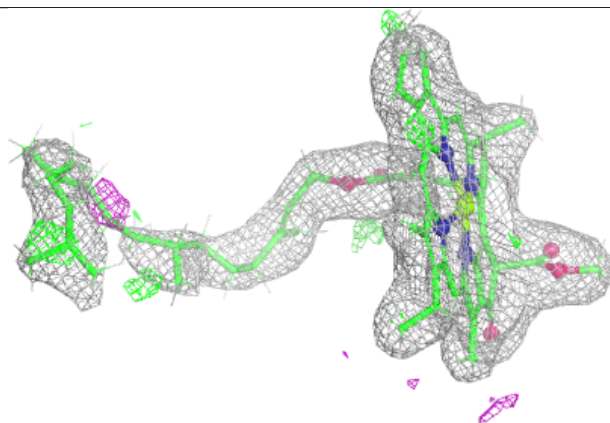
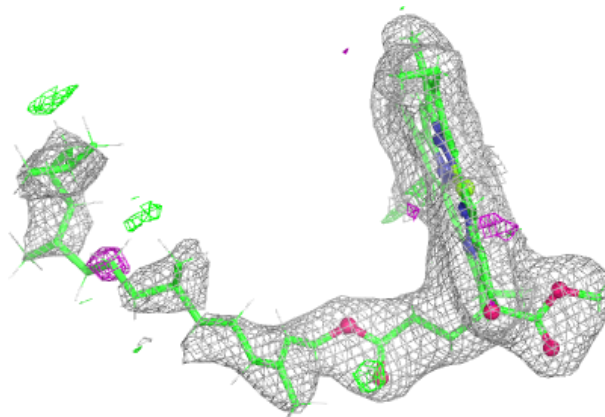
Electron density around CLA c 510:

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

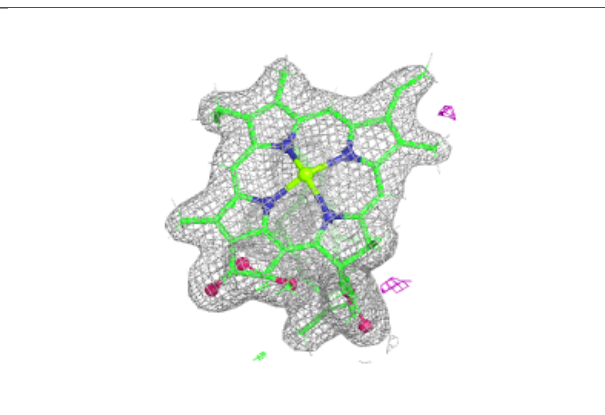
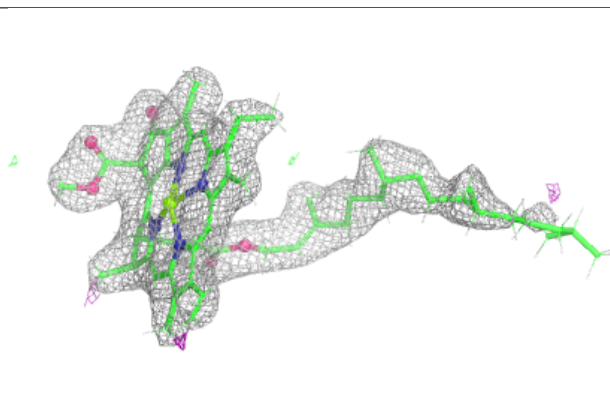
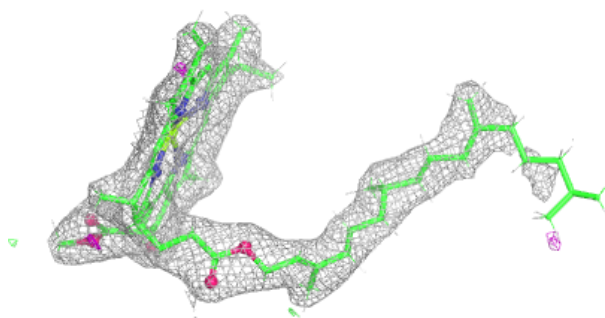


Electron density around CLA C 506:

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

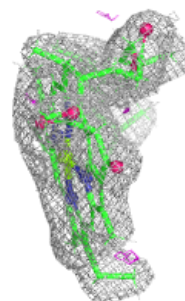
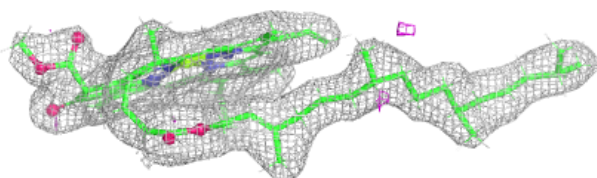
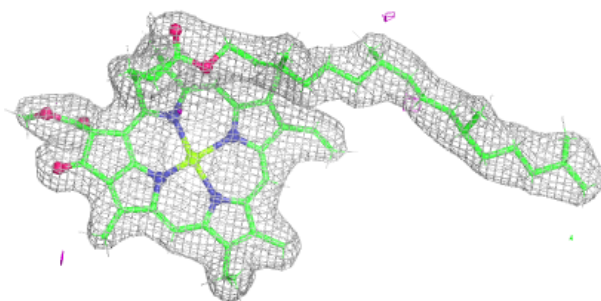
**Electron density around CLA C 508:**

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

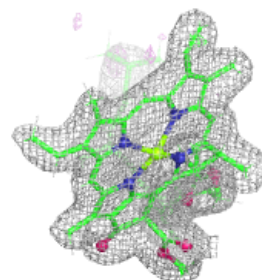
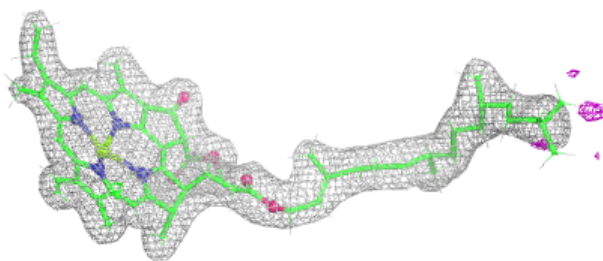
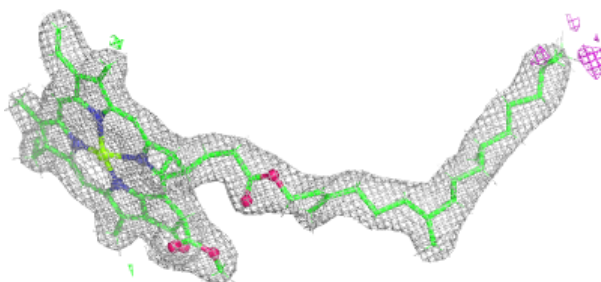


Electron density around CLA C 501:

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

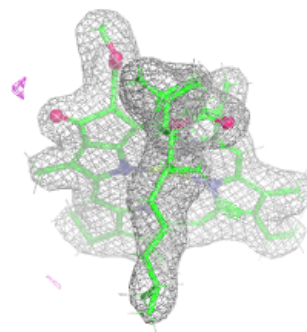
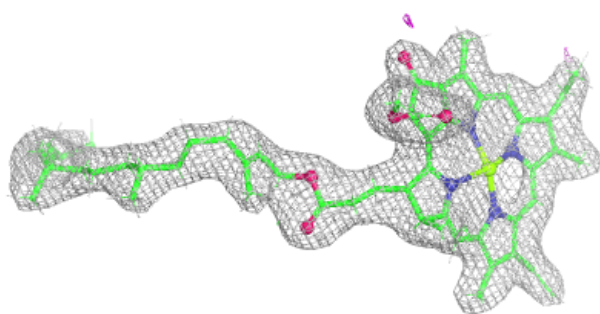
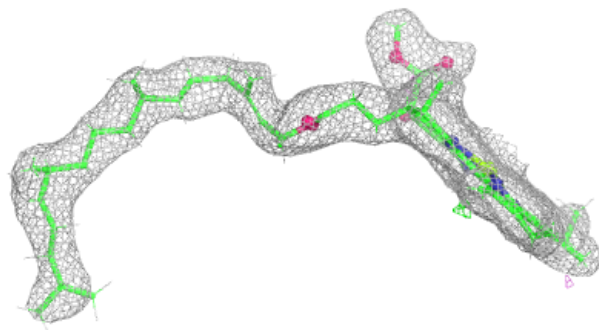
**Electron density around CLA a 402:**

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

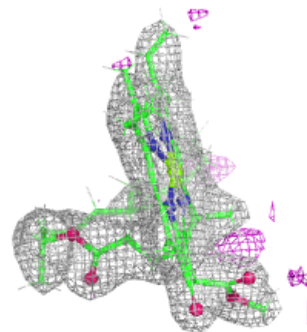
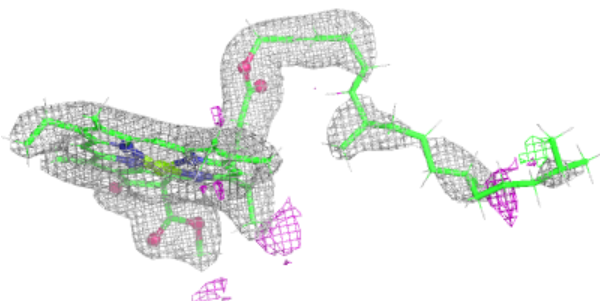
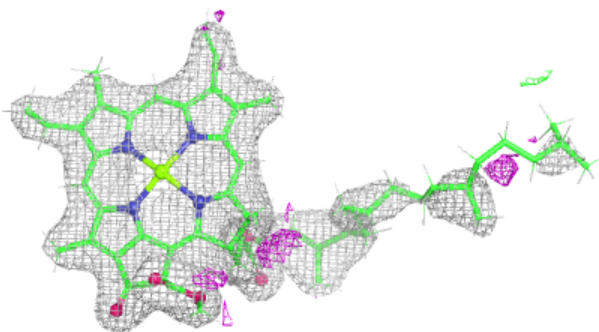


Electron density around CLA d 403:

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

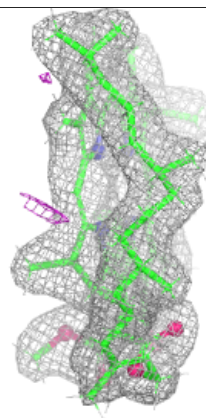
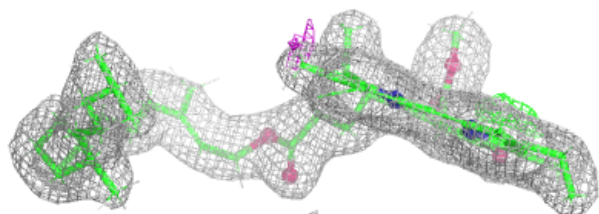
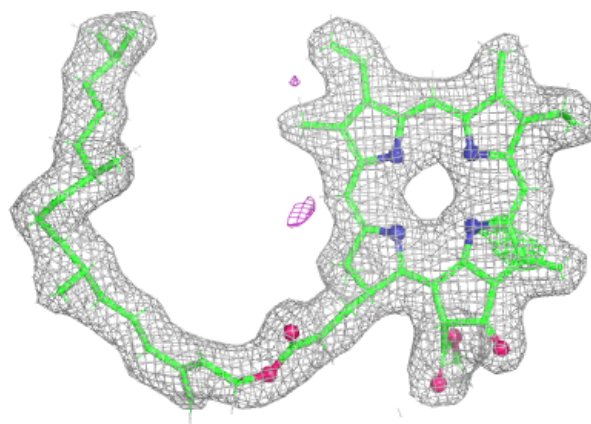
**Electron density around CLA a 403:**

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



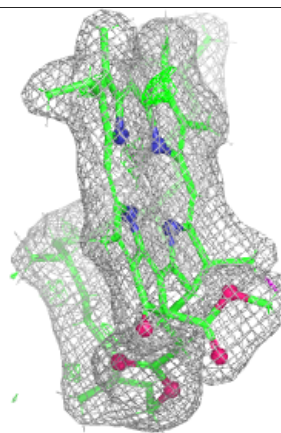
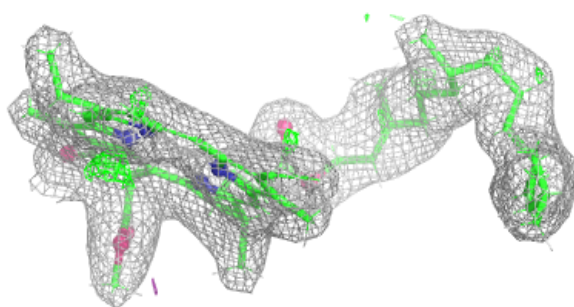
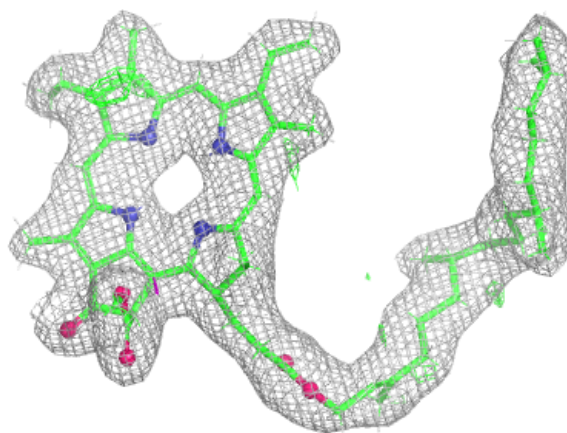
Electron density around PHO A 404:

