



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 09:00 PM EDT

PDB ID : 5KAI
Title : NH3-bound RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 2.8 Å resolution
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2016-06-01
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1

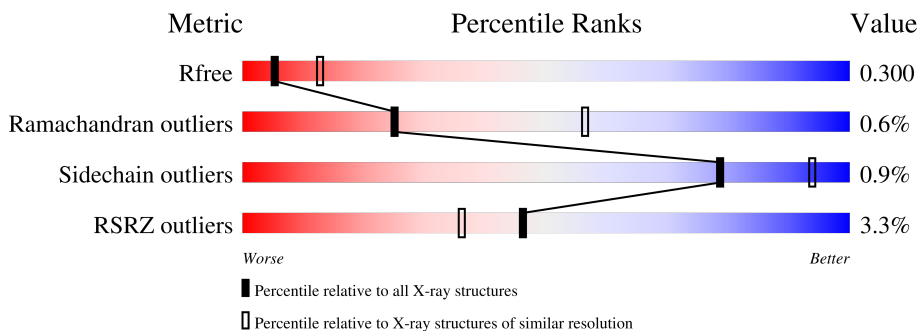
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

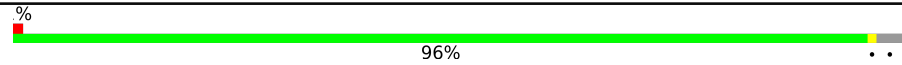
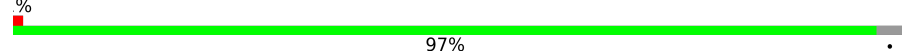
The reported resolution of this entry is 2.80 Å.

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}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	 96%
1	a	344	 97%

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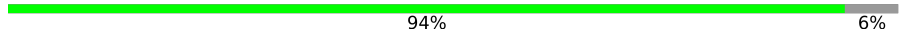












buster-report : 1.1.7 (2018)
 Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
 Refmac : 5.8.0158
 CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
2	B	510	2% 98%
2	b	510	5% 98%
3	C	461	% 97%
3	c	461	% 97%
4	D	352	% 96%
4	d	352	% 96%
5	E	84	10% 96%
5	e	84	14% 96%
6	F	45	76% 24%
6	f	45	76% 24%
7	H	63	3% 97%
7	h	63	98%
8	I	38	5% 95% 5%
8	i	38	8% 89% 5% 5%
9	J	40	5% 88% 10%
9	j	40	5% 88% 10%
10	K	46	9% 78% 20%
10	k	46	78% 20%
11	L	37	100%
11	l	37	3% 100%
12	M	36	3% 89% 8%
12	m	36	3% 89% 8%
13	O	272	4% 89% 10%
13	o	272	3% 86% 10%
14	T	32	3% 94% 6%

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Mol	Chain	Length	Quality of chain
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	B	602	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	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	616	X	-	-	-
25	CLA	B	617	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	508	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	C	514	X	-	-	-
25	CLA	a	707	X	-	-	-
25	CLA	a	708	X	-	-	-
25	CLA	a	711	X	-	-	-
25	CLA	a	719	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	b	618	X	-	-	-
25	CLA	b	619	X	-	-	-
25	CLA	b	620	X	-	-	-
25	CLA	b	621	X	-	-	-
25	CLA	b	622	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	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	-	-	-
29	SQD	I	102	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 50284 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
			Total	C	N	O	S			
1	A	334	Total 2622	C 1717	N 431	O 459	S 15	0	0	0
1	a	334	Total 2622	C 1717	N 431	O 459	S 15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	Total 3969	C 2605	N 661	O 690	S 13	0	0	0
2	b	504	Total 3968	C 2605	N 661	O 689	S 13	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3486	C 2281	N 584	O 608	S 13	0	0	0
3	c	451	Total 3486	C 2281	N 584	O 608	S 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	Total 2716	C 1800	N 444	O 460	S 12	0	0	0
4	d	341	Total 2716	C 1800	N 444	O 460	S 12	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			661	432	107	122			
5	e	82	Total	C	N	O	0	0	0
			665	434	108	123			

- 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	63	Total	C	N	O	S	0	0	0
			498	333	80	83	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	expression tag	UNP Q8DJZ6
i	1	FME	-	expression tag	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	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
			Total	C	N	O			
10	K	37	293	204	43	46	0	0	0
10	k	37	293	204	43	46	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	260	173	38	48	1	0	0	0
12	m	33	260	173	38	48	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	expression tag	UNP Q8DHA7
m	1	FME	-	expression tag	UNP Q8DHA7

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	expression tag	UNP Q8DIQ0
t	1	FME	-	expression tag	UNP Q8DIQ0

- 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
			200	131	35	31	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	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	38	Total	C	N	O	0	0	0
			279	187	45	47			

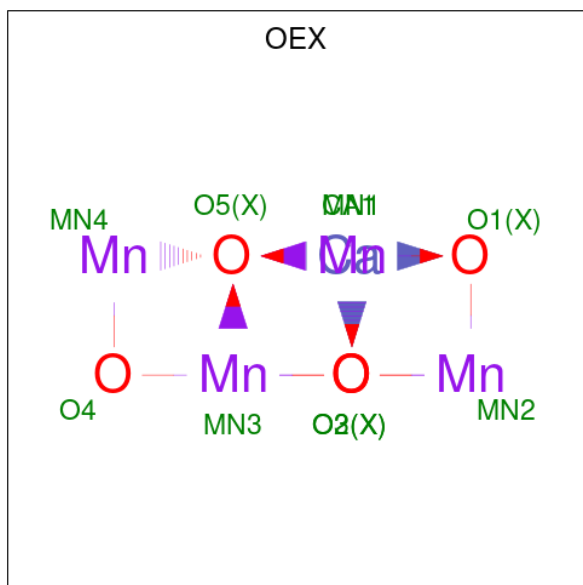
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			478	328	72	76	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
			273	186	47	40			
20	r	34	Total	C	N	O	0	0	0
			270	183	47	40			

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

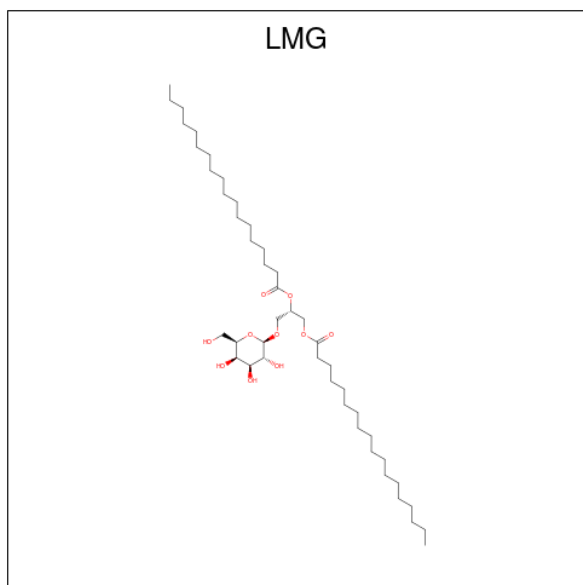
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
23	A	1	51	41	10	0	0
23	B	1	51	41	10	0	0
23	C	1	51	41	10	0	0
23	C	1	51	41	10	0	0
23	C	1	51	41	10	0	0
23	D	1	51	41	10	0	0
23	M	1	51	41	10	0	0
23	a	1	51	41	10	0	0
23	a	1	51	41	10	0	0
23	b	1	51	41	10	0	0

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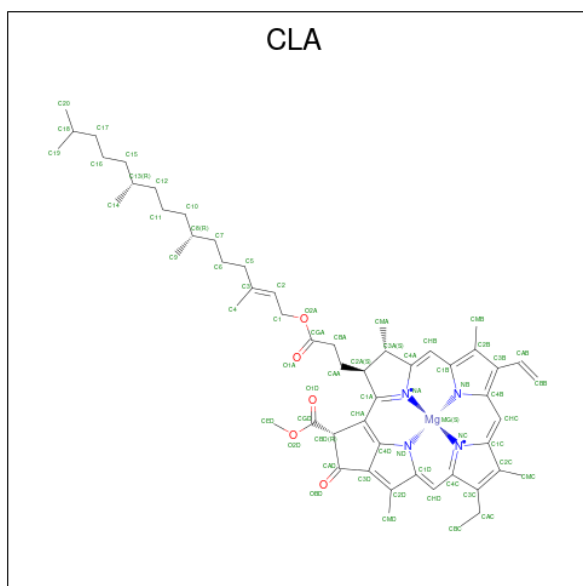
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	b	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C		0	0
			9	9			
23	c	1	Total	C	O	0	0
			51	41	10		
23	c	1	Total	C	O	0	0
			51	41	10		
23	d	1	Total	C	O	0	0
			40	35	5		
23	f	1	Total	C	O	0	0
			51	41	10		

- Molecule 24 is CHLORIDE ION (three-letter code: 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 (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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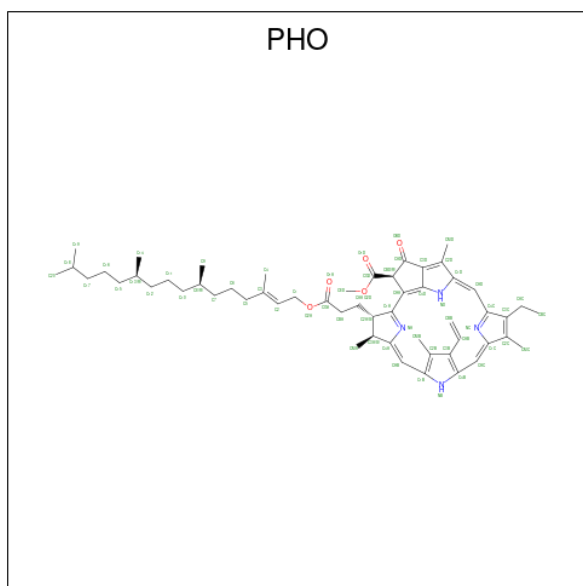
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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
			47	37	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
			58	48	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
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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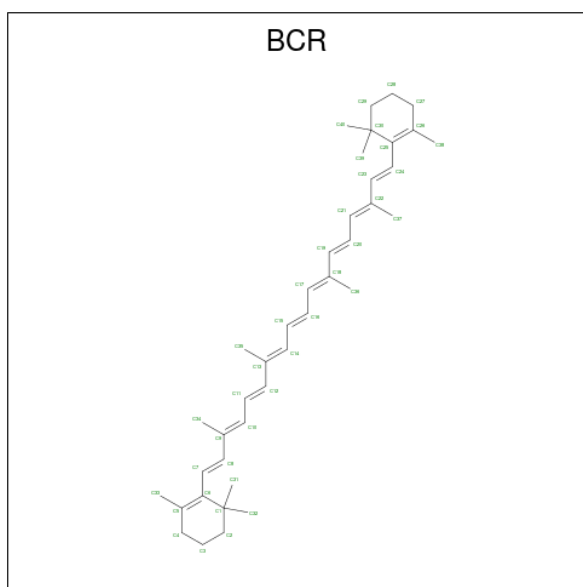
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (three-letter code: 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	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



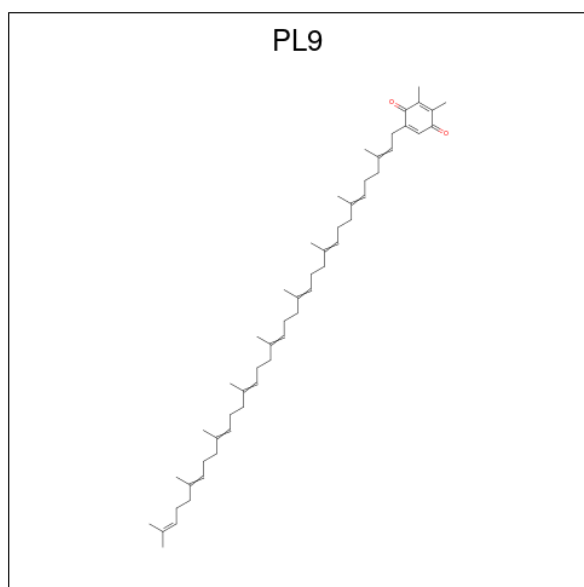
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
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 (three-letter code: PL9) (formula: C₅₃H₈₀O₂).



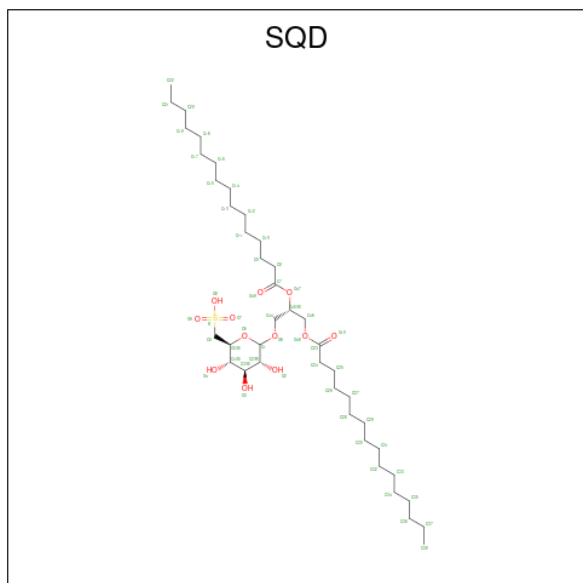
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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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-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

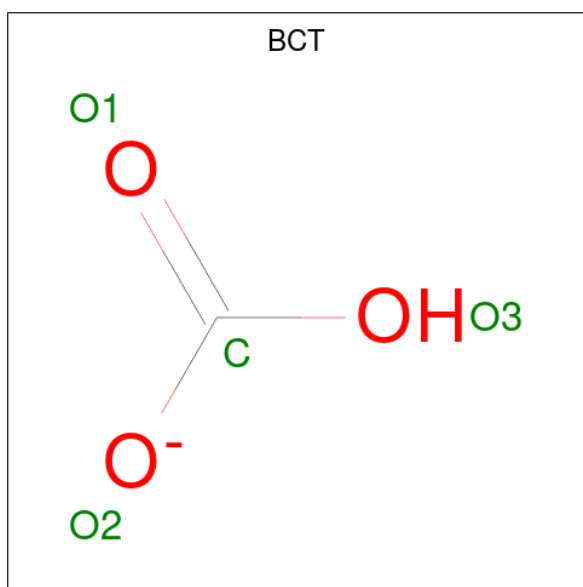


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			40	35	5			
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	I	1	Total	C	O		0	0
			40	35	5			
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O	S	0	0
			54	41	12	1		
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

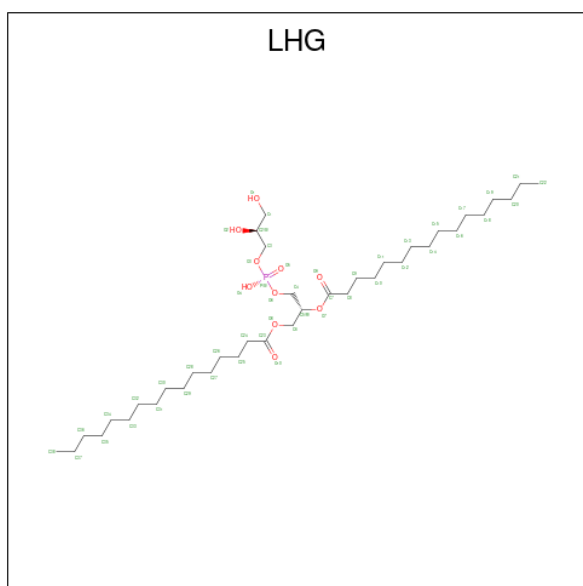
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C 7 7	0	0
30	B	3	Total C 29 29	0	0
30	H	1	Total C 8 8	0	0
30	I	1	Total C 9 9	0	0
30	M	2	Total C 22 22	0	0
30	a	3	Total C 24 24	0	0
30	b	4	Total C 48 48	0	0
30	d	1	Total C 22 22	0	0
30	i	1	Total C 22 22	0	0
30	j	1	Total C 9 9	0	0
30	m	2	Total C 17 17	0	0
30	t	2	Total C 15 15	0	0
30	z	1	Total C 11 11	0	0

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

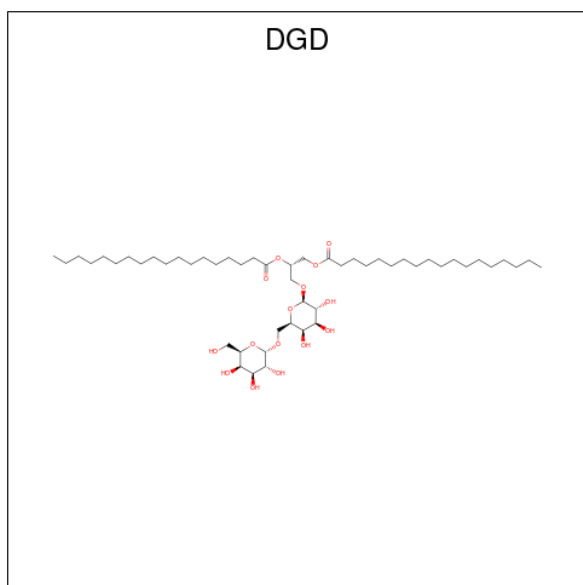
- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



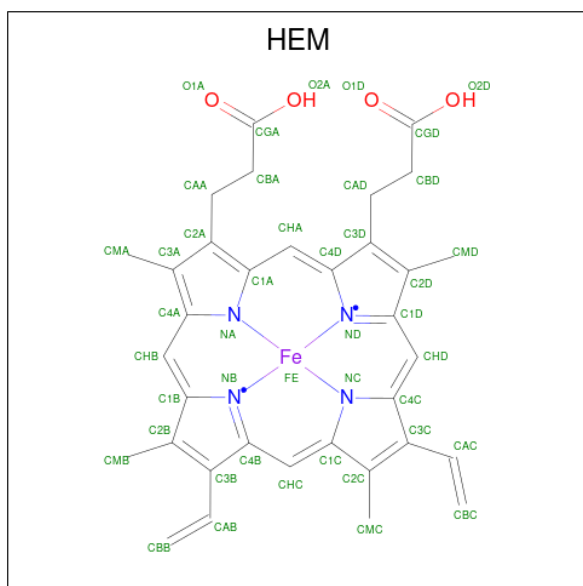
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

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



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

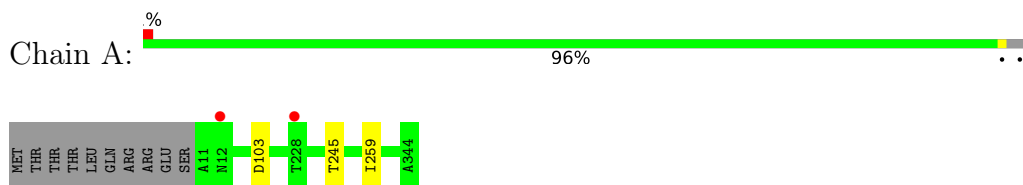
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	V	6	Total O 6 6	0	0
36	a	13	Total O 13 13	0	0
36	b	12	Total O 12 12	0	0
36	c	8	Total O 8 8	0	0
36	d	11	Total O 11 11	0	0
36	e	1	Total O 1 1	0	0
36	h	1	Total O 1 1	0	0
36	l	1	Total O 1 1	0	0
36	o	5	Total O 5 5	0	0
36	u	5	Total O 5 5	0	0
36	v	3	Total O 3 3	0	0
36	z	1	Total O 1 1	0	0

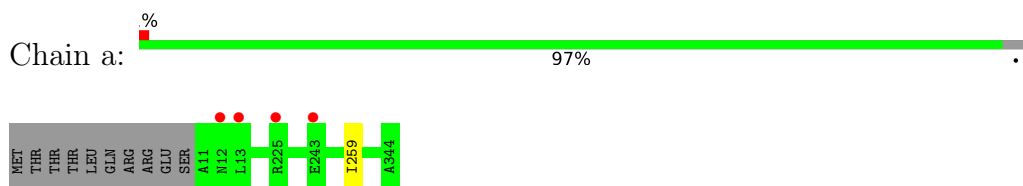
3 Residue-property plots [i](#)

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.

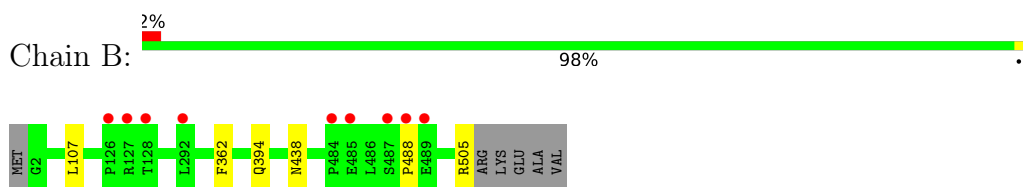
- Molecule 1: Photosystem II protein D1 1



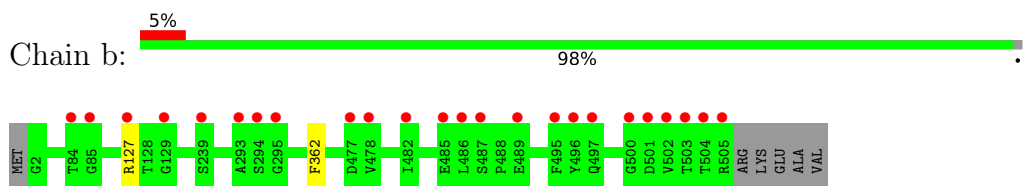
- Molecule 1: Photosystem II protein D1 1



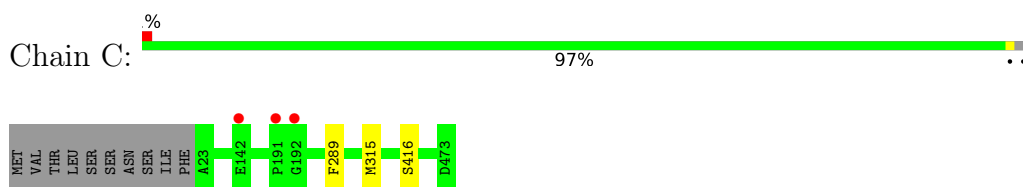
- Molecule 2: Photosystem II CP47 reaction center protein



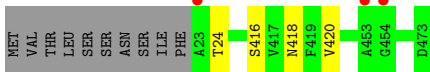
- Molecule 2: Photosystem II CP47 reaction center protein



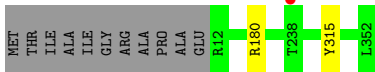
- Molecule 3: Photosystem II CP43 reaction center protein



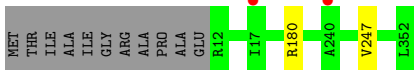
- Molecule 3: Photosystem II CP43 reaction center protein



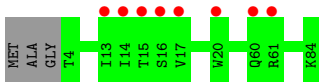
- Molecule 4: Photosystem II D2 protein



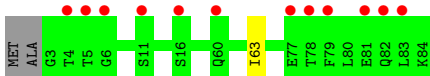
- Molecule 4: Photosystem II D2 protein



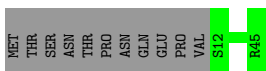
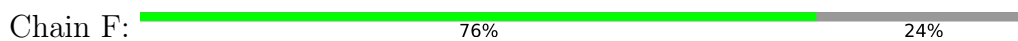
- Molecule 5: Cytochrome b559 subunit alpha



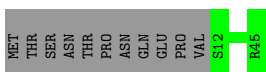
- Molecule 5: Cytochrome b559 subunit alpha



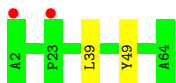
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



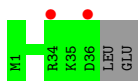
- Molecule 7: Photosystem II reaction center protein H



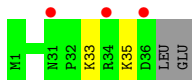
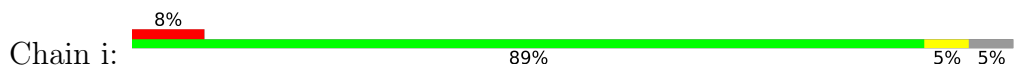
- Molecule 7: Photosystem II reaction center protein H



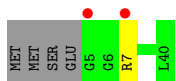
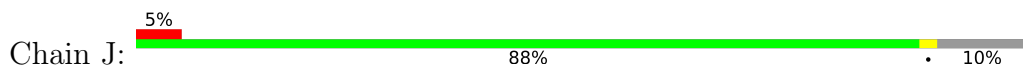
- Molecule 8: Photosystem II reaction center protein I



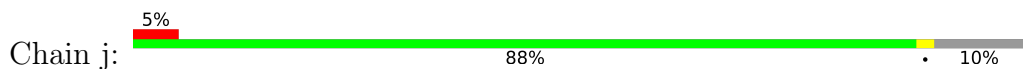
- Molecule 8: Photosystem II reaction center protein I



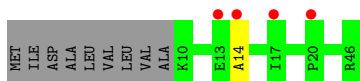
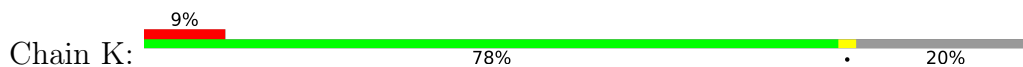
- Molecule 9: Photosystem II reaction center protein J




- Molecule 9: Photosystem II reaction center protein J

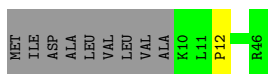


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%

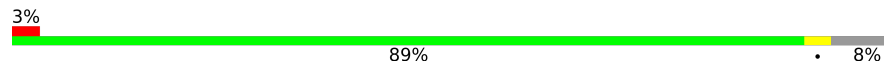
There are no outlier residues recorded for this chain.

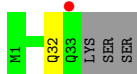
- Molecule 11: Photosystem II reaction center protein L

Chain l:  3% 100%

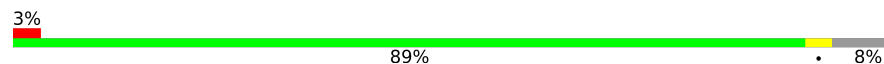


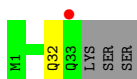
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 89% 8%



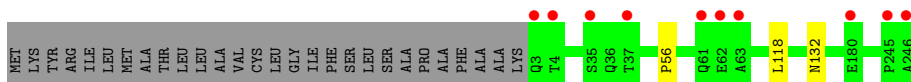
- Molecule 12: Photosystem II reaction center protein M

Chain m:  3% 89% 8%




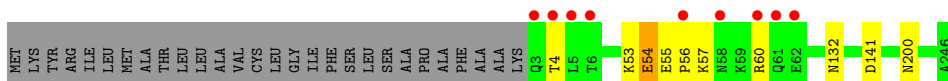
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  4% 89% 10%

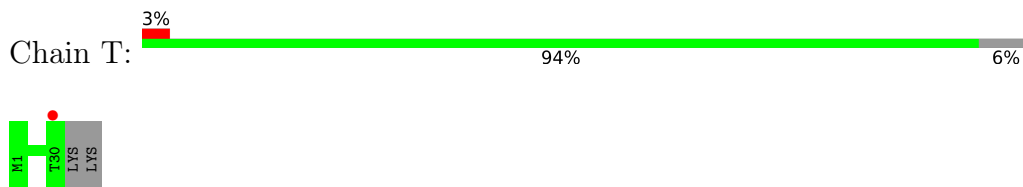


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

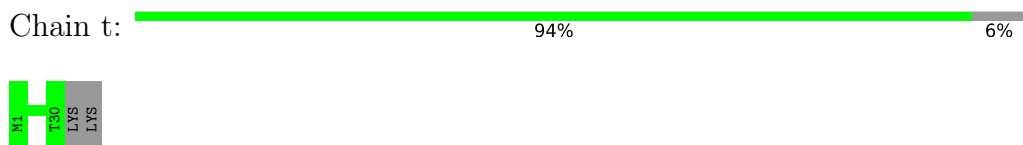
Chain o:  3% 86% 10%



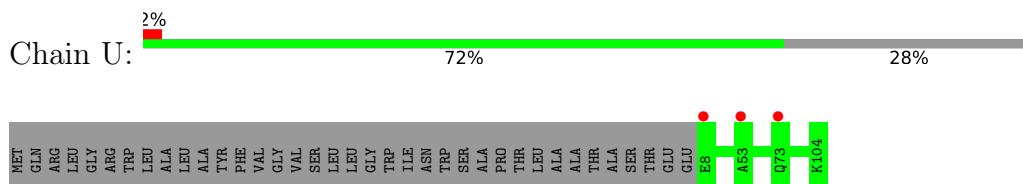
- Molecule 14: Photosystem II reaction center protein T



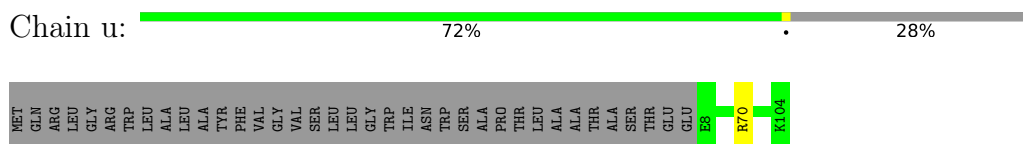
- Molecule 14: Photosystem II reaction center protein T



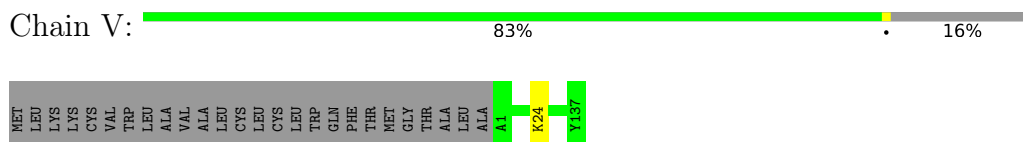
- Molecule 15: Photosystem II 12 kDa extrinsic protein



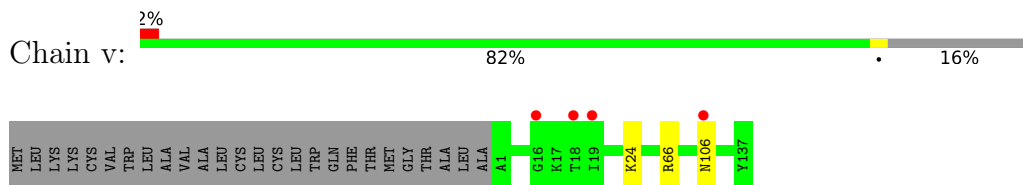
- Molecule 15: Photosystem II 12 kDa extrinsic protein



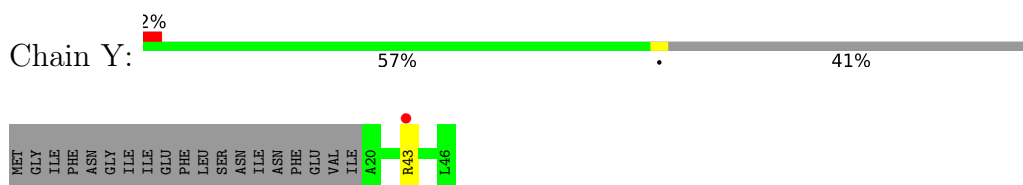
- Molecule 16: Cytochrome c-550



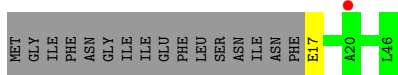
- Molecule 16: Cytochrome c-550



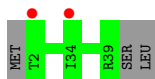
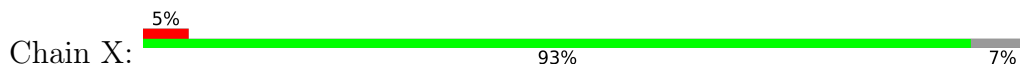
- Molecule 17: Photosystem II reaction center protein Ycf12



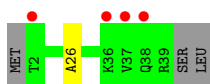
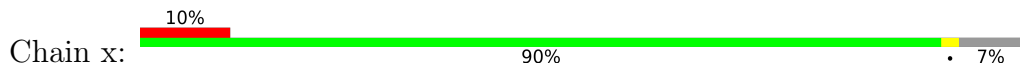
- Molecule 17: Photosystem II reaction center protein Ycf12



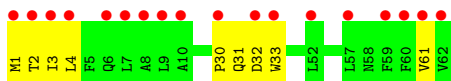
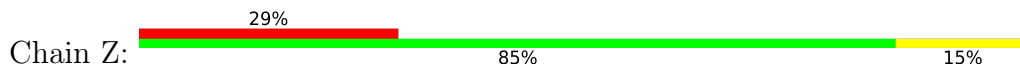
- Molecule 18: Photosystem II reaction center X protein



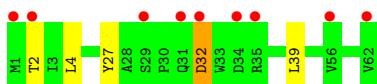
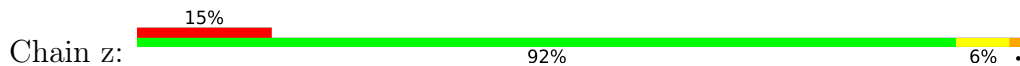
- Molecule 18: Photosystem II reaction center X protein



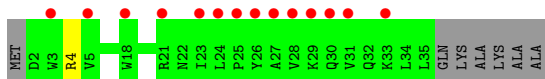
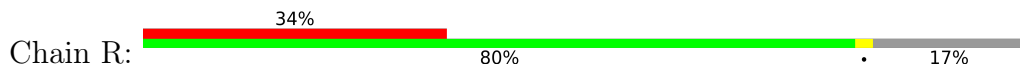
- Molecule 19: Photosystem II reaction center protein Z



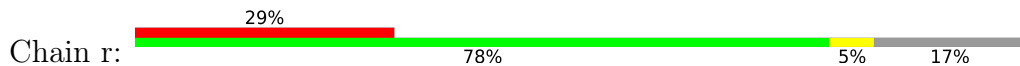
- Molecule 19: Photosystem II reaction center protein Z

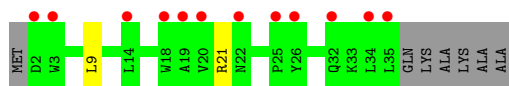


- Molecule 20: Photosystem II protein Y



- 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	117.91Å 224.27Å 331.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.57 – 2.80 43.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.57-2.80) 87.7 (43.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.81Å)	Xtrriage
Refinement program	PHENIX dev_2411	Depositor
R, R_{free}	0.250 , 0.300 0.250 , 0.300	Depositor DCC
R_{free} test set	1792 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50284	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: BCT, DGD, CL, CLA, FME, LHG, PL9, SQD, FE2, UNL, OEX, PHO, HEC, BCR, LMG, HEM

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	0.26	0/2707	0.42	0/3692
1	a	0.25	0/2707	0.40	0/3692
2	B	0.26	0/4109	0.41	0/5600
2	b	0.25	0/4111	0.41	0/5603
3	C	0.25	0/3599	0.40	0/4900
3	c	0.26	0/3599	0.43	0/4900
4	D	0.25	0/2811	0.40	0/3830
4	d	0.25	0/2811	0.40	0/3830
5	E	0.26	0/680	0.42	0/928
5	e	0.32	1/684 (0.1%)	0.40	0/933
6	F	0.25	0/284	0.40	0/387
6	f	0.24	0/284	0.36	0/387
7	H	0.27	0/511	0.44	0/697
7	h	0.24	0/511	0.41	0/697
8	I	0.26	0/293	0.40	0/396
8	i	0.56	1/293 (0.3%)	0.54	0/396
9	J	0.24	0/263	0.38	0/356
9	j	0.24	0/263	0.38	0/356
10	K	0.30	0/303	0.50	0/416
10	k	0.43	0/303	0.45	0/416
11	L	0.27	0/311	0.43	0/422
11	l	0.24	0/311	0.38	0/422
12	M	0.24	0/253	0.35	0/346
12	m	0.24	0/253	0.33	0/346
13	O	0.26	0/1905	0.46	0/2583
13	o	0.27	0/1905	0.52	1/2583 (0.0%)
14	T	0.27	0/257	0.36	0/349
14	t	0.26	0/257	0.36	0/349
15	U	0.24	0/785	0.43	0/1064
15	u	0.26	0/785	0.48	0/1064
16	V	0.23	0/1085	0.43	0/1473
16	v	0.23	0/1085	0.44	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.23	0/201	0.41	0/268
17	y	0.35	0/225	0.45	0/301
18	X	0.25	0/284	0.42	0/384
18	x	0.24	0/282	0.39	0/381
19	Z	0.30	0/490	0.51	0/669
19	z	0.35	0/489	0.52	0/669
20	R	0.27	0/279	0.52	0/383
20	r	0.25	0/276	0.51	0/379
All	All	0.26	2/42844 (0.0%)	0.42	1/58320 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	33	LYS	CB-CG	-6.06	1.36	1.52
5	e	63	ILE	C-N	5.53	1.44	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	54	GLU	C-N-CA	5.75	136.08	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	4	THR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	324 (98%)	7 (2%)	1 (0%)	41	72
1	a	332/344 (96%)	325 (98%)	6 (2%)	1 (0%)	41	72
2	B	502/510 (98%)	482 (96%)	19 (4%)	1 (0%)	47	78
2	b	503/510 (99%)	484 (96%)	19 (4%)	0	100	100
3	C	449/461 (97%)	431 (96%)	17 (4%)	1 (0%)	47	78
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	34	66
4	D	339/352 (96%)	325 (96%)	14 (4%)	0	100	100
4	d	339/352 (96%)	323 (95%)	16 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
7	h	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	29 (85%)	5 (15%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	4	15
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	4	15
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	4	15
11	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	4	13
12	m	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	4	13
13	O	242/272 (89%)	230 (95%)	10 (4%)	2 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	223 (92%)	15 (6%)	4 (2%)	9	29
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	88 (93%)	7 (7%)	0	100	100
16	V	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	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	36/41 (88%)	32 (89%)	3 (8%)	1 (3%)	5	17
19	Z	60/62 (97%)	51 (85%)	1 (2%)	8 (13%)	0	0
19	z	60/62 (97%)	53 (88%)	4 (7%)	3 (5%)	2	6
20	R	32/41 (78%)	29 (91%)	3 (9%)	0	100	100
20	r	32/41 (78%)	30 (94%)	1 (3%)	1 (3%)	4	14
All	All	5237/5694 (92%)	4987 (95%)	220 (4%)	30 (1%)	25	56

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	Z	30	PRO
19	Z	31	GLN
19	Z	33	TRP
19	Z	61	VAL
3	c	24	THR
10	k	12	PRO
13	o	53	LYS
13	o	55	GLU
19	z	32	ASP
3	C	416	SER
10	K	14	ALA
12	M	32	GLN
19	Z	3	ILE
19	Z	32	ASP
3	c	416	SER
18	x	26	ALA
13	O	132	ASN

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Mol	Chain	Res	Type
19	Z	2	THR
13	o	54	GLU
1	a	259	ILE
19	z	2	THR
19	z	4	LEU
20	r	21	ARG
13	O	56	PRO
19	Z	4	LEU
12	m	32	GLN
2	B	488	PRO
9	j	6	GLY
1	A	259	ILE
13	o	56	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	268 (99%)	2 (1%)	84	95
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	402/407 (99%)	397 (99%)	5 (1%)	71	92
2	b	402/407 (99%)	400 (100%)	2 (0%)	88	96
3	C	352/362 (97%)	350 (99%)	2 (1%)	86	96
3	c	352/362 (97%)	350 (99%)	2 (1%)	86	96
4	D	276/283 (98%)	274 (99%)	2 (1%)	84	95
4	d	276/283 (98%)	274 (99%)	2 (1%)	84	95
5	E	72/73 (99%)	72 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	53/53 (100%)	51 (96%)	2 (4%)	33	67
7	h	53/53 (100%)	52 (98%)	1 (2%)	57	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	74
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	63
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	207/228 (91%)	206 (100%)	1 (0%)	88	96
13	o	207/228 (91%)	202 (98%)	5 (2%)	49	81
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	92
16	V	117/138 (85%)	116 (99%)	1 (1%)	78	94
16	v	117/138 (85%)	114 (97%)	3 (3%)	46	79
17	Y	20/37 (54%)	19 (95%)	1 (5%)	24	56
17	y	23/37 (62%)	22 (96%)	1 (4%)	29	62
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	30/34 (88%)	30 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	85
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	50
20	R	29/33 (88%)	28 (97%)	1 (3%)	37	71
20	r	28/33 (85%)	27 (96%)	1 (4%)	35	69
All	All	4339/4650 (93%)	4298 (99%)	41 (1%)	78	94

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASP
1	A	245	THR

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Mol	Chain	Res	Type
2	B	107	LEU
2	B	362	PHE
2	B	394	GLN
2	B	438	ASN
2	B	505	ARG
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
4	D	315	TYR
7	H	39	LEU
7	H	49	TYR
9	J	7	ARG
13	O	118	LEU
16	V	24	LYS
17	Y	43	ARG
19	Z	1	MET
20	R	4	ARG
2	b	127	ARG
2	b	362	PHE
3	c	418	ASN
3	c	420	VAL
4	d	180	ARG
4	d	247	VAL
7	h	49	TYR
8	i	35	LYS
13	o	57	LYS
13	o	60	ARG
13	o	132	ASN
13	o	141	ASP
13	o	200	ASN
15	u	70	ARG
16	v	24	LYS
16	v	66	ARG
16	v	106	ASN
17	y	17	GLU
19	z	27	TYR
19	z	32	ASP
19	z	39	LEU
20	r	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	252	HIS
1	A	312	ASN
2	B	216	HIS
2	B	409	GLN
3	C	201	ASN
3	C	311	GLN
4	D	98	GLN
5	E	74	GLN
11	L	6	ASN
13	O	82	GLN
13	O	130	GLN
13	O	200	ASN
15	U	29	ASN
16	V	106	ASN
20	R	32	GLN
1	a	261	GLN
1	a	335	ASN
2	b	216	HIS
2	b	223	GLN
2	b	409	GLN
3	c	311	GLN
4	d	239	GLN
5	e	74	GLN
13	o	46	GLN
13	o	61	GLN
13	o	147	ASN
13	o	236	GLN
16	v	25	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	I	1	8	8,9,10	0.95	0	7,9,11	1.08	0
12	FME	m	1	12	8,9,10	0.94	0	7,9,11	0.89	0
8	FME	i	1	8	8,9,10	0.94	0	7,9,11	0.92	0
12	FME	M	1	12	8,9,10	0.90	0	7,9,11	0.86	0
14	FME	T	1	14	8,9,10	0.95	0	7,9,11	0.92	0
14	FME	t	1	14	8,9,10	0.94	0	7,9,11	0.86	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
8	I	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 6 are monoatomic and 23 are unknown - leaving 151 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
23	LMG	A	603	-	51,51,55	0.95	2 (3%)	59,59,63	1.40	7 (11%)
25	CLA	B	602	36	65,73,73	1.48	5 (7%)	76,113,113	1.33	8 (10%)
32	LHG	L	101	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
33	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.41	11 (14%)
33	DGD	C	518	-	63,63,67	0.92	4 (6%)	77,77,81	1.44	9 (11%)
32	LHG	d	407	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
29	SQD	A	614	-	39,39,54	0.88	2 (5%)	41,41,65	1.19	3 (7%)
25	CLA	A	606	-	65,73,73	1.47	6 (9%)	76,113,113	1.25	9 (11%)
25	CLA	C	503	-	65,73,73	1.47	5 (7%)	76,113,113	1.33	8 (10%)
25	CLA	b	610	-	65,73,73	1.47	5 (7%)	76,113,113	1.45	10 (13%)
23	LMG	c	519	-	51,51,55	0.71	0	59,59,63	1.32	5 (8%)
25	CLA	A	609	-	54,62,73	1.63	5 (9%)	62,99,113	1.40	8 (12%)
25	CLA	B	603	-	65,73,73	1.49	5 (7%)	76,113,113	1.29	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	609	-	65,73,73	1.47	6 (9%)	76,113,113	1.27	8 (10%)
32	LHG	D	407	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
25	CLA	C	512	3	65,73,73	1.47	5 (7%)	76,113,113	1.38	8 (10%)
23	LMG	b	627	-	51,51,55	0.78	0	59,59,63	1.27	4 (6%)
25	CLA	A	607	36	65,73,73	1.48	5 (7%)	76,113,113	1.30	9 (11%)
32	LHG	e	101	-	41,41,48	0.68	1 (2%)	44,47,54	1.32	7 (15%)
25	CLA	c	511	3	65,73,73	1.46	6 (9%)	76,113,113	1.36	8 (10%)
27	BCR	a	712	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	6 (10%)
25	CLA	d	403	-	65,73,73	1.46	5 (7%)	76,113,113	1.34	8 (10%)
23	LMG	f	101	-	51,51,55	0.71	0	59,59,63	1.35	7 (11%)
26	PHO	a	709	-	51,69,69	1.00	3 (5%)	47,99,99	1.12	6 (12%)
25	CLA	c	502	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	8 (10%)
29	SQD	A	612	-	51,52,54	0.96	5 (9%)	60,63,65	1.67	12 (20%)
29	SQD	f	102	-	40,41,54	1.09	5 (12%)	49,52,65	1.60	9 (18%)
32	LHG	B	625	-	48,48,48	0.62	2 (4%)	51,54,54	1.27	6 (11%)
27	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	5 (8%)
25	CLA	B	617	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
23	LMG	a	701	-	51,51,55	0.80	0	59,59,63	1.32	7 (11%)
29	SQD	I	102	-	39,39,54	0.86	2 (5%)	41,41,65	1.22	2 (4%)
27	BCR	t	103	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
27	BCR	H	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
28	PL9	d	405	-	55,55,55	0.94	3 (5%)	68,69,69	1.51	11 (16%)
25	CLA	D	403	-	65,73,73	1.50	6 (9%)	76,113,113	1.26	7 (9%)
23	LMG	M	101	-	51,51,55	0.74	0	59,59,63	1.32	5 (8%)
25	CLA	B	613	-	65,73,73	1.45	5 (7%)	76,113,113	1.38	8 (10%)
25	CLA	C	508	36	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
25	CLA	C	504	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
34	HEM	e	102	5,6	41,50,50	1.52	5 (12%)	45,82,82	1.48	7 (15%)
25	CLA	b	611	-	65,73,73	1.49	6 (9%)	76,113,113	1.29	8 (10%)
33	DGD	C	519	-	63,63,67	0.88	1 (1%)	77,77,81	1.41	9 (11%)
25	CLA	c	504	36	58,66,73	1.54	5 (8%)	67,104,113	1.41	8 (11%)
29	SQD	b	601	-	53,54,54	0.94	3 (5%)	62,65,65	1.72	10 (16%)
25	CLA	c	507	36	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
28	PL9	A	611	-	55,55,55	1.04	4 (7%)	68,69,69	1.51	11 (16%)
33	DGD	c	517	-	63,63,67	0.95	4 (6%)	77,77,81	1.41	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMG	D	409	-	51,51,55	0.72	0	59,59,63	1.30	5 (8%)
27	BCR	B	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	8 (14%)
25	CLA	B	607	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	7 (9%)
23	LMG	C	521	-	51,51,55	0.79	1 (1%)	59,59,63	1.37	6 (10%)
25	CLA	B	604	-	65,73,73	1.47	6 (9%)	76,113,113	1.31	8 (10%)
27	BCR	K	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	6 (10%)
25	CLA	c	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.26	7 (9%)
27	BCR	A	610	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	5 (8%)
27	BCR	c	514	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	7 (12%)
27	BCR	b	624	-	41,41,41	1.10	2 (4%)	56,56,56	1.19	5 (8%)
32	LHG	d	406	-	48,48,48	0.61	0	51,54,54	1.28	6 (11%)
27	BCR	b	602	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	6 (10%)
29	SQD	B	626	-	53,54,54	0.95	5 (9%)	62,65,65	1.71	10 (16%)
27	BCR	b	625	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	8 (14%)
32	LHG	D	408	-	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
27	BCR	B	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	4 (7%)
25	CLA	C	509	-	65,73,73	1.47	5 (7%)	76,113,113	1.36	8 (10%)
21	OEX	A	601	36,3,1	0,15,15	-	-	-	-	-
25	CLA	D	404	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	8 (10%)
29	SQD	D	410	-	42,43,54	1.06	5 (11%)	51,54,65	1.63	10 (19%)
25	CLA	a	711	-	65,73,73	1.49	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	B	616	-	65,73,73	1.50	5 (7%)	76,113,113	1.34	7 (9%)
26	PHO	D	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.15	5 (10%)
23	LMG	C	501	-	51,51,55	0.73	0	59,59,63	1.31	5 (8%)
25	CLA	B	608	36	65,73,73	1.47	5 (7%)	76,113,113	1.26	8 (10%)
25	CLA	c	503	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
25	CLA	C	511	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	9 (11%)
33	DGD	h	102	-	63,63,67	0.89	0	77,77,81	1.29	7 (9%)
33	DGD	H	103	-	63,63,67	0.87	1 (1%)	77,77,81	1.34	7 (9%)
27	BCR	Y	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	5 (8%)
33	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.41	9 (11%)
25	CLA	C	505	36	65,73,73	1.46	5 (7%)	76,113,113	1.29	8 (10%)
25	CLA	b	613	36	65,73,73	1.47	5 (7%)	76,113,113	1.25	8 (10%)
31	BCT	A	615	22	2,3,3	1.25	0	2,3,3	2.64	2 (100%)
25	CLA	b	608	-	65,73,73	1.49	5 (7%)	76,113,113	1.24	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	618	-	65,73,73	1.47	6 (9%)	76,113,113	1.33	8 (10%)
25	CLA	C	510	-	65,73,73	1.47	5 (7%)	76,113,113	1.32	7 (9%)
21	OEX	a	702	36,3,1	0,15,15	-	-	-	-	-
25	CLA	B	615	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	8 (10%)
35	HEC	V	201	16	32,50,50	2.15	5 (15%)	24,82,82	1.55	4 (16%)
27	BCR	c	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
25	CLA	D	402	36	65,73,73	1.46	5 (7%)	76,113,113	1.32	8 (10%)
31	BCT	a	706	22	2,3,3	1.25	0	2,3,3	2.70	2 (100%)
25	CLA	b	612	-	65,73,73	1.48	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	c	512	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
23	LMG	a	715	-	51,51,55	0.75	0	59,59,63	1.32	6 (10%)
25	CLA	c	508	-	65,73,73	1.48	5 (7%)	76,113,113	1.31	9 (11%)
23	LMG	C	520	-	51,51,55	0.75	1 (1%)	59,59,63	1.31	5 (8%)
25	CLA	a	707	-	65,73,73	1.47	6 (9%)	76,113,113	1.29	8 (10%)
35	HEC	v	201	16	32,50,50	2.13	5 (15%)	24,82,82	1.53	4 (16%)
25	CLA	B	606	-	65,73,73	1.49	5 (7%)	76,113,113	1.27	7 (9%)
25	CLA	C	514	-	65,73,73	1.44	5 (7%)	76,113,113	1.38	8 (10%)
25	CLA	c	506	-	65,73,73	1.48	5 (7%)	76,113,113	1.29	8 (10%)
25	CLA	a	708	36	65,73,73	1.46	5 (7%)	76,113,113	1.29	7 (9%)
28	PL9	a	713	-	55,55,55	0.98	3 (5%)	68,69,69	1.51	12 (17%)
25	CLA	C	506	-	65,73,73	1.49	6 (9%)	76,113,113	1.33	7 (9%)
27	BCR	k	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	6 (10%)
25	CLA	b	622	-	47,55,73	1.70	5 (10%)	54,91,113	1.55	8 (14%)
27	BCR	k	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.13	2 (3%)
33	DGD	c	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.41	9 (11%)
32	LHG	E	101	-	48,48,48	0.67	1 (2%)	51,54,54	1.22	6 (11%)
25	CLA	c	501	-	65,73,73	1.46	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	B	610	-	65,73,73	1.52	5 (7%)	76,113,113	1.31	8 (10%)
23	LMG	d	408	-	39,39,55	0.53	1 (2%)	41,41,63	1.29	4 (9%)
25	CLA	b	607	36	65,73,73	1.47	5 (7%)	76,113,113	1.36	9 (11%)
26	PHO	a	710	-	51,69,69	0.98	3 (5%)	47,99,99	1.17	4 (8%)
32	LHG	a	720	-	38,38,48	0.68	0	41,44,54	1.17	3 (7%)
25	CLA	b	619	-	65,73,73	1.45	5 (7%)	76,113,113	1.39	9 (11%)
34	HEM	E	102	5,6	41,50,50	1.52	6 (14%)	45,82,82	1.31	4 (8%)
25	CLA	C	502	-	65,73,73	1.47	5 (7%)	76,113,113	1.32	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	h	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	6 (10%)
27	BCR	C	516	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
25	CLA	B	605	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	10 (13%)
25	CLA	c	513	-	65,73,73	1.44	5 (7%)	76,113,113	1.37	8 (10%)
25	CLA	c	510	-	65,73,73	1.44	6 (9%)	76,113,113	1.34	7 (9%)
25	CLA	C	513	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
32	LHG	b	629	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	a	719	36	65,73,73	1.48	5 (7%)	76,113,113	1.28	8 (10%)
25	CLA	B	614	-	65,73,73	1.47	5 (7%)	76,113,113	1.34	8 (10%)
25	CLA	C	507	-	65,73,73	1.51	5 (7%)	76,113,113	1.27	8 (10%)
25	CLA	b	620	-	65,73,73	1.48	5 (7%)	76,113,113	1.26	8 (10%)
29	SQD	B	623	-	46,47,54	1.01	3 (6%)	55,58,65	1.82	12 (21%)
28	PL9	D	406	-	55,55,55	0.98	3 (5%)	68,69,69	1.53	13 (19%)
27	BCR	b	623	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	7 (12%)
25	CLA	b	615	-	65,73,73	1.50	5 (7%)	76,113,113	1.32	9 (11%)
25	CLA	d	402	-	65,73,73	1.49	6 (9%)	76,113,113	1.28	8 (10%)
25	CLA	b	614	-	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	c	509	-	65,73,73	1.47	5 (7%)	76,113,113	1.37	8 (10%)
26	PHO	A	608	-	51,69,69	0.99	2 (3%)	47,99,99	1.11	5 (10%)
23	LMG	B	621	-	51,51,55	0.73	0	59,59,63	1.37	7 (11%)
25	CLA	b	616	36	65,73,73	1.47	5 (7%)	76,113,113	1.27	7 (9%)
27	BCR	C	515	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	8 (14%)
29	SQD	a	714	-	53,54,54	0.95	5 (9%)	62,65,65	1.63	12 (19%)
23	LMG	b	626	-	51,51,55	0.81	2 (3%)	59,59,63	1.53	9 (15%)
25	CLA	b	609	-	65,73,73	1.49	6 (9%)	76,113,113	1.25	7 (9%)
27	BCR	D	405	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
25	CLA	b	617	-	65,73,73	1.44	5 (7%)	76,113,113	1.39	9 (11%)
25	CLA	b	621	-	65,73,73	1.47	5 (7%)	76,113,113	1.35	9 (11%)
27	BCR	d	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	8 (14%)
25	CLA	B	611	36	65,73,73	1.47	5 (7%)	76,113,113	1.30	9 (11%)
23	LMG	b	628	-	8,8,55	0.15	0	7,7,63	0.92	0
25	CLA	B	612	-	65,73,73	1.45	5 (7%)	76,113,113	1.37	9 (11%)
23	LMG	c	520	-	51,51,55	0.82	1 (1%)	59,59,63	1.36	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMG	A	603	-	-	24/46/66/70	0/1/1/1
25	CLA	B	602	36	1/1/15/20	15/37/115/115	-
32	LHG	L	101	-	-	18/53/53/53	-
33	DGD	c	518	-	-	11/51/91/95	0/2/2/2
33	DGD	C	518	-	-	24/51/91/95	0/2/2/2
32	LHG	d	407	-	-	14/53/53/53	-
29	SQD	A	614	-	-	21/41/41/69	-
25	CLA	A	606	-	1/1/15/20	2/37/115/115	-
25	CLA	C	503	-	1/1/15/20	17/37/115/115	-
25	CLA	b	610	-	1/1/15/20	11/37/115/115	-
23	LMG	c	519	-	-	23/46/66/70	0/1/1/1
25	CLA	A	609	-	1/1/12/20	0/24/102/115	-
25	CLA	B	603	-	-	8/37/115/115	-
25	CLA	B	609	-	1/1/15/20	12/37/115/115	-
32	LHG	D	407	-	-	18/53/53/53	-
25	CLA	C	512	3	1/1/15/20	14/37/115/115	-
25	CLA	A	607	36	1/1/15/20	7/37/115/115	-
23	LMG	b	627	-	-	18/46/66/70	0/1/1/1
32	LHG	e	101	-	-	22/46/46/53	-
25	CLA	c	511	3	1/1/15/20	10/37/115/115	-
27	BCR	a	712	-	-	5/29/63/63	0/2/2/2
25	CLA	d	403	-	-	9/37/115/115	-
23	LMG	f	101	-	-	16/46/66/70	0/1/1/1
26	PHO	a	709	-	-	5/37/103/103	0/5/6/6
25	CLA	c	502	-	1/1/15/20	13/37/115/115	-
29	SQD	A	612	-	-	18/47/67/69	0/1/1/1
29	SQD	f	102	-	-	11/36/56/69	0/1/1/1
32	LHG	B	625	-	-	19/53/53/53	-
27	BCR	B	619	-	-	5/29/63/63	0/2/2/2
25	CLA	B	617	-	1/1/15/20	11/37/115/115	-
23	LMG	a	701	-	-	26/46/66/70	0/1/1/1
29	SQD	I	102	-	-	25/41/41/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	t	103	-	-	8/29/63/63	0/2/2/2
27	BCR	H	102	-	-	7/29/63/63	0/2/2/2
28	PL9	d	405	-	-	8/53/73/73	0/1/1/1
25	CLA	D	403	-	-	10/37/115/115	-
25	CLA	B	613	-	1/1/15/20	10/37/115/115	-
23	LMG	M	101	-	-	13/46/66/70	0/1/1/1
25	CLA	C	508	36	1/1/15/20	9/37/115/115	-
25	CLA	C	504	-	1/1/15/20	13/37/115/115	-
34	HEM	e	102	5,6	-	6/12/54/54	-
25	CLA	b	611	-	-	11/37/115/115	-
33	DGD	C	519	-	-	16/51/91/95	0/2/2/2
25	CLA	c	504	36	1/1/13/20	5/29/107/115	-
29	SQD	b	601	-	-	25/49/69/69	0/1/1/1
25	CLA	c	507	36	1/1/15/20	8/37/115/115	-
28	PL9	A	611	-	-	8/53/73/73	0/1/1/1
33	DGD	c	517	-	-	19/51/91/95	0/2/2/2
23	LMG	D	409	-	-	19/46/66/70	0/1/1/1
27	BCR	B	618	-	-	4/29/63/63	0/2/2/2
25	CLA	B	607	-	1/1/15/20	16/37/115/115	-
25	CLA	B	604	-	1/1/15/20	18/37/115/115	-
23	LMG	C	521	-	-	18/46/66/70	0/1/1/1
27	BCR	K	101	-	-	4/29/63/63	0/2/2/2
25	CLA	c	505	-	-	7/37/115/115	-
27	BCR	A	610	-	-	4/29/63/63	0/2/2/2
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
27	BCR	b	624	-	-	7/29/63/63	0/2/2/2
32	LHG	d	406	-	-	16/53/53/53	-
27	BCR	b	602	-	-	6/29/63/63	0/2/2/2
29	SQD	B	626	-	-	23/49/69/69	0/1/1/1
27	BCR	b	625	-	-	7/29/63/63	0/2/2/2
32	LHG	D	408	-	-	25/53/53/53	-
27	BCR	B	620	-	-	6/29/63/63	0/2/2/2
25	CLA	C	509	-	1/1/15/20	7/37/115/115	-
25	CLA	D	404	-	-	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	D	410	-	-	16/38/58/69	0/1/1/1
25	CLA	a	711	-	1/1/15/20	11/37/115/115	-
25	CLA	B	616	-	1/1/15/20	11/37/115/115	-
26	PHO	D	401	-	-	6/37/103/103	0/5/6/6
25	CLA	c	503	-	1/1/15/20	9/37/115/115	-
25	CLA	B	608	36	1/1/15/20	11/37/115/115	-
23	LMG	C	501	-	-	22/46/66/70	0/1/1/1
25	CLA	C	511	-	1/1/15/20	11/37/115/115	-
33	DGD	h	102	-	-	16/51/91/95	0/2/2/2
33	DGD	H	103	-	-	10/51/91/95	0/2/2/2
27	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
33	DGD	C	517	-	-	17/51/91/95	0/2/2/2
25	CLA	C	505	36	1/1/15/20	11/37/115/115	-
25	CLA	b	613	36	1/1/15/20	9/37/115/115	-
25	CLA	b	608	-	1/1/15/20	9/37/115/115	-
25	CLA	b	618	-	1/1/15/20	12/37/115/115	-
25	CLA	C	510	-	1/1/15/20	17/37/115/115	-
25	CLA	B	615	-	1/1/15/20	16/37/115/115	-
35	HEC	V	201	16	-	1/10/54/54	-
27	BCR	c	515	-	-	6/29/63/63	0/2/2/2
25	CLA	D	402	36	-	6/37/115/115	-
25	CLA	b	612	-	1/1/15/20	12/37/115/115	-
25	CLA	c	512	-	1/1/15/20	15/37/115/115	-
23	LMG	a	715	-	-	25/46/66/70	0/1/1/1
25	CLA	c	508	-	-	14/37/115/115	-
23	LMG	C	520	-	-	25/46/66/70	0/1/1/1
25	CLA	a	707	-	1/1/15/20	6/37/115/115	-
35	HEC	v	201	16	-	0/10/54/54	-
25	CLA	B	606	-	1/1/15/20	15/37/115/115	-
25	CLA	C	514	-	1/1/15/20	7/37/115/115	-
25	CLA	c	506	-	-	14/37/115/115	-
25	CLA	a	708	36	1/1/15/20	8/37/115/115	-
28	PL9	a	713	-	-	13/53/73/73	0/1/1/1
25	CLA	C	506	-	-	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	k	102	-	-	4/29/63/63	0/2/2/2
25	CLA	b	622	-	1/1/11/20	2/16/94/115	-
27	BCR	k	101	-	-	8/29/63/63	0/2/2/2
33	DGD	c	516	-	-	15/51/91/95	0/2/2/2
32	LHG	E	101	-	-	28/53/53/53	-
25	CLA	c	501	-	1/1/15/20	8/37/115/115	-
25	CLA	B	610	-	-	11/37/115/115	-
23	LMG	d	408	-	-	19/41/41/70	-
25	CLA	b	607	36	1/1/15/20	16/37/115/115	-
26	PHO	a	710	-	-	7/37/103/103	0/5/6/6
32	LHG	a	720	-	-	18/43/43/53	-
25	CLA	b	619	-	1/1/15/20	10/37/115/115	-
34	HEM	E	102	5,6	-	3/12/54/54	-
25	CLA	C	502	-	1/1/15/20	8/37/115/115	-
27	BCR	h	101	-	-	6/29/63/63	0/2/2/2
27	BCR	C	516	-	-	6/29/63/63	0/2/2/2
25	CLA	B	605	-	1/1/15/20	10/37/115/115	-
25	CLA	c	513	-	1/1/15/20	17/37/115/115	-
25	CLA	c	510	-	1/1/15/20	16/37/115/115	-
25	CLA	C	513	-	1/1/15/20	12/37/115/115	-
32	LHG	b	629	-	-	20/53/53/53	-
25	CLA	a	719	36	1/1/15/20	9/37/115/115	-
25	CLA	B	614	-	1/1/15/20	9/37/115/115	-
25	CLA	C	507	-	-	14/37/115/115	-
25	CLA	b	620	-	1/1/15/20	12/37/115/115	-
29	SQD	B	623	-	-	23/42/62/69	0/1/1/1
28	PL9	D	406	-	-	9/53/73/73	0/1/1/1
27	BCR	b	623	-	-	3/29/63/63	0/2/2/2
25	CLA	b	615	-	-	11/37/115/115	-
25	CLA	d	402	-	-	9/37/115/115	-
25	CLA	b	614	-	1/1/15/20	3/37/115/115	-
25	CLA	c	509	-	1/1/15/20	5/37/115/115	-
26	PHO	A	608	-	-	9/37/103/103	0/5/6/6
23	LMG	B	621	-	-	19/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	616	36	1/1/15/20	5/37/115/115	-
27	BCR	C	515	-	-	4/29/63/63	0/2/2/2
29	SQD	a	714	-	-	16/49/69/69	0/1/1/1
23	LMG	b	626	-	-	16/46/66/70	0/1/1/1
25	CLA	b	609	-	1/1/15/20	17/37/115/115	-
27	BCR	D	405	-	-	8/29/63/63	0/2/2/2
25	CLA	b	617	-	1/1/15/20	16/37/115/115	-
25	CLA	b	621	-	1/1/15/20	9/37/115/115	-
27	BCR	d	404	-	-	7/29/63/63	0/2/2/2
25	CLA	B	611	36	1/1/15/20	10/37/115/115	-
23	LMG	b	628	-	-	3/6/6/70	-
25	CLA	B	612	-	1/1/15/20	5/37/115/115	-
23	LMG	c	520	-	-	16/46/66/70	0/1/1/1

