



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:23 PM UTC

PDB ID : 8F4G / pdb_00008f4g
Title : RT XFEL structure of Photosystem II 730 microseconds after the third illumination at 2.03 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.03 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

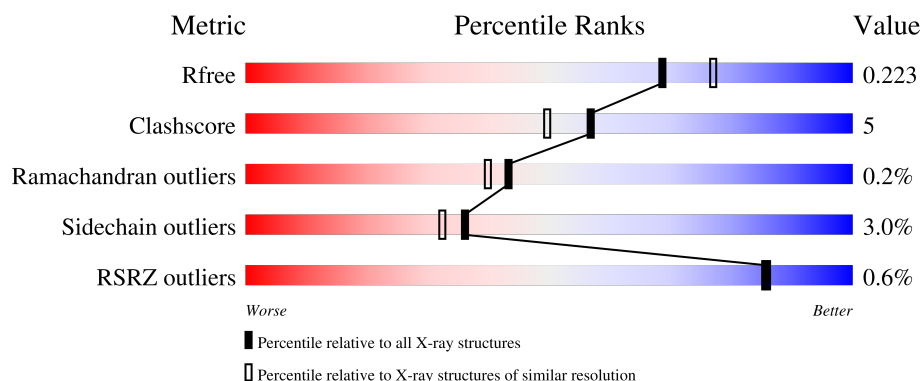
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

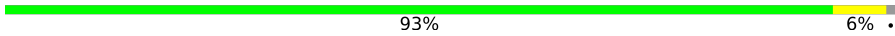
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	 90% 7% •

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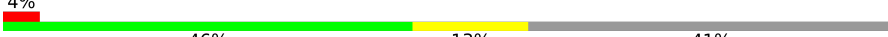
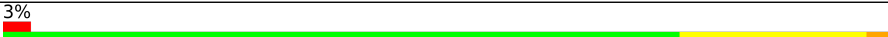
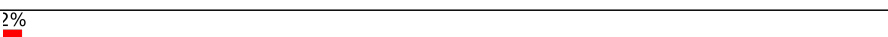
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	a	344	 85% 10% . .
2	B	510	 93% 6% .
2	b	510	 91% 8% .
3	C	461	 89% 6% .
3	c	461	 90% 8% .
4	D	352	 89% 8% .
4	d	352	 89% 7% . .
5	E	84	 87% 10% . .
5	e	84	 79% 19% .
6	F	45	 71% . . 24%
6	f	45	 49% 22% . 24%
7	H	66	 86% 11% . .
7	h	66	 89% 6% 5%
8	I	38	 84% 11% 5%
8	i	38	 89% 5% 5%
9	J	40	 80% 10% 10%
9	j	40	 65% 22% . 10%
10	K	46	 78% . 20%
10	k	46	 67% 13% 20%
11	L	37	 86% 14%
11	l	37	 81% 14% . .
12	M	36	 72% 19% 8%
12	m	36	 75% 14% 11%
13	O	272	 81% 8% . 10%
13	o	272	 83% 6% . 10%

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Mol	Chain	Length	Quality of chain
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	612	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	H	101	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	h	101	X	-	-	-

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 54517 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	64	0
			3604	2343	595	643	23			
1	a	334	Total	C	N	O	S	0	64	0
			3601	2340	595	643	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	4	0
			4005	2631	666	695	13			
2	b	505	Total	C	N	O	S	0	0	0
			3978	2610	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	N	O	S	0	11	0
			3592	2355	601	621	15			
3	c	451	Total	C	N	O	S	0	12	0
			3666	2396	617	638	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2745	1818	448	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2751	1822	448	469	12			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

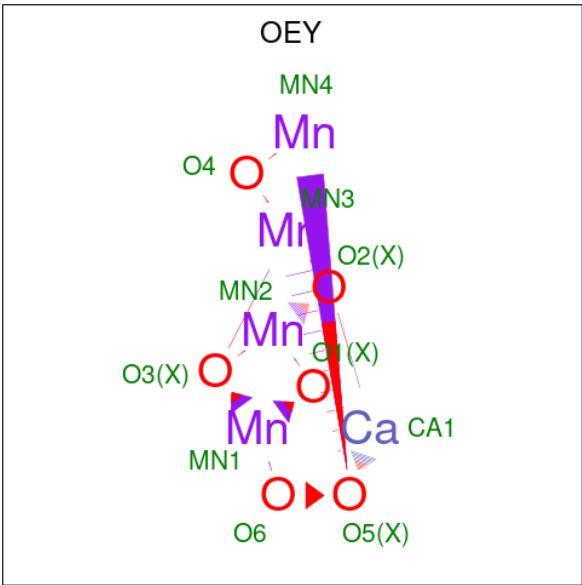
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

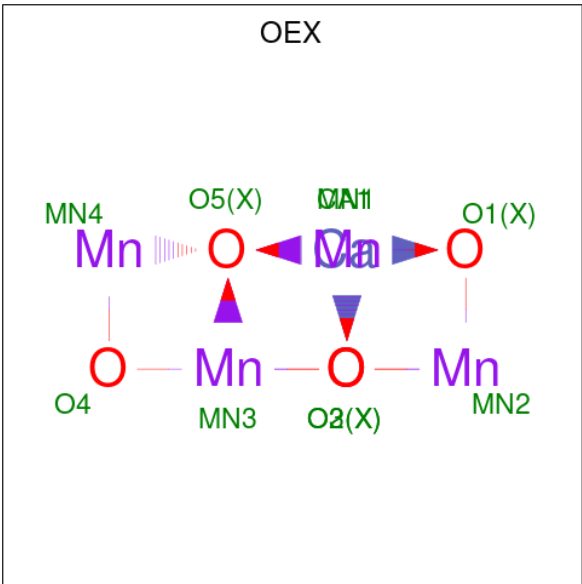
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			22	2	8	12		
21	a	1	Total	Ca	Mn	O	0	1
			22	2	8	12		

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



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

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

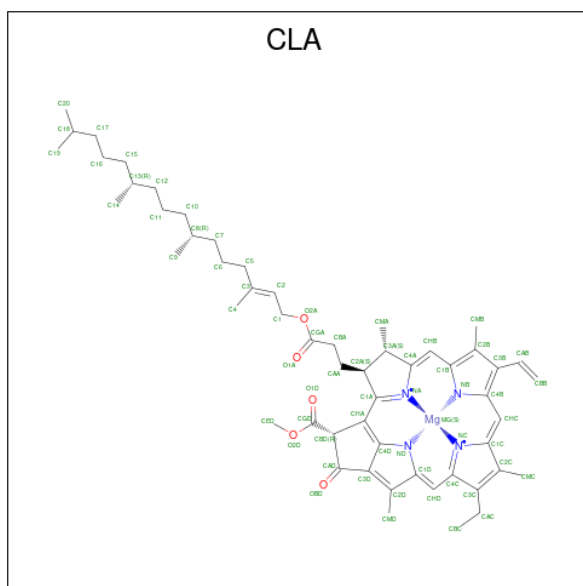
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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

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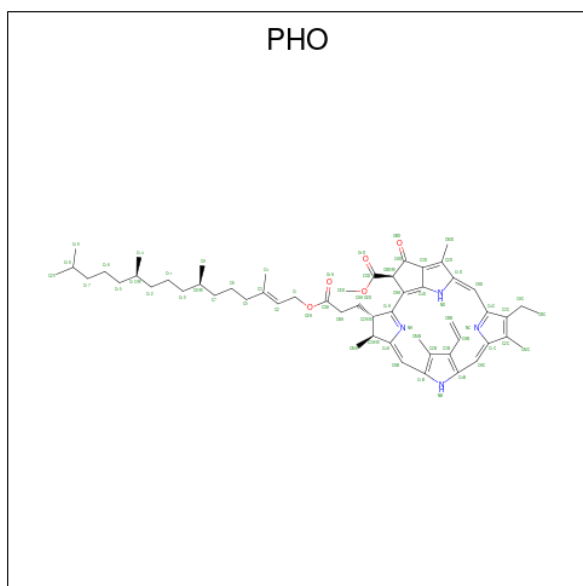
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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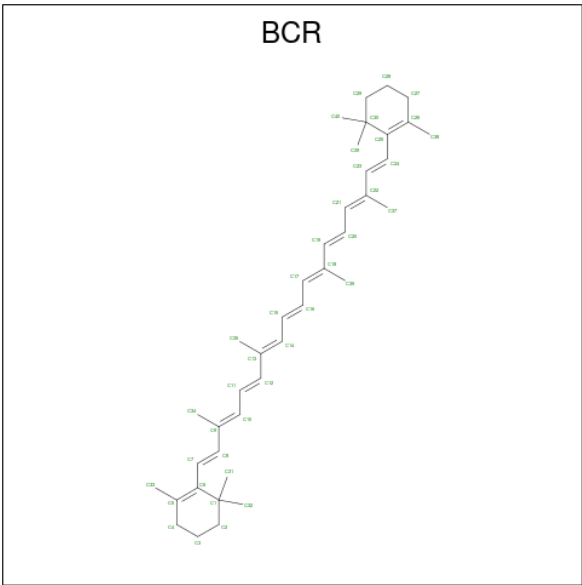
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



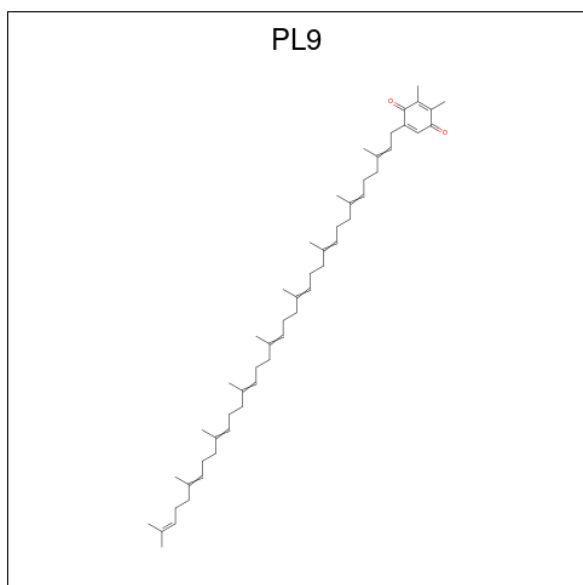
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



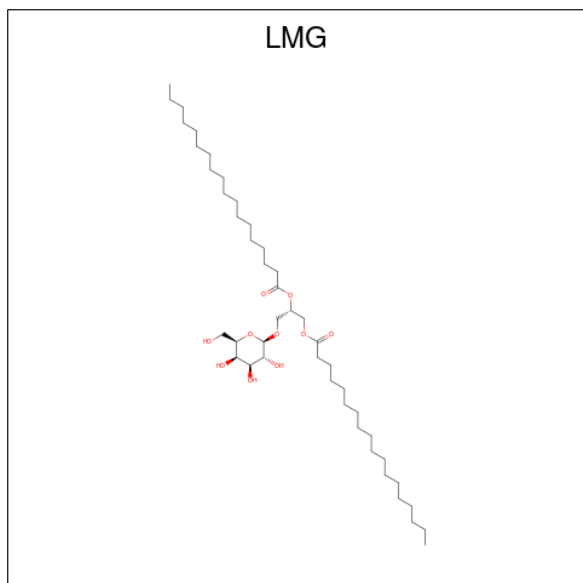
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



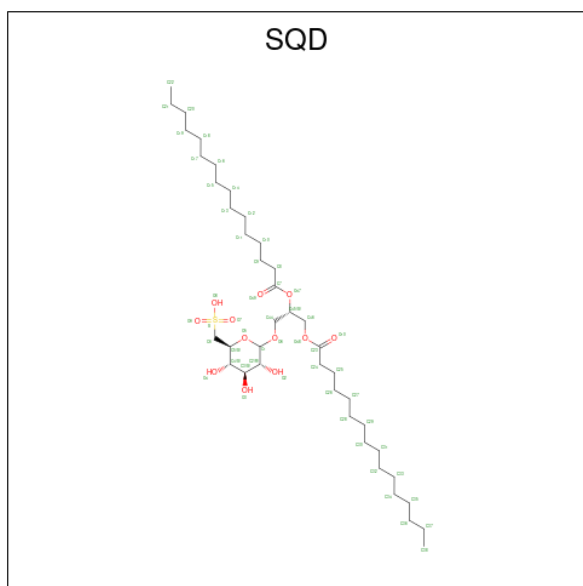
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C	O	0	0
			37	27	10		
29	c	1	Total	C	O	0	0
			48	38	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			49	39	10		
29	d	1	Total	C	O	0	0
			23	21	2		
29	d	1	Total	C	O	0	0
			44	34	10		
29	m	1	Total	C	O	0	0
			51	41	10		

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



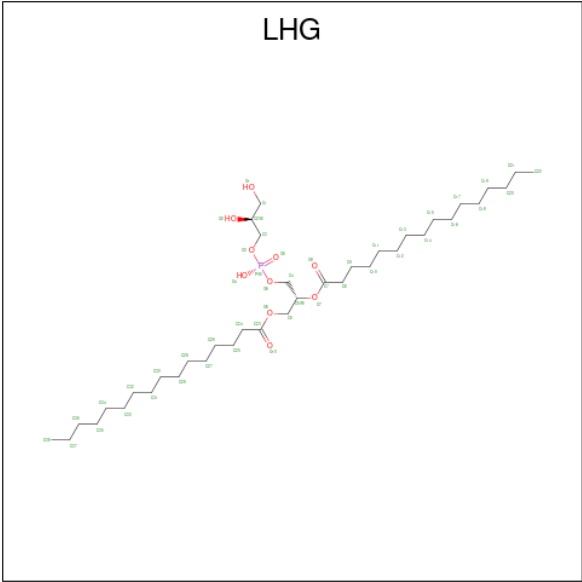
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	F	1	Total	C	O	S	0	0
			36	25	10	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36	31	5			
30	b	1	Total	C	O	S	0	0
			49	36	12	1		

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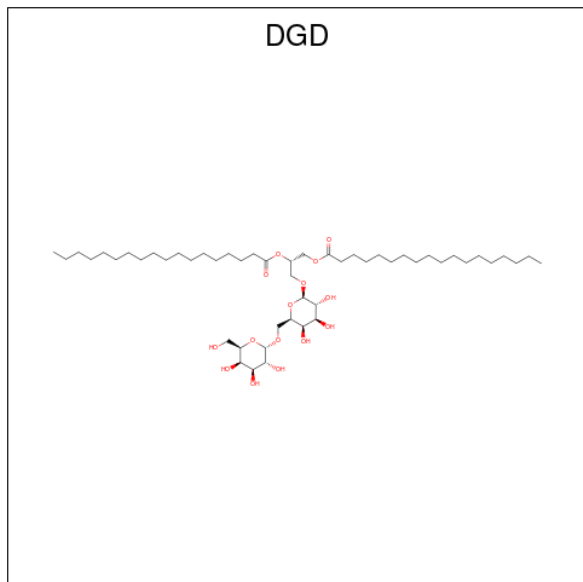
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



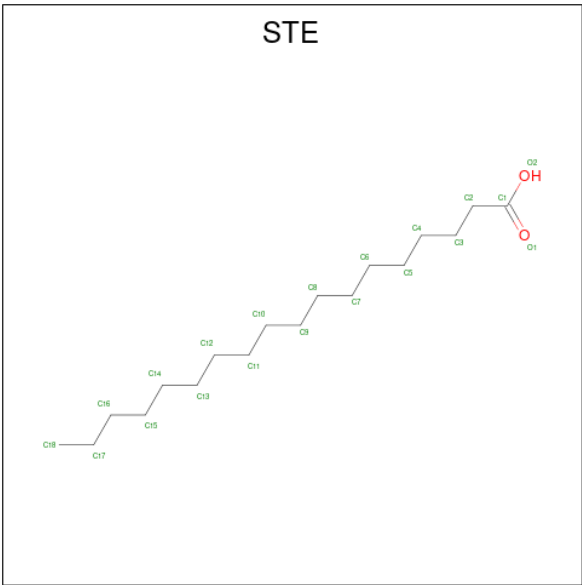
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			47	36	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	b	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			66	51	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	H	1	Total	C	O	0	0
			62	47	15		
32	a	1	Total	C	O	0	0
			44	39	5		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



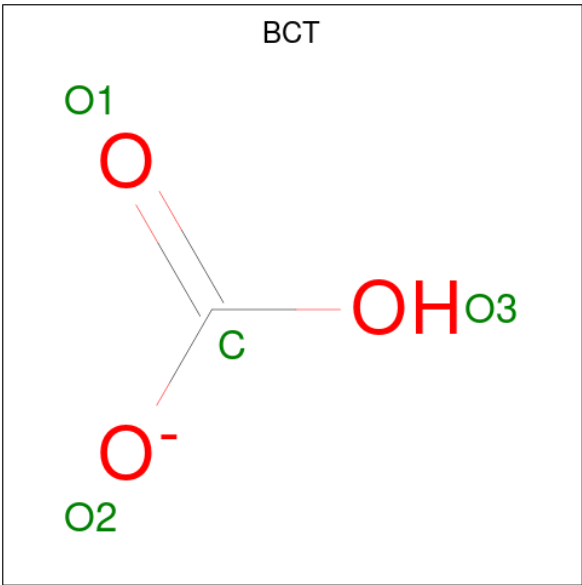
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			17	15	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C	O	0	0
			18	16	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C		0	0
			16	16			
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C		0	0
			16	16			
33	E	1	Total	C	O	0	0
			12	10	2		
33	H	1	Total	C		0	0
			18	18			
33	I	1	Total	C		0	0
			15	15			
33	J	1	Total	C	O	0	0
			12	10	2		
33	M	1	Total	C	O	0	0
			15	13	2		
33	M	1	Total	C		0	0
			10	10			

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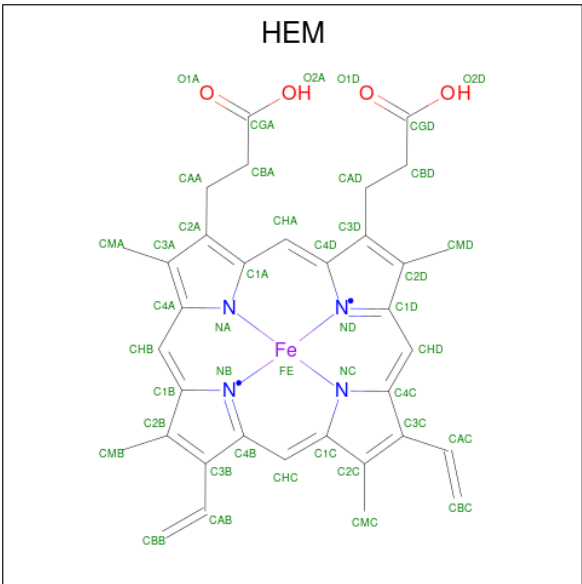
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	1	Total C O 20 18 2	0	0
33	a	1	Total C O 12 10 2	0	0
33	b	1	Total C 16 16	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 15 15	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 10 10	0	0
33	c	1	Total C O 20 18 2	0	0
33	d	1	Total C O 16 14 2	0	0
33	d	1	Total C O 17 15 2	0	0
33	j	1	Total C O 12 10 2	0	0
33	k	1	Total C O 12 10 2	0	0
33	l	1	Total C 18 18	0	0
33	m	1	Total C O 12 10 2	0	0
33	t	1	Total C O 14 12 2	0	0
33	t	1	Total C 10 10	0	0
33	x	1	Total C O 20 18 2	0	0

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



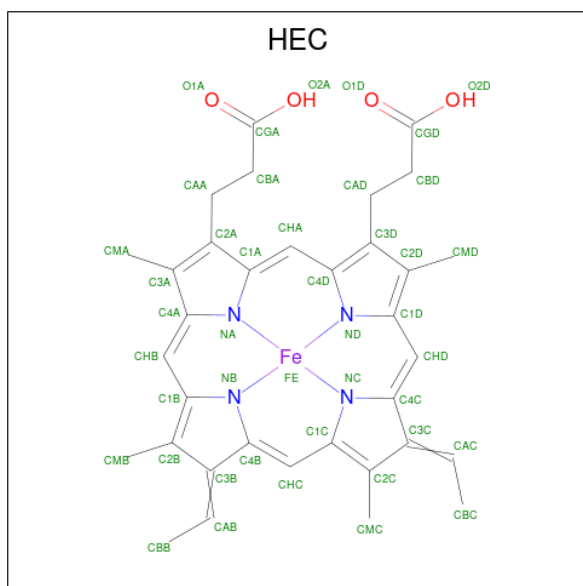
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	142	Total O 150 150	0	4
37	B	204	Total O 204 204	0	0
37	C	184	Total O 184 184	0	0
37	D	133	Total O 133 133	0	0
37	E	21	Total O 21 21	0	0
37	F	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	28	Total 28	O 28	0	0
37	I	12	Total 12	O 12	0	0
37	J	10	Total 10	O 10	0	0
37	K	1	Total 1	O 1	0	0
37	L	10	Total 10	O 10	0	0
37	M	7	Total 7	O 7	0	0
37	O	93	Total 93	O 93	0	0
37	T	8	Total 8	O 8	0	0
37	U	43	Total 43	O 43	0	0
37	V	69	Total 69	O 69	0	0
37	Y	3	Total 3	O 3	0	0
37	X	15	Total 15	O 15	0	0
37	Z	4	Total 4	O 4	0	0
37	R	1	Total 1	O 1	0	0
37	a	115	Total 123	O 123	0	4
37	b	189	Total 189	O 189	0	0
37	c	175	Total 175	O 175	0	0
37	d	112	Total 112	O 112	0	0
37	e	18	Total 18	O 18	0	0
37	f	7	Total 7	O 7	0	0
37	h	18	Total 18	O 18	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	7	Total 7	O 7	0	0
37	j	4	Total 4	O 4	0	0
37	k	7	Total 7	O 7	0	0
37	l	8	Total 8	O 8	0	0
37	m	7	Total 7	O 7	0	0
37	o	99	Total 99	O 99	0	0
37	t	11	Total 11	O 11	0	0
37	u	55	Total 55	O 55	0	0
37	v	58	Total 58	O 58	0	0
37	y	1	Total 1	O 1	0	0
37	x	10	Total 10	O 10	0	0
37	z	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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

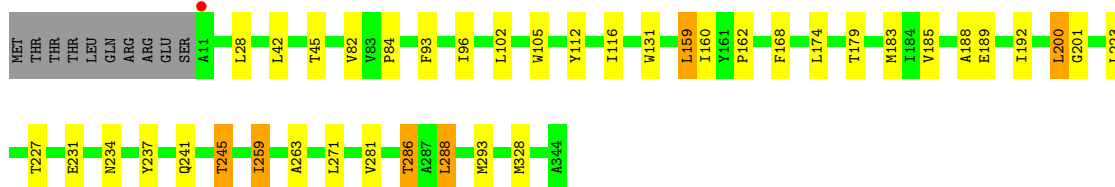
- Molecule 1: Photosystem II protein D1 1

Chain A: 



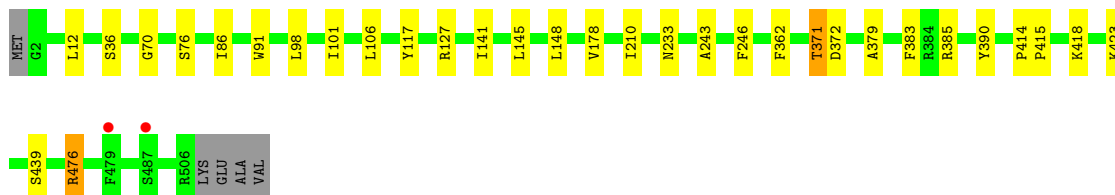
- Molecule 1: Photosystem II protein D1 1

Chain a: 



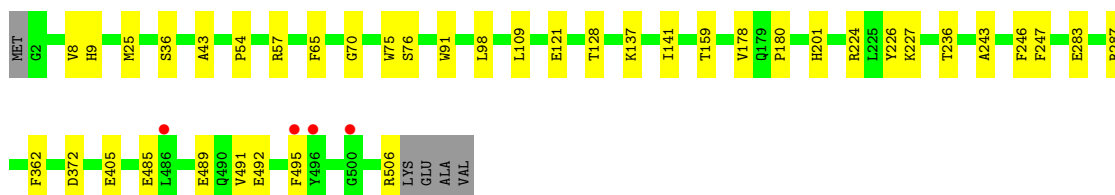
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

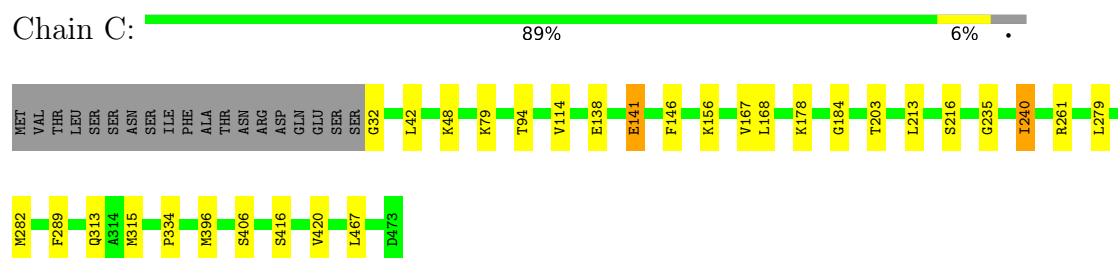


- Molecule 2: Photosystem II CP47 reaction center protein

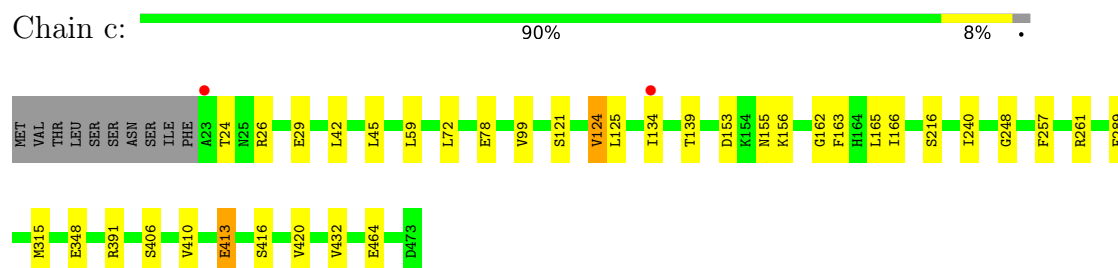
Chain b: 



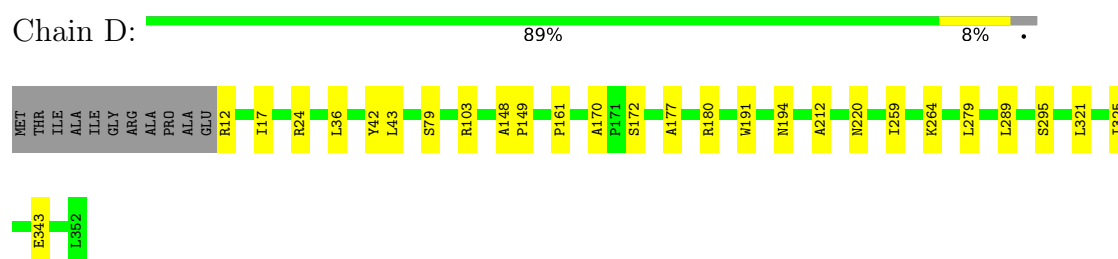
- Molecule 3: Photosystem II CP43 reaction center protein



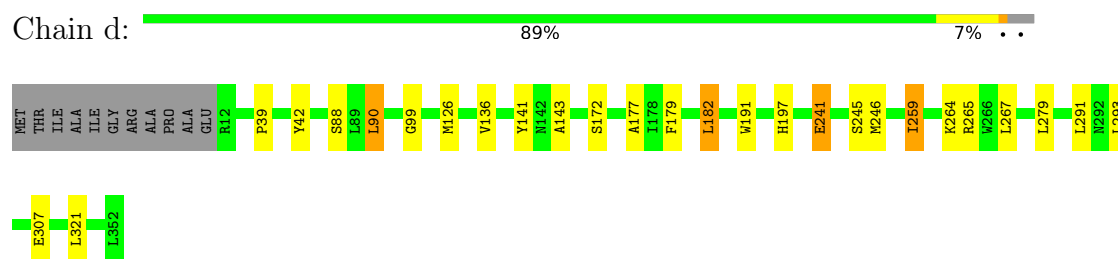
- Molecule 3: Photosystem II CP43 reaction center protein



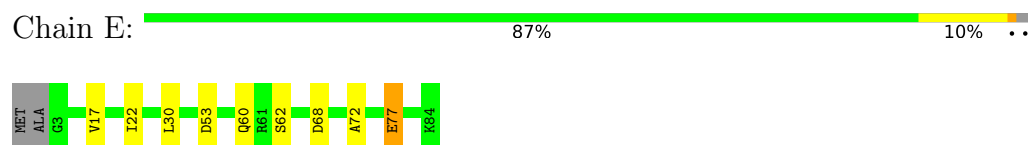
- Molecule 4: Photosystem II D2 protein



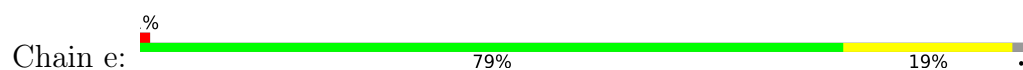
- Molecule 4: Photosystem II D2 protein



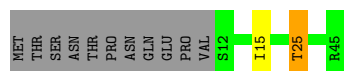
- Molecule 5: Cytochrome b559 subunit alpha



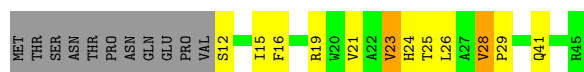
- Molecule 5: Cytochrome b559 subunit alpha



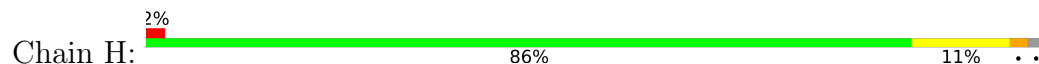
- Molecule 6: Cytochrome b559 subunit beta



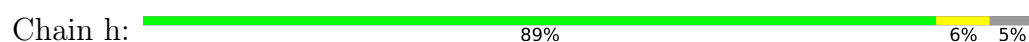
- Molecule 6: Cytochrome b559 subunit beta



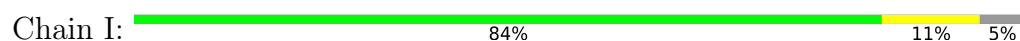
- Molecule 7: Photosystem II reaction center protein H



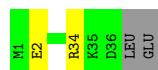
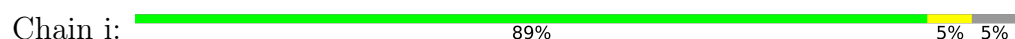
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

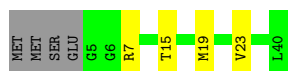


- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

Chain J:  80% 10% 10%



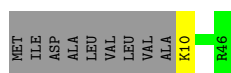
- Molecule 9: Photosystem II reaction center protein J

Chain j:  65% 22% 10%



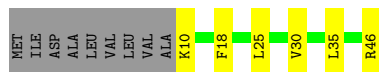
- Molecule 10: Photosystem II reaction center protein K

Chain K:  78% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  67% 13% 20%



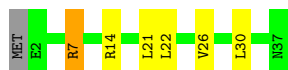
- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  81% 14% 2%



- Molecule 12: Photosystem II reaction center protein M

Chain M:  72% 19% 8%



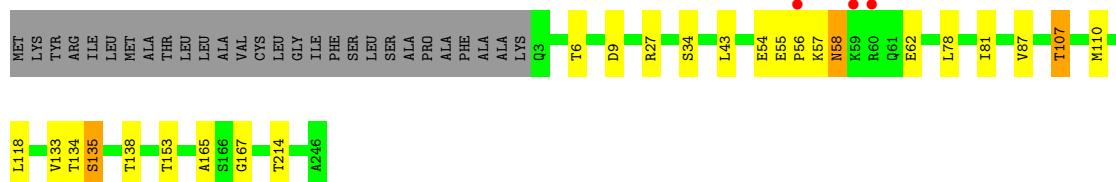
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 14% 11%



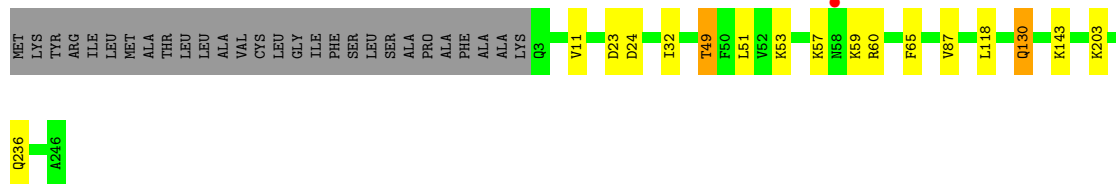
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  81% 8% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  83% 6% 10%



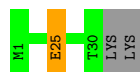
- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 9% 6%



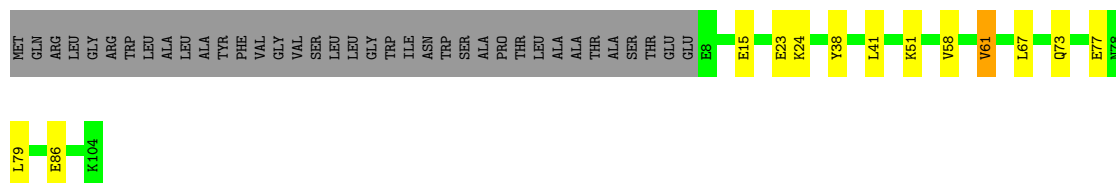
- Molecule 14: Photosystem II reaction center protein T

Chain t:  91% 6%

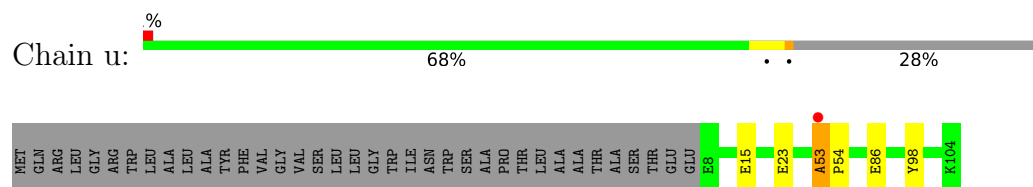


- Molecule 15: Photosystem II 12 kDa extrinsic protein

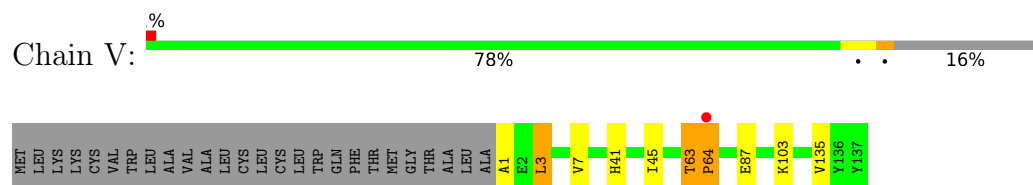
Chain U:  63% 9% 28%



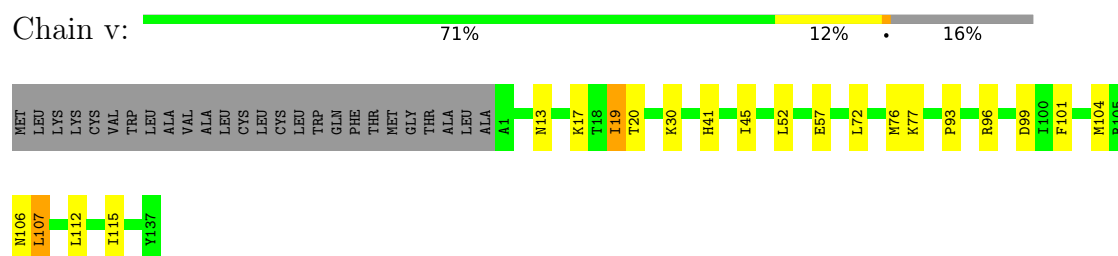
- Molecule 15: Photosystem II 12 kDa extrinsic protein



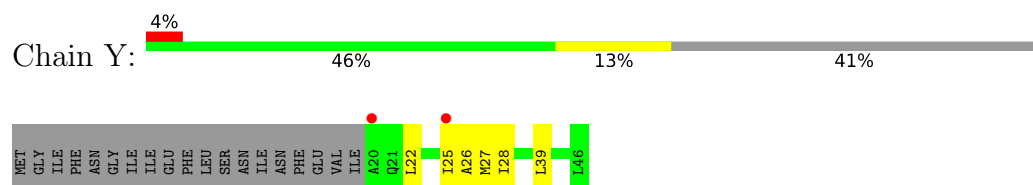
- Molecule 16: Cytochrome c-550



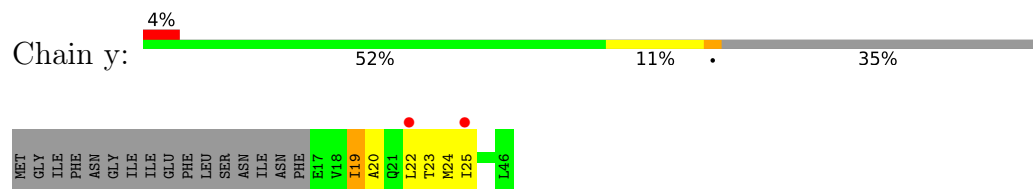
- Molecule 16: Cytochrome c-550



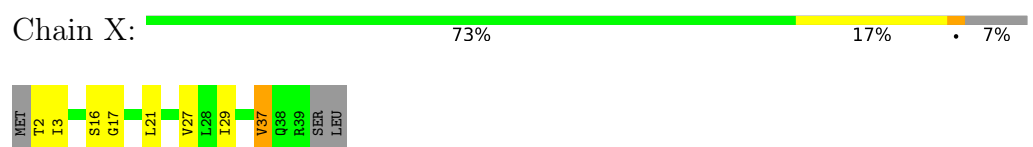
- Molecule 17: Photosystem II reaction center protein Ycf12



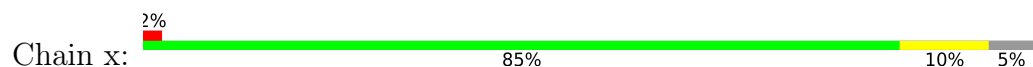
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

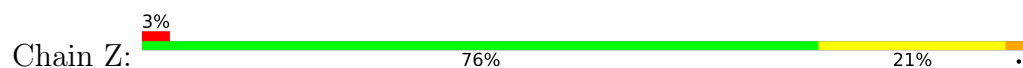


- Molecule 18: Photosystem II reaction center X protein

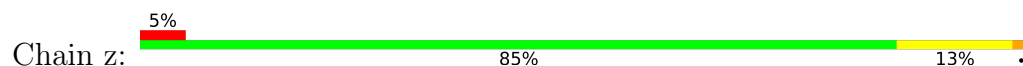




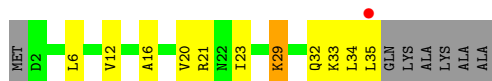
- Molecule 19: Photosystem II reaction center protein Z



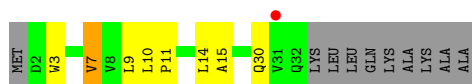
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.57Å 222.91Å 310.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.03 29.87 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.87-2.03) 87.2 (29.87-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.26 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.223 0.180 , 0.223	Depositor DCC
R_{free} test set	4628 reflections (0.74%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.5	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	0.96	EDS
Total number of atoms	54517	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/3717	0.45	0/5060
1	a	0.28	0/3714	0.44	0/5056
2	B	0.32	0/4155	0.48	0/5661
2	b	0.31	0/4118	0.46	0/5611
3	C	0.30	0/3711	0.44	0/5051
3	c	0.29	0/3791	0.45	0/5158
4	D	0.35	0/2838	0.49	0/3862
4	d	0.34	0/2847	0.49	0/3874
5	E	0.25	0/688	0.41	0/940
5	e	0.23	0/683	0.41	0/932
6	F	0.25	0/284	0.42	0/387
6	f	0.24	0/284	0.48	0/387
7	H	0.30	0/523	0.45	0/713
7	h	0.27	0/511	0.47	0/697
8	I	0.28	0/293	0.46	0/396
8	i	0.31	0/293	0.46	0/396
9	J	0.25	0/263	0.40	0/356
9	j	0.23	0/263	0.38	0/356
10	K	0.24	0/303	0.41	0/416
10	k	0.22	0/303	0.38	0/416
11	L	0.33	0/311	0.45	0/422
11	l	0.35	0/303	0.45	0/412
12	M	0.32	0/249	0.50	0/341
12	m	0.33	0/244	0.51	0/334
13	O	0.29	0/1904	0.50	0/2585
13	o	0.30	0/1905	0.49	0/2583
14	T	0.31	0/257	0.48	0/349
14	t	0.29	0/255	0.46	0/346
15	U	0.28	0/785	0.45	0/1064
15	u	0.29	0/785	0.48	0/1064
16	V	0.30	0/1085	0.51	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1085	0.42	0/1473
17	Y	0.21	0/197	0.37	0/264
17	y	0.17	0/219	0.32	0/294
18	X	0.23	0/284	0.38	0/384
18	x	0.20	0/289	0.28	0/391
19	Z	0.21	0/490	0.43	0/669
19	z	0.16	0/488	0.28	0/666
20	R	0.24	0/277	0.36	0/380
20	r	0.23	0/252	0.38	0/347
All	All	0.30	0/45246	0.46	0/61566

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3604	0	3445	17	0
1	a	3601	0	3436	35	0
2	B	4005	0	3871	19	0
2	b	3978	0	3836	26	0
3	C	3592	0	3501	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3666	0	3574	21	0
4	D	2745	0	2653	20	0
4	d	2751	0	2659	21	0
5	E	666	0	651	6	0
5	e	664	0	648	11	0
6	F	275	0	282	2	0
6	f	275	0	282	12	0
7	H	510	0	532	7	0
7	h	498	0	518	3	0
8	I	296	0	311	1	0
8	i	296	0	311	1	0
9	J	257	0	268	3	0
9	j	257	0	268	7	0
10	K	293	0	305	0	0
10	k	293	0	305	3	0
11	L	304	0	316	5	0
11	l	296	0	304	4	0
12	M	256	0	269	3	0
12	m	251	0	267	3	0
13	O	1870	0	1830	16	0
13	o	1874	0	1846	10	0
14	T	258	0	261	3	0
14	t	256	0	256	1	0
15	U	774	0	773	5	0
15	u	774	0	773	3	0
16	V	1064	0	1073	7	0
16	v	1064	0	1073	15	0
17	Y	196	0	217	5	0
17	y	218	0	241	3	0
18	X	281	0	312	6	0
18	x	286	0	314	4	0
19	Z	479	0	516	8	0
19	z	477	0	509	7	0
20	R	271	0	298	8	0
20	r	246	0	263	6	0
21	A	22	0	0	2	0
21	a	22	0	0	2	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	7	0
25	B	970	0	1067	27	0
25	C	839	0	922	18	0
25	D	130	0	144	3	0
25	H	65	0	72	1	0
25	a	260	0	288	4	0
25	b	970	0	1067	28	0
25	c	839	0	919	17	0
25	d	130	0	144	1	0
25	h	65	0	72	2	0
26	A	64	0	74	1	0
26	D	64	0	74	0	0
26	a	64	0	74	0	0
26	d	64	0	74	1	0
27	A	40	0	56	1	0
27	B	120	0	168	4	0
27	C	80	0	112	4	0
27	D	40	0	56	0	0
27	H	40	0	56	1	0
27	K	80	0	112	4	0
27	T	40	0	56	2	0
27	a	40	0	56	0	0
27	b	120	0	168	4	0
27	c	80	0	112	3	0
27	d	40	0	56	0	0
27	h	40	0	56	3	0
27	k	80	0	112	3	0
27	t	40	0	56	2	0
28	A	55	0	80	7	0
28	D	55	0	80	1	0
28	a	55	0	80	5	0
28	d	55	0	80	1	0
29	A	48	0	66	2	0
29	B	28	0	40	1	0
29	C	48	0	66	1	0
29	D	84	0	117	2	0
29	M	51	0	72	2	0
29	b	55	0	86	0	0
29	c	134	0	181	1	0
29	d	67	0	92	1	0
29	m	51	0	72	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	91	0	136	3	0
30	B	54	0	78	2	0
30	F	36	0	46	1	0
30	a	90	0	134	4	0
30	b	49	0	65	1	0
30	f	41	0	49	1	0
31	A	49	0	74	3	0
31	D	145	0	215	12	0
31	L	49	0	74	1	0
31	b	49	0	74	4	0
31	d	137	0	199	7	0
31	e	42	0	57	3	0
32	A	66	0	96	4	0
32	C	186	0	246	12	0
32	H	62	0	82	5	0
32	a	44	0	75	2	0
32	c	186	0	246	6	0
32	h	62	0	82	1	0
33	B	75	0	117	3	0
33	C	40	0	63	1	0
33	E	12	0	16	0	0
33	H	18	0	35	1	0
33	I	15	0	26	2	0
33	J	12	0	16	2	0
33	M	25	0	38	1	0
33	X	20	0	35	5	0
33	a	12	0	16	0	0
33	b	81	0	146	4	0
33	c	20	0	35	1	0
33	d	33	0	50	2	0
33	j	12	0	16	0	0
33	k	12	0	16	0	0
33	l	18	0	35	1	0
33	m	12	0	16	1	0
33	t	24	0	36	0	0
33	x	20	0	35	2	0
34	D	4	0	1	1	0
34	d	4	0	1	0	0
35	F	43	0	30	2	0
35	f	43	0	30	3	0
36	V	43	0	30	0	0
36	v	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A	150	0	0	3	0
37	B	204	0	0	3	0
37	C	184	0	0	3	0
37	D	133	0	0	2	0
37	E	21	0	0	0	0
37	F	6	0	0	0	0
37	H	28	0	0	0	0
37	I	12	0	0	0	0
37	J	10	0	0	0	0
37	K	1	0	0	0	0
37	L	10	0	0	0	0
37	M	7	0	0	0	0
37	O	93	0	0	2	0
37	R	1	0	0	0	0
37	T	8	0	0	1	0
37	U	43	0	0	0	0
37	V	69	0	0	1	0
37	X	15	0	0	0	0
37	Y	3	0	0	2	0
37	Z	4	0	0	0	0
37	a	123	0	0	0	0
37	b	189	0	0	3	0
37	c	175	0	0	5	0
37	d	112	0	0	1	0
37	e	18	0	0	0	0
37	f	7	0	0	1	0
37	h	18	0	0	0	0
37	i	7	0	0	1	0
37	j	4	0	0	0	0
37	k	7	0	0	0	0
37	l	8	0	0	0	0
37	m	7	0	0	0	0
37	o	99	0	0	0	0
37	t	11	0	0	0	0
37	u	55	0	0	1	0
37	v	58	0	0	1	0
37	x	10	0	0	1	0
37	y	1	0	0	0	0
37	z	1	0	0	0	0
All	All	54517	0	53863	485	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 (485) 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)
21:a:601[C]:OEY:O5	21:a:601[C]:OEY:O6	1.86	0.93
21:A:601[C]:OEY:O6	21:A:601[C]:OEY:O5	1.87	0.92
3:c:153:ASP:OD1	37:c:601:HOH:O	1.98	0.80
21:A:601[A]:OEY:O6	21:A:601[A]:OEY:O5	2.03	0.76
21:a:601[A]:OEY:O5	21:a:601[A]:OEY:O6	2.02	0.76
26:A:608:PHO:HBC3	4:D:279:LEU:HD22	1.67	0.74
13:O:27:ARG:NH1	37:O:301:HOH:O	2.20	0.74
2:B:91:TRP:HE1	33:B:619:STE:H32	1.55	0.71
5:E:60:GLN:NE2	5:E:62:SER:O	2.22	0.71
18:X:16:SER:HB3	33:X:101:STE:H92	1.74	0.69
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.75	0.69
3:C:32:GLY:N	37:C:601:HOH:O	2.24	0.68
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.59	0.68
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.77	0.67
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.75	0.67
4:d:259:ILE:HD12	31:d:408:LHG:H291	1.77	0.67
6:f:16:PHE:H	20:r:30:GLN:HE22	1.42	0.66
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.30	0.66
4:D:264:LYS:NZ	34:D:401:BCT:O3	2.29	0.66
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.77	0.65
19:Z:29:SER:HB3	19:Z:31:GLN:HE21	1.59	0.65
25:b:606:CLA:H142	25:b:612:CLA:H203	1.77	0.65
15:U:23:GLU:HG3	15:U:24:LYS:HG2	1.77	0.65
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.79	0.65
15:u:86:GLU:H	15:u:86:GLU:CD	2.06	0.64
25:b:601:CLA:H203	32:h:103:DGD:HBT1	1.77	0.64
35:f:101:HEM:HBC2	35:f:101:HEM:HMC2	1.80	0.64
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.80	0.64
1:a:188[C]:ALA:HB2	1:a:328[C]:MET:HB2	1.79	0.64
28:A:611:PL9:H28	31:A:615:LHG:H202	1.81	0.63
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.81	0.63
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.64	0.63
30:A:614:SQD:H262	31:D:409:LHG:H151	1.81	0.63
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.80	0.62
25:H:101:CLA:HBD	25:H:101:CLA:HBA1	1.80	0.62
19:z:1:MET:SD	19:z:1:MET:N	2.71	0.62
4:D:12:ARG:HH11	4:D:17:ILE:HD13	1.65	0.62
2:b:489:GLU:HA	2:b:495:PHE:HD2	1.64	0.62
7:H:56:ASP:OD2	18:X:2:THR:N	2.33	0.61
3:c:78:GLU:OE1	16:v:106:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:615:LHG:HC42	31:A:615:LHG:HC2	1.82	0.61
3:c:406:SER:HA	3:c:420:VAL:HG23	1.81	0.61
30:F:102:SQD:H301	18:X:27:VAL:HG11	1.82	0.60
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.82	0.60
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.84	0.60
2:B:371:THR:HG23	2:B:372:ASP:O	2.02	0.59
30:a:613:SQD:H381	9:j:22:ILE:HD11	1.83	0.59
18:X:17:GLY:HA2	33:X:101:STE:H142	1.83	0.59
29:A:613:LMG:HC72	3:C:216:SER:HB2	1.84	0.59
25:b:612:CLA:H171	31:d:407:LHG:H212	1.86	0.58
25:B:601:CLA:H43	7:H:45:ILE:HG22	1.86	0.58
13:O:34:SER:HB3	13:O:87:VAL:HG11	1.86	0.58
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.86	0.57
25:C:504:CLA:H101	32:C:518:DGD:HB2	1.85	0.57
31:b:623:LHG:H241	31:b:623:LHG:H101	1.86	0.57
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.86	0.57
32:A:617:DGD:HB41	33:I:101:STE:H42	1.87	0.57
30:B:621:SQD:O2	37:B:701:HOH:O	2.17	0.57
2:b:91:TRP:HE1	33:b:621:STE:H111	1.69	0.57
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.87	0.56
31:d:407:LHG:H351	31:d:407:LHG:H102	1.87	0.56
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.20	0.56
33:d:412:STE:H21	33:d:413:STE:O2	2.05	0.56
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.87	0.56
12:M:8:LEU:HD11	33:b:624:STE:H142	1.86	0.56
1:a:227:THR:HB	1:a:231:GLU:HG3	1.87	0.55
32:c:517:DGD:HAN1	32:c:518:DGD:HAE1	1.88	0.55
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.88	0.55
25:b:614:CLA:H2	25:b:615:CLA:HBB2	1.87	0.55
27:t:101:BCR:H321	27:t:101:BCR:HC8	1.87	0.55
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.36	0.55
5:e:33:ALA:HB2	20:r:11:PRO:HG2	1.88	0.55
32:C:518:DGD:HA31	29:D:407:LMG:H111	1.89	0.55
11:l:7:ARG:HH12	33:l:101:STE:C1	2.20	0.55
25:B:606:CLA:H192	31:D:411:LHG:H162	1.88	0.55
9:j:9:PRO:HG2	9:j:12:ILE:HG13	1.88	0.55
3:c:257:PHE:O	3:c:261:ARG:HG3	2.07	0.54
28:A:611:PL9:H272	31:A:615:LHG:H223	1.89	0.54
1:a:263:ALA:HA	31:e:101:LHG:H291	1.88	0.54
29:B:620:LMG:H392	4:D:36:LEU:HB2	1.90	0.54
25:C:504:CLA:H143	25:C:508:CLA:H141	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.08	0.54
3:C:406:SER:HA	3:C:420:VAL:HG23	1.89	0.54
3:C:167:VAL:HG13	25:C:512:CLA:H62	1.89	0.54
1:a:200:LEU:HD13	32:c:518:DGD:HAW2	1.90	0.54
4:d:126:MET:HE3	4:d:143:ALA:O	2.08	0.54
15:U:58:VAL:O	15:U:61:VAL:HG22	2.09	0.53
3:c:391[B]:ARG:NE	37:c:608:HOH:O	2.42	0.53
2:b:372:ASP:OD2	37:b:703:HOH:O	2.17	0.53
16:v:76:MET:HE3	36:v:201:HEC:HBB3	1.91	0.53
1:A:188[C]:ALA:HB2	1:A:328[C]:MET:HB2	1.90	0.53
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.91	0.53
3:c:45:LEU:HA	3:c:139:THR:HG22	1.89	0.53
25:b:601:CLA:HBB1	25:b:601:CLA:HMB3	1.91	0.53
3:c:163:PHE:CD2	25:c:512:CLA:HAB	2.44	0.53
6:f:24:HIS:O	6:f:28:VAL:HG13	2.07	0.53
28:D:406:PL9:H412	11:L:29:LEU:HD23	1.90	0.53
8:I:2:GLU:O	8:I:6:ILE:HG12	2.09	0.53
16:v:76:MET:HE1	16:v:115:ILE:HD12	1.90	0.52
4:d:241:GLU:CD	4:d:241:GLU:H	2.17	0.52
5:e:10:PHE:N	31:e:101:LHG:O4	2.40	0.52
31:b:623:LHG:H212	11:l:26:VAL:HG11	1.91	0.52
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.91	0.52
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.90	0.52
3:C:42:LEU:HD21	25:C:511:CLA:H2A	1.91	0.52
8:i:34:ARG:NH2	37:i:101:HOH:O	2.43	0.52
32:A:617:DGD:HE4	2:b:76:SER:HB3	1.91	0.52
27:T:101:BCR:H321	27:T:101:BCR:HC8	1.91	0.52
1:a:45:THR:HG23	25:a:612:CLA:H201	1.92	0.52
2:b:226:TYR:OH	37:b:701:HOH:O	2.17	0.52
1:a:259:ILE:HG21	28:a:611:PL9:H202	1.91	0.52
2:b:43:ALA:HB2	33:b:625:STE:H32	1.92	0.52
7:H:46:LEU:HD11	32:H:103:DGD:HA31	1.92	0.52
32:C:517:DGD:O2D	33:J:101:STE:O2	2.26	0.51
5:e:68:ASP:O	5:e:72:ALA:HB2	2.10	0.51
7:H:49:TYR:CE2	32:H:103:DGD:HB41	2.45	0.51
3:C:168:LEU:HD21	25:C:509:CLA:H61	1.92	0.51
1:a:281:VAL:HG11	30:a:613:SQD:H182	1.91	0.51
14:T:25:GLU:HB3	37:T:206:HOH:O	2.11	0.51
1:a:234:ASN:OD1	31:d:407:LHG:O1	2.27	0.51
2:B:414:PRO:O	2:B:418:LYS:HG3	2.10	0.51
25:B:613:CLA:HMD2	33:M:102:STE:H41	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:GLU:H	3:C:141:GLU:CD	2.17	0.51
18:X:21:LEU:HD11	33:X:101:STE:H172	1.93	0.51
25:B:609:CLA:H122	25:B:614:CLA:HAA1	1.93	0.51
27:K:101:BCR:H322	19:Z:17:PHE:CE2	2.46	0.51
7:H:17:GLU:OE2	7:H:20:LYS:NZ	2.39	0.50
28:a:611:PL9:H503	4:d:39:PRO:HG3	1.92	0.50
6:f:21:VAL:O	6:f:25:THR:OG1	2.25	0.50
16:v:41:HIS:HA	16:v:45:ILE:O	2.12	0.50
25:C:512:CLA:H121	25:C:513:CLA:H141	1.93	0.50
1:A:201:GLY:HA3	1:A:286:THR:HB	1.93	0.50
4:d:99:GLY:HA3	33:x:101:STE:H162	1.92	0.50
10:k:18:PHE:HE2	19:z:13:VAL:HG21	1.76	0.50
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.92	0.50
4:d:279:LEU:HD22	26:d:402:PHO:HBC3	1.92	0.50
25:B:613:CLA:H42	33:m:102:STE:H22	1.93	0.50
3:C:94:THR:HG22	25:C:501:CLA:HED1	1.93	0.50
12:m:4:ASN:ND2	29:m:101:LMG:O10	2.43	0.50
15:U:73:GLN:O	15:U:77:GLU:HG3	2.12	0.50
32:A:617:DGD:HB91	32:A:617:DGD:HB42	1.93	0.50
1:a:245:THR:HB	4:d:265:ARG:HE	1.77	0.50
13:O:56:PRO:O	13:O:58:ASN:ND2	2.45	0.49
2:B:36:SER:OG	27:B:617:BCR:H362	2.13	0.49
19:Z:55:GLY:HA2	19:Z:58:ASN:HB3	1.94	0.49
25:b:613:CLA:H43	30:b:619:SQD:H102	1.93	0.49
3:c:134:ILE:HD12	25:c:511:CLA:H43	1.95	0.49
25:c:512:CLA:H142	25:c:513:CLA:H151	1.94	0.49
25:A:607:CLA:HED1	32:C:518:DGD:HAH2	1.94	0.49
13:O:133:VAL:C	13:O:135:SER:H	2.20	0.49
5:E:17:VAL:HG23	9:J:7:ARG:HG3	1.94	0.49
5:E:53:ASP:O	16:V:1:ALA:N	2.46	0.49
19:Z:23:VAL:HG22	19:Z:40:ILE:HD12	1.93	0.49
3:c:464:GLU:OE2	4:d:245:SER:OG	2.28	0.49
19:z:32:ASP:OD1	19:z:32:ASP:N	2.43	0.49
3:C:261:ARG:NE	37:C:605:HOH:O	2.42	0.49
11:L:14:ARG:HB3	14:T:25:GLU:HG2	1.94	0.49
2:b:65:PHE:HE1	25:b:603:CLA:HED2	1.77	0.49
25:b:606:CLA:H142	25:b:612:CLA:H162	1.95	0.49
33:I:101:STE:H111	25:b:605:CLA:H192	1.95	0.49
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.94	0.49
13:O:27:ARG:HG3	37:O:301:HOH:O	2.12	0.49
31:D:408:LHG:H321	14:T:21:ILE:HD11	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:ARG:NH2	37:D:503:HOH:O	2.39	0.48
31:b:623:LHG:H172	11:l:22:LEU:HD23	1.95	0.48
15:u:98:TYR:O	37:u:201:HOH:O	2.20	0.48
30:f:102:SQD:H312	18:x:27:VAL:HG11	1.96	0.48
3:C:313:GLN:HB2	3:C:396:MET:HG3	1.96	0.48
25:C:502:CLA:H61	25:C:512:CLA:H42	1.95	0.48
4:d:141:TYR:OH	31:d:407:LHG:O4	2.17	0.48
2:b:36:SER:OG	27:b:617:BCR:H362	2.13	0.48
3:c:59:LEU:HD21	27:k:102:BCR:H372	1.96	0.48
32:C:516:DGD:HA91	32:C:516:DGD:HAW2	1.78	0.48
19:Z:46:LEU:HD22	19:Z:50:LEU:HD22	1.94	0.48
1:a:102:LEU:HD12	32:a:615:DGD:HB22	1.96	0.48
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.96	0.48
25:B:612:CLA:HBB1	25:B:612:CLA:HMB1	1.96	0.48
4:D:343:GLU:HG2	16:V:135:VAL:HG11	1.96	0.48
25:B:612:CLA:H161	31:D:411:LHG:H201	1.95	0.48
3:C:213:LEU:HG	25:C:506:CLA:H193	1.95	0.48
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.49	0.48
1:A:334[A]:ARG:NH2	37:A:710:HOH:O	2.46	0.47
2:B:141:ILE:O	2:B:145:LEU:HG	2.14	0.47
3:C:146:PHE:O	3:C:156:LYS:NZ	2.42	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.49	0.47
32:c:517:DGD:HA91	32:c:518:DGD:HB71	1.95	0.47
32:C:517:DGD:HG32	29:C:519:LMG:HC92	1.95	0.47
5:e:57:ALA:H	5:e:60:GLN:NE2	2.12	0.47
1:a:102:LEU:H	32:a:615:DGD:HA22	1.79	0.47
5:E:30:LEU:HD11	35:F:101:HEM:HAB	1.96	0.47
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.94	0.47
13:o:24:ASP:HA	13:o:203:LYS:HE2	1.97	0.47
25:A:606:CLA:HBD	25:A:612:CLA:HAC2	1.95	0.47
1:a:160[A]:ILE:HD11	32:c:516:DGD:HB92	1.96	0.47
25:b:612:CLA:H192	31:d:407:LHG:H212	1.97	0.47
28:A:611:PL9:H371	28:A:611:PL9:H351	1.75	0.47
25:b:614:CLA:H52	25:b:615:CLA:HBB1	1.97	0.47
3:c:26:ARG:HD3	10:k:46:ARG:NH2	2.30	0.47
25:c:507:CLA:H61	25:c:507:CLA:H92	1.70	0.47
25:A:612:CLA:H192	25:A:612:CLA:H162	1.76	0.47
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.50	0.47
29:D:407:LMG:H112	37:D:507:HOH:O	2.14	0.47
16:V:87:GLU:OE2	37:V:301:HOH:O	2.20	0.47
1:a:84:PRO:HA	1:a:112:TYR:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:613:CLA:H202	25:B:613:CLA:H141	1.97	0.47
1:A:84:PRO:HA	1:A:112:TYR:CG	2.51	0.46
37:A:751:HOH:O	13:O:107:THR:HG21	2.15	0.46
1:a:179[B]:THR:O	1:a:183[B]:MET:HG3	2.16	0.46
5:e:56:TYR:HA	5:e:60:GLN:HE21	1.81	0.46
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.97	0.46
3:C:203:THR:O	3:C:235:GLY:HA3	2.15	0.46
25:a:609:CLA:H41	25:a:609:CLA:H142	1.98	0.46
25:c:509:CLA:H92	25:c:509:CLA:H61	1.71	0.46
1:A:25:ASP:OD1	37:A:701:HOH:O	2.21	0.46
2:B:12:LEU:HB2	25:B:611:CLA:HMC2	1.97	0.46
25:B:605:CLA:H121	37:B:898:HOH:O	2.15	0.46
3:C:178:LYS:NZ	3:C:184:GLY:O	2.45	0.46
27:B:617:BCR:H15C	27:B:617:BCR:H351	1.82	0.46
1:a:271:LEU:HD21	28:a:611:PL9:C3	2.46	0.46
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.96	0.46
25:A:609:CLA:H41	25:A:609:CLA:H61	1.64	0.46
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.51	0.46
19:Z:2:THR:HG22	19:Z:6:GLN:OE1	2.15	0.46
2:b:287:ARG:HD3	37:b:704:HOH:O	2.15	0.46
1:A:211:PHE:CD1	28:A:611:PL9:H111	2.50	0.46
25:B:606:CLA:H193	11:L:27:LEU:HD11	1.98	0.46
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.98	0.46
13:o:57:LYS:HB3	13:o:59:LYS:HE3	1.97	0.46
25:b:613:CLA:H61	25:b:613:CLA:H93	1.61	0.45
1:a:82:VAL:HB	1:a:174[C]:LEU:HB2	1.98	0.45
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.16	0.45
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.52	0.45
25:C:512:CLA:H193	25:C:512:CLA:H161	1.71	0.45
13:O:110:MET:HE2	13:O:110:MET:HB3	1.83	0.45
3:c:153:ASP:CG	37:c:601:HOH:O	2.56	0.45
30:A:616:SQD:H383	25:b:605:CLA:H93	1.98	0.45
25:B:608:CLA:HBC1	33:H:104:STE:H72	1.98	0.45
25:C:510:CLA:H122	25:C:510:CLA:H162	1.74	0.45
2:b:247:PHE:CE1	25:b:601:CLA:H102	2.52	0.45
5:e:26:THR:HA	20:r:15:ALA:HB1	1.98	0.45
27:k:102:BCR:H24C	27:k:102:BCR:H371	1.80	0.45
13:o:23:ASP:OD1	13:o:24:ASP:N	2.50	0.45
25:A:606:CLA:CBD	25:A:612:CLA:HAC2	2.47	0.45
25:C:506:CLA:H91	25:C:506:CLA:H203	1.98	0.45
25:C:507:CLA:H142	25:C:507:CLA:H111	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:K:101:BCR:H10C	17:Y:28:ILE:HG23	1.98	0.45
2:b:121:GLU:OE2	7:h:12:ARG:NH1	2.39	0.45
33:c:520:STE:H52	33:c:520:STE:H21	1.80	0.45
31:d:409:LHG:H242	31:d:409:LHG:H272	1.61	0.45
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.99	0.45
1:a:185[C]:VAL:O	1:a:189[C]:GLU:HG3	2.16	0.45
2:b:25:MET:HG2	27:b:616:BCR:H23C	1.97	0.45
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.98	0.45
32:A:617:DGD:HD5	2:b:75:TRP:HB3	1.99	0.45
1:a:162[C]:PRO:HB3	1:a:168[C]:PHE:HA	1.98	0.45
3:c:121:SER:O	3:c:124:VAL:HG13	2.17	0.45
25:B:609:CLA:HHC	25:B:609:CLA:HBB1	1.99	0.45
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.98	0.45
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.52	0.45
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.79	0.45
25:h:101:CLA:H92	27:h:102:BCR:H402	1.99	0.45
9:j:19:MET:O	9:j:23:VAL:HG23	2.17	0.45
29:m:101:LMG:H411	29:m:101:LMG:H381	1.88	0.45
31:D:411:LHG:H221	12:M:18:PRO:HG3	1.99	0.45
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.99	0.45
20:R:16:ALA:O	20:R:20:VAL:HG23	2.17	0.45
2:b:8:VAL:HG23	2:b:9:HIS:CD2	2.52	0.45
27:h:102:BCR:H15C	27:h:102:BCR:H351	1.88	0.45
13:o:130:GLN:OE1	13:o:143:LYS:NZ	2.49	0.45
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.82	0.45
25:A:606:CLA:H192	31:D:408:LHG:H331	1.99	0.44
32:C:517:DGD:HA82	32:C:517:DGD:HAE2	1.72	0.44
9:J:15:THR:HG22	9:J:19:MET:HE3	1.99	0.44
27:h:102:BCR:H24C	27:h:102:BCR:H371	1.75	0.44
13:o:53:LYS:HE3	13:o:65:PHE:CZ	2.52	0.44
4:D:194:ASN:HA	4:D:295:SER:OG	2.17	0.44
20:R:34:LEU:O	20:R:35:LEU:HG	2.16	0.44
25:b:614:CLA:H152	25:b:614:CLA:H112	1.66	0.44
25:B:612:CLA:H192	31:D:411:LHG:H201	1.99	0.44
13:O:56:PRO:O	13:O:58:ASN:N	2.41	0.44
25:b:601:CLA:H43	7:h:45:ILE:HG22	2.00	0.44
9:j:18:GLY:O	9:j:21:VAL:HG13	2.17	0.44
25:B:610:CLA:H112	25:B:610:CLA:H72	1.53	0.44
32:C:518:DGD:HA91	32:C:518:DGD:HAW1	1.62	0.44
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.84	0.44
25:B:601:CLA:H171	32:H:103:DGD:HAE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:29:LYS:HE2	20:R:33:LYS:HD2	1.99	0.44
2:b:283:GLU:O	2:b:287:ARG:HG3	2.18	0.44
6:f:12:SER:N	37:f:201:HOH:O	2.50	0.44
29:m:101:LMG:H322	29:m:101:LMG:H291	1.60	0.44
18:x:17:GLY:HA2	33:x:101:STE:H41	1.99	0.44
20:r:3:TRP:O	20:r:7:VAL:HG13	2.18	0.44
25:B:601:CLA:H152	25:B:601:CLA:H18	1.64	0.44
17:Y:26:ALA:HB3	37:Y:101:HOH:O	2.18	0.44
20:R:32:GLN:C	20:R:34:LEU:H	2.25	0.44
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.99	0.44
3:C:114:VAL:HG22	33:C:522:STE:H102	1.99	0.44
1:a:93:PHE:HZ	25:a:609:CLA:HAA1	1.83	0.44
2:b:141:ILE:HD13	25:b:614:CLA:HBB1	2.00	0.44
25:c:506:CLA:H162	25:c:506:CLA:H122	1.40	0.44
27:c:514:BCR:H15C	27:c:514:BCR:H351	1.85	0.44
16:V:3:LEU:HD23	16:V:3:LEU:HA	1.89	0.44
25:c:504:CLA:H92	25:c:504:CLA:H62	1.74	0.44
32:c:516:DGD:HAH2	32:c:516:DGD:HAT2	1.90	0.44
9:j:16:VAL:HA	9:j:19:MET:HE2	2.00	0.44
2:B:233:ASN:HD21	2:B:476:ARG:NH1	2.16	0.44
25:B:607:CLA:H141	25:B:607:CLA:H161	1.67	0.44
28:a:611:PL9:H322	28:a:611:PL9:H301	1.74	0.44
29:m:101:LMG:H392	29:m:101:LMG:H361	1.70	0.44
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.00	0.43
29:A:613:LMG:H111	29:A:613:LMG:O10	2.18	0.43
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.00	0.43
20:R:32:GLN:C	20:R:34:LEU:N	2.76	0.43
1:a:288:LEU:HG	3:c:432:VAL:HG22	2.01	0.43
31:b:623:LHG:H271	12:m:22:LEU:HD21	2.01	0.43
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.19	0.43
5:e:30:LEU:HD11	35:f:101:HEM:CBB	2.49	0.43
4:D:12:ARG:NE	4:D:12:ARG:HA	2.33	0.43
31:D:411:LHG:H212	31:D:411:LHG:H182	1.84	0.43
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.71	0.43
25:b:602:CLA:H141	25:b:602:CLA:H161	1.71	0.43
1:A:183[A]:MET:HA	25:A:606:CLA:HMD1	2.00	0.43
2:B:439:SER:O	37:B:702:HOH:O	2.21	0.43
4:d:191:TRP:CZ2	4:d:197:HIS:HB2	2.53	0.43
4:d:267:LEU:C	4:d:267:LEU:HD23	2.43	0.43
29:d:410:LMG:O9	33:d:412:STE:H32	2.18	0.43
10:k:18:PHE:CE2	19:z:13:VAL:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:19:ILE:HG12	16:v:20:THR:N	2.33	0.43
16:v:104:MET:HA	16:v:107:LEU:HD22	2.01	0.43
33:B:623:STE:H111	12:m:8:LEU:HD11	1.99	0.43
25:b:614:CLA:H2	25:b:615:CLA:CBB	2.49	0.43
16:v:41:HIS:CD2	36:v:201:HEC:NB	2.86	0.43
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.53	0.43
25:B:604:CLA:H41	25:B:611:CLA:H161	2.00	0.43
6:f:15:ILE:H	20:r:30:GLN:NE2	2.15	0.43
7:H:49:TYR:CD2	32:H:103:DGD:HB41	2.53	0.43
2:B:385:ARG:HB2	13:O:165:ALA:O	2.19	0.43
5:E:68:ASP:O	5:E:72:ALA:HB2	2.18	0.43
27:H:102:BCR:H20C	27:H:102:BCR:H361	1.86	0.43
25:b:607:CLA:H92	25:b:607:CLA:H62	1.88	0.43
28:d:406:PL9:H421	28:d:406:PL9:H401	1.88	0.43
17:y:20:ALA:O	17:y:24:MET:HG2	2.18	0.43
19:z:32:ASP:HB2	19:z:35:ARG:HB2	2.01	0.43
25:C:512:CLA:H93	25:C:512:CLA:H61	1.66	0.43
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.01	0.43
20:R:34:LEU:HD12	20:R:34:LEU:HA	1.82	0.43
25:b:609:CLA:H203	25:b:609:CLA:H162	1.83	0.43
25:c:501:CLA:C4D	25:c:503:CLA:H2	2.49	0.43
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.00	0.43
13:o:53:LYS:HB2	13:o:65:PHE:CE1	2.54	0.43
16:v:30:LYS:NZ	37:v:304:HOH:O	2.52	0.43
6:f:26:LEU:O	6:f:29:PRO:HD2	2.18	0.43
16:v:99:ASP:OD1	16:v:99:ASP:N	2.51	0.43
1:A:297:LEU:HD23	32:C:517:DGD:HB1	2.01	0.42
27:C:514:BCR:H361	27:C:514:BCR:H20C	1.82	0.42
28:a:611:PL9:H28	31:e:101:LHG:H201	2.01	0.42
25:c:509:CLA:H13	25:c:509:CLA:H172	1.80	0.42
4:d:307:GLU:OE1	37:d:501:HOH:O	2.21	0.42
28:A:611:PL9:H401	28:A:611:PL9:H422	1.67	0.42
25:B:604:CLA:H41	25:B:604:CLA:H61	1.83	0.42
7:H:59:ASN:OD1	7:H:61:SER:HB3	2.19	0.42
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.55	0.42
25:b:606:CLA:H93	25:b:606:CLA:H111	1.85	0.42
27:b:617:BCR:H15C	27:b:617:BCR:H351	1.87	0.42
28:A:611:PL9:H451	28:A:611:PL9:H471	1.65	0.42
2:B:117:TYR:HA	11:L:1:MET:HE1	2.02	0.42
25:B:602:CLA:C2D	25:B:604:CLA:H2	2.49	0.42
27:B:616:BCR:H371	27:B:616:BCR:H24C	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:19:MET:O	9:J:23:VAL:HG23	2.19	0.42
27:K:102:BCR:H20C	27:K:102:BCR:H361	1.80	0.42
16:V:41:HIS:HA	16:V:45:ILE:O	2.19	0.42
1:a:162[B]:PRO:HB3	1:a:168[B]:PHE:HA	2.00	0.42
33:b:625:STE:H51	33:b:625:STE:H22	1.93	0.42
29:c:521:LMG:HO4	29:c:521:LMG:HO5	1.67	0.42
1:A:234:ASN:ND2	31:D:411:LHG:HC11	2.35	0.42
27:A:610:BCR:H371	27:A:610:BCR:H24C	1.84	0.42
25:B:603:CLA:H62	25:B:603:CLA:H92	1.82	0.42
13:O:57:LYS:HE2	13:O:57:LYS:HB3	1.85	0.42
3:c:348:GLU:OE2	13:o:11:VAL:HA	2.19	0.42
27:k:101:BCR:HC7	27:k:102:BCR:H353	2.00	0.42
4:D:321:LEU:O	4:D:325:ILE:HG13	2.18	0.42
31:D:409:LHG:H141	31:D:409:LHG:H341	2.02	0.42
32:c:518:DGD:HAE2	32:c:518:DGD:HA82	1.78	0.42
25:C:508:CLA:H192	25:C:508:CLA:H162	1.74	0.42
1:a:237:TYR:CZ	4:d:264:LYS:HG3	2.54	0.42
25:b:610:CLA:H143	25:b:610:CLA:H162	1.83	0.42
25:c:511:CLA:HBB1	25:c:511:CLA:HMB3	2.01	0.42
18:x:8:LYS:HA	18:x:8:LYS:HD2	1.76	0.42
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.00	0.42
25:B:606:CLA:H111	25:B:612:CLA:H202	2.02	0.42
25:B:610:CLA:HBB1	25:B:610:CLA:HMB3	2.02	0.42
25:D:404:CLA:C1D	33:X:101:STE:H102	2.49	0.42
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.01	0.42
25:B:612:CLA:H62	25:B:612:CLA:H41	1.87	0.42
25:D:404:CLA:H142	25:D:404:CLA:H111	1.86	0.42
27:c:515:BCR:H15C	27:c:515:BCR:H351	1.93	0.42
6:f:19:ARG:O	6:f:23:VAL:HG13	2.19	0.42
3:C:261:ARG:HB3	37:C:749:HOH:O	2.20	0.42
25:C:511:CLA:H141	25:C:511:CLA:H162	1.82	0.42
31:D:411:LHG:H172	31:L:101:LHG:H292	2.01	0.42
3:c:166:ILE:HG21	25:c:512:CLA:H202	2.01	0.42
4:d:179:PHE:HA	4:d:182:LEU:HD22	2.00	0.42
25:D:404:CLA:H51	33:X:101:STE:H182	2.01	0.42
16:V:63:THR:HG22	16:V:64:PRO:CD	2.50	0.42
17:Y:27:MET:HG3	37:Y:101:HOH:O	2.19	0.42
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.89	0.41
32:C:517:DGD:HB31	32:C:517:DGD:HB62	1.86	0.41
31:D:411:LHG:H192	31:D:411:LHG:H161	1.77	0.41
19:Z:31:GLN:H	19:Z:31:GLN:HG3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:26:THR:HG22	20:r:15:ALA:HB1	2.01	0.41
13:o:32:ILE:HD13	13:o:32:ILE:HA	1.96	0.41
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.55	0.41
5:e:30:LEU:HD11	6:f:28:VAL:HB	2.02	0.41
30:B:621:SQD:H172	30:B:621:SQD:H341	2.02	0.41
3:C:79:LYS:HG2	16:V:103:LYS:HD3	2.02	0.41
2:b:201:HIS:HB2	25:b:601:CLA:CHB	2.50	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.54	0.41
3:c:155:ASN:HB3	37:c:601:HOH:O	2.20	0.41
11:l:14:ARG:HB3	14:t:25:GLU:HG2	2.02	0.41
25:C:506:CLA:H91	25:C:506:CLA:H111	1.77	0.41
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.91	0.41
27:T:101:BCR:H15C	27:T:101:BCR:H351	1.89	0.41
28:A:611:PL9:H271	28:A:611:PL9:H251	1.84	0.41
30:a:613:SQD:H171	30:a:613:SQD:H202	1.80	0.41
25:b:606:CLA:H161	25:b:606:CLA:H141	1.59	0.41
25:b:613:CLA:H41	25:b:613:CLA:H62	1.36	0.41
27:t:101:BCR:H24C	27:t:101:BCR:H371	1.85	0.41
2:B:106:LEU:HD11	30:a:614:SQD:H211	2.01	0.41
25:B:614:CLA:H2	25:B:615:CLA:HBB2	2.01	0.41
25:h:101:CLA:CHA	25:h:101:CLA:HBA2	2.50	0.41
30:A:616:SQD:H282	2:b:109:LEU:HD13	2.02	0.41
32:C:517:DGD:HA32	33:J:101:STE:H81	2.03	0.41
4:D:79:SER:HA	4:D:172:SER:HB3	2.02	0.41
32:H:103:DGD:HBT1	32:H:103:DGD:HBH2	1.99	0.41
13:O:133:VAL:O	13:O:135:SER:N	2.53	0.41
1:a:112:TYR:O	1:a:116:ILE:HG12	2.20	0.41
25:b:602:CLA:C4D	25:b:604:CLA:H43	2.51	0.41
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.82	0.41
9:j:9:PRO:HG2	9:j:12:ILE:CG1	2.48	0.41
16:v:77:LYS:O	16:v:96:ARG:HB2	2.20	0.41
19:z:1:MET:HB2	19:z:4:LEU:HB3	2.03	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.41
4:D:42:TYR:CE1	6:F:25:THR:HG23	2.55	0.41
1:a:159[C]:LEU:C	1:a:162[C]:PRO:HD2	2.46	0.41
1:a:183[B]:MET:HA	25:a:606:CLA:HMD1	2.01	0.41
1:a:231:GLU:H	1:a:231:GLU:HG2	1.74	0.41
1:a:237:TYR:HB2	1:a:245:THR:HG21	2.02	0.41
25:c:512:CLA:H92	25:c:512:CLA:H61	1.81	0.41
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.51	0.41
18:x:8:LYS:NZ	37:x:202:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190[A]:HIS:ND1	1:A:298:ASN:OD1	2.54	0.41
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.02	0.41
2:B:414:PRO:N	2:B:415:PRO:HD2	2.35	0.41
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.87	0.41
27:K:102:BCR:H24C	27:K:102:BCR:H371	1.91	0.41
25:b:606:CLA:H41	25:b:606:CLA:H62	1.89	0.41
16:v:57:GLU:H	16:v:57:GLU:CD	2.29	0.41
27:B:618:BCR:H20C	27:B:618:BCR:H361	1.85	0.40
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.87	0.40
3:C:467:LEU:HD23	3:C:467:LEU:HA	1.82	0.40
11:L:27:LEU:HD23	11:L:27:LEU:HA	1.94	0.40
12:M:6:LEU:HD12	29:M:101:LMG:HC92	2.03	0.40
27:b:618:BCR:H20C	27:b:618:BCR:H361	1.92	0.40
17:y:19:ILE:O	17:y:23:THR:HG22	2.22	0.40
25:B:603:CLA:H11	25:B:604:CLA:H42	2.02	0.40
20:R:34:LEU:C	20:R:35:LEU:HG	2.47	0.40
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.56	0.40
2:b:489:GLU:HA	2:b:495:PHE:CD2	2.50	0.40
33:B:622:STE:H42	33:B:622:STE:H72	1.91	0.40
27:C:514:BCR:H24C	27:C:514:BCR:H371	1.79	0.40
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	2.03	0.40
2:b:54:PRO:HD2	2:b:57:ARG:HG3	2.02	0.40
2:B:148:LEU:HD23	2:B:210:ILE:HD11	2.03	0.40
32:C:518:DGD:HA51	32:C:518:DGD:HA22	1.72	0.40
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.02	0.40
29:M:101:LMG:H421	29:M:101:LMG:H391	1.79	0.40
13:O:55:GLU:HA	13:O:56:PRO:HD3	1.92	0.40
1:a:201:GLY:HA3	1:a:286:THR:HB	2.03	0.40
2:b:159:THR:O	2:b:180:PRO:HB3	2.21	0.40
3:c:156:LYS:N	37:c:601:HOH:O	2.22	0.40
25:d:404:CLA:H162	25:d:404:CLA:H192	1.84	0.40
29:m:101:LMG:H371	29:m:101:LMG:H342	1.42	0.40
1:A:343[A]:LEU:HD23	1:A:343[A]:LEU:HA	1.93	0.40
25:C:503:CLA:HBB2	25:C:512:CLA:H92	2.03	0.40
25:c:502:CLA:HBA2	25:c:503:CLA:H171	2.03	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	458/344 (133%)	448 (98%)	9 (2%)	1 (0%)	43	40
1	a	458/344 (133%)	448 (98%)	9 (2%)	1 (0%)	43	40
2	B	507/510 (99%)	500 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	461/461 (100%)	452 (98%)	8 (2%)	1 (0%)	43	40
3	c	471/461 (102%)	454 (96%)	16 (3%)	1 (0%)	43	40
4	D	341/352 (97%)	331 (97%)	10 (3%)	0	100	100
4	d	342/352 (97%)	332 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	229 (94%)	10 (4%)	4 (2%)	7	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	233 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	5
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	10
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5534/5700 (97%)	5386 (97%)	138 (2%)	10 (0%)	43	40

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	58	ASN
16	V	64	PRO
13	O	62	GLU
3	c	416	SER
15	u	53	ALA
13	O	134	THR
13	O	138	THR
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/280 (134%)	370 (99%)	4 (1%)	65	68
1	a	373/280 (133%)	363 (97%)	10 (3%)	39	37
2	B	407/407 (100%)	399 (98%)	8 (2%)	48	48
2	b	402/407 (99%)	393 (98%)	9 (2%)	45	45
3	C	361/362 (100%)	357 (99%)	4 (1%)	65	68
3	c	370/362 (102%)	357 (96%)	13 (4%)	32	27
4	D	278/283 (98%)	276 (99%)	2 (1%)	76	77
4	d	279/283 (99%)	272 (98%)	7 (2%)	42	40
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	20
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	12
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	26
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	7
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	50
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	50
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	31
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	31
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	5
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	29
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	34
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	4
12	M	28/32 (88%)	25 (89%)	3 (11%)	6	2
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	7
13	O	206/228 (90%)	200 (97%)	6 (3%)	37	34
13	o	207/228 (91%)	202 (98%)	5 (2%)	43	41
14	T	26/28 (93%)	24 (92%)	2 (8%)	12	6
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	22
15	U	84/112 (75%)	79 (94%)	5 (6%)	17	10
15	u	84/112 (75%)	82 (98%)	2 (2%)	43	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	53
16	v	117/138 (85%)	114 (97%)	3 (3%)	40	38
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	17
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	2
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	30
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	3
19	z	51/52 (98%)	48 (94%)	3 (6%)	18	10
20	R	28/33 (85%)	24 (86%)	4 (14%)	3	1
20	r	25/33 (76%)	21 (84%)	4 (16%)	2	0
All	All	4572/4654 (98%)	4438 (97%)	134 (3%)	36	34

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	243	GLU
1	A	244	GLU
1	A	270	SER
2	B	76	SER
2	B	86	ILE
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	141	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	43	LEU
4	D	259	ILE
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	77	GLU
6	F	25	THR
7	H	20	LYS

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Mol	Chain	Res	Type
8	I	4	LEU
10	K	10	LYS
11	L	10	VAL
12	M	2	GLU
12	M	20	VAL
12	M	25	LEU
13	O	54	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	214	THR
14	T	25	GLU
14	T	30	THR
15	U	15	GLU
15	U	51	LYS
15	U	61	VAL
15	U	67	LEU
15	U	86	GLU
16	V	3	LEU
16	V	7	VAL
18	X	3	ILE
18	X	29	ILE
18	X	37	VAL
19	Z	15	LEU
19	Z	19	MET
19	Z	35	ARG
19	Z	46	LEU
19	Z	50	LEU
20	R	6	LEU
20	R	12	VAL
20	R	21	ARG
20	R	29	LYS
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	159[C]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	245	THR
1	a	286	THR

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Mol	Chain	Res	Type
1	a	288	LEU
2	b	98	LEU
2	b	128	THR
2	b	137	LYS
2	b	236	THR
2	b	362	PHE
2	b	405	GLU
2	b	485	GLU
2	b	492	GLU
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	216	SER
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	182	LEU
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
5	e	4	THR
5	e	8	ARG
5	e	65	LEU
5	e	83	LEU
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
8	i	2	GLU
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	25	LEU

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Mol	Chain	Res	Type
10	k	30	VAL
10	k	35	LEU
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	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
14	t	25	GLU
15	u	15	GLU
15	u	23	GLU
16	v	19	ILE
16	v	52	LEU
16	v	107	LEU
17	y	19	ILE
18	x	15	LEU
19	z	1	MET
19	z	42	LEU
19	z	46	LEU
20	r	7	VAL
20	r	9	LEU
20	r	10	LEU
20	r	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN
2	B	374	ASN
2	B	394	GLN
2	B	409	GLN
3	C	201	ASN
3	C	311	GLN
3	C	385	GLN
6	F	44	GLN
12	M	5	GLN
13	O	88	ASN
13	O	155	ASN

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Mol	Chain	Res	Type
16	V	86	GLN
17	Y	45	ASN
19	Z	31	GLN
19	Z	38	GLN
1	a	19	ASN
2	b	338	GLN
2	b	409	GLN
3	c	311	GLN
3	c	322	GLN
5	e	60	GLN
5	e	82	GLN
7	h	59	ASN
13	o	155	ASN
18	x	33	GLN
20	r	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.88	0	8,9,11	1.00	0
8	FME	i	1	8	8,9,10	1.04	0	8,9,11	0.97	0
12	FME	M	1	12	8,9,10	1.01	1 (12%)	8,9,11	1.15	0
8	FME	I	1	8	8,9,10	0.93	0	8,9,11	0.97	1 (12%)
12	FME	m	1	12	8,9,10	1.00	0	8,9,11	0.59	0
14	FME	T	1	14	8,9,10	1.11	1 (12%)	8,9,11	1.21	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
14	FME	t	1	14	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.20	1.43	1.46
12	M	1	FME	CA-N	-2.12	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.26	113.86	109.50
8	I	1	FME	C-CA-N	2.04	113.43	109.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 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$
33	STE	C	520	-	11,11,19	0.64	0	11,11,19	1.56	2 (18%)
31	LHG	D	408	-	48,48,48	0.68	1 (2%)	51,54,54	1.27	7 (13%)
33	STE	M	103	-	9,9,19	0.37	0	8,8,19	0.70	0
31	LHG	d	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.39	7 (13%)
25	CLA	a	606	-	69,73,73	1.38	9 (13%)	82,113,113	1.35	8 (9%)
25	CLA	c	504	37	64,68,73	1.24	6 (9%)	76,107,113	1.37	9 (11%)
25	CLA	C	507	37	69,73,73	1.24	7 (10%)	82,113,113	1.37	5 (6%)
33	STE	C	522	-	15,15,19	0.32	0	14,14,19	0.90	0
22	OEX	A	602[B]	1,3,37	0,15,15	-	-	-	-	-
27	BCR	H	102	-	41,41,41	0.96	1 (2%)	56,56,56	1.19	6 (10%)
25	CLA	c	508	-	68,72,73	1.34	8 (11%)	80,111,113	1.42	10 (12%)
32	DGD	c	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.42	9 (11%)
31	LHG	d	409	-	38,38,48	0.82	1 (2%)	41,44,54	1.16	3 (7%)
25	CLA	B	612	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
29	LMG	c	519	-	37,37,55	0.91	1 (2%)	45,45,63	1.34	6 (13%)
34	BCT	D	401	23	3,3,3	1.24	0	2,3,3	2.92	1 (50%)
27	BCR	k	101	-	41,41,41	1.02	3 (7%)	56,56,56	1.03	2 (3%)
32	DGD	A	617	-	67,67,67	1.06	6 (8%)	81,81,81	1.32	12 (14%)
25	CLA	b	609	37	69,73,73	1.39	7 (10%)	82,113,113	1.39	8 (9%)
27	BCR	K	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.10	2 (3%)
29	LMG	D	410	-	31,31,55	0.70	1 (3%)	33,33,63	1.21	3 (9%)
33	STE	b	624	-	14,14,19	0.32	0	13,13,19	0.90	0
29	LMG	m	101	-	51,51,55	0.73	1 (1%)	59,59,63	1.41	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	D	407	-	51,51,55	0.81	2 (3%)	59,59,63	1.34	5 (8%)
25	CLA	A	607	37	69,73,73	1.14	5 (7%)	82,113,113	1.18	8 (9%)
26	PHO	d	402	-	58,69,69	2.13	8 (13%)	55,99,99	1.57	9 (16%)
25	CLA	B	615	-	64,68,73	1.48	9 (14%)	76,107,113	1.49	7 (9%)
25	CLA	b	611	-	69,73,73	1.20	9 (13%)	82,113,113	1.38	11 (13%)
25	CLA	h	101	37	69,73,73	1.26	7 (10%)	82,113,113	1.33	7 (8%)
36	HEC	v	201	16	46,50,50	1.89	5 (10%)	58,82,82	1.81	4 (6%)
27	BCR	k	102	-	41,41,41	1.01	3 (7%)	56,56,56	1.21	5 (8%)
32	DGD	h	103	-	63,63,67	0.98	5 (7%)	77,77,81	1.45	12 (15%)
25	CLA	a	607	37	69,73,73	1.17	6 (8%)	82,113,113	1.34	10 (12%)
27	BCR	d	405	-	41,41,41	1.06	2 (4%)	56,56,56	1.12	4 (7%)
25	CLA	C	504	37	63,67,73	1.39	9 (14%)	74,105,113	1.35	10 (13%)
25	CLA	b	610	-	69,73,73	1.30	6 (8%)	82,113,113	1.29	8 (9%)
25	CLA	d	404	-	69,73,73	1.11	7 (10%)	82,113,113	1.19	8 (9%)
25	CLA	a	612	37	69,73,73	1.40	7 (10%)	82,113,113	1.32	5 (6%)
26	PHO	A	608	-	58,69,69	2.03	9 (15%)	55,99,99	1.39	6 (10%)
29	LMG	B	620	-	26,26,55	0.72	2 (7%)	26,26,63	1.24	2 (7%)
29	LMG	c	521	-	48,48,55	0.89	1 (2%)	56,56,63	1.28	6 (10%)
30	SQD	a	614	-	35,35,54	1.73	6 (17%)	37,37,65	1.37	3 (8%)
25	CLA	b	614	-	69,73,73	1.39	8 (11%)	82,113,113	1.39	5 (6%)
25	CLA	C	503	-	69,73,73	1.35	9 (13%)	82,113,113	1.46	8 (9%)
33	STE	x	101	-	19,19,19	0.53	0	19,19,19	1.27	1 (5%)
25	CLA	B	606	37	69,73,73	1.33	8 (11%)	82,113,113	1.35	6 (7%)
33	STE	c	520	-	19,19,19	0.61	0	19,19,19	0.98	0
29	LMG	M	101	-	51,51,55	0.85	2 (3%)	59,59,63	1.45	7 (11%)
25	CLA	c	501	-	69,73,73	1.18	8 (11%)	82,113,113	1.45	9 (10%)
25	CLA	B	604	-	69,73,73	1.22	7 (10%)	82,113,113	1.35	8 (9%)
25	CLA	C	505	-	69,73,73	1.20	6 (8%)	82,113,113	1.27	8 (9%)
33	STE	H	104	-	17,17,19	0.38	0	16,16,19	0.77	0
25	CLA	C	511	3	69,73,73	1.33	8 (11%)	82,113,113	1.39	4 (4%)
27	BCR	t	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.30	5 (8%)
28	PL9	D	406	-	55,55,55	1.07	4 (7%)	68,69,69	1.49	14 (20%)
34	BCT	d	401	23	3,3,3	1.20	0	2,3,3	2.88	1 (50%)
32	DGD	c	516	-	63,63,67	0.99	4 (6%)	77,77,81	1.48	13 (16%)
27	BCR	a	610	-	41,41,41	0.93	2 (4%)	56,56,56	1.15	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	609	37	69,73,73	1.26	8 (11%)	82,113,113	1.27	10 (12%)
25	CLA	B	608	-	69,73,73	1.36	8 (11%)	82,113,113	1.42	7 (8%)
32	DGD	H	103	-	63,63,67	1.08	8 (12%)	77,77,81	1.43	12 (15%)
33	STE	d	413	-	16,16,19	0.58	0	16,16,19	1.35	2 (12%)
25	CLA	c	509	-	69,73,73	1.18	5 (7%)	82,113,113	1.39	5 (6%)
27	BCR	c	515	-	41,41,41	1.14	3 (7%)	56,56,56	1.19	6 (10%)
25	CLA	A	612	37	69,73,73	1.32	8 (11%)	82,113,113	1.28	7 (8%)
31	LHG	e	101	-	41,41,48	0.77	1 (2%)	44,47,54	1.31	6 (13%)
27	BCR	D	405	-	41,41,41	1.05	2 (4%)	56,56,56	1.17	5 (8%)
33	STE	b	620	-	15,15,19	0.37	0	14,14,19	0.85	0
25	CLA	C	502	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
33	STE	B	619	-	16,16,19	0.68	0	16,16,19	1.08	0
31	LHG	A	615	-	48,48,48	0.81	3 (6%)	51,54,54	1.19	5 (9%)
25	CLA	b	604	-	69,73,73	1.30	9 (13%)	82,113,113	1.43	9 (10%)
30	SQD	a	613	-	52,54,54	1.57	7 (13%)	62,65,65	1.89	12 (19%)
35	HEM	f	101	5,6	50,50,50	1.48	9 (18%)	67,82,82	1.25	7 (10%)
21	OEY	A	601[A]	1,3,37	0,16,16	-	-	-	-	-
32	DGD	C	517	-	63,63,67	1.03	6 (9%)	77,77,81	1.33	10 (12%)
25	CLA	b	606	37	69,73,73	1.07	5 (7%)	82,113,113	1.22	9 (10%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.15	5 (8%)
27	BCR	b	618	-	41,41,41	0.97	2 (4%)	56,56,56	1.15	3 (5%)
33	STE	m	102	-	11,11,19	0.65	0	11,11,19	1.64	3 (27%)
25	CLA	C	508	-	69,73,73	1.29	7 (10%)	82,113,113	1.38	10 (12%)
25	CLA	A	606	-	69,73,73	1.23	6 (8%)	82,113,113	1.15	6 (7%)
25	CLA	c	506	-	69,73,73	1.26	8 (11%)	82,113,113	1.26	4 (4%)
33	STE	t	102	-	13,13,19	0.64	0	13,13,19	1.31	2 (15%)
25	CLA	b	613	-	69,73,73	1.24	9 (13%)	82,113,113	1.31	9 (10%)
29	LMG	C	519	-	48,48,55	0.86	2 (4%)	56,56,63	1.29	7 (12%)
25	CLA	b	612	-	69,73,73	1.33	8 (11%)	82,113,113	1.33	12 (14%)
25	CLA	c	513	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	8 (9%)
33	STE	E	101	-	11,11,19	0.74	0	11,11,19	1.17	1 (9%)
29	LMG	d	411	-	44,44,55	0.85	1 (2%)	52,52,63	1.26	6 (11%)
33	STE	b	621	-	19,19,19	0.58	0	19,19,19	1.14	1 (5%)
25	CLA	B	610	-	69,73,73	1.31	7 (10%)	82,113,113	1.32	6 (7%)
22	OEX	a	602[B]	1,3,37	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.35	8 (10%)
25	CLA	c	510	-	69,73,73	1.27	9 (13%)	82,113,113	1.37	9 (10%)
25	CLA	C	501	-	69,73,73	1.52	9 (13%)	82,113,113	1.49	9 (10%)
21	OEY	a	601[A]	1,3,37	0,16,16	-	-	-		
25	CLA	b	602	-	69,73,73	1.30	9 (13%)	82,113,113	1.38	11 (13%)
25	CLA	b	603	-	69,73,73	1.28	7 (10%)	82,113,113	1.56	9 (10%)
33	STE	j	101	-	11,11,19	0.79	0	11,11,19	1.00	0
33	STE	B	624	-	11,11,19	0.73	0	11,11,19	1.22	1 (9%)
27	BCR	b	616	-	41,41,41	0.98	2 (4%)	56,56,56	1.30	7 (12%)
29	LMG	b	622	-	55,55,55	0.77	3 (5%)	63,63,63	1.30	7 (11%)
30	SQD	f	102	-	39,41,54	1.67	8 (20%)	49,52,65	1.80	11 (22%)
25	CLA	c	503	-	69,73,73	1.23	7 (10%)	82,113,113	1.42	7 (8%)
27	BCR	b	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.08	2 (3%)
25	CLA	B	613	-	69,73,73	1.24	6 (8%)	82,113,113	1.33	10 (12%)
25	CLA	b	607	-	69,73,73	1.20	6 (8%)	82,113,113	1.32	12 (14%)
33	STE	k	103	-	11,11,19	0.73	0	11,11,19	1.20	0
25	CLA	a	609	-	69,73,73	1.15	7 (10%)	82,113,113	1.29	5 (6%)
25	CLA	D	404	-	69,73,73	1.34	8 (11%)	82,113,113	1.22	8 (9%)
25	CLA	b	605	-	69,73,73	1.28	7 (10%)	82,113,113	1.36	9 (10%)
25	CLA	c	512	-	69,73,73	1.31	9 (13%)	82,113,113	1.36	8 (9%)
31	LHG	d	408	-	48,48,48	0.63	0	51,54,54	1.20	4 (7%)
25	CLA	c	502	-	69,73,73	1.54	9 (13%)	82,113,113	1.34	9 (10%)
27	BCR	c	514	-	41,41,41	1.03	2 (4%)	56,56,56	1.20	6 (10%)
27	BCR	h	102	-	41,41,41	1.01	2 (4%)	56,56,56	1.19	4 (7%)
35	HEM	F	101	5,6	50,50,50	1.45	6 (12%)	67,82,82	1.17	3 (4%)
25	CLA	B	602	-	69,73,73	1.17	6 (8%)	82,113,113	1.39	9 (10%)
25	CLA	C	506	-	69,73,73	1.30	8 (11%)	82,113,113	1.24	6 (7%)
25	CLA	B	607	-	69,73,73	1.22	9 (13%)	82,113,113	1.28	8 (9%)
30	SQD	b	619	-	47,49,54	1.65	8 (17%)	57,60,65	1.47	7 (12%)
31	LHG	D	409	-	46,46,48	0.87	3 (6%)	49,52,54	1.21	6 (12%)
33	STE	X	101	-	19,19,19	0.55	0	19,19,19	1.19	1 (5%)
29	LMG	c	522	-	49,49,55	0.78	1 (2%)	57,57,63	1.34	6 (10%)
33	STE	a	616	-	11,11,19	0.74	0	11,11,19	1.23	2 (18%)
27	BCR	B	616	-	41,41,41	1.04	3 (7%)	56,56,56	1.23	7 (12%)
25	CLA	C	512	-	69,73,73	1.33	10 (14%)	82,113,113	1.34	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	605	-	69,73,73	1.47	8 (11%)	82,113,113	1.48	9 (10%)
29	LMG	d	410	-	21,21,55	0.54	1 (4%)	20,20,63	1.21	2 (10%)
26	PHO	D	402	-	58,69,69	1.97	10 (17%)	55,99,99	1.41	6 (10%)
32	DGD	C	516	-	63,63,67	1.02	4 (6%)	77,77,81	1.31	11 (14%)
28	PL9	d	406	-	55,55,55	1.08	3 (5%)	68,69,69	1.58	14 (20%)
28	PL9	A	611	-	55,55,55	1.02	3 (5%)	68,69,69	1.54	12 (17%)
25	CLA	D	403	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	7 (8%)
29	LMG	A	613	-	48,48,55	0.80	0	56,56,63	1.41	9 (16%)
30	SQD	A	614	-	50,52,54	1.57	7 (14%)	60,63,65	1.93	11 (18%)
33	STE	b	626	-	9,9,19	0.36	0	8,8,19	0.72	0
27	BCR	B	618	-	41,41,41	1.05	2 (4%)	56,56,56	1.18	3 (5%)
33	STE	C	521	-	11,11,19	0.75	0	11,11,19	1.20	1 (9%)
33	STE	d	412	-	15,15,19	0.79	0	15,15,19	0.85	0
21	OXY	a	601[C]	1,3,37	0,16,16	-	-	-	-	-
30	SQD	F	102	-	34,36,54	1.52	5 (14%)	42,45,65	1.79	9 (21%)
27	BCR	C	514	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	7 (12%)
28	PL9	a	611	-	55,55,55	0.69	1 (1%)	68,69,69	1.54	10 (14%)
31	LHG	D	411	-	48,48,48	0.81	1 (2%)	51,54,54	1.32	7 (13%)
25	CLA	C	510	-	69,73,73	1.26	8 (11%)	82,113,113	1.38	8 (9%)
33	STE	b	625	-	19,19,19	0.60	0	19,19,19	1.01	0
27	BCR	T	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.25	8 (14%)
25	CLA	C	509	-	69,73,73	1.29	8 (11%)	82,113,113	1.36	10 (12%)
27	BCR	A	610	-	41,41,41	0.96	2 (4%)	56,56,56	1.24	6 (10%)
33	STE	I	101	-	14,14,19	0.38	0	13,13,19	0.73	0
25	CLA	b	601	-	69,73,73	1.13	7 (10%)	82,113,113	1.36	10 (12%)
33	STE	t	103	-	9,9,19	0.34	0	8,8,19	0.81	0
25	CLA	B	611	-	69,73,73	1.16	8 (11%)	82,113,113	1.46	10 (12%)
25	CLA	c	505	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	5 (6%)
32	DGD	a	615	-	43,43,67	0.67	1 (2%)	45,45,81	1.47	6 (13%)
30	SQD	A	616	-	38,38,54	1.76	5 (13%)	40,40,65	1.12	2 (5%)
36	HEC	V	201	16	46,50,50	1.84	5 (10%)	58,82,82	1.79	4 (6%)
25	CLA	C	513	-	69,73,73	1.26	8 (11%)	82,113,113	1.37	6 (7%)
30	SQD	B	621	-	52,54,54	1.58	8 (15%)	62,65,65	1.71	12 (19%)
33	STE	l	101	-	17,17,19	0.31	0	16,16,19	0.95	0
31	LHG	L	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.19	3 (5%)
25	CLA	c	507	37	69,73,73	1.21	7 (10%)	82,113,113	1.37	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	614	-	69,73,73	1.45	6 (8%)	82,113,113	1.38	6 (7%)
25	CLA	d	403	-	69,73,73	1.27	7 (10%)	82,113,113	1.22	7 (8%)
33	STE	B	625	-	15,15,19	0.36	0	14,14,19	0.80	0
33	STE	B	622	-	11,11,19	0.79	0	11,11,19	1.13	0
25	CLA	b	608	-	69,73,73	1.21	8 (11%)	82,113,113	1.35	11 (13%)
25	CLA	B	603	-	69,73,73	1.40	6 (8%)	82,113,113	1.58	10 (12%)
21	OEY	A	601[C]	1,3,37	0,16,16	-	-	-		
32	DGD	c	517	-	63,63,67	0.97	4 (6%)	77,77,81	1.32	10 (12%)
33	STE	B	623	-	17,17,19	0.62	0	17,17,19	1.17	0
25	CLA	H	101	37	69,73,73	1.38	9 (13%)	82,113,113	1.49	10 (12%)
25	CLA	b	615	-	64,68,73	1.09	5 (7%)	76,107,113	1.39	10 (13%)
25	CLA	A	609	-	58,62,73	1.22	5 (8%)	68,99,113	1.37	9 (13%)
25	CLA	B	601	-	69,73,73	1.28	7 (10%)	82,113,113	1.31	9 (10%)
27	BCR	B	617	-	41,41,41	1.04	3 (7%)	56,56,56	1.16	4 (7%)
25	CLA	c	511	3	69,73,73	1.55	9 (13%)	82,113,113	1.38	6 (7%)
31	LHG	b	623	-	48,48,48	0.70	0	51,54,54	1.19	5 (9%)
33	STE	J	101	-	11,11,19	0.72	0	11,11,19	1.12	0
27	BCR	C	515	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	3 (5%)
26	PHO	a	608	-	58,69,69	2.11	9 (15%)	55,99,99	1.57	8 (14%)
33	STE	M	102	-	14,14,19	0.62	0	14,14,19	1.24	1 (7%)

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
33	STE	C	520	-	-	5/9/9/17	-
31	LHG	D	408	-	-	25/53/53/53	-
33	STE	M	103	-	-	2/7/7/17	-
31	LHG	d	407	-	-	18/53/53/53	-
25	CLA	a	606	-	1/1/15/20	1/39/115/115	-
25	CLA	c	504	37	1/1/14/20	9/33/109/115	-
25	CLA	C	507	37	1/1/15/20	9/39/115/115	-
33	STE	C	522	-	-	9/13/13/17	-
27	BCR	H	102	-	-	3/29/63/63	0/2/2/2
25	CLA	c	508	-	-	8/38/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	DGD	c	518	-	-	19/51/91/95	0/2/2/2
31	LHG	d	409	-	-	11/43/43/53	-
25	CLA	B	612	-	1/1/15/20	15/39/115/115	-
29	LMG	c	519	-	-	12/31/51/70	0/1/1/1
27	BCR	k	101	-	-	10/29/63/63	0/2/2/2
32	DGD	A	617	-	-	28/55/95/95	0/2/2/2
25	CLA	b	609	37	1/1/15/20	7/39/115/115	-
27	BCR	K	102	-	-	4/29/63/63	0/2/2/2
29	LMG	D	410	-	-	17/33/33/70	-
33	STE	b	624	-	-	10/12/12/17	-
29	LMG	m	101	-	-	22/46/66/70	0/1/1/1
29	LMG	D	407	-	-	16/46/66/70	0/1/1/1
25	CLA	A	607	37	1/1/15/20	12/39/115/115	-
26	PHO	d	402	-	-	5/37/103/103	0/5/6/6
25	CLA	B	615	-	1/1/14/20	12/33/109/115	-
25	CLA	b	611	-	1/1/15/20	8/39/115/115	-
25	CLA	h	101	37	1/1/15/20	18/39/115/115	-
36	HEC	v	201	16	-	6/14/54/54	-
27	BCR	k	102	-	-	0/29/63/63	0/2/2/2
32	DGD	h	103	-	-	20/51/91/95	0/2/2/2
25	CLA	a	607	37	1/1/15/20	9/39/115/115	-
27	BCR	d	405	-	-	7/29/63/63	0/2/2/2
25	CLA	C	504	37	1/1/13/20	9/32/108/115	-
25	CLA	b	610	-	1/1/15/20	6/39/115/115	-
25	CLA	d	404	-	1/1/15/20	8/39/115/115	-
25	CLA	a	612	37	1/1/15/20	2/39/115/115	-
26	PHO	A	608	-	-	1/37/103/103	0/5/6/6
29	LMG	B	620	-	-	9/22/22/70	-
29	LMG	c	521	-	-	24/43/63/70	0/1/1/1
30	SQD	a	614	-	-	22/37/37/69	-
25	CLA	b	614	-	1/1/15/20	11/39/115/115	-
25	CLA	C	503	-	1/1/15/20	6/39/115/115	-
33	STE	x	101	-	-	10/17/17/17	-
25	CLA	B	606	37	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	c	520	-	-	8/17/17/17	-
29	LMG	M	101	-	-	14/46/66/70	0/1/1/1
25	CLA	c	501	-	1/1/15/20	4/39/115/115	-
25	CLA	B	604	-	1/1/15/20	8/39/115/115	-
25	CLA	C	505	-	1/1/15/20	12/39/115/115	-
33	STE	H	104	-	-	12/15/15/17	-
25	CLA	C	511	3	1/1/15/20	7/39/115/115	-
27	BCR	t	101	-	-	5/29/63/63	0/2/2/2
28	PL9	D	406	-	-	6/53/73/73	0/1/1/1
32	DGD	c	516	-	-	28/51/91/95	0/2/2/2
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2
25	CLA	B	609	37	1/1/15/20	7/39/115/115	-
25	CLA	B	608	-	-	6/39/115/115	-
32	DGD	H	103	-	-	14/51/91/95	0/2/2/2
33	STE	d	413	-	-	9/14/14/17	-
25	CLA	c	509	-	1/1/15/20	16/39/115/115	-
27	BCR	c	515	-	-	3/29/63/63	0/2/2/2
25	CLA	A	612	37	1/1/15/20	7/39/115/115	-
31	LHG	e	101	-	-	23/46/46/53	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
33	STE	b	620	-	-	4/13/13/17	-
25	CLA	C	502	-	1/1/15/20	7/39/115/115	-
33	STE	B	619	-	-	7/14/14/17	-
31	LHG	A	615	-	-	21/53/53/53	-
25	CLA	b	604	-	1/1/15/20	7/39/115/115	-
30	SQD	a	613	-	-	21/49/69/69	0/1/1/1
35	HEM	f	101	5,6	-	5/14/54/54	-
32	DGD	C	517	-	-	16/51/91/95	0/2/2/2
25	CLA	b	606	37	1/1/15/20	15/39/115/115	-
27	BCR	K	101	-	-	6/29/63/63	0/2/2/2
27	BCR	b	618	-	-	1/29/63/63	0/2/2/2
33	STE	m	102	-	-	5/9/9/17	-
25	CLA	C	508	-	-	9/39/115/115	-
25	CLA	A	606	-	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	506	-	1/1/15/20	13/39/115/115	-
33	STE	t	102	-	-	5/11/11/17	-
25	CLA	b	613	-	1/1/15/20	16/39/115/115	-
29	LMG	C	519	-	-	18/43/63/70	0/1/1/1
25	CLA	b	612	-	1/1/15/20	10/39/115/115	-
25	CLA	c	513	-	1/1/15/20	8/39/115/115	-
33	STE	E	101	-	-	6/9/9/17	-
29	LMG	d	411	-	-	14/39/59/70	0/1/1/1
33	STE	b	621	-	-	11/17/17/17	-
25	CLA	B	610	-	1/1/15/20	6/39/115/115	-
32	DGD	C	518	-	-	16/51/91/95	0/2/2/2
25	CLA	c	510	-	1/1/15/20	14/39/115/115	-
25	CLA	C	501	-	1/1/15/20	5/39/115/115	-
25	CLA	b	602	-	1/1/15/20	10/39/115/115	-
25	CLA	b	603	-	1/1/15/20	5/39/115/115	-
33	STE	j	101	-	-	5/9/9/17	-
33	STE	B	624	-	-	1/9/9/17	-
27	BCR	b	616	-	-	5/29/63/63	0/2/2/2
29	LMG	b	622	-	-	27/50/70/70	0/1/1/1
30	SQD	f	102	-	-	12/36/56/69	0/1/1/1
25	CLA	c	503	-	1/1/15/20	7/39/115/115	-
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
25	CLA	B	613	-	1/1/15/20	10/39/115/115	-
25	CLA	b	607	-	1/1/15/20	5/39/115/115	-
33	STE	k	103	-	-	4/9/9/17	-
25	CLA	a	609	-	1/1/15/20	10/39/115/115	-
25	CLA	b	605	-	1/1/15/20	9/39/115/115	-
25	CLA	c	512	-	1/1/15/20	20/39/115/115	-
25	CLA	D	404	-	-	11/39/115/115	-
31	LHG	d	408	-	-	14/53/53/53	-
25	CLA	c	502	-	-	2/39/115/115	-
27	BCR	c	514	-	-	3/29/63/63	0/2/2/2
27	BCR	h	102	-	-	3/29/63/63	0/2/2/2
35	HEM	F	101	5,6	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	602	-	1/1/15/20	5/39/115/115	-
25	CLA	C	506	-	1/1/15/20	10/39/115/115	-
25	CLA	B	607	-	1/1/15/20	5/39/115/115	-
30	SQD	b	619	-	-	18/44/64/69	0/1/1/1
31	LHG	D	409	-	-	17/51/51/53	-
33	STE	X	101	-	-	12/17/17/17	-
29	LMG	c	522	-	-	23/44/64/70	0/1/1/1
33	STE	a	616	-	-	3/9/9/17	-
27	BCR	B	616	-	-	3/29/63/63	0/2/2/2
25	CLA	C	512	-	1/1/15/20	13/39/115/115	-
25	CLA	B	605	-	1/1/15/20	8/39/115/115	-
29	LMG	d	410	-	-	10/17/17/70	-
26	PHO	D	402	-	-	1/37/103/103	0/5/6/6
32	DGD	C	516	-	-	18/51/91/95	0/2/2/2
28	PL9	d	406	-	-	14/53/73/73	0/1/1/1
28	PL9	A	611	-	-	24/53/73/73	0/1/1/1
25	CLA	D	403	-	-	9/39/115/115	-
29	LMG	A	613	-	-	21/43/63/70	0/1/1/1
30	SQD	A	614	-	-	18/47/67/69	0/1/1/1
33	STE	b	626	-	-	4/7/7/17	-
27	BCR	B	618	-	-	2/29/63/63	0/2/2/2
33	STE	C	521	-	-	6/9/9/17	-
33	STE	d	412	-	-	6/13/13/17	-
30	SQD	F	102	-	-	14/28/48/69	0/1/1/1
27	BCR	C	514	-	-	3/29/63/63	0/2/2/2
28	PL9	a	611	-	-	24/53/73/73	0/1/1/1
31	LHG	D	411	-	-	18/53/53/53	-
25	CLA	C	510	-	1/1/15/20	7/39/115/115	-
33	STE	b	625	-	-	10/17/17/17	-
27	BCR	T	101	-	-	7/29/63/63	0/2/2/2
25	CLA	C	509	-	1/1/15/20	13/39/115/115	-
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
33	STE	I	101	-	-	6/12/12/17	-
25	CLA	b	601	-	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	t	103	-	-	3/7/7/17	-
25	CLA	B	611	-	1/1/15/20	7/39/115/115	-
25	CLA	c	505	-	1/1/15/20	8/39/115/115	-
32	DGD	a	615	-	-	22/45/45/95	-
30	SQD	A	616	-	-	15/39/39/69	-
36	HEC	V	201	16	-	6/14/54/54	-
25	CLA	C	513	-	1/1/15/20	9/39/115/115	-
30	SQD	B	621	-	-	21/49/69/69	0/1/1/1
33	STE	l	101	-	-	8/15/15/17	-
31	LHG	L	101	-	-	19/53/53/53	-
25	CLA	c	507	37	1/1/15/20	13/39/115/115	-
25	CLA	B	614	-	1/1/15/20	14/39/115/115	-
25	CLA	d	403	-	-	6/39/115/115	-
33	STE	B	625	-	-	6/13/13/17	-
33	STE	B	622	-	-	7/9/9/17	-
25	CLA	b	608	-	1/1/15/20	7/39/115/115	-
25	CLA	B	603	-	1/1/15/20	8/39/115/115	-
32	DGD	c	517	-	-	15/51/91/95	0/2/2/2
33	STE	B	623	-	-	7/15/15/17	-
25	CLA	H	101	37	1/1/15/20	18/39/115/115	-
25	CLA	b	615	-	1/1/14/20	7/33/109/115	-
25	CLA	A	609	-	1/1/12/20	3/26/102/115	-
25	CLA	B	601	-	1/1/15/20	7/39/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	CLA	c	511	3	1/1/15/20	9/39/115/115	-
31	LHG	b	623	-	-	12/53/53/53	-
33	STE	J	101	-	-	4/9/9/17	-
27	BCR	C	515	-	-	2/29/63/63	0/2/2/2
26	PHO	a	608	-	-	2/37/103/103	0/5/6/6
33	STE	M	102	-	-	5/12/12/17	-