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



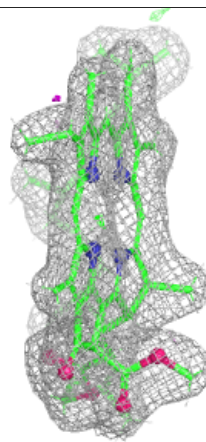
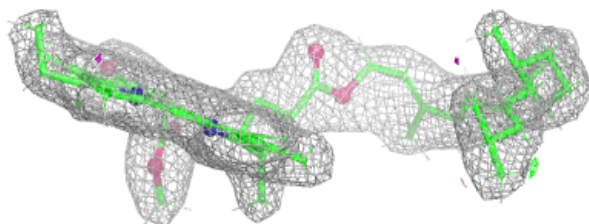
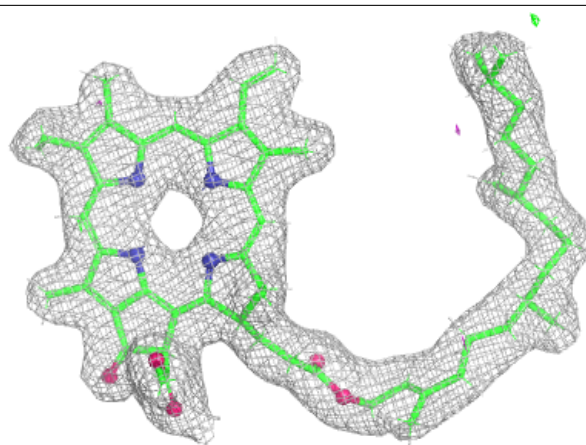
Electron density around PHO D 401:

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



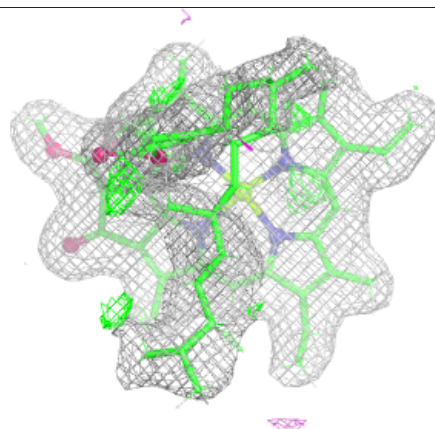
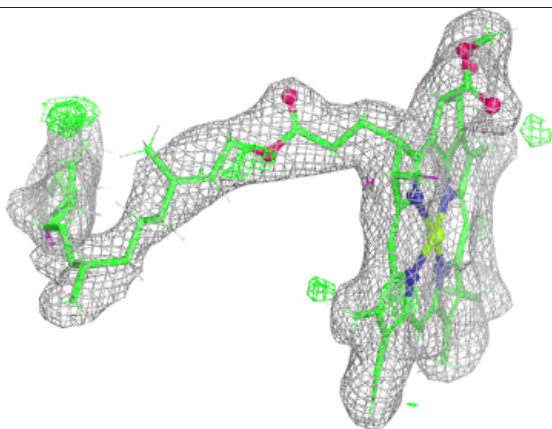
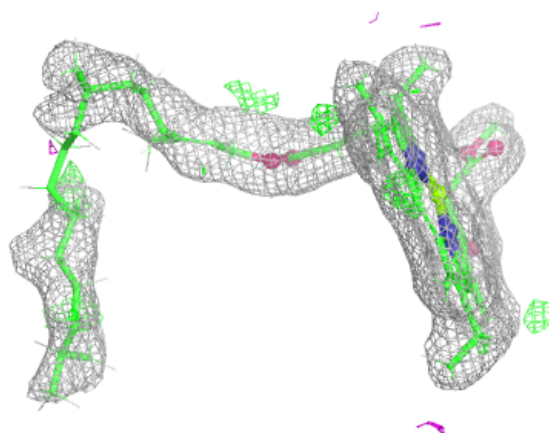
Electron density around PHO a 404:

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

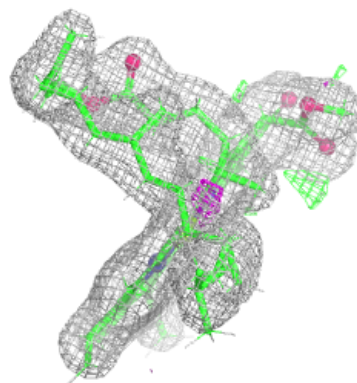
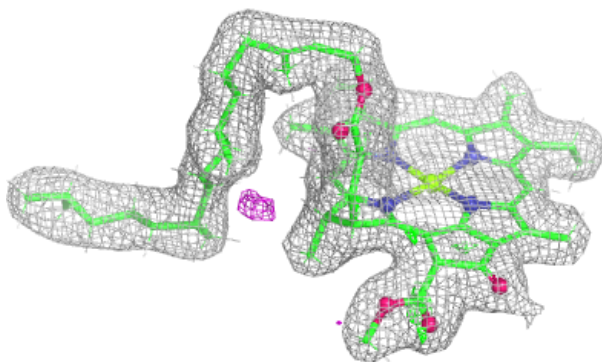
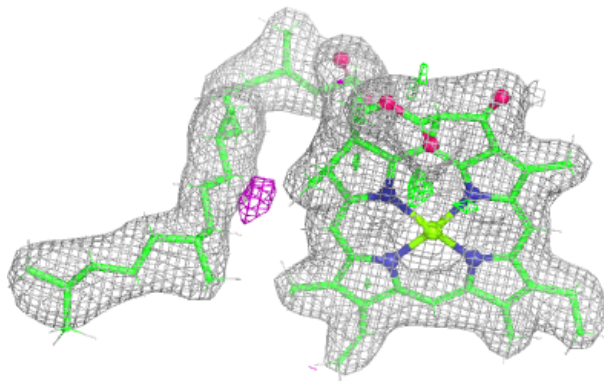


Electron density around CLA a 405:

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

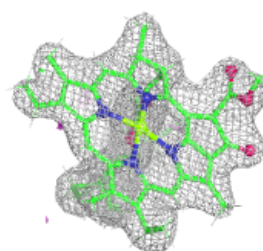
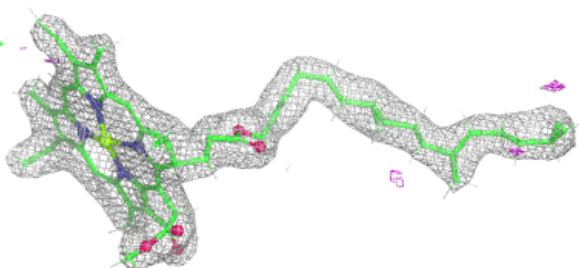
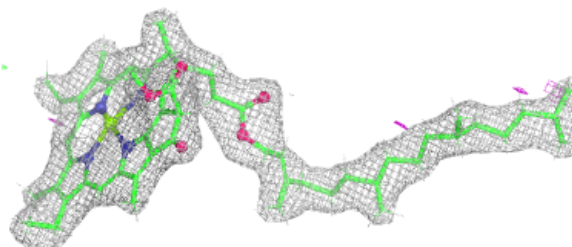
**Electron density around CLA a 410:**

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

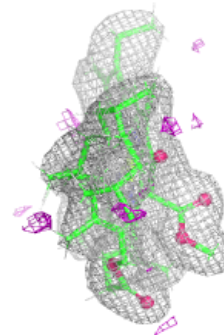
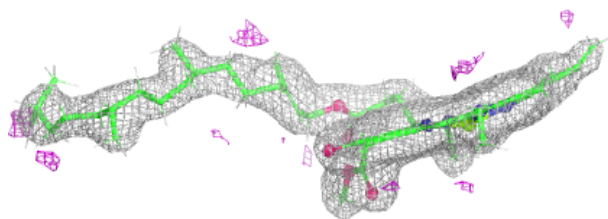
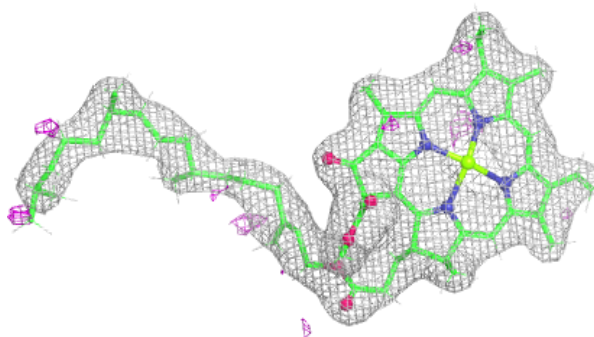


Electron density around CLA C 502:

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

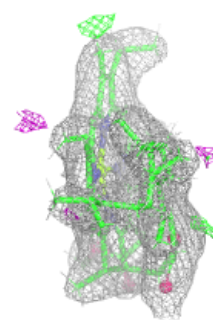
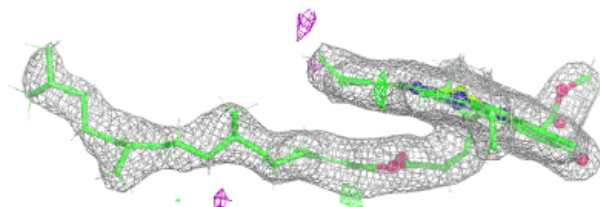
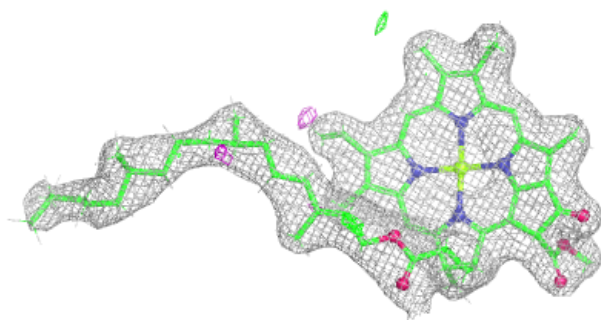
**Electron density around CLA b 602:**

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

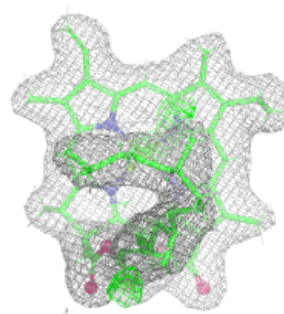
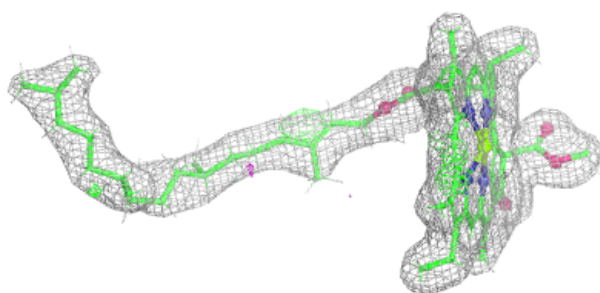
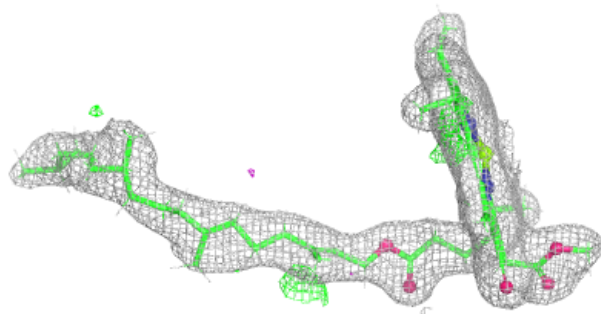


Electron density around CLA b 603:

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

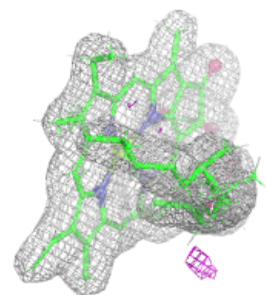
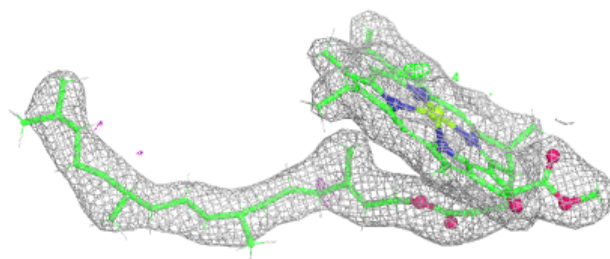
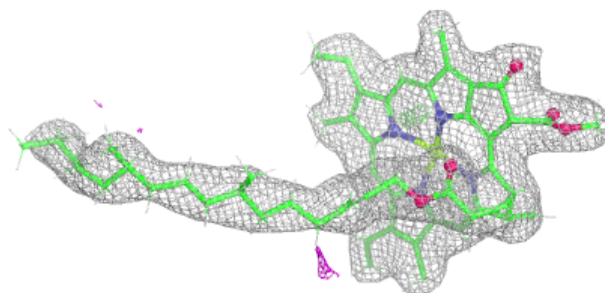
**Electron density around CLA B 605:**