All (523) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	C4B-NB	7.76	1.42	1.35
25	C	507	CLA	C4B-NB	7.73	1.42	1.35
25	c	505	CLA	C4B-NB	7.72	1.42	1.35
25	D	403	CLA	C4B-NB	7.70	1.42	1.35
25	b	615	CLA	C4B-NB	7.68	1.42	1.35
25	C	506	CLA	C4B-NB	7.66	1.42	1.35
25	d	402	CLA	C4B-NB	7.66	1.42	1.35
25	b	609	CLA	C4B-NB	7.64	1.42	1.35
25	B	607	CLA	C4B-NB	7.64	1.42	1.35
25	A	609	CLA	C4B-NB	7.60	1.42	1.35
25	c	506	CLA	C4B-NB	7.59	1.42	1.35
25	b	612	CLA	C4B-NB	7.58	1.42	1.35
25	B	616	CLA	C4B-NB	7.57	1.42	1.35
25	B	606	CLA	C4B-NB	7.55	1.41	1.35
25	b	608	CLA	C4B-NB	7.55	1.41	1.35
25	a	711	CLA	C4B-NB	7.54	1.41	1.35
25	B	615	CLA	C4B-NB	7.54	1.41	1.35
25	B	603	CLA	C4B-NB	7.52	1.41	1.35
25	a	719	CLA	C4B-NB	7.52	1.41	1.35
25	D	404	CLA	C4B-NB	7.52	1.41	1.35
25	b	611	CLA	C4B-NB	7.51	1.41	1.35
25	B	604	CLA	C4B-NB	7.50	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	620	CLA	C4B-NB	7.50	1.41	1.35
25	c	508	CLA	C4B-NB	7.50	1.41	1.35
25	b	614	CLA	C4B-NB	7.49	1.41	1.35
25	a	707	CLA	C4B-NB	7.48	1.41	1.35
25	C	504	CLA	C4B-NB	7.46	1.41	1.35
25	b	621	CLA	C4B-NB	7.45	1.41	1.35
25	c	507	CLA	C4B-NB	7.44	1.41	1.35
25	b	616	CLA	C4B-NB	7.44	1.41	1.35
25	B	602	CLA	C4B-NB	7.43	1.41	1.35
25	B	611	CLA	C4B-NB	7.43	1.41	1.35
25	C	509	CLA	C4B-NB	7.43	1.41	1.35
25	C	508	CLA	C4B-NB	7.42	1.41	1.35
25	C	513	CLA	C4B-NB	7.42	1.41	1.35
25	d	403	CLA	C4B-NB	7.42	1.41	1.35
25	C	503	CLA	C4B-NB	7.42	1.41	1.35
25	b	607	CLA	C4B-NB	7.42	1.41	1.35
25	b	618	CLA	C4B-NB	7.42	1.41	1.35
25	b	610	CLA	C4B-NB	7.40	1.41	1.35
25	B	608	CLA	C4B-NB	7.39	1.41	1.35
25	A	606	CLA	C4B-NB	7.39	1.41	1.35
25	B	617	CLA	C4B-NB	7.37	1.41	1.35
25	c	512	CLA	C4B-NB	7.37	1.41	1.35
25	c	503	CLA	C4B-NB	7.37	1.41	1.35
25	C	505	CLA	C4B-NB	7.36	1.41	1.35
25	b	613	CLA	C4B-NB	7.35	1.41	1.35
25	B	614	CLA	C4B-NB	7.35	1.41	1.35
25	C	512	CLA	C4B-NB	7.35	1.41	1.35
25	c	509	CLA	C4B-NB	7.35	1.41	1.35
25	B	609	CLA	C4B-NB	7.35	1.41	1.35
25	B	605	CLA	C4B-NB	7.32	1.41	1.35
25	C	502	CLA	C4B-NB	7.32	1.41	1.35
25	c	501	CLA	C4B-NB	7.32	1.41	1.35
25	B	612	CLA	C4B-NB	7.31	1.41	1.35
25	b	622	CLA	C4B-NB	7.31	1.41	1.35
25	A	607	CLA	C4B-NB	7.30	1.41	1.35
25	c	511	CLA	C4B-NB	7.29	1.41	1.35
25	B	613	CLA	C4B-NB	7.29	1.41	1.35
25	C	511	CLA	C4B-NB	7.29	1.41	1.35
25	D	402	CLA	C4B-NB	7.27	1.41	1.35
25	b	619	CLA	C4B-NB	7.26	1.41	1.35
25	C	510	CLA	C4B-NB	7.26	1.41	1.35
25	c	502	CLA	C4B-NB	7.25	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	708	CLA	C4B-NB	7.22	1.41	1.35
25	c	504	CLA	C4B-NB	7.20	1.41	1.35
25	b	617	CLA	C4B-NB	7.17	1.41	1.35
25	c	510	CLA	C4B-NB	7.13	1.41	1.35
25	C	514	CLA	C4B-NB	7.13	1.41	1.35
25	c	513	CLA	C4B-NB	7.11	1.41	1.35
35	V	201	HEC	C3C-C2C	-6.58	1.33	1.40
35	v	201	HEC	C3C-C2C	-6.41	1.34	1.40
35	v	201	HEC	C2B-C3B	-5.34	1.35	1.40
35	V	201	HEC	C2B-C3B	-5.33	1.35	1.40
34	E	102	HEM	C3C-C2C	-4.61	1.34	1.40
34	e	102	HEM	C3C-C2C	-4.52	1.34	1.40
35	V	201	HEC	CBC-CAC	-4.15	1.33	1.49
35	v	201	HEC	CBC-CAC	-4.11	1.34	1.49
28	A	611	PL9	C7-C3	-4.09	1.47	1.51
35	V	201	HEC	CBB-CAB	-4.05	1.34	1.49
35	v	201	HEC	CBB-CAB	-4.04	1.34	1.49
25	B	610	CLA	C1D-ND	3.95	1.42	1.37
25	C	508	CLA	C1D-ND	3.95	1.42	1.37
25	B	605	CLA	C1D-ND	3.93	1.42	1.37
25	B	614	CLA	C1D-ND	3.90	1.42	1.37
25	B	617	CLA	C1D-ND	3.90	1.42	1.37
25	c	509	CLA	C1D-ND	3.89	1.42	1.37
25	b	615	CLA	C1D-ND	3.88	1.42	1.37
25	c	507	CLA	C1D-ND	3.88	1.42	1.37
25	B	616	CLA	C1D-ND	3.87	1.42	1.37
25	C	510	CLA	C1D-ND	3.87	1.42	1.37
25	B	611	CLA	C1D-ND	3.87	1.42	1.37
25	b	622	CLA	C1D-ND	3.86	1.42	1.37
25	D	404	CLA	C1D-ND	3.86	1.42	1.37
25	b	619	CLA	C1D-ND	3.86	1.42	1.37
25	b	616	CLA	C1D-ND	3.84	1.42	1.37
25	c	511	CLA	C1D-ND	3.84	1.42	1.37
25	B	603	CLA	C1D-ND	3.83	1.42	1.37
25	B	602	CLA	C1D-ND	3.82	1.42	1.37
25	C	507	CLA	C1D-ND	3.81	1.42	1.37
25	b	610	CLA	C1D-ND	3.81	1.42	1.37
25	C	513	CLA	C1D-ND	3.81	1.42	1.37
25	C	512	CLA	C1D-ND	3.81	1.42	1.37
25	B	606	CLA	C1D-ND	3.81	1.42	1.37
25	B	613	CLA	C1D-ND	3.81	1.42	1.37
25	a	719	CLA	C1D-ND	3.80	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	606	CLA	C1D-ND	3.80	1.42	1.37
25	c	504	CLA	C1D-ND	3.79	1.42	1.37
25	b	611	CLA	C1D-ND	3.78	1.42	1.37
25	A	607	CLA	C1D-ND	3.78	1.42	1.37
25	D	403	CLA	C1D-ND	3.77	1.42	1.37
25	c	503	CLA	C1D-ND	3.77	1.42	1.37
25	a	711	CLA	C1D-ND	3.77	1.42	1.37
25	C	511	CLA	C1D-ND	3.77	1.42	1.37
25	b	608	CLA	C1D-ND	3.77	1.42	1.37
25	c	501	CLA	C1D-ND	3.77	1.42	1.37
25	B	615	CLA	C1D-ND	3.77	1.42	1.37
25	C	509	CLA	C1D-ND	3.76	1.42	1.37
25	C	504	CLA	C1D-ND	3.76	1.42	1.37
25	a	708	CLA	C1D-ND	3.75	1.42	1.37
25	C	506	CLA	C1D-ND	3.75	1.42	1.37
25	A	609	CLA	C1D-ND	3.75	1.42	1.37
25	b	618	CLA	C1D-ND	3.74	1.42	1.37
25	d	403	CLA	C1D-ND	3.74	1.42	1.37
25	D	402	CLA	C1D-ND	3.73	1.42	1.37
25	B	607	CLA	C1D-ND	3.73	1.42	1.37
25	c	513	CLA	C1D-ND	3.73	1.42	1.37
34	e	102	HEM	C3C-CAC	3.73	1.55	1.47
34	E	102	HEM	C3C-CAC	3.72	1.55	1.47
25	d	402	CLA	C1D-ND	3.72	1.42	1.37
25	b	621	CLA	C1D-ND	3.72	1.42	1.37
25	C	502	CLA	C1D-ND	3.71	1.42	1.37
25	B	612	CLA	C1D-ND	3.71	1.42	1.37
27	d	404	BCR	C1-C6	-3.71	1.48	1.53
25	c	508	CLA	C1D-ND	3.71	1.42	1.37
25	c	510	CLA	C1D-ND	3.70	1.42	1.37
25	a	707	CLA	C1D-ND	3.70	1.42	1.37
25	c	505	CLA	C1D-ND	3.70	1.42	1.37
25	c	512	CLA	C1D-ND	3.70	1.42	1.37
25	b	607	CLA	C1D-ND	3.69	1.42	1.37
25	b	613	CLA	C1D-ND	3.69	1.42	1.37
25	B	608	CLA	C1D-ND	3.68	1.42	1.37
25	C	503	CLA	C1D-ND	3.68	1.42	1.37
25	c	502	CLA	C1D-ND	3.68	1.42	1.37
25	b	617	CLA	C1D-ND	3.67	1.42	1.37
25	b	614	CLA	C1D-ND	3.67	1.42	1.37
25	c	506	CLA	C1D-ND	3.66	1.42	1.37
25	b	609	CLA	C1D-ND	3.66	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	620	CLA	C1D-ND	3.66	1.42	1.37
25	B	604	CLA	C1D-ND	3.66	1.42	1.37
27	D	405	BCR	C30-C25	-3.65	1.48	1.53
25	B	609	CLA	C1D-ND	3.65	1.42	1.37
25	C	514	CLA	C1D-ND	3.65	1.42	1.37
25	b	612	CLA	C1D-ND	3.63	1.42	1.37
25	C	505	CLA	C1D-ND	3.63	1.42	1.37
28	a	713	PL9	C7-C3	-3.57	1.47	1.51
27	D	405	BCR	C1-C6	-3.56	1.48	1.53
23	A	603	LMG	C4-C5	3.56	1.60	1.53
27	b	623	BCR	C1-C6	-3.55	1.48	1.53
27	k	101	BCR	C1-C6	-3.48	1.49	1.53
27	c	515	BCR	C1-C6	-3.47	1.49	1.53
27	C	516	BCR	C1-C6	-3.46	1.49	1.53
27	Y	101	BCR	C1-C6	-3.42	1.49	1.53
27	t	103	BCR	C1-C6	-3.42	1.49	1.53
27	b	602	BCR	C1-C6	-3.42	1.49	1.53
27	B	620	BCR	C1-C6	-3.42	1.49	1.53
27	a	712	BCR	C1-C6	-3.39	1.49	1.53
27	c	514	BCR	C30-C25	-3.37	1.49	1.53
27	b	624	BCR	C1-C6	-3.36	1.49	1.53
27	B	618	BCR	C1-C6	-3.36	1.49	1.53
27	k	102	BCR	C1-C6	-3.36	1.49	1.53
27	K	101	BCR	C1-C6	-3.35	1.49	1.53
27	b	625	BCR	C1-C6	-3.34	1.49	1.53
27	c	514	BCR	C1-C6	-3.34	1.49	1.53
27	B	619	BCR	C1-C6	-3.31	1.49	1.53
27	b	623	BCR	C30-C25	-3.29	1.49	1.53
28	D	406	PL9	C7-C3	-3.28	1.47	1.51
29	A	614	SQD	O48-C23	3.28	1.42	1.33
25	c	503	CLA	CHC-C1C	3.27	1.43	1.35
25	B	609	CLA	CHC-C1C	3.27	1.43	1.35
25	B	613	CLA	CHC-C1C	3.25	1.43	1.35
25	b	620	CLA	CHC-C1C	3.25	1.43	1.35
25	B	615	CLA	CHC-C1C	3.25	1.43	1.35
27	A	610	BCR	C1-C6	-3.24	1.49	1.53
25	A	607	CLA	CHC-C1C	3.23	1.43	1.35
25	C	512	CLA	CHC-C1C	3.23	1.43	1.35
25	C	504	CLA	CHC-C1C	3.23	1.43	1.35
25	C	509	CLA	CHC-C1C	3.23	1.43	1.35
25	b	613	CLA	CHC-C1C	3.22	1.43	1.35
25	b	609	CLA	CHC-C1C	3.22	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	CLA	CHC-C1C	3.22	1.43	1.35
25	C	511	CLA	CHC-C1C	3.22	1.43	1.35
25	c	508	CLA	CHC-C1C	3.22	1.43	1.35
25	b	614	CLA	CHC-C1C	3.21	1.43	1.35
25	B	614	CLA	CHC-C1C	3.21	1.43	1.35
25	c	511	CLA	CHC-C1C	3.21	1.43	1.35
25	b	611	CLA	CHC-C1C	3.21	1.43	1.35
25	B	607	CLA	CHC-C1C	3.21	1.43	1.35
25	B	602	CLA	CHC-C1C	3.20	1.43	1.35
25	C	507	CLA	CHC-C1C	3.20	1.43	1.35
25	b	618	CLA	CHC-C1C	3.20	1.43	1.35
25	A	609	CLA	CHC-C1C	3.20	1.43	1.35
25	B	603	CLA	CHC-C1C	3.20	1.43	1.35
25	c	509	CLA	CHC-C1C	3.20	1.43	1.35
25	b	616	CLA	CHC-C1C	3.20	1.43	1.35
25	C	506	CLA	CHC-C1C	3.19	1.43	1.35
25	C	502	CLA	C4D-ND	-3.19	1.33	1.37
25	C	514	CLA	CHC-C1C	3.19	1.43	1.35
25	C	503	CLA	CHC-C1C	3.19	1.43	1.35
25	A	606	CLA	CHC-C1C	3.19	1.43	1.35
25	D	403	CLA	CHC-C1C	3.19	1.43	1.35
25	d	402	CLA	CHC-C1C	3.19	1.43	1.35
25	c	502	CLA	CHC-C1C	3.19	1.43	1.35
25	c	506	CLA	CHC-C1C	3.18	1.43	1.35
25	C	505	CLA	CHC-C1C	3.18	1.43	1.35
25	C	505	CLA	C4D-ND	-3.18	1.33	1.37
25	a	708	CLA	CHC-C1C	3.18	1.43	1.35
25	D	402	CLA	CHC-C1C	3.18	1.43	1.35
25	a	711	CLA	CHC-C1C	3.17	1.43	1.35
25	C	513	CLA	CHC-C1C	3.17	1.43	1.35
25	a	719	CLA	CHC-C1C	3.17	1.43	1.35
25	B	610	CLA	CHC-C1C	3.17	1.43	1.35
25	c	510	CLA	CHC-C1C	3.17	1.43	1.35
25	B	606	CLA	CHC-C1C	3.16	1.43	1.35
27	b	625	BCR	C30-C25	-3.16	1.49	1.53
25	B	616	CLA	CHC-C1C	3.16	1.43	1.35
29	D	410	SQD	O48-C23	3.16	1.42	1.33
25	b	622	CLA	CHC-C1C	3.16	1.43	1.35
25	c	505	CLA	CHC-C1C	3.16	1.43	1.35
25	C	502	CLA	CHC-C1C	3.16	1.43	1.35
25	a	707	CLA	CHC-C1C	3.16	1.43	1.35
25	c	504	CLA	CHC-C1C	3.16	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	CHC-C1C	3.16	1.43	1.35
25	b	615	CLA	CHC-C1C	3.16	1.43	1.35
29	a	714	SQD	O48-C23	3.16	1.42	1.33
25	b	607	CLA	CHC-C1C	3.15	1.43	1.35
25	B	612	CLA	CHC-C1C	3.15	1.43	1.35
25	b	620	CLA	C4D-ND	-3.15	1.33	1.37
25	B	617	CLA	CHC-C1C	3.15	1.43	1.35
25	C	514	CLA	C4D-ND	-3.15	1.33	1.37
25	b	613	CLA	C4D-ND	-3.15	1.33	1.37
29	B	623	SQD	O48-C23	3.15	1.42	1.33
25	b	617	CLA	CHC-C1C	3.15	1.43	1.35
25	B	611	CLA	CHC-C1C	3.15	1.43	1.35
25	b	608	CLA	CHC-C1C	3.15	1.43	1.35
29	f	102	SQD	O48-C23	3.15	1.42	1.33
25	b	610	CLA	CHC-C1C	3.15	1.43	1.35
25	A	607	CLA	C4D-ND	-3.14	1.33	1.37
25	c	501	CLA	CHC-C1C	3.14	1.43	1.35
25	d	403	CLA	C4D-ND	-3.14	1.33	1.37
25	b	619	CLA	CHC-C1C	3.14	1.43	1.35
25	a	708	CLA	C4D-ND	-3.14	1.33	1.37
25	B	608	CLA	CHC-C1C	3.14	1.43	1.35
25	C	509	CLA	C4D-ND	-3.14	1.33	1.37
27	C	515	BCR	C30-C25	-3.14	1.49	1.53
25	c	512	CLA	CHC-C1C	3.13	1.43	1.35
25	c	507	CLA	CHC-C1C	3.13	1.43	1.35
25	B	604	CLA	CHC-C1C	3.12	1.43	1.35
25	c	513	CLA	C4D-ND	-3.12	1.33	1.37
25	c	513	CLA	CHC-C1C	3.11	1.43	1.35
25	D	404	CLA	CHC-C1C	3.11	1.42	1.35
25	B	609	CLA	C4D-ND	-3.11	1.33	1.37
27	C	515	BCR	C1-C6	-3.11	1.49	1.53
25	c	506	CLA	C4D-ND	-3.11	1.33	1.37
25	b	612	CLA	CHC-C1C	3.11	1.42	1.35
25	b	611	CLA	C4D-ND	-3.10	1.33	1.37
25	c	508	CLA	C4D-ND	-3.10	1.33	1.37
29	B	626	SQD	O48-C23	3.10	1.42	1.33
29	I	102	SQD	O48-C23	3.09	1.42	1.33
25	b	622	CLA	C4D-ND	-3.09	1.33	1.37
25	c	504	CLA	C4D-ND	-3.09	1.33	1.37
27	C	516	BCR	C30-C25	-3.09	1.49	1.53
25	C	503	CLA	C4D-ND	-3.09	1.33	1.37
29	A	612	SQD	O48-C23	3.08	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	CHC-C1C	3.08	1.42	1.35
25	c	502	CLA	C4D-ND	-3.08	1.33	1.37
25	b	621	CLA	C4D-ND	-3.08	1.33	1.37
29	b	601	SQD	O48-C23	3.08	1.42	1.33
27	B	620	BCR	C30-C25	-3.08	1.49	1.53
25	B	615	CLA	C4D-ND	-3.08	1.33	1.37
25	b	617	CLA	C4D-ND	-3.08	1.33	1.37
25	D	403	CLA	C4D-ND	-3.08	1.33	1.37
25	d	402	CLA	C4D-ND	-3.07	1.33	1.37
25	a	711	CLA	C4D-ND	-3.07	1.33	1.37
25	c	501	CLA	C4D-ND	-3.07	1.33	1.37
25	b	607	CLA	C4D-ND	-3.07	1.33	1.37
25	B	612	CLA	C4D-ND	-3.07	1.33	1.37
25	b	621	CLA	CHC-C1C	3.07	1.42	1.35
25	b	608	CLA	C4D-ND	-3.06	1.33	1.37
27	c	515	BCR	C30-C25	-3.06	1.49	1.53
25	b	614	CLA	C4D-ND	-3.05	1.33	1.37
25	B	617	CLA	C4D-ND	-3.05	1.33	1.37
27	H	102	BCR	C1-C6	-3.04	1.49	1.53
25	C	507	CLA	C4D-ND	-3.04	1.33	1.37
25	B	606	CLA	C4D-ND	-3.04	1.33	1.37
25	B	605	CLA	CHC-C1C	3.04	1.42	1.35
25	B	614	CLA	C4D-ND	-3.04	1.33	1.37
25	a	707	CLA	C4D-ND	-3.04	1.33	1.37
23	A	603	LMG	C4-C3	3.04	1.60	1.52
27	b	624	BCR	C30-C25	-3.03	1.49	1.53
27	a	712	BCR	C30-C25	-3.03	1.49	1.53
27	d	404	BCR	C30-C25	-3.03	1.49	1.53
27	Y	101	BCR	C30-C25	-3.03	1.49	1.53
25	a	719	CLA	C4D-ND	-3.03	1.33	1.37
28	d	405	PL9	C7-C3	-3.03	1.48	1.51
25	B	602	CLA	C4D-ND	-3.03	1.33	1.37
25	c	503	CLA	C4D-ND	-3.03	1.33	1.37
25	A	606	CLA	C4D-ND	-3.03	1.33	1.37
25	B	613	CLA	C4D-ND	-3.01	1.33	1.37
34	E	102	HEM	CAB-C3B	3.01	1.55	1.47
25	D	404	CLA	C4D-ND	-3.01	1.33	1.37
25	D	402	CLA	C4D-ND	-3.01	1.33	1.37
25	C	511	CLA	C4D-ND	-3.01	1.33	1.37
25	C	512	CLA	C4D-ND	-3.01	1.33	1.37
25	B	616	CLA	C4D-ND	-3.00	1.33	1.37
25	B	603	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	614	SQD	O47-C7	3.00	1.42	1.34
25	b	615	CLA	C4D-ND	-3.00	1.33	1.37
25	B	610	CLA	C4D-ND	-2.99	1.33	1.37
25	c	510	CLA	C4D-ND	-2.99	1.33	1.37
25	c	509	CLA	C4D-ND	-2.99	1.33	1.37
29	B	623	SQD	O47-C7	2.99	1.42	1.34
25	A	609	CLA	C4D-ND	-2.98	1.33	1.37
25	C	510	CLA	C4D-ND	-2.98	1.33	1.37
25	b	612	CLA	C4D-ND	-2.98	1.33	1.37
25	C	504	CLA	C4D-ND	-2.98	1.33	1.37
25	B	604	CLA	C4D-ND	-2.97	1.33	1.37
25	b	618	CLA	C4D-ND	-2.97	1.33	1.37
25	b	609	CLA	C4D-ND	-2.96	1.33	1.37
27	B	619	BCR	C30-C25	-2.96	1.49	1.53
25	B	608	CLA	C4D-ND	-2.95	1.33	1.37
25	C	513	CLA	C4D-ND	-2.95	1.33	1.37
25	c	507	CLA	C4D-ND	-2.95	1.33	1.37
25	c	505	CLA	C4D-ND	-2.95	1.33	1.37
27	h	101	BCR	C1-C6	-2.95	1.49	1.53
27	k	102	BCR	C30-C25	-2.94	1.49	1.53
27	A	610	BCR	C30-C25	-2.94	1.49	1.53
27	b	602	BCR	C30-C25	-2.93	1.49	1.53
25	B	607	CLA	C4D-ND	-2.93	1.33	1.37
25	B	611	CLA	C4D-ND	-2.93	1.33	1.37
27	h	101	BCR	C30-C25	-2.92	1.49	1.53
25	b	616	CLA	C4D-ND	-2.92	1.33	1.37
25	c	511	CLA	C4D-ND	-2.92	1.33	1.37
25	c	512	CLA	C4D-ND	-2.92	1.33	1.37
25	C	508	CLA	C4D-ND	-2.91	1.33	1.37
25	b	619	CLA	C4D-ND	-2.91	1.33	1.37
29	I	102	SQD	O47-C7	2.90	1.42	1.34
27	B	618	BCR	C30-C25	-2.89	1.49	1.53
27	k	101	BCR	C30-C25	-2.89	1.49	1.53
25	C	506	CLA	C4D-ND	-2.88	1.33	1.37
29	f	102	SQD	O47-C7	2.87	1.42	1.34
27	K	101	BCR	C30-C25	-2.87	1.49	1.53
29	B	626	SQD	O47-C7	2.85	1.42	1.34
27	H	102	BCR	C30-C25	-2.85	1.49	1.53
27	t	103	BCR	C30-C25	-2.84	1.49	1.53
29	D	410	SQD	O47-C7	2.84	1.42	1.34
29	A	612	SQD	O47-C7	2.83	1.42	1.34
34	e	102	HEM	CAB-C3B	2.83	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	C4D-ND	-2.82	1.33	1.37
29	a	714	SQD	O47-C7	2.81	1.42	1.34
25	B	605	CLA	C4D-ND	-2.80	1.33	1.37
29	b	601	SQD	O47-C7	2.78	1.42	1.34
28	D	406	PL9	C3-C4	-2.77	1.45	1.49
28	A	611	PL9	C3-C4	-2.75	1.45	1.49
26	a	709	PHO	CAC-C3C	-2.65	1.47	1.52
26	A	608	PHO	CAC-C3C	-2.63	1.47	1.52
26	a	710	PHO	CAC-C3C	-2.57	1.47	1.52
26	D	401	PHO	CAC-C3C	-2.57	1.47	1.52
28	d	405	PL9	C3-C4	-2.56	1.45	1.49
28	a	713	PL9	C3-C4	-2.53	1.45	1.49
23	c	520	LMG	C1-C2	2.49	1.59	1.52
25	c	501	CLA	CMB-C2B	-2.49	1.46	1.51
25	C	507	CLA	CMB-C2B	-2.49	1.46	1.51
25	b	617	CLA	CMB-C2B	-2.46	1.46	1.51
23	C	521	LMG	C1-C2	2.46	1.59	1.52
25	b	607	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.45	1.46	1.51
25	a	708	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	616	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	605	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	612	CLA	CMB-C2B	-2.43	1.46	1.51
25	a	711	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	510	CLA	CMB-C2B	-2.43	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.43	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	511	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.41	1.46	1.51
25	b	614	CLA	CMB-C2B	-2.40	1.46	1.51
25	a	719	CLA	CMB-C2B	-2.40	1.46	1.51
25	B	611	CLA	CMB-C2B	-2.40	1.46	1.51
25	B	607	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	502	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	506	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	504	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.39	1.46	1.51
25	A	609	CLA	CMB-C2B	-2.39	1.46	1.51
25	C	503	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	506	CLA	CMB-C2B	-2.39	1.46	1.51
25	A	607	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	CMB-C2B	-2.39	1.46	1.51
25	B	608	CLA	CMB-C2B	-2.39	1.46	1.51
25	b	618	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	508	CLA	CMB-C2B	-2.39	1.46	1.51
25	B	613	CLA	CMB-C2B	-2.38	1.46	1.51
25	D	404	CLA	CMB-C2B	-2.38	1.46	1.51
25	D	403	CLA	CMB-C2B	-2.38	1.46	1.51
25	b	611	CLA	CMB-C2B	-2.38	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	615	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	621	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	613	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	604	CLA	CMB-C2B	-2.37	1.46	1.51
25	a	707	CLA	CMB-C2B	-2.37	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.37	1.46	1.51
25	D	402	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	620	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.36	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.36	1.46	1.51
25	C	513	CLA	CMB-C2B	-2.36	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.36	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.36	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.35	1.46	1.51
25	b	608	CLA	CMB-C2B	-2.35	1.46	1.51
25	d	402	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.35	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.35	1.46	1.51
25	A	606	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.34	1.46	1.51
25	C	504	CLA	CMB-C2B	-2.34	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.34	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.34	1.46	1.51
25	b	619	CLA	CMB-C2B	-2.33	1.46	1.51
25	B	609	CLA	CMB-C2B	-2.33	1.46	1.51
25	d	403	CLA	CMB-C2B	-2.33	1.46	1.51
33	c	517	DGD	O1G-C1G	-2.33	1.39	1.45
25	C	509	CLA	CMB-C2B	-2.32	1.46	1.51
25	B	617	CLA	CMB-C2B	-2.31	1.46	1.51
33	C	518	DGD	O1G-C1G	-2.31	1.39	1.45
25	C	512	CLA	CMB-C2B	-2.30	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	514	CLA	CMB-C2B	-2.28	1.46	1.51
25	b	622	CLA	CMB-C2B	-2.28	1.46	1.51
32	E	101	LHG	P-O6	2.27	1.68	1.59
33	C	518	DGD	O2G-C2G	-2.25	1.41	1.46
33	c	517	DGD	O2G-C2G	-2.25	1.41	1.46
35	V	201	HEC	CAD-C3D	2.25	1.55	1.52
29	A	612	SQD	O2-C2	-2.23	1.37	1.43
29	a	714	SQD	O2-C2	-2.21	1.37	1.43
33	C	518	DGD	O6D-C5D	-2.21	1.39	1.44
32	b	629	LHG	O7-C5	-2.18	1.41	1.46
29	D	410	SQD	O2-C2	-2.18	1.37	1.43
29	b	601	SQD	O2-C2	-2.17	1.37	1.43
32	D	407	LHG	O7-C5	-2.17	1.41	1.46
32	L	101	LHG	O7-C5	-2.17	1.41	1.46
23	b	626	LMG	O6-C1	2.16	1.47	1.41
29	f	102	SQD	O2-C2	-2.16	1.37	1.43
25	c	510	CLA	CMD-C2D	-2.16	1.46	1.50
35	v	201	HEC	CAD-C3D	2.16	1.55	1.52
29	B	626	SQD	O2-C2	-2.16	1.37	1.43
33	H	103	DGD	O2G-C2G	-2.16	1.41	1.46
33	C	517	DGD	O1G-C1G	-2.15	1.40	1.45
25	c	505	CLA	CMD-C2D	-2.14	1.46	1.50
32	e	101	LHG	P-O6	2.14	1.68	1.59
32	d	407	LHG	O7-C5	-2.14	1.41	1.46
34	E	102	HEM	FE-ND	2.14	2.07	1.96
32	B	625	LHG	O7-C5	-2.10	1.41	1.46
25	C	506	CLA	CMD-C2D	-2.10	1.46	1.50
33	c	516	DGD	O1G-C1G	-2.09	1.40	1.45
34	e	102	HEM	FE-NB	2.09	2.07	1.96
25	B	604	CLA	CMD-C2D	-2.08	1.46	1.50
29	B	623	SQD	O2-C2	-2.08	1.38	1.43
25	b	618	CLA	CMD-C2D	-2.08	1.46	1.50
26	a	710	PHO	CMC-C2C	-2.08	1.46	1.51
25	a	707	CLA	CMD-C2D	-2.07	1.46	1.50
33	c	516	DGD	O2G-C2G	-2.06	1.41	1.46
33	C	518	DGD	O5D-C6D	-2.06	1.40	1.43
26	a	709	PHO	CMC-C2C	-2.06	1.46	1.51
34	E	102	HEM	CMD-C2D	2.06	1.55	1.50
29	a	714	SQD	O3-C3	-2.06	1.38	1.43
25	B	617	CLA	CMC-C2C	-2.06	1.46	1.50
28	d	405	PL9	C53-C6	-2.05	1.46	1.50
34	E	102	HEM	CMB-C2B	2.05	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	102	SQD	O4-C4	-2.05	1.38	1.43
25	A	606	CLA	CMD-C2D	-2.05	1.46	1.50
33	c	517	DGD	C1E-C2E	2.05	1.58	1.52
26	A	608	PHO	CMC-C2C	-2.05	1.46	1.51
33	c	517	DGD	O6E-C5E	-2.05	1.39	1.44
29	B	626	SQD	O3-C3	-2.04	1.38	1.43
26	D	401	PHO	CMC-C2C	-2.04	1.46	1.51
28	A	611	PL9	C53-C6	-2.04	1.46	1.50
25	b	609	CLA	CMD-C2D	-2.03	1.46	1.50
25	c	503	CLA	CMD-C2D	-2.03	1.46	1.50
25	d	402	CLA	CMD-C2D	-2.03	1.46	1.50
29	D	410	SQD	O3-C3	-2.03	1.38	1.43
25	D	403	CLA	CMD-C2D	-2.03	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.03	1.46	1.50
29	A	612	SQD	O3-C3	-2.03	1.38	1.43
26	D	401	PHO	CMD-C2D	-2.02	1.46	1.51
29	D	410	SQD	O4-C4	-2.02	1.38	1.43
28	a	713	PL9	C53-C6	-2.02	1.46	1.50
33	C	517	DGD	O2G-C2G	-2.02	1.41	1.46
25	b	611	CLA	CMD-C2D	-2.02	1.46	1.50
33	c	518	DGD	O1G-C1G	-2.02	1.40	1.45
29	f	102	SQD	O3-C3	-2.02	1.38	1.43
26	a	709	PHO	CMB-C2B	-2.02	1.46	1.51
29	A	612	SQD	O4-C4	-2.02	1.38	1.43
28	D	406	PL9	C53-C6	-2.02	1.46	1.50
25	c	512	CLA	CMD-C2D	-2.02	1.46	1.50
29	B	626	SQD	O4-C4	-2.02	1.38	1.43
25	B	609	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	626	LMG	O8-C9	-2.01	1.40	1.45
23	d	408	LMG	C7-C8	2.01	1.56	1.51
26	a	710	PHO	CMD-C2D	-2.01	1.46	1.51
23	C	520	LMG	C4-C5	2.01	1.57	1.53
33	C	519	DGD	O1G-C1G	-2.01	1.40	1.45
33	c	518	DGD	O2G-C2G	-2.01	1.41	1.46
32	B	625	LHG	P-O6	2.01	1.67	1.59
25	C	504	CLA	CMD-C2D	-2.01	1.46	1.50
29	a	714	SQD	O4-C4	-2.01	1.38	1.43
28	A	611	PL9	C6-C1	-2.00	1.45	1.48
34	e	102	HEM	CMD-C2D	2.00	1.55	1.50