All (770) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	608	PHO	C1B-C2B	9.86	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	402	PHO	C1B-C2B	9.42	1.49	1.39
26	d	402	PHO	C3B-C4B	9.05	1.50	1.41
26	A	608	PHO	C1B-C2B	8.83	1.49	1.39
26	D	402	PHO	C1B-C2B	8.24	1.48	1.39
26	A	608	PHO	C3B-C4B	8.21	1.49	1.41
25	c	511	CLA	MG-NA	8.09	2.25	2.06
25	B	605	CLA	MG-NA	8.06	2.25	2.06
26	a	608	PHO	C3B-C4B	7.96	1.49	1.41
26	D	402	PHO	C3B-C4B	7.45	1.49	1.41
25	a	612	CLA	MG-NA	6.81	2.22	2.06
36	V	201	HEC	CAC-C3C	6.76	1.56	1.35
25	c	502	CLA	MG-NB	-6.67	1.92	2.05
36	v	201	HEC	CAB-C3B	6.37	1.55	1.35
36	v	201	HEC	CAC-C3C	6.35	1.55	1.35
36	V	201	HEC	CAB-C3B	6.21	1.55	1.35
25	b	614	CLA	MG-NA	5.85	2.20	2.06
25	C	501	CLA	MG-NA	5.84	2.20	2.06
25	b	610	CLA	MG-NA	5.71	2.19	2.06
25	B	603	CLA	MG-NC	5.55	2.19	2.06
25	b	609	CLA	MG-NB	-5.48	1.94	2.05
36	v	201	HEC	C3D-C2D	5.46	1.53	1.38
30	A	616	SQD	O47-C45	-5.38	1.37	1.47
25	B	614	CLA	MG-NC	5.31	2.18	2.06
25	B	610	CLA	MG-NA	5.22	2.18	2.06
25	B	615	CLA	MG-NA	5.14	2.18	2.06
30	b	619	SQD	O48-C23	5.07	1.48	1.33
30	a	613	SQD	O48-C23	5.06	1.48	1.33
25	H	101	CLA	MG-NA	4.99	2.18	2.06
25	b	602	CLA	MG-NA	4.95	2.18	2.06
36	V	201	HEC	C3D-C2D	4.93	1.51	1.38
25	C	504	CLA	MG-NB	4.84	2.15	2.05
25	B	608	CLA	MG-NA	4.83	2.17	2.06
25	D	404	CLA	MG-NB	-4.82	1.96	2.05
25	b	605	CLA	MG-NA	4.81	2.17	2.06
30	F	102	SQD	O48-C23	4.78	1.47	1.33
25	C	510	CLA	MG-NA	4.77	2.17	2.06
30	B	621	SQD	O48-C23	4.76	1.47	1.33
35	F	101	HEM	FE-NC	4.76	2.10	1.95
25	b	603	CLA	MG-NA	4.72	2.17	2.06
30	a	614	SQD	O48-C23	4.66	1.46	1.33
30	A	616	SQD	O48-C23	4.66	1.46	1.33
25	A	612	CLA	MG-NA	4.65	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	MG-NB	4.64	2.15	2.05
25	c	510	CLA	MG-NA	4.64	2.17	2.06
30	A	614	SQD	O48-C23	4.64	1.46	1.33
25	b	612	CLA	MG-NA	4.63	2.17	2.06
30	f	102	SQD	O48-C23	4.59	1.46	1.33
25	A	606	CLA	MG-NA	4.57	2.17	2.06
25	C	503	CLA	MG-NA	4.55	2.17	2.06
25	C	507	CLA	MG-NA	4.55	2.17	2.06
25	B	603	CLA	MG-NA	4.54	2.17	2.06
25	C	509	CLA	MG-NB	-4.49	1.96	2.05
25	C	508	CLA	MG-NA	4.49	2.16	2.06
35	f	101	HEM	FE-NA	4.46	2.09	1.95
25	B	614	CLA	MG-NA	4.45	2.16	2.06
26	d	402	PHO	C1D-C2D	4.41	1.44	1.39
25	B	606	CLA	C1D-ND	4.38	1.43	1.37
25	a	606	CLA	MG-NA	4.38	2.16	2.06
25	B	608	CLA	C1D-ND	4.37	1.43	1.37
25	C	506	CLA	MG-NA	4.35	2.16	2.06
25	c	502	CLA	MG-ND	4.33	2.14	2.05
25	C	511	CLA	MG-NA	4.31	2.16	2.06
25	C	501	CLA	MG-NB	4.30	2.14	2.05
25	B	601	CLA	MG-NA	4.28	2.16	2.06
25	h	101	CLA	MG-NA	4.25	2.16	2.06
25	c	502	CLA	MG-NA	4.23	2.16	2.06
27	c	515	BCR	C1-C6	-4.16	1.48	1.53
25	c	512	CLA	MG-NB	4.15	2.14	2.05
26	A	608	PHO	C1D-C2D	4.15	1.44	1.39
25	C	512	CLA	MG-NB	4.13	2.14	2.05
25	a	606	CLA	C1D-ND	4.13	1.43	1.37
28	A	611	PL9	C7-C3	-4.06	1.45	1.51
25	B	615	CLA	C1D-ND	4.05	1.43	1.37
25	B	613	CLA	MG-NA	4.03	2.15	2.06
25	b	609	CLA	C1D-ND	4.00	1.43	1.37
25	C	501	CLA	MG-ND	-4.00	1.97	2.05
25	A	612	CLA	C1D-ND	3.99	1.43	1.37
25	D	404	CLA	C1D-ND	3.98	1.43	1.37
25	D	404	CLA	MG-NC	3.98	2.15	2.06
25	B	602	CLA	MG-NA	3.92	2.15	2.06
25	B	606	CLA	MG-NA	3.91	2.15	2.06
25	C	513	CLA	C1D-ND	3.89	1.43	1.37
25	c	509	CLA	C1D-ND	3.88	1.43	1.37
25	C	505	CLA	MG-NA	3.86	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	406	PL9	C3-C4	-3.84	1.43	1.49
25	C	509	CLA	C1D-ND	3.84	1.42	1.37
30	A	614	SQD	O47-C45	-3.84	1.37	1.46
25	d	403	CLA	MG-NC	3.83	2.15	2.06
25	C	506	CLA	C1D-ND	3.83	1.42	1.37
25	C	502	CLA	MG-NA	3.81	2.15	2.06
28	d	406	PL9	C3-C4	-3.81	1.43	1.49
25	H	101	CLA	C1D-ND	3.79	1.42	1.37
25	b	614	CLA	MG-NB	3.79	2.13	2.05
25	B	605	CLA	C1D-ND	3.78	1.42	1.37
25	B	606	CLA	MG-NC	3.78	2.15	2.06
25	B	604	CLA	C1D-ND	3.78	1.42	1.37
26	a	608	PHO	C4D-CHA	3.77	1.45	1.39
25	B	603	CLA	C1D-ND	3.77	1.42	1.37
25	d	403	CLA	MG-NA	3.76	2.15	2.06
25	c	508	CLA	C1D-ND	3.76	1.42	1.37
25	B	601	CLA	C1D-ND	3.75	1.42	1.37
25	b	613	CLA	C1D-ND	3.74	1.42	1.37
25	c	504	CLA	MG-NB	3.72	2.13	2.05
25	B	607	CLA	MG-NA	3.72	2.15	2.06
26	a	608	PHO	C1D-C2D	3.71	1.43	1.39
25	c	510	CLA	C1D-ND	3.71	1.42	1.37
25	b	602	CLA	C1D-ND	3.71	1.42	1.37
25	C	511	CLA	C1D-ND	3.70	1.42	1.37
25	C	503	CLA	MG-ND	3.69	2.13	2.05
25	B	614	CLA	C4B-NB	3.69	1.42	1.37
25	C	504	CLA	MG-ND	-3.69	1.98	2.05
25	a	606	CLA	MG-NB	3.68	2.13	2.05
25	b	607	CLA	MG-NA	3.67	2.15	2.06
31	d	407	LHG	O7-C5	-3.66	1.38	1.46
30	a	614	SQD	O47-C7	3.66	1.44	1.34
25	B	615	CLA	C1B-C2B	3.64	1.51	1.43
25	H	101	CLA	C4B-NB	3.64	1.42	1.37
31	D	409	LHG	P-O6	3.64	1.73	1.59
25	c	513	CLA	C1D-ND	3.63	1.42	1.37
25	b	611	CLA	C1D-ND	3.62	1.42	1.37
25	C	510	CLA	C1D-ND	3.61	1.42	1.37
30	B	621	SQD	O47-C7	3.61	1.44	1.34
25	C	501	CLA	C1D-ND	3.61	1.42	1.37
25	c	506	CLA	C1D-ND	3.60	1.42	1.37
25	b	605	CLA	C1D-ND	3.59	1.42	1.37
25	B	614	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	606	CLA	C1D-ND	3.58	1.42	1.37
25	c	505	CLA	MG-NA	3.56	2.14	2.06
27	K	101	BCR	C1-C6	-3.54	1.49	1.53
30	f	102	SQD	O47-C7	3.54	1.44	1.34
27	b	617	BCR	C30-C25	-3.53	1.49	1.53
25	b	612	CLA	C1D-ND	3.53	1.42	1.37
25	B	615	CLA	MG-ND	3.52	2.12	2.05
30	b	619	SQD	O47-C7	3.52	1.44	1.34
30	b	619	SQD	O5-C1	3.50	1.50	1.41
25	B	609	CLA	C4B-NB	3.50	1.42	1.37
25	B	604	CLA	C1B-C2B	3.49	1.51	1.43
25	c	507	CLA	C1D-ND	3.49	1.42	1.37
25	B	609	CLA	MG-NA	3.48	2.14	2.06
27	B	618	BCR	C1-C6	-3.47	1.49	1.53
25	c	512	CLA	C1D-ND	3.46	1.42	1.37
25	c	501	CLA	C1D-ND	3.46	1.42	1.37
25	C	501	CLA	C4B-NB	3.46	1.42	1.37
30	a	613	SQD	O47-C7	3.45	1.44	1.34
27	C	515	BCR	C1-C6	-3.44	1.49	1.53
25	B	613	CLA	C1D-ND	3.43	1.42	1.37
25	b	608	CLA	C1D-ND	3.42	1.42	1.37
25	b	612	CLA	C4B-NB	3.42	1.42	1.37
25	C	512	CLA	MG-ND	-3.41	1.99	2.05
25	b	601	CLA	C1D-ND	3.41	1.42	1.37
25	b	603	CLA	C1D-ND	3.41	1.42	1.37
25	b	608	CLA	MG-NA	3.40	2.14	2.06
26	D	402	PHO	C1D-C2D	3.40	1.43	1.39
25	c	511	CLA	C1D-ND	3.39	1.42	1.37
25	c	501	CLA	MG-NC	3.39	2.14	2.06
30	a	613	SQD	O47-C45	-3.38	1.38	1.46
25	c	503	CLA	C1D-ND	3.38	1.42	1.37
25	a	609	CLA	C1D-ND	3.37	1.42	1.37
25	b	613	CLA	C4B-NB	3.36	1.42	1.37
30	f	102	SQD	O47-C45	-3.36	1.38	1.46
25	C	502	CLA	C1D-ND	3.36	1.42	1.37
25	h	101	CLA	C4B-NB	3.35	1.42	1.37
25	b	609	CLA	MG-NA	3.35	2.14	2.06
25	B	602	CLA	C1D-ND	3.35	1.42	1.37
25	b	603	CLA	MG-NC	3.35	2.14	2.06
25	c	504	CLA	C4B-NB	3.35	1.42	1.37
25	B	611	CLA	C1D-ND	3.34	1.42	1.37
25	A	607	CLA	C1D-ND	3.34	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	MG-NA	3.33	2.14	2.06
25	C	512	CLA	C1D-ND	3.33	1.42	1.37
30	a	614	SQD	C24-C23	3.33	1.60	1.50
30	A	616	SQD	O47-C7	3.32	1.43	1.34
35	f	101	HEM	FE-NB	3.32	2.05	1.94
25	b	604	CLA	C1D-ND	3.30	1.42	1.37
25	h	101	CLA	C1D-ND	3.30	1.42	1.37
25	B	610	CLA	C1D-ND	3.29	1.42	1.37
25	C	508	CLA	C1D-ND	3.29	1.42	1.37
25	d	403	CLA	C1D-ND	3.29	1.42	1.37
25	c	512	CLA	C1B-C2B	3.28	1.50	1.43
25	c	506	CLA	C4B-NB	3.28	1.42	1.37
30	a	614	SQD	O47-C45	-3.27	1.38	1.46
26	A	608	PHO	C4D-CHA	3.27	1.44	1.39
25	A	606	CLA	C1B-C2B	3.26	1.50	1.43
25	B	613	CLA	MG-ND	-3.26	1.99	2.05
25	A	609	CLA	C1D-ND	3.25	1.42	1.37
25	B	609	CLA	C1D-ND	3.25	1.42	1.37
25	B	601	CLA	C4B-NB	3.24	1.42	1.37
25	c	507	CLA	C1B-C2B	3.24	1.50	1.43
27	B	616	BCR	C1-C6	-3.24	1.49	1.53
30	B	621	SQD	O47-C45	-3.23	1.39	1.46
25	b	612	CLA	MG-NC	3.23	2.13	2.06
35	F	101	HEM	FE-NB	3.23	2.04	1.94
28	A	611	PL9	C3-C4	-3.23	1.44	1.49
25	c	502	CLA	C1D-ND	3.22	1.42	1.37
30	F	102	SQD	C24-C23	3.22	1.60	1.50
25	a	609	CLA	C1B-C2B	3.22	1.50	1.43
25	C	504	CLA	C1D-ND	3.22	1.42	1.37
25	B	612	CLA	C1D-ND	3.21	1.42	1.37
25	a	606	CLA	C1B-C2B	3.19	1.50	1.43
27	d	405	BCR	C1-C6	-3.19	1.49	1.53
25	b	615	CLA	C1D-ND	3.19	1.42	1.37
32	h	103	DGD	C4D-C3D	3.19	1.60	1.52
25	A	606	CLA	C1D-ND	3.18	1.42	1.37
35	f	101	HEM	FE-ND	3.18	2.04	1.94
25	c	508	CLA	MG-NC	3.18	2.13	2.06
27	k	101	BCR	C1-C6	-3.17	1.49	1.53
30	A	616	SQD	C24-C23	3.16	1.59	1.50
30	A	614	SQD	C24-C23	3.16	1.59	1.50
26	d	402	PHO	C4D-CHA	3.15	1.44	1.39
27	H	102	BCR	C30-C25	-3.15	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	C4B-NB	3.15	1.42	1.37
25	c	509	CLA	C1B-C2B	3.14	1.50	1.43
25	C	513	CLA	MG-NA	3.14	2.13	2.06
25	b	614	CLA	C1D-ND	3.13	1.42	1.37
25	c	507	CLA	C4B-NB	3.13	1.42	1.37
25	c	508	CLA	MG-NA	3.13	2.13	2.06
25	b	604	CLA	C1B-C2B	3.13	1.50	1.43
25	b	602	CLA	C4B-NB	3.13	1.42	1.37
25	b	603	CLA	C4B-NB	3.13	1.42	1.37
25	b	604	CLA	C4B-NB	3.12	1.42	1.37
27	A	610	BCR	C1-C6	-3.11	1.49	1.53
25	C	506	CLA	MG-NB	3.11	2.12	2.05
27	C	514	BCR	C30-C25	-3.11	1.49	1.53
25	B	615	CLA	C4B-NB	3.11	1.41	1.37
25	C	511	CLA	C1B-C2B	3.11	1.50	1.43
25	d	403	CLA	C1B-C2B	3.11	1.50	1.43
27	h	102	BCR	C30-C25	-3.10	1.49	1.53
25	C	507	CLA	C1D-ND	3.10	1.41	1.37
25	B	608	CLA	MG-NC	3.10	2.13	2.06
30	f	102	SQD	C24-C23	3.10	1.59	1.50
25	C	508	CLA	C4B-NB	3.10	1.41	1.37
25	c	513	CLA	C4B-NB	3.10	1.41	1.37
25	A	607	CLA	C1B-C2B	3.09	1.50	1.43
25	a	607	CLA	C4B-NB	3.09	1.41	1.37
25	A	609	CLA	C4B-NB	3.08	1.41	1.37
27	K	102	BCR	C1-C6	-3.08	1.49	1.53
25	C	507	CLA	C4B-NB	3.07	1.41	1.37
25	b	610	CLA	C1B-C2B	3.07	1.50	1.43
25	b	612	CLA	MG-NB	-3.06	1.99	2.05
25	c	506	CLA	MG-ND	-3.06	1.99	2.05
25	C	505	CLA	C4B-NB	3.06	1.41	1.37
27	c	514	BCR	C1-C6	-3.06	1.49	1.53
26	D	402	PHO	C4D-CHA	3.05	1.44	1.39
27	c	515	BCR	C30-C25	-3.05	1.49	1.53
30	B	621	SQD	O5-C1	3.05	1.49	1.41
32	c	516	DGD	O2G-C2G	-3.04	1.39	1.46
25	a	612	CLA	C1B-C2B	3.04	1.50	1.43
25	C	503	CLA	C1B-C2B	3.04	1.50	1.43
25	a	612	CLA	C1D-ND	3.04	1.41	1.37
25	c	508	CLA	C1B-C2B	3.04	1.50	1.43
27	C	515	BCR	C30-C25	-3.03	1.49	1.53
25	B	610	CLA	C1B-C2B	3.03	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	CHC-C1C	3.03	1.44	1.38
27	b	618	BCR	C1-C6	-3.02	1.49	1.53
25	b	610	CLA	C1D-ND	3.02	1.41	1.37
27	d	405	BCR	C30-C25	-3.01	1.49	1.53
25	B	607	CLA	C1D-ND	3.01	1.41	1.37
25	b	607	CLA	C4B-NB	3.01	1.41	1.37
25	B	601	CLA	C1B-C2B	3.01	1.50	1.43
30	f	102	SQD	O5-C1	3.01	1.49	1.41
31	d	409	LHG	P-O6	3.01	1.71	1.59
30	b	619	SQD	O47-C45	-3.01	1.39	1.46
31	L	101	LHG	O7-C5	-3.01	1.39	1.46
30	a	613	SQD	C24-C23	3.01	1.59	1.50
35	f	101	HEM	CAC-C3C	3.00	1.55	1.47
25	a	607	CLA	C1D-ND	3.00	1.41	1.37
25	C	512	CLA	MG-NA	3.00	2.13	2.06
27	D	405	BCR	C1-C6	-3.00	1.49	1.53
27	B	617	BCR	C30-C25	-3.00	1.49	1.53
25	c	507	CLA	MG-NA	2.99	2.13	2.06
25	c	512	CLA	C4B-NB	2.99	1.41	1.37
25	b	613	CLA	CHC-C1C	2.99	1.44	1.38
25	b	613	CLA	MG-NC	2.98	2.13	2.06
26	D	402	PHO	C4D-ND	-2.98	1.34	1.38
25	a	607	CLA	CHC-C1C	2.98	1.44	1.38
25	c	502	CLA	C4B-NB	2.98	1.41	1.37
25	a	612	CLA	C4B-NB	2.97	1.41	1.37
25	c	505	CLA	C4B-NB	2.97	1.41	1.37
25	A	609	CLA	MG-NB	-2.96	1.99	2.05
25	c	505	CLA	C1D-ND	2.96	1.41	1.37
25	c	506	CLA	MG-NC	2.96	2.13	2.06
30	F	102	SQD	O5-C1	2.96	1.49	1.41
32	A	617	DGD	C4D-C5D	2.96	1.59	1.53
25	B	608	CLA	MG-NB	-2.95	1.99	2.05
32	C	518	DGD	O2G-C2G	-2.95	1.39	1.46
27	D	405	BCR	C30-C25	-2.95	1.50	1.53
27	K	101	BCR	C30-C25	-2.95	1.50	1.53
25	c	509	CLA	C4B-NB	2.95	1.41	1.37
25	A	612	CLA	MG-NB	2.94	2.11	2.05
28	d	406	PL9	C6-C1	-2.93	1.43	1.48
25	c	511	CLA	C1B-C2B	2.93	1.50	1.43
27	K	102	BCR	C30-C25	-2.93	1.50	1.53
27	b	617	BCR	C1-C6	-2.93	1.50	1.53
28	D	406	PL9	C6-C1	-2.92	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	C1B-C2B	2.92	1.50	1.43
25	d	403	CLA	C4B-NB	2.92	1.41	1.37
25	B	610	CLA	MG-ND	2.92	2.11	2.05
25	C	511	CLA	MG-NC	2.92	2.13	2.06
25	B	611	CLA	MG-NA	2.92	2.13	2.06
25	C	513	CLA	C4B-NB	2.91	1.41	1.37
27	T	101	BCR	C30-C25	-2.91	1.50	1.53
25	C	511	CLA	C4B-NB	2.91	1.41	1.37
30	b	619	SQD	C24-C23	2.91	1.59	1.50
31	D	411	LHG	O7-C5	-2.91	1.39	1.46
30	B	621	SQD	C24-C23	2.90	1.59	1.50
25	C	505	CLA	C1D-ND	2.90	1.41	1.37
31	A	615	LHG	P-O6	2.90	1.70	1.59
27	C	514	BCR	C1-C6	-2.90	1.50	1.53
25	H	101	CLA	C1B-C2B	2.90	1.49	1.43
27	b	616	BCR	C1-C6	-2.90	1.50	1.53
25	c	503	CLA	C1B-C2B	2.89	1.49	1.43
25	D	403	CLA	C1B-C2B	2.88	1.49	1.43
25	c	508	CLA	C4B-NB	2.88	1.41	1.37
25	D	403	CLA	MG-NC	2.88	2.13	2.06
30	A	614	SQD	O47-C7	2.88	1.42	1.34
25	b	607	CLA	CHC-C1C	2.87	1.44	1.38
25	b	609	CLA	C4B-NB	2.87	1.41	1.37
25	B	612	CLA	C1B-C2B	2.87	1.49	1.43
25	B	609	CLA	MG-ND	-2.87	2.00	2.05
25	C	505	CLA	C1B-C2B	2.87	1.49	1.43
25	c	506	CLA	C1B-C2B	2.87	1.49	1.43
26	D	402	PHO	C3D-C4D	2.86	1.45	1.41
27	c	514	BCR	C30-C25	-2.86	1.50	1.53
25	b	609	CLA	C1B-C2B	2.86	1.49	1.43
25	C	507	CLA	C1B-C2B	2.86	1.49	1.43
25	C	503	CLA	C1D-ND	2.86	1.41	1.37
25	c	503	CLA	MG-NC	2.85	2.13	2.06
25	b	614	CLA	C1B-C2B	2.84	1.49	1.43
25	B	612	CLA	C4B-NB	2.84	1.41	1.37
27	k	101	BCR	C30-C25	-2.84	1.50	1.53
30	A	614	SQD	O5-C1	2.84	1.49	1.41
32	c	518	DGD	O2G-C2G	-2.84	1.39	1.46
25	b	615	CLA	C1B-C2B	2.83	1.49	1.43
29	c	521	LMG	C3-C2	2.83	1.59	1.52
25	B	614	CLA	C1B-C2B	2.83	1.49	1.43
25	c	513	CLA	C1B-C2B	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	609	CLA	C4B-NB	2.82	1.41	1.37
25	c	513	CLA	MG-NA	2.82	2.13	2.06
25	B	606	CLA	MG-ND	-2.82	2.00	2.05
25	A	612	CLA	CHC-C1C	2.82	1.44	1.38
35	F	101	HEM	CAC-C3C	2.82	1.54	1.47
25	c	511	CLA	C4B-NB	2.81	1.41	1.37
25	C	503	CLA	C4B-NB	2.81	1.41	1.37
25	b	605	CLA	C4B-NB	2.81	1.41	1.37
25	a	612	CLA	CHC-C1C	2.81	1.44	1.38
25	B	604	CLA	MG-NA	2.81	2.12	2.06
25	b	608	CLA	C4B-NB	2.81	1.41	1.37
26	D	402	PHO	CMC-C2C	-2.80	1.46	1.50
25	D	403	CLA	C1D-ND	2.80	1.41	1.37
32	A	617	DGD	C4D-C3D	2.80	1.59	1.52
25	c	504	CLA	C1B-C2B	2.80	1.49	1.43
25	c	508	CLA	CHC-C1C	2.80	1.44	1.38
27	B	617	BCR	C1-C6	-2.80	1.50	1.53
25	b	611	CLA	MG-NB	2.79	2.11	2.05
35	F	101	HEM	CAB-C3B	2.79	1.54	1.47
27	k	102	BCR	C1-C6	-2.79	1.50	1.53
25	B	604	CLA	CHC-C1C	2.79	1.44	1.38
25	C	506	CLA	C1B-C2B	2.78	1.49	1.43
25	c	510	CLA	C1B-C2B	2.77	1.49	1.43
25	b	605	CLA	C1B-C2B	2.77	1.49	1.43
32	c	516	DGD	C3G-C2G	2.77	1.59	1.50
30	a	613	SQD	O5-C1	2.77	1.49	1.41
25	C	501	CLA	CHC-C1C	2.76	1.44	1.38
25	b	603	CLA	C1B-C2B	2.76	1.49	1.43
25	c	502	CLA	C1B-C2B	2.76	1.49	1.43
25	C	506	CLA	C3B-C4B	2.76	1.50	1.42
25	B	608	CLA	C1B-C2B	2.76	1.49	1.43
30	A	616	SQD	C46-C45	2.75	1.56	1.50
25	b	607	CLA	C1D-ND	2.75	1.41	1.37
27	B	616	BCR	C30-C25	-2.74	1.50	1.53
27	a	610	BCR	C1-C6	-2.74	1.50	1.53
25	h	101	CLA	C1B-C2B	2.74	1.49	1.43
25	C	502	CLA	C4B-NB	2.73	1.41	1.37
25	C	508	CLA	C3B-C4B	2.73	1.50	1.42
25	C	503	CLA	MG-NC	2.73	2.12	2.06
25	C	512	CLA	C1B-C2B	2.73	1.49	1.43
25	C	502	CLA	C1B-C2B	2.73	1.49	1.43
25	B	603	CLA	C3B-C4B	2.73	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	C4E-C3E	2.72	1.59	1.52
25	c	505	CLA	C1B-C2B	2.72	1.49	1.43
25	D	404	CLA	C1B-C2B	2.72	1.49	1.43
25	A	606	CLA	C4B-NB	2.71	1.41	1.37
25	c	510	CLA	C4B-NB	2.71	1.41	1.37
28	d	406	PL9	C53-C6	-2.71	1.45	1.50
25	C	508	CLA	C1B-C2B	2.71	1.49	1.43
25	C	510	CLA	C1B-C2B	2.70	1.49	1.43
28	A	611	PL9	C7-C8	-2.70	1.46	1.50
25	c	503	CLA	C4B-NB	2.70	1.41	1.37
25	b	601	CLA	MG-ND	2.70	2.11	2.05
25	C	509	CLA	C4B-NB	2.70	1.41	1.37
25	b	610	CLA	MG-ND	2.70	2.11	2.05
31	d	407	LHG	C24-C23	2.70	1.58	1.50
25	B	605	CLA	C1B-C2B	2.70	1.49	1.43
25	B	614	CLA	CHC-C1C	2.69	1.43	1.38
25	b	601	CLA	C1B-C2B	2.68	1.49	1.43
26	D	402	PHO	C3B-C2B	-2.67	1.36	1.40
25	b	605	CLA	MG-NC	2.66	2.12	2.06
25	A	607	CLA	C4B-NB	2.66	1.41	1.37
29	D	407	LMG	C4-C5	2.66	1.58	1.53
25	C	511	CLA	C3B-C4B	2.66	1.50	1.42
25	b	608	CLA	MG-NC	2.66	2.12	2.06
25	C	504	CLA	MG-NA	2.66	2.12	2.06
25	B	604	CLA	C3B-C4B	2.66	1.50	1.42
25	B	606	CLA	C1B-C2B	2.65	1.49	1.43
35	f	101	HEM	CAB-C3B	2.65	1.54	1.47
29	d	411	LMG	O7-C8	-2.65	1.40	1.46
25	A	612	CLA	C1B-C2B	2.65	1.49	1.43
25	B	610	CLA	C4B-NB	2.64	1.41	1.37
25	B	605	CLA	C4B-NB	2.64	1.41	1.37
25	b	614	CLA	C4B-NB	2.64	1.41	1.37
25	d	404	CLA	C4B-NB	2.63	1.41	1.37
25	B	602	CLA	C1B-C2B	2.63	1.49	1.43
25	B	601	CLA	CHC-C1C	2.63	1.43	1.38
25	C	506	CLA	CHC-C1C	2.63	1.43	1.38
25	B	609	CLA	C3B-C4B	2.63	1.50	1.42
25	c	513	CLA	C3B-C4B	2.63	1.50	1.42
25	B	607	CLA	C1B-C2B	2.63	1.49	1.43
25	b	613	CLA	C1B-C2B	2.63	1.49	1.43
29	b	622	LMG	C9-C8	2.62	1.59	1.50
25	b	607	CLA	C3B-C4B	2.61	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	518	DGD	C4D-C5D	2.61	1.58	1.53
25	B	603	CLA	C1B-C2B	2.61	1.49	1.43
26	a	608	PHO	CAC-C3C	-2.61	1.47	1.51
25	b	604	CLA	CHC-C1C	2.60	1.43	1.38
32	h	103	DGD	O2G-C2G	-2.60	1.40	1.46
25	b	601	CLA	C4B-NB	2.60	1.41	1.37
32	C	516	DGD	C3E-C2E	2.60	1.59	1.52
25	c	512	CLA	MG-NA	2.60	2.12	2.06
25	C	508	CLA	CHC-C1C	2.60	1.43	1.38
25	d	404	CLA	C1D-ND	2.60	1.41	1.37
25	C	507	CLA	CHC-C1C	2.60	1.43	1.38
27	t	101	BCR	C30-C25	-2.60	1.50	1.53
27	B	618	BCR	C30-C25	-2.59	1.50	1.53
25	C	506	CLA	C4B-NB	2.59	1.41	1.37
25	b	611	CLA	MG-NA	2.58	2.12	2.06
25	c	511	CLA	CHC-C1C	2.58	1.43	1.38
25	a	607	CLA	C1B-C2B	2.58	1.49	1.43
25	C	512	CLA	C4B-NB	2.57	1.41	1.37
25	A	607	CLA	CHC-C1C	2.57	1.43	1.38
25	c	501	CLA	C1B-C2B	2.57	1.49	1.43
25	C	504	CLA	C3B-C4B	2.57	1.50	1.42
27	k	102	BCR	C30-C25	-2.57	1.50	1.53
25	d	404	CLA	C1B-C2B	2.56	1.49	1.43
30	A	614	SQD	O9-S	2.56	1.52	1.45
25	d	404	CLA	MG-NA	2.56	2.12	2.06
25	B	605	CLA	CHC-C1C	2.55	1.43	1.38
25	C	501	CLA	C3B-C4B	2.55	1.50	1.42
25	C	503	CLA	C3B-C4B	2.54	1.50	1.42
32	A	617	DGD	C1E-C2E	2.53	1.59	1.52
25	B	608	CLA	C4B-NB	2.53	1.41	1.37
25	H	101	CLA	CHC-C1C	2.53	1.43	1.38
25	b	614	CLA	C3B-C4B	2.53	1.50	1.42
25	c	504	CLA	C1D-ND	2.53	1.41	1.37
25	b	606	CLA	C3B-C4B	2.52	1.50	1.42
26	a	608	PHO	C3D-C4D	2.52	1.44	1.41
32	C	517	DGD	C4D-C3D	2.52	1.58	1.52
25	c	504	CLA	CHC-C1C	2.52	1.43	1.38
32	C	517	DGD	C1G-C2G	2.52	1.58	1.50
27	b	616	BCR	C30-C25	-2.52	1.50	1.53
27	T	101	BCR	C1-C6	-2.51	1.50	1.53
25	b	607	CLA	C1B-C2B	2.51	1.49	1.43
25	b	602	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	607	CLA	C3B-C4B	2.50	1.50	1.42
25	B	611	CLA	C1B-C2B	2.50	1.49	1.43
25	C	509	CLA	MG-ND	2.50	2.10	2.05
25	C	504	CLA	C4B-NB	2.50	1.41	1.37
25	C	509	CLA	C1B-C2B	2.50	1.49	1.43
25	c	508	CLA	C3B-C4B	2.50	1.50	1.42
25	B	612	CLA	MG-NC	2.49	2.12	2.06
25	C	513	CLA	MG-NC	2.49	2.12	2.06
27	h	102	BCR	C1-C6	-2.49	1.50	1.53
25	B	609	CLA	CHC-C1C	2.49	1.43	1.38
25	c	505	CLA	C3B-C4B	2.49	1.50	1.42
25	h	101	CLA	CHC-C1C	2.48	1.43	1.38
25	b	608	CLA	C1B-C2B	2.47	1.48	1.43
25	C	511	CLA	CHC-C1C	2.47	1.43	1.38
25	h	101	CLA	C3B-C4B	2.47	1.49	1.42
25	B	609	CLA	C1B-C2B	2.46	1.48	1.43
28	a	611	PL9	C53-C6	-2.46	1.45	1.50
25	a	606	CLA	CHC-C1C	2.46	1.43	1.38
26	A	608	PHO	CMD-C2D	-2.45	1.46	1.51
25	c	508	CLA	MG-ND	2.45	2.10	2.05
25	B	612	CLA	MG-NA	2.45	2.12	2.06
25	c	512	CLA	C3B-C4B	2.45	1.49	1.42
25	D	403	CLA	MG-NB	2.45	2.10	2.05
25	C	512	CLA	C3B-C4B	2.44	1.49	1.42
25	b	606	CLA	C1B-C2B	2.44	1.48	1.43
25	d	404	CLA	MG-ND	-2.44	2.01	2.05
25	a	606	CLA	C4B-NB	2.44	1.41	1.37
25	c	506	CLA	CHC-C1C	2.43	1.43	1.38
25	B	611	CLA	C4B-NB	2.43	1.41	1.37
25	B	611	CLA	CHC-C1C	2.43	1.43	1.38
25	a	606	CLA	MG-NC	2.42	2.12	2.06
25	B	604	CLA	MG-NB	2.42	2.10	2.05
25	b	611	CLA	C1B-C2B	2.42	1.48	1.43
25	b	611	CLA	CHC-C1C	2.42	1.43	1.38
25	B	611	CLA	C3B-C4B	2.42	1.49	1.42
25	b	612	CLA	C1B-C2B	2.42	1.48	1.43
25	B	615	CLA	C3B-C4B	2.41	1.49	1.42
25	B	607	CLA	C4B-NB	2.41	1.41	1.37
25	C	509	CLA	C3B-C4B	2.41	1.49	1.42
25	d	403	CLA	CHC-C1C	2.41	1.43	1.38
25	B	604	CLA	C4B-NB	2.41	1.41	1.37
25	B	607	CLA	MG-ND	-2.41	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	519	LMG	C4-C5	2.40	1.58	1.53
25	C	510	CLA	C3B-C4B	2.40	1.49	1.42
25	b	615	CLA	C4B-NB	2.40	1.41	1.37
25	c	511	CLA	MG-ND	-2.40	2.01	2.05
25	B	607	CLA	C3B-C4B	2.40	1.49	1.42
25	B	612	CLA	MG-ND	-2.39	2.01	2.05
25	A	612	CLA	C3B-C4B	2.39	1.49	1.42
32	H	103	DGD	O1G-C1G	-2.39	1.39	1.45
25	B	601	CLA	C3B-C4B	2.39	1.49	1.42
25	b	611	CLA	C3B-C4B	2.39	1.49	1.42
25	d	403	CLA	C3B-C4B	2.39	1.49	1.42
25	B	602	CLA	C4B-NB	2.39	1.41	1.37
32	C	517	DGD	C1E-C2E	2.38	1.59	1.52
25	C	501	CLA	C1B-C2B	2.38	1.48	1.43
25	A	607	CLA	C3B-C4B	2.38	1.49	1.42
25	b	605	CLA	C3B-C4B	2.38	1.49	1.42
25	b	613	CLA	C3B-C4B	2.38	1.49	1.42
25	D	404	CLA	C4B-NB	2.38	1.41	1.37
25	B	607	CLA	MG-NC	2.38	2.11	2.06
29	b	622	LMG	C4-C5	2.38	1.58	1.53
25	H	101	CLA	C3B-C4B	2.38	1.49	1.42
25	C	508	CLA	C1D-C2D	2.37	1.50	1.45
31	e	101	LHG	P-O6	2.37	1.68	1.59
25	C	503	CLA	CHC-C1C	2.37	1.43	1.38
26	A	608	PHO	CMB-C2B	-2.37	1.46	1.51
36	V	201	HEC	CMB-C2B	2.37	1.55	1.50
25	C	501	CLA	C1D-C2D	2.37	1.50	1.45
25	c	513	CLA	CHC-C1C	2.37	1.43	1.38
25	D	403	CLA	C3B-C4B	2.37	1.49	1.42
25	b	604	CLA	C3B-C4B	2.37	1.49	1.42
25	b	602	CLA	CMB-C2B	-2.36	1.45	1.50
26	d	402	PHO	CMC-C2C	-2.36	1.46	1.50
29	B	620	LMG	O8-C28	2.36	1.38	1.30
25	B	610	CLA	CHC-C1C	2.36	1.43	1.38
25	B	607	CLA	CMD-C2D	-2.35	1.45	1.50
25	B	611	CLA	CMC-C2C	-2.35	1.45	1.50
27	t	101	BCR	C1-C6	-2.35	1.50	1.53
25	c	501	CLA	CHC-C1C	2.35	1.43	1.38
25	c	510	CLA	CMB-C2B	-2.34	1.46	1.50
25	A	609	CLA	C1B-C2B	2.34	1.48	1.43
25	c	510	CLA	C3B-C4B	2.34	1.49	1.42
25	C	510	CLA	C4B-NB	2.34	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	CHC-C1C	2.33	1.43	1.38
30	f	102	SQD	O7-S	2.33	1.51	1.45
25	C	510	CLA	CHC-C1C	2.33	1.43	1.38
32	a	615	DGD	O1G-C1A	2.33	1.40	1.33
25	D	403	CLA	MG-NA	2.33	2.11	2.06
25	c	509	CLA	C3B-C4B	2.32	1.49	1.42
30	b	619	SQD	O7-S	2.32	1.51	1.45
30	b	619	SQD	O9-S	2.32	1.51	1.45
25	A	606	CLA	C3B-C4B	2.31	1.49	1.42
25	b	614	CLA	CHC-C1C	2.31	1.43	1.38
32	H	103	DGD	C4D-C5D	2.31	1.57	1.53
25	c	512	CLA	CHC-C1C	2.31	1.43	1.38
25	b	603	CLA	C3B-C4B	2.31	1.49	1.42
25	C	505	CLA	C3B-C4B	2.30	1.49	1.42
25	B	602	CLA	C3B-C4B	2.30	1.49	1.42
30	B	621	SQD	O9-S	2.30	1.51	1.45
30	f	102	SQD	O9-S	2.30	1.51	1.45
29	D	407	LMG	C7-C8	2.29	1.58	1.50
25	b	604	CLA	MG-NA	2.29	2.11	2.06
25	B	615	CLA	MG-NC	2.29	2.11	2.06
32	H	103	DGD	C4E-C5E	2.29	1.57	1.53
25	C	502	CLA	C3B-C4B	2.28	1.49	1.42
32	C	516	DGD	O1G-C1A	2.28	1.40	1.33
25	B	607	CLA	CHC-C1C	2.28	1.43	1.38
25	B	613	CLA	C1B-C2B	2.28	1.48	1.43
25	d	404	CLA	C3B-C4B	2.28	1.49	1.42
25	c	511	CLA	MG-NB	2.28	2.10	2.05
25	b	601	CLA	C3B-C4B	2.27	1.49	1.42
25	c	507	CLA	C3D-C4D	2.27	1.49	1.44
32	A	617	DGD	C3G-C2G	2.27	1.57	1.50
25	c	510	CLA	CHC-C1C	2.27	1.43	1.38
25	c	511	CLA	C3B-C4B	2.27	1.49	1.42
27	b	618	BCR	C30-C25	-2.27	1.50	1.53
32	H	103	DGD	C6D-C5D	2.27	1.58	1.51
25	a	607	CLA	MG-NC	2.27	2.11	2.06
25	b	604	CLA	CMD-C2D	-2.26	1.46	1.50
28	D	406	PL9	C11-C9	-2.26	1.46	1.51
36	v	201	HEC	CMD-C2D	2.26	1.55	1.50
25	C	513	CLA	C3B-C4B	2.26	1.49	1.42
32	A	617	DGD	C6E-C5E	2.25	1.59	1.51
32	H	103	DGD	C1E-C2E	2.25	1.59	1.52
35	F	101	HEM	CMD-C2D	2.25	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	516	DGD	C4D-C3D	2.25	1.58	1.52
31	A	615	LHG	O7-C5	-2.25	1.41	1.46
25	b	602	CLA	CMD-C2D	-2.24	1.46	1.50
35	f	101	HEM	CMC-C2C	2.24	1.55	1.50
25	c	502	CLA	CHC-C1C	2.24	1.43	1.38
30	a	613	SQD	O7-S	2.24	1.51	1.45
26	d	402	PHO	CMD-C2D	-2.24	1.47	1.51
36	v	201	HEC	CMA-C3A	2.24	1.55	1.50
30	a	614	SQD	C44-C45	2.24	1.56	1.51
25	B	609	CLA	MG-NC	-2.23	2.01	2.06
25	c	509	CLA	CHC-C1C	2.23	1.42	1.38
26	A	608	PHO	CAC-C3C	-2.23	1.47	1.51
25	B	612	CLA	CHC-C1C	2.22	1.42	1.38
25	B	608	CLA	C3B-C4B	2.22	1.49	1.42
25	C	509	CLA	CHC-C1C	2.22	1.42	1.38
36	V	201	HEC	CMC-C2C	2.22	1.55	1.50
25	c	504	CLA	C3B-C4B	2.22	1.49	1.42
25	C	512	CLA	CHC-C1C	2.22	1.42	1.38
25	C	512	CLA	CMD-C2D	-2.22	1.46	1.50
31	D	409	LHG	O3-C3	-2.22	1.36	1.44
25	B	610	CLA	C3B-C4B	2.22	1.49	1.42
25	C	503	CLA	C1D-C2D	2.21	1.49	1.45
26	A	608	PHO	CMC-C2C	-2.21	1.47	1.50
25	C	507	CLA	C3B-C4B	2.21	1.49	1.42
32	H	103	DGD	O5D-C1E	2.21	1.43	1.40
25	H	101	CLA	CMB-C2B	-2.21	1.46	1.50
32	h	103	DGD	C6D-C5D	2.21	1.58	1.51
25	D	403	CLA	CHC-C1C	2.21	1.42	1.38
25	b	601	CLA	CHC-C1C	2.21	1.42	1.38
25	C	509	CLA	CMD-C2D	-2.21	1.46	1.50
25	B	605	CLA	C3B-C4B	2.21	1.49	1.42
30	F	102	SQD	O9-S	2.21	1.51	1.45
30	B	621	SQD	C8-C7	2.21	1.57	1.50
25	b	612	CLA	CMD-C2D	-2.20	1.46	1.50
25	b	614	CLA	CMD-C2D	-2.20	1.46	1.50
32	c	518	DGD	C6D-C5D	2.20	1.58	1.51
28	D	406	PL9	C52-C5	-2.20	1.46	1.50
32	c	517	DGD	C3D-C2D	2.20	1.58	1.52
25	b	615	CLA	C3B-C4B	2.20	1.49	1.42
25	A	609	CLA	C1D-C2D	2.20	1.49	1.45
29	c	522	LMG	C4-C5	2.19	1.57	1.53
25	a	609	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	609	CLA	C3D-C4D	2.19	1.49	1.44
29	b	622	LMG	C4-C3	2.19	1.58	1.52
25	a	612	CLA	C3B-C4B	2.19	1.49	1.42
29	D	410	LMG	C7-C8	2.19	1.56	1.51
25	b	606	CLA	C4B-NB	2.19	1.40	1.37
25	B	603	CLA	CHC-C1C	2.19	1.42	1.38
25	c	505	CLA	CHC-C1C	2.19	1.42	1.38
25	B	615	CLA	CHC-C1C	2.19	1.42	1.38
25	a	606	CLA	C3B-C4B	2.19	1.49	1.42
25	b	611	CLA	MG-ND	-2.18	2.01	2.05
25	b	613	CLA	C1D-C2D	2.18	1.49	1.45
25	b	604	CLA	MG-NC	2.18	2.11	2.06
25	C	506	CLA	CMC-C2C	-2.18	1.46	1.50
25	c	506	CLA	C3B-C4B	2.18	1.49	1.42
32	H	103	DGD	O2D-C2D	-2.18	1.37	1.43
25	B	613	CLA	CHC-C1C	2.17	1.42	1.38
25	B	606	CLA	C3B-C4B	2.17	1.49	1.42
25	c	501	CLA	C4B-NB	2.17	1.40	1.37
31	A	615	LHG	O8-C23	2.17	1.39	1.33
25	b	609	CLA	C3B-C4B	2.17	1.49	1.42
25	a	609	CLA	C3B-C4B	2.17	1.49	1.42
26	a	608	PHO	C4D-ND	-2.17	1.35	1.38
29	C	519	LMG	O7-C8	-2.17	1.41	1.46
25	B	606	CLA	C4B-NB	2.17	1.40	1.37
25	c	501	CLA	C1D-C2D	2.17	1.49	1.45
31	d	407	LHG	P-O6	2.16	1.67	1.59
26	a	608	PHO	CMB-C2B	-2.16	1.47	1.51
25	B	611	CLA	MG-ND	-2.16	2.01	2.05
25	C	504	CLA	CHC-C1C	2.16	1.42	1.38
25	b	611	CLA	C4B-NB	2.16	1.40	1.37
32	A	617	DGD	C3E-C2E	2.16	1.57	1.52
25	b	605	CLA	CHC-C1C	2.16	1.42	1.38
25	b	613	CLA	CMC-C2C	-2.15	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.15	1.46	1.50
32	H	103	DGD	O2G-C2G	-2.15	1.41	1.46
25	C	504	CLA	CMD-C2D	-2.15	1.46	1.50
32	c	516	DGD	C4E-C3E	2.15	1.57	1.52
25	D	403	CLA	C4B-NB	2.15	1.40	1.37
32	h	103	DGD	C4D-C5D	2.14	1.57	1.53
32	c	517	DGD	C4D-C5D	2.14	1.57	1.53
29	B	620	LMG	O7-C10	2.14	1.37	1.30
27	a	610	BCR	C30-C25	-2.14	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	C4D-ND	-2.14	1.35	1.38
31	D	408	LHG	O8-C6	-2.13	1.40	1.45
25	D	404	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	615	CLA	CMC-C2C	-2.13	1.46	1.50
25	H	101	CLA	CMC-C2C	-2.13	1.46	1.50
25	c	502	CLA	CMC-C2C	-2.13	1.46	1.50
27	B	616	BCR	C33-C5	-2.12	1.47	1.50
30	B	621	SQD	O5-C5	2.12	1.49	1.44
32	h	103	DGD	C1E-C2E	2.12	1.58	1.52
32	C	516	DGD	C4D-C5D	2.12	1.57	1.53
32	C	517	DGD	O2G-C2G	-2.12	1.41	1.46
25	c	503	CLA	CHC-C1C	2.12	1.42	1.38
25	c	510	CLA	CMC-C2C	-2.12	1.46	1.50
25	B	608	CLA	C3D-C4D	2.12	1.49	1.44
30	F	102	SQD	O7-S	2.11	1.51	1.45
29	M	101	LMG	C1-C2	2.11	1.58	1.52
26	a	608	PHO	O2D-CGD	2.11	1.38	1.33
26	D	402	PHO	CMD-C2D	-2.11	1.47	1.51
31	D	409	LHG	O7-C7	2.11	1.40	1.34
25	b	608	CLA	C3B-C4B	2.10	1.48	1.42
35	f	101	HEM	C3B-C2B	-2.10	1.32	1.37
25	b	608	CLA	CHC-C1C	2.10	1.42	1.38
25	D	404	CLA	CMD-C2D	-2.10	1.46	1.50
25	c	503	CLA	C3B-C4B	2.10	1.48	1.42
25	b	602	CLA	CHC-C1C	2.10	1.42	1.38
25	c	507	CLA	CMC-C2C	-2.10	1.46	1.50
25	b	603	CLA	CHC-C1C	2.09	1.42	1.38
35	f	101	HEM	CMA-C3A	2.09	1.55	1.50
25	C	507	CLA	CMC-C2C	-2.09	1.46	1.50
25	b	608	CLA	CMB-C2B	-2.09	1.46	1.50
25	a	609	CLA	MG-ND	-2.09	2.01	2.05
32	c	517	DGD	C6E-C5E	2.09	1.58	1.51
35	F	101	HEM	CMA-C3A	2.09	1.55	1.50
25	b	613	CLA	MG-NA	2.08	2.11	2.06
25	c	501	CLA	CMC-C2C	-2.08	1.46	1.50
29	d	410	LMG	O7-C10	2.08	1.37	1.30
25	C	511	CLA	CMD-C2D	-2.08	1.46	1.50
35	f	101	HEM	FE-NC	2.08	2.02	1.95
25	b	606	CLA	C1D-C2D	2.08	1.49	1.45
29	M	101	LMG	C9-C8	2.08	1.57	1.50
25	c	502	CLA	C3B-C4B	2.08	1.48	1.42
25	B	601	CLA	C3C-C2C	2.07	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	612	CLA	MG-NC	2.07	2.11	2.06
25	C	510	CLA	CMD-C2D	-2.07	1.46	1.50
29	m	101	LMG	C4-C5	2.07	1.57	1.53
26	d	402	PHO	CMB-C2B	-2.07	1.47	1.51
25	c	510	CLA	CMD-C2D	-2.07	1.46	1.50
32	C	517	DGD	C4D-C5D	2.07	1.57	1.53
25	a	606	CLA	C3D-C4D	2.07	1.48	1.44
25	A	612	CLA	C4B-NB	2.06	1.40	1.37
25	C	513	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	602	CLA	C3B-C4B	2.06	1.48	1.42
30	b	619	SQD	C46-C45	2.06	1.57	1.50
25	a	612	CLA	C1D-C2D	2.06	1.49	1.45
27	A	610	BCR	C33-C5	-2.06	1.47	1.50
27	k	102	BCR	C38-C26	-2.05	1.47	1.50
32	C	518	DGD	O3G-C3G	-2.05	1.40	1.43
25	c	512	CLA	C1D-C2D	2.05	1.49	1.45
32	C	517	DGD	C6E-C5E	2.05	1.58	1.51
25	b	602	CLA	CMC-C2C	-2.05	1.46	1.50
30	a	613	SQD	O9-S	2.04	1.50	1.45
25	B	606	CLA	CHC-C1C	2.04	1.42	1.38
25	D	404	CLA	C3B-C4B	2.04	1.48	1.42
25	B	605	CLA	C3D-C4D	2.04	1.48	1.44
27	B	617	BCR	C33-C5	-2.04	1.47	1.50
25	C	510	CLA	C3D-C4D	2.04	1.48	1.44
25	A	606	CLA	CHC-C1C	2.04	1.42	1.38
29	c	519	LMG	C4-C5	2.03	1.57	1.53
25	b	615	CLA	CHC-C1C	2.03	1.42	1.38
25	c	512	CLA	CMD-C2D	-2.03	1.46	1.50
32	c	517	DGD	O3E-C3E	-2.03	1.37	1.43
25	C	512	CLA	CMB-C2B	-2.03	1.46	1.50
25	C	504	CLA	C1B-C2B	2.03	1.47	1.43
26	D	402	PHO	CMB-C2B	-2.02	1.47	1.51
27	k	101	BCR	C33-C5	-2.02	1.47	1.50
25	a	609	CLA	CMD-C2D	-2.02	1.46	1.50
27	c	515	BCR	C33-C5	-2.02	1.47	1.50
25	b	610	CLA	C4B-NB	2.02	1.40	1.37
25	h	101	CLA	CMC-C2C	-2.02	1.46	1.50
25	C	513	CLA	MG-ND	2.02	2.09	2.05
25	c	507	CLA	CHC-C1C	2.01	1.42	1.38
25	B	612	CLA	CMD-C2D	-2.01	1.46	1.50
25	d	404	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	513	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	CHC-C1C	2.01	1.42	1.38
30	A	614	SQD	C8-C7	2.01	1.56	1.50
25	c	501	CLA	CMB-C2B	-2.01	1.46	1.50
26	d	402	PHO	C4D-ND	-2.01	1.35	1.38
30	a	614	SQD	C25-C24	2.01	1.59	1.52
25	b	612	CLA	CHC-C1C	2.01	1.42	1.38
30	f	102	SQD	O5-C5	2.01	1.49	1.44
25	B	602	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	611	CLA	CMC-C2C	-2.01	1.46	1.50
25	b	601	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.01	1.46	1.50
25	B	605	CLA	CMD-C2D	-2.00	1.46	1.50
25	H	101	CLA	C3D-C4D	2.00	1.48	1.44

All (1082) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	603	CLA	C4A-NA-C1A	9.62	111.07	106.68
25	B	615	CLA	C4A-NA-C1A	9.03	110.80	106.68
36	V	201	HEC	CBB-CAB-C3B	-8.89	109.66	127.43
25	C	511	CLA	C4A-NA-C1A	8.70	110.65	106.68
25	b	603	CLA	C4A-NA-C1A	8.54	110.58	106.68
25	B	608	CLA	C4A-NA-C1A	8.47	110.54	106.68
36	v	201	HEC	CBB-CAB-C3B	-8.25	110.94	127.43
25	H	101	CLA	C4A-NA-C1A	8.21	110.43	106.68
25	C	503	CLA	C4A-NA-C1A	8.08	110.36	106.68
25	B	605	CLA	C4A-NA-C1A	8.07	110.36	106.68
25	c	511	CLA	C4A-NA-C1A	8.03	110.34	106.68
25	c	509	CLA	C4A-NA-C1A	7.93	110.30	106.68
25	C	513	CLA	C4A-NA-C1A	7.88	110.28	106.68
25	c	507	CLA	C4A-NA-C1A	7.73	110.20	106.68
25	b	614	CLA	C4A-NA-C1A	7.69	110.19	106.68
25	C	501	CLA	C4A-NA-C1A	7.65	110.17	106.68
25	C	510	CLA	C4A-NA-C1A	7.61	110.15	106.68
25	B	606	CLA	C4A-NA-C1A	7.58	110.14	106.68
25	c	503	CLA	C4A-NA-C1A	7.58	110.14	106.68
25	B	614	CLA	C4A-NA-C1A	7.56	110.13	106.68
30	a	613	SQD	O6-C1-C2	7.44	119.57	108.27
25	a	606	CLA	C4A-NA-C1A	7.40	110.05	106.68
25	C	507	CLA	C4A-NA-C1A	7.24	109.98	106.68
36	v	201	HEC	CBC-CAC-C3C	-7.20	113.04	127.43
25	c	510	CLA	C4A-NA-C1A	6.98	109.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	501	CLA	C4A-NA-C1A	6.88	109.82	106.68
25	c	504	CLA	C4A-NA-C1A	6.85	109.81	106.68
25	b	604	CLA	C4A-NA-C1A	6.84	109.80	106.68
25	c	506	CLA	C4A-NA-C1A	6.70	109.73	106.68
26	D	402	PHO	C4D-CHA-CBD	-6.68	105.25	108.45
25	c	508	CLA	C4A-NA-C1A	6.67	109.72	106.68
26	a	608	PHO	C4D-CHA-CBD	-6.63	105.27	108.45
25	C	508	CLA	C4A-NA-C1A	6.55	109.67	106.68
25	A	612	CLA	C4A-NA-C1A	6.52	109.66	106.68
25	B	610	CLA	C4A-NA-C1A	6.47	109.63	106.68
25	a	612	CLA	C4A-NA-C1A	6.44	109.62	106.68
25	h	101	CLA	C4A-NA-C1A	6.43	109.61	106.68
25	C	509	CLA	C4A-NA-C1A	6.41	109.61	106.68
30	A	614	SQD	O6-C1-C2	6.39	117.98	108.27
25	b	605	CLA	C4A-NA-C1A	6.30	109.55	106.68
28	a	611	PL9	C7-C3-C4	6.20	122.01	116.91
25	B	604	CLA	C4A-NA-C1A	6.12	109.47	106.68
25	b	615	CLA	C4A-NA-C1A	6.11	109.47	106.68
30	a	613	SQD	C1-O5-C5	-6.10	101.80	113.72
25	C	506	CLA	C4A-NA-C1A	6.07	109.45	106.68
25	d	403	CLA	C4A-NA-C1A	6.06	109.44	106.68
25	c	512	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	B	612	CLA	C4A-NA-C1A	5.92	109.38	106.68
25	c	502	CLA	C4A-NA-C1A	5.89	109.37	106.68
25	b	610	CLA	C4A-NA-C1A	5.89	109.37	106.68
25	B	611	CLA	C4A-NA-C1A	5.83	109.34	106.68
25	a	609	CLA	C4A-NA-C1A	5.78	109.32	106.68
25	b	612	CLA	C4A-NA-C1A	5.77	109.31	106.68
25	C	505	CLA	C4A-NA-C1A	5.73	109.29	106.68
25	b	609	CLA	C4A-NA-C1A	5.72	109.29	106.68
25	a	607	CLA	C4A-NA-C1A	5.69	109.28	106.68
25	b	611	CLA	C4A-NA-C1A	5.67	109.27	106.68
25	b	608	CLA	C4A-NA-C1A	5.64	109.25	106.68
25	b	602	CLA	C4A-NA-C1A	5.64	109.25	106.68
25	b	601	CLA	C4A-NA-C1A	5.63	109.25	106.68
25	c	505	CLA	C4A-NA-C1A	5.61	109.24	106.68
25	C	502	CLA	C4A-NA-C1A	5.56	109.22	106.68
25	B	602	CLA	C4A-NA-C1A	5.54	109.21	106.68
25	B	607	CLA	C4A-NA-C1A	5.50	109.19	106.68
36	V	201	HEC	CBC-CAC-C3C	-5.47	116.50	127.43
25	C	512	CLA	C4A-NA-C1A	5.43	109.16	106.68
25	A	606	CLA	C4A-NA-C1A	5.32	109.11	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	C4A-NA-C1A	5.32	109.11	106.68
25	B	613	CLA	C4A-NA-C1A	5.25	109.08	106.68
25	C	504	CLA	C4A-NA-C1A	5.08	109.00	106.68
25	D	403	CLA	C4A-NA-C1A	5.05	108.98	106.68
25	b	613	CLA	C4A-NA-C1A	5.02	108.97	106.68
25	B	611	CLA	C1-C2-C3	-5.00	118.01	126.20
30	F	102	SQD	O6-C1-C2	4.98	115.84	108.27
30	A	614	SQD	C1-C2-C3	-4.98	99.53	110.01
30	f	102	SQD	O6-C1-C2	4.88	115.69	108.27
25	B	601	CLA	C4A-NA-C1A	4.87	108.90	106.68
30	a	614	SQD	O47-C7-C8	4.80	121.87	111.48
32	a	615	DGD	O3G-C3G-C2G	-4.79	99.47	111.77
30	B	621	SQD	O47-C7-C8	4.74	121.72	111.48
25	D	404	CLA	C4A-NA-C1A	4.70	108.82	106.68
28	d	406	PL9	C7-C3-C4	4.69	120.77	116.91
30	F	102	SQD	C1-O5-C5	-4.67	104.60	113.72
28	a	611	PL9	C7-C3-C2	-4.63	117.93	123.39
25	c	501	CLA	O2D-CGD-O1D	-4.63	114.84	123.85
26	d	402	PHO	C1-C2-C3	-4.61	118.64	126.20
25	B	612	CLA	C1-C2-C3	-4.59	118.68	126.20
28	D	406	PL9	C7-C3-C4	4.49	120.61	116.91
28	A	611	PL9	C7-C3-C4	4.43	120.56	116.91
25	b	602	CLA	O2D-CGD-O1D	-4.40	115.29	123.85
26	d	402	PHO	C4D-CHA-CBD	-4.40	106.35	108.45
31	d	408	LHG	O4-P-O5	4.40	132.90	112.44
30	f	102	SQD	O7-S-C6	4.39	113.31	106.76
31	e	101	LHG	O4-P-O5	4.36	132.71	112.44
32	H	103	DGD	O3G-C3G-C2G	-4.33	100.30	110.82
30	B	621	SQD	O6-C1-C2	4.32	114.84	108.27
31	b	623	LHG	O4-P-O5	4.31	132.50	112.44
30	A	614	SQD	C1-O5-C5	-4.29	105.34	113.72
30	f	102	SQD	O9-S-O7	-4.27	99.93	113.82
31	L	101	LHG	O4-P-O5	4.24	132.19	112.44
30	f	102	SQD	C1-O5-C5	-4.23	105.47	113.72
32	C	518	DGD	O3G-C3G-C2G	-4.22	100.56	110.82
31	d	407	LHG	O4-P-O5	4.20	132.00	112.44
25	b	615	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
31	A	615	LHG	O4-P-O5	4.20	131.97	112.44
30	A	614	SQD	O9-S-O7	-4.20	100.17	113.82
31	D	411	LHG	O4-P-O5	4.19	131.94	112.44
30	A	614	SQD	O47-C7-C8	4.18	120.53	111.48
25	A	609	CLA	C4A-NA-C1A	4.18	108.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	409	LHG	O4-P-O5	4.15	131.74	112.44
25	b	607	CLA	C3B-C4B-NB	-4.10	106.87	110.53
25	C	508	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
32	c	516	DGD	O3G-C3G-C2G	-4.02	101.03	110.82
28	A	611	PL9	C7-C3-C2	-4.01	118.66	123.39
27	b	616	BCR	C2-C1-C6	4.01	116.26	110.44
31	d	409	LHG	O4-P-O5	3.99	131.00	112.44
31	D	408	LHG	O4-P-O5	3.99	130.99	112.44
25	d	404	CLA	C4A-NA-C1A	3.98	108.49	106.68
30	a	613	SQD	O47-C7-C8	3.95	120.03	111.48
25	b	614	CLA	C3B-C4B-NB	-3.95	107.00	110.53
25	b	609	CLA	O2D-CGD-O1D	-3.94	116.17	123.85
34	D	401	BCT	O2-C-O1	3.92	129.72	119.68
32	c	518	DGD	O3G-C3G-C2G	-3.92	101.28	110.82
25	b	613	CLA	C1-C2-C3	-3.91	119.79	126.20
25	c	509	CLA	O2A-CGA-O1A	-3.89	113.90	123.63
28	d	406	PL9	C7-C8-C9	-3.89	120.14	126.83
27	B	616	BCR	C2-C1-C6	3.87	116.06	110.44
25	A	609	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
26	A	608	PHO	C1-C2-C3	-3.84	119.90	126.20
25	b	601	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
25	c	512	CLA	C1-C2-C3	-3.84	119.91	126.20
25	b	611	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
25	b	605	CLA	O2D-CGD-O1D	-3.82	116.42	123.85
34	d	401	BCT	O2-C-O1	3.78	129.36	119.68
30	B	621	SQD	C1-O5-C5	-3.77	106.35	113.72
25	b	604	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
25	A	612	CLA	C3B-C4B-NB	-3.76	107.17	110.53
25	B	605	CLA	C3B-C4B-NB	-3.74	107.19	110.53
26	d	402	PHO	C2B-C1B-NB	-3.72	106.74	109.43
25	C	501	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
25	C	508	CLA	C3B-C4B-NB	-3.70	107.22	110.53
25	b	607	CLA	C4A-NA-C1A	3.68	108.36	106.68
28	d	406	PL9	C7-C3-C2	-3.68	119.05	123.39
25	B	602	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
30	a	614	SQD	O48-C23-C24	3.66	123.00	111.83
30	A	614	SQD	O9-S-C6	3.66	112.21	106.76
26	a	608	PHO	CBC-CAC-C3C	-3.65	107.64	112.87
30	b	619	SQD	O48-C23-C24	3.65	122.96	111.83
25	B	602	CLA	C3B-C4B-NB	-3.63	107.29	110.53
25	b	603	CLA	C3B-C4B-NB	-3.62	107.30	110.53
25	B	609	CLA	C4A-NA-C1A	3.62	108.33	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	606	CLA	C4A-NA-C1A	3.62	108.33	106.68
25	B	609	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
30	b	619	SQD	O9-S-O7	-3.60	102.12	113.82
25	B	605	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
32	C	516	DGD	O3G-C3G-C2G	-3.58	102.11	110.82
25	c	512	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
25	a	609	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
25	c	502	CLA	C1-C2-C3	-3.57	120.35	126.20
30	b	619	SQD	O7-S-C6	3.56	112.07	106.76
33	x	101	STE	C3-C2-C1	-3.54	105.26	114.51
25	b	601	CLA	CHB-C4A-NA	3.54	129.51	124.40
25	B	603	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	B	613	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	B	604	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
25	B	613	CLA	C1-C2-C3	-3.51	120.45	126.20
25	a	609	CLA	O2D-CGD-CBD	3.51	117.36	111.23
30	b	619	SQD	O47-C7-C8	3.51	119.07	111.48
25	B	611	CLA	C3B-C4B-NB	-3.51	107.40	110.53
25	b	604	CLA	C3B-C4B-NB	-3.51	107.40	110.53
25	b	605	CLA	O2D-CGD-CBD	3.50	117.35	111.23
25	b	609	CLA	O1D-CGD-CBD	3.49	131.40	124.52
36	V	201	HEC	C4D-ND-C1D	3.48	111.49	105.82
25	b	611	CLA	C3B-C4B-NB	-3.47	107.43	110.53
25	b	610	CLA	O2D-CGD-CBD	3.46	117.28	111.23
30	A	614	SQD	O5-C1-C2	-3.46	103.25	110.37
25	C	501	CLA	C3B-C4B-NB	-3.45	107.45	110.53
26	a	608	PHO	C2B-C1B-NB	-3.44	106.94	109.43
25	B	610	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
25	h	101	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
25	d	403	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
32	h	103	DGD	O6E-C5E-C4E	3.41	115.85	109.70
35	F	101	HEM	CBD-CAD-C3D	-3.41	103.10	112.53
30	a	613	SQD	O9-S-O7	-3.40	102.76	113.82
25	c	508	CLA	C3B-C4B-NB	-3.40	107.49	110.53
25	a	607	CLA	C3B-C4B-NB	-3.39	107.50	110.53
25	c	505	CLA	C3B-C4B-NB	-3.39	107.50	110.53
28	D	406	PL9	C37-C38-C39	-3.39	119.87	127.62
25	B	614	CLA	C3B-C4B-NB	-3.38	107.51	110.53
30	B	621	SQD	C3-C4-C5	3.38	116.35	110.23
30	B	621	SQD	O7-S-C6	3.37	111.79	106.76
30	B	621	SQD	O9-S-O7	-3.36	102.88	113.82
25	B	613	CLA	O2D-CGD-O1D	-3.36	117.31	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C3B-C4B-NB	-3.36	107.53	110.53
26	A	608	PHO	O1D-CGD-CBD	3.35	129.81	124.72
28	A	611	PL9	O1-C4-C3	-3.35	117.19	120.73
25	B	611	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
26	D	402	PHO	CMA-C3A-C4A	-3.33	107.43	114.61
30	A	616	SQD	O47-C7-C8	3.33	118.69	111.48
25	C	503	CLA	C3B-C4B-NB	-3.33	107.56	110.53
25	b	609	CLA	C1-C2-C3	-3.32	120.75	126.20
35	f	101	HEM	CBD-CAD-C3D	-3.32	103.35	112.53
30	A	614	SQD	O7-S-C6	3.31	111.70	106.76
25	B	609	CLA	CHB-C4A-NA	3.31	129.18	124.40
27	B	618	BCR	C2-C1-C6	3.30	115.24	110.44
25	C	505	CLA	C3B-C4B-NB	-3.30	107.59	110.53
25	C	510	CLA	C3B-C4B-NB	-3.29	107.59	110.53
25	c	508	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	c	510	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	c	502	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	D	403	CLA	C3B-C4B-NB	-3.29	107.59	110.53
25	B	607	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
26	d	402	PHO	O1D-CGD-CBD	3.28	129.69	124.72
25	C	506	CLA	C3B-C4B-NB	-3.28	107.61	110.53
25	B	601	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
28	d	406	PL9	C40-C39-C41	3.27	120.90	115.23
30	F	102	SQD	O8-S-C6	3.27	112.28	105.97
28	D	406	PL9	C7-C3-C2	-3.27	119.54	123.39
31	D	411	LHG	O8-C23-C24	3.26	121.77	111.83
30	B	621	SQD	O5-C5-C4	3.25	115.55	109.70
30	B	621	SQD	O48-C23-C24	3.24	121.72	111.83
25	D	403	CLA	O2A-CGA-O1A	-3.24	115.53	123.63
25	b	610	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
26	d	402	PHO	CMB-C2B-C3B	3.23	131.13	124.68
32	c	517	DGD	O6D-C1D-O3G	-3.22	102.44	110.04
30	a	613	SQD	O48-C23-C24	3.20	121.61	111.83
33	m	102	STE	C3-C2-C1	-3.20	106.15	114.51
25	c	512	CLA	CHB-C4A-NA	3.20	129.01	124.40
25	C	512	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
25	H	101	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
25	C	512	CLA	CHB-C4A-NA	3.18	128.99	124.40
27	C	514	BCR	C24-C23-C22	-3.18	121.53	126.23
25	B	607	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	h	101	CLA	C3B-C4B-NB	-3.18	107.69	110.53
30	F	102	SQD	O9-S-C6	3.17	111.49	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	v	201	HEC	C4D-ND-C1D	3.17	110.99	105.82
32	c	518	DGD	O6D-C1D-O3G	-3.17	102.55	110.04
27	A	610	BCR	C27-C26-C25	3.17	126.99	122.70
31	d	407	LHG	O8-C23-C24	3.17	121.49	111.83
29	b	622	LMG	C1-O6-C5	-3.16	107.55	113.72
36	V	201	HEC	CBD-CAD-C3D	-3.15	103.81	112.53
25	B	615	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
25	H	101	CLA	CAA-C2A-C3A	-3.15	104.50	113.00
25	C	507	CLA	C3B-C4B-NB	-3.14	107.73	110.53
25	c	505	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
25	b	603	CLA	C1-C2-C3	-3.13	121.07	126.20
25	C	513	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
25	c	513	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
25	c	501	CLA	O2D-CGD-CBD	3.12	116.68	111.23
25	B	609	CLA	C3B-C4B-NB	-3.12	107.75	110.53
25	B	610	CLA	O2D-CGD-CBD	3.12	116.68	111.23
25	b	605	CLA	C3B-C4B-NB	-3.12	107.75	110.53
26	A	608	PHO	CMB-C2B-C3B	3.11	130.91	124.68
25	c	503	CLA	C3B-C4B-NB	-3.11	107.75	110.53
30	b	619	SQD	C4-C3-C2	3.11	116.28	110.83
28	D	406	PL9	C40-C39-C41	3.10	120.61	115.23
25	H	101	CLA	C3B-C4B-NB	-3.10	107.77	110.53
26	A	608	PHO	O2D-CGD-O1D	-3.10	117.82	123.85
25	B	601	CLA	CHB-C4A-NA	3.09	128.87	124.40
27	d	405	BCR	C2-C1-C6	3.09	114.93	110.44
32	c	516	DGD	O3E-C3E-C2E	-3.09	103.08	110.38
33	M	102	STE	C3-C2-C1	-3.09	106.44	114.51
27	D	405	BCR	C2-C1-C6	3.09	114.92	110.44
26	A	608	PHO	C2B-C1B-NB	-3.09	107.20	109.43
29	c	522	LMG	O6-C1-O1	-3.09	102.75	110.04
25	a	606	CLA	CHB-C4A-NA	3.08	128.85	124.40
25	a	607	CLA	CHB-C4A-NA	3.08	128.85	124.40
28	A	611	PL9	C22-C23-C24	-3.08	120.57	127.62
30	a	613	SQD	C1-C2-C3	-3.08	103.53	110.01
26	A	608	PHO	C4D-CHA-CBD	-3.06	106.98	108.45
25	c	507	CLA	CHB-C4A-NA	3.06	128.82	124.40
25	C	512	CLA	C1-C2-C3	-3.06	121.18	126.20
25	b	608	CLA	C3B-C4B-NB	-3.06	107.80	110.53
25	B	607	CLA	O2D-CGD-CBD	3.05	116.57	111.23
25	b	602	CLA	C3B-C4B-NB	-3.04	107.81	110.53
25	b	607	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
25	B	609	CLA	C1-C2-C3	-3.04	121.21	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	612	CLA	C1-C2-C3	-3.04	121.22	126.20
25	A	607	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
25	D	404	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	b	606	CLA	C3B-C4B-NB	-3.03	107.83	110.53
32	C	518	DGD	O6D-C1D-O3G	-3.02	102.90	110.04
25	c	504	CLA	CHB-C4A-NA	3.02	128.76	124.40
27	K	101	BCR	C27-C26-C25	3.02	126.79	122.70
25	B	611	CLA	O2A-CGA-O1A	-3.02	116.08	123.63
31	d	409	LHG	O8-C23-C24	3.02	121.03	111.83
26	a	608	PHO	CMB-C2B-C3B	3.02	130.71	124.68
28	a	611	PL9	C40-C39-C41	3.01	120.46	115.23
30	F	102	SQD	O9-S-O7	-3.00	104.06	113.82
32	A	617	DGD	C3G-C2G-C1G	-3.00	104.79	111.78
25	B	603	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
25	c	507	CLA	C3B-C4B-NB	-2.98	107.87	110.53
25	C	507	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
31	e	101	LHG	O8-C23-C24	2.98	120.92	111.83
28	d	406	PL9	C22-C23-C24	-2.98	120.81	127.62
25	c	510	CLA	CMB-C2B-C1B	-2.97	120.89	125.42
27	c	514	BCR	C27-C26-C25	2.97	126.72	122.70
25	a	606	CLA	C3B-C4B-NB	-2.96	107.88	110.53
25	b	613	CLA	C3B-C4B-NB	-2.96	107.89	110.53
25	A	607	CLA	C3B-C4B-NB	-2.96	107.89	110.53
25	a	609	CLA	CHB-C4A-NA	2.96	128.67	124.40
25	C	501	CLA	O2D-CGD-CBD	2.96	116.40	111.23
27	a	610	BCR	C27-C26-C25	2.95	126.69	122.70
33	m	102	STE	O2-C1-C2	2.94	123.30	114.00
25	b	613	CLA	O2A-CGA-O1A	-2.94	116.27	123.63
33	C	520	STE	C3-C2-C1	-2.94	106.84	114.51
30	f	102	SQD	C1-C2-C3	-2.92	103.86	110.01
29	c	519	LMG	O6-C1-O1	-2.92	103.15	110.04
25	B	609	CLA	O2A-CGA-O1A	-2.92	116.33	123.63
25	b	606	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
25	a	607	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
28	A	611	PL9	O2-C1-C6	2.91	125.11	120.48
25	C	504	CLA	C3B-C4B-NB	-2.91	107.93	110.53
30	F	102	SQD	O48-C23-C24	2.90	120.69	111.83
25	B	601	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	C	502	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
31	d	407	LHG	O8-C23-O10	-2.90	116.37	123.63
32	c	517	DGD	O3G-C3G-C2G	-2.90	103.77	110.82
32	c	516	DGD	CDB-CCB-CBB	-2.90	99.73	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	406	PL9	C37-C38-C39	-2.89	121.01	127.62
27	K	102	BCR	C27-C26-C25	2.88	126.60	122.70
31	d	407	LHG	C11-C10-C9	-2.87	99.84	114.37
27	b	616	BCR	C11-C10-C9	-2.87	123.25	127.28
25	C	511	CLA	C3B-C4B-NB	-2.87	107.97	110.53
27	C	515	BCR	C2-C1-C6	2.87	114.61	110.44
25	b	606	CLA	CMB-C2B-C1B	-2.87	121.05	125.42
27	d	405	BCR	C27-C26-C25	2.86	126.58	122.70
26	d	402	PHO	O2D-CGD-O1D	-2.86	118.28	123.85
25	C	512	CLA	O2D-CGD-CBD	2.86	116.23	111.23
27	h	102	BCR	C27-C26-C25	2.86	126.56	122.70
25	a	612	CLA	O2D-CGD-CBD	2.86	116.22	111.23
32	h	103	DGD	C1E-O6E-C5E	2.85	119.28	113.72
25	A	607	CLA	C4A-NA-C1A	2.85	107.98	106.68
31	D	408	LHG	O8-C23-C24	2.85	120.51	111.83
25	b	607	CLA	CHB-C4A-NA	2.84	128.50	124.40
27	T	101	BCR	C33-C5-C6	-2.84	121.38	124.48
25	C	509	CLA	C3B-C4B-NB	-2.84	107.99	110.53
32	a	615	DGD	CDB-CCB-CBB	-2.84	100.01	114.37
32	h	103	DGD	C4E-C3E-C2E	-2.84	105.84	110.83
27	C	514	BCR	C11-C10-C9	-2.84	123.29	127.28
27	c	515	BCR	C11-C10-C9	-2.84	123.30	127.28
25	C	509	CLA	CHB-C4A-NA	2.84	128.49	124.40
25	a	612	CLA	C3B-C4B-NB	-2.84	108.00	110.53
25	b	602	CLA	O2D-CGD-CBD	2.84	116.19	111.23
27	B	617	BCR	C15-C14-C13	-2.83	123.30	127.28
28	A	611	PL9	C27-C28-C29	-2.83	121.15	127.62
28	d	406	PL9	C36-C34-C33	-2.83	114.82	121.17
27	T	101	BCR	C7-C8-C9	-2.82	122.06	126.23
25	c	512	CLA	C3B-C4B-NB	-2.82	108.01	110.53
25	B	606	CLA	C3B-C4B-NB	-2.82	108.01	110.53
27	D	405	BCR	C27-C26-C25	2.81	126.50	122.70
25	b	609	CLA	CAA-CBA-CGA	-2.81	105.22	113.21
27	k	102	BCR	C27-C26-C25	2.81	126.50	122.70
25	c	508	CLA	O2D-CGD-CBD	2.81	116.14	111.23
25	A	606	CLA	CHB-C4A-NA	2.80	128.44	124.40
30	F	102	SQD	C44-O6-C1	-2.80	108.90	113.68
25	a	606	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
25	B	612	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	A	607	CLA	CAC-C3C-C4C	2.79	128.42	124.79
25	c	504	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	C	517	DGD	CDB-CCB-CBB	-2.79	100.28	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	411	LMG	O6-C1-O1	-2.79	103.46	110.04
32	c	517	DGD	CDB-CCB-CBB	-2.78	100.30	114.37
25	h	101	CLA	CHB-C4A-NA	2.78	128.42	124.40
32	c	518	DGD	CDB-CCB-CBB	-2.78	100.30	114.37
25	c	508	CLA	C1-C2-C3	-2.78	121.64	126.20
25	B	614	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
30	F	102	SQD	C1-C2-C3	-2.77	104.19	110.01
25	h	101	CLA	O2D-CGD-CBD	2.76	116.06	111.23
32	h	103	DGD	O3G-C3G-C2G	-2.76	104.10	110.82
25	B	610	CLA	CHB-C4A-NA	2.76	128.38	124.40
25	C	504	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
27	c	515	BCR	C7-C8-C9	-2.76	122.16	126.23
28	A	611	PL9	C20-C19-C21	2.76	120.01	115.23
25	b	604	CLA	C1-C2-C3	-2.75	121.69	126.20
30	f	102	SQD	O9-S-C6	2.75	110.86	106.76
35	f	101	HEM	C3B-C2B-C1B	2.75	108.47	106.41
25	A	609	CLA	O2D-CGD-CBD	2.75	116.03	111.23
25	C	505	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
25	A	609	CLA	C3B-C4B-NB	-2.74	108.08	110.53
25	B	610	CLA	C3B-C4B-NB	-2.74	108.08	110.53
28	a	611	PL9	C37-C38-C39	-2.74	121.34	127.62
25	C	506	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
28	a	611	PL9	C22-C23-C24	-2.73	121.37	127.62
26	D	402	PHO	CMB-C2B-C3B	2.73	130.14	124.68
25	A	609	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
28	D	406	PL9	C22-C23-C24	-2.73	121.38	127.62
25	b	606	CLA	O1D-CGD-CBD	2.73	129.90	124.52
25	C	504	CLA	CHB-C4A-NA	2.72	128.33	124.40
25	a	607	CLA	O2D-CGD-CBD	2.72	115.98	111.23
25	c	511	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
29	m	101	LMG	O7-C10-O9	-2.72	117.35	123.70
25	c	504	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
32	h	103	DGD	C1D-C2D-C3D	-2.71	104.30	110.01
29	m	101	LMG	O1-C7-C8	-2.71	104.23	110.82
25	b	604	CLA	O1D-CGD-CBD	2.71	129.86	124.52
25	B	608	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
25	C	502	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
32	C	517	DGD	O6D-C1D-O3G	-2.70	103.67	110.04
25	A	609	CLA	CHB-C4A-NA	2.69	128.29	124.40
29	A	613	LMG	O7-C10-O9	-2.69	117.41	123.70
25	b	615	CLA	CAA-CBA-CGA	-2.69	105.56	113.21
33	d	413	STE	C3-C2-C1	-2.69	107.48	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	O2A-CGA-O1A	-2.69	116.91	123.63
25	B	611	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	b	609	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
25	C	503	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
25	B	601	CLA	O2D-CGD-CBD	2.67	115.90	111.23
27	B	616	BCR	C29-C30-C25	2.67	114.32	110.44
29	m	101	LMG	O1-C1-C2	-2.67	104.22	108.27
27	t	101	BCR	C7-C8-C9	-2.67	122.29	126.23
32	C	517	DGD	O3G-C3G-C2G	-2.66	104.34	110.82
27	H	102	BCR	C2-C1-C6	2.66	114.31	110.44
25	b	611	CLA	C11-C12-C13	-2.66	107.14	115.97
31	d	408	LHG	O8-C23-C24	2.65	119.93	111.83
25	b	602	CLA	CHB-C1B-NB	2.65	128.03	124.05
25	B	608	CLA	CHC-C4B-NB	2.65	128.03	124.05
27	H	102	BCR	C27-C26-C25	2.65	126.29	122.70
25	C	510	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
25	b	612	CLA	C3B-C4B-NB	-2.65	108.16	110.53
32	H	103	DGD	C4E-C3E-C2E	-2.65	106.18	110.83
25	b	611	CLA	O1D-CGD-CBD	2.64	129.73	124.52
25	C	504	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
27	T	101	BCR	C27-C26-C25	2.64	126.27	122.70
31	D	411	LHG	C20-C19-C18	-2.64	101.02	114.37
25	b	603	CLA	CHB-C4A-NA	2.64	128.21	124.40
33	b	621	STE	C3-C2-C1	-2.63	107.64	114.51
27	D	405	BCR	C7-C8-C9	-2.63	122.34	126.23
25	c	503	CLA	CHB-C4A-NA	2.63	128.19	124.40
32	H	103	DGD	C3E-C4E-C5E	-2.63	105.47	110.23
25	c	501	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
25	c	504	CLA	C3B-C4B-NB	-2.63	108.18	110.53
30	A	614	SQD	O48-C23-C24	2.63	119.84	111.83
32	C	516	DGD	O6D-C1D-O3G	-2.62	103.84	110.04
25	B	608	CLA	C3B-C4B-NB	-2.62	108.19	110.53
25	B	604	CLA	O1D-CGD-CBD	2.62	129.69	124.52
25	b	614	CLA	CHB-C4A-NA	2.62	128.18	124.40
25	C	502	CLA	C3B-C4B-NB	-2.62	108.19	110.53
27	A	610	BCR	C11-C10-C9	-2.62	123.61	127.28
25	A	609	CLA	CMB-C2B-C3B	2.62	132.70	126.55
32	h	103	DGD	C6D-C5D-C4D	2.62	117.56	112.07
25	d	404	CLA	CHB-C4A-NA	2.62	128.17	124.40
27	b	616	BCR	C27-C26-C25	2.61	126.24	122.70
25	B	601	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
25	C	507	CLA	CHB-C4A-NA	2.61	128.17	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	514	BCR	C27-C26-C25	2.61	126.23	122.70
33	C	521	STE	C3-C2-C1	-2.61	107.70	114.51
25	b	612	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
25	b	607	CLA	O2D-CGD-CBD	2.60	115.78	111.23
27	k	102	BCR	C11-C10-C9	-2.60	123.63	127.28
25	b	603	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
25	d	404	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
25	B	611	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
29	M	101	LMG	O1-C1-C2	-2.60	104.32	108.27
25	b	613	CLA	CHD-C1D-ND	-2.60	121.15	124.80
25	C	505	CLA	C1-C2-C3	-2.60	121.94	126.20
25	C	512	CLA	C3B-C4B-NB	-2.60	108.21	110.53
25	A	607	CLA	O2A-CGA-O1A	-2.60	117.14	123.63
25	c	513	CLA	C3B-C4B-NB	-2.60	108.21	110.53
32	A	617	DGD	CDB-CCB-CBB	-2.60	101.25	114.37
25	b	611	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
25	c	506	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
25	c	507	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
29	m	101	LMG	O3-C3-C2	-2.59	104.28	110.38
25	b	611	CLA	C1-C2-C3	-2.59	121.96	126.20
31	D	411	LHG	C11-C10-C9	-2.59	101.30	114.37
28	A	611	PL9	C7-C8-C9	-2.59	122.38	126.83
29	A	613	LMG	O6-C1-O1	-2.58	103.94	110.04
28	a	611	PL9	O2-C1-C6	2.58	124.59	120.48
25	b	610	CLA	CHD-C1D-ND	-2.58	121.17	124.80
27	B	618	BCR	C29-C30-C25	2.58	114.19	110.44
32	C	518	DGD	CDB-CCB-CBB	-2.58	101.33	114.37
27	k	101	BCR	C27-C26-C25	2.58	126.19	122.70
27	A	610	BCR	C2-C1-C6	2.58	114.18	110.44
27	C	514	BCR	C2-C1-C6	2.58	114.18	110.44
32	c	516	DGD	CBB-CAB-C9B	-2.58	101.35	114.37
30	A	616	SQD	O48-C23-C24	2.57	119.68	111.83
32	c	516	DGD	C3G-C2G-C1G	-2.57	105.79	111.78
25	B	614	CLA	CHB-C4A-NA	2.57	128.11	124.40
25	b	610	CLA	C3B-C4B-NB	-2.57	108.24	110.53
27	k	101	BCR	C33-C5-C6	-2.57	121.69	124.48
25	d	403	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
25	B	603	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
29	m	101	LMG	O6-C1-O1	-2.56	104.00	110.04
25	b	615	CLA	O1D-CGD-CBD	2.55	129.56	124.52
25	h	101	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
25	b	601	CLA	O2D-CGD-CBD	2.55	115.69	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	102	SQD	O5-C5-C4	2.55	114.30	109.70
32	C	517	DGD	C1D-C2D-C3D	-2.55	104.65	110.01
25	B	602	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
27	b	618	BCR	C29-C30-C25	2.55	114.14	110.44
25	c	513	CLA	CHB-C4A-NA	2.55	128.08	124.40
31	D	408	LHG	C27-C26-C25	-2.54	101.51	114.37
27	c	515	BCR	C27-C26-C25	2.54	126.14	122.70
25	B	601	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
29	m	101	LMG	O8-C28-O10	-2.54	117.28	123.63
25	b	604	CLA	CHB-C4A-NA	2.54	128.06	124.40
28	A	611	PL9	O2-C1-C2	-2.54	116.06	121.83
29	M	101	LMG	C40-C39-C38	-2.54	101.55	114.37
27	b	616	BCR	C29-C30-C25	2.53	114.12	110.44
30	f	102	SQD	O5-C1-C2	-2.53	105.16	110.37
25	b	612	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
27	A	610	BCR	C7-C8-C9	-2.53	122.49	126.23
25	C	506	CLA	CHB-C4A-NA	2.53	128.06	124.40
25	a	606	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
29	D	407	LMG	O3-C3-C2	-2.53	104.41	110.38
27	B	616	BCR	C3-C4-C5	-2.53	109.55	114.06
27	B	618	BCR	C3-C4-C5	-2.53	109.55	114.06
32	H	103	DGD	C1D-C2D-C3D	-2.53	104.70	110.01
25	b	602	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
25	C	508	CLA	O1D-CGD-CBD	2.52	129.50	124.52
25	C	509	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
32	C	518	DGD	O3E-C3E-C2E	-2.52	104.43	110.38
35	f	101	HEM	C3B-C4B-NB	-2.52	107.66	109.47
27	B	617	BCR	C7-C8-C9	-2.52	122.51	126.23
25	c	502	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
25	b	608	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
30	a	613	SQD	O8-S-C6	2.52	110.84	105.97
25	b	609	CLA	CHB-C4A-NA	2.52	128.03	124.40
27	k	102	BCR	C24-C23-C22	-2.52	122.51	126.23
25	B	602	CLA	O2D-CGD-CBD	2.52	115.63	111.23
36	v	201	HEC	CBD-CAD-C3D	-2.52	105.57	112.53
31	A	615	LHG	O8-C23-C24	2.52	119.51	111.83
35	f	101	HEM	CBA-CAA-C2A	-2.52	105.57	112.53
28	d	406	PL9	C27-C28-C29	-2.52	121.86	127.62
28	d	406	PL9	C42-C43-C44	-2.51	121.87	127.62
25	C	504	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
25	B	605	CLA	O2D-CGD-CBD	2.51	115.62	111.23
29	b	622	LMG	C40-C39-C38	-2.51	101.67	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	612	CLA	CMB-C2B-C3B	2.51	132.46	126.55
25	c	512	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
27	b	617	BCR	C27-C26-C25	2.51	126.09	122.70
25	C	501	CLA	CHB-C1B-NB	2.51	127.81	124.05
25	B	605	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	c	511	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	A	612	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
25	c	513	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
25	c	510	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	A	614	SQD	O8-S-C6	2.50	110.80	105.97
25	b	605	CLA	C1-C2-C3	-2.50	122.10	126.20
25	c	508	CLA	C1D-ND-C4D	2.50	108.06	106.31
30	a	613	SQD	O7-S-C6	2.50	110.48	106.76
25	b	605	CLA	CHC-C4B-NB	2.50	127.79	124.05
25	C	509	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
27	C	515	BCR	C27-C26-C25	2.49	126.07	122.70
32	C	517	DGD	C6D-O5D-C1E	2.49	119.14	113.80
27	t	101	BCR	C11-C10-C9	-2.49	123.78	127.28
27	d	405	BCR	C38-C26-C25	-2.49	121.77	124.48
25	C	508	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
25	a	612	CLA	CHB-C4A-NA	2.49	127.99	124.40
32	A	617	DGD	O6D-C1D-O3G	-2.49	104.17	110.04
32	c	516	DGD	O6E-C5E-C4E	2.49	114.18	109.70
25	b	613	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
25	b	615	CLA	CHB-C4A-NA	2.49	127.99	124.40
25	C	501	CLA	CHD-C1D-ND	-2.49	121.30	124.80
27	C	514	BCR	C33-C5-C6	-2.49	121.77	124.48
25	b	610	CLA	CHB-C4A-NA	2.48	127.98	124.40
27	B	617	BCR	C27-C26-C25	2.48	126.06	122.70
25	b	606	CLA	CMB-C2B-C3B	2.48	132.38	126.55
28	a	611	PL9	O2-C1-C2	-2.48	116.19	121.83
25	b	608	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
26	d	402	PHO	CMA-C3A-C4A	-2.48	109.27	114.61
28	d	406	PL9	C8-C7-C3	2.48	118.43	112.03
30	b	619	SQD	O9-S-C6	2.48	110.45	106.76
25	C	510	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
32	c	516	DGD	O3G-C1D-C2D	-2.47	104.52	108.27
30	f	102	SQD	O48-C23-C24	2.47	119.38	111.83
25	d	404	CLA	CMB-C2B-C3B	2.47	132.37	126.55
25	C	512	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
32	a	615	DGD	C1G-C2G-C3G	-2.47	106.09	111.80
25	c	502	CLA	C3B-C4B-NB	-2.47	108.32	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	612	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
32	h	103	DGD	CDB-CCB-CBB	-2.47	101.88	114.37
32	C	516	DGD	C3G-C2G-C1G	-2.47	106.03	111.78
25	B	604	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
29	A	613	LMG	C40-C39-C38	-2.47	101.90	114.37
25	B	601	CLA	C1-C2-C3	-2.47	122.16	126.20
32	A	617	DGD	C3E-C4E-C5E	-2.47	105.76	110.23
28	A	611	PL9	C12-C13-C14	-2.47	121.98	127.62
25	b	607	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
25	d	404	CLA	C3B-C4B-NB	-2.46	108.33	110.53
27	c	514	BCR	C2-C1-C6	2.46	114.01	110.44
25	b	606	CLA	CHD-C1D-ND	-2.46	121.34	124.80
25	d	404	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
27	t	101	BCR	C27-C26-C25	2.46	126.03	122.70
25	B	612	CLA	CAC-C3C-C4C	2.46	127.99	124.79
32	C	517	DGD	C3E-C4E-C5E	-2.46	105.78	110.23
29	D	407	LMG	O6-C1-O1	-2.46	104.24	110.04
25	C	513	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
32	h	103	DGD	O6D-C1D-O3G	-2.46	104.24	110.04
25	C	511	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
29	A	613	LMG	O1-C7-C8	-2.45	104.85	110.82
29	d	411	LMG	C40-C39-C38	-2.45	101.98	114.37
25	C	513	CLA	C3B-C4B-NB	-2.45	108.34	110.53
27	t	101	BCR	C33-C5-C6	-2.45	121.81	124.48
25	C	510	CLA	CHB-C4A-NA	2.45	127.93	124.40
25	C	505	CLA	CMB-C2B-C1B	-2.45	121.70	125.42
25	B	605	CLA	CGD-CBD-CAD	-2.44	102.94	110.85
30	A	614	SQD	O47-C7-O49	-2.44	118.00	123.70
32	H	103	DGD	CDB-CCB-CBB	-2.44	102.05	114.37
25	B	611	CLA	CMB-C2B-C3B	2.44	132.28	126.55
30	b	619	SQD	O5-C5-C4	2.43	114.08	109.70
32	H	103	DGD	O6D-C1D-O3G	-2.43	104.30	110.04
25	c	501	CLA	C3B-C4B-NB	-2.43	108.36	110.53
29	M	101	LMG	O6-C1-O1	-2.43	104.30	110.04
25	B	615	CLA	CHB-C4A-NA	2.43	127.90	124.40
33	t	102	STE	C3-C2-C1	-2.43	108.18	114.51
28	D	406	PL9	O1-C4-C3	-2.43	118.17	120.73
32	c	518	DGD	C3G-C2G-C1G	-2.42	106.13	111.78
25	D	403	CLA	CHB-C4A-NA	2.42	127.90	124.40
27	c	514	BCR	C15-C14-C13	-2.42	123.88	127.28
25	A	607	CLA	O2D-CGD-CBD	2.42	115.46	111.23
30	a	613	SQD	O9-S-C6	2.42	110.36	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	C3B-C4B-NB	-2.41	108.38	110.53
27	h	102	BCR	C24-C23-C22	-2.41	122.67	126.23
25	B	603	CLA	CHB-C4A-NA	2.41	127.87	124.40
25	B	606	CLA	CHB-C1B-NB	2.40	127.66	124.05
25	H	101	CLA	C2A-C1A-CHA	2.40	128.04	123.87
27	h	102	BCR	C2-C1-C6	2.40	113.93	110.44
30	a	613	SQD	C3-C4-C5	2.40	114.58	110.23
25	b	602	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
25	B	603	CLA	O2D-CGD-CBD	2.39	115.41	111.23
25	C	509	CLA	C1-C2-C3	-2.39	122.28	126.20
25	b	611	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
30	a	614	SQD	O48-C23-O10	-2.39	117.66	123.63
29	c	521	LMG	C40-C39-C38	-2.39	102.31	114.37
30	a	613	SQD	O5-C1-C2	-2.38	105.47	110.37
31	e	101	LHG	C11-C10-C9	-2.38	102.31	114.37
28	d	406	PL9	O2-C1-C6	2.38	124.27	120.48
32	h	103	DGD	CBB-CAB-C9B	-2.38	102.31	114.37
25	c	506	CLA	C3B-C4B-NB	-2.38	108.40	110.53
33	t	102	STE	O2-C1-C2	2.38	121.53	114.00
25	b	612	CLA	C7-C6-C5	-2.38	106.91	113.26
25	B	604	CLA	CHD-C1D-ND	-2.38	121.46	124.80
32	A	617	DGD	O2D-C2D-C1D	-2.38	104.41	110.08
28	d	406	PL9	C20-C19-C21	2.38	119.35	115.23
25	a	607	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
25	A	612	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
27	B	616	BCR	C27-C26-C25	2.37	125.91	122.70
31	D	411	LHG	O8-C23-O10	-2.37	117.69	123.63
27	K	101	BCR	C33-C5-C6	-2.37	121.89	124.48
29	C	519	LMG	O6-C1-O1	-2.37	104.44	110.04
25	c	509	CLA	C3B-C4B-NB	-2.37	108.41	110.53
25	B	605	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
25	d	403	CLA	C3B-C4B-NB	-2.37	108.42	110.53
25	b	603	CLA	O2D-CGD-CBD	2.36	115.36	111.23
29	d	411	LMG	O3-C3-C2	-2.36	104.81	110.38
29	c	519	LMG	C40-C39-C38	-2.36	102.44	114.37
33	d	413	STE	O2-C1-C2	2.36	121.44	114.00
28	D	406	PL9	C50-C49-C48	-2.36	115.59	122.66
27	c	514	BCR	C7-C8-C9	-2.35	122.75	126.23
32	A	617	DGD	O3G-C3G-C2G	-2.35	105.09	110.82
27	C	514	BCR	C15-C16-C17	-2.35	118.70	123.52
27	b	618	BCR	C27-C26-C25	2.35	125.88	122.70
26	D	402	PHO	O2A-CGA-O1A	-2.35	117.75	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	102	SQD	O47-C7-C8	2.35	119.57	110.93
28	D	406	PL9	C12-C13-C14	-2.35	122.24	127.62
32	c	517	DGD	O2D-C2D-C1D	-2.35	104.48	110.08
29	d	411	LMG	C38-C37-C36	-2.35	102.49	114.37
25	B	612	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	b	612	CLA	CHA-C1A-NA	-2.35	121.08	126.39
27	c	515	BCR	C33-C5-C6	-2.35	121.92	124.48
25	c	501	CLA	CHB-C4A-NA	2.35	127.78	124.40
31	L	101	LHG	C20-C19-C18	-2.34	102.52	114.37
25	B	601	CLA	CMB-C2B-C3B	2.34	132.06	126.55
32	c	518	DGD	C1D-C2D-C3D	-2.34	105.08	110.01
25	C	511	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	c	506	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	c	502	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
25	a	612	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
25	C	509	CLA	CMB-C2B-C3B	2.34	132.05	126.55
27	D	405	BCR	C3-C4-C5	-2.34	109.89	114.06
25	b	611	CLA	CMB-C2B-C3B	2.33	132.04	126.55
25	D	404	CLA	CHB-C4A-NA	2.33	127.77	124.40
25	B	607	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
25	C	503	CLA	CHD-C1D-ND	-2.33	121.52	124.80
25	d	404	CLA	CHD-C1D-ND	-2.33	121.53	124.80
25	c	503	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
32	A	617	DGD	CBB-CAB-C9B	-2.33	102.61	114.37
29	d	411	LMG	O2-C2-C1	-2.33	104.53	110.08
29	C	519	LMG	O7-C10-O9	-2.33	118.27	123.70
27	b	618	BCR	C7-C8-C9	-2.33	122.79	126.23
27	C	514	BCR	C15-C14-C13	-2.33	124.02	127.28
25	b	601	CLA	C3B-C4B-NB	-2.32	108.45	110.53
25	c	512	CLA	O2D-CGD-CBD	2.32	115.29	111.23
29	D	407	LMG	C38-C37-C36	-2.32	102.63	114.37
30	f	102	SQD	C46-C45-C44	-2.32	106.38	111.78
25	C	513	CLA	CHB-C4A-NA	2.32	127.74	124.40
25	a	609	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
29	A	613	LMG	C38-C37-C36	-2.32	102.66	114.37
25	b	607	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
27	H	102	BCR	C16-C17-C18	-2.31	124.03	127.28
35	f	101	HEM	CAB-C3B-C2B	-2.31	120.91	128.43
27	A	610	BCR	C33-C5-C6	-2.31	121.96	124.48
25	C	509	CLA	CED-O2D-CGD	2.31	121.15	115.92
27	H	102	BCR	C16-C15-C14	-2.31	118.79	123.52
25	b	604	CLA	O2A-CGA-O1A	-2.31	117.85	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	508	CLA	CHB-C4A-NA	2.31	127.73	124.40
26	D	402	PHO	O2D-CGD-O1D	-2.31	119.36	123.85
25	b	608	CLA	CHC-C4B-NB	2.30	127.51	124.05
31	D	408	LHG	C11-C10-C9	-2.30	102.72	114.37
31	D	408	LHG	C20-C19-C18	-2.30	102.72	114.37
25	b	612	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
31	D	408	LHG	C18-C17-C16	-2.30	102.72	114.37
27	k	102	BCR	C33-C5-C6	-2.30	121.97	124.48
29	M	101	LMG	C38-C37-C36	-2.30	102.74	114.37
31	d	408	LHG	C20-C19-C18	-2.30	102.74	114.37
25	C	508	CLA	CHB-C1B-NB	2.30	127.50	124.05
27	a	610	BCR	C2-C1-C6	2.30	113.78	110.44
25	D	404	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
25	c	503	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
25	B	602	CLA	C4-C3-C5	2.30	119.21	115.23
31	e	101	LHG	C20-C19-C18	-2.29	102.77	114.37
29	B	620	LMG	C38-C37-C36	-2.29	102.77	114.37
25	b	608	CLA	C6-C5-C3	2.29	119.05	113.47
25	b	606	CLA	CHB-C4A-NA	2.29	127.71	124.40
29	b	622	LMG	C38-C37-C36	-2.29	102.78	114.37
31	A	615	LHG	C20-C19-C18	-2.29	102.79	114.37
29	m	101	LMG	C38-C37-C36	-2.29	102.79	114.37
25	c	502	CLA	CMB-C2B-C3B	2.29	131.94	126.55
27	A	610	BCR	C38-C26-C25	-2.29	121.98	124.48
25	b	601	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
25	c	502	CLA	CHD-C1D-ND	-2.29	121.58	124.80
25	A	607	CLA	CHB-C4A-NA	2.29	127.70	124.40
25	c	510	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
25	b	609	CLA	C3B-C4B-NB	-2.28	108.49	110.53
25	a	607	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	C	510	CLA	CMB-C2B-C3B	2.28	131.92	126.55
25	C	506	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
25	b	605	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
25	D	404	CLA	CMB-C2B-C3B	2.28	131.91	126.55
28	d	406	PL9	O1-C4-C3	-2.28	118.33	120.73
25	b	604	CLA	C4-C3-C5	2.28	119.18	115.23
32	c	518	DGD	CAB-C9B-C8B	-2.28	102.86	114.37
29	d	411	LMG	O1-C7-C8	-2.28	105.28	110.82
29	c	519	LMG	C38-C37-C36	-2.28	102.86	114.37
32	C	517	DGD	CBB-CAB-C9B	-2.28	102.86	114.37
25	B	608	CLA	C1-C2-C3	-2.27	122.47	126.20
28	A	611	PL9	C40-C39-C41	2.27	119.17	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	615	DGD	CBB-CAB-C9B	-2.27	102.88	114.37
25	A	609	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
31	d	407	LHG	C20-C19-C18	-2.27	102.89	114.37
33	C	520	STE	C4-C3-C2	-2.27	104.79	113.13
25	H	101	CLA	CAA-CBA-CGA	-2.27	106.77	113.21
25	b	603	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
25	b	601	CLA	CMB-C2B-C3B	2.27	131.88	126.55
25	H	101	CLA	C4-C3-C5	2.27	119.16	115.23
25	a	606	CLA	O1D-CGD-CBD	2.27	128.99	124.52
25	D	404	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
25	c	513	CLA	C1-C2-C3	-2.26	122.49	126.20
25	A	606	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
25	c	501	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
29	c	522	LMG	C38-C37-C36	-2.26	102.94	114.37
33	B	624	STE	O2-C1-C2	2.26	121.13	114.00
29	D	410	LMG	O1-C7-C8	-2.26	105.97	111.77
25	B	615	CLA	C3B-C4B-NB	-2.26	108.52	110.53
25	B	614	CLA	CHC-C4B-NB	2.25	127.43	124.05
28	D	406	PL9	C20-C19-C21	2.25	119.14	115.23
26	a	608	PHO	CMA-C3A-C4A	-2.25	109.76	114.61
31	D	409	LHG	O8-C23-C24	2.25	118.69	111.83
25	C	508	CLA	CHD-C1D-ND	-2.25	121.64	124.80
25	b	615	CLA	C1-C2-C3	-2.25	122.52	126.20
25	B	615	CLA	O1D-CGD-CBD	2.24	128.94	124.52
25	C	502	CLA	CHD-C1D-ND	-2.24	121.65	124.80
29	m	101	LMG	C9-C8-C7	-2.24	106.56	111.78
29	c	519	LMG	O3-C3-C2	-2.24	105.10	110.38
27	K	101	BCR	C30-C25-C26	-2.24	119.58	122.64
28	D	406	PL9	C36-C34-C33	-2.24	116.14	121.17
32	C	516	DGD	O1G-C1A-C2A	-2.24	105.02	111.83
25	b	607	CLA	CHB-C1B-NB	2.24	127.40	124.05
25	b	607	CLA	CMB-C2B-C3B	2.23	131.81	126.55
25	B	611	CLA	O2D-CGD-CBD	2.23	115.13	111.23
29	c	522	LMG	O1-C7-C8	-2.23	105.39	110.82
30	F	102	SQD	C3-C4-C5	2.23	114.28	110.23
25	H	101	CLA	CHB-C4A-NA	2.23	127.62	124.40
29	M	101	LMG	O2-C2-C1	-2.23	104.76	110.08
32	c	518	DGD	O6E-C1E-O5D	-2.23	104.78	110.04
25	B	609	CLA	CHA-C1A-NA	-2.23	121.34	126.39
31	b	623	LHG	O8-C23-C24	2.22	118.61	111.83
25	b	613	CLA	CHB-C4A-NA	2.22	127.61	124.40
25	c	509	CLA	CHB-C4A-NA	2.22	127.61	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	406	PL9	C27-C28-C29	-2.22	122.54	127.62
32	C	516	DGD	C6B-C5B-C4B	-2.22	103.14	114.37
25	B	604	CLA	CHB-C4A-NA	2.22	127.60	124.40
25	c	504	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
25	c	508	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
25	d	403	CLA	O2D-CGD-CBD	2.22	115.11	111.23
25	B	609	CLA	CHD-C1D-ND	-2.22	121.68	124.80
25	c	507	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
29	c	522	LMG	C40-C39-C38	-2.21	103.18	114.37
32	c	516	DGD	C2G-O2G-C1B	2.21	123.09	117.80
25	c	504	CLA	CHD-C1D-ND	-2.21	121.69	124.80
29	b	622	LMG	O2-C2-C1	-2.21	104.81	110.08
31	A	615	LHG	C11-C10-C9	-2.21	103.20	114.37
35	F	101	HEM	CHC-C4B-NB	2.21	126.80	124.42
29	d	410	LMG	C38-C37-C36	-2.21	103.20	114.37
25	B	605	CLA	C1-C2-C3	-2.21	122.58	126.20
30	B	621	SQD	O8-S-C6	2.21	110.23	105.97
25	c	511	CLA	C2A-C1A-CHA	2.21	127.69	123.87
25	C	501	CLA	CHD-C1D-C2D	2.20	130.07	125.49
32	c	517	DGD	O3D-C3D-C4D	-2.20	105.18	110.38
29	D	407	LMG	O1-C1-C2	-2.20	104.93	108.27
25	B	613	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
32	A	617	DGD	C4E-C3E-C2E	-2.20	106.97	110.83
33	a	616	STE	C3-C2-C1	-2.20	108.77	114.51
32	a	615	DGD	CFB-CEB-CDB	-2.20	103.25	114.37
26	a	608	PHO	O2A-CGA-O1A	-2.20	118.13	123.63
25	c	510	CLA	CMB-C2B-C3B	2.20	131.72	126.55
25	B	607	CLA	CMB-C2B-C3B	2.20	131.72	126.55
32	A	617	DGD	C1D-C2D-C3D	-2.20	105.39	110.01
25	c	504	CLA	O2D-CGD-CBD	2.19	115.07	111.23
25	B	613	CLA	CMB-C2B-C3B	2.19	131.71	126.55
25	c	510	CLA	C16-C15-C13	-2.19	108.68	115.97
32	H	103	DGD	C7B-C6B-C5B	-2.19	103.29	114.37
25	b	612	CLA	CHB-C1B-NB	2.19	127.33	124.05
32	C	516	DGD	CDB-CCB-CBB	-2.19	103.30	114.37
25	C	505	CLA	CMB-C2B-C3B	2.19	131.70	126.55
25	B	614	CLA	C7-C6-C5	-2.19	107.43	113.26
29	C	519	LMG	O3-C3-C2	-2.19	105.22	110.38
25	a	607	CLA	C1-C2-C3	-2.19	122.61	126.20
25	c	503	CLA	C7-C6-C5	-2.19	107.43	113.26
25	b	611	CLA	CHB-C4A-NA	2.19	127.56	124.40
29	c	519	LMG	O1-C7-C8	-2.19	105.50	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	402	PHO	O2D-CGD-CBD	2.18	113.35	110.95
26	d	402	PHO	C3B-C4B-NB	-2.18	106.04	107.46
27	C	515	BCR	C15-C16-C17	-2.18	119.05	123.52
30	a	613	SQD	C44-O6-C1	-2.18	109.12	113.80
25	b	613	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
25	B	607	CLA	CHB-C4A-NA	2.18	127.55	124.40
32	H	103	DGD	CAB-C9B-C8B	-2.18	103.35	114.37
25	B	610	CLA	CHD-C1D-ND	-2.18	121.73	124.80
29	A	613	LMG	O8-C28-O10	-2.18	118.18	123.63
25	C	508	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
25	C	512	CLA	C6-C5-C3	-2.18	108.17	113.47
28	d	406	PL9	O2-C1-C2	-2.18	116.88	121.83
25	B	604	CLA	C16-C15-C13	-2.18	108.73	115.97
25	b	603	CLA	CHB-C1B-NB	2.18	127.31	124.05
31	d	407	LHG	C18-C17-C16	-2.17	103.38	114.37
31	D	411	LHG	C18-C17-C16	-2.17	103.38	114.37
27	K	101	BCR	C16-C15-C14	-2.17	119.08	123.52
32	H	103	DGD	C1D-O6D-C5D	-2.17	109.48	113.72
25	c	508	CLA	C2D-C1D-ND	-2.17	107.98	110.13
28	a	611	PL9	C27-C28-C29	-2.17	122.66	127.62
25	B	603	CLA	C2D-C1D-ND	-2.17	107.98	110.13
25	B	613	CLA	CHB-C1B-NB	2.17	127.30	124.05
25	B	613	CLA	O1D-CGD-CBD	2.17	128.80	124.52
32	H	103	DGD	C3G-C2G-C1G	-2.17	106.73	111.78
25	H	101	CLA	O2D-CGD-CBD	2.17	115.02	111.23
27	b	616	BCR	C24-C23-C22	-2.17	123.03	126.23
27	H	102	BCR	C24-C23-C22	-2.16	123.04	126.23
25	c	511	CLA	CHA-C1A-NA	-2.16	121.50	126.39
25	d	404	CLA	CHA-C1A-NA	-2.16	121.50	126.39
28	a	611	PL9	C7-C8-C9	-2.16	123.11	126.83
32	C	518	DGD	CAB-C9B-C8B	-2.16	103.45	114.37
27	B	616	BCR	C15-C16-C17	-2.16	119.10	123.52
25	b	602	CLA	CHC-C4B-NB	2.16	127.29	124.05
25	c	502	CLA	CHB-C1B-NB	2.16	127.29	124.05
35	f	101	HEM	C1B-NB-C4B	2.16	107.76	105.21
25	C	513	CLA	O2D-CGD-CBD	2.16	115.00	111.23
32	h	103	DGD	CAB-C9B-C8B	-2.16	103.47	114.37
25	A	612	CLA	CHB-C4A-NA	2.16	127.51	124.40
25	B	609	CLA	O1D-CGD-CBD	2.15	128.77	124.52
25	c	501	CLA	CHD-C1D-ND	-2.15	121.77	124.80
25	A	607	CLA	C1D-ND-C4D	2.15	107.82	106.31
25	b	601	CLA	O2A-CGA-O1A	-2.15	118.24	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	BCR	C2-C1-C6	2.15	113.56	110.44
27	c	514	BCR	C33-C5-C6	-2.15	122.14	124.48
32	c	517	DGD	O5D-C6D-C5D	-2.15	104.57	109.42
25	b	614	CLA	CAA-CBA-CGA	-2.15	107.10	113.21
31	D	409	LHG	O8-C6-C5	-2.15	102.20	108.40
25	C	506	CLA	O1D-CGD-CBD	2.15	128.76	124.52
25	h	101	CLA	CHD-C1D-ND	-2.15	121.78	124.80
25	D	403	CLA	C4-C3-C5	2.15	118.96	115.23
31	e	101	LHG	C18-C17-C16	-2.15	103.51	114.37
25	b	615	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
31	d	408	LHG	C18-C17-C16	-2.15	103.52	114.37
27	a	610	BCR	C38-C26-C25	-2.14	122.14	124.48
25	C	503	CLA	C7-C6-C5	-2.14	107.55	113.26
29	M	101	LMG	O1-C7-C8	-2.14	105.60	110.82
32	a	615	DGD	C5B-C4B-C3B	-2.14	103.53	114.37
27	a	610	BCR	C11-C10-C9	-2.14	124.27	127.28
25	B	602	CLA	CHB-C1B-NB	2.14	127.26	124.05
25	D	403	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
25	b	607	CLA	CHD-C1D-ND	-2.14	121.79	124.80
25	b	612	CLA	CHC-C4B-NB	2.14	127.26	124.05
25	c	510	CLA	C3B-C4B-NB	-2.14	108.62	110.53
29	d	410	LMG	C40-C39-C38	-2.14	103.56	114.37
27	b	617	BCR	C15-C14-C13	-2.14	124.28	127.28
31	D	409	LHG	C11-C10-C9	-2.14	103.57	114.37
25	b	607	CLA	CHD-C4C-NC	2.14	127.54	124.23
27	b	616	BCR	C33-C5-C6	-2.13	122.16	124.48
27	T	101	BCR	C1-C6-C5	-2.13	119.72	122.64
29	C	519	LMG	C40-C39-C38	-2.13	103.58	114.37
29	b	622	LMG	C42-C41-C40	-2.13	103.58	114.37
31	d	407	LHG	O8-C6-C5	-2.13	102.25	108.40
32	c	516	DGD	O6D-C1D-O3G	-2.13	105.00	110.04
25	B	603	CLA	C1-C2-C3	-2.13	122.71	126.20
32	c	518	DGD	C8B-C7B-C6B	-2.13	103.61	114.37
31	b	623	LHG	C20-C19-C18	-2.13	103.61	114.37
31	L	101	LHG	O8-C23-C24	2.13	118.32	111.83
32	C	516	DGD	C6D-O5D-C1E	2.13	118.36	113.80
25	C	510	CLA	O2D-CGD-CBD	2.13	114.95	111.23
35	f	101	HEM	CHB-C1B-NB	2.13	127.00	124.37
25	C	503	CLA	O1D-CGD-CBD	2.12	128.71	124.52
25	A	612	CLA	O2D-CGD-CBD	2.12	114.94	111.23
25	B	611	CLA	C11-C12-C13	-2.12	108.91	115.97
27	H	102	BCR	C1-C6-C5	-2.12	119.73	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	CHD-C1D-C2D	2.12	129.90	125.49
29	c	519	LMG	O8-C28-O10	-2.12	118.33	123.63
32	C	518	DGD	C3G-C2G-C1G	-2.12	106.84	111.78
32	h	103	DGD	O5E-C6E-C5E	-2.12	104.12	111.33
25	B	603	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
27	t	101	BCR	C1-C6-C5	-2.12	119.74	122.64
25	d	403	CLA	CHA-C4D-ND	2.12	136.92	132.55
25	D	403	CLA	O2D-CGD-CBD	2.12	114.93	111.23
25	b	608	CLA	CMB-C2B-C3B	2.12	131.53	126.55
33	E	101	STE	O2-C1-C2	2.11	120.68	114.00
25	c	513	CLA	CMB-C2B-C3B	2.11	131.52	126.55
29	C	519	LMG	O2-C2-C1	-2.11	105.04	110.08
25	b	610	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
25	c	508	CLA	CHD-C1D-C2D	2.11	129.88	125.49
25	C	507	CLA	O2D-CGD-CBD	2.11	114.92	111.23
29	c	521	LMG	O2-C2-C1	-2.11	105.04	110.08
32	C	517	DGD	C5B-C4B-C3B	-2.11	103.69	114.37
25	C	503	CLA	CHB-C4A-NA	2.11	127.45	124.40
25	B	612	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
26	a	608	PHO	CMD-C2D-C3D	2.11	128.90	124.68
27	b	616	BCR	C15-C14-C13	-2.11	124.32	127.28
35	F	101	HEM	O2D-CGD-CBD	2.11	120.66	114.00
25	b	608	CLA	C1-C2-C3	-2.11	122.75	126.20
25	b	605	CLA	CHB-C4A-NA	2.11	127.44	124.40
27	B	616	BCR	C11-C10-C9	-2.10	124.33	127.28
25	b	608	CLA	O1D-CGD-CBD	2.10	128.67	124.52
25	c	504	CLA	CHD-C4C-NC	2.10	127.49	124.23
25	c	512	CLA	CHD-C1D-ND	-2.10	121.84	124.80
25	b	602	CLA	CHB-C4A-NA	2.10	127.43	124.40
25	b	608	CLA	CHB-C4A-NA	2.10	127.43	124.40
31	b	623	LHG	C11-C10-C9	-2.10	103.74	114.37
31	D	409	LHG	C18-C17-C16	-2.10	103.75	114.37
32	C	516	DGD	O2D-C2D-C1D	-2.10	105.07	110.08
32	C	517	DGD	O3E-C3E-C2E	-2.10	105.43	110.38
29	c	521	LMG	O6-C1-O1	-2.10	105.08	110.04
29	D	410	LMG	O7-C10-O9	-2.10	118.80	123.70
25	D	404	CLA	CHC-C4B-NB	2.10	127.20	124.05
25	B	606	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	b	602	CLA	CMB-C2B-C3B	2.09	131.47	126.55
25	b	606	CLA	C6-C7-C8	-2.09	109.01	115.97
25	B	606	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
27	T	101	BCR	C31-C1-C6	2.09	113.52	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	519	LMG	C38-C37-C36	-2.09	103.79	114.37
29	A	613	LMG	C1-C2-C3	-2.09	105.61	110.01
25	B	613	CLA	CHB-C4A-NA	2.09	127.42	124.40
25	A	606	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
25	B	609	CLA	CHD-C4C-NC	2.09	127.47	124.23
29	A	613	LMG	C9-C8-C7	-2.09	106.91	111.78
25	a	606	CLA	C2A-C1A-CHA	2.09	127.49	123.87
32	h	103	DGD	C7B-C6B-C5B	-2.09	103.82	114.37
32	C	518	DGD	O3D-C3D-C4D	-2.09	105.46	110.38
32	c	517	DGD	C5B-C4B-C3B	-2.09	103.82	114.37
25	b	607	CLA	C1-C2-C3	-2.08	122.78	126.20
25	b	604	CLA	CHC-C1C-NC	2.08	127.45	124.31
29	c	521	LMG	O7-C10-O9	-2.08	118.84	123.70
29	b	622	LMG	O8-C28-O10	-2.08	118.42	123.63
32	c	516	DGD	C5B-C4B-C3B	-2.08	103.84	114.37
25	c	503	CLA	C1-C2-C3	-2.08	122.79	126.20
25	c	510	CLA	O2D-CGD-CBD	2.08	114.87	111.23
32	c	516	DGD	C3D-C4D-C5D	-2.08	106.46	110.23
25	C	501	CLA	CHB-C4A-NA	2.08	127.40	124.40
25	C	504	CLA	CHC-C1C-NC	2.08	127.44	124.31
27	T	101	BCR	C35-C13-C14	-2.08	119.45	122.82
25	B	606	CLA	CMB-C2B-C3B	2.08	131.44	126.55
25	A	606	CLA	C7-C6-C5	-2.07	107.73	113.26
33	m	102	STE	O1-C1-C2	-2.07	116.52	123.09
25	b	615	CLA	CMB-C2B-C3B	2.07	131.43	126.55
32	c	517	DGD	C8B-C7B-C6B	-2.07	103.89	114.37
25	C	510	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	C	509	CLA	C2A-C1A-CHA	2.07	127.46	123.87
25	C	504	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	B	607	CLA	CHB-C1B-NB	2.07	127.15	124.05
25	B	613	CLA	CHC-C4B-NB	2.07	127.15	124.05
25	b	614	CLA	C2A-C1A-CHA	2.07	127.45	123.87
25	d	403	CLA	C4-C3-C5	2.07	118.82	115.23
25	b	611	CLA	CAC-C3C-C4C	2.07	127.48	124.79
25	D	404	CLA	O2D-CGD-CBD	2.07	114.84	111.23
27	B	617	BCR	C2-C1-C6	2.07	113.44	110.44
29	b	622	LMG	C8-O7-C10	2.06	122.74	117.80
29	c	522	LMG	O8-C28-O10	-2.06	118.46	123.63
25	B	605	CLA	CHC-C4B-NB	2.06	127.14	124.05
25	B	602	CLA	CMB-C2B-C3B	2.06	131.40	126.55
30	B	621	SQD	C1-C2-C3	-2.06	105.67	110.01
25	a	607	CLA	CHD-C1D-C2D	2.06	129.77	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	605	CLA	C11-C12-C13	-2.06	109.12	115.97
32	C	516	DGD	C8B-C7B-C6B	-2.06	103.96	114.37
31	d	409	LHG	C27-C26-C25	-2.06	103.96	114.37
30	B	621	SQD	C9-C8-C7	-2.06	106.15	113.69
32	c	516	DGD	C7B-C6B-C5B	-2.06	103.97	114.37
31	D	408	LHG	O8-C23-O10	-2.05	118.49	123.63
27	c	515	BCR	C15-C16-C17	-2.05	119.32	123.52
25	b	608	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
25	B	608	CLA	C7-C6-C5	-2.05	107.79	113.26
25	C	505	CLA	CHB-C4A-NA	2.05	127.36	124.40
31	D	409	LHG	C27-C26-C25	-2.05	104.00	114.37
29	A	613	LMG	C4-C3-C2	-2.05	107.23	110.83
32	C	518	DGD	CBB-CAB-C9B	-2.05	104.01	114.37
25	A	609	CLA	CHC-C4B-NB	2.05	127.12	124.05
29	c	521	LMG	C42-C41-C40	-2.05	104.01	114.37
32	C	517	DGD	CAB-C9B-C8B	-2.05	104.02	114.37
25	a	607	CLA	C1D-ND-C4D	2.05	107.75	106.31
25	c	501	CLA	CHD-C1D-C2D	2.05	129.75	125.49
31	D	411	LHG	C15-C14-C13	-2.05	104.02	114.37
32	A	617	DGD	C8B-C7B-C6B	-2.05	104.03	114.37
25	B	608	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
29	B	620	LMG	O7-C10-O9	-2.04	118.08	123.33
28	D	406	PL9	C35-C34-C36	2.04	118.77	115.23
28	D	406	PL9	C32-C33-C34	-2.04	122.95	127.62
28	D	406	PL9	C42-C43-C44	-2.04	122.95	127.62
32	H	103	DGD	C3D-C4D-C5D	-2.04	106.53	110.23
32	c	517	DGD	C3D-C4D-C5D	-2.04	106.53	110.23
25	b	601	CLA	C16-C15-C13	-2.04	109.18	115.97
29	c	522	LMG	C9-C8-C7	-2.04	107.03	111.78
32	c	518	DGD	CBB-CAB-C9B	-2.04	104.06	114.37
32	H	103	DGD	CBB-CAB-C9B	-2.04	104.06	114.37
25	H	101	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
25	b	603	CLA	CHC-C4B-NB	2.04	127.10	124.05
25	B	615	CLA	CAA-CBA-CGA	-2.03	107.43	113.21
25	C	508	CLA	CHD-C1D-C2D	2.03	129.71	125.49
26	a	608	PHO	OBD-CAD-CBD	-2.03	122.84	125.82
25	C	512	CLA	CHA-C1A-NA	-2.03	121.80	126.39
32	A	617	DGD	CAB-C9B-C8B	-2.03	104.12	114.37
27	c	515	BCR	C2-C1-C6	2.03	113.38	110.44
25	C	504	CLA	O2D-CGD-CBD	2.03	114.77	111.23
33	a	616	STE	O2-C1-C2	2.02	120.40	114.00
25	c	505	CLA	CHB-C4A-NA	2.02	127.32	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	517	DGD	CBB-CAB-C9B	-2.02	104.14	114.37
31	b	623	LHG	C27-C26-C25	-2.02	104.14	114.37
26	d	402	PHO	C11-C12-C13	-2.02	109.24	115.97
25	c	505	CLA	O2D-CGD-CBD	2.02	114.77	111.23
27	D	405	BCR	C38-C26-C25	-2.02	122.28	124.48
27	K	101	BCR	C1-C6-C5	-2.02	119.87	122.64
27	c	514	BCR	C30-C25-C26	-2.02	119.87	122.64
25	c	511	CLA	CHB-C4A-NA	2.02	127.32	124.40
25	b	602	CLA	O1D-CGD-CBD	2.02	128.50	124.52
25	c	513	CLA	O2D-CGD-CBD	2.02	114.76	111.23
25	B	603	CLA	C6-C5-C3	-2.02	108.55	113.47
25	C	505	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
29	D	407	LMG	O7-C10-O9	-2.02	118.98	123.70
25	b	615	CLA	O2D-CGD-CBD	2.02	114.76	111.23
25	A	606	CLA	C3B-C4B-NB	-2.02	108.73	110.53
27	a	610	BCR	C3-C4-C5	-2.02	110.46	114.06
32	C	516	DGD	O5D-C6D-C5D	-2.02	104.87	109.42
25	b	612	CLA	CMB-C2B-C3B	2.02	131.30	126.55
25	b	613	CLA	CMD-C2D-C1D	2.02	128.28	124.73
32	c	516	DGD	C1D-C2D-C3D	-2.02	105.77	110.01
27	d	405	BCR	C3-C4-C5	-2.02	110.46	114.06
25	b	612	CLA	C2A-C1A-CHA	2.02	127.37	123.87
27	h	102	BCR	C16-C17-C18	-2.02	124.45	127.28
33	X	101	STE	C3-C2-C1	-2.02	109.25	114.51
25	C	508	CLA	CMB-C2B-C3B	2.02	131.29	126.55
27	T	101	BCR	C15-C14-C13	-2.01	124.45	127.28
25	C	504	CLA	C4-C3-C5	2.01	118.72	115.23
25	B	615	CLA	CHC-C4B-NB	2.01	127.07	124.05
28	a	611	PL9	C35-C34-C36	2.01	118.72	115.23
30	B	621	SQD	O5-C1-C2	-2.01	106.24	110.37
28	A	611	PL9	C31-C29-C28	2.01	125.68	121.17
29	D	410	LMG	C38-C37-C36	-2.01	104.22	114.37
25	B	602	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
29	C	519	LMG	C1-O6-C5	-2.01	109.80	113.72
29	M	101	LMG	O3-C3-C2	-2.01	105.65	110.38
25	c	509	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
27	k	102	BCR	C7-C8-C9	-2.01	123.27	126.23
29	c	521	LMG	O3-C3-C2	-2.01	105.65	110.38
31	e	101	LHG	C27-C26-C25	-2.01	104.23	114.37
25	C	503	CLA	CHD-C1D-C2D	2.00	129.66	125.49
31	A	615	LHG	C27-C26-C25	-2.00	104.24	114.37
25	a	606	CLA	CAC-C3C-C4C	2.00	127.40	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	509	CLA	O1D-CGD-CBD	2.00	128.47	124.52
32	A	617	DGD	CFB-CEB-CDB	-2.00	104.24	114.37
27	T	101	BCR	C4-C5-C6	2.00	125.41	122.70
25	c	507	CLA	C2A-C1A-CHA	2.00	127.34	123.87
32	C	516	DGD	CAB-C9B-C8B	-2.00	104.25	114.37
25	b	601	CLA	C1-C2-C3	-2.00	122.92	126.20
27	B	616	BCR	C30-C25-C26	-2.00	119.90	122.64