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



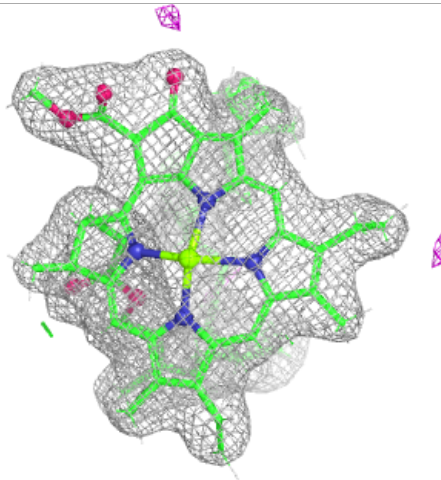
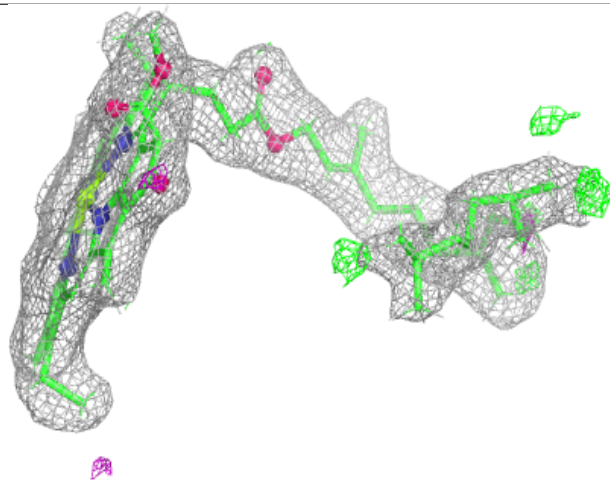
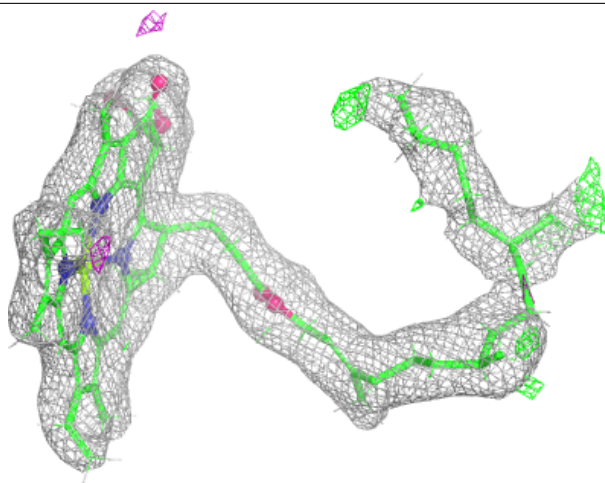
Electron density around CLA b 608:

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



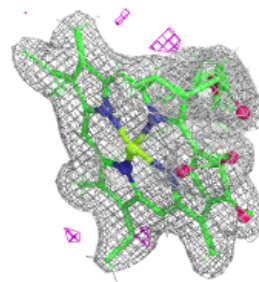
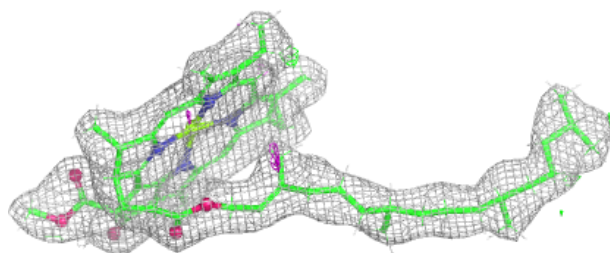
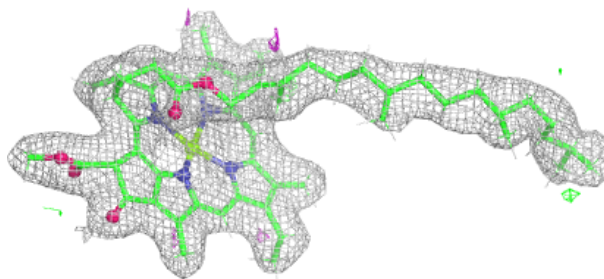
Electron density around CLA B 606:

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



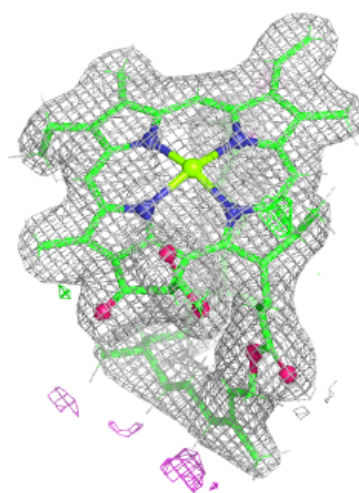
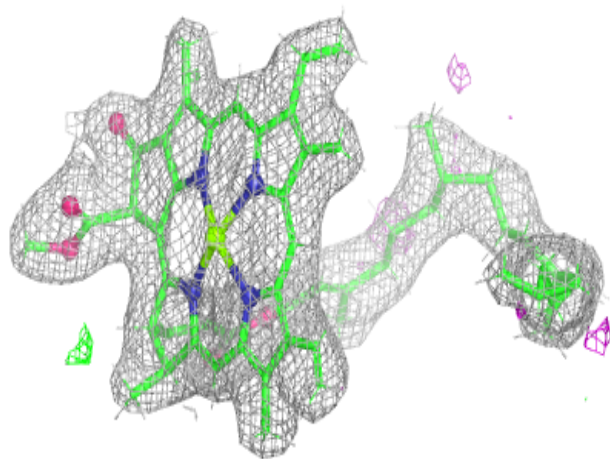
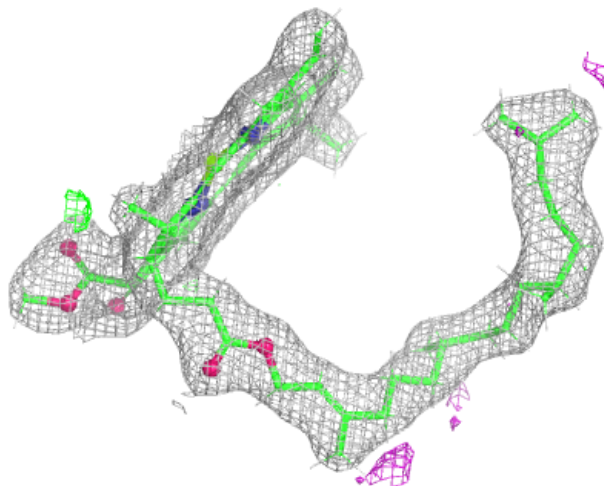
Electron density around CLA B 608:

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



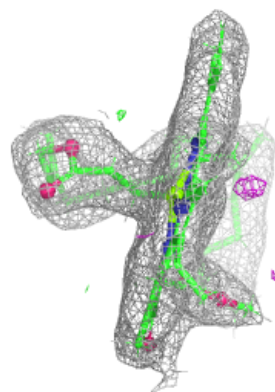
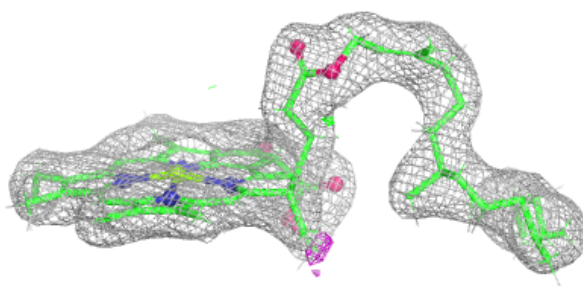
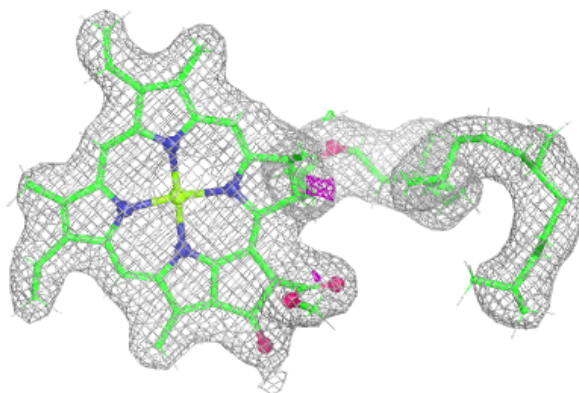
Electron density around CLA b 611:

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

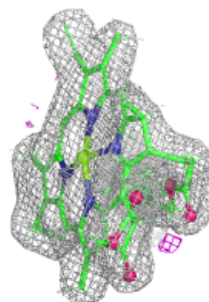
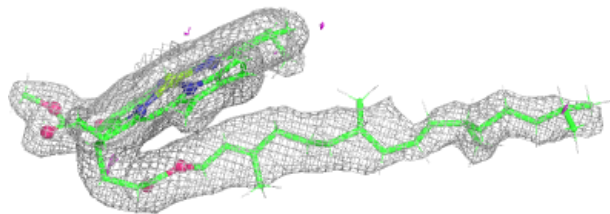
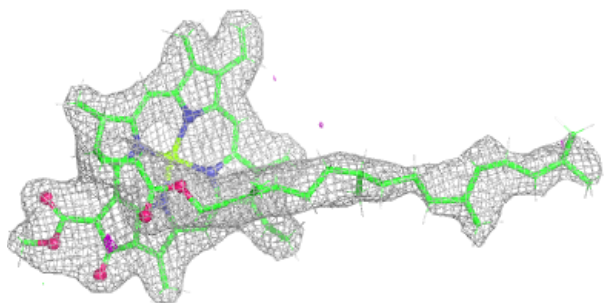


Electron density around CLA b 612:

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

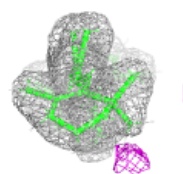
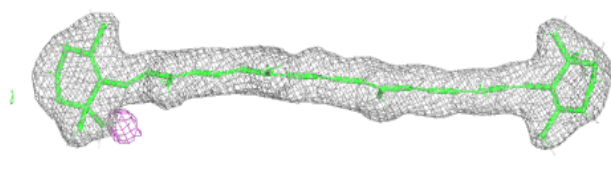
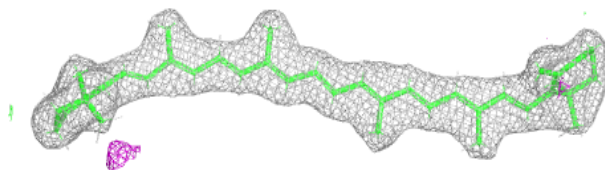
**Electron density around CLA b 614:**

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



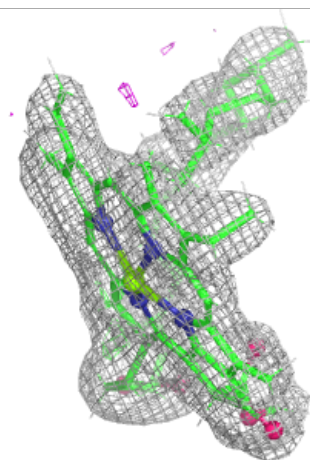
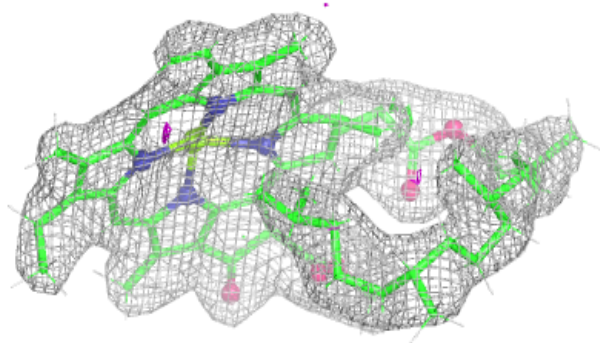
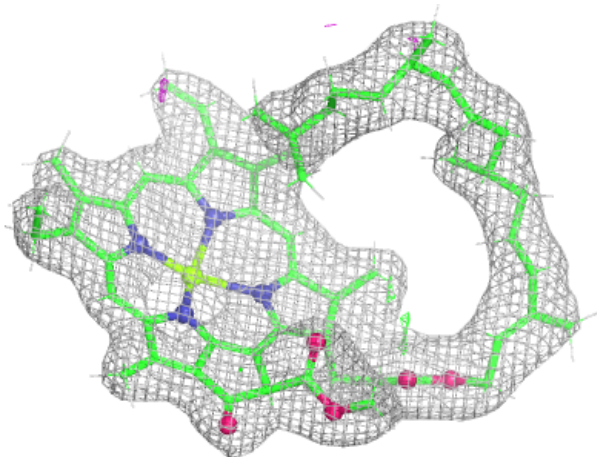
Electron density around BCR a 406:

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



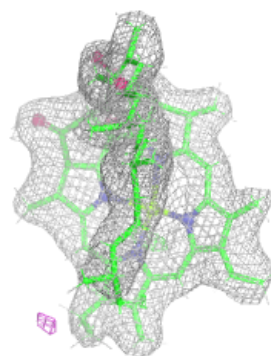
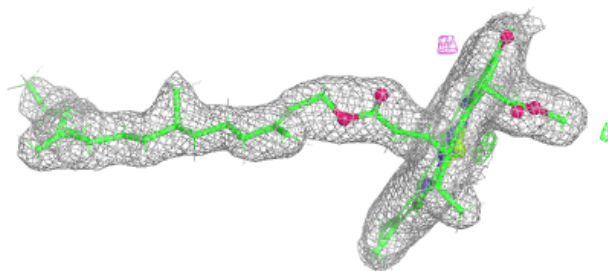
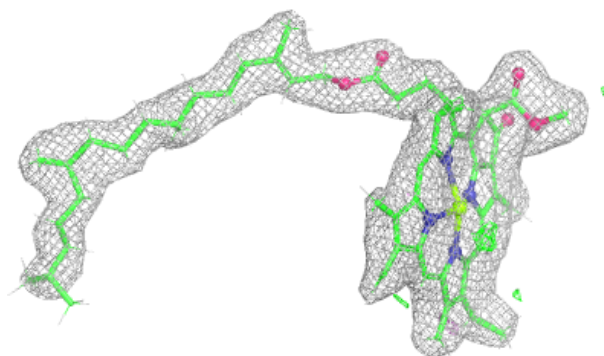
Electron density around CLA b 615:

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

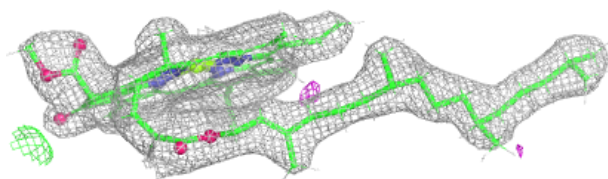
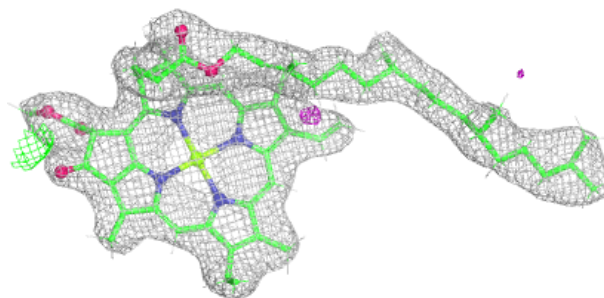


Electron density around CLA B 609:

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

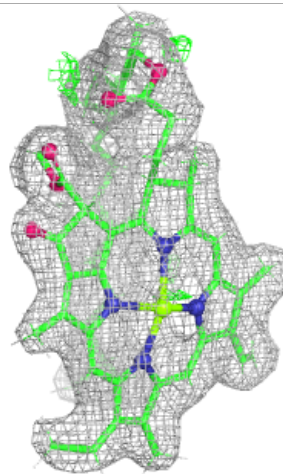
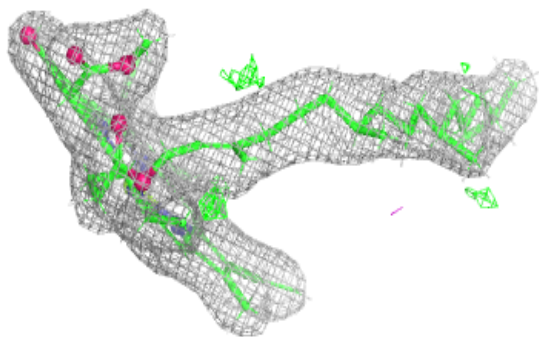
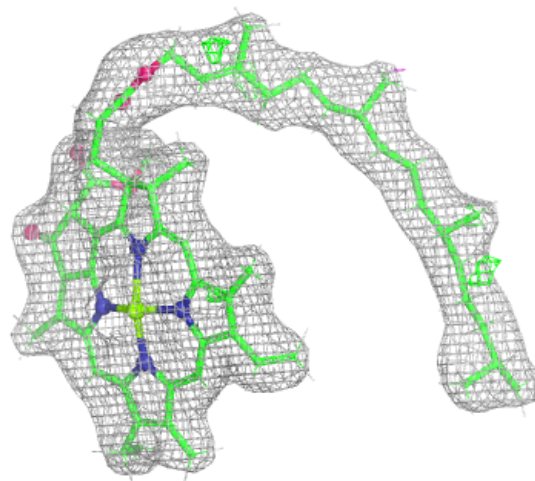
**Electron density around CLA c 502:**

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



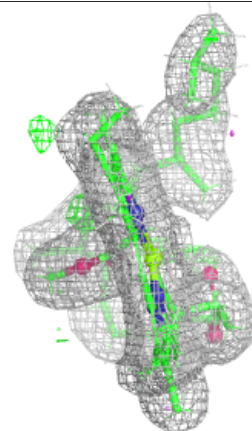
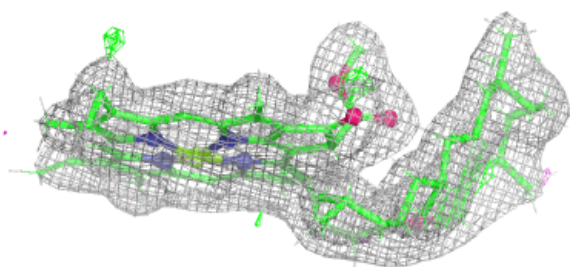
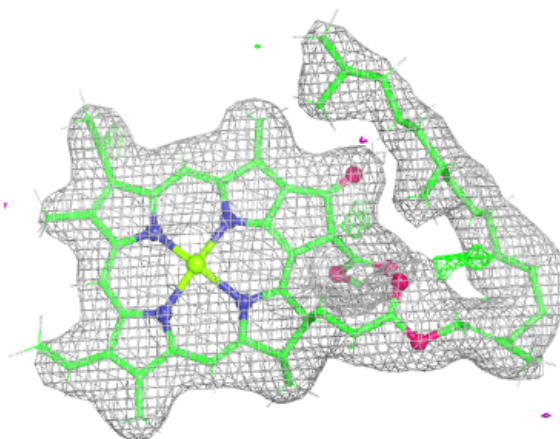
Electron density around CLA C 507:

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

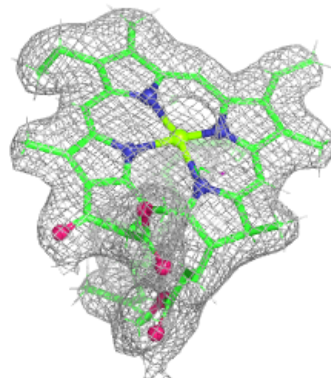
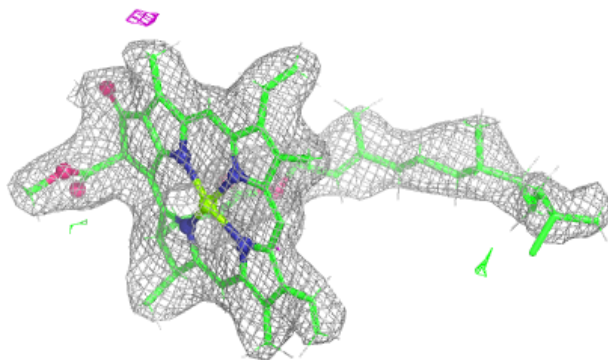
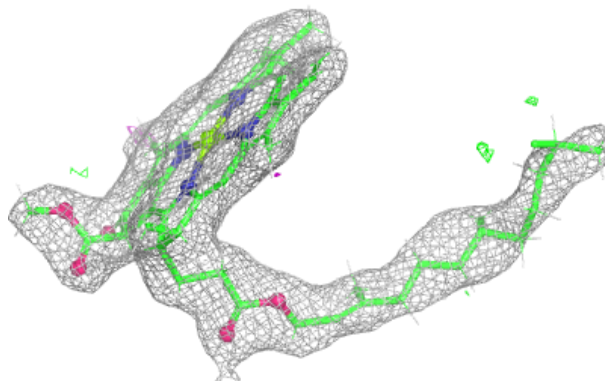


Electron density around CLA B 610:

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

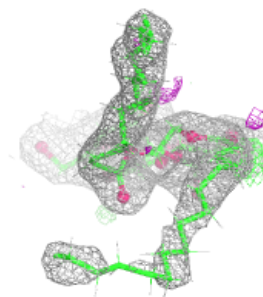
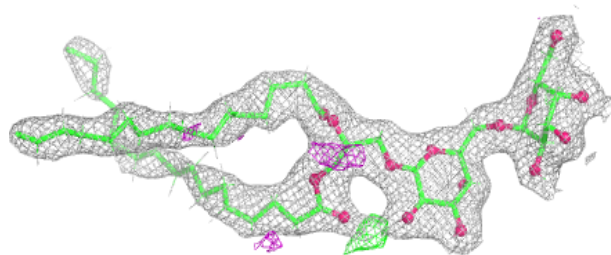
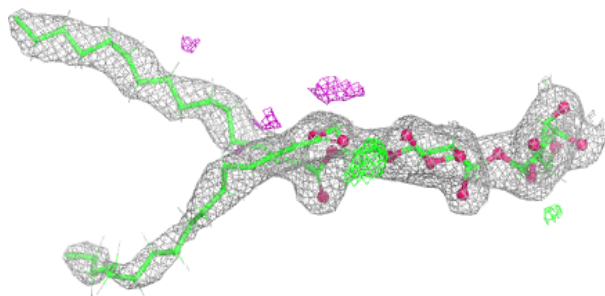
**Electron density around CLA c 505:**

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



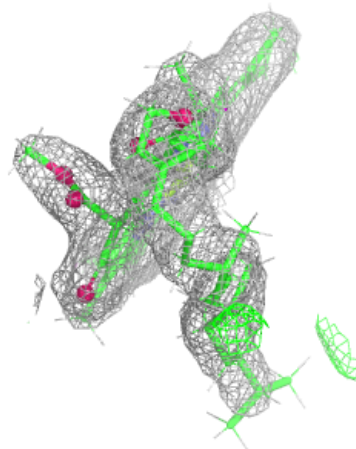
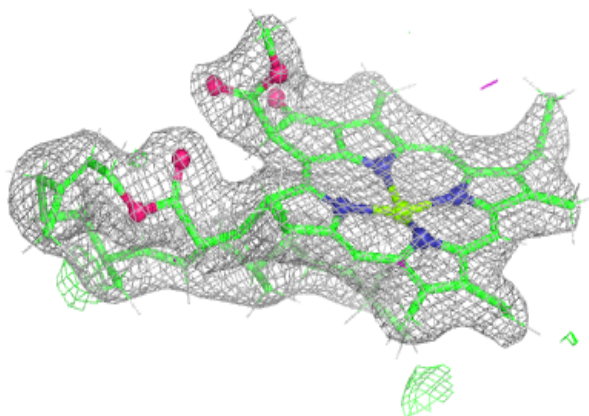
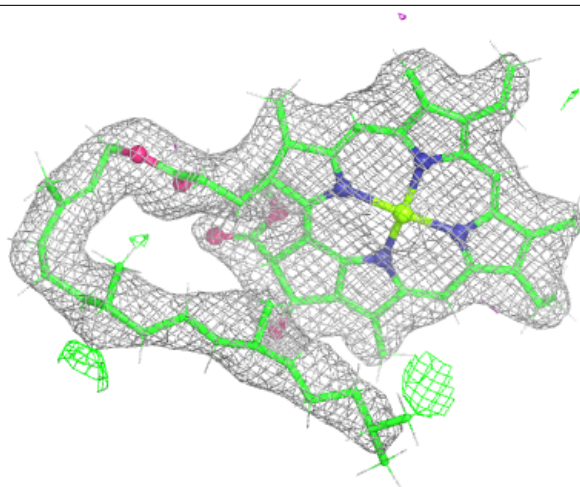
Electron density around DGD c 517:

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



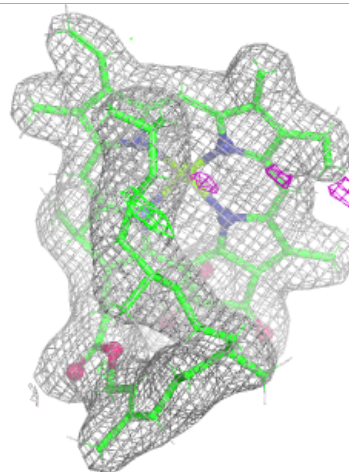
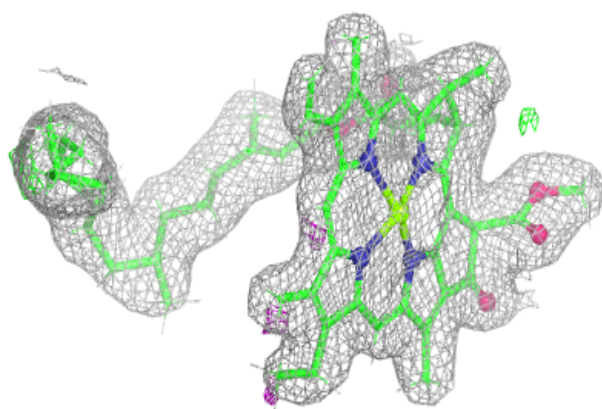
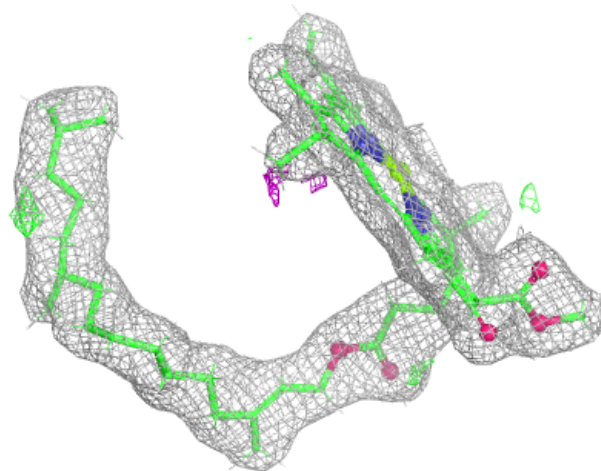
Electron density around CLA C 509:

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



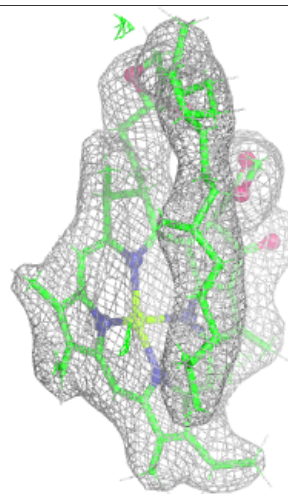
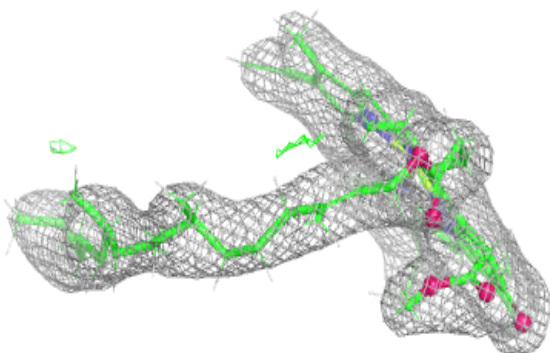
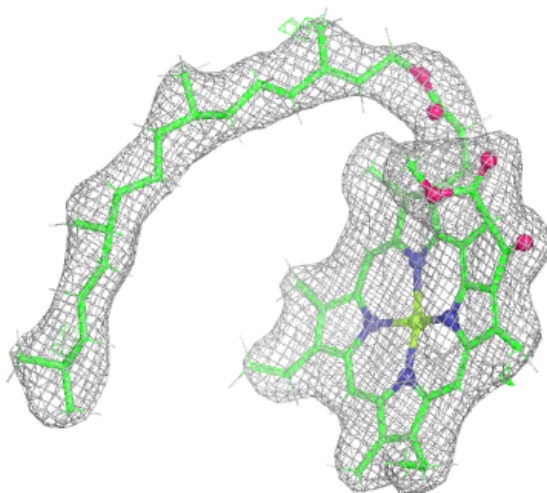
Electron density around CLA B 611:

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



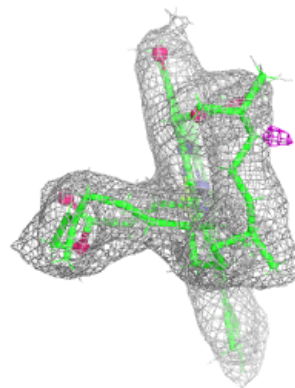
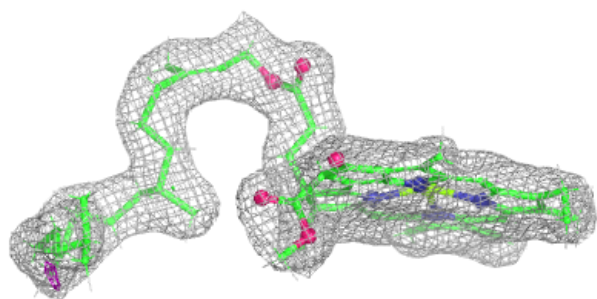
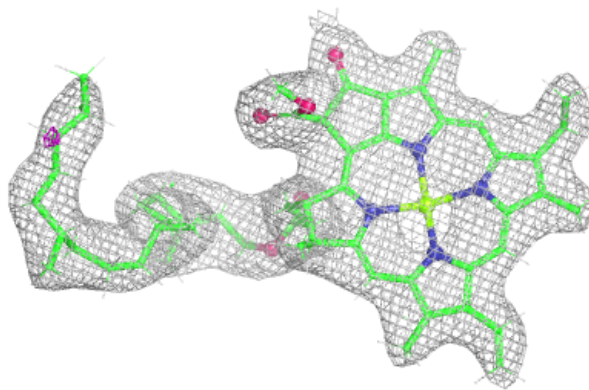
Electron density around CLA c 508:

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

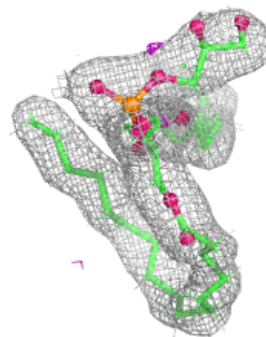
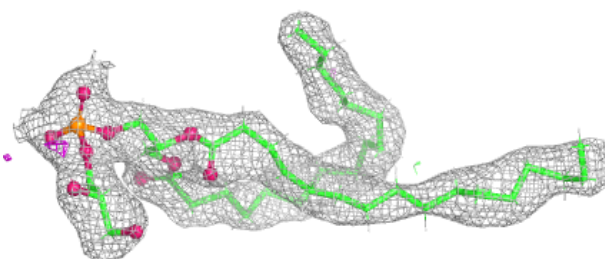
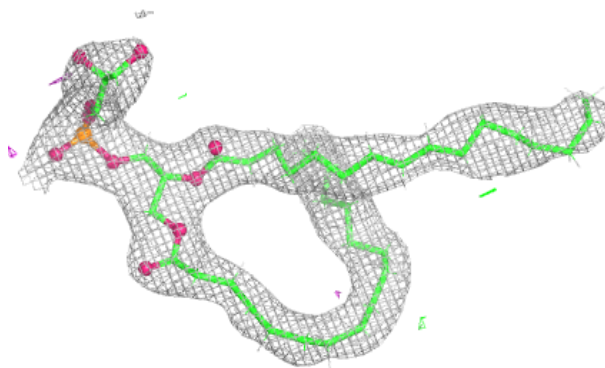


Electron density around CLA B 612:

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

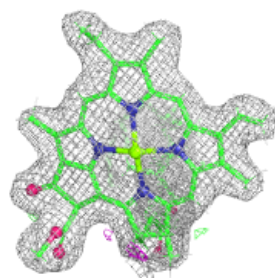
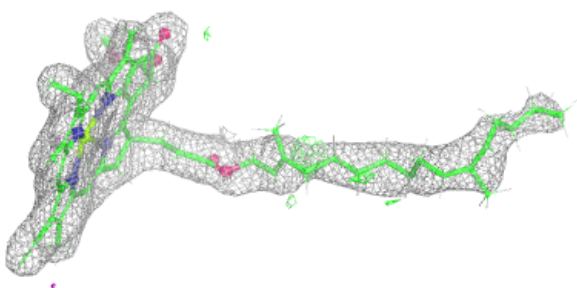
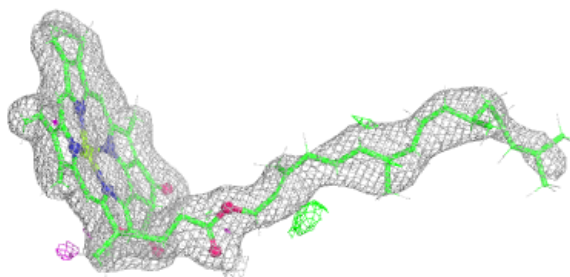
**Electron density around LHG D 412:**

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



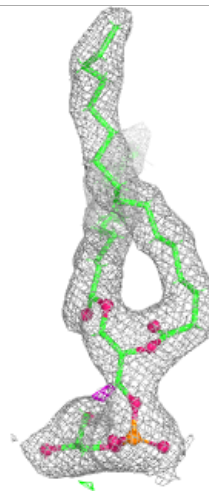
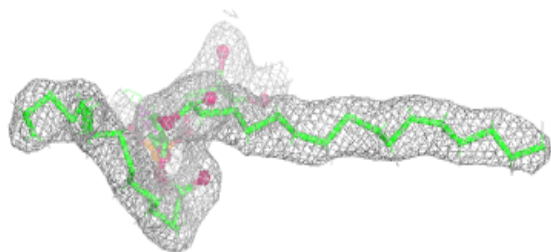
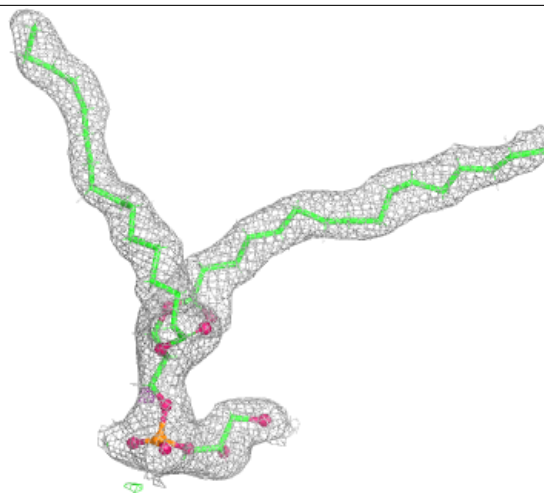
Electron density around CLA B 604:

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



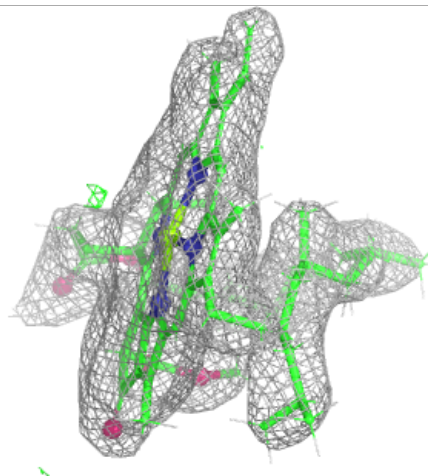
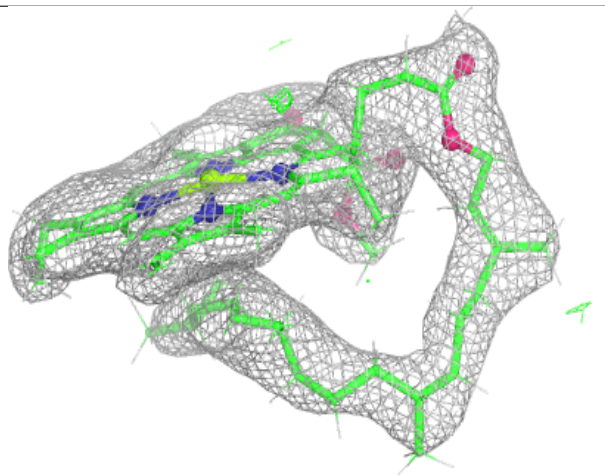
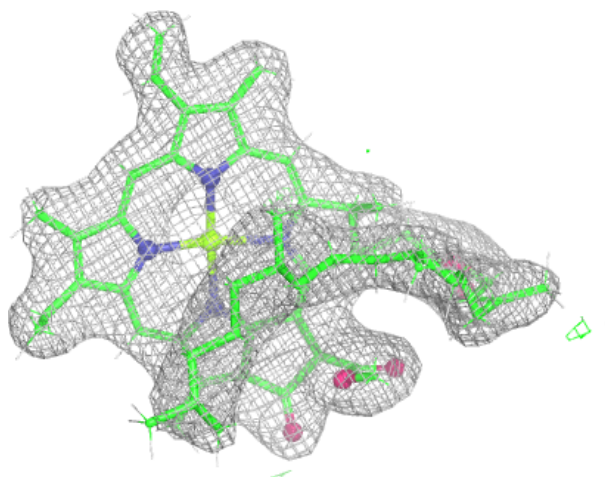
Electron density around LHG L 102:

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



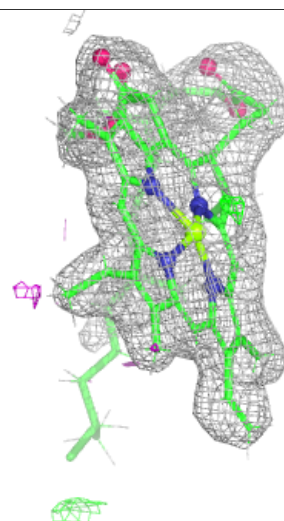
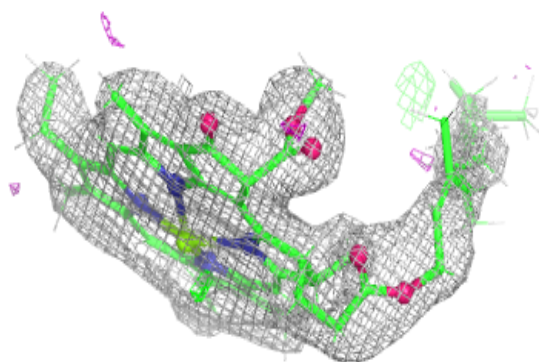
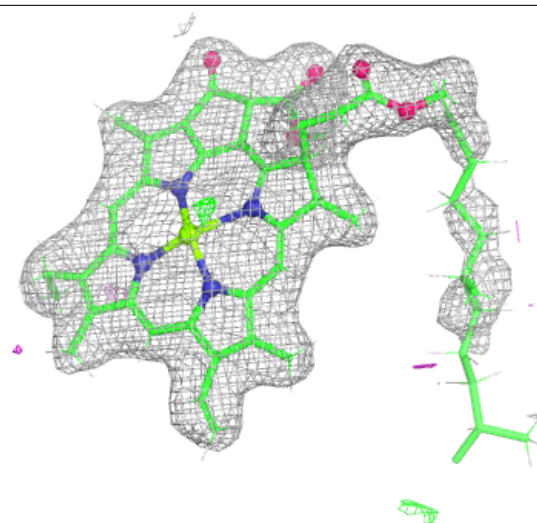
Electron density around CLA c 511:

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



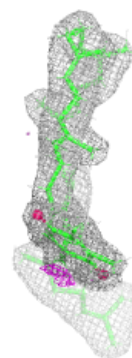
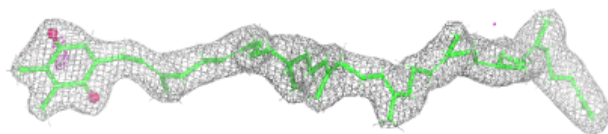
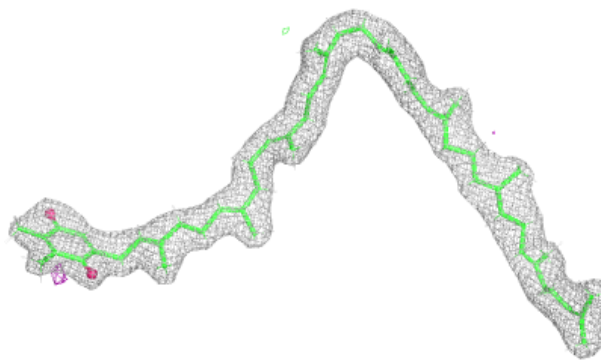
Electron density around CLA B 616:

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



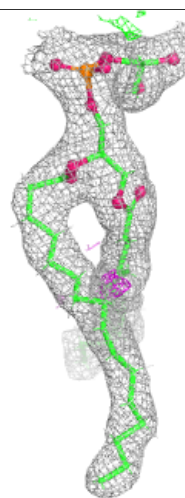
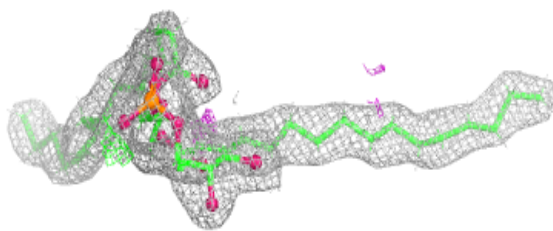
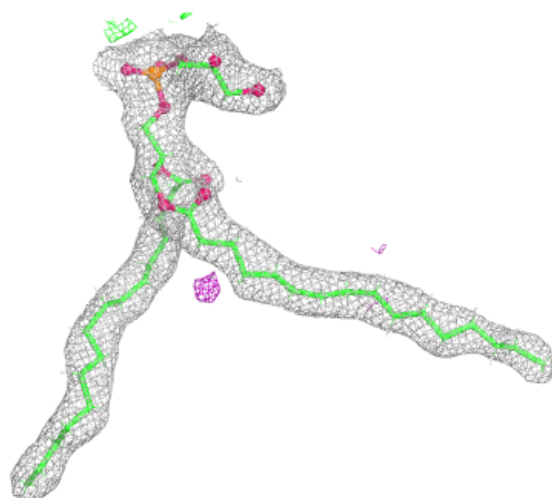
Electron density around PL9 d 406:

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



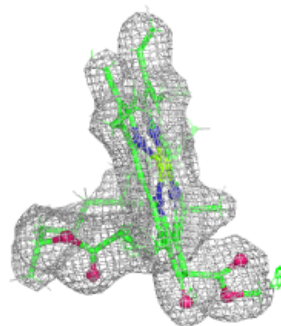
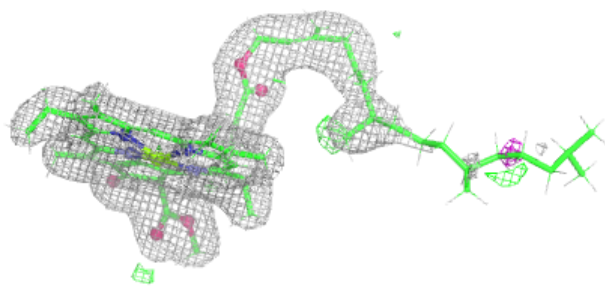
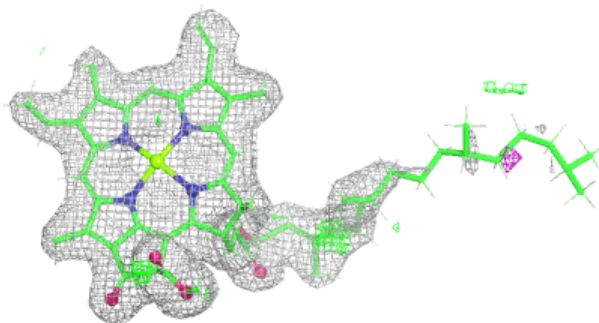
Electron density around LHG 1 101:

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

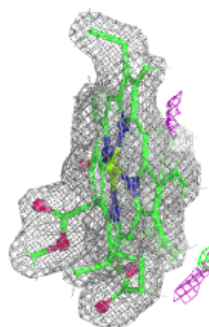
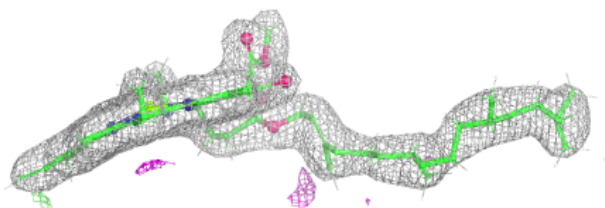
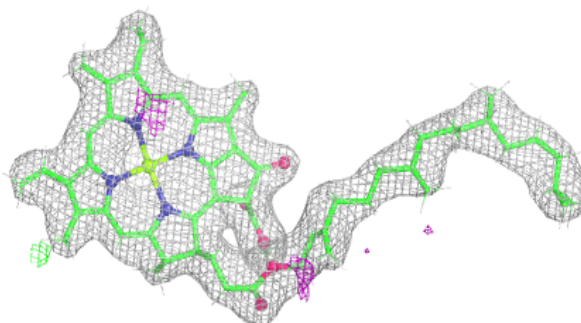


Electron density around CLA A 403:

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

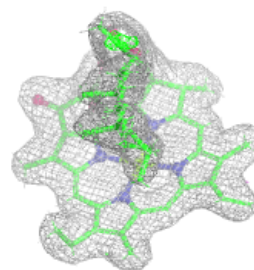
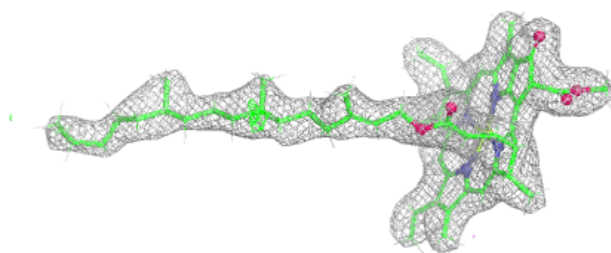
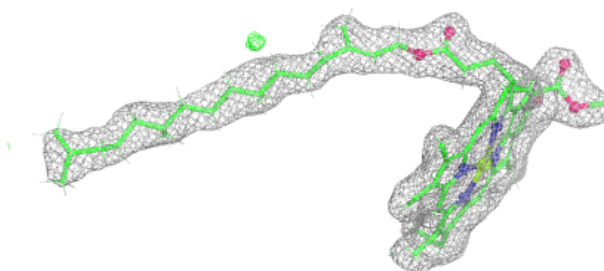
**Electron density around CLA B 602:**

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



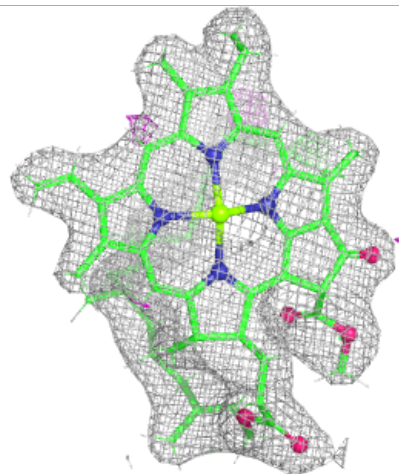
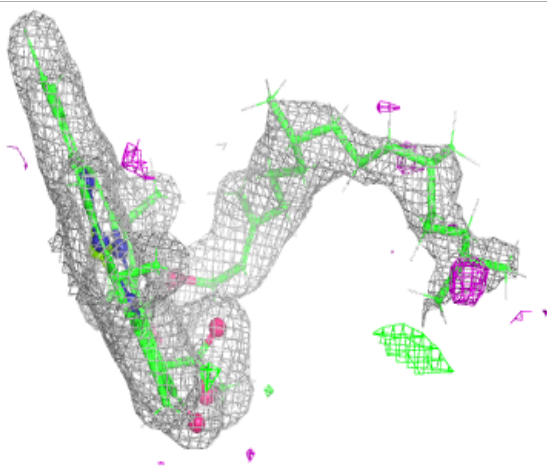
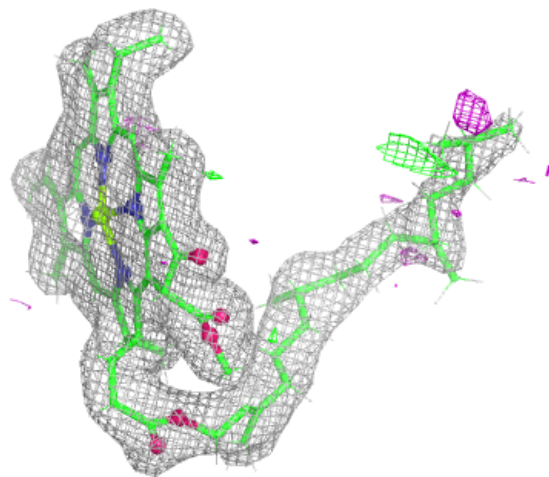
Electron density around CLA B 607:

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



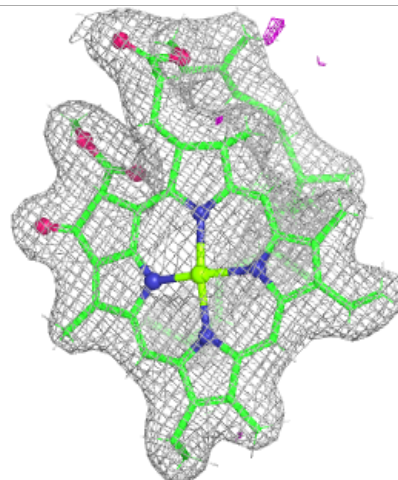
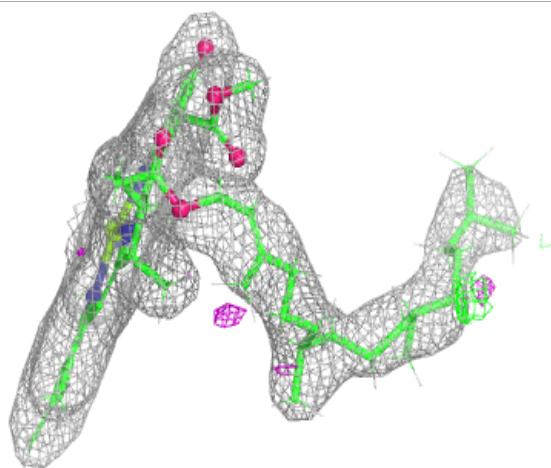
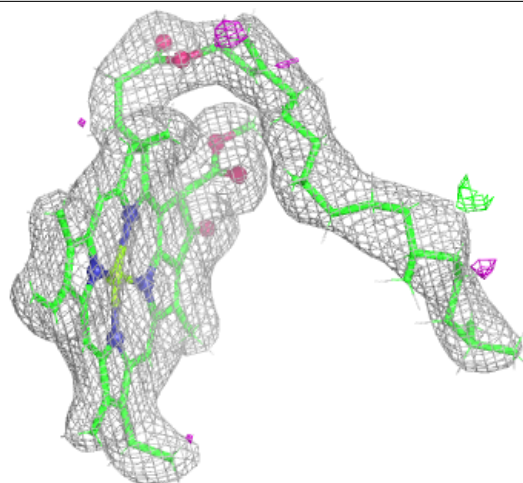
Electron density around CLA b 613:

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



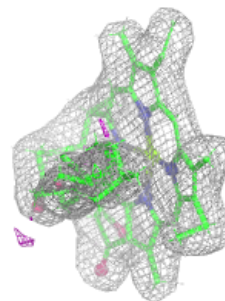
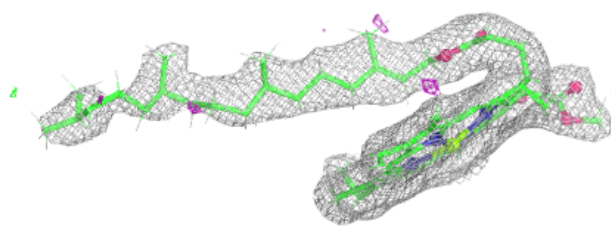
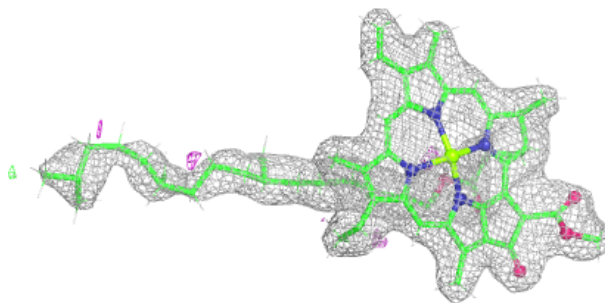
Electron density around CLA B 613:

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



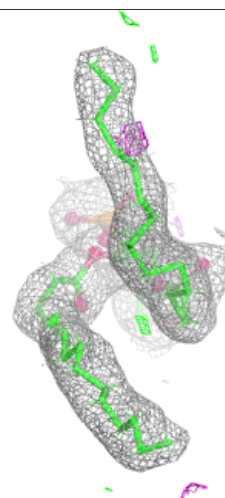
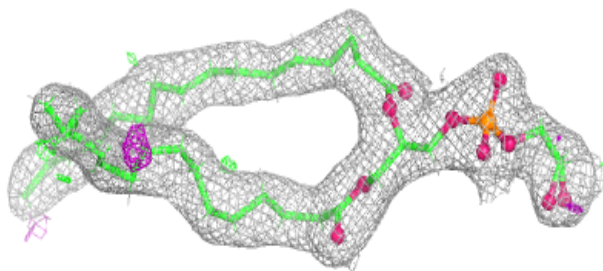
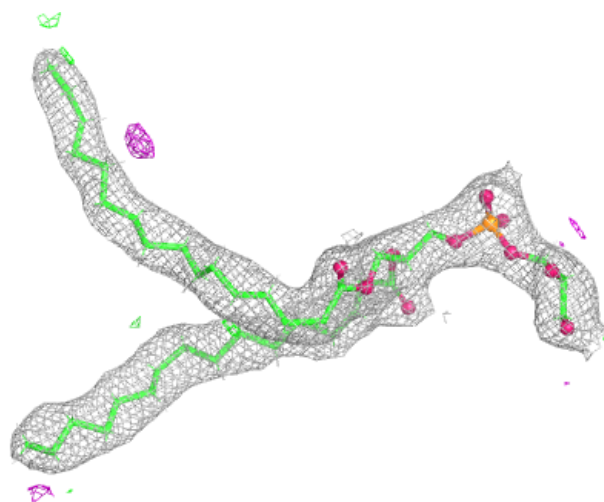
Electron density around CLA B 614:

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



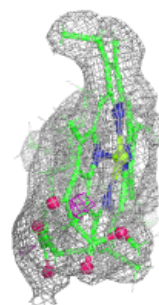
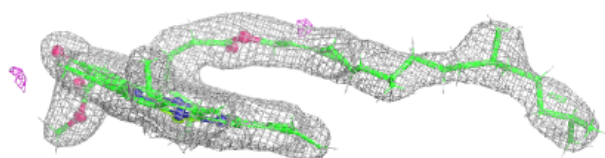
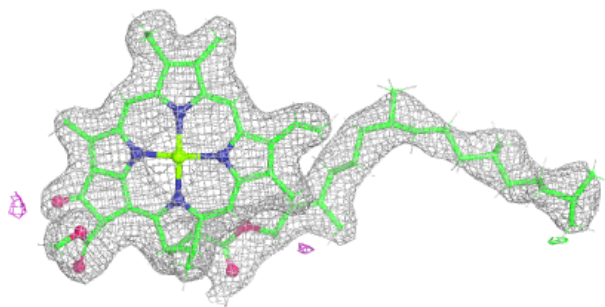
Electron density around LHG D 409:

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

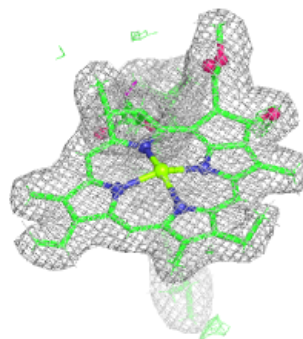
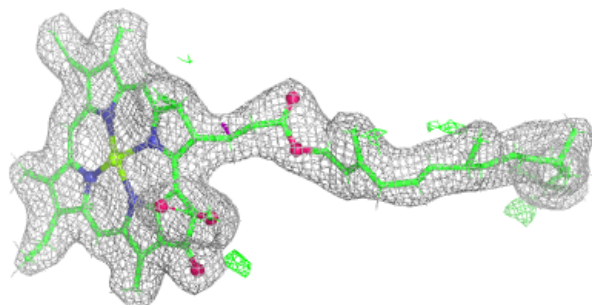
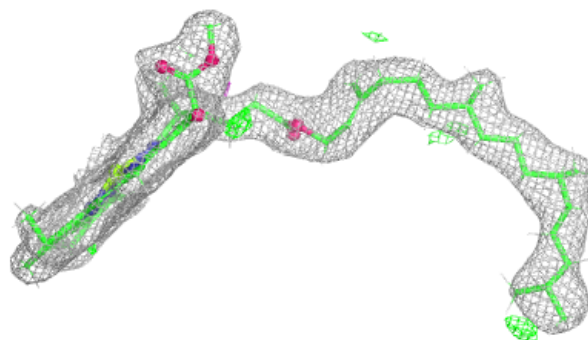


Electron density around CLA B 603:

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

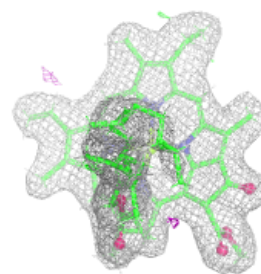
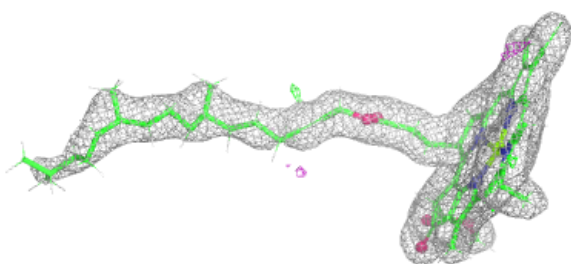
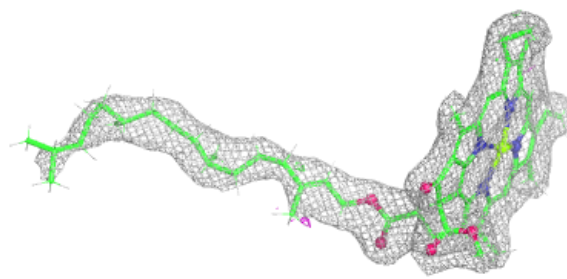
**Electron density around CLA D 403:**

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

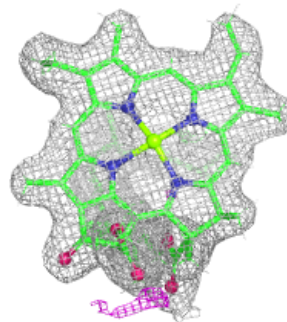
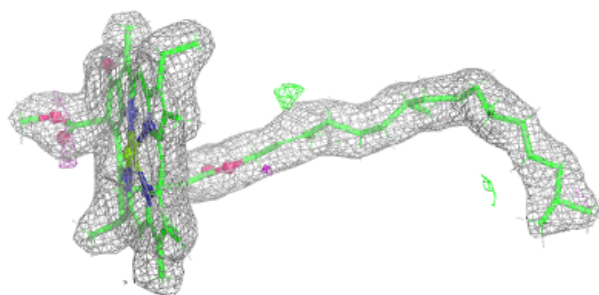
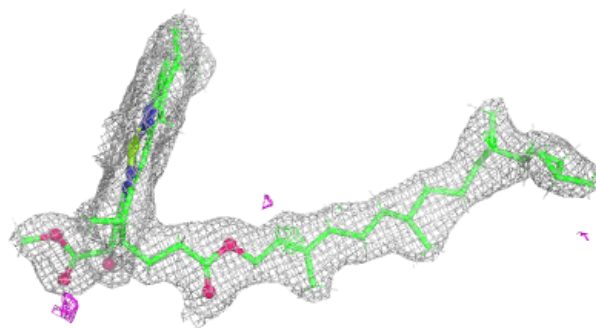


Electron density around CLA b 604:

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

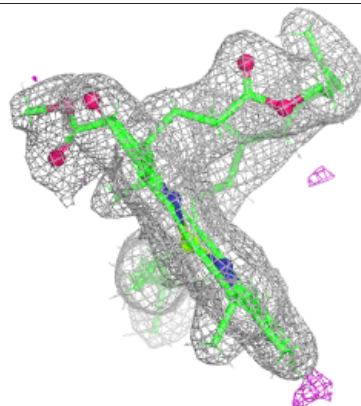
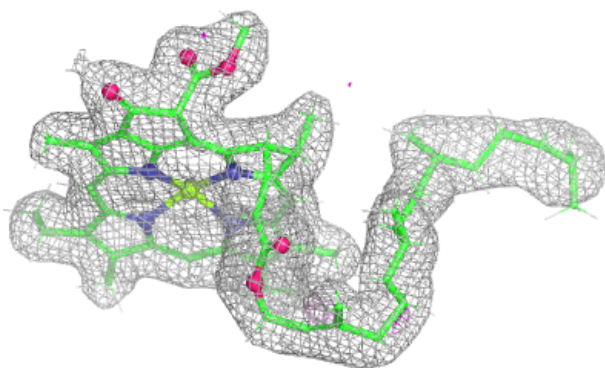
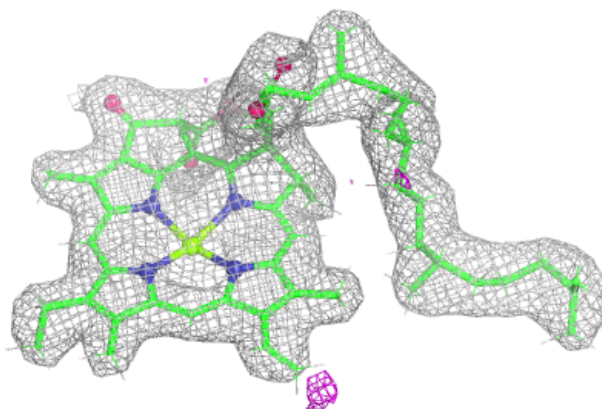
**Electron density around CLA b 605:**

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

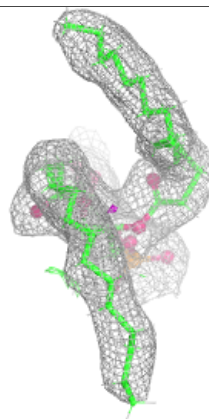
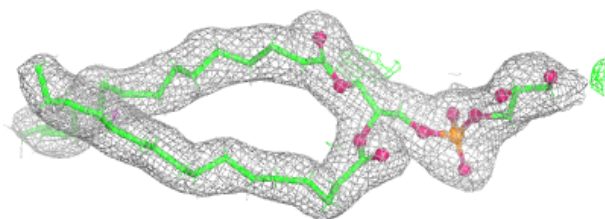
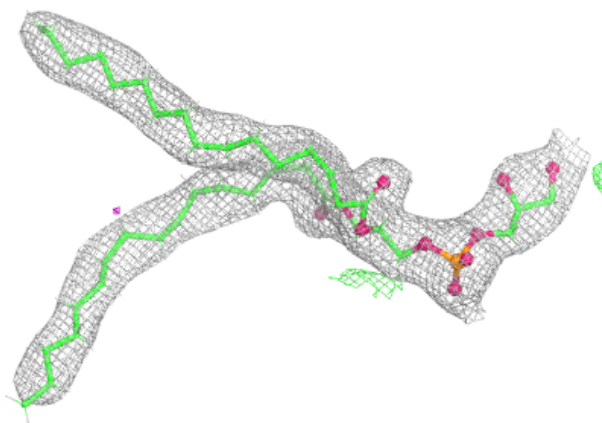


Electron density around CLA D 404:

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

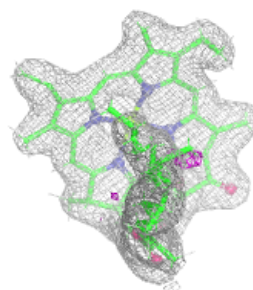
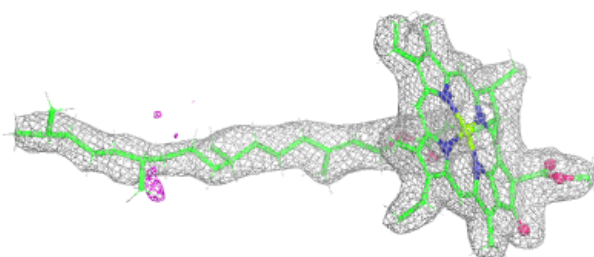
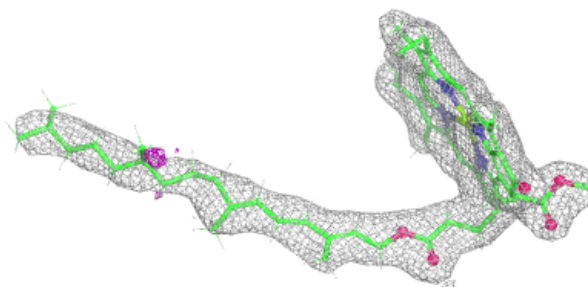
**Electron density around LHG d 408:**