All (1076) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	605	CLA	C4A-NA-C1A	6.61	109.68	106.71
25	b	610	CLA	C4A-NA-C1A	6.40	109.58	106.71
25	C	508	CLA	C4A-NA-C1A	6.36	109.57	106.71
25	C	513	CLA	C4A-NA-C1A	6.29	109.53	106.71
25	b	619	CLA	C4A-NA-C1A	6.21	109.50	106.71
25	b	621	CLA	C4A-NA-C1A	6.17	109.48	106.71
25	c	507	CLA	C4A-NA-C1A	6.13	109.46	106.71
25	C	504	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	c	509	CLA	C4A-NA-C1A	6.07	109.44	106.71
25	c	511	CLA	C4A-NA-C1A	6.06	109.43	106.71
25	c	513	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	c	503	CLA	C4A-NA-C1A	6.03	109.42	106.71
25	c	512	CLA	C4A-NA-C1A	5.97	109.39	106.71
25	b	615	CLA	C4A-NA-C1A	5.93	109.37	106.71
25	C	510	CLA	C4A-NA-C1A	5.91	109.36	106.71
25	B	616	CLA	C4A-NA-C1A	5.90	109.36	106.71
25	B	610	CLA	C4A-NA-C1A	5.89	109.36	106.71
25	C	512	CLA	C4A-NA-C1A	5.87	109.34	106.71
25	b	607	CLA	C4A-NA-C1A	5.86	109.34	106.71
25	B	617	CLA	C4A-NA-C1A	5.84	109.33	106.71
25	B	613	CLA	C4A-NA-C1A	5.80	109.31	106.71
25	c	502	CLA	C4A-NA-C1A	5.79	109.31	106.71
25	b	618	CLA	C4A-NA-C1A	5.78	109.31	106.71
25	B	612	CLA	C4A-NA-C1A	5.75	109.29	106.71
25	C	506	CLA	C4A-NA-C1A	5.73	109.28	106.71
25	B	602	CLA	C4A-NA-C1A	5.73	109.28	106.71
25	b	622	CLA	C4A-NA-C1A	5.68	109.26	106.71
25	B	614	CLA	C4A-NA-C1A	5.67	109.26	106.71
25	C	502	CLA	C4A-NA-C1A	5.64	109.24	106.71
25	C	503	CLA	C4A-NA-C1A	5.59	109.22	106.71
25	d	402	CLA	C4A-NA-C1A	5.56	109.21	106.71
25	c	510	CLA	C4A-NA-C1A	5.55	109.20	106.71
29	B	626	SQD	O9-S-C6	5.54	113.53	106.94
25	B	607	CLA	C4A-NA-C1A	5.51	109.18	106.71
25	C	509	CLA	C4A-NA-C1A	5.46	109.16	106.71
25	D	404	CLA	C4A-NA-C1A	5.45	109.16	106.71
25	C	507	CLA	C4A-NA-C1A	5.43	109.15	106.71
25	C	514	CLA	C4A-NA-C1A	5.42	109.14	106.71
25	c	501	CLA	C4A-NA-C1A	5.41	109.14	106.71
25	C	511	CLA	C4A-NA-C1A	5.39	109.13	106.71
29	b	601	SQD	O7-S-C6	5.38	113.34	106.94
25	b	617	CLA	C4A-NA-C1A	5.37	109.12	106.71
25	B	606	CLA	C4A-NA-C1A	5.36	109.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	713	PL9	C7-C3-C4	5.33	121.21	116.88
25	c	508	CLA	C4A-NA-C1A	5.32	109.10	106.71
25	a	711	CLA	C4A-NA-C1A	5.27	109.08	106.71
25	D	403	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	A	609	CLA	C4A-NA-C1A	5.23	109.06	106.71
28	d	405	PL9	C7-C3-C4	5.22	121.12	116.88
25	b	611	CLA	C4A-NA-C1A	5.22	109.05	106.71
25	c	504	CLA	C4A-NA-C1A	5.19	109.04	106.71
25	d	403	CLA	C4A-NA-C1A	5.17	109.03	106.71
25	B	611	CLA	C4A-NA-C1A	5.14	109.02	106.71
25	B	604	CLA	C4A-NA-C1A	5.14	109.02	106.71
25	c	506	CLA	C4A-NA-C1A	5.13	109.01	106.71
25	B	615	CLA	C4A-NA-C1A	5.13	109.01	106.71
28	D	406	PL9	C7-C3-C4	5.09	121.01	116.88
25	c	505	CLA	C4A-NA-C1A	5.08	108.99	106.71
25	b	614	CLA	C4A-NA-C1A	5.02	108.96	106.71
28	A	611	PL9	C7-C3-C4	5.00	120.94	116.88
25	b	616	CLA	C4A-NA-C1A	4.94	108.92	106.71
25	A	607	CLA	C4A-NA-C1A	4.92	108.92	106.71
25	B	603	CLA	C4A-NA-C1A	4.91	108.91	106.71
25	a	708	CLA	C4A-NA-C1A	4.89	108.91	106.71
25	b	612	CLA	C4A-NA-C1A	4.87	108.89	106.71
29	A	612	SQD	O9-S-C6	4.86	112.71	106.94
29	b	601	SQD	O6-C1-C2	4.82	115.82	108.30
25	D	402	CLA	C4A-NA-C1A	4.74	108.84	106.71
25	a	719	CLA	C4A-NA-C1A	4.73	108.83	106.71
25	a	707	CLA	C4A-NA-C1A	4.63	108.79	106.71
29	B	626	SQD	O5-C5-C4	4.54	117.93	109.69
29	b	601	SQD	O9-S-C6	4.52	112.31	106.94
29	B	623	SQD	C4-C3-C2	4.48	118.64	110.82
33	C	519	DGD	O3G-C3G-C2G	-4.39	100.32	110.90
25	B	608	CLA	C4A-NA-C1A	4.32	108.65	106.71
25	b	617	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
25	d	403	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
33	C	517	DGD	O3G-C3G-C2G	-4.29	100.56	110.90
25	C	514	CLA	CMB-C2B-C1B	-4.27	121.89	128.46
33	c	516	DGD	O3G-C3G-C2G	-4.27	100.60	110.90
25	B	617	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
33	C	518	DGD	O3G-C3G-C2G	-4.23	100.70	110.90
25	b	608	CLA	C4A-NA-C1A	4.23	108.61	106.71
29	B	626	SQD	O7-S-C6	4.22	111.96	106.94
25	B	612	CLA	CMB-C2B-C1B	-4.22	121.98	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	613	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
32	D	408	LHG	O4-P-O5	4.20	133.01	112.24
25	c	512	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
25	C	512	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
33	c	518	DGD	O3G-C3G-C2G	-4.19	100.78	110.90
32	B	625	LHG	O4-P-O5	4.19	132.94	112.24
32	L	101	LHG	O4-P-O5	4.19	132.94	112.24
29	a	714	SQD	O7-S-C6	4.18	111.91	106.94
32	d	407	LHG	O4-P-O5	4.18	132.91	112.24
32	d	406	LHG	O4-P-O5	4.18	132.91	112.24
32	b	629	LHG	O4-P-O5	4.18	132.90	112.24
29	a	714	SQD	O5-C5-C4	4.18	117.28	109.69
33	c	517	DGD	O3G-C3G-C2G	-4.18	100.82	110.90
32	a	720	LHG	O4-P-O5	4.18	132.89	112.24
32	D	407	LHG	O4-P-O5	4.18	132.88	112.24
25	C	505	CLA	C4A-NA-C1A	4.17	108.58	106.71
25	b	622	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
32	e	101	LHG	O4-P-O5	4.16	132.79	112.24
25	b	620	CLA	C4A-NA-C1A	4.15	108.57	106.71
32	E	101	LHG	O4-P-O5	4.12	132.62	112.24
25	b	619	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
25	c	513	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
29	I	102	SQD	O47-C7-C8	4.09	120.33	111.50
29	f	102	SQD	O7-S-C6	4.08	111.79	106.94
29	D	410	SQD	O7-S-C6	4.05	111.75	106.94
25	c	510	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
23	c	520	LMG	O6-C1-O1	-4.03	100.42	109.97
29	A	612	SQD	O5-C5-C4	4.02	116.99	109.69
25	b	612	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
25	c	509	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
29	D	410	SQD	O9-S-C6	3.99	111.68	106.94
29	f	102	SQD	O9-S-C6	3.99	111.68	106.94
23	b	626	LMG	O6-C1-C2	3.97	118.76	110.35
25	a	707	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
25	C	511	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
29	B	626	SQD	O6-C1-C2	3.94	114.46	108.30
29	D	410	SQD	O6-C1-C2	3.94	114.46	108.30
25	A	606	CLA	C4A-NA-C1A	3.93	108.47	106.71
25	B	614	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
29	A	612	SQD	O9-S-O7	-3.87	100.56	113.95
25	c	503	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
25	C	513	CLA	CMB-C2B-C1B	-3.86	122.53	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	609	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
25	b	613	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
25	B	604	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
25	C	509	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
29	a	714	SQD	O9-S-C6	3.84	111.51	106.94
25	D	402	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
29	B	626	SQD	O9-S-O7	-3.84	100.66	113.95
23	C	521	LMG	O6-C1-O1	-3.83	100.91	109.97
25	c	506	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
33	H	103	DGD	O3G-C3G-C2G	-3.81	101.71	110.90
25	b	609	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
25	c	511	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
29	B	623	SQD	O9-S-O7	-3.79	100.84	113.95
25	B	609	CLA	C4A-NA-C1A	3.79	108.41	106.71
25	C	504	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
25	A	606	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
25	b	609	CLA	C4A-NA-C1A	3.73	108.38	106.71
29	B	623	SQD	O47-C7-C8	3.73	119.54	111.50
29	B	623	SQD	O9-S-C6	3.72	111.36	106.94
29	f	102	SQD	O9-S-O7	-3.70	101.13	113.95
29	A	612	SQD	O47-C7-C8	3.70	119.47	111.50
25	c	507	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
27	H	102	BCR	C2-C1-C6	3.69	116.16	110.48
29	D	410	SQD	O9-S-O7	-3.68	101.21	113.95
25	b	614	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
29	A	612	SQD	O7-S-C6	3.68	111.31	106.94
25	b	610	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
25	C	514	CLA	CMB-C2B-C3B	3.66	131.53	124.68
34	e	102	HEM	C4B-CHC-C1C	3.66	127.39	122.56
25	B	607	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
25	c	504	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
29	B	623	SQD	O5-C5-C4	3.63	116.29	109.69
29	a	714	SQD	O9-S-O7	-3.63	101.37	113.95
23	b	626	LMG	O6-C5-C4	3.63	116.28	109.69
28	a	713	PL9	C7-C3-C2	-3.63	118.53	123.30
25	C	506	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
25	B	617	CLA	CMB-C2B-C3B	3.60	131.42	124.68
25	C	510	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
25	d	403	CLA	CMB-C2B-C3B	3.60	131.41	124.68
29	A	614	SQD	O47-C7-C8	3.59	119.24	111.50
25	B	608	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
25	b	620	CLA	CMB-C2B-C1B	-3.59	122.95	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	CMB-C2B-C3B	3.58	131.38	124.68
35	v	201	HEC	CMB-C2B-C1B	-3.57	122.97	128.46
25	b	622	CLA	CMB-C2B-C3B	3.57	131.35	124.68
25	c	508	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	c	513	CLA	CMB-C2B-C3B	3.52	131.27	124.68
25	C	507	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
25	b	613	CLA	C4A-NA-C1A	3.52	108.29	106.71
25	c	501	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
29	a	714	SQD	O47-C7-C8	3.51	119.06	111.50
25	C	505	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
28	A	611	PL9	C7-C3-C2	-3.50	118.70	123.30
25	B	615	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
25	C	512	CLA	CMB-C2B-C3B	3.49	131.22	124.68
33	C	519	DGD	O6D-C1D-O3G	-3.49	101.72	109.97
35	V	201	HEC	CMB-C2B-C1B	-3.48	123.11	128.46
25	b	617	CLA	CMB-C2B-C3B	3.48	131.19	124.68
25	b	608	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
25	C	503	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
28	D	406	PL9	C7-C3-C2	-3.46	118.75	123.30
29	B	623	SQD	C3-C4-C5	3.46	116.41	110.24
25	C	508	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
33	h	102	DGD	O3G-C3G-C2G	-3.45	102.56	110.90
25	b	611	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
25	B	613	CLA	CMB-C2B-C3B	3.45	131.14	124.68
28	d	405	PL9	C7-C3-C2	-3.45	118.77	123.30
29	B	623	SQD	O7-S-C6	3.43	111.02	106.94
33	c	518	DGD	O6D-C1D-O3G	-3.43	101.85	109.97
29	D	410	SQD	O47-C7-C8	3.43	118.89	111.50
25	b	607	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
25	b	619	CLA	CMB-C2B-C3B	3.41	131.05	124.68
25	a	708	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
25	b	618	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
33	c	517	DGD	O6D-C1D-O3G	-3.39	101.94	109.97
25	a	711	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
25	B	612	CLA	CMB-C2B-C3B	3.39	131.02	124.68
29	b	601	SQD	O47-C7-C8	3.39	118.81	111.50
25	C	502	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
33	C	518	DGD	O5D-C6D-C5D	-3.38	102.80	109.05
25	c	510	CLA	CMB-C2B-C3B	3.37	130.99	124.68
25	A	609	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
29	A	612	SQD	O6-C1-C2	3.37	113.56	108.30
25	D	404	CLA	CMB-C2B-C1B	-3.36	123.29	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	626	SQD	O47-C7-C8	3.36	118.75	111.50
33	C	518	DGD	O6D-C1D-O3G	-3.36	102.02	109.97
25	b	616	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
25	b	621	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
25	c	509	CLA	CMB-C2B-C3B	3.33	130.90	124.68
33	C	517	DGD	O6D-C1D-O3G	-3.33	102.09	109.97
33	c	516	DGD	O6D-C1D-O3G	-3.32	102.10	109.97
25	B	606	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
29	a	714	SQD	C3-C4-C5	3.32	116.15	110.24
25	C	511	CLA	CMB-C2B-C3B	3.31	130.87	124.68
25	B	611	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	a	719	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	B	602	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
26	a	710	PHO	CMB-C2B-C3B	3.30	130.84	124.68
25	B	616	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
25	a	707	CLA	CMB-C2B-C3B	3.29	130.83	124.68
25	b	612	CLA	CMB-C2B-C3B	3.29	130.83	124.68
25	B	610	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
29	b	601	SQD	O9-S-O7	-3.28	102.61	113.95
25	c	502	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
25	C	513	CLA	CMB-C2B-C3B	3.27	130.79	124.68
25	b	615	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
25	D	403	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
25	B	603	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
25	B	609	CLA	CMB-C2B-C3B	3.25	130.77	124.68
25	d	402	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
25	B	605	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
25	A	607	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
25	D	402	CLA	CMB-C2B-C3B	3.24	130.74	124.68
29	B	623	SQD	O8-S-C6	3.23	110.89	105.74
25	C	509	CLA	CMB-C2B-C3B	3.23	130.72	124.68
31	a	706	BCT	O2-C-O1	-3.23	111.16	119.55
25	B	614	CLA	CMB-C2B-C3B	3.23	130.71	124.68
25	c	503	CLA	CMB-C2B-C3B	3.21	130.68	124.68
25	B	604	CLA	CMB-C2B-C3B	3.21	130.68	124.68
23	B	621	LMG	O6-C1-O1	-3.20	102.39	109.97
27	C	516	BCR	C15-C16-C17	-3.20	116.91	123.47
25	c	507	CLA	CMB-C2B-C3B	3.19	130.64	124.68
29	f	102	SQD	O6-C1-C2	3.18	113.27	108.30
25	b	613	CLA	CMB-C2B-C3B	3.18	130.63	124.68
25	c	505	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
25	b	609	CLA	CMB-C2B-C3B	3.17	130.60	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	CMB-C2B-C3B	3.16	130.59	124.68
26	D	401	PHO	CMB-C2B-C3B	3.16	130.59	124.68
25	c	511	CLA	CMB-C2B-C3B	3.15	130.57	124.68
25	C	505	CLA	CHB-C4A-NA	3.14	128.85	124.51
33	H	103	DGD	O6D-C1D-O3G	-3.14	102.55	109.97
25	C	513	CLA	CHB-C4A-NA	3.13	128.84	124.51
29	B	626	SQD	C1-O5-C5	3.13	119.82	113.69
25	B	605	CLA	CHB-C4A-NA	3.12	128.82	124.51
31	A	615	BCT	O2-C-O1	-3.12	111.46	119.55
25	D	402	CLA	CHB-C4A-NA	3.11	128.81	124.51
25	b	607	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
25	B	608	CLA	CHB-C4A-NA	3.10	128.81	124.51
29	D	410	SQD	O5-C5-C4	3.10	115.33	109.69
25	A	606	CLA	CMB-C2B-C3B	3.10	130.48	124.68
34	e	102	HEM	C1B-NB-C4B	3.10	108.27	105.07
34	E	102	HEM	C4B-CHC-C1C	3.09	126.64	122.56
25	C	506	CLA	CMB-C2B-C3B	3.09	130.46	124.68
25	B	602	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
25	C	504	CLA	CMB-C2B-C3B	3.07	130.42	124.68
26	a	709	PHO	CMB-C2B-C3B	3.07	130.41	124.68
29	a	714	SQD	O6-C1-C2	3.07	113.09	108.30
25	b	612	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	B	607	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
29	A	612	SQD	C3-C4-C5	3.04	115.67	110.24
26	a	710	PHO	O1D-CGD-CBD	3.04	129.80	124.74
23	b	626	LMG	C1-O6-C5	3.04	119.65	113.69
25	A	606	CLA	CHB-C4A-NA	3.04	128.71	124.51
25	b	610	CLA	CMB-C2B-C3B	3.03	130.35	124.68
25	C	510	CLA	CMB-C2B-C3B	3.02	130.32	124.68
29	B	623	SQD	C1-O5-C5	3.00	119.58	113.69
29	f	102	SQD	O47-C7-C8	3.00	119.18	110.80
25	B	604	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
25	b	610	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
25	b	621	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
25	b	613	CLA	CHB-C4A-NA	2.99	128.65	124.51
25	c	504	CLA	CMB-C2B-C3B	2.99	130.28	124.68
25	b	614	CLA	CMB-C2B-C3B	2.99	130.27	124.68
25	b	610	CLA	CHB-C4A-NA	2.99	128.64	124.51
25	c	507	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	a	708	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
28	A	611	PL9	C7-C8-C9	-2.97	121.85	126.79
29	b	601	SQD	C44-O6-C1	2.97	119.54	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	101	BCR	C2-C1-C6	2.97	115.05	110.48
25	C	502	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
25	b	620	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	C	508	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	C	508	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	b	608	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	c	508	CLA	CMB-C2B-C3B	2.96	130.21	124.68
25	B	608	CLA	CMB-C2B-C3B	2.96	130.21	124.68
25	D	402	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
25	D	404	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
26	D	401	PHO	O1D-CGD-CBD	2.95	129.66	124.74
25	B	605	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
25	c	504	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	A	607	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	a	719	CLA	CHB-C4A-NA	2.95	128.59	124.51
33	h	102	DGD	O6D-C1D-O3G	-2.94	103.00	109.97
25	c	504	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
27	c	515	BCR	C15-C16-C17	-2.94	117.45	123.47
25	B	607	CLA	CMB-C2B-C3B	2.94	130.18	124.68
25	b	613	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	C	506	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
25	c	508	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
25	C	505	CLA	CHD-C1D-ND	-2.93	121.76	124.45
25	C	505	CLA	CMB-C2B-C3B	2.93	130.16	124.68
26	a	709	PHO	O1D-CGD-CBD	2.93	129.61	124.74
25	C	508	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	A	608	PHO	CMB-C2B-C3B	2.92	130.14	124.68
25	c	501	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	c	502	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	C	509	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	C	513	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	H	102	BCR	C24-C23-C22	-2.90	121.85	126.23
25	C	507	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	A	609	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	A	607	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	A	609	CLA	CMB-C2B-C3B	2.90	130.10	124.68
25	B	616	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	b	617	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
25	B	616	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	C	503	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	b	620	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	C	503	CLA	CMB-C2B-C3B	2.89	130.08	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	t	103	BCR	C15-C14-C13	-2.89	123.19	127.31
28	d	405	PL9	C40-C39-C41	2.89	120.13	115.27
25	B	615	CLA	CMB-C2B-C3B	2.88	130.07	124.68
25	B	604	CLA	CHB-C4A-NA	2.88	128.50	124.51
27	b	602	BCR	C33-C5-C6	-2.88	121.29	124.53
25	c	505	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
27	t	103	BCR	C33-C5-C6	-2.88	121.30	124.53
29	B	626	SQD	C3-C4-C5	2.88	115.37	110.24
28	A	611	PL9	C40-C39-C41	2.87	120.11	115.27
25	B	603	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	C	505	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	a	711	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	a	710	PHO	O2D-CGD-O1D	-2.86	118.24	123.84
25	A	607	CLA	CHD-C1D-ND	-2.86	121.82	124.45
25	B	609	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
27	B	618	BCR	C15-C16-C17	-2.86	117.61	123.47
25	d	403	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	D	402	CLA	CHD-C1D-ND	-2.86	121.83	124.45
25	b	609	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	b	620	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	B	613	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	C	510	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	a	711	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	b	616	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	a	719	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	a	707	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	c	507	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	c	512	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	c	513	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	B	609	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	C	514	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	b	618	CLA	CHB-C4A-NA	2.84	128.45	124.51
25	b	618	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	b	621	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	c	501	CLA	CMB-C2B-C3B	2.84	129.99	124.68
25	d	402	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	A	608	PHO	O2D-CGD-O1D	-2.84	118.29	123.84
25	a	711	CLA	CMB-C2B-C3B	2.84	129.99	124.68
25	c	505	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
25	C	509	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	a	708	CLA	CMB-C2B-C3B	2.84	129.99	124.68
25	c	509	CLA	CHB-C4A-NA	2.84	128.43	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	607	CLA	CHB-C4A-NA	2.83	128.43	124.51
23	A	603	LMG	O6-C5-C4	2.83	114.84	109.69
33	h	102	DGD	CDB-CCB-CBB	-2.83	100.04	114.42
25	B	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
25	B	615	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
25	A	609	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
32	a	720	LHG	O8-C23-C24	2.83	120.78	111.91
25	c	511	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	a	719	CLA	CHD-C1D-ND	-2.83	121.86	124.45
32	B	625	LHG	O8-C23-C24	2.82	120.76	111.91
25	B	603	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	D	404	CLA	CMB-C2B-C3B	2.82	129.94	124.68
33	c	517	DGD	CDB-CCB-CBB	-2.81	100.14	114.42
25	b	611	CLA	CMB-C2B-C3B	2.81	129.94	124.68
25	a	708	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	B	606	CLA	CMB-C2B-C3B	2.81	129.93	124.68
25	b	618	CLA	CMB-C2B-C3B	2.81	129.93	124.68
25	b	612	CLA	CHD-C1D-ND	-2.81	121.87	124.45
29	f	102	SQD	O5-C5-C4	2.81	114.79	109.69
25	C	511	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	A	603	LMG	O6-C1-O1	-2.80	103.33	109.97
25	c	512	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	b	626	LMG	C4-C3-C2	-2.80	105.94	110.82
27	b	623	BCR	C15-C16-C17	-2.79	117.75	123.47
25	b	611	CLA	CHD-C1D-ND	-2.79	121.89	124.45
25	b	614	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	C	504	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	B	611	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
27	b	602	BCR	C15-C14-C13	-2.79	123.33	127.31
25	c	503	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
34	E	102	HEM	C4D-ND-C1D	2.79	107.95	105.07
25	b	609	CLA	CHB-C4A-NA	2.79	128.36	124.51
33	C	519	DGD	CDB-CCB-CBB	-2.79	100.28	114.42
25	b	620	CLA	CHD-C1D-ND	-2.78	121.90	124.45
25	b	616	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	B	616	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	B	602	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	B	603	CLA	CMB-C2B-C3B	2.78	129.87	124.68
32	D	407	LHG	O8-C23-C24	2.78	120.62	111.91
25	c	510	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	d	402	CLA	CMB-C2B-C3B	2.77	129.87	124.68
25	b	621	CLA	CMB-C2B-C3B	2.77	129.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	613	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	b	619	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	C	502	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	D	403	CLA	CMB-C2B-C3B	2.77	129.85	124.68
25	a	719	CLA	CMB-C2B-C3B	2.77	129.85	124.68
25	D	403	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
25	c	505	CLA	CMB-C2B-C3B	2.77	129.85	124.68
33	C	518	DGD	CDB-CCB-CBB	-2.77	100.38	114.42
33	c	518	DGD	O5D-C6D-C5D	-2.77	103.93	109.05
25	b	614	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	b	615	CLA	CMB-C2B-C3B	2.76	129.85	124.68
25	c	508	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	B	602	CLA	CMB-C2B-C3B	2.76	129.85	124.68
25	b	614	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	B	611	CLA	CMB-C2B-C3B	2.76	129.85	124.68
25	b	608	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	b	622	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	B	612	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
27	b	623	BCR	C33-C5-C6	-2.76	121.43	124.53
25	C	506	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
27	t	103	BCR	C15-C16-C17	-2.76	117.83	123.47
33	c	516	DGD	O5D-C6D-C5D	-2.76	103.95	109.05
25	B	614	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
25	B	611	CLA	CHB-C4A-NA	2.75	128.31	124.51
25	b	619	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
33	c	516	DGD	CDB-CCB-CBB	-2.75	100.48	114.42
25	c	501	CLA	CHD-C1D-ND	-2.74	121.93	124.45
25	c	504	CLA	CHD-C1D-ND	-2.74	121.93	124.45
25	c	501	CLA	CHB-C4A-NA	2.74	128.30	124.51
32	E	101	LHG	O8-C23-C24	2.74	120.51	111.91
25	B	606	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	B	608	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	c	503	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	b	616	CLA	CMB-C2B-C3B	2.74	129.80	124.68
25	C	502	CLA	CMB-C2B-C3B	2.74	129.80	124.68
27	b	602	BCR	C15-C16-C17	-2.74	117.87	123.47
25	B	610	CLA	CMB-C2B-C3B	2.73	129.79	124.68
25	C	510	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	C	504	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
25	c	506	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
25	B	609	CLA	CHD-C1D-ND	-2.73	121.95	124.45
26	D	401	PHO	O2D-CGD-O1D	-2.73	118.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	404	BCR	C27-C26-C25	2.73	126.69	122.73
25	C	512	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
32	D	408	LHG	C11-C10-C9	-2.72	100.59	114.42
25	B	610	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
25	C	507	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
25	C	514	CLA	CHD-C1D-ND	-2.72	121.95	124.45
25	b	609	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
25	C	514	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	A	607	CLA	CMB-C2B-C3B	2.72	129.76	124.68
25	B	615	CLA	CHD-C1D-ND	-2.71	121.96	124.45
25	B	612	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	B	617	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
32	d	406	LHG	O8-C23-C24	2.71	120.42	111.91
29	B	623	SQD	C44-O6-C1	2.71	119.04	113.74
33	c	518	DGD	CDB-CCB-CBB	-2.71	100.66	114.42
28	A	611	PL9	C22-C23-C24	-2.71	121.13	127.66
25	d	403	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	C	509	CLA	CHD-C1D-ND	-2.71	121.96	124.45
25	A	609	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
27	B	618	BCR	C33-C5-C6	-2.71	121.49	124.53
25	c	502	CLA	CMB-C2B-C3B	2.71	129.74	124.68
33	H	103	DGD	CDB-CCB-CBB	-2.71	100.69	114.42
34	e	102	HEM	CBA-CAA-C2A	-2.71	108.00	112.62
34	e	102	HEM	C4D-ND-C1D	2.71	107.87	105.07
27	b	625	BCR	C27-C26-C25	2.70	126.66	122.73
28	a	713	PL9	C40-C39-C41	2.70	119.82	115.27
29	b	601	SQD	O8-S-C6	2.70	110.05	105.74
26	A	608	PHO	O1D-CGD-CBD	2.70	129.24	124.74
25	b	607	CLA	CMB-C2B-C3B	2.70	129.73	124.68
25	B	607	CLA	CHB-C4A-NA	2.70	128.24	124.51
25	B	615	CLA	CHB-C4A-NA	2.70	128.24	124.51
25	B	614	CLA	CHB-C4A-NA	2.70	128.24	124.51
25	b	617	CLA	CHB-C4A-NA	2.70	128.24	124.51
25	d	402	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
27	B	620	BCR	C27-C26-C25	2.69	126.64	122.73
25	B	617	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	b	615	CLA	CHB-C4A-NA	2.69	128.23	124.51
27	B	618	BCR	C11-C10-C9	-2.69	123.47	127.31
25	c	506	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	B	605	CLA	C1-C2-C3	-2.69	121.39	126.04
23	f	101	LMG	O6-C1-O1	-2.69	103.61	109.97
25	c	502	CLA	CHB-C4A-NA	2.69	128.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	617	CLA	CHD-C1D-ND	-2.68	121.99	124.45
32	d	407	LHG	O8-C23-C24	2.68	120.33	111.91
27	B	618	BCR	C29-C30-C25	2.68	114.61	110.48
27	k	101	BCR	C33-C5-C6	-2.68	121.52	124.53
25	d	403	CLA	CHD-C1D-ND	-2.68	121.99	124.45
25	b	612	CLA	CHB-C4A-NA	2.68	128.22	124.51
34	E	102	HEM	C1B-NB-C4B	2.68	107.84	105.07
25	a	708	CLA	CHD-C1D-ND	-2.68	121.99	124.45
25	C	503	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	b	611	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	c	510	CLA	CHB-C4A-NA	2.67	128.21	124.51
27	b	623	BCR	C15-C14-C13	-2.67	123.50	127.31
25	c	513	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
33	C	519	DGD	C3G-C2G-C1G	-2.67	105.48	111.79
25	a	711	CLA	CHD-C1D-ND	-2.66	122.00	124.45
25	B	603	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
27	C	515	BCR	C2-C1-C6	2.66	114.58	110.48
25	b	622	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
28	D	406	PL9	C7-C8-C9	-2.66	122.36	126.79
25	D	403	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
25	b	615	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
28	D	406	PL9	C40-C39-C41	2.66	119.74	115.27
25	C	511	CLA	CHB-C4A-NA	2.66	128.18	124.51
27	b	623	BCR	C27-C26-C25	2.65	126.58	122.73
25	B	603	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	c	511	CLA	CHB-C4A-NA	2.65	128.18	124.51
27	D	405	BCR	C33-C5-C6	-2.65	121.56	124.53
25	B	606	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	b	617	CLA	C1-C2-C3	-2.65	121.47	126.04
25	b	608	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
25	b	611	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
29	D	410	SQD	O8-S-C6	2.64	109.95	105.74
27	c	515	BCR	C15-C14-C13	-2.64	123.54	127.31
25	B	605	CLA	CMB-C2B-C3B	2.64	129.62	124.68
25	c	509	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	D	404	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
27	C	515	BCR	C11-C10-C9	-2.63	123.55	127.31
35	V	201	HEC	CMB-C2B-C3B	2.63	128.91	125.82
25	C	507	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
25	C	507	CLA	CHB-C4A-NA	2.63	128.14	124.51
29	I	102	SQD	O48-C23-C24	2.62	120.14	111.91
25	C	512	CLA	CHD-C1D-ND	-2.62	122.05	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	627	LMG	O6-C1-O1	-2.62	103.77	109.97
25	b	608	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	B	606	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	c	506	CLA	CHD-C1D-ND	-2.61	122.06	124.45
34	e	102	HEM	C3B-C2B-C1B	2.61	108.42	106.49
25	B	611	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
29	A	612	SQD	O8-S-C6	2.61	109.89	105.74
25	b	609	CLA	CHD-C1D-ND	-2.60	122.06	124.45
27	c	514	BCR	C27-C26-C25	2.60	126.51	122.73
25	B	612	CLA	CHD-C1D-ND	-2.60	122.06	124.45
33	C	517	DGD	CDB-CCB-CBB	-2.60	101.22	114.42
32	L	101	LHG	O8-C23-C24	2.60	120.06	111.91
25	C	512	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	a	709	PHO	O2D-CGD-O1D	-2.60	118.76	123.84
25	c	506	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
27	B	620	BCR	C33-C5-C6	-2.60	121.61	124.53
25	C	511	CLA	CHD-C1D-ND	-2.60	122.07	124.45
25	B	610	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	b	607	CLA	CHD-C1D-ND	-2.60	122.07	124.45
25	D	404	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	a	701	LMG	O6-C1-O1	-2.59	103.84	109.97
27	D	405	BCR	C27-C26-C25	2.59	126.49	122.73
27	b	624	BCR	C27-C26-C25	2.59	126.49	122.73
27	Y	101	BCR	C33-C5-C6	-2.59	121.62	124.53
25	A	609	CLA	CHD-C1D-ND	-2.59	122.08	124.45
29	f	102	SQD	O8-S-C6	2.59	109.86	105.74
25	C	502	CLA	CHB-C4A-NA	2.59	128.09	124.51
29	f	102	SQD	C44-O6-C1	2.58	118.79	113.74
29	b	601	SQD	C4-C3-C2	2.58	115.33	110.82
29	B	623	SQD	O48-C23-C24	2.58	120.01	111.91
25	B	609	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
28	a	713	PL9	C22-C23-C24	-2.58	121.44	127.66
25	C	506	CLA	CHB-C4A-NA	2.58	128.07	124.51
25	b	622	CLA	CHB-C4A-NA	2.58	128.07	124.51
28	D	406	PL9	C27-C28-C29	-2.57	121.46	127.66
27	b	625	BCR	C33-C5-C6	-2.57	121.64	124.53
33	C	519	DGD	O5D-C6D-C5D	-2.57	104.29	109.05
29	a	714	SQD	O8-S-C6	2.57	109.83	105.74
25	d	402	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	B	608	CLA	CHD-C1D-ND	-2.57	122.10	124.45
25	D	403	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	A	603	LMG	O6-C1-C2	-2.56	104.92	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	624	BCR	C15-C16-C17	-2.56	118.22	123.47
32	B	625	LHG	C11-C10-C9	-2.56	101.42	114.42
25	B	613	CLA	CHD-C1D-ND	-2.56	122.10	124.45
25	c	508	CLA	CHD-C1D-ND	-2.56	122.10	124.45
28	d	405	PL9	C22-C23-C24	-2.56	121.50	127.66
25	B	602	CLA	CHD-C1D-ND	-2.56	122.11	124.45
25	D	402	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
29	A	612	SQD	O48-C23-C24	2.55	119.92	111.91
27	D	405	BCR	C15-C16-C17	-2.55	118.25	123.47
29	a	714	SQD	O48-C23-C24	2.55	119.91	111.91
27	t	103	BCR	C24-C23-C22	-2.55	122.38	126.23
25	a	707	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
27	C	516	BCR	C15-C14-C13	-2.55	123.67	127.31
35	v	201	HEC	CMB-C2B-C3B	2.55	128.81	125.82
32	d	406	LHG	C11-C10-C9	-2.55	101.50	114.42
25	C	504	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	c	503	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	A	606	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
28	a	713	PL9	C7-C8-C9	-2.54	122.56	126.79
27	B	619	BCR	C27-C26-C25	2.54	126.42	122.73
29	A	614	SQD	O48-C23-C24	2.54	119.87	111.91
27	c	514	BCR	C33-C5-C6	-2.54	121.68	124.53
29	a	714	SQD	C4-C3-C2	2.54	115.25	110.82
25	B	617	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
25	D	403	CLA	CHD-C1D-ND	-2.53	122.12	124.45
25	a	711	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
25	B	608	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
25	b	608	CLA	CHD-C1D-ND	-2.53	122.13	124.45
23	c	519	LMG	O6-C1-O1	-2.53	103.99	109.97
27	D	405	BCR	C24-C23-C22	-2.53	122.42	126.23
27	h	101	BCR	C27-C26-C25	2.53	126.40	122.73
25	B	604	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
25	b	615	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
25	D	404	CLA	CHD-C1D-ND	-2.52	122.13	124.45
28	d	405	PL9	C27-C28-C29	-2.52	121.58	127.66
25	B	610	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
25	B	606	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
32	L	101	LHG	C11-C10-C9	-2.52	101.63	114.42
23	a	701	LMG	C38-C37-C36	-2.52	101.63	114.42
33	c	517	DGD	O5D-C6D-C5D	-2.52	104.38	109.05
23	C	501	LMG	C38-C37-C36	-2.52	101.64	114.42
29	B	626	SQD	O48-C23-C24	2.52	119.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	518	DGD	C3G-C2G-C1G	-2.52	105.84	111.79
27	c	514	BCR	C15-C16-C17	-2.52	118.32	123.47
27	A	610	BCR	C24-C23-C22	-2.51	122.44	126.23
25	b	610	CLA	CHD-C1D-ND	-2.51	122.14	124.45
27	C	516	BCR	C33-C5-C6	-2.51	121.71	124.53
23	a	701	LMG	C40-C39-C38	-2.51	101.67	114.42
27	c	515	BCR	C33-C5-C6	-2.51	121.71	124.53
27	c	515	BCR	C27-C26-C25	2.51	126.37	122.73
33	C	517	DGD	O5D-C6D-C5D	-2.51	104.41	109.05
23	M	101	LMG	O6-C1-O1	-2.51	104.04	109.97
25	c	502	CLA	CHD-C1D-ND	-2.50	122.15	124.45
25	A	606	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
25	C	508	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
25	a	707	CLA	CHD-C1D-ND	-2.50	122.16	124.45
28	d	405	PL9	C20-C19-C21	2.50	119.48	115.27
25	B	615	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	a	715	LMG	O6-C1-O1	-2.50	104.06	109.97
32	b	629	LHG	O8-C23-C24	2.49	119.73	111.91
32	b	629	LHG	C11-C10-C9	-2.49	101.78	114.42
32	D	408	LHG	O8-C23-C24	2.49	119.72	111.91
25	A	606	CLA	CHD-C1D-ND	-2.49	122.17	124.45
29	B	623	SQD	C1-C2-C3	2.49	115.18	110.00
33	C	517	DGD	C3G-C2G-C1G	-2.49	105.91	111.79
25	C	505	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
27	a	712	BCR	C27-C26-C25	2.48	126.34	122.73
25	B	607	CLA	CHD-C1D-ND	-2.48	122.17	124.45
23	M	101	LMG	C38-C37-C36	-2.48	101.83	114.42
25	c	507	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
25	C	510	CLA	CHD-C1D-ND	-2.48	122.17	124.45
25	a	719	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
27	h	101	BCR	C15-C14-C13	-2.48	123.78	127.31
25	b	616	CLA	CHD-C1D-ND	-2.48	122.18	124.45
29	a	714	SQD	C44-O6-C1	2.47	118.57	113.74
28	D	406	PL9	C20-C19-C21	2.47	119.43	115.27
25	b	612	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
25	a	707	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
25	b	611	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
27	b	624	BCR	C15-C14-C13	-2.47	123.79	127.31
27	k	102	BCR	C29-C30-C25	2.46	114.27	110.48
27	K	101	BCR	C27-C26-C25	2.46	126.30	122.73
27	c	514	BCR	C11-C10-C9	-2.46	123.80	127.31
28	A	611	PL9	C27-C28-C29	-2.46	121.75	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	403	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
27	k	102	BCR	C33-C5-C6	-2.45	121.77	124.53
23	C	501	LMG	O6-C1-O1	-2.45	104.16	109.97
27	H	102	BCR	C27-C26-C25	2.45	126.29	122.73
32	D	408	LHG	C20-C19-C18	-2.45	101.98	114.42
25	b	620	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	C	507	CLA	CHD-C1D-ND	-2.45	122.20	124.45
25	B	611	CLA	CHD-C1D-ND	-2.45	122.20	124.45
25	d	402	CLA	CHD-C1D-ND	-2.45	122.20	124.45
25	b	614	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
25	c	511	CLA	CHD-C1D-ND	-2.44	122.21	124.45
23	B	621	LMG	O1-C7-C8	-2.44	105.01	110.90
32	D	407	LHG	C20-C19-C18	-2.44	102.03	114.42
25	b	616	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
32	d	406	LHG	C20-C19-C18	-2.44	102.04	114.42
25	B	602	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
25	B	616	CLA	CHD-C1D-ND	-2.44	122.22	124.45
32	D	407	LHG	C11-C10-C9	-2.44	102.06	114.42
23	M	101	LMG	C40-C39-C38	-2.43	102.08	114.42
32	d	407	LHG	C20-C19-C18	-2.43	102.08	114.42
27	K	101	BCR	C24-C23-C22	-2.43	122.56	126.23
25	c	512	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	f	101	LMG	C40-C39-C38	-2.42	102.12	114.42
27	d	404	BCR	C7-C8-C9	-2.42	122.57	126.23
27	C	515	BCR	C27-C26-C25	2.42	126.25	122.73
23	D	409	LMG	O6-C1-O1	-2.42	104.24	109.97
27	B	618	BCR	C15-C14-C13	-2.42	123.86	127.31
25	C	509	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	C	501	LMG	C40-C39-C38	-2.42	102.15	114.42
32	B	625	LHG	C20-C19-C18	-2.42	102.15	114.42
23	A	603	LMG	C40-C39-C38	-2.42	102.15	114.42
27	a	712	BCR	C24-C23-C22	-2.42	122.58	126.23
23	B	621	LMG	C38-C37-C36	-2.41	102.18	114.42
27	h	101	BCR	C24-C23-C22	-2.41	122.59	126.23
25	c	508	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
27	c	514	BCR	C15-C14-C13	-2.41	123.88	127.31
23	C	521	LMG	C40-C39-C38	-2.40	102.23	114.42
27	a	712	BCR	C33-C5-C6	-2.40	121.83	124.53
23	B	621	LMG	C40-C39-C38	-2.40	102.24	114.42
32	e	101	LHG	C11-C10-C9	-2.40	102.24	114.42
23	C	520	LMG	O6-C1-O1	-2.40	104.30	109.97
27	c	514	BCR	C24-C23-C22	-2.40	122.61	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	101	BCR	C11-C10-C9	-2.39	123.89	127.31
23	b	626	LMG	O3-C3-C2	-2.39	104.82	110.35
32	e	101	LHG	O8-C23-C24	2.39	119.42	111.91
28	d	405	PL9	C7-C8-C9	-2.39	122.81	126.79
25	c	502	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
27	Y	101	BCR	C27-C26-C25	2.39	126.20	122.73
27	b	624	BCR	C33-C5-C6	-2.39	121.84	124.53
23	b	627	LMG	C38-C37-C36	-2.39	102.30	114.42
23	c	520	LMG	C40-C39-C38	-2.39	102.30	114.42
25	c	505	CLA	CHD-C1D-ND	-2.39	122.26	124.45
27	K	101	BCR	C15-C14-C13	-2.39	123.90	127.31
25	c	505	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	c	519	LMG	C40-C39-C38	-2.39	102.31	114.42
27	K	101	BCR	C33-C5-C6	-2.38	121.85	124.53
25	a	708	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
27	a	712	BCR	C15-C16-C17	-2.38	118.59	123.47
23	b	626	LMG	O2-C2-C1	-2.38	104.26	110.05
25	C	503	CLA	CHD-C1D-ND	-2.38	122.26	124.45
27	A	610	BCR	C27-C26-C25	2.38	126.19	122.73
25	c	501	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
25	A	607	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	a	715	LMG	C40-C39-C38	-2.38	102.34	114.42
25	C	514	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	D	409	LMG	C40-C39-C38	-2.38	102.35	114.42
25	b	617	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	b	627	LMG	C40-C39-C38	-2.38	102.36	114.42
32	L	101	LHG	C20-C19-C18	-2.38	102.36	114.42
27	B	619	BCR	C33-C5-C6	-2.38	121.86	124.53
25	B	616	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
23	d	408	LMG	O7-C10-O9	-2.37	117.97	123.70
32	d	407	LHG	C11-C10-C9	-2.37	102.38	114.42
32	e	101	LHG	C20-C19-C18	-2.37	102.40	114.42
27	d	404	BCR	C2-C3-C4	2.37	116.67	111.38
32	b	629	LHG	C20-C19-C18	-2.37	102.41	114.42
25	b	613	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
25	c	509	CLA	CHD-C1D-ND	-2.36	122.28	124.45
35	V	201	HEC	CMD-C2D-C1D	-2.36	124.83	128.46
25	b	618	CLA	CHD-C1D-ND	-2.36	122.29	124.45
29	D	410	SQD	C3-C4-C5	2.36	114.45	110.24
23	c	519	LMG	C38-C37-C36	-2.36	102.45	114.42
27	K	101	BCR	C15-C16-C17	-2.36	118.65	123.47
25	B	607	CLA	C1B-CHB-C4A	-2.35	125.45	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	503	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
25	B	605	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
33	c	516	DGD	C3G-C2G-C1G	-2.35	106.23	111.79
27	C	515	BCR	C33-C5-C6	-2.35	121.89	124.53
25	C	506	CLA	CHD-C1D-ND	-2.35	122.30	124.45
27	C	516	BCR	C27-C26-C25	2.35	126.14	122.73
27	b	625	BCR	C24-C23-C22	-2.34	122.69	126.23
32	E	101	LHG	C20-C19-C18	-2.34	102.53	114.42
27	A	610	BCR	C33-C5-C6	-2.34	121.90	124.53
25	C	503	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
27	A	610	BCR	C15-C16-C17	-2.34	118.68	123.47
28	D	406	PL9	C22-C23-C24	-2.34	122.03	127.66
25	B	612	CLA	C1-C2-C3	-2.34	122.00	126.04
27	Y	101	BCR	C15-C16-C17	-2.33	118.69	123.47
27	b	623	BCR	C11-C10-C9	-2.33	123.98	127.31
34	E	102	HEM	CBA-CAA-C2A	-2.33	108.64	112.62
23	B	621	LMG	O7-C10-O9	-2.33	118.06	123.70
25	c	510	CLA	CHD-C1D-ND	-2.33	122.31	124.45
25	B	613	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	b	626	LMG	C40-C39-C38	-2.33	102.58	114.42
27	k	101	BCR	C27-C26-C25	2.33	126.12	122.73
25	b	621	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
27	A	610	BCR	C15-C14-C13	-2.33	123.98	127.31
25	b	610	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	f	101	LMG	C38-C37-C36	-2.33	102.60	114.42
26	a	710	PHO	CMC-C2C-C3C	2.33	129.33	124.94
25	B	604	CLA	CHD-C1D-ND	-2.33	122.31	124.45
23	a	715	LMG	C38-C37-C36	-2.32	102.62	114.42
25	b	615	CLA	CHD-C1D-ND	-2.32	122.32	124.45
29	A	612	SQD	C1-O5-C5	2.32	118.25	113.69
23	A	603	LMG	O3-C3-C2	-2.32	104.99	110.35
25	C	510	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
27	b	625	BCR	C15-C16-C17	-2.31	118.74	123.47
25	C	513	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
27	H	102	BCR	C15-C14-C13	-2.31	124.01	127.31
25	b	622	CLA	CHD-C1D-ND	-2.31	122.33	124.45
23	B	621	LMG	O3-C3-C2	-2.31	105.02	110.35
33	c	518	DGD	C3D-C4D-C5D	-2.30	106.13	110.24
25	b	607	CLA	O2D-CGD-CBD	2.30	115.36	111.27
25	C	502	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	c	520	LMG	C38-C37-C36	-2.30	102.76	114.42
27	k	102	BCR	C15-C16-C17	-2.30	118.77	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	515	BCR	C15-C14-C13	-2.30	124.03	127.31
27	b	602	BCR	C11-C10-C9	-2.30	124.03	127.31
23	C	520	LMG	C38-C37-C36	-2.30	102.76	114.42
25	c	504	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
25	C	511	CLA	C1-C2-C3	-2.30	122.07	126.04
23	A	603	LMG	C38-C37-C36	-2.30	102.77	114.42
23	C	521	LMG	C38-C37-C36	-2.30	102.77	114.42
23	A	603	LMG	C1-C2-C3	-2.29	105.22	110.00
25	B	614	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
25	c	513	CLA	CHD-C1D-ND	-2.29	122.35	124.45
23	f	101	LMG	O1-C7-C8	-2.29	105.37	110.90
26	D	401	PHO	CMC-C2C-C3C	2.29	129.26	124.94
25	c	513	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	C	520	LMG	O3-C3-C2	-2.29	105.06	110.35
23	a	701	LMG	O1-C7-C8	-2.29	105.38	110.90
29	b	601	SQD	O5-C5-C4	2.29	113.85	109.69
27	H	102	BCR	C3-C4-C5	-2.29	109.99	114.08
27	C	515	BCR	C15-C16-C17	-2.29	118.79	123.47
25	B	602	CLA	O2D-CGD-CBD	2.28	115.33	111.27
27	t	103	BCR	C27-C26-C25	2.28	126.05	122.73
25	C	504	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
33	c	517	DGD	CBB-CAB-C9B	-2.28	102.84	114.42
27	b	602	BCR	C27-C26-C25	2.28	126.04	122.73
27	B	620	BCR	C24-C23-C22	-2.28	122.79	126.23
25	b	607	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
25	c	509	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
27	a	712	BCR	C15-C14-C13	-2.28	124.06	127.31
23	C	520	LMG	C40-C39-C38	-2.28	102.86	114.42
27	k	102	BCR	C27-C26-C25	2.28	126.03	122.73
23	D	409	LMG	C38-C37-C36	-2.27	102.88	114.42
32	d	406	LHG	C18-C17-C16	-2.27	102.89	114.42
32	e	101	LHG	C5-O7-C7	-2.27	112.20	117.79
28	a	713	PL9	C27-C28-C29	-2.27	122.20	127.66
27	B	619	BCR	C15-C14-C13	-2.26	124.08	127.31
23	f	101	LMG	O3-C3-C2	-2.26	105.12	110.35
27	B	618	BCR	C7-C8-C9	-2.26	122.82	126.23
29	f	102	SQD	O48-C23-C24	2.26	119.00	111.91
27	k	102	BCR	C24-C23-C22	-2.26	122.82	126.23
25	C	511	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
27	B	619	BCR	C15-C16-C17	-2.26	118.85	123.47
25	B	612	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
27	Y	101	BCR	C24-C23-C22	-2.25	122.83	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	h	102	DGD	C3G-C2G-C1G	-2.25	106.47	111.79
25	B	610	CLA	CHD-C1D-ND	-2.25	122.39	124.45
25	c	510	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
25	b	618	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
27	d	404	BCR	C1-C6-C5	-2.24	119.45	122.61
25	c	507	CLA	CHD-C1D-ND	-2.24	122.40	124.45
27	d	404	BCR	C11-C10-C9	-2.24	124.12	127.31
27	D	405	BCR	C7-C8-C9	-2.23	122.86	126.23
28	a	713	PL9	C20-C19-C21	2.23	119.03	115.27
25	B	605	CLA	CHD-C1D-ND	-2.23	122.41	124.45
28	D	406	PL9	C36-C34-C33	-2.23	116.61	121.12
28	D	406	PL9	C37-C38-C39	-2.23	122.30	127.66
25	b	619	CLA	CHD-C1D-ND	-2.22	122.41	124.45
27	H	102	BCR	C11-C10-C9	-2.22	124.14	127.31
23	b	626	LMG	C38-C37-C36	-2.22	103.14	114.42
29	b	601	SQD	O48-C23-O10	-2.22	117.99	123.59
33	C	518	DGD	C3D-C4D-C5D	-2.22	106.28	110.24
27	d	404	BCR	C24-C23-C22	-2.22	122.89	126.23
33	C	517	DGD	O6E-C5E-C4E	2.21	113.71	109.69
25	b	610	CLA	C1-C2-C3	-2.21	122.22	126.04
23	c	519	LMG	O3-C3-C2	-2.21	105.24	110.35
27	h	101	BCR	C15-C16-C17	-2.21	118.94	123.47
23	a	715	LMG	O3-C3-C2	-2.21	105.24	110.35
32	D	408	LHG	C18-C17-C16	-2.21	103.22	114.42
25	B	614	CLA	CHD-C1D-ND	-2.21	122.43	124.45
23	C	521	LMG	O3-C3-C2	-2.21	105.25	110.35
33	H	103	DGD	C3G-C2G-C1G	-2.20	106.58	111.79
25	b	619	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
23	b	626	LMG	O6-C1-O1	-2.20	104.77	109.97
26	A	608	PHO	CMC-C2C-C3C	2.20	129.08	124.94
32	D	408	LHG	C27-C26-C25	-2.20	103.28	114.42
25	C	504	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
33	c	517	DGD	O3E-C3E-C2E	-2.19	105.28	110.35
25	B	605	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
28	A	611	PL9	C20-C19-C21	2.19	118.96	115.27
27	b	624	BCR	C11-C10-C9	-2.19	124.18	127.31
25	b	618	CLA	C1-C2-C3	-2.19	122.25	126.04
32	L	101	LHG	C18-C17-C16	-2.19	103.30	114.42
33	c	516	DGD	O6E-C5E-C4E	2.19	113.67	109.69
32	e	101	LHG	C27-C26-C25	-2.19	103.32	114.42
32	B	625	LHG	C27-C26-C25	-2.19	103.33	114.42
25	C	509	CLA	O2A-CGA-O1A	-2.19	118.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	L	101	LHG	C27-C26-C25	-2.19	103.33	114.42
25	C	512	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
23	C	501	LMG	O3-C3-C2	-2.18	105.30	110.35
25	c	511	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
32	E	101	LHG	C11-C10-C9	-2.18	103.35	114.42
25	C	507	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
32	b	629	LHG	C18-C17-C16	-2.18	103.35	114.42
28	a	713	PL9	O2-C1-C6	2.18	124.36	120.59
25	b	617	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
32	d	406	LHG	C27-C26-C25	-2.18	103.37	114.42
28	A	611	PL9	O2-C1-C6	2.18	124.36	120.59
32	B	625	LHG	C18-C17-C16	-2.18	103.38	114.42
23	d	408	LMG	O1-C7-C8	-2.17	106.02	111.78
23	M	101	LMG	O3-C3-C2	-2.17	105.33	110.35
26	a	709	PHO	CMC-C2C-C3C	2.17	129.04	124.94
23	a	701	LMG	C1-O6-C5	-2.17	109.42	113.69
27	H	102	BCR	C20-C21-C22	-2.17	124.21	127.31
27	B	618	BCR	C24-C23-C22	-2.17	122.96	126.23
23	C	521	LMG	O2-C2-C3	-2.17	105.34	110.35
33	C	518	DGD	CBB-CAB-C9B	-2.17	103.42	114.42
32	a	720	LHG	C27-C26-C25	-2.17	103.43	114.42
35	v	201	HEC	CMD-C2D-C1D	-2.16	125.14	128.46
33	c	516	DGD	CBB-CAB-C9B	-2.16	103.46	114.42
25	C	508	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	D	406	PL9	C31-C32-C33	-2.16	104.79	111.88
35	v	201	HEC	CBA-CAA-C2A	-2.16	108.97	112.60
32	d	407	LHG	C18-C17-C16	-2.16	103.48	114.42
25	b	615	CLA	C1-C2-C3	-2.16	122.31	126.04
32	e	101	LHG	C18-C17-C16	-2.16	103.48	114.42
33	C	519	DGD	CAB-C9B-C8B	-2.15	103.49	114.42
25	c	508	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
25	C	503	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
25	B	608	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
27	C	516	BCR	C11-C10-C9	-2.15	124.24	127.31
25	B	610	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
25	D	404	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
25	B	612	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
27	d	404	BCR	C33-C5-C6	-2.15	122.11	124.53
28	D	406	PL9	O2-C1-C6	2.15	124.31	120.59
27	t	103	BCR	C35-C13-C14	-2.15	119.92	122.92
28	d	405	PL9	O2-C1-C6	2.15	124.31	120.59
25	B	611	CLA	C1-C2-C3	-2.15	122.33	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	606	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
25	c	512	CLA	CHD-C1D-ND	-2.14	122.49	124.45
25	B	617	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
29	D	410	SQD	O48-C23-C24	2.14	118.62	111.91
25	B	617	CLA	CHD-C1D-ND	-2.14	122.49	124.45
33	c	517	DGD	C3G-C2G-C1G	-2.14	106.73	111.79
23	c	520	LMG	C7-O1-C1	2.14	117.92	113.74
25	B	614	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
29	A	614	SQD	C45-O47-C7	2.14	123.05	117.79
27	c	514	BCR	C2-C1-C6	2.14	113.77	110.48
25	C	514	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	c	503	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	c	502	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
23	B	621	LMG	C3-C4-C5	-2.14	106.43	110.24
33	C	517	DGD	CAB-C9B-C8B	-2.13	103.59	114.42
32	d	407	LHG	C27-C26-C25	-2.13	103.59	114.42
23	C	521	LMG	C7-O1-C1	2.13	117.91	113.74
23	f	101	LMG	O1-C1-C2	-2.13	104.98	108.30
33	h	102	DGD	C1D-C2D-C3D	-2.13	105.56	110.00
25	C	511	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	f	101	LMG	O2-C2-C1	-2.13	104.87	110.05
27	b	625	BCR	C15-C14-C13	-2.13	124.27	127.31
28	a	713	PL9	O2-C1-C2	-2.13	116.90	121.78
28	d	405	PL9	O1-C4-C3	-2.13	118.38	120.72
27	k	102	BCR	C15-C14-C13	-2.13	124.27	127.31
23	c	520	LMG	O2-C2-C3	-2.13	105.43	110.35
33	C	518	DGD	C3G-C2G-C1G	-2.12	106.76	111.79
32	b	629	LHG	C27-C26-C25	-2.12	103.65	114.42
28	a	713	PL9	C37-C38-C39	-2.12	122.55	127.66
33	H	103	DGD	CBB-CAB-C9B	-2.12	103.66	114.42
25	C	512	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	b	619	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
33	c	518	DGD	CBB-CAB-C9B	-2.12	103.68	114.42
29	B	626	SQD	C44-O6-C1	2.12	117.87	113.74
32	D	407	LHG	C27-C26-C25	-2.12	103.69	114.42
27	C	515	BCR	C24-C23-C22	-2.11	123.04	126.23
35	V	201	HEC	C1D-C2D-C3D	2.11	108.47	107.00
23	c	520	LMG	O3-C3-C2	-2.11	105.46	110.35
23	a	701	LMG	O2-C2-C1	-2.11	104.91	110.05
27	C	515	BCR	C7-C8-C9	-2.11	123.05	126.23
33	c	518	DGD	CAB-C9B-C8B	-2.11	103.72	114.42
27	d	404	BCR	C16-C15-C14	-2.11	119.15	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	405	BCR	C11-C10-C9	-2.11	124.30	127.31
25	c	506	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
32	E	101	LHG	C18-C17-C16	-2.11	103.73	114.42
25	C	505	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
28	A	611	PL9	O2-C1-C2	-2.10	116.96	121.78
25	A	609	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	C	513	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	C	520	LMG	O2-C2-C1	-2.10	104.95	110.05
34	e	102	HEM	CHC-C4B-C3B	2.10	127.78	124.57
25	c	504	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
33	h	102	DGD	CBB-CAB-C9B	-2.10	103.78	114.42
32	D	407	LHG	C18-C17-C16	-2.09	103.79	114.42
27	D	405	BCR	C15-C14-C13	-2.09	124.32	127.31
28	A	611	PL9	O1-C4-C3	-2.09	118.42	120.72
28	D	406	PL9	O2-C1-C2	-2.09	116.99	121.78
27	c	515	BCR	C11-C10-C9	-2.09	124.33	127.31
27	Y	101	BCR	C15-C14-C13	-2.09	124.33	127.31
25	B	613	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
27	b	625	BCR	C11-C10-C9	-2.09	124.33	127.31
23	M	101	LMG	O2-C2-C1	-2.09	104.97	110.05
33	C	519	DGD	O6E-C1E-O5D	-2.09	105.03	109.97
28	D	406	PL9	O1-C4-C3	-2.09	118.42	120.72
29	A	612	SQD	O48-C23-O10	-2.09	118.33	123.59
33	H	103	DGD	C1D-C2D-C3D	-2.08	105.66	110.00
25	b	621	CLA	CHD-C1D-ND	-2.08	122.54	124.45
28	a	713	PL9	O1-C4-C3	-2.08	118.43	120.72
27	b	623	BCR	C24-C23-C22	-2.08	123.09	126.23
23	b	627	LMG	O2-C2-C1	-2.08	104.99	110.05
25	c	513	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	B	618	BCR	C27-C26-C25	2.08	125.75	122.73
25	b	615	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	A	607	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
29	D	410	SQD	C4-C3-C2	2.08	114.45	110.82
33	H	103	DGD	CAB-C9B-C8B	-2.08	103.87	114.42
33	C	518	DGD	CAB-C9B-C8B	-2.08	103.88	114.42
25	B	605	CLA	O2D-CGD-CBD	2.08	114.96	111.27
28	d	405	PL9	O2-C1-C2	-2.08	117.02	121.78
33	c	517	DGD	CAB-C9B-C8B	-2.08	103.89	114.42
25	A	607	CLA	C1-C2-C3	-2.08	122.45	126.04
23	a	715	LMG	O2-C2-C1	-2.07	105.01	110.05
25	a	707	CLA	O1D-CGD-CBD	2.07	128.72	124.48
26	D	401	PHO	O2A-CGA-O1A	-2.07	118.36	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	517	DGD	CBB-CAB-C9B	-2.07	103.91	114.42
23	D	409	LMG	O3-C3-C2	-2.07	105.56	110.35
32	E	101	LHG	C27-C26-C25	-2.07	103.93	114.42
25	b	613	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
25	B	603	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
25	b	607	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
25	b	621	CLA	O2D-CGD-CBD	2.07	114.94	111.27
25	b	614	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
27	b	602	BCR	C7-C8-C9	-2.06	123.12	126.23
33	C	518	DGD	O3E-C3E-C2E	-2.06	105.58	110.35
23	D	409	LMG	O2-C2-C1	-2.06	105.04	110.05
25	b	610	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
27	b	623	BCR	C7-C8-C9	-2.06	123.12	126.23
23	a	715	LMG	C1-C2-C3	-2.06	105.71	110.00
31	A	615	BCT	O3-C-O1	-2.06	114.21	119.55
25	b	621	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
27	B	619	BCR	C24-C23-C22	-2.06	123.13	126.23
34	e	102	HEM	C4C-CHD-C1D	2.06	125.27	122.56
25	d	403	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	b	612	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	b	610	CLA	O2D-CGD-CBD	2.05	114.91	111.27
27	b	625	BCR	C2-C1-C6	2.05	113.64	110.48
27	b	625	BCR	C38-C26-C25	-2.05	122.23	124.53
25	a	711	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
33	c	516	DGD	CAB-C9B-C8B	-2.05	104.03	114.42
23	d	408	LMG	C38-C37-C36	-2.05	104.03	114.42
33	c	517	DGD	C3D-C4D-C5D	-2.05	106.59	110.24
28	d	405	PL9	C37-C38-C39	-2.05	122.73	127.66
25	B	609	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
27	a	712	BCR	C11-C10-C9	-2.04	124.39	127.31
25	c	511	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	d	402	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
33	h	102	DGD	CAB-C9B-C8B	-2.04	104.07	114.42
23	d	408	LMG	C40-C39-C38	-2.04	104.08	114.42
33	C	517	DGD	C5B-C4B-C3B	-2.04	104.08	114.42
33	c	516	DGD	C5B-C4B-C3B	-2.04	104.08	114.42
33	c	518	DGD	O6E-C1E-O5D	-2.04	105.15	109.97
23	C	501	LMG	C1-C2-C3	-2.03	105.76	110.00
25	D	402	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
33	c	518	DGD	O2D-C2D-C1D	-2.03	105.11	110.05
25	b	622	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
33	C	519	DGD	C5B-C4B-C3B	-2.02	104.15	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	706	BCT	O3-C-O1	-2.02	114.30	119.55
33	C	519	DGD	CBB-CAB-C9B	-2.02	104.16	114.42
23	a	701	LMG	O3-C3-C2	-2.02	105.67	110.35
25	a	719	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	b	620	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
27	B	620	BCR	C38-C26-C25	-2.02	122.26	124.53
23	c	519	LMG	O2-C2-C1	-2.02	105.14	110.05
25	B	611	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
33	c	518	DGD	C5B-C4B-C3B	-2.02	104.19	114.42
29	A	612	SQD	C4-C3-C2	2.02	114.34	110.82
25	c	508	CLA	C1-C2-C3	-2.02	122.56	126.04
25	B	604	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
25	B	615	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	c	501	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	c	509	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
28	a	713	PL9	C32-C33-C34	-2.01	122.81	127.66
27	K	101	BCR	C11-C10-C9	-2.01	124.44	127.31
25	A	606	CLA	O1D-CGD-CBD	2.01	128.60	124.48
26	a	709	PHO	C1-C2-C3	-2.01	122.57	126.04
25	b	611	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
29	a	714	SQD	C1-O5-C5	2.01	117.63	113.69
26	A	608	PHO	O2A-CGA-O1A	-2.01	118.53	123.59
28	A	611	PL9	C36-C34-C33	-2.00	117.06	121.12
25	b	619	CLA	C1-C2-C3	-2.00	122.58	126.04
26	a	709	PHO	O2A-CGA-O1A	-2.00	118.54	123.59

All (56) 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	B	602	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	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	B	617	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	508	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	C	514	CLA	ND
25	a	707	CLA	ND
25	a	708	CLA	ND
25	a	711	CLA	ND
25	a	719	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	616	CLA	ND
25	b	617	CLA	ND
25	b	618	CLA	ND
25	b	619	CLA	ND
25	b	620	CLA	ND
25	b	621	CLA	ND
25	b	622	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	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

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Mol	Chain	Res	Type	Atom
25	c	513	CLA	ND