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	609	CLA	ND
25	A	612	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	H	101	CLA	ND

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Mol	Chain	Res	Type	Atom
25	a	606	CLA	ND
25	a	607	CLA	ND
25	a	609	CLA	ND
25	a	612	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	c	501	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	404	CLA	ND
25	h	101	CLA	ND

All (1743) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C4B-C3B-CAB-CBB
25	C	504	CLA	C2-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	C11-C10-C8-C9
25	H	101	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C11-C12-C13-C14
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
25	c	513	CLA	CBD-CGD-O2D-CED
25	h	101	CLA	C1A-C2A-CAA-CBA
25	h	101	CLA	C11-C10-C8-C9
27	D	405	BCR	C23-C24-C25-C26
27	K	101	BCR	C16-C17-C18-C36
27	K	101	BCR	C20-C21-C22-C37
27	K	101	BCR	C37-C22-C23-C24
27	d	405	BCR	C21-C22-C23-C24
27	d	405	BCR	C37-C22-C23-C24
27	d	405	BCR	C22-C23-C24-C25
27	k	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C17-C18-C19-C20
28	A	611	PL9	C32-C33-C34-C36
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C37-C38-C39-C41
28	A	611	PL9	C43-C44-C46-C47
28	D	406	PL9	C32-C33-C34-C36
28	a	611	PL9	C12-C13-C14-C15
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C32-C33-C34-C35
28	a	611	PL9	C33-C34-C36-C37
28	a	611	PL9	C47-C48-C49-C50
28	d	406	PL9	C40-C39-C41-C42
28	d	406	PL9	C42-C43-C44-C46
29	A	613	LMG	O6-C1-O1-C7
29	A	613	LMG	O9-C10-O7-C8
29	A	613	LMG	C11-C10-O7-C8
29	C	519	LMG	O9-C10-O7-C8
29	C	519	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
29	D	410	LMG	C11-C10-O7-C8
29	c	521	LMG	C11-C10-O7-C8
29	c	522	LMG	O6-C1-O1-C7
30	B	621	SQD	O6-C44-C45-O47
30	B	621	SQD	O49-C7-O47-C45
30	B	621	SQD	C8-C7-O47-C45
30	a	613	SQD	O6-C44-C45-O47
30	a	614	SQD	C8-C7-O47-C45
30	b	619	SQD	O5-C1-O6-C44
30	b	619	SQD	C8-C7-O47-C45
30	b	619	SQD	O10-C23-O48-C46
30	b	619	SQD	C24-C23-O48-C46
30	f	102	SQD	C2-C1-O6-C44
30	f	102	SQD	O5-C1-O6-C44
31	D	408	LHG	C1-C2-C3-O3
31	D	408	LHG	C3-O3-P-O4
31	D	408	LHG	C3-O3-P-O5
31	D	408	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
31	D	408	LHG	C4-O6-P-O4
31	D	409	LHG	C3-O3-P-O6
31	D	411	LHG	C3-O3-P-O4
31	D	411	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
31	b	623	LHG	C4-O6-P-O5
31	d	407	LHG	O1-C1-C2-C3
31	d	407	LHG	C3-O3-P-O4
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C4-O6-P-O3
31	d	408	LHG	C4-O6-P-O4
31	e	101	LHG	C1-C2-C3-O3
31	e	101	LHG	C3-O3-P-O5
31	e	101	LHG	C3-O3-P-O6
31	e	101	LHG	C24-C23-O8-C6
32	A	617	DGD	C2B-C1B-O2G-C2G
32	A	617	DGD	O1B-C1B-O2G-C2G
32	A	617	DGD	O2G-C2G-C3G-O3G
36	V	201	HEC	C2B-C3B-CAB-CBB
36	V	201	HEC	C4B-C3B-CAB-CBB
36	V	201	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
36	V	201	HEC	C4C-C3C-CAC-CBC
36	v	201	HEC	C2B-C3B-CAB-CBB
36	v	201	HEC	C4B-C3B-CAB-CBB
36	v	201	HEC	C2C-C3C-CAC-CBC
36	v	201	HEC	C4C-C3C-CAC-CBC
25	h	101	CLA	O1D-CGD-O2D-CED
25	h	101	CLA	CBD-CGD-O2D-CED
30	f	102	SQD	O10-C23-O48-C46
31	e	101	LHG	O10-C23-O8-C6
28	a	611	PL9	C47-C48-C49-C51
30	f	102	SQD	C24-C23-O48-C46
29	M	101	LMG	O10-C28-O8-C9
29	c	521	LMG	O10-C28-O8-C9
29	D	410	LMG	O9-C10-O7-C8
30	a	614	SQD	O49-C7-O47-C45
30	b	619	SQD	O49-C7-O47-C45
32	a	615	DGD	O1B-C1B-O2G-C2G
25	B	615	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	d	404	CLA	C3-C5-C6-C7
29	M	101	LMG	C29-C28-O8-C9
29	c	521	LMG	C29-C28-O8-C9
30	F	102	SQD	C24-C23-O48-C46
25	c	510	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	C15-C16-C17-C18
25	A	609	CLA	C4-C3-C5-C6
25	B	613	CLA	C4-C3-C5-C6
25	C	507	CLA	C4-C3-C5-C6
25	b	613	CLA	C4-C3-C5-C6
28	A	611	PL9	C20-C19-C21-C22
28	A	611	PL9	C35-C34-C36-C37
28	A	611	PL9	C40-C39-C41-C42
28	a	611	PL9	C30-C29-C31-C32
28	a	611	PL9	C35-C34-C36-C37
25	A	609	CLA	C2-C3-C5-C6
25	C	507	CLA	C2-C3-C5-C6
25	b	613	CLA	C2-C3-C5-C6
28	A	611	PL9	C18-C19-C21-C22
28	d	406	PL9	C38-C39-C41-C42
28	A	611	PL9	C32-C33-C34-C35
28	d	406	PL9	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
29	c	522	LMG	O10-C28-O8-C9
31	A	615	LHG	O10-C23-O8-C6
29	c	521	LMG	O9-C10-O7-C8
31	A	615	LHG	C32-C33-C34-C35
28	D	406	PL9	C47-C48-C49-C51
25	h	101	CLA	C3-C5-C6-C7
25	c	512	CLA	CBD-CGD-O2D-CED
31	D	408	LHG	O2-C2-C3-O3
31	e	101	LHG	O2-C2-C3-O3
29	c	522	LMG	C29-C28-O8-C9
30	a	614	SQD	C24-C23-O48-C46
30	F	102	SQD	O10-C23-O48-C46
32	h	103	DGD	C4E-C5E-C6E-O5E
29	c	519	LMG	O6-C5-C6-O5
25	C	509	CLA	CBD-CGD-O2D-CED
25	H	101	CLA	CBD-CGD-O2D-CED
26	d	402	PHO	CBD-CGD-O2D-CED
25	B	602	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	B	602	CLA	C2-C3-C5-C6
25	B	613	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
28	A	611	PL9	C33-C34-C36-C37
28	A	611	PL9	C34-C36-C37-C38
28	A	611	PL9	C44-C46-C47-C48
28	a	611	PL9	C24-C26-C27-C28
25	C	511	CLA	CBD-CGD-O2D-CED
30	a	614	SQD	O10-C23-O48-C46
29	b	622	LMG	O6-C1-O1-C7
30	B	621	SQD	O5-C1-O6-C44
25	B	615	CLA	CBD-CGD-O2D-CED
25	D	404	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	CBD-CGD-O2D-CED
32	C	516	DGD	O6E-C5E-C6E-O5E
25	H	101	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
29	m	101	LMG	C29-C28-O8-C9
30	B	621	SQD	C24-C23-O48-C46
31	A	615	LHG	C24-C23-O8-C6
29	m	101	LMG	C38-C39-C40-C41
25	b	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C15-C16-C17-C18
25	c	507	CLA	C4-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
25	C	513	CLA	CBD-CGD-O2D-CED
25	A	607	CLA	C14-C13-C15-C16
25	B	606	CLA	C14-C13-C15-C16
25	B	614	CLA	C11-C10-C8-C9
25	C	503	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	b	606	CLA	C14-C13-C15-C16
25	b	609	CLA	C14-C13-C15-C16
25	b	610	CLA	C14-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C9
25	c	509	CLA	C6-C7-C8-C9
25	c	511	CLA	C14-C13-C15-C16
25	c	512	CLA	C6-C7-C8-C9
25	d	404	CLA	C6-C7-C8-C9
25	h	101	CLA	C14-C13-C15-C16
30	A	614	SQD	C30-C31-C32-C33
25	c	510	CLA	O1D-CGD-O2D-CED
29	b	622	LMG	C2-C1-O1-C7
30	B	621	SQD	C2-C1-O6-C44
32	h	103	DGD	O6E-C5E-C6E-O5E
25	c	506	CLA	O1A-CGA-O2A-C1
27	B	617	BCR	C7-C8-C9-C34
27	C	515	BCR	C11-C12-C13-C35
27	D	405	BCR	C37-C22-C23-C24
27	T	101	BCR	C7-C8-C9-C34
27	c	515	BCR	C11-C12-C13-C35
27	k	101	BCR	C7-C8-C9-C34
27	t	101	BCR	C7-C8-C9-C34
29	A	613	LMG	O1-C7-C8-O7
25	c	512	CLA	CBA-CGA-O2A-C1
25	A	612	CLA	C15-C16-C17-C18
25	D	404	CLA	C10-C11-C12-C13
25	a	609	CLA	C5-C6-C7-C8
25	c	503	CLA	C8-C10-C11-C12
25	c	510	CLA	C15-C16-C17-C18
31	d	407	LHG	C7-C8-C9-C10
25	C	501	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	A	611	PL9	C12-C13-C14-C15
25	b	606	CLA	C8-C10-C11-C12
25	b	615	CLA	C5-C6-C7-C8
31	e	101	LHG	C23-C24-C25-C26
25	H	101	CLA	C15-C16-C17-C18
25	B	610	CLA	C11-C10-C8-C7
25	B	610	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C15
25	c	506	CLA	C12-C13-C15-C16
25	c	510	CLA	C11-C10-C8-C7
29	d	411	LMG	C28-C29-C30-C31
30	A	614	SQD	C7-C8-C9-C10
33	x	101	STE	C1-C2-C3-C4
28	a	611	PL9	C34-C36-C37-C38
28	a	611	PL9	C39-C41-C42-C43
25	a	607	CLA	C8-C10-C11-C12
29	b	622	LMG	O6-C5-C6-O5
29	c	519	LMG	C4-C5-C6-O5
29	A	613	LMG	C10-C11-C12-C13
31	D	411	LHG	C7-C8-C9-C10
31	d	407	LHG	C23-C24-C25-C26
32	H	103	DGD	C1A-C2A-C3A-C4A
32	c	516	DGD	C1B-C2B-C3B-C4B
33	X	101	STE	C1-C2-C3-C4
33	b	625	STE	C1-C2-C3-C4
25	H	101	CLA	O1A-CGA-O2A-C1
25	A	607	CLA	C10-C11-C12-C13
25	A	612	CLA	C13-C15-C16-C17
25	C	506	CLA	C8-C10-C11-C12
25	C	513	CLA	C15-C16-C17-C18
25	b	613	CLA	C5-C6-C7-C8
25	d	404	CLA	C15-C16-C17-C18
25	b	605	CLA	C2A-CAA-CBA-CGA
25	h	101	CLA	C2A-CAA-CBA-CGA
25	B	602	CLA	C13-C15-C16-C17
25	B	606	CLA	C5-C6-C7-C8
25	B	612	CLA	C8-C10-C11-C12
25	C	508	CLA	C15-C16-C17-C18
25	c	506	CLA	C8-C10-C11-C12
25	c	511	CLA	C13-C15-C16-C17
29	D	410	LMG	C28-C29-C30-C31
29	c	521	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	m	101	LMG	C10-C11-C12-C13
30	A	614	SQD	C23-C24-C25-C26
31	A	615	LHG	C7-C8-C9-C10
33	B	622	STE	C1-C2-C3-C4
32	a	615	DGD	O1A-C1A-O1G-C1G
25	B	601	CLA	C13-C15-C16-C17
25	B	607	CLA	C15-C16-C17-C18
25	C	512	CLA	C5-C6-C7-C8
25	b	610	CLA	C13-C15-C16-C17
25	b	614	CLA	C5-C6-C7-C8
25	b	614	CLA	C15-C16-C17-C18
25	c	506	CLA	C13-C15-C16-C17
25	c	510	CLA	C10-C11-C12-C13
29	D	407	LMG	C10-C11-C12-C13
25	c	509	CLA	C10-C11-C12-C13
25	C	504	CLA	C8-C10-C11-C12
25	C	509	CLA	C5-C6-C7-C8
25	H	101	CLA	C5-C6-C7-C8
25	c	509	CLA	C5-C6-C7-C8
25	c	511	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	C4-C3-C5-C6
25	c	512	CLA	O1A-CGA-O2A-C1
30	B	621	SQD	O10-C23-O48-C46
32	c	518	DGD	O1A-C1A-O1G-C1G
30	B	621	SQD	C23-C24-C25-C26
32	A	617	DGD	C1B-C2B-C3B-C4B
33	b	621	STE	C1-C2-C3-C4
33	c	520	STE	C1-C2-C3-C4
25	B	613	CLA	C13-C15-C16-C17
25	B	614	CLA	C15-C16-C17-C18
25	H	101	CLA	C8-C10-C11-C12
32	a	615	DGD	C2B-C1B-O2G-C2G
30	f	102	SQD	C23-C24-C25-C26
25	A	609	CLA	C3-C5-C6-C7
25	c	512	CLA	O1D-CGD-O2D-CED
31	d	407	LHG	C1-C2-C3-O3
25	B	605	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
32	a	615	DGD	C2A-C1A-O1G-C1G
33	b	625	STE	C2-C3-C4-C5
25	B	613	CLA	C8-C10-C11-C12
25	C	503	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	C5-C6-C7-C8
25	C	507	CLA	C10-C11-C12-C13
25	C	509	CLA	C13-C15-C16-C17
25	c	507	CLA	C5-C6-C7-C8
25	c	509	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
25	c	503	CLA	CBD-CGD-O2D-CED
25	H	101	CLA	O1D-CGD-O2D-CED
33	j	101	STE	C1-C2-C3-C4
25	B	610	CLA	C8-C10-C11-C12
25	c	508	CLA	C13-C15-C16-C17
25	B	615	CLA	C5-C6-C7-C8
25	C	509	CLA	C10-C11-C12-C13
25	a	606	CLA	C15-C16-C17-C18
25	b	607	CLA	C13-C15-C16-C17
25	c	503	CLA	C5-C6-C7-C8
25	b	603	CLA	C4-C3-C5-C6
25	b	606	CLA	C11-C10-C8-C9
26	d	402	PHO	O1D-CGD-O2D-CED
28	D	406	PL9	C32-C33-C34-C35
31	d	409	LHG	C24-C25-C26-C27
32	C	517	DGD	C2E-C1E-O5D-C6D
32	c	517	DGD	C2E-C1E-O5D-C6D
25	C	505	CLA	C5-C6-C7-C8
27	B	616	BCR	C35-C13-C14-C15
27	C	514	BCR	C16-C17-C18-C36
27	C	514	BCR	C20-C21-C22-C37
27	D	405	BCR	C20-C21-C22-C37
27	K	102	BCR	C11-C10-C9-C34
27	a	610	BCR	C16-C17-C18-C36
27	b	616	BCR	C20-C21-C22-C37
27	b	617	BCR	C11-C10-C9-C34
27	b	618	BCR	C20-C21-C22-C37
27	k	101	BCR	C16-C17-C18-C36
29	B	620	LMG	C28-C29-C30-C31
27	d	405	BCR	C7-C8-C9-C34
27	C	514	BCR	C21-C22-C23-C24
27	D	405	BCR	C7-C8-C9-C10
27	b	616	BCR	C21-C22-C23-C24
25	B	611	CLA	C10-C11-C12-C13
31	d	409	LHG	O1-C1-C2-C3
29	D	410	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
30	b	619	SQD	C46-C45-O47-C7
25	B	605	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C20
29	c	521	LMG	C41-C42-C43-C44
25	C	509	CLA	O1D-CGD-O2D-CED
29	A	613	LMG	O6-C5-C6-O5
27	K	102	BCR	C11-C10-C9-C8
27	h	102	BCR	C11-C10-C9-C8
30	B	621	SQD	C29-C30-C31-C32
32	c	517	DGD	O6E-C1E-O5D-C6D
29	b	622	LMG	C11-C10-O7-C8
33	m	102	STE	C6-C7-C8-C9
25	B	606	CLA	C8-C10-C11-C12
25	C	509	CLA	C8-C10-C11-C12
33	c	520	STE	C2-C3-C4-C5
28	a	611	PL9	C16-C17-C18-C19
25	B	615	CLA	O1D-CGD-O2D-CED
32	c	517	DGD	C1A-C2A-C3A-C4A
25	A	606	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C20
25	b	606	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
30	a	613	SQD	C34-C35-C36-C37
32	A	617	DGD	CCA-CDA-CEA-CFA
33	b	621	STE	C14-C15-C16-C17
29	B	620	LMG	C11-C12-C13-C14
29	D	407	LMG	C35-C36-C37-C38
29	d	410	LMG	C35-C36-C37-C38
31	D	408	LHG	C30-C31-C32-C33
31	d	407	LHG	C32-C33-C34-C35
32	A	617	DGD	C2B-C3B-C4B-C5B
32	C	517	DGD	C2A-C3A-C4A-C5A
32	C	517	DGD	C3A-C4A-C5A-C6A
32	h	103	DGD	C5B-C6B-C7B-C8B
33	I	101	STE	C11-C12-C13-C14
33	X	101	STE	C4-C5-C6-C7
33	a	616	STE	C5-C6-C7-C8
33	x	101	STE	C6-C7-C8-C9
29	C	519	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	A	617	DGD	CBA-CCA-CDA-CEA
32	C	516	DGD	C5A-C6A-C7A-C8A
33	H	104	STE	C13-C14-C15-C16
25	B	603	CLA	CBA-CGA-O2A-C1
29	A	613	LMG	C38-C39-C40-C41
29	c	522	LMG	C18-C19-C20-C21
30	a	614	SQD	C11-C12-C13-C14
31	D	411	LHG	C29-C30-C31-C32
31	d	409	LHG	C32-C33-C34-C35
32	c	518	DGD	CCB-CDB-CEB-CFB
33	B	623	STE	C5-C6-C7-C8
33	C	522	STE	C4-C5-C6-C7
33	J	101	STE	C5-C6-C7-C8
33	d	413	STE	C5-C6-C7-C8
30	F	102	SQD	C45-C44-O6-C1
31	d	407	LHG	O1-C1-C2-O2
29	M	101	LMG	C12-C13-C14-C15
29	M	101	LMG	C37-C38-C39-C40
30	a	614	SQD	C14-C15-C16-C17
30	b	619	SQD	C16-C17-C18-C19
31	e	101	LHG	C16-C17-C18-C19
25	C	511	CLA	O1D-CGD-O2D-CED
25	H	101	CLA	C10-C11-C12-C13
25	B	605	CLA	C4B-C3B-CAB-CBB
25	C	512	CLA	C4B-C3B-CAB-CBB
25	b	609	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
29	d	411	LMG	C32-C33-C34-C35
32	A	617	DGD	C8B-C9B-CAB-CBB
25	B	605	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
25	c	507	CLA	C16-C17-C18-C20
30	b	619	SQD	C18-C19-C20-C21
31	D	409	LHG	C28-C29-C30-C31
31	d	407	LHG	C11-C10-C9-C8
32	c	516	DGD	CCB-CDB-CEB-CFB
25	B	613	CLA	C15-C16-C17-C18
25	b	614	CLA	C10-C11-C12-C13
31	D	408	LHG	C12-C13-C14-C15
25	C	508	CLA	C12-C13-C15-C16
25	C	510	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	B	621	SQD	C11-C12-C13-C14
33	b	625	STE	C11-C12-C13-C14
33	b	625	STE	C12-C13-C14-C15
28	D	406	PL9	C47-C48-C49-C50
30	F	102	SQD	C23-C24-C25-C26
25	b	614	CLA	C8-C10-C11-C12
25	b	615	CLA	C10-C11-C12-C13
25	d	404	CLA	C8-C10-C11-C12
29	d	410	LMG	C37-C38-C39-C40
29	m	101	LMG	C17-C18-C19-C20
30	a	614	SQD	C10-C11-C12-C13
31	L	101	LHG	C15-C16-C17-C18
31	L	101	LHG	C32-C33-C34-C35
31	e	101	LHG	C11-C10-C9-C8
33	B	625	STE	C12-C13-C14-C15
25	c	512	CLA	C3A-C2A-CAA-CBA
25	h	101	CLA	C3A-C2A-CAA-CBA
29	D	407	LMG	C20-C21-C22-C23
29	c	519	LMG	C36-C37-C38-C39
30	A	616	SQD	C28-C29-C30-C31
30	f	102	SQD	C32-C33-C34-C35
33	B	625	STE	C5-C6-C7-C8
29	C	519	LMG	C17-C18-C19-C20
25	A	606	CLA	C15-C16-C17-C18
25	H	101	CLA	C16-C17-C18-C20
25	b	613	CLA	CBD-CGD-O2D-CED
32	a	615	DGD	C6A-C7A-C8A-C9A
29	A	613	LMG	C18-C19-C20-C21
29	b	622	LMG	C32-C33-C34-C35
29	c	519	LMG	C31-C32-C33-C34
29	c	521	LMG	C39-C40-C41-C42
30	A	616	SQD	C11-C12-C13-C14
32	A	617	DGD	C4B-C5B-C6B-C7B
32	A	617	DGD	C5B-C6B-C7B-C8B
32	A	617	DGD	C6B-C7B-C8B-C9B
32	C	518	DGD	CBA-CCA-CDA-CEA
32	c	516	DGD	C9B-CAB-CBB-CCB
33	B	622	STE	C5-C6-C7-C8
33	j	101	STE	C5-C6-C7-C8
25	b	608	CLA	C3-C5-C6-C7
29	C	519	LMG	C30-C31-C32-C33
29	D	407	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	D	407	LMG	C21-C22-C23-C24
30	a	613	SQD	C13-C14-C15-C16
31	L	101	LHG	C27-C28-C29-C30
32	c	518	DGD	C4A-C5A-C6A-C7A
33	b	620	STE	C11-C12-C13-C14
33	j	101	STE	C2-C3-C4-C5
30	A	616	SQD	C14-C15-C16-C17
31	e	101	LHG	C27-C28-C29-C30
32	C	517	DGD	CAB-CBB-CCB-CDB
29	b	622	LMG	C16-C17-C18-C19
30	A	616	SQD	C9-C10-C11-C12
31	L	101	LHG	C12-C13-C14-C15
33	X	101	STE	C9-C10-C11-C12
25	c	508	CLA	O1D-CGD-O2D-CED
29	b	622	LMG	C40-C41-C42-C43
30	f	102	SQD	C30-C31-C32-C33
31	D	409	LHG	C24-C25-C26-C27
31	L	101	LHG	C33-C34-C35-C36
31	d	408	LHG	C29-C30-C31-C32
33	B	624	STE	C2-C3-C4-C5
33	d	412	STE	C5-C6-C7-C8
25	b	606	CLA	C16-C17-C18-C19
25	B	614	CLA	C2B-C3B-CAB-CBB
27	D	405	BCR	C23-C24-C25-C30
27	K	101	BCR	C1-C6-C7-C8
27	K	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
33	C	522	STE	C7-C8-C9-C10
29	c	519	LMG	C29-C28-O8-C9
25	B	606	CLA	C13-C15-C16-C17
25	b	605	CLA	C15-C16-C17-C18
29	c	519	LMG	C33-C34-C35-C36
29	c	522	LMG	C33-C34-C35-C36
29	d	410	LMG	C33-C34-C35-C36
33	b	625	STE	C9-C10-C11-C12
25	c	501	CLA	O1D-CGD-O2D-CED
29	c	519	LMG	C38-C39-C40-C41
29	c	521	LMG	C14-C15-C16-C17
33	d	413	STE	C10-C11-C12-C13
32	A	617	DGD	C1A-C2A-C3A-C4A
32	H	103	DGD	C1B-C2B-C3B-C4B
32	a	615	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	C10-C11-C12-C13
32	c	516	DGD	C4A-C5A-C6A-C7A
29	M	101	LMG	O6-C5-C6-O5
29	M	101	LMG	C13-C14-C15-C16
29	c	521	LMG	C36-C37-C38-C39
31	D	409	LHG	C9-C10-C11-C12
29	b	622	LMG	O9-C10-O7-C8
30	A	614	SQD	C11-C10-C9-C8
31	D	409	LHG	C11-C12-C13-C14
32	C	518	DGD	C5A-C6A-C7A-C8A
27	d	405	BCR	C18-C19-C20-C21
25	C	508	CLA	C10-C11-C12-C13
28	A	611	PL9	C23-C24-C26-C27
29	d	410	LMG	C31-C32-C33-C34
31	A	615	LHG	C24-C25-C26-C27
31	d	408	LHG	C16-C17-C18-C19
32	A	617	DGD	C5A-C6A-C7A-C8A
32	c	518	DGD	CBA-CCA-CDA-CEA
33	H	104	STE	C14-C15-C16-C17
33	J	101	STE	C3-C4-C5-C6
33	c	520	STE	C7-C8-C9-C10
33	k	103	STE	C2-C3-C4-C5
29	b	622	LMG	C28-C29-C30-C31
29	c	522	LMG	C12-C13-C14-C15
30	A	614	SQD	C27-C28-C29-C30
31	D	408	LHG	C32-C33-C34-C35
31	d	408	LHG	C15-C16-C17-C18
32	h	103	DGD	C3B-C4B-C5B-C6B
33	X	101	STE	C11-C12-C13-C14
25	D	404	CLA	O1D-CGD-O2D-CED
29	c	521	LMG	C34-C35-C36-C37
30	a	613	SQD	C12-C13-C14-C15
32	C	517	DGD	O6E-C1E-O5D-C6D
29	c	519	LMG	C39-C40-C41-C42
29	c	522	LMG	C15-C16-C17-C18
31	d	409	LHG	C26-C27-C28-C29
32	A	617	DGD	CEB-CFB-CGB-CHB
32	C	517	DGD	C6A-C7A-C8A-C9A
33	C	520	STE	C6-C7-C8-C9
25	b	610	CLA	C15-C16-C17-C18
30	A	614	SQD	C10-C11-C12-C13
31	d	407	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	B	620	LMG	C36-C37-C38-C39
29	d	411	LMG	C33-C34-C35-C36
30	A	616	SQD	C15-C16-C17-C18
30	a	613	SQD	C29-C30-C31-C32
31	A	615	LHG	C34-C35-C36-C37
31	D	408	LHG	C16-C17-C18-C19
32	c	516	DGD	CAA-CBA-CCA-CDA
33	x	101	STE	C11-C12-C13-C14
29	d	410	LMG	C32-C33-C34-C35
31	D	408	LHG	C15-C16-C17-C18
31	L	101	LHG	C18-C19-C20-C21
31	d	408	LHG	C32-C33-C34-C35
32	a	615	DGD	C2B-C3B-C4B-C5B
33	I	101	STE	C11-C10-C9-C8
33	b	624	STE	C12-C13-C14-C15
25	B	603	CLA	O1A-CGA-O2A-C1
33	B	619	STE	C1-C2-C3-C4
33	C	520	STE	C1-C2-C3-C4
32	A	617	DGD	CAB-CBB-CCB-CDB
33	b	624	STE	C5-C6-C7-C8
33	l	101	STE	C3-C4-C5-C6
25	b	608	CLA	CBD-CGD-O2D-CED
31	d	408	LHG	C34-C35-C36-C37
32	H	103	DGD	C7B-C8B-C9B-CAB
33	m	102	STE	C4-C5-C6-C7
31	D	408	LHG	C11-C12-C13-C14
32	c	516	DGD	C3B-C4B-C5B-C6B
25	C	502	CLA	C16-C17-C18-C20
25	H	101	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C20
29	C	519	LMG	C18-C19-C20-C21
30	A	616	SQD	C16-C17-C18-C19
30	a	613	SQD	C9-C10-C11-C12
31	d	408	LHG	C12-C13-C14-C15
33	b	624	STE	C14-C15-C16-C17
33	b	625	STE	C4-C5-C6-C7
32	c	516	DGD	O6D-C5D-C6D-O5D
29	C	519	LMG	C33-C34-C35-C36
33	c	520	STE	C9-C10-C11-C12
33	l	101	STE	C12-C13-C14-C15
31	A	615	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	B	621	SQD	C28-C29-C30-C31
25	B	604	CLA	C15-C16-C17-C18
29	D	407	LMG	C18-C19-C20-C21
32	c	518	DGD	C9B-CAB-CBB-CCB
29	C	519	LMG	C28-C29-C30-C31
29	D	407	LMG	C28-C29-C30-C31
33	H	104	STE	C2-C3-C4-C5
33	H	104	STE	C3-C4-C5-C6
33	X	101	STE	C5-C6-C7-C8
29	c	521	LMG	C16-C17-C18-C19
32	c	516	DGD	CBB-CCB-CDB-CEB
32	h	103	DGD	C2B-C3B-C4B-C5B
28	a	611	PL9	C19-C21-C22-C23
30	A	616	SQD	C19-C20-C21-C22
25	B	612	CLA	C5-C6-C7-C8
25	B	615	CLA	C10-C11-C12-C13
35	F	101	HEM	C4C-C3C-CAC-CBC
25	c	509	CLA	C16-C17-C18-C20
30	A	614	SQD	C26-C27-C28-C29
30	A	616	SQD	C32-C33-C34-C35
30	a	614	SQD	C9-C10-C11-C12
33	X	101	STE	C6-C7-C8-C9
33	k	103	STE	C3-C4-C5-C6
29	D	407	LMG	C17-C18-C19-C20
30	a	614	SQD	C18-C19-C20-C21
32	a	615	DGD	C4A-C5A-C6A-C7A
33	C	522	STE	C11-C10-C9-C8
33	b	624	STE	C11-C10-C9-C8
29	b	622	LMG	C10-C11-C12-C13
33	H	104	STE	C9-C10-C11-C12
33	b	621	STE	C5-C6-C7-C8
29	m	101	LMG	C15-C16-C17-C18
30	b	619	SQD	C14-C15-C16-C17
32	H	103	DGD	C6B-C7B-C8B-C9B
29	A	613	LMG	C11-C12-C13-C14
29	A	613	LMG	C35-C36-C37-C38
30	a	613	SQD	C17-C18-C19-C20
32	C	516	DGD	CCB-CDB-CEB-CFB
32	c	518	DGD	C5A-C6A-C7A-C8A
32	h	103	DGD	CBA-CCA-CDA-CEA
33	H	104	STE	C11-C12-C13-C14
33	a	616	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	D	410	LMG	C11-C12-C13-C14
30	b	619	SQD	C11-C12-C13-C14
30	A	614	SQD	C12-C13-C14-C15
31	A	615	LHG	C11-C10-C9-C8
32	C	516	DGD	C5B-C6B-C7B-C8B
25	c	506	CLA	C2-C1-O2A-CGA
29	D	407	LMG	O6-C5-C6-O5
25	b	601	CLA	C16-C17-C18-C20
25	c	507	CLA	C16-C17-C18-C19
29	B	620	LMG	C29-C30-C31-C32
31	D	411	LHG	C14-C15-C16-C17
32	c	516	DGD	C9A-CAA-CBA-CCA
29	d	411	LMG	O6-C5-C6-O5
30	a	613	SQD	C26-C27-C28-C29
31	A	615	LHG	C17-C18-C19-C20
33	X	101	STE	C10-C11-C12-C13
32	c	518	DGD	C2A-C1A-O1G-C1G
30	F	102	SQD	C26-C27-C28-C29
25	c	506	CLA	C5-C6-C7-C8
29	m	101	LMG	C34-C35-C36-C37
32	A	617	DGD	CBB-CCB-CDB-CEB
32	c	518	DGD	C3B-C4B-C5B-C6B
33	b	621	STE	C15-C16-C17-C18
29	A	613	LMG	C31-C32-C33-C34
29	c	522	LMG	C36-C37-C38-C39
29	m	101	LMG	C14-C15-C16-C17
31	D	411	LHG	C31-C32-C33-C34
31	L	101	LHG	C17-C18-C19-C20
31	d	407	LHG	C17-C18-C19-C20
33	B	623	STE	C10-C11-C12-C13
32	c	516	DGD	O6E-C5E-C6E-O5E
30	a	614	SQD	C11-C10-C9-C8
30	B	621	SQD	C33-C34-C35-C36
25	a	609	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	C5-C6-C7-C8
30	f	102	SQD	C25-C26-C27-C28
33	B	622	STE	C6-C7-C8-C9
33	c	520	STE	C11-C12-C13-C14
30	A	614	SQD	C24-C25-C26-C27
33	d	413	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
31	b	623	LHG	O6-C4-C5-C6
30	A	614	SQD	C14-C15-C16-C17
31	D	409	LHG	C31-C32-C33-C34
32	C	516	DGD	C4B-C5B-C6B-C7B
30	a	613	SQD	C7-C8-C9-C10
25	A	607	CLA	C11-C10-C8-C7
25	A	607	CLA	C12-C13-C15-C16
25	B	601	CLA	C11-C12-C13-C15
25	B	603	CLA	C11-C12-C13-C15
25	B	614	CLA	C11-C12-C13-C15
25	C	503	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	C	511	CLA	C6-C7-C8-C10
25	C	512	CLA	C6-C7-C8-C10
25	C	513	CLA	C11-C10-C8-C7
25	a	607	CLA	C11-C10-C8-C7
25	b	601	CLA	C12-C13-C15-C16
25	b	612	CLA	C12-C13-C15-C16
25	c	508	CLA	C12-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C10
25	d	404	CLA	C6-C7-C8-C10
33	C	522	STE	C5-C6-C7-C8
30	F	102	SQD	C44-C45-C46-O48
33	C	520	STE	C3-C4-C5-C6
25	C	512	CLA	C10-C11-C12-C13
31	d	409	LHG	C27-C28-C29-C30
28	a	611	PL9	C13-C14-C16-C17
32	c	516	DGD	CAB-CBB-CCB-CDB
25	C	510	CLA	CBD-CGD-O2D-CED
25	B	601	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C12-C13-C14
25	B	603	CLA	C14-C13-C15-C16
25	B	610	CLA	C14-C13-C15-C16
25	C	513	CLA	C11-C10-C8-C9
25	D	404	CLA	C6-C7-C8-C9
25	a	607	CLA	C11-C10-C8-C9
25	a	609	CLA	C14-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C9
25	b	614	CLA	C11-C12-C13-C14
25	c	506	CLA	C14-C13-C15-C16
25	c	510	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	511	CLA	C11-C10-C8-C9
30	b	619	SQD	C26-C27-C28-C29
31	D	408	LHG	C25-C26-C27-C28
33	t	103	STE	C5-C6-C7-C8
32	h	103	DGD	C6B-C7B-C8B-C9B
29	m	101	LMG	C30-C31-C32-C33
30	B	621	SQD	C9-C10-C11-C12
31	e	101	LHG	C4-C5-C6-O8
32	A	617	DGD	C1G-C2G-C3G-O3G
33	B	625	STE	C6-C7-C8-C9
33	b	620	STE	C7-C8-C9-C10
31	A	615	LHG	C13-C14-C15-C16
31	d	407	LHG	C16-C17-C18-C19
33	B	623	STE	C9-C10-C11-C12
25	c	512	CLA	C10-C11-C12-C13
30	F	102	SQD	C34-C35-C36-C37
31	e	101	LHG	C18-C19-C20-C21
32	c	518	DGD	C6A-C7A-C8A-C9A
32	c	518	DGD	CCA-CDA-CEA-CFA
33	H	104	STE	C10-C11-C12-C13
33	t	102	STE	C6-C7-C8-C9
31	A	615	LHG	C23-C24-C25-C26
25	B	609	CLA	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C20
29	D	407	LMG	C36-C37-C38-C39
29	m	101	LMG	C11-C12-C13-C14
30	b	619	SQD	C15-C16-C17-C18
31	A	615	LHG	C27-C28-C29-C30
32	A	617	DGD	C2A-C3A-C4A-C5A
32	c	518	DGD	C3A-C4A-C5A-C6A
33	b	624	STE	C13-C14-C15-C16
33	j	101	STE	C4-C5-C6-C7
29	b	622	LMG	C29-C30-C31-C32
31	d	409	LHG	C25-C26-C27-C28
28	a	611	PL9	C32-C33-C34-C36
27	C	515	BCR	C20-C21-C22-C37
32	C	518	DGD	C7B-C8B-C9B-CAB
32	c	516	DGD	C4B-C5B-C6B-C7B
29	b	622	LMG	C13-C14-C15-C16
28	A	611	PL9	C45-C44-C46-C47
28	d	406	PL9	C43-C44-C46-C47
25	a	609	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	d	411	LMG	C35-C36-C37-C38
32	C	517	DGD	C6B-C7B-C8B-C9B
33	H	104	STE	C7-C8-C9-C10
33	c	520	STE	C4-C5-C6-C7
29	m	101	LMG	O10-C28-O8-C9
29	D	410	LMG	C33-C34-C35-C36
29	D	407	LMG	C34-C35-C36-C37
29	M	101	LMG	C18-C19-C20-C21
32	C	517	DGD	C5A-C6A-C7A-C8A
31	D	411	LHG	C23-C24-C25-C26
31	D	411	LHG	C27-C28-C29-C30
32	H	103	DGD	C9A-CAA-CBA-CCA
25	C	513	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	B	615	CLA	CBA-CGA-O2A-C1
29	b	622	LMG	C9-C8-O7-C10
29	c	519	LMG	C37-C38-C39-C40
32	C	518	DGD	C3A-C4A-C5A-C6A
33	b	624	STE	C7-C8-C9-C10
33	k	103	STE	C5-C6-C7-C8
32	A	617	DGD	O6D-C5D-C6D-O5D
25	C	510	CLA	C10-C11-C12-C13
29	b	622	LMG	C17-C18-C19-C20
29	c	522	LMG	C32-C33-C34-C35
29	d	410	LMG	C39-C40-C41-C42
33	t	102	STE	C3-C4-C5-C6
25	D	403	CLA	C2C-C3C-CAC-CBC
33	C	521	STE	C4-C5-C6-C7
33	t	102	STE	C1-C2-C3-C4
32	h	103	DGD	CAB-CBB-CCB-CDB
33	X	101	STE	C3-C4-C5-C6
33	d	413	STE	C9-C10-C11-C12
29	c	521	LMG	C30-C31-C32-C33
33	B	622	STE	C4-C5-C6-C7
32	A	617	DGD	CAA-CBA-CCA-CDA
29	d	410	LMG	C34-C35-C36-C37
30	A	614	SQD	C16-C17-C18-C19
32	C	518	DGD	CAA-CBA-CCA-CDA
25	c	506	CLA	C2-C3-C5-C6
30	B	621	SQD	C14-C15-C16-C17
30	b	619	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
32	h	103	DGD	C9A-CAA-CBA-CCA
25	B	610	CLA	C16-C17-C18-C20
29	b	622	LMG	C39-C40-C41-C42
32	a	615	DGD	C5A-C6A-C7A-C8A
33	l	101	STE	C11-C12-C13-C14
33	x	101	STE	C11-C10-C9-C8
31	D	408	LHG	C35-C36-C37-C38
33	B	619	STE	C12-C13-C14-C15
33	I	101	STE	C12-C13-C14-C15
32	c	516	DGD	C1A-C2A-C3A-C4A
32	C	518	DGD	C6A-C7A-C8A-C9A
33	b	624	STE	C6-C7-C8-C9
29	D	410	LMG	C30-C31-C32-C33
29	c	521	LMG	C15-C16-C17-C18
30	A	616	SQD	C10-C11-C12-C13
31	b	623	LHG	C9-C10-C11-C12
32	H	103	DGD	C5A-C6A-C7A-C8A
30	a	613	SQD	C24-C23-O48-C46
32	A	617	DGD	C2A-C1A-O1G-C1G
32	C	518	DGD	C7A-C8A-C9A-CAA
33	b	621	STE	C12-C13-C14-C15
31	A	615	LHG	C11-C12-C13-C14
32	a	615	DGD	C3B-C4B-C5B-C6B
32	c	518	DGD	C4B-C5B-C6B-C7B
33	I	101	STE	C4-C5-C6-C7
31	D	408	LHG	C18-C19-C20-C21
33	l	101	STE	C15-C16-C17-C18
29	d	411	LMG	C38-C39-C40-C41
32	c	517	DGD	CAB-CBB-CCB-CDB
29	M	101	LMG	C40-C41-C42-C43
33	H	104	STE	C1-C2-C3-C4
33	b	626	STE	C7-C8-C9-C10
31	d	408	LHG	C14-C15-C16-C17
29	d	411	LMG	C10-C11-C12-C13
32	a	615	DGD	C5B-C6B-C7B-C8B
32	a	615	DGD	C6B-C7B-C8B-C9B
32	h	103	DGD	CCA-CDA-CEA-CFA
25	C	501	CLA	O1D-CGD-O2D-CED
29	d	410	LMG	C40-C41-C42-C43
30	A	614	SQD	C17-C18-C19-C20
31	e	101	LHG	C24-C25-C26-C27
33	b	626	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	e	101	LHG	C28-C29-C30-C31
33	t	103	STE	C7-C8-C9-C10
28	d	406	PL9	C37-C38-C39-C40
29	A	613	LMG	C39-C40-C41-C42
25	B	607	CLA	C13-C15-C16-C17
29	c	521	LMG	C32-C33-C34-C35
32	c	517	DGD	CAA-CBA-CCA-CDA
29	D	410	LMG	C10-C11-C12-C13
31	D	411	LHG	C24-C25-C26-C27
33	b	620	STE	C13-C14-C15-C16
25	A	607	CLA	C16-C17-C18-C20
25	C	506	CLA	C4-C3-C5-C6
28	d	406	PL9	C28-C29-C31-C32
30	A	614	SQD	C11-C12-C13-C14
31	d	409	LHG	C35-C36-C37-C38
31	d	408	LHG	C33-C34-C35-C36
33	X	101	STE	C14-C15-C16-C17
31	D	408	LHG	O1-C1-C2-O2
25	A	607	CLA	C11-C10-C8-C9
25	A	612	CLA	C11-C12-C13-C14
25	B	614	CLA	C11-C12-C13-C14
25	C	504	CLA	C11-C10-C8-C9
25	b	601	CLA	C14-C13-C15-C16
25	b	606	CLA	C11-C12-C13-C14
25	b	608	CLA	C14-C13-C15-C16
25	b	612	CLA	C14-C13-C15-C16
25	c	508	CLA	C14-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C9
25	h	101	CLA	C11-C12-C13-C14
32	C	518	DGD	C2B-C3B-C4B-C5B
25	c	511	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	C10-C11-C12-C13
25	c	504	CLA	C5-C6-C7-C8
25	C	503	CLA	C4B-C3B-CAB-CBB
25	a	607	CLA	C4B-C3B-CAB-CBB
25	h	101	CLA	C4B-C3B-CAB-CBB
29	d	411	LMG	C37-C38-C39-C40
32	c	517	DGD	CBB-CCB-CDB-CEB
33	m	102	STE	C3-C4-C5-C6
33	m	102	STE	C7-C8-C9-C10
33	B	625	STE	C13-C14-C15-C16
25	C	506	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	b	601	CLA	C10-C11-C12-C13
29	M	101	LMG	C29-C30-C31-C32
31	D	408	LHG	C29-C30-C31-C32
33	B	625	STE	C7-C8-C9-C10
32	c	516	DGD	C4D-C5D-C6D-O5D
31	D	411	LHG	C28-C29-C30-C31
33	M	102	STE	C11-C10-C9-C8
31	d	409	LHG	C9-C10-C11-C12
33	J	101	STE	C7-C8-C9-C10
32	h	103	DGD	O2G-C1B-C2B-C3B
25	A	612	CLA	C11-C12-C13-C15
25	B	603	CLA	C12-C13-C15-C16
25	B	604	CLA	C11-C10-C8-C7
25	B	607	CLA	C11-C12-C13-C15
25	B	612	CLA	C12-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C7
25	D	404	CLA	C6-C7-C8-C10
25	H	101	CLA	C11-C10-C8-C7
25	a	607	CLA	C12-C13-C15-C16
25	a	609	CLA	C12-C13-C15-C16
25	b	602	CLA	C6-C7-C8-C10
25	b	603	CLA	C12-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C10
25	b	606	CLA	C11-C12-C13-C15
25	b	608	CLA	C12-C13-C15-C16
25	b	610	CLA	C11-C12-C13-C15
25	c	509	CLA	C11-C12-C13-C15
25	c	512	CLA	C6-C7-C8-C10
25	b	602	CLA	C13-C15-C16-C17
25	c	512	CLA	C5-C6-C7-C8
25	B	615	CLA	O1A-CGA-O2A-C1
31	d	407	LHG	O2-C2-C3-O3
31	L	101	LHG	C34-C35-C36-C37
32	c	516	DGD	C2B-C3B-C4B-C5B
32	C	518	DGD	CDA-CEA-CFA-CGA
30	F	102	SQD	C30-C31-C32-C33
32	H	103	DGD	CCA-CDA-CEA-CFA
33	l	101	STE	C7-C8-C9-C10
28	d	406	PL9	C45-C44-C46-C47
32	H	103	DGD	C8A-C9A-CAA-CBA
29	c	522	LMG	C40-C41-C42-C43
25	a	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	C	521	STE	C6-C7-C8-C9
29	C	519	LMG	C31-C32-C33-C34
33	C	522	STE	C9-C10-C11-C12
31	b	623	LHG	C19-C20-C21-C22
27	B	618	BCR	C11-C12-C13-C35
32	C	518	DGD	O6D-C5D-C6D-O5D
32	C	517	DGD	CDA-CEA-CFA-CGA
33	B	619	STE	C7-C8-C9-C10
32	A	617	DGD	CFA-CGA-CHA-CIA
29	A	613	LMG	O1-C7-C8-C9
29	b	622	LMG	O1-C7-C8-C9
29	c	521	LMG	C7-C8-C9-O8
30	a	613	SQD	O6-C44-C45-C46
30	a	614	SQD	C44-C45-C46-O48
31	A	615	LHG	C4-C5-C6-O8
32	A	617	DGD	O1G-C1G-C2G-C3G
33	C	521	STE	C7-C8-C9-C10
33	M	102	STE	C10-C11-C12-C13
29	m	101	LMG	C21-C22-C23-C24
32	a	615	DGD	C8A-C9A-CAA-CBA
33	C	521	STE	C2-C3-C4-C5
33	M	102	STE	C6-C7-C8-C9
29	b	622	LMG	C37-C38-C39-C40
31	d	407	LHG	C12-C13-C14-C15
33	a	616	STE	C2-C3-C4-C5
33	l	101	STE	C14-C15-C16-C17
25	B	608	CLA	C4-C3-C5-C6
25	C	505	CLA	C4-C3-C5-C6
32	h	103	DGD	CCB-CDB-CEB-CFB
30	F	102	SQD	C27-C28-C29-C30
30	a	613	SQD	C11-C12-C13-C14
25	b	608	CLA	O1D-CGD-O2D-CED
25	B	610	CLA	C16-C17-C18-C19
25	b	615	CLA	C11-C12-C13-C15
25	B	611	CLA	C13-C15-C16-C17
31	e	101	LHG	O6-C4-C5-O7
25	h	101	CLA	C2B-C3B-CAB-CBB
27	b	616	BCR	C1-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
25	c	511	CLA	C15-C16-C17-C18
25	c	512	CLA	C8-C10-C11-C12
25	h	101	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	D	407	LMG	C30-C31-C32-C33
31	L	101	LHG	C25-C26-C27-C28
31	b	623	LHG	C10-C11-C12-C13
32	C	518	DGD	C6B-C7B-C8B-C9B
33	M	102	STE	C3-C4-C5-C6
33	x	101	STE	C9-C10-C11-C12
32	a	615	DGD	CFB-CGB-CHB-CIB
30	f	102	SQD	C31-C32-C33-C34
31	L	101	LHG	C13-C14-C15-C16
32	a	615	DGD	CCB-CDB-CEB-CFB
25	C	505	CLA	C15-C16-C17-C18
30	a	614	SQD	C19-C20-C21-C22
31	A	615	LHG	C14-C15-C16-C17
33	k	103	STE	C6-C7-C8-C9
29	b	622	LMG	C18-C19-C20-C21
33	B	625	STE	C4-C5-C6-C7
25	B	609	CLA	C16-C17-C18-C20
25	B	611	CLA	C16-C17-C18-C19
25	a	607	CLA	C16-C17-C18-C20
25	b	601	CLA	C16-C17-C18-C19
25	b	612	CLA	C16-C17-C18-C20
25	c	505	CLA	C10-C11-C12-C13
29	M	101	LMG	O7-C8-C9-O8
29	b	622	LMG	O1-C7-C8-O7
29	c	522	LMG	O7-C8-C9-O8
30	a	613	SQD	O47-C45-C46-O48
30	f	102	SQD	O6-C44-C45-O47
32	A	617	DGD	O1G-C1G-C2G-O2G
28	A	611	PL9	C4-C3-C7-C8
28	a	611	PL9	C4-C3-C7-C8
32	h	103	DGD	C4A-C5A-C6A-C7A
33	b	621	STE	C6-C7-C8-C9
25	B	604	CLA	C8-C10-C11-C12
31	D	409	LHG	C35-C36-C37-C38
27	t	101	BCR	C18-C19-C20-C21
25	b	609	CLA	C15-C16-C17-C18
25	C	505	CLA	C2-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
28	a	611	PL9	C28-C29-C31-C32
31	d	407	LHG	C33-C34-C35-C36
29	D	410	LMG	C34-C35-C36-C37
25	D	404	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	C	508	CLA	C11-C10-C8-C9
25	a	607	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C9
25	b	612	CLA	C11-C12-C13-C14
25	b	614	CLA	C11-C10-C8-C9
32	c	517	DGD	C5B-C6B-C7B-C8B
25	C	513	CLA	C13-C15-C16-C17
27	k	101	BCR	C14-C15-C16-C17
25	A	606	CLA	C16-C17-C18-C20
25	A	607	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C19
25	c	513	CLA	C3-C5-C6-C7
31	e	101	LHG	C14-C15-C16-C17
29	c	522	LMG	C2-C1-O1-C7
29	C	519	LMG	C37-C38-C39-C40
28	d	406	PL9	C34-C36-C37-C38
32	A	617	DGD	C4D-C5D-C6D-O5D
33	t	103	STE	C3-C4-C5-C6
29	d	411	LMG	C40-C41-C42-C43
25	C	509	CLA	C3-C5-C6-C7
31	e	101	LHG	C11-C12-C13-C14
25	C	504	CLA	C11-C12-C13-C14
29	b	622	LMG	C24-C25-C26-C27
32	a	615	DGD	CFA-CGA-CHA-CIA
25	a	607	CLA	C16-C17-C18-C19
29	d	411	LMG	C30-C31-C32-C33
31	D	408	LHG	C28-C29-C30-C31
25	b	613	CLA	O1D-CGD-O2D-CED
33	b	620	STE	C11-C10-C9-C8
25	b	606	CLA	C5-C6-C7-C8
29	b	622	LMG	C30-C31-C32-C33
30	a	613	SQD	C11-C10-C9-C8
31	A	615	LHG	C26-C27-C28-C29
31	L	101	LHG	C30-C31-C32-C33
32	A	617	DGD	CCB-CDB-CEB-CFB
33	d	412	STE	C3-C4-C5-C6
27	D	405	BCR	C11-C10-C9-C34
27	T	101	BCR	C20-C21-C22-C37
27	d	405	BCR	C11-C10-C9-C34
27	k	101	BCR	C35-C13-C14-C15
27	k	101	BCR	C20-C21-C22-C37
27	t	101	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	CBA-CGA-O2A-C1
32	c	518	DGD	C1B-C2B-C3B-C4B
32	H	103	DGD	C4B-C5B-C6B-C7B
25	B	613	CLA	C16-C17-C18-C20
29	b	622	LMG	C36-C37-C38-C39
32	C	518	DGD	O1A-C1A-O1G-C1G
27	b	616	BCR	C37-C22-C23-C24
25	A	607	CLA	C11-C12-C13-C15
25	B	615	CLA	C6-C7-C8-C10
25	C	509	CLA	C12-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C7
25	b	605	CLA	C12-C13-C15-C16
25	b	613	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C10-C8-C7
25	c	513	CLA	C11-C12-C13-C15
25	d	404	CLA	C12-C13-C15-C16
25	h	101	CLA	C11-C12-C13-C15
29	c	522	LMG	C31-C32-C33-C34
31	D	411	LHG	C25-C26-C27-C28
29	c	521	LMG	C29-C30-C31-C32
30	a	613	SQD	O10-C23-O48-C46
32	C	517	DGD	C5D-C6D-O5D-C1E
33	X	101	STE	C13-C14-C15-C16
25	b	612	CLA	C16-C17-C18-C19
28	d	406	PL9	C15-C14-C16-C17
25	B	608	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6
32	c	516	DGD	C2A-C3A-C4A-C5A
29	c	521	LMG	C17-C18-C19-C20
31	D	409	LHG	O1-C1-C2-C3
29	B	620	LMG	C35-C36-C37-C38
31	e	101	LHG	C17-C18-C19-C20
33	b	621	STE	C7-C8-C9-C10
25	B	612	CLA	C15-C16-C17-C18
25	C	506	CLA	C15-C16-C17-C18
30	a	614	SQD	C46-C45-O47-C7
32	a	615	DGD	C1G-C2G-O2G-C1B
25	C	505	CLA	C10-C11-C12-C13
33	B	623	STE	C11-C10-C9-C8
30	a	614	SQD	C25-C26-C27-C28
31	D	411	LHG	C11-C10-C9-C8
33	I	101	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	C	516	DGD	CDB-CEB-CFB-CGB
25	D	404	CLA	O1A-CGA-O2A-C1
32	C	517	DGD	CDB-CEB-CFB-CGB
25	b	608	CLA	C15-C16-C17-C18
29	D	410	LMG	C36-C37-C38-C39
29	C	519	LMG	O1-C7-C8-C9
29	M	101	LMG	C7-C8-C9-O8
29	c	521	LMG	O1-C7-C8-C9
30	B	621	SQD	O6-C44-C45-C46
35	f	101	HEM	C4B-C3B-CAB-CBB
33	t	102	STE	C9-C10-C11-C12
25	c	505	CLA	C15-C16-C17-C18
32	C	516	DGD	CAA-CBA-CCA-CDA
25	c	510	CLA	C4-C3-C5-C6
28	a	611	PL9	C15-C14-C16-C17
25	c	509	CLA	CAA-CBA-CGA-O2A
28	A	611	PL9	C38-C39-C41-C42
30	a	614	SQD	C17-C18-C19-C20
32	C	518	DGD	C3B-C4B-C5B-C6B
33	C	520	STE	C5-C6-C7-C8
29	c	521	LMG	O7-C8-C9-O8
30	a	614	SQD	O47-C45-C46-O48
31	A	615	LHG	O7-C5-C6-O8
32	C	516	DGD	O1G-C1G-C2G-O2G
25	A	607	CLA	C11-C12-C13-C14
25	b	603	CLA	C14-C13-C15-C16
25	b	604	CLA	C11-C10-C8-C9
25	b	610	CLA	C11-C12-C13-C14
25	b	613	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C14
32	c	518	DGD	C7A-C8A-C9A-CAA
29	A	613	LMG	C29-C30-C31-C32
30	a	614	SQD	C24-C25-C26-C27
32	A	617	DGD	CDB-CEB-CFB-CGB
32	H	103	DGD	C3A-C4A-C5A-C6A
32	h	103	DGD	C9B-CAB-CBB-CCB
33	E	101	STE	C4-C5-C6-C7
33	d	413	STE	C11-C12-C13-C14
32	c	517	DGD	C6A-C7A-C8A-C9A
25	B	608	CLA	C13-C15-C16-C17
30	A	616	SQD	C11-C10-C9-C8
30	B	621	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
32	A	617	DGD	CEA-CFA-CGA-CHA
33	C	521	STE	C1-C2-C3-C4
30	A	616	SQD	C17-C18-C19-C20
31	A	615	LHG	C28-C29-C30-C31
29	C	519	LMG	C32-C33-C34-C35
25	B	613	CLA	C16-C17-C18-C19
25	b	609	CLA	C16-C17-C18-C20
25	C	513	CLA	C8-C10-C11-C12
33	E	101	STE	C6-C7-C8-C9
33	M	102	STE	C5-C6-C7-C8
33	x	101	STE	C12-C13-C14-C15
25	c	512	CLA	C4-C3-C5-C6
25	B	603	CLA	C15-C16-C17-C18
25	C	512	CLA	C13-C15-C16-C17
25	b	606	CLA	C13-C15-C16-C17
25	C	501	CLA	C2A-CAA-CBA-CGA
31	L	101	LHG	C28-C29-C30-C31
25	C	511	CLA	C16-C17-C18-C19
25	B	609	CLA	C13-C15-C16-C17
33	B	619	STE	C9-C10-C11-C12
33	C	521	STE	C3-C4-C5-C6
33	b	625	STE	C14-C15-C16-C17
29	m	101	LMG	C37-C38-C39-C40
31	D	409	LHG	C11-C10-C9-C8
32	c	518	DGD	C2B-C3B-C4B-C5B
27	T	101	BCR	C11-C12-C13-C35
25	C	504	CLA	C4B-C3B-CAB-CBB
25	D	403	CLA	C4B-C3B-CAB-CBB
25	H	101	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	C4B-C3B-CAB-CBB
25	C	510	CLA	O1D-CGD-O2D-CED
25	a	609	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	C15-C16-C17-C18
32	C	516	DGD	O1G-C1A-C2A-C3A
28	d	406	PL9	C33-C34-C36-C37
32	H	103	DGD	CDB-CEB-CFB-CGB
33	b	625	STE	C15-C16-C17-C18
25	b	612	CLA	CBD-CGD-O2D-CED
31	D	408	LHG	O9-C7-O7-C5
32	a	615	DGD	C7B-C8B-C9B-CAB
33	j	101	STE	C3-C4-C5-C6
32	c	517	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
25	A	612	CLA	C12-C13-C15-C16
25	B	609	CLA	C12-C13-C15-C16
25	B	612	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C10-C8-C7
25	b	605	CLA	C11-C10-C8-C7
25	b	606	CLA	C12-C13-C15-C16
25	b	613	CLA	C11-C10-C8-C7
25	c	505	CLA	C6-C7-C8-C10
25	c	510	CLA	C12-C13-C15-C16
25	B	612	CLA	C16-C17-C18-C19
25	B	612	CLA	C16-C17-C18-C20
32	C	516	DGD	C7A-C8A-C9A-CAA
25	c	504	CLA	O1A-CGA-O2A-C1
32	C	517	DGD	C8B-C9B-CAB-CBB
31	d	409	LHG	C2-C3-O3-P
29	A	613	LMG	C13-C14-C15-C16
31	L	101	LHG	C11-C12-C13-C14
32	c	516	DGD	C6B-C7B-C8B-C9B
32	h	103	DGD	C6A-C7A-C8A-C9A
29	M	101	LMG	C20-C21-C22-C23
31	b	623	LHG	O6-C4-C5-O7
32	C	518	DGD	C4A-C5A-C6A-C7A
25	B	604	CLA	C11-C10-C8-C9
25	B	607	CLA	C11-C12-C13-C14
25	B	615	CLA	C6-C7-C8-C9
25	C	511	CLA	C6-C7-C8-C9
25	b	602	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	611	CLA	C14-C13-C15-C16
25	c	513	CLA	C11-C12-C13-C14
30	F	102	SQD	C25-C26-C27-C28
31	D	408	LHG	C14-C15-C16-C17
25	B	609	CLA	C5-C6-C7-C8
25	C	502	CLA	C13-C15-C16-C17
31	D	411	LHG	C32-C33-C34-C35
25	C	513	CLA	C16-C17-C18-C19
29	b	622	LMG	C34-C35-C36-C37
33	t	102	STE	C7-C8-C9-C10
33	x	101	STE	C13-C14-C15-C16
33	b	626	STE	C4-C5-C6-C7
29	C	519	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
32	a	615	DGD	CDB-CEB-CFB-CGB
25	b	603	CLA	C13-C15-C16-C17
30	F	102	SQD	C32-C33-C34-C35
25	C	505	CLA	C16-C17-C18-C19
25	b	604	CLA	C16-C17-C18-C20
31	D	411	LHG	C26-C27-C28-C29
29	A	613	LMG	C7-C8-C9-O8
29	c	522	LMG	O1-C7-C8-C9
29	c	522	LMG	C7-C8-C9-O8
32	C	516	DGD	O1G-C1G-C2G-C3G
32	a	615	DGD	CBA-CCA-CDA-CEA
33	E	101	STE	C5-C6-C7-C8
25	C	502	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	a	609	CLA	O1A-CGA-O2A-C1
29	d	410	LMG	C36-C37-C38-C39
29	C	519	LMG	C29-C28-O8-C9
29	C	519	LMG	O6-C1-O1-C7
25	B	606	CLA	C10-C11-C12-C13
25	a	609	CLA	C16-C17-C18-C20
32	h	103	DGD	C8A-C9A-CAA-CBA
29	m	101	LMG	C40-C41-C42-C43
30	A	614	SQD	C33-C34-C35-C36
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	b	615	CLA	CHA-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O2D
27	a	610	BCR	C20-C21-C22-C37
30	A	616	SQD	C46-C45-O47-C7
31	D	408	LHG	C4-O6-P-O5
31	D	409	LHG	C3-O3-P-O5
31	D	411	LHG	C3-O3-P-O5
31	d	408	LHG	C4-O6-P-O5
31	e	101	LHG	C3-O3-P-O4
28	d	406	PL9	C30-C29-C31-C32
25	B	605	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C2B-C3B-CAB-CBB
25	H	101	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	a	607	CLA	C2B-C3B-CAB-CBB
25	b	604	CLA	C2B-C3B-CAB-CBB
25	b	609	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C2B-C3B-CAB-CBB
27	t	101	BCR	C5-C6-C7-C8
31	d	407	LHG	C25-C26-C27-C28
28	d	406	PL9	C13-C14-C16-C17
33	b	624	STE	C11-C12-C13-C14
30	A	616	SQD	C13-C14-C15-C16
25	B	614	CLA	C16-C17-C18-C20
30	A	616	SQD	C23-C24-C25-C26
31	b	623	LHG	C14-C15-C16-C17
29	m	101	LMG	C16-C17-C18-C19
32	c	516	DGD	C5B-C6B-C7B-C8B
29	c	519	LMG	O9-C10-O7-C8
30	a	614	SQD	C16-C17-C18-C19
32	C	518	DGD	C8B-C9B-CAB-CBB
33	d	413	STE	C2-C3-C4-C5
29	c	521	LMG	C42-C43-C44-C45
30	b	619	SQD	C30-C31-C32-C33
33	b	625	STE	C13-C14-C15-C16
25	B	605	CLA	C15-C16-C17-C18
29	D	407	LMG	C32-C33-C34-C35
29	d	410	LMG	C38-C39-C40-C41
32	c	518	DGD	C2A-C3A-C4A-C5A
32	C	516	DGD	O6D-C5D-C6D-O5D
29	m	101	LMG	C22-C23-C24-C25
25	c	510	CLA	C2-C3-C5-C6
31	e	101	LHG	O6-C4-C5-C6
29	C	519	LMG	C11-C12-C13-C14
25	c	505	CLA	C3-C5-C6-C7
25	A	612	CLA	C14-C13-C15-C16
25	B	612	CLA	C11-C12-C13-C14
25	B	612	CLA	C14-C13-C15-C16
25	C	505	CLA	C11-C10-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	H	101	CLA	C11-C10-C8-C9
25	c	504	CLA	C11-C10-C8-C9
25	c	510	CLA	C11-C10-C8-C9
26	a	608	PHO	C14-C13-C15-C16
25	C	512	CLA	C11-C10-C8-C7
25	b	611	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	507	CLA	C11-C10-C8-C7
25	c	509	CLA	C12-C13-C15-C16
25	h	101	CLA	C6-C7-C8-C10
25	C	508	CLA	C16-C17-C18-C19
33	C	520	STE	C4-C5-C6-C7
32	H	103	DGD	C9B-CAB-CBB-CCB
29	D	410	LMG	C37-C38-C39-C40
31	b	623	LHG	C34-C35-C36-C37
25	B	614	CLA	C16-C17-C18-C19
25	C	512	CLA	C16-C17-C18-C19
25	b	605	CLA	C16-C17-C18-C19
30	F	102	SQD	C24-C25-C26-C27
32	c	517	DGD	C9A-CAA-CBA-CCA
31	e	101	LHG	O7-C5-C6-O8
32	c	516	DGD	O1G-C1G-C2G-O2G
29	d	411	LMG	C15-C16-C17-C18
25	B	612	CLA	C13-C15-C16-C17
31	d	407	LHG	C26-C27-C28-C29
25	b	605	CLA	C16-C17-C18-C20
33	H	104	STE	C6-C7-C8-C9
33	M	103	STE	C1-C2-C3-C4
33	x	101	STE	C2-C3-C4-C5
25	D	404	CLA	C16-C17-C18-C20
32	H	103	DGD	O2G-C1B-C2B-C3B
29	d	411	LMG	C14-C15-C16-C17
26	d	402	PHO	C2C-C3C-CAC-CBC
27	c	515	BCR	C7-C8-C9-C34
27	h	102	BCR	C7-C8-C9-C34
32	C	516	DGD	C4E-C5E-C6E-O5E
29	c	522	LMG	C14-C15-C16-C17
27	T	101	BCR	C11-C12-C13-C14
25	a	612	CLA	C2C-C3C-CAC-CBC
32	c	516	DGD	C5D-C6D-O5D-C1E
33	b	624	STE	C15-C16-C17-C18
29	D	407	LMG	C38-C39-C40-C41
30	b	619	SQD	C29-C30-C31-C32
30	B	621	SQD	C35-C36-C37-C38
32	C	516	DGD	C1B-C2B-C3B-C4B
33	b	626	STE	C1-C2-C3-C4
25	A	612	CLA	C16-C17-C18-C19
25	C	506	CLA	C14-C13-C15-C16
25	C	508	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	C14-C13-C15-C16
25	b	613	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	d	404	CLA	O1D-CGD-O2D-CED
31	d	407	LHG	C27-C28-C29-C30
33	x	101	STE	C5-C6-C7-C8
29	c	522	LMG	C29-C30-C31-C32
29	c	522	LMG	C34-C35-C36-C37
33	I	101	STE	C1-C2-C3-C4
28	a	611	PL9	C42-C43-C44-C46
25	b	611	CLA	C10-C11-C12-C13
25	c	504	CLA	C8-C10-C11-C12
30	F	102	SQD	O48-C23-C24-C25
25	c	512	CLA	C2-C3-C5-C6
33	b	621	STE	C4-C5-C6-C7
25	B	614	CLA	C13-C15-C16-C17
29	d	411	LMG	C11-C12-C13-C14
31	D	408	LHG	C11-C10-C9-C8
33	l	101	STE	C9-C10-C11-C12
25	C	506	CLA	C11-C12-C13-C15
25	C	506	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C15
25	b	610	CLA	C12-C13-C15-C16
25	c	511	CLA	C12-C13-C15-C16
29	D	410	LMG	C31-C32-C33-C34
32	c	518	DGD	C7B-C8B-C9B-CAB
32	c	516	DGD	CBA-CCA-CDA-CEA
32	C	516	DGD	C4D-C5D-C6D-O5D
29	D	407	LMG	C15-C16-C17-C18
29	c	521	LMG	O1-C7-C8-O7
29	c	522	LMG	O1-C7-C8-O7
30	A	614	SQD	O6-C44-C45-O47
30	b	619	SQD	C28-C29-C30-C31
25	B	614	CLA	C4-C3-C5-C6
28	d	406	PL9	C32-C33-C34-C36
31	L	101	LHG	C10-C11-C12-C13
31	d	408	LHG	C28-C29-C30-C31
25	c	503	CLA	C15-C16-C17-C18
25	c	513	CLA	C8-C10-C11-C12
32	C	516	DGD	C6A-C7A-C8A-C9A
32	c	517	DGD	C9B-CAB-CBB-CCB
27	k	101	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
33	B	619	STE	C10-C11-C12-C13
33	B	622	STE	C7-C8-C9-C10
31	L	101	LHG	C19-C20-C21-C22
36	v	201	HEC	CAD-CBD-CGD-O1D
25	B	604	CLA	C4-C3-C5-C6
25	D	404	CLA	C16-C17-C18-C19
25	c	501	CLA	C2A-CAA-CBA-CGA
29	D	410	LMG	C7-C8-C9-O8
30	a	613	SQD	C44-C45-C46-O48
29	B	620	LMG	O7-C10-C11-C12
33	d	413	STE	O1-C1-C2-C3
25	B	607	CLA	C14-C13-C15-C16
25	B	608	CLA	C11-C10-C8-C9
25	B	609	CLA	C11-C12-C13-C14
25	C	502	CLA	C11-C12-C13-C14
25	C	506	CLA	C11-C12-C13-C14
25	b	602	CLA	C14-C13-C15-C16
25	c	508	CLA	C11-C12-C13-C14
25	c	513	CLA	C6-C7-C8-C9
33	d	412	STE	C10-C11-C12-C13
33	x	101	STE	C10-C11-C12-C13
30	B	621	SQD	C46-C45-O47-C7
29	D	410	LMG	O1-C7-C8-C9
33	B	623	STE	C3-C4-C5-C6
33	d	413	STE	C6-C7-C8-C9
28	A	611	PL9	C28-C29-C31-C32
30	a	614	SQD	C13-C14-C15-C16
33	J	101	STE	C4-C5-C6-C7
33	d	413	STE	O2-C1-C2-C3
36	v	201	HEC	CAD-CBD-CGD-O2D
31	d	409	LHG	C11-C10-C9-C8
33	c	520	STE	C10-C11-C12-C13
31	D	411	LHG	C30-C31-C32-C33
25	B	601	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
27	K	101	BCR	C16-C17-C18-C19
27	T	101	BCR	C20-C21-C22-C23
25	b	602	CLA	C16-C17-C18-C20
35	f	101	HEM	CAD-CBD-CGD-O1D
31	b	623	LHG	C27-C28-C29-C30
33	H	104	STE	C11-C10-C9-C8
25	B	608	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	C	504	CLA	C2B-C3B-CAB-CBB
25	b	602	CLA	C2B-C3B-CAB-CBB
27	B	616	BCR	C1-C6-C7-C8
27	H	102	BCR	C23-C24-C25-C30
27	K	102	BCR	C1-C6-C7-C8
27	T	101	BCR	C1-C6-C7-C8
27	b	617	BCR	C23-C24-C25-C30
32	c	517	DGD	C1B-C2B-C3B-C4B
25	D	403	CLA	C15-C16-C17-C18
28	a	611	PL9	C40-C39-C41-C42
29	A	613	LMG	C4-C5-C6-O5
25	B	614	CLA	C2-C3-C5-C6
33	B	619	STE	C5-C6-C7-C8
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C12-C13-C15-C16
25	B	606	CLA	C12-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C15
25	C	507	CLA	C11-C10-C8-C7
25	D	403	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C10-C8-C7
25	b	611	CLA	C11-C10-C8-C7
25	c	504	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	d	403	CLA	C6-C7-C8-C10
25	C	513	CLA	C16-C17-C18-C20
25	b	609	CLA	C2A-CAA-CBA-CGA
29	D	410	LMG	O7-C8-C9-O8
29	B	620	LMG	O10-C28-C29-C30
35	F	101	HEM	CAD-CBD-CGD-O1D
32	c	517	DGD	C5A-C6A-C7A-C8A
30	B	621	SQD	C24-C25-C26-C27
31	D	409	LHG	C25-C26-C27-C28
32	h	103	DGD	C1A-C2A-C3A-C4A
33	B	622	STE	O2-C1-C2-C3
28	A	611	PL9	C12-C11-C9-C10
28	A	611	PL9	C15-C14-C16-C17
28	a	611	PL9	C38-C39-C41-C42
32	h	103	DGD	CAA-CBA-CCA-CDA
25	c	512	CLA	C13-C15-C16-C17
25	c	504	CLA	C11-C12-C13-C15
30	a	613	SQD	C10-C11-C12-C13
31	e	101	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	b	619	SQD	C19-C20-C21-C22
29	B	620	LMG	O9-C10-C11-C12
25	B	614	CLA	C6-C7-C8-C9
25	H	101	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C9
25	b	601	CLA	C15-C16-C17-C18
29	c	521	LMG	C12-C13-C14-C15
25	b	612	CLA	C8-C10-C11-C12
29	D	410	LMG	C13-C14-C15-C16
32	H	103	DGD	CBB-CCB-CDB-CEB
25	b	605	CLA	C13-C15-C16-C17
25	B	604	CLA	C2-C3-C5-C6
29	c	522	LMG	C20-C21-C22-C23
25	A	606	CLA	C13-C15-C16-C17
25	a	609	CLA	C16-C17-C18-C19
30	A	614	SQD	C35-C36-C37-C38
35	F	101	HEM	CAD-CBD-CGD-O2D
32	c	516	DGD	O1A-C1A-O1G-C1G
33	C	522	STE	C15-C16-C17-C18
29	D	407	LMG	C33-C34-C35-C36
32	c	516	DGD	O1G-C1G-C2G-C3G
32	h	103	DGD	C1G-C2G-C3G-O3G
35	f	101	HEM	CAD-CBD-CGD-O2D
29	D	410	LMG	O1-C7-C8-O7
30	a	614	SQD	O6-C44-C45-O47
32	a	615	DGD	C3A-C4A-C5A-C6A
25	B	611	CLA	O1A-CGA-O2A-C1
33	m	102	STE	C5-C6-C7-C8
25	B	603	CLA	C13-C15-C16-C17
29	A	613	LMG	C15-C16-C17-C18
25	H	101	CLA	C4-C3-C5-C6
29	c	519	LMG	C34-C35-C36-C37
30	a	614	SQD	C15-C16-C17-C18
33	B	619	STE	C2-C3-C4-C5
25	b	602	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
29	B	620	LMG	O8-C28-C29-C30
25	c	506	CLA	C10-C11-C12-C13
35	f	101	HEM	CAA-CBA-CGA-O2A
26	D	402	PHO	CHA-CBD-CGD-O1D
27	B	617	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
27	h	102	BCR	C20-C21-C22-C37
32	h	103	DGD	CDB-CEB-CFB-CGB
25	a	612	CLA	C4C-C3C-CAC-CBC
33	H	104	STE	C5-C6-C7-C8
33	b	621	STE	O2-C1-C2-C3
33	b	625	STE	C3-C4-C5-C6
25	b	613	CLA	C10-C11-C12-C13
31	D	409	LHG	C2-C3-O3-P
30	b	619	SQD	C12-C13-C14-C15
32	C	517	DGD	C2B-C3B-C4B-C5B
25	B	614	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C12-C13-C15
25	C	512	CLA	C12-C13-C15-C16
33	M	103	STE	C7-C8-C9-C10
33	B	623	STE	C11-C12-C13-C14
32	C	517	DGD	C8A-C9A-CAA-CBA
31	A	615	LHG	C10-C11-C12-C13
33	b	621	STE	O1-C1-C2-C3
33	d	412	STE	O1-C1-C2-C3
25	B	612	CLA	C6-C7-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	D	404	CLA	C11-C10-C8-C9
29	M	101	LMG	C8-C7-O1-C1
32	C	517	DGD	C2G-C3G-O3G-C1D
32	c	517	DGD	C5D-C6D-O5D-C1E
32	a	615	DGD	CEB-CFB-CGB-CHB
33	B	622	STE	O1-C1-C2-C3
25	C	506	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
25	C	511	CLA	C8-C10-C11-C12
25	b	612	CLA	O1D-CGD-O2D-CED
29	d	411	LMG	C36-C37-C38-C39
30	f	102	SQD	C27-C28-C29-C30
25	B	601	CLA	C3A-C2A-CAA-CBA
30	a	613	SQD	C30-C31-C32-C33
28	D	406	PL9	C38-C39-C41-C42
25	B	611	CLA	CBA-CGA-O2A-C1
29	c	521	LMG	C11-C12-C13-C14
32	c	516	DGD	C3A-C4A-C5A-C6A
25	B	615	CLA	O2A-C1-C2-C3
26	a	608	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	B	621	SQD	C44-C45-O47-C7
33	b	621	STE	C10-C11-C12-C13
28	a	611	PL9	C17-C18-C19-C20
32	c	516	DGD	O1G-C1A-C2A-C3A
28	A	611	PL9	C30-C29-C31-C32
32	c	518	DGD	CBB-CCB-CDB-CEB
27	B	618	BCR	C12-C13-C14-C15
35	f	101	HEM	CAA-CBA-CGA-O1A
25	c	509	CLA	C3-C5-C6-C7
30	A	616	SQD	C7-C8-C9-C10
33	d	412	STE	C6-C7-C8-C9
29	b	622	LMG	C4-C5-C6-O5
28	A	611	PL9	C9-C11-C12-C13
29	m	101	LMG	C7-C8-C9-O8
30	f	102	SQD	O6-C44-C45-C46
26	d	402	PHO	C5-C6-C7-C8
33	X	101	STE	C7-C8-C9-C10
29	A	613	LMG	C17-C18-C19-C20
31	b	623	LHG	C11-C12-C13-C14
25	C	512	CLA	C4-C3-C5-C6
29	m	101	LMG	O8-C28-C29-C30
32	C	518	DGD	C5B-C6B-C7B-C8B
29	A	613	LMG	O7-C8-C9-O8
25	B	606	CLA	C11-C10-C8-C9
25	B	609	CLA	C14-C13-C15-C16
25	C	501	CLA	C14-C13-C15-C16
25	D	403	CLA	C11-C10-C8-C9
25	b	611	CLA	C11-C10-C8-C9
25	c	505	CLA	C6-C7-C8-C9
25	c	507	CLA	C6-C7-C8-C9
25	c	507	CLA	C11-C10-C8-C9
25	c	509	CLA	C11-C10-C8-C9
25	b	609	CLA	C16-C17-C18-C19
31	D	409	LHG	C12-C13-C14-C15
25	A	606	CLA	C2C-C3C-CAC-CBC
31	A	615	LHG	C16-C17-C18-C19
29	c	519	LMG	O10-C28-O8-C9
36	V	201	HEC	CAD-CBD-CGD-O2D
25	B	614	CLA	C6-C7-C8-C10
25	C	505	CLA	C12-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C10
25	D	404	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	c	501	CLA	C11-C12-C13-C15
25	h	101	CLA	C12-C13-C15-C16
29	A	613	LMG	C33-C34-C35-C36
25	b	611	CLA	C3-C5-C6-C7
31	D	409	LHG	C17-C18-C19-C20
36	V	201	HEC	CAD-CBD-CGD-O1D
25	C	503	CLA	C2B-C3B-CAB-CBB
25	D	403	CLA	C2B-C3B-CAB-CBB
25	c	507	CLA	C2B-C3B-CAB-CBB
27	B	616	BCR	C5-C6-C7-C8
27	H	102	BCR	C23-C24-C25-C26
27	K	102	BCR	C5-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	b	616	BCR	C5-C6-C7-C8
27	b	617	BCR	C23-C24-C25-C26
27	c	514	BCR	C23-C24-C25-C26
27	c	514	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C30
33	C	522	STE	C3-C4-C5-C6
25	b	611	CLA	CAA-CBA-CGA-O2A
25	B	612	CLA	C2-C1-O2A-CGA
33	C	522	STE	C12-C13-C14-C15
25	B	615	CLA	C11-C12-C13-C14
28	A	611	PL9	C14-C16-C17-C18
32	c	516	DGD	O2G-C1B-C2B-C3B
25	c	509	CLA	CAA-CBA-CGA-O1A
26	A	608	PHO	C8-C10-C11-C12
33	b	624	STE	C9-C10-C11-C12
25	C	511	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
25	B	605	CLA	C8-C10-C11-C12
28	a	611	PL9	C23-C24-C26-C27
30	a	613	SQD	C27-C28-C29-C30
31	D	411	LHG	C10-C11-C12-C13
33	d	412	STE	O2-C1-C2-C3
30	a	613	SQD	O47-C7-C8-C9
31	b	623	LHG	C25-C26-C27-C28
25	B	612	CLA	C10-C11-C12-C13
29	c	521	LMG	C35-C36-C37-C38
27	c	514	BCR	C16-C17-C18-C36
25	b	601	CLA	C2A-CAA-CBA-CGA
30	F	102	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C15-C16-C17-C18
31	D	409	LHG	C29-C30-C31-C32
25	C	505	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C10-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	c	504	CLA	C6-C7-C8-C9
31	D	408	LHG	C17-C18-C19-C20
33	c	520	STE	C11-C10-C9-C8
31	A	615	LHG	C2-C3-O3-P
25	B	611	CLA	CAA-CBA-CGA-O2A
32	c	517	DGD	CCB-CDB-CEB-CFB
25	h	101	CLA	C13-C15-C16-C17
25	B	608	CLA	C4B-C3B-CAB-CBB
25	b	614	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C1A-C2A-CAA-CBA
28	A	611	PL9	C25-C24-C26-C27
32	C	516	DGD	O6E-C1E-O5D-C6D
29	b	622	LMG	O7-C8-C9-O8
27	H	102	BCR	C11-C12-C13-C14
27	c	515	BCR	C7-C8-C9-C10
31	d	408	LHG	C25-C26-C27-C28
25	B	602	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	C2A-CAA-CBA-CGA
33	X	101	STE	C2-C3-C4-C5
25	d	404	CLA	C16-C17-C18-C19
29	b	622	LMG	O7-C10-C11-C12
25	b	604	CLA	C10-C11-C12-C13
25	b	612	CLA	CAA-CBA-CGA-O2A
29	M	101	LMG	C33-C34-C35-C36
25	B	606	CLA	C11-C10-C8-C7
25	C	505	CLA	C6-C7-C8-C10
25	b	601	CLA	C11-C10-C8-C7
25	c	507	CLA	C12-C13-C15-C16
25	c	509	CLA	C6-C7-C8-C10
25	h	101	CLA	C11-C10-C8-C7
29	c	522	LMG	C11-C12-C13-C14
29	C	519	LMG	O9-C10-C11-C12
33	C	522	STE	C11-C12-C13-C14
25	B	612	CLA	CAA-CBA-CGA-O2A
29	m	101	LMG	C33-C34-C35-C36
31	D	411	LHG	C33-C34-C35-C36
33	B	623	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	c	509	CLA	C2A-CAA-CBA-CGA
32	c	518	DGD	O1B-C1B-O2G-C2G
31	d	409	LHG	C23-C24-C25-C26
33	E	101	STE	O1-C1-C2-C3
25	b	608	CLA	C13-C15-C16-C17
33	E	101	STE	C7-C8-C9-C10
32	c	516	DGD	O1B-C1B-C2B-C3B
29	c	522	LMG	C19-C20-C21-C22
25	B	601	CLA	C8-C10-C11-C12
25	C	501	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
29	C	519	LMG	C16-C17-C18-C19
27	k	101	BCR	C20-C21-C22-C23
30	a	614	SQD	C12-C13-C14-C15
33	l	101	STE	C13-C14-C15-C16
29	m	101	LMG	C29-C30-C31-C32
25	B	604	CLA	C14-C13-C15-C16
25	c	509	CLA	C14-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C9
25	h	101	CLA	C6-C7-C8-C9
30	A	614	SQD	C34-C35-C36-C37
30	B	621	SQD	C13-C14-C15-C16
25	b	614	CLA	C16-C17-C18-C19
28	D	406	PL9	C15-C14-C16-C17
25	b	611	CLA	CAA-CBA-CGA-O1A
25	b	613	CLA	C13-C15-C16-C17
29	m	101	LMG	C12-C13-C14-C15
25	c	508	CLA	C10-C11-C12-C13
25	c	505	CLA	C13-C15-C16-C17
29	c	522	LMG	C8-C7-O1-C1
29	m	101	LMG	O7-C8-C9-O8
25	b	613	CLA	C8-C10-C11-C12
30	A	614	SQD	O6-C44-C45-C46
30	a	613	SQD	O49-C7-C8-C9
25	b	602	CLA	C10-C11-C12-C13
29	m	101	LMG	O9-C10-C11-C12
31	D	409	LHG	O2-C2-C3-O3
31	D	409	LHG	C33-C34-C35-C36
25	b	606	CLA	C10-C11-C12-C13
31	b	623	LHG	C28-C29-C30-C31
32	c	516	DGD	O6E-C1E-O5D-C6D
25	A	606	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	D	403	CLA	C2-C1-O2A-CGA
31	L	101	LHG	O7-C7-C8-C9
31	e	101	LHG	O8-C23-C24-C25
32	C	516	DGD	O2G-C1B-C2B-C3B
25	B	615	CLA	C11-C12-C13-C15
32	C	517	DGD	C9A-CAA-CBA-CCA
25	C	508	CLA	C13-C15-C16-C17
31	d	407	LHG	C10-C11-C12-C13
25	H	101	CLA	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
33	E	101	STE	O2-C1-C2-C3
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
29	b	622	LMG	O9-C10-C11-C12

There are no ring outliers.

149 monomers are involved in 250 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	408	LHG	2	0
31	d	407	LHG	5	0
25	a	606	CLA	1	0
25	c	504	CLA	1	0
25	C	507	CLA	1	0
33	C	522	STE	1	0
27	H	102	BCR	1	0
32	c	518	DGD	4	0
31	d	409	LHG	1	0
25	B	612	CLA	5	0
34	D	401	BCT	1	0
27	k	101	BCR	1	0
32	A	617	DGD	4	0
25	b	609	CLA	1	0
27	K	102	BCR	2	0
33	b	624	STE	1	0
29	m	101	LMG	5	0
29	D	407	LMG	2	0
25	A	607	CLA	1	0
26	d	402	PHO	1	0
25	B	615	CLA	1	0
25	h	101	CLA	2	0
36	v	201	HEC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	k	102	BCR	3	0
32	h	103	DGD	1	0
25	C	504	CLA	2	0
25	b	610	CLA	1	0
25	d	404	CLA	1	0
25	a	612	CLA	1	0
26	A	608	PHO	1	0
29	B	620	LMG	1	0
29	c	521	LMG	1	0
30	a	614	SQD	1	0
25	b	614	CLA	5	0
25	C	503	CLA	1	0
33	x	101	STE	2	0
25	B	606	CLA	3	0
33	c	520	STE	1	0
29	M	101	LMG	2	0
25	c	501	CLA	3	0
25	B	604	CLA	4	0
33	H	104	STE	1	0
25	C	511	CLA	2	0
27	t	101	BCR	2	0
28	D	406	PL9	1	0
32	c	516	DGD	2	0
25	B	609	CLA	2	0
25	B	608	CLA	1	0
32	H	103	DGD	5	0
33	d	413	STE	1	0
25	c	509	CLA	2	0
27	c	515	BCR	1	0
25	A	612	CLA	3	0
31	e	101	LHG	3	0
25	C	502	CLA	1	0
33	B	619	STE	1	0
31	A	615	LHG	3	0
25	b	604	CLA	1	0
30	a	613	SQD	3	0
35	f	101	HEM	3	0
21	A	601[A]	OEY	1	0
32	C	517	DGD	6	0
25	b	606	CLA	5	0
27	K	101	BCR	2	0
27	b	618	BCR	1	0

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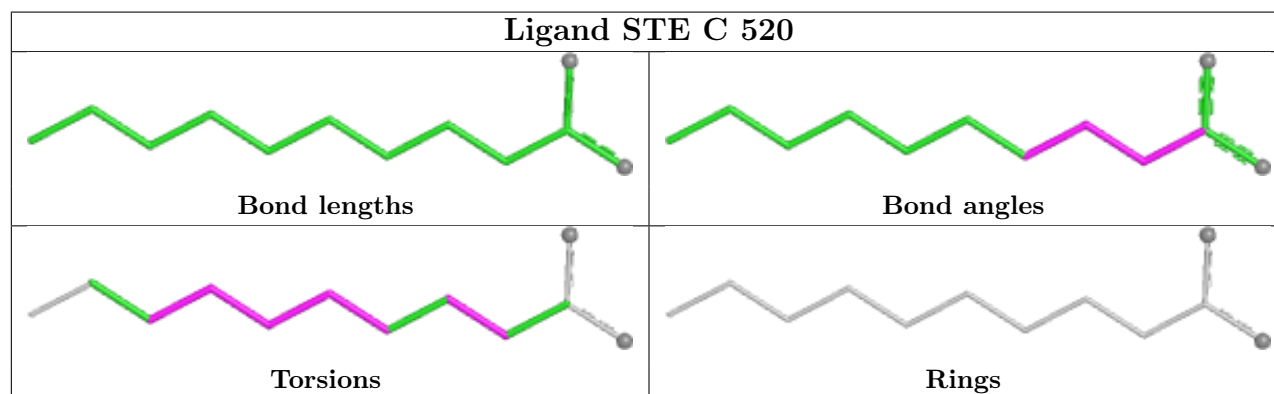
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33	m	102	STE	1	0
25	C	508	CLA	2	0
25	A	606	CLA	4	0
25	c	506	CLA	1	0
25	b	613	CLA	3	0
29	C	519	LMG	1	0
25	b	612	CLA	4	0
25	c	513	CLA	1	0
33	b	621	STE	1	0
25	B	610	CLA	2	0
32	C	518	DGD	5	0
25	C	501	CLA	1	0
21	a	601[A]	OEY	1	0
25	b	602	CLA	2	0
25	b	603	CLA	1	0
27	b	616	BCR	1	0
30	f	102	SQD	1	0
25	c	503	CLA	3	0
27	b	617	BCR	2	0
25	B	613	CLA	3	0
25	b	607	CLA	1	0
25	a	609	CLA	2	0
25	D	404	CLA	3	0
25	b	605	CLA	2	0
25	c	512	CLA	4	0
31	d	408	LHG	1	0
25	c	502	CLA	1	0
27	c	514	BCR	2	0
27	h	102	BCR	3	0
35	F	101	HEM	2	0
25	B	602	CLA	1	0
25	C	506	CLA	3	0
25	B	607	CLA	1	0
30	b	619	SQD	1	0
31	D	409	LHG	2	0
33	X	101	STE	5	0
27	B	616	BCR	1	0
25	C	512	CLA	6	0
25	B	605	CLA	1	0
29	d	410	LMG	1	0
32	C	516	DGD	1	0
28	d	406	PL9	1	0

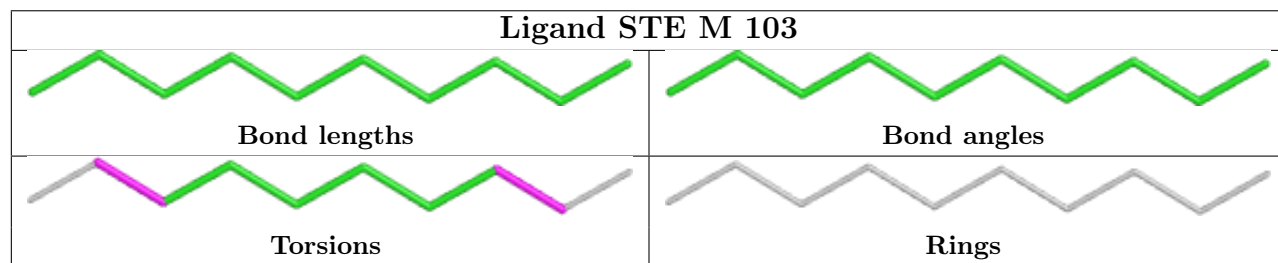
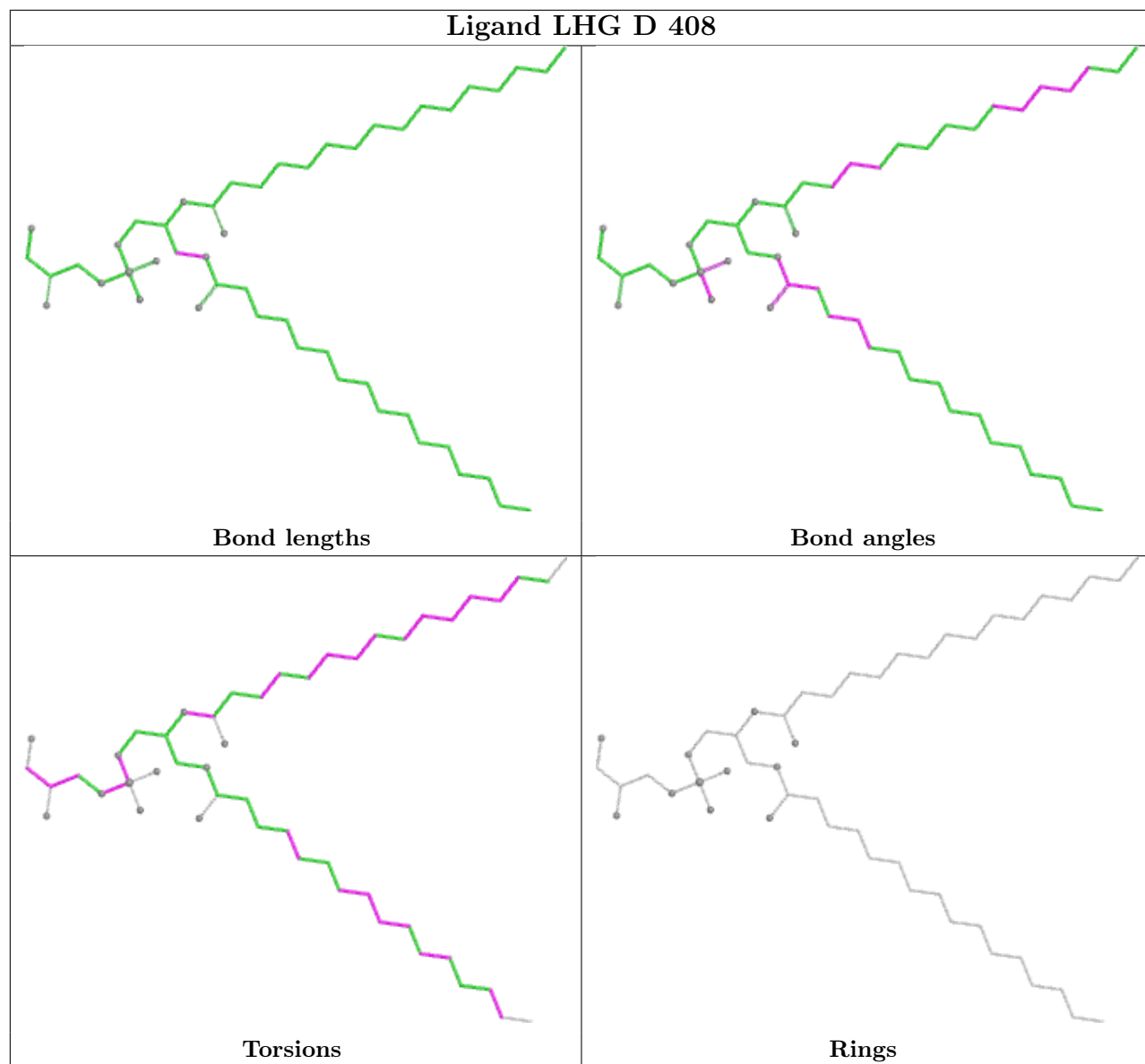
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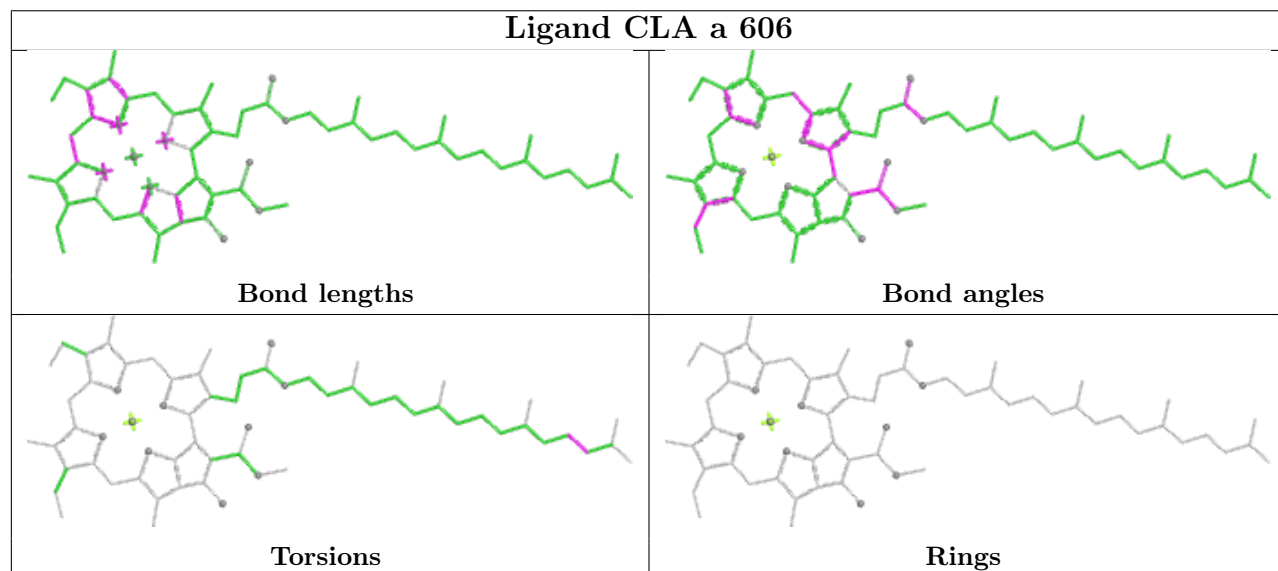
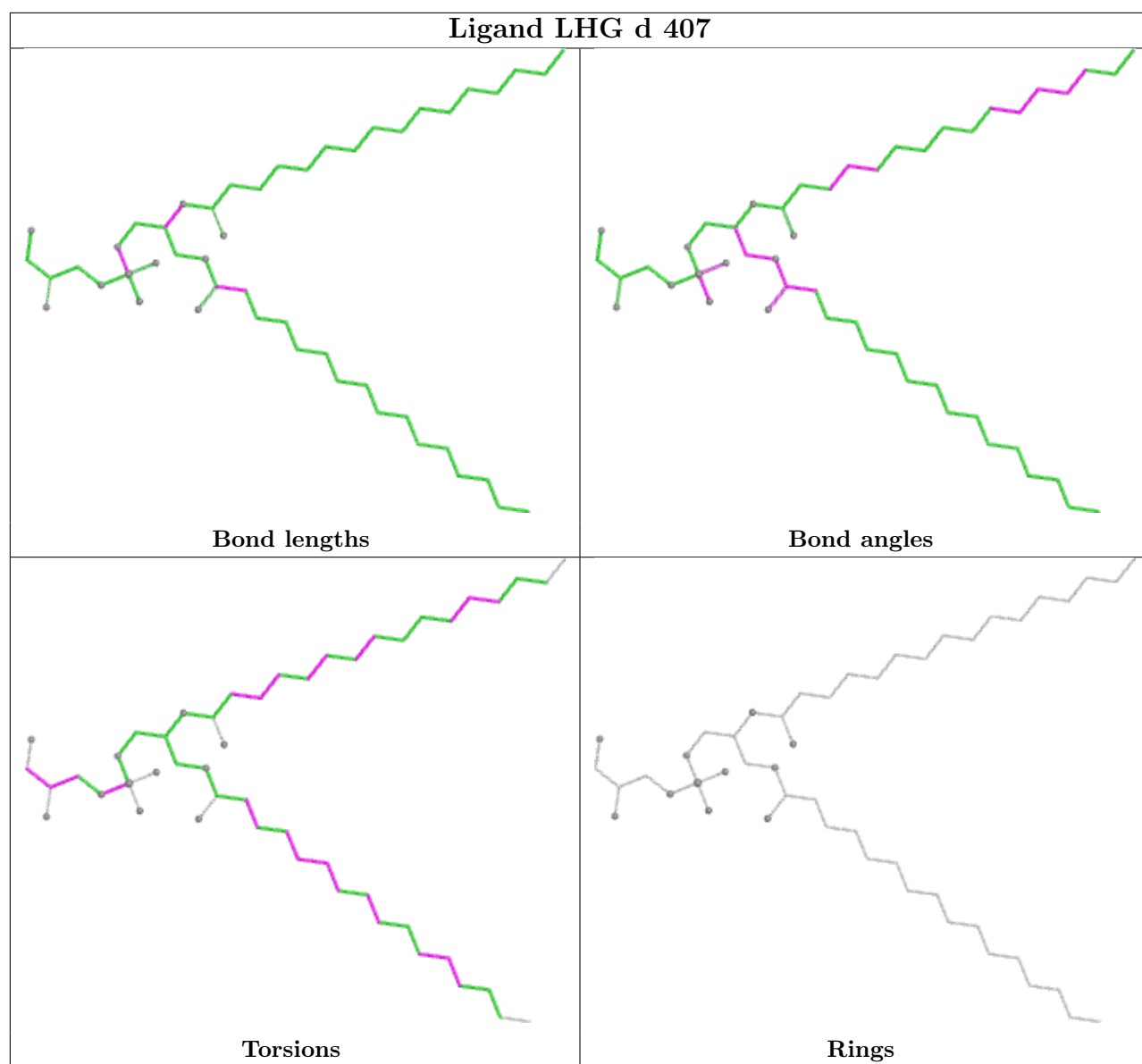
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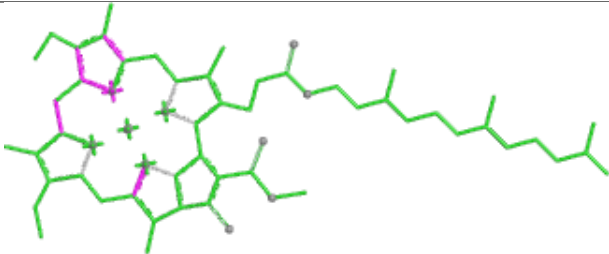
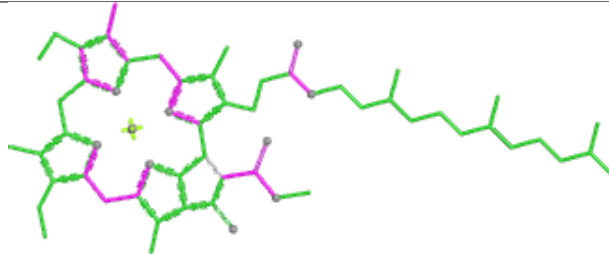
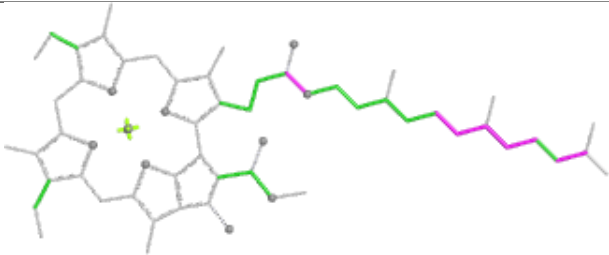
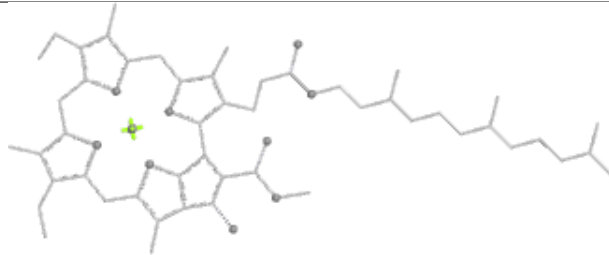
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	611	PL9	7	0
29	A	613	LMG	2	0
30	A	614	SQD	1	0
27	B	618	BCR	1	0
33	d	412	STE	2	0
21	a	601[C]	OEY	1	0
30	F	102	SQD	1	0
27	C	514	BCR	2	0
28	a	611	PL9	5	0
31	D	411	LHG	8	0
25	C	510	CLA	1	0
33	b	625	STE	2	0
27	T	101	BCR	2	0
25	C	509	CLA	1	0
27	A	610	BCR	1	0
33	I	101	STE	2	0
25	b	601	CLA	5	0
25	B	611	CLA	2	0
25	c	505	CLA	1	0
32	a	615	DGD	2	0
30	A	616	SQD	2	0
25	C	513	CLA	1	0
30	B	621	SQD	2	0
33	l	101	STE	1	0
31	L	101	LHG	1	0
25	c	507	CLA	2	0
25	B	614	CLA	2	0
33	B	622	STE	1	0
25	B	603	CLA	2	0
21	A	601[C]	OEY	1	0
32	c	517	DGD	2	0
33	B	623	STE	1	0
25	H	101	CLA	1	0
25	b	615	CLA	3	0
25	A	609	CLA	1	0
25	B	601	CLA	3	0
27	B	617	BCR	2	0
25	c	511	CLA	3	0
31	b	623	LHG	4	0
33	J	101	STE	2	0
27	C	515	BCR	2	0
33	M	102	STE	1	0

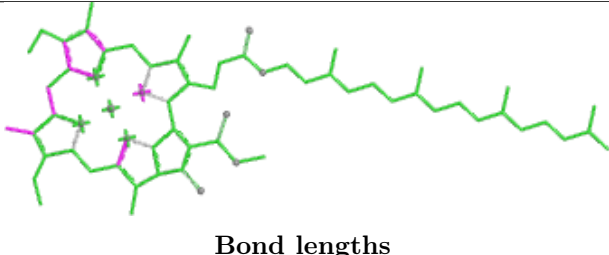
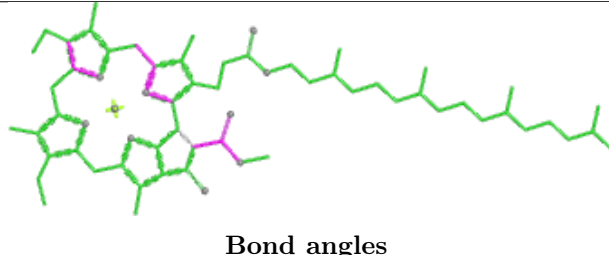
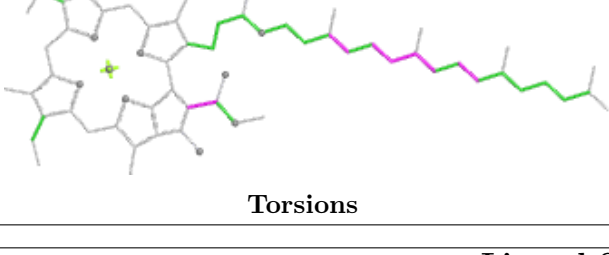
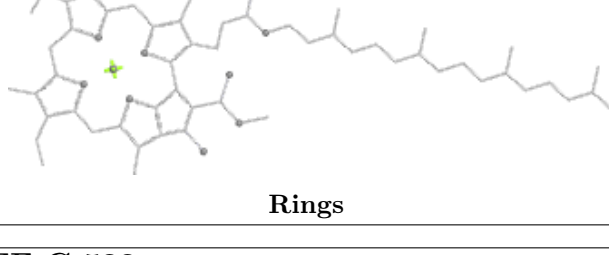
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.