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

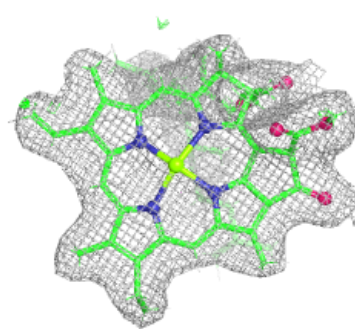
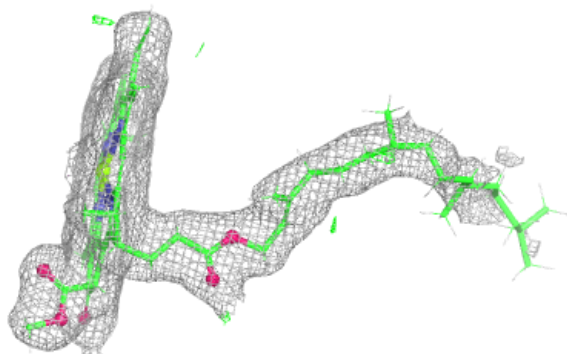
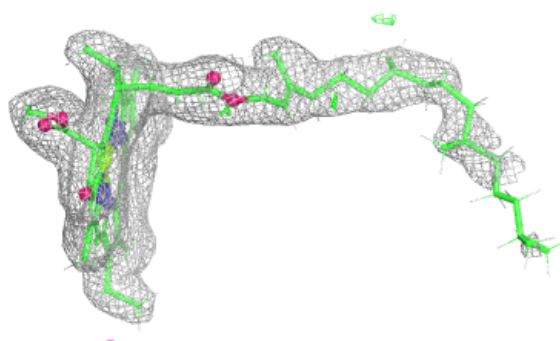


Electron density around CLA b 607:

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

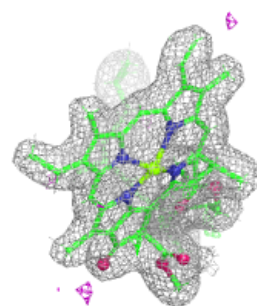
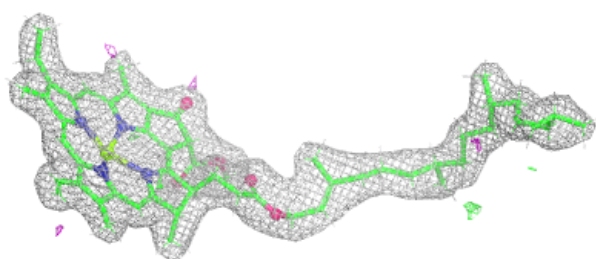
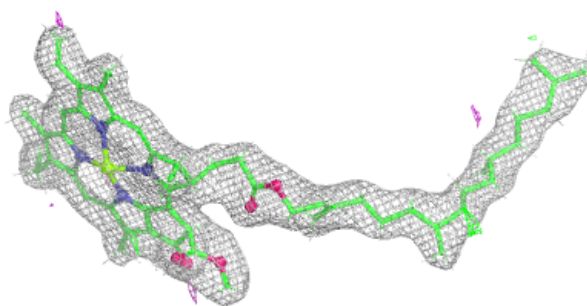
**Electron density around CLA D 405:**

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



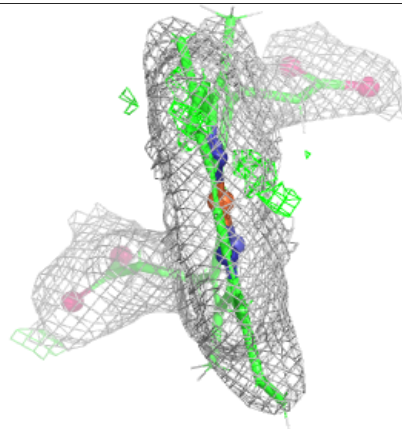
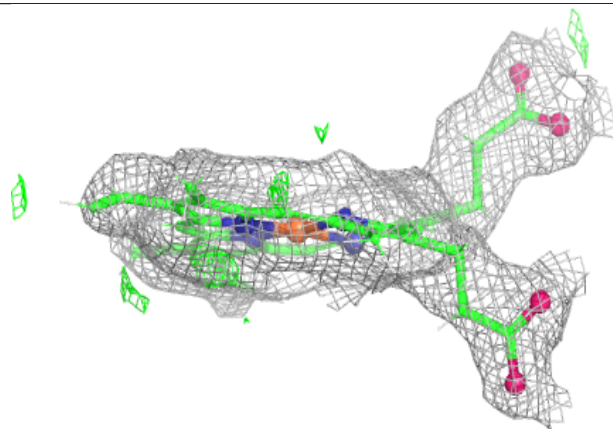
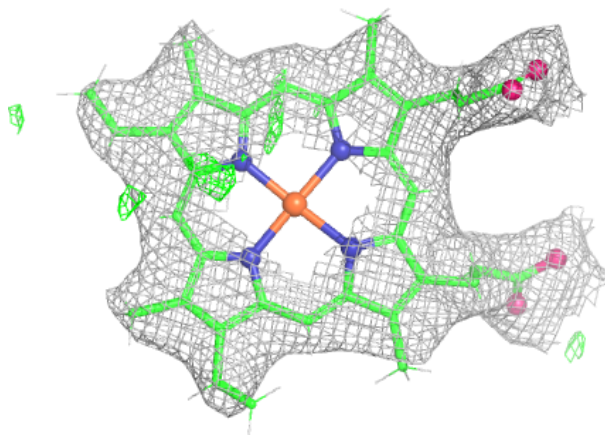
Electron density around CLA A 402:

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



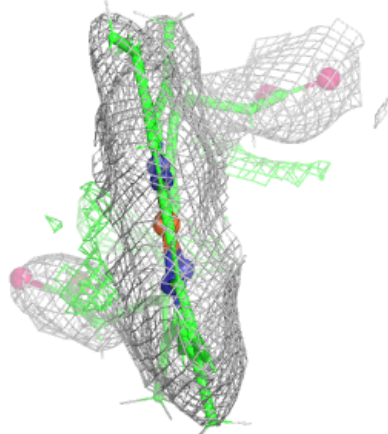
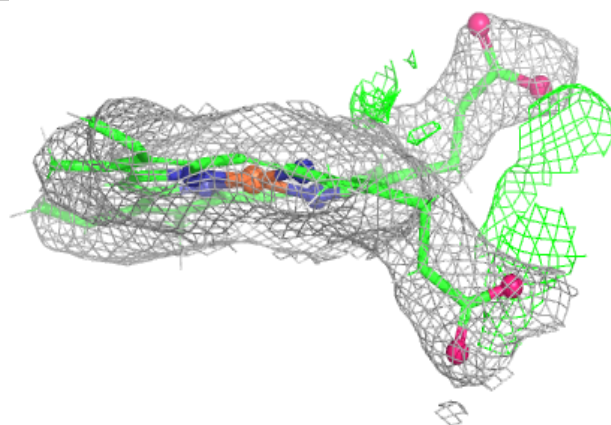
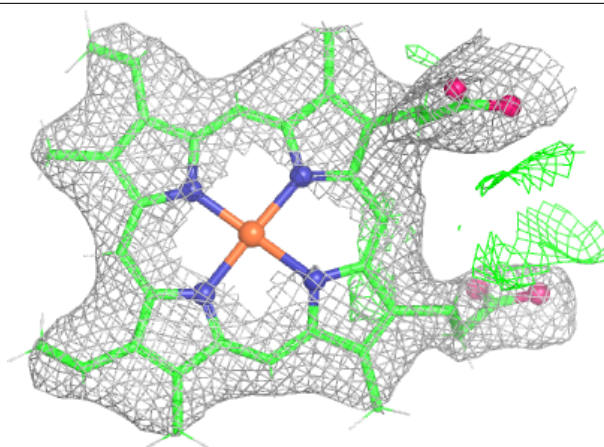
Electron density around HEC F 102:

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



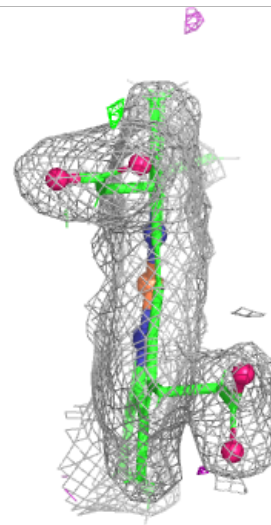
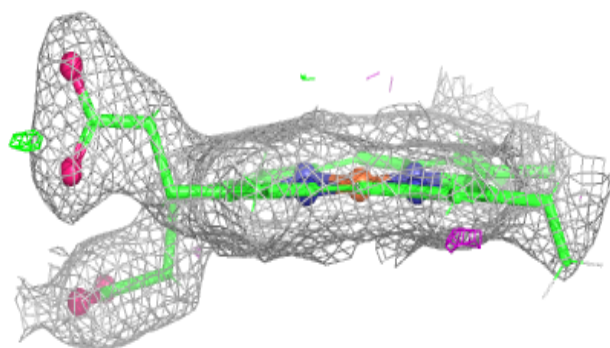
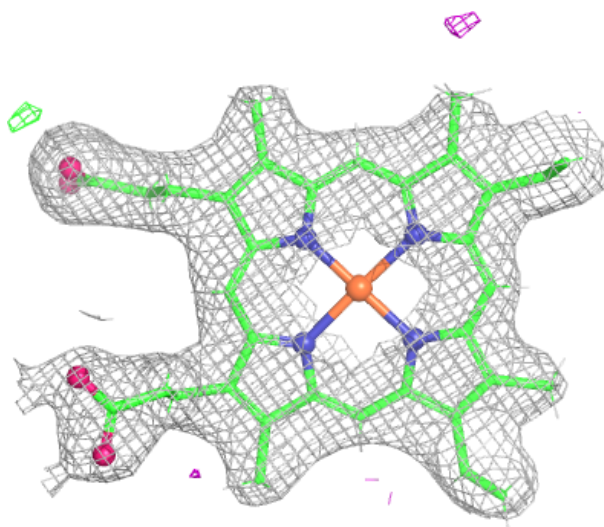
Electron density around HEC f 101:

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



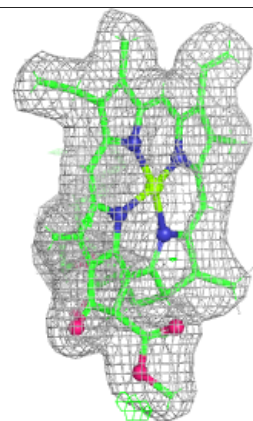
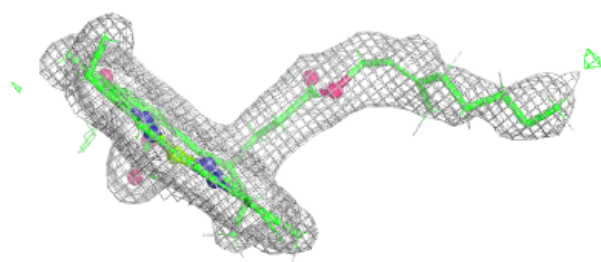
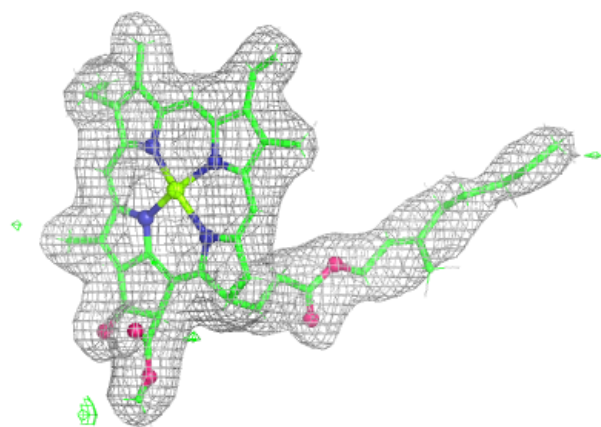
Electron density around HEC V 201:

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



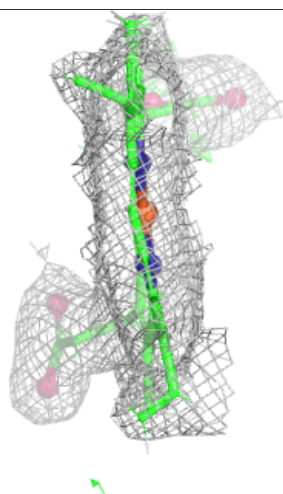
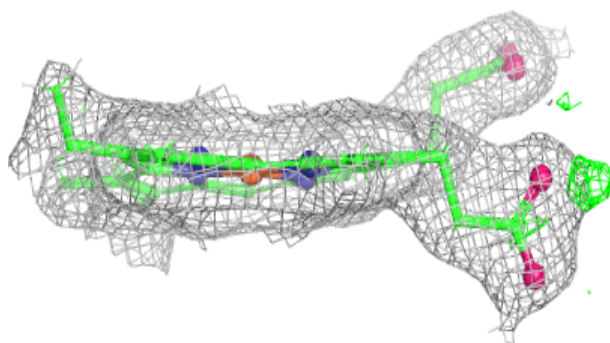
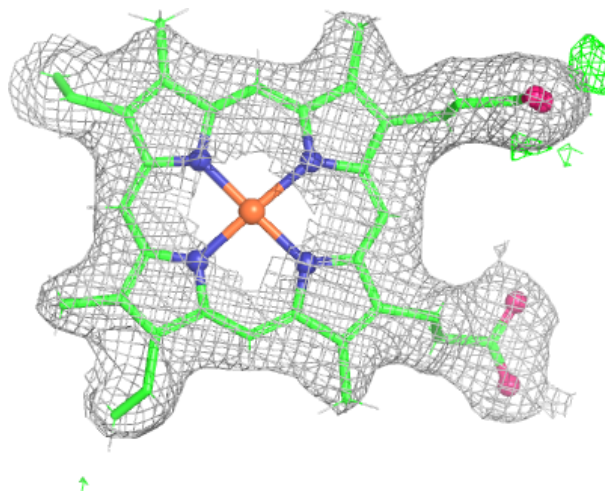
Electron density around CLA A 405:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.