All (1743) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	621	LMG	C2-C1-O1-C7
23	B	621	LMG	O6-C1-O1-C7
23	C	501	LMG	C2-C1-O1-C7
23	C	501	LMG	O6-C1-O1-C7
23	C	521	LMG	O6-C1-O1-C7
23	c	520	LMG	O6-C1-O1-C7
23	d	408	LMG	C11-C10-O7-C8
25	A	607	CLA	CHA-CBD-CGD-O1D
25	A	607	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CAD-CBD-CGD-O1D
25	B	602	CLA	CAD-CBD-CGD-O2D
25	B	602	CLA	C11-C10-C8-C9
25	B	603	CLA	CHA-CBD-CGD-O1D
25	B	603	CLA	CHA-CBD-CGD-O2D
25	B	603	CLA	C4-C3-C5-C6
25	B	604	CLA	CHA-CBD-CGD-O1D
25	B	604	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	CHA-CBD-CGD-O1D
25	B	607	CLA	CHA-CBD-CGD-O2D
25	B	608	CLA	CHA-CBD-CGD-O1D
25	B	608	CLA	CHA-CBD-CGD-O2D
25	B	608	CLA	CAD-CBD-CGD-O1D
25	B	608	CLA	CAD-CBD-CGD-O2D
25	B	615	CLA	CHA-CBD-CGD-O1D
25	B	615	CLA	CHA-CBD-CGD-O2D
25	B	615	CLA	C2-C3-C5-C6
25	B	615	CLA	C4-C3-C5-C6
25	C	503	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O1D
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	D	402	CLA	CHA-CBD-CGD-O1D
25	D	402	CLA	CHA-CBD-CGD-O2D
25	D	404	CLA	C2-C3-C5-C6
25	D	404	CLA	C4-C3-C5-C6
25	a	707	CLA	CBD-CGD-O2D-CED
25	a	708	CLA	CHA-CBD-CGD-O1D
25	a	708	CLA	CHA-CBD-CGD-O2D
25	a	711	CLA	C2-C3-C5-C6
25	a	711	CLA	C4-C3-C5-C6
25	a	719	CLA	CHA-CBD-CGD-O1D
25	a	719	CLA	CHA-CBD-CGD-O2D
25	b	607	CLA	CHA-CBD-CGD-O1D
25	b	607	CLA	CHA-CBD-CGD-O2D
25	b	610	CLA	CHA-CBD-CGD-O1D
25	b	610	CLA	CHA-CBD-CGD-O2D
25	b	612	CLA	CHA-CBD-CGD-O1D
25	b	612	CLA	CHA-CBD-CGD-O2D
25	b	613	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C3A-C2A-CAA-CBA
25	b	613	CLA	CHA-CBD-CGD-O1D
25	b	613	CLA	CHA-CBD-CGD-O2D
25	b	617	CLA	CHA-CBD-CGD-O1D
25	b	617	CLA	CHA-CBD-CGD-O2D
25	b	620	CLA	CHA-CBD-CGD-O1D
25	b	620	CLA	CHA-CBD-CGD-O2D
25	b	620	CLA	CAD-CBD-CGD-O1D
25	b	620	CLA	CAD-CBD-CGD-O2D
25	c	501	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	C6-C7-C8-C9
25	d	402	CLA	CBD-CGD-O2D-CED
27	B	619	BCR	C7-C8-C9-C34
27	B	620	BCR	C1-C6-C7-C8
27	B	620	BCR	C7-C8-C9-C34
27	B	620	BCR	C23-C24-C25-C30
27	D	405	BCR	C1-C6-C7-C8
27	D	405	BCR	C7-C8-C9-C10
27	D	405	BCR	C7-C8-C9-C34
27	D	405	BCR	C21-C22-C23-C24
27	H	102	BCR	C7-C8-C9-C34
27	Y	101	BCR	C7-C8-C9-C34
27	b	602	BCR	C5-C6-C7-C8
27	b	602	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	b	602	BCR	C21-C22-C23-C24
27	b	602	BCR	C37-C22-C23-C24
27	b	624	BCR	C7-C8-C9-C10
27	b	624	BCR	C7-C8-C9-C34
27	b	625	BCR	C1-C6-C7-C8
27	b	625	BCR	C37-C22-C23-C24
27	c	514	BCR	C7-C8-C9-C34
27	c	515	BCR	C1-C6-C7-C8
27	h	101	BCR	C7-C8-C9-C10
27	h	101	BCR	C7-C8-C9-C34
27	k	101	BCR	C20-C21-C22-C37
27	t	103	BCR	C21-C22-C23-C24
28	A	611	PL9	C9-C11-C12-C13
28	D	406	PL9	C33-C34-C36-C37
28	D	406	PL9	C35-C34-C36-C37
29	A	612	SQD	C5-C6-S-O8
29	A	612	SQD	C5-C6-S-O9
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O5-C5-C6-S
29	B	626	SQD	O5-C1-O6-C44
29	B	626	SQD	O49-C7-O47-C45
29	B	626	SQD	O10-C23-O48-C46
29	D	410	SQD	C8-C7-O47-C45
29	I	102	SQD	O6-C44-C45-O47
29	I	102	SQD	C8-C7-O47-C45
29	a	714	SQD	C5-C6-S-O7
29	b	601	SQD	O5-C1-O6-C44
29	b	601	SQD	C8-C7-O47-C45
29	b	601	SQD	C4-C5-C6-S
29	f	102	SQD	C2-C1-O6-C44
29	f	102	SQD	O5-C1-O6-C44
32	B	625	LHG	C3-O3-P-O6
32	B	625	LHG	C4-O6-P-O5
32	D	407	LHG	O1-C1-C2-C3
32	D	407	LHG	O2-C2-C3-O3
32	D	407	LHG	C4-O6-P-O3
32	D	408	LHG	O1-C1-C2-O2
32	D	408	LHG	O1-C1-C2-C3
32	D	408	LHG	C4-O6-P-O4
32	E	101	LHG	O1-C1-C2-C3
32	E	101	LHG	C3-O3-P-O5
32	a	720	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
32	a	720	LHG	C4-O6-P-O5
32	b	629	LHG	C4-O6-P-O5
32	d	407	LHG	C4-O6-P-O3
33	C	518	DGD	C2E-C1E-O5D-C6D
25	c	513	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	O1D-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	B	611	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	b	620	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	O1D-CGD-O2D-CED
25	c	501	CLA	O1D-CGD-O2D-CED
25	d	402	CLA	O1D-CGD-O2D-CED
29	A	614	SQD	C24-C23-O48-C46
29	B	626	SQD	C24-C23-O48-C46
25	B	604	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	607	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	CBD-CGD-O2D-CED
25	C	507	CLA	CBD-CGD-O2D-CED
25	b	612	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
29	A	614	SQD	O10-C23-O48-C46
29	B	623	SQD	O10-C23-O48-C46
32	e	101	LHG	O10-C23-O8-C6
25	a	707	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	614	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
23	a	701	LMG	O9-C10-O7-C8
29	B	623	SQD	O49-C7-O47-C45
29	I	102	SQD	O49-C7-O47-C45
25	B	602	CLA	C3-C5-C6-C7
25	C	503	CLA	C3-C5-C6-C7
33	C	518	DGD	O6E-C5E-C6E-O5E
29	A	614	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	C8-C7-O47-C45
29	B	626	SQD	C8-C7-O47-C45
25	B	611	CLA	O1D-CGD-O2D-CED
25	B	604	CLA	C4-C3-C5-C6
25	B	603	CLA	C2-C3-C5-C6
25	B	607	CLA	C2A-CAA-CBA-CGA
25	B	611	CLA	C2A-CAA-CBA-CGA
25	b	613	CLA	O1D-CGD-O2D-CED
29	B	623	SQD	C24-C23-O48-C46
25	B	615	CLA	O1D-CGD-O2D-CED
28	A	611	PL9	C42-C43-C44-C45
25	B	613	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
23	d	408	LMG	O9-C10-O7-C8
29	A	614	SQD	O49-C7-O47-C45
28	A	611	PL9	C42-C43-C44-C46
25	D	404	CLA	O1A-CGA-O2A-C1
25	b	620	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	CBD-CGD-O2D-CED
25	c	505	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
26	a	710	PHO	CBD-CGD-O2D-CED
32	d	407	LHG	O2-C2-C3-O3
25	b	610	CLA	C3-C5-C6-C7
33	C	517	DGD	O6E-C5E-C6E-O5E
33	h	102	DGD	C4E-C5E-C6E-O5E
23	a	701	LMG	C11-C10-O7-C8
25	D	404	CLA	CBD-CGD-O2D-CED
25	b	607	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
23	a	701	LMG	O6-C5-C6-O5
23	b	626	LMG	O6-C5-C6-O5
23	a	715	LMG	O6-C5-C6-O5
23	b	626	LMG	C4-C5-C6-O5
25	D	404	CLA	CBA-CGA-O2A-C1
32	e	101	LHG	C24-C23-O8-C6
23	A	603	LMG	O6-C5-C6-O5
33	c	517	DGD	O6E-C5E-C6E-O5E
25	b	609	CLA	C4-C3-C5-C6
25	b	611	CLA	C4-C3-C5-C6
33	C	518	DGD	C4E-C5E-C6E-O5E
25	b	609	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	611	CLA	C2-C3-C5-C6
25	c	510	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	O1D-CGD-O2D-CED
23	b	627	LMG	O10-C28-O8-C9
29	I	102	SQD	O10-C23-O48-C46
32	E	101	LHG	O10-C23-O8-C6
33	C	518	DGD	O6E-C1E-O5D-C6D
28	A	611	PL9	C24-C26-C27-C28
28	a	713	PL9	C9-C11-C12-C13
23	b	627	LMG	C29-C28-O8-C9
25	c	512	CLA	CBA-CGA-O2A-C1
25	b	619	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	O1D-CGD-O2D-CED
32	D	407	LHG	C28-C29-C30-C31
25	c	502	CLA	O1D-CGD-O2D-CED
32	D	407	LHG	C1-C2-C3-O3
32	d	406	LHG	C1-C2-C3-O3
33	C	517	DGD	C4E-C5E-C6E-O5E
33	c	517	DGD	C4E-C5E-C6E-O5E
25	c	512	CLA	O1A-CGA-O2A-C1
25	C	505	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
23	a	701	LMG	C29-C28-O8-C9
25	C	513	CLA	CBA-CGA-O2A-C1
25	b	607	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
29	I	102	SQD	C24-C23-O48-C46
32	E	101	LHG	C24-C23-O8-C6
32	B	625	LHG	C23-C24-C25-C26
23	a	715	LMG	C4-C5-C6-O5
32	E	101	LHG	O6-C4-C5-O7
25	C	510	CLA	C8-C10-C11-C12
25	c	506	CLA	C5-C6-C7-C8
25	c	502	CLA	C3-C5-C6-C7
23	a	715	LMG	C10-C11-C12-C13
23	D	409	LMG	C16-C17-C18-C19
25	b	607	CLA	O1A-CGA-O2A-C1
25	B	604	CLA	C2-C3-C5-C6
28	A	611	PL9	C38-C39-C41-C42
25	B	607	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C10-C8-C9
25	B	617	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	504	CLA	C11-C10-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C12-C13-C14
25	D	403	CLA	C6-C7-C8-C9
25	b	611	CLA	C14-C13-C15-C16
25	b	612	CLA	C11-C10-C8-C9
25	b	616	CLA	C14-C13-C15-C16
25	c	502	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C10-C8-C9
25	b	612	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	d	403	CLA	C13-C15-C16-C17
27	D	405	BCR	C37-C22-C23-C24
27	c	515	BCR	C7-C8-C9-C34
27	d	404	BCR	C37-C22-C23-C24
27	k	101	BCR	C11-C12-C13-C35
27	t	103	BCR	C7-C8-C9-C34
27	b	602	BCR	C7-C8-C9-C10
27	d	404	BCR	C21-C22-C23-C24
27	t	103	BCR	C7-C8-C9-C10
29	b	601	SQD	O49-C7-O47-C45
29	I	102	SQD	C23-C24-C25-C26
32	a	720	LHG	C7-C8-C9-C10
32	e	101	LHG	C23-C24-C25-C26
25	C	513	CLA	O1A-CGA-O2A-C1
25	C	512	CLA	C10-C11-C12-C13
26	a	709	PHO	C13-C15-C16-C17
23	c	520	LMG	O6-C5-C6-O5
23	f	101	LMG	O6-C5-C6-O5
25	B	607	CLA	O1D-CGD-O2D-CED
25	d	403	CLA	C3-C5-C6-C7
25	C	508	CLA	C15-C16-C17-C18
25	b	607	CLA	C5-C6-C7-C8
25	b	608	CLA	C13-C15-C16-C17
25	c	506	CLA	C15-C16-C17-C18
23	B	621	LMG	O6-C5-C6-O5
33	H	103	DGD	O6E-C5E-C6E-O5E
29	B	623	SQD	C23-C24-C25-C26
32	b	629	LHG	C23-C24-C25-C26
26	D	401	PHO	CBD-CGD-O2D-CED
25	B	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C8-C10-C11-C12
25	B	604	CLA	C15-C16-C17-C18
25	B	607	CLA	C8-C10-C11-C12
25	C	514	CLA	C15-C16-C17-C18
25	a	711	CLA	C8-C10-C11-C12
25	b	612	CLA	C8-C10-C11-C12
25	b	612	CLA	C13-C15-C16-C17
25	b	617	CLA	C8-C10-C11-C12
25	c	503	CLA	C15-C16-C17-C18
25	c	505	CLA	C15-C16-C17-C18
25	c	512	CLA	C10-C11-C12-C13
25	d	403	CLA	C15-C16-C17-C18
23	d	408	LMG	C10-C11-C12-C13
23	d	408	LMG	C28-C29-C30-C31
29	A	614	SQD	C7-C8-C9-C10
29	A	614	SQD	C23-C24-C25-C26
29	b	601	SQD	C7-C8-C9-C10
32	E	101	LHG	C23-C24-C25-C26
33	C	518	DGD	C1A-C2A-C3A-C4A
23	a	701	LMG	C4-C5-C6-O5
25	C	504	CLA	C15-C16-C17-C18
25	C	512	CLA	C15-C16-C17-C18
25	a	711	CLA	C13-C15-C16-C17
25	b	610	CLA	C10-C11-C12-C13
25	b	616	CLA	C15-C16-C17-C18
25	C	503	CLA	C13-C15-C16-C17
25	D	404	CLA	C8-C10-C11-C12
25	c	508	CLA	C15-C16-C17-C18
23	C	501	LMG	C28-C29-C30-C31
23	c	519	LMG	C10-C11-C12-C13
25	B	605	CLA	CBD-CGD-O2D-CED
34	e	102	HEM	C3D-CAD-CBD-CGD
25	B	604	CLA	C5-C6-C7-C8
25	B	609	CLA	C15-C16-C17-C18
25	b	607	CLA	C13-C15-C16-C17
25	b	608	CLA	C10-C11-C12-C13
25	b	611	CLA	C13-C15-C16-C17
25	b	614	CLA	C15-C16-C17-C18
25	B	611	CLA	C12-C13-C15-C16
25	C	505	CLA	C12-C13-C15-C16
32	e	101	LHG	C7-C8-C9-C10
25	b	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	O1D-CGD-O2D-CED
25	D	404	CLA	C10-C11-C12-C13
25	a	719	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18
25	c	511	CLA	C15-C16-C17-C18
25	c	513	CLA	C13-C15-C16-C17
33	h	102	DGD	O6E-C5E-C6E-O5E
23	a	715	LMG	O10-C28-O8-C9
25	c	510	CLA	O1A-CGA-O2A-C1
23	C	520	LMG	O6-C1-O1-C7
23	a	715	LMG	O6-C1-O1-C7
25	b	621	CLA	C5-C6-C7-C8
28	A	611	PL9	C44-C46-C47-C48
28	D	406	PL9	C39-C41-C42-C43
28	a	713	PL9	C24-C26-C27-C28
27	h	101	BCR	C18-C19-C20-C21
32	d	406	LHG	O2-C2-C3-O3
29	D	410	SQD	O49-C7-O47-C45
25	B	607	CLA	C3-C5-C6-C7
25	A	606	CLA	C15-C16-C17-C18
25	C	512	CLA	C13-C15-C16-C17
25	b	607	CLA	C8-C10-C11-C12
25	b	615	CLA	C13-C15-C16-C17
25	b	617	CLA	C13-C15-C16-C17
25	c	508	CLA	C8-C10-C11-C12
25	c	511	CLA	C8-C10-C11-C12
25	B	603	CLA	C5-C6-C7-C8
25	B	616	CLA	C5-C6-C7-C8
25	B	616	CLA	C15-C16-C17-C18
25	C	507	CLA	C10-C11-C12-C13
25	C	514	CLA	C13-C15-C16-C17
25	B	609	CLA	CBD-CGD-O2D-CED
23	D	409	LMG	C11-C10-O7-C8
25	b	609	CLA	O1D-CGD-O2D-CED
25	B	602	CLA	C10-C11-C12-C13
25	B	602	CLA	C15-C16-C17-C18
25	B	607	CLA	C10-C11-C12-C13
25	b	607	CLA	C10-C11-C12-C13
25	c	509	CLA	C13-C15-C16-C17
25	c	510	CLA	C5-C6-C7-C8
25	c	511	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	a	720	LHG	C3-O3-P-O6
32	a	720	LHG	C4-O6-P-O3
32	d	406	LHG	C3-O3-P-O6
32	d	406	LHG	C23-C24-C25-C26
25	b	615	CLA	C3-C5-C6-C7
29	f	102	SQD	C24-C23-O48-C46
25	B	605	CLA	C13-C15-C16-C17
25	B	615	CLA	C8-C10-C11-C12
25	b	621	CLA	C10-C11-C12-C13
26	a	709	PHO	C15-C16-C17-C18
23	C	520	LMG	C28-C29-C30-C31
32	d	407	LHG	C1-C2-C3-O3
25	C	508	CLA	C4-C3-C5-C6
25	b	610	CLA	C4-C3-C5-C6
25	b	620	CLA	C4-C3-C5-C6
25	b	619	CLA	C8-C10-C11-C12
25	B	605	CLA	CBA-CGA-O2A-C1
25	a	711	CLA	CBA-CGA-O2A-C1
29	D	410	SQD	C24-C23-O48-C46
29	b	601	SQD	C24-C23-O48-C46
29	A	612	SQD	C29-C30-C31-C32
29	B	623	SQD	C30-C31-C32-C33
32	d	406	LHG	C32-C33-C34-C35
27	d	404	BCR	C20-C21-C22-C37
23	B	621	LMG	C18-C19-C20-C21
23	C	520	LMG	C15-C16-C17-C18
23	C	520	LMG	C16-C17-C18-C19
23	a	715	LMG	C20-C21-C22-C23
23	b	627	LMG	C17-C18-C19-C20
23	b	627	LMG	C29-C30-C31-C32
29	B	623	SQD	C28-C29-C30-C31
32	e	101	LHG	C15-C16-C17-C18
33	C	518	DGD	C8B-C9B-CAB-CBB
33	H	103	DGD	C7A-C8A-C9A-CAA
33	h	102	DGD	C5B-C6B-C7B-C8B
25	B	613	CLA	O1D-CGD-O2D-CED
25	C	507	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C19
23	a	715	LMG	C29-C28-O8-C9
23	C	501	LMG	C18-C19-C20-C21
23	C	521	LMG	C15-C16-C17-C18
23	D	409	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	b	627	LMG	C13-C14-C15-C16
23	c	519	LMG	C31-C32-C33-C34
29	B	623	SQD	C11-C10-C9-C8
29	B	626	SQD	C13-C14-C15-C16
33	C	519	DGD	C6B-C7B-C8B-C9B
33	c	516	DGD	C5B-C6B-C7B-C8B
23	a	701	LMG	C7-C8-O7-C10
29	A	614	SQD	C44-C45-O47-C7
29	B	623	SQD	C46-C45-O47-C7
25	C	512	CLA	O1D-CGD-O2D-CED
23	A	603	LMG	C10-C11-C12-C13
23	b	627	LMG	C28-C29-C30-C31
23	M	101	LMG	C30-C31-C32-C33
29	I	102	SQD	C13-C14-C15-C16
23	B	621	LMG	C29-C30-C31-C32
23	D	409	LMG	C20-C21-C22-C23
29	B	626	SQD	C31-C32-C33-C34
29	I	102	SQD	C10-C11-C12-C13
29	b	601	SQD	C12-C13-C14-C15
32	D	407	LHG	C32-C33-C34-C35
25	C	507	CLA	C13-C15-C16-C17
23	a	715	LMG	C13-C14-C15-C16
23	b	627	LMG	C14-C15-C16-C17
29	b	601	SQD	C11-C12-C13-C14
32	B	625	LHG	C30-C31-C32-C33
23	C	520	LMG	C2-C1-O1-C7
23	a	715	LMG	C2-C1-O1-C7
27	k	101	BCR	C20-C21-C22-C23
33	c	517	DGD	C2E-C1E-O5D-C6D
25	c	504	CLA	CBA-CGA-O2A-C1
33	C	519	DGD	C2A-C1A-O1G-C1G
23	A	603	LMG	C19-C20-C21-C22
23	C	501	LMG	C31-C32-C33-C34
23	b	627	LMG	C33-C34-C35-C36
23	f	101	LMG	C21-C22-C23-C24
29	I	102	SQD	C11-C12-C13-C14
29	a	714	SQD	C15-C16-C17-C18
29	f	102	SQD	C27-C28-C29-C30
32	D	408	LHG	C17-C18-C19-C20
33	C	517	DGD	C5B-C6B-C7B-C8B
33	C	518	DGD	C2A-C3A-C4A-C5A
33	C	518	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
33	C	519	DGD	CBA-CCA-CDA-CEA
33	c	516	DGD	C4A-C5A-C6A-C7A
25	D	404	CLA	C15-C16-C17-C18
33	C	518	DGD	O1A-C1A-O1G-C1G
25	C	512	CLA	C16-C17-C18-C20
25	b	617	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
23	M	101	LMG	C35-C36-C37-C38
23	c	519	LMG	C32-C33-C34-C35
23	d	408	LMG	C30-C31-C32-C33
29	D	410	SQD	C33-C34-C35-C36
32	D	408	LHG	C30-C31-C32-C33
32	e	101	LHG	C18-C19-C20-C21
33	c	516	DGD	C4B-C5B-C6B-C7B
25	B	605	CLA	C14-C13-C15-C16
25	B	606	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
25	b	610	CLA	C11-C12-C13-C14
25	b	617	CLA	C11-C12-C13-C14
25	c	508	CLA	C14-C13-C15-C16
26	a	709	PHO	C14-C13-C15-C16
23	M	101	LMG	C28-C29-C30-C31
23	a	715	LMG	C28-C29-C30-C31
29	I	102	SQD	C7-C8-C9-C10
23	A	603	LMG	C18-C19-C20-C21
23	C	501	LMG	C15-C16-C17-C18
23	C	501	LMG	C29-C30-C31-C32
23	D	409	LMG	C11-C12-C13-C14
23	a	701	LMG	C32-C33-C34-C35
29	A	614	SQD	C9-C10-C11-C12
29	A	614	SQD	C24-C25-C26-C27
33	C	518	DGD	CBA-CCA-CDA-CEA
33	h	102	DGD	C9A-CAA-CBA-CCA
25	b	607	CLA	C15-C16-C17-C18
25	b	618	CLA	C15-C16-C17-C18
25	c	501	CLA	C2A-CAA-CBA-CGA
27	t	103	BCR	C37-C22-C23-C24
23	C	521	LMG	C30-C31-C32-C33
23	b	627	LMG	C34-C35-C36-C37
23	c	520	LMG	C19-C20-C21-C22
23	f	101	LMG	C16-C17-C18-C19
29	D	410	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
32	L	101	LHG	C32-C33-C34-C35
32	a	720	LHG	O1-C1-C2-C3
32	e	101	LHG	O1-C1-C2-C3
27	H	102	BCR	C7-C8-C9-C10
23	D	409	LMG	C31-C32-C33-C34
23	b	626	LMG	C16-C17-C18-C19
23	b	627	LMG	C35-C36-C37-C38
29	B	626	SQD	C14-C15-C16-C17
29	B	626	SQD	C34-C35-C36-C37
32	D	408	LHG	C25-C26-C27-C28
32	E	101	LHG	C13-C14-C15-C16
29	D	410	SQD	C23-C24-C25-C26
25	c	511	CLA	O1D-CGD-O2D-CED
23	A	603	LMG	C15-C16-C17-C18
23	B	621	LMG	C33-C34-C35-C36
23	C	521	LMG	C35-C36-C37-C38
23	M	101	LMG	C31-C32-C33-C34
23	a	701	LMG	C13-C14-C15-C16
23	a	715	LMG	C16-C17-C18-C19
23	b	626	LMG	C32-C33-C34-C35
23	b	627	LMG	C37-C38-C39-C40
29	I	102	SQD	C9-C10-C11-C12
32	D	407	LHG	C30-C31-C32-C33
32	D	408	LHG	C29-C30-C31-C32
32	E	101	LHG	C32-C33-C34-C35
32	a	720	LHG	C30-C31-C32-C33
32	b	629	LHG	C32-C33-C34-C35
32	e	101	LHG	C14-C15-C16-C17
32	e	101	LHG	C24-C25-C26-C27
33	C	519	DGD	C7B-C8B-C9B-CAB
33	H	103	DGD	C5B-C6B-C7B-C8B
33	c	517	DGD	C9A-CAA-CBA-CCA
33	c	518	DGD	CBA-CCA-CDA-CEA
25	B	604	CLA	C16-C17-C18-C20
25	C	505	CLA	C16-C17-C18-C20
25	C	507	CLA	C16-C17-C18-C20
25	b	619	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C20
26	A	608	PHO	C16-C17-C18-C20
23	c	519	LMG	O6-C1-O1-C7
25	B	606	CLA	C15-C16-C17-C18
25	c	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	C	501	LMG	C17-C18-C19-C20
23	C	521	LMG	C20-C21-C22-C23
23	D	409	LMG	C19-C20-C21-C22
23	a	701	LMG	C30-C31-C32-C33
29	B	626	SQD	C24-C25-C26-C27
29	f	102	SQD	C32-C33-C34-C35
32	B	625	LHG	C11-C10-C9-C8
32	D	408	LHG	C32-C33-C34-C35
33	C	517	DGD	C4B-C5B-C6B-C7B
23	D	409	LMG	C15-C16-C17-C18
23	a	701	LMG	C21-C22-C23-C24
29	A	614	SQD	C15-C16-C17-C18
29	B	626	SQD	C29-C30-C31-C32
29	I	102	SQD	C14-C15-C16-C17
29	a	714	SQD	C13-C14-C15-C16
25	c	513	CLA	C8-C10-C11-C12
23	C	521	LMG	C21-C22-C23-C24
23	d	408	LMG	C31-C32-C33-C34
29	a	714	SQD	C28-C29-C30-C31
32	D	408	LHG	C18-C19-C20-C21
32	d	406	LHG	C25-C26-C27-C28
25	D	404	CLA	C3-C5-C6-C7
26	D	401	PHO	C3-C5-C6-C7
25	C	504	CLA	CBA-CGA-O2A-C1
25	b	622	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
23	c	520	LMG	C20-C21-C22-C23
29	a	714	SQD	C9-C10-C11-C12
32	b	629	LHG	C10-C11-C12-C13
33	C	517	DGD	C6A-C7A-C8A-C9A
25	B	614	CLA	O1D-CGD-O2D-CED
26	a	710	PHO	O1D-CGD-O2D-CED
25	D	403	CLA	C3A-C2A-CAA-CBA
25	B	606	CLA	C8-C10-C11-C12
23	C	520	LMG	C29-C30-C31-C32
23	C	520	LMG	C35-C36-C37-C38
23	C	521	LMG	C38-C39-C40-C41
23	f	101	LMG	C19-C20-C21-C22
29	B	626	SQD	C18-C19-C20-C21
29	I	102	SQD	C30-C31-C32-C33
32	B	625	LHG	C32-C33-C34-C35
33	C	517	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C16-C17-C18-C19
25	b	617	CLA	C16-C17-C18-C20
25	b	619	CLA	C16-C17-C18-C19
25	c	507	CLA	C16-C17-C18-C20
23	f	101	LMG	C12-C13-C14-C15
29	I	102	SQD	C31-C32-C33-C34
32	b	629	LHG	C34-C35-C36-C37
32	e	101	LHG	C12-C13-C14-C15
25	b	617	CLA	CBD-CGD-O2D-CED
29	A	614	SQD	C13-C14-C15-C16
28	d	405	PL9	C15-C14-C16-C17
26	A	608	PHO	C2-C3-C5-C6
28	a	713	PL9	C43-C44-C46-C47
23	B	621	LMG	C30-C31-C32-C33
23	C	521	LMG	C19-C20-C21-C22
32	b	629	LHG	C27-C28-C29-C30
25	c	505	CLA	O1D-CGD-O2D-CED
23	A	603	LMG	C14-C15-C16-C17
23	B	621	LMG	C12-C13-C14-C15
23	C	501	LMG	C32-C33-C34-C35
23	C	520	LMG	C17-C18-C19-C20
23	a	701	LMG	C31-C32-C33-C34
23	a	715	LMG	C32-C33-C34-C35
23	d	408	LMG	C11-C12-C13-C14
29	A	612	SQD	C12-C13-C14-C15
29	A	612	SQD	C25-C26-C27-C28
29	I	102	SQD	C26-C27-C28-C29
29	b	601	SQD	C24-C25-C26-C27
33	C	518	DGD	C4A-C5A-C6A-C7A
33	c	517	DGD	C5A-C6A-C7A-C8A
33	c	518	DGD	C2B-C3B-C4B-C5B
25	a	711	CLA	O1A-CGA-O2A-C1
25	d	403	CLA	C16-C17-C18-C20
23	c	520	LMG	C14-C15-C16-C17
25	a	707	CLA	C13-C15-C16-C17
29	I	102	SQD	C17-C18-C19-C20
32	D	408	LHG	C9-C10-C11-C12
32	L	101	LHG	C10-C11-C12-C13
25	c	504	CLA	O1D-CGD-O2D-CED
29	I	102	SQD	C27-C28-C29-C30
32	e	101	LHG	C9-C10-C11-C12
33	h	102	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
32	D	408	LHG	C15-C16-C17-C18
25	C	506	CLA	C13-C15-C16-C17
25	D	404	CLA	C5-C6-C7-C8
25	B	605	CLA	O1A-CGA-O2A-C1
25	b	622	CLA	O1A-CGA-O2A-C1
25	c	504	CLA	O1A-CGA-O2A-C1
23	A	603	LMG	C32-C33-C34-C35
23	C	520	LMG	C36-C37-C38-C39
23	c	519	LMG	C17-C18-C19-C20
29	A	614	SQD	C11-C10-C9-C8
32	D	408	LHG	C11-C12-C13-C14
32	d	406	LHG	C11-C12-C13-C14
33	C	519	DGD	CBB-CCB-CDB-CEB
25	C	507	CLA	C3-C5-C6-C7
27	B	618	BCR	C1-C6-C7-C8
27	B	618	BCR	C5-C6-C7-C8
27	B	620	BCR	C5-C6-C7-C8
27	B	620	BCR	C23-C24-C25-C26
27	D	405	BCR	C5-C6-C7-C8
27	Y	101	BCR	C1-C6-C7-C8
27	Y	101	BCR	C5-C6-C7-C8
27	b	602	BCR	C1-C6-C7-C8
27	b	623	BCR	C1-C6-C7-C8
27	b	623	BCR	C5-C6-C7-C8
27	b	625	BCR	C5-C6-C7-C8
27	b	625	BCR	C23-C24-C25-C26
27	b	625	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
27	c	515	BCR	C5-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	t	103	BCR	C1-C6-C7-C8
27	t	103	BCR	C5-C6-C7-C8
23	C	520	LMG	C29-C28-O8-C9
23	C	521	LMG	C29-C28-O8-C9
25	b	620	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	C10-C11-C12-C13
25	c	507	CLA	C15-C16-C17-C18
23	C	520	LMG	C32-C33-C34-C35
29	B	623	SQD	C32-C33-C34-C35
32	a	720	LHG	C31-C32-C33-C34
33	h	102	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	O1A-CGA-O2A-C1
29	b	601	SQD	C23-C24-C25-C26
33	c	516	DGD	O6E-C5E-C6E-O5E
23	A	603	LMG	C31-C32-C33-C34
25	b	615	CLA	C4-C3-C5-C6
28	D	406	PL9	C15-C14-C16-C17
25	b	607	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	C11-C10-C8-C7
25	B	607	CLA	C11-C12-C13-C15
25	C	504	CLA	C11-C10-C8-C7
25	C	511	CLA	C6-C7-C8-C10
25	b	609	CLA	C6-C7-C8-C10
25	b	612	CLA	C11-C10-C8-C7
25	c	508	CLA	C12-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C10
25	c	511	CLA	C6-C7-C8-C10
25	d	402	CLA	C12-C13-C15-C16
25	C	504	CLA	O1A-CGA-O2A-C1
23	c	520	LMG	C32-C33-C34-C35
25	B	614	CLA	C13-C15-C16-C17
25	c	508	CLA	C16-C17-C18-C19
23	b	627	LMG	O9-C10-O7-C8
29	A	614	SQD	C16-C17-C18-C19
32	a	720	LHG	C27-C28-C29-C30
32	e	101	LHG	C26-C27-C28-C29
25	b	620	CLA	C2A-CAA-CBA-CGA
25	C	513	CLA	C10-C11-C12-C13
25	c	510	CLA	C8-C10-C11-C12
25	D	404	CLA	O1D-CGD-O2D-CED
29	b	601	SQD	C30-C31-C32-C33
23	a	701	LMG	C28-C29-C30-C31
32	L	101	LHG	C23-C24-C25-C26
32	E	101	LHG	C24-C25-C26-C27
33	C	518	DGD	CCB-CDB-CEB-CFB
33	H	103	DGD	CBA-CCA-CDA-CEA
33	H	103	DGD	CCA-CDA-CEA-CFA
32	d	406	LHG	C10-C11-C12-C13
25	C	507	CLA	CBA-CGA-O2A-C1
25	B	614	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C20
33	C	519	DGD	O6D-C1D-O3G-C3G
33	c	517	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
25	b	609	CLA	C15-C16-C17-C18
25	c	510	CLA	O1D-CGD-O2D-CED
28	a	713	PL9	C39-C41-C42-C43
23	c	519	LMG	C19-C20-C21-C22
29	b	601	SQD	C32-C33-C34-C35
32	E	101	LHG	C8-C7-O7-C5
23	C	501	LMG	C13-C14-C15-C16
23	C	520	LMG	C13-C14-C15-C16
32	d	407	LHG	C16-C17-C18-C19
25	b	615	CLA	C15-C16-C17-C18
25	C	509	CLA	CBD-CGD-O2D-CED
23	c	519	LMG	C20-C21-C22-C23
23	d	408	LMG	C18-C19-C20-C21
32	d	407	LHG	C34-C35-C36-C37
33	H	103	DGD	C4D-C5D-C6D-O5D
23	a	701	LMG	C17-C18-C19-C20
32	D	408	LHG	C12-C13-C14-C15
23	c	519	LMG	C2-C1-O1-C7
23	c	520	LMG	C2-C1-O1-C7
29	B	623	SQD	C2-C1-O6-C44
25	c	508	CLA	CBA-CGA-O2A-C1
23	C	521	LMG	C37-C38-C39-C40
23	a	715	LMG	C21-C22-C23-C24
25	C	504	CLA	C5-C6-C7-C8
25	B	606	CLA	C4-C3-C5-C6
26	A	608	PHO	C4-C3-C5-C6
28	D	406	PL9	C30-C29-C31-C32
28	a	713	PL9	C15-C14-C16-C17
23	B	621	LMG	C10-C11-C12-C13
29	B	626	SQD	C7-C8-C9-C10
25	b	610	CLA	C2-C3-C5-C6
25	b	615	CLA	C2-C3-C5-C6
28	a	713	PL9	C38-C39-C41-C42
25	A	607	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	605	CLA	C11-C10-C8-C9
25	B	607	CLA	C6-C7-C8-C9
25	B	616	CLA	C11-C12-C13-C14
25	B	616	CLA	C14-C13-C15-C16
25	B	617	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	b	609	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	510	CLA	C6-C7-C8-C9
25	c	511	CLA	C6-C7-C8-C9
23	M	101	LMG	C16-C17-C18-C19
25	C	512	CLA	C3-C5-C6-C7
25	c	512	CLA	C2A-CAA-CBA-CGA
23	a	701	LMG	O10-C28-O8-C9
25	b	620	CLA	O1A-CGA-O2A-C1
25	C	504	CLA	C1A-C2A-CAA-CBA
25	a	719	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C1A-C2A-CAA-CBA
25	B	614	CLA	C16-C17-C18-C19
25	C	512	CLA	C16-C17-C18-C19
25	c	508	CLA	C16-C17-C18-C20
23	D	409	LMG	O9-C10-O7-C8
23	b	628	LMG	C11-C12-C13-C14
32	E	101	LHG	C28-C29-C30-C31
33	C	519	DGD	C5A-C6A-C7A-C8A
25	B	608	CLA	O1D-CGD-O2D-CED
25	b	619	CLA	O1D-CGD-O2D-CED
32	D	407	LHG	C3-O3-P-O6
32	E	101	LHG	C4-O6-P-O3
23	f	101	LMG	C31-C32-C33-C34
29	B	626	SQD	C27-C28-C29-C30
29	b	601	SQD	C33-C34-C35-C36
29	f	102	SQD	C31-C32-C33-C34
32	D	407	LHG	C34-C35-C36-C37
32	a	720	LHG	C25-C26-C27-C28
33	C	518	DGD	C6A-C7A-C8A-C9A
33	C	519	DGD	C4B-C5B-C6B-C7B
23	C	520	LMG	C31-C32-C33-C34
32	b	629	LHG	C33-C34-C35-C36
23	b	626	LMG	C30-C31-C32-C33
32	B	625	LHG	C27-C28-C29-C30
25	b	611	CLA	C16-C17-C18-C19
23	C	521	LMG	O6-C5-C6-O5
23	C	520	LMG	C12-C13-C14-C15
33	C	519	DGD	C8A-C9A-CAA-CBA
25	c	507	CLA	C3-C5-C6-C7
23	c	519	LMG	C29-C30-C31-C32
35	V	201	HEC	C3D-CAD-CBD-CGD
23	b	626	LMG	C37-C38-C39-C40
29	I	102	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	b	601	SQD	C27-C28-C29-C30
25	a	707	CLA	C15-C16-C17-C18
26	A	608	PHO	C15-C16-C17-C18
29	A	614	SQD	C14-C15-C16-C17
23	f	101	LMG	C11-C12-C13-C14
32	E	101	LHG	C31-C32-C33-C34
25	B	611	CLA	C15-C16-C17-C18
29	f	102	SQD	C44-C45-C46-O48
32	E	101	LHG	C4-C5-C6-O8
32	e	101	LHG	C4-C5-C6-O8
32	e	101	LHG	C19-C20-C21-C22
23	b	627	LMG	O6-C5-C6-O5
25	d	403	CLA	C10-C11-C12-C13
23	A	603	LMG	C20-C21-C22-C23
23	C	501	LMG	C38-C39-C40-C41
23	C	521	LMG	C8-C7-O1-C1
29	b	601	SQD	C45-C44-O6-C1
23	C	501	LMG	C22-C23-C24-C25
33	C	519	DGD	C2B-C3B-C4B-C5B
25	C	502	CLA	O1D-CGD-O2D-CED
26	D	401	PHO	O1D-CGD-O2D-CED
23	c	520	LMG	C17-C18-C19-C20
23	f	101	LMG	C33-C34-C35-C36
32	B	625	LHG	C10-C11-C12-C13
23	B	621	LMG	C28-C29-C30-C31
29	A	612	SQD	C30-C31-C32-C33
23	M	101	LMG	C19-C20-C21-C22
29	A	612	SQD	C32-C33-C34-C35
25	C	506	CLA	CBD-CGD-O2D-CED
32	E	101	LHG	O1-C1-C2-O2
32	a	720	LHG	O1-C1-C2-O2
32	e	101	LHG	O1-C1-C2-O2
32	b	629	LHG	C9-C10-C11-C12
32	e	101	LHG	C28-C29-C30-C31
23	D	409	LMG	O6-C5-C6-O5
23	A	603	LMG	C38-C39-C40-C41
33	c	517	DGD	C3B-C4B-C5B-C6B
29	D	410	SQD	O48-C23-C24-C25
23	A	603	LMG	C4-C5-C6-O5
23	b	626	LMG	C40-C41-C42-C43
25	c	503	CLA	C5-C6-C7-C8
25	c	505	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	a	713	PL9	C20-C19-C21-C22
28	a	713	PL9	C45-C44-C46-C47
25	C	508	CLA	C2-C3-C5-C6
25	b	620	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
23	D	409	LMG	C28-C29-C30-C31
25	C	508	CLA	C16-C17-C18-C19
25	C	511	CLA	CBA-CGA-O2A-C1
29	B	626	SQD	C11-C12-C13-C14
29	I	102	SQD	C18-C19-C20-C21
33	C	518	DGD	C9B-CAB-CBB-CCB
25	c	512	CLA	C2-C1-O2A-CGA
23	b	626	LMG	C31-C32-C33-C34
32	E	101	LHG	C12-C13-C14-C15
33	h	102	DGD	CBB-CCB-CDB-CEB
33	C	518	DGD	C2A-C1A-O1G-C1G
25	C	507	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	O1A-CGA-O2A-C1
32	D	407	LHG	C27-C28-C29-C30
23	b	626	LMG	C19-C20-C21-C22
29	I	102	SQD	C11-C10-C9-C8
25	B	612	CLA	C13-C15-C16-C17
23	C	521	LMG	C2-C1-O1-C7
23	B	621	LMG	O1-C7-C8-O7
23	a	715	LMG	O7-C8-C9-O8
29	a	714	SQD	O6-C44-C45-O47
23	b	626	LMG	C34-C35-C36-C37
25	B	617	CLA	C15-C16-C17-C18
26	a	710	PHO	CHA-CBD-CGD-O1D
26	a	710	PHO	CHA-CBD-CGD-O2D
29	f	102	SQD	C35-C36-C37-C38
23	B	621	LMG	C40-C41-C42-C43
32	L	101	LHG	C34-C35-C36-C37
25	B	610	CLA	C15-C16-C17-C18
25	b	620	CLA	C10-C11-C12-C13
25	A	607	CLA	C6-C7-C8-C10
25	A	607	CLA	C12-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C11-C12-C13-C15
25	B	607	CLA	C6-C7-C8-C10
25	B	609	CLA	C11-C12-C13-C15
25	B	616	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	C12-C13-C15-C16
25	B	617	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C10-C8-C7
25	C	513	CLA	C11-C10-C8-C7
25	a	711	CLA	C11-C12-C13-C15
25	b	610	CLA	C11-C12-C13-C15
25	b	611	CLA	C12-C13-C15-C16
25	b	612	CLA	C6-C7-C8-C10
25	b	621	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	507	CLA	C12-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C10
28	D	406	PL9	C28-C29-C31-C32
23	C	520	LMG	O10-C28-O8-C9
32	b	629	LHG	C16-C17-C18-C19
33	c	517	DGD	CCB-CDB-CEB-CFB
25	B	604	CLA	C6-C7-C8-C9
25	B	612	CLA	C14-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C9
25	C	513	CLA	C11-C10-C8-C9
25	a	708	CLA	C6-C7-C8-C9
25	a	711	CLA	C11-C12-C13-C14
25	b	617	CLA	C6-C7-C8-C9
25	b	621	CLA	C11-C10-C8-C9
25	b	621	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C12-C13-C14
25	c	512	CLA	C14-C13-C15-C16
25	c	513	CLA	C11-C12-C13-C14
25	d	403	CLA	C6-C7-C8-C9
23	b	626	LMG	C17-C18-C19-C20
29	B	626	SQD	C32-C33-C34-C35
23	A	603	LMG	C29-C28-O8-C9
23	c	519	LMG	C29-C28-O8-C9
25	C	503	CLA	C5-C6-C7-C8
25	C	505	CLA	C8-C10-C11-C12
29	A	612	SQD	C9-C10-C11-C12
29	B	623	SQD	C7-C8-C9-C10
23	a	715	LMG	C29-C30-C31-C32
32	D	408	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	c	503	CLA	CBA-CGA-O2A-C1
32	D	407	LHG	C14-C15-C16-C17
33	h	102	DGD	C7A-C8A-C9A-CAA
33	h	102	DGD	C2B-C3B-C4B-C5B
23	C	501	LMG	C21-C22-C23-C24
29	B	623	SQD	C12-C13-C14-C15
29	a	714	SQD	C14-C15-C16-C17
32	e	101	LHG	C27-C28-C29-C30
27	t	103	BCR	C22-C23-C24-C25
33	c	518	DGD	C9B-CAB-CBB-CCB
32	E	101	LHG	O6-C4-C5-C6
32	b	629	LHG	O6-C4-C5-C6
32	d	407	LHG	O6-C4-C5-C6
23	c	519	LMG	C30-C31-C32-C33
23	d	408	LMG	C12-C13-C14-C15
23	A	603	LMG	C16-C17-C18-C19
25	B	604	CLA	CBA-CGA-O2A-C1
25	C	504	CLA	C4-C3-C5-C6
23	f	101	LMG	C10-C11-C12-C13
23	C	501	LMG	C36-C37-C38-C39
32	L	101	LHG	C31-C32-C33-C34
25	C	511	CLA	O1A-CGA-O2A-C1
23	C	521	LMG	C12-C13-C14-C15
23	C	520	LMG	C30-C31-C32-C33
23	f	101	LMG	C13-C14-C15-C16
23	f	101	LMG	C4-C5-C6-O5
32	b	629	LHG	C29-C30-C31-C32
33	h	102	DGD	CBA-CCA-CDA-CEA
29	A	612	SQD	C10-C11-C12-C13
25	B	616	CLA	C13-C15-C16-C17
25	b	608	CLA	C8-C10-C11-C12
25	c	506	CLA	C8-C10-C11-C12
33	c	516	DGD	C5A-C6A-C7A-C8A
25	c	507	CLA	C16-C17-C18-C19
25	C	502	CLA	CBA-CGA-O2A-C1
29	B	623	SQD	C33-C34-C35-C36
32	L	101	LHG	C16-C17-C18-C19
25	B	616	CLA	C8-C10-C11-C12
25	C	510	CLA	C13-C15-C16-C17
25	B	609	CLA	O1D-CGD-O2D-CED
23	B	621	LMG	O1-C7-C8-C9
23	C	520	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	a	715	LMG	C7-C8-C9-O8
29	A	614	SQD	C44-C45-C46-O48
29	D	410	SQD	C44-C45-C46-O48
29	a	714	SQD	O6-C44-C45-C46
33	c	516	DGD	C1G-C2G-C3G-O3G
23	c	520	LMG	C30-C31-C32-C33
32	B	625	LHG	C11-C12-C13-C14
32	L	101	LHG	C9-C10-C11-C12
25	c	508	CLA	C10-C11-C12-C13
23	c	519	LMG	C34-C35-C36-C37
25	B	611	CLA	C13-C15-C16-C17
25	b	611	CLA	CBA-CGA-O2A-C1
23	c	519	LMG	C14-C15-C16-C17
23	a	701	LMG	C36-C37-C38-C39
32	D	408	LHG	C4-O6-P-O3
23	C	521	LMG	C10-C11-C12-C13
23	C	521	LMG	C36-C37-C38-C39
32	D	407	LHG	O1-C1-C2-O2
25	b	621	CLA	C15-C16-C17-C18
23	C	501	LMG	C16-C17-C18-C19
23	c	519	LMG	C15-C16-C17-C18
33	H	103	DGD	C5A-C6A-C7A-C8A
32	D	407	LHG	O6-C4-C5-O7
32	a	720	LHG	O6-C4-C5-O7
33	c	516	DGD	O6D-C5D-C6D-O5D
25	C	508	CLA	C16-C17-C18-C20
32	a	720	LHG	C9-C10-C11-C12
32	L	101	LHG	O2-C2-C3-O3
23	a	701	LMG	C18-C19-C20-C21
32	d	406	LHG	C18-C19-C20-C21
23	a	715	LMG	C37-C38-C39-C40
23	A	603	LMG	C34-C35-C36-C37
29	a	714	SQD	C16-C17-C18-C19
23	C	501	LMG	O1-C7-C8-O7
23	a	715	LMG	O1-C7-C8-O7
29	B	623	SQD	O47-C45-C46-O48
29	b	601	SQD	O6-C44-C45-O47
32	E	101	LHG	O7-C5-C6-O8
33	c	516	DGD	O2G-C2G-C3G-O3G
25	B	608	CLA	CBA-CGA-O2A-C1
23	M	101	LMG	C38-C39-C40-C41
33	C	519	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
33	c	517	DGD	C4B-C5B-C6B-C7B
23	a	715	LMG	C11-C10-O7-C8
26	A	608	PHO	C16-C17-C18-C19
26	a	710	PHO	C16-C17-C18-C20
23	b	626	LMG	C35-C36-C37-C38
29	A	614	SQD	C33-C34-C35-C36
28	d	405	PL9	C39-C41-C42-C43
29	I	102	SQD	O6-C44-C45-C46
23	C	520	LMG	C38-C39-C40-C41
29	B	623	SQD	C31-C32-C33-C34
25	B	609	CLA	C2-C1-O2A-CGA
25	B	614	CLA	C2-C1-O2A-CGA
28	a	713	PL9	C18-C19-C21-C22
25	B	612	CLA	C11-C12-C13-C14
25	C	512	CLA	C11-C10-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	c	505	CLA	C11-C10-C8-C9
25	c	513	CLA	C14-C13-C15-C16
25	d	402	CLA	C6-C7-C8-C9
29	I	102	SQD	C35-C36-C37-C38
32	E	101	LHG	C2-C3-O3-P
23	C	501	LMG	C33-C34-C35-C36
25	B	609	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C16-C17-C18-C20
25	a	711	CLA	C16-C17-C18-C20
25	a	719	CLA	C16-C17-C18-C20
27	A	610	BCR	C1-C6-C7-C8
27	A	610	BCR	C5-C6-C7-C8
27	B	619	BCR	C1-C6-C7-C8
27	B	619	BCR	C5-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C26
27	B	619	BCR	C23-C24-C25-C30
27	C	515	BCR	C1-C6-C7-C8
27	C	516	BCR	C1-C6-C7-C8
27	D	405	BCR	C23-C24-C25-C26
27	D	405	BCR	C23-C24-C25-C30
27	H	102	BCR	C23-C24-C25-C26
27	H	102	BCR	C23-C24-C25-C30
27	K	101	BCR	C1-C6-C7-C8
27	K	101	BCR	C23-C24-C25-C26
27	a	712	BCR	C1-C6-C7-C8
27	a	712	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	b	624	BCR	C1-C6-C7-C8
27	b	624	BCR	C5-C6-C7-C8
27	b	624	BCR	C23-C24-C25-C26
27	c	514	BCR	C5-C6-C7-C8
27	c	515	BCR	C23-C24-C25-C26
27	c	515	BCR	C23-C24-C25-C30
27	d	404	BCR	C1-C6-C7-C8
27	d	404	BCR	C5-C6-C7-C8
27	h	101	BCR	C23-C24-C25-C26
27	k	102	BCR	C1-C6-C7-C8
27	k	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C30
25	C	509	CLA	C5-C6-C7-C8
25	c	513	CLA	C15-C16-C17-C18
23	D	409	LMG	C30-C31-C32-C33
25	b	617	CLA	O1D-CGD-O2D-CED
23	f	101	LMG	C14-C15-C16-C17
32	D	408	LHG	C24-C23-O8-C6
27	Y	101	BCR	C7-C8-C9-C10
27	b	623	BCR	C21-C22-C23-C24
27	c	514	BCR	C21-C22-C23-C24
33	c	516	DGD	C4D-C5D-C6D-O5D
25	B	602	CLA	C8-C10-C11-C12
23	C	501	LMG	C12-C13-C14-C15
23	d	408	LMG	C20-C21-C22-C23
25	B	604	CLA	C16-C17-C18-C19
25	B	609	CLA	C16-C17-C18-C20
23	C	521	LMG	C39-C40-C41-C42
32	D	407	LHG	C11-C10-C9-C8
33	c	516	DGD	C2A-C3A-C4A-C5A
25	B	605	CLA	O1D-CGD-O2D-CED
25	B	607	CLA	C13-C15-C16-C17
25	C	504	CLA	C8-C10-C11-C12
32	D	407	LHG	O6-C4-C5-C6
25	B	604	CLA	C6-C7-C8-C10
25	B	612	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C10-C8-C7
25	B	617	CLA	C11-C12-C13-C15
25	C	503	CLA	C6-C7-C8-C10
25	C	503	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C12-C13-C15
25	C	511	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C6-C7-C8-C10
25	C	512	CLA	C11-C10-C8-C7
25	C	513	CLA	C12-C13-C15-C16
25	a	708	CLA	C6-C7-C8-C10
25	a	708	CLA	C12-C13-C15-C16
25	b	617	CLA	C6-C7-C8-C10
25	b	617	CLA	C11-C12-C13-C15
25	b	617	CLA	C12-C13-C15-C16
25	b	621	CLA	C12-C13-C15-C16
25	c	502	CLA	C11-C10-C8-C7
25	c	513	CLA	C6-C7-C8-C10
25	c	513	CLA	C11-C12-C13-C15
25	c	513	CLA	C12-C13-C15-C16
33	C	518	DGD	C4B-C5B-C6B-C7B
33	c	518	DGD	C7A-C8A-C9A-CAA
25	C	514	CLA	C8-C10-C11-C12
23	a	715	LMG	C33-C34-C35-C36
23	B	621	LMG	C14-C15-C16-C17
25	C	510	CLA	C5-C6-C7-C8
25	C	511	CLA	C8-C10-C11-C12
23	C	501	LMG	C11-C10-O7-C8
33	C	517	DGD	C4D-C5D-C6D-O5D
27	C	516	BCR	C16-C17-C18-C36
27	a	712	BCR	C16-C17-C18-C36
29	a	714	SQD	C26-C27-C28-C29
25	C	506	CLA	CBA-CGA-O2A-C1
32	L	101	LHG	C33-C34-C35-C36
23	B	621	LMG	C34-C35-C36-C37
23	D	409	LMG	C18-C19-C20-C21
23	b	628	LMG	C13-C14-C15-C16
25	c	512	CLA	C5-C6-C7-C8
23	a	715	LMG	C38-C39-C40-C41
29	A	612	SQD	C14-C15-C16-C17
25	B	609	CLA	CAD-CBD-CGD-O2D
25	C	514	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
29	B	626	SQD	C46-C45-O47-C7
25	C	507	CLA	C5-C6-C7-C8
23	B	621	LMG	C39-C40-C41-C42
23	M	101	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
29	A	612	SQD	C13-C14-C15-C16
23	c	520	LMG	C29-C28-O8-C9
33	C	517	DGD	O6D-C5D-C6D-O5D
25	B	616	CLA	C10-C11-C12-C13
23	D	409	LMG	C22-C23-C24-C25
23	a	701	LMG	O1-C7-C8-C9
23	b	627	LMG	C7-C8-C9-O8
29	B	623	SQD	C44-C45-C46-O48
32	L	101	LHG	C4-C5-C6-O8
32	a	720	LHG	C4-C5-C6-O8
32	b	629	LHG	C4-C5-C6-O8
25	B	604	CLA	O1A-CGA-O2A-C1
32	b	629	LHG	O6-C4-C5-O7
25	c	508	CLA	C13-C15-C16-C17
23	a	715	LMG	C15-C16-C17-C18
33	C	519	DGD	CAA-CBA-CCA-CDA
34	e	102	HEM	C4B-C3B-CAB-CBB
25	B	615	CLA	C16-C17-C18-C19
25	C	509	CLA	O1D-CGD-O2D-CED
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	610	CLA	CHA-CBD-CGD-O1D
25	B	610	CLA	CHA-CBD-CGD-O2D
25	B	613	CLA	CHA-CBD-CGD-O1D
25	C	504	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	b	618	CLA	CHA-CBD-CGD-O1D
25	b	618	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
23	a	715	LMG	C36-C37-C38-C39
25	C	502	CLA	O1A-CGA-O2A-C1
25	c	503	CLA	O1A-CGA-O2A-C1
23	c	520	LMG	O7-C8-C9-O8
32	a	720	LHG	O7-C5-C6-O8
25	b	611	CLA	O1A-CGA-O2A-C1
23	D	409	LMG	C32-C33-C34-C35
32	B	625	LHG	C24-C25-C26-C27
33	c	517	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
23	A	603	LMG	O10-C28-O8-C9
28	d	405	PL9	C4-C3-C7-C8
25	C	503	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	514	CLA	C11-C10-C8-C9
25	b	617	CLA	C14-C13-C15-C16
25	B	608	CLA	O1A-CGA-O2A-C1
32	e	101	LHG	C25-C26-C27-C28
33	c	518	DGD	C4A-C5A-C6A-C7A
29	a	714	SQD	C5-C6-S-O8
23	C	520	LMG	C11-C12-C13-C14
23	c	520	LMG	C33-C34-C35-C36
25	C	506	CLA	O1A-CGA-O2A-C1
23	D	409	LMG	C34-C35-C36-C37
23	f	101	LMG	C18-C19-C20-C21
25	D	403	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C16-C17-C18-C19
25	C	503	CLA	C16-C17-C18-C20
25	b	618	CLA	CBD-CGD-O2D-CED
29	b	601	SQD	C11-C10-C9-C8
32	E	101	LHG	C3-O3-P-O6
25	B	611	CLA	C5-C6-C7-C8
25	c	513	CLA	C3-C5-C6-C7
25	B	606	CLA	C2-C3-C5-C6
33	h	102	DGD	O1A-C1A-O1G-C1G
32	B	625	LHG	C3-O3-P-O5
32	D	407	LHG	C3-O3-P-O4
32	D	407	LHG	C4-O6-P-O5
32	E	101	LHG	C4-O6-P-O4
32	a	720	LHG	C3-O3-P-O5
32	d	406	LHG	C3-O3-P-O5
32	d	407	LHG	C4-O6-P-O5
25	C	510	CLA	C16-C17-C18-C20
25	a	711	CLA	C16-C17-C18-C19
25	a	719	CLA	C16-C17-C18-C19
25	b	609	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C20
29	A	612	SQD	O5-C1-O6-C44
25	B	606	CLA	C10-C11-C12-C13
23	M	101	LMG	C20-C21-C22-C23
29	b	601	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	b	609	CLA	C2A-CAA-CBA-CGA
32	D	408	LHG	C10-C11-C12-C13
25	B	604	CLA	CAD-CBD-CGD-O1D
25	B	606	CLA	CAD-CBD-CGD-O1D
25	B	610	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	615	CLA	CAD-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	b	610	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	618	CLA	CAD-CBD-CGD-O1D
29	A	612	SQD	C5-C6-S-O7
25	B	613	CLA	C10-C11-C12-C13
23	a	701	LMG	C20-C21-C22-C23
32	L	101	LHG	C1-C2-C3-O3
32	L	101	LHG	C17-C18-C19-C20
25	B	610	CLA	C16-C17-C18-C20
25	B	615	CLA	C6-C7-C8-C10
25	B	616	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C12-C13-C15
25	C	514	CLA	C11-C10-C8-C7
25	b	607	CLA	C11-C12-C13-C15
25	b	609	CLA	C11-C10-C8-C7
25	b	610	CLA	C11-C10-C8-C7
25	b	619	CLA	C6-C7-C8-C10
25	c	502	CLA	C6-C7-C8-C10
25	c	509	CLA	C11-C10-C8-C7
26	A	608	PHO	C6-C7-C8-C10
32	d	407	LHG	O6-C4-C5-O7
33	c	517	DGD	C6A-C7A-C8A-C9A
33	c	518	DGD	C6A-C7A-C8A-C9A
23	M	101	LMG	C34-C35-C36-C37
23	M	101	LMG	C32-C33-C34-C35
23	a	701	LMG	C37-C38-C39-C40
25	D	404	CLA	C16-C17-C18-C20
23	C	501	LMG	O1-C7-C8-C9
23	a	715	LMG	O1-C7-C8-C9
29	D	410	SQD	C2-C1-O6-C44
29	b	601	SQD	O6-C44-C45-C46
32	d	406	LHG	C17-C18-C19-C20
23	C	520	LMG	O1-C7-C8-O7
23	a	701	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
29	A	614	SQD	O47-C45-C46-O48
29	B	623	SQD	O6-C44-C45-O47
29	D	410	SQD	O47-C45-C46-O48
32	L	101	LHG	O7-C5-C6-O8
32	e	101	LHG	O7-C5-C6-O8
33	C	517	DGD	O2G-C2G-C3G-O3G
29	B	623	SQD	C25-C26-C27-C28
23	a	701	LMG	C39-C40-C41-C42
32	D	408	LHG	C13-C14-C15-C16
32	d	406	LHG	C27-C28-C29-C30
29	D	410	SQD	O10-C23-O48-C46
23	a	701	LMG	C8-C7-O1-C1
26	a	710	PHO	C16-C17-C18-C19
23	d	408	LMG	C37-C38-C39-C40
25	C	506	CLA	O1D-CGD-O2D-CED
23	f	101	LMG	C30-C31-C32-C33
25	a	711	CLA	C10-C11-C12-C13
25	c	510	CLA	C4-C3-C5-C6
25	C	512	CLA	CBA-CGA-O2A-C1
23	c	519	LMG	C37-C38-C39-C40
32	b	629	LHG	C30-C31-C32-C33
33	c	517	DGD	C3A-C4A-C5A-C6A
28	D	406	PL9	C13-C14-C16-C17
33	H	103	DGD	O2G-C1B-C2B-C3B
25	B	605	CLA	C10-C11-C12-C13
25	B	609	CLA	C11-C12-C13-C14
25	C	511	CLA	C11-C10-C8-C9
25	a	708	CLA	C14-C13-C15-C16
25	b	612	CLA	C14-C13-C15-C16
25	b	617	CLA	C11-C10-C8-C9
25	b	618	CLA	C6-C7-C8-C9
25	c	501	CLA	C11-C12-C13-C14
25	c	502	CLA	C11-C10-C8-C9
26	A	608	PHO	C6-C7-C8-C9
23	C	521	LMG	O10-C28-O8-C9
23	C	520	LMG	C37-C38-C39-C40
23	c	520	LMG	C15-C16-C17-C18
29	b	601	SQD	C18-C19-C20-C21
33	C	518	DGD	C1B-C2B-C3B-C4B
33	h	102	DGD	C4D-C5D-C6D-O5D
29	f	102	SQD	C8-C7-O47-C45
23	B	621	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	C	520	LMG	C22-C23-C24-C25
23	c	519	LMG	C38-C39-C40-C41
33	C	518	DGD	CDA-CEA-CFA-CGA
25	C	504	CLA	C2-C3-C5-C6
23	a	701	LMG	C15-C16-C17-C18
33	C	519	DGD	O6E-C5E-C6E-O5E
25	C	512	CLA	O1A-CGA-O2A-C1
32	E	101	LHG	C30-C31-C32-C33
25	C	506	CLA	C2A-CAA-CBA-CGA
25	D	402	CLA	C15-C16-C17-C18
25	D	403	CLA	C2-C1-O2A-CGA
25	a	707	CLA	C2-C1-O2A-CGA
25	b	619	CLA	C2-C1-O2A-CGA
33	c	516	DGD	C7B-C8B-C9B-CAB
25	D	403	CLA	C3-C5-C6-C7
23	c	520	LMG	C31-C32-C33-C34
32	D	408	LHG	C34-C35-C36-C37
32	d	406	LHG	C15-C16-C17-C18
23	C	501	LMG	C29-C28-O8-C9
32	e	101	LHG	O6-C4-C5-O7
23	c	520	LMG	C40-C41-C42-C43
25	b	618	CLA	O1D-CGD-O2D-CED
27	A	610	BCR	C23-C24-C25-C26
27	A	610	BCR	C23-C24-C25-C30
27	C	515	BCR	C5-C6-C7-C8
27	C	516	BCR	C5-C6-C7-C8
27	C	516	BCR	C23-C24-C25-C30
27	K	101	BCR	C5-C6-C7-C8
27	K	101	BCR	C23-C24-C25-C30
27	a	712	BCR	C23-C24-C25-C30
27	b	624	BCR	C23-C24-C25-C30
27	h	101	BCR	C23-C24-C25-C30
27	k	102	BCR	C23-C24-C25-C26
32	E	101	LHG	O9-C7-O7-C5
34	e	102	HEM	C2D-C3D-CAD-CBD
25	C	508	CLA	C13-C15-C16-C17
29	b	601	SQD	C2-C1-O6-C44
33	C	519	DGD	C2D-C1D-O3G-C3G
32	L	101	LHG	C4-O6-P-O3
32	b	629	LHG	C4-O6-P-O3
32	d	407	LHG	C3-O3-P-O6
26	D	401	PHO	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
33	C	517	DGD	C7A-C8A-C9A-CAA
33	C	517	DGD	C3B-C4B-C5B-C6B
23	c	519	LMG	O1-C7-C8-C9
33	C	517	DGD	C1G-C2G-C3G-O3G
23	C	520	LMG	C20-C21-C22-C23
23	D	409	LMG	C39-C40-C41-C42
32	D	407	LHG	C12-C13-C14-C15
32	d	406	LHG	C12-C13-C14-C15
25	C	502	CLA	C12-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C10
25	b	617	CLA	C11-C10-C8-C7
25	b	618	CLA	C6-C7-C8-C10
25	c	512	CLA	C12-C13-C15-C16
25	A	607	CLA	C14-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C14
25	B	606	CLA	C6-C7-C8-C9
25	B	616	CLA	C11-C10-C8-C9
25	B	617	CLA	C11-C12-C13-C14
25	b	609	CLA	C11-C10-C8-C9
25	b	619	CLA	C6-C7-C8-C9
25	c	501	CLA	C11-C10-C8-C9
25	c	508	CLA	C11-C12-C13-C14
25	d	402	CLA	C14-C13-C15-C16
27	d	404	BCR	C19-C20-C21-C22
25	B	608	CLA	C16-C17-C18-C20
23	a	701	LMG	C34-C35-C36-C37
33	h	102	DGD	CCB-CDB-CEB-CFB
25	B	613	CLA	C13-C15-C16-C17
25	C	510	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C19
23	d	408	LMG	C36-C37-C38-C39
32	d	406	LHG	O1-C1-C2-C3
32	d	407	LHG	C25-C26-C27-C28
29	f	102	SQD	O10-C23-O48-C46
27	b	625	BCR	C21-C22-C23-C24
33	C	517	DGD	C7B-C8B-C9B-CAB
25	B	606	CLA	C5-C6-C7-C8
25	C	511	CLA	C4-C3-C5-C6
28	d	405	PL9	C13-C14-C16-C17
28	d	405	PL9	C28-C29-C31-C32
25	B	610	CLA	C16-C17-C18-C19
23	b	628	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	B	625	LHG	C25-C26-C27-C28
33	h	102	DGD	C5A-C6A-C7A-C8A
23	b	626	LMG	O8-C28-C29-C30
25	B	606	CLA	C13-C15-C16-C17
25	B	617	CLA	C5-C6-C7-C8
33	C	517	DGD	O1A-C1A-O1G-C1G
25	C	502	CLA	C2A-CAA-CBA-CGA
25	D	404	CLA	C16-C17-C18-C19
23	b	627	LMG	O6-C1-O1-C7
29	a	714	SQD	O5-C1-O6-C44
33	c	517	DGD	CBA-CCA-CDA-CEA
27	B	618	BCR	C10-C11-C12-C13
27	b	624	BCR	C10-C11-C12-C13
27	k	101	BCR	C10-C11-C12-C13
27	t	103	BCR	C10-C11-C12-C13
25	A	607	CLA	C3-C5-C6-C7
29	A	614	SQD	C34-C35-C36-C37
28	D	406	PL9	C45-C44-C46-C47
25	C	505	CLA	C15-C16-C17-C18
25	C	511	CLA	C2-C3-C5-C6
28	a	713	PL9	C13-C14-C16-C17
25	B	613	CLA	C15-C16-C17-C18
33	c	517	DGD	C8B-C9B-CAB-CBB
25	C	504	CLA	C2-C1-O2A-CGA
33	C	518	DGD	CBB-CCB-CDB-CEB
33	C	518	DGD	C7B-C8B-C9B-CAB
23	b	627	LMG	O7-C8-C9-O8
23	c	519	LMG	O1-C7-C8-O7
25	B	615	CLA	C2A-CAA-CBA-CGA
25	a	707	CLA	C2A-CAA-CBA-CGA
32	b	629	LHG	O7-C5-C6-O8
33	c	517	DGD	C1B-C2B-C3B-C4B
25	b	611	CLA	C15-C16-C17-C18
26	D	401	PHO	C16-C17-C18-C20
23	d	408	LMG	C29-C30-C31-C32
23	f	101	LMG	C39-C40-C41-C42
25	C	513	CLA	C4-C3-C5-C6
29	A	614	SQD	C11-C12-C13-C14
25	c	510	CLA	C2-C3-C5-C6
28	a	713	PL9	C4-C3-C7-C8
23	d	408	LMG	C14-C15-C16-C17
32	d	407	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
25	B	611	CLA	C11-C12-C13-C14
25	B	611	CLA	C14-C13-C15-C16
25	b	609	CLA	C14-C13-C15-C16
25	b	613	CLA	C11-C12-C13-C14
25	b	615	CLA	C11-C10-C8-C9
25	c	507	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	512	CLA	C11-C12-C13-C14
34	E	102	HEM	C3D-CAD-CBD-CGD
23	c	519	LMG	C7-C8-C9-O8
33	H	103	DGD	O1A-C1A-O1G-C1G
23	c	519	LMG	C4-C5-C6-O5
25	a	708	CLA	C16-C17-C18-C19
25	b	615	CLA	CBA-CGA-O2A-C1
33	c	516	DGD	O6D-C1D-O3G-C3G
33	c	518	DGD	O6D-C1D-O3G-C3G
33	C	519	DGD	CCB-CDB-CEB-CFB
27	C	516	BCR	C7-C8-C9-C34
32	b	629	LHG	C17-C18-C19-C20
33	c	516	DGD	CAA-CBA-CCA-CDA
27	B	620	BCR	C7-C8-C9-C10
23	d	408	LMG	C16-C17-C18-C19
32	a	720	LHG	C35-C36-C37-C38
33	C	518	DGD	C6B-C7B-C8B-C9B
25	D	404	CLA	C1A-C2A-CAA-CBA
32	b	629	LHG	C11-C10-C9-C8
25	B	608	CLA	C12-C13-C15-C16
25	D	403	CLA	C6-C7-C8-C10
25	D	403	CLA	C11-C12-C13-C15
25	c	506	CLA	C12-C13-C15-C16
23	B	621	LMG	C19-C20-C21-C22
23	b	627	LMG	C40-C41-C42-C43
32	E	101	LHG	C10-C11-C12-C13
33	c	518	DGD	O6E-C5E-C6E-O5E
29	B	626	SQD	C10-C11-C12-C13
25	C	502	CLA	C15-C16-C17-C18
25	B	602	CLA	C16-C17-C18-C20
23	f	101	LMG	C20-C21-C22-C23
32	d	406	LHG	C33-C34-C35-C36
32	d	407	LHG	C26-C27-C28-C29
25	B	615	CLA	C13-C15-C16-C17
23	a	715	LMG	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
34	e	102	HEM	C4D-C3D-CAD-CBD
25	B	610	CLA	C8-C10-C11-C12
23	b	626	LMG	C20-C21-C22-C23
23	d	408	LMG	C15-C16-C17-C18
25	C	513	CLA	C5-C6-C7-C8
25	b	609	CLA	C10-C11-C12-C13
32	D	408	LHG	C27-C28-C29-C30
23	A	603	LMG	C37-C38-C39-C40
25	C	510	CLA	C3-C5-C6-C7
29	f	102	SQD	O47-C45-C46-O48
23	b	627	LMG	C16-C17-C18-C19
25	B	617	CLA	C13-C15-C16-C17
23	b	626	LMG	C18-C19-C20-C21
32	E	101	LHG	C26-C27-C28-C29
25	b	615	CLA	O1A-CGA-O2A-C1
25	D	404	CLA	C6-C7-C8-C9
25	c	502	CLA	O1A-CGA-O2A-C1
26	a	709	PHO	C1A-C2A-CAA-CBA
33	c	518	DGD	C5B-C6B-C7B-C8B
23	A	603	LMG	C13-C14-C15-C16
32	D	408	LHG	C33-C34-C35-C36
27	B	618	BCR	C23-C24-C25-C30
27	C	515	BCR	C23-C24-C25-C26
27	C	515	BCR	C23-C24-C25-C30
27	C	516	BCR	C23-C24-C25-C26
27	H	102	BCR	C1-C6-C7-C8
27	Y	101	BCR	C23-C24-C25-C30
27	a	712	BCR	C23-C24-C25-C26
27	h	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C23-C24-C25-C30
29	D	410	SQD	C31-C32-C33-C34
32	L	101	LHG	C28-C29-C30-C31
33	h	102	DGD	C6A-C7A-C8A-C9A
25	B	612	CLA	C8-C10-C11-C12
25	B	617	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17
23	D	409	LMG	C8-C7-O1-C1
29	B	626	SQD	C26-C27-C28-C29
29	D	410	SQD	C27-C28-C29-C30
33	C	517	DGD	C8A-C9A-CAA-CBA
25	c	502	CLA	CBA-CGA-O2A-C1
34	E	102	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	d	408	LMG	O7-C10-C11-C12
25	B	603	CLA	C16-C17-C18-C20
25	b	608	CLA	O1D-CGD-O2D-CED
29	A	612	SQD	C34-C35-C36-C37
29	B	626	SQD	C12-C13-C14-C15
25	B	607	CLA	CBA-CGA-O2A-C1
33	c	517	DGD	CDB-CEB-CFB-CGB
25	B	607	CLA	O1A-CGA-O2A-C1
23	d	408	LMG	O9-C10-C11-C12
29	D	410	SQD	O5-C1-O6-C44
25	C	503	CLA	C4-C3-C5-C6
25	C	505	CLA	C4-C3-C5-C6
25	b	608	CLA	C4-C3-C5-C6
25	d	402	CLA	C4-C3-C5-C6
25	B	610	CLA	C11-C12-C13-C15
25	b	612	CLA	C12-C13-C15-C16
25	b	615	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C10-C8-C7
25	c	508	CLA	C11-C12-C13-C15
25	c	510	CLA	C12-C13-C15-C16
33	c	517	DGD	C4A-C5A-C6A-C7A
25	a	719	CLA	C13-C15-C16-C17
25	b	619	CLA	CAA-CBA-CGA-O2A
33	h	102	DGD	O2G-C1B-C2B-C3B
29	B	626	SQD	C19-C20-C21-C22
29	B	626	SQD	O47-C45-C46-O48
33	C	519	DGD	O1A-C1A-O1G-C1G
29	I	102	SQD	C33-C34-C35-C36
33	c	516	DGD	C6A-C7A-C8A-C9A
23	c	520	LMG	C16-C17-C18-C19
23	B	621	LMG	C29-C28-O8-C9
27	b	625	BCR	C20-C21-C22-C37
27	c	514	BCR	C20-C21-C22-C37
25	b	618	CLA	CAA-CBA-CGA-O2A
28	A	611	PL9	C40-C39-C41-C42
28	d	405	PL9	C35-C34-C36-C37
25	c	502	CLA	C8-C10-C11-C12
25	B	615	CLA	C6-C7-C8-C9
25	C	510	CLA	C6-C7-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	b	607	CLA	C6-C7-C8-C9
25	b	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	b	601	SQD	C31-C32-C33-C34
33	c	517	DGD	CBB-CCB-CDB-CEB
25	c	506	CLA	C3A-C2A-CAA-CBA
26	a	709	PHO	C3A-C2A-CAA-CBA
29	b	601	SQD	O48-C23-C24-C25
25	B	611	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	507	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	b	611	CLA	CAD-CBD-CGD-O2D
25	b	615	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	d	403	CLA	CAD-CBD-CGD-O2D
23	d	408	LMG	C29-C28-O8-C9
25	B	602	CLA	C16-C17-C18-C19
23	A	603	LMG	C11-C12-C13-C14
25	c	503	CLA	C8-C10-C11-C12
25	d	402	CLA	C2-C1-O2A-CGA
23	A	603	LMG	O7-C10-C11-C12
25	c	510	CLA	CAA-CBA-CGA-O2A
29	A	614	SQD	C10-C11-C12-C13
28	D	406	PL9	C43-C44-C46-C47
23	C	501	LMG	O8-C28-C29-C30
25	B	614	CLA	CAA-CBA-CGA-O2A
29	I	102	SQD	C12-C13-C14-C15
23	M	101	LMG	C33-C34-C35-C36
32	B	625	LHG	C9-C10-C11-C12
29	D	410	SQD	C29-C30-C31-C32
29	a	714	SQD	C30-C31-C32-C33
23	A	603	LMG	O8-C28-C29-C30
29	D	410	SQD	C7-C8-C9-C10
29	B	623	SQD	C11-C12-C13-C14
25	A	606	CLA	O2A-C1-C2-C3
25	C	514	CLA	O2A-C1-C2-C3
25	c	512	CLA	O2A-C1-C2-C3
23	A	603	LMG	C22-C23-C24-C25
25	B	613	CLA	CHA-CBD-CGD-O2D
25	B	617	CLA	CHA-CBD-CGD-O2D
25	C	505	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	CHA-CBD-CGD-O1D
25	C	510	CLA	CHA-CBD-CGD-O2D
25	b	608	CLA	CHA-CBD-CGD-O1D
25	b	608	CLA	CHA-CBD-CGD-O2D
25	b	609	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CHA-CBD-CGD-O2D
25	c	512	CLA	CHA-CBD-CGD-O1D
25	D	402	CLA	C4C-C3C-CAC-CBC
23	C	520	LMG	C10-C11-C12-C13
34	E	102	HEM	CAD-CBD-CGD-O1D
34	e	102	HEM	CAD-CBD-CGD-O2D
33	C	517	DGD	O1G-C1A-C2A-C3A
23	D	409	LMG	C37-C38-C39-C40
23	c	519	LMG	O7-C8-C9-O8
32	d	407	LHG	C10-C11-C12-C13
25	B	617	CLA	C10-C11-C12-C13
23	a	701	LMG	C40-C41-C42-C43
29	A	612	SQD	C33-C34-C35-C36
32	B	625	LHG	C29-C30-C31-C32
25	B	610	CLA	C13-C15-C16-C17
25	C	511	CLA	CAA-CBA-CGA-O2A
29	a	714	SQD	O47-C7-C8-C9
26	A	608	PHO	CHA-CBD-CGD-O1D
26	D	401	PHO	CHA-CBD-CGD-O1D
25	D	403	CLA	CAA-CBA-CGA-O2A
32	L	101	LHG	O7-C7-C8-C9
25	d	402	CLA	C11-C10-C8-C7
28	A	611	PL9	C4-C3-C7-C8
32	b	629	LHG	O7-C7-C8-C9
25	D	402	CLA	C2C-C3C-CAC-CBC
25	b	607	CLA	C11-C12-C13-C14
25	b	609	CLA	C11-C12-C13-C14
32	B	625	LHG	C28-C29-C30-C31
26	a	710	PHO	C8-C10-C11-C12
25	a	708	CLA	C16-C17-C18-C20
23	c	519	LMG	O10-C28-O8-C9
25	C	508	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	O49-C7-C8-C9
33	c	516	DGD	CBA-CCA-CDA-CEA
25	C	503	CLA	O1A-CGA-O2A-C1
25	B	614	CLA	CAA-CBA-CGA-O1A
27	d	404	BCR	C7-C8-C9-C10
25	C	503	CLA	CBA-CGA-O2A-C1
25	b	618	CLA	CBA-CGA-O2A-C1
23	b	626	LMG	C38-C39-C40-C41
33	C	517	DGD	C2B-C3B-C4B-C5B
25	B	609	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA
29	A	614	SQD	C25-C26-C27-C28
29	a	714	SQD	O49-C7-C8-C9
32	D	408	LHG	O10-C23-C24-C25
33	C	518	DGD	O1B-C1B-C2B-C3B
25	b	613	CLA	C10-C11-C12-C13
28	d	405	PL9	C11-C12-C13-C14
25	b	621	CLA	C13-C15-C16-C17
23	A	603	LMG	O10-C28-C29-C30
25	b	618	CLA	CAA-CBA-CGA-O1A
25	b	619	CLA	CAA-CBA-CGA-O1A
32	e	101	LHG	O10-C23-C24-C25
33	c	518	DGD	C8A-C9A-CAA-CBA
25	b	616	CLA	C2A-CAA-CBA-CGA
29	b	601	SQD	C29-C30-C31-C32
23	A	603	LMG	O9-C10-C11-C12
23	M	101	LMG	O10-C28-C29-C30
29	I	102	SQD	C28-C29-C30-C31
32	D	408	LHG	C2-C3-O3-P
25	C	511	CLA	CAA-CBA-CGA-O1A
29	A	612	SQD	O49-C7-C8-C9
32	D	408	LHG	C4-O6-P-O5
32	E	101	LHG	C4-O6-P-O5
32	L	101	LHG	C4-O6-P-O5
32	d	407	LHG	C3-O3-P-O5
32	a	720	LHG	O6-C4-C5-C6
29	B	626	SQD	C35-C36-C37-C38
27	H	102	BCR	C5-C6-C7-C8
27	Y	101	BCR	C23-C24-C25-C26
27	k	101	BCR	C23-C24-C25-C26
32	L	101	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	B	625	LHG	O8-C23-C24-C25
27	c	514	BCR	C18-C19-C20-C21
25	c	510	CLA	CAA-CBA-CGA-O1A
25	b	609	CLA	C5-C6-C7-C8
25	b	621	CLA	C8-C10-C11-C12
32	B	625	LHG	C17-C18-C19-C20
34	e	102	HEM	CAD-CBD-CGD-O1D
33	c	518	DGD	O1G-C1A-C2A-C3A
25	C	507	CLA	C15-C16-C17-C18
32	e	101	LHG	C11-C12-C13-C14
33	c	517	DGD	C1A-C2A-C3A-C4A
28	a	713	PL9	C21-C22-C23-C24
23	a	701	LMG	C22-C23-C24-C25
25	B	605	CLA	C2C-C3C-CAC-CBC
25	C	505	CLA	CAD-CBD-CGD-O1D
25	D	404	CLA	CAD-CBD-CGD-O1D
25	b	609	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	510	CLA	CAD-CBD-CGD-O1D
25	c	511	CLA	CAD-CBD-CGD-O1D
29	a	714	SQD	O5-C5-C6-S
29	b	601	SQD	O5-C5-C6-S
25	b	618	CLA	O1A-CGA-O2A-C1
32	B	625	LHG	O10-C23-C24-C25
25	B	608	CLA	C14-C13-C15-C16
25	B	613	CLA	C11-C10-C8-C9
25	a	719	CLA	C11-C10-C8-C9
25	b	615	CLA	C6-C7-C8-C9
23	C	520	LMG	C14-C15-C16-C17
25	c	505	CLA	CAA-CBA-CGA-O2A
29	A	612	SQD	O47-C7-C8-C9
33	H	103	DGD	C6A-C7A-C8A-C9A
25	b	608	CLA	CBD-CGD-O2D-CED
23	A	603	LMG	C33-C34-C35-C36
32	B	625	LHG	C33-C34-C35-C36
25	C	502	CLA	CAA-CBA-CGA-O2A
32	D	408	LHG	O8-C23-C24-C25
33	C	518	DGD	C5A-C6A-C7A-C8A
28	d	405	PL9	C30-C29-C31-C32
25	B	602	CLA	C11-C10-C8-C7
25	B	606	CLA	C11-C12-C13-C15
25	B	613	CLA	C11-C10-C8-C7