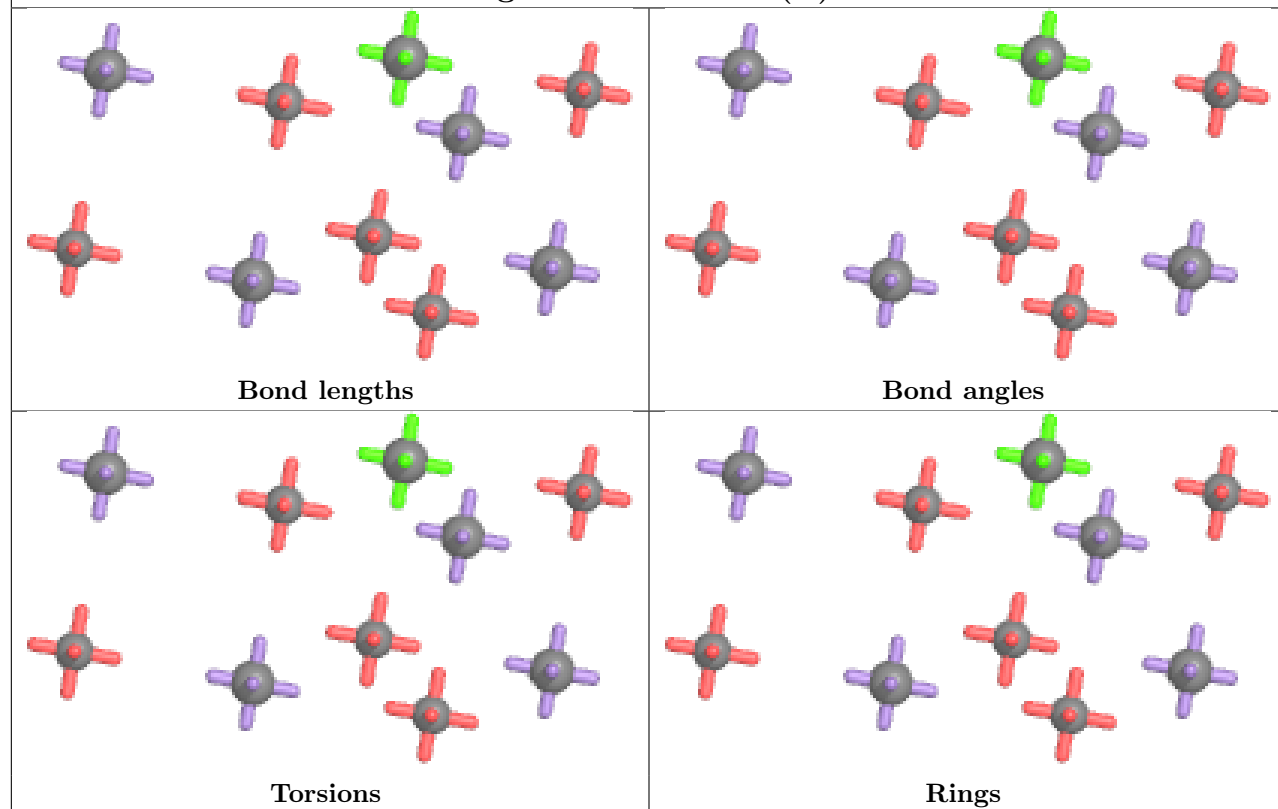


Ligand CLA c 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

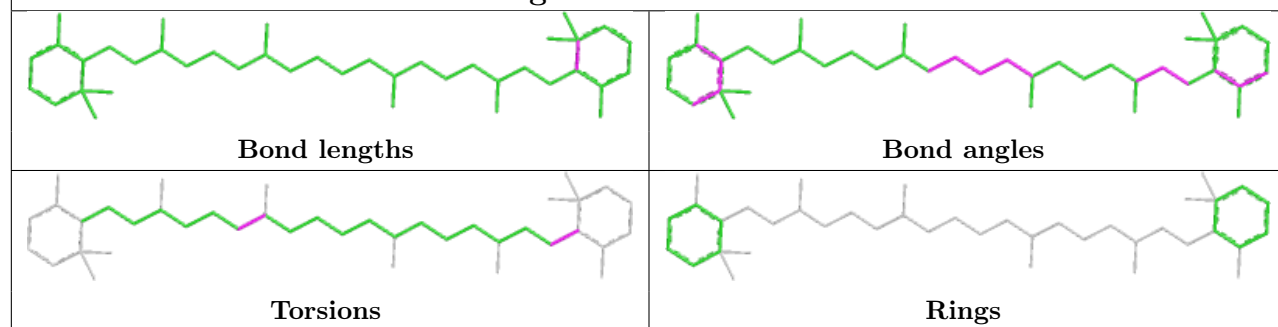
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

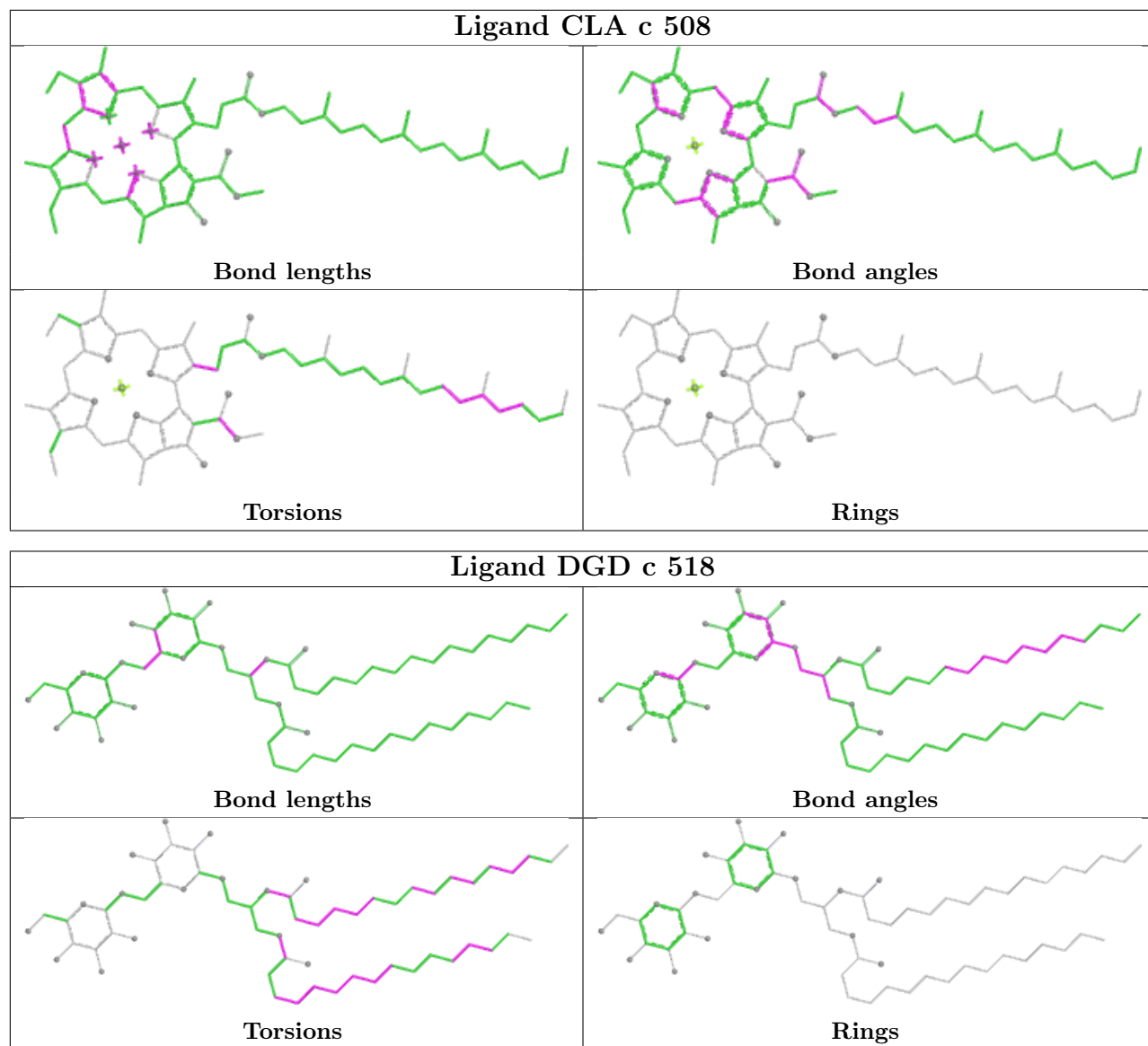
Ligand STE C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand OEX A 602 (B)

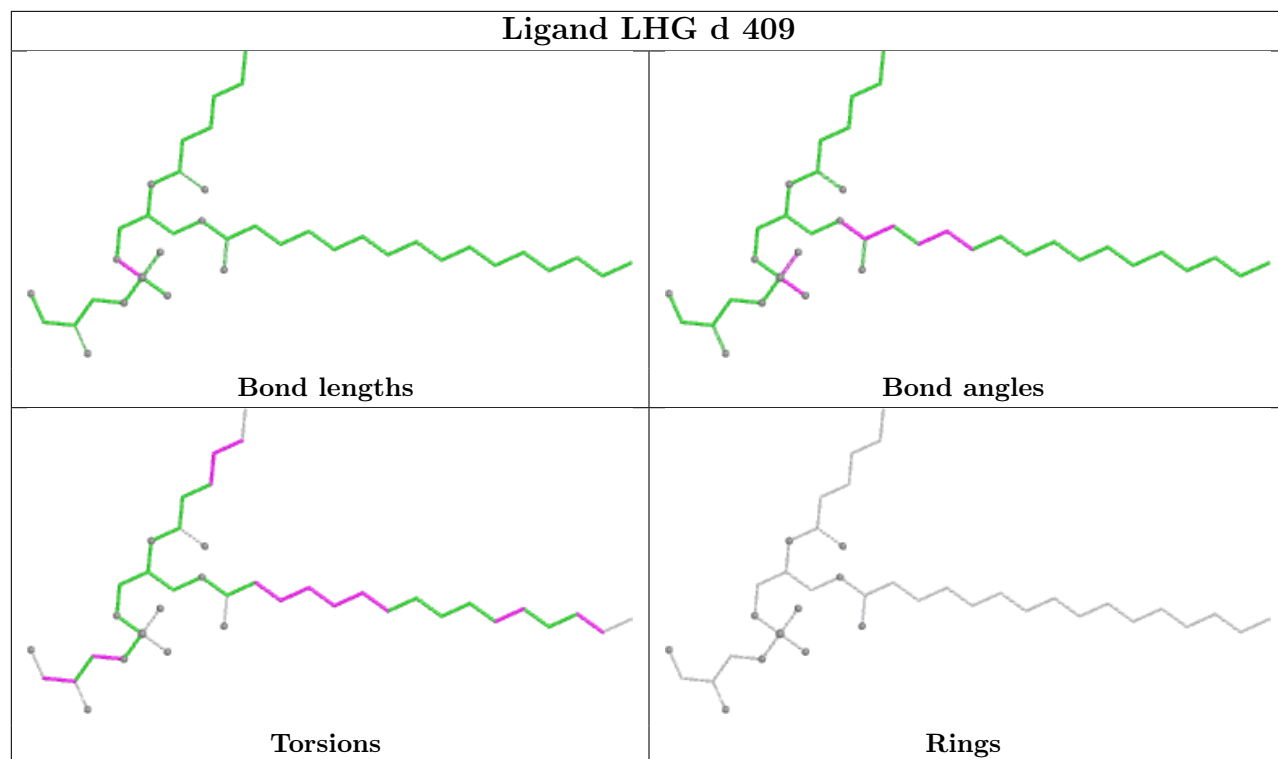


Ligand BCR H 102

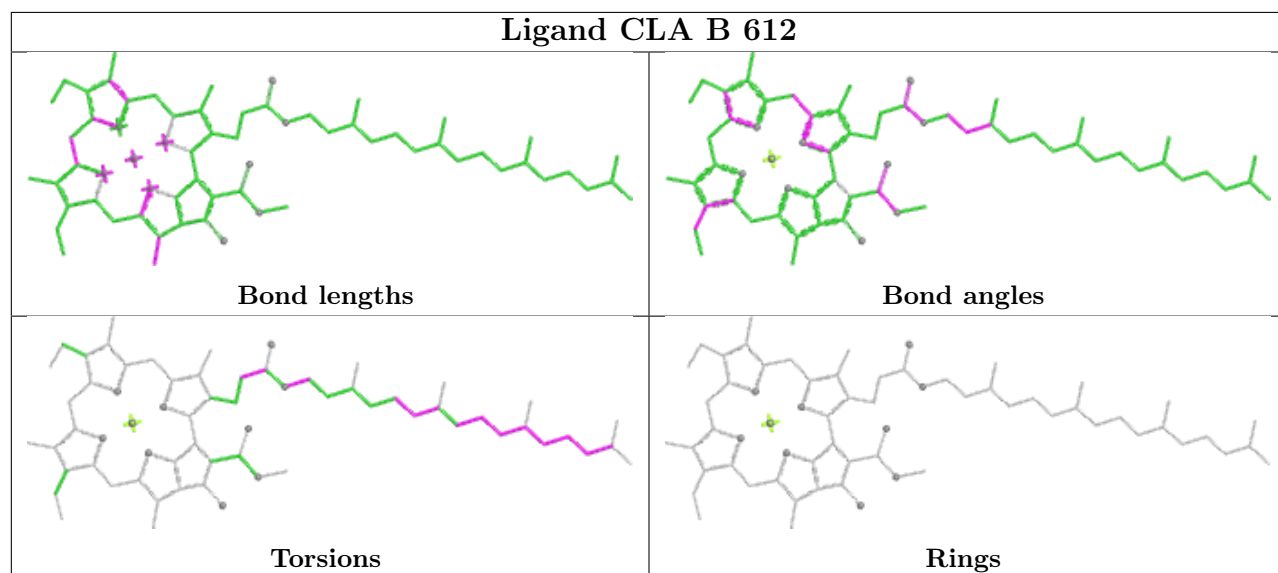




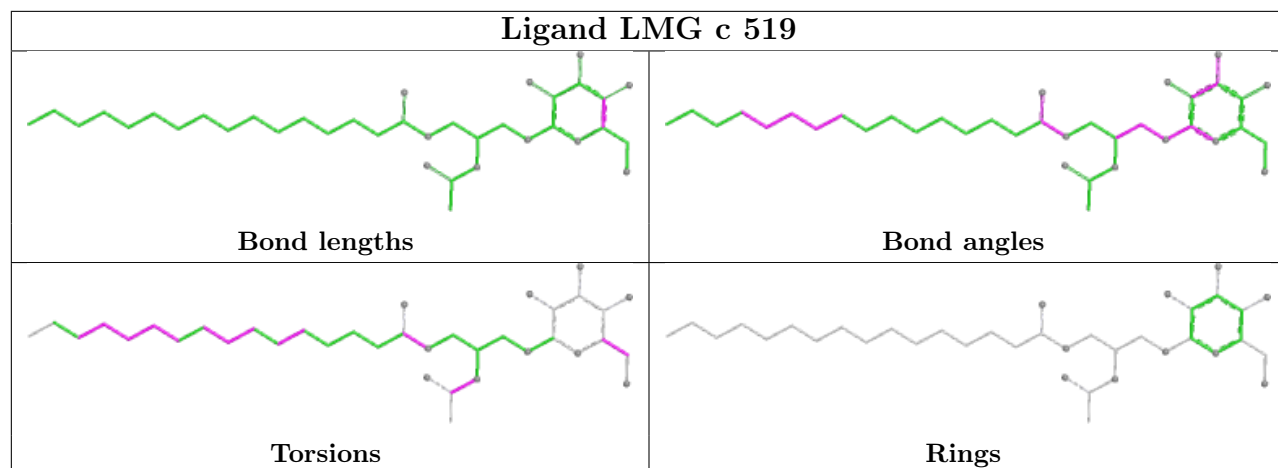
Ligand LHG d 409



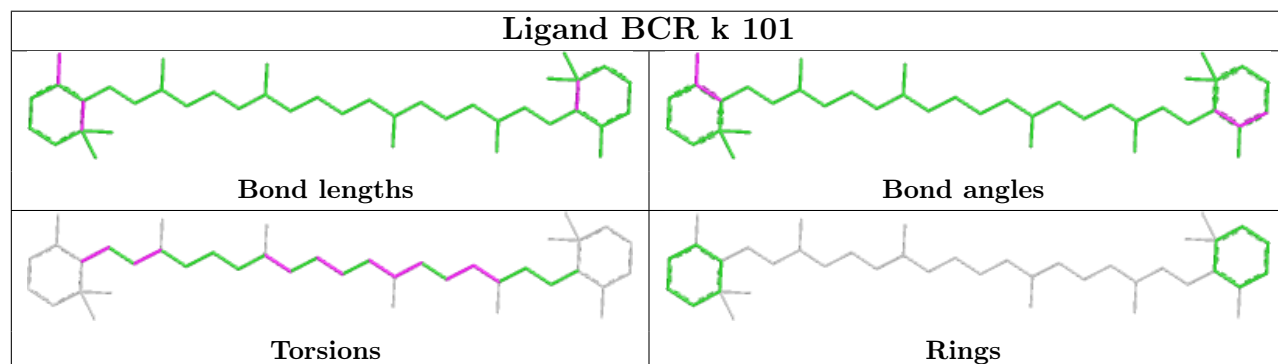
Ligand CLA B 612



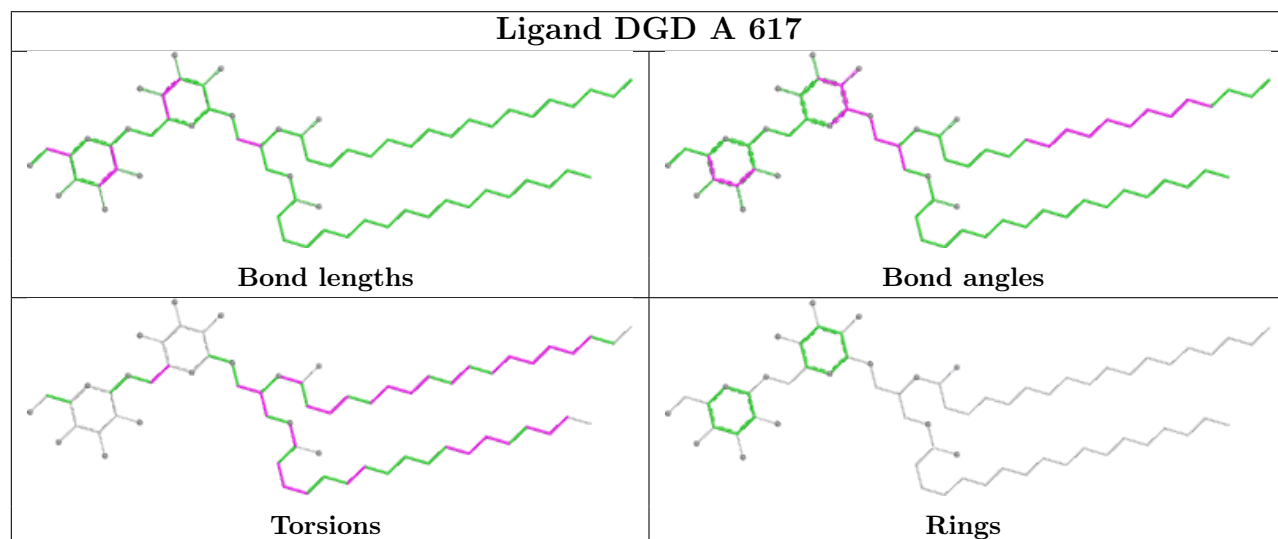
Ligand LMG c 519



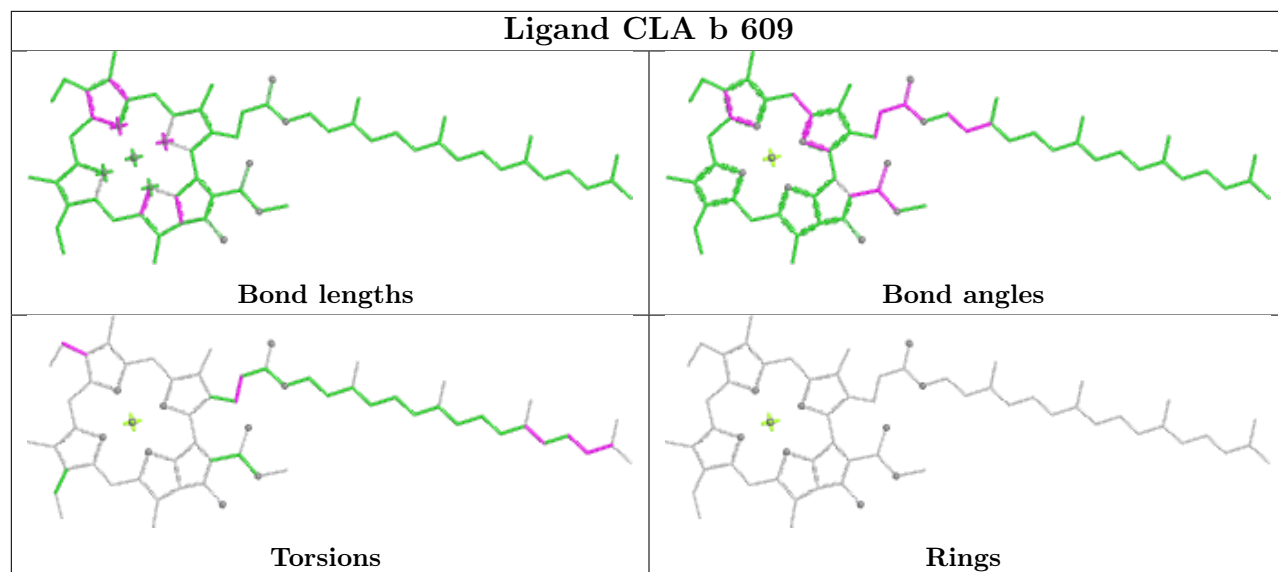
Ligand BCR k 101



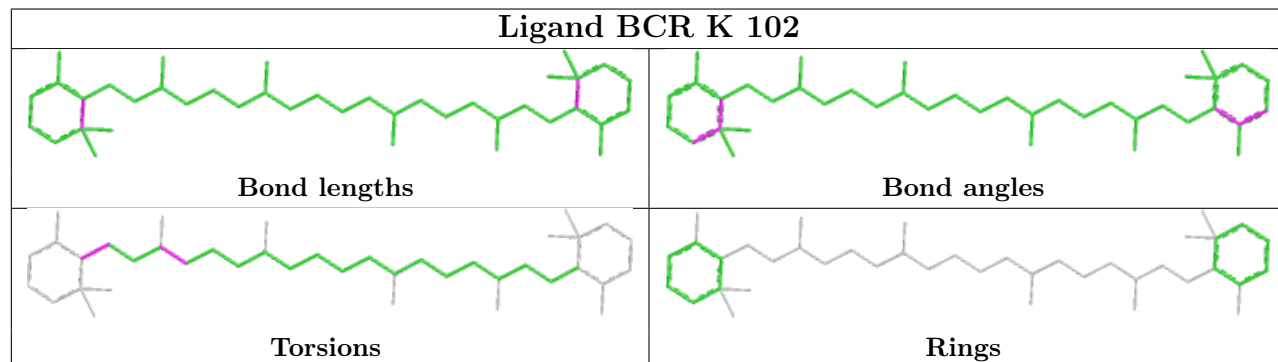
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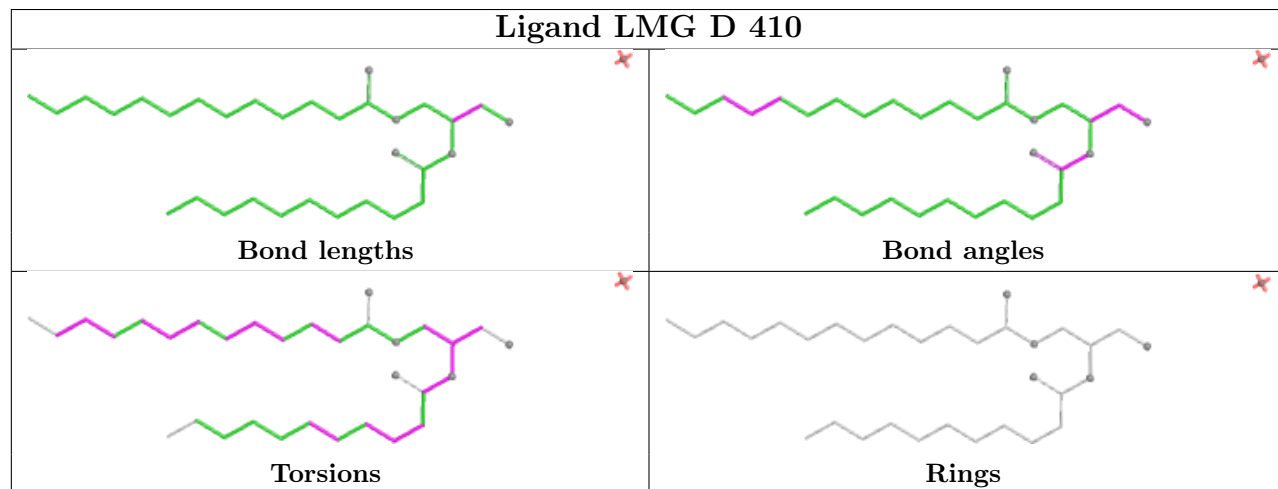
Ligand CLA b 609



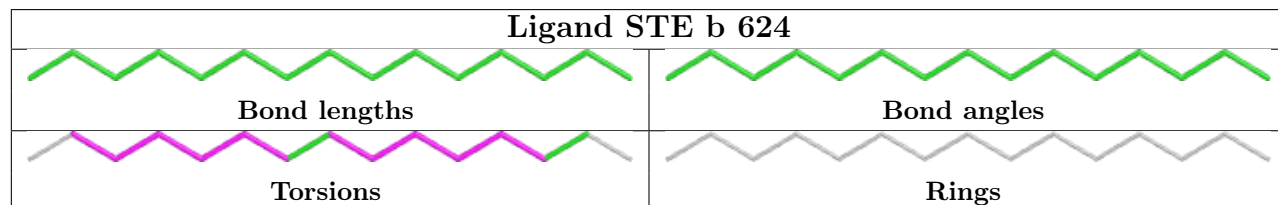
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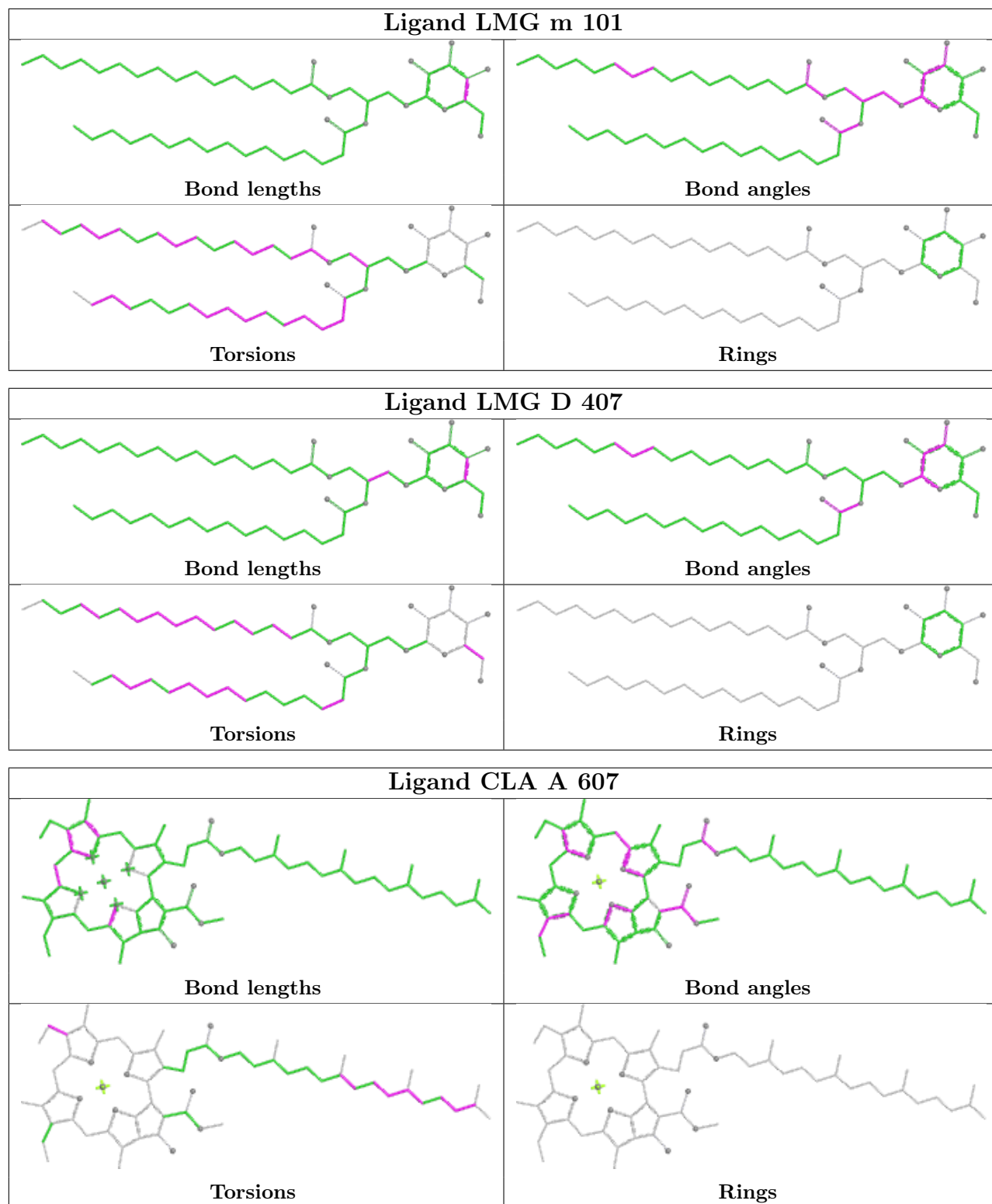


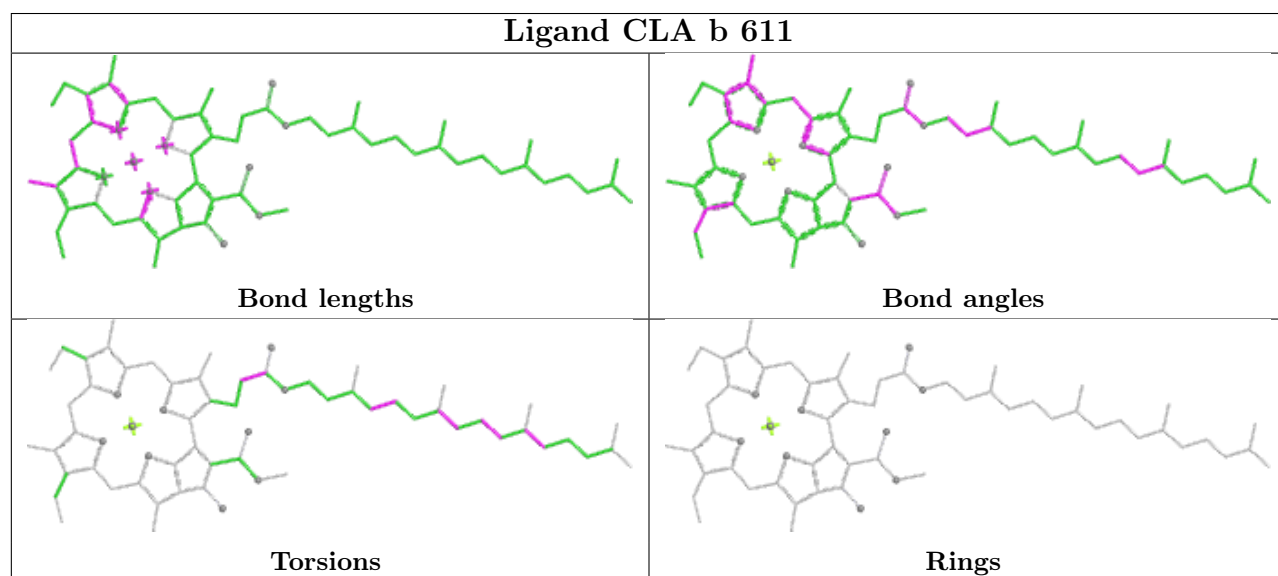
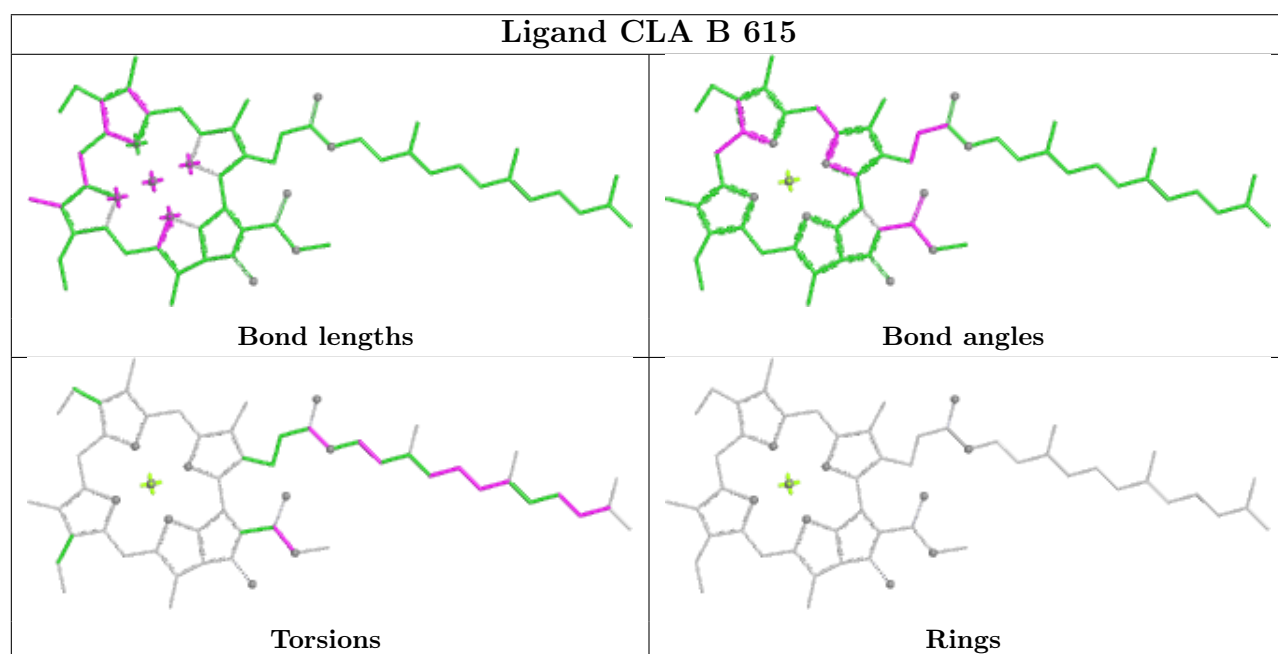
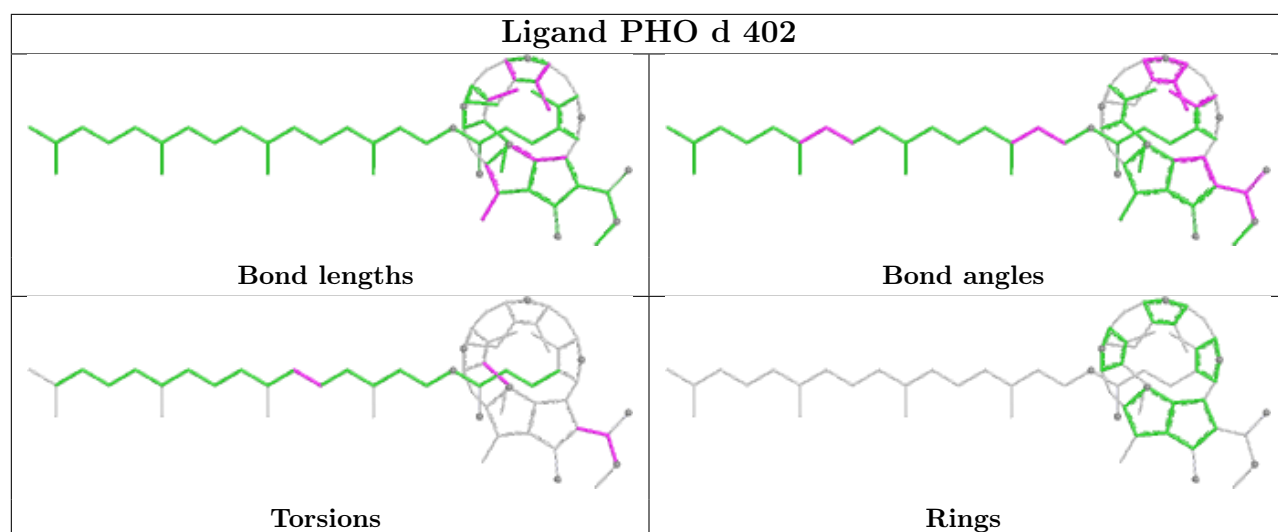
Ligand LMG D 410



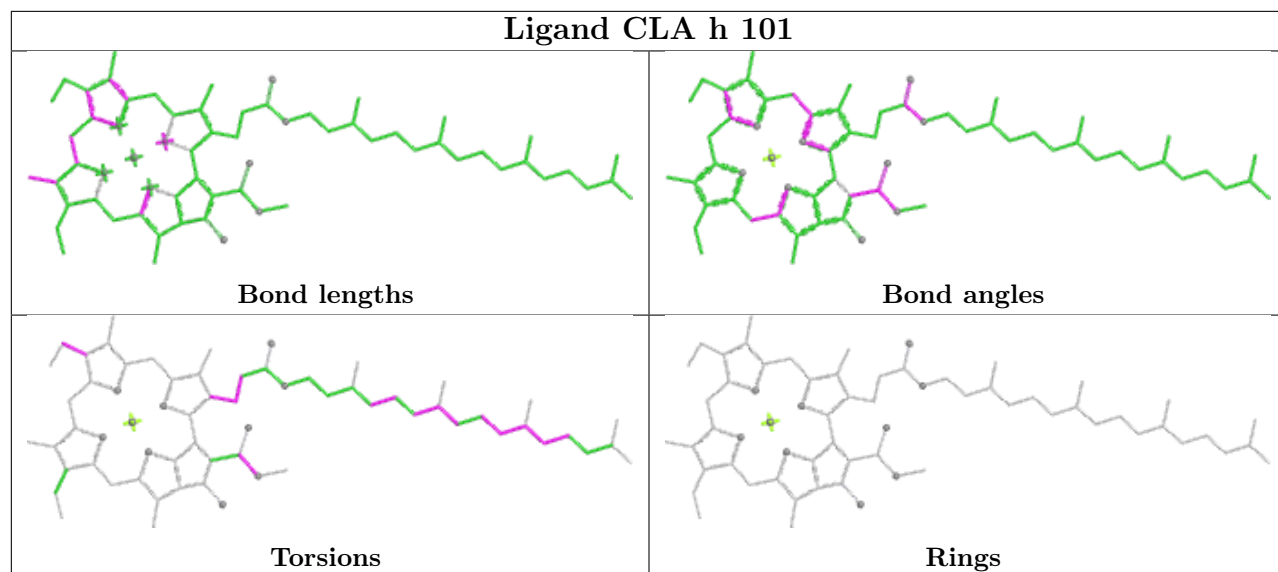
Ligand STE b 624



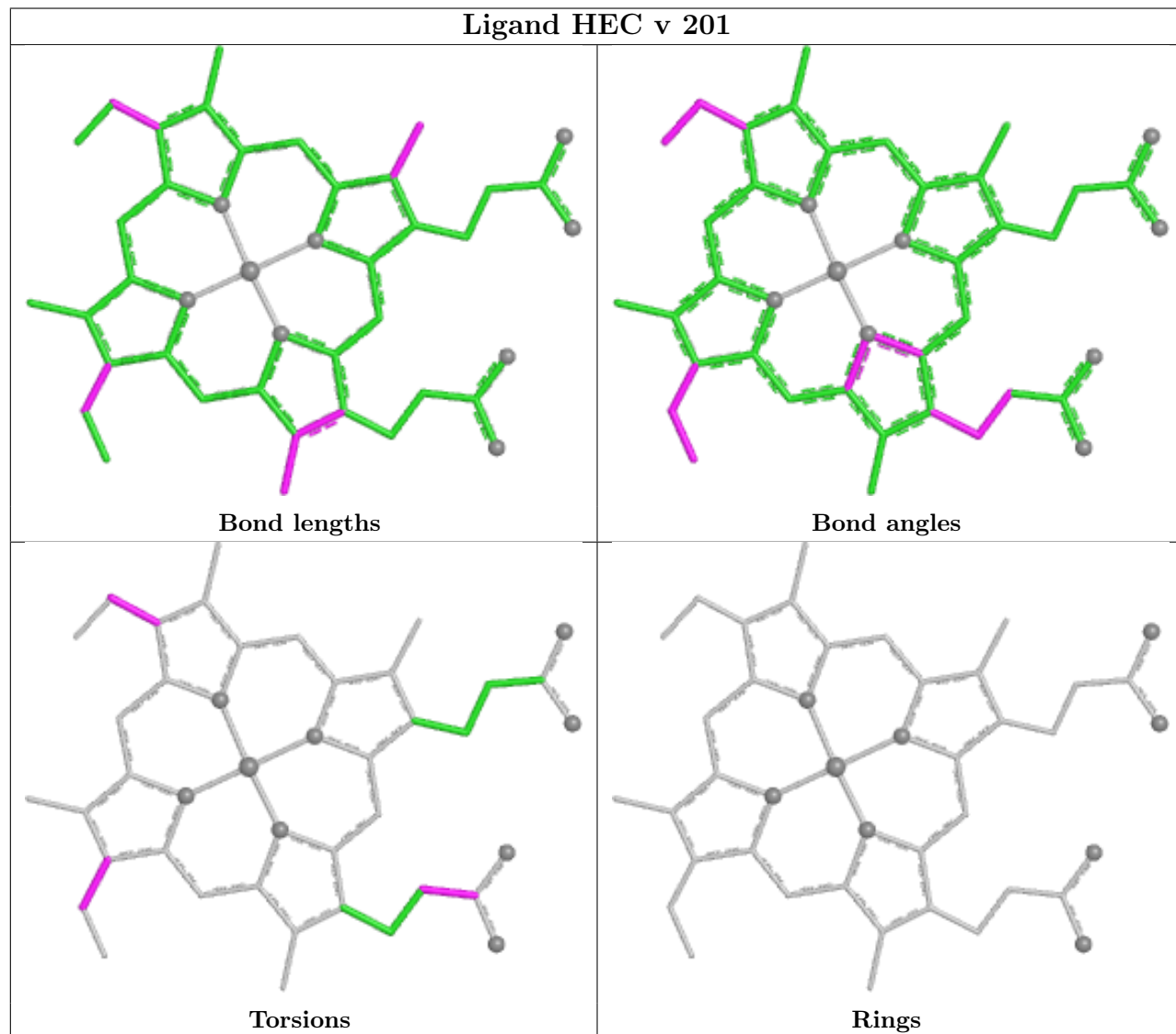




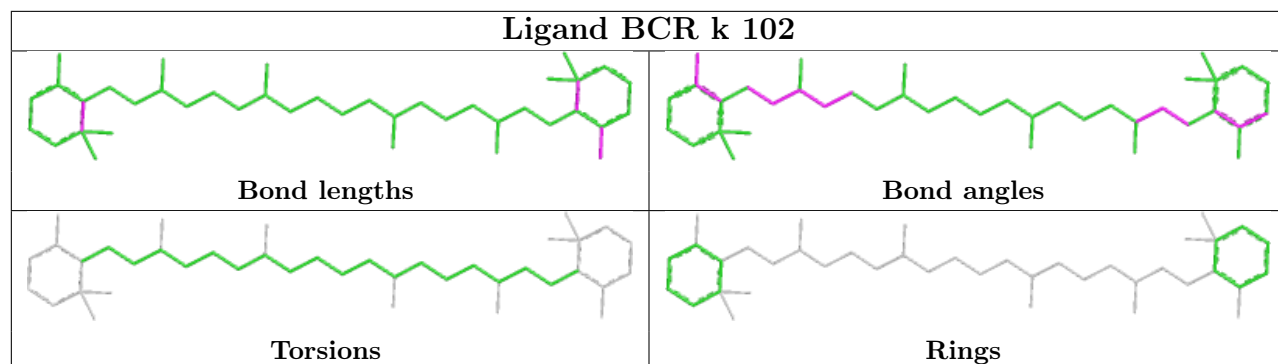
Ligand CLA h 101



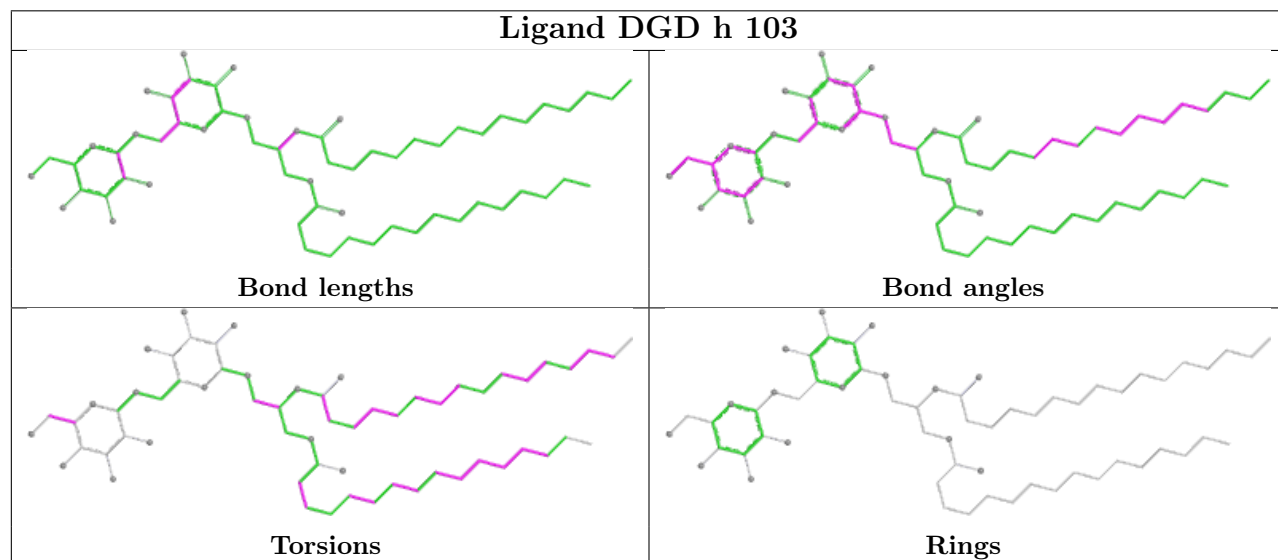
Ligand HEC v 201



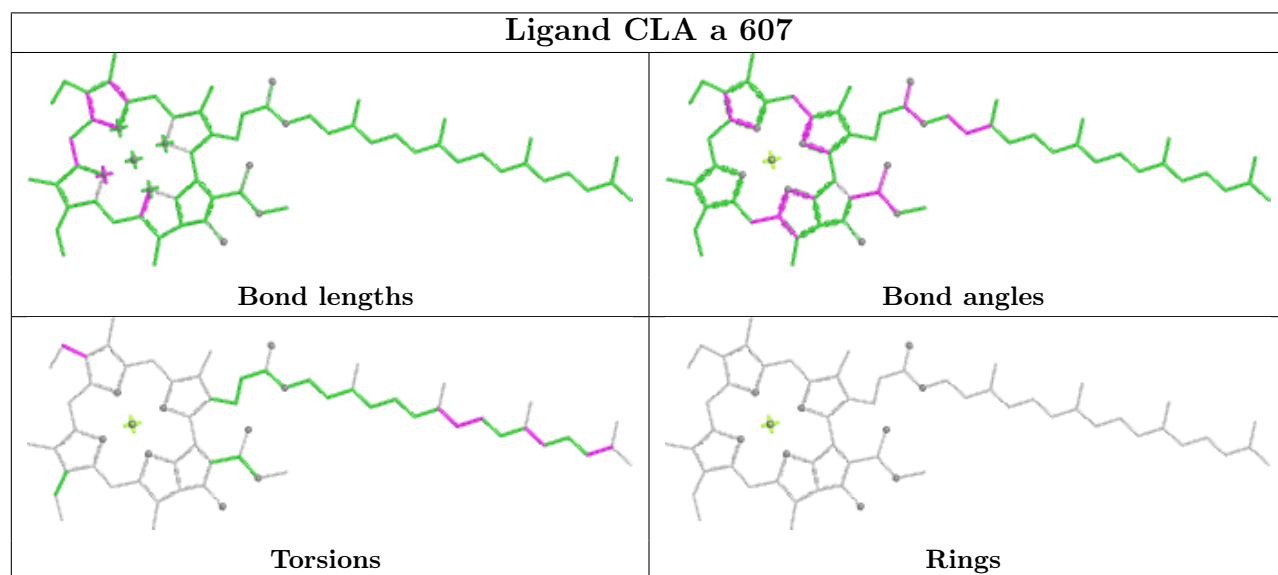
Ligand BCR k 102



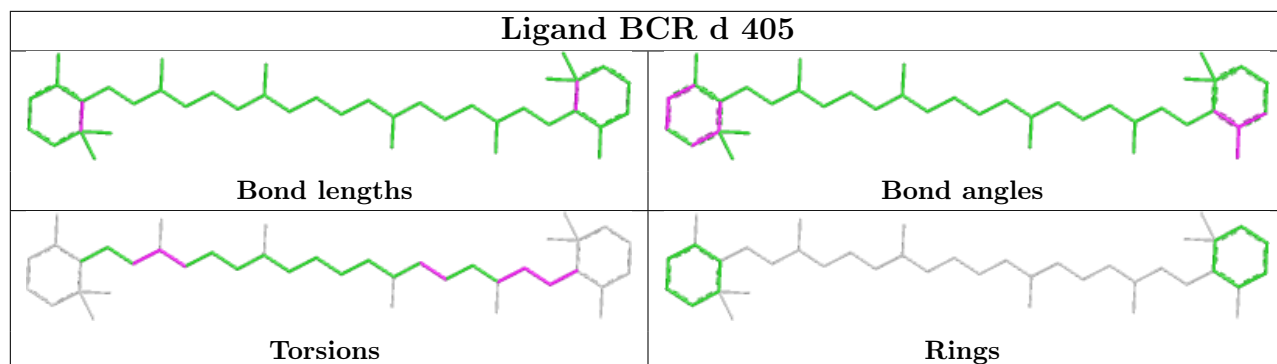
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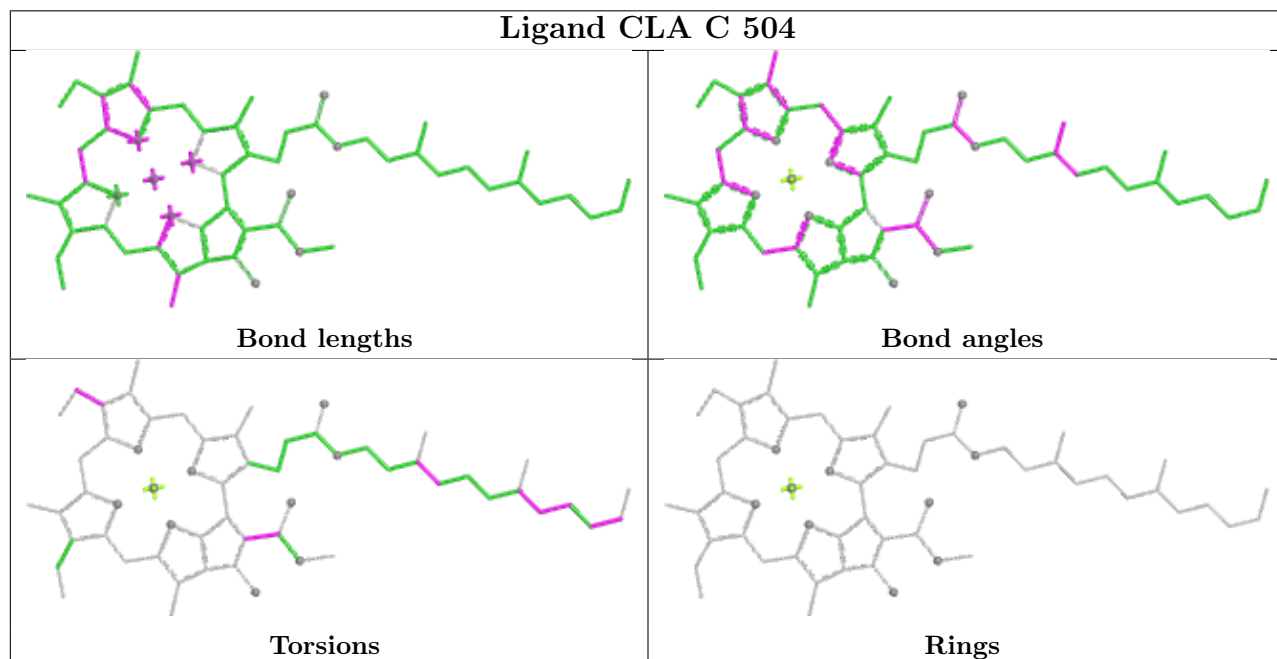
Ligand CLA a 607



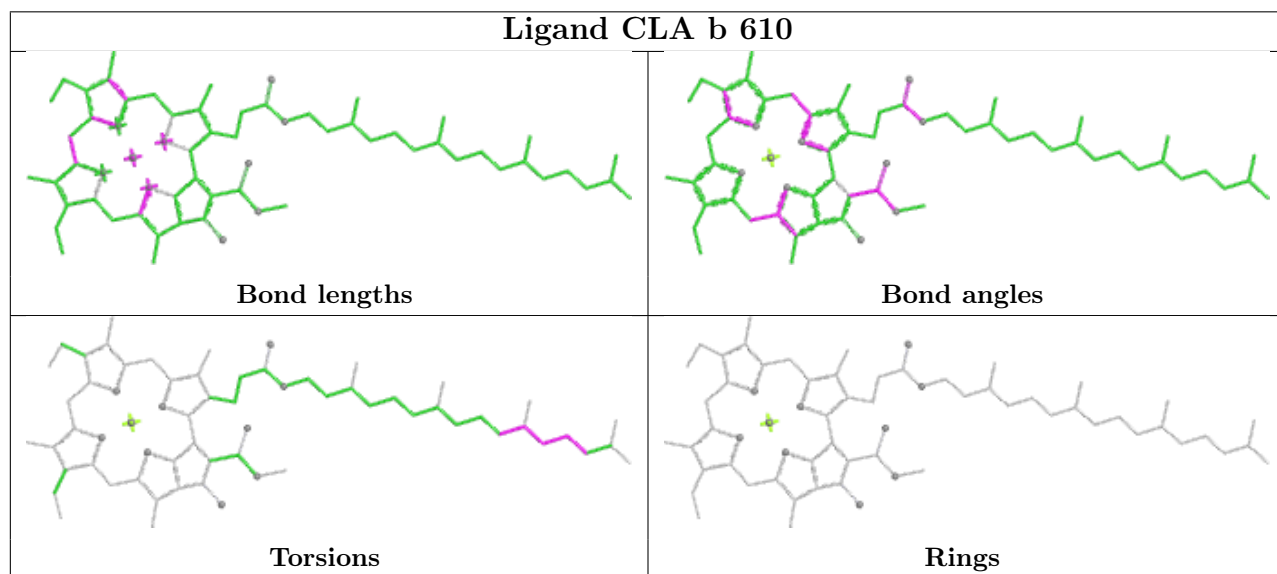
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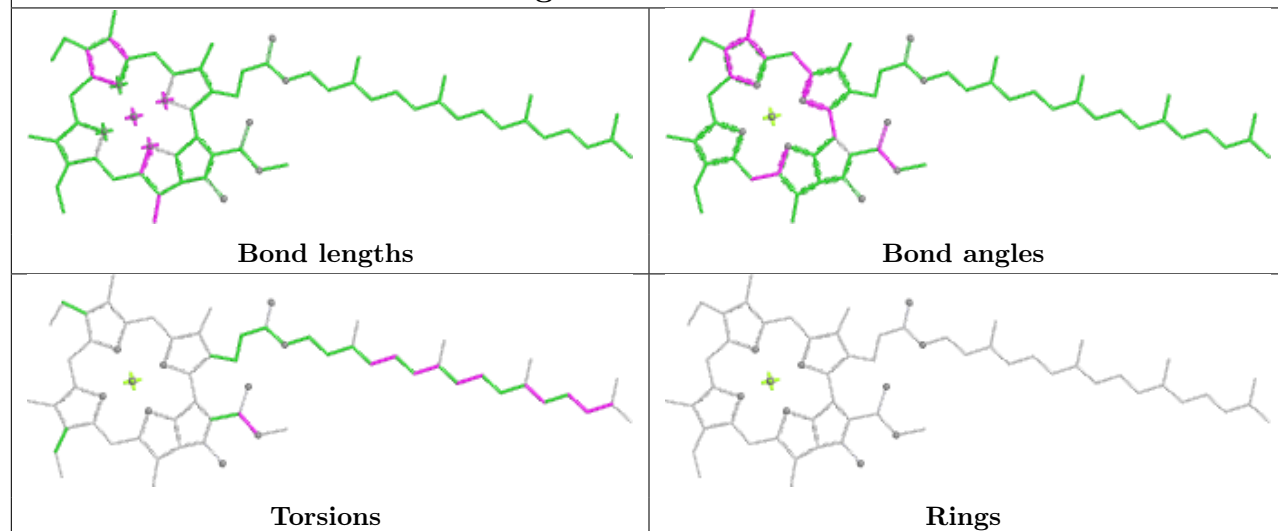
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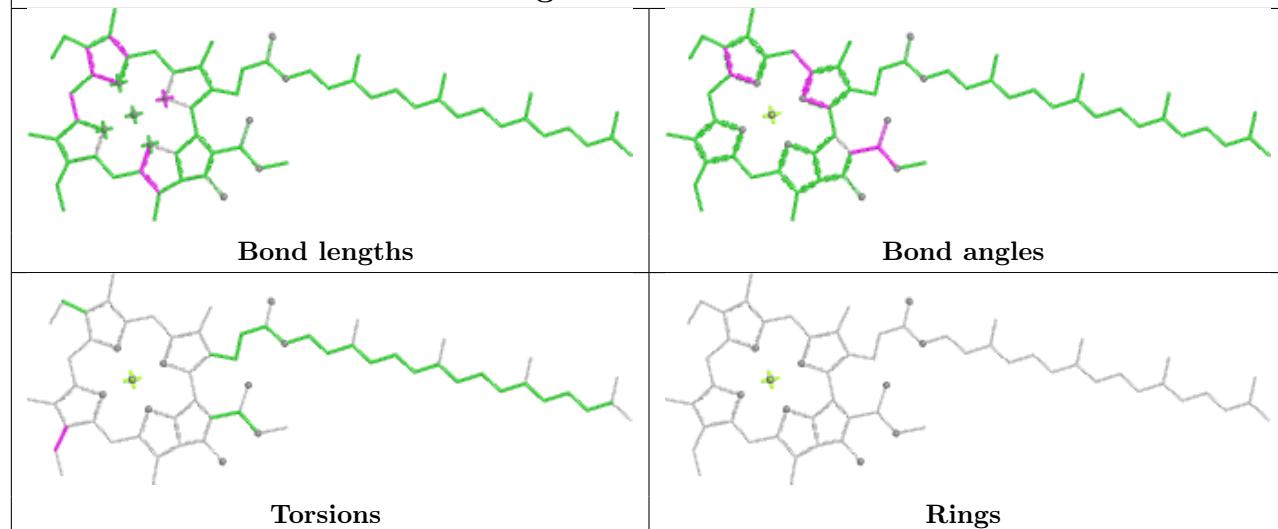
Ligand CLA b 610



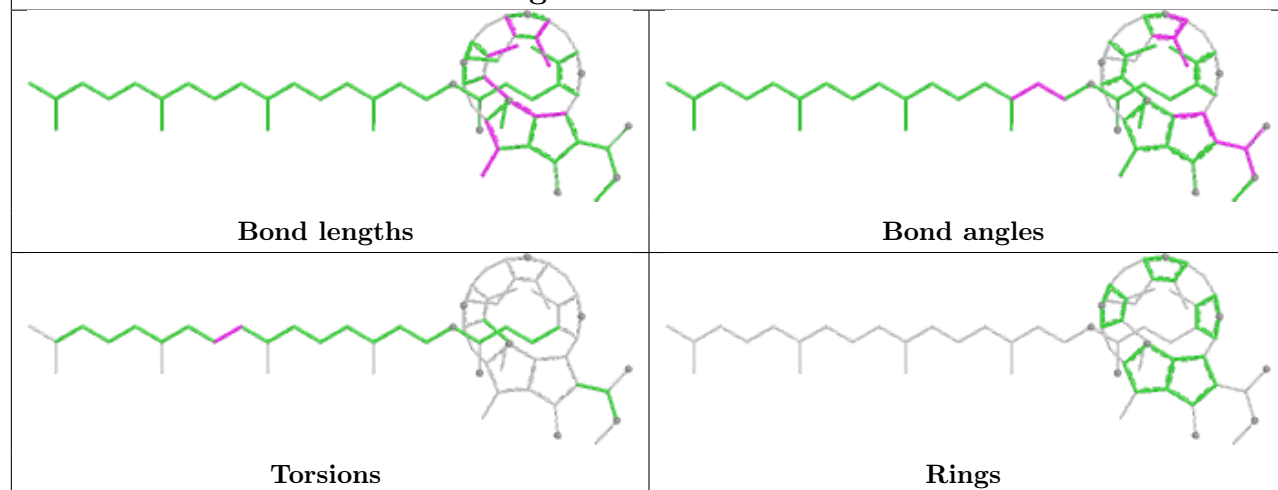
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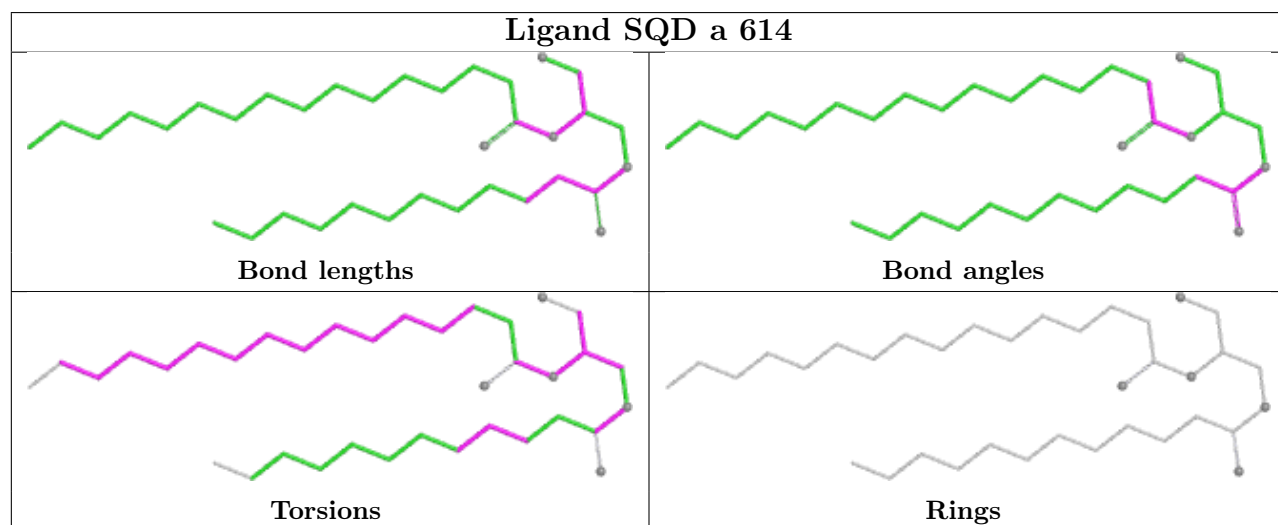
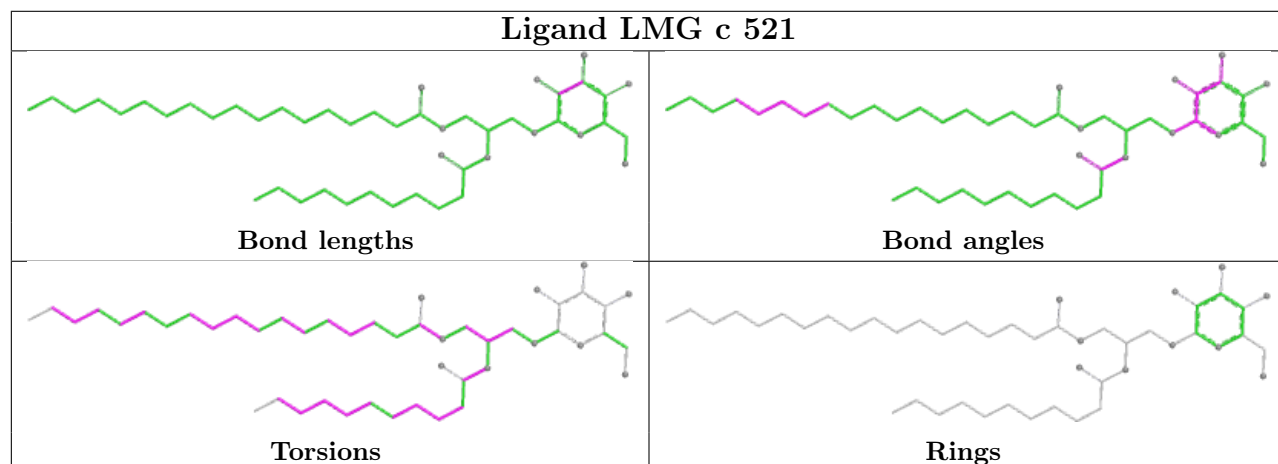
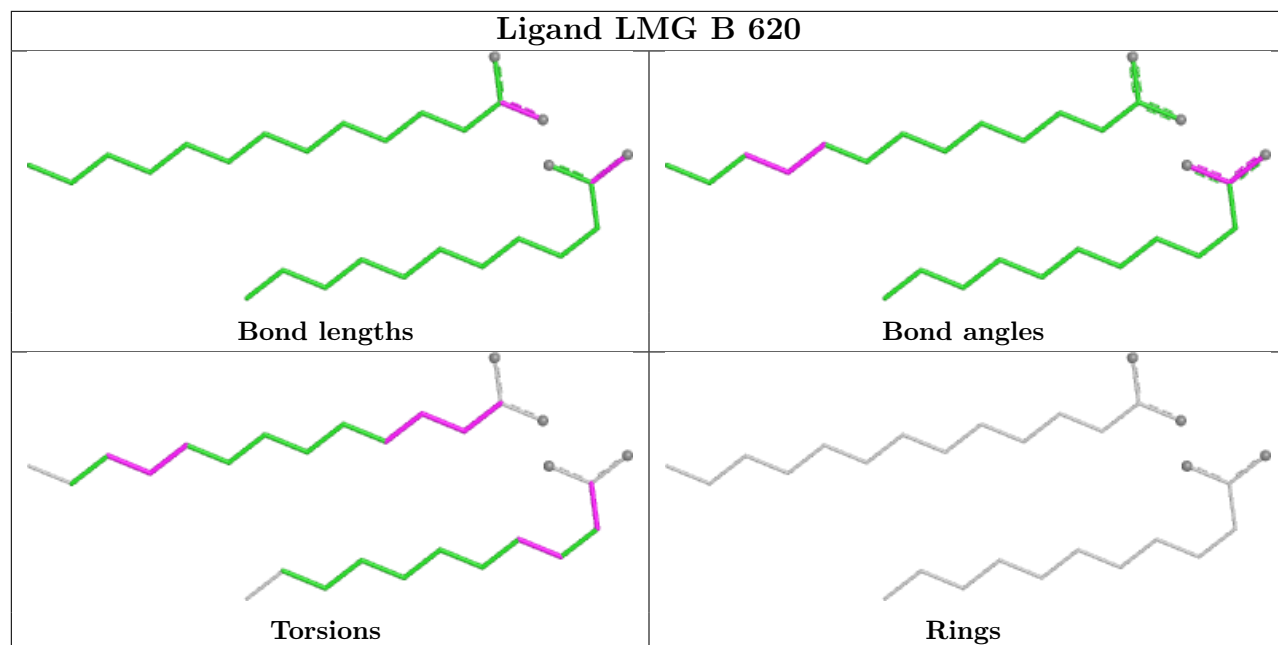


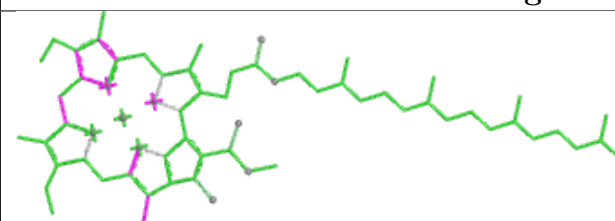
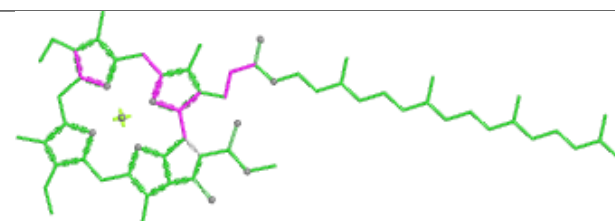
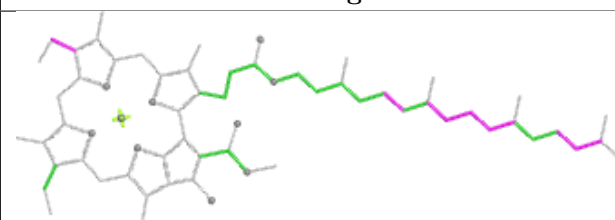
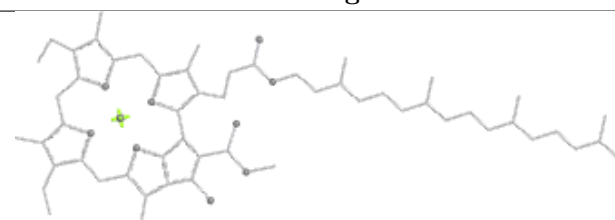
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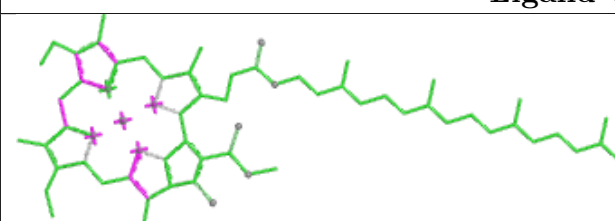
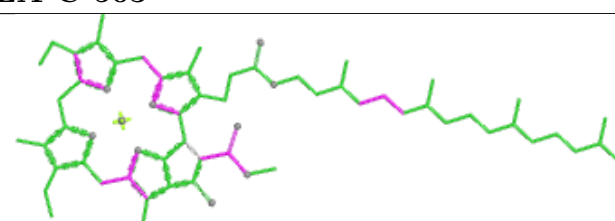
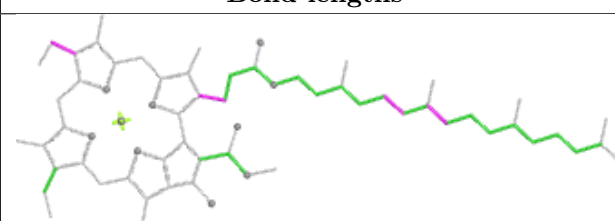
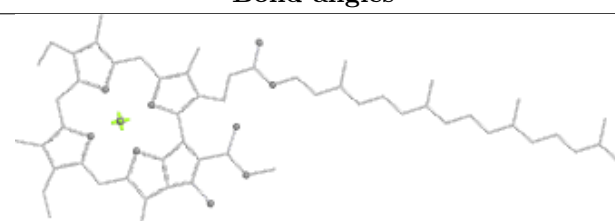


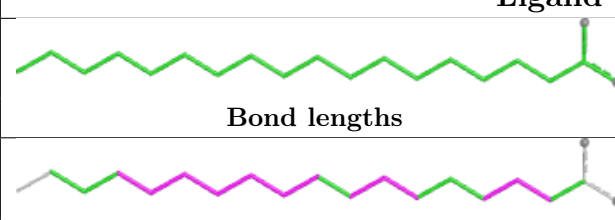
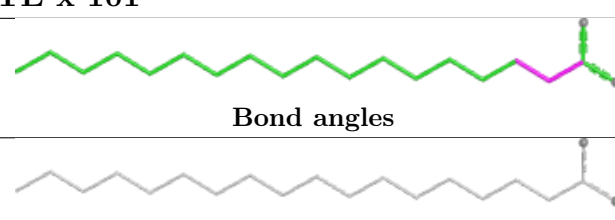
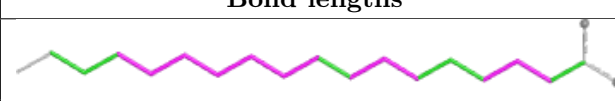
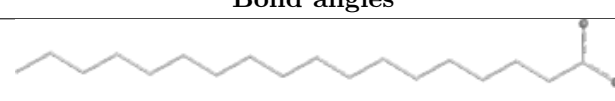
Ligand PHO A 608

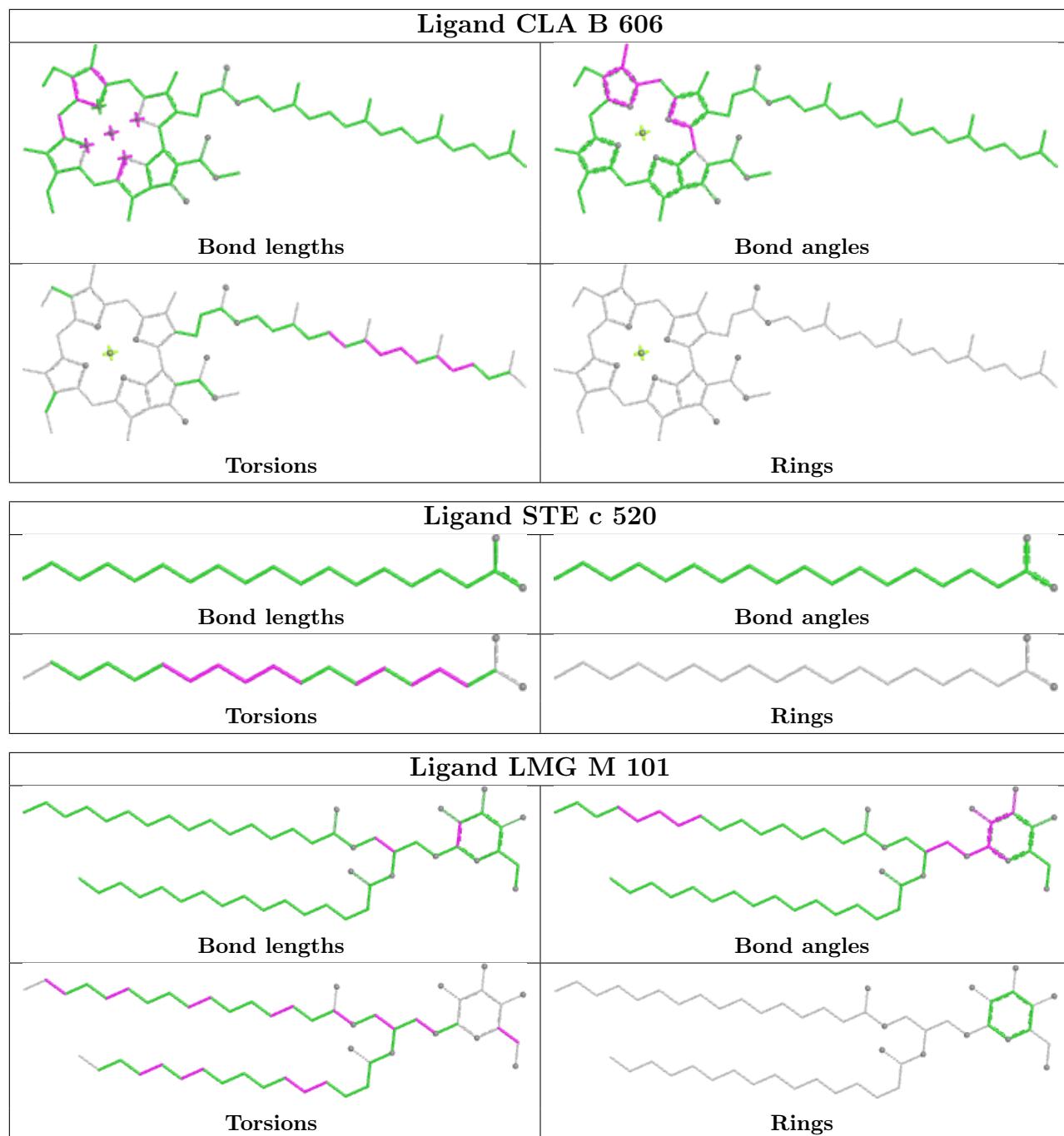




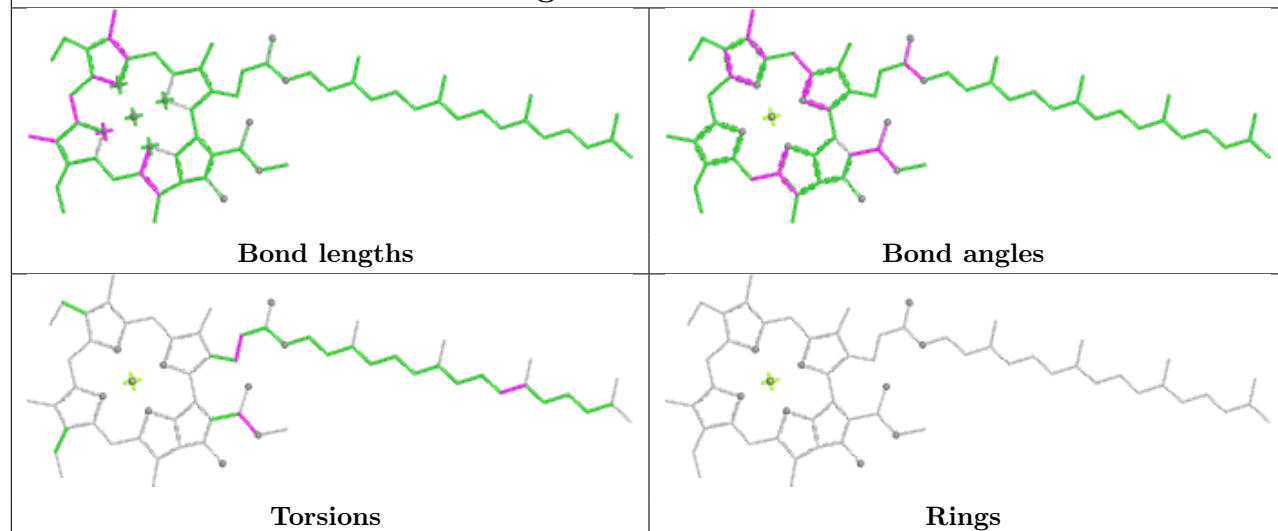
Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

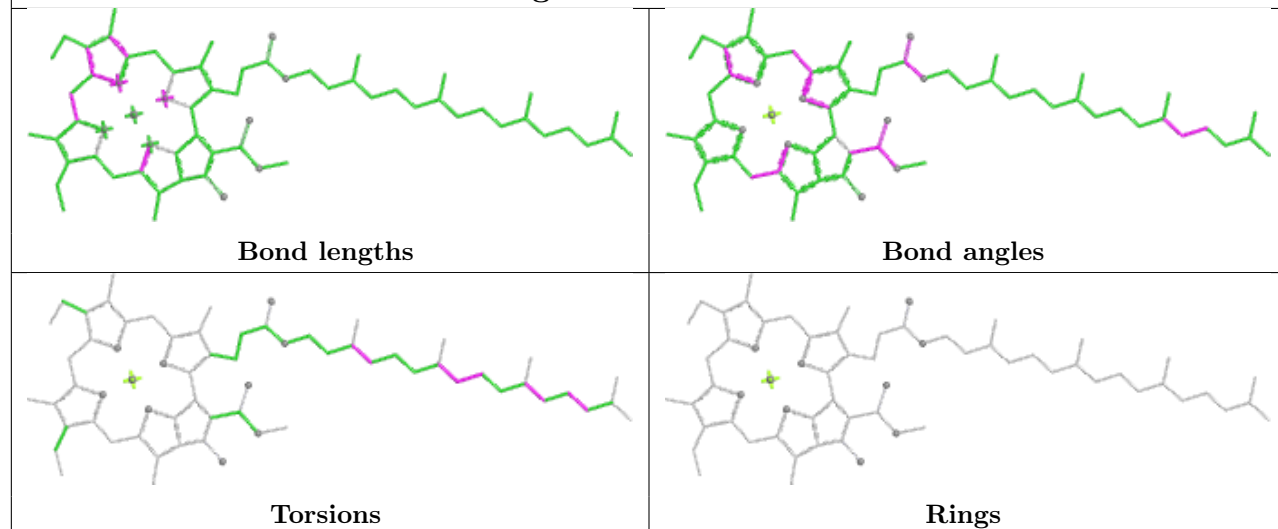
Ligand STE x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



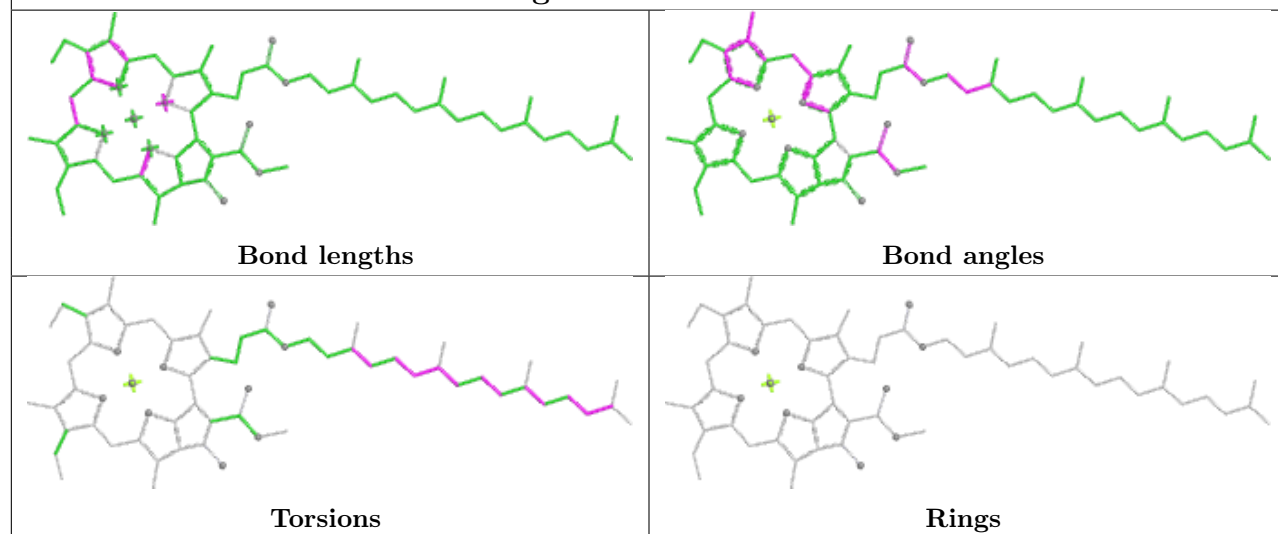
Ligand CLA c 501

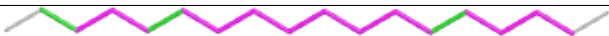


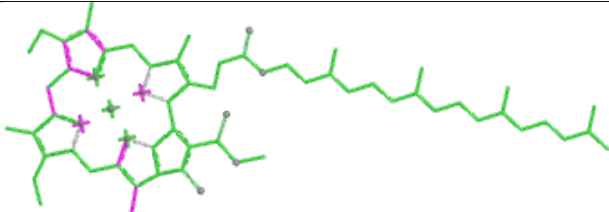
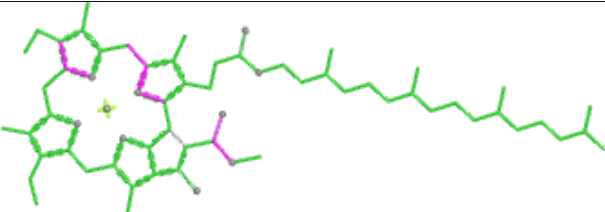
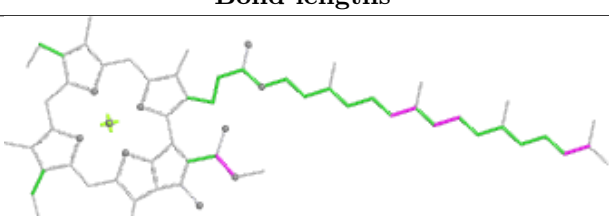
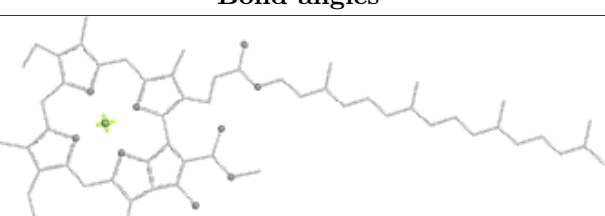
Ligand CLA B 604

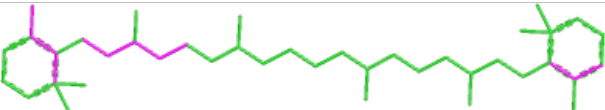
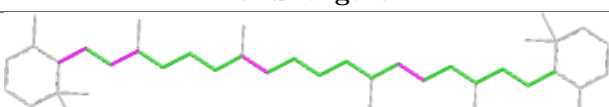
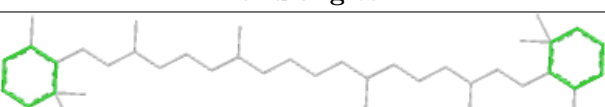


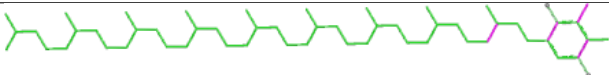
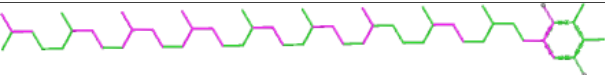
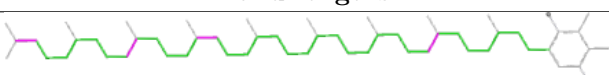
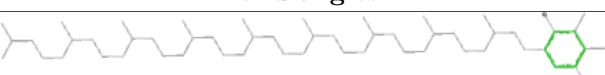
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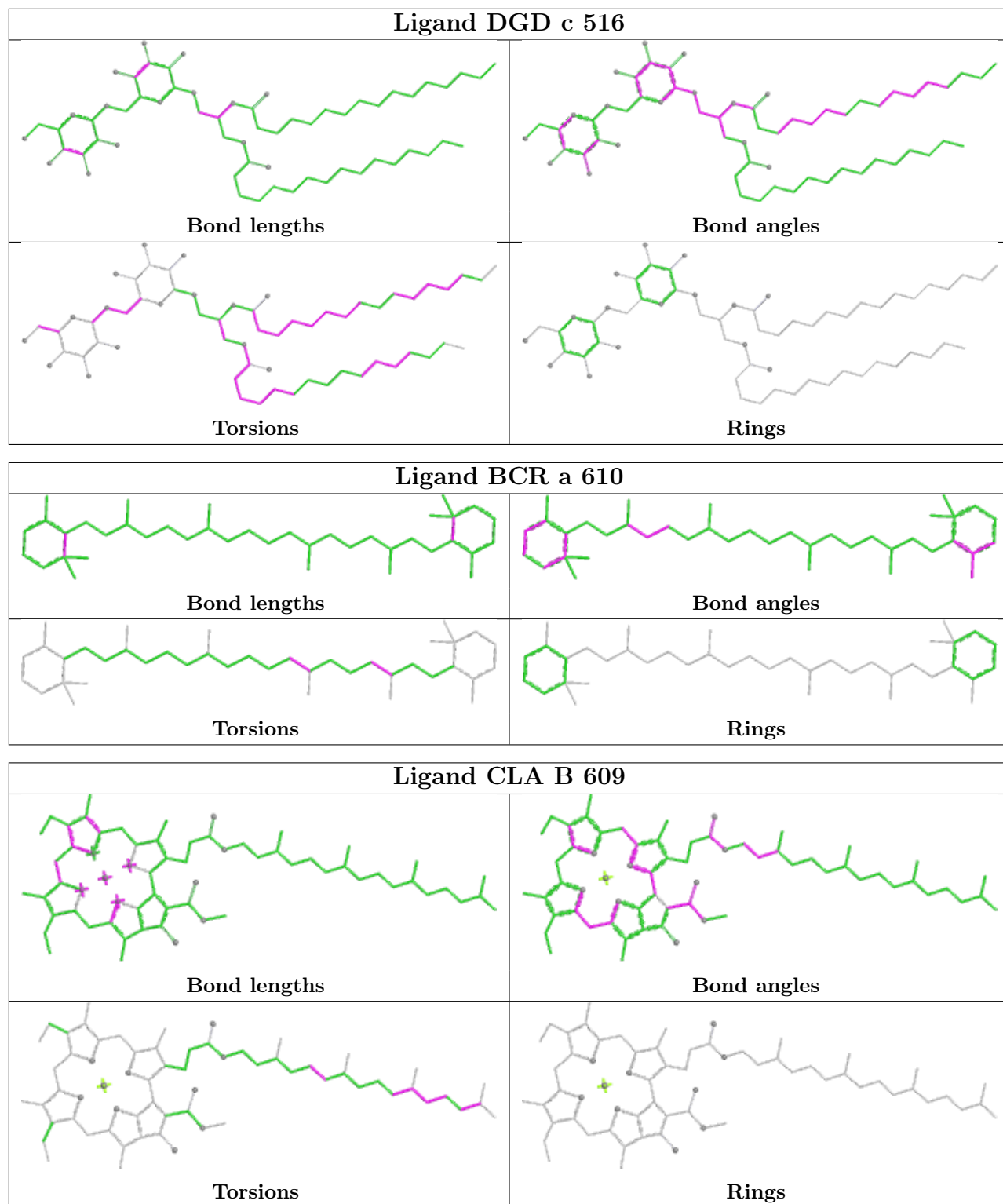


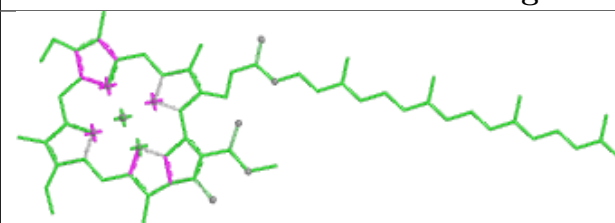
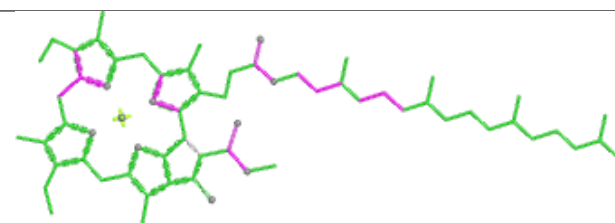
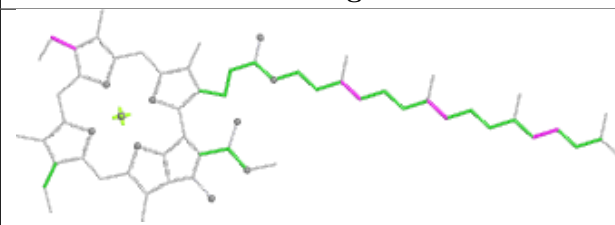
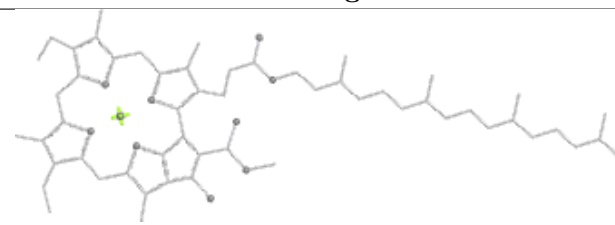
Ligand STE H 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

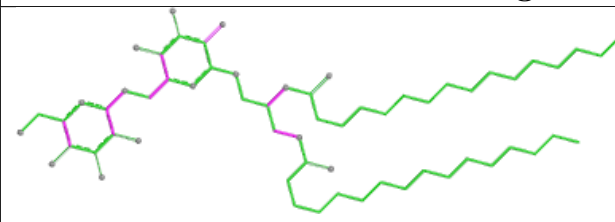
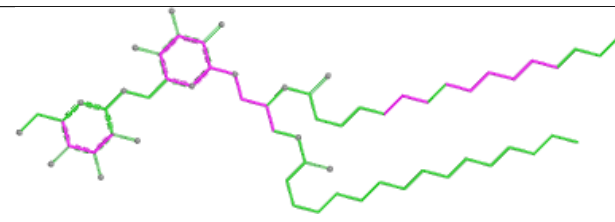
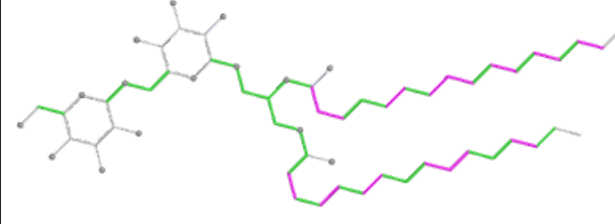
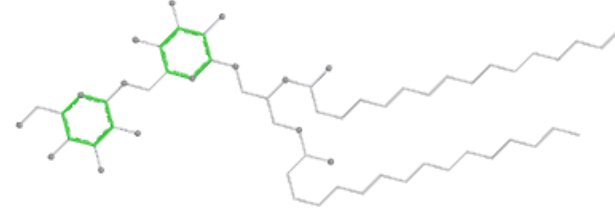
Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

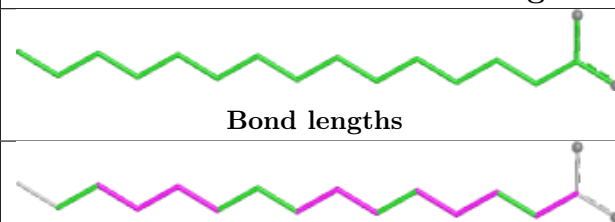
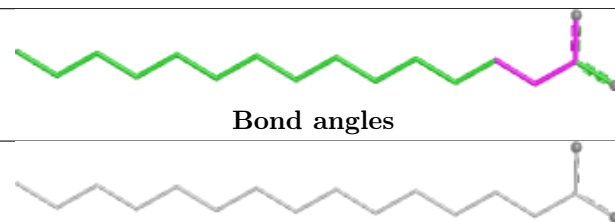
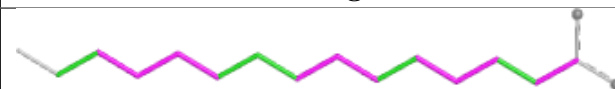
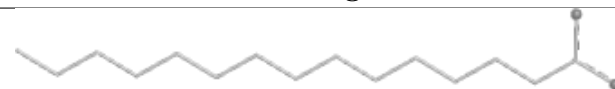
Ligand BCR t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

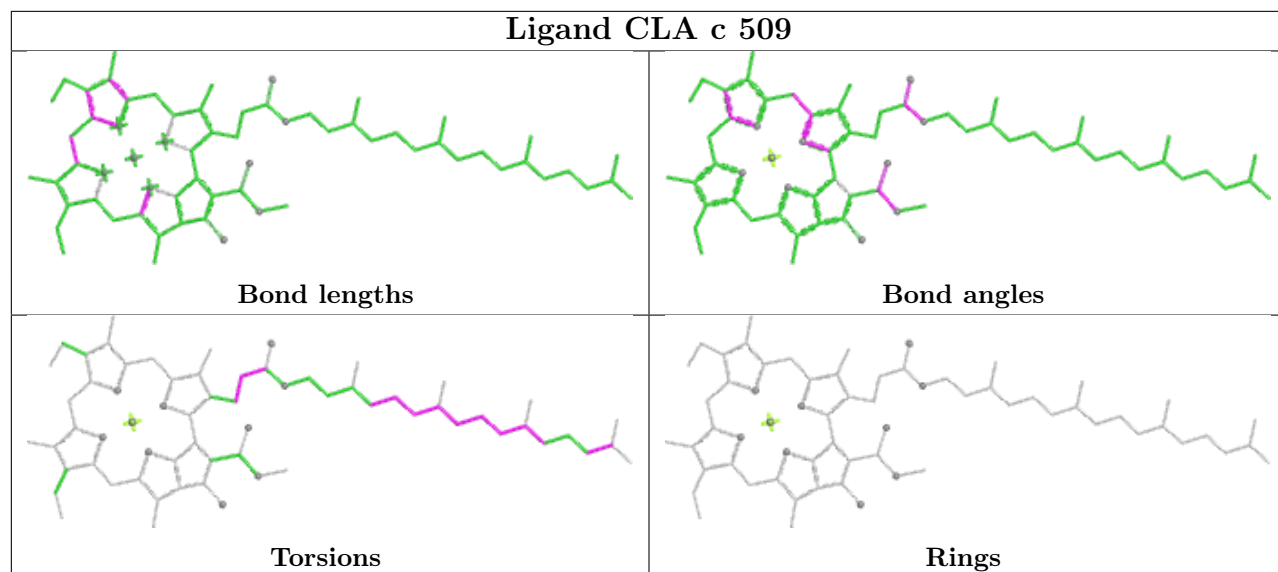


Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

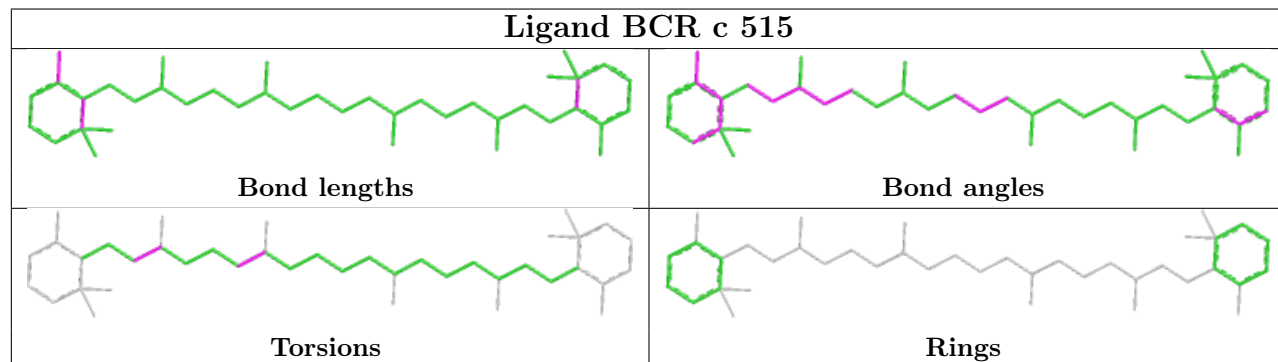
Ligand DGD H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE d 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

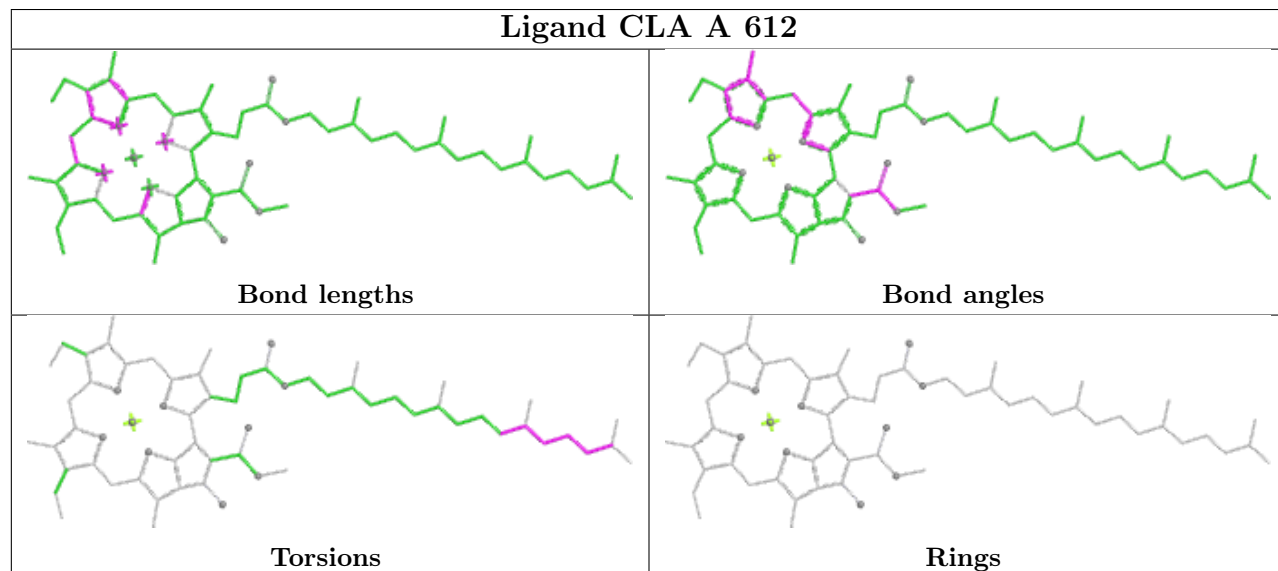
Ligand CLA c 509

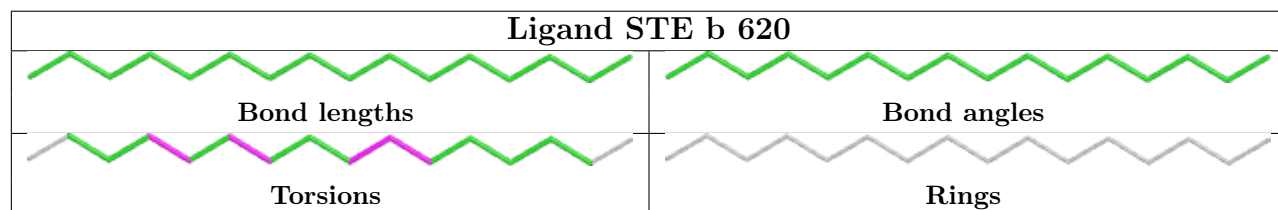
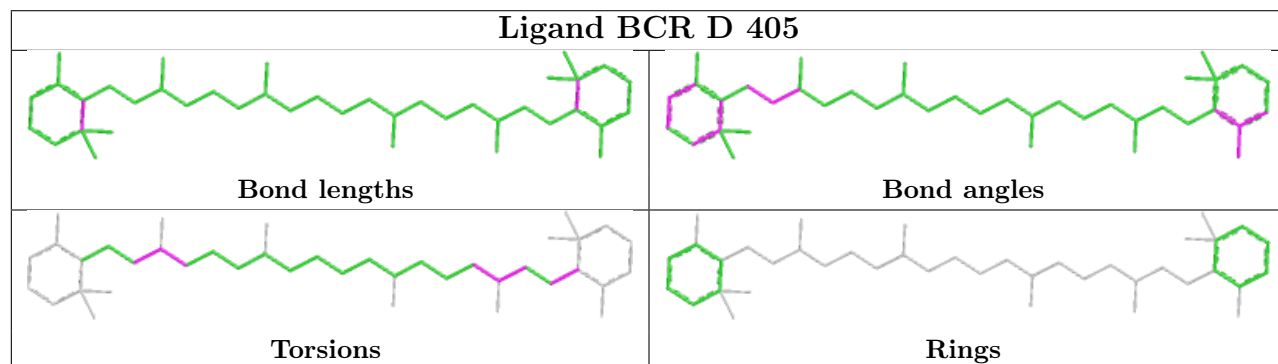
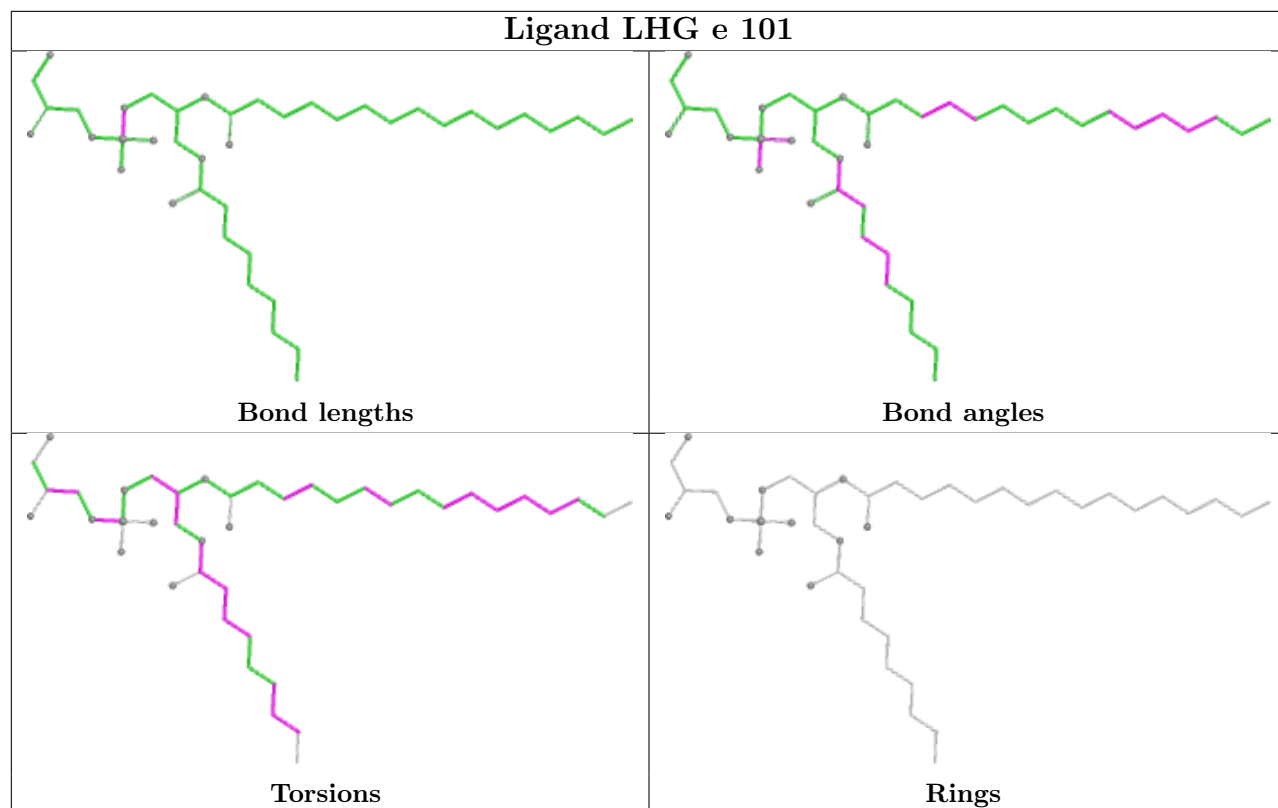


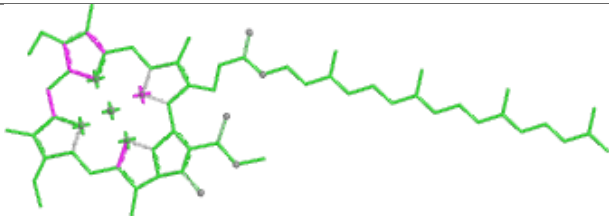
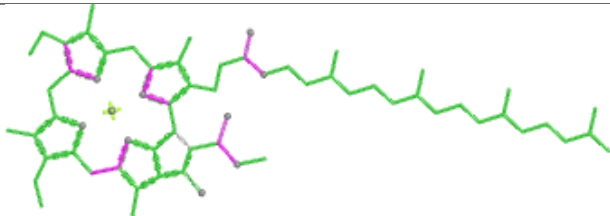
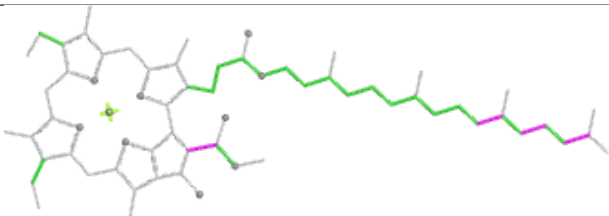
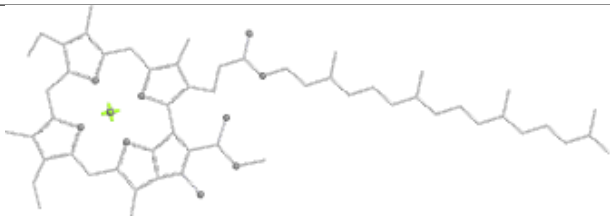
Ligand BCR c 515

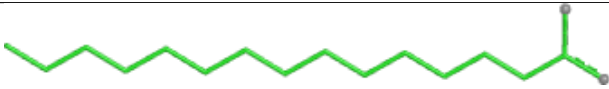
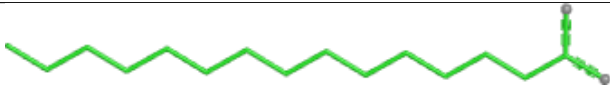
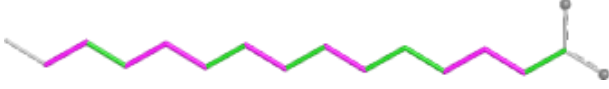
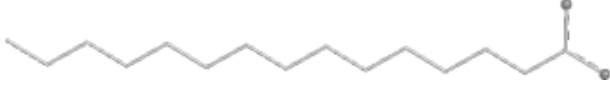


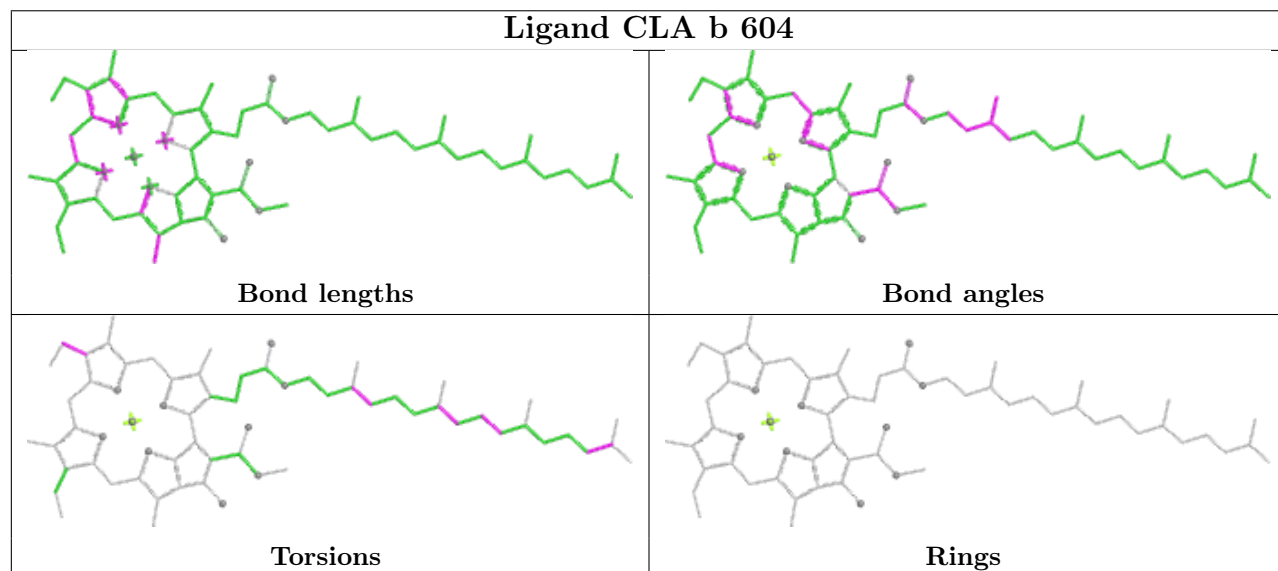
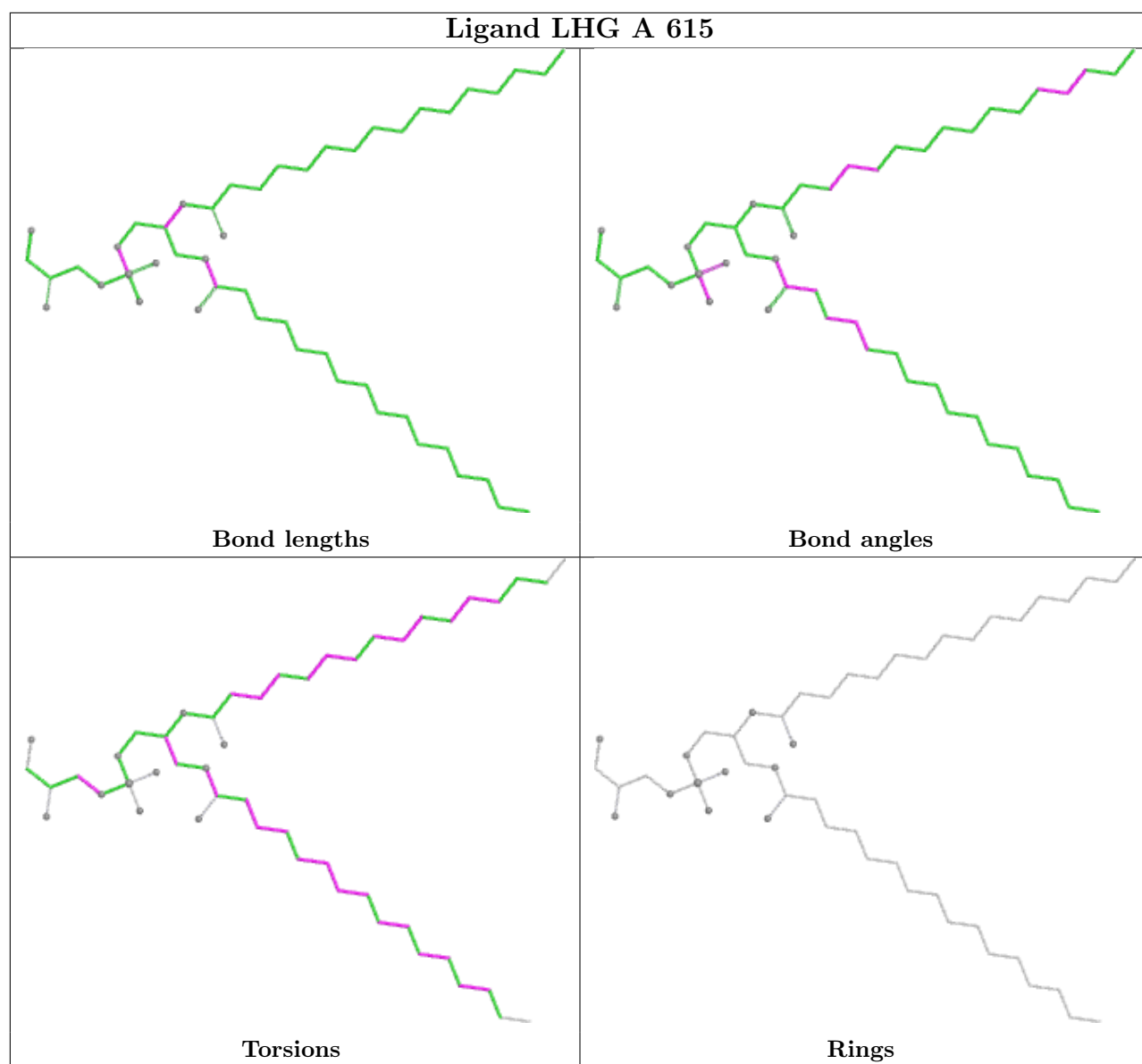
Ligand CLA A 612

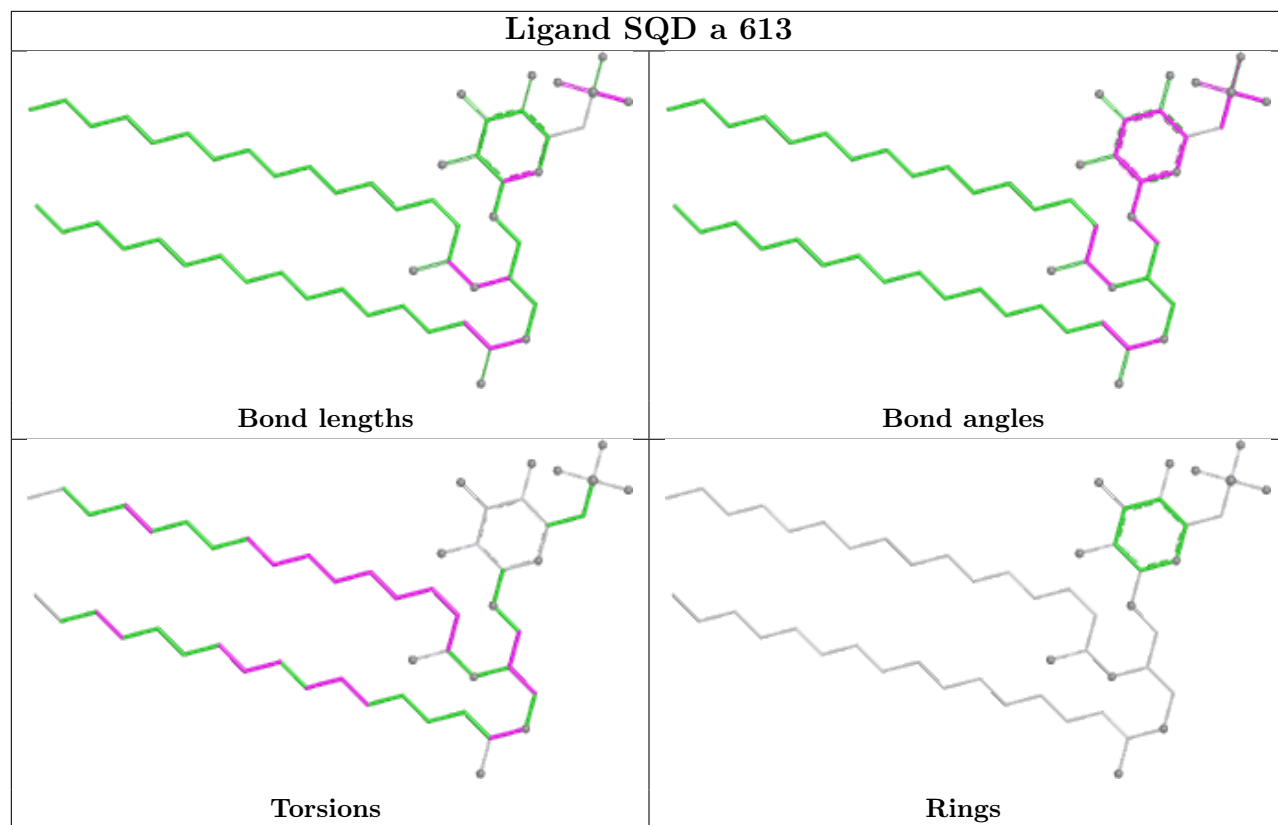




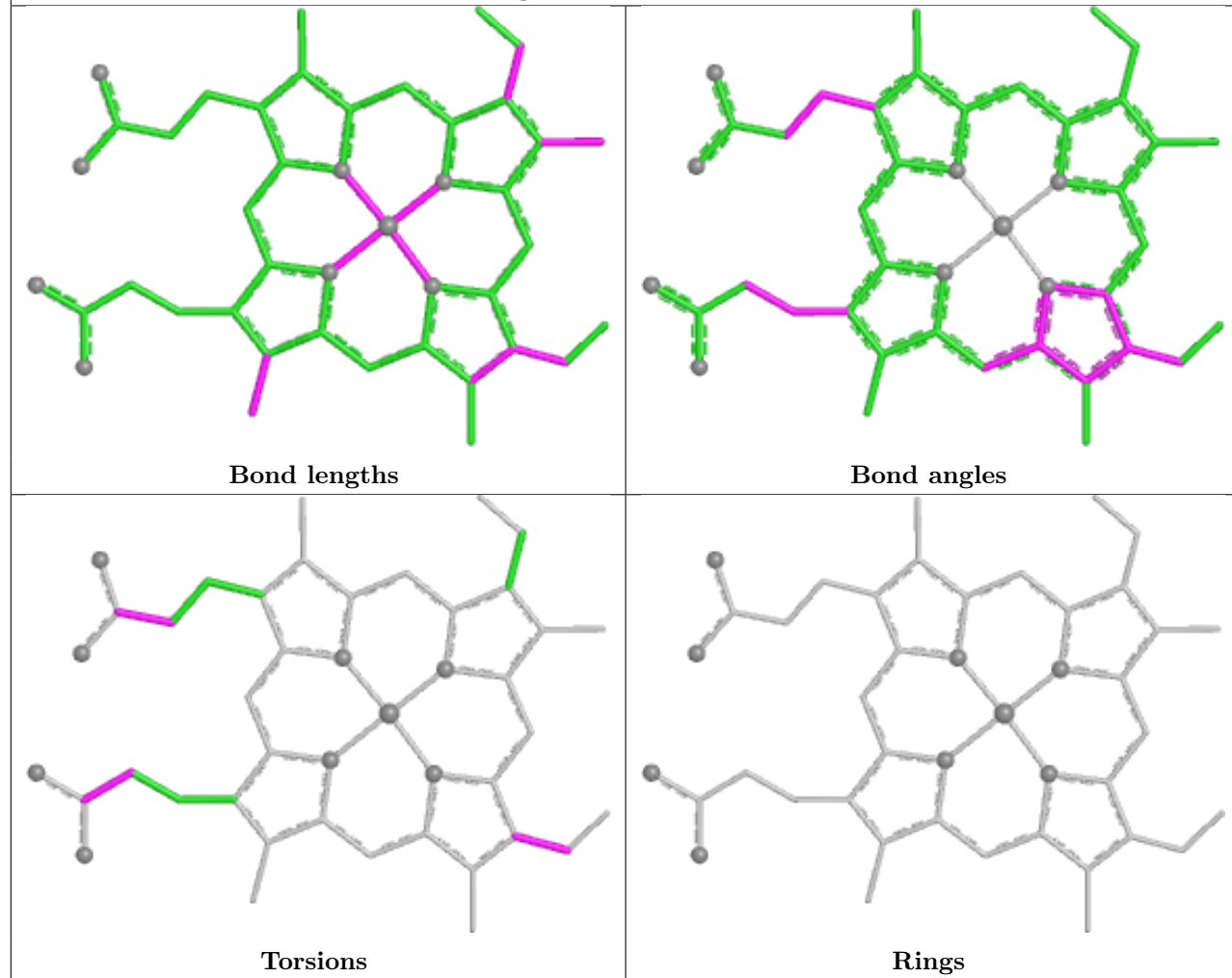
Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

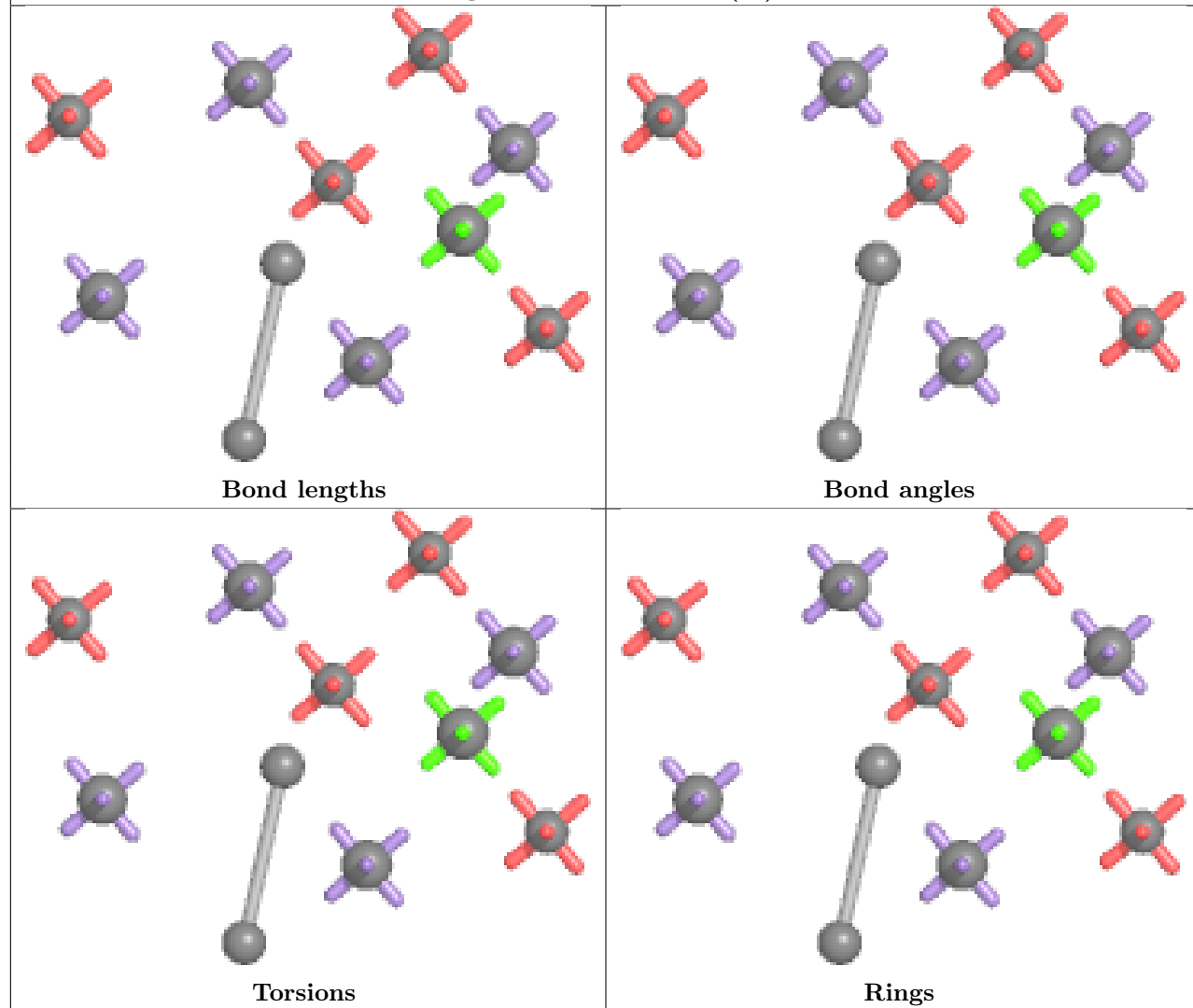




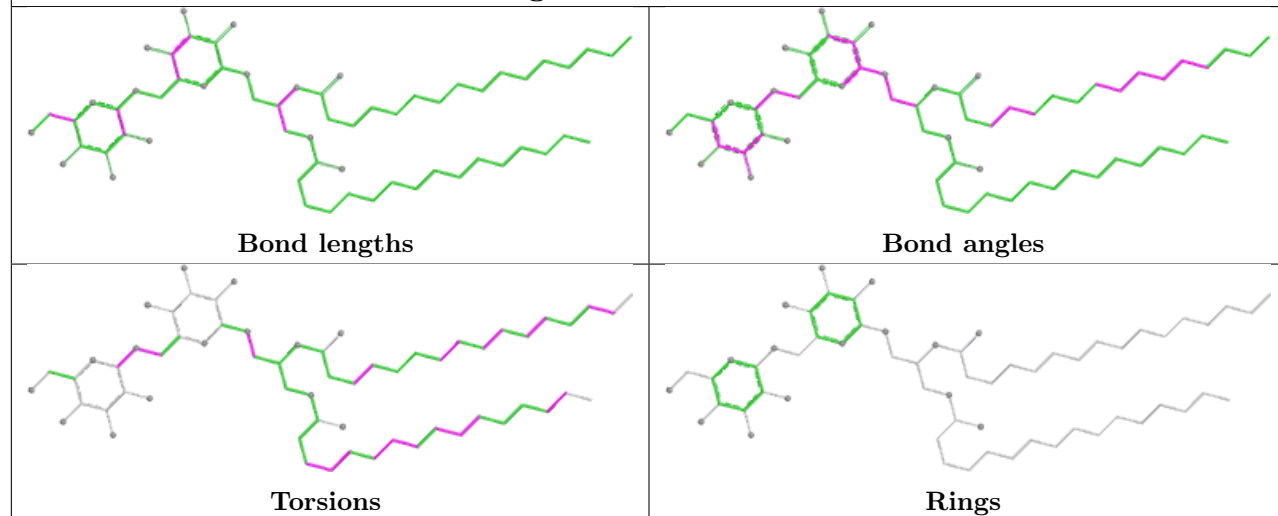
Ligand HEM f 101



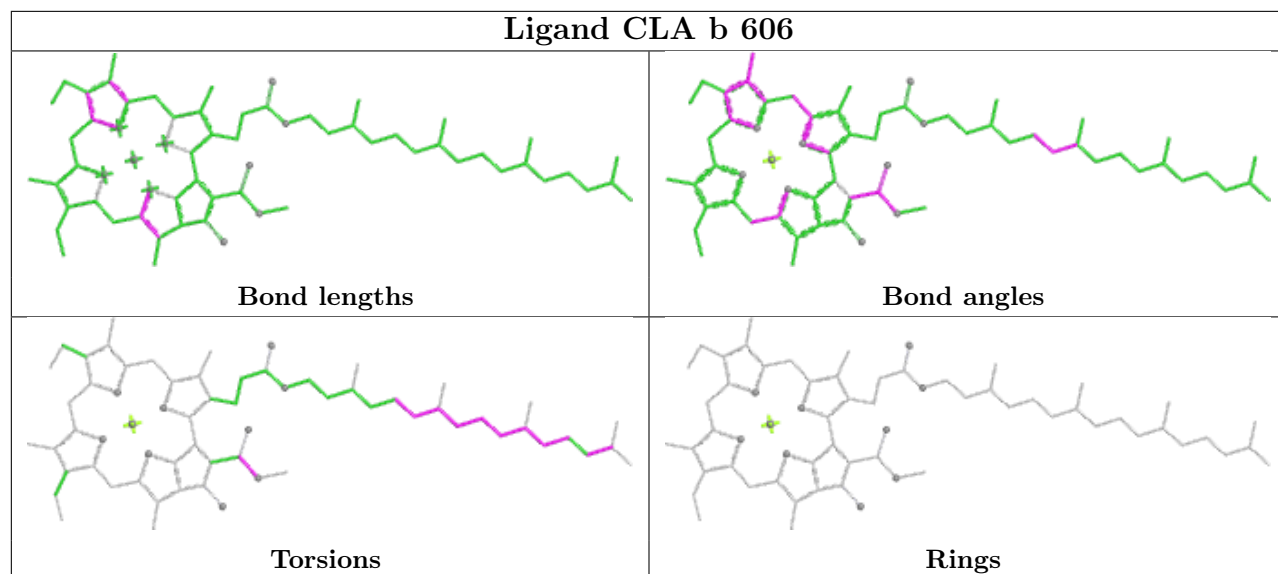
Ligand OEY A 601 (A)



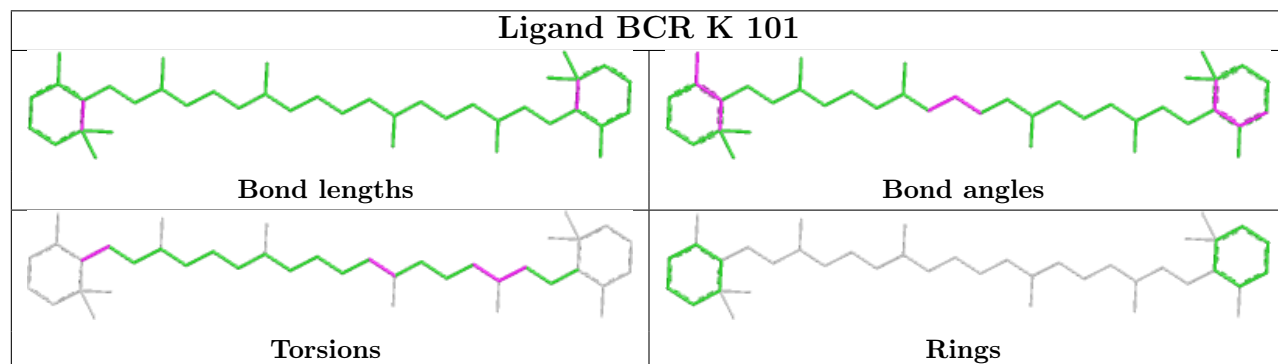
Ligand DGD C 517



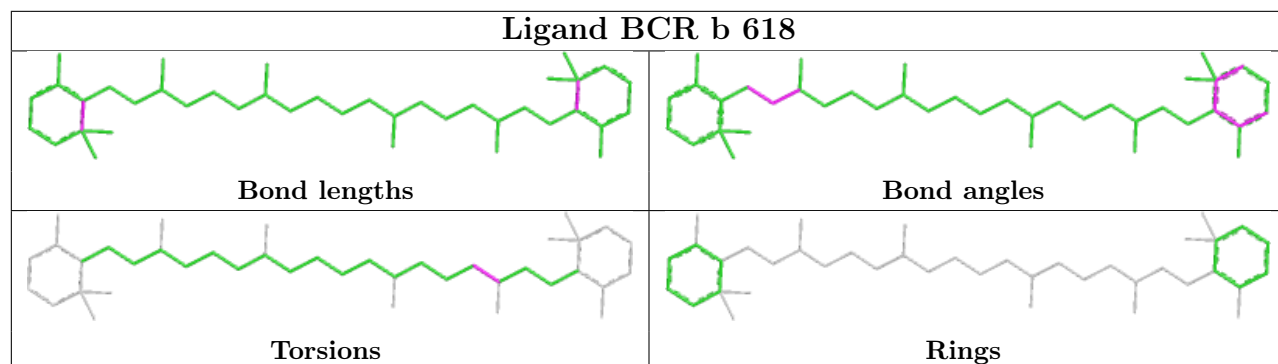
Ligand CLA b 606



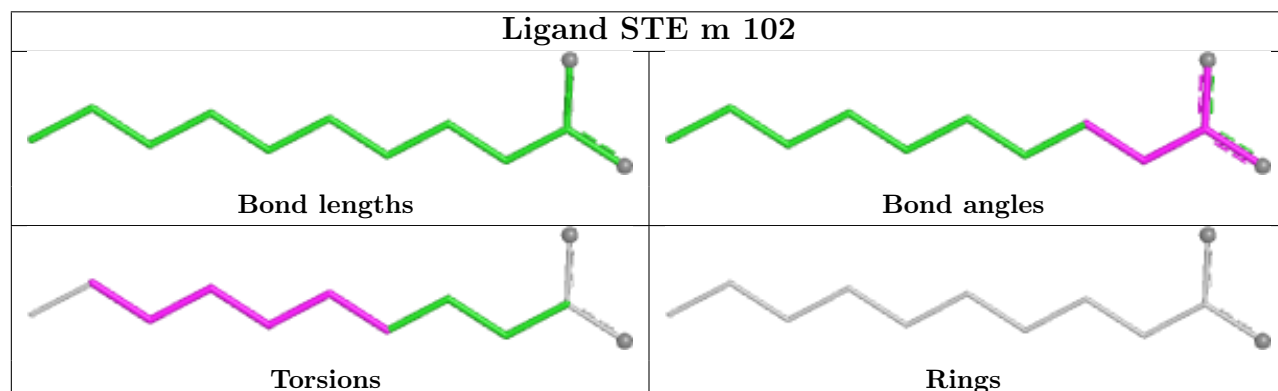
Ligand BCR K 101



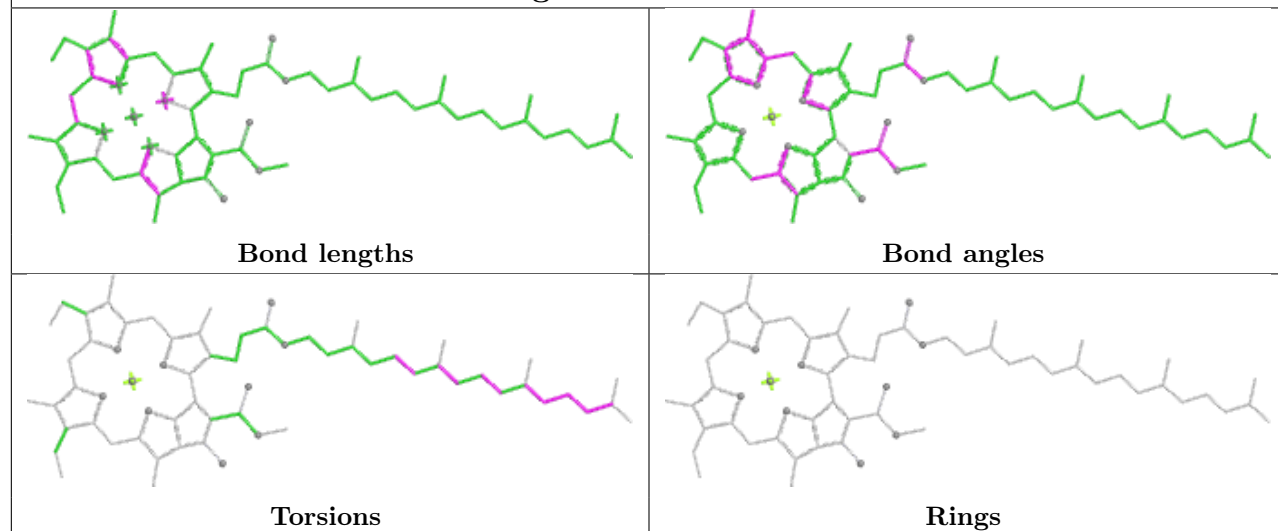
Ligand BCR b 618



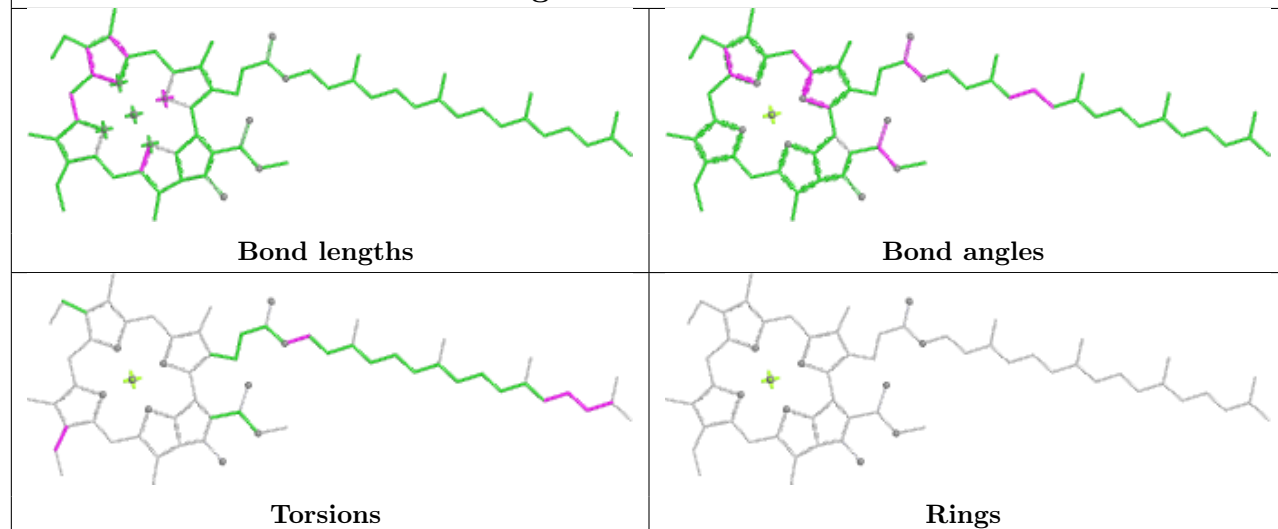
Ligand STE m 102



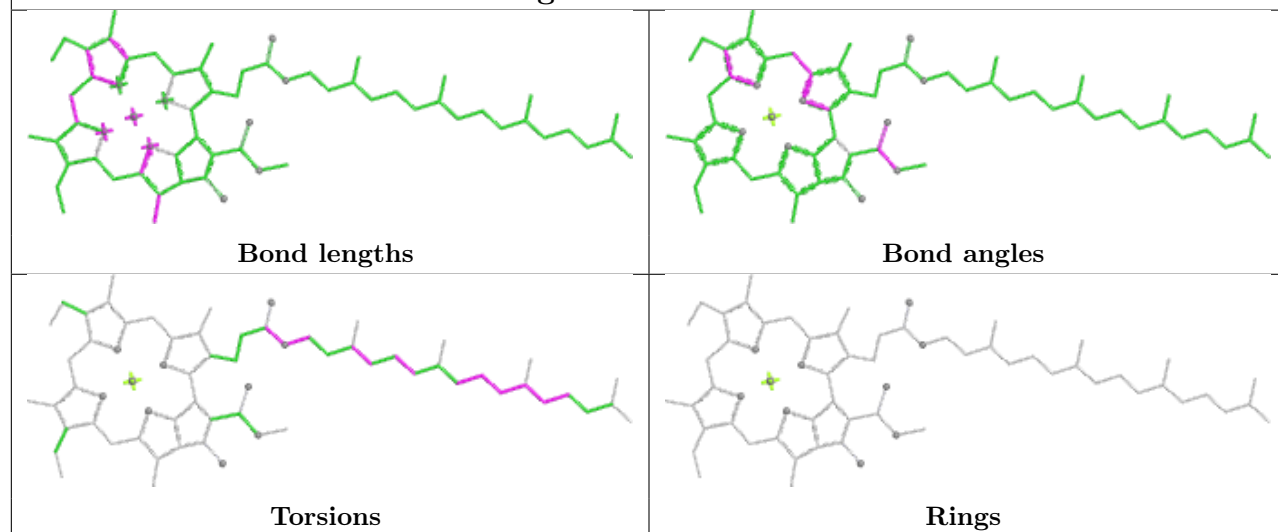
Ligand CLA C 508

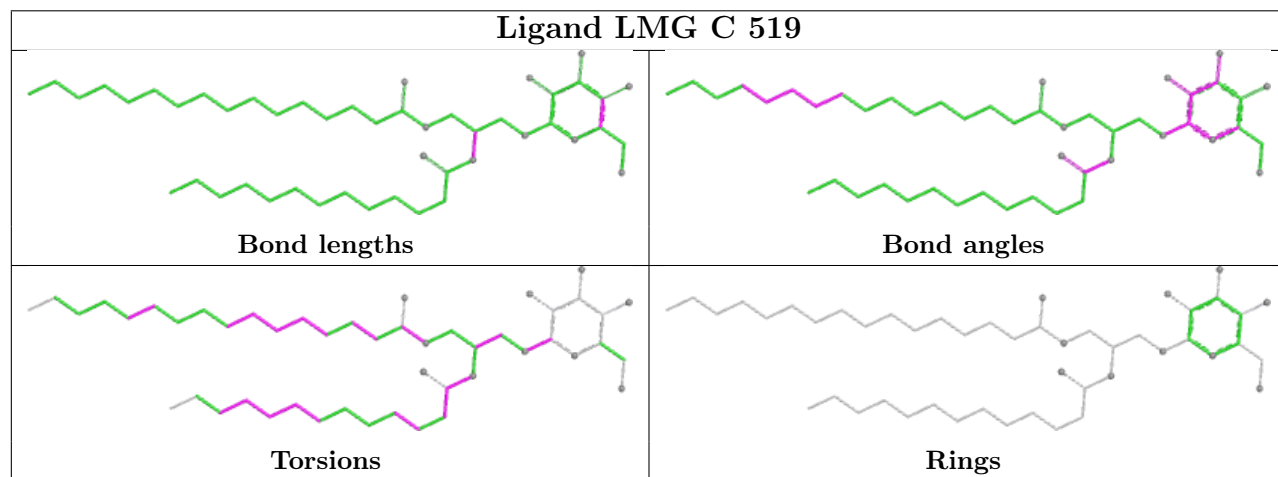
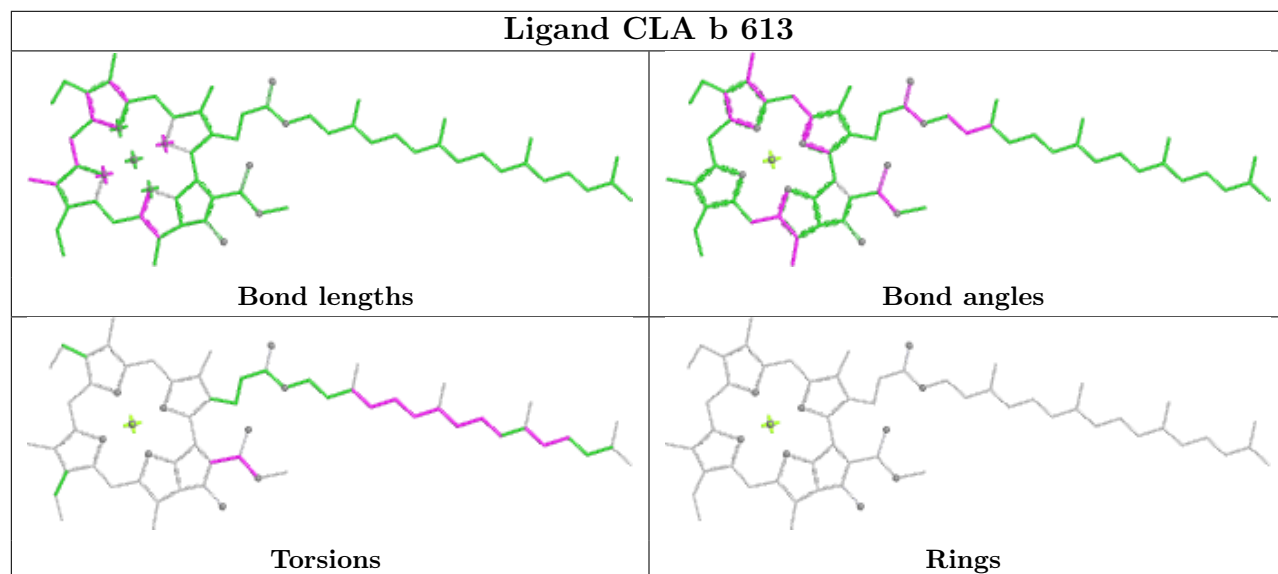
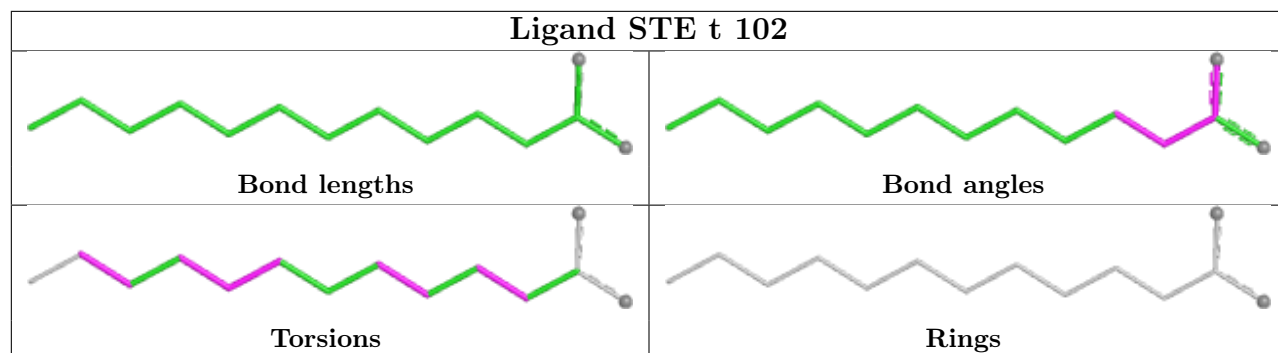


Ligand CLA A 606

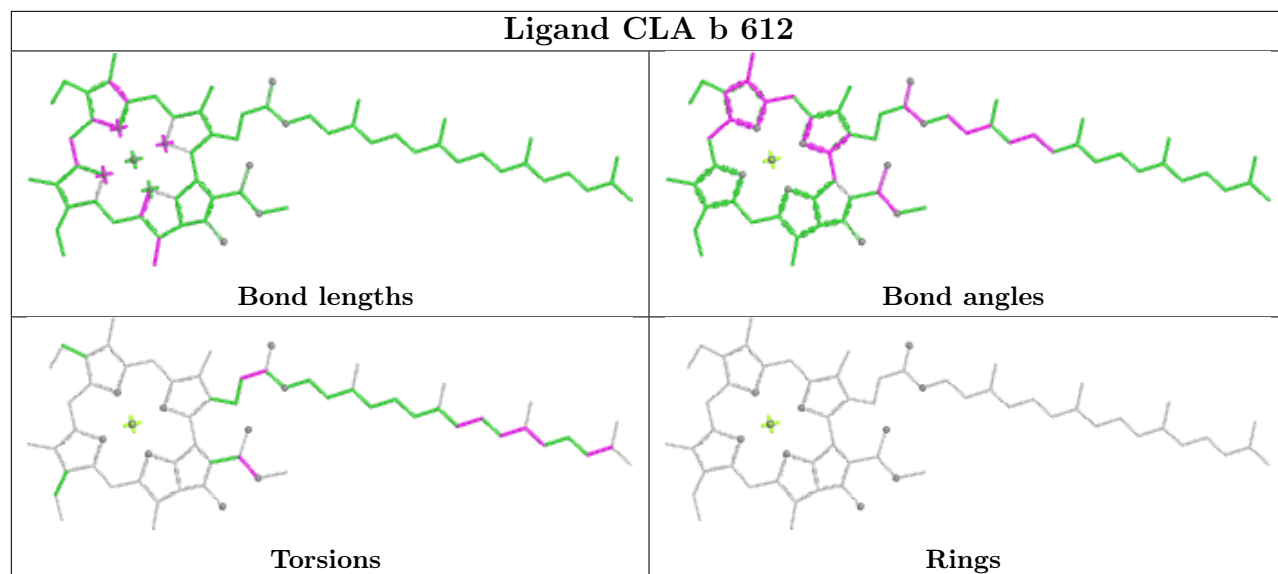


Ligand CLA c 506

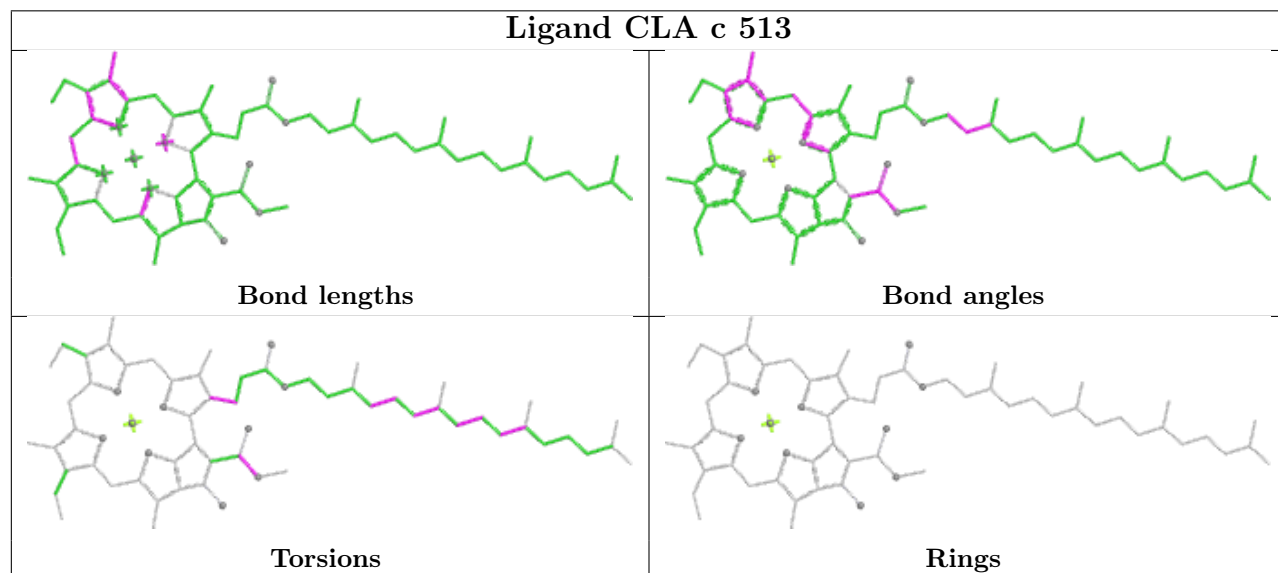




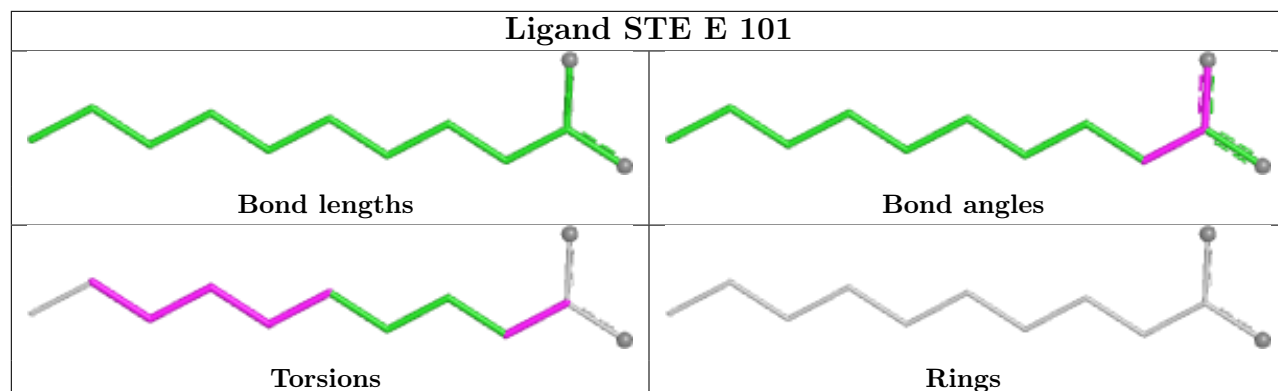
Ligand CLA b 612

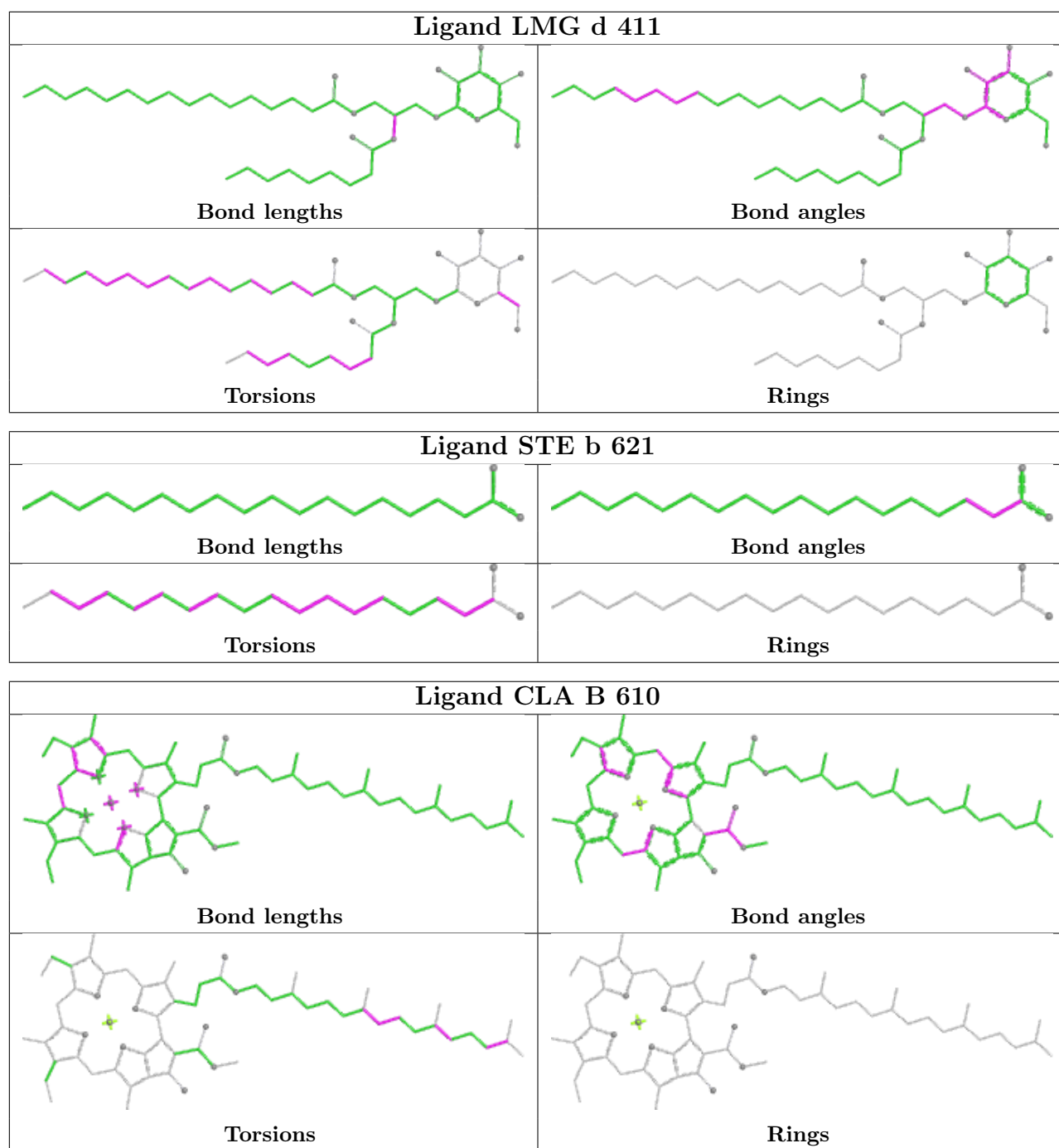


Ligand CLA c 513

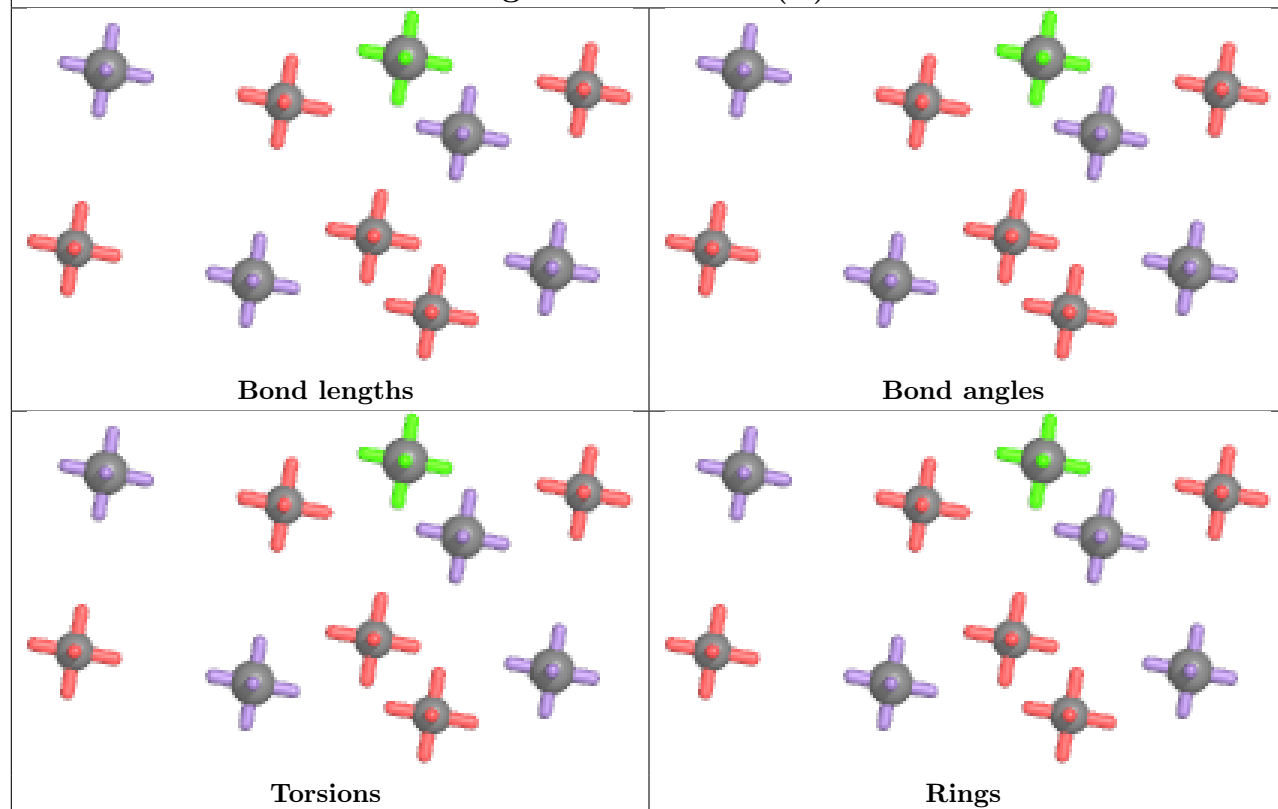


Ligand STE E 101

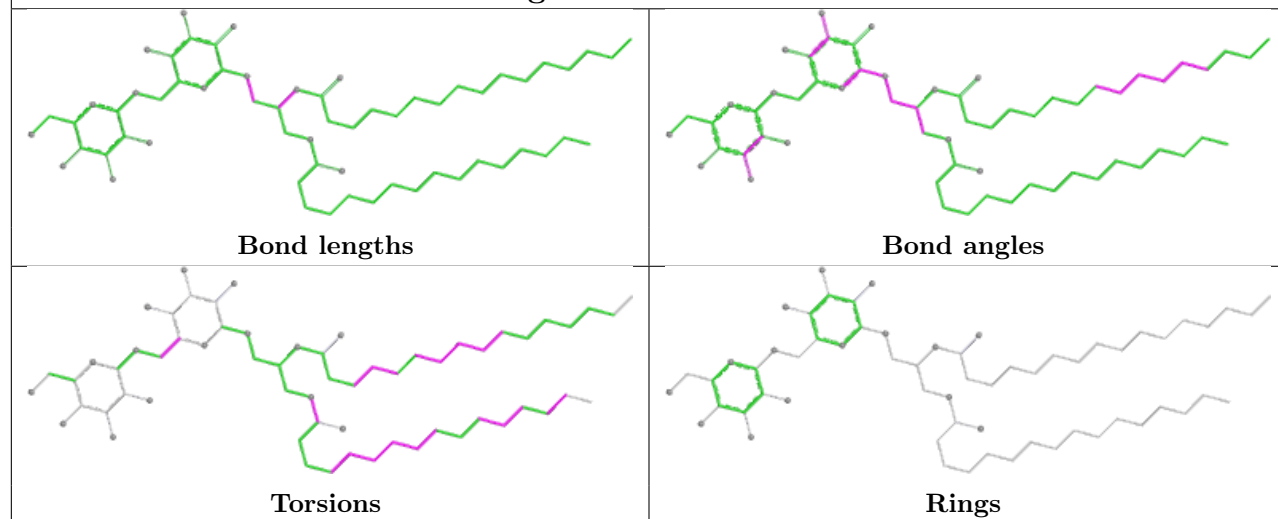




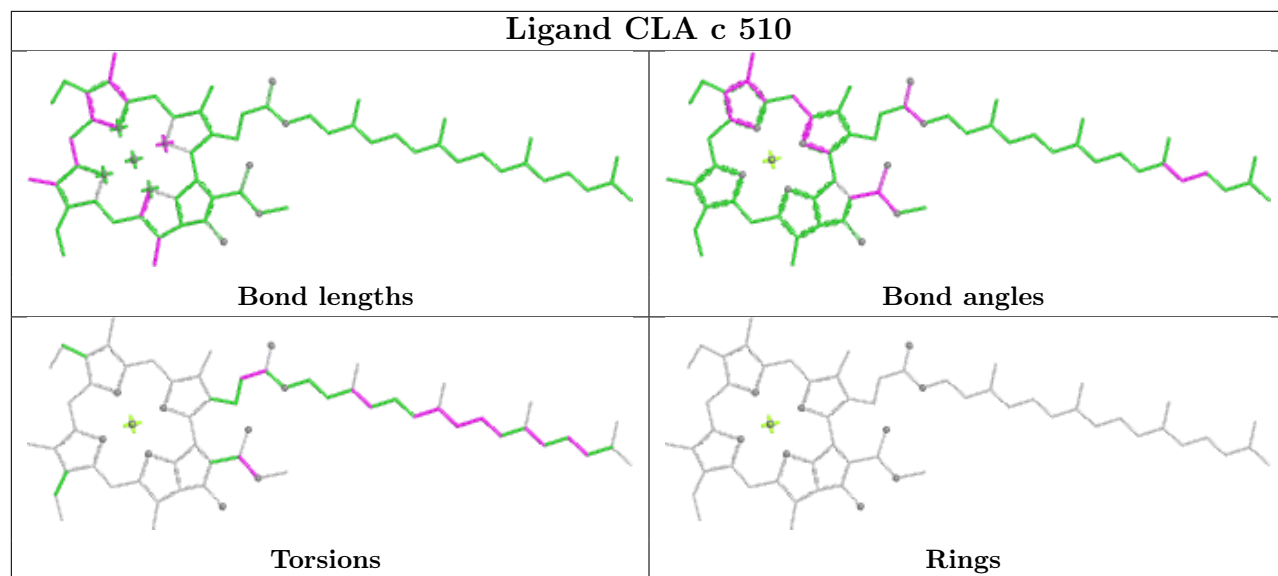
Ligand OEX a 602 (B)



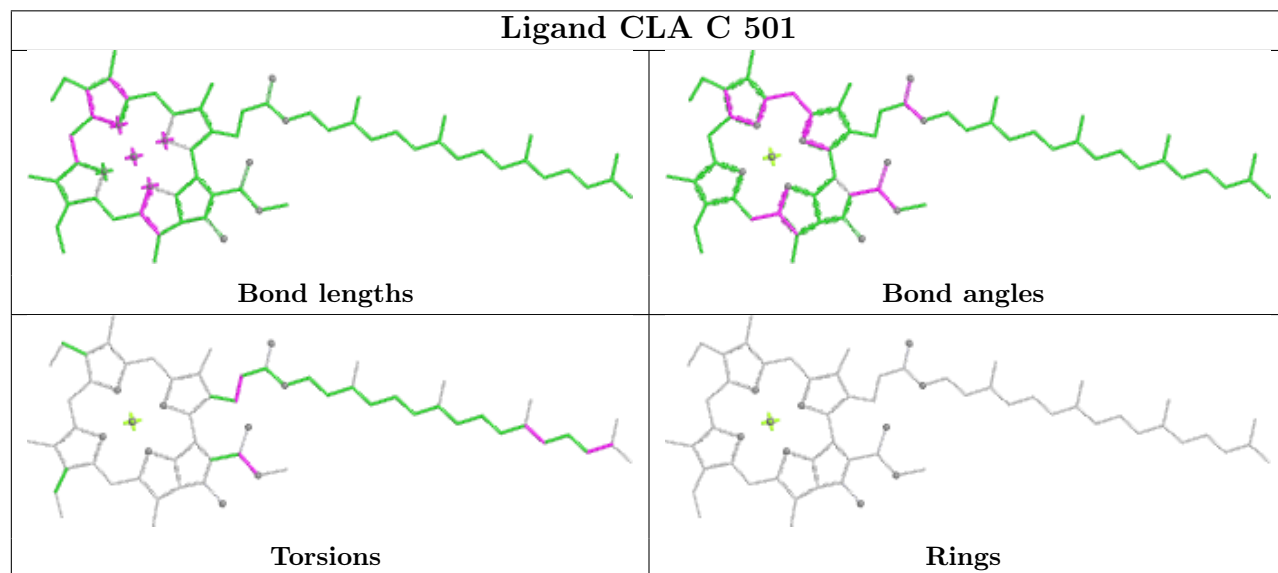
Ligand DGD C 518



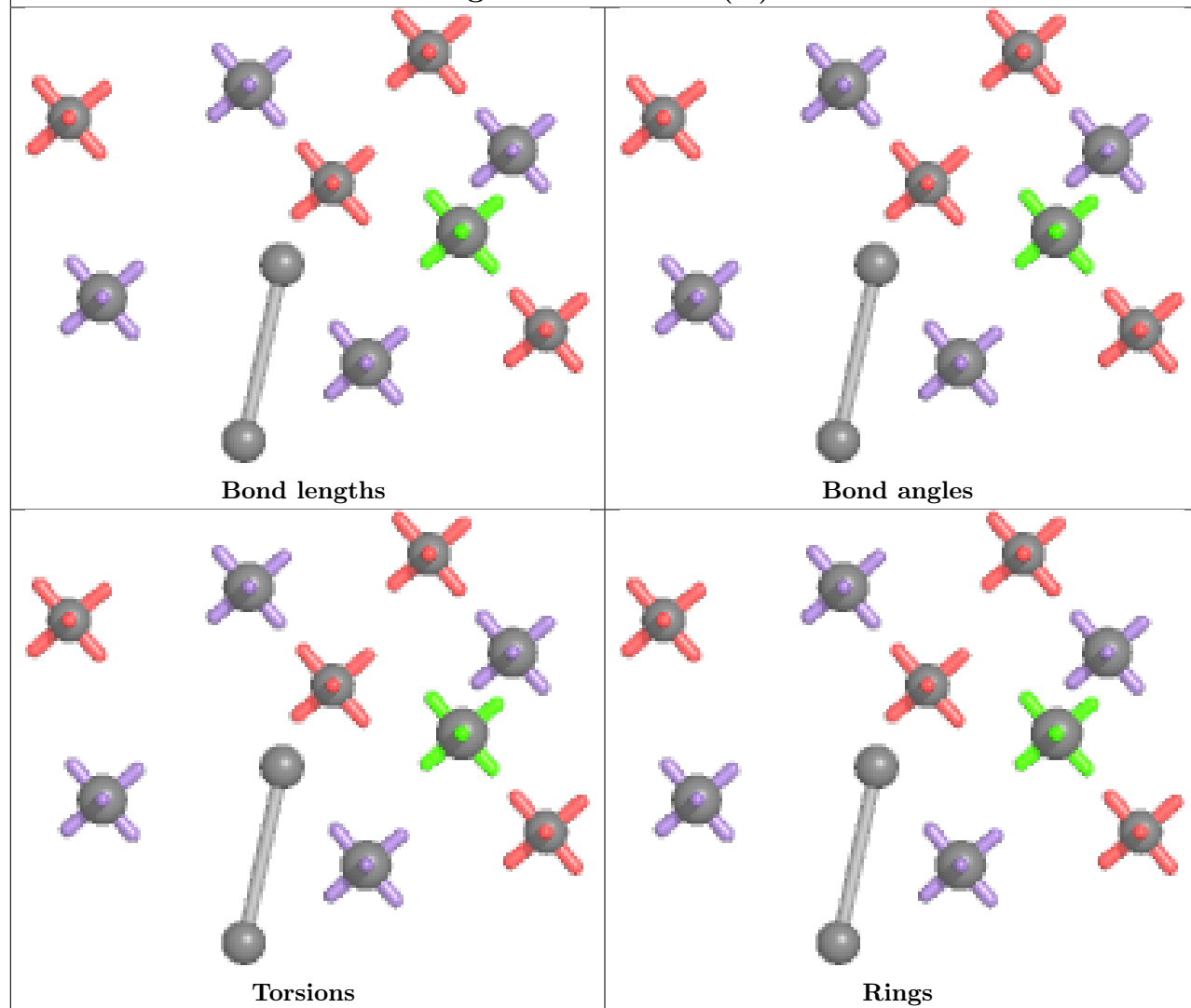
Ligand CLA c 510



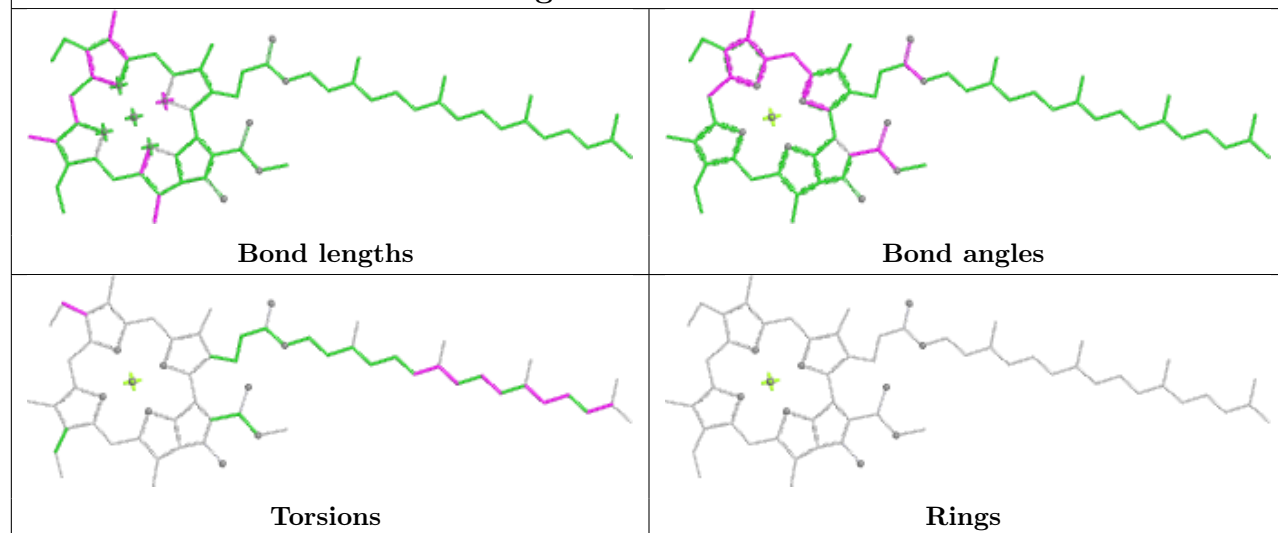
Ligand CLA C 501

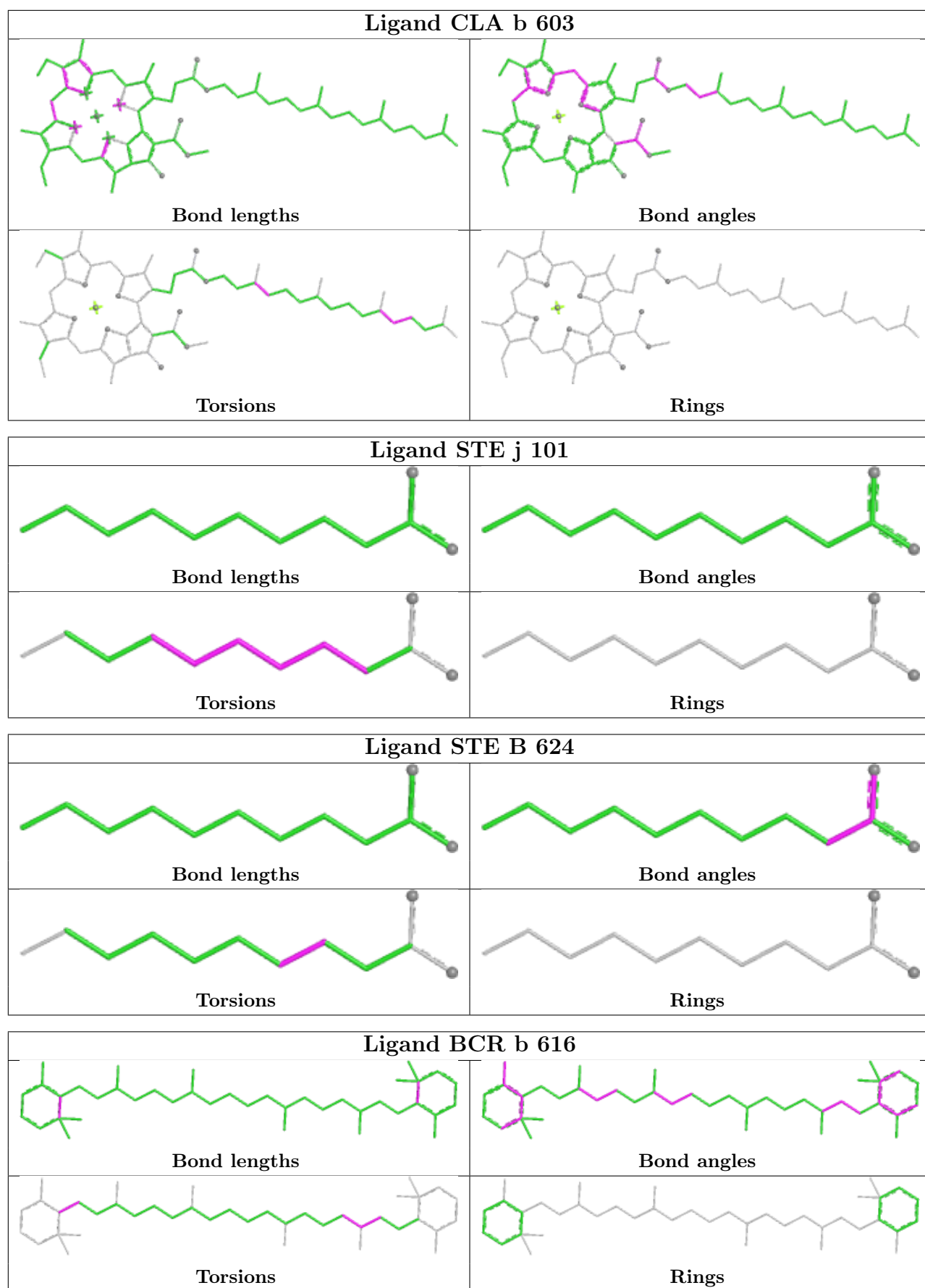


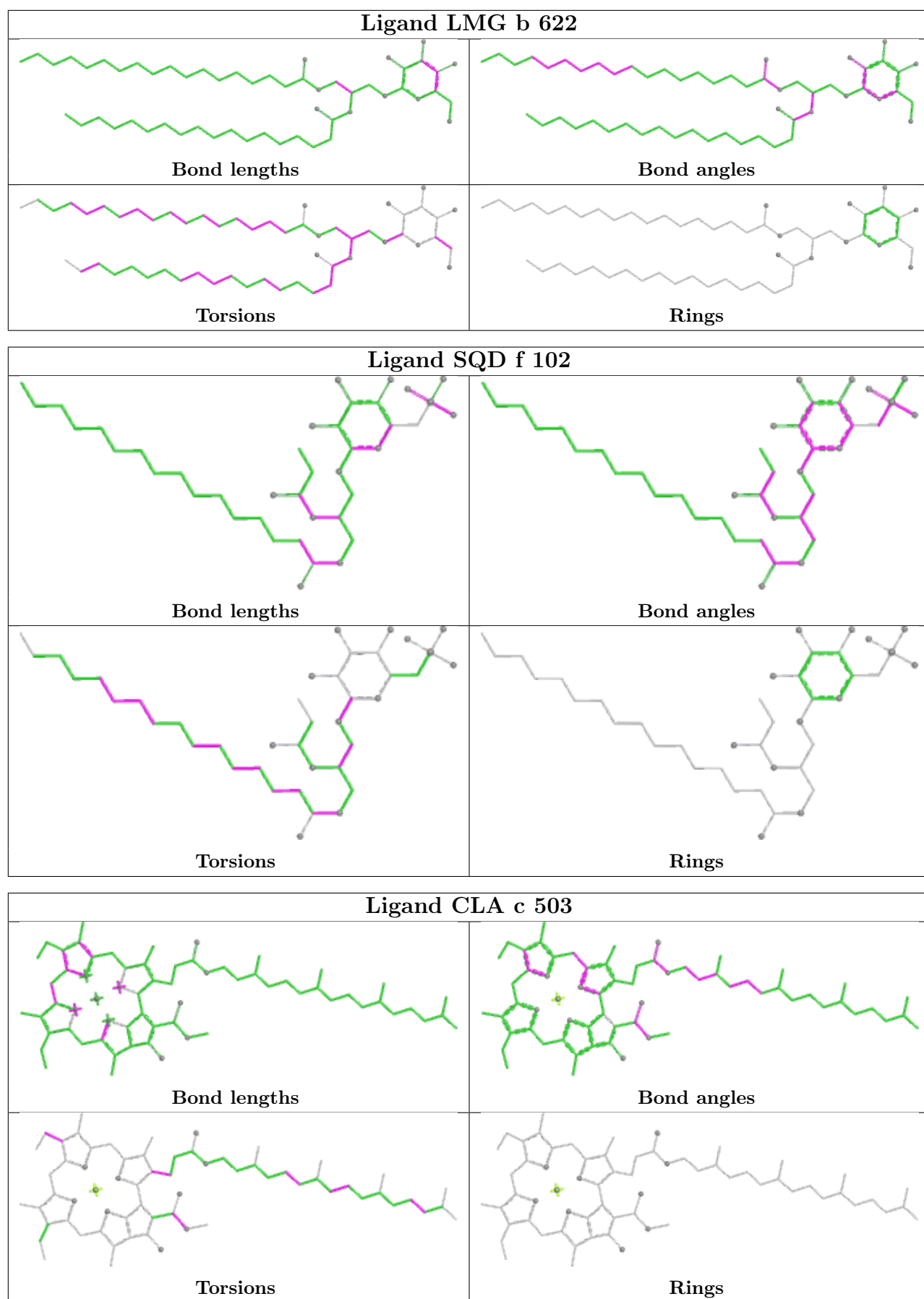
Ligand OEY a 601 (A)



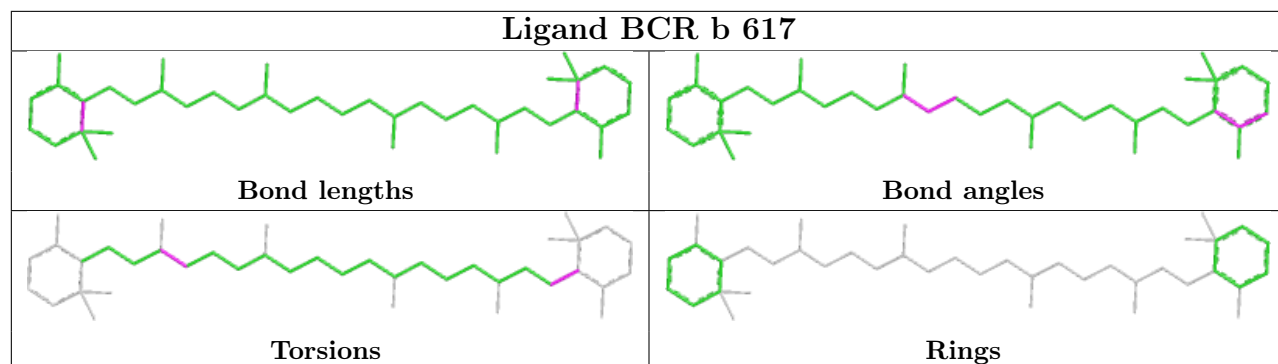
Ligand CLA b 602



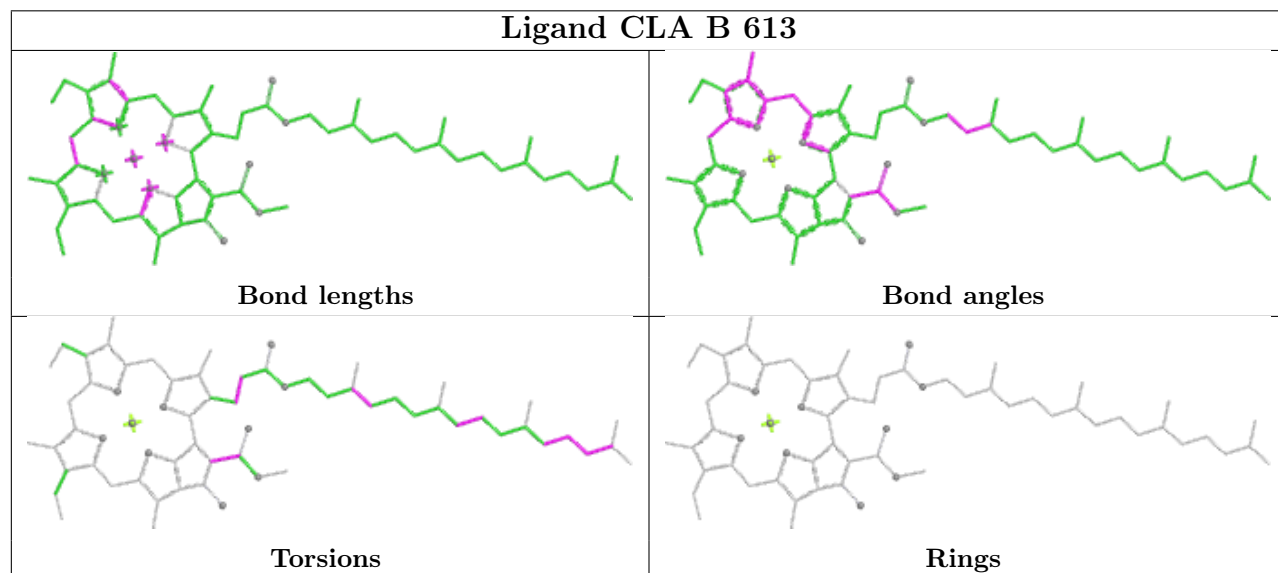




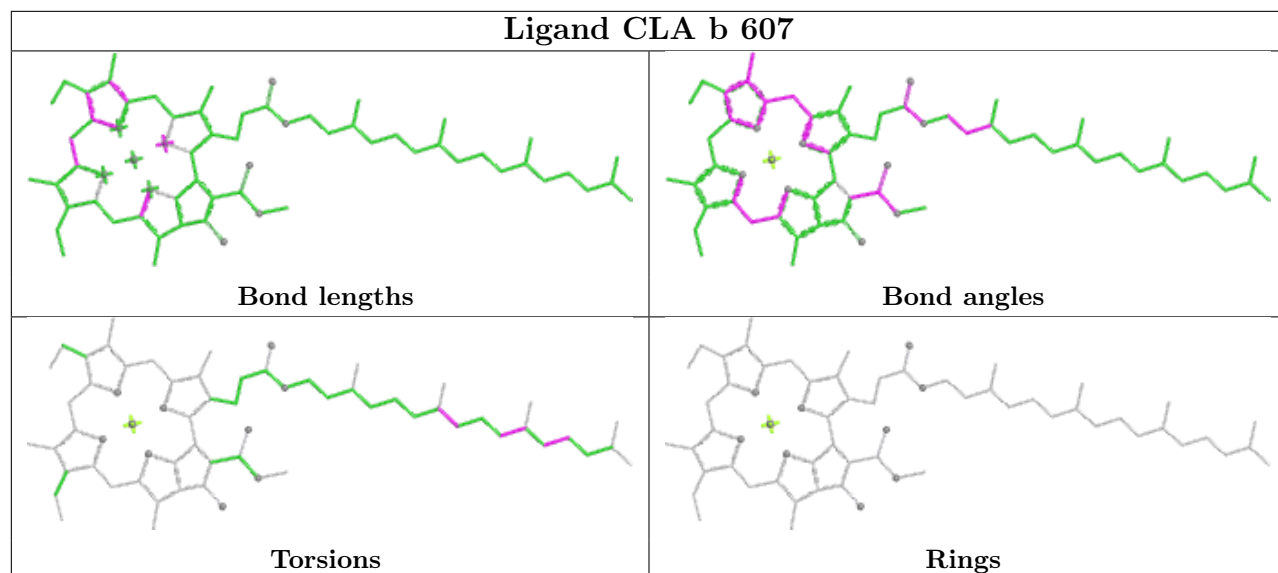
Ligand BCR b 617

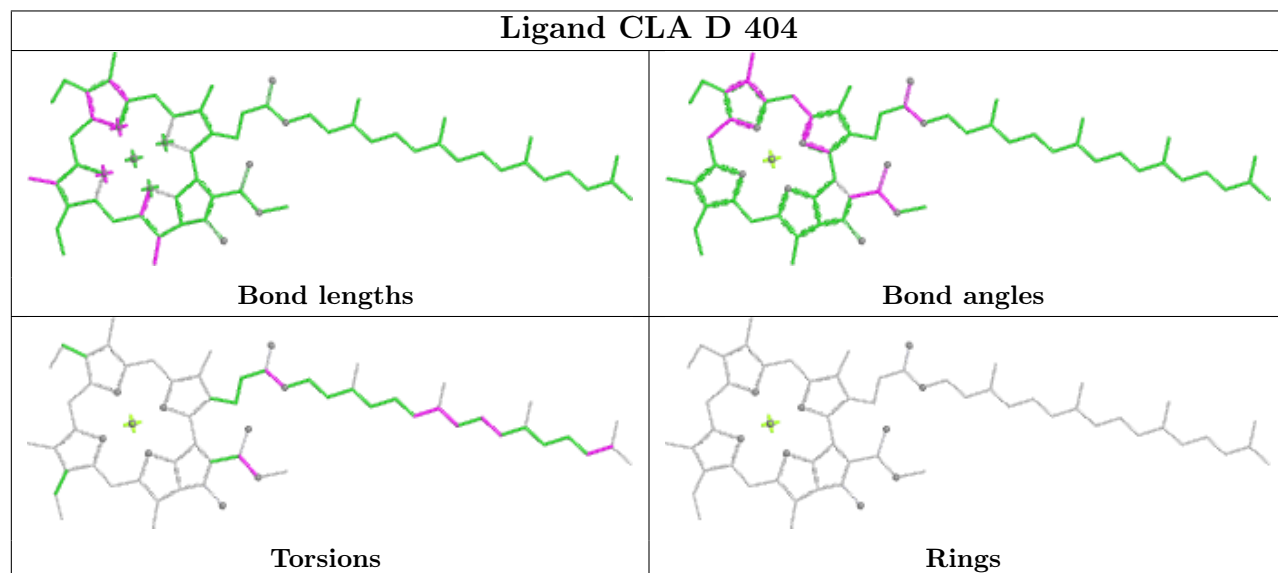
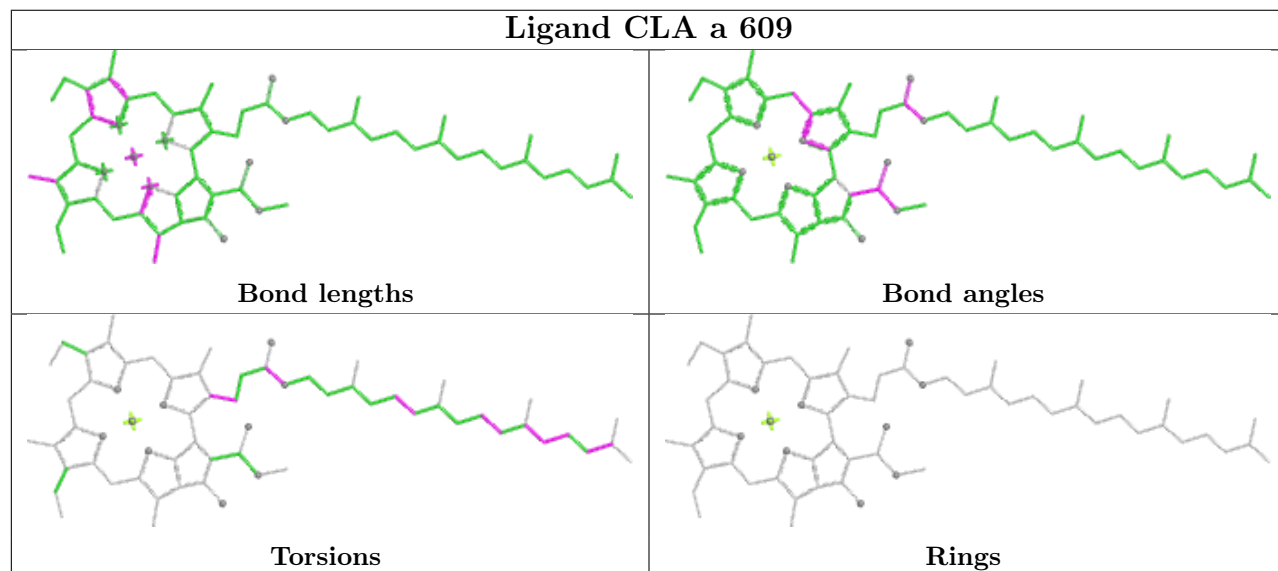
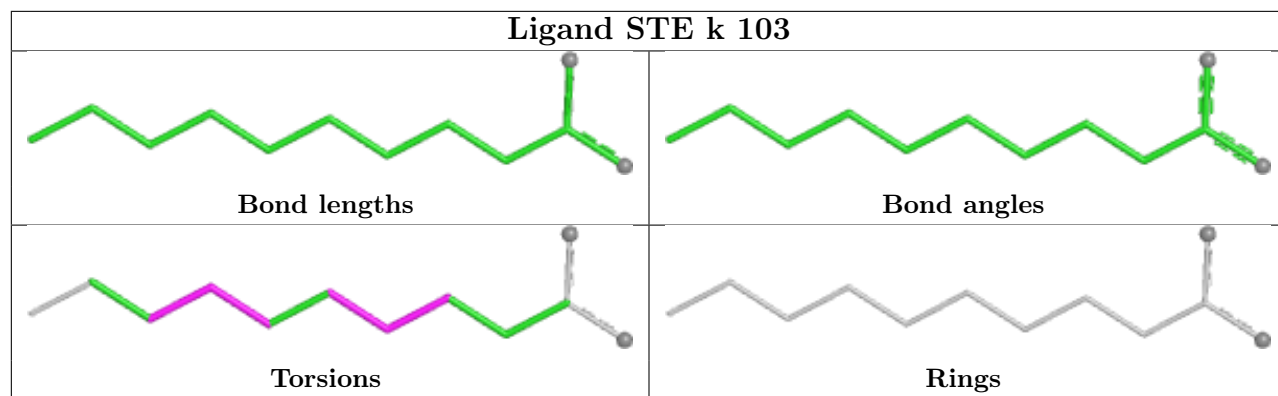


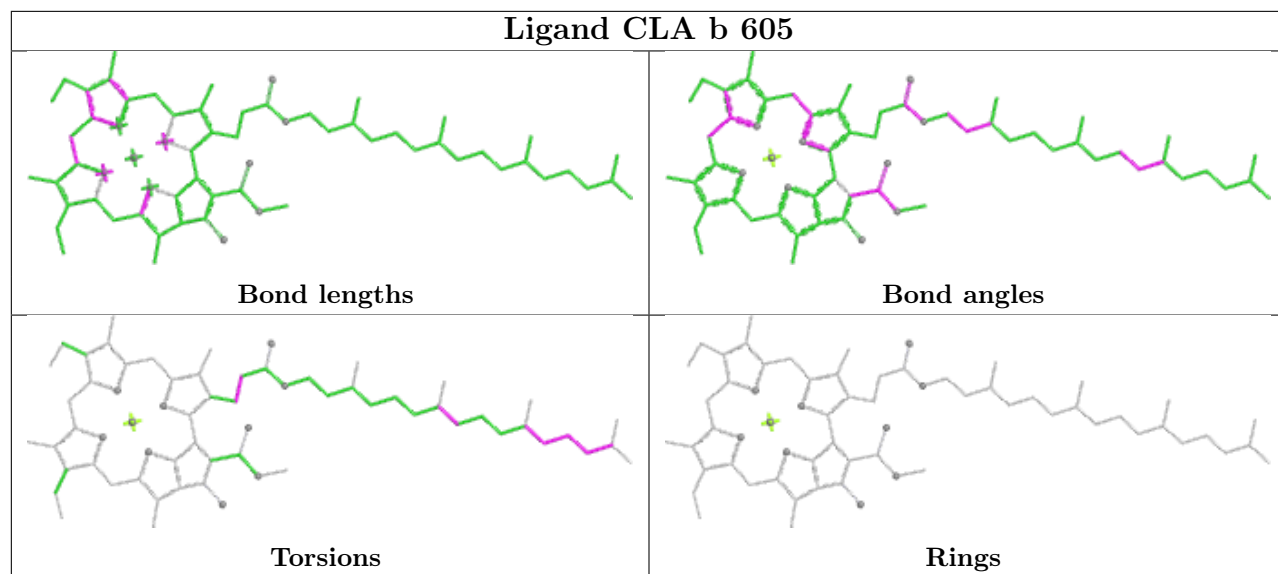
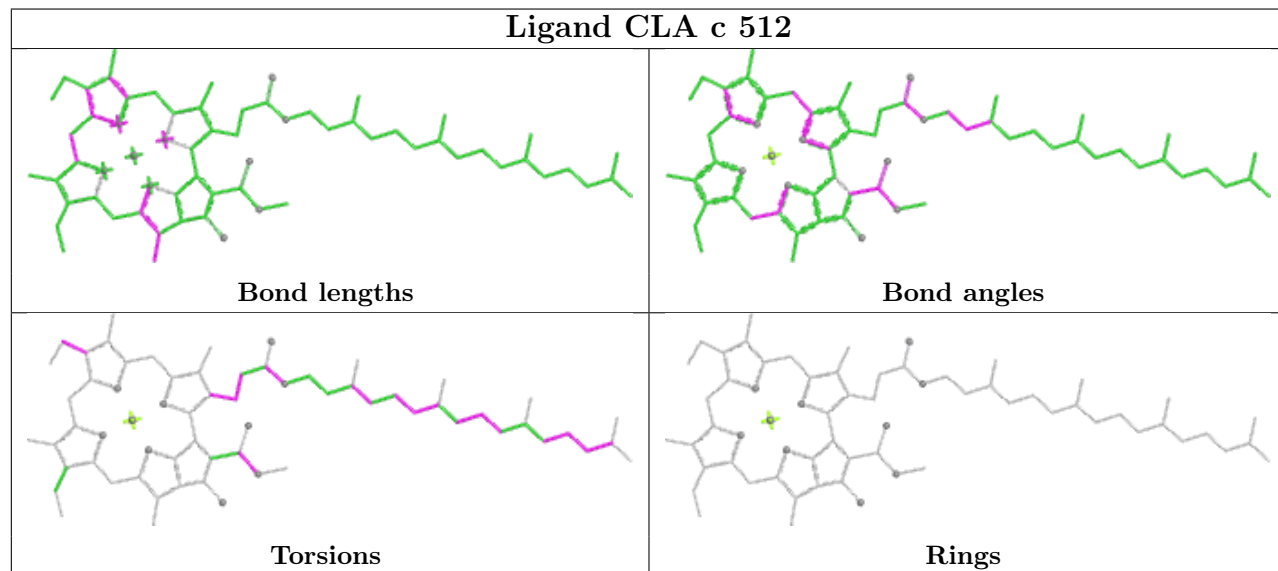
Ligand CLA B 613

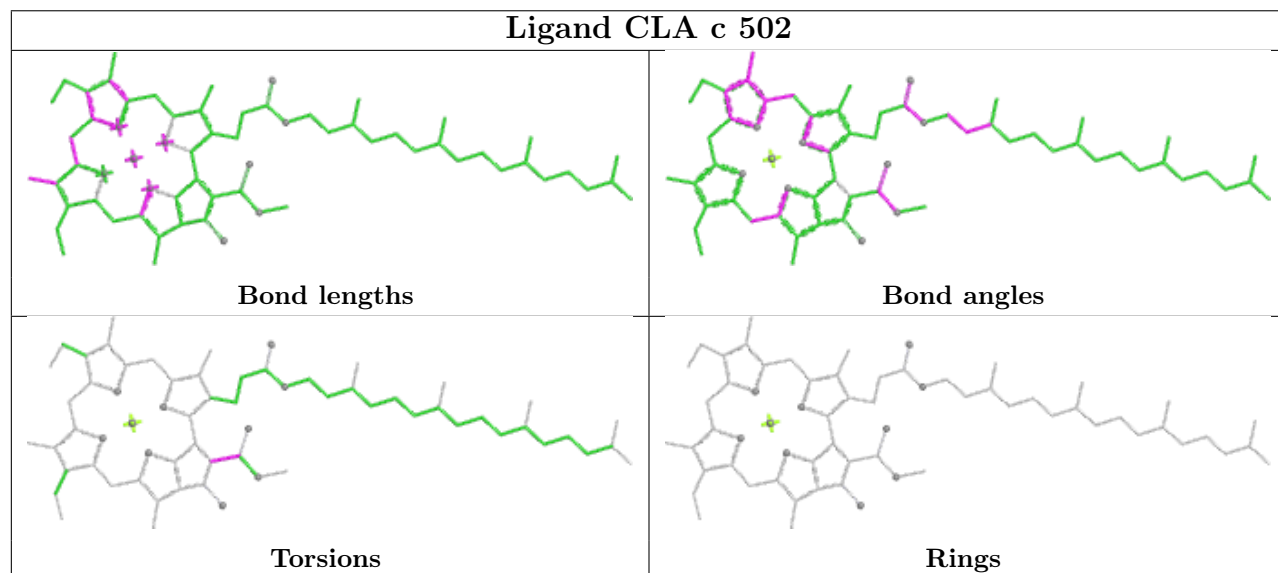
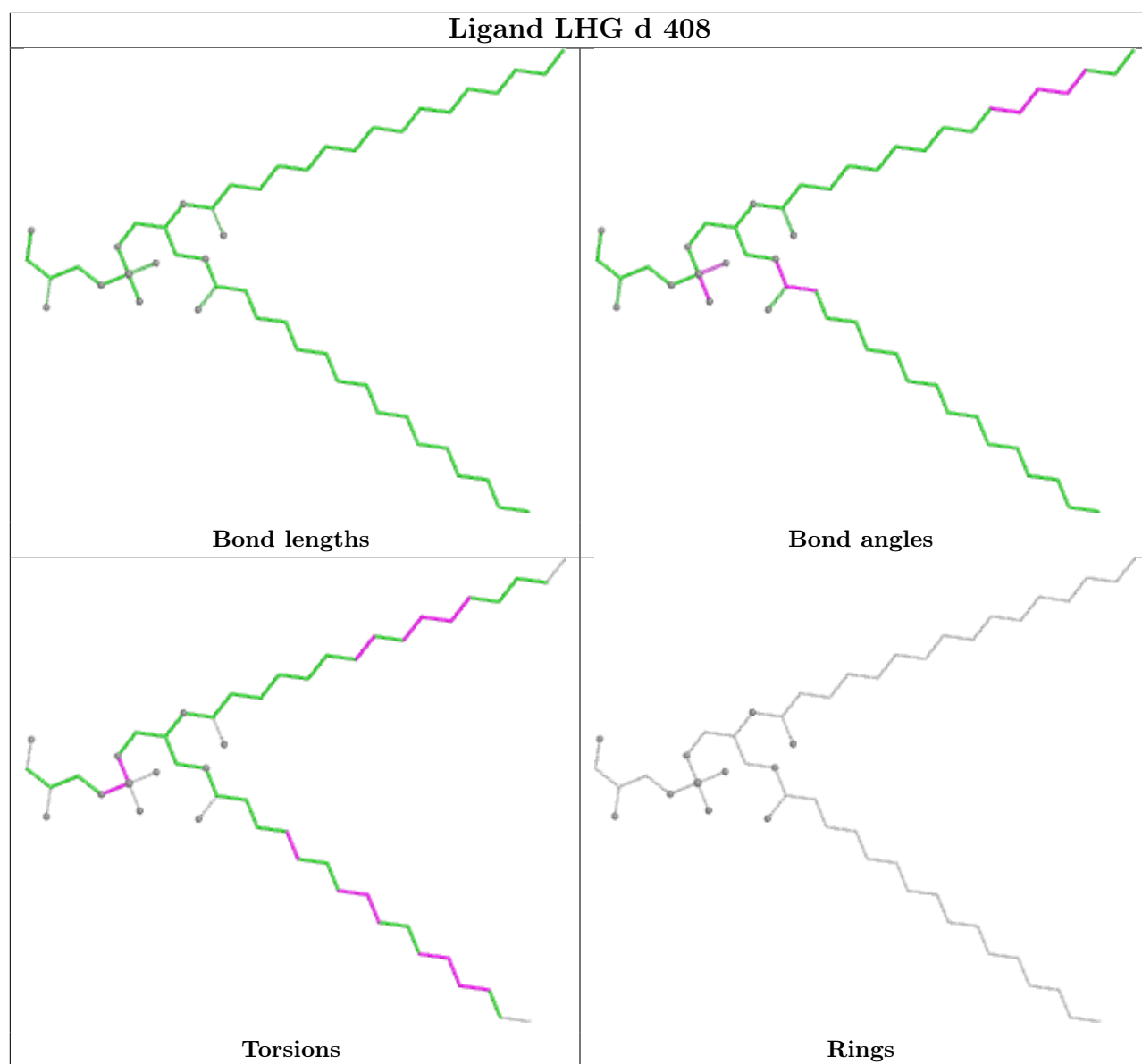


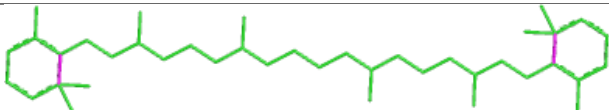
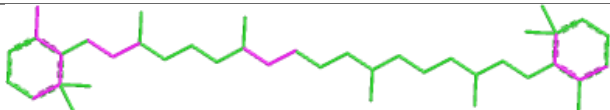
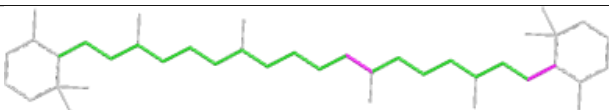
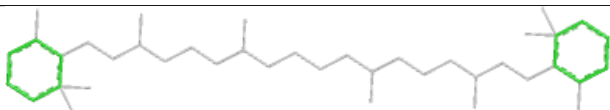
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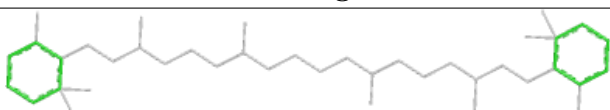


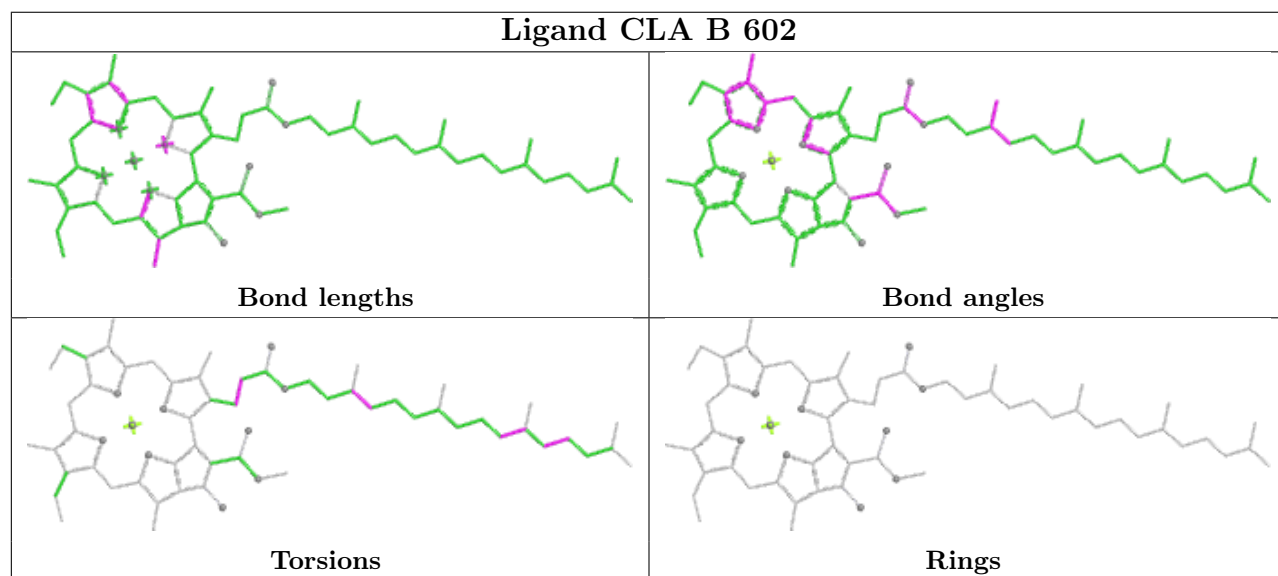
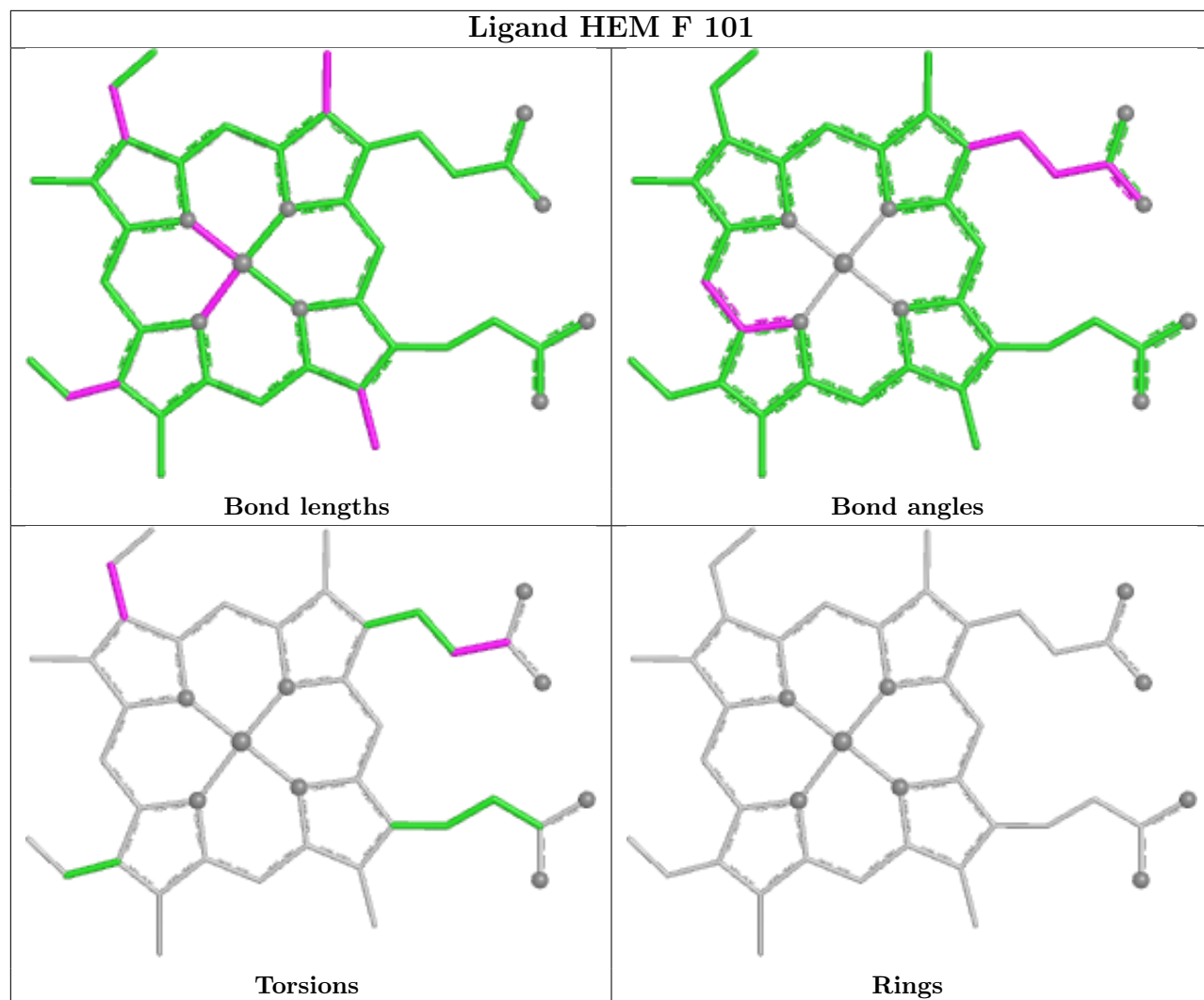


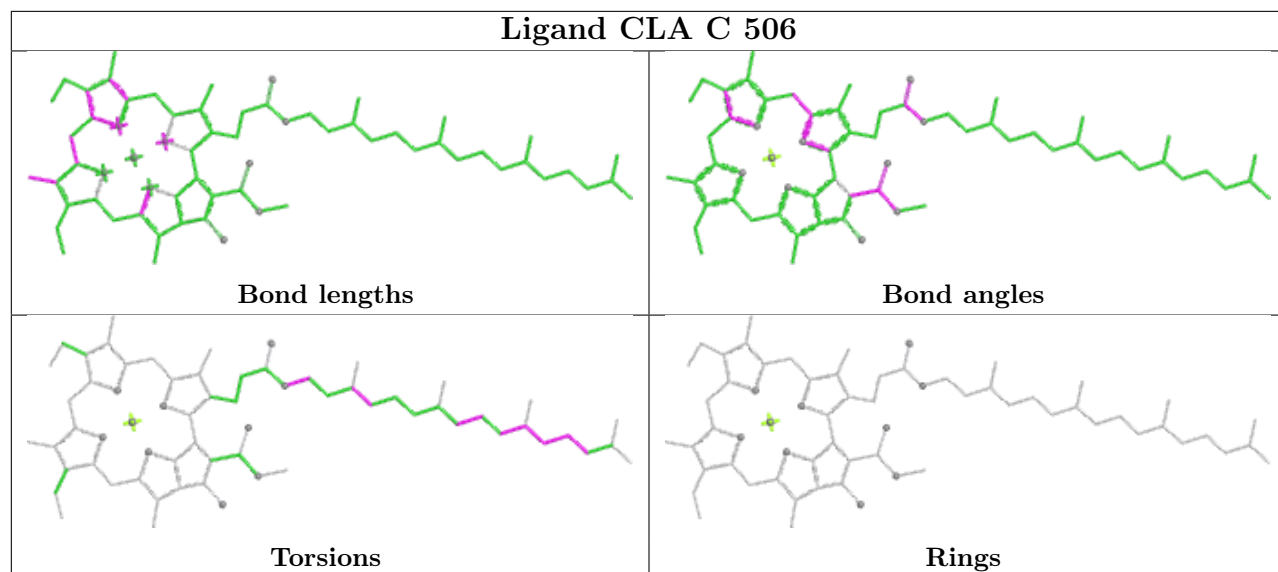
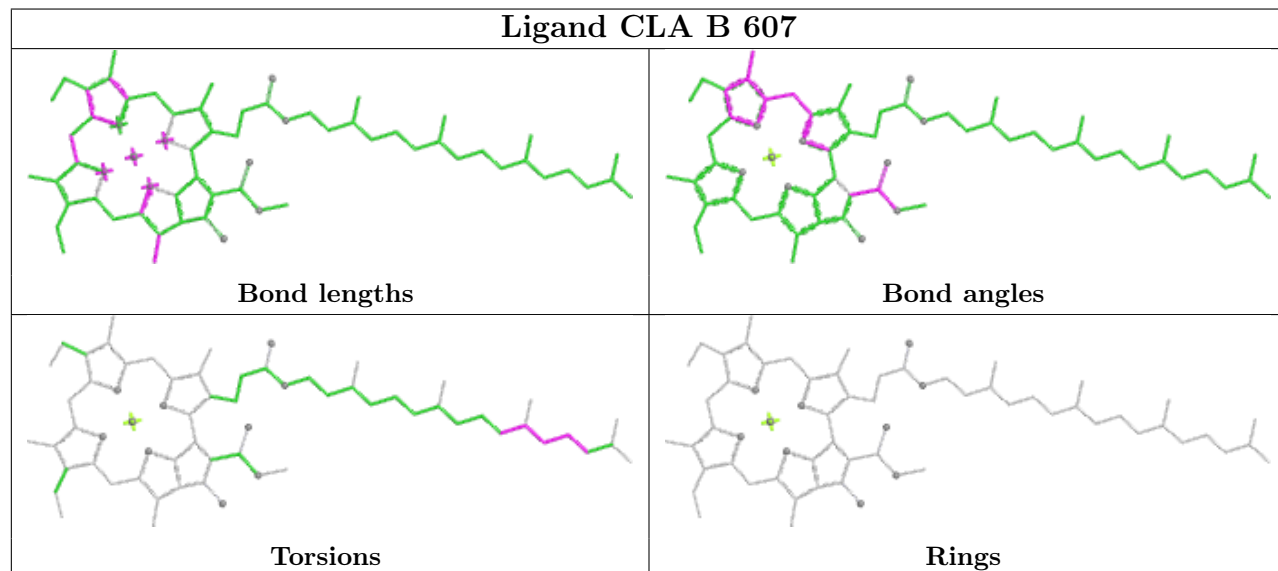
Ligand CLA b 605**Ligand CLA c 512**

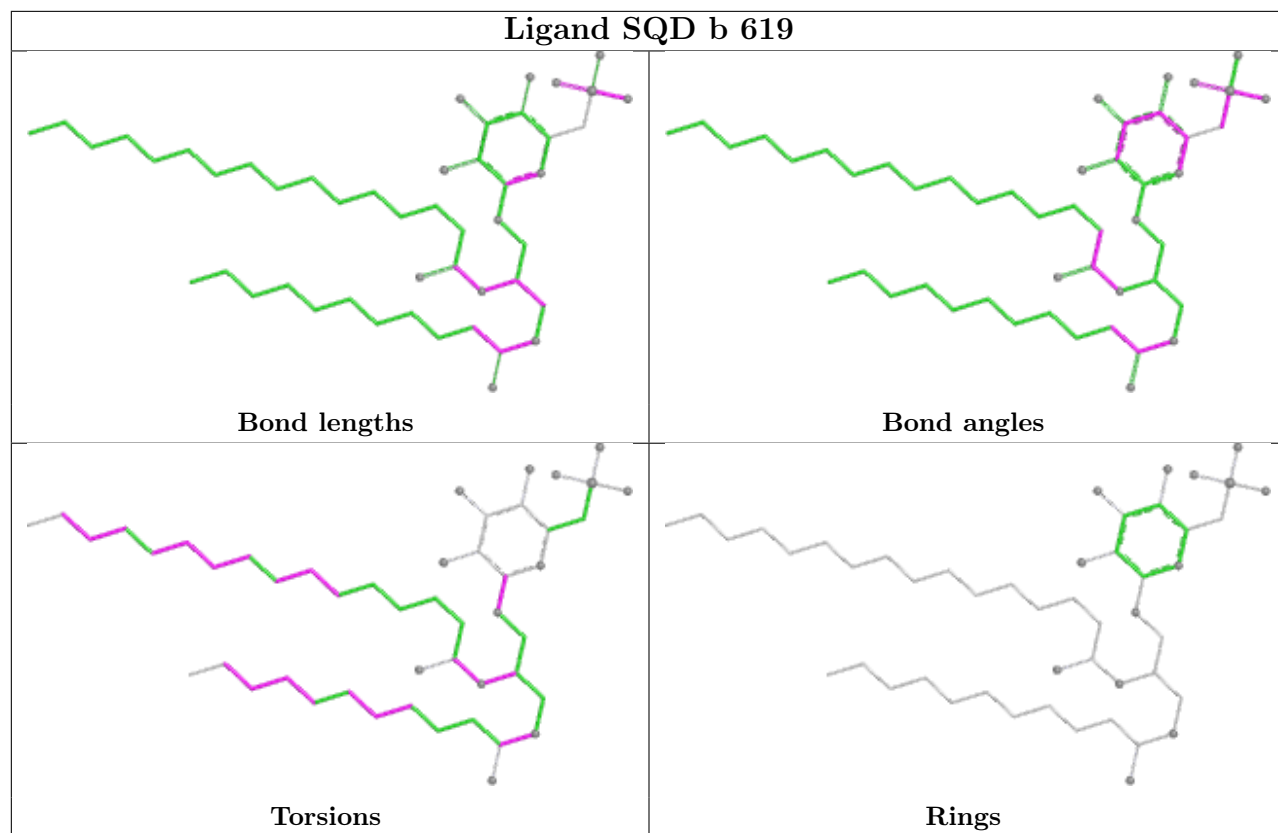


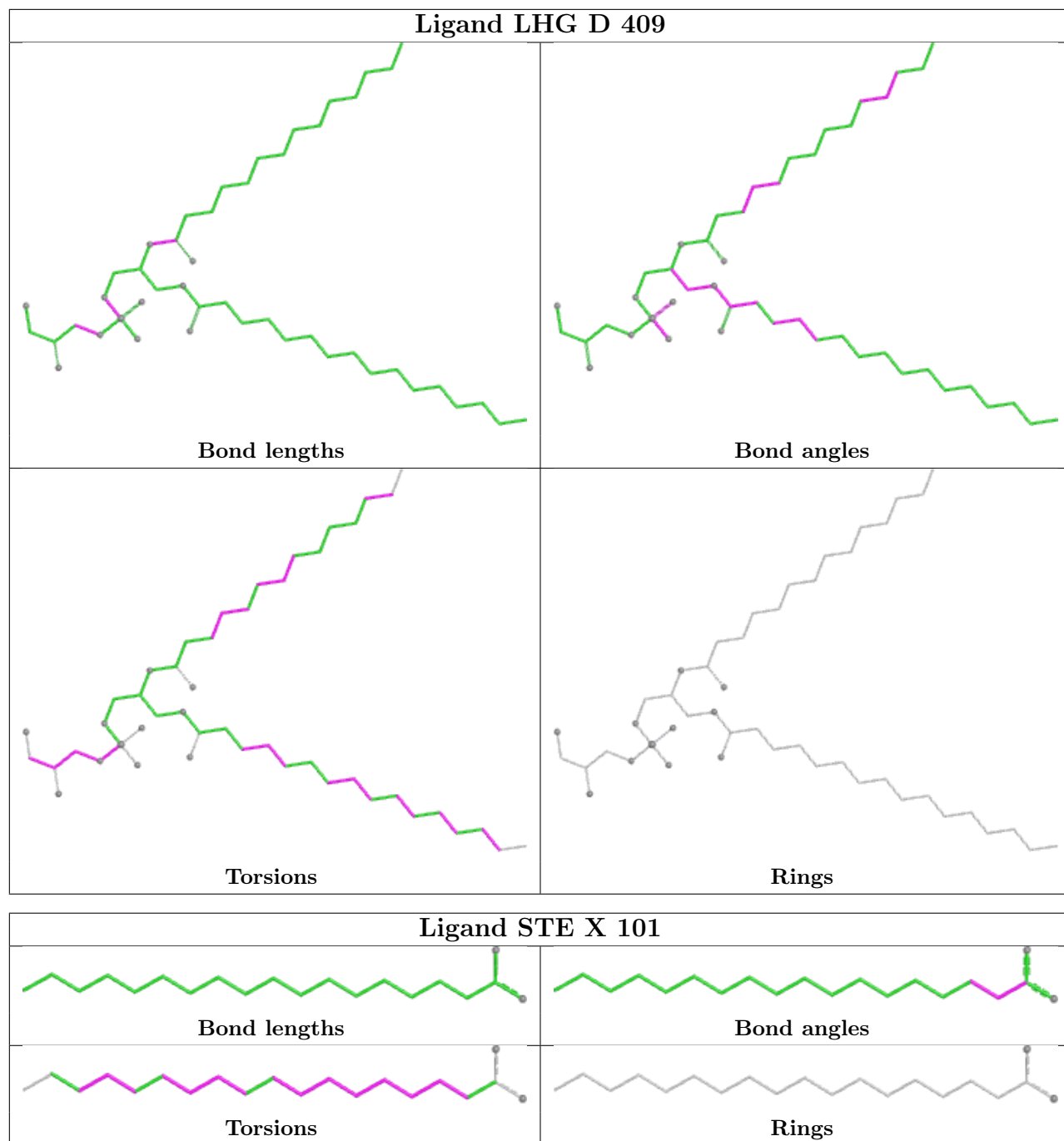
Ligand BCR c 514	
	Bond lengths
	Bond angles
	Torsions
	Rings

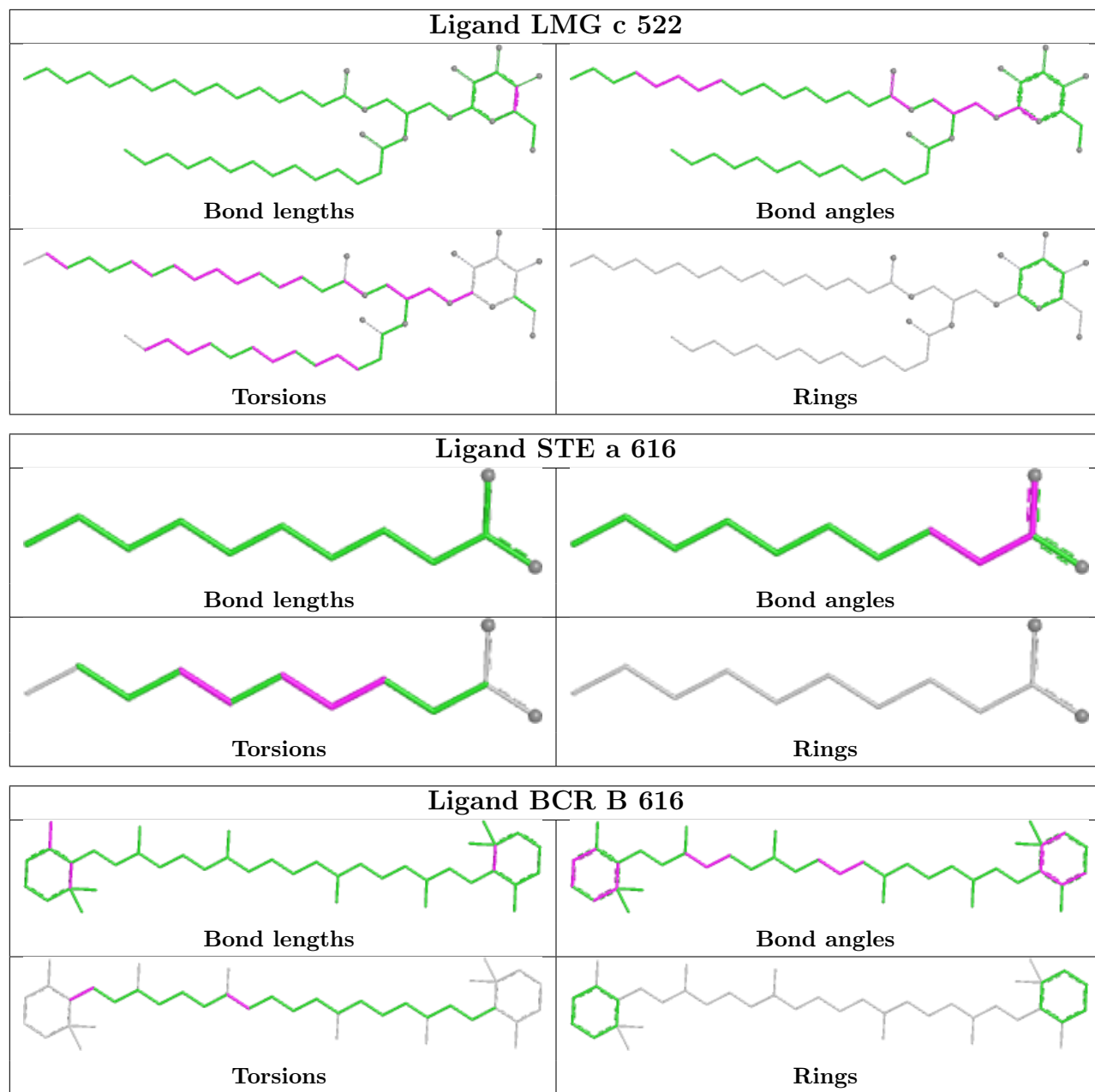
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	Bond lengths
	Bond angles
	Torsions
	Rings

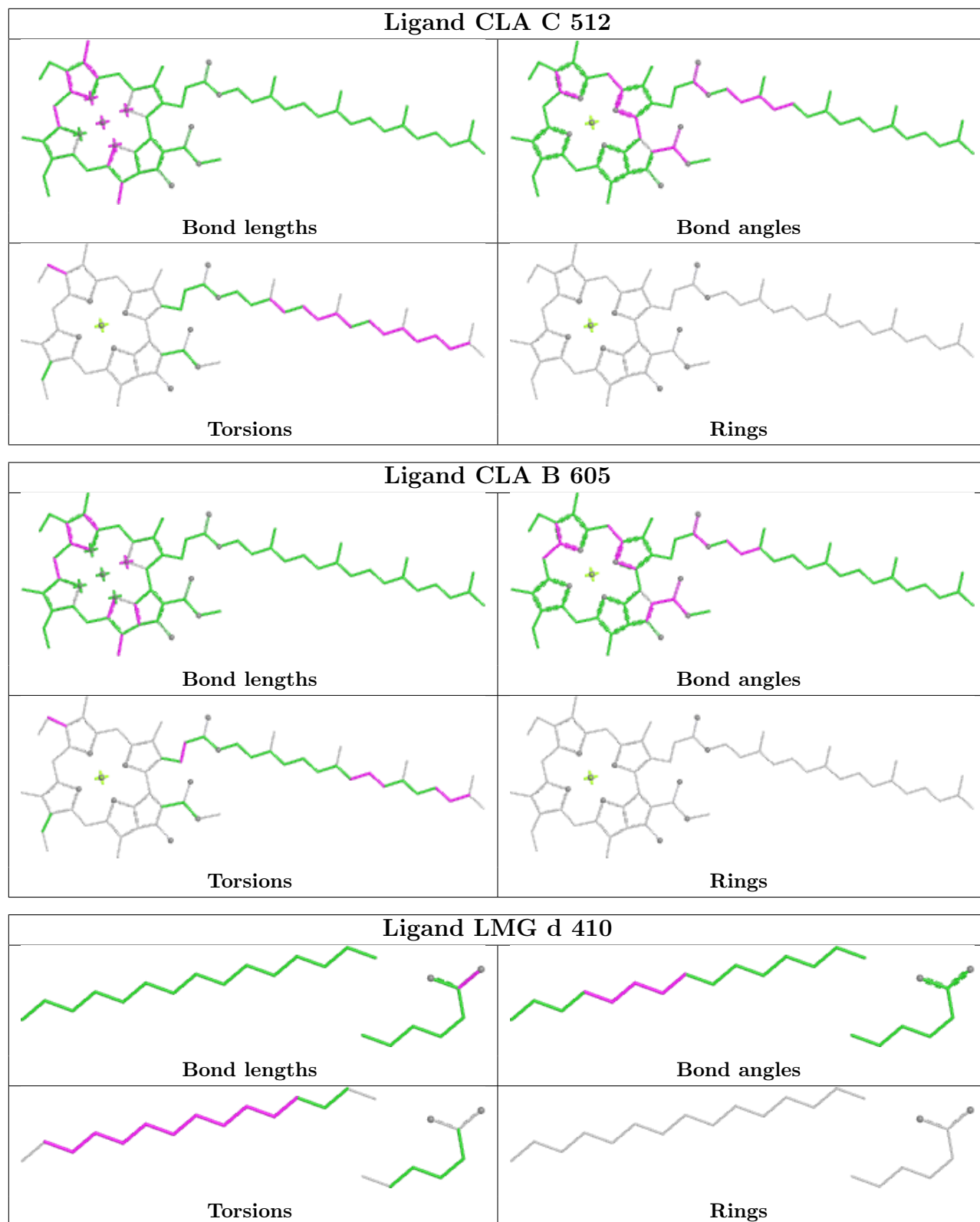


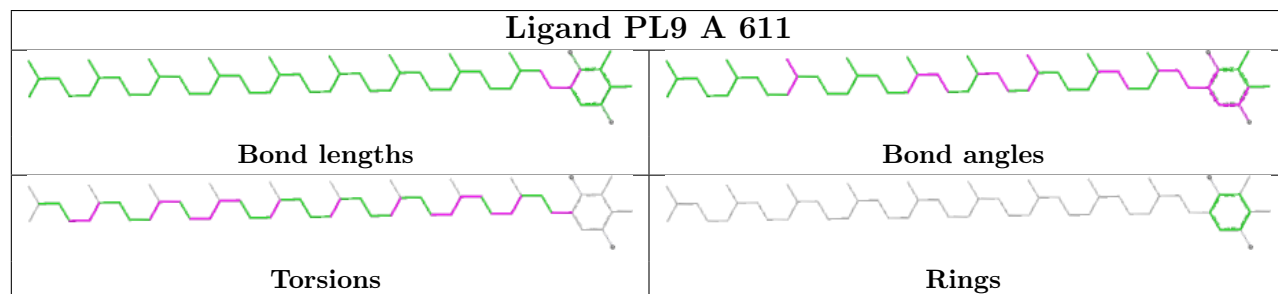
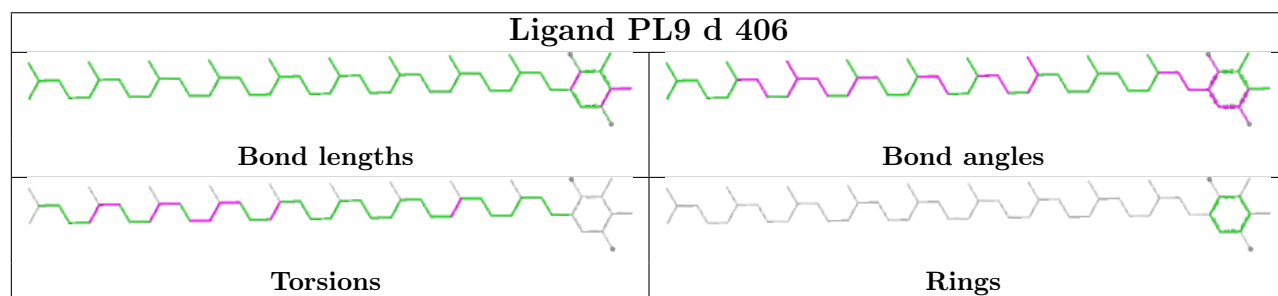
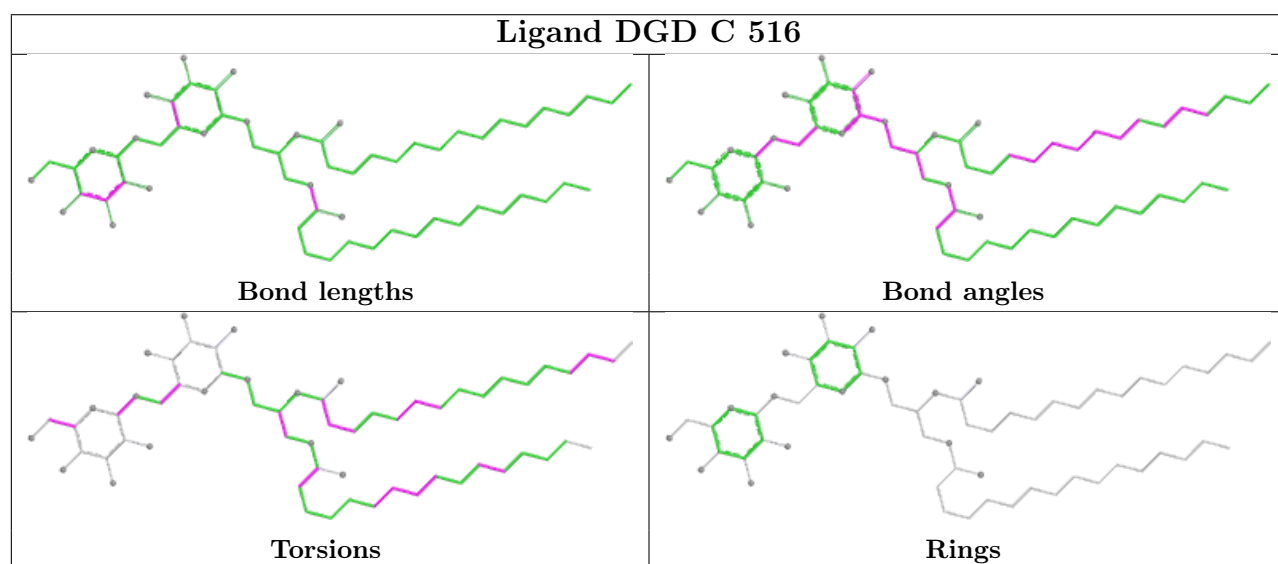
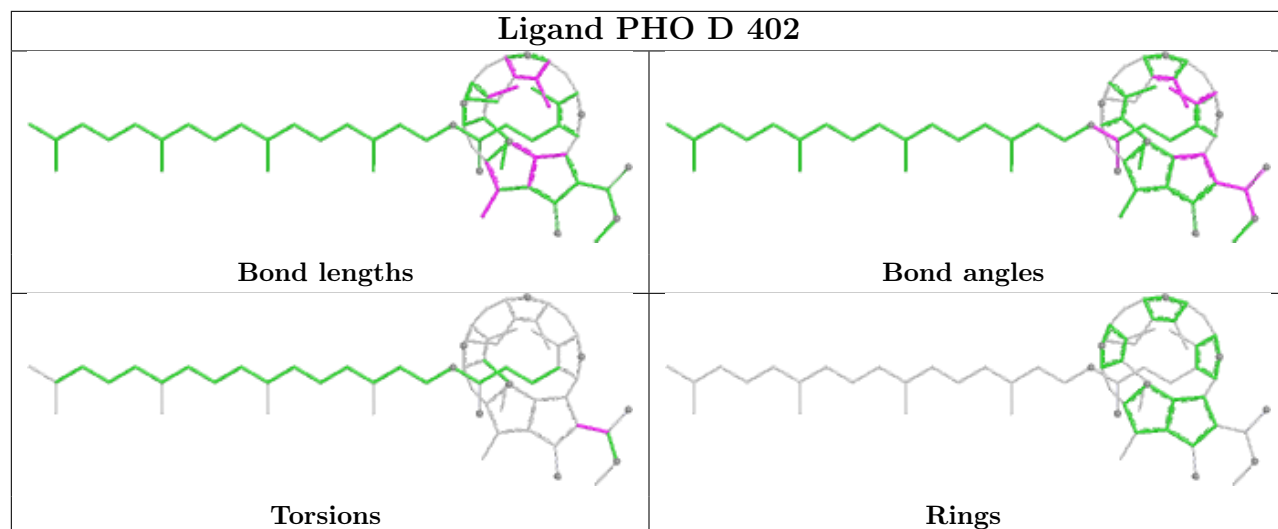
Ligand CLA C 506**Ligand CLA B 607**

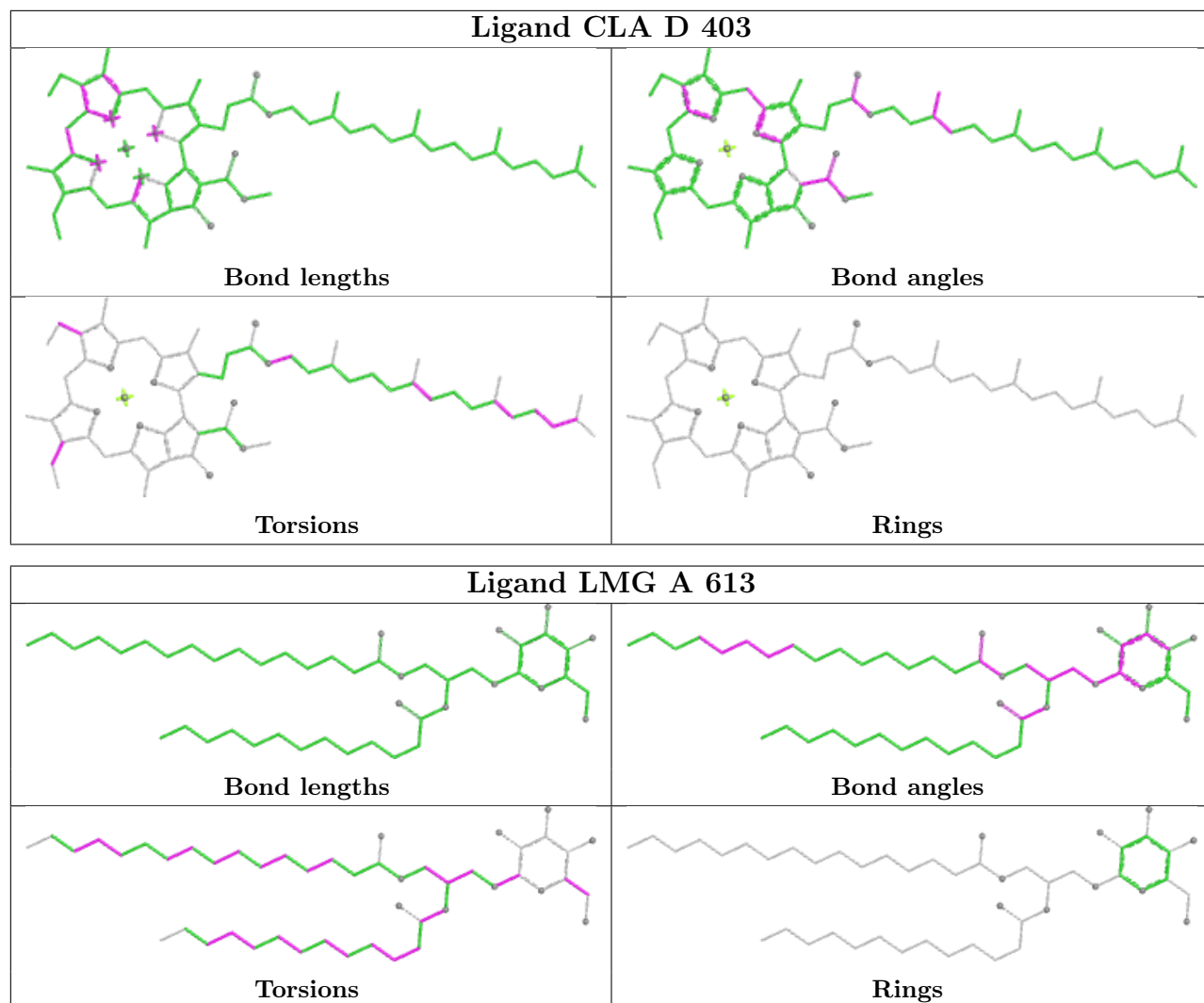


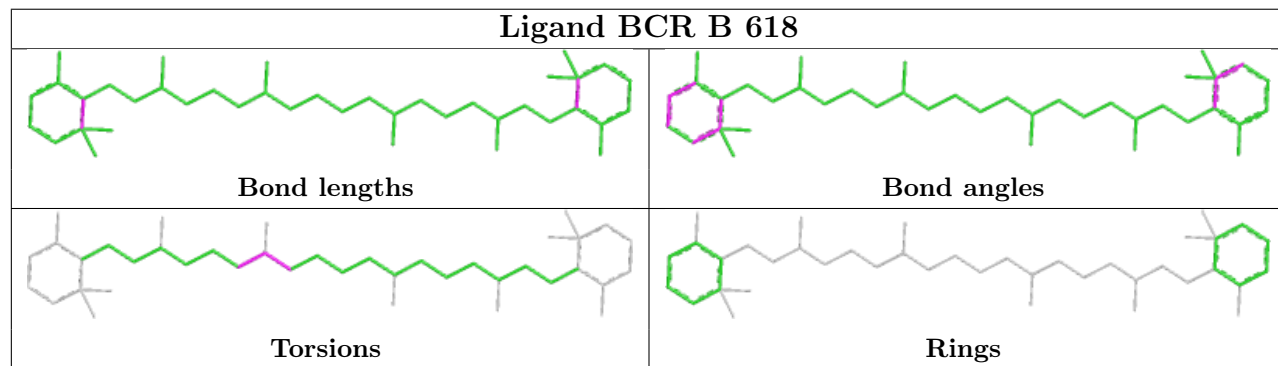
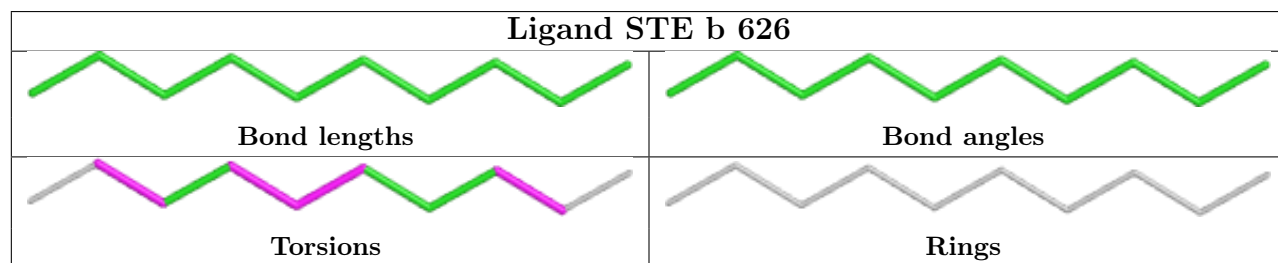
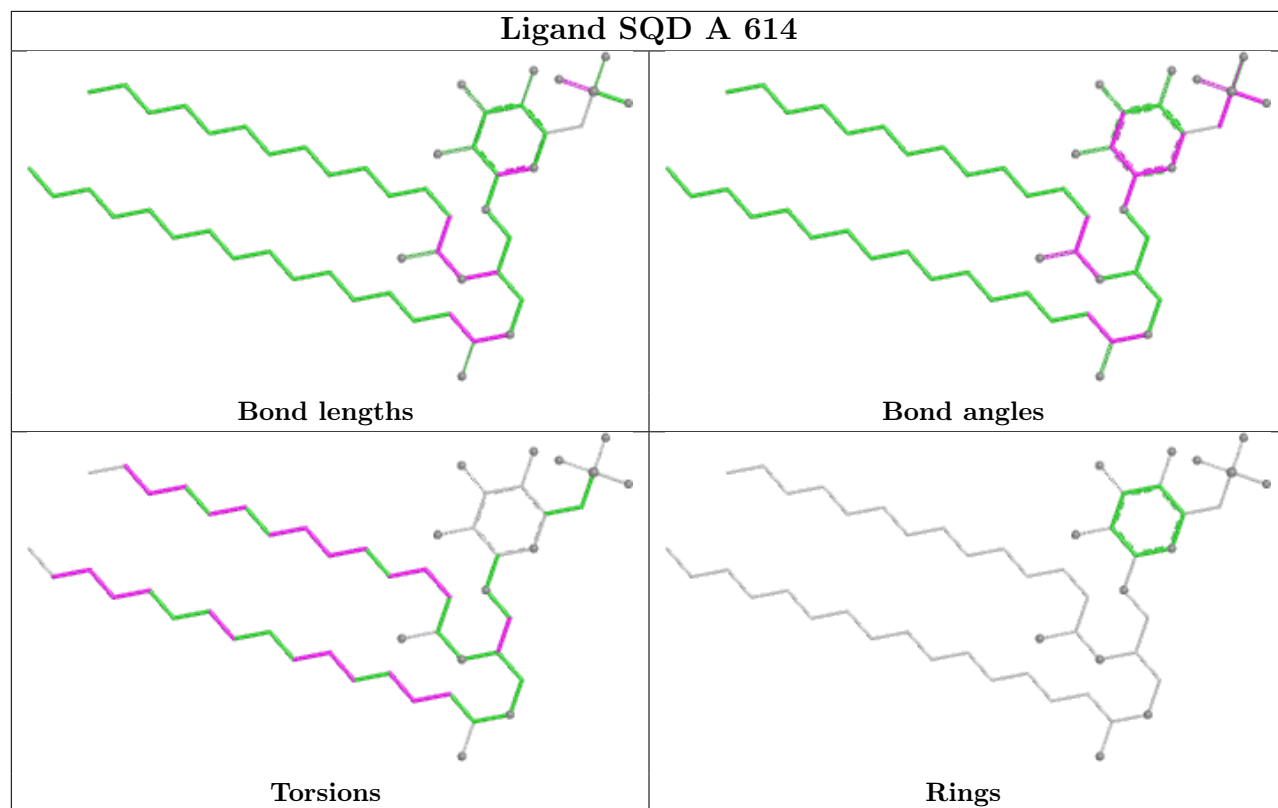


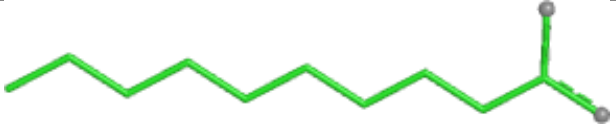
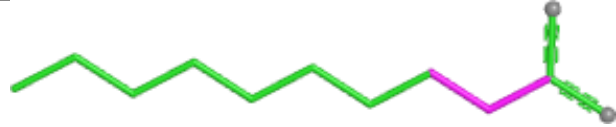
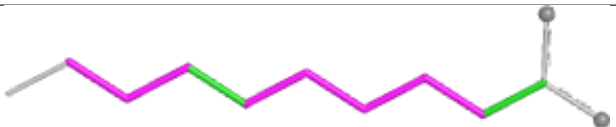
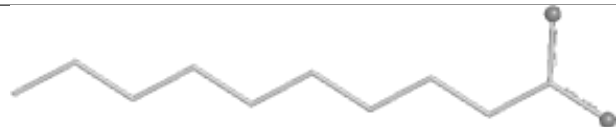
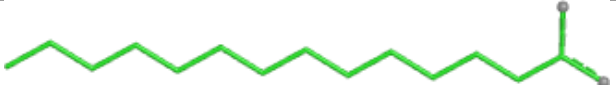
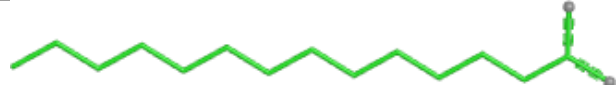
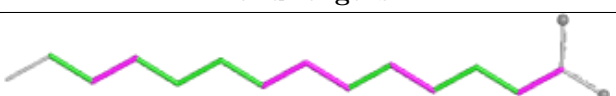
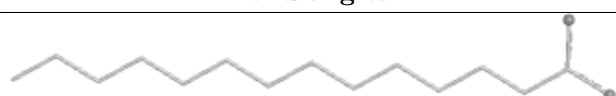


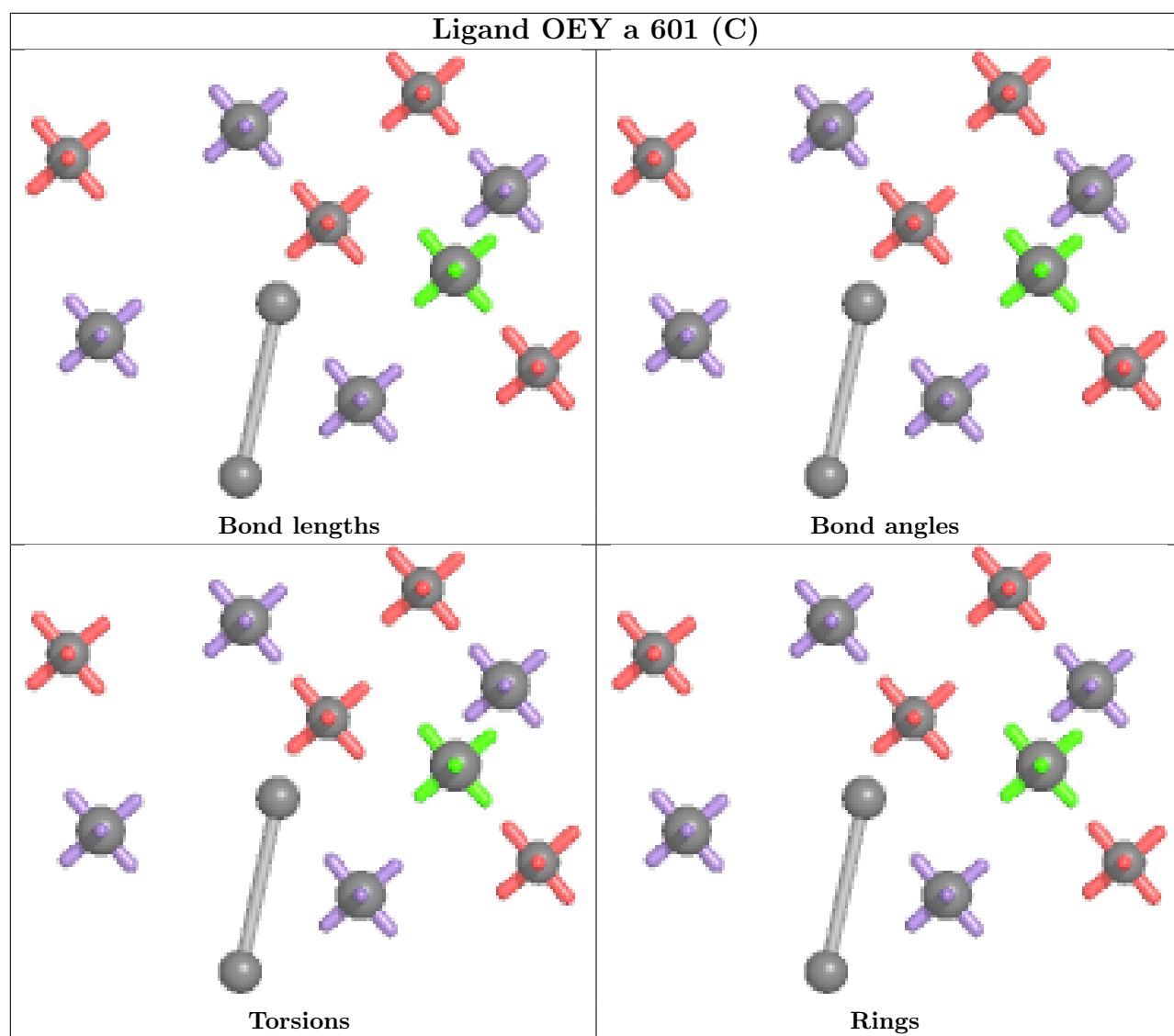


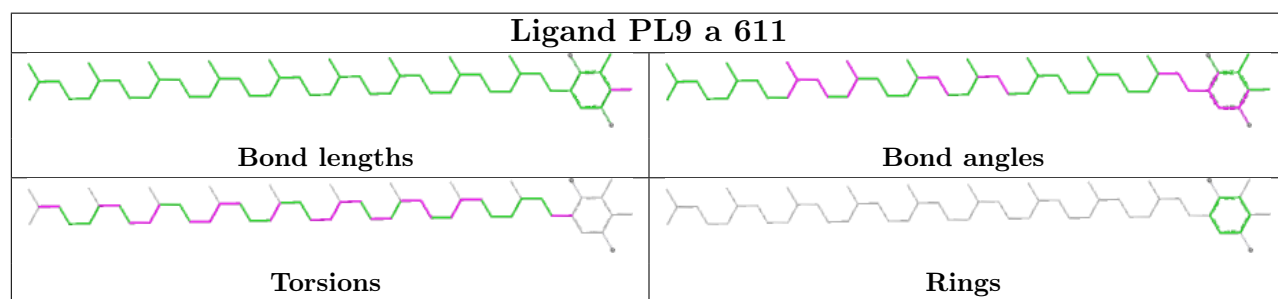
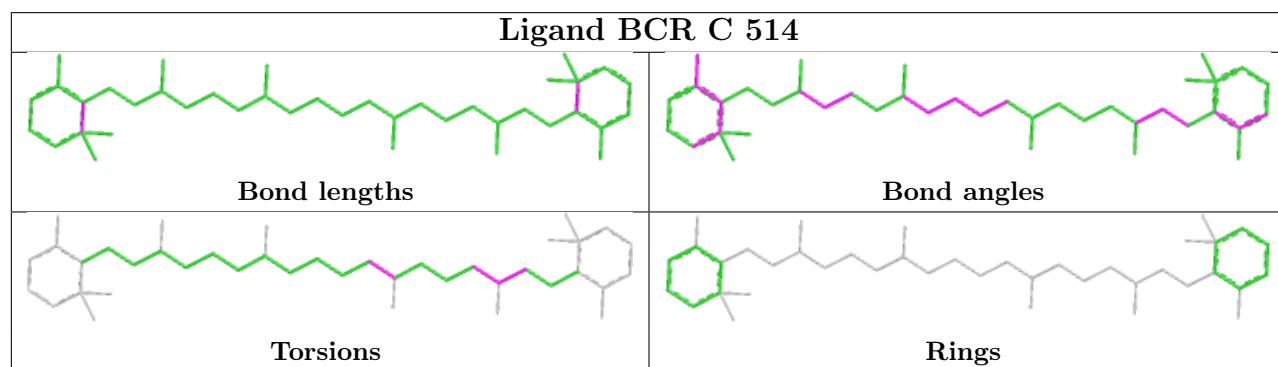
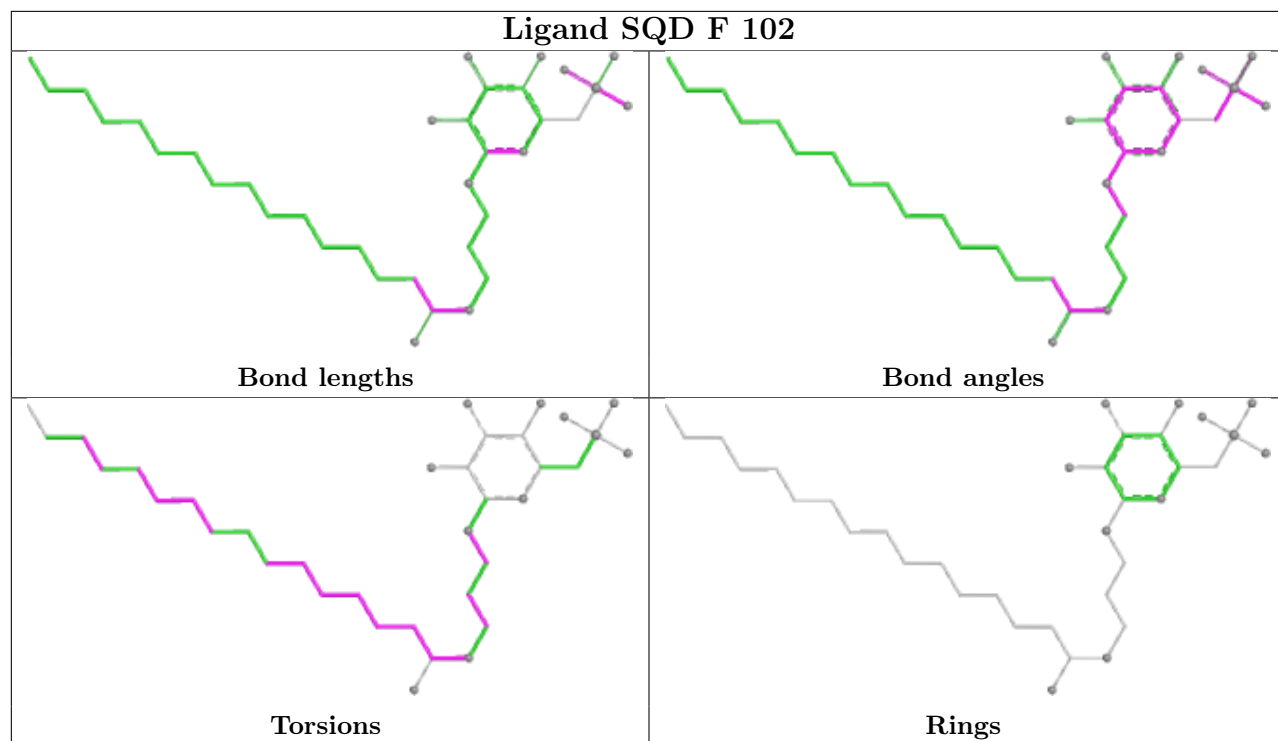