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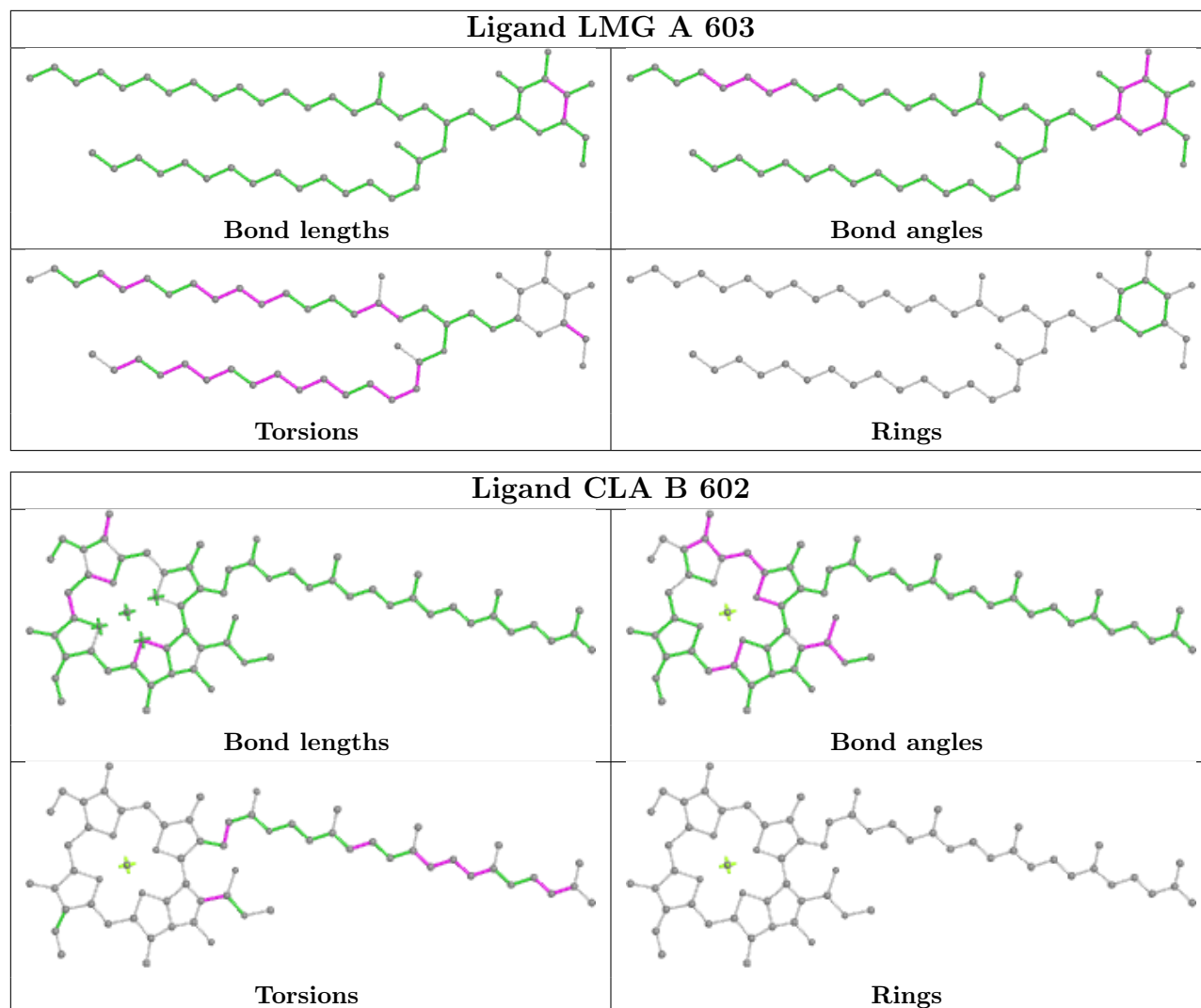
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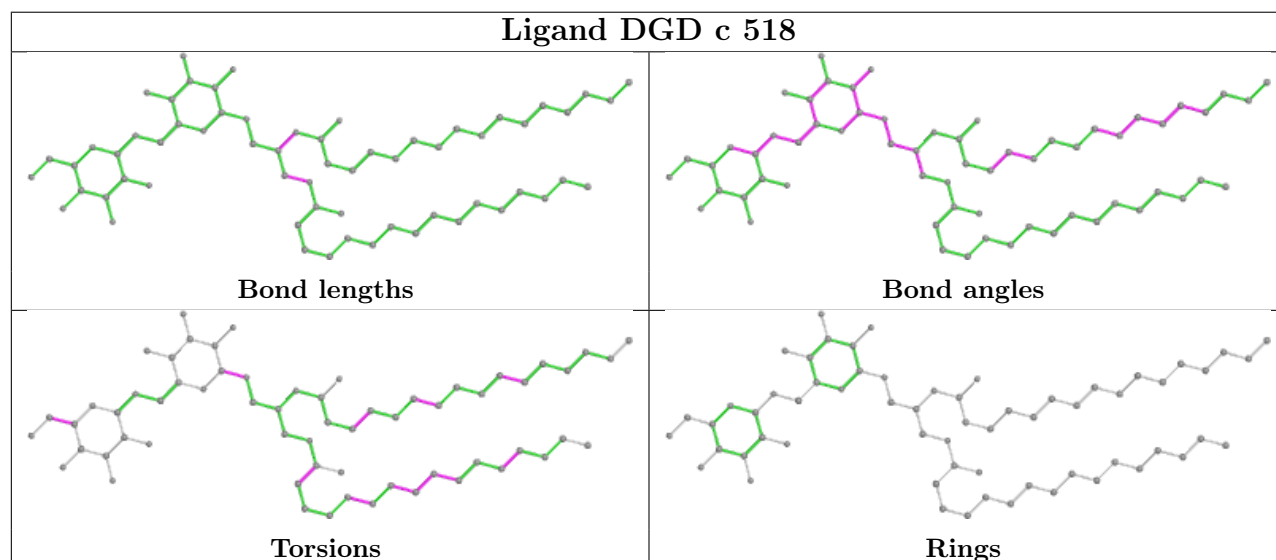
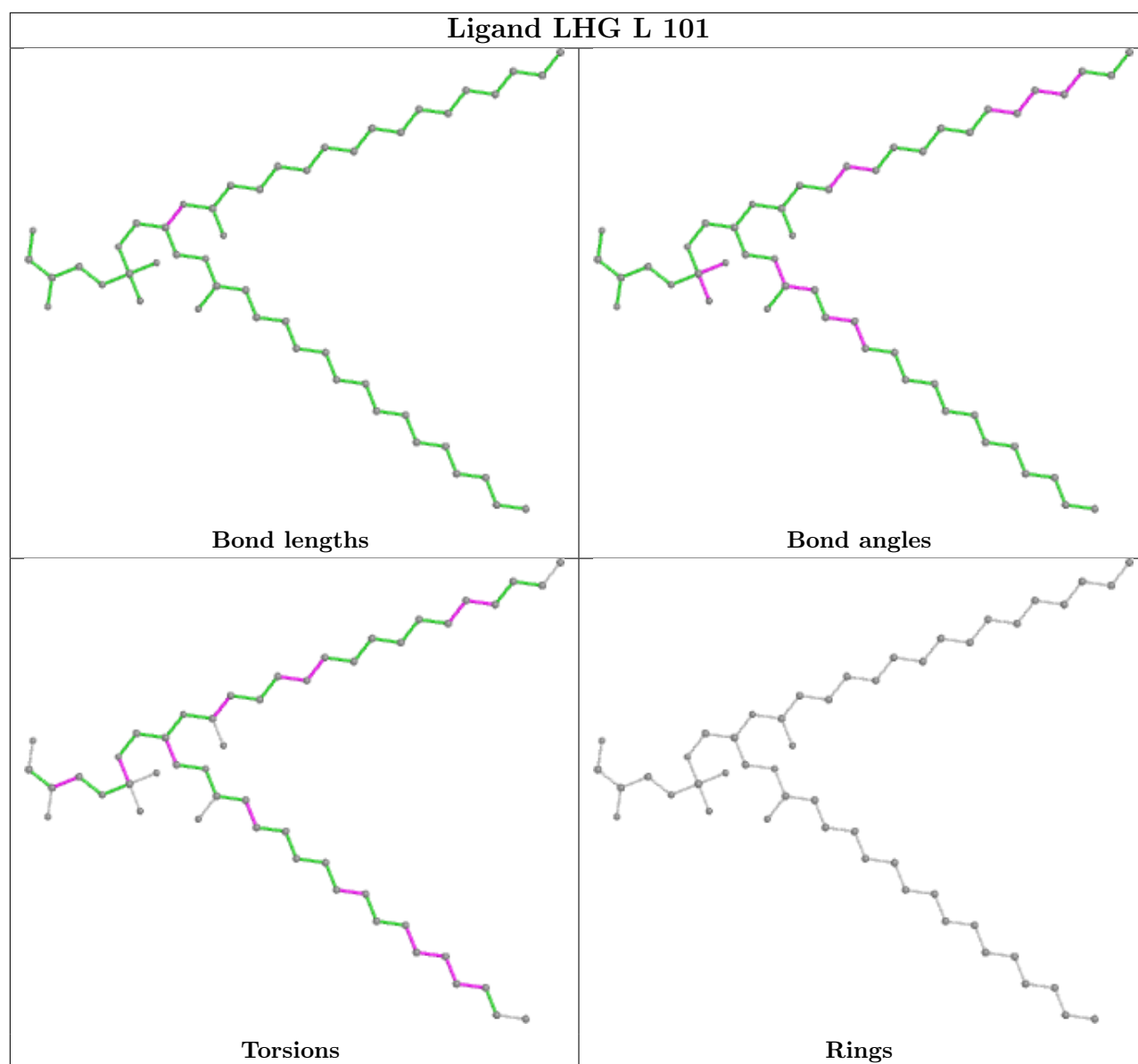
Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C2-C3-C5-C6
25	D	404	CLA	C6-C7-C8-C10
25	a	719	CLA	C11-C10-C8-C7
25	b	616	CLA	C12-C13-C15-C16
25	c	513	CLA	C11-C10-C8-C7
28	a	713	PL9	C33-C34-C36-C37
29	A	612	SQD	C7-C8-C9-C10
25	D	403	CLA	CAA-CBA-CGA-O1A
25	B	603	CLA	CAA-CBA-CGA-O2A
25	c	501	CLA	C15-C16-C17-C18
27	c	515	BCR	C7-C8-C9-C10
32	b	629	LHG	O9-C7-C8-C9
27	H	102	BCR	C9-C10-C11-C12
33	C	518	DGD	O2G-C1B-C2B-C3B
25	d	402	CLA	C2C-C3C-CAC-CBC
25	B	607	CLA	C15-C16-C17-C18
25	D	402	CLA	C13-C15-C16-C17
23	c	519	LMG	O9-C10-C11-C12
32	E	101	LHG	C17-C18-C19-C20
32	E	101	LHG	C29-C30-C31-C32
25	B	603	CLA	C13-C15-C16-C17
25	B	609	CLA	C13-C15-C16-C17
25	b	607	CLA	CAA-CBA-CGA-O2A
25	B	602	CLA	C2A-CAA-CBA-CGA
25	c	510	CLA	C2A-CAA-CBA-CGA
25	C	513	CLA	CAA-CBA-CGA-O2A

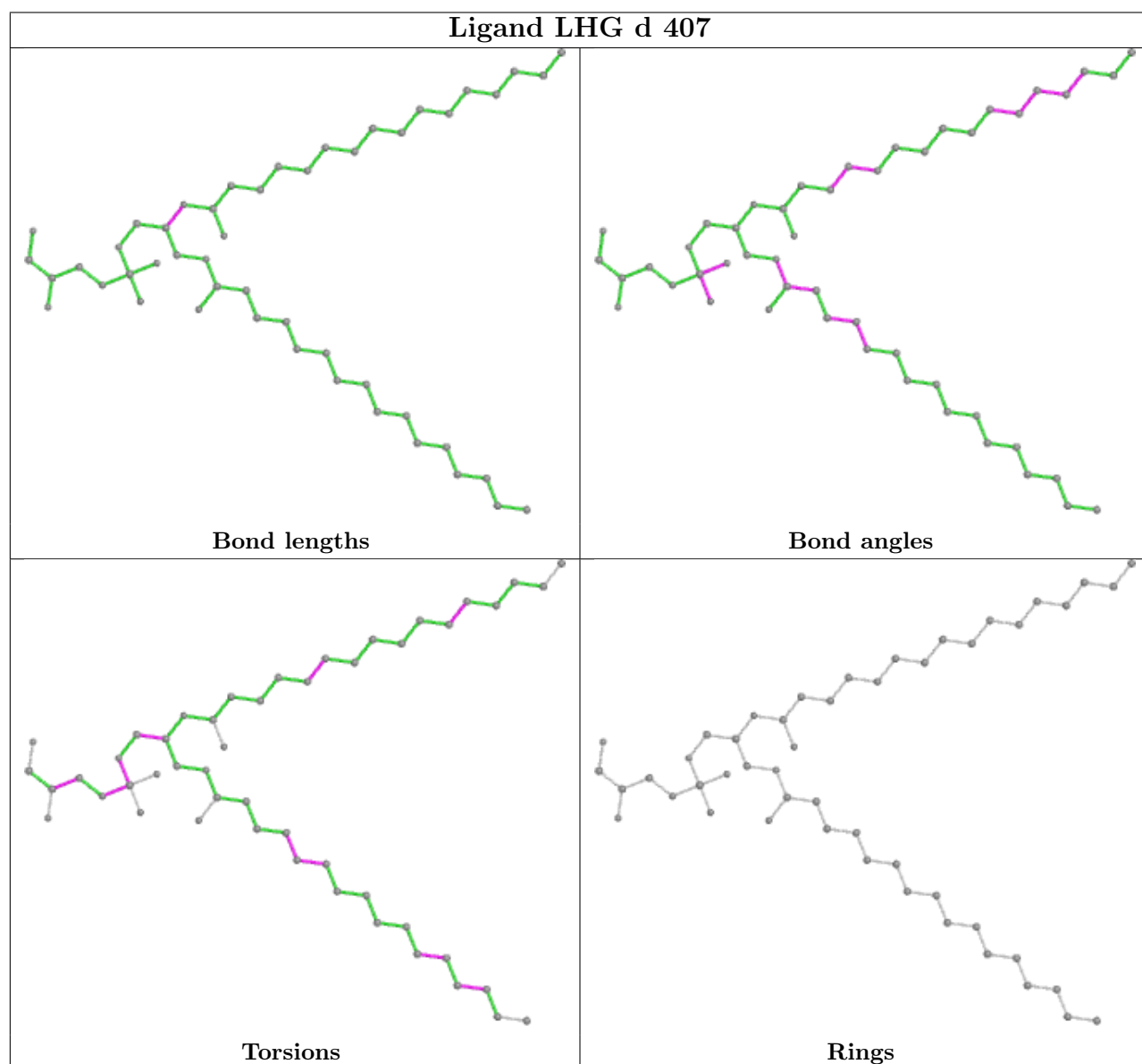
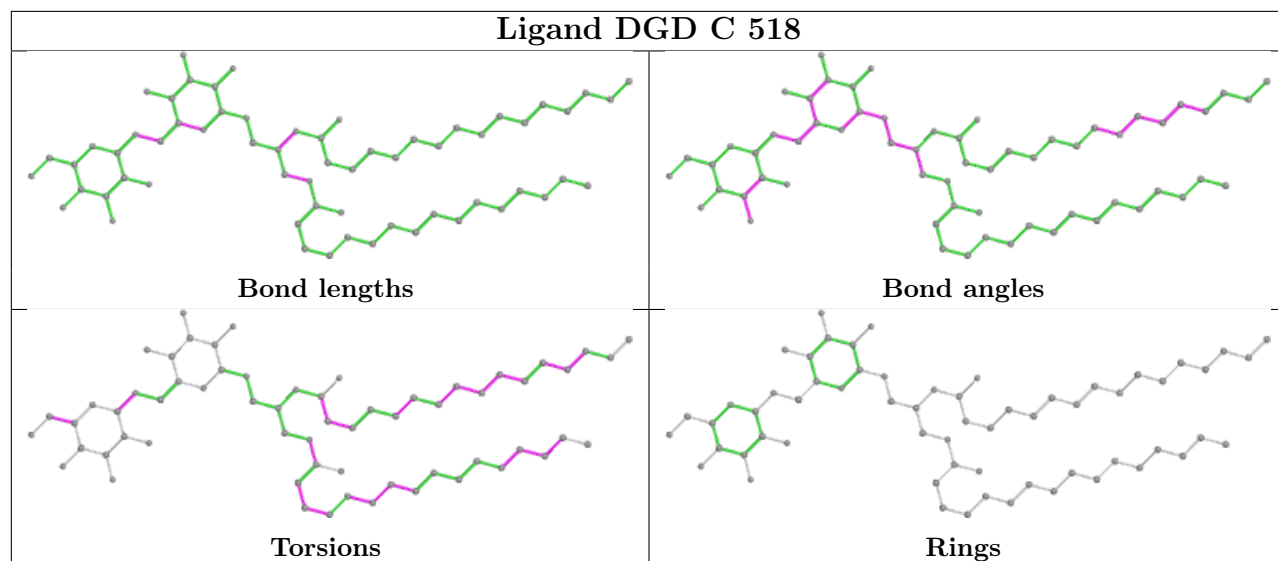
There are no ring outliers.

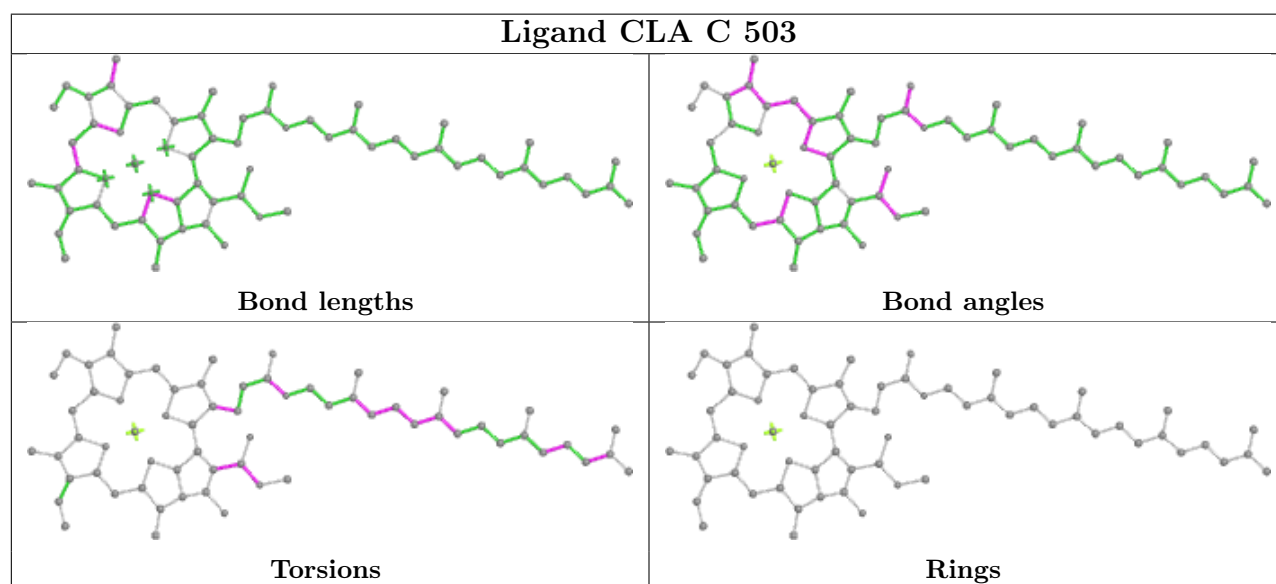
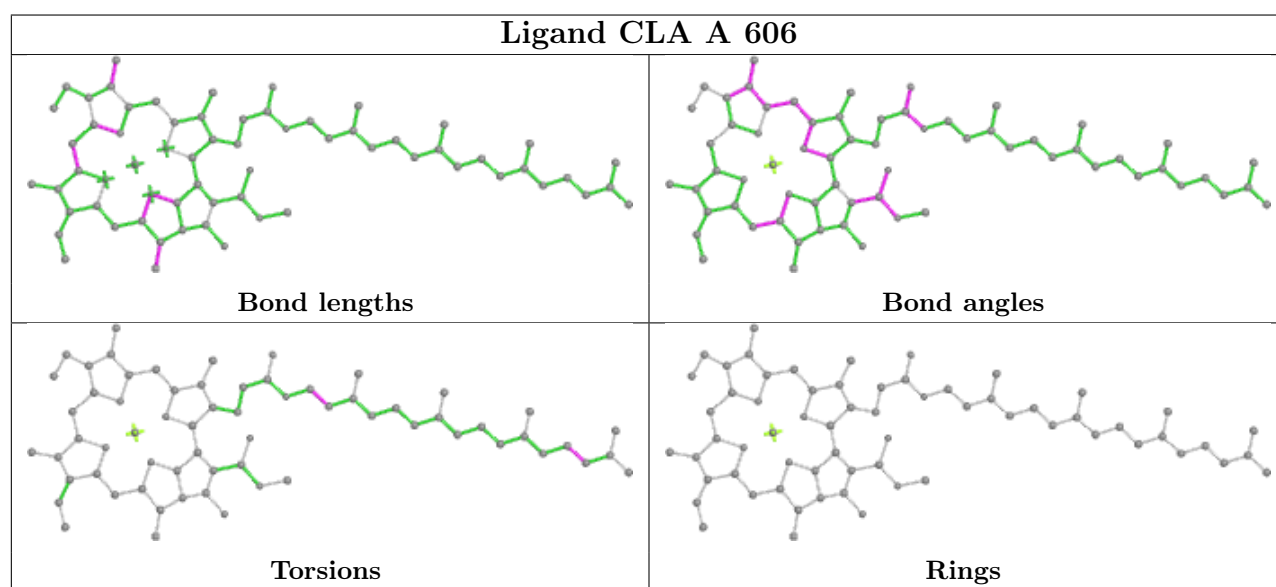
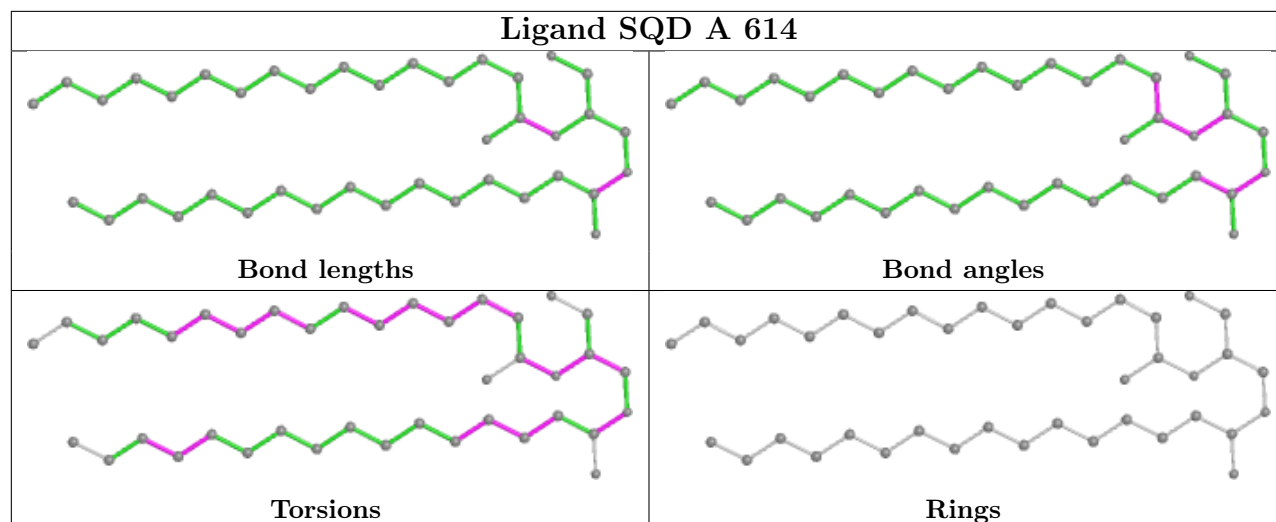
No monomer is involved in short contacts.

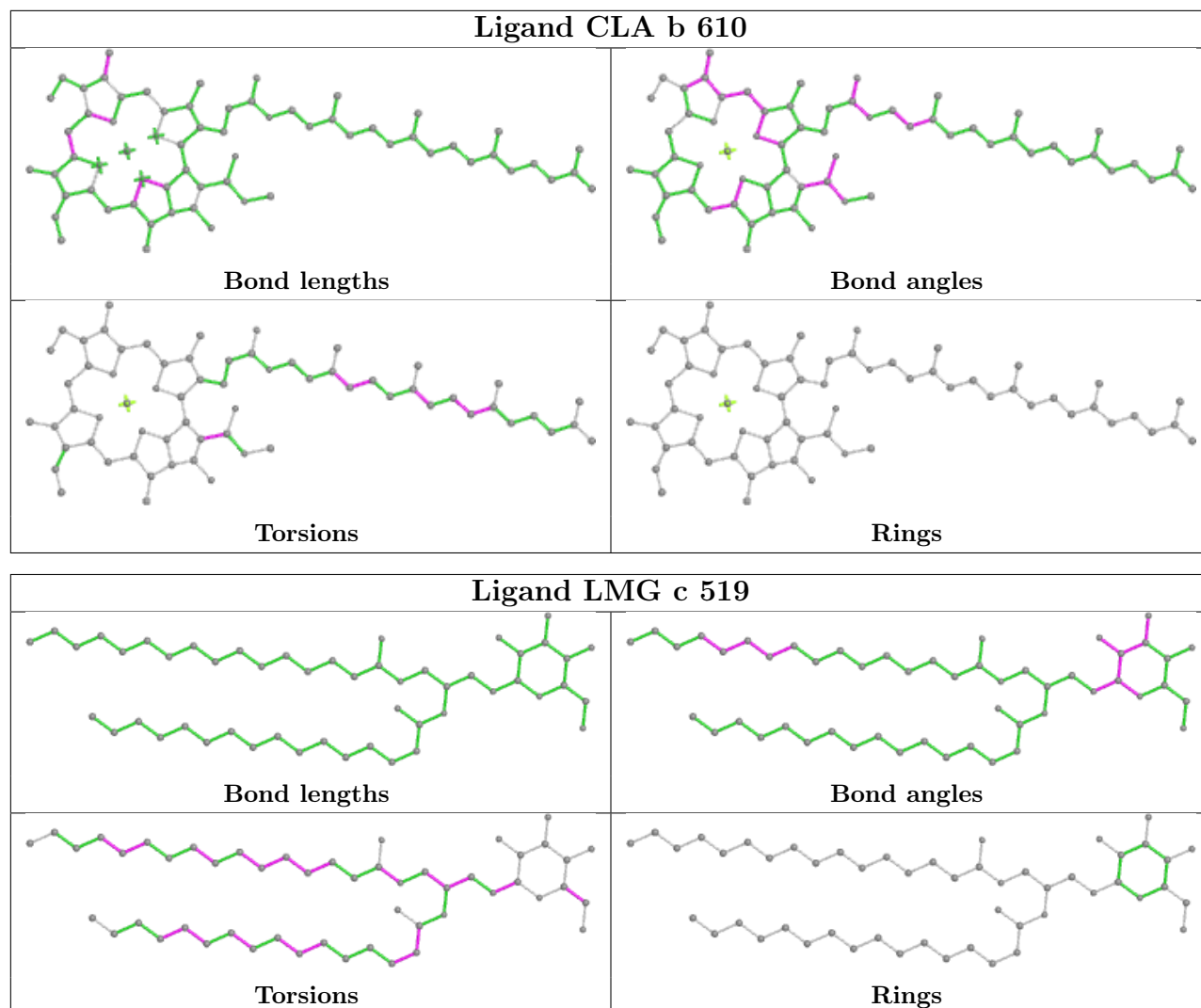
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

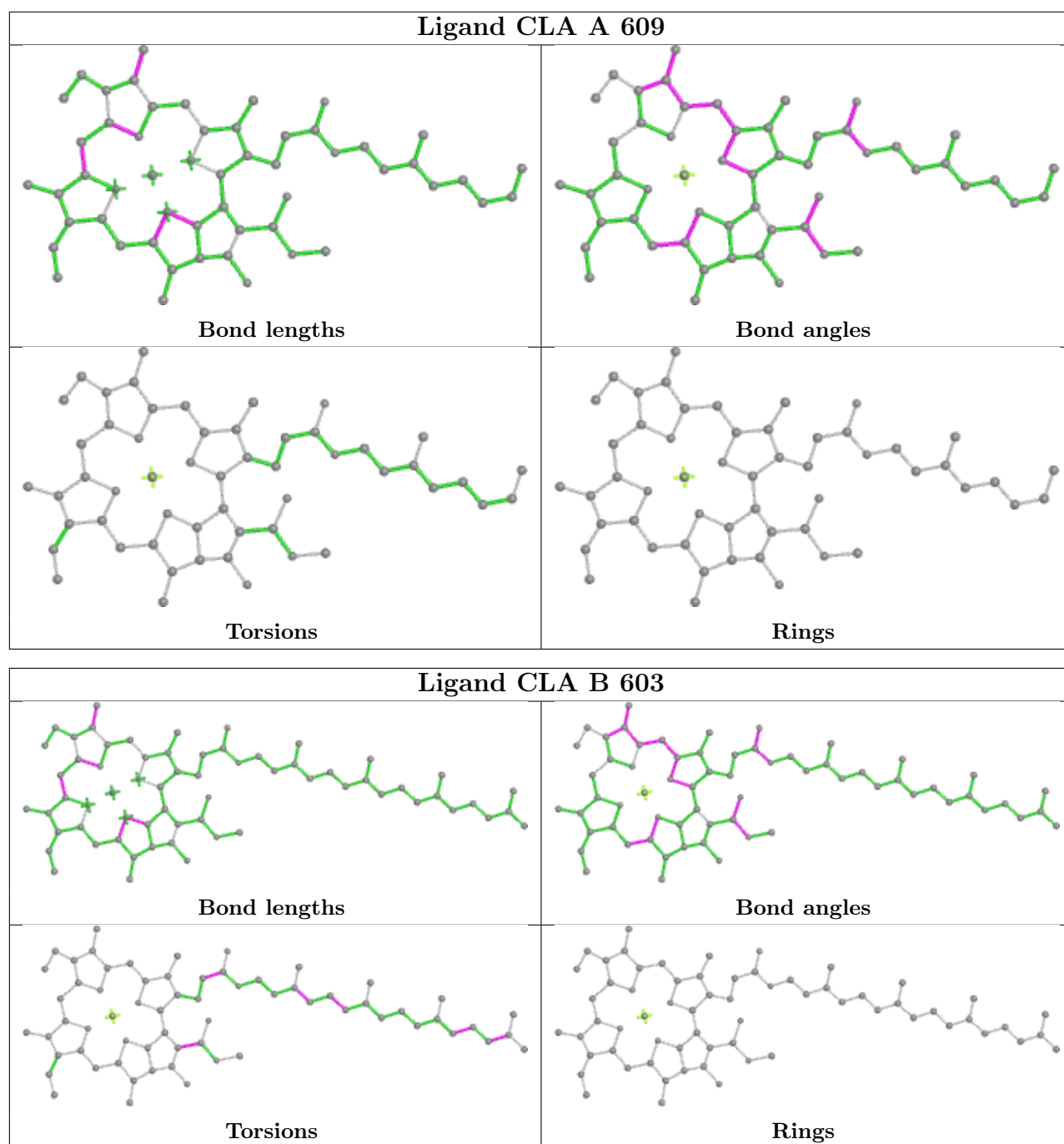


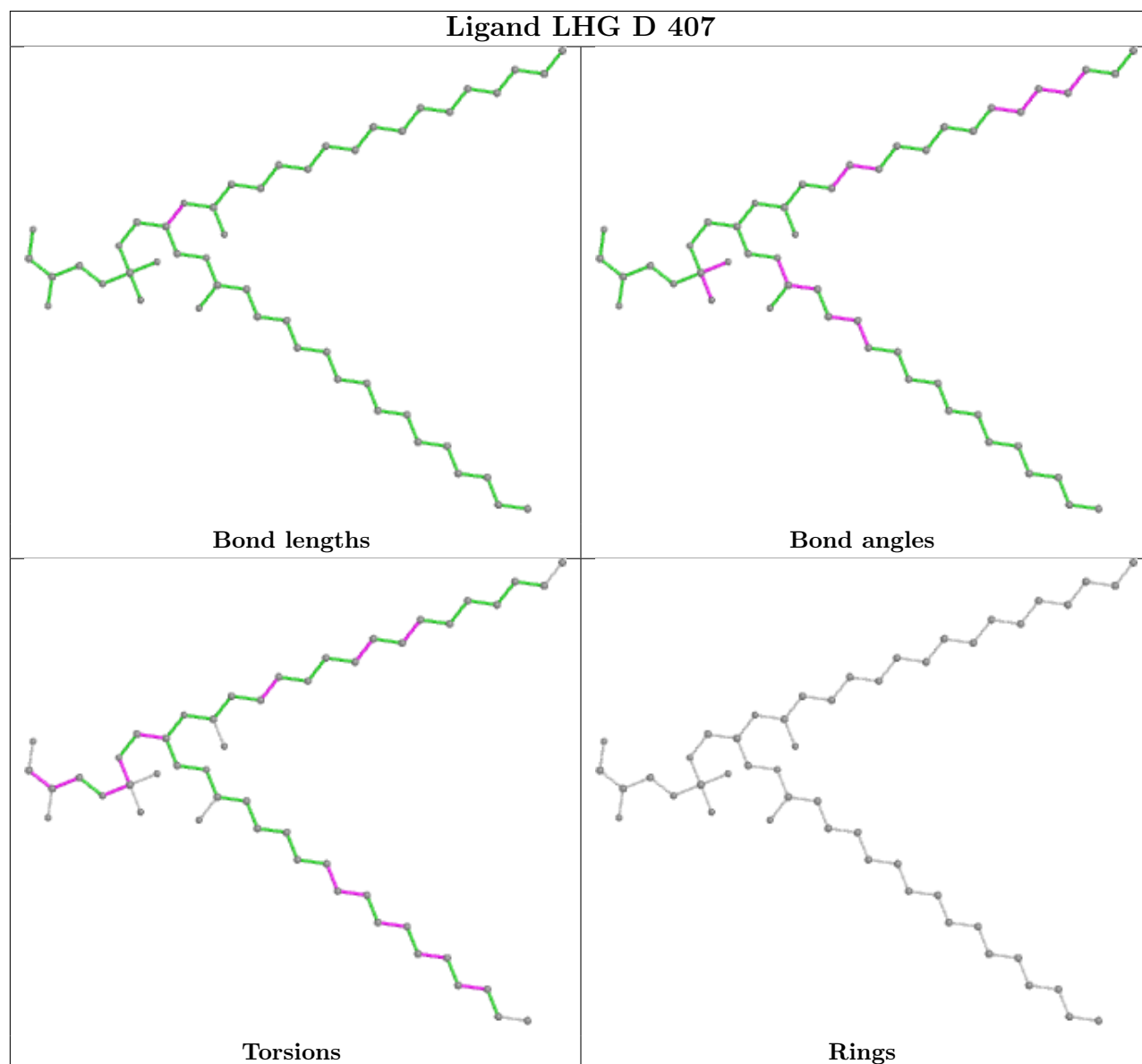
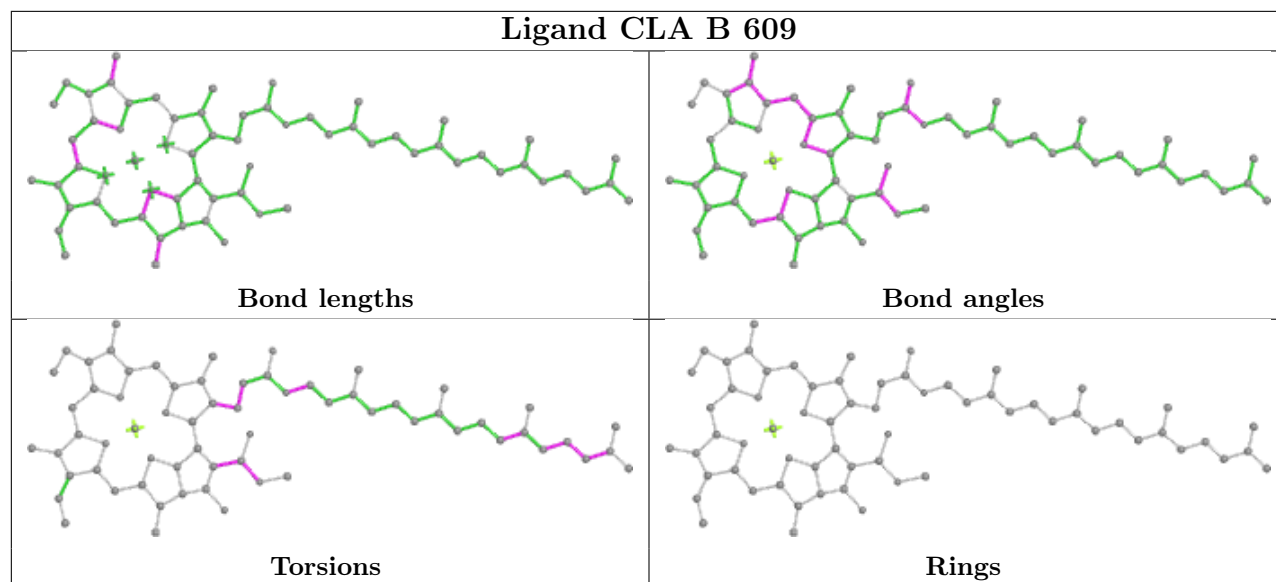


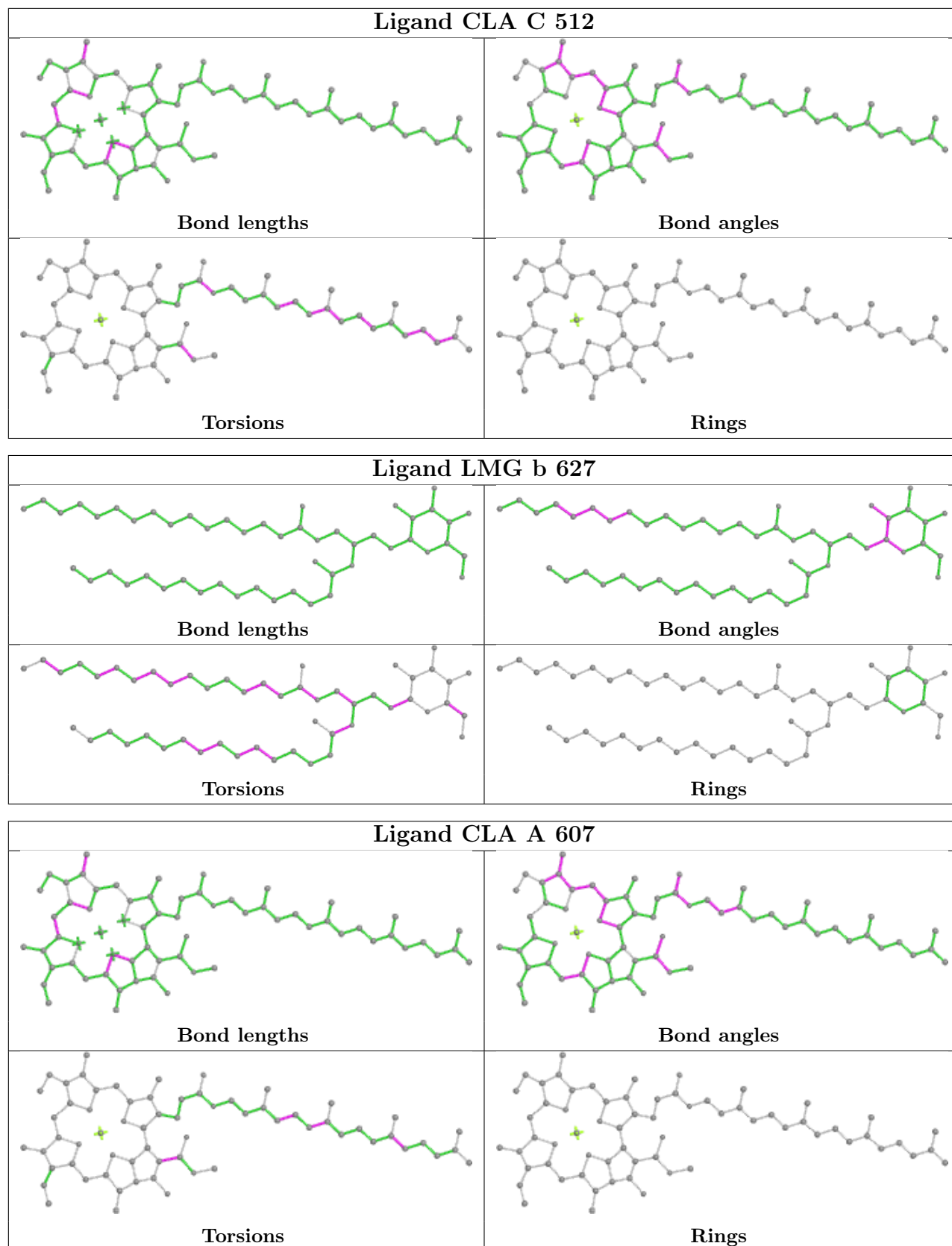


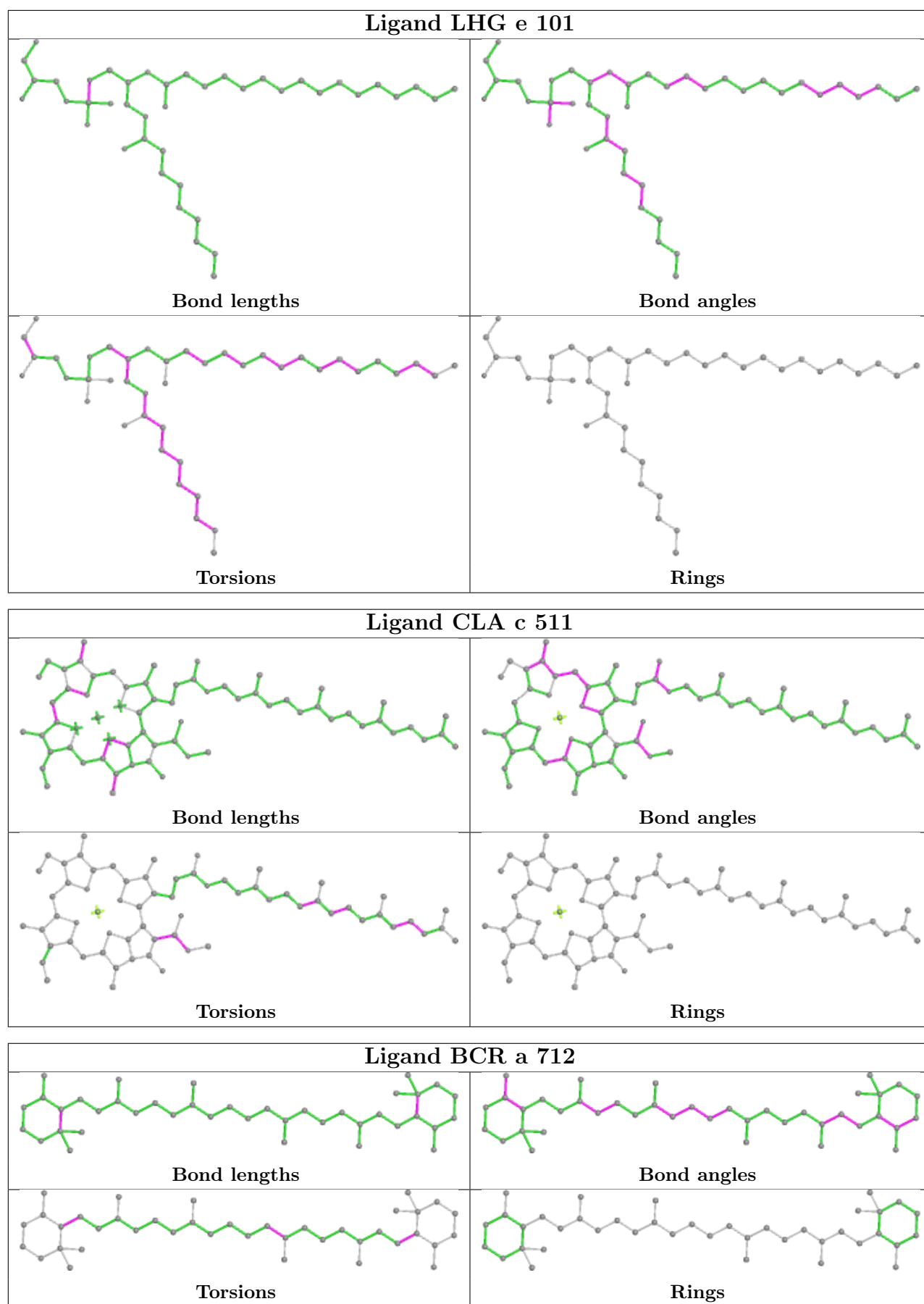


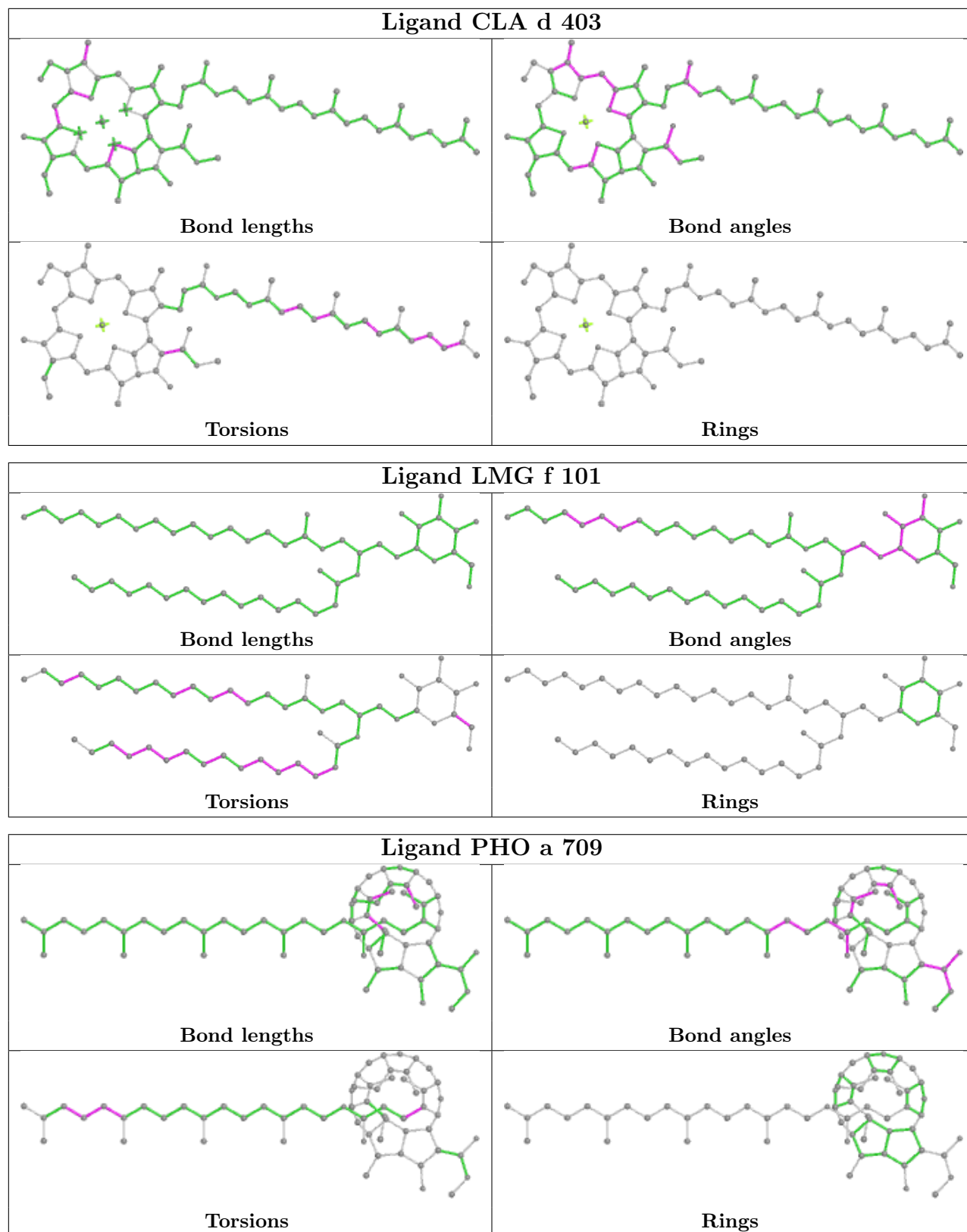


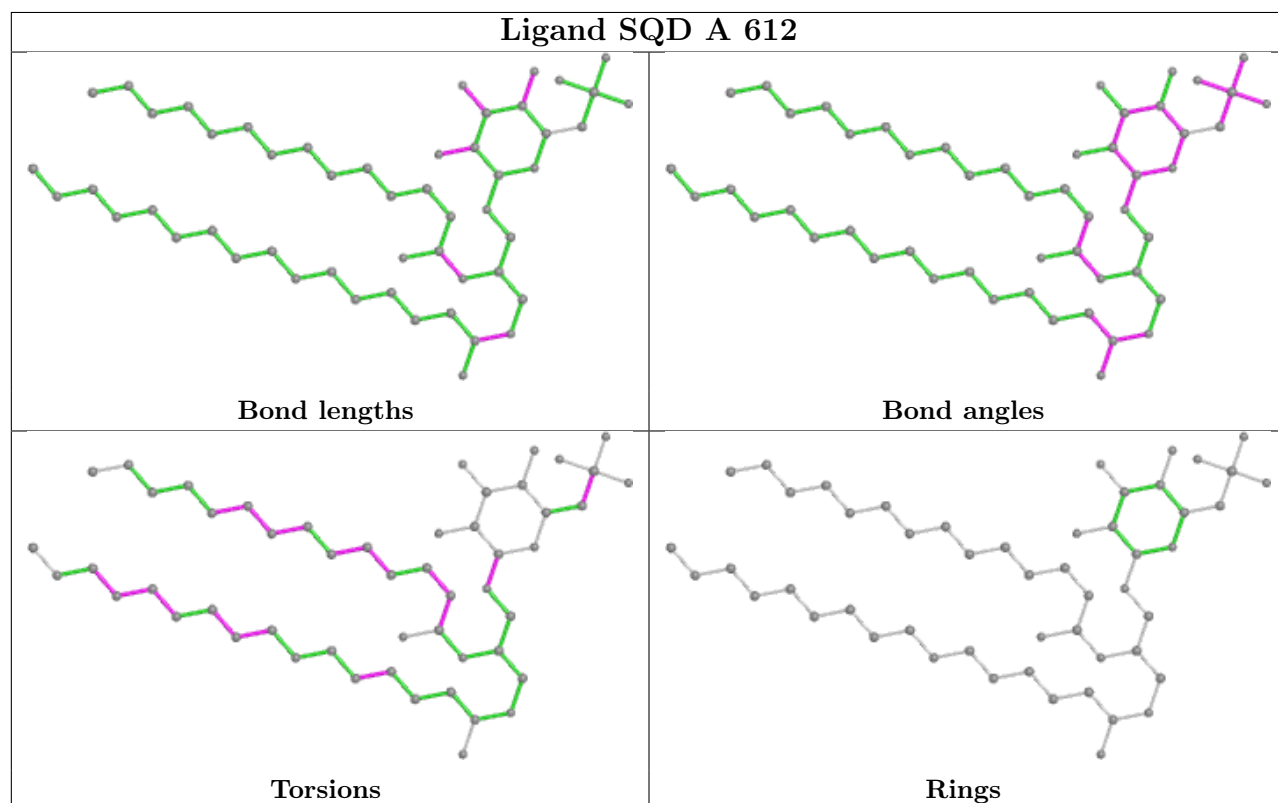
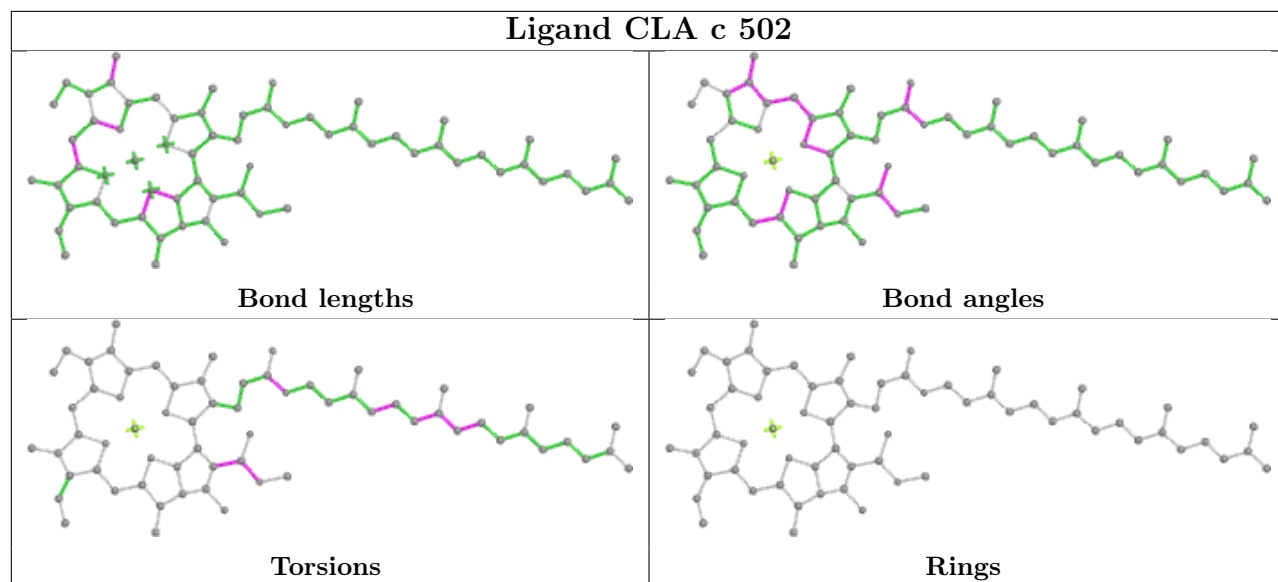


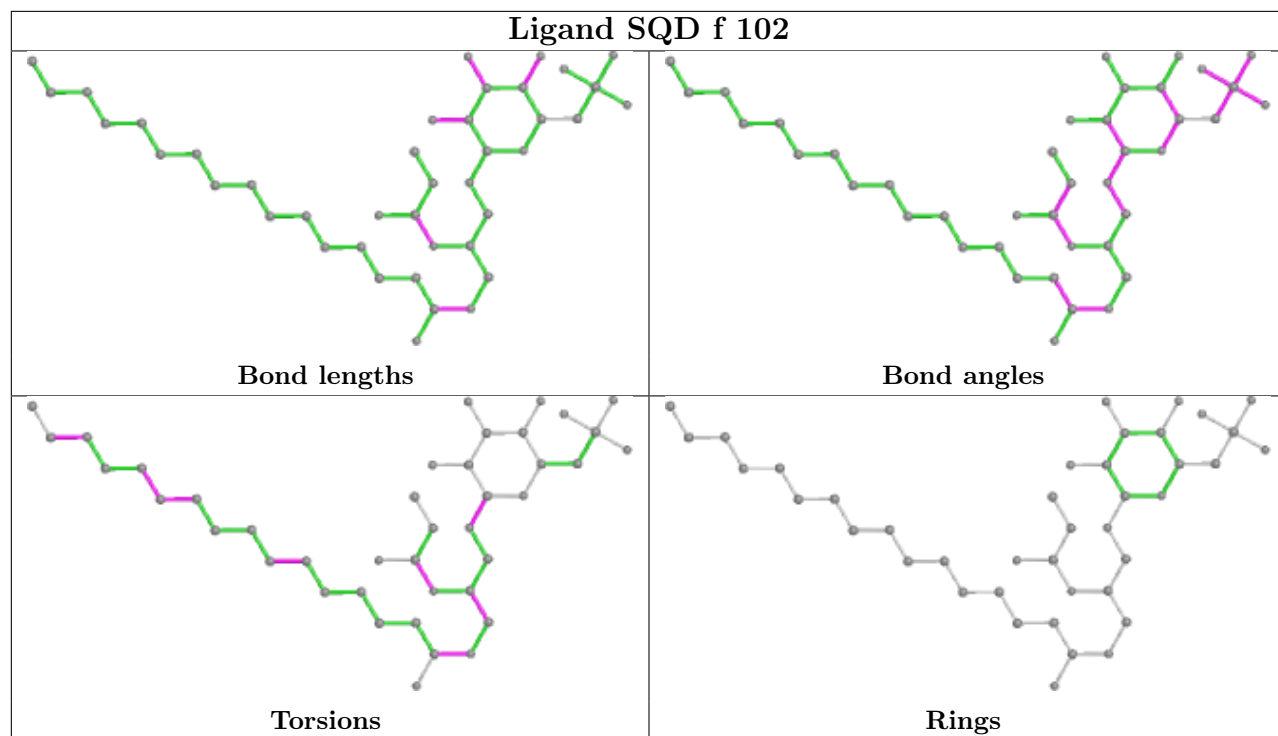


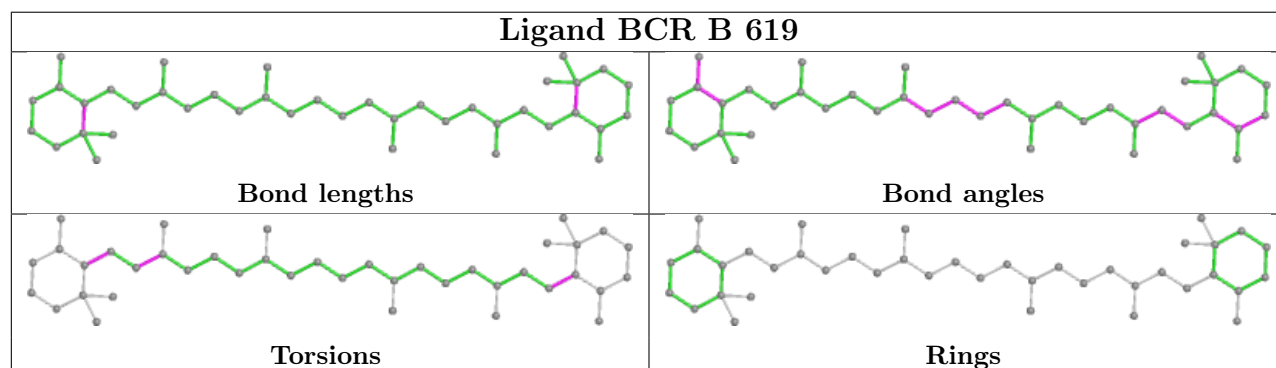
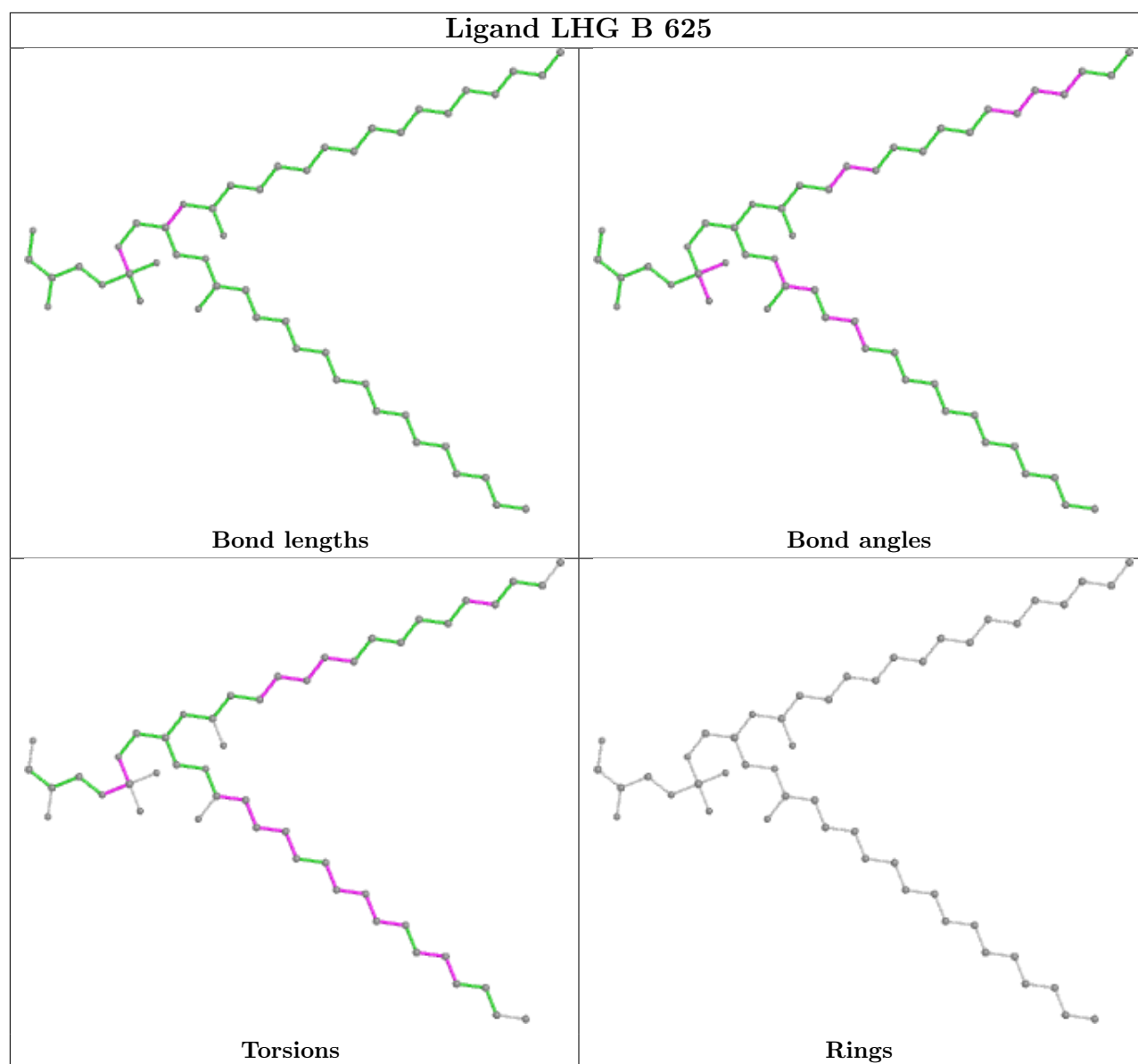


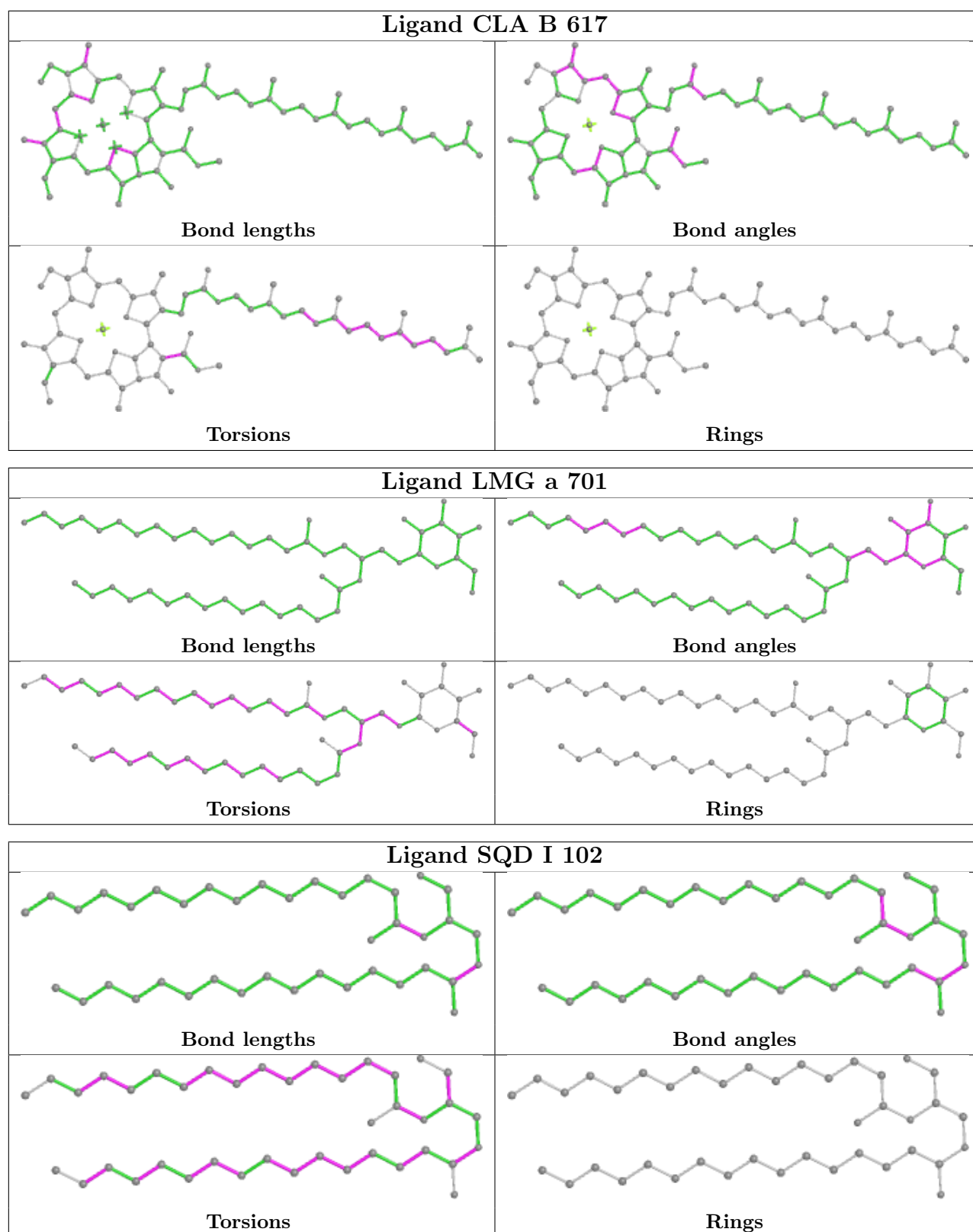


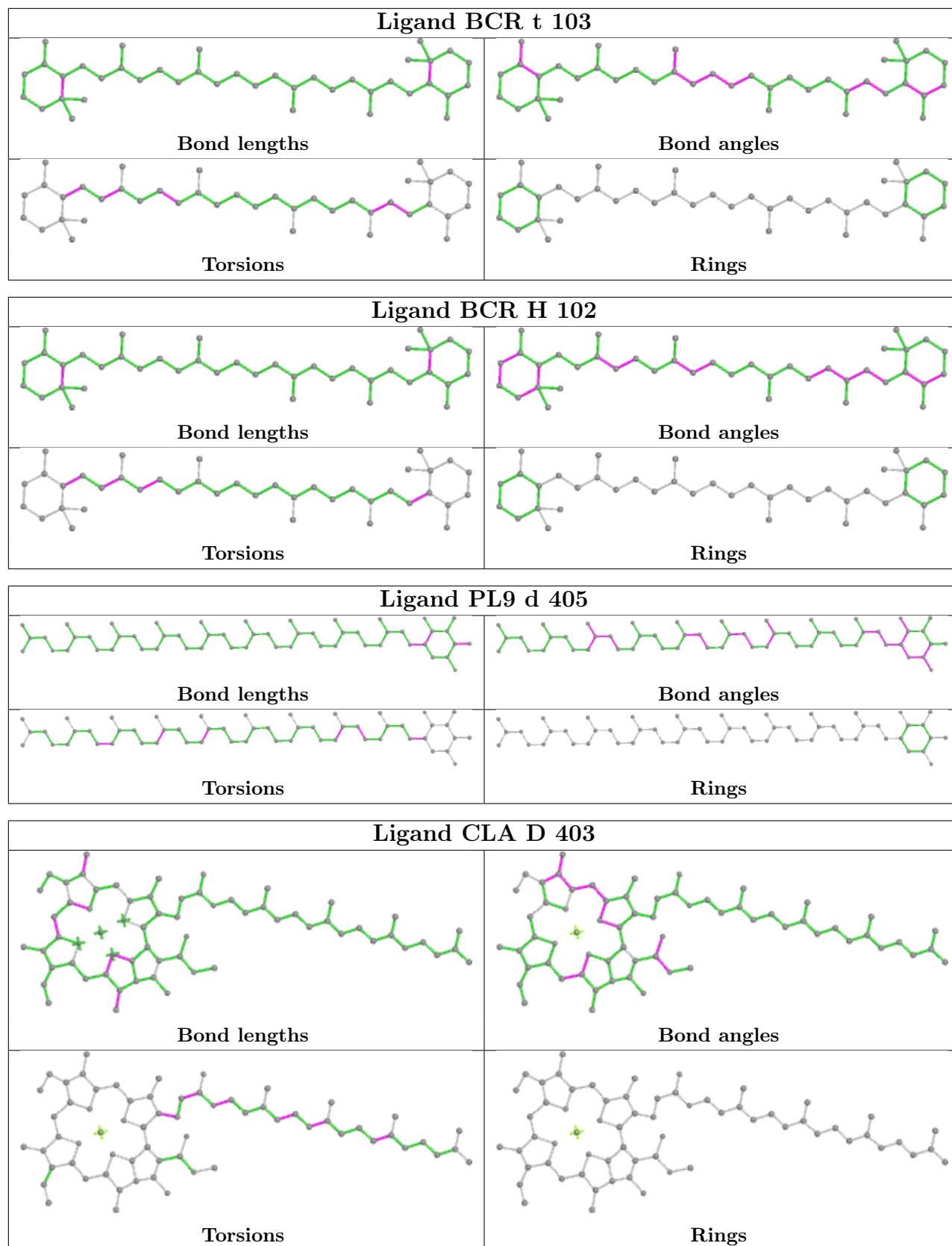


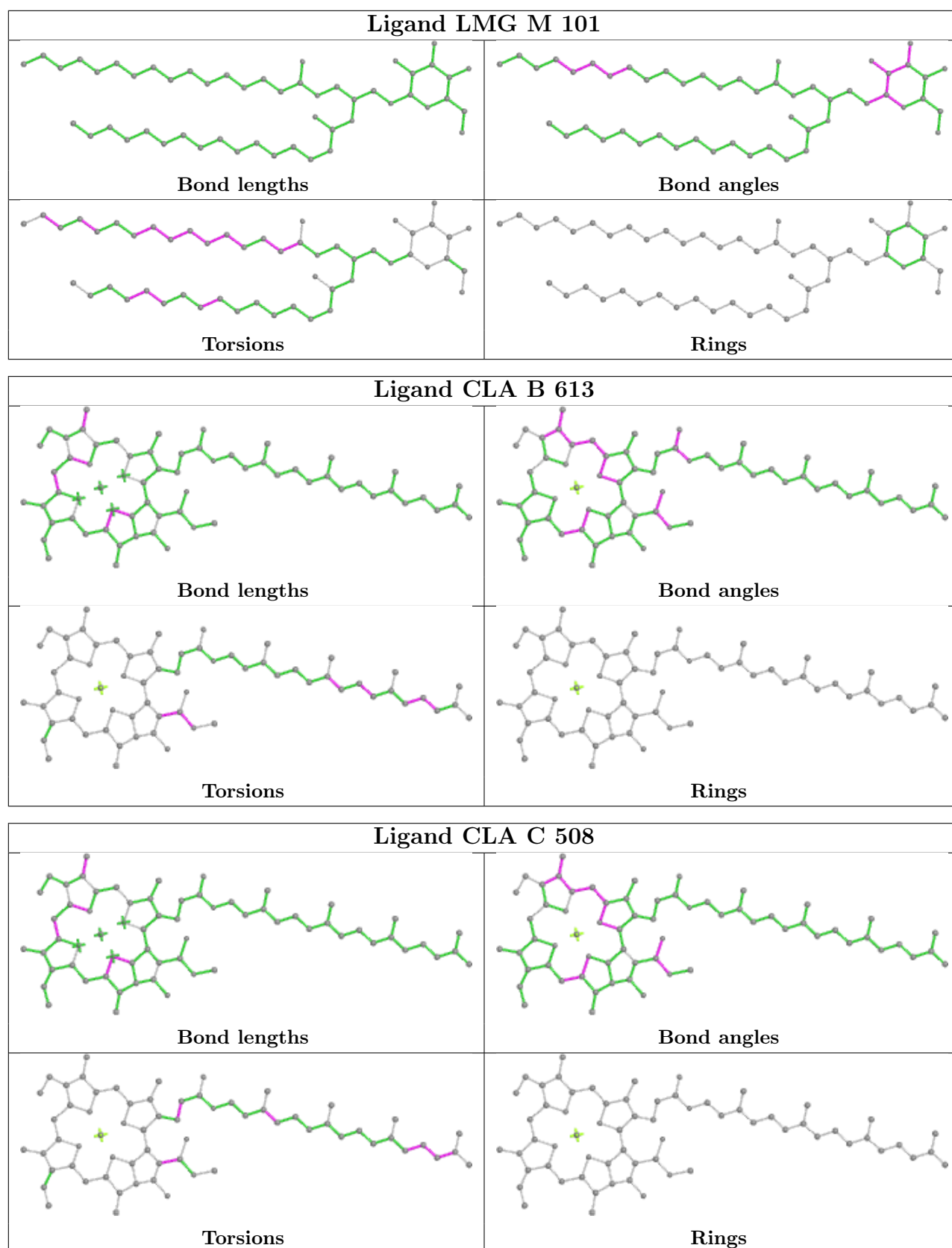


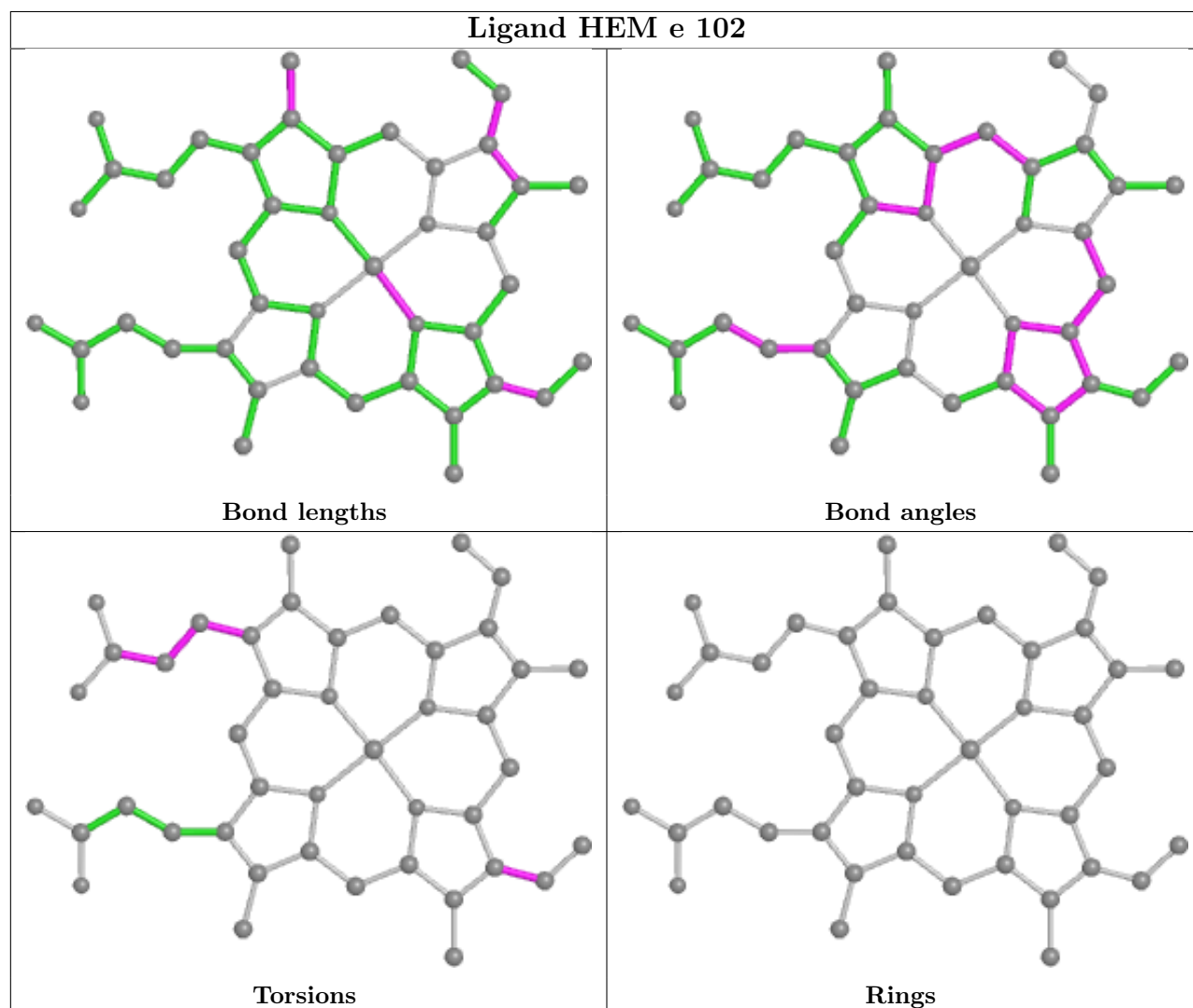
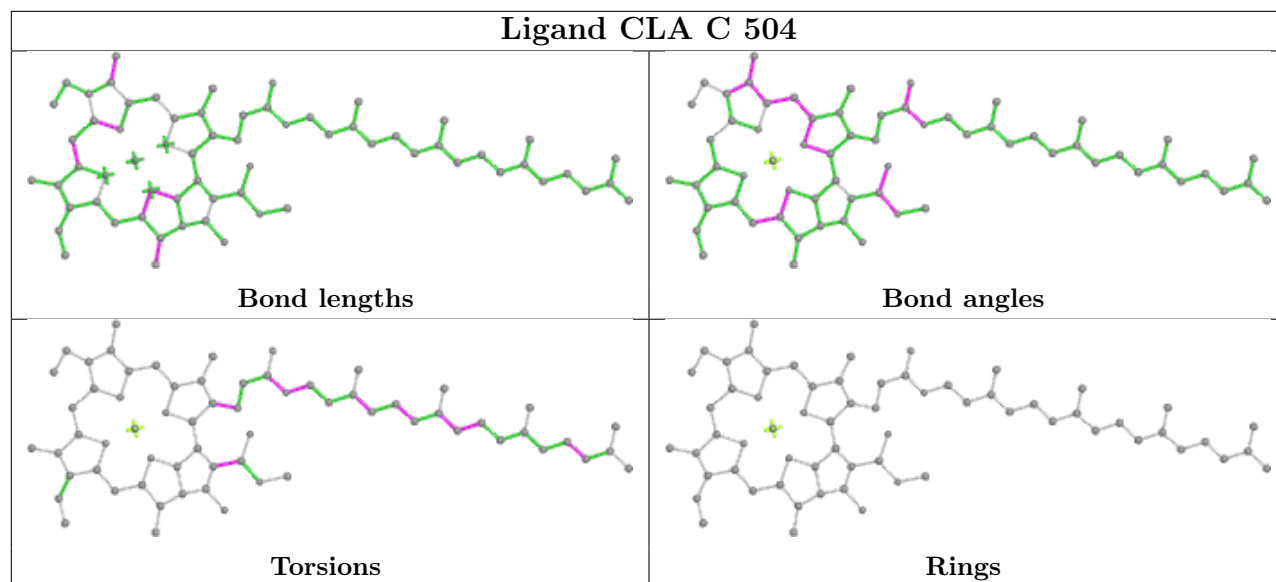


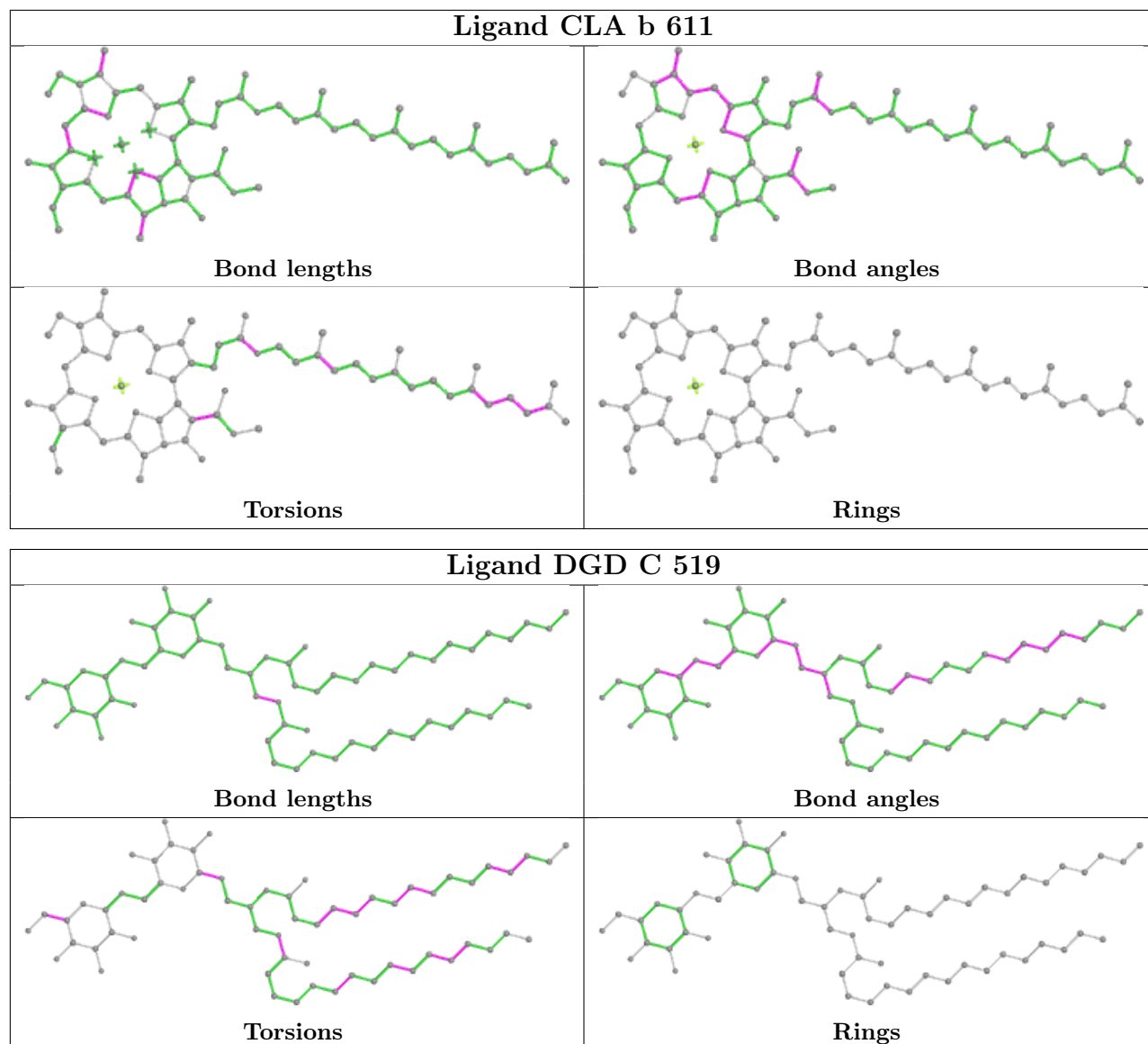


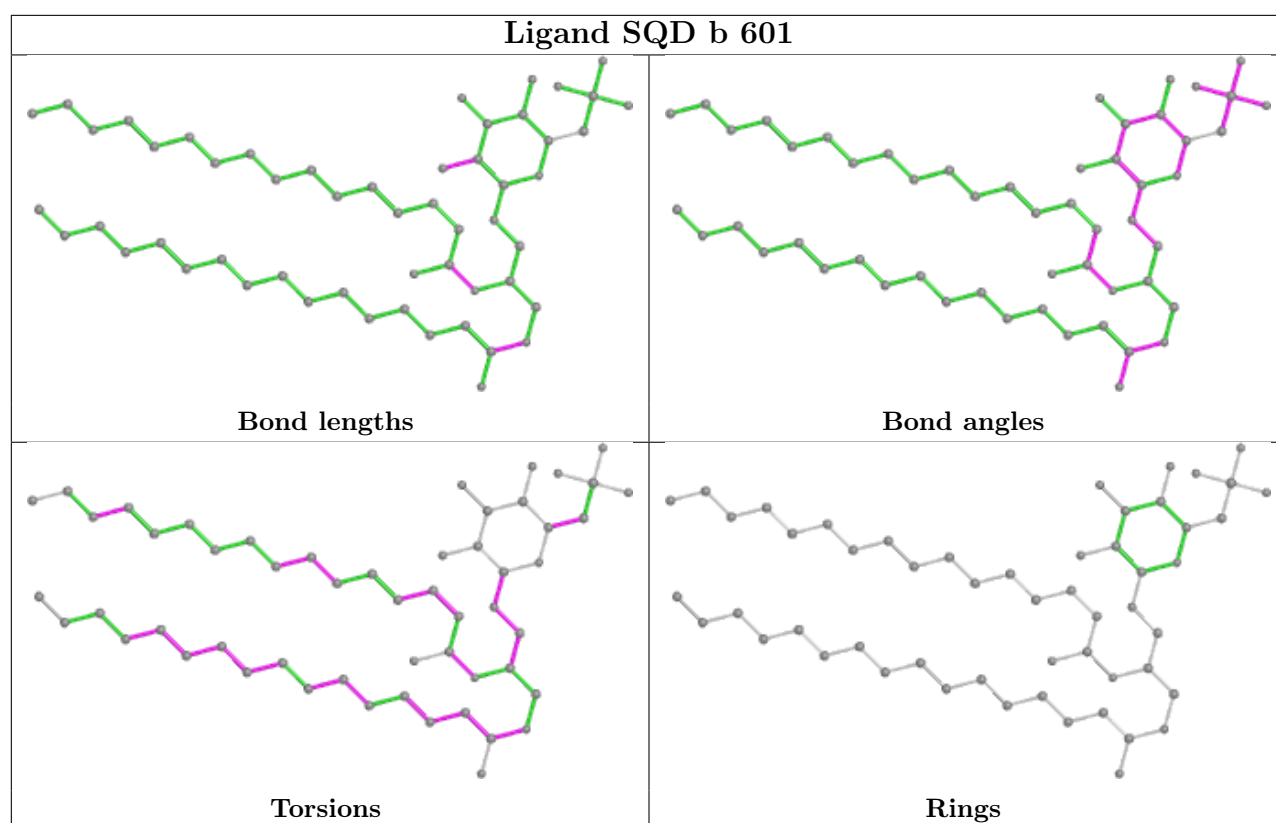
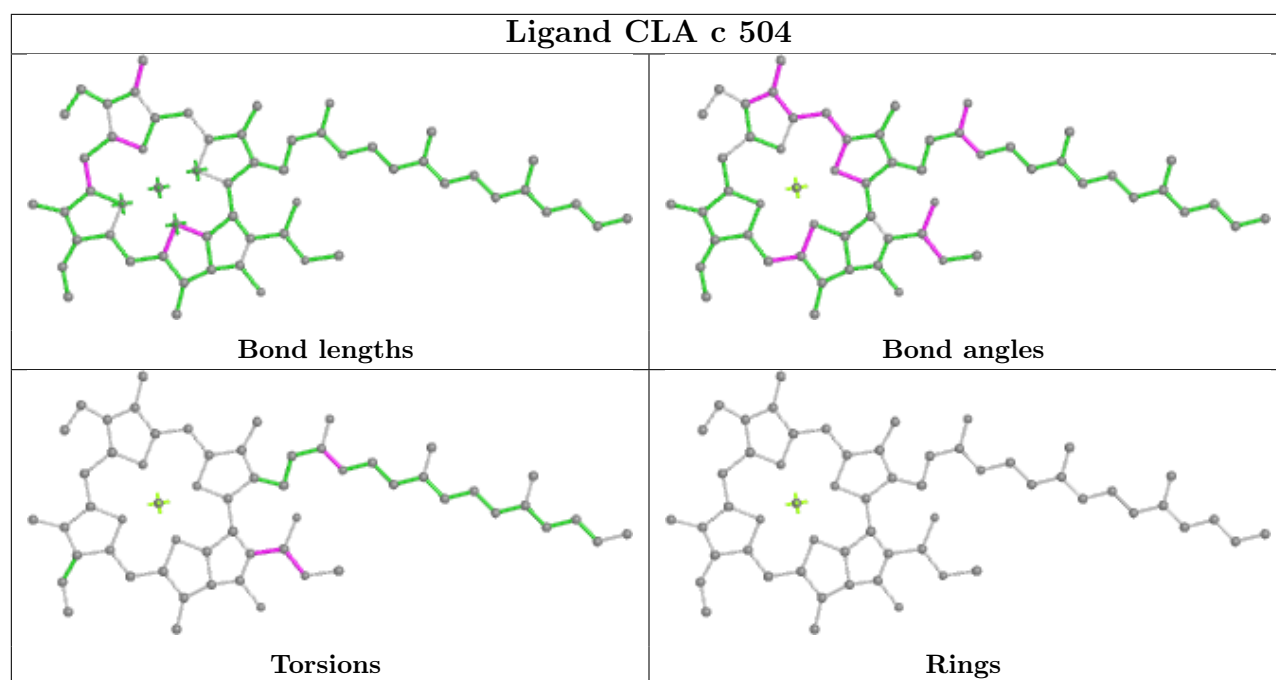


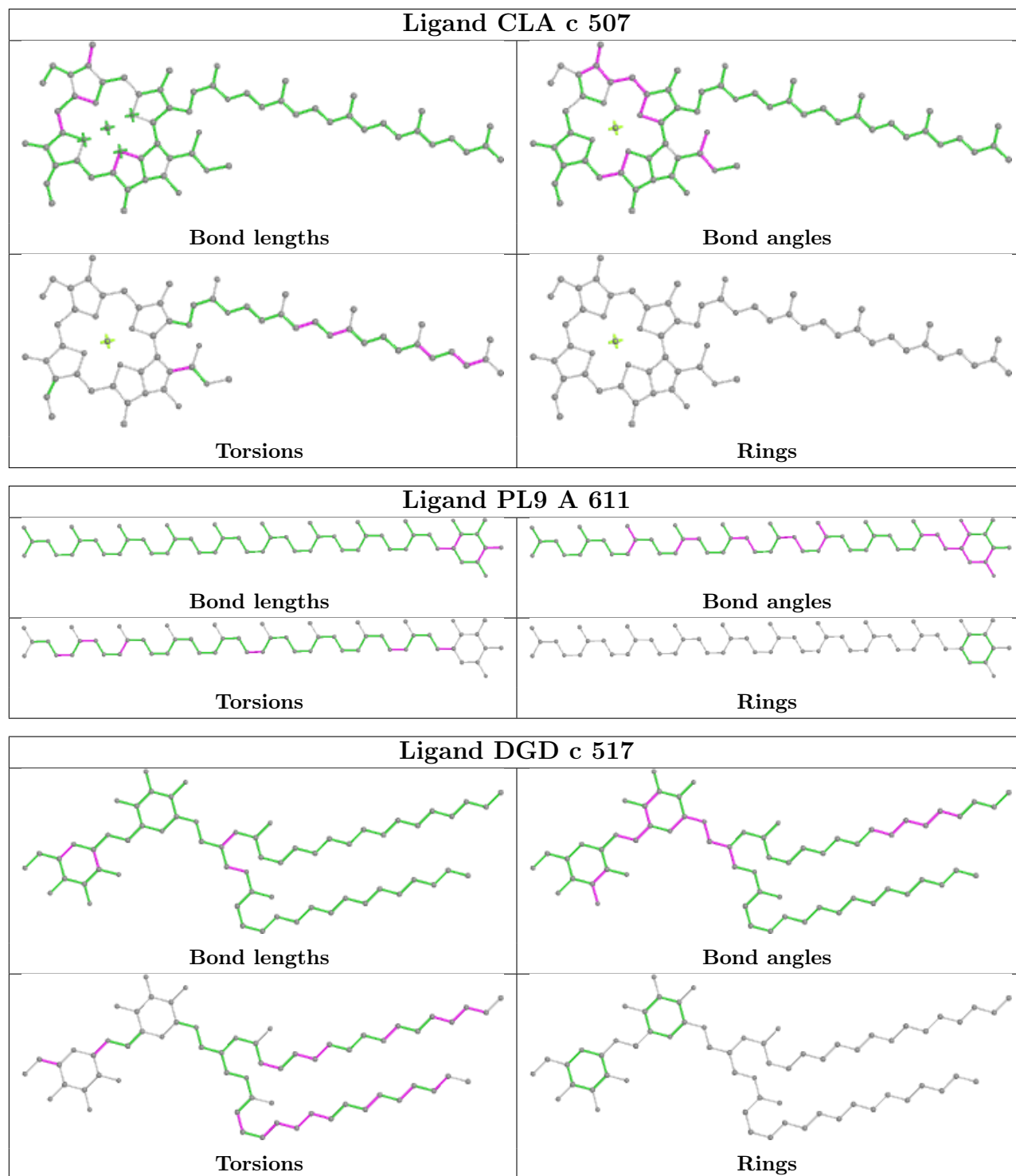


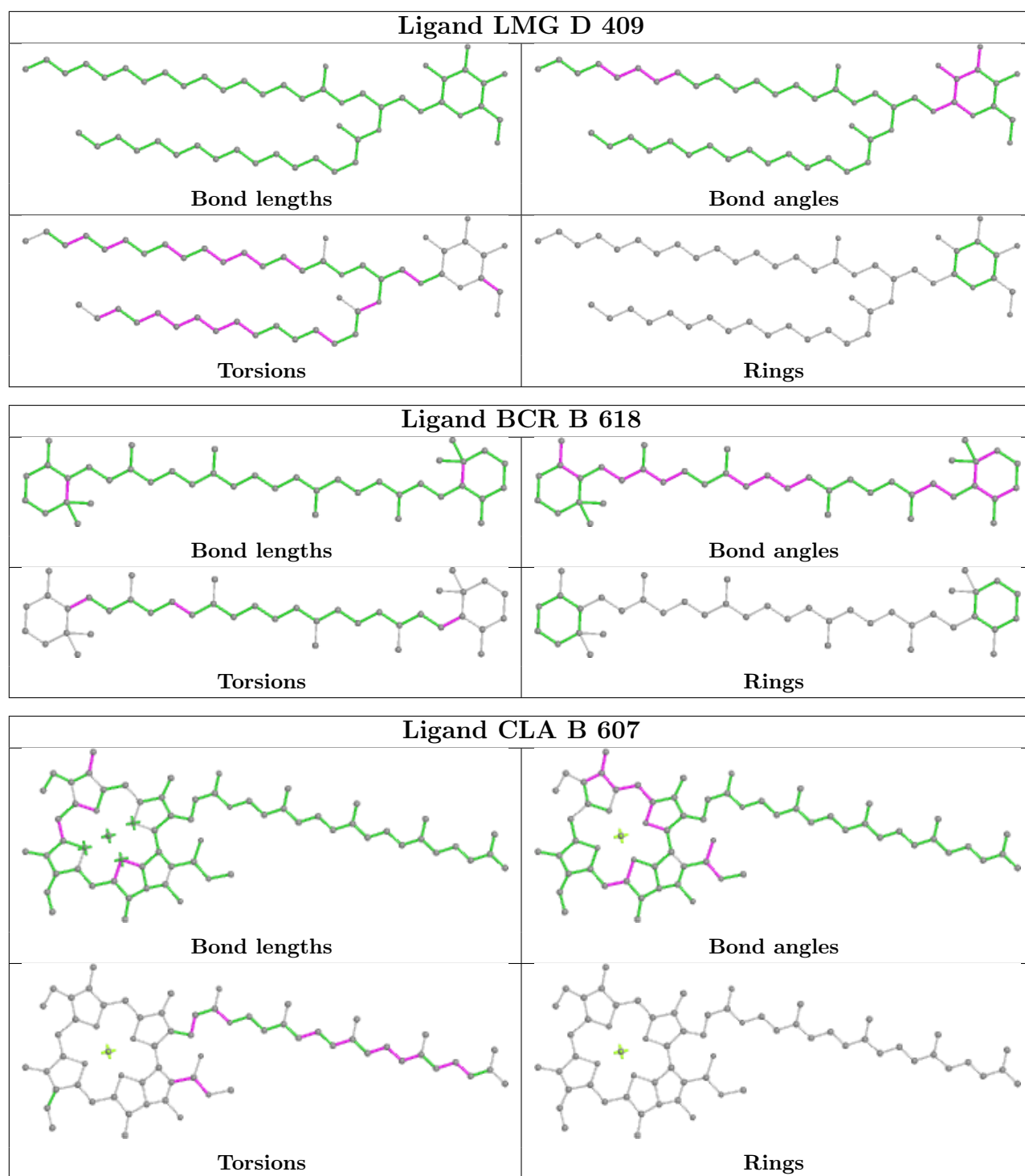


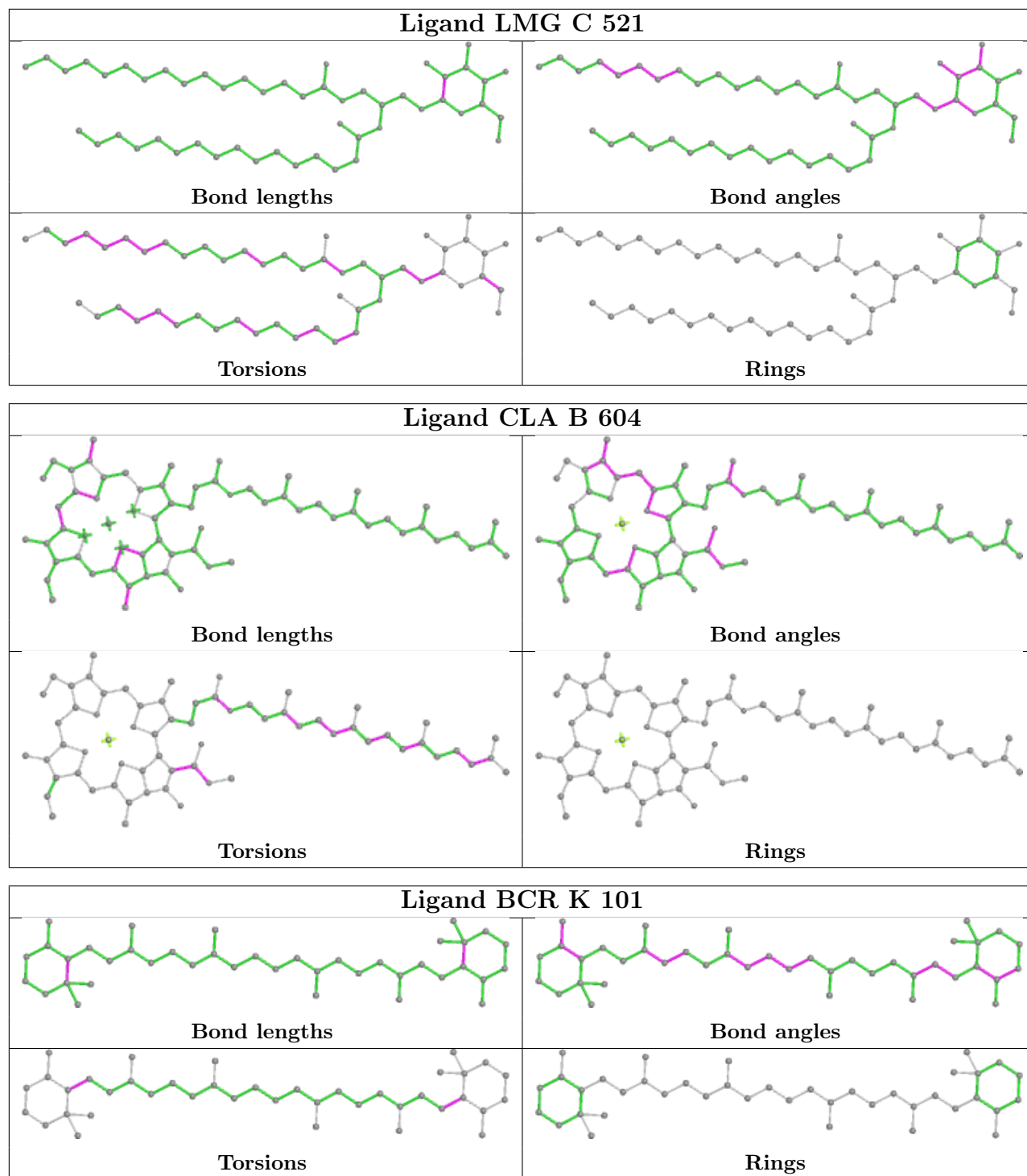


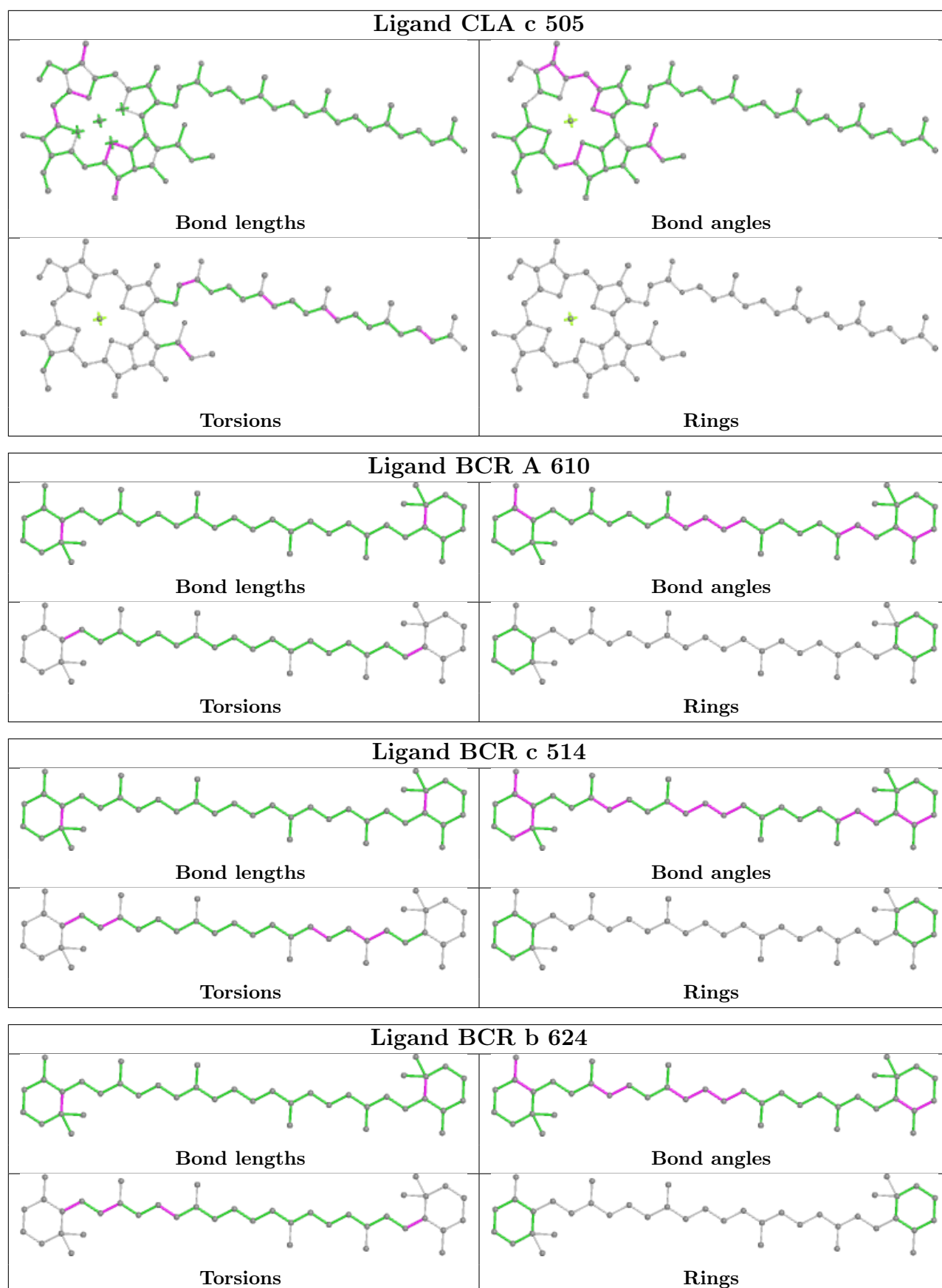


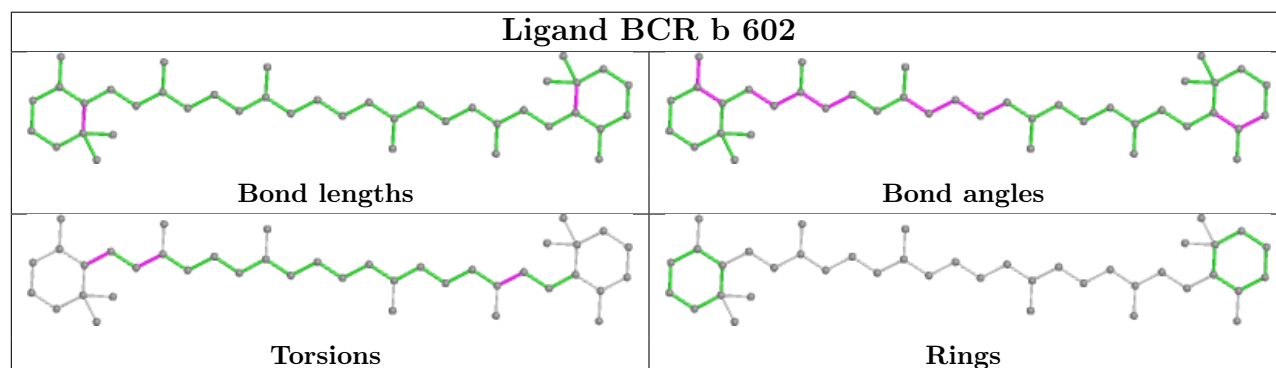
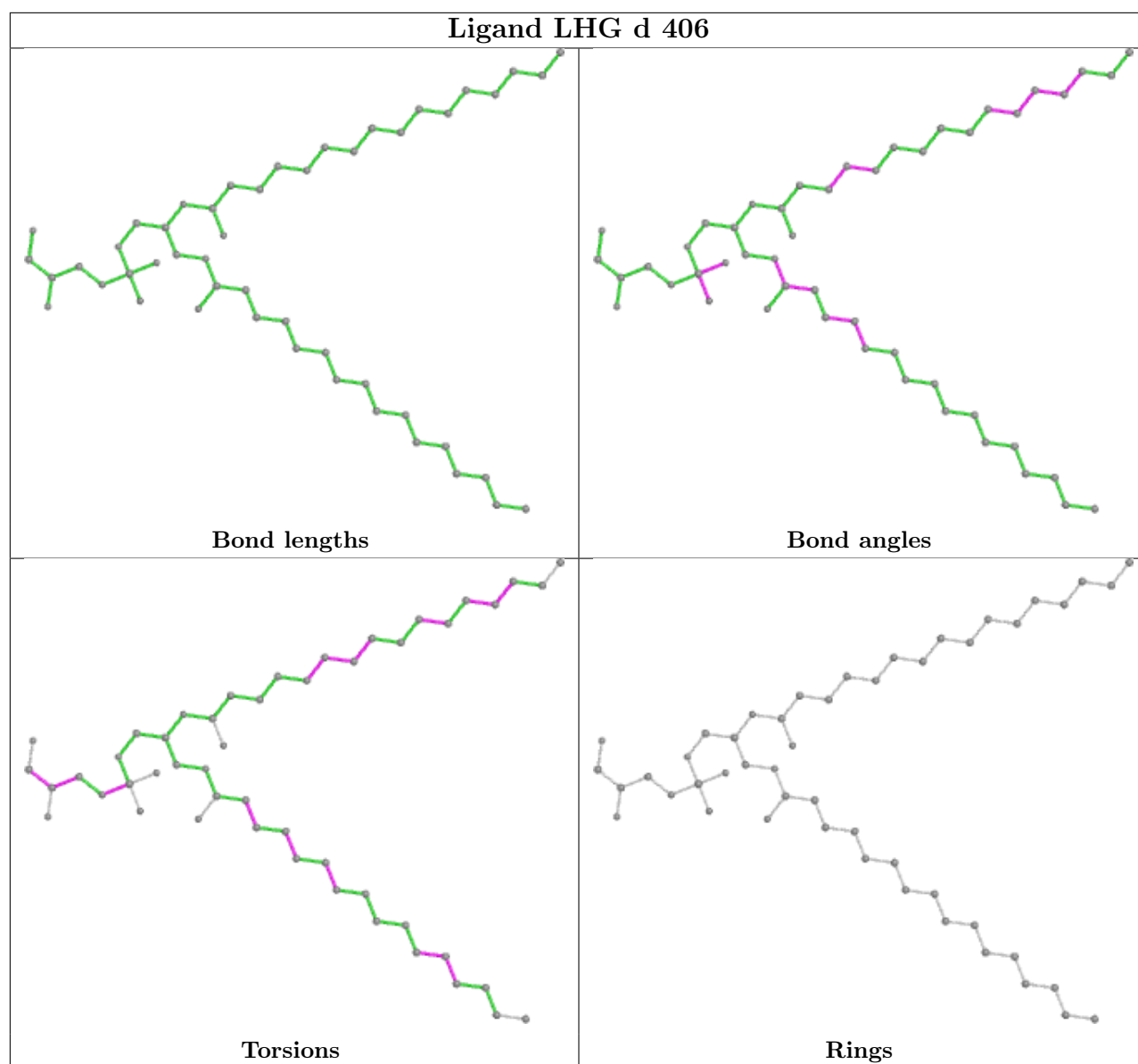


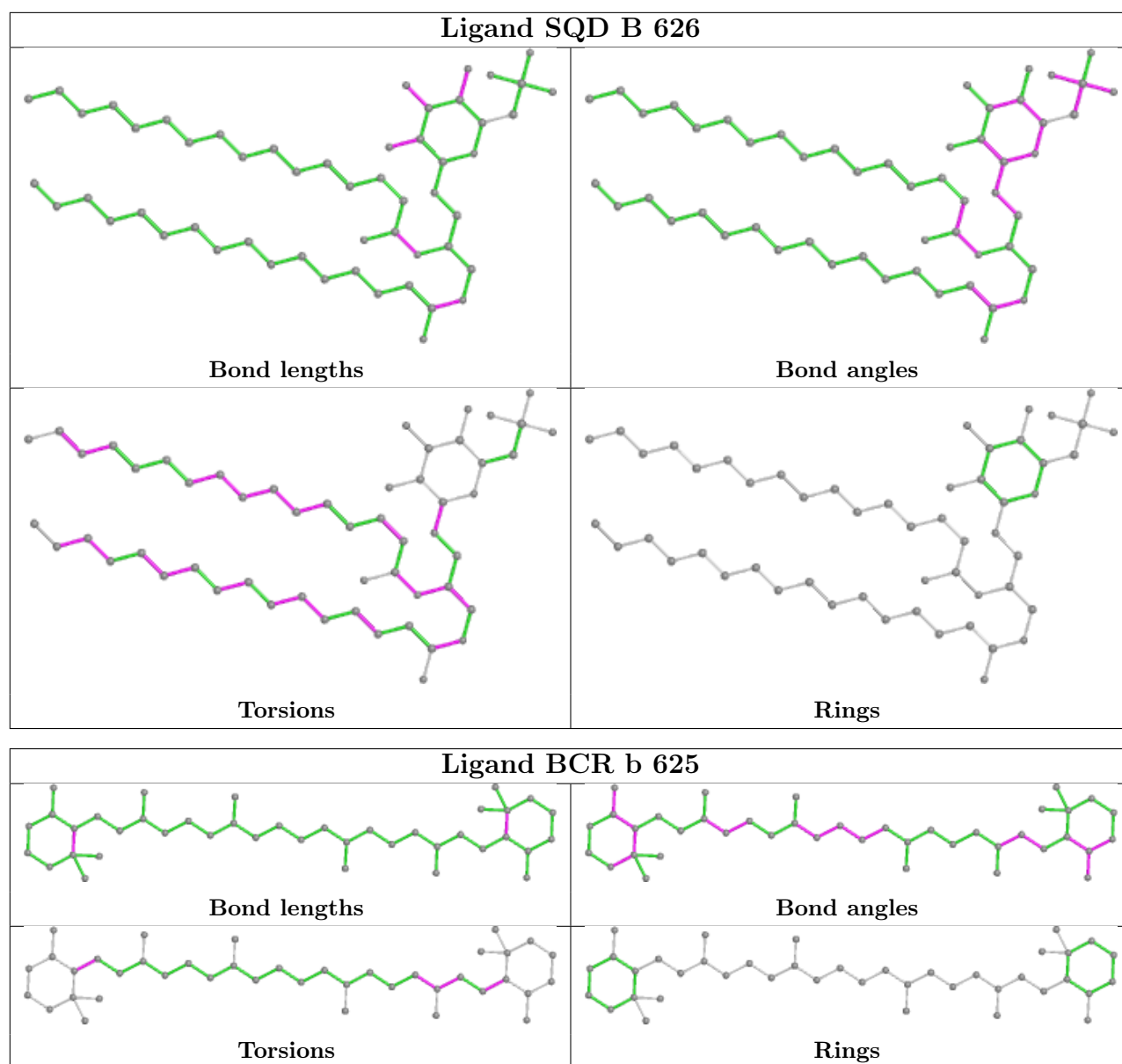


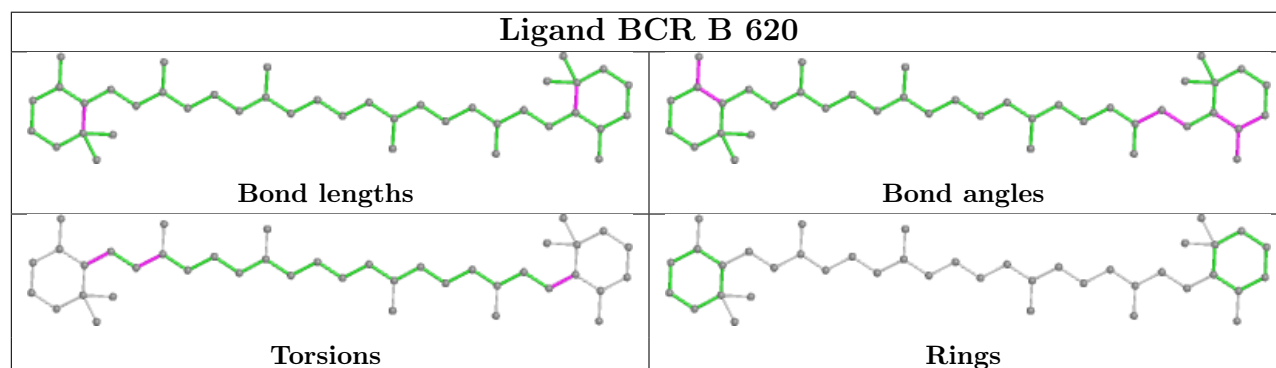
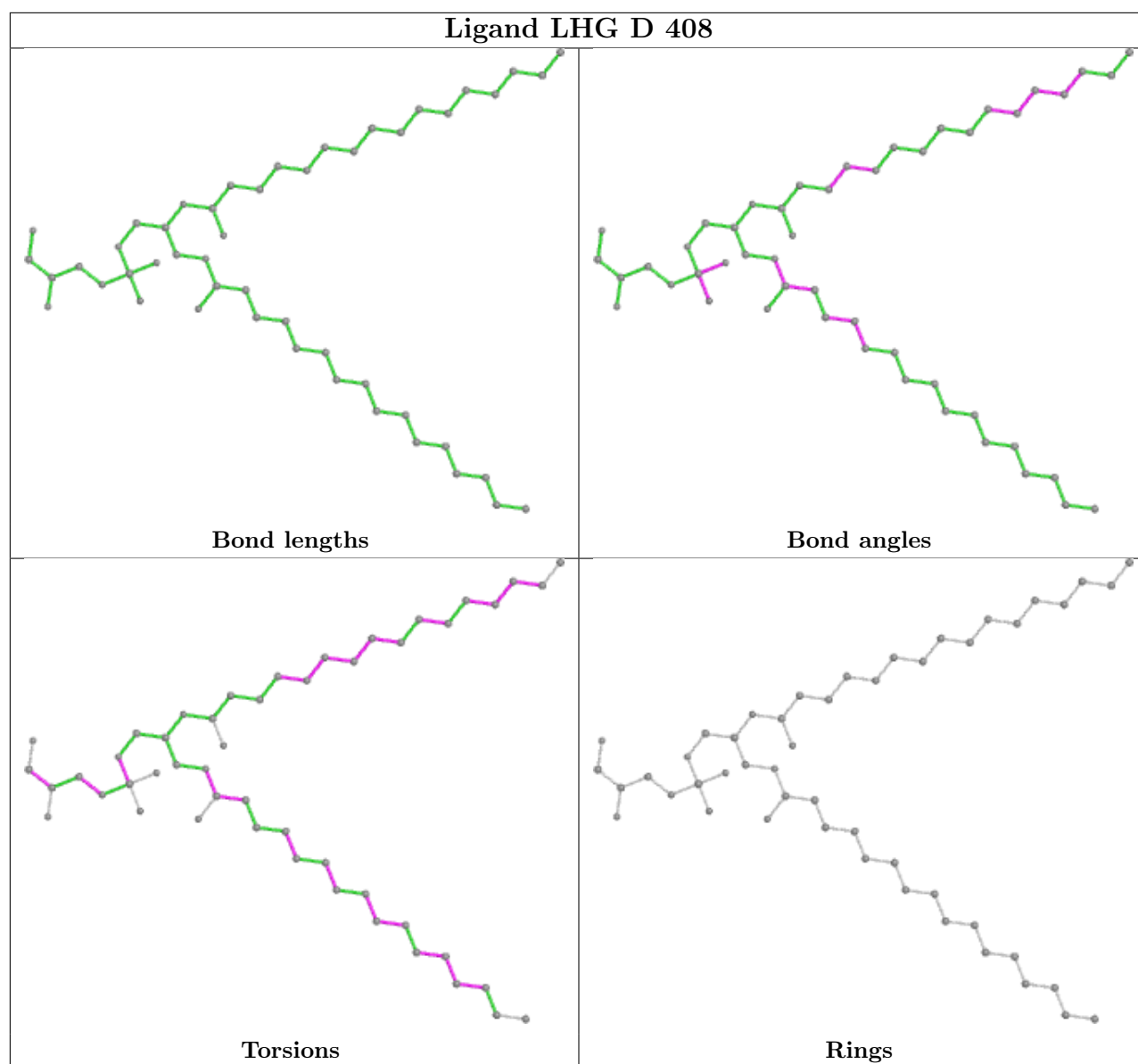


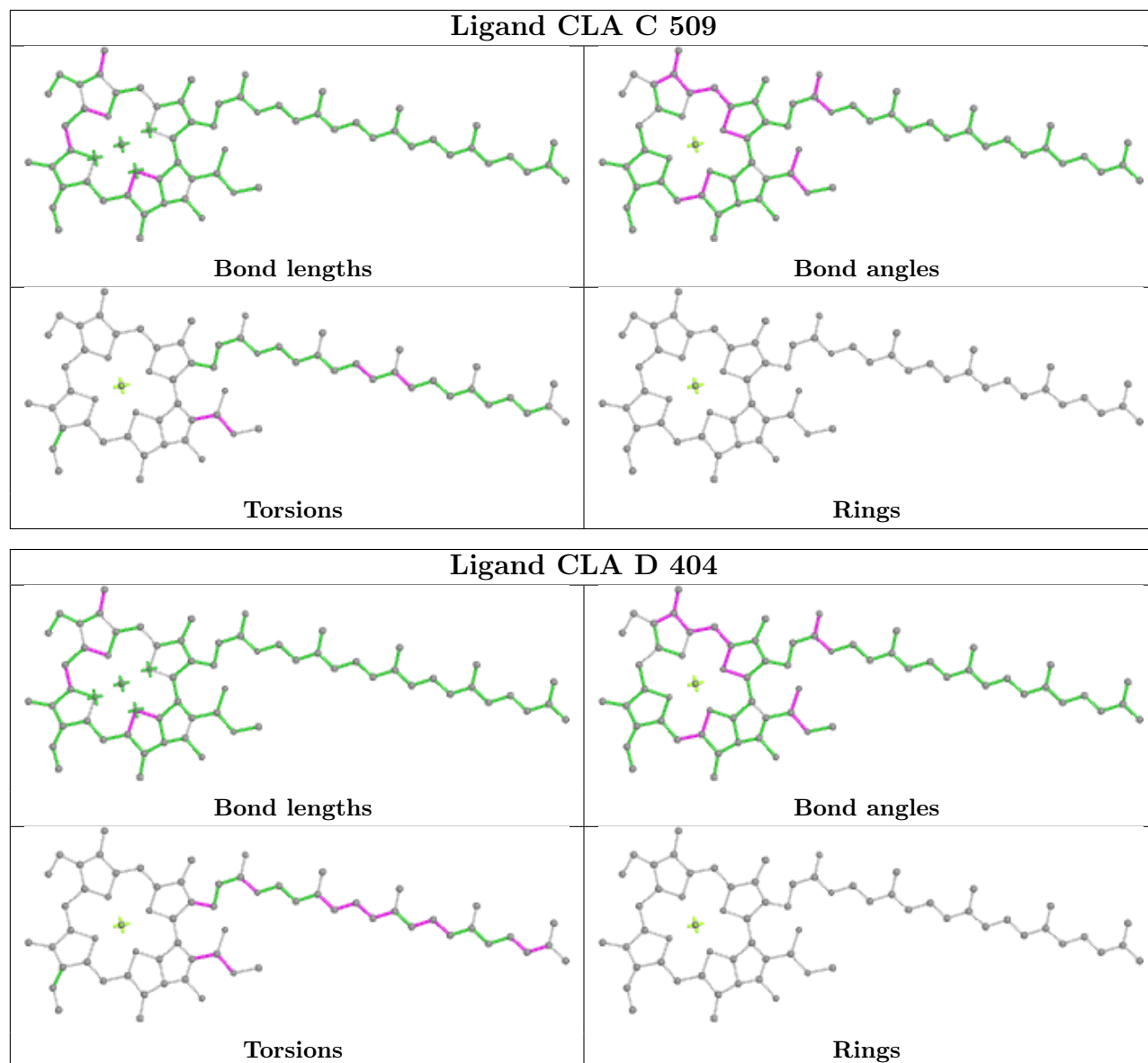


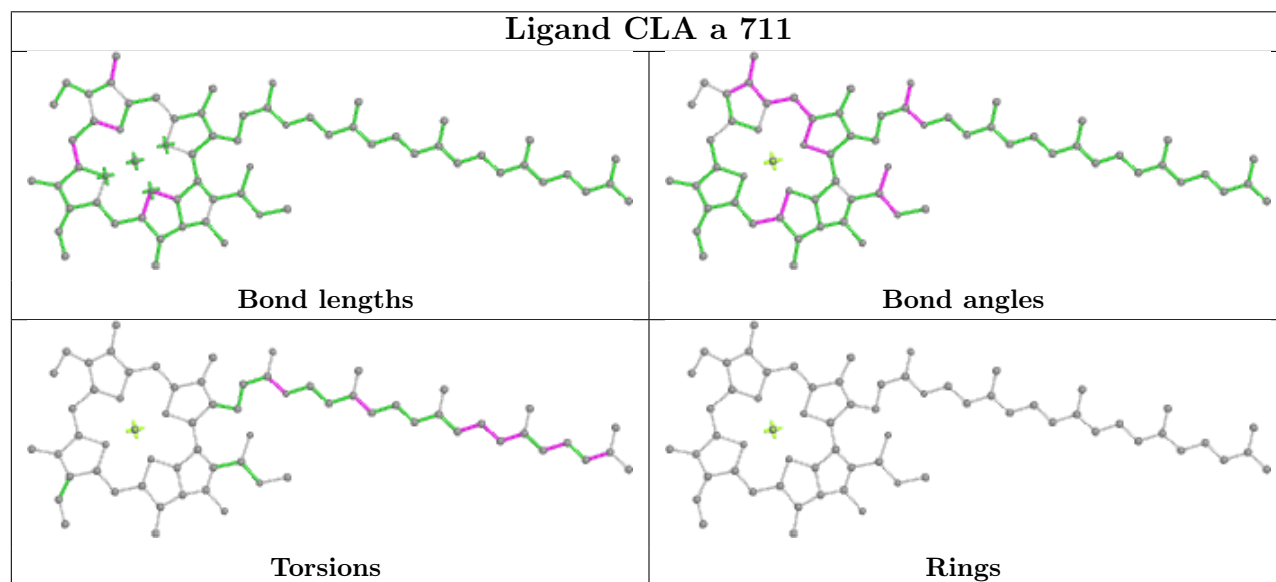
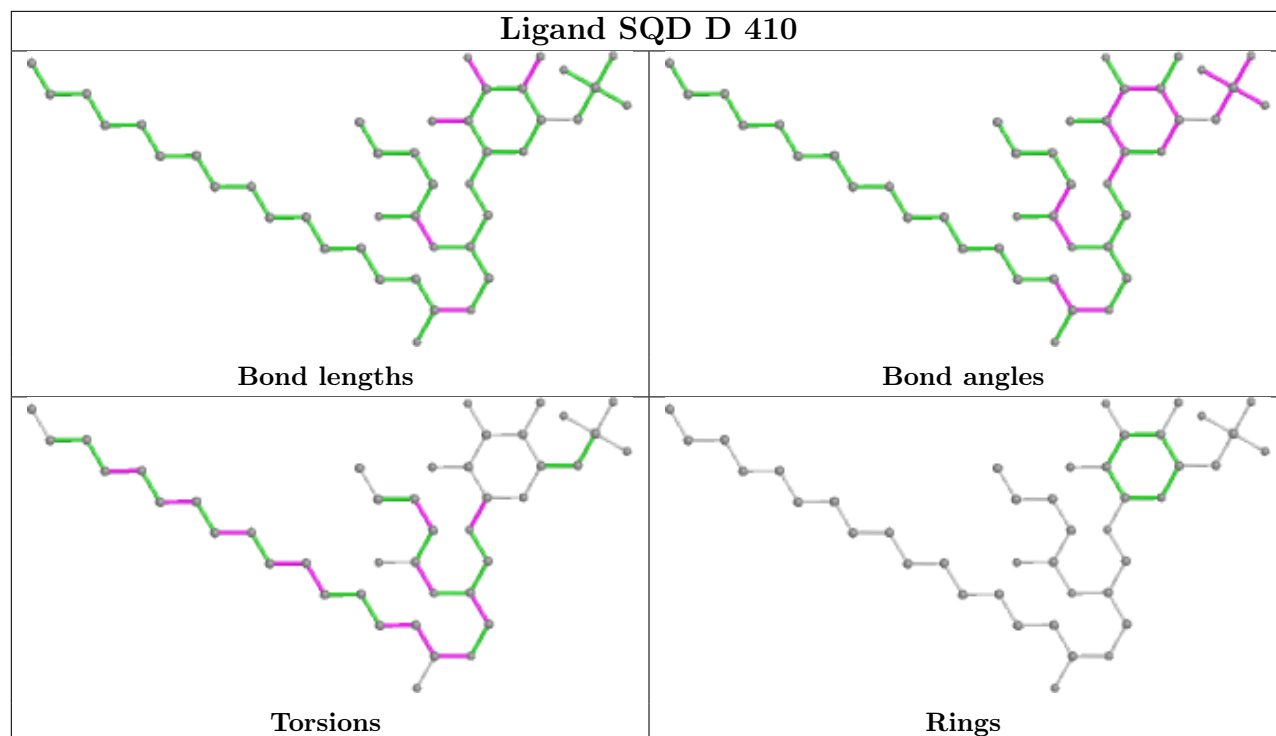


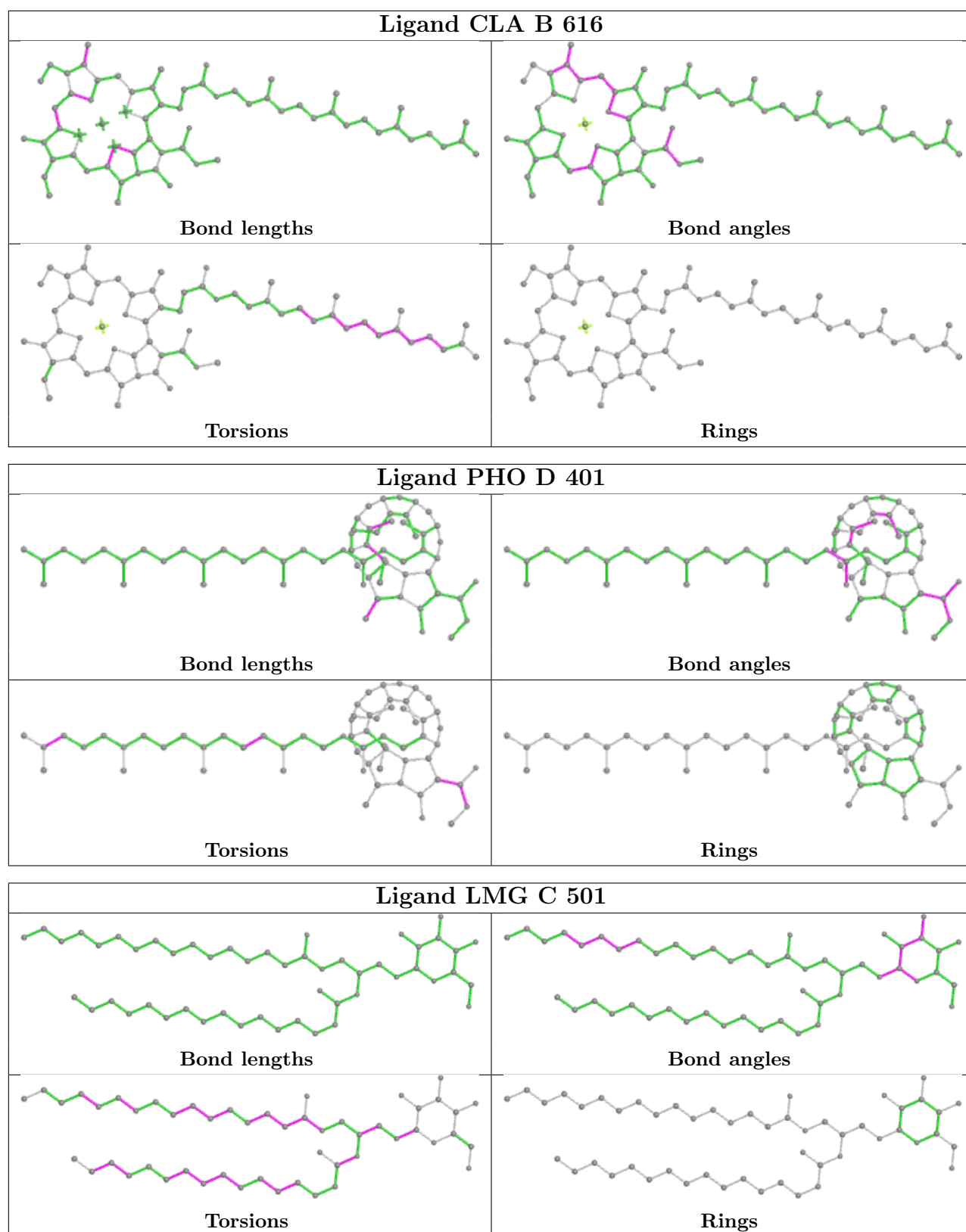


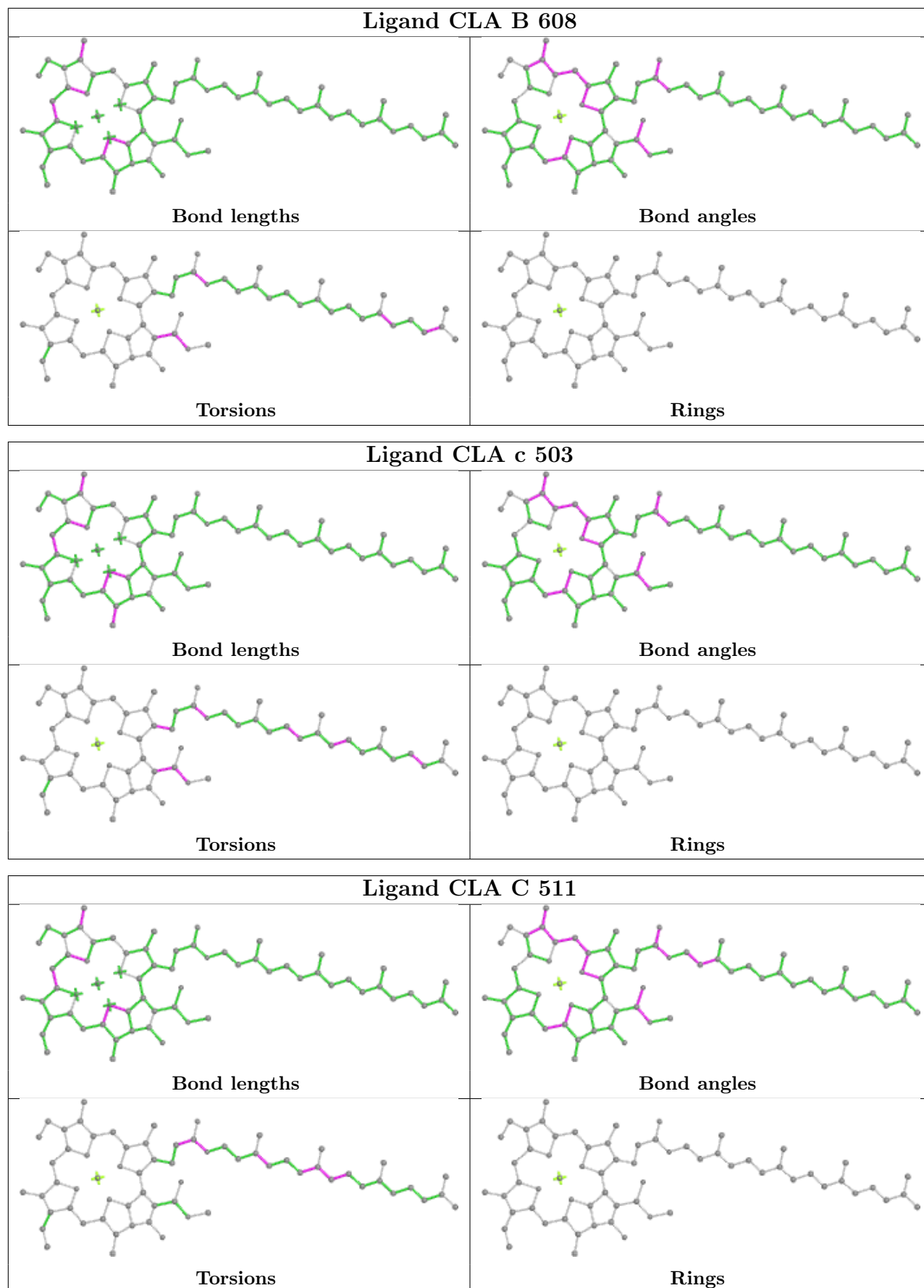


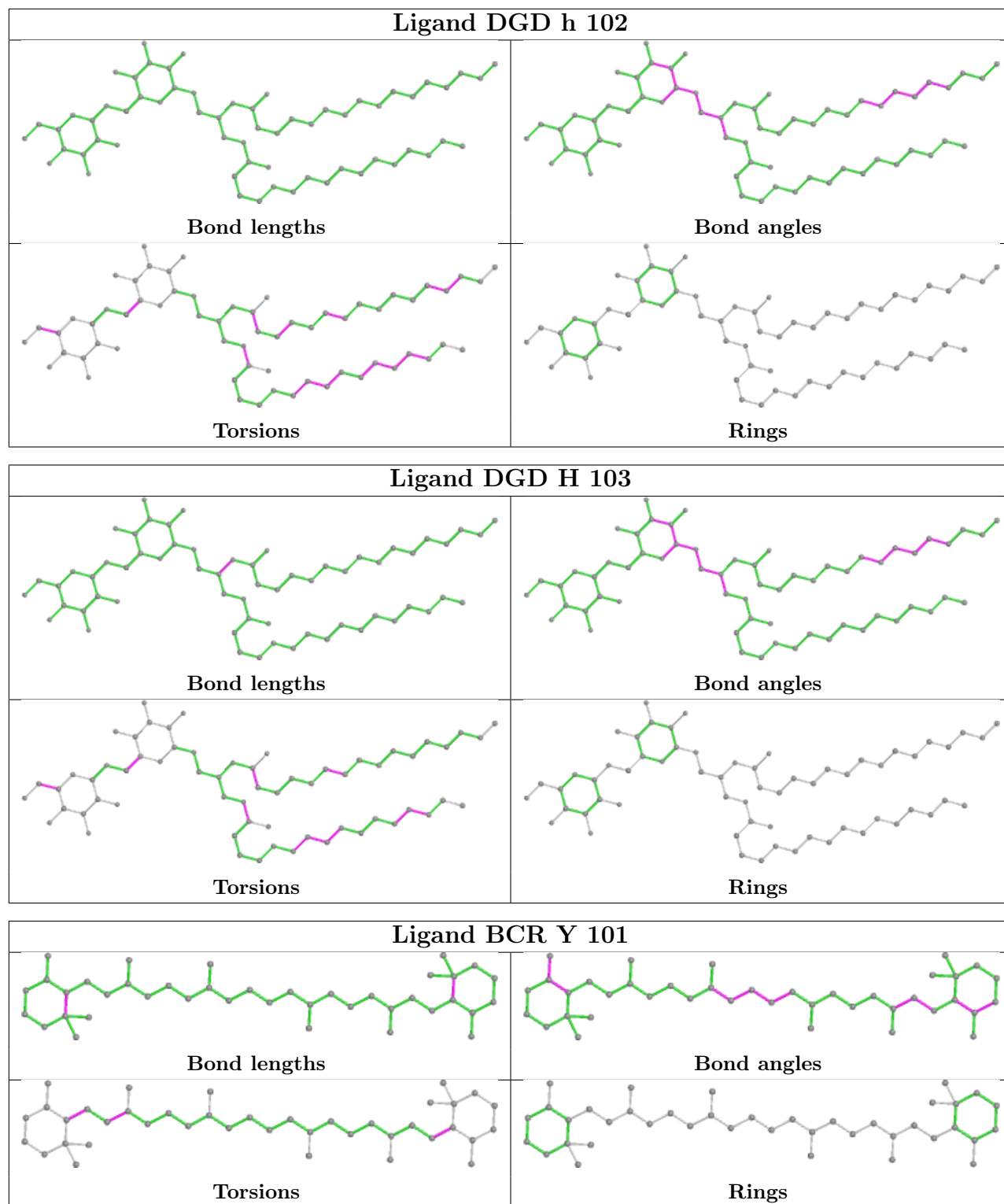


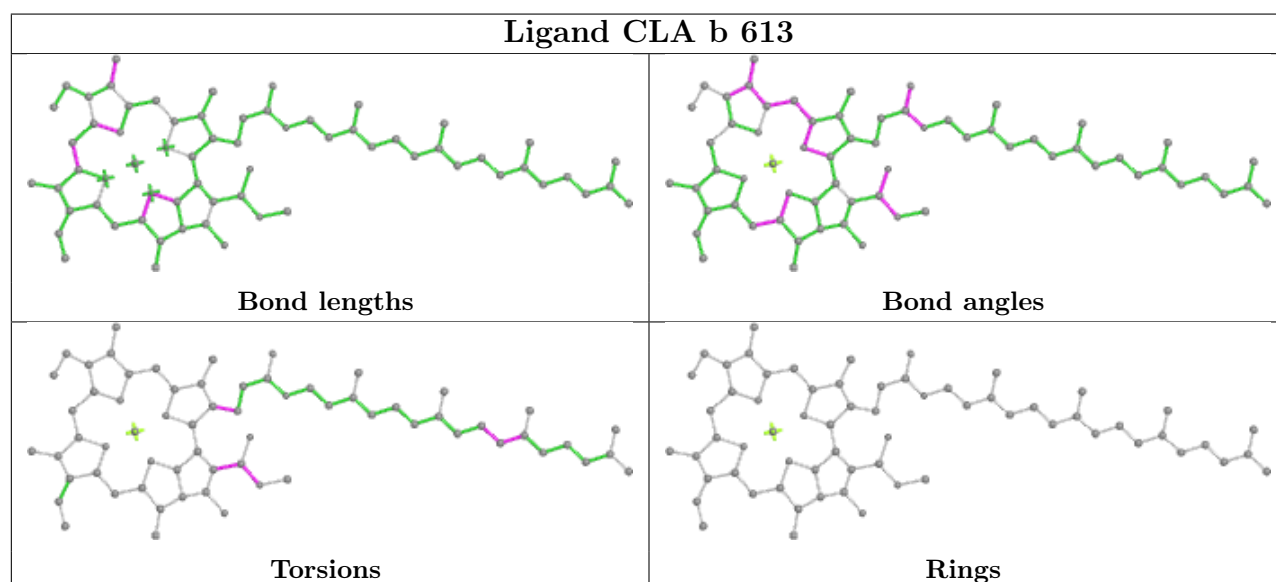
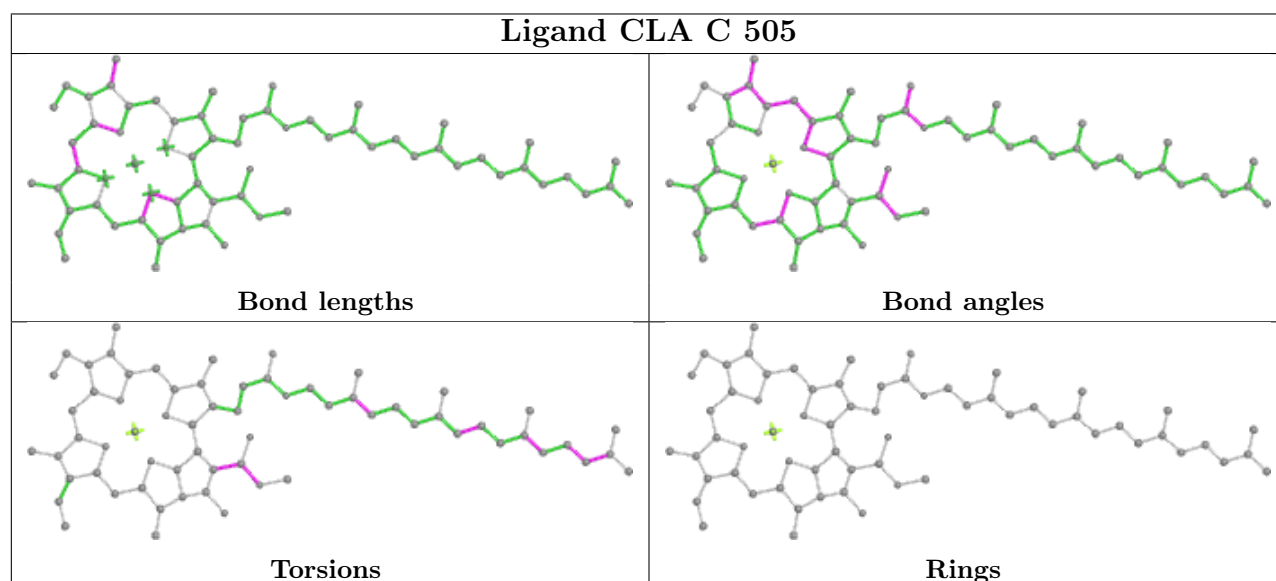
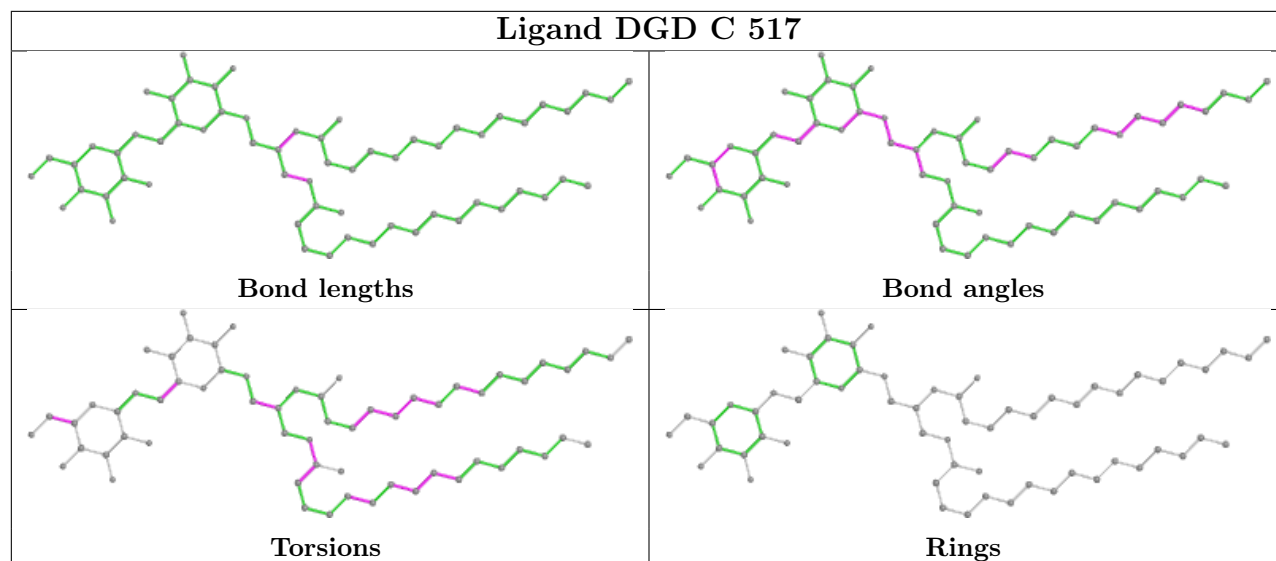


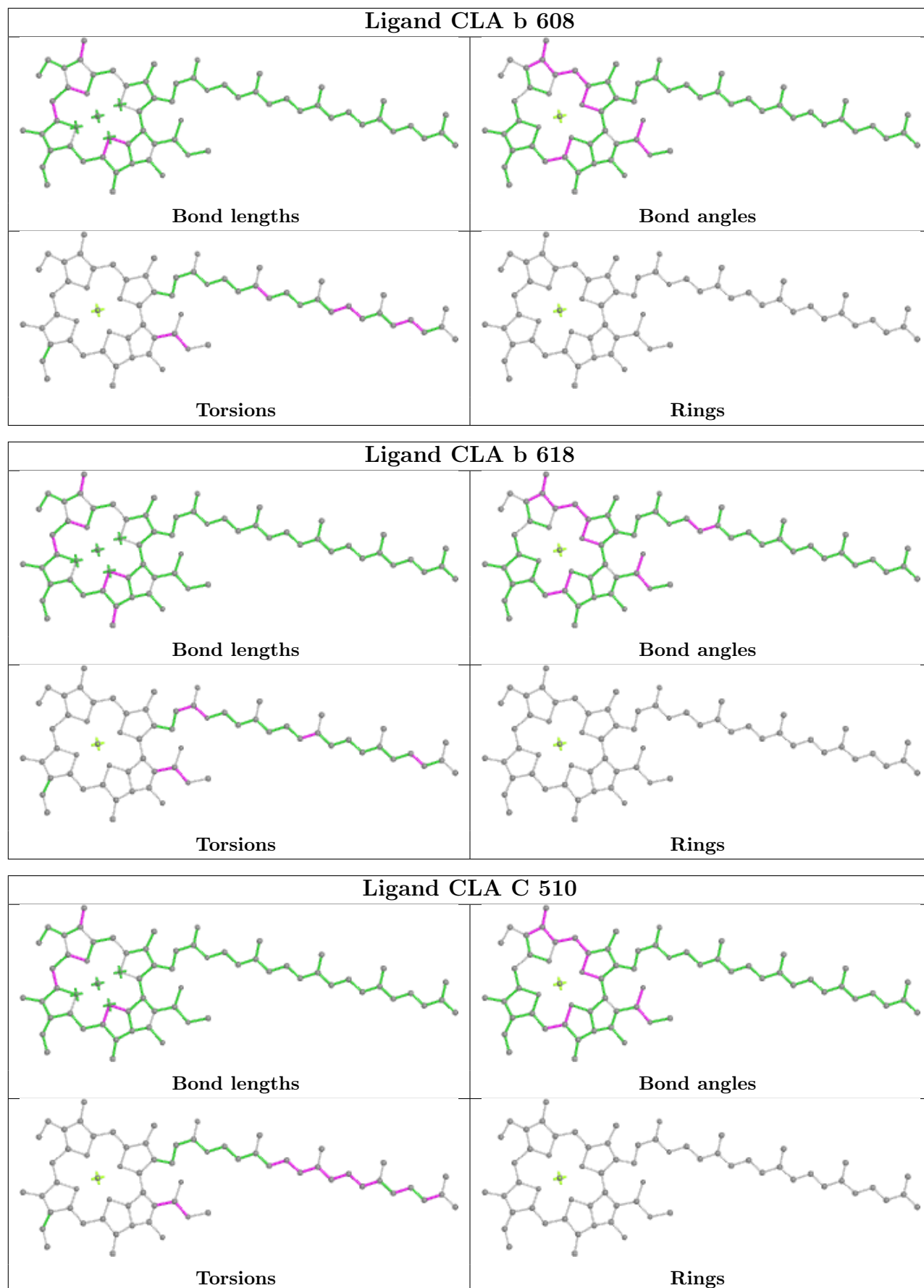


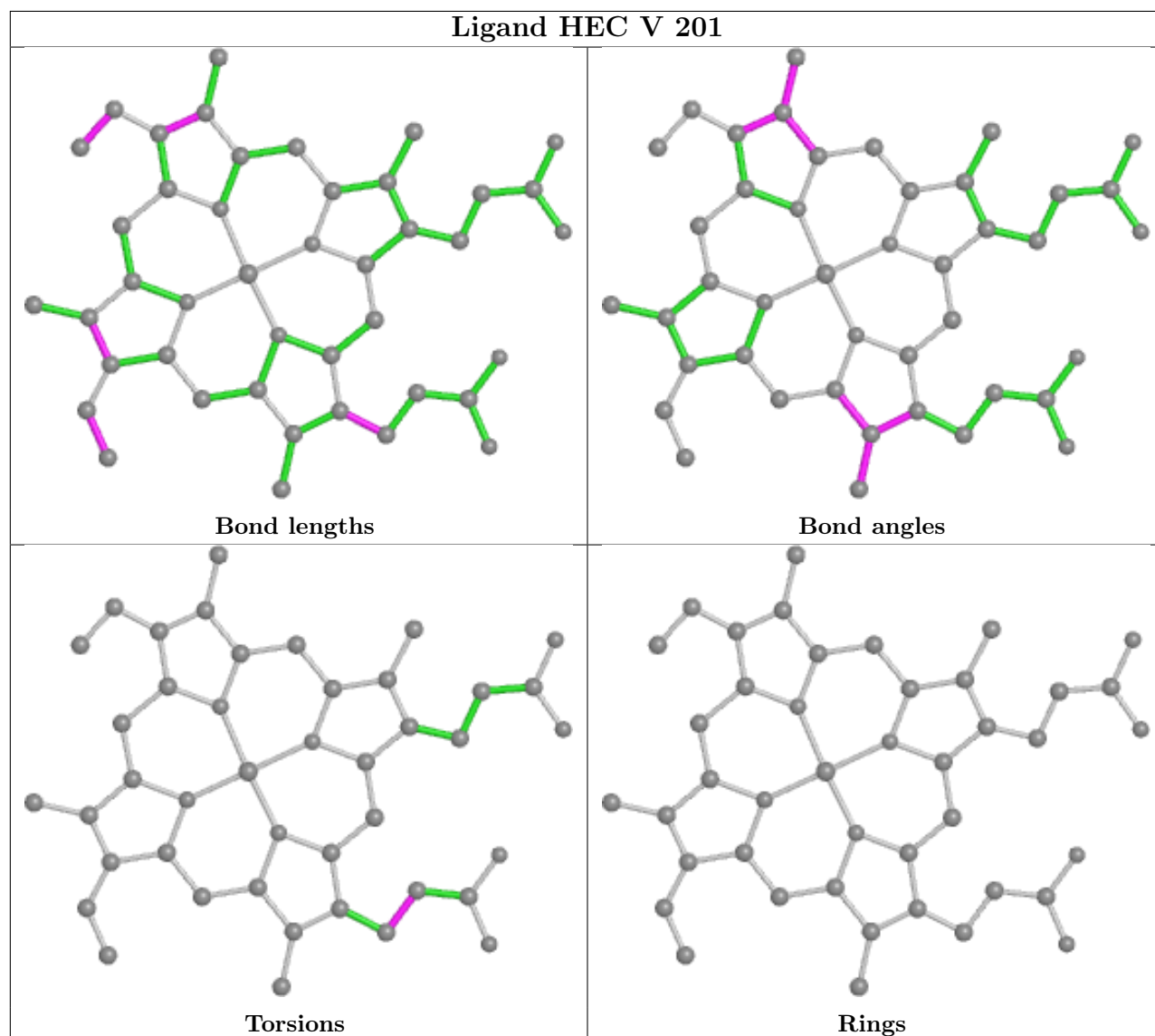
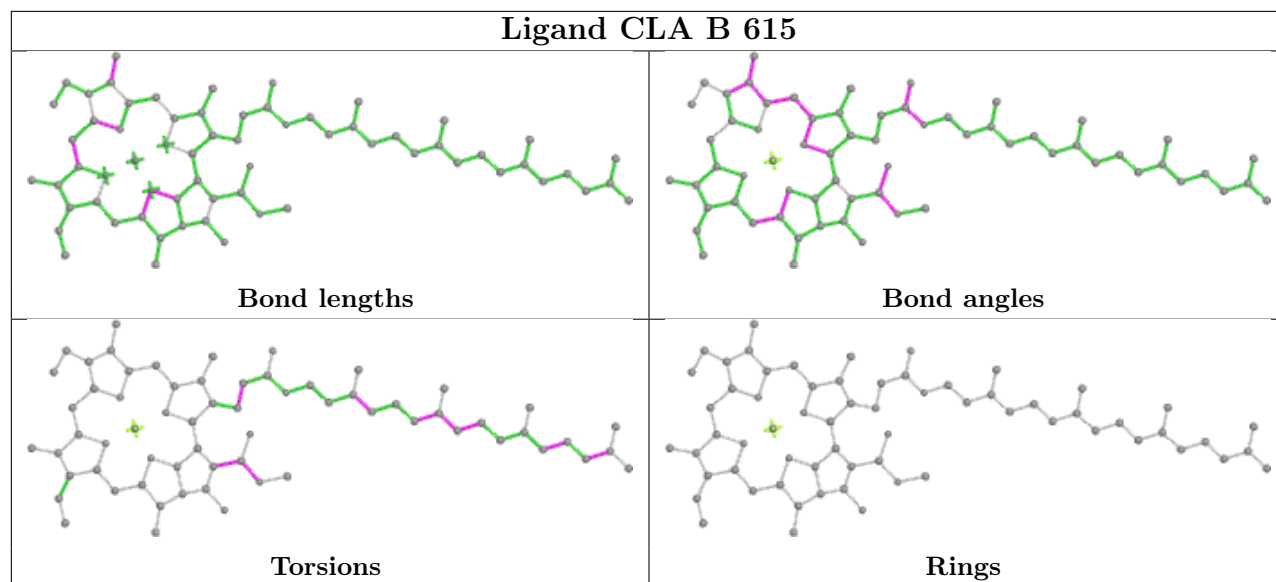


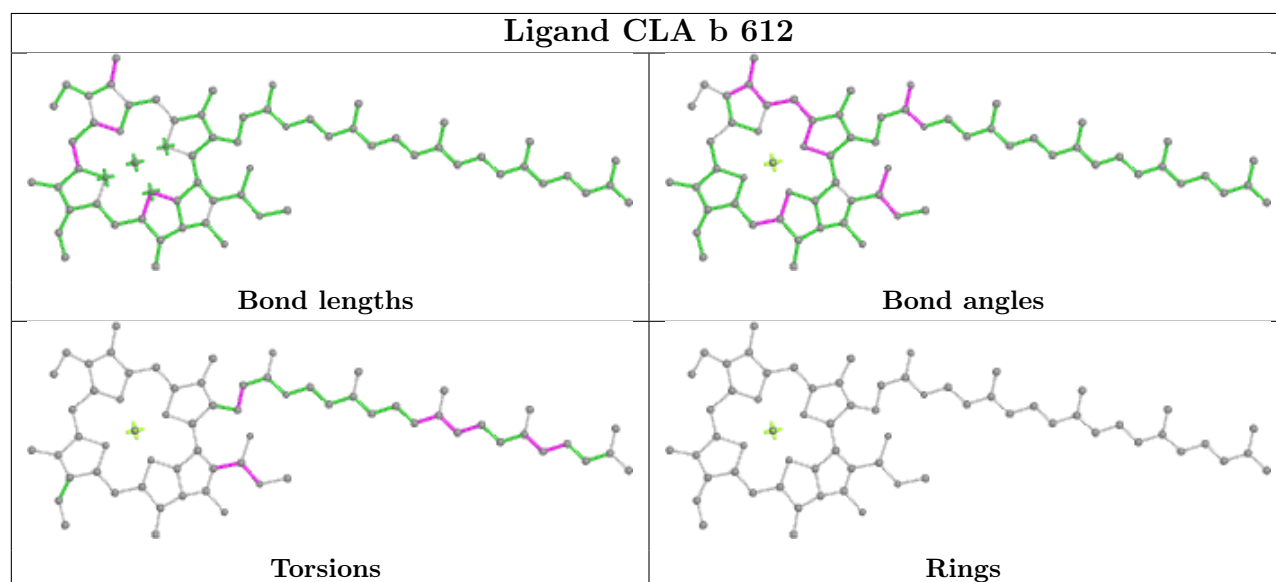
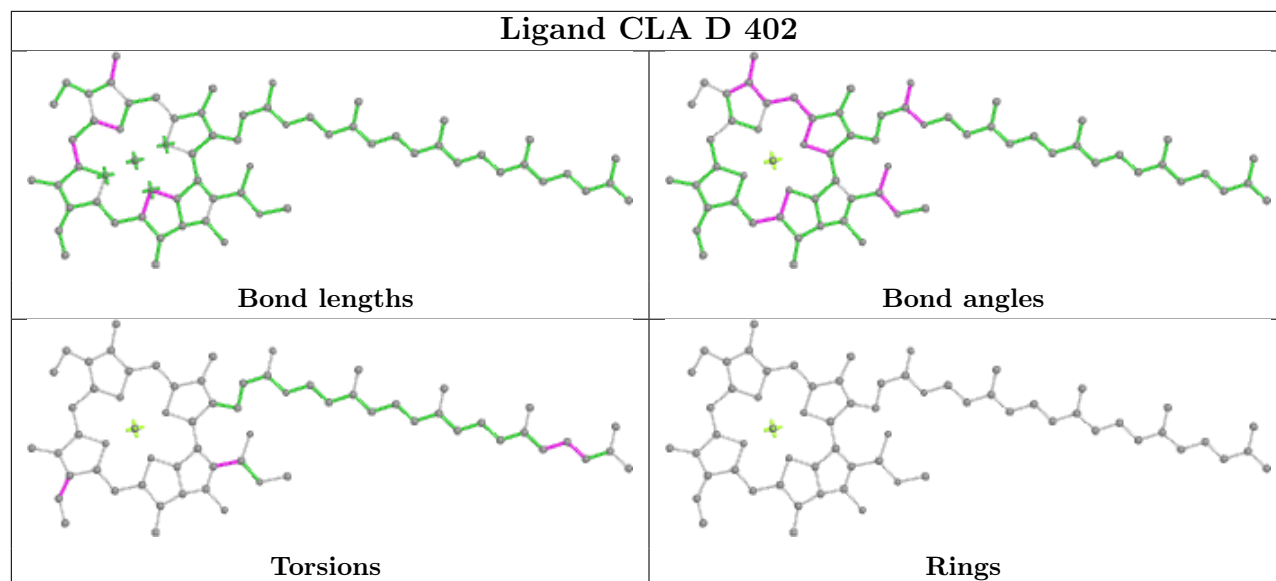
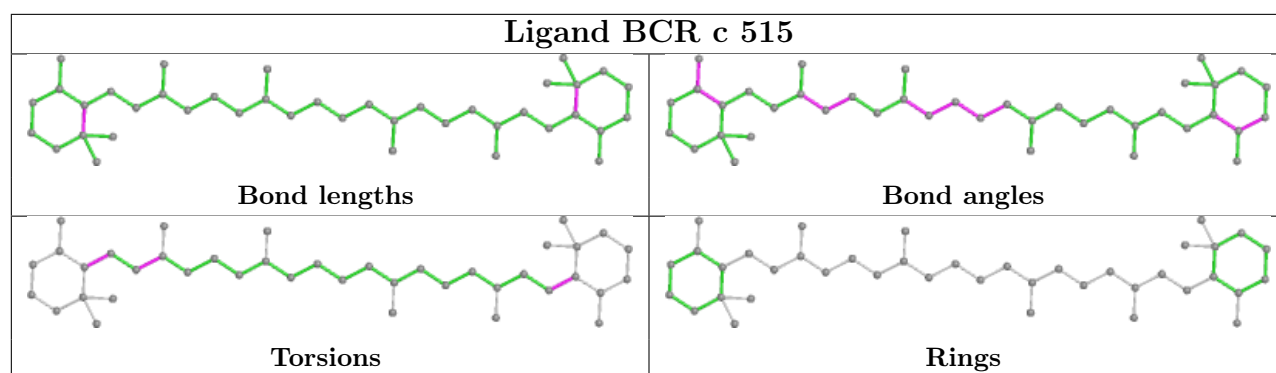


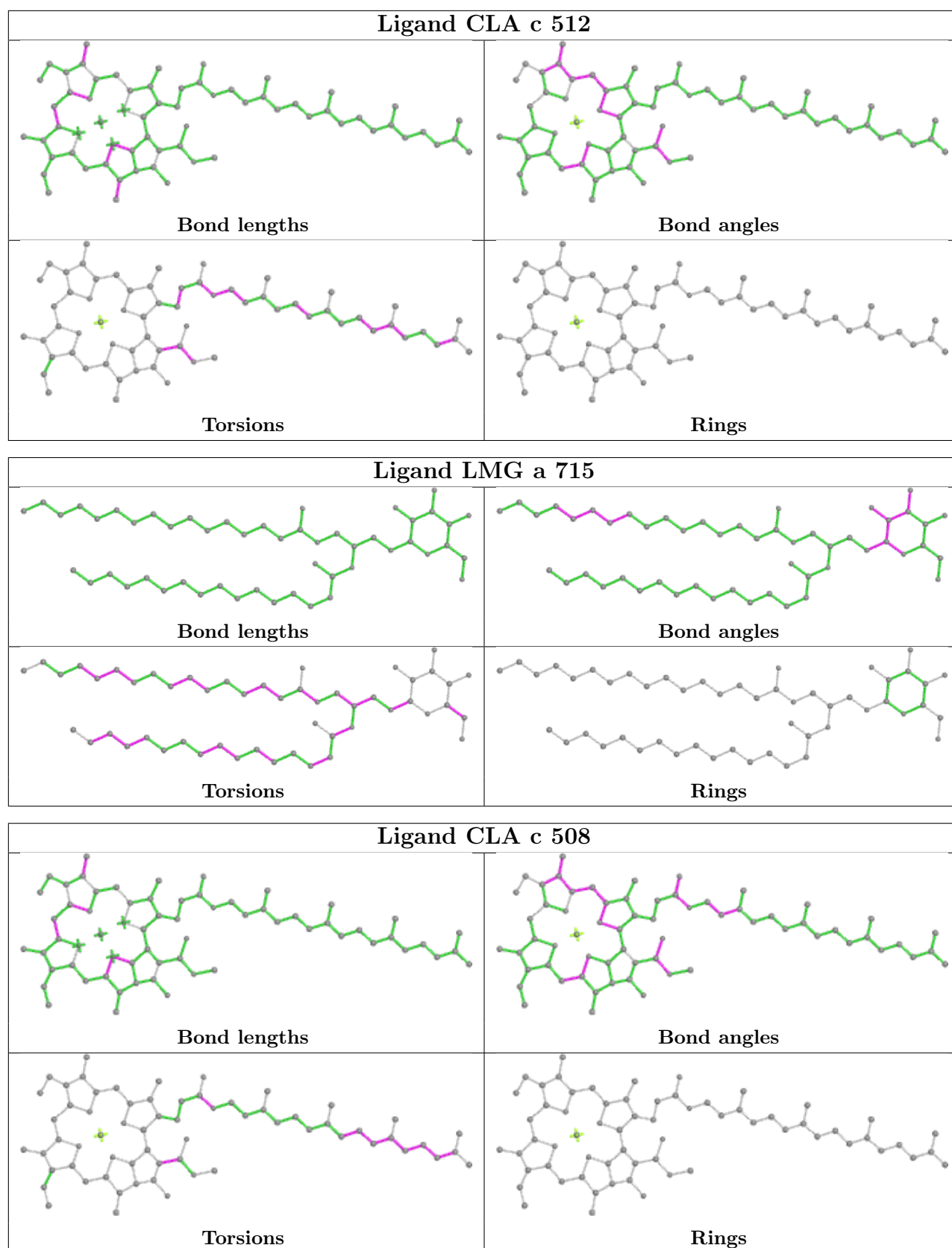


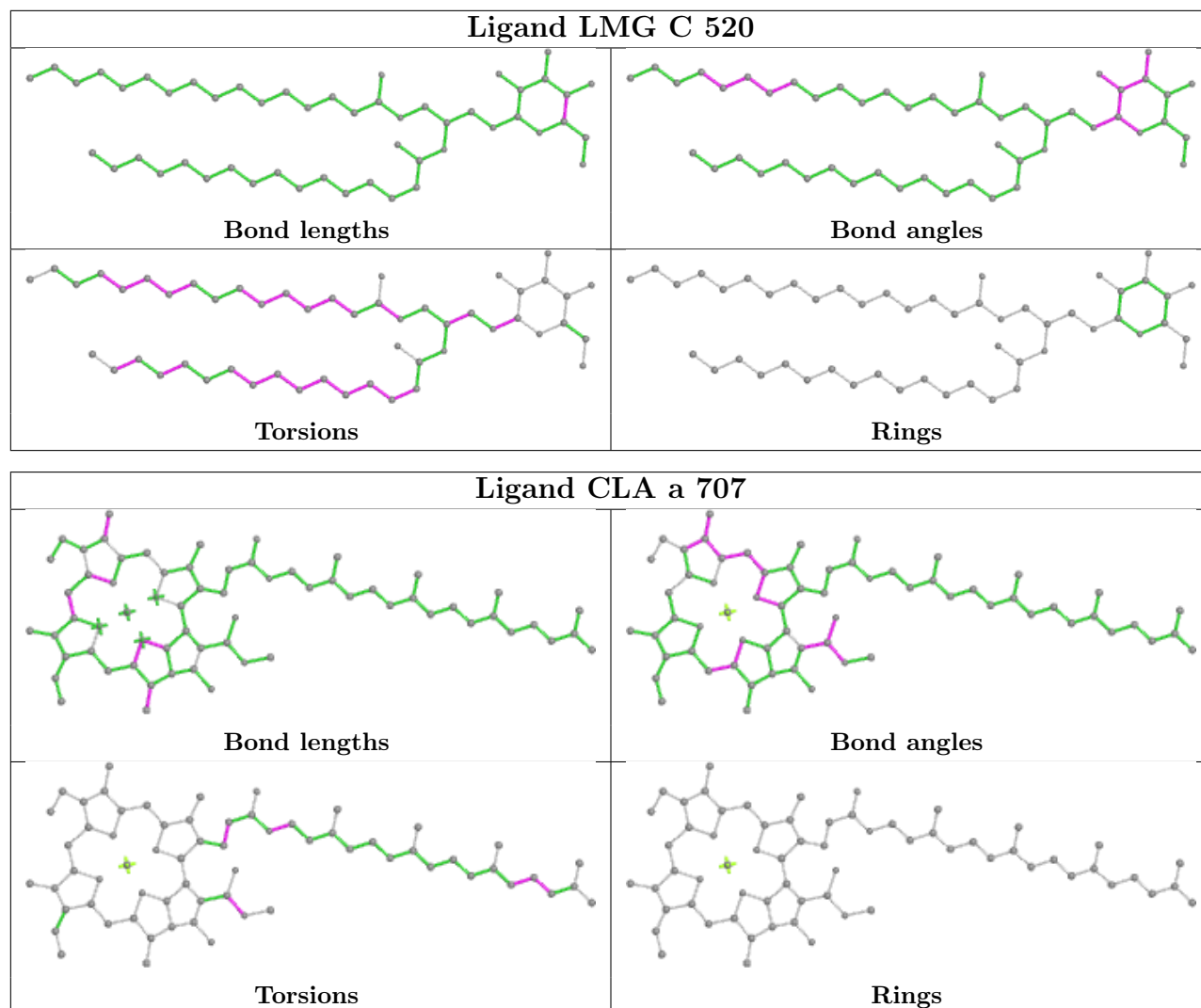


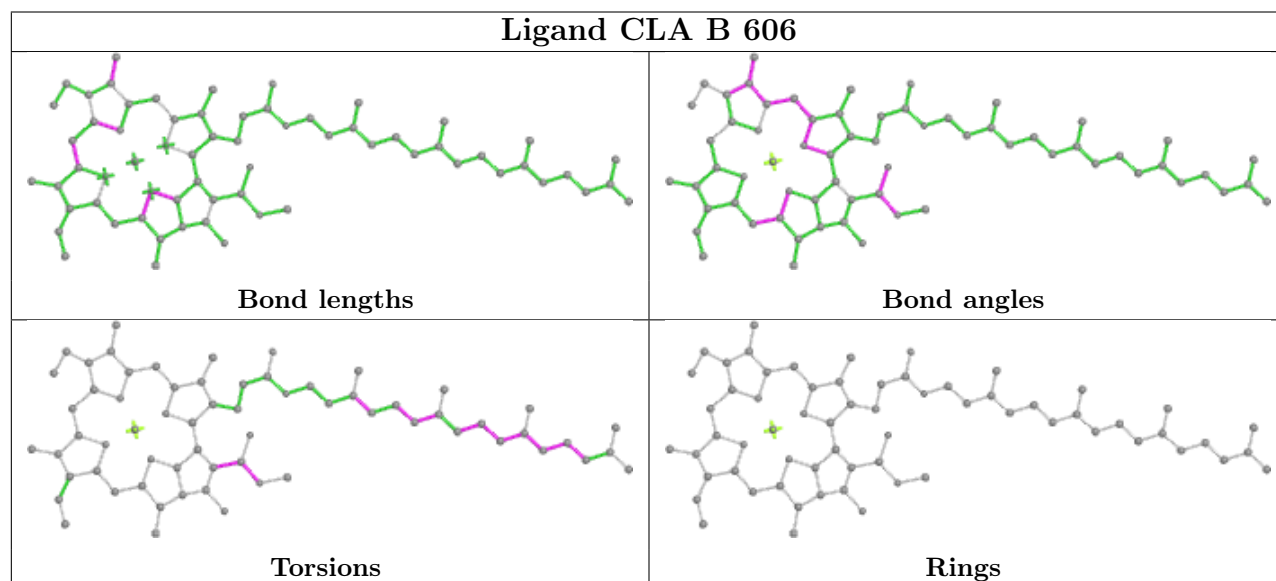
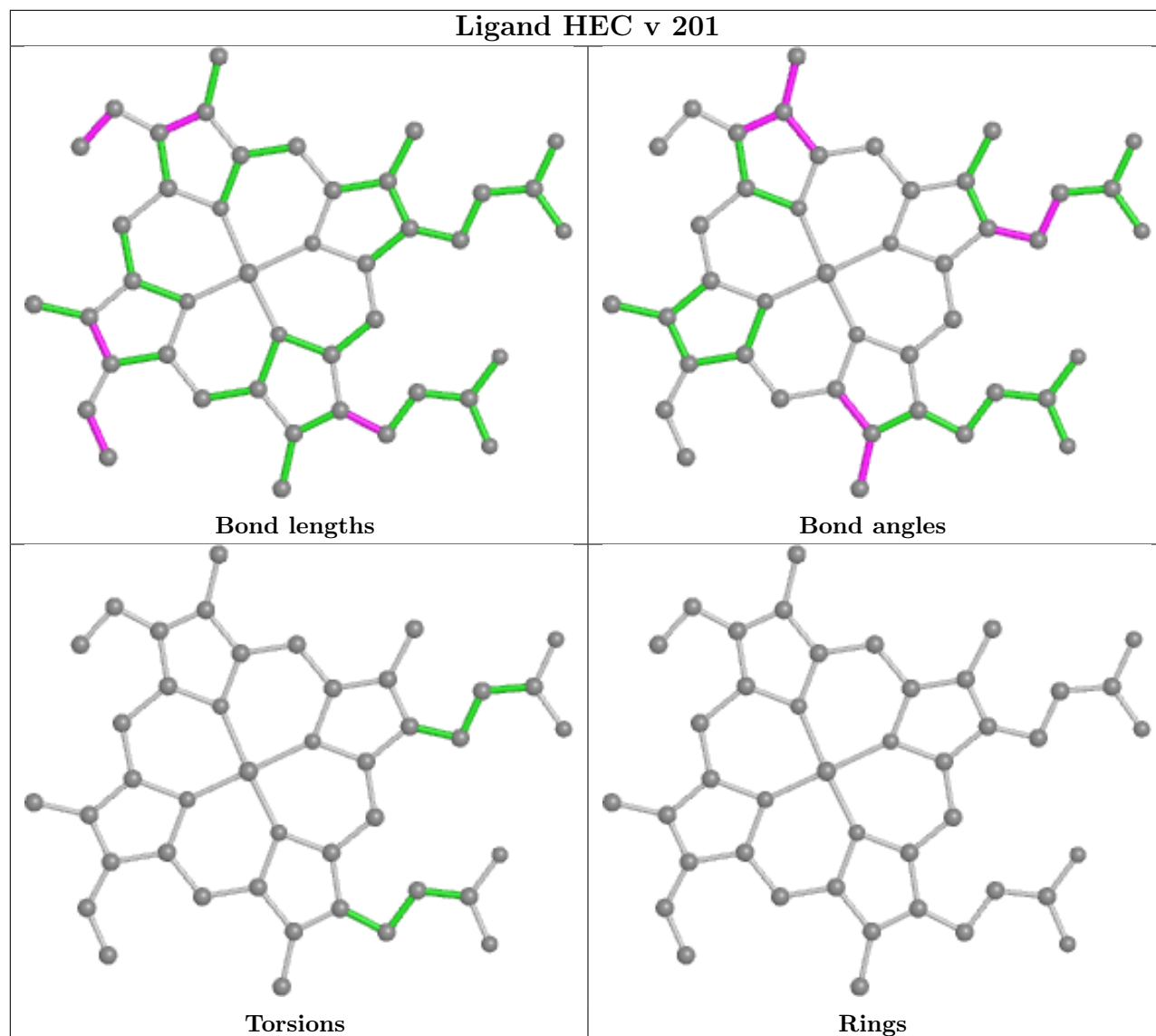


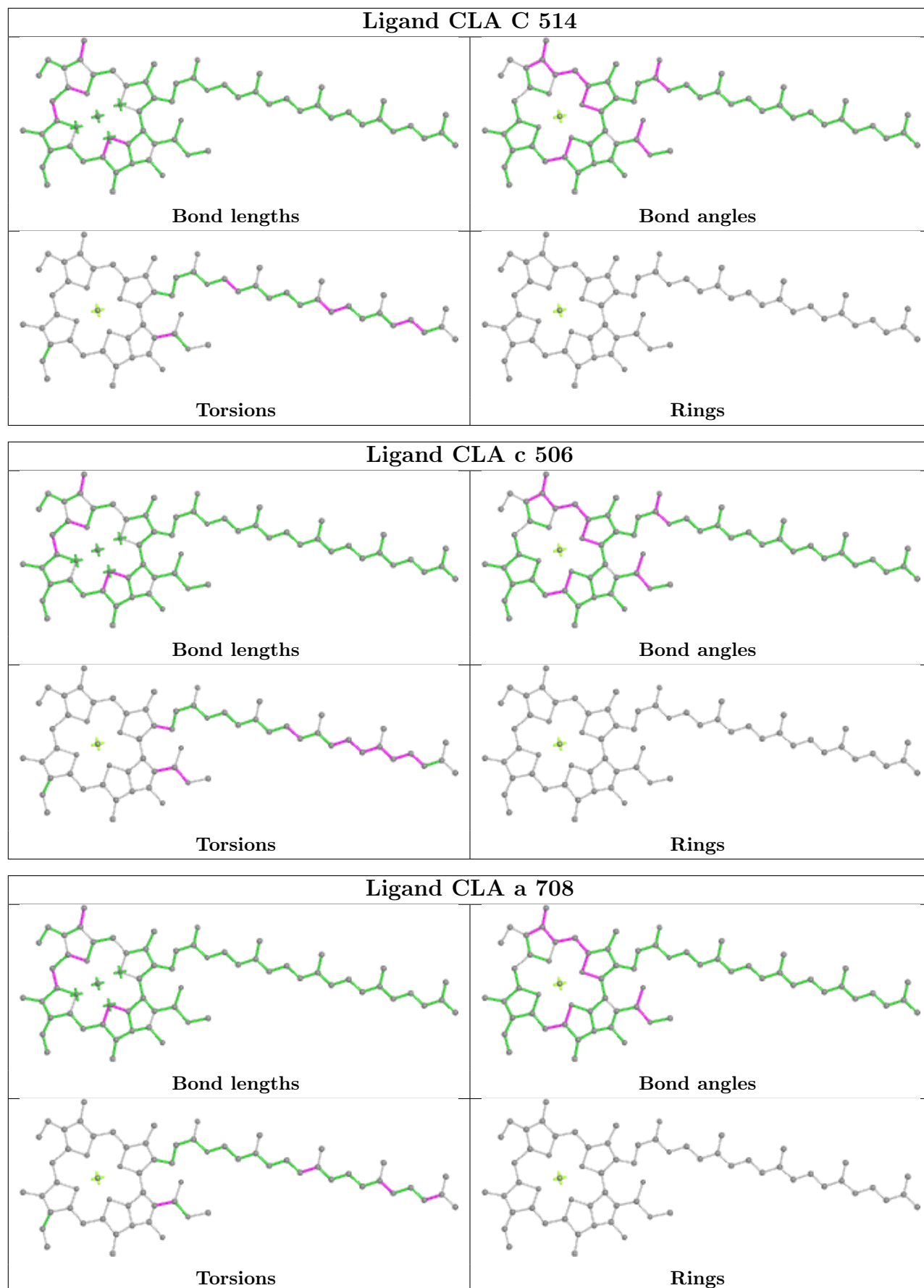


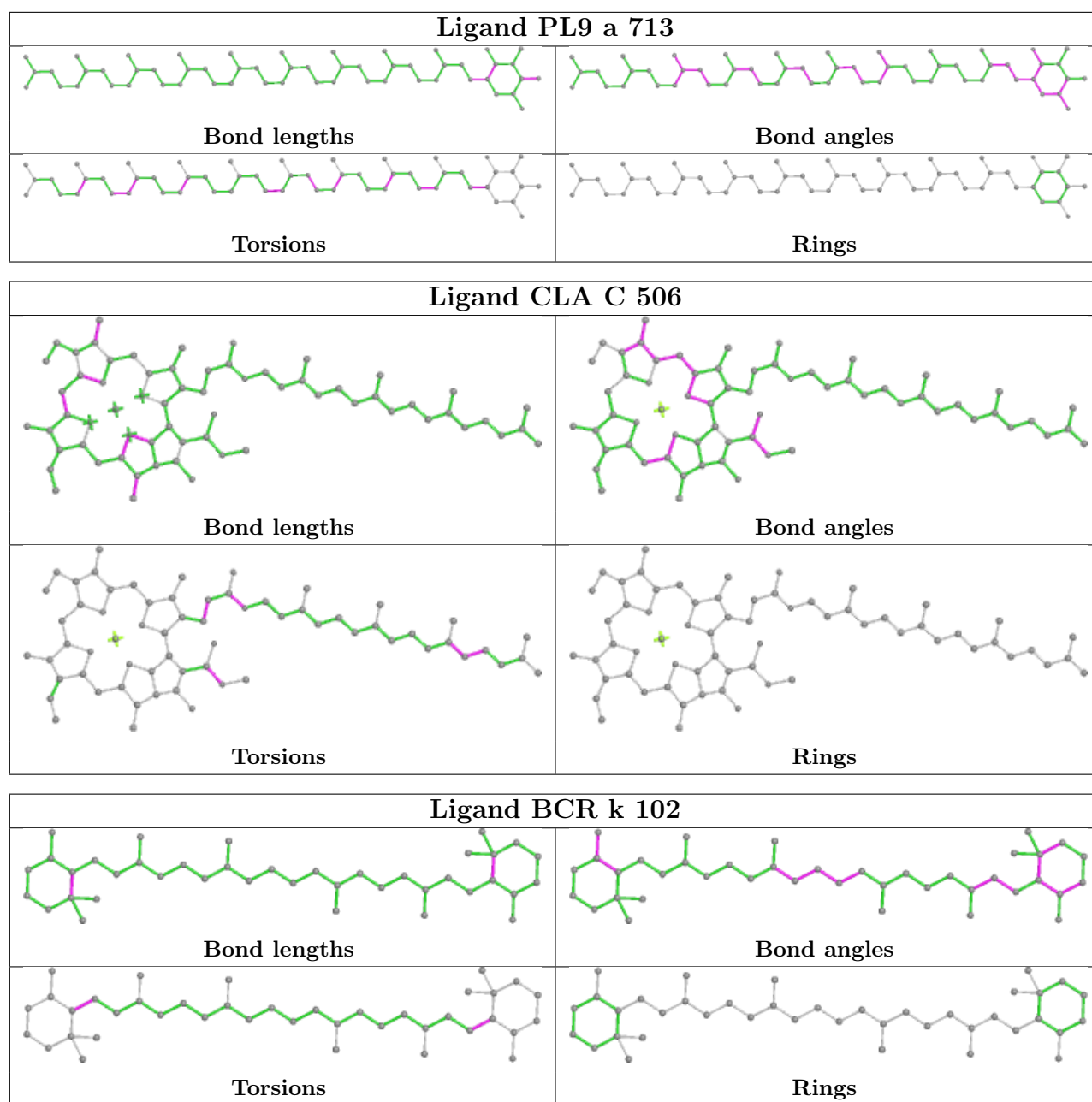


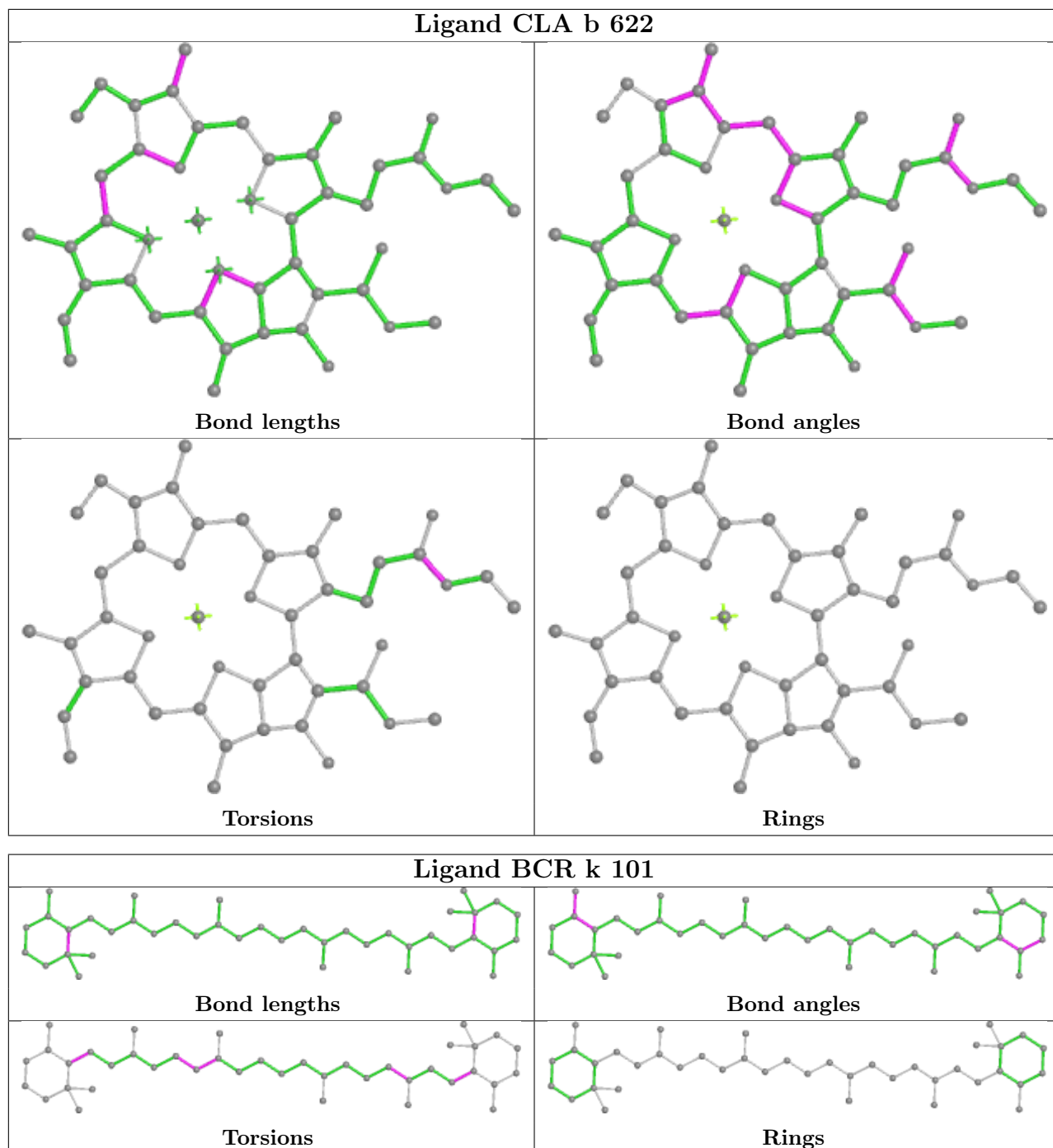


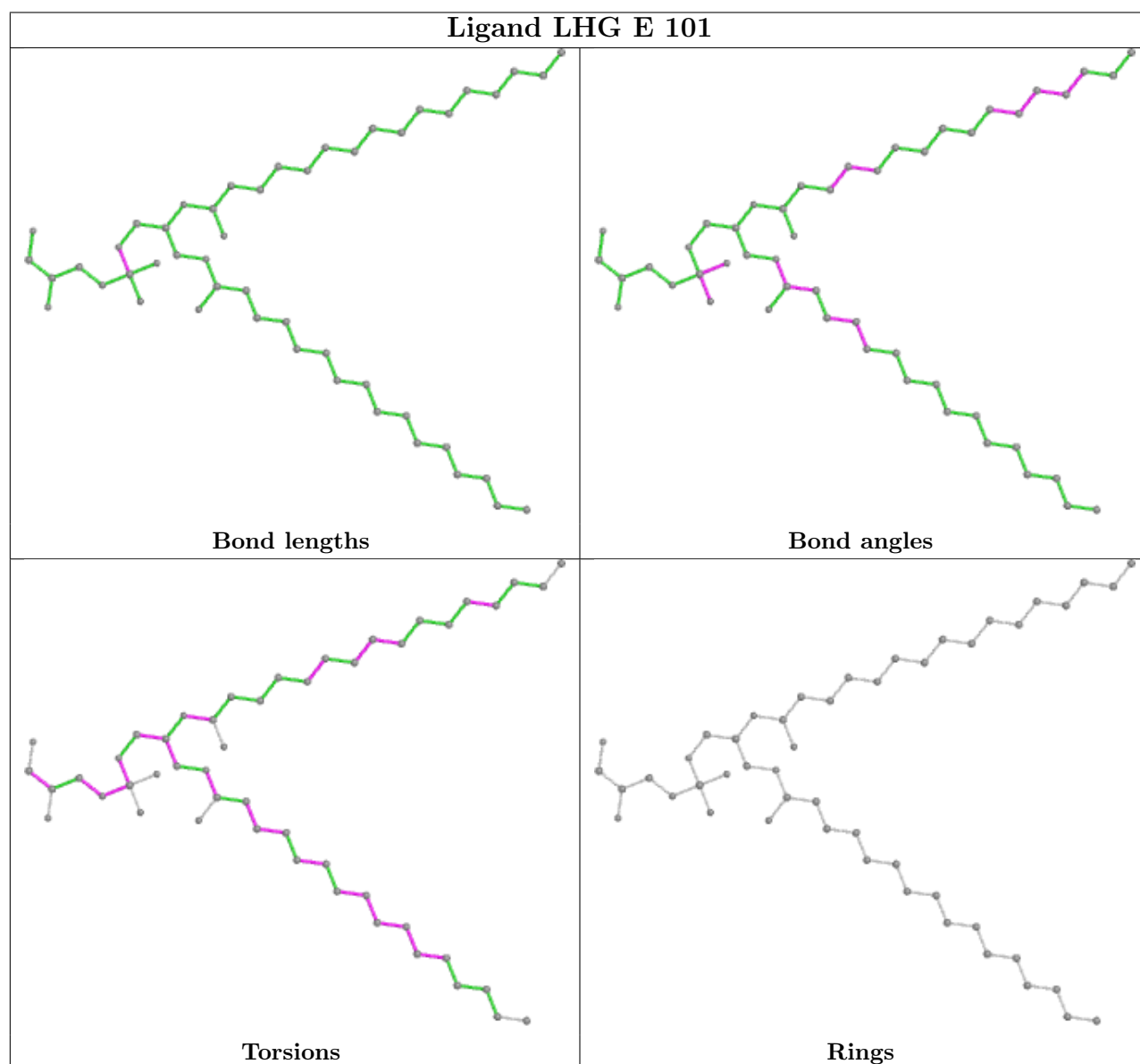
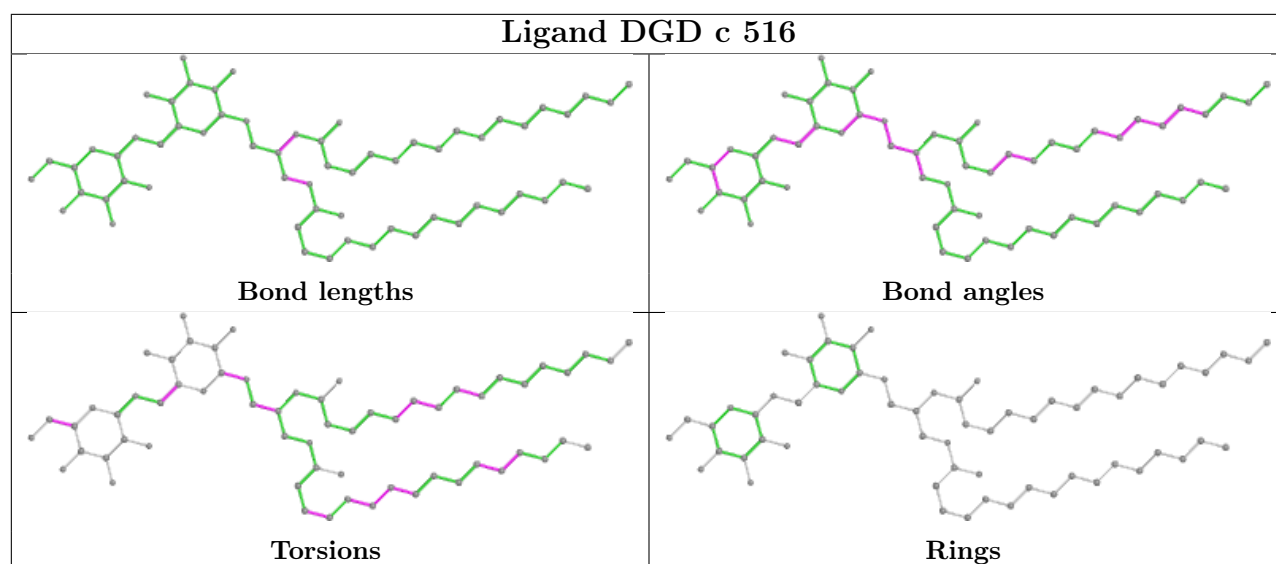


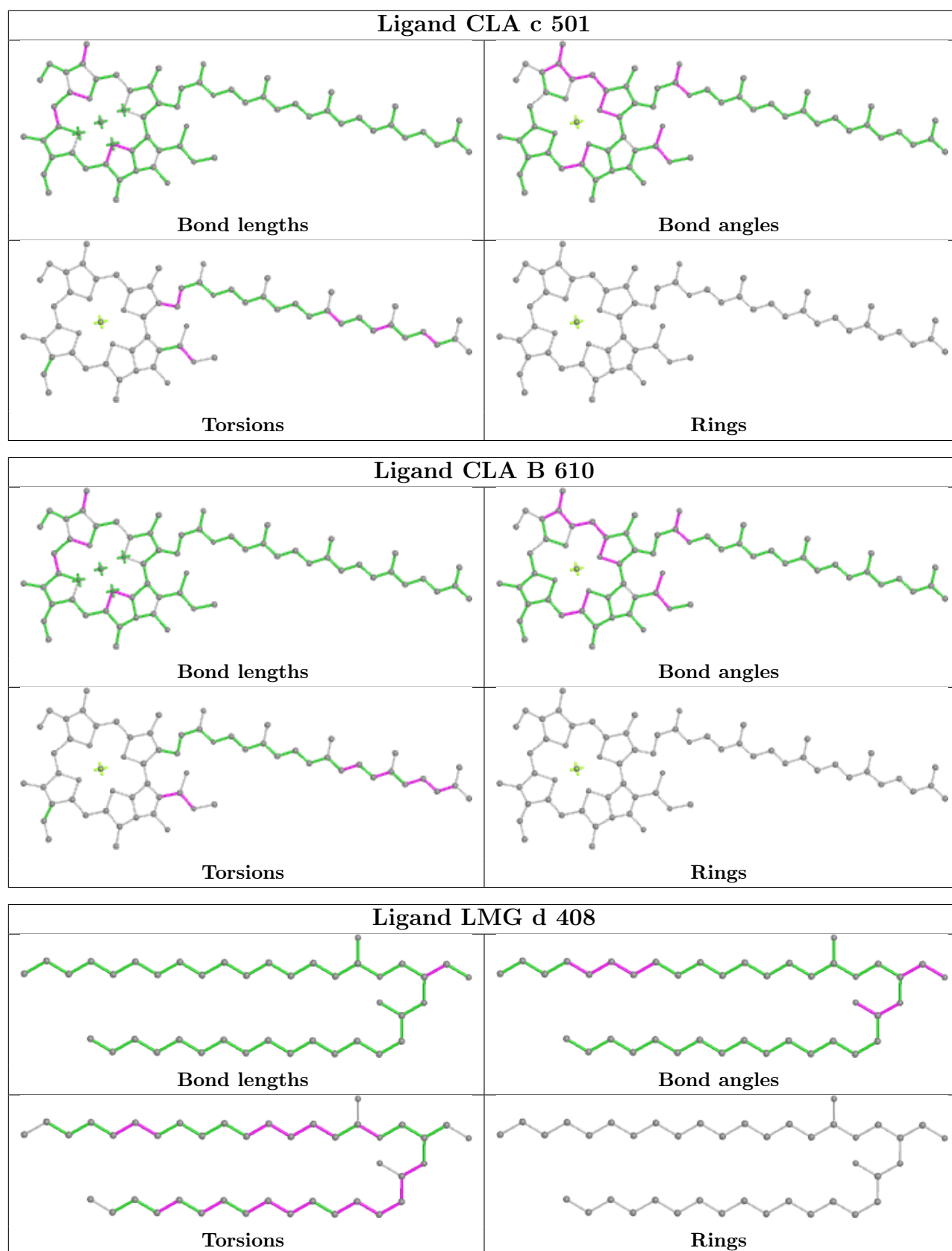


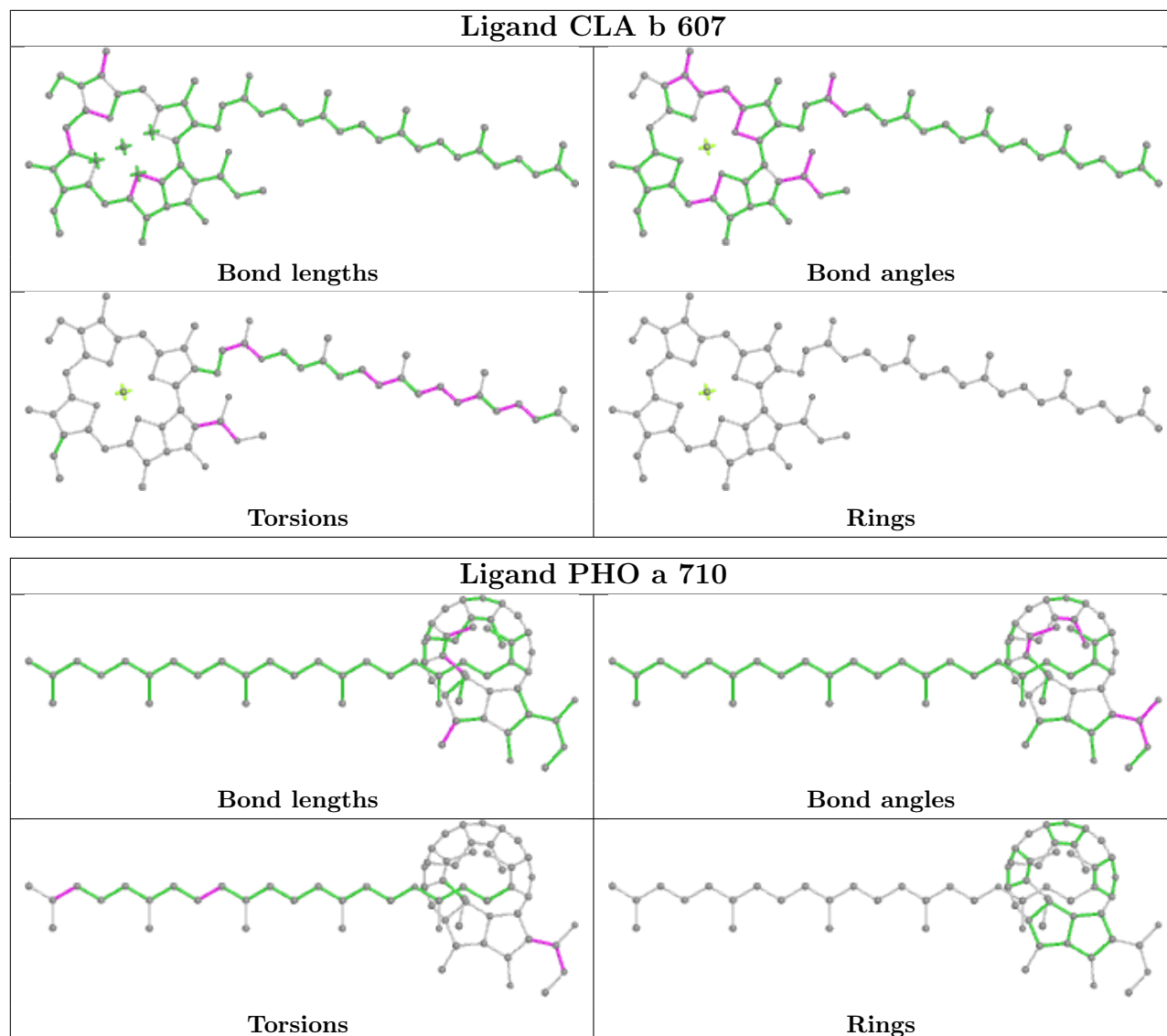


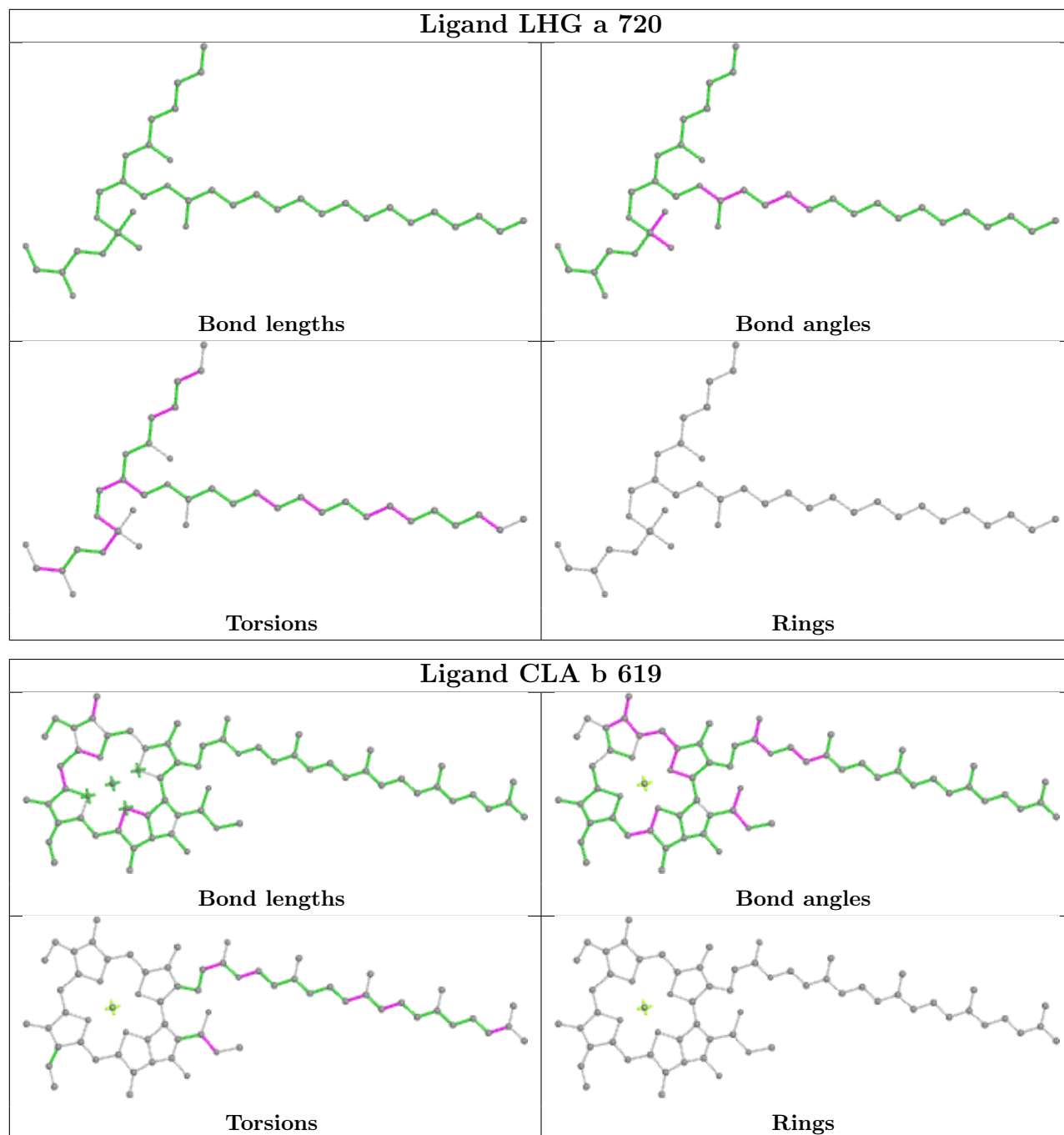


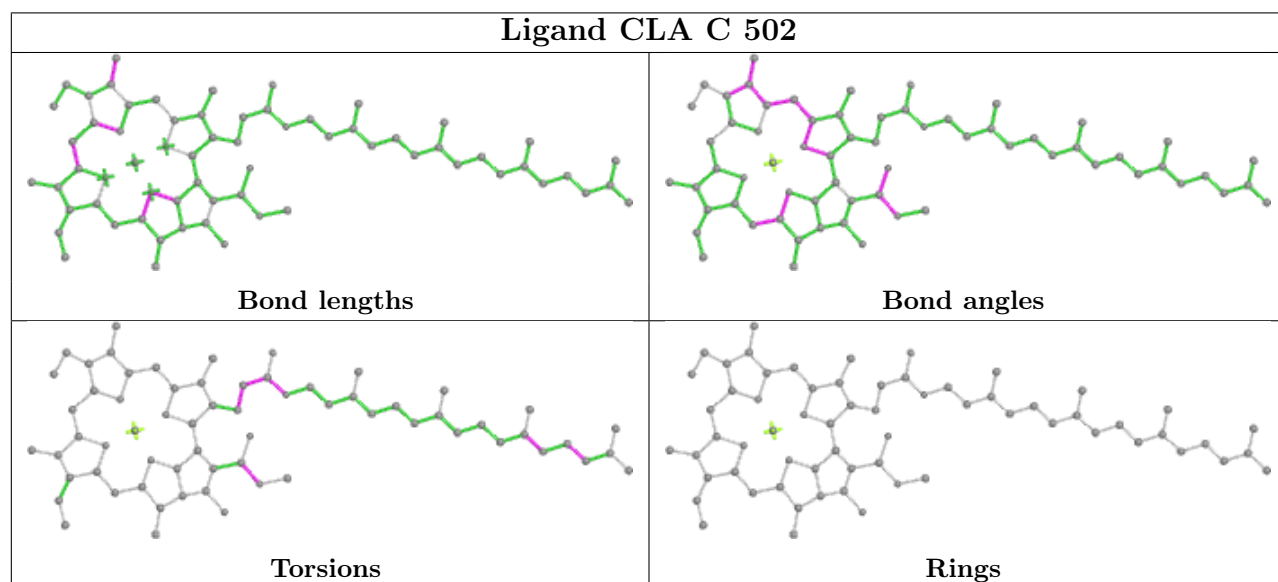
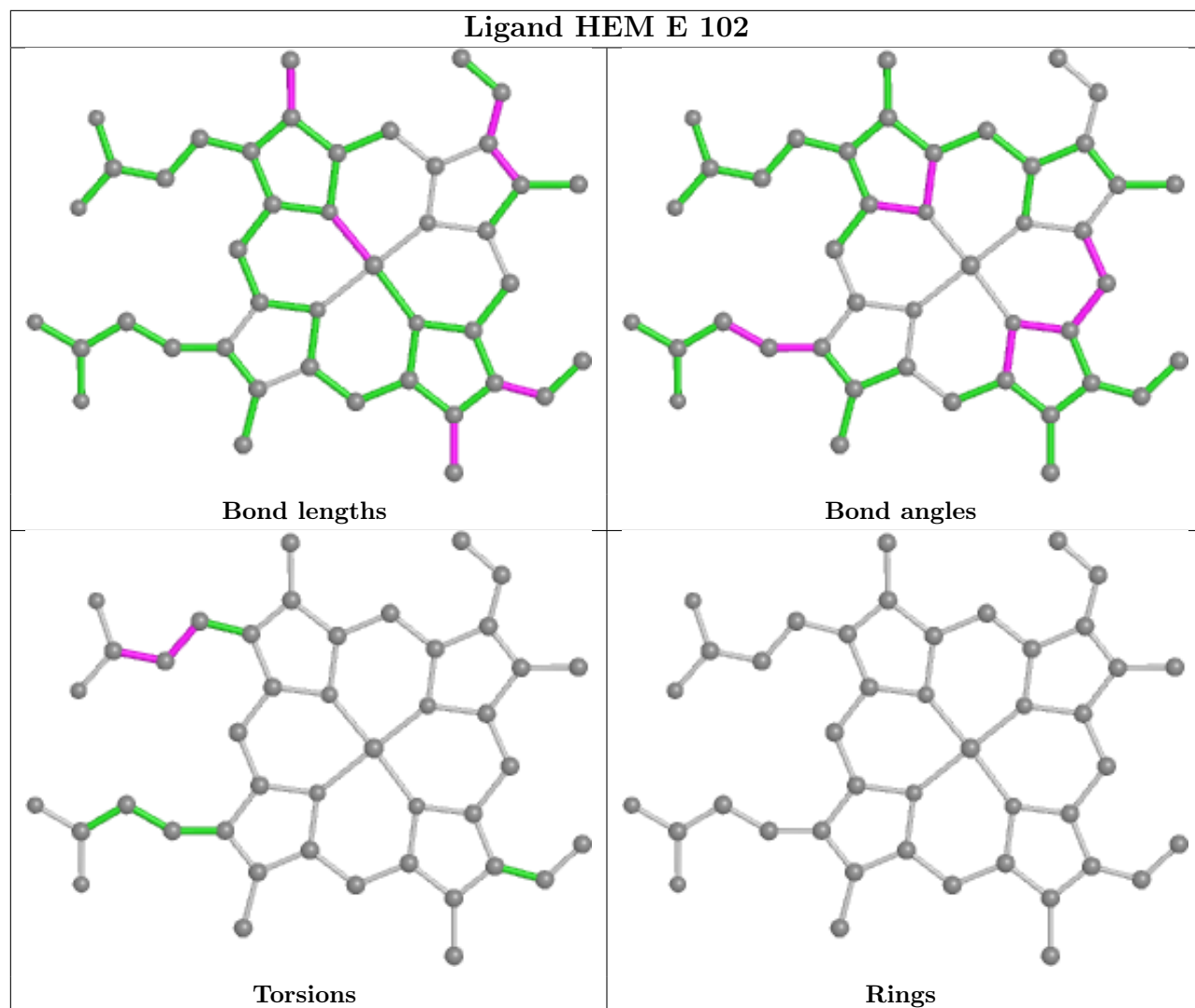


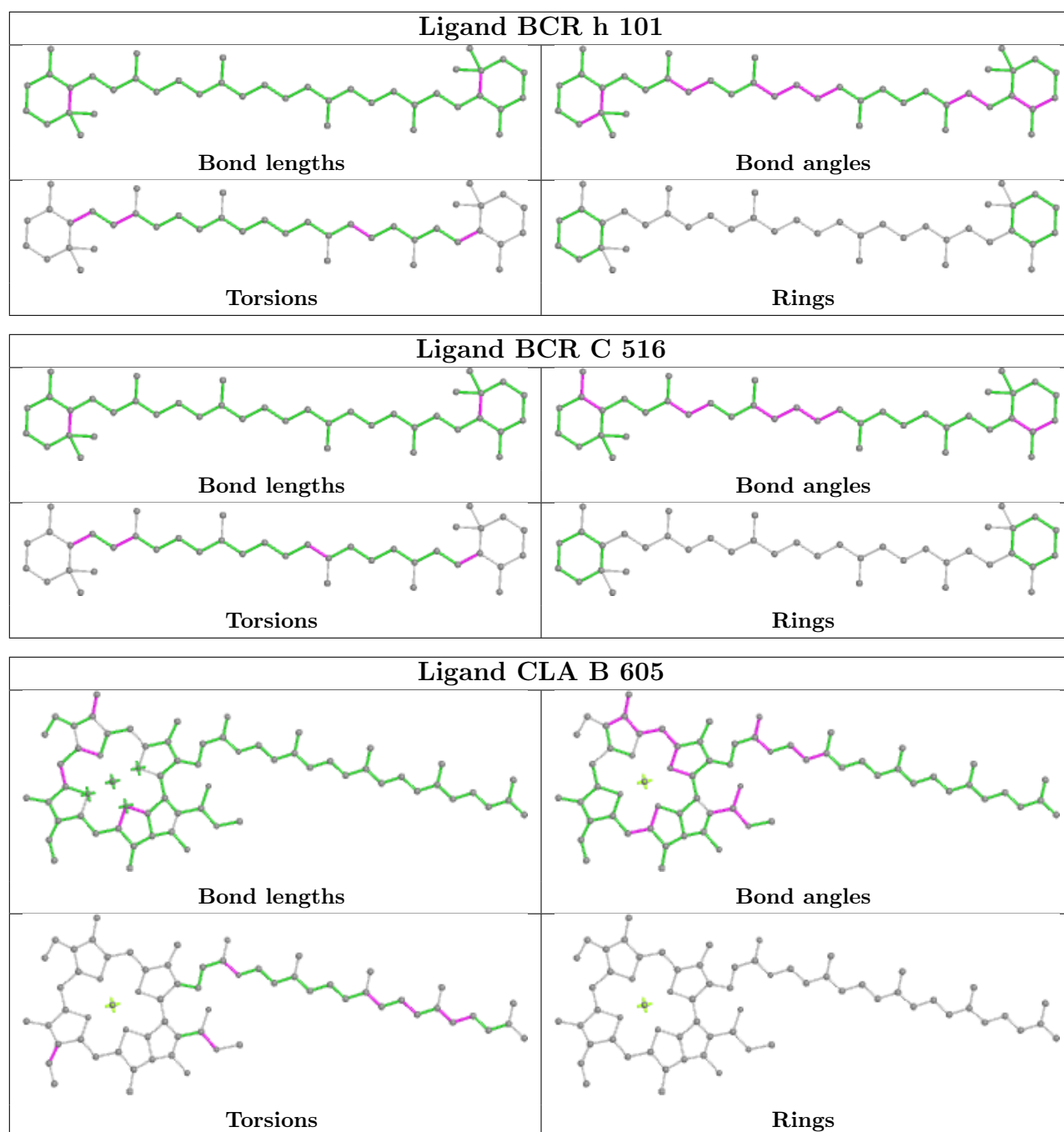


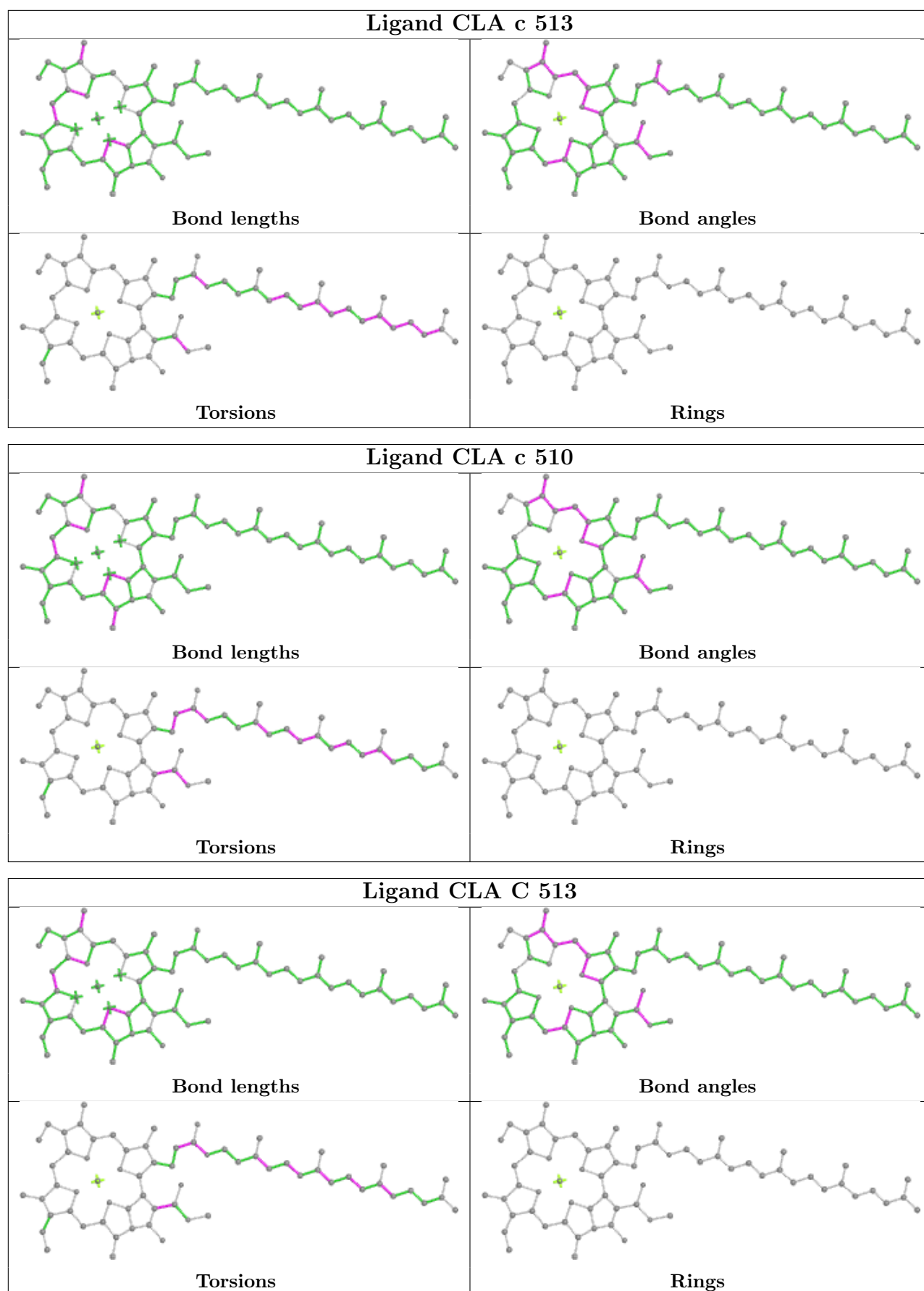


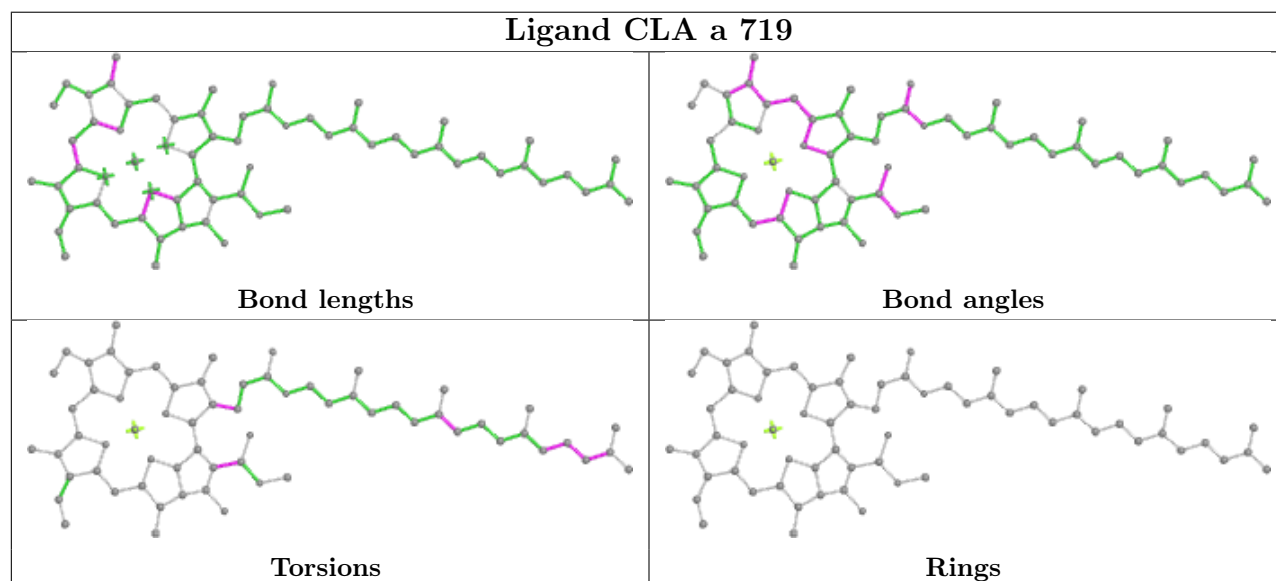