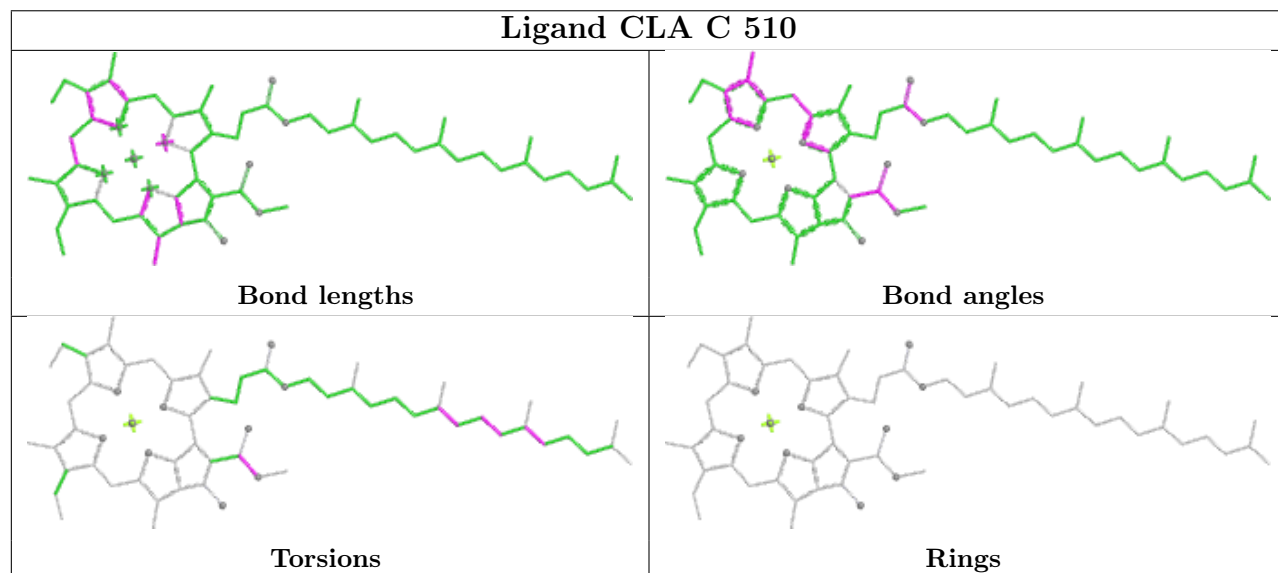
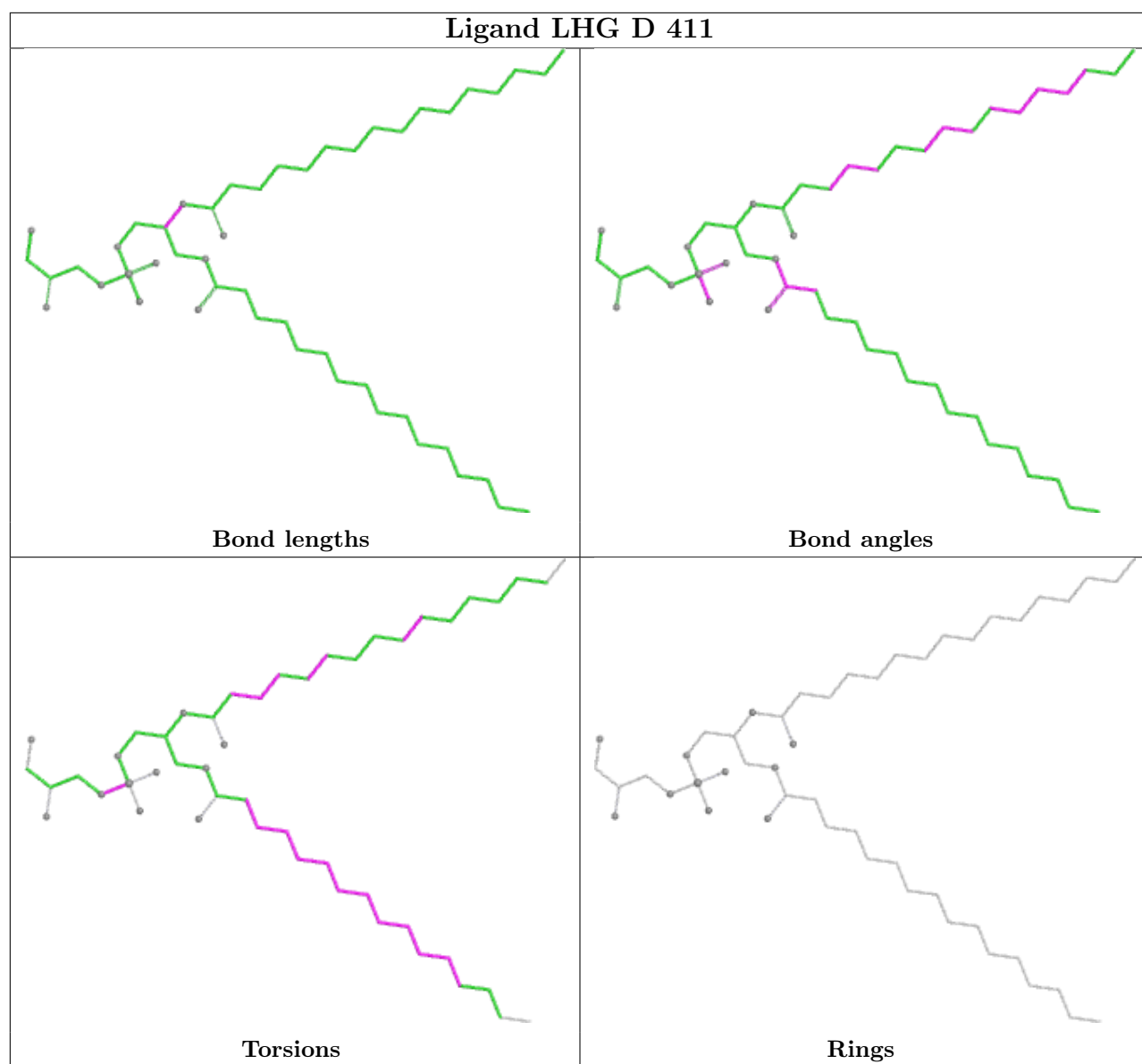


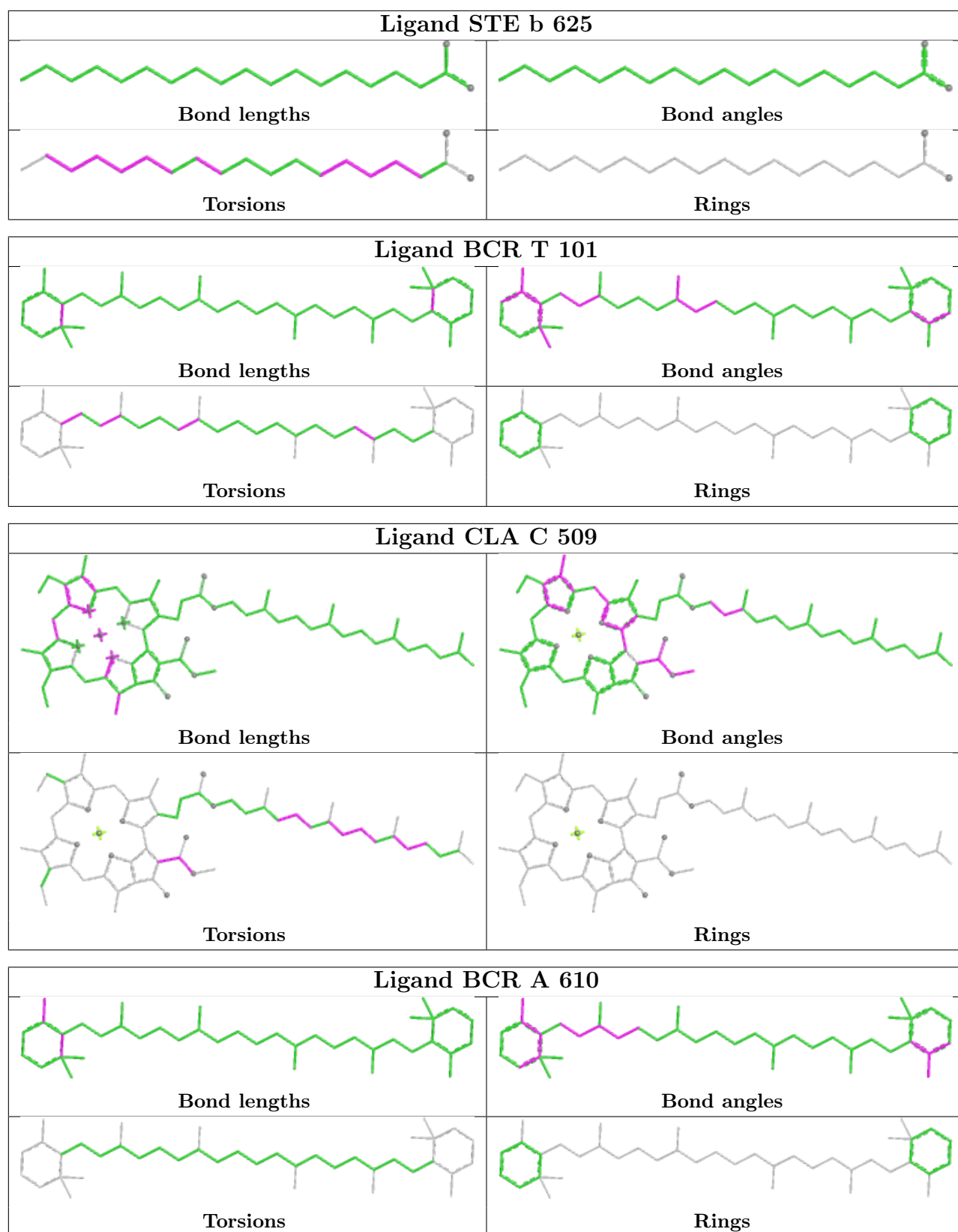


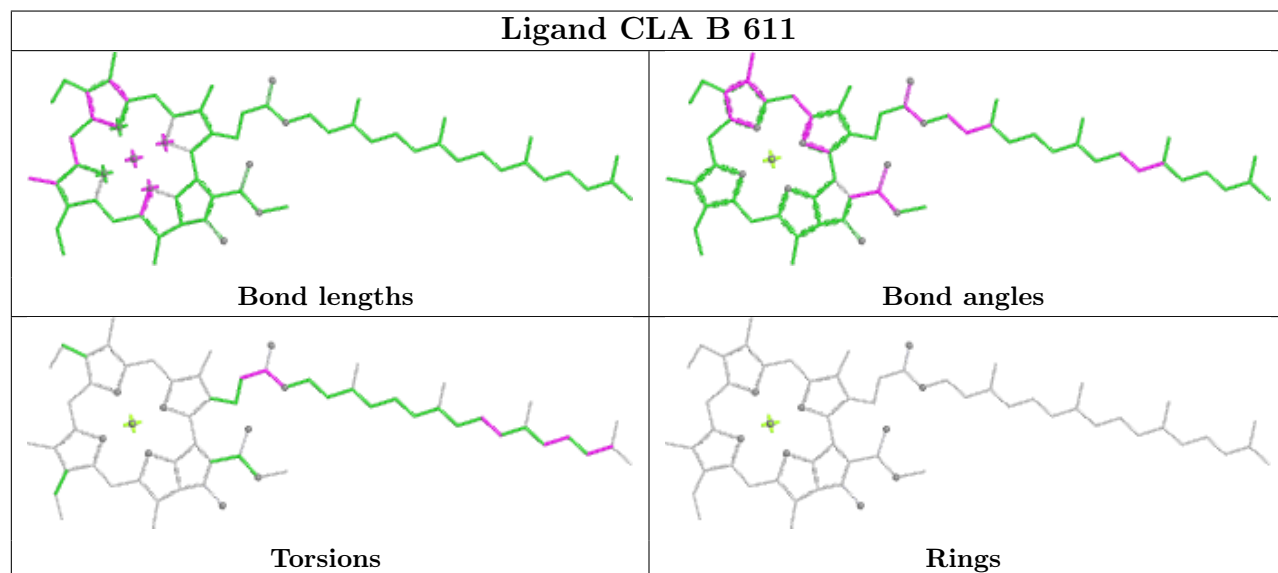
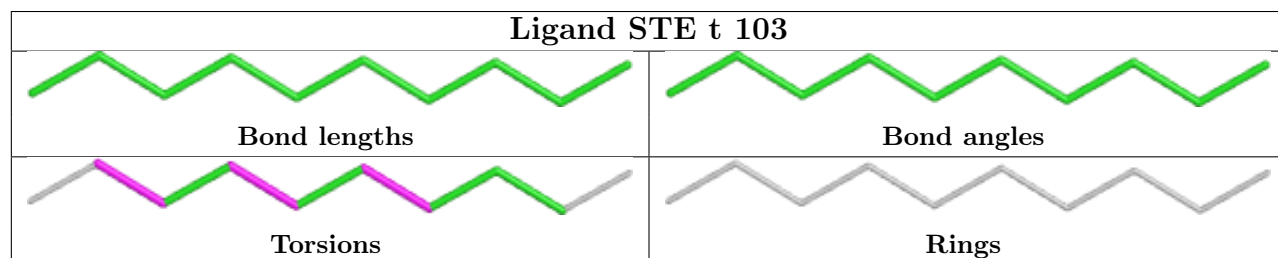
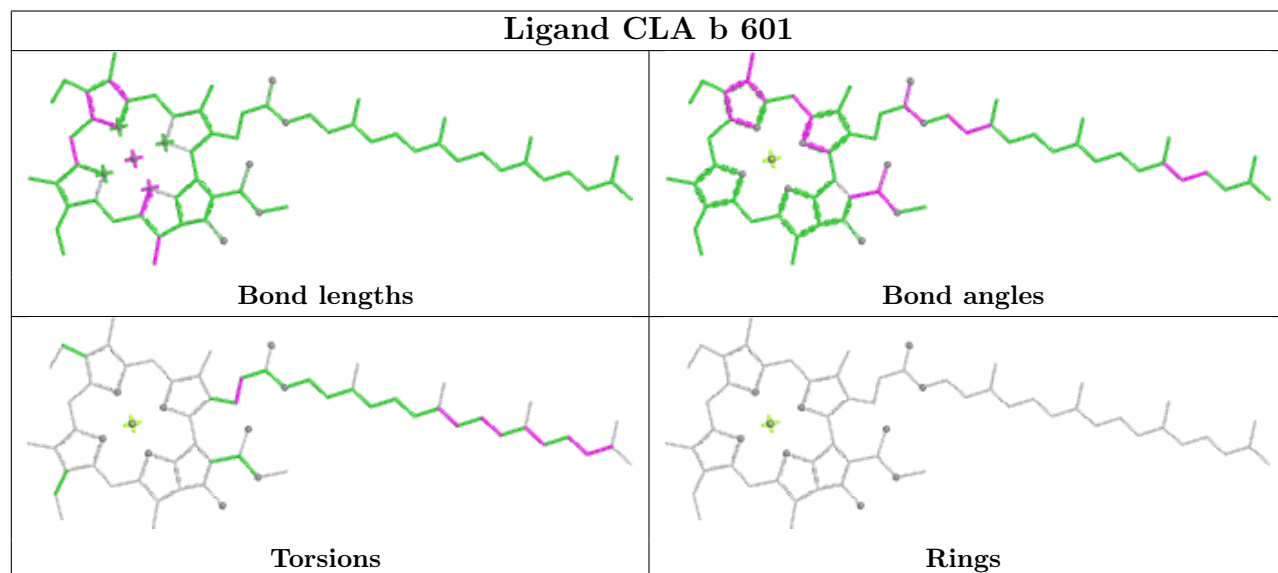
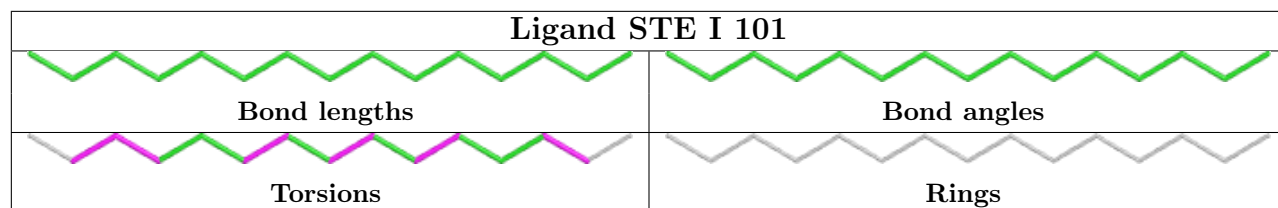
Ligand STE C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

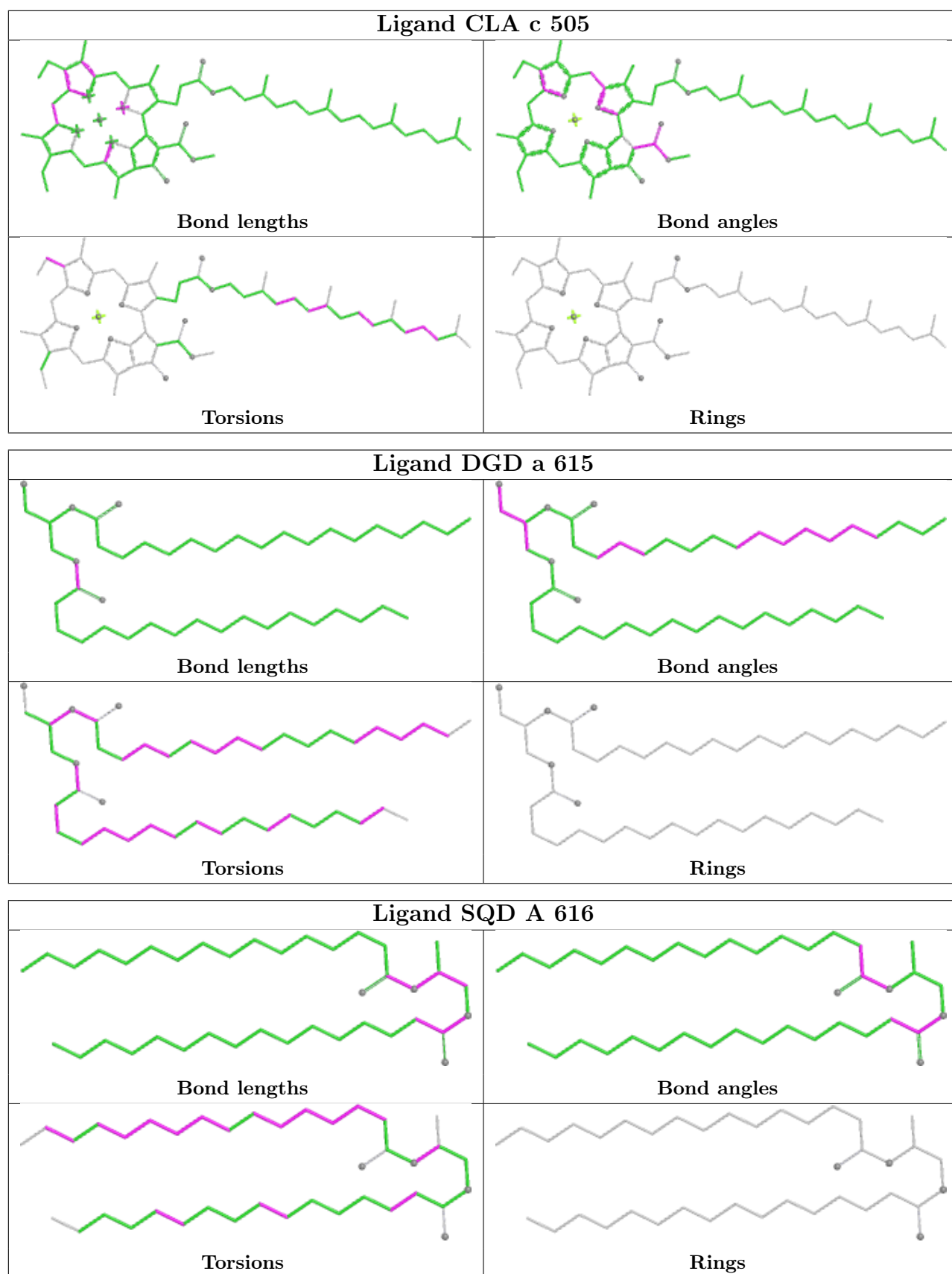




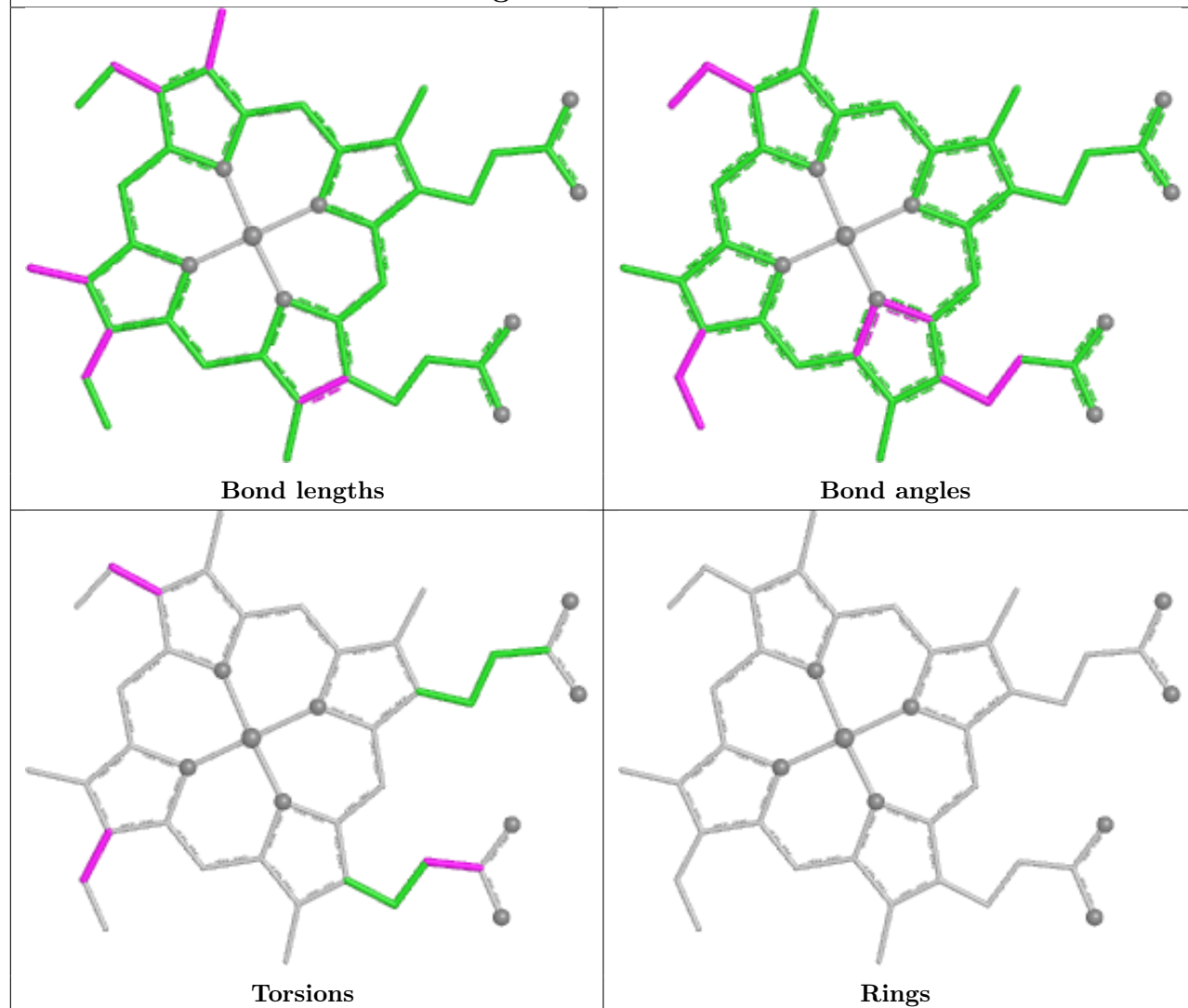




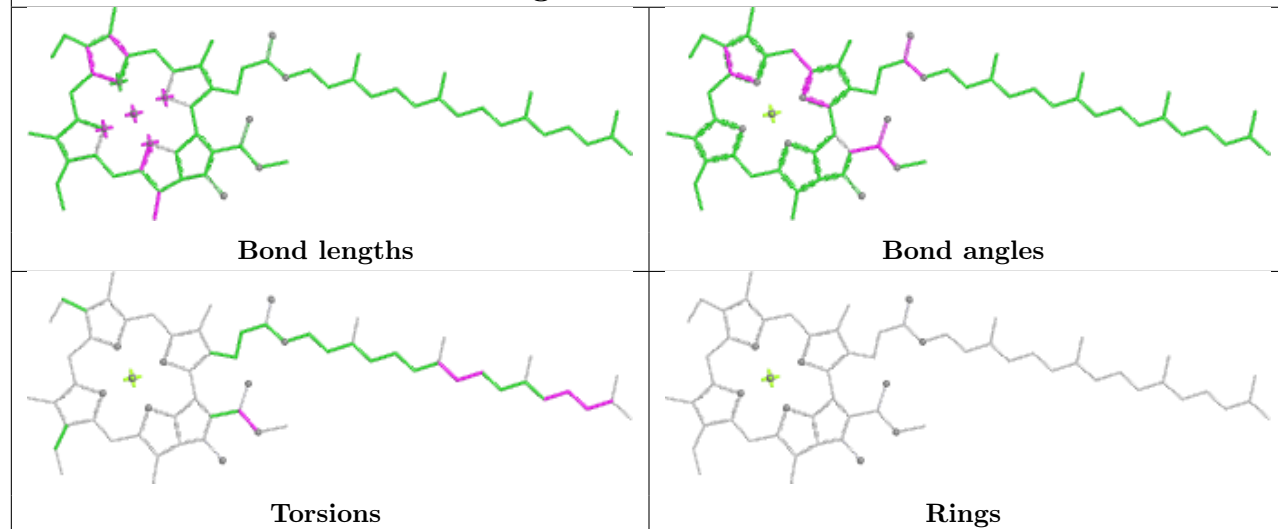


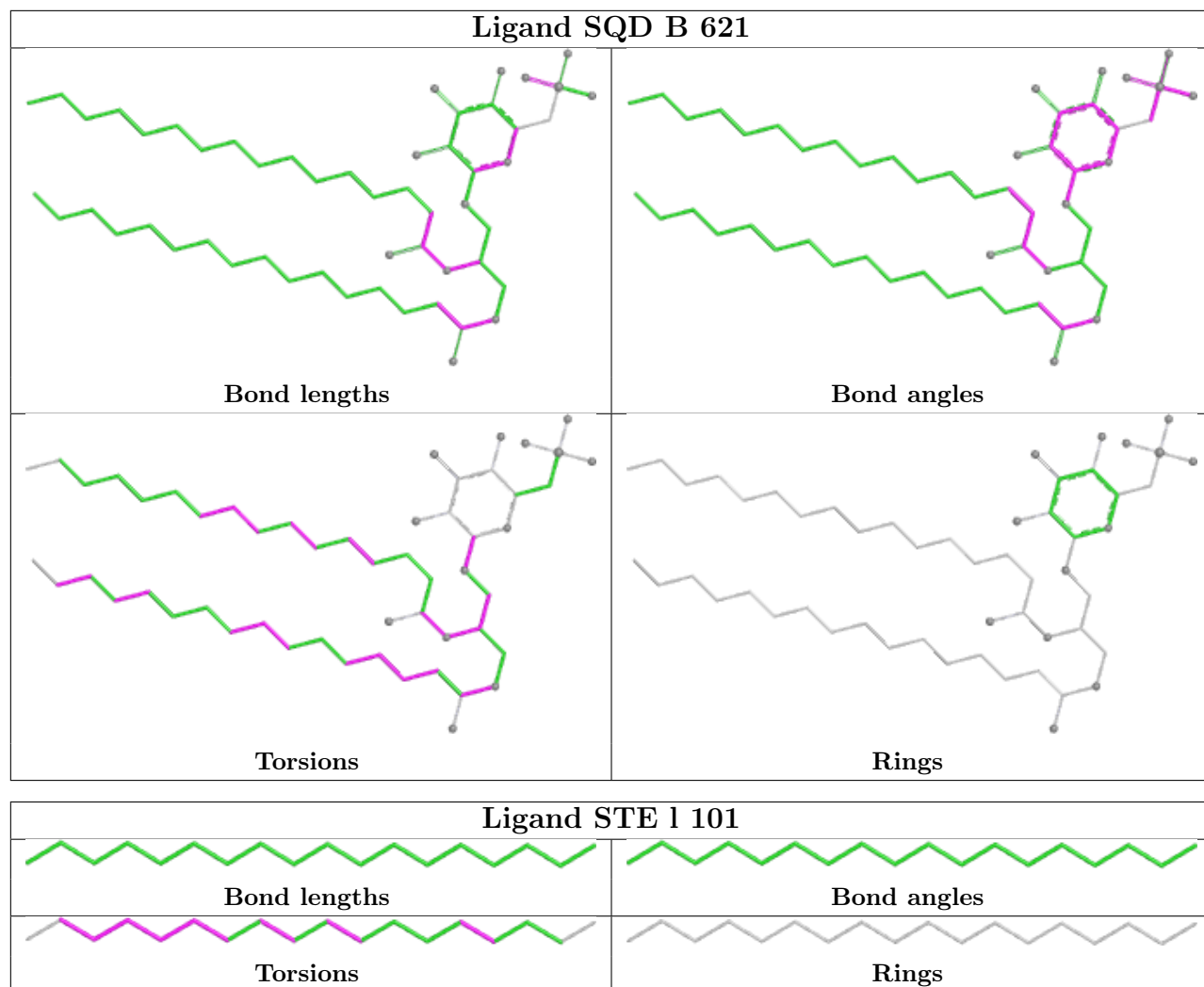


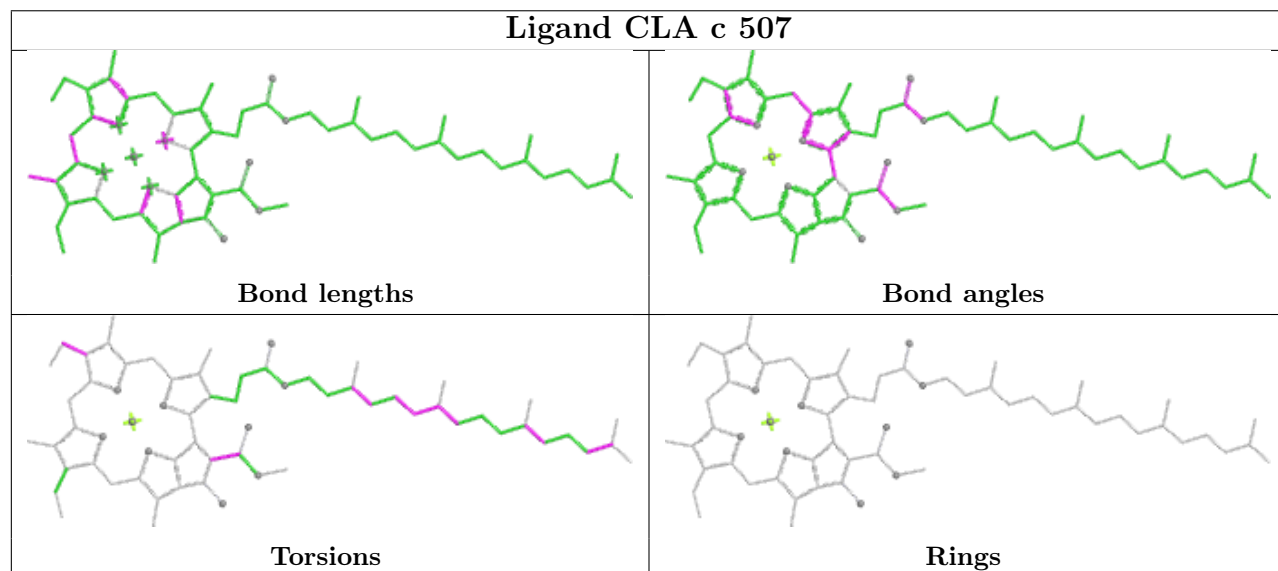
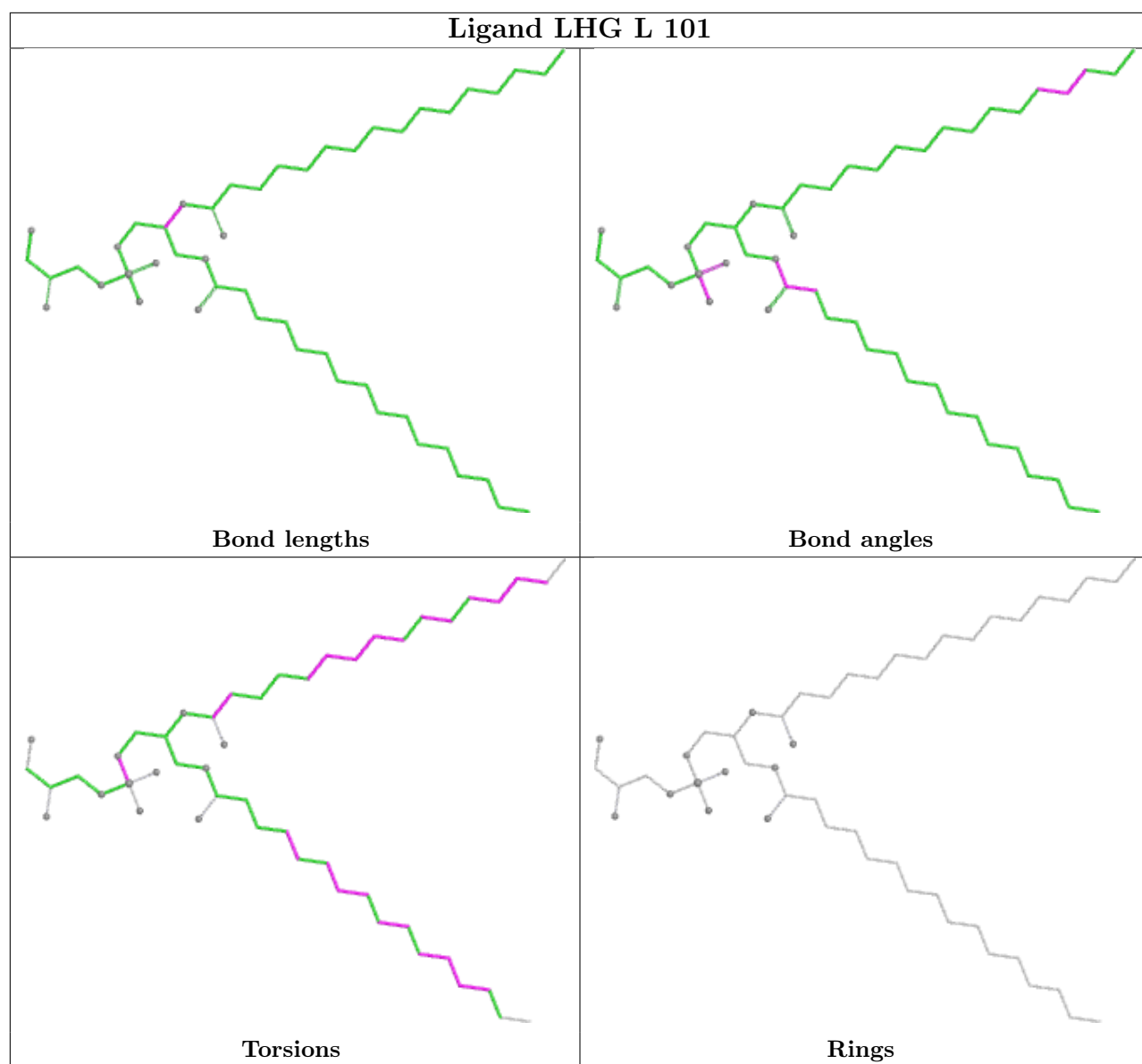
Ligand HEC V 201

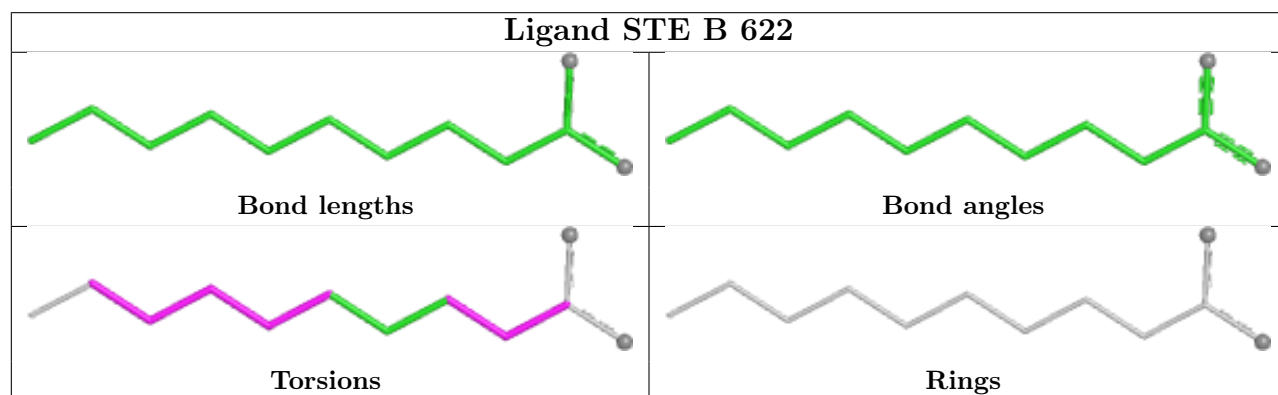
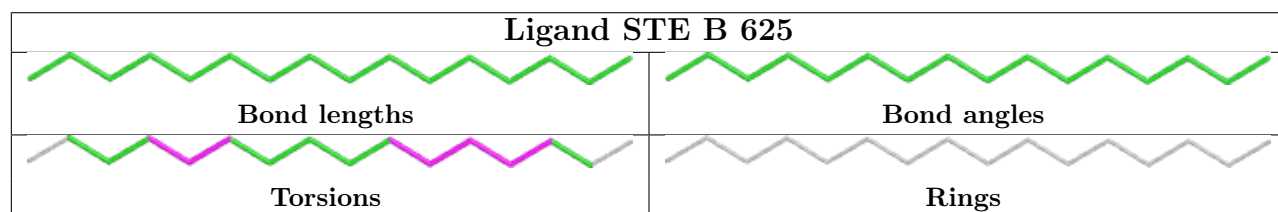
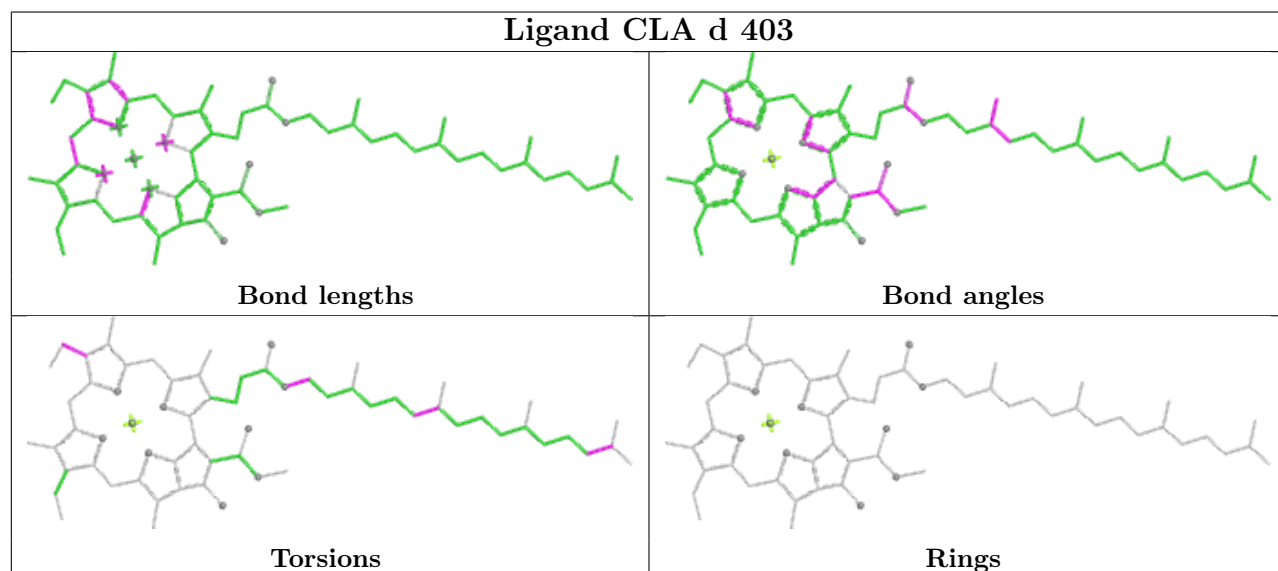
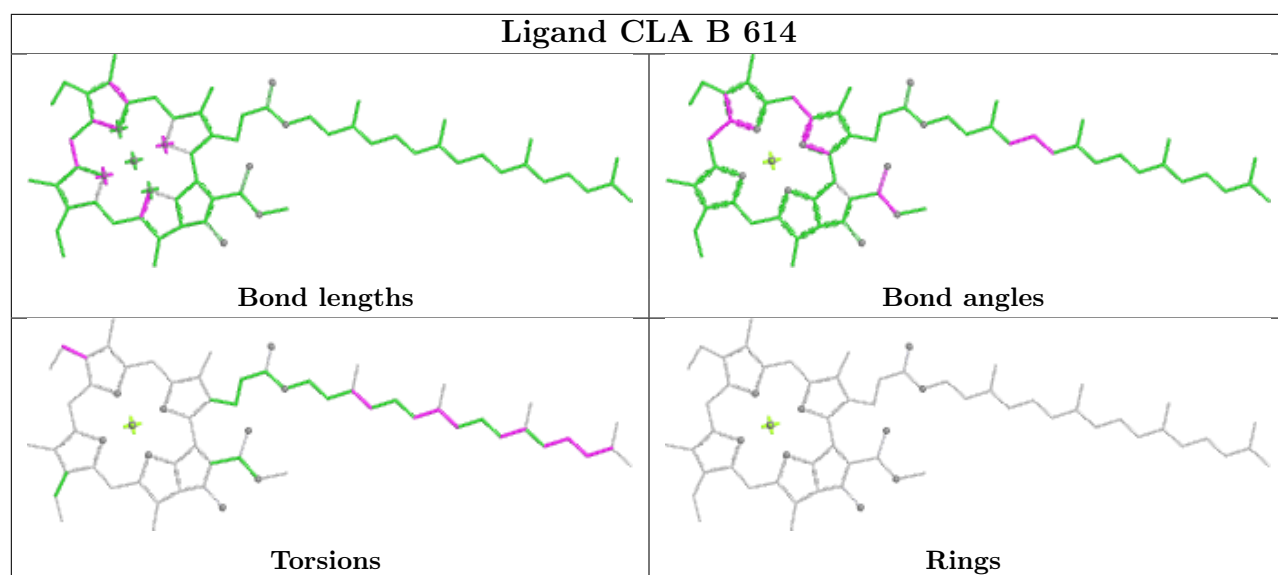


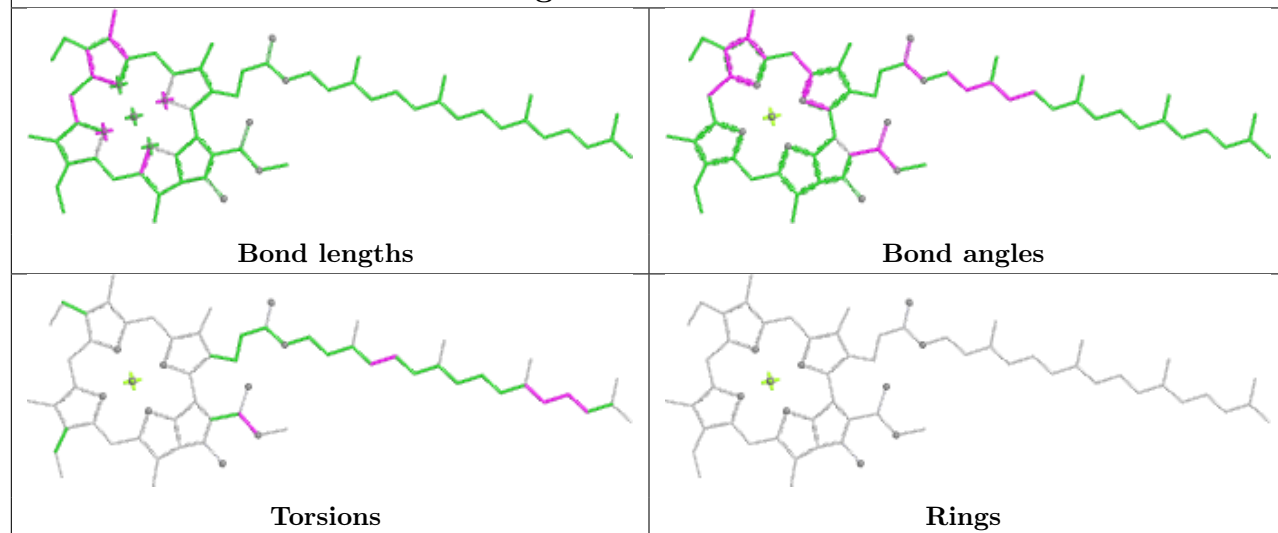
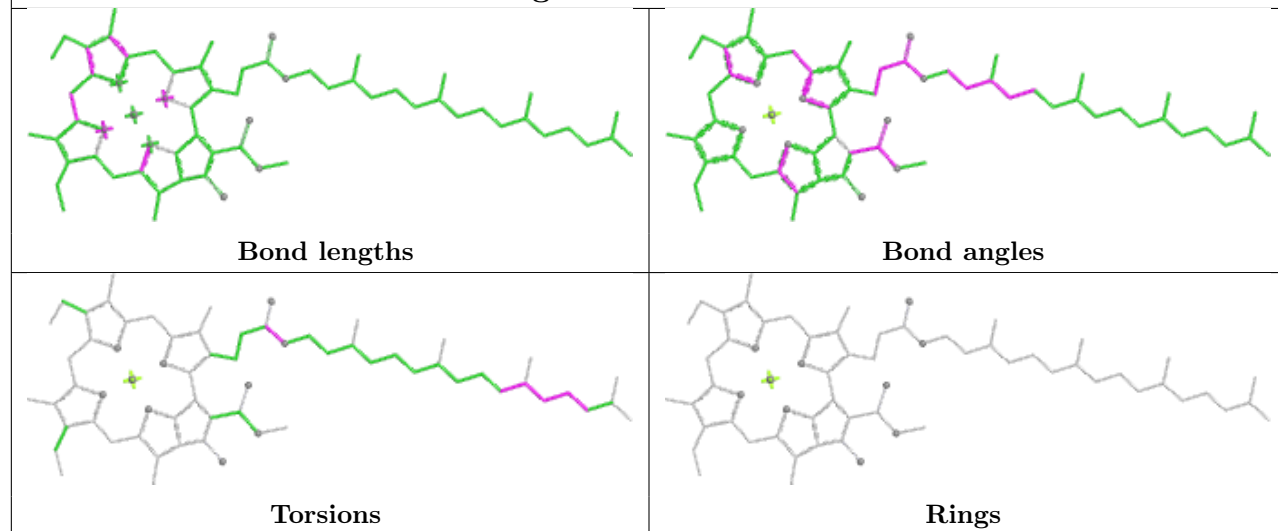
Ligand CLA C 513



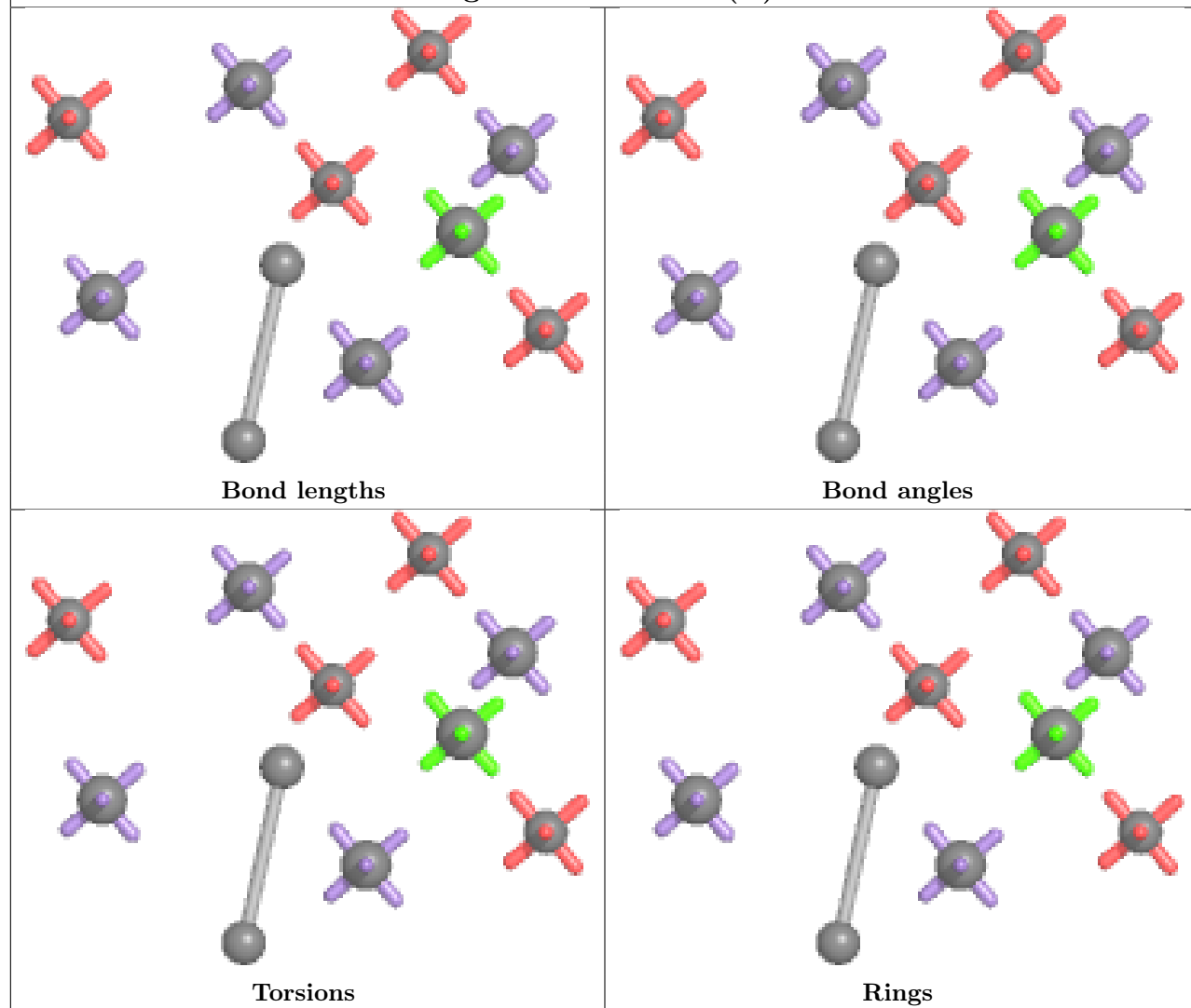




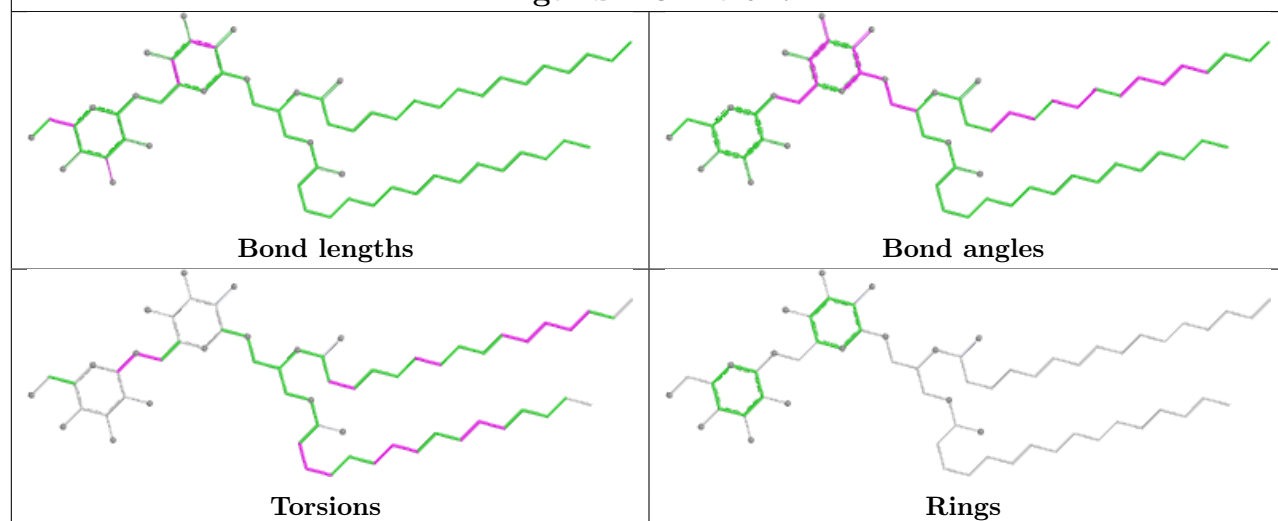


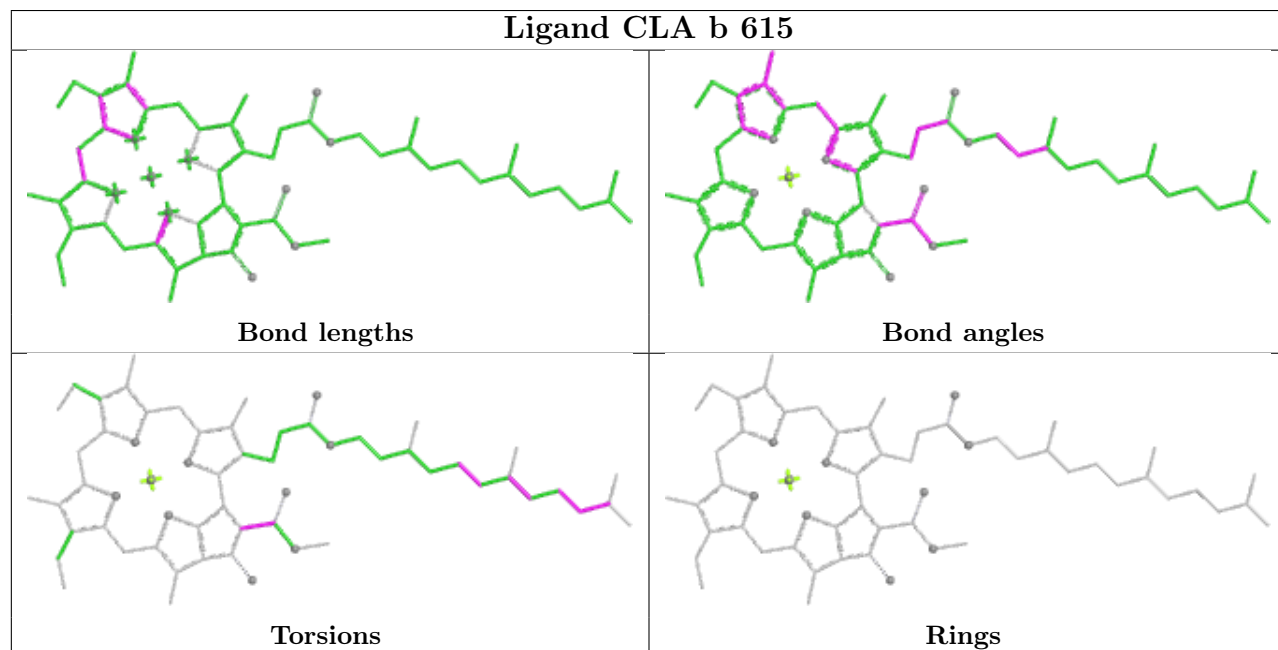
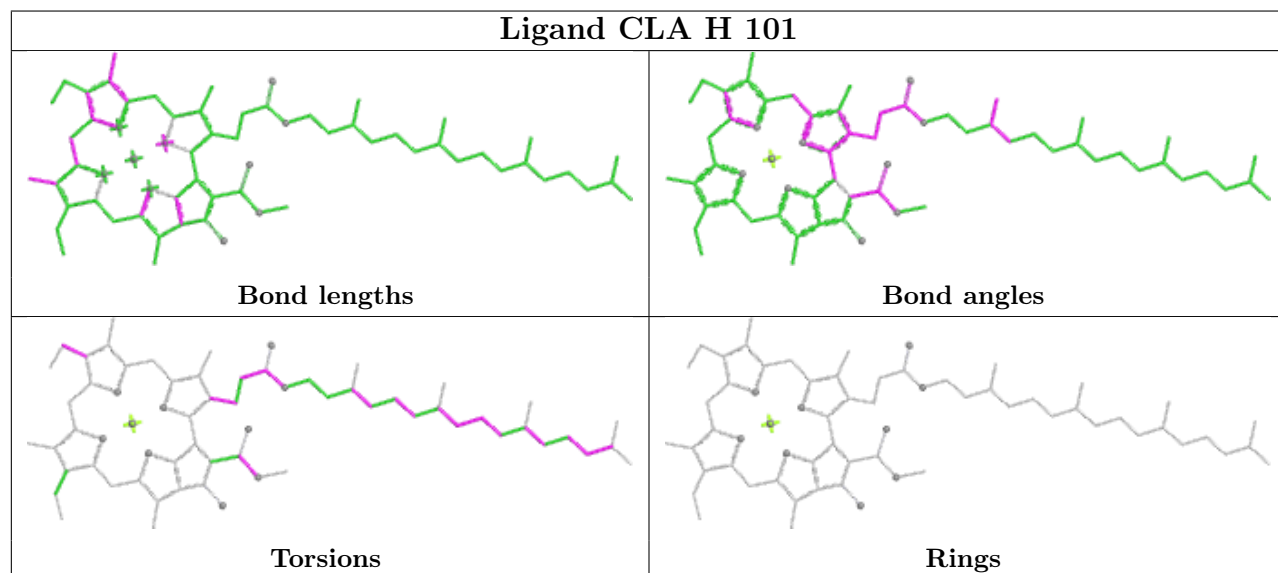
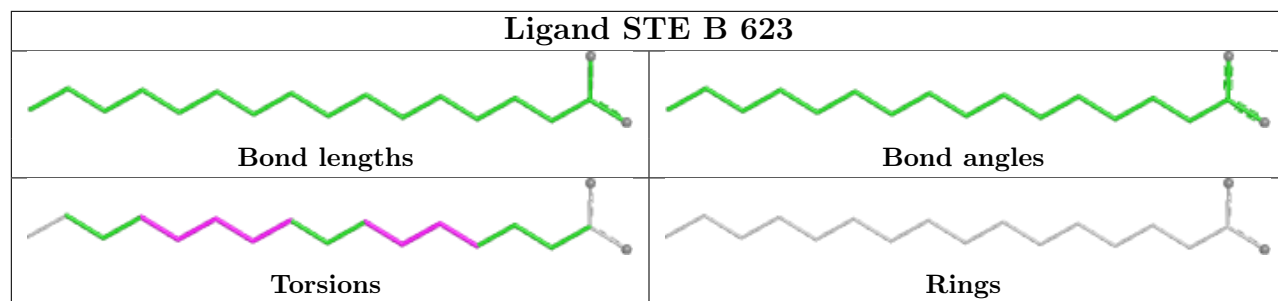
Ligand CLA b 608**Ligand CLA B 603**

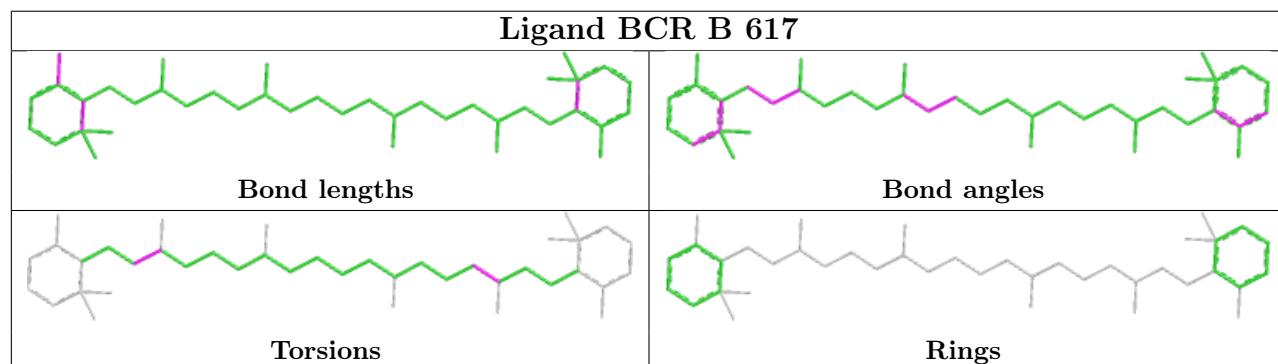
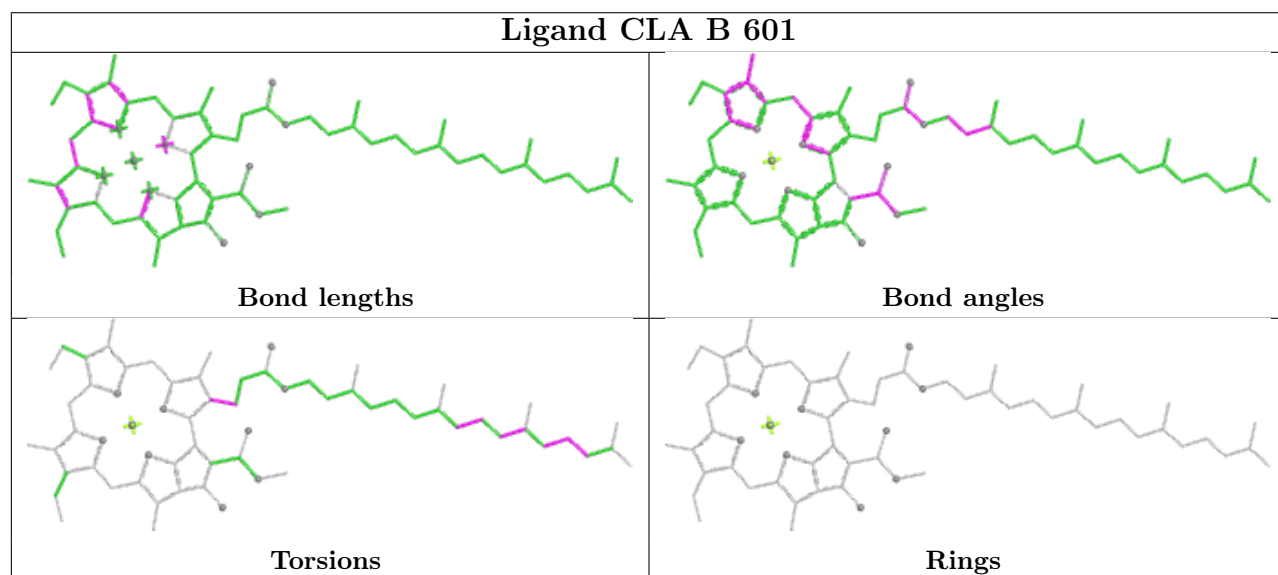
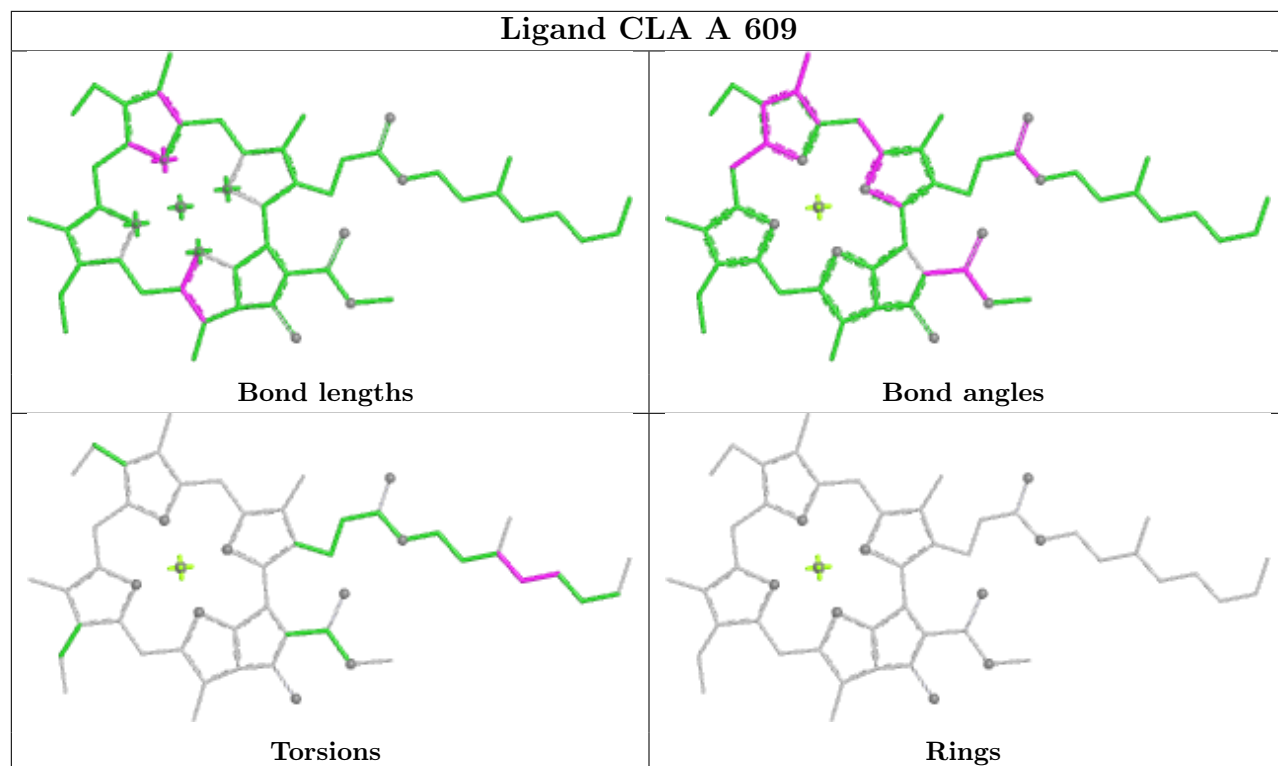
Ligand OEY A 601 (C)

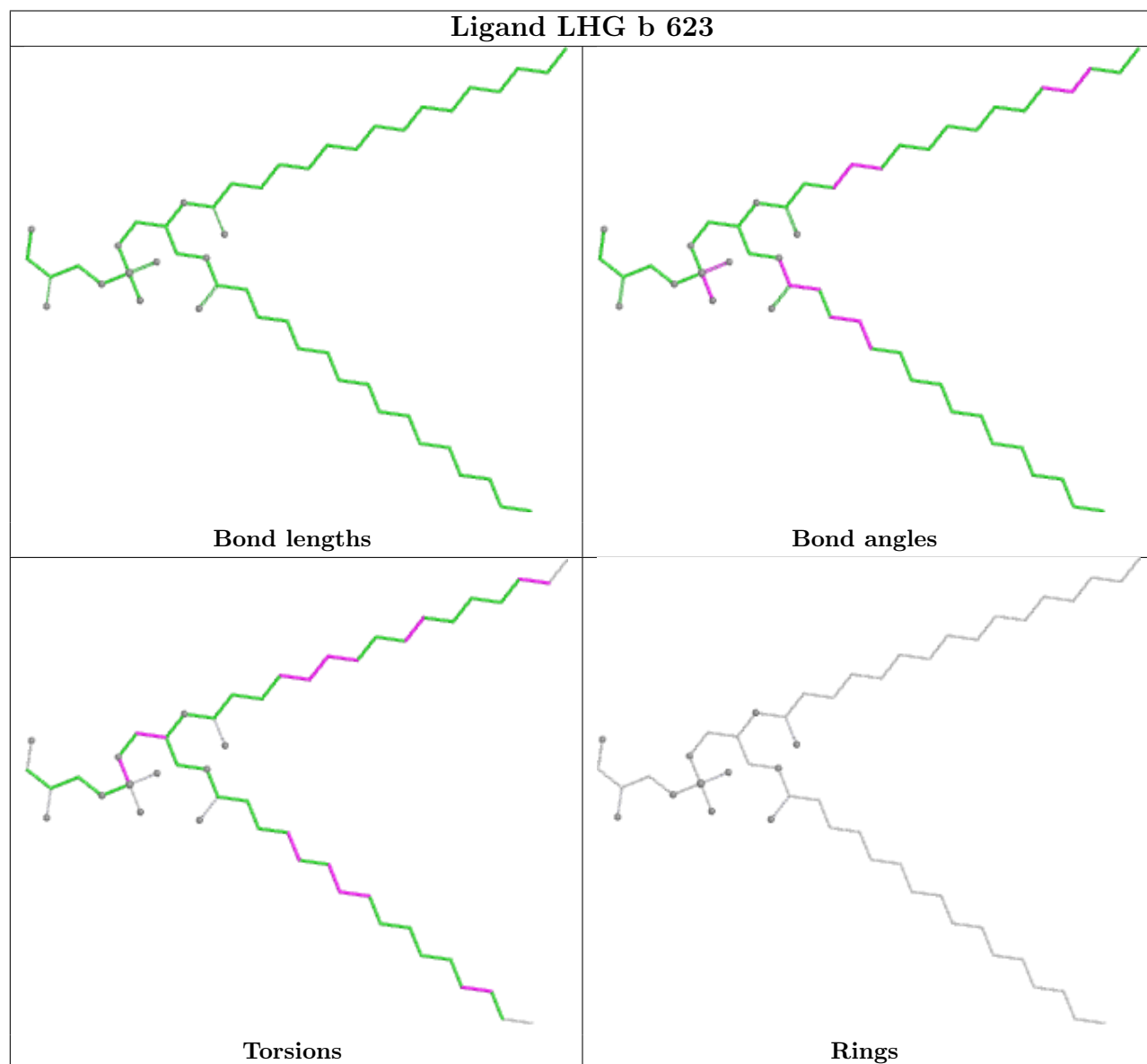
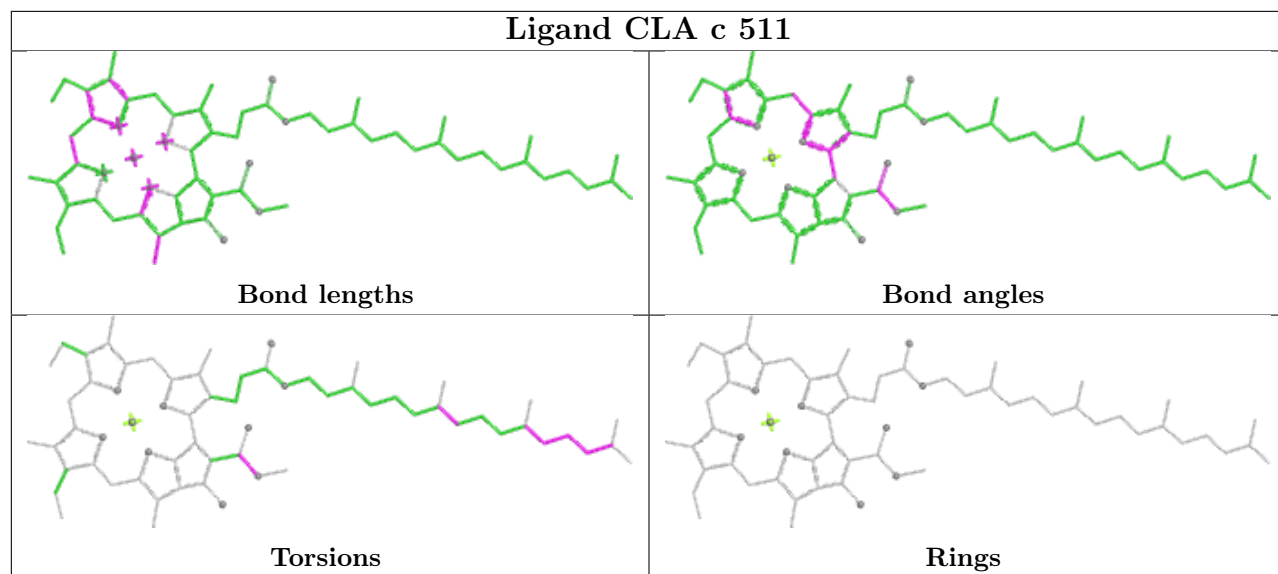


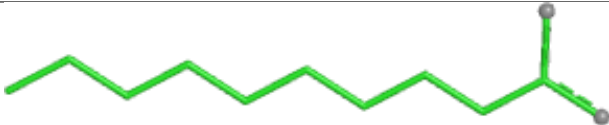
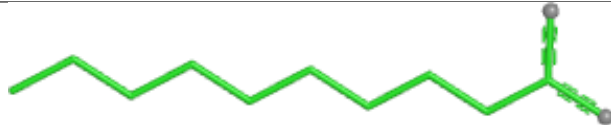
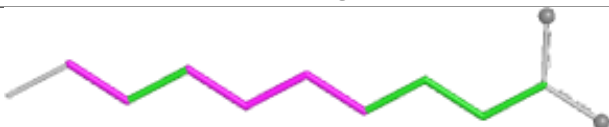
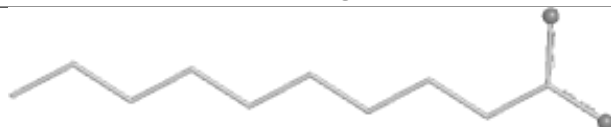
Ligand DGD c 517

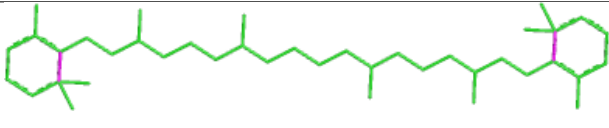
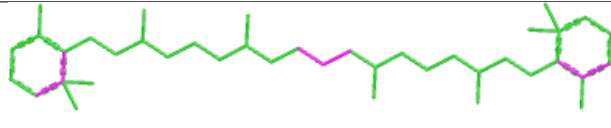
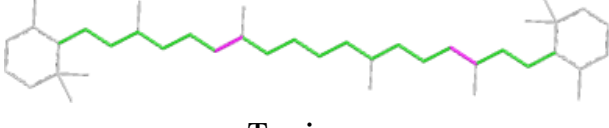
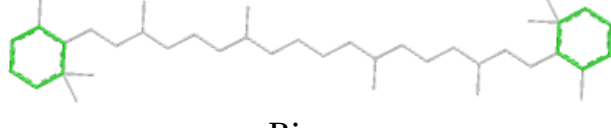


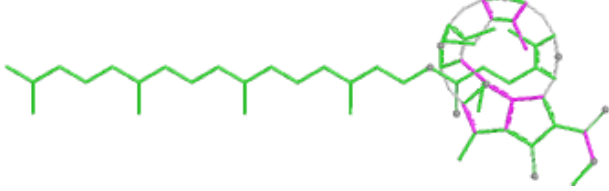
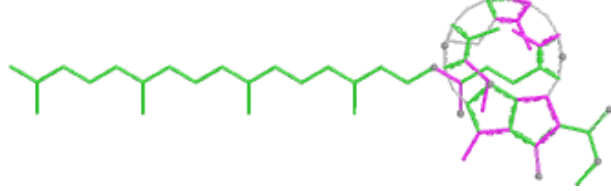
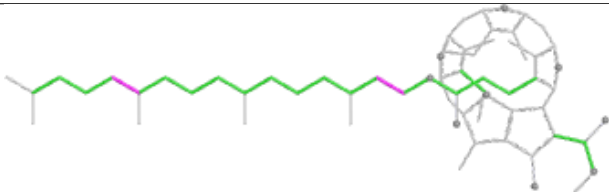
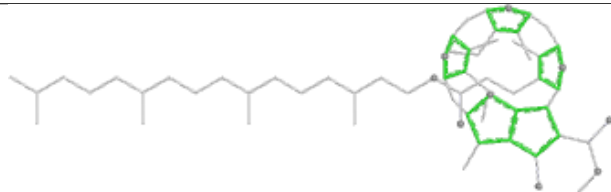


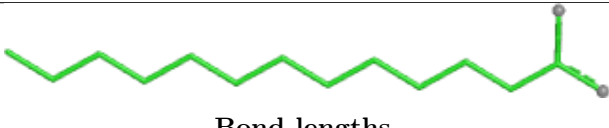
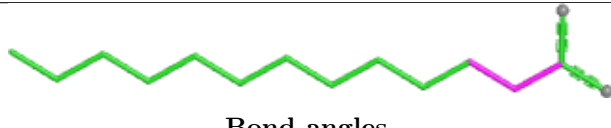
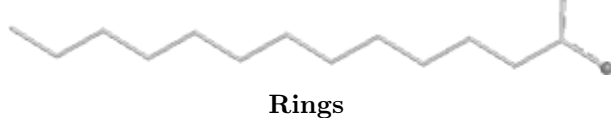




Ligand STE J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO a 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE M 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.51	1 (0%) 90 90	8, 28, 48, 77	64 (19%)
1	a	334/344 (97%)	-0.43	1 (0%) 90 90	8, 30, 55, 76	64 (19%)
2	B	505/510 (99%)	-0.42	2 (0%) 88 89	18, 32, 60, 83	4 (0%)
2	b	505/510 (99%)	-0.31	4 (0%) 82 83	23, 35, 67, 104	0
3	C	442/461 (95%)	-0.38	0 100 100	9, 35, 51, 71	11 (2%)
3	c	451/461 (97%)	-0.25	2 (0%) 88 89	9, 39, 60, 91	12 (2%)
4	D	341/352 (96%)	-0.56	0 100 100	10, 30, 48, 74	2 (0%)
4	d	341/352 (96%)	-0.42	0 100 100	10, 33, 55, 78	3 (0%)
5	E	82/84 (97%)	0.18	0 100 100	31, 48, 66, 78	1 (1%)
5	e	82/84 (97%)	0.41	1 (1%) 76 76	39, 56, 73, 84	0
6	F	34/45 (75%)	-0.08	0 100 100	37, 44, 57, 78	0
6	f	34/45 (75%)	0.16	0 100 100	40, 49, 73, 88	0
7	H	65/66 (98%)	-0.11	1 (1%) 72 72	34, 41, 55, 67	0
7	h	63/66 (95%)	0.12	0 100 100	40, 51, 60, 62	0
8	I	35/38 (92%)	-0.19	0 100 100	32, 39, 61, 78	0
8	i	35/38 (92%)	-0.25	0 100 100	29, 38, 69, 84	0
9	J	36/40 (90%)	0.10	0 100 100	35, 49, 77, 86	0
9	j	36/40 (90%)	0.26	0 100 100	41, 54, 87, 93	0
10	K	37/46 (80%)	0.06	0 100 100	42, 50, 65, 72	0
10	k	37/46 (80%)	0.21	0 100 100	48, 55, 72, 80	0
11	L	37/37 (100%)	-0.50	0 100 100	24, 29, 58, 64	0
11	l	36/37 (97%)	-0.51	0 100 100	26, 30, 62, 73	0
12	M	32/36 (88%)	-0.49	0 100 100	28, 32, 53, 66	0
12	m	31/36 (86%)	-0.44	0 100 100	29, 32, 48, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.23	3 (1%) 76 76	24, 40, 74, 124	1 (0%)
13	o	244/272 (89%)	-0.23	1 (0%) 88 89	25, 39, 73, 109	0
14	T	29/32 (90%)	-0.54	0 100 100	27, 31, 55, 70	0
14	t	29/32 (90%)	-0.51	0 100 100	27, 31, 66, 82	0
15	U	97/134 (72%)	-0.23	0 100 100	32, 41, 65, 83	0
15	u	97/134 (72%)	-0.24	1 (1%) 79 80	32, 39, 55, 80	0
16	V	137/163 (84%)	-0.36	1 (0%) 84 84	29, 39, 54, 70	0
16	v	137/163 (84%)	-0.05	0 100 100	33, 47, 67, 83	0
17	Y	27/46 (58%)	0.91	2 (7%) 20 19	50, 67, 94, 100	0
17	y	30/46 (65%)	0.71	2 (6%) 24 23	61, 74, 94, 99	0
18	X	38/41 (92%)	-0.00	0 100 100	40, 50, 68, 75	0
18	x	39/41 (95%)	0.23	1 (2%) 57 57	50, 59, 81, 92	0
19	Z	62/62 (100%)	0.59	2 (3%) 50 49	53, 67, 100, 114	0
19	z	62/62 (100%)	0.69	3 (4%) 35 35	60, 72, 105, 111	0
20	R	34/41 (82%)	0.63	1 (2%) 53 53	56, 64, 74, 79	0
20	r	31/41 (75%)	1.02	1 (3%) 50 49	64, 77, 93, 97	0
All	All	5302/5700 (93%)	-0.26	30 (0%) 85 86	8, 37, 70, 124	162 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	3.5
20	R	35	LEU	3.1
1	A	13	LEU	3.1
17	Y	25	ILE	2.9
2	b	495	PHE	2.9
15	u	53	ALA	2.9
2	b	496	TYR	2.8
3	c	23	ALA	2.8
3	c	134	ILE	2.7
7	H	41	PHE	2.6
2	b	486	LEU	2.6
20	r	31	VAL	2.5
13	O	59	LYS	2.4
19	Z	33	TRP	2.4
1	a	11	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
17	y	22	LEU	2.3
5	e	79	PHE	2.3
16	V	64	PRO	2.3
19	z	33	TRP	2.3
2	B	479[A]	PHE	2.2
17	Y	20	ALA	2.2
13	o	58	ASN	2.2
19	z	27	TYR	2.2
18	x	40	SER	2.2
19	z	3	ILE	2.1
2	b	500	GLY	2.1
2	B	487	SER	2.1
13	O	60	ARG	2.0
17	y	25	ILE	2.0
13	O	56	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.90	0.10	29,35,51,61	0
12	FME	M	1	10/11	0.93	0.10	38,44,61,66	0
14	FME	T	1	10/11	0.94	0.10	33,37,56,65	0
8	FME	i	1	10/11	0.96	0.07	35,47,49,49	0
8	FME	I	1	10/11	0.96	0.08	36,45,50,52	0
12	FME	m	1	10/11	0.97	0.07	31,44,62,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LHG	A	615	49/49	0.73	0.16	51,71,91,96	0
33	STE	H	104	18/20	0.74	0.17	56,64,68,70	0
29	LMG	d	410	23/55	0.75	0.20	45,65,73,75	0
29	LMG	b	622	55/55	0.76	0.17	49,63,72,77	0
28	PL9	A	611	55/55	0.78	0.15	43,60,70,73	0
33	STE	b	625	20/20	0.78	0.14	46,55,63,71	0
29	LMG	c	521	48/55	0.79	0.14	53,68,79,83	0
33	STE	d	412	16/20	0.79	0.17	51,58,80,82	0
32	DGD	a	615	44/66	0.81	0.13	36,49,61,69	0
25	CLA	h	101	65/65	0.81	0.12	47,62,78,88	0
28	PL9	a	611	55/55	0.81	0.14	42,61,73,74	0
31	LHG	e	101	42/49	0.81	0.13	57,76,89,100	0
33	STE	a	616	12/20	0.82	0.12	52,58,69,73	0
33	STE	k	103	12/20	0.82	0.13	59,71,78,80	0
29	LMG	A	613	48/55	0.83	0.11	38,52,65,68	0
33	STE	B	625	16/20	0.83	0.14	41,51,62,64	0
32	DGD	A	617	66/66	0.83	0.12	49,58,64,67	0
33	STE	J	101	12/20	0.83	0.13	49,56,60,63	0
33	STE	m	102	12/20	0.83	0.17	49,57,62,65	0
33	STE	b	624	15/20	0.84	0.14	44,48,58,59	0
33	STE	B	623	18/20	0.84	0.14	43,53,74,75	0
33	STE	b	626	10/20	0.84	0.14	45,51,59,61	0
29	LMG	D	410	33/55	0.84	0.13	31,53,76,77	0
33	STE	C	521	12/20	0.84	0.12	45,52,57,59	0
33	STE	b	621	20/20	0.84	0.12	40,51,61,68	0
33	STE	B	624	12/20	0.85	0.12	49,54,68,72	0
29	LMG	c	519	37/55	0.85	0.12	48,63,75,76	0
29	LMG	B	620	28/55	0.85	0.13	40,48,58,70	0
33	STE	E	101	12/20	0.85	0.12	57,62,76,78	0
29	LMG	C	519	48/55	0.85	0.13	43,63,75,78	0
30	SQD	A	616	39/54	0.85	0.12	42,52,70,72	0
30	SQD	a	614	36/54	0.85	0.12	36,55,67,70	0
33	STE	x	101	20/20	0.85	0.12	41,51,60,61	0
33	STE	B	622	12/20	0.86	0.12	45,50,58,62	0
33	STE	B	619	17/20	0.86	0.11	35,48,63,64	0
33	STE	C	520	12/20	0.86	0.14	40,44,52,55	0
33	STE	c	520	20/20	0.86	0.12	47,53,76,77	0
30	SQD	b	619	49/54	0.87	0.11	40,53,77,85	0
30	SQD	f	102	41/54	0.87	0.13	61,73,84,90	0
29	LMG	c	522	49/55	0.87	0.10	39,51,74,79	0
29	LMG	m	101	51/55	0.87	0.10	34,47,59,65	0
33	STE	X	101	20/20	0.87	0.11	40,49,63,69	0
33	STE	b	620	16/20	0.88	0.12	39,44,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	STE	I	101	15/20	0.88	0.13	43,49,56,57	0
33	STE	d	413	17/20	0.88	0.12	46,50,60,62	0
33	STE	j	101	12/20	0.88	0.11	50,55,58,58	0
29	LMG	M	101	51/55	0.88	0.10	31,46,60,64	0
25	CLA	H	101	65/65	0.88	0.10	36,51,74,82	0
33	STE	t	102	14/20	0.88	0.10	35,42,51,54	0
33	STE	t	103	10/20	0.88	0.11	43,55,61,62	0
27	BCR	k	101	40/40	0.88	0.11	48,57,64,65	0
33	STE	C	522	16/20	0.89	0.10	42,46,50,51	0
32	DGD	h	103	62/66	0.89	0.11	38,48,56,60	0
30	SQD	B	621	54/54	0.89	0.10	33,55,73,75	0
32	DGD	H	103	62/66	0.90	0.10	35,44,51,57	0
27	BCR	K	101	40/40	0.90	0.10	44,48,57,61	0
32	DGD	c	517	62/66	0.90	0.10	37,47,73,75	0
27	BCR	c	514	40/40	0.90	0.10	49,55,61,62	0
27	BCR	C	514	40/40	0.91	0.10	44,51,58,60	0
33	STE	M	103	10/20	0.91	0.12	44,47,53,56	0
30	SQD	F	102	36/54	0.91	0.12	45,64,68,70	0
30	SQD	a	613	54/54	0.91	0.10	37,55,72,75	0
27	BCR	d	405	40/40	0.91	0.09	38,46,77,84	0
27	BCR	h	102	40/40	0.91	0.10	40,50,61,63	0
27	BCR	D	405	40/40	0.91	0.09	34,41,69,77	0
27	BCR	H	102	40/40	0.91	0.09	33,45,51,56	0
25	CLA	C	513	65/65	0.91	0.10	45,54,76,81	0
34	BCT	d	401	4/4	0.91	0.11	34,37,41,47	0
25	CLA	c	512	65/65	0.92	0.10	43,55,73,79	0
27	BCR	B	618	40/40	0.92	0.08	27,37,49,51	0
32	DGD	C	517	62/66	0.92	0.09	36,45,80,87	0
27	BCR	k	102	40/40	0.92	0.10	43,51,59,64	0
33	STE	l	101	18/20	0.92	0.11	35,43,59,61	0
27	BCR	b	616	40/40	0.93	0.08	27,38,45,46	0
27	BCR	b	617	40/40	0.93	0.07	27,35,44,47	0
30	SQD	A	614	52/54	0.93	0.09	32,49,67,71	0
27	BCR	b	618	40/40	0.93	0.08	31,40,56,58	0
25	CLA	c	513	65/65	0.93	0.09	47,60,81,87	0
29	LMG	D	407	51/55	0.93	0.10	29,48,68,74	0
33	STE	M	102	15/20	0.93	0.09	34,40,52,63	0
27	BCR	C	515	40/40	0.93	0.08	28,38,46,52	0
25	CLA	c	503	65/65	0.93	0.08	33,41,49,54	0
27	BCR	B	617	40/40	0.93	0.07	26,34,44,50	0
25	CLA	C	503	65/65	0.93	0.08	34,39,45,51	0
27	BCR	t	101	40/40	0.93	0.07	29,35,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	BCR	T	101	40/40	0.93	0.07	29,35,45,49	0
25	CLA	C	508	65/65	0.94	0.09	29,36,84,88	0
28	PL9	D	406	55/55	0.94	0.07	23,29,36,38	0
31	LHG	D	409	47/49	0.94	0.10	30,38,65,73	0
31	LHG	d	407	49/49	0.94	0.09	31,44,60,64	0
27	BCR	A	610	40/40	0.94	0.06	25,31,35,37	0
25	CLA	C	510	65/65	0.94	0.08	30,38,49,52	0
32	DGD	C	516	62/66	0.94	0.09	24,34,63,68	0
25	CLA	c	504	60/65	0.94	0.07	31,43,64,68	0
25	CLA	c	508	64/65	0.94	0.09	33,41,71,84	0
25	CLA	c	509	65/65	0.94	0.09	36,42,54,56	0
25	CLA	c	511	65/65	0.94	0.10	36,50,61,66	0
32	DGD	c	518	62/66	0.94	0.08	31,45,64,69	0
25	CLA	C	512	65/65	0.94	0.09	38,46,68,74	0
25	CLA	B	605	65/65	0.94	0.08	24,32,57,61	0
27	BCR	K	102	40/40	0.94	0.09	39,47,56,60	0
25	CLA	c	505	65/65	0.95	0.07	30,37,51,56	0
25	CLA	c	506	65/65	0.95	0.08	33,41,72,76	0
25	CLA	C	502	65/65	0.95	0.07	27,35,45,50	0
31	LHG	D	411	49/49	0.95	0.08	30,39,57,64	0
31	LHG	b	623	49/49	0.95	0.08	31,40,46,50	0
25	CLA	C	504	59/65	0.95	0.07	32,39,66,70	0
31	LHG	d	409	39/49	0.95	0.08	32,41,54,59	0
25	CLA	c	510	65/65	0.95	0.07	31,43,52,56	0
25	CLA	a	606	65/65	0.95	0.06	21,27,38,49	0
25	CLA	b	608	65/65	0.95	0.07	32,40,57,63	0
25	CLA	b	611	65/65	0.95	0.07	25,31,40,46	0
32	DGD	C	518	62/66	0.95	0.07	29,41,66,72	0
25	CLA	d	404	65/65	0.95	0.08	28,40,75,79	0
27	BCR	c	515	40/40	0.95	0.08	33,42,48,54	0
32	DGD	c	516	62/66	0.95	0.08	25,35,59,68	0
25	CLA	b	613	65/65	0.95	0.08	25,33,59,69	0
29	LMG	d	411	44/55	0.95	0.08	35,45,66,71	0
26	PHO	d	402	64/64	0.95	0.06	29,35,40,44	0
25	CLA	b	614	65/65	0.95	0.07	25,36,48,51	0
27	BCR	B	616	40/40	0.95	0.07	28,36,42,46	0
25	CLA	b	615	60/65	0.95	0.08	29,38,75,78	0
25	CLA	c	502	65/65	0.95	0.07	30,37,49,54	0
25	CLA	C	511	65/65	0.95	0.08	36,45,54,56	0
25	CLA	C	506	65/65	0.95	0.09	27,40,71,75	0
28	PL9	d	406	55/55	0.95	0.07	23,30,36,38	0
25	CLA	C	505	65/65	0.96	0.07	26,34,53,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	606	65/65	0.96	0.07	17,27,50,54	0
25	CLA	C	507	65/65	0.96	0.07	26,34,46,49	0
27	BCR	a	610	40/40	0.96	0.06	22,29,41,43	0
25	CLA	B	608	65/65	0.96	0.06	23,34,47,52	0
25	CLA	C	509	65/65	0.96	0.08	29,36,53,58	0
25	CLA	B	609	65/65	0.96	0.06	21,29,35,37	0
25	CLA	c	507	65/65	0.96	0.07	29,38,48,54	0
25	CLA	B	610	65/65	0.96	0.06	23,28,40,44	0
25	CLA	B	611	65/65	0.96	0.06	21,29,38,41	0
25	CLA	B	613	65/65	0.96	0.07	23,30,61,68	0
25	CLA	B	614	65/65	0.96	0.07	24,33,51,60	0
25	CLA	B	615	60/65	0.96	0.07	26,34,65,70	0
25	CLA	a	607	65/65	0.96	0.08	27,34,78,86	0
25	CLA	d	403	65/65	0.96	0.07	23,29,48,56	0
31	LHG	d	408	49/49	0.96	0.08	28,37,44,50	0
25	CLA	a	609	65/65	0.96	0.08	21,28,63,67	0
25	CLA	a	612	65/65	0.96	0.06	22,27,35,42	0
26	PHO	A	608	64/64	0.96	0.05	24,30,36,38	0
26	PHO	D	402	64/64	0.96	0.05	20,26,32,36	0
26	PHO	a	608	64/64	0.96	0.05	23,28,34,36	0
25	CLA	b	601	65/65	0.96	0.07	31,36,52,57	0
25	CLA	b	605	65/65	0.96	0.07	27,35,60,64	0
25	CLA	b	607	65/65	0.96	0.07	32,37,52,54	0
25	CLA	C	501	65/65	0.96	0.06	25,32,44,46	0
25	CLA	b	609	65/65	0.96	0.07	26,33,40,45	0
25	CLA	B	601	65/65	0.96	0.06	26,32,48,54	0
25	CLA	b	612	65/65	0.96	0.07	22,28,55,66	0
25	CLA	B	603	65/65	0.96	0.07	24,28,58,65	0
25	CLA	A	607	65/65	0.96	0.07	21,30,74,81	0
31	LHG	L	101	49/49	0.97	0.07	27,36,47,52	0
25	CLA	c	501	65/65	0.97	0.06	30,35,45,49	0
25	CLA	b	603	65/65	0.97	0.07	23,29,61,72	0
25	CLA	b	604	65/65	0.97	0.06	23,32,41,43	0
25	CLA	D	403	65/65	0.97	0.06	19,26,44,51	0
25	CLA	b	606	65/65	0.97	0.06	22,31,51,57	0
25	CLA	D	404	65/65	0.97	0.07	29,33,83,88	0
25	CLA	B	602	65/65	0.97	0.06	22,28,50,53	0
25	CLA	B	612	65/65	0.97	0.06	20,27,55,62	0
25	CLA	b	610	65/65	0.97	0.05	24,31,44,51	0
25	CLA	B	607	65/65	0.97	0.06	23,30,47,52	0
25	CLA	A	612	65/65	0.97	0.06	18,25,38,47	0
25	CLA	B	604	65/65	0.97	0.06	22,27,38,41	0

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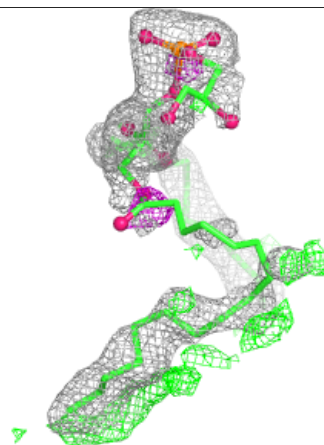
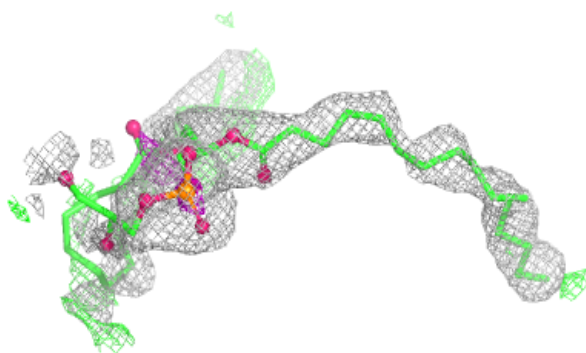
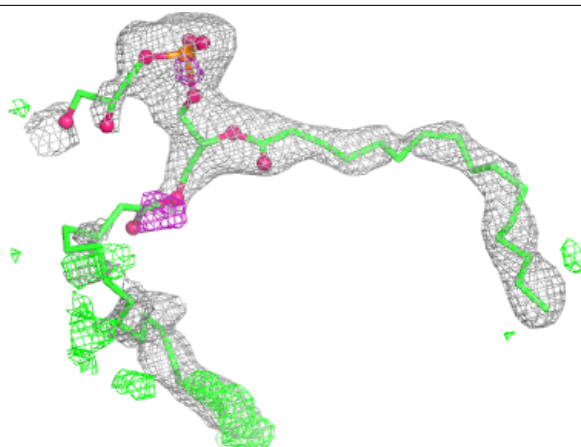
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	LHG	D	408	49/49	0.97	0.06	25,34,44,50	0
25	CLA	A	606	65/65	0.97	0.06	18,25,38,41	0
25	CLA	b	602	65/65	0.97	0.07	25,31,52,63	0
35	HEM	F	101	43/43	0.97	0.08	39,45,54,59	0
35	HEM	f	101	43/43	0.97	0.09	51,55,67,76	0
25	CLA	A	609	54/65	0.98	0.05	20,27,54,60	0
24	CL	A	604	1/1	0.98	0.05	27,27,27,27	0
34	BCT	D	401	4/4	0.98	0.06	33,34,35,38	0
36	HEC	V	201	43/43	0.98	0.06	24,30,37,41	0
36	HEC	v	201	43/43	0.98	0.06	28,36,41,45	0
24	CL	a	604	1/1	0.99	0.04	29,29,29,29	0
24	CL	a	605	1/1	0.99	0.07	30,30,30,30	0
21	OEY	A	601[C]	11/11	0.99	0.03	24,26,30,31	11
21	OEY	a	601[A]	11/11	0.99	0.03	27,31,33,34	11
21	OEY	a	601[C]	11/11	0.99	0.03	24,27,32,32	11
22	OEX	A	602[B]	10/10	0.99	0.03	25,29,32,32	10
22	OEX	a	602[B]	10/10	0.99	0.03	25,29,31,32	10
23	FE2	a	603	1/1	0.99	0.03	32,32,32,32	0
21	OEY	A	601[A]	11/11	0.99	0.03	28,31,33,34	11
23	FE2	A	603	1/1	1.00	0.01	30,30,30,30	0
24	CL	A	605	1/1	1.00	0.06	28,28,28,28	0

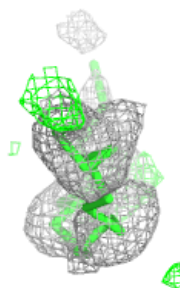
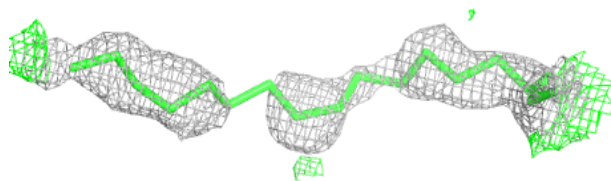
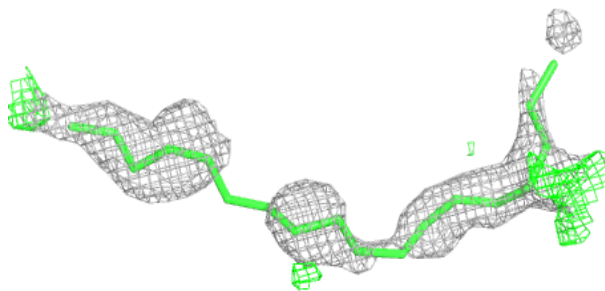
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LHG A 615:

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

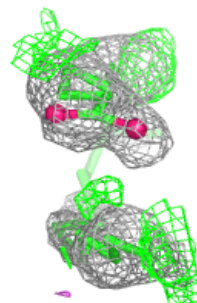
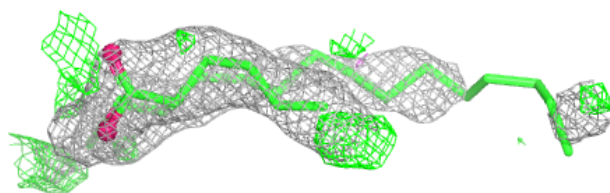
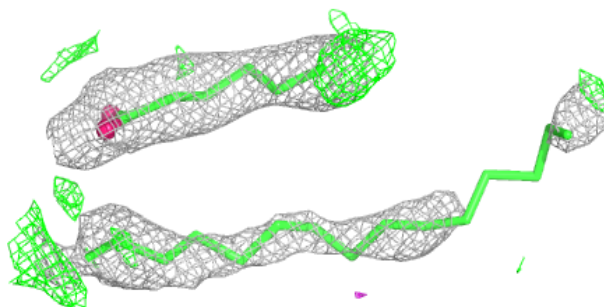
**Electron density around STE H 104:**

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

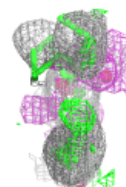
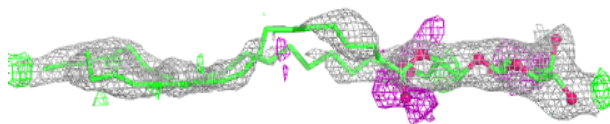
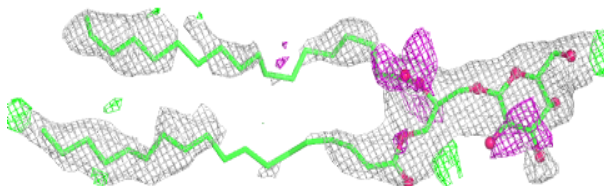


Electron density around LMG d 410:

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

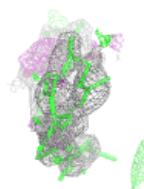
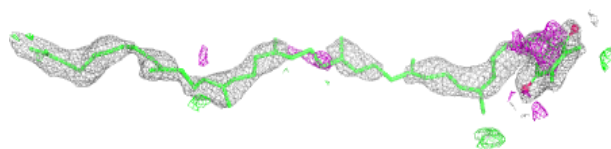
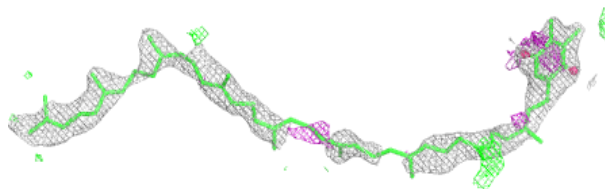
**Electron density around LMG b 622:**

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

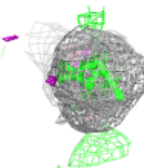
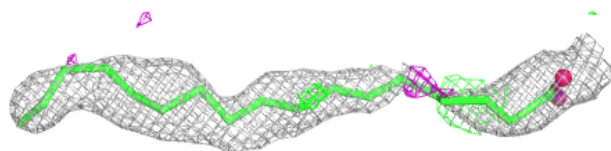
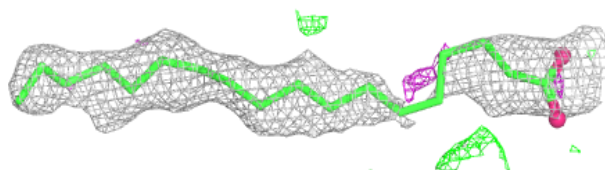


Electron density around PL9 A 611:

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

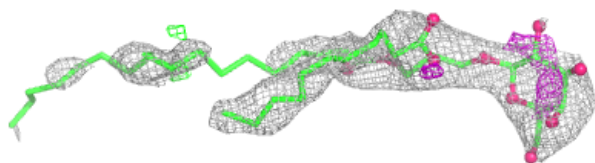
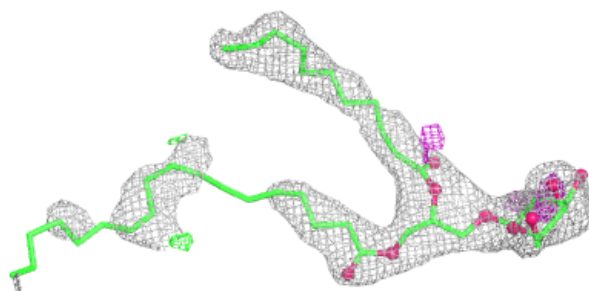
**Electron density around STE b 625:**

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

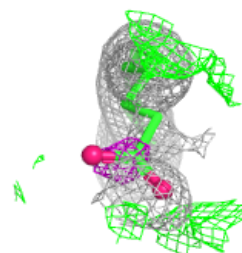
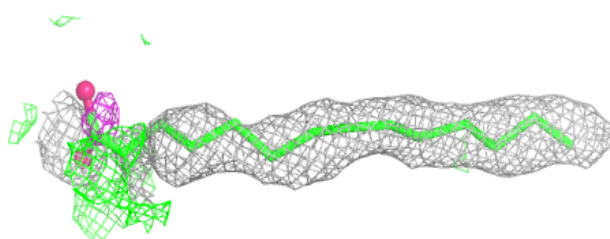
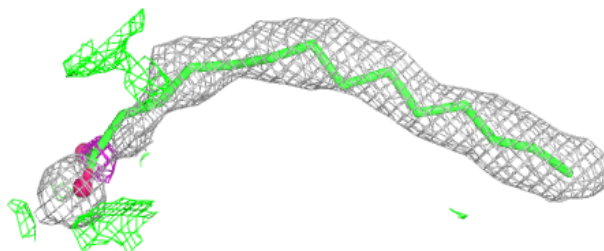


Electron density around LMG c 521:

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

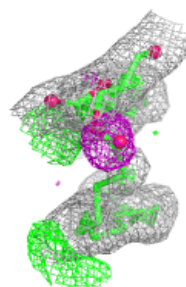
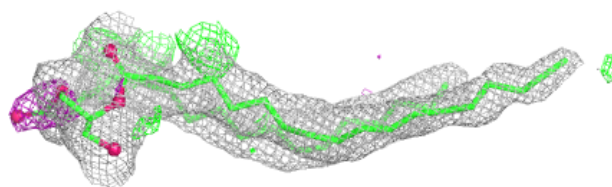
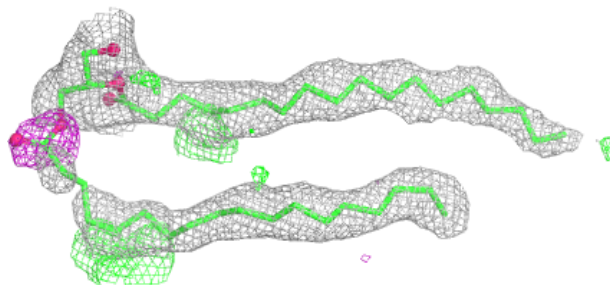
**Electron density around STE d 412:**

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

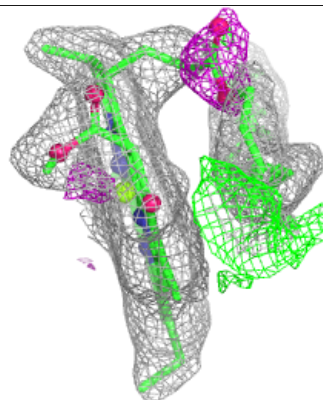
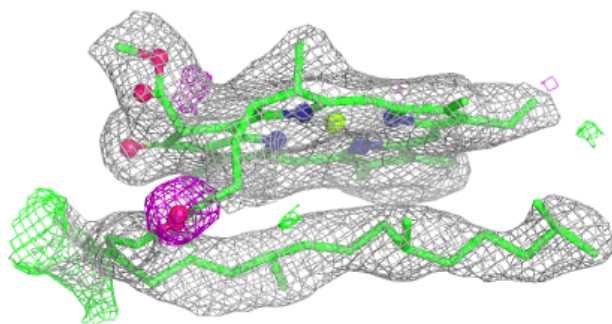
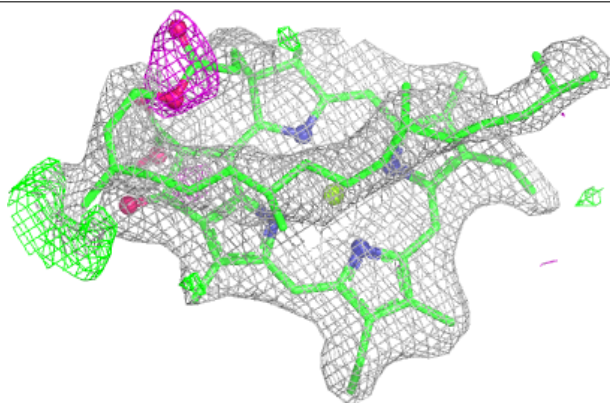


Electron density around DGD a 615:

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

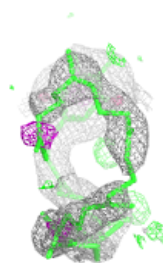
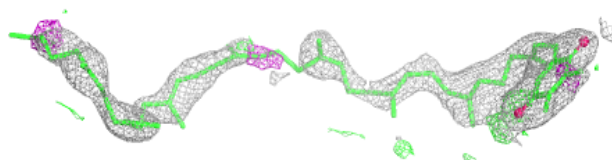
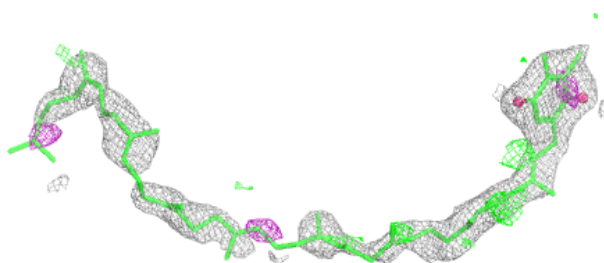
**Electron density around CLA h 101:**

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

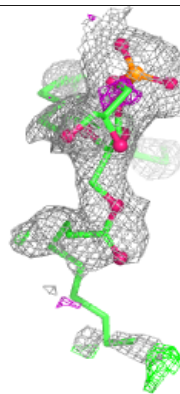
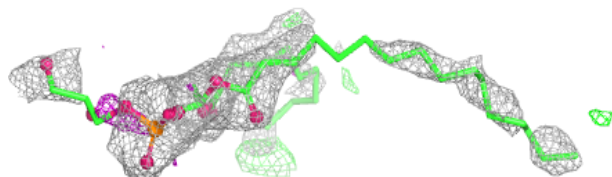
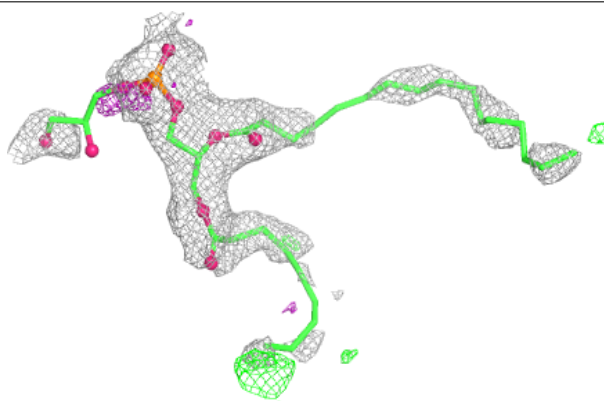


Electron density around PL9 a 611:

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

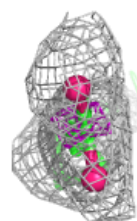
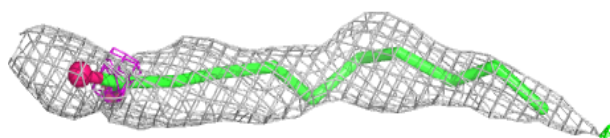
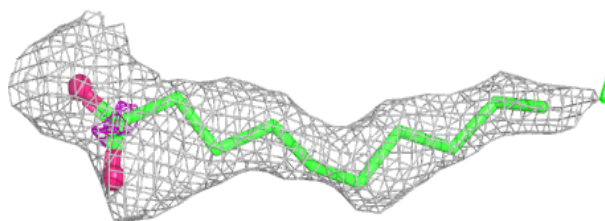
**Electron density around LHG e 101:**

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

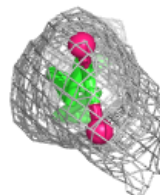
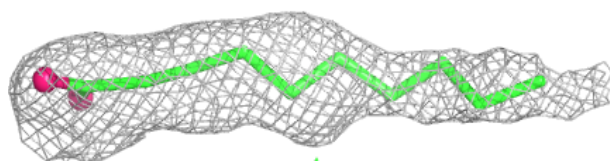
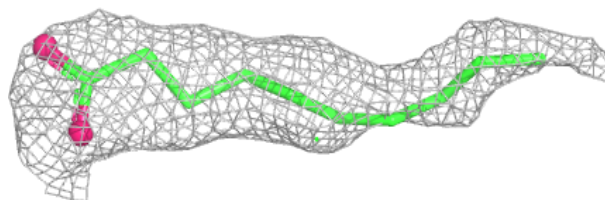


Electron density around STE a 616:

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

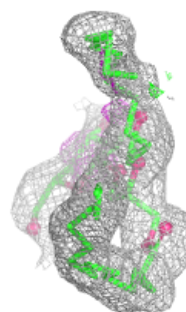
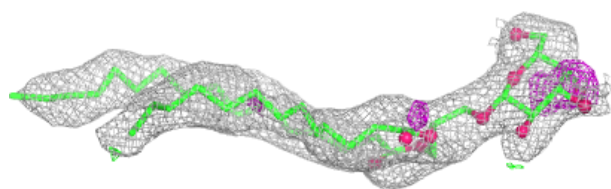
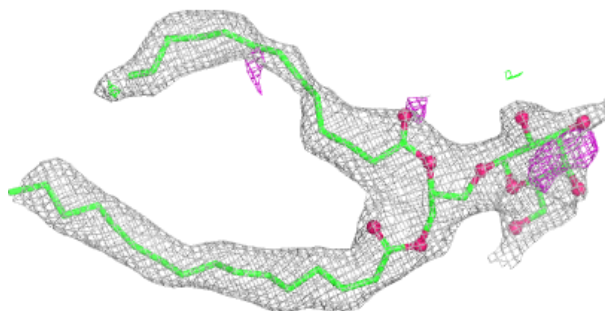
**Electron density around STE k 103:**

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

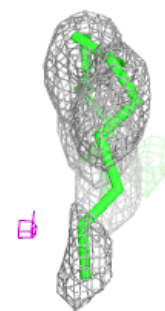
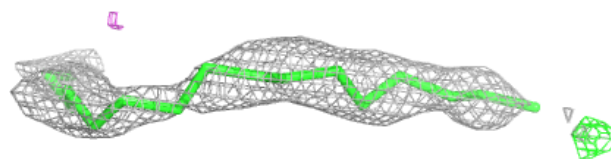
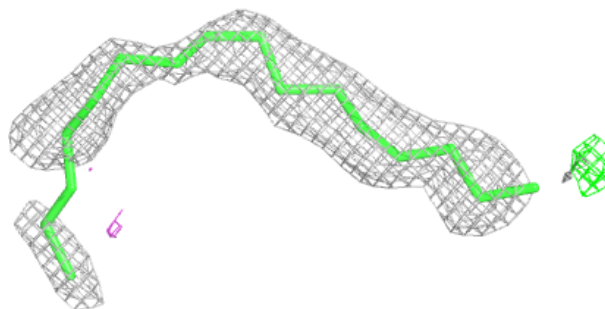


Electron density around LMG A 613:

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

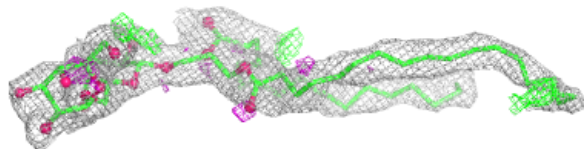
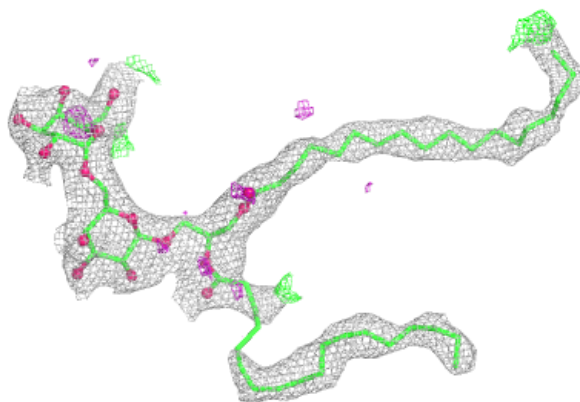
**Electron density around STE B 625:**

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

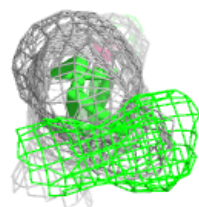
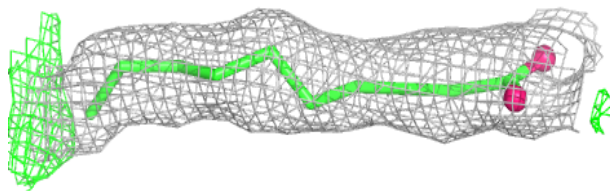
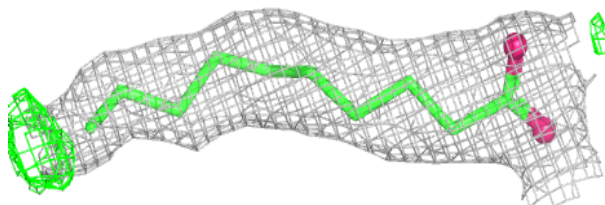


Electron density around DGD A 617:

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

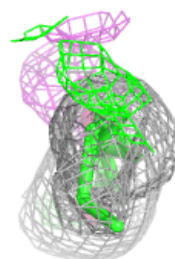
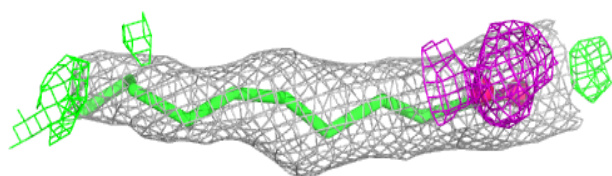
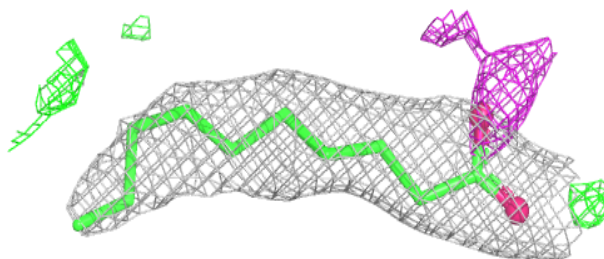
**Electron density around STE J 101:**

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

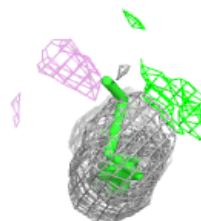
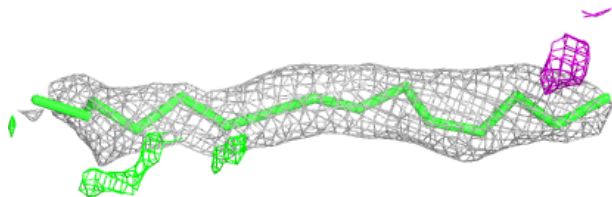
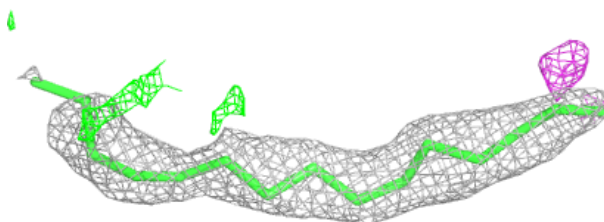


Electron density around STE m 102:

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

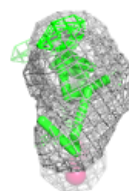
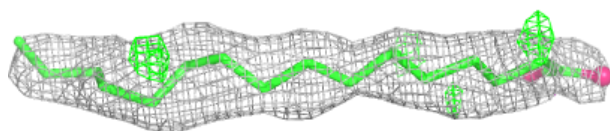
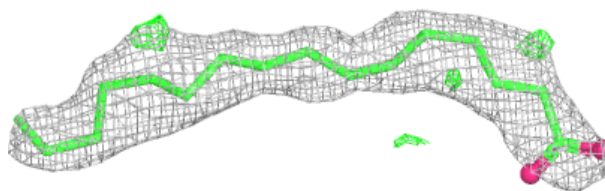
**Electron density around STE b 624:**

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

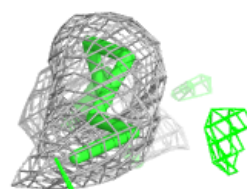
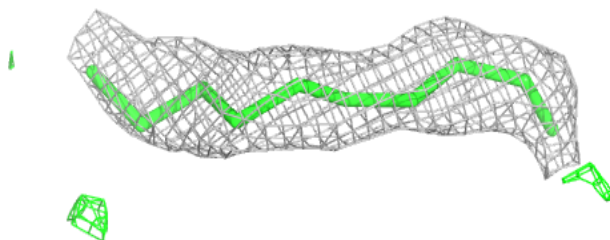
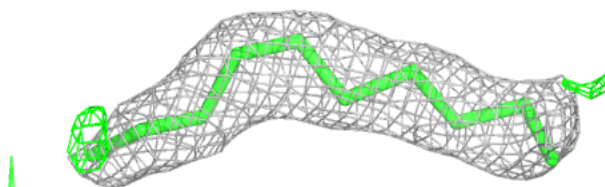


Electron density around STE B 623:

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

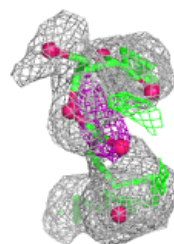
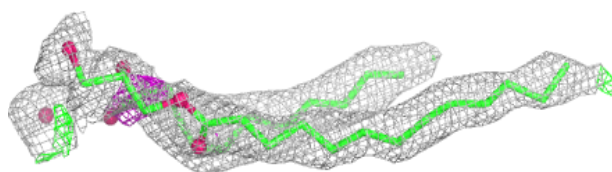
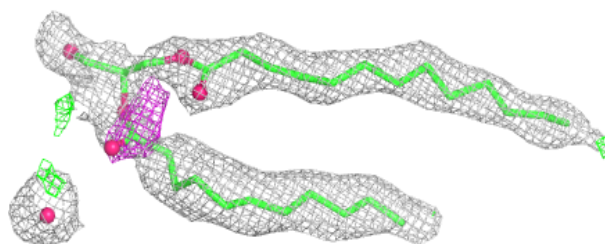
**Electron density around STE b 626:**

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

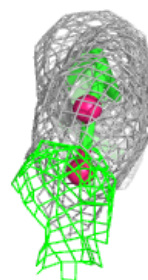
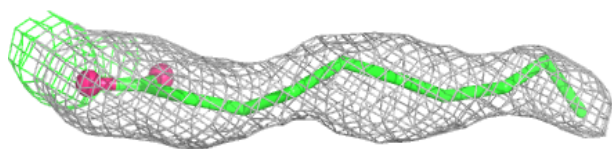
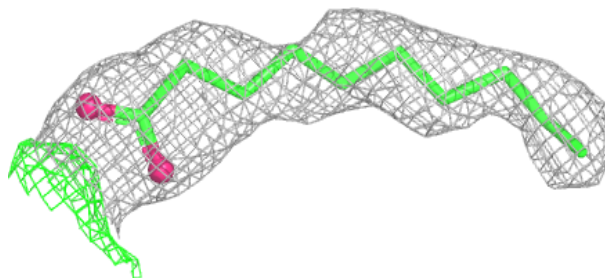


Electron density around LMG D 410:

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

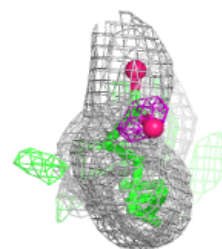
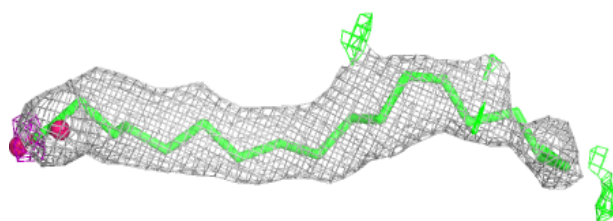
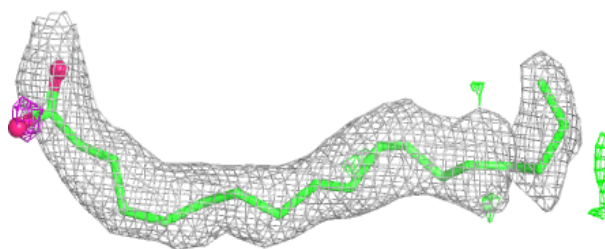
**Electron density around STE C 521:**

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

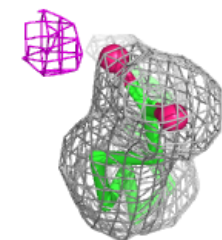
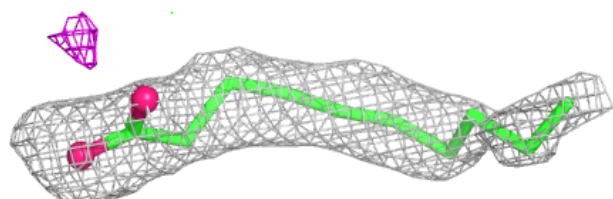
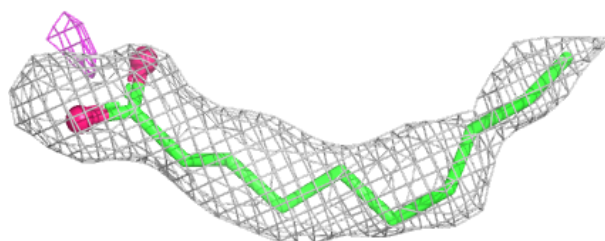


Electron density around STE b 621:

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

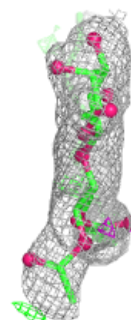
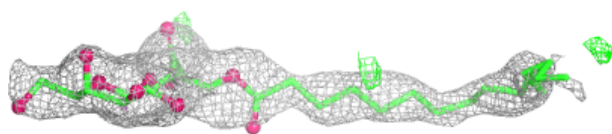
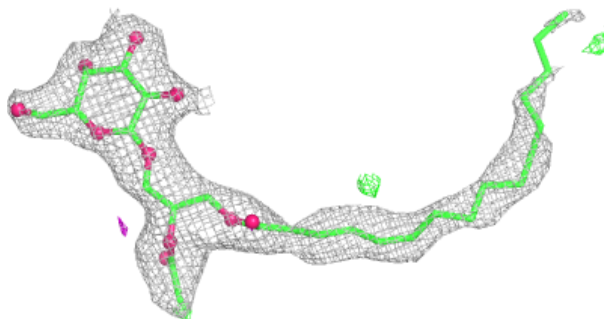
**Electron density around STE B 624:**

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

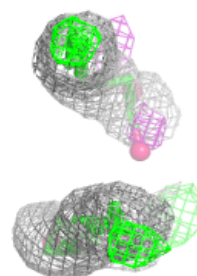
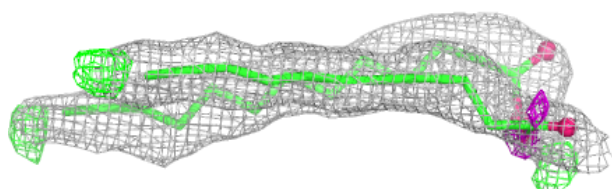
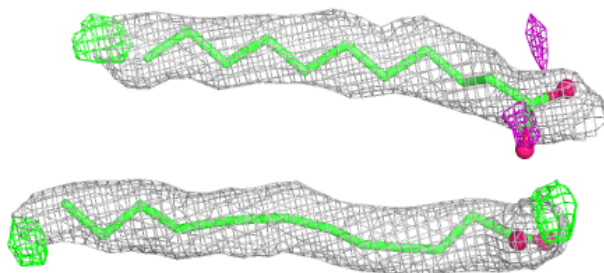


Electron density around LMG c 519:

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

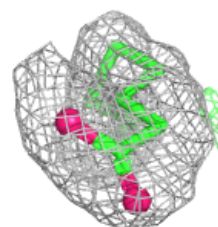
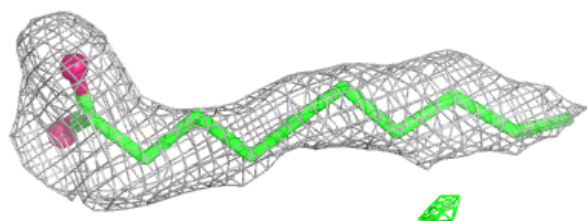
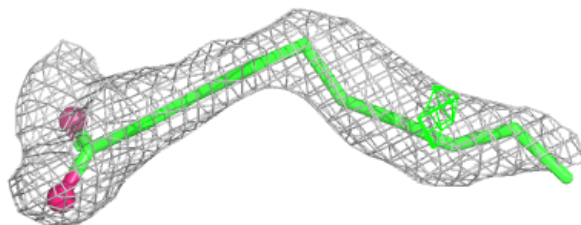
**Electron density around LMG B 620:**

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



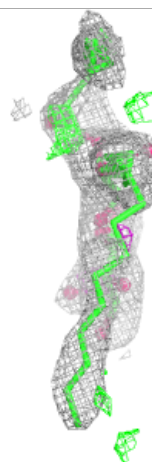
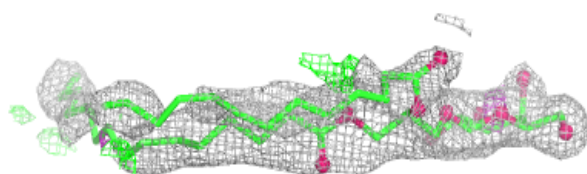
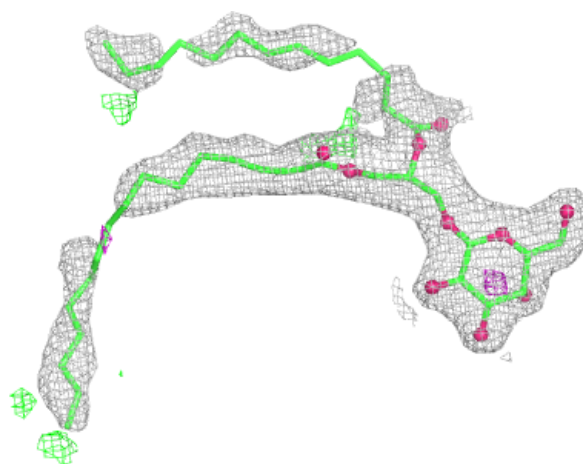
Electron density around STE E 101:

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



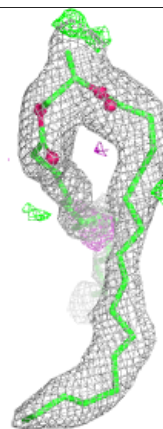
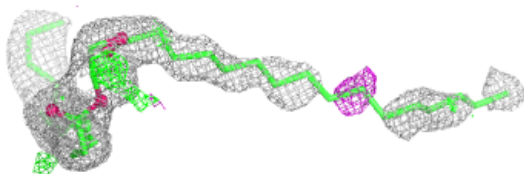
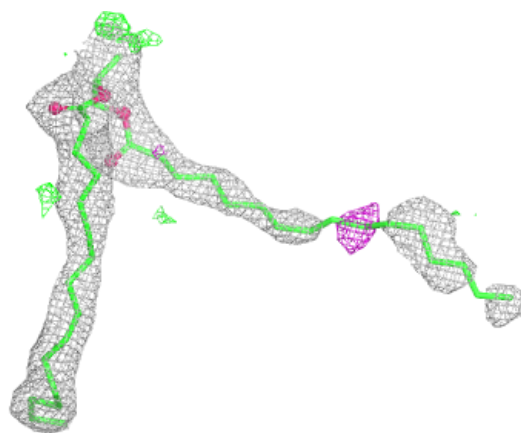
Electron density around LMG C 519:

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



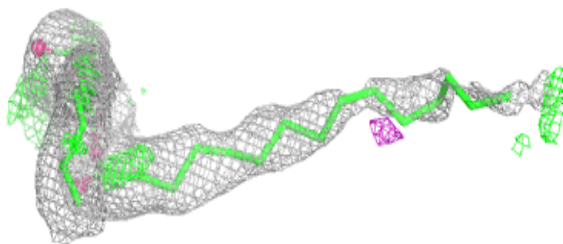
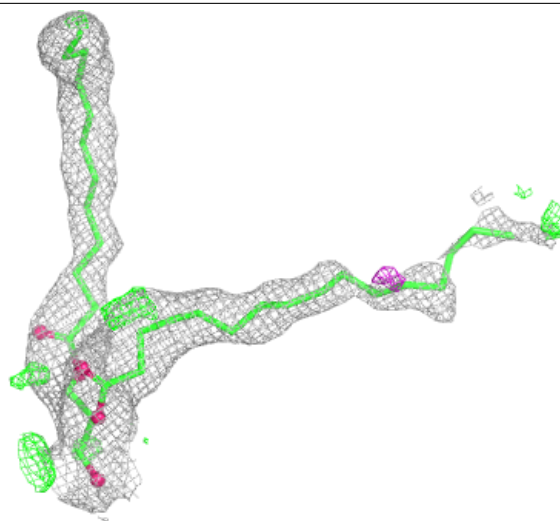
Electron density around SQD A 616:

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



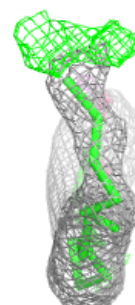
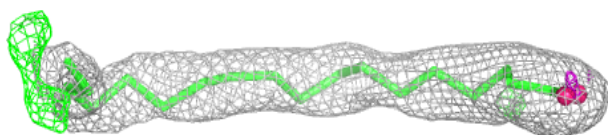
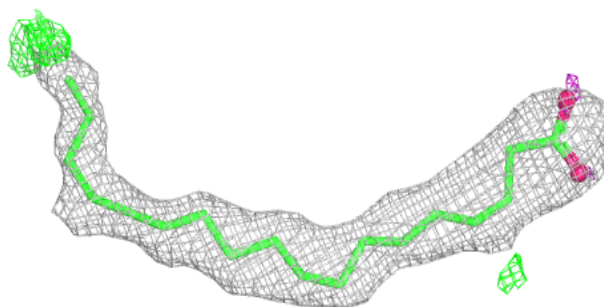
Electron density around SQD a 614:

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

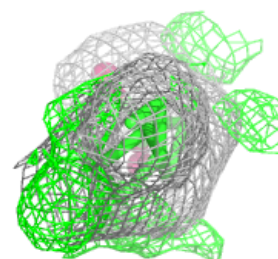
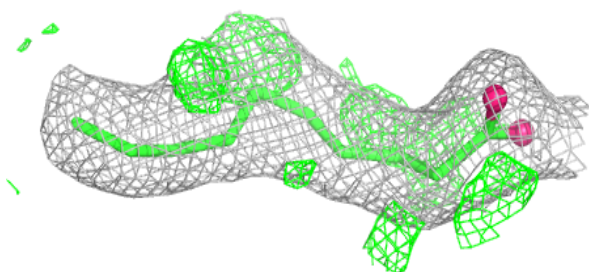
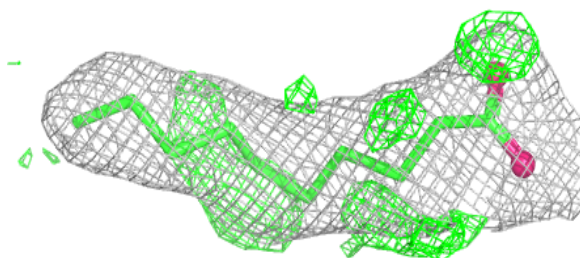


Electron density around STE x 101:

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

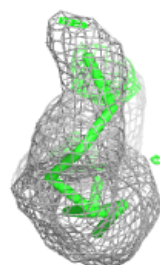
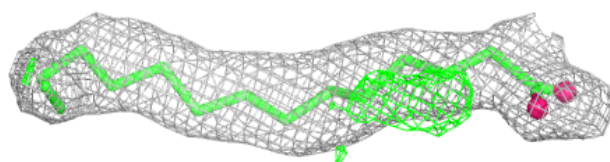
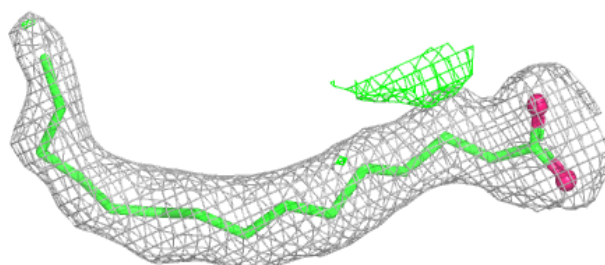
**Electron density around STE B 622:**

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

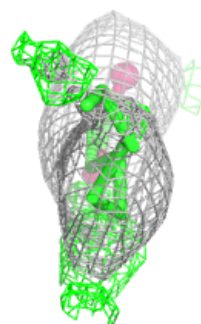
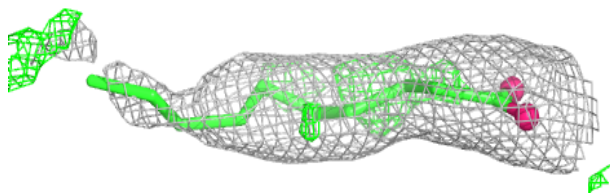
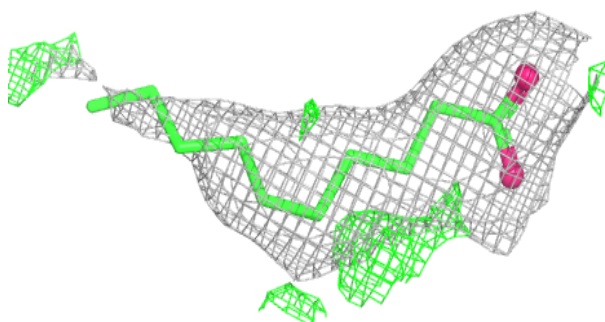


Electron density around STE B 619:

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

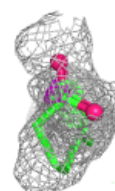
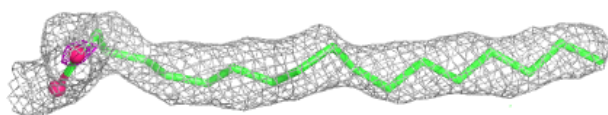
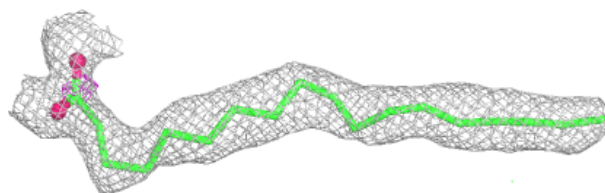
**Electron density around STE C 520:**

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

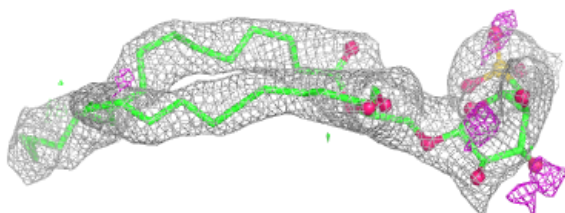
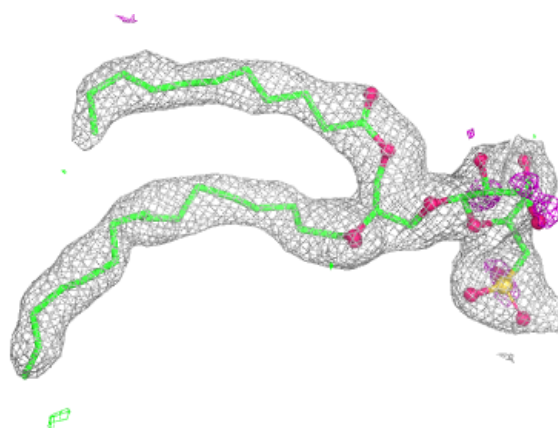


Electron density around STE c 520:

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

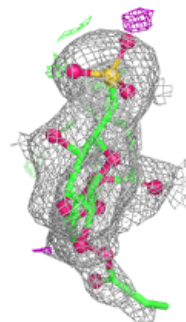
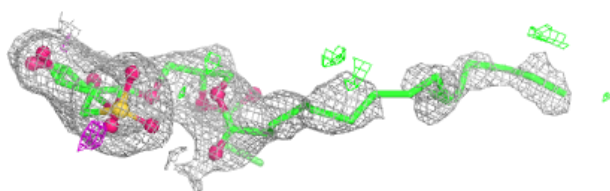
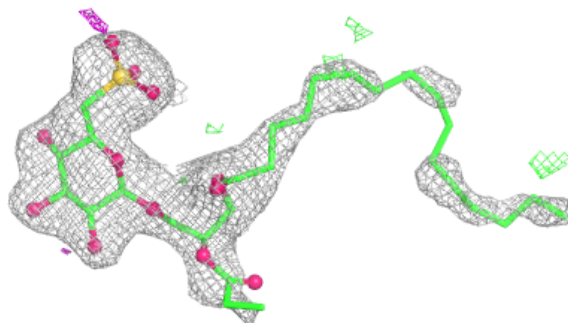
**Electron density around SQD b 619:**

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

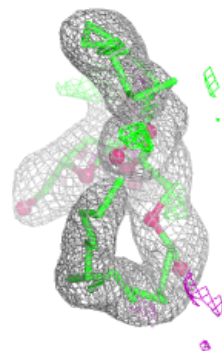
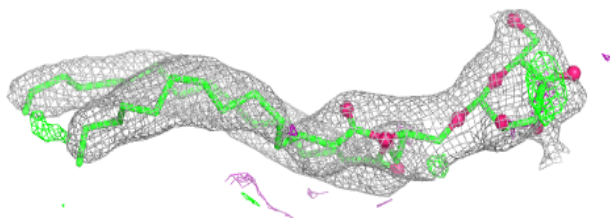
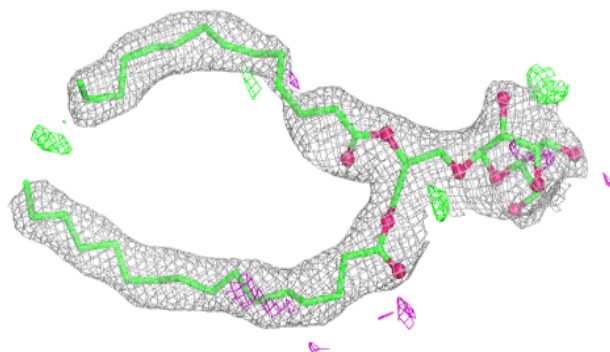


Electron density around SQD f 102:

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

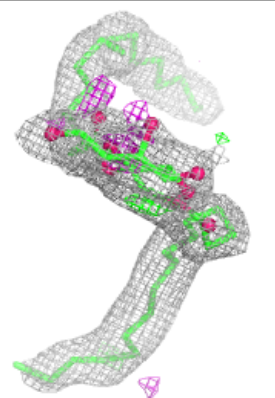
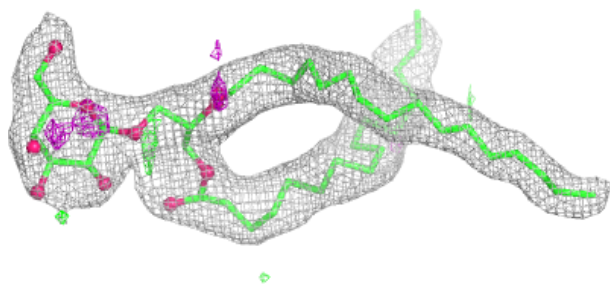
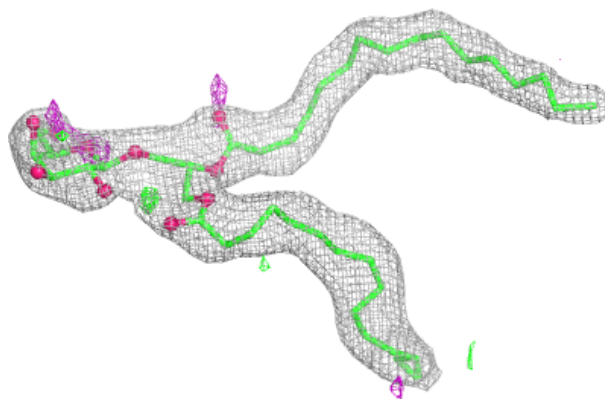
**Electron density around LMG c 522:**

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

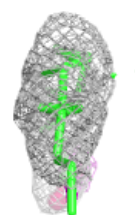
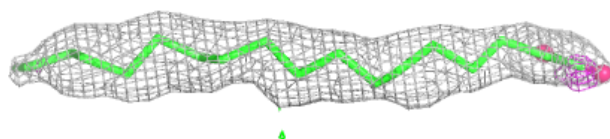
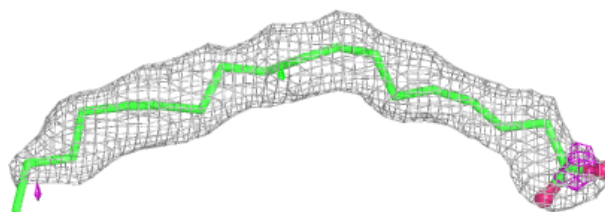


Electron density around LMG m 101:

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

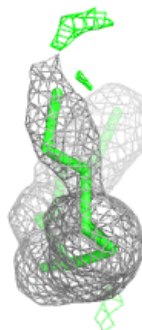
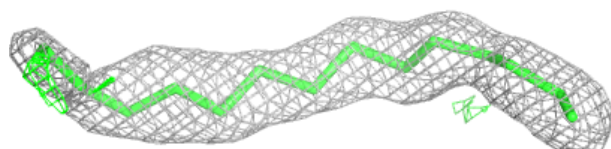
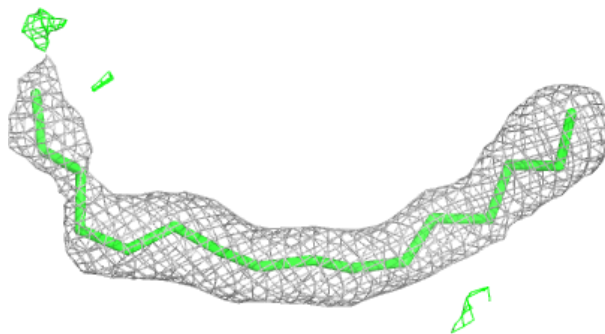
**Electron density around STE X 101:**

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

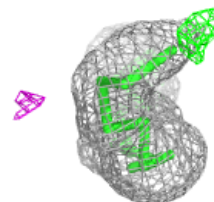
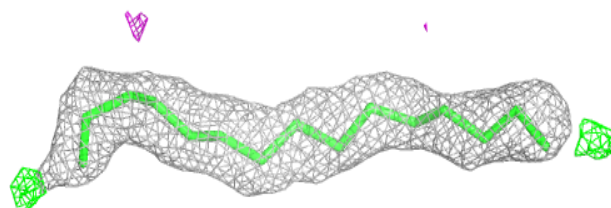
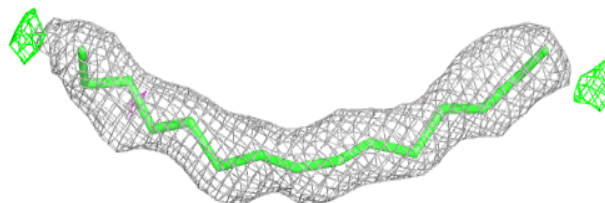


Electron density around STE b 620:

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

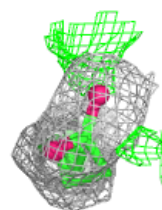
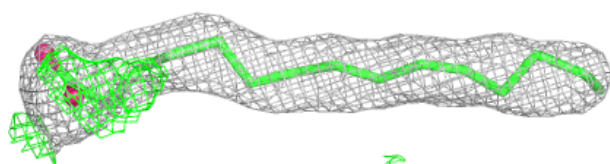
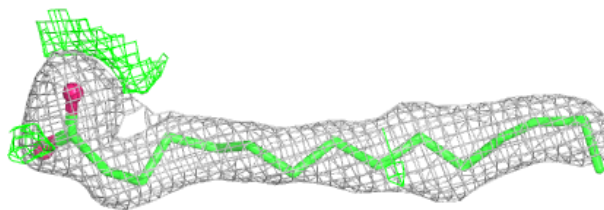
**Electron density around STE I 101:**

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

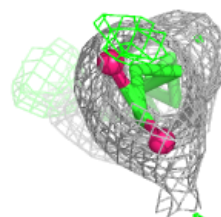
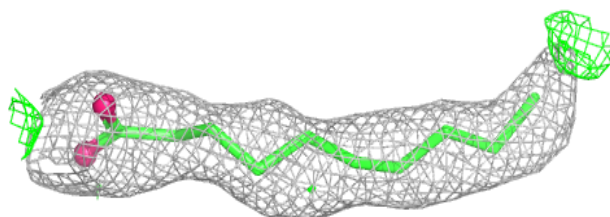
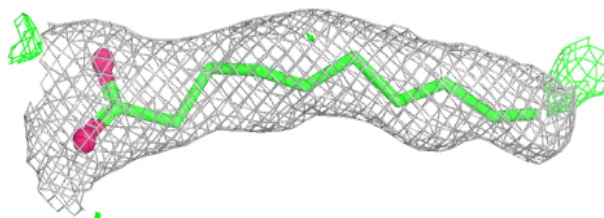


Electron density around STE d 413:

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

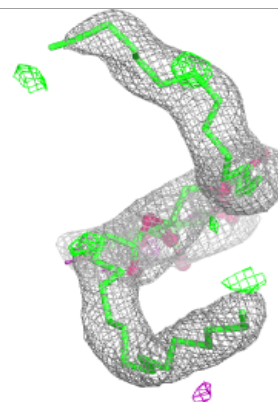
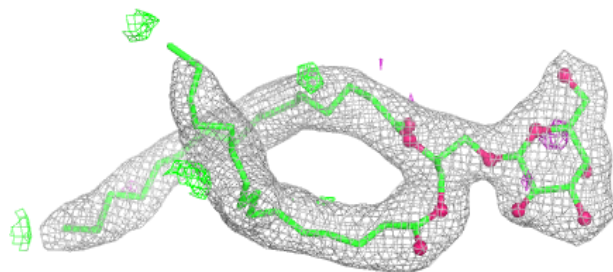
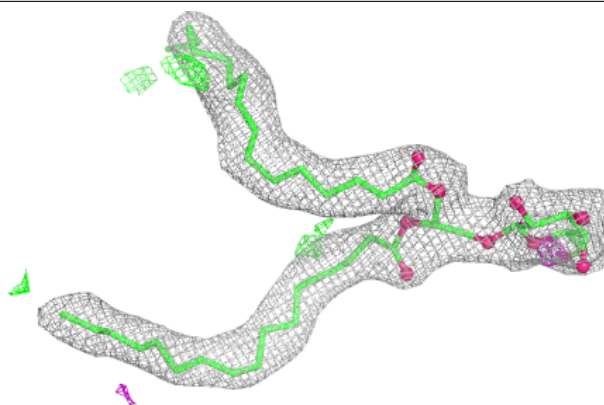
**Electron density around STE j 101:**

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

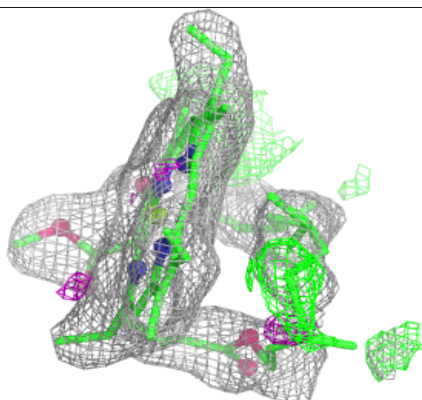
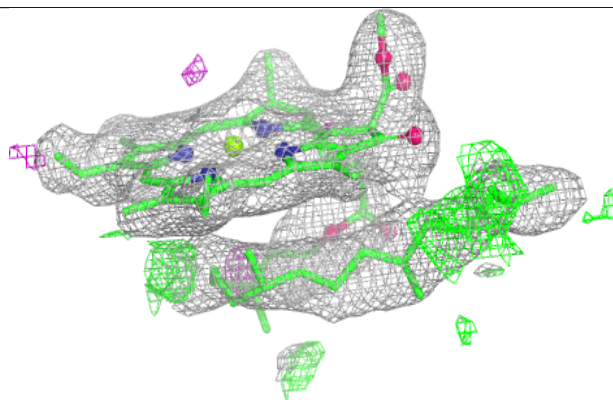
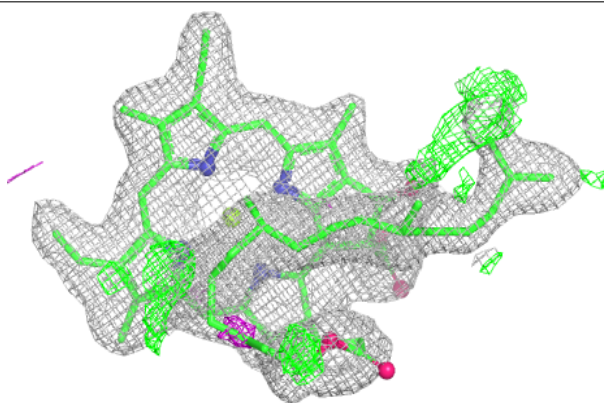


Electron density around LMG M 101:

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

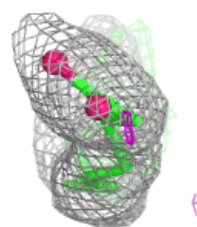
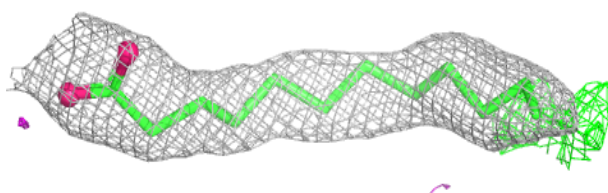
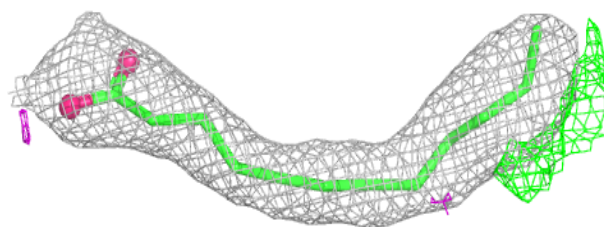
**Electron density around CLA H 101:**

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

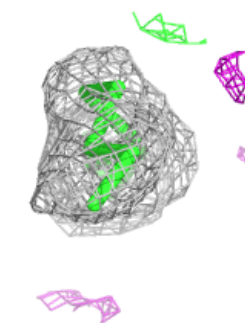
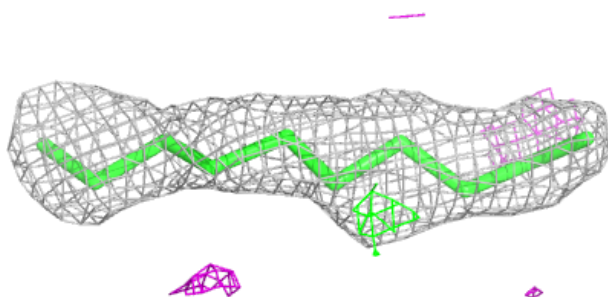


Electron density around STE t 102:

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

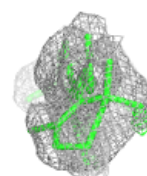
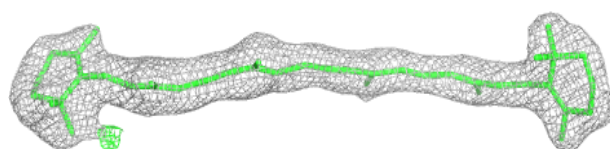
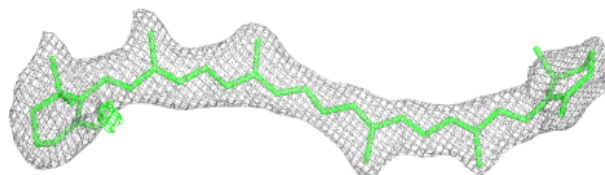
**Electron density around STE t 103:**

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

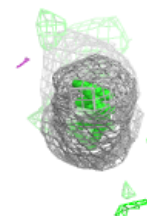
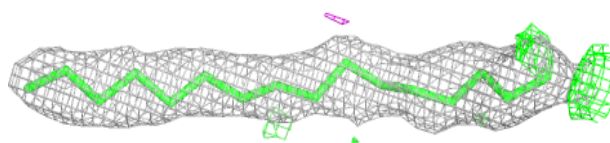
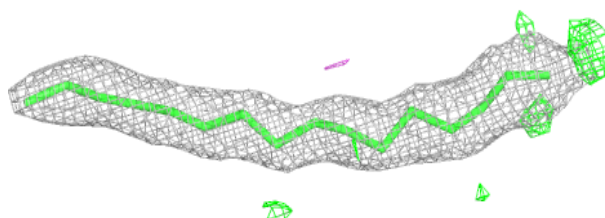


Electron density around BCR k 101:

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

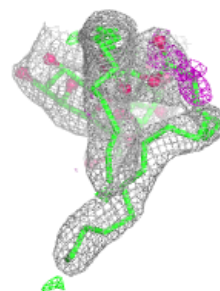
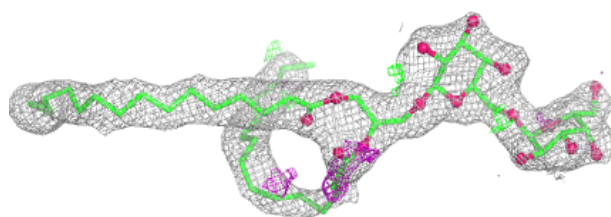
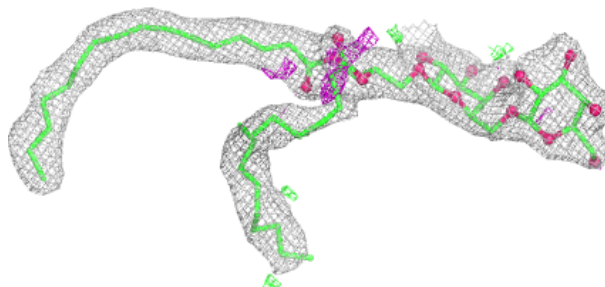
**Electron density around STE C 522:**

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

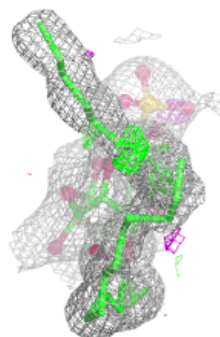
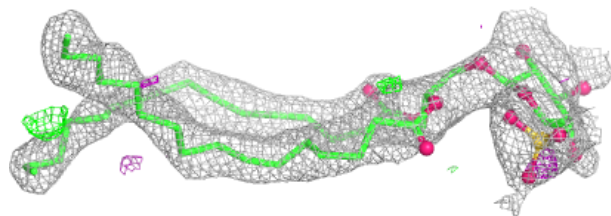
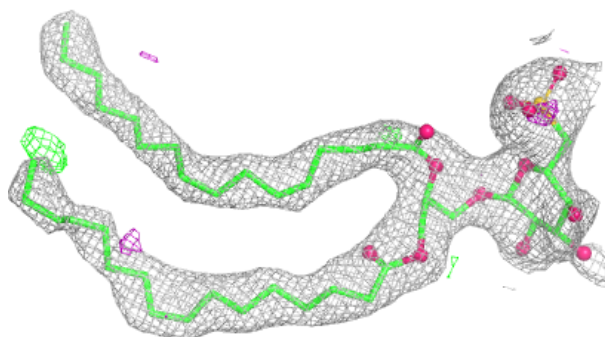


Electron density around DGD h 103:

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

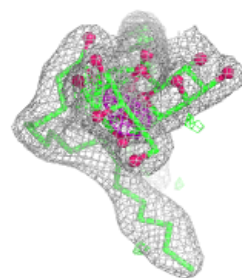
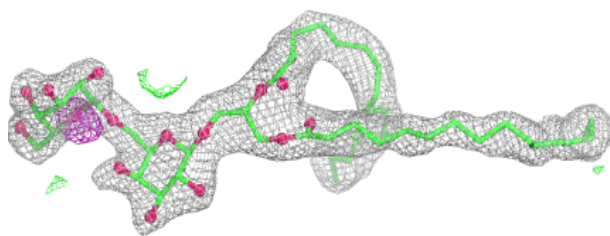
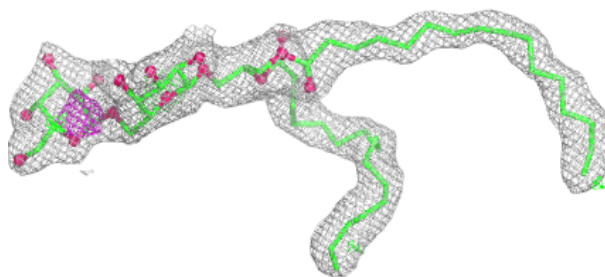
**Electron density around SQD B 621:**

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

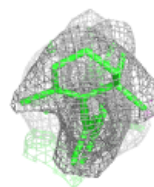
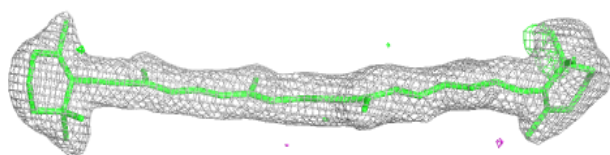
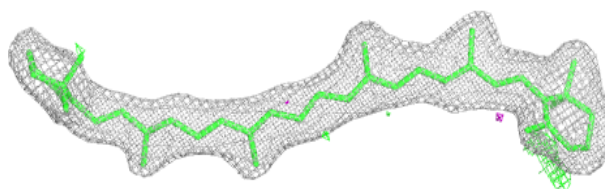


Electron density around DGD H 103:

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

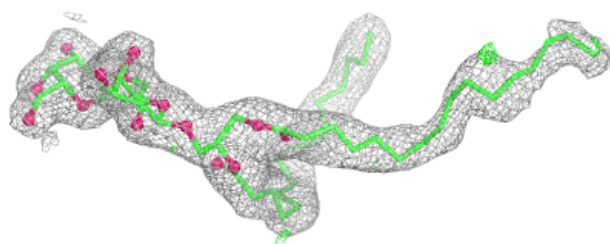
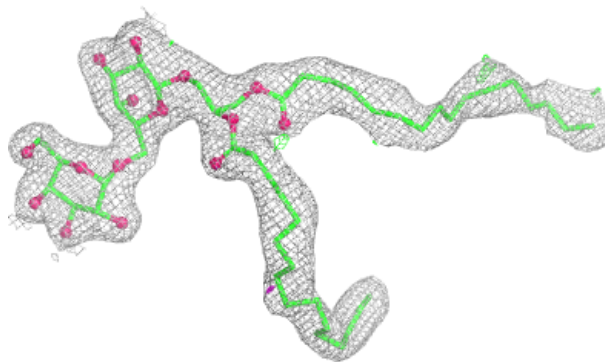
**Electron density around BCR K 101:**

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

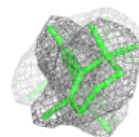
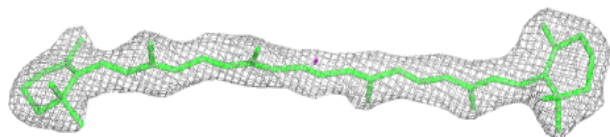
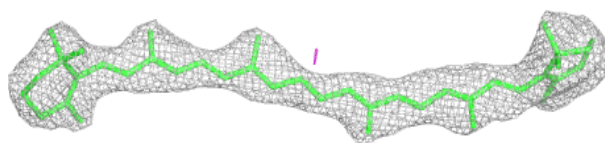


Electron density around DGD c 517:

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

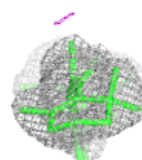
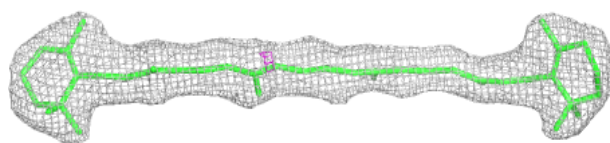
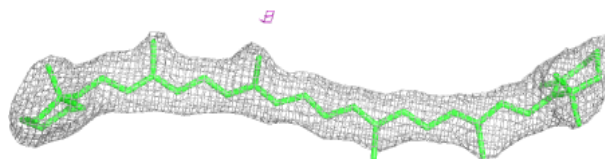
**Electron density around BCR c 514:**

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

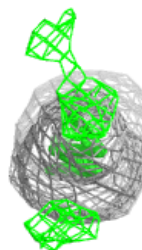
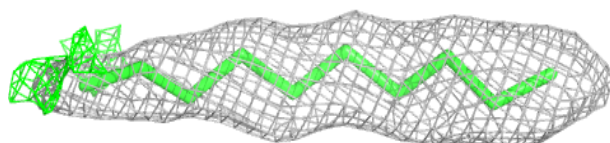
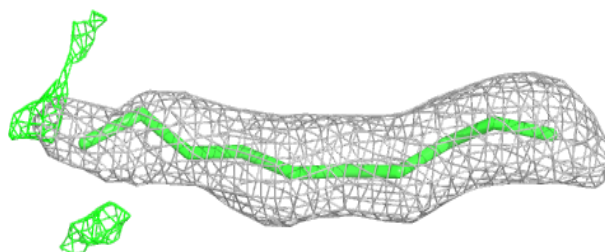


Electron density around BCR C 514:

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

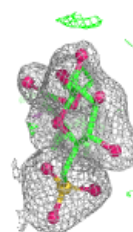
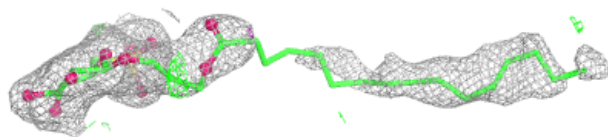
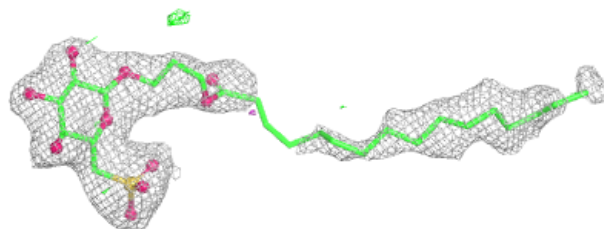
**Electron density around STE M 103:**

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



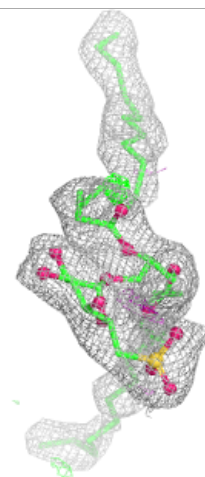
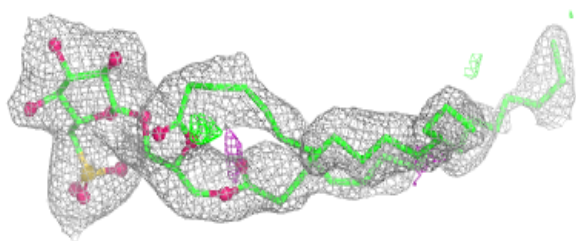
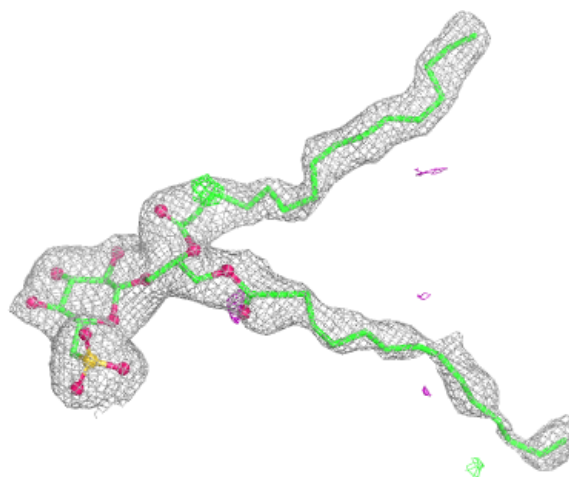
Electron density around SQD F 102:

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



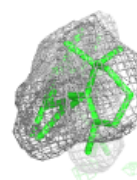
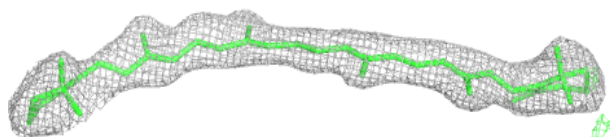
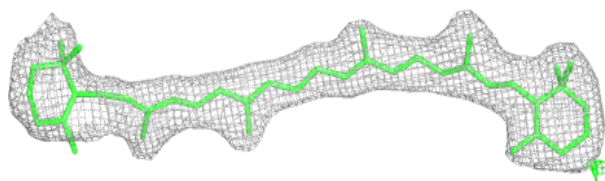
Electron density around SQD a 613:

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

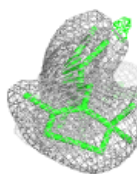
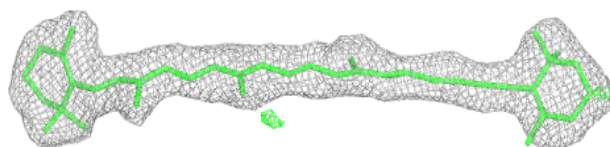
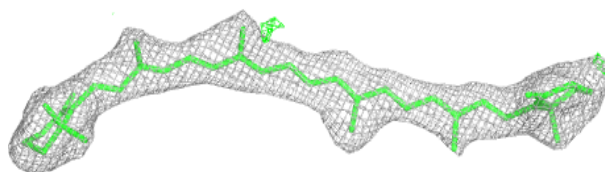


Electron density around BCR d 405:

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

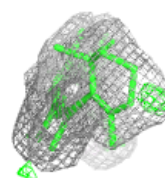
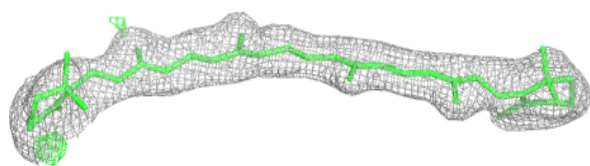
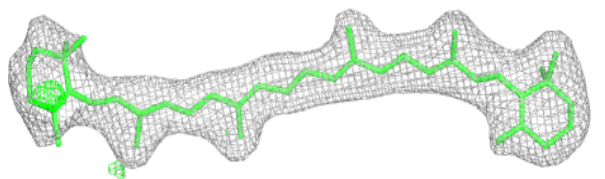
**Electron density around BCR h 102:**

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

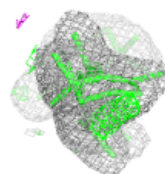
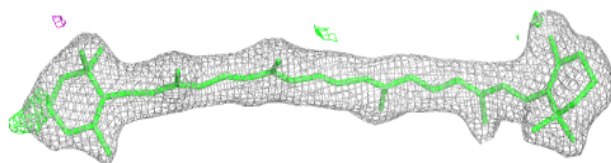
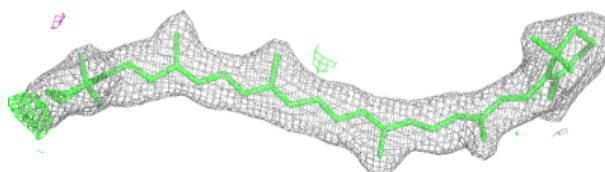


Electron density around BCR D 405:

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

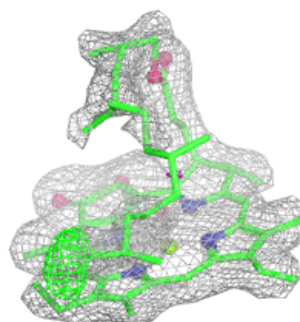
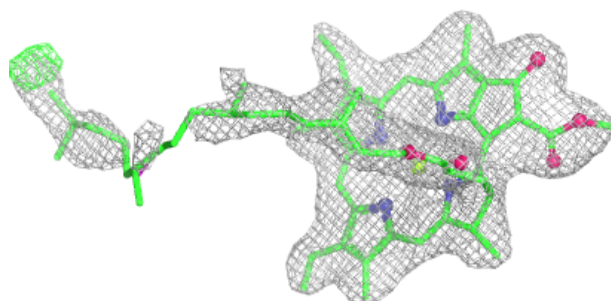
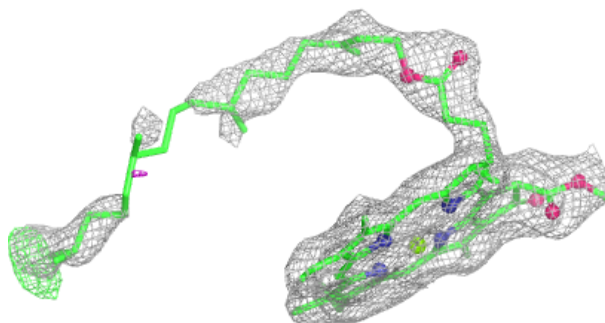
**Electron density around BCR H 102:**

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



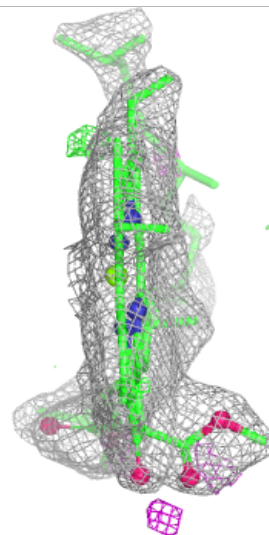
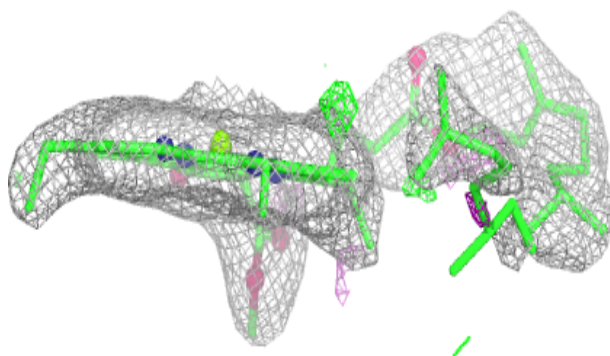
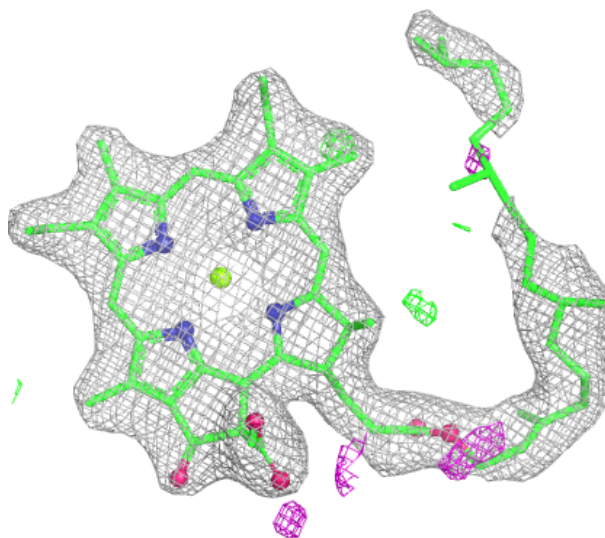
Electron density around CLA C 513:

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



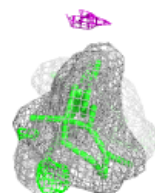
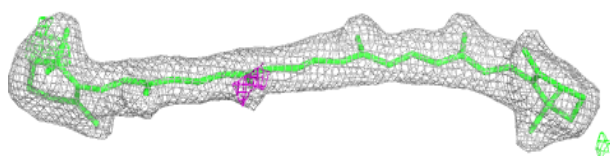
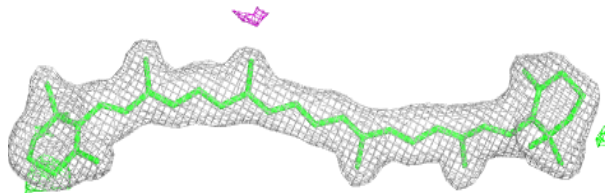
Electron density around CLA c 512:

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

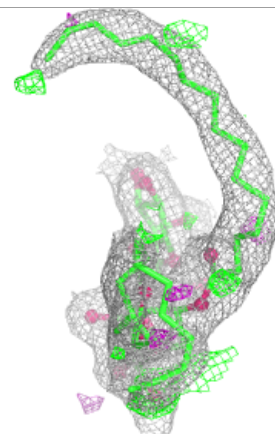
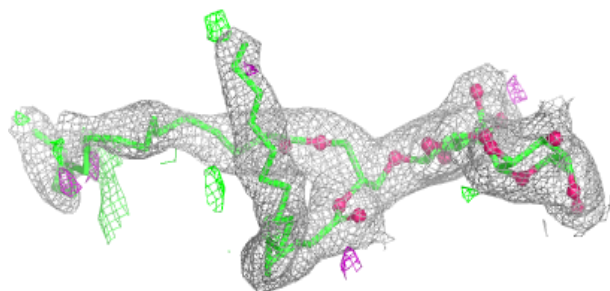
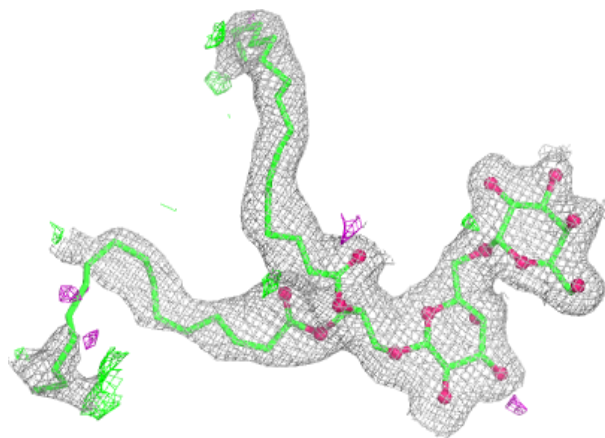


Electron density around BCR B 618:

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

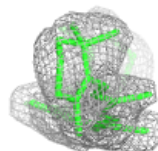
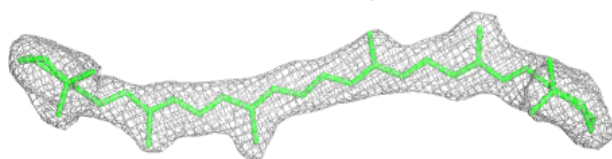
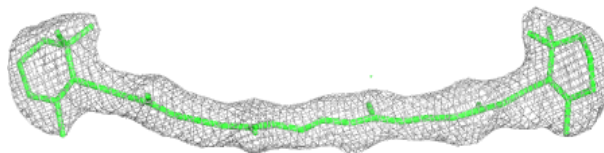
**Electron density around DGD C 517:**

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

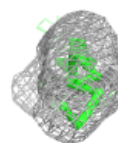
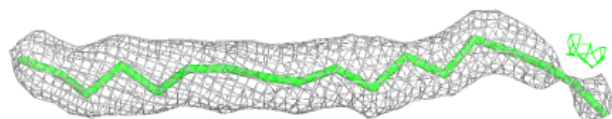
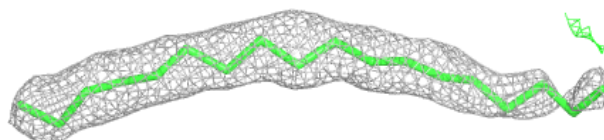


Electron density around BCR k 102:

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

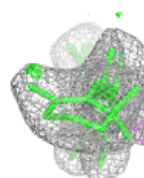
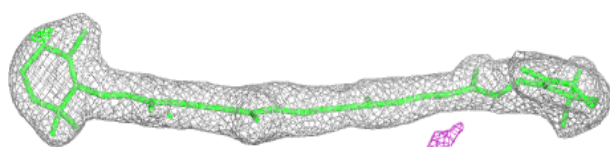
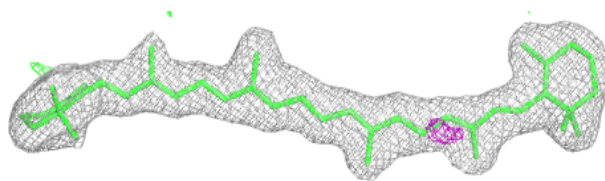
**Electron density around STE l 101:**

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

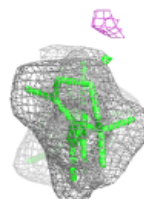
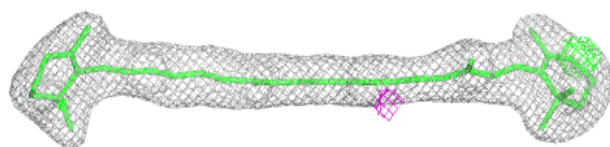
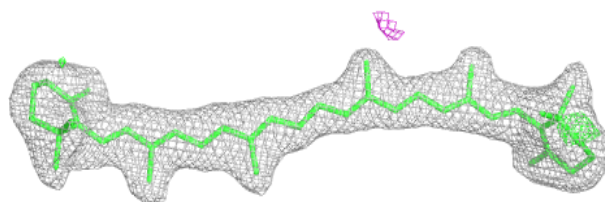


Electron density around BCR b 616:

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

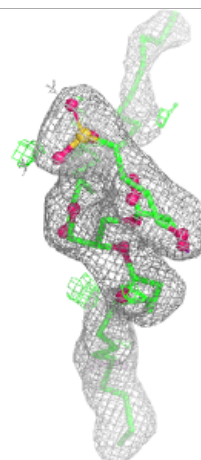
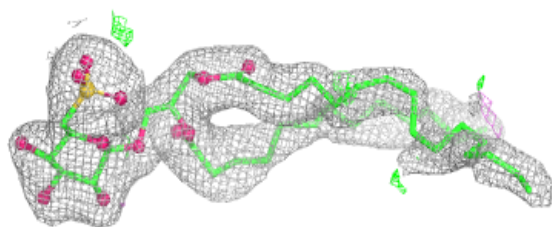
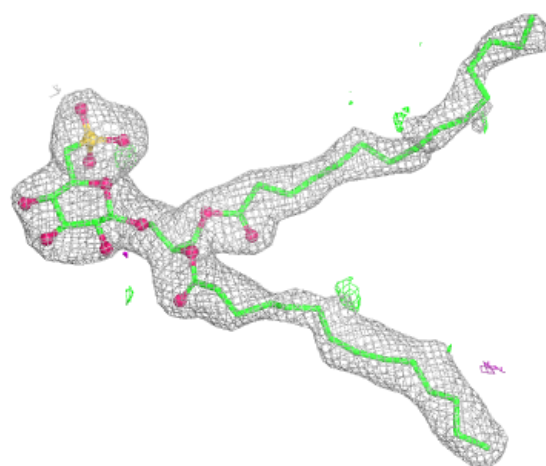
**Electron density around BCR b 617:**

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



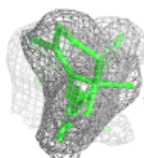
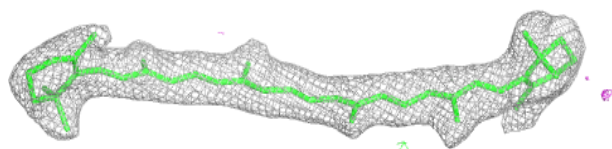
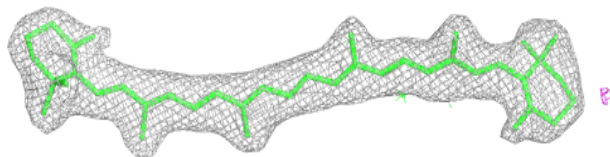
Electron density around SQD A 614:

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

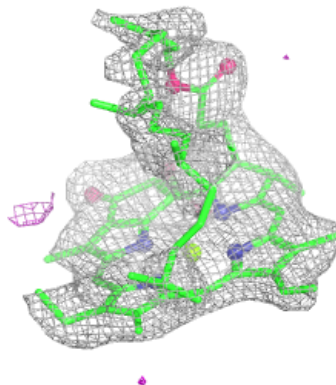
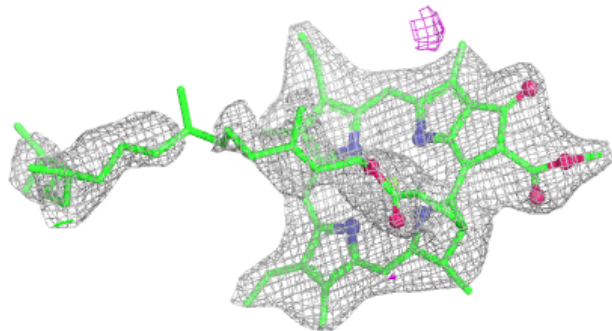
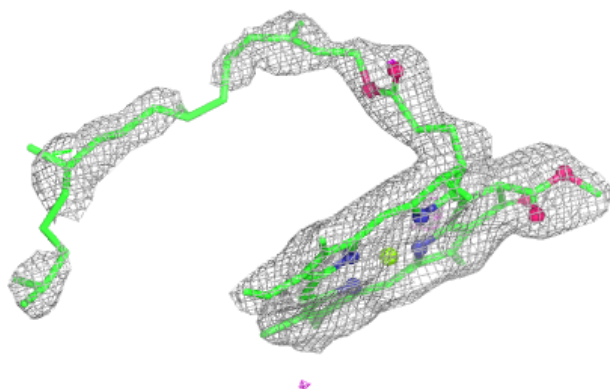


Electron density around BCR b 618:

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

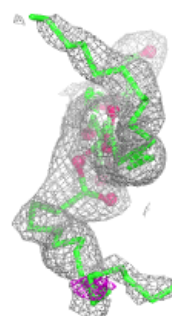
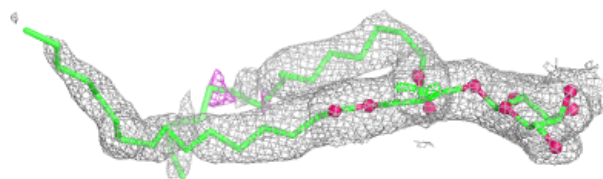
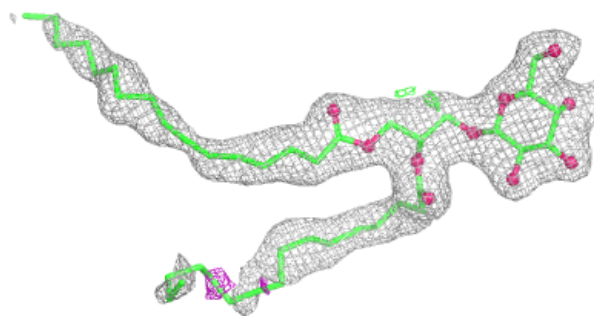
**Electron density around CLA c 513:**

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

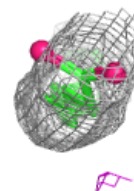
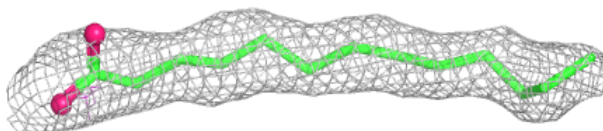
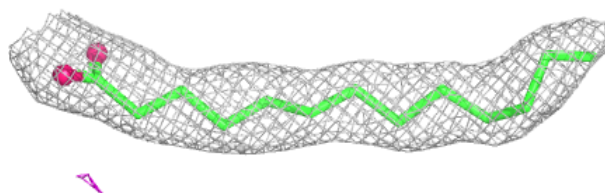


Electron density around LMG D 407:

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

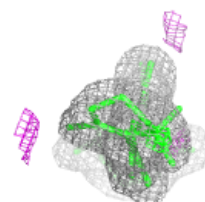
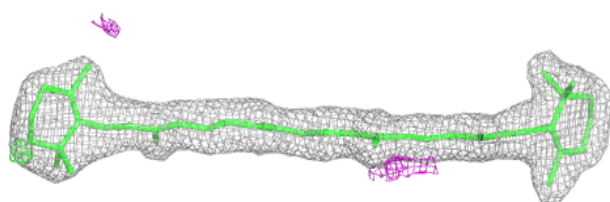
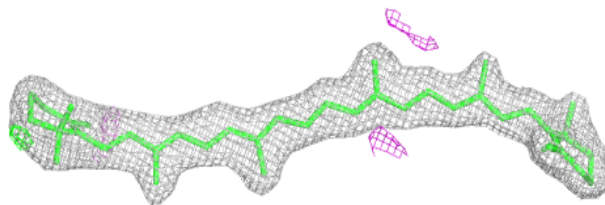
**Electron density around STE M 102:**

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

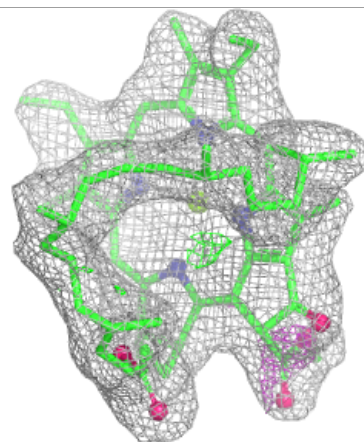
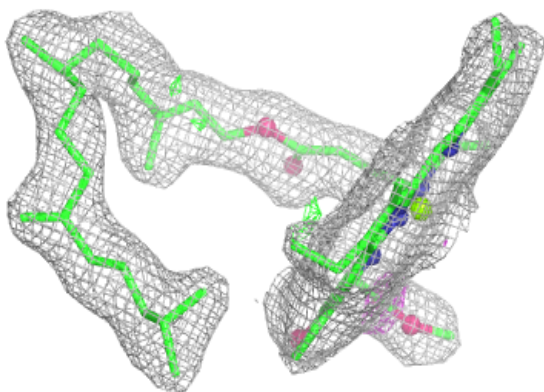
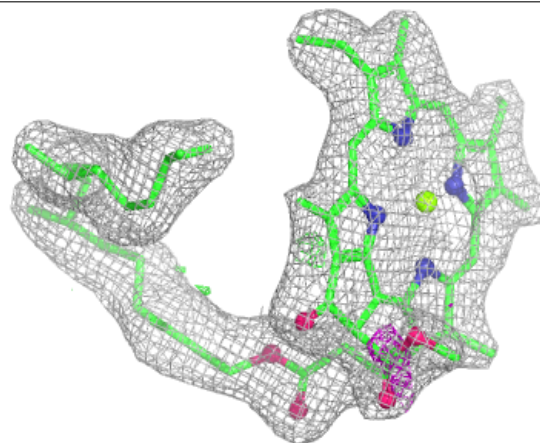


Electron density around BCR C 515:

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

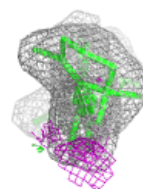
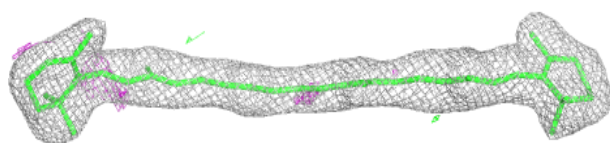
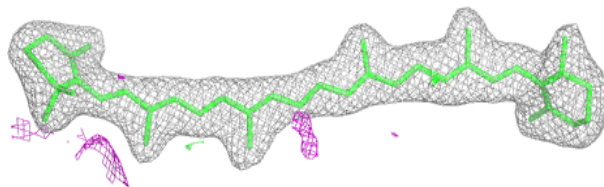
**Electron density around CLA c 503:**

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



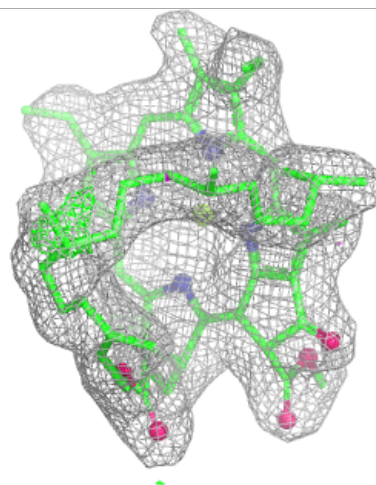
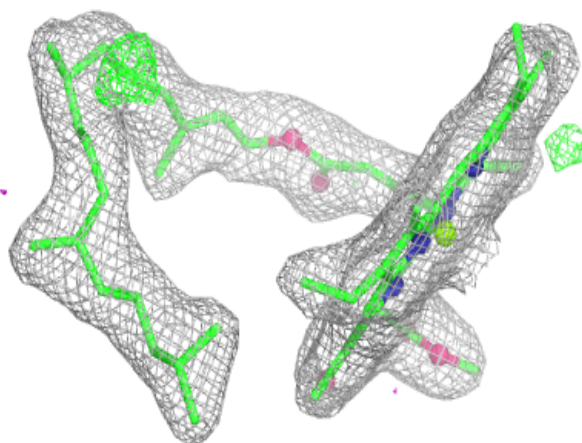
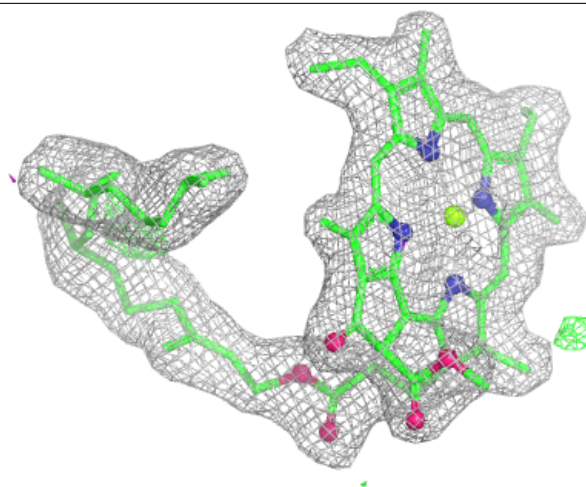
Electron density around BCR B 617:

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



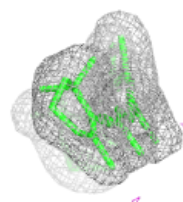
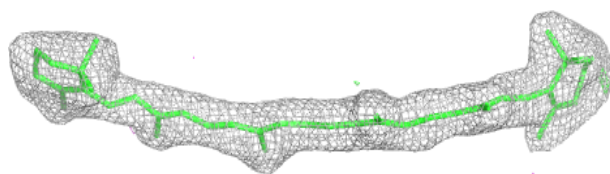
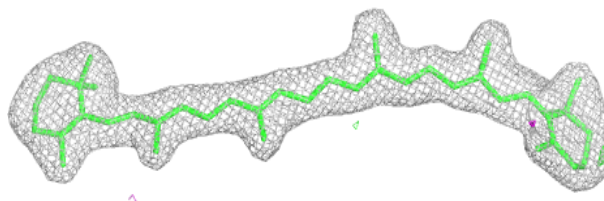
Electron density around CLA C 503:

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

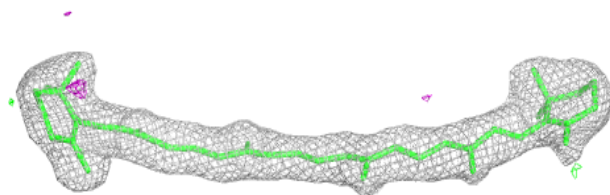
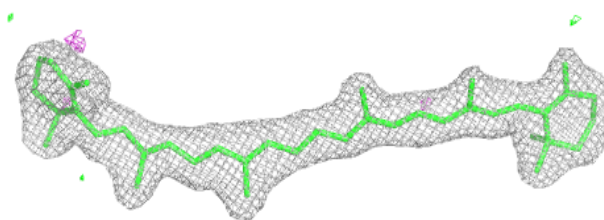


Electron density around BCR t 101:

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

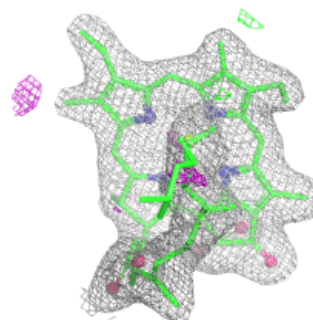
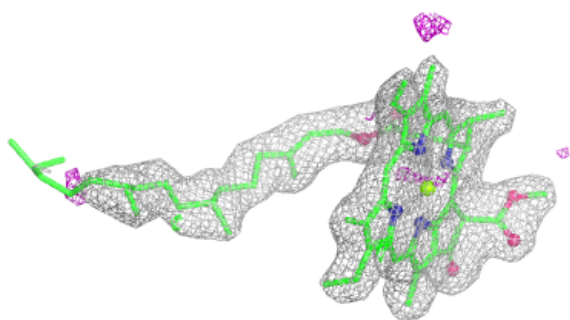
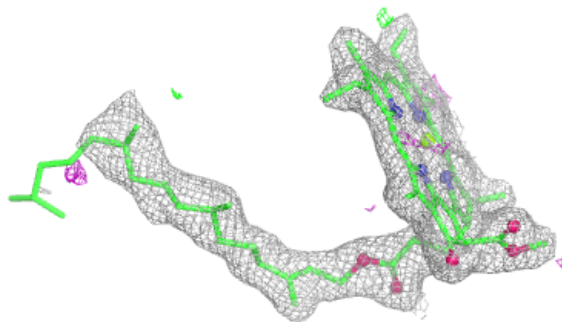
**Electron density around BCR T 101:**

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

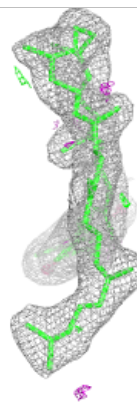
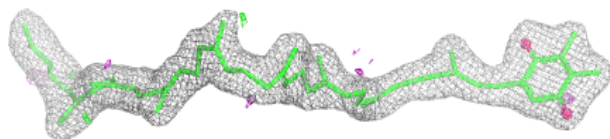
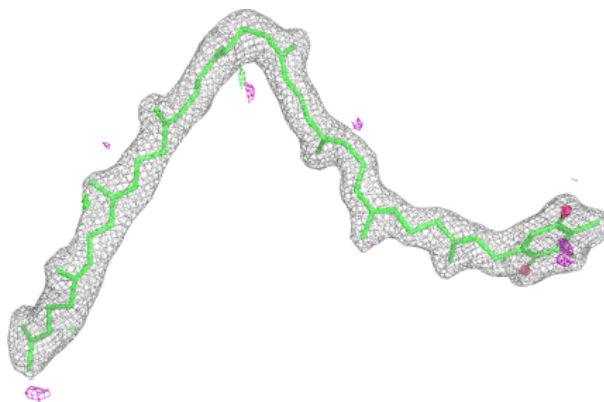


Electron density around CLA C 508:

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

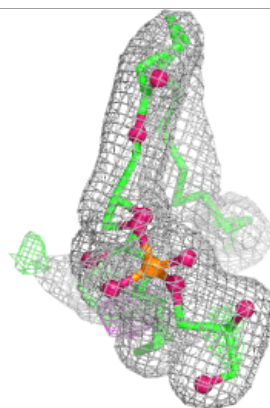
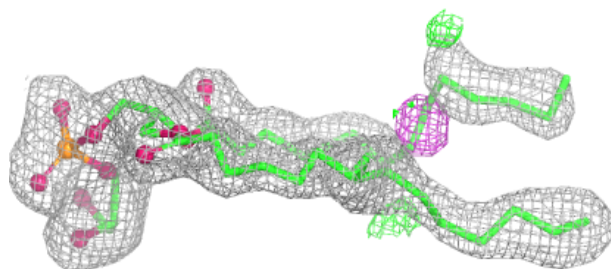
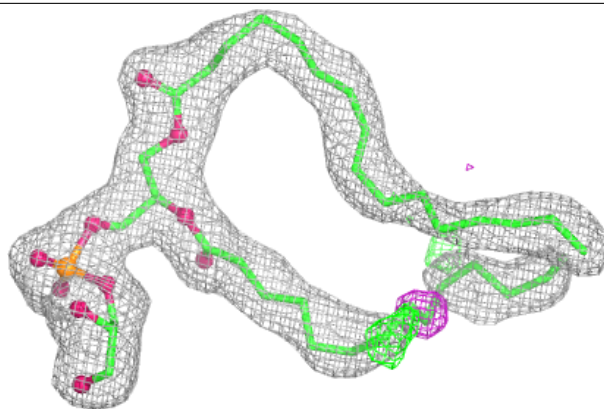
**Electron density around PL9 D 406:**

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

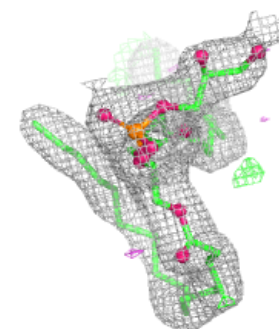
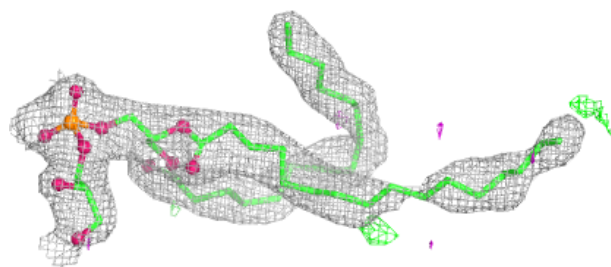
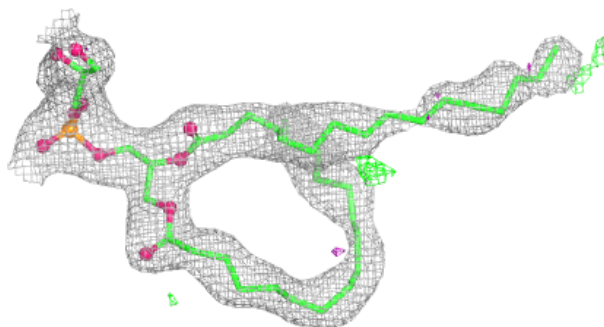


Electron density around LHG D 409:

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

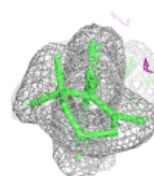
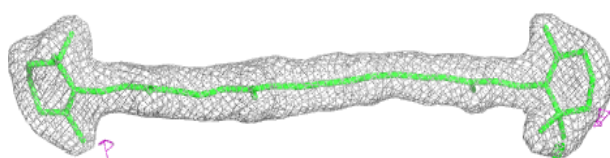
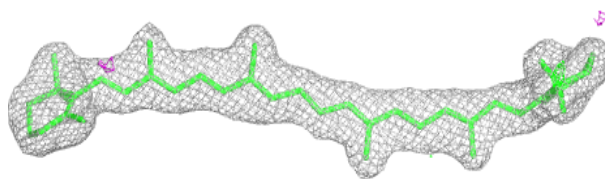
**Electron density around LHG d 407:**

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

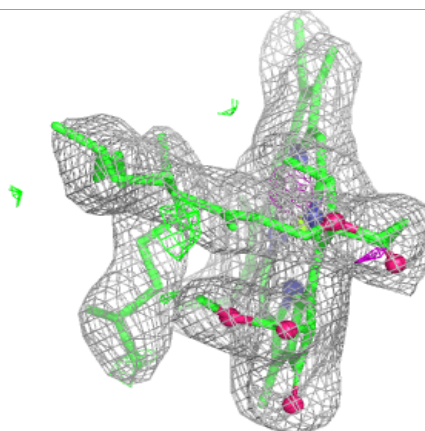
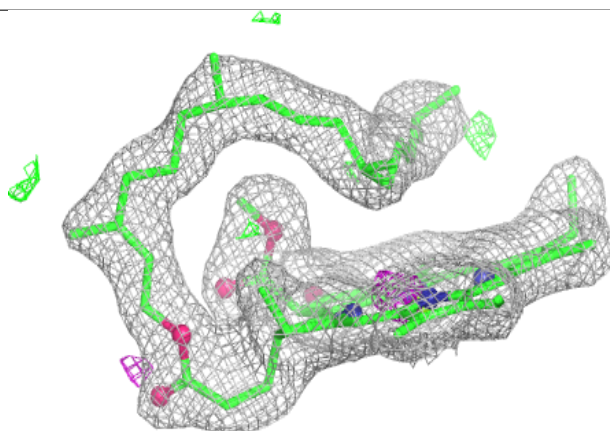
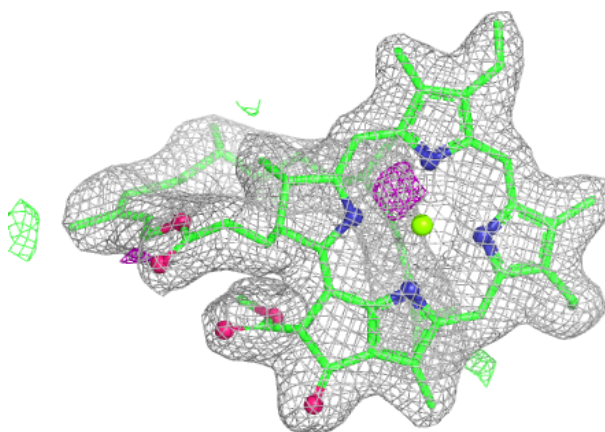


Electron density around BCR A 610:

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

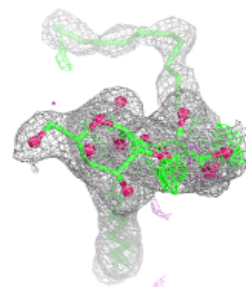
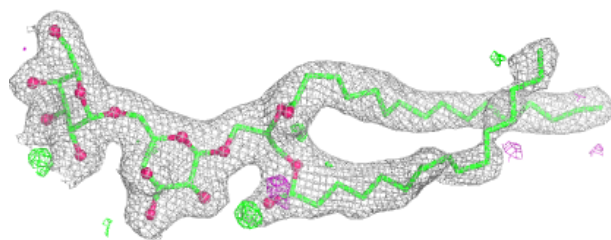
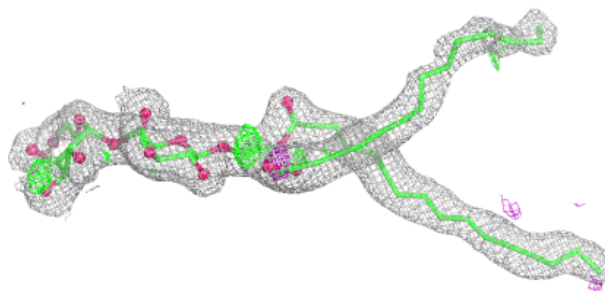
**Electron density around CLA C 510:**

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

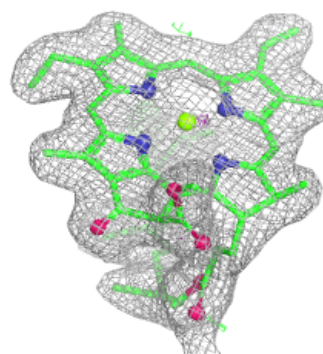
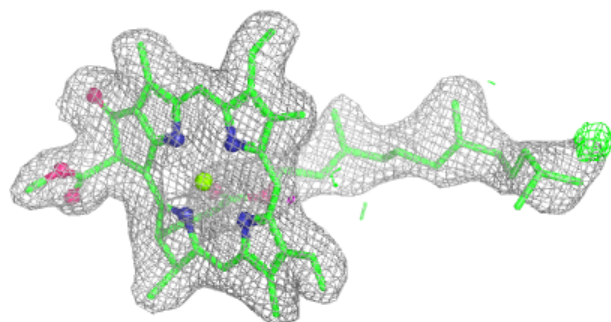
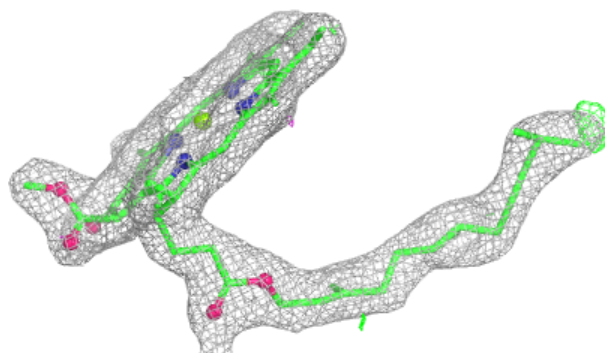


Electron density around DGD C 516:

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

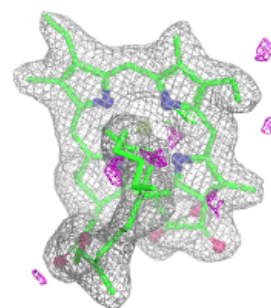
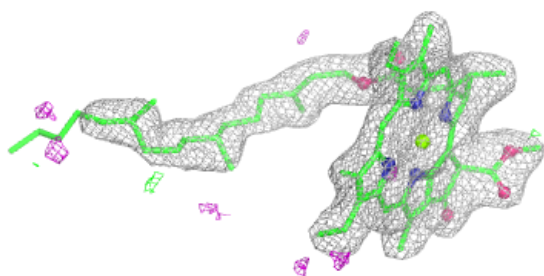
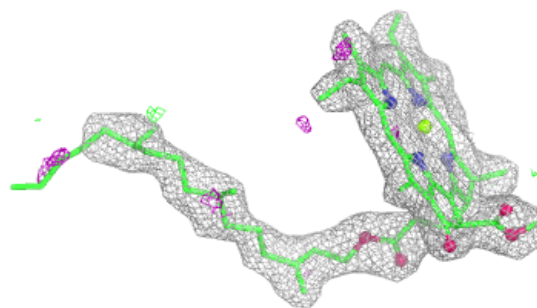
**Electron density around CLA c 504:**

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



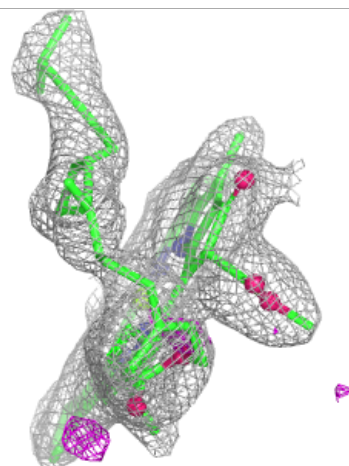
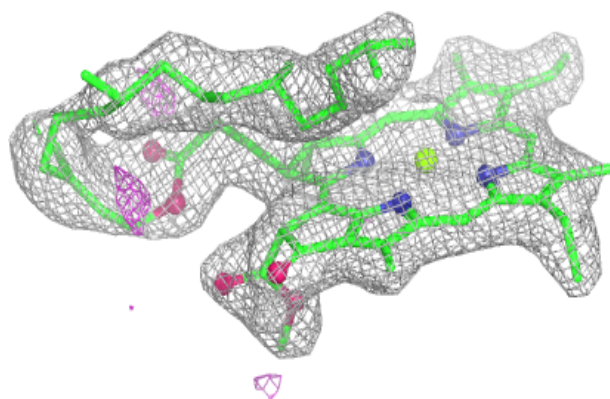
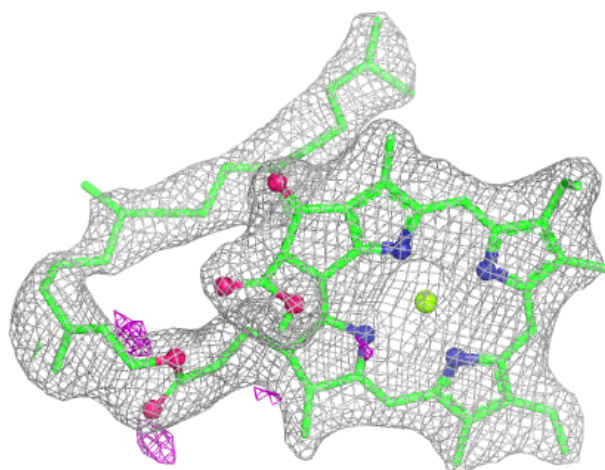
Electron density around CLA c 508:

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



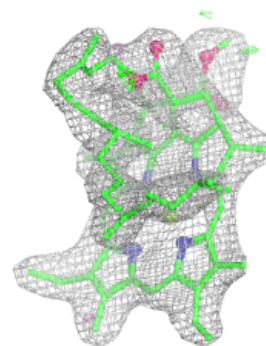
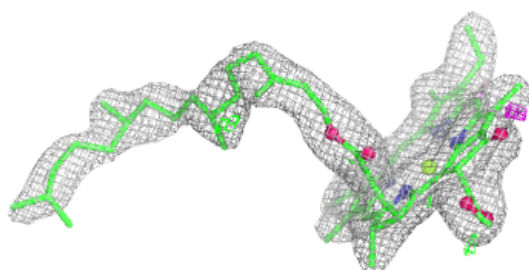
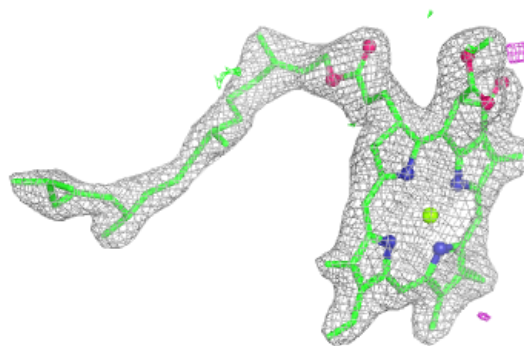
Electron density around CLA c 509:

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

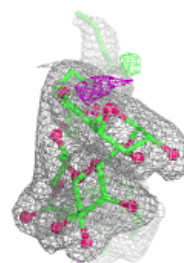
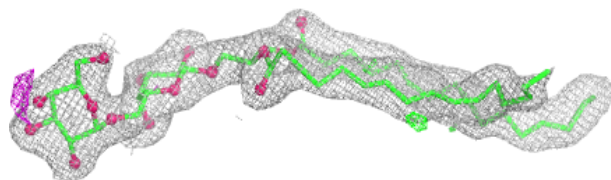
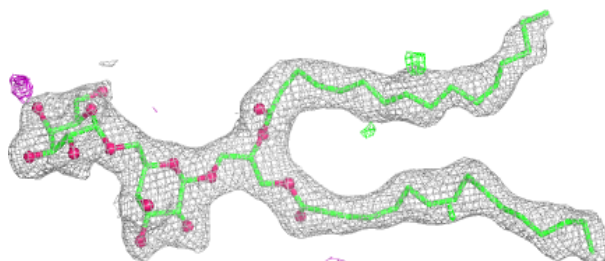


Electron density around CLA c 511:

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

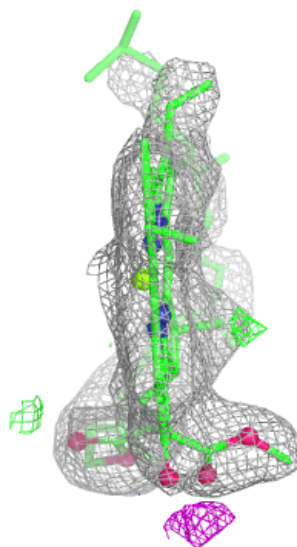
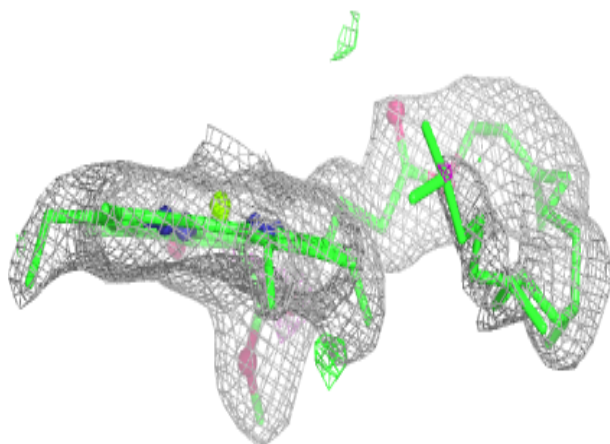
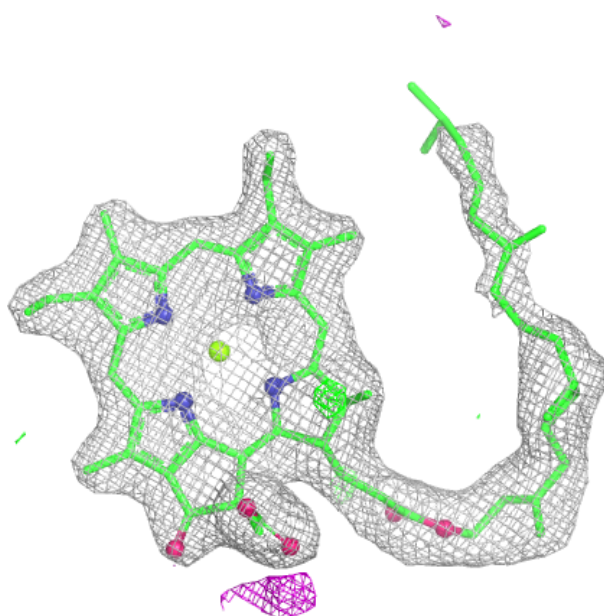
**Electron density around DGD c 518:**

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



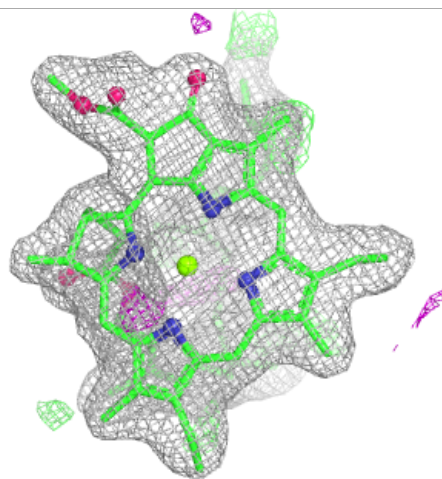
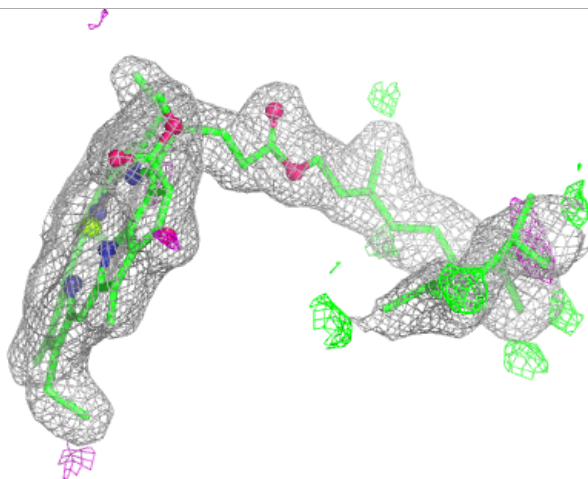
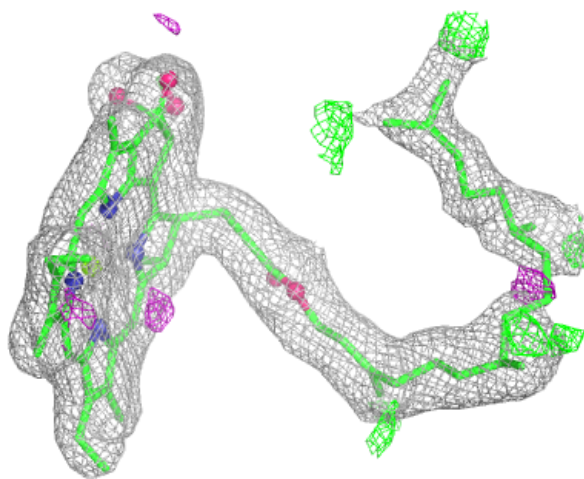
Electron density around CLA C 512:

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



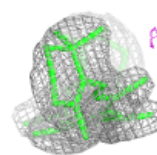
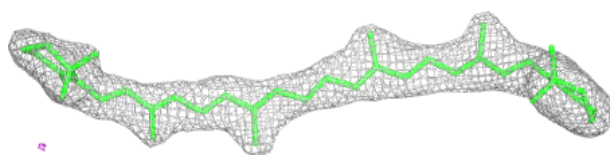
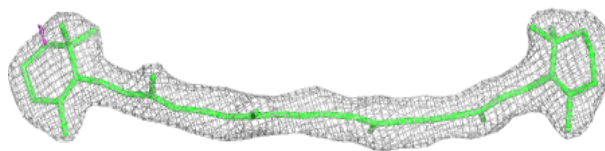
Electron density around CLA B 605:

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

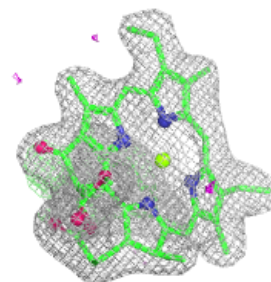
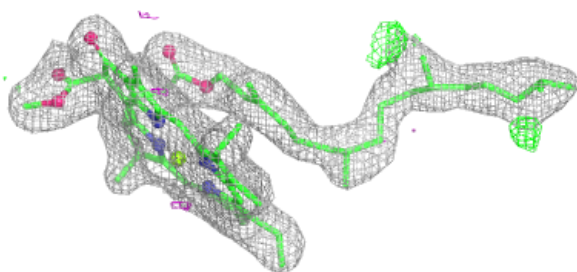
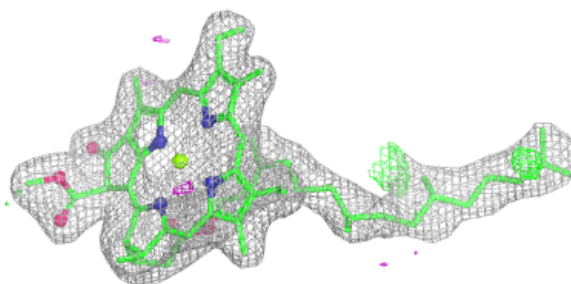


Electron density around BCR K 102:

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

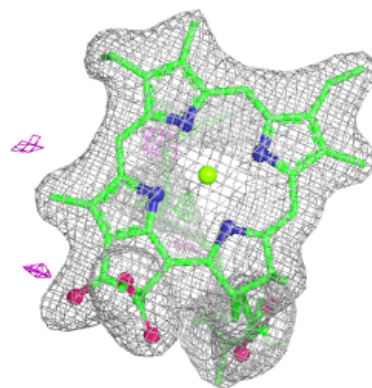
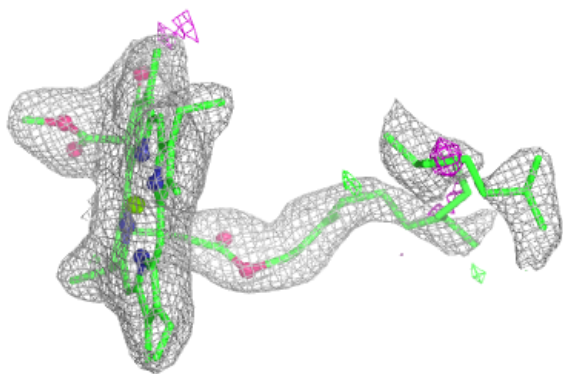
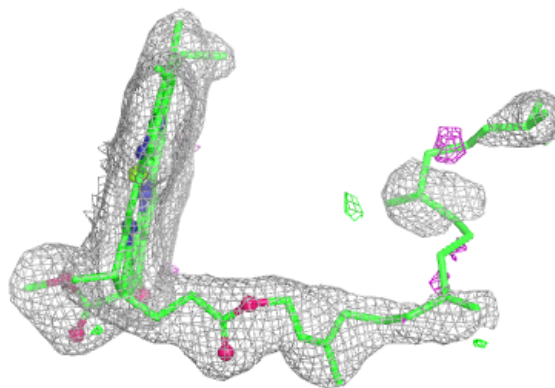
**Electron density around CLA c 505:**

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

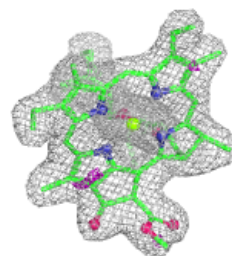
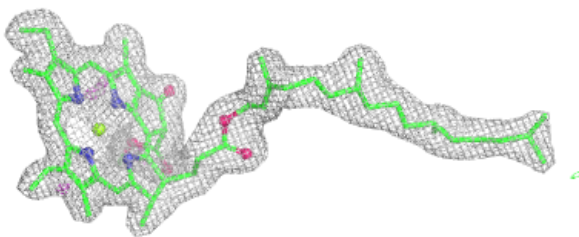
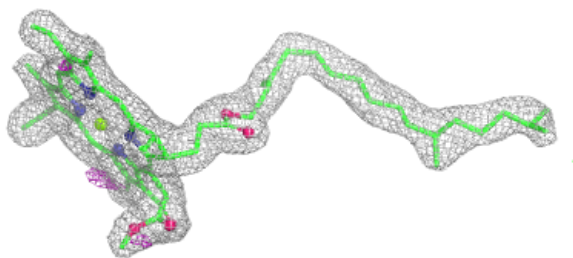


Electron density around CLA c 506:

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

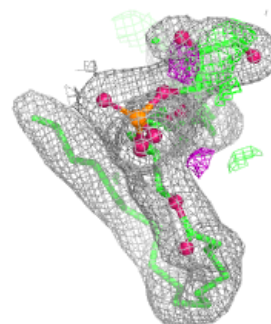
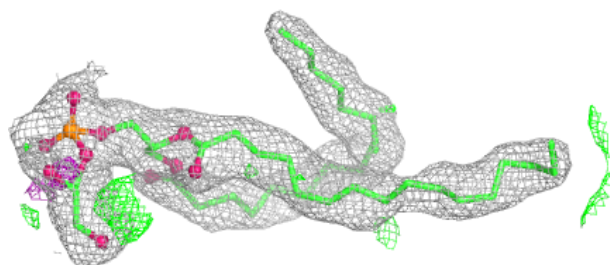
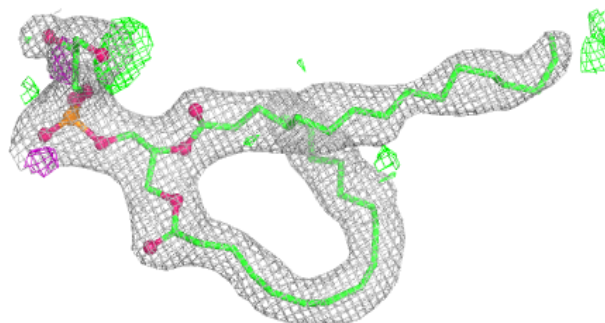
**Electron density around CLA C 502:**

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



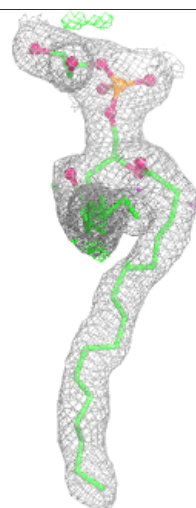
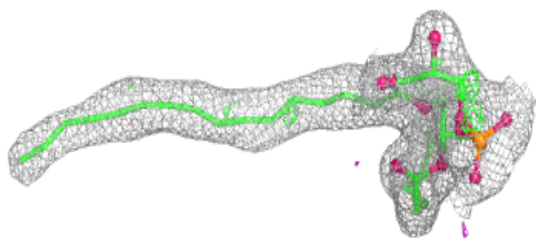
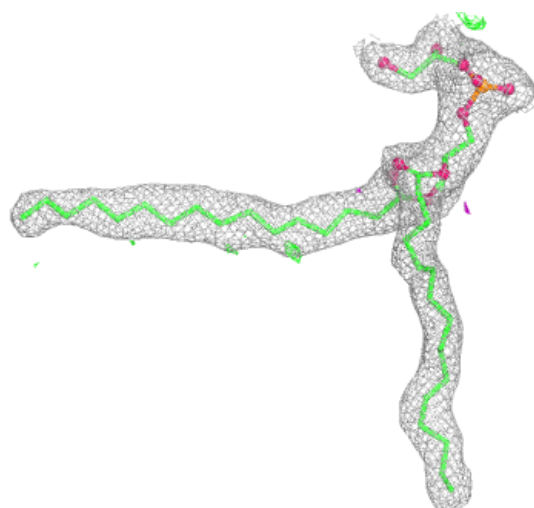
Electron density around LHG D 411:

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



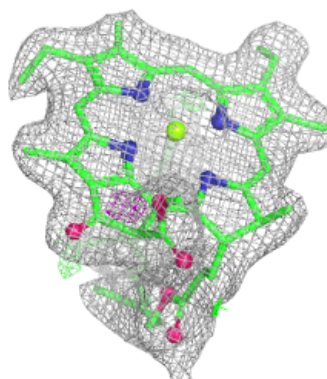
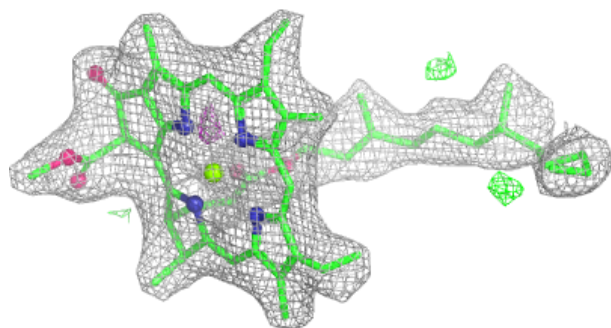
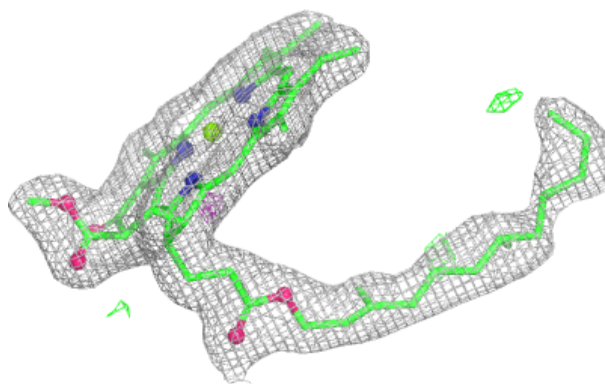
Electron density around LHG b 623:

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

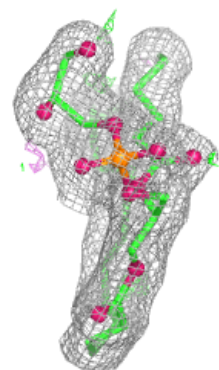
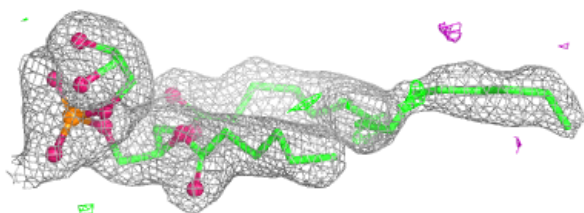
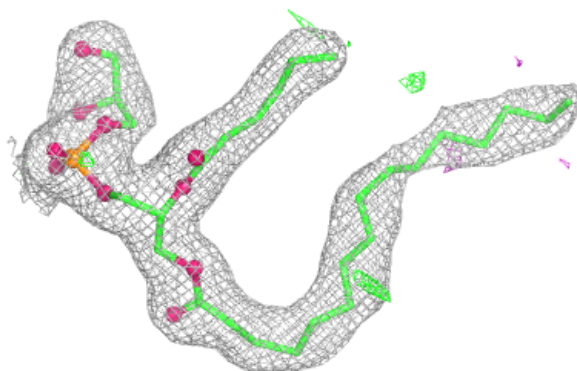


Electron density around CLA C 504:

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

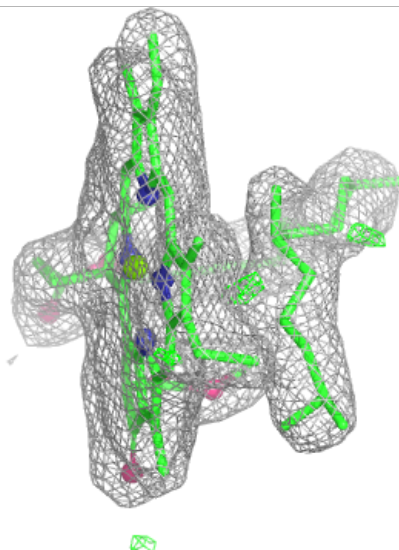
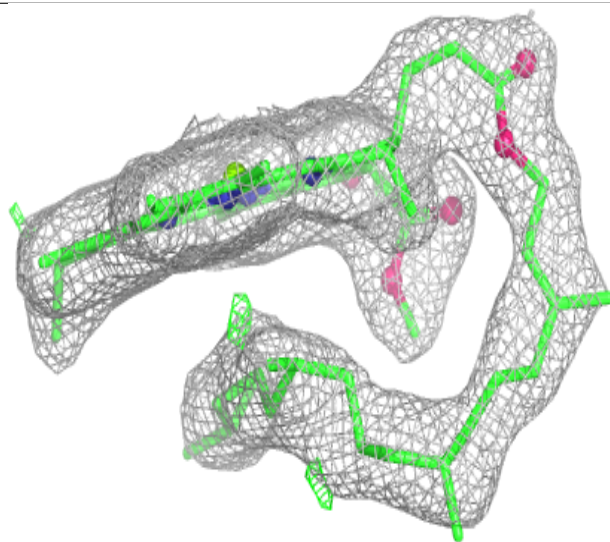
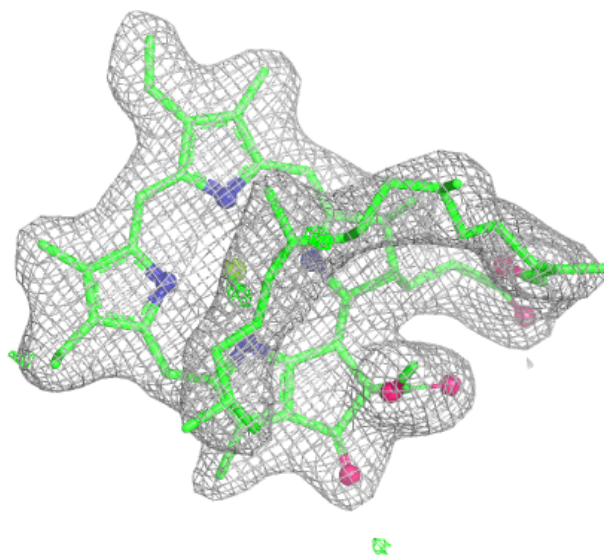
**Electron density around LHG d 409:**

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



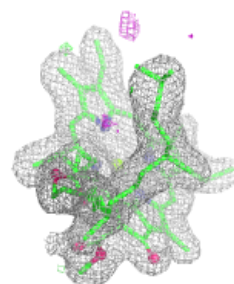
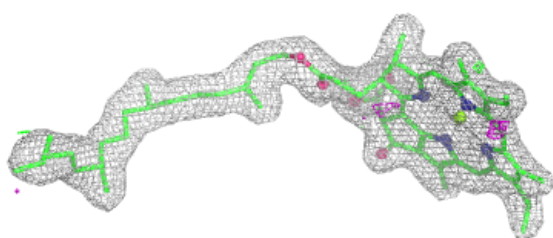
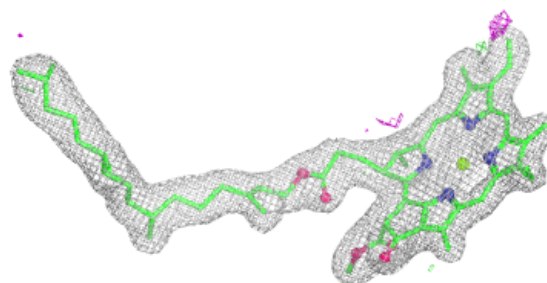
Electron density around CLA c 510:

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

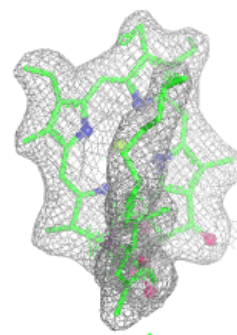
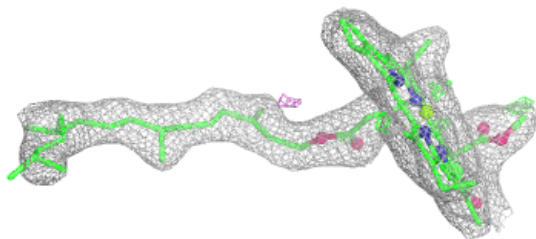
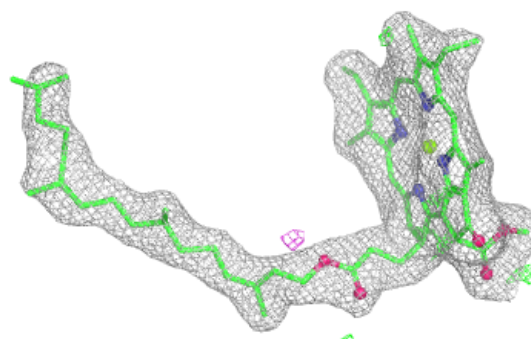


Electron density around CLA a 606:

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

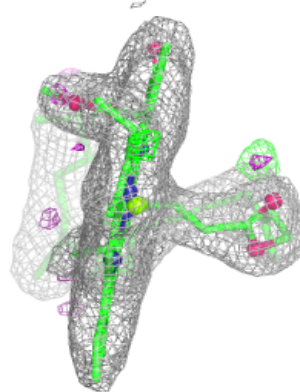
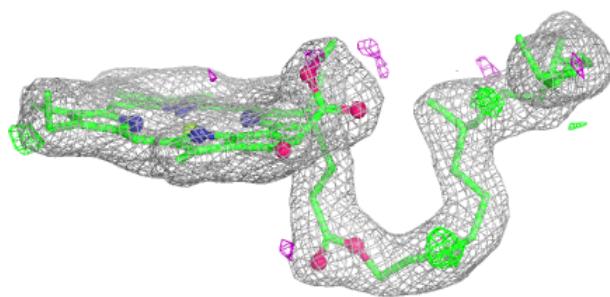
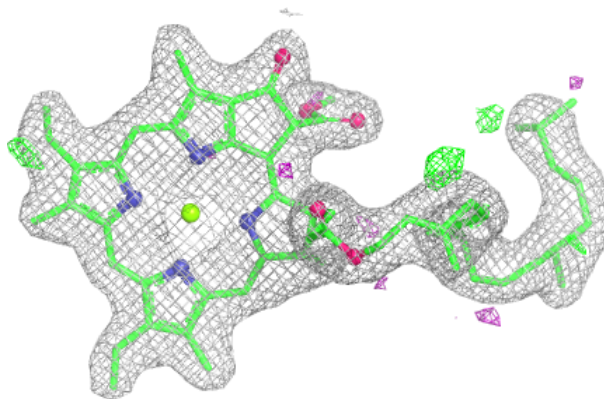
**Electron density around CLA b 608:**

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

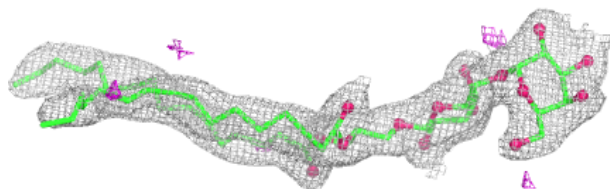
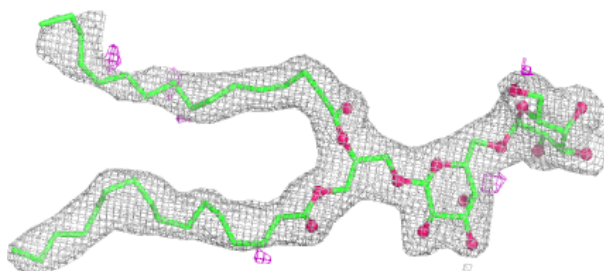


Electron density around CLA b 611:

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

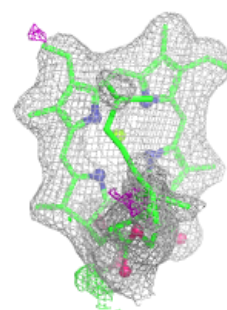
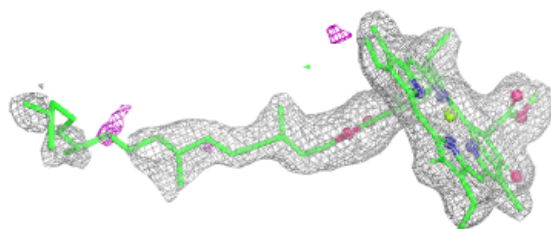
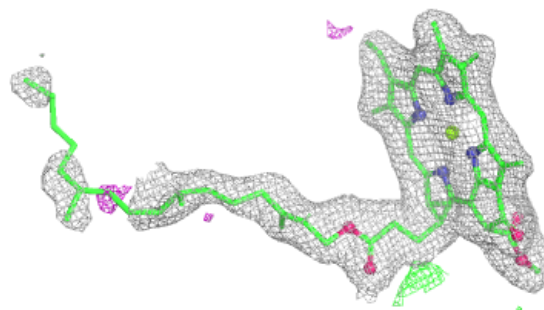
**Electron density around DGD C 518:**

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

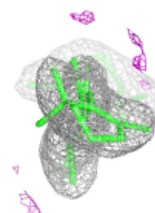
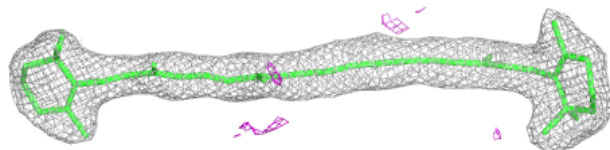
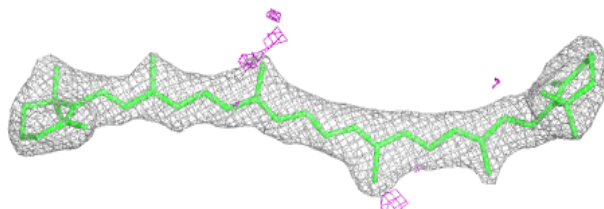


Electron density around CLA d 404:

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

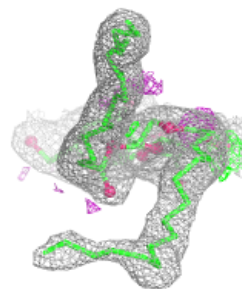
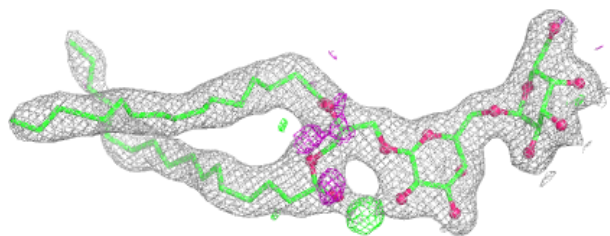
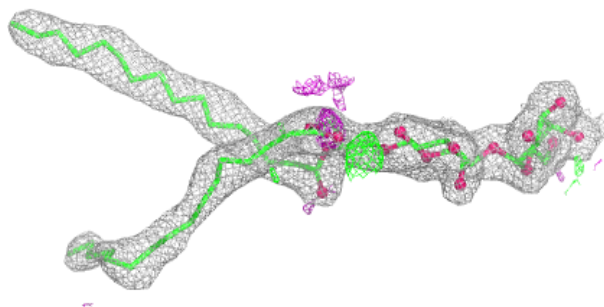
**Electron density around BCR c 515:**

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

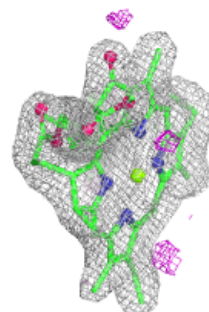
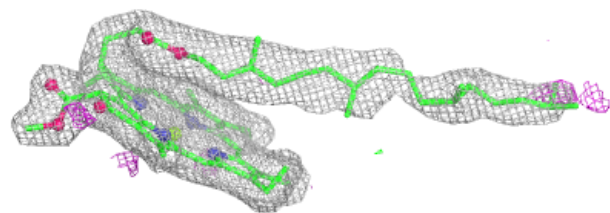
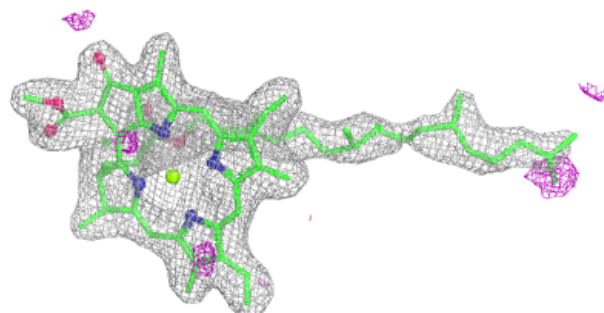


Electron density around DGD c 516:

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

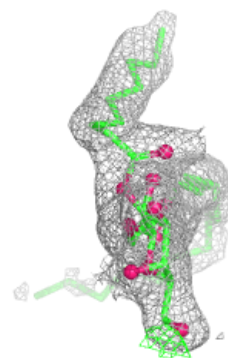
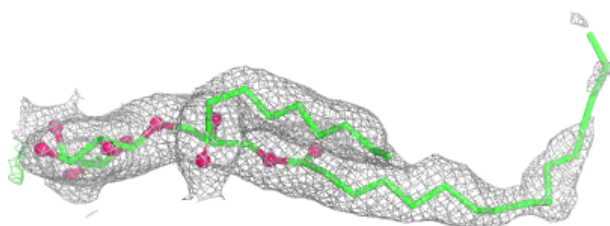
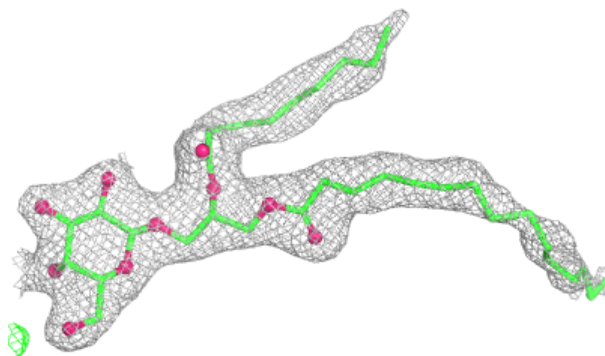
**Electron density around CLA b 613:**

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

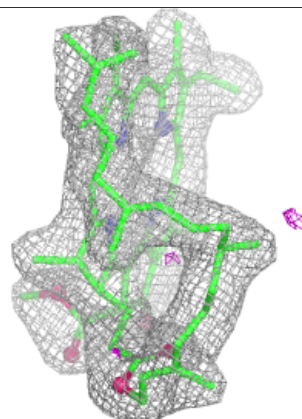
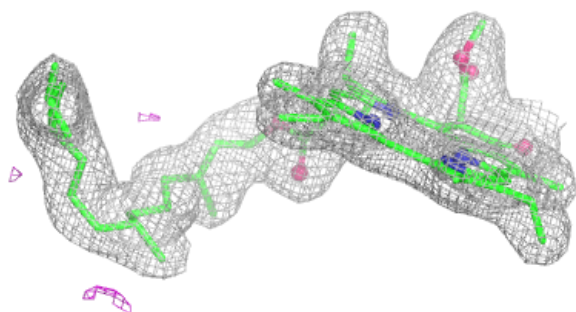
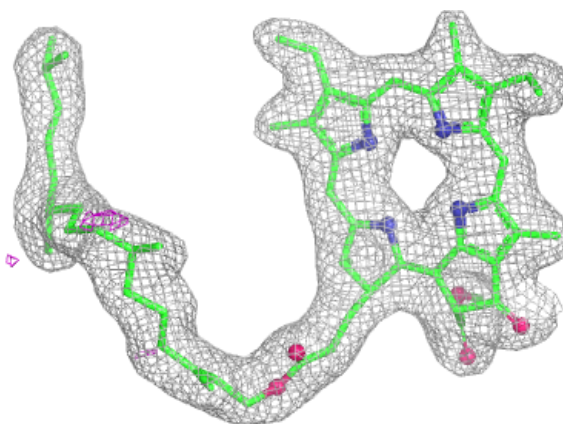


Electron density around LMG d 411:

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

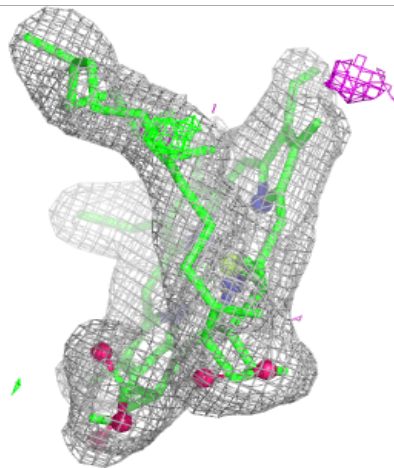
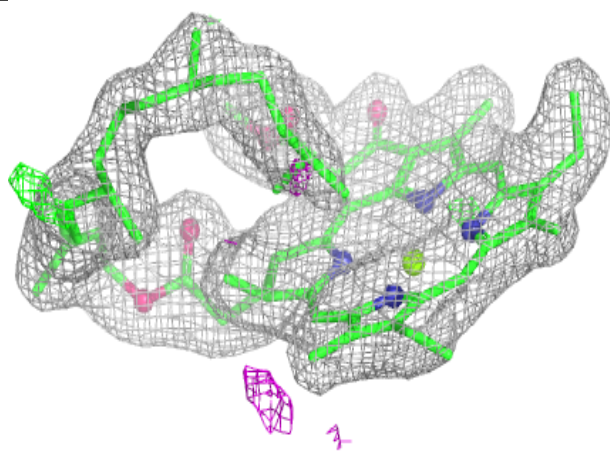
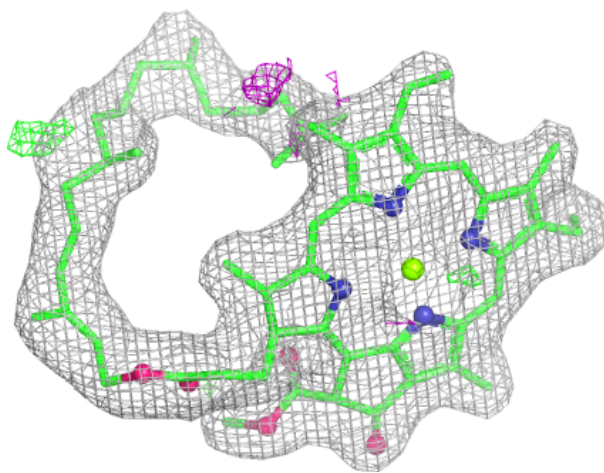
**Electron density around PHO d 402:**

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



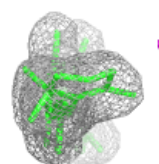
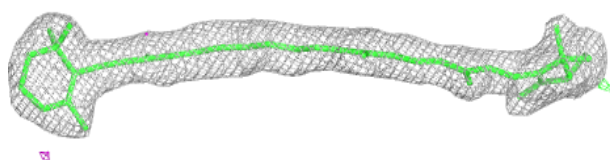
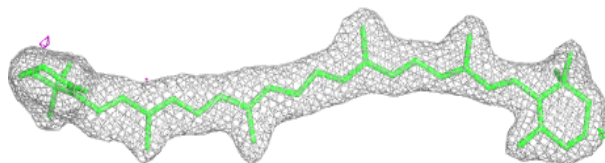
Electron density around CLA b 614:

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



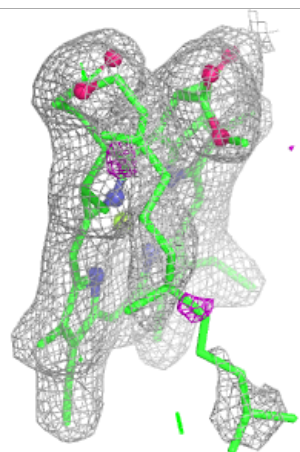
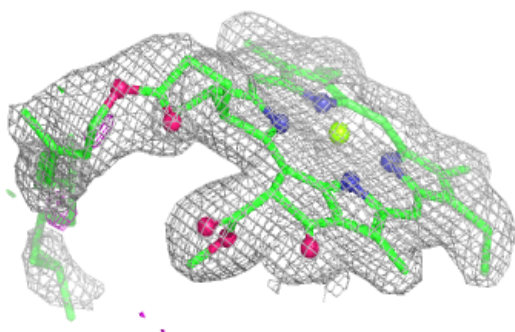
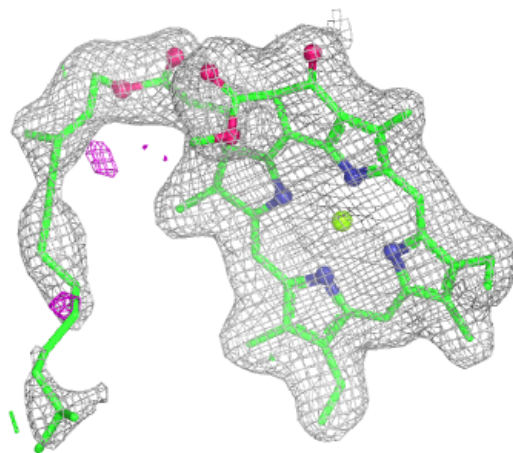
Electron density around BCR B 616:

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



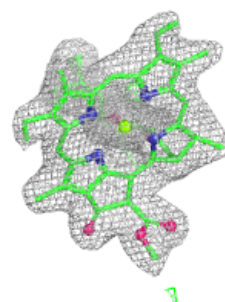
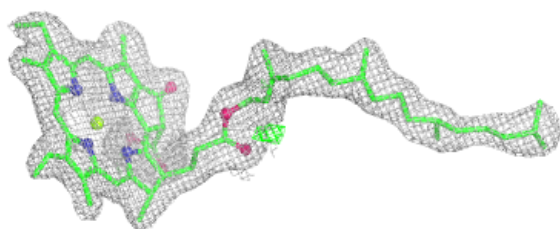
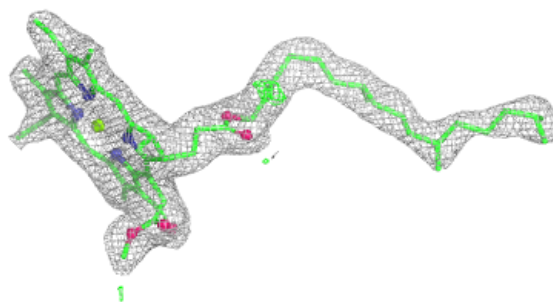
Electron density around CLA b 615:

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

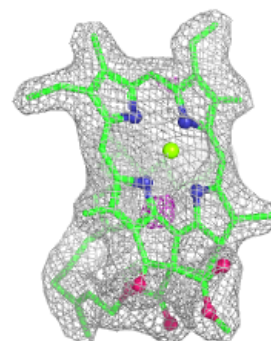
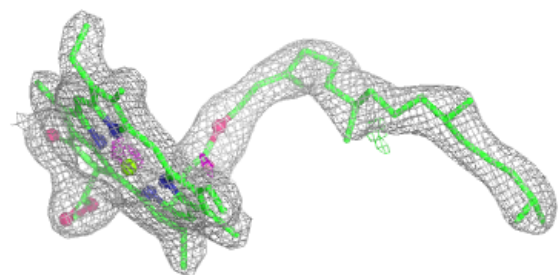
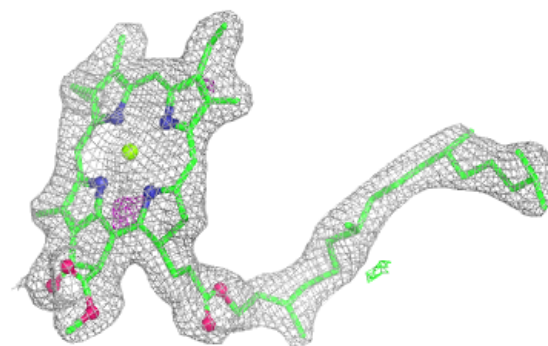


Electron density around CLA c 502:

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

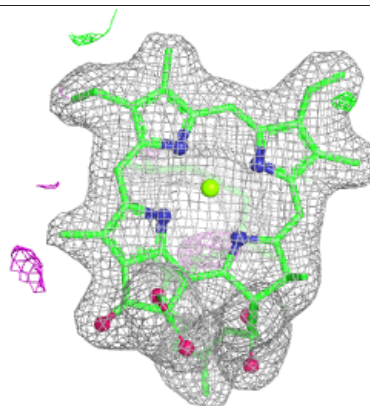
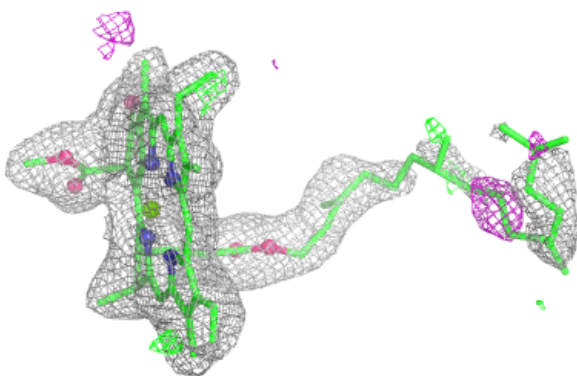
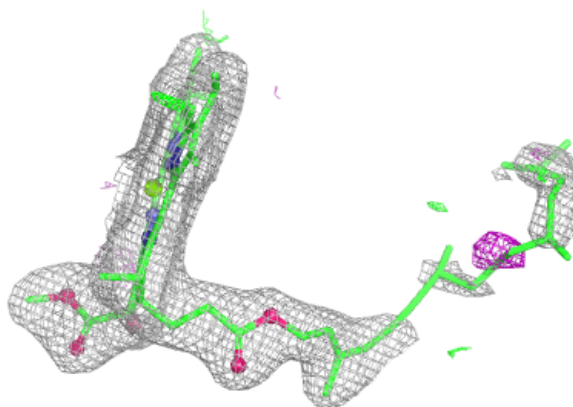
**Electron density around CLA C 511:**

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

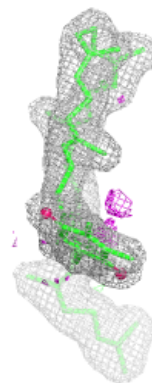
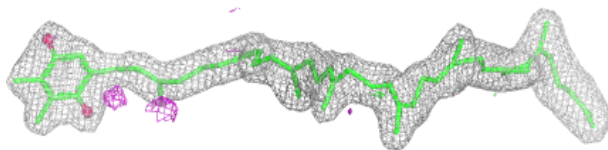
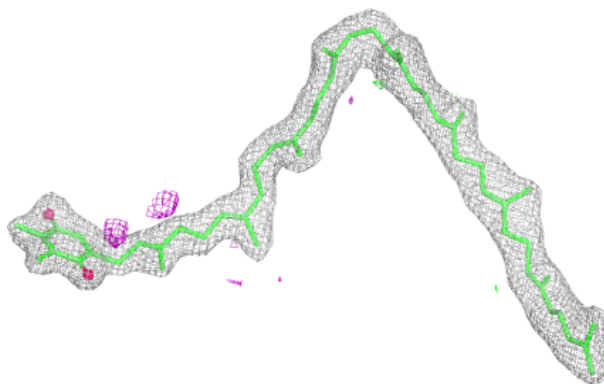


Electron density around CLA C 506:

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

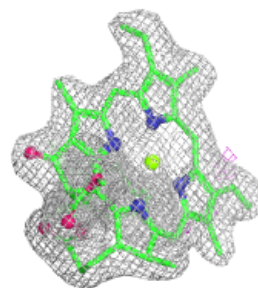
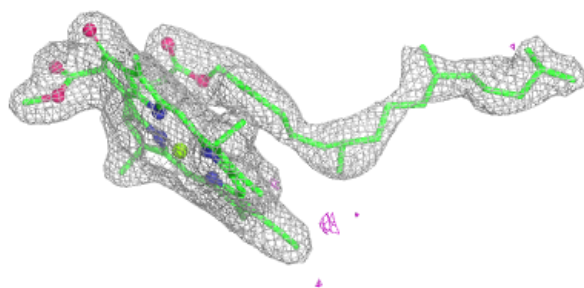
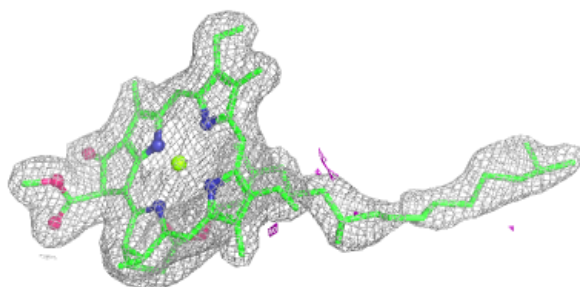
**Electron density around PL9 d 406:**

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

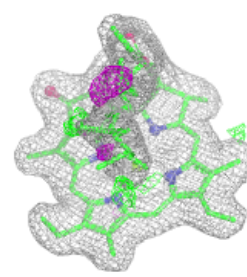
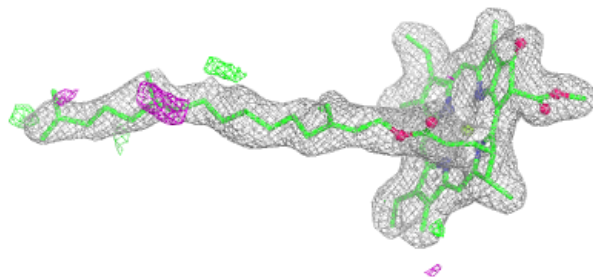
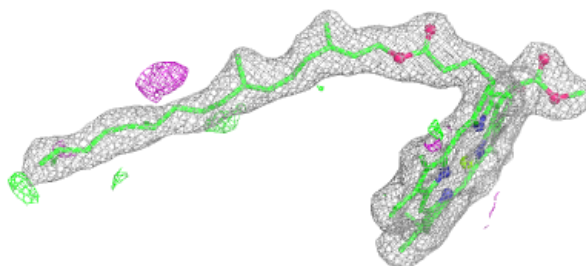


Electron density around CLA C 505:

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

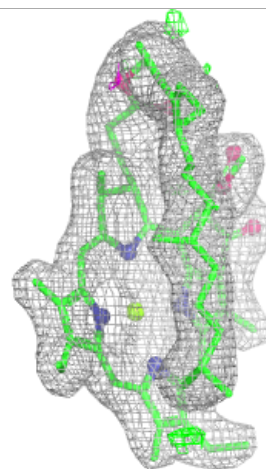
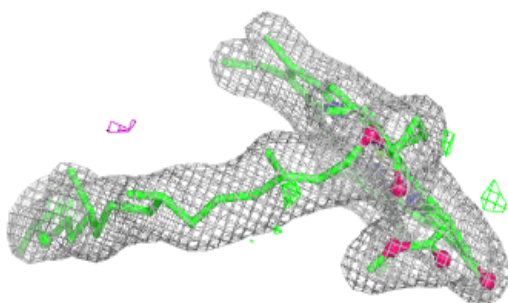
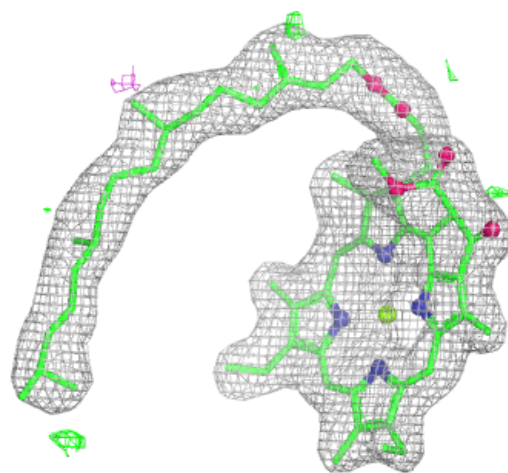
**Electron density around CLA B 606:**

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



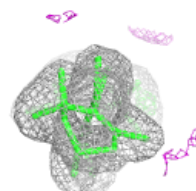
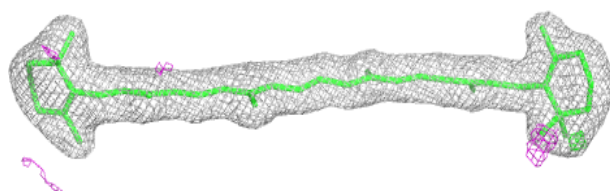
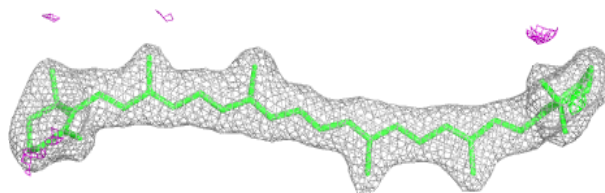
Electron density around CLA C 507:

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

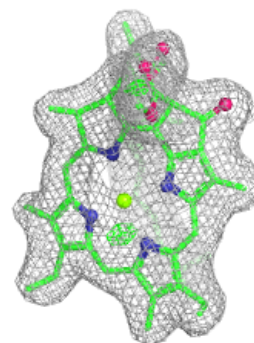
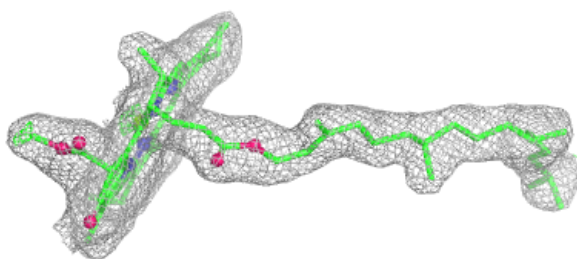
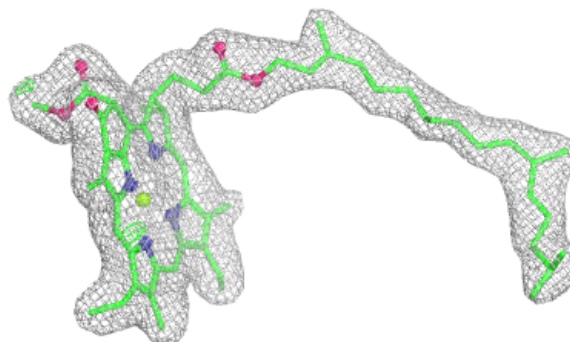


Electron density around BCR a 610:

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

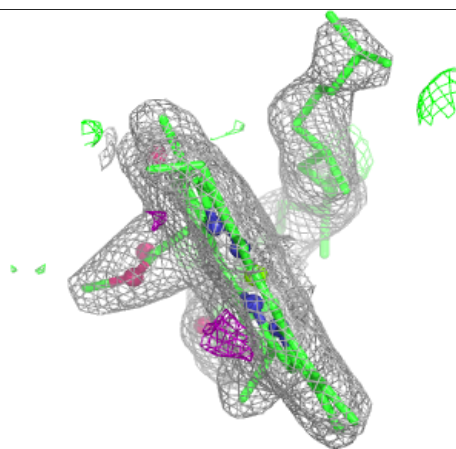
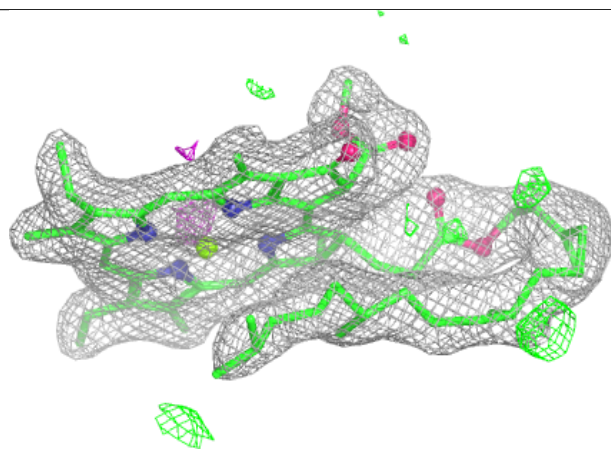
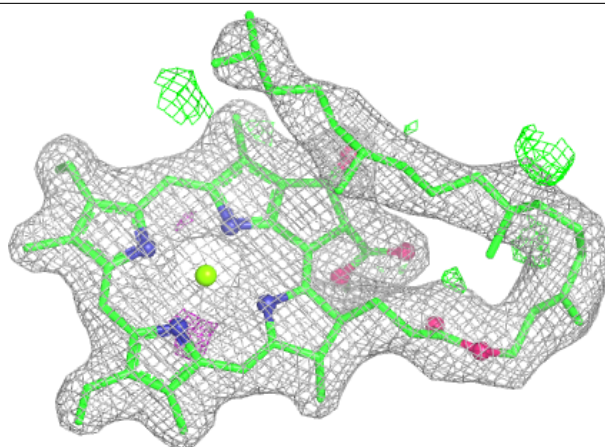
**Electron density around CLA B 608:**

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



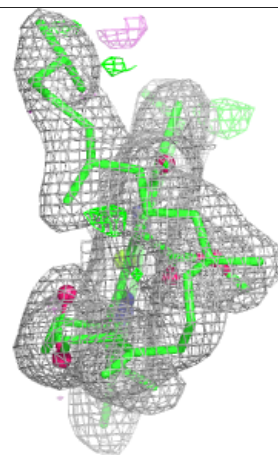
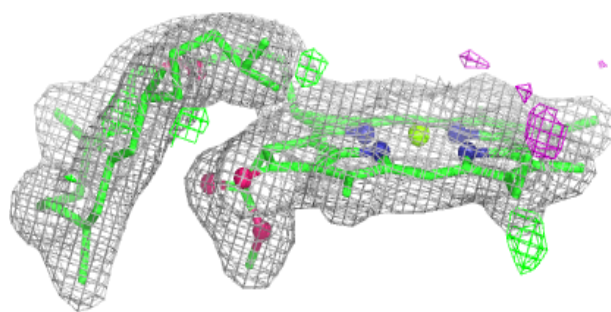
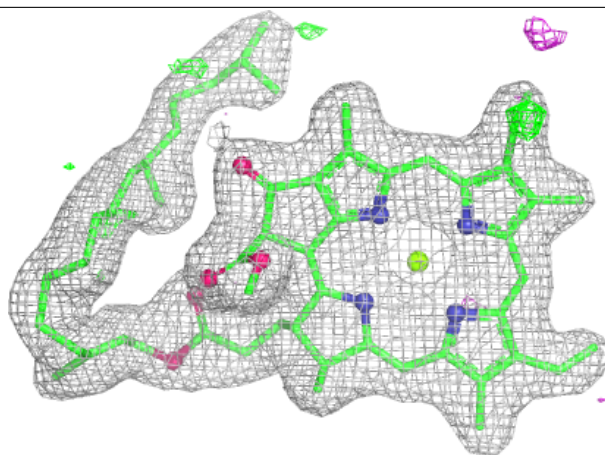
Electron density around CLA C 509:

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



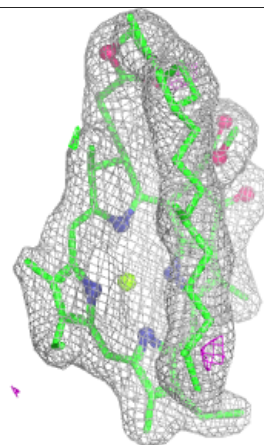
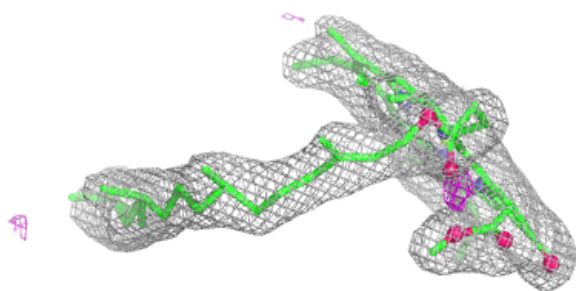
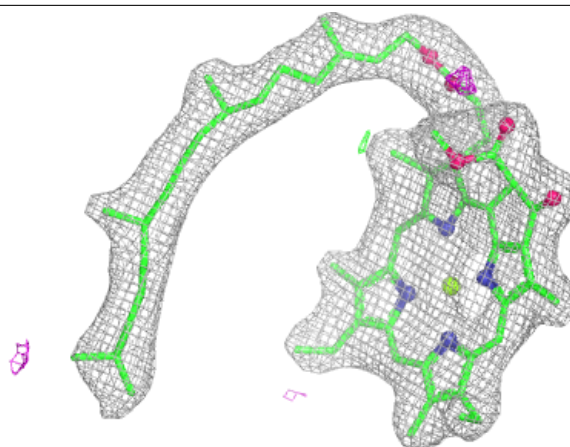
Electron density around CLA B 609:

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



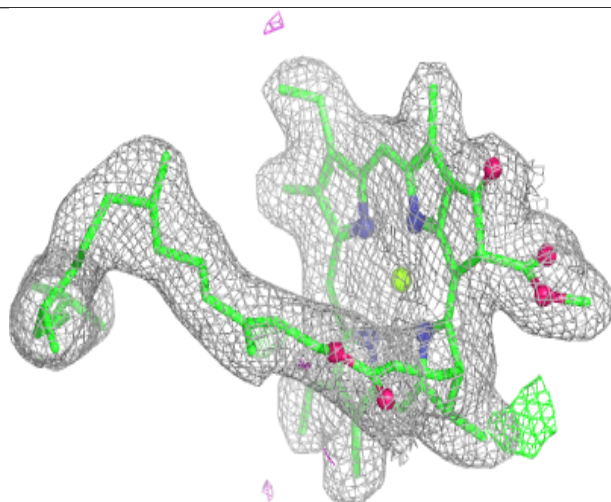
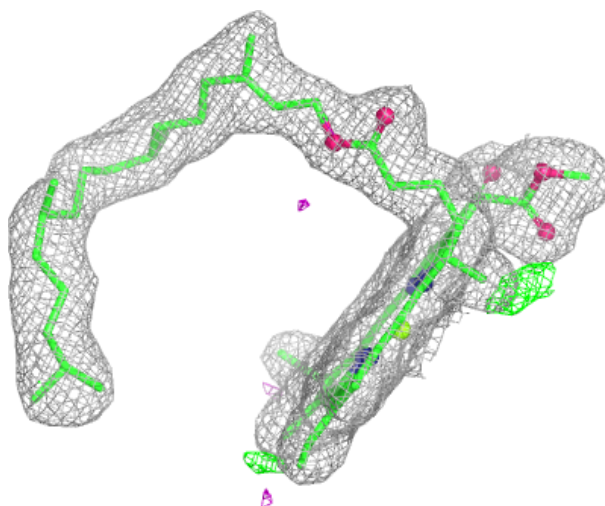
Electron density around CLA c 507:

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



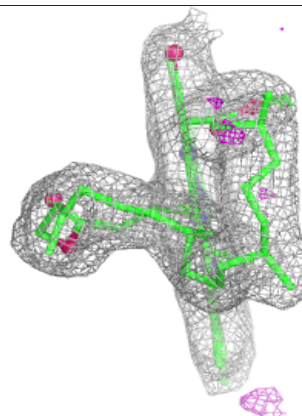
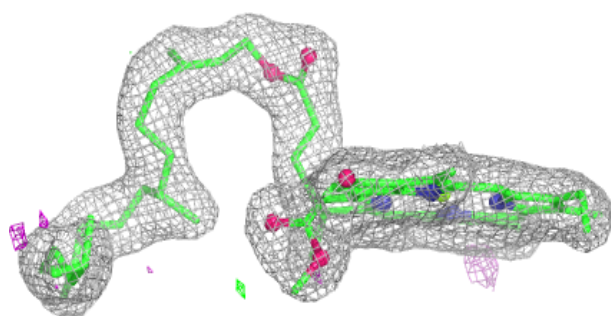
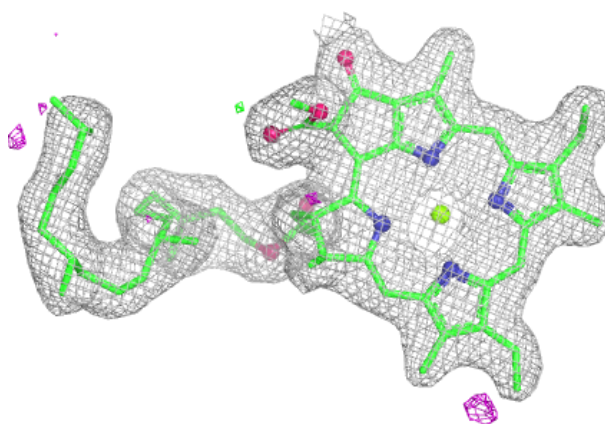
Electron density around CLA B 610:

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

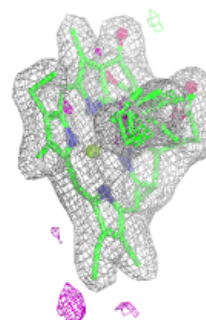
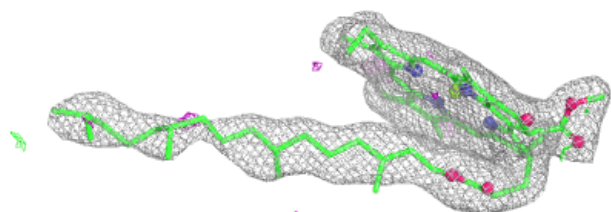
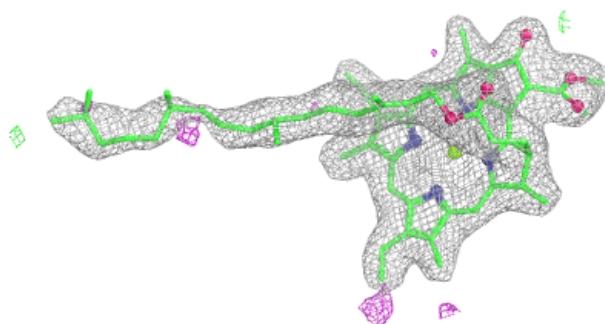


Electron density around CLA B 611:

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

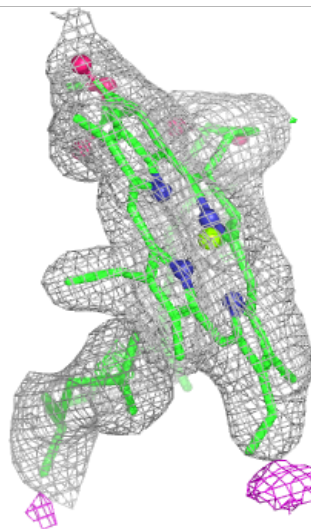
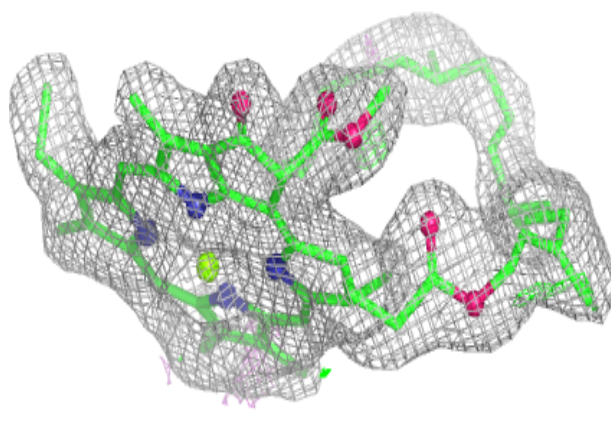
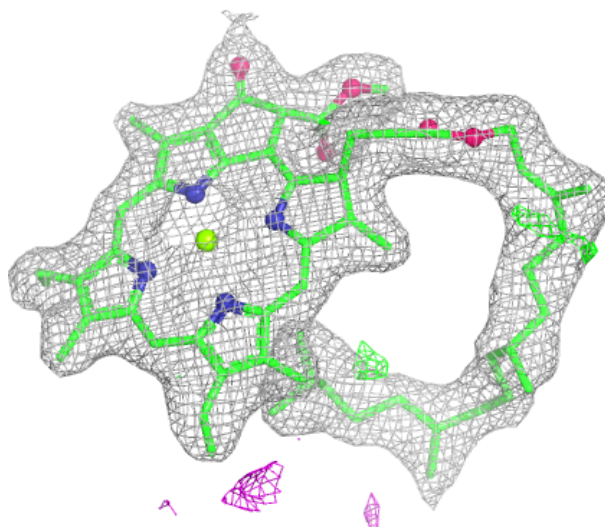
**Electron density around CLA B 613:**

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



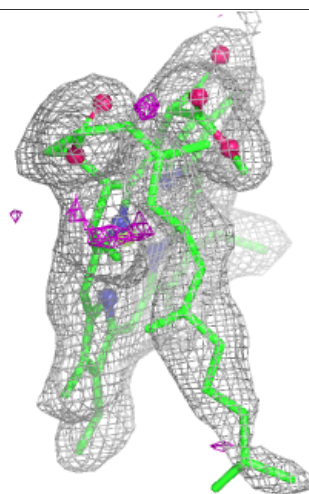
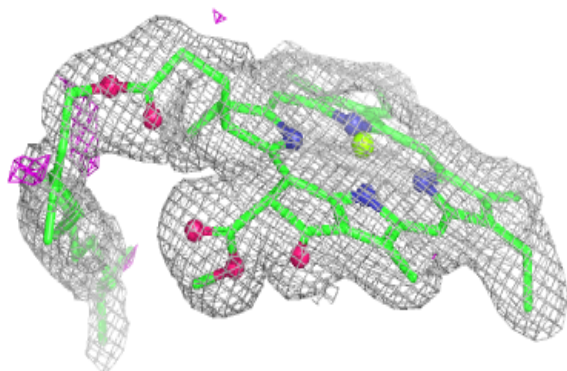
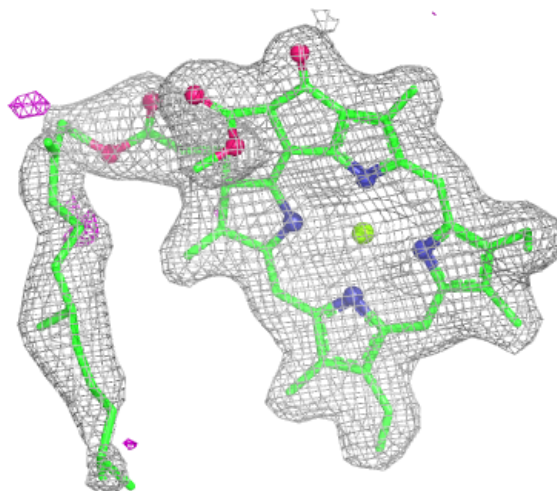
Electron density around CLA B 614:

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



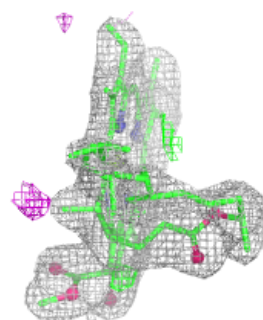
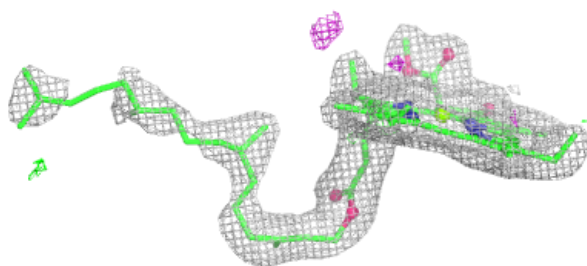
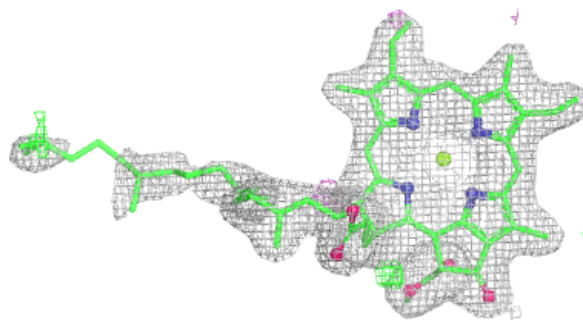
Electron density around CLA B 615:

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

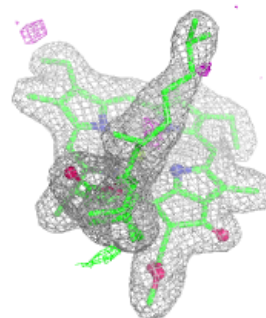
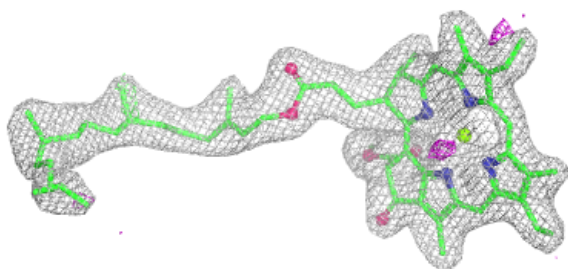
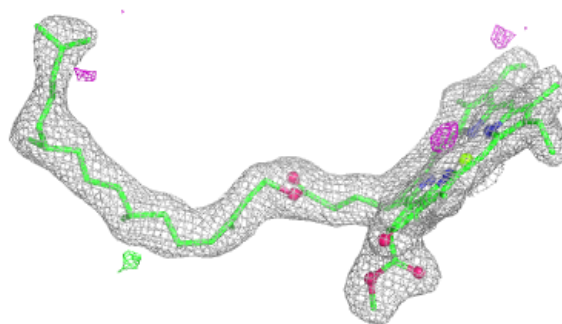


Electron density around CLA a 607:

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

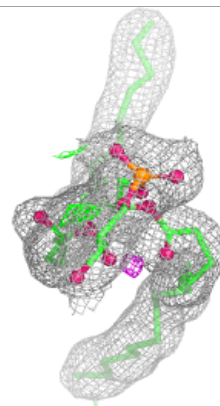
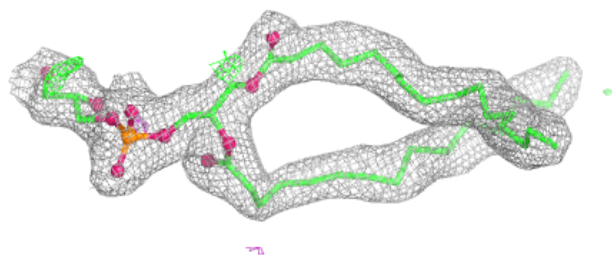
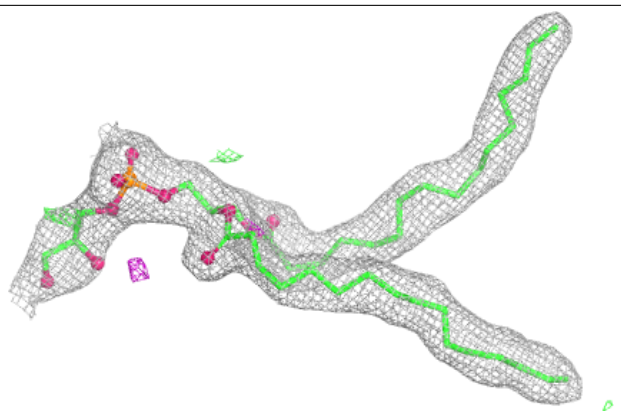
**Electron density around CLA d 403:**

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

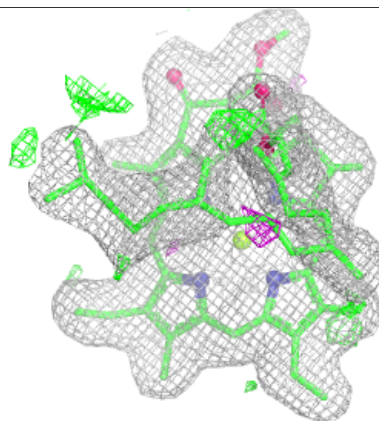
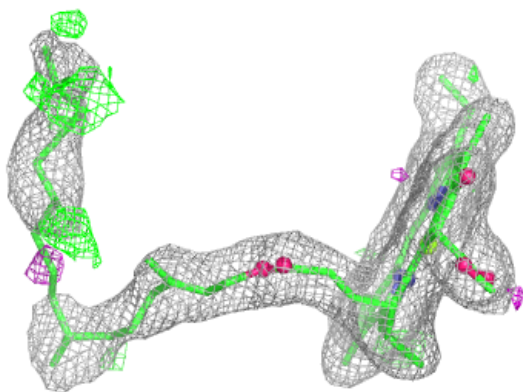
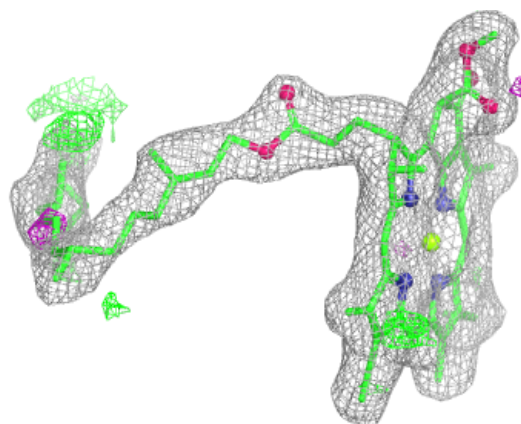


Electron density around LHG d 408:

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

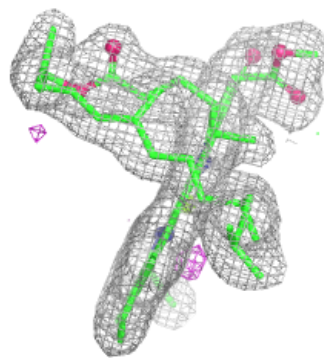
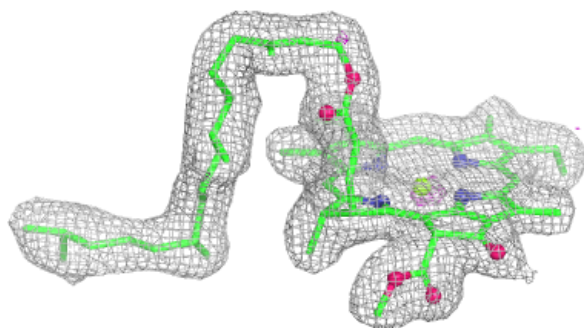
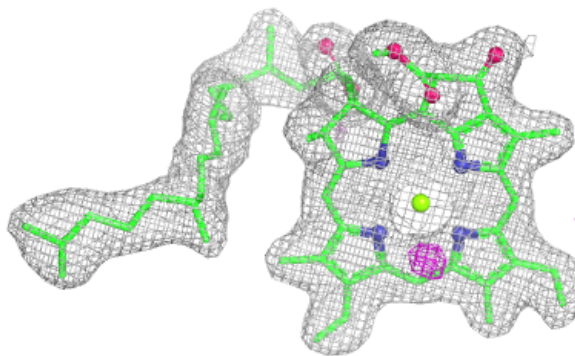
**Electron density around CLA a 609:**

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

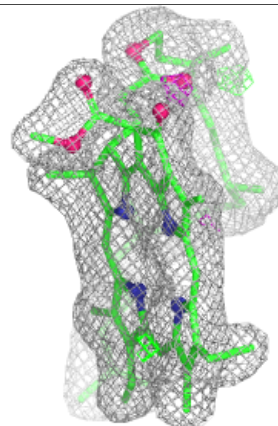
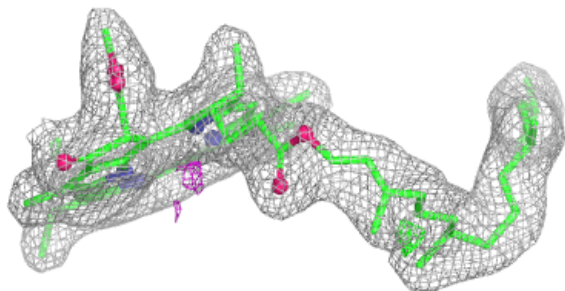
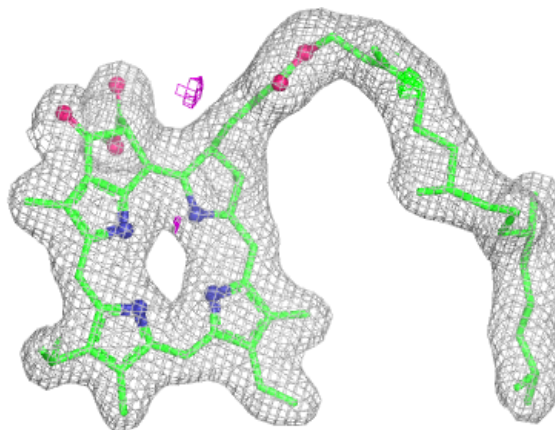


Electron density around CLA a 612:

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

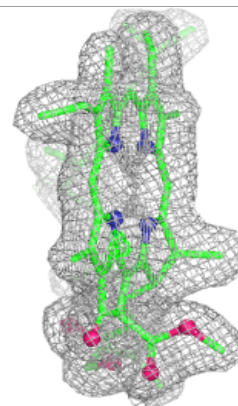
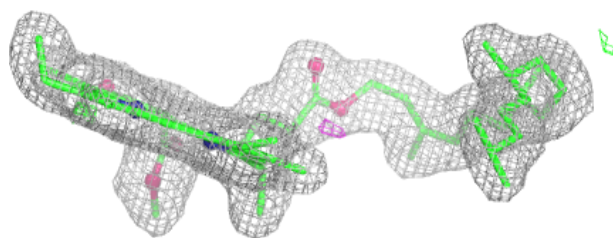
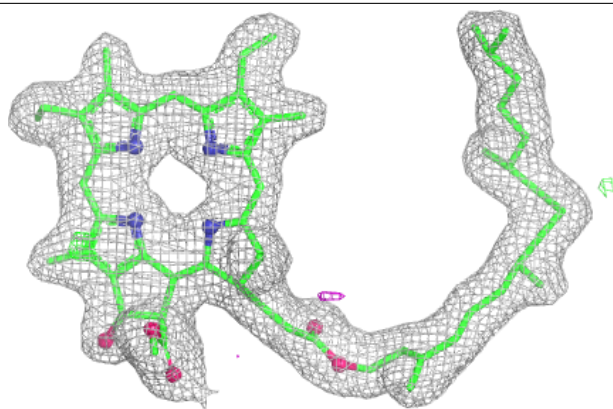
**Electron density around PHO A 608:**

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

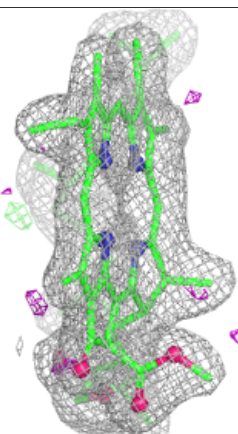
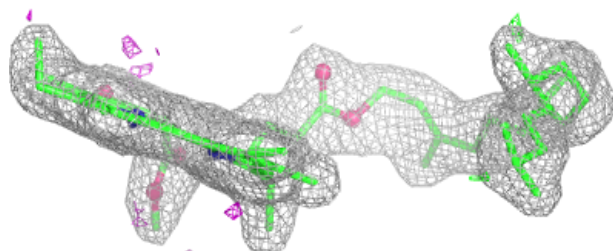
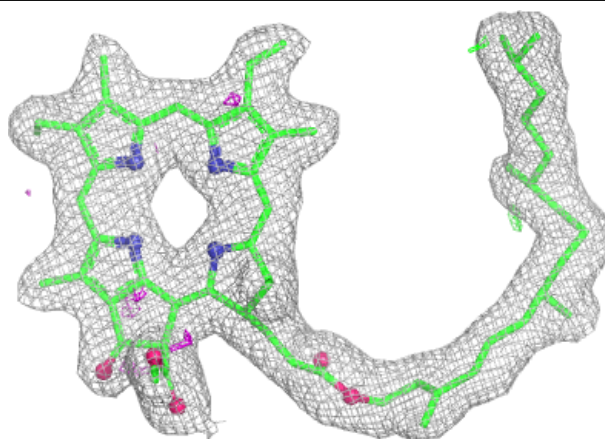


Electron density around PHO D 402:

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

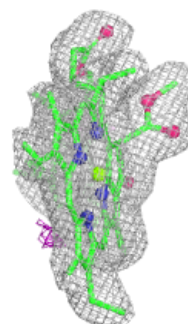
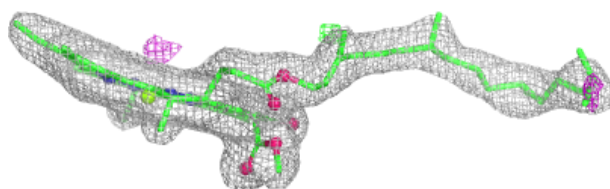
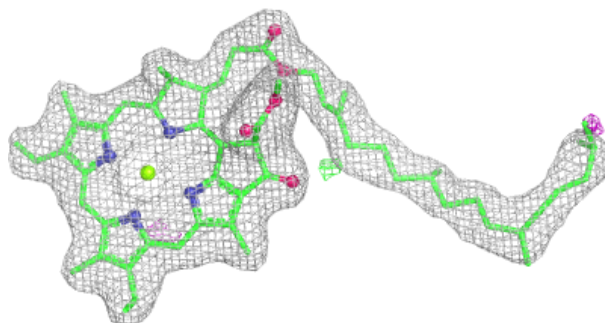
**Electron density around PHO a 608:**

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

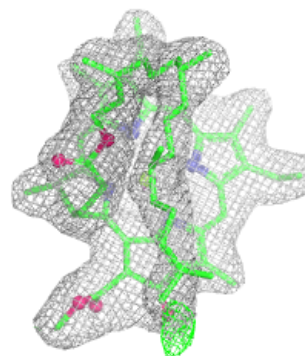
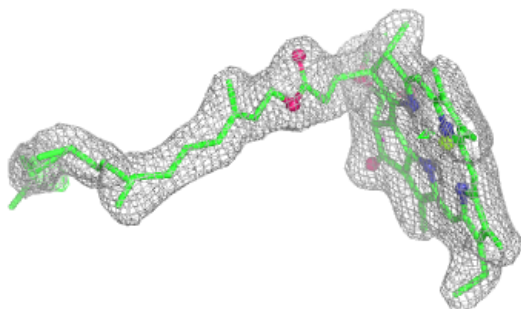
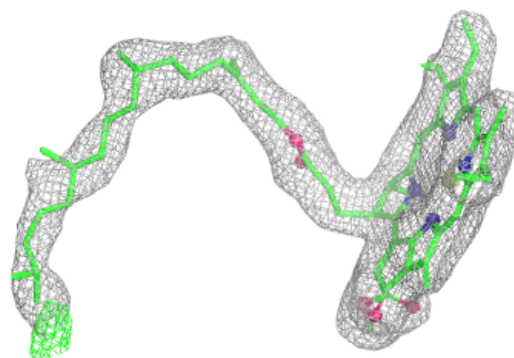


Electron density around CLA b 601:

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

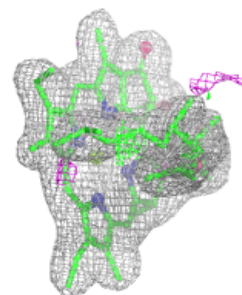
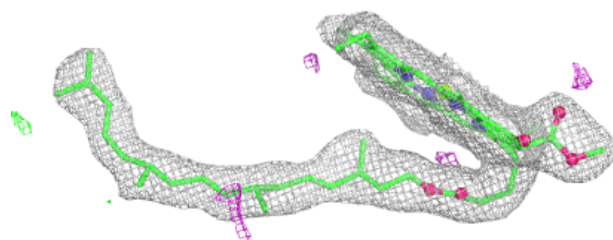
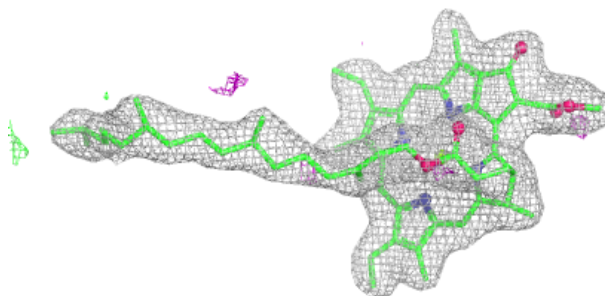
**Electron density around CLA b 605:**

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

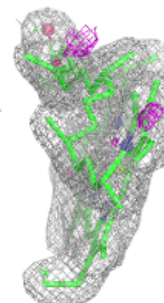
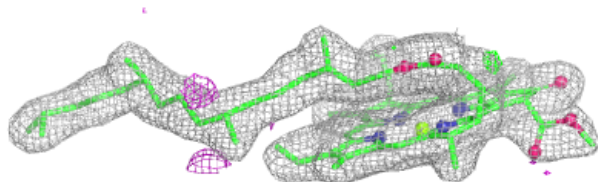
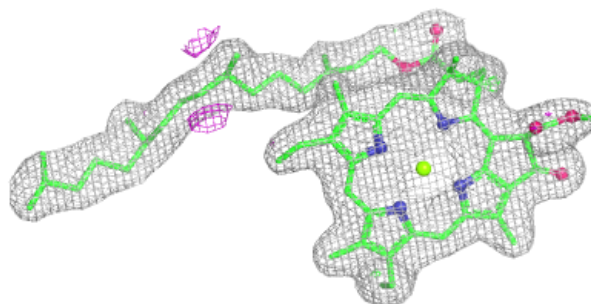


Electron density around CLA b 607:

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

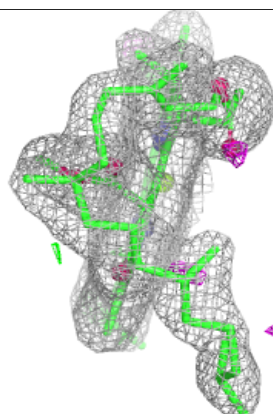
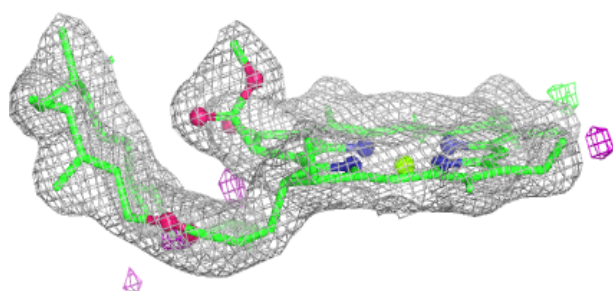
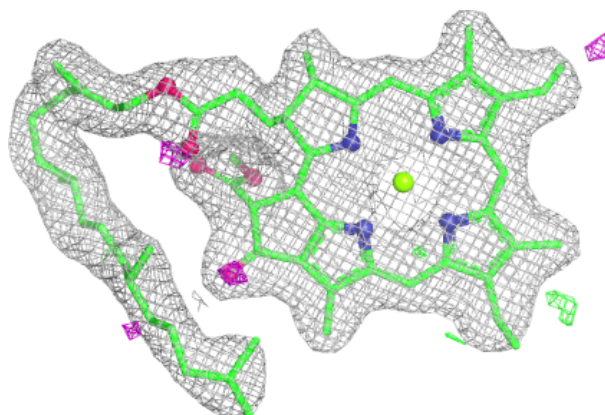
**Electron density around CLA C 501:**

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

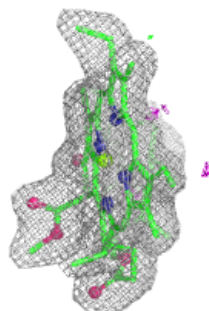
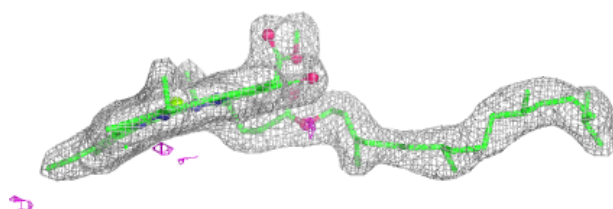
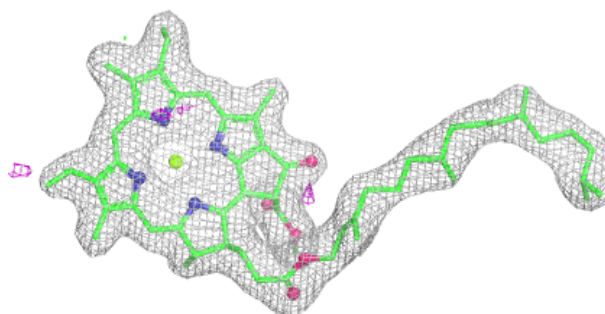


Electron density around CLA b 609:

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

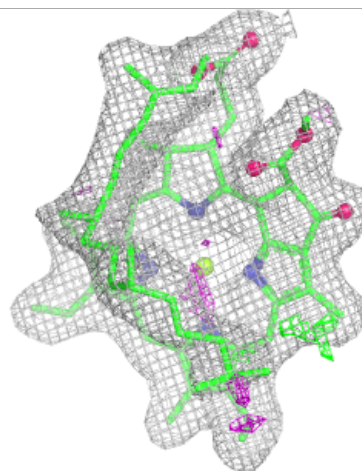
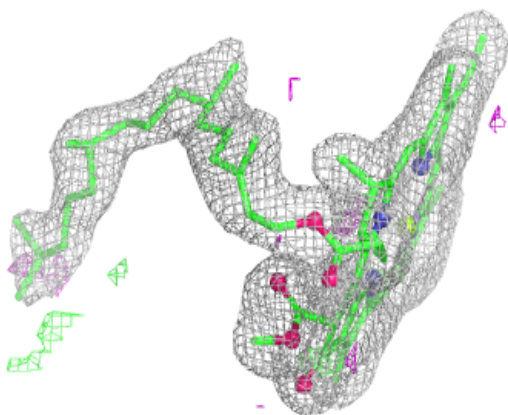
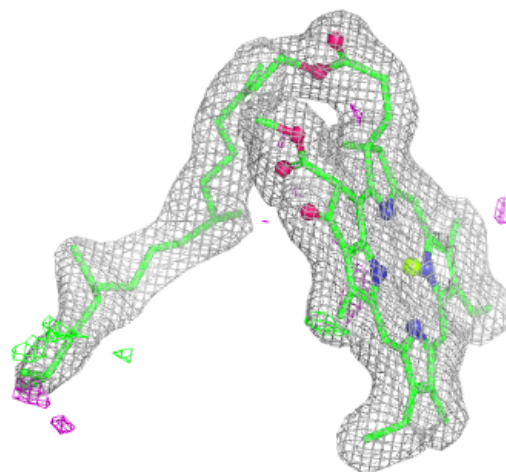
**Electron density around CLA B 601:**

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



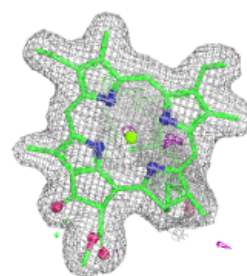
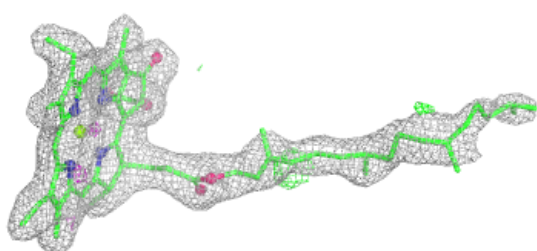
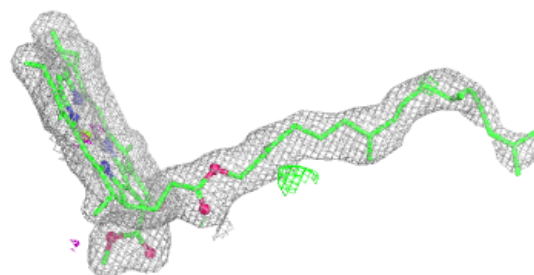
Electron density around CLA b 612:

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

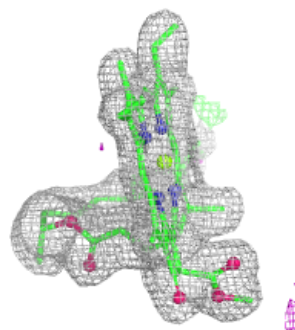
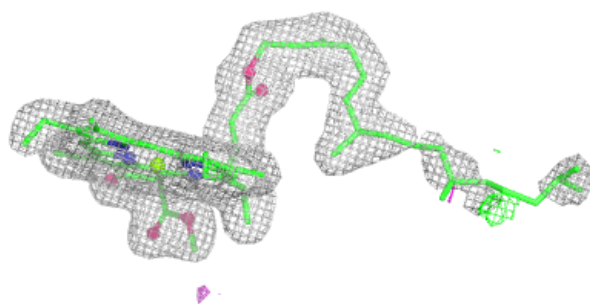
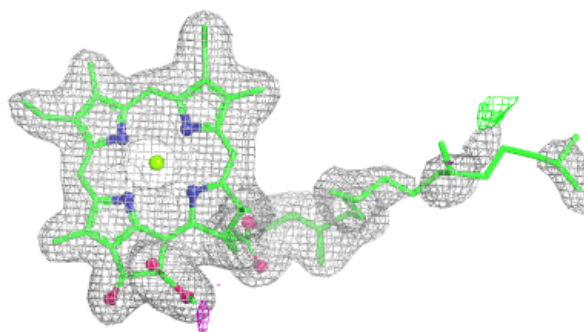


Electron density around CLA B 603:

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

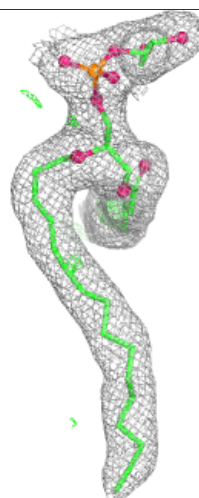
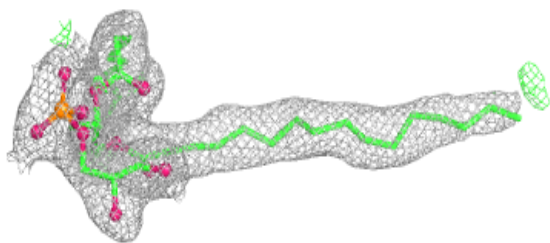
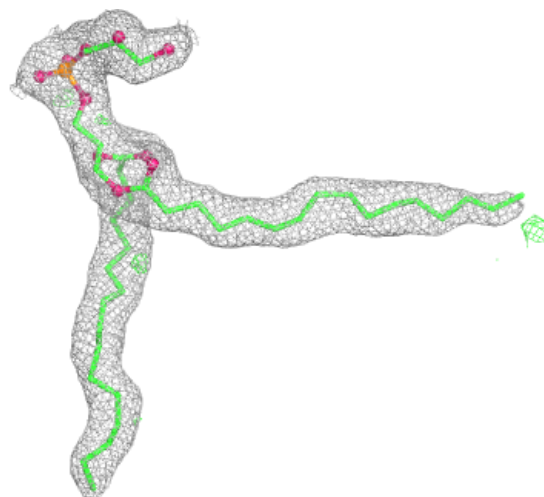
**Electron density around CLA A 607:**

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



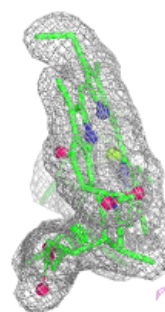
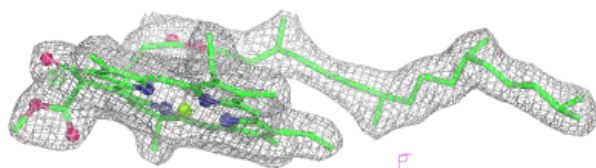
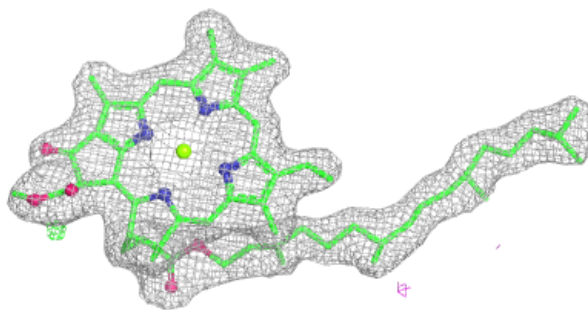
Electron density around LHG L 101:

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

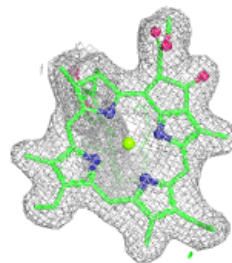
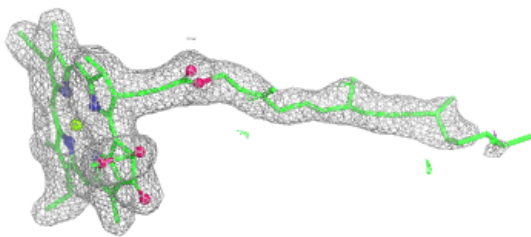
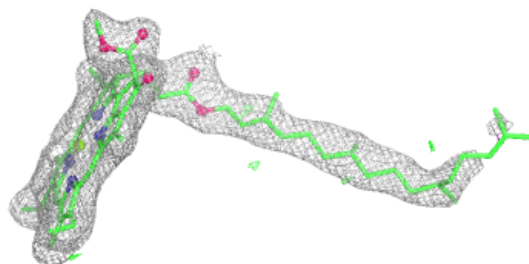


Electron density around CLA c 501:

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

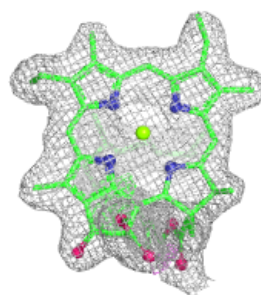
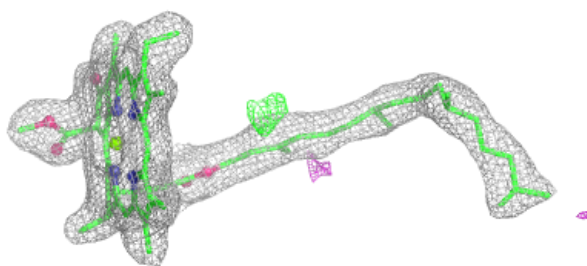
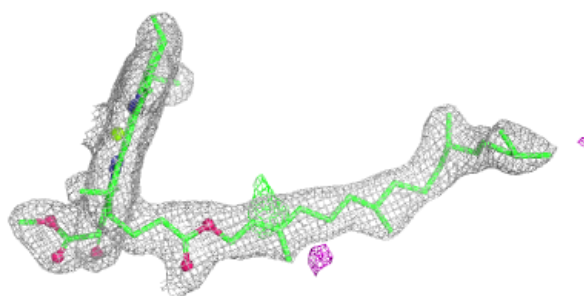
**Electron density around CLA b 603:**

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

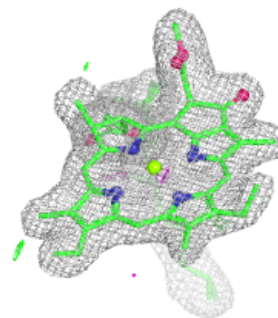
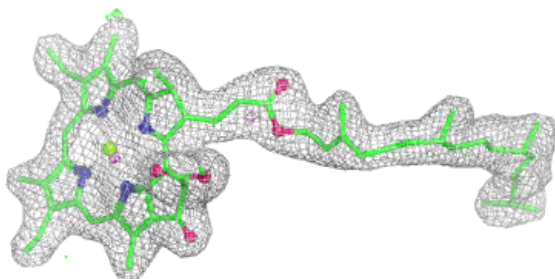
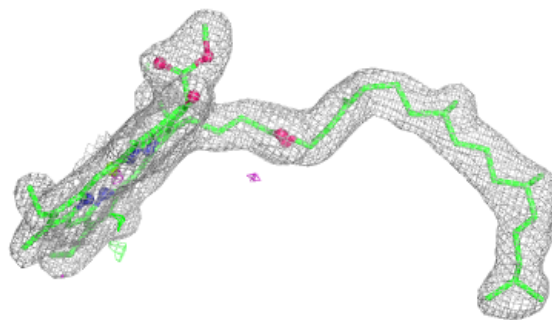


Electron density around CLA b 604:

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

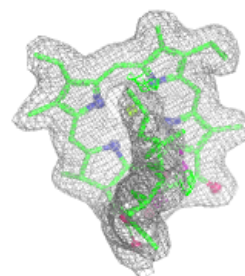
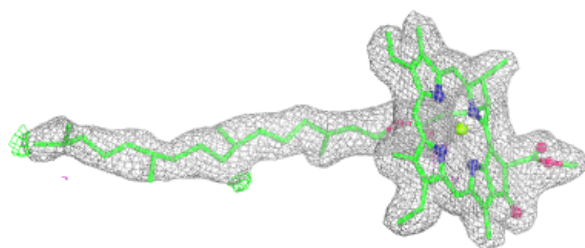
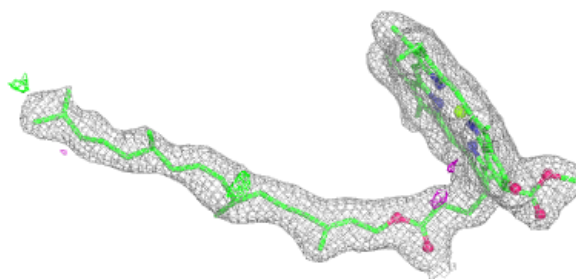
**Electron density around CLA D 403:**

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

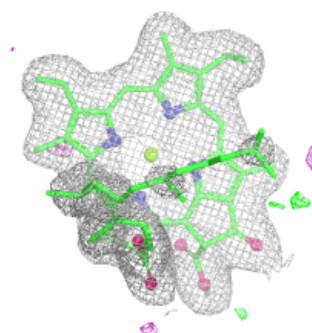
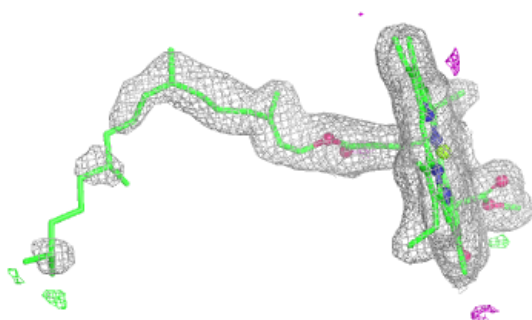
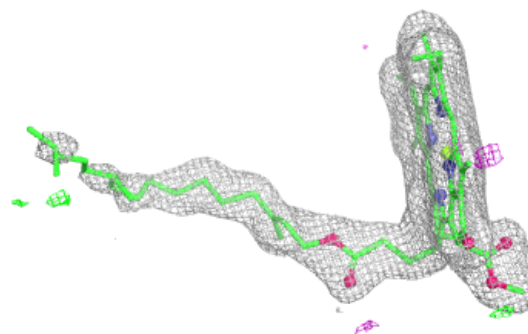


Electron density around CLA b 606:

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

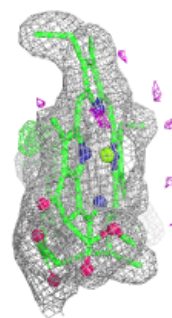
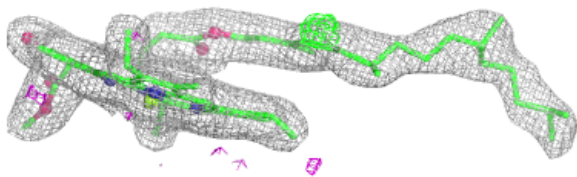
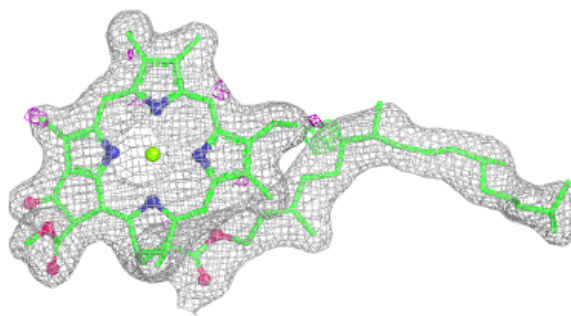
**Electron density around CLA D 404:**

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



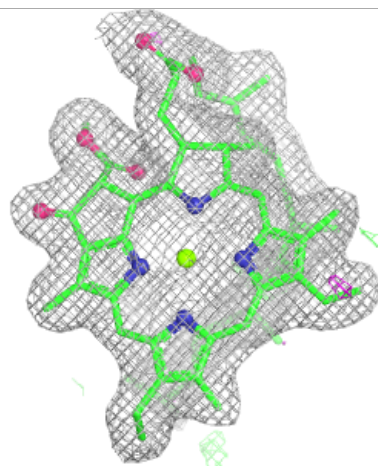
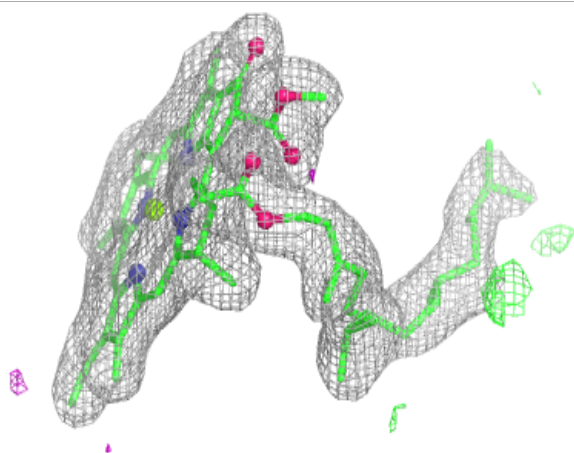
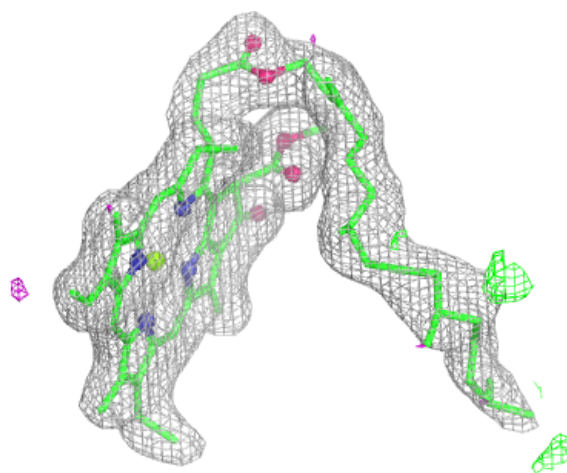
Electron density around CLA B 602:

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



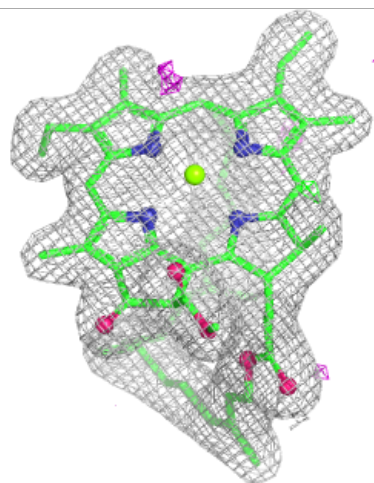
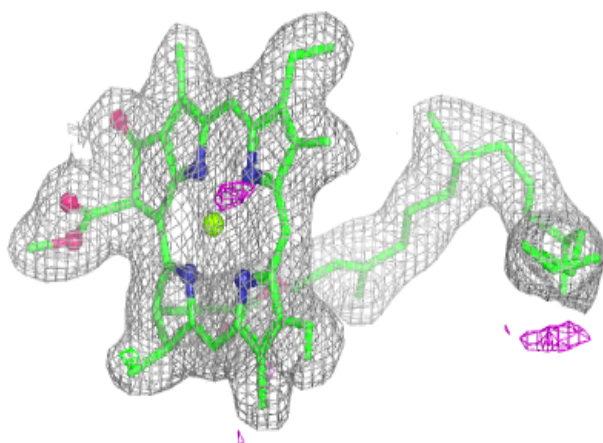
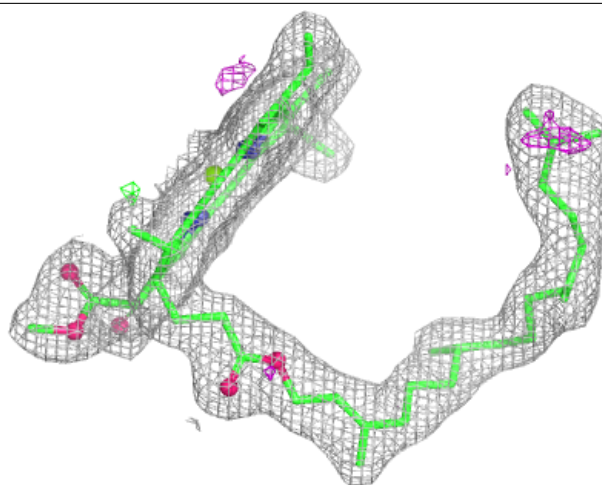
Electron density around CLA B 612:

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



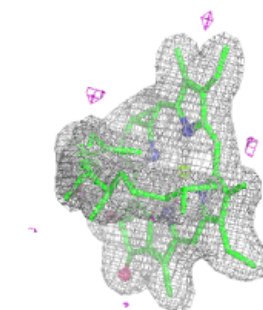
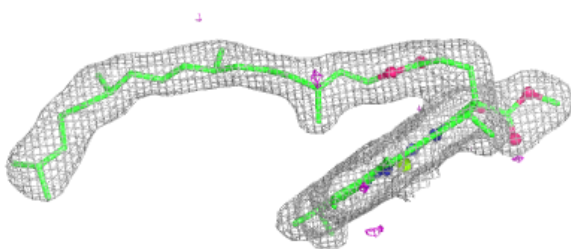
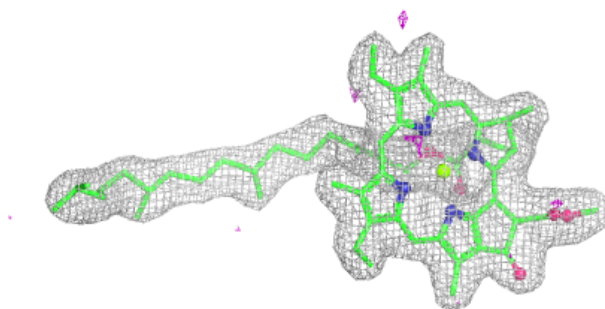
Electron density around CLA b 610:

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

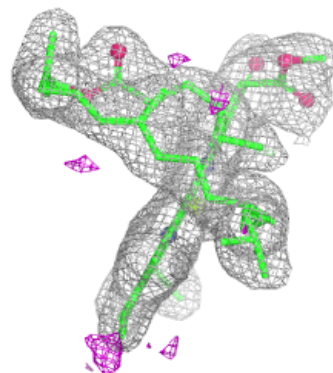
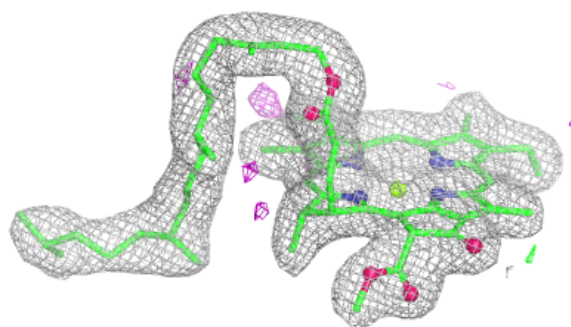
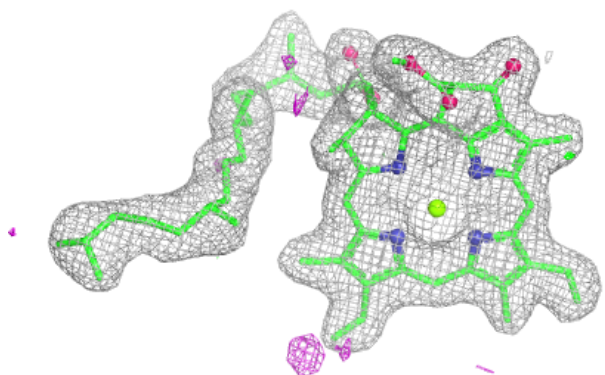


Electron density around CLA B 607:

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

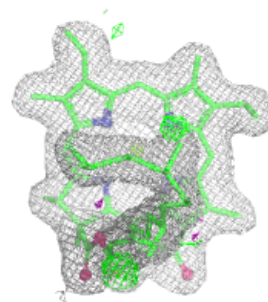
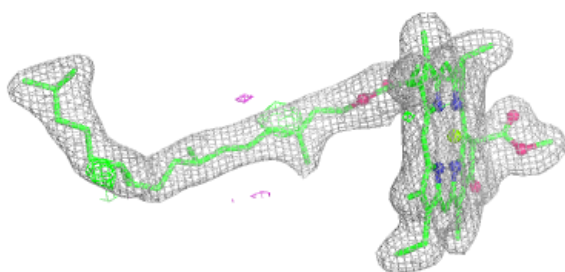
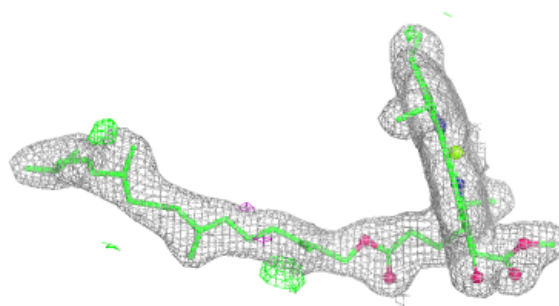
**Electron density around CLA A 612:**

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



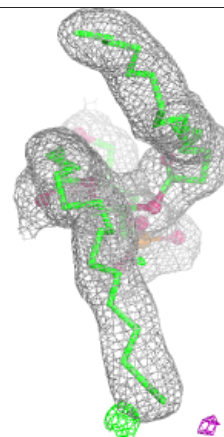
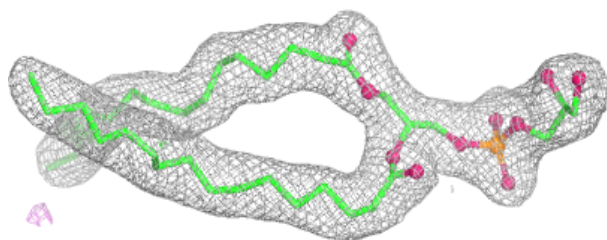
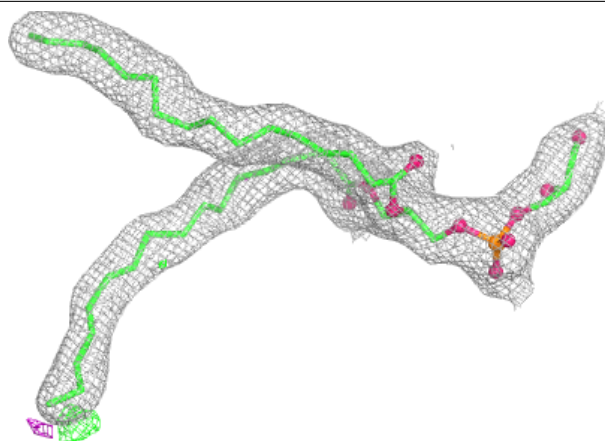
Electron density around CLA B 604:

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



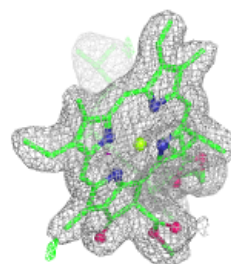
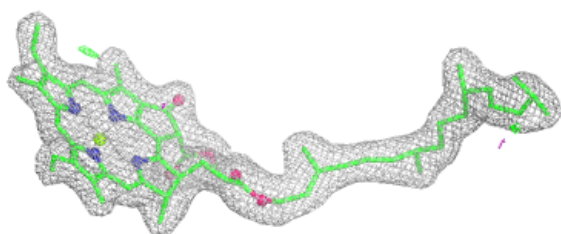
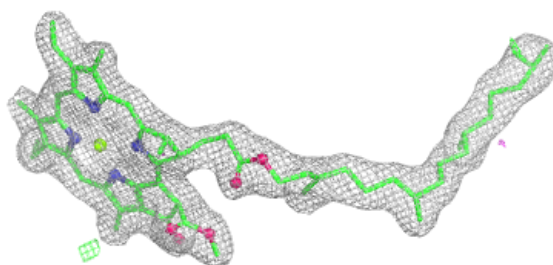
Electron density around LHG D 408:

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

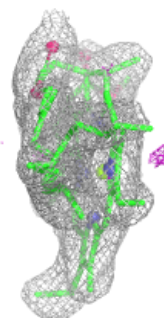
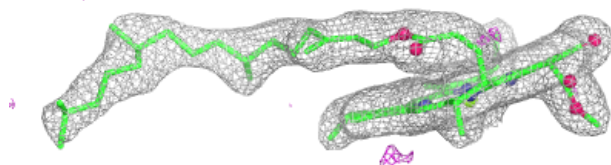
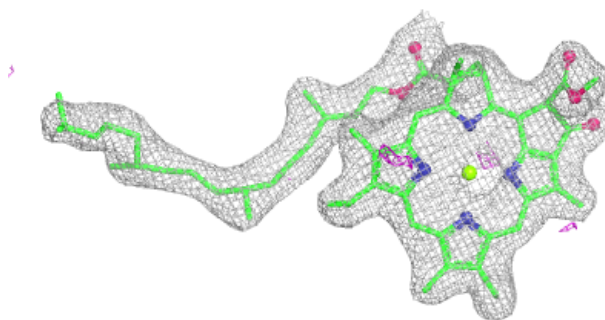


Electron density around CLA A 606:

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

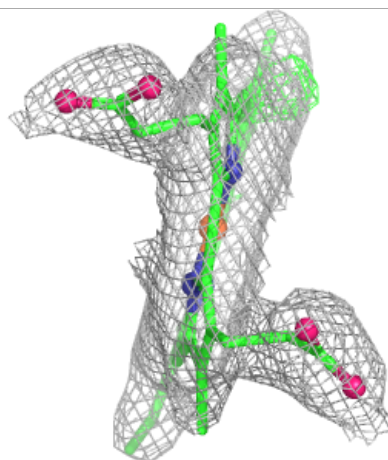
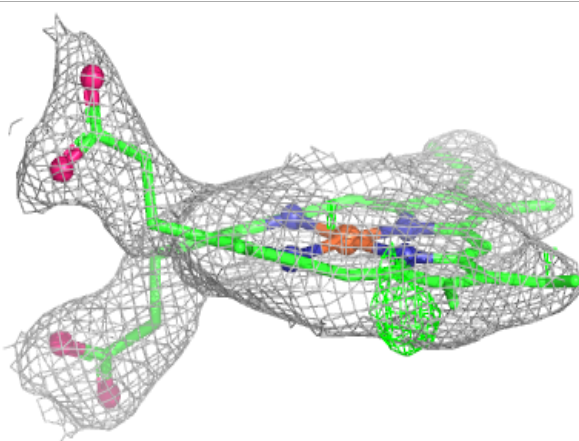
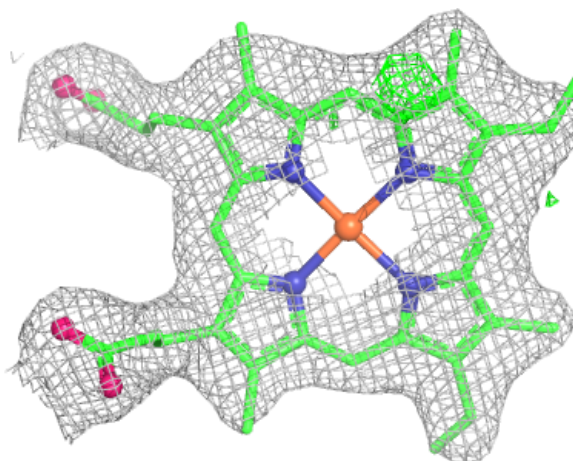
**Electron density around CLA b 602:**

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



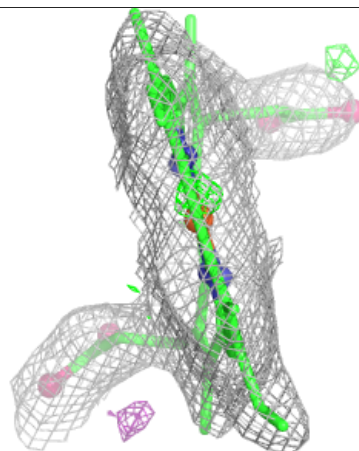
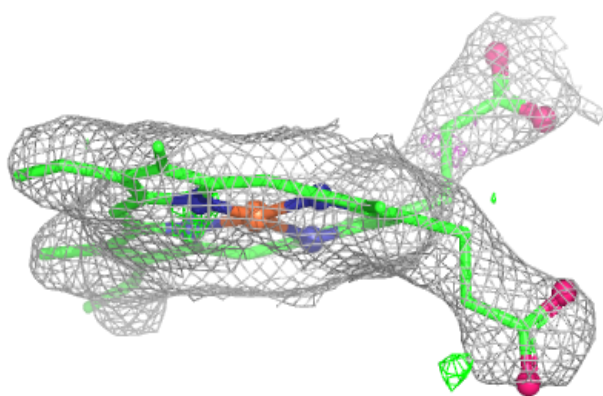
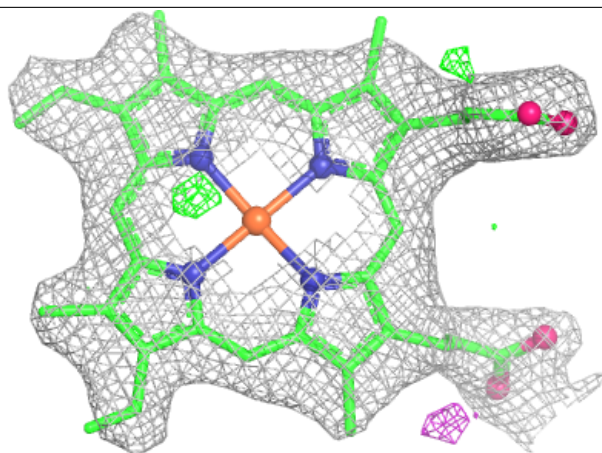
Electron density around HEM F 101:

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



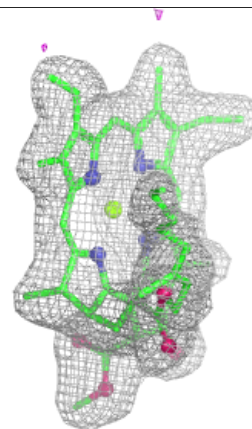
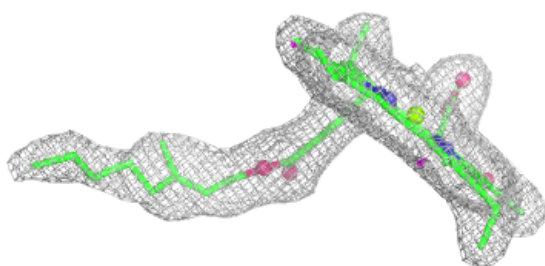
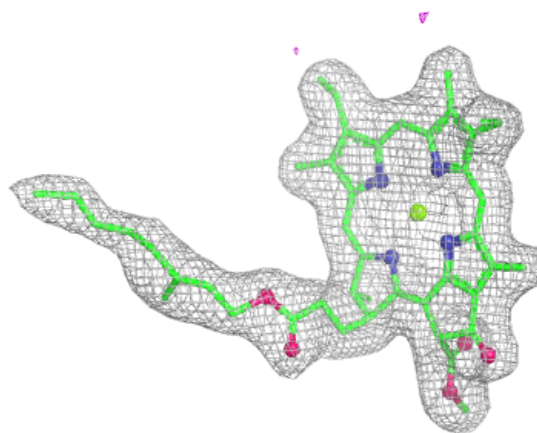
Electron density around HEM f 101:

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



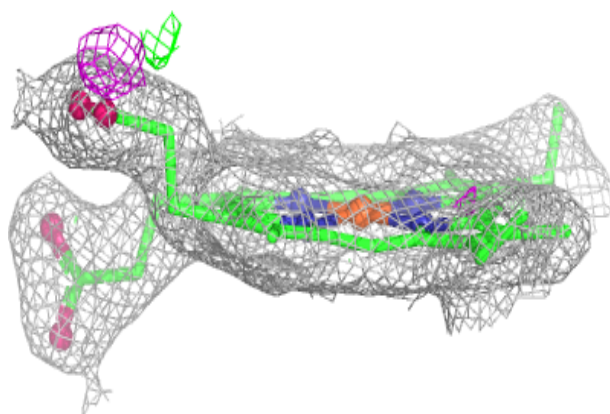
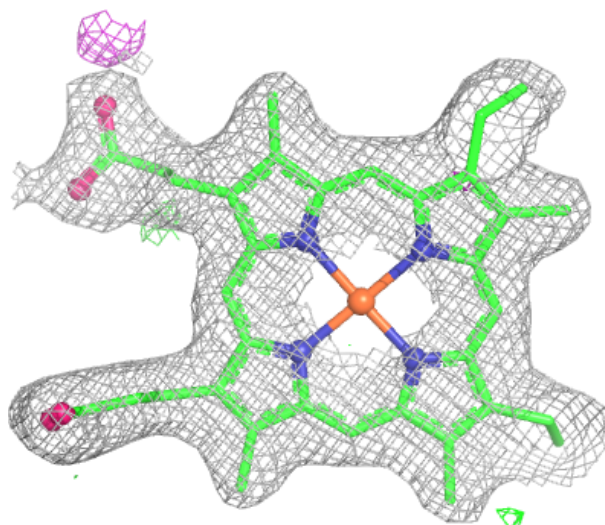
Electron density around CLA A 609:

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



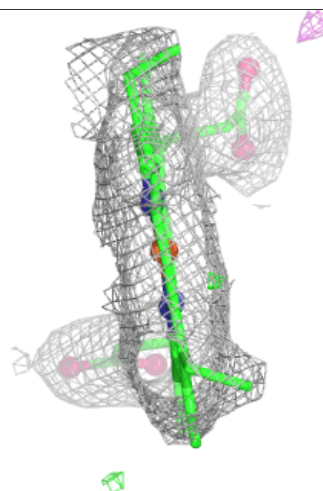
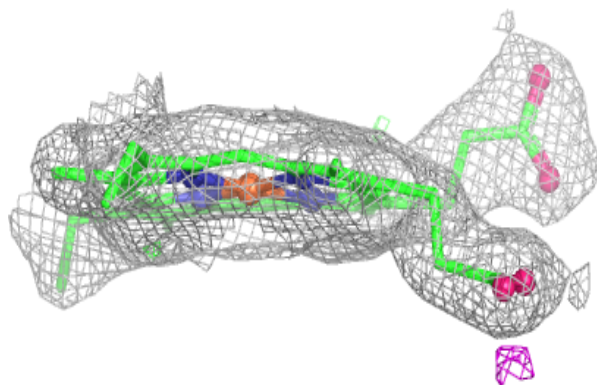
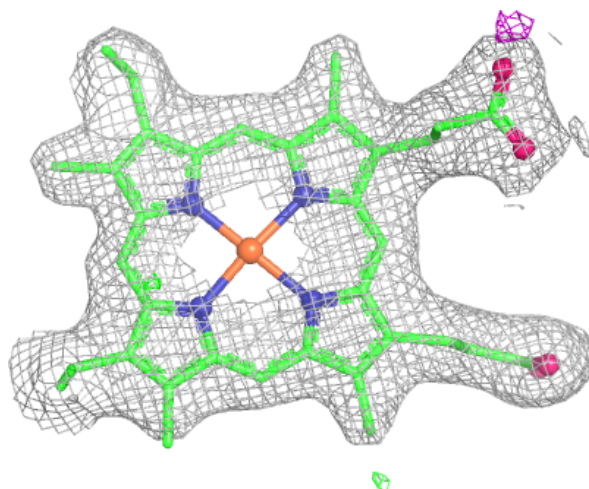
Electron density around HEC V 201:

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



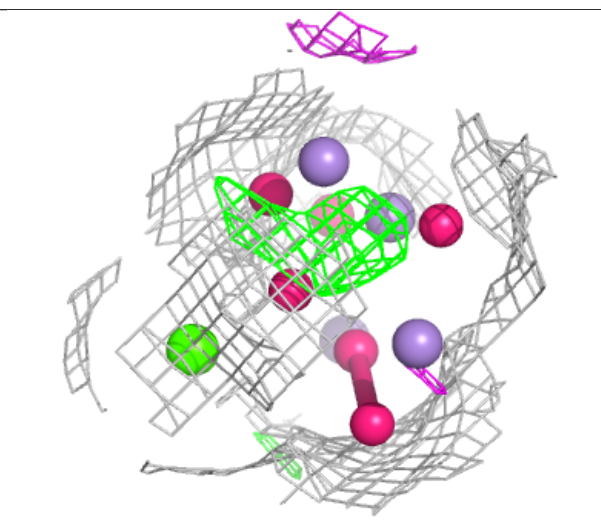
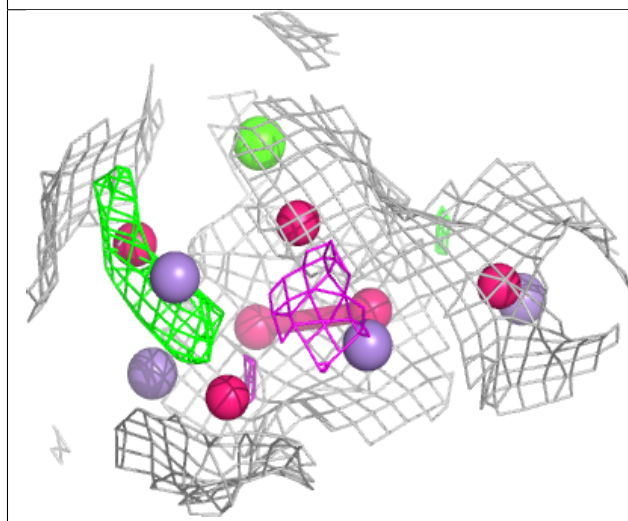
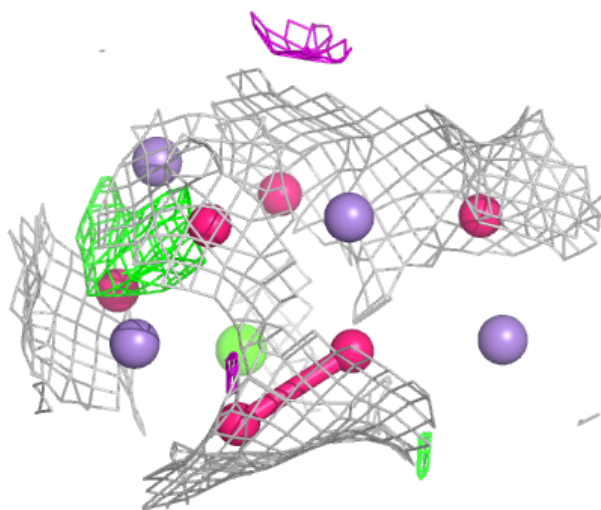
Electron density around HEC v 201:

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



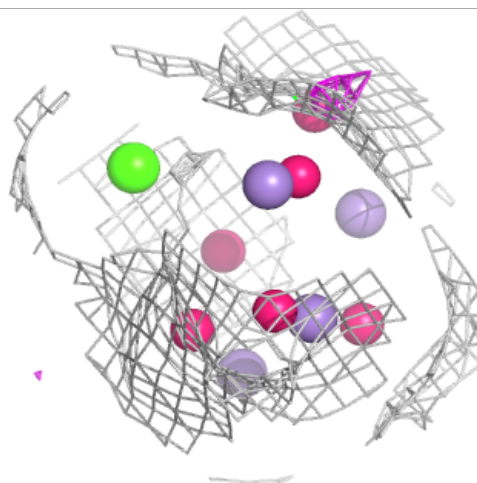
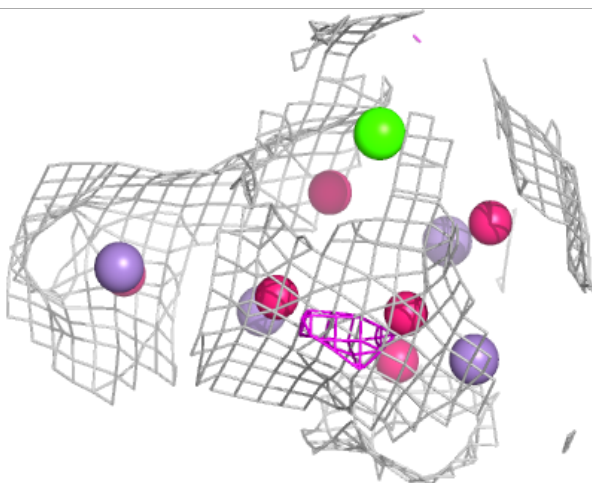
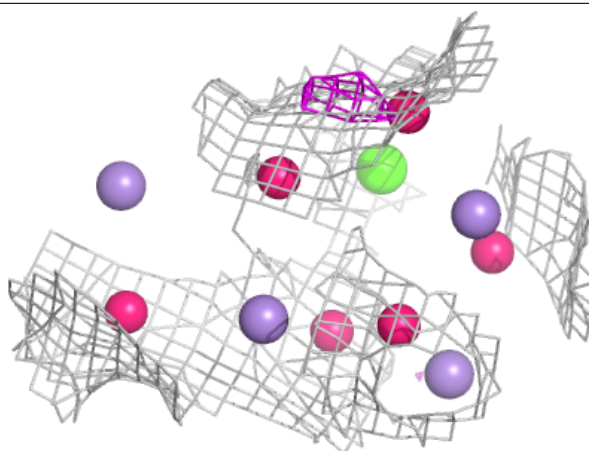
Electron density around OEY A 601 (C):

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



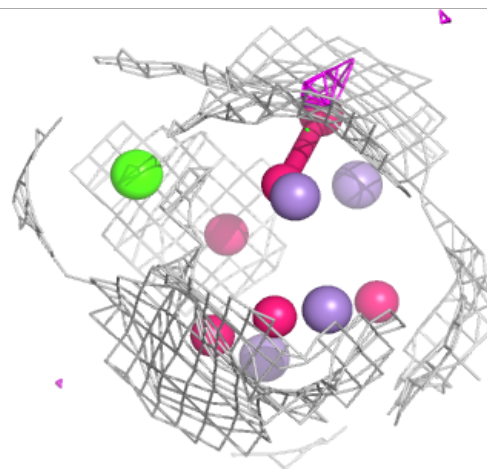
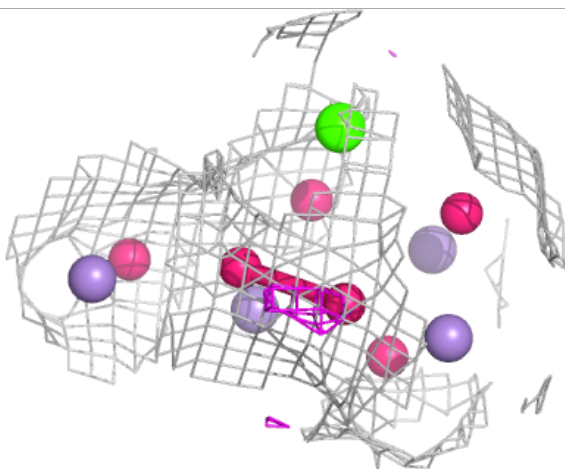
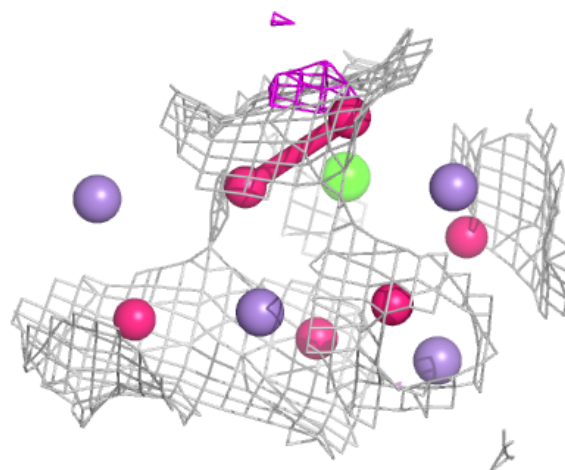
Electron density around OEY a 601 (A):

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



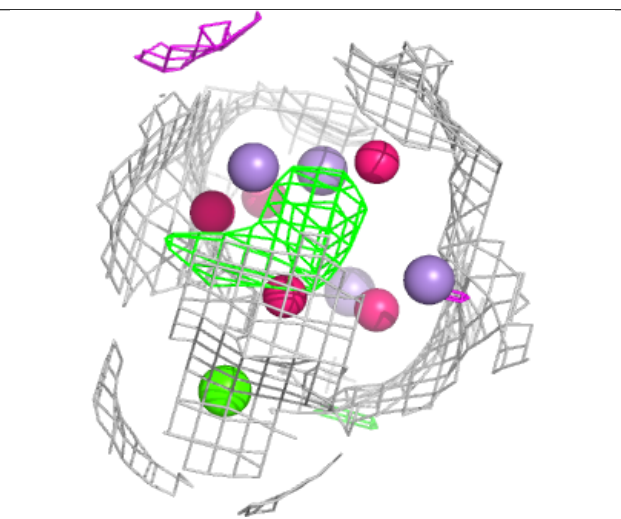
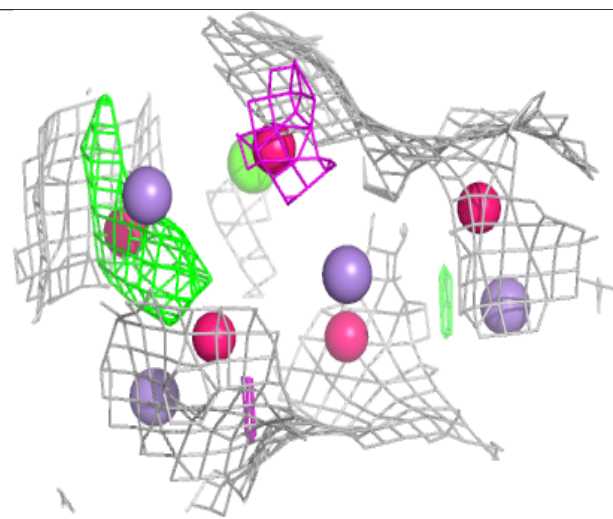
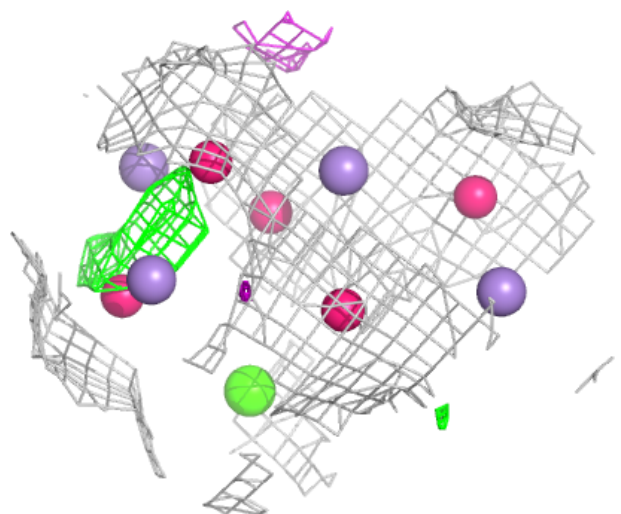
Electron density around OEY a 601 (C):

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



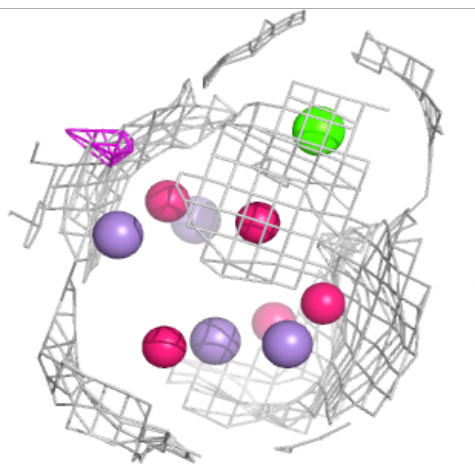
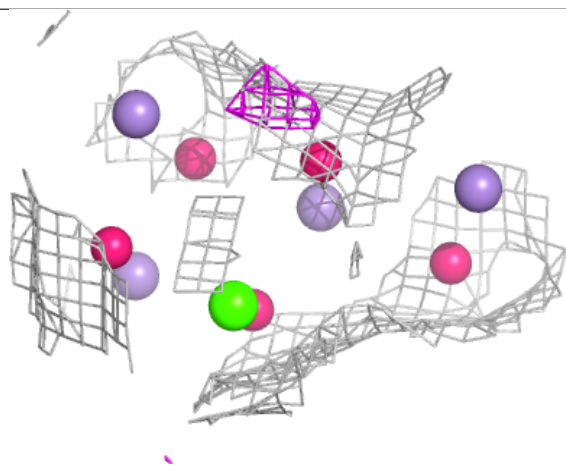
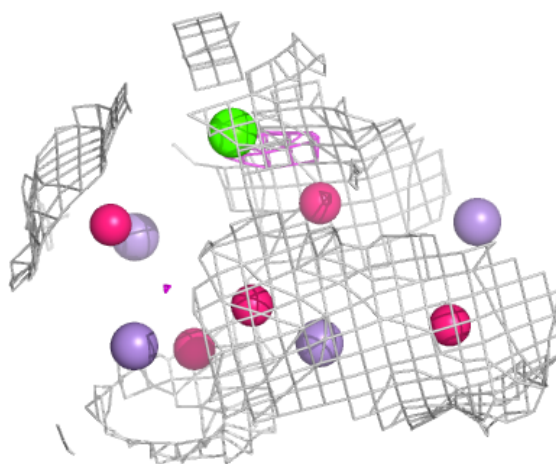
Electron density around OEX A 602 (B):

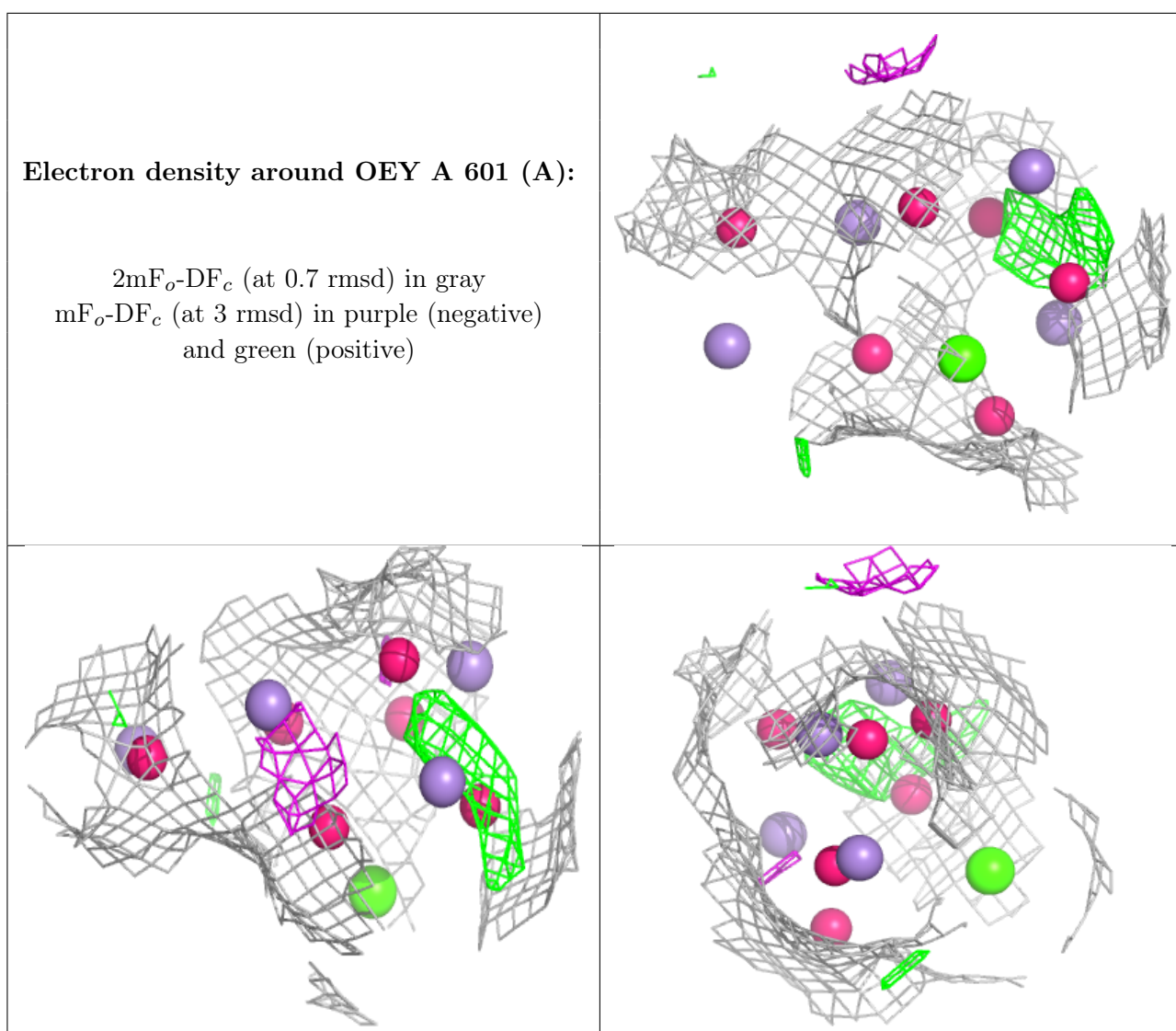
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX a 602 (B):

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





6.5 Other polymers ⓘ

There are no such residues in this entry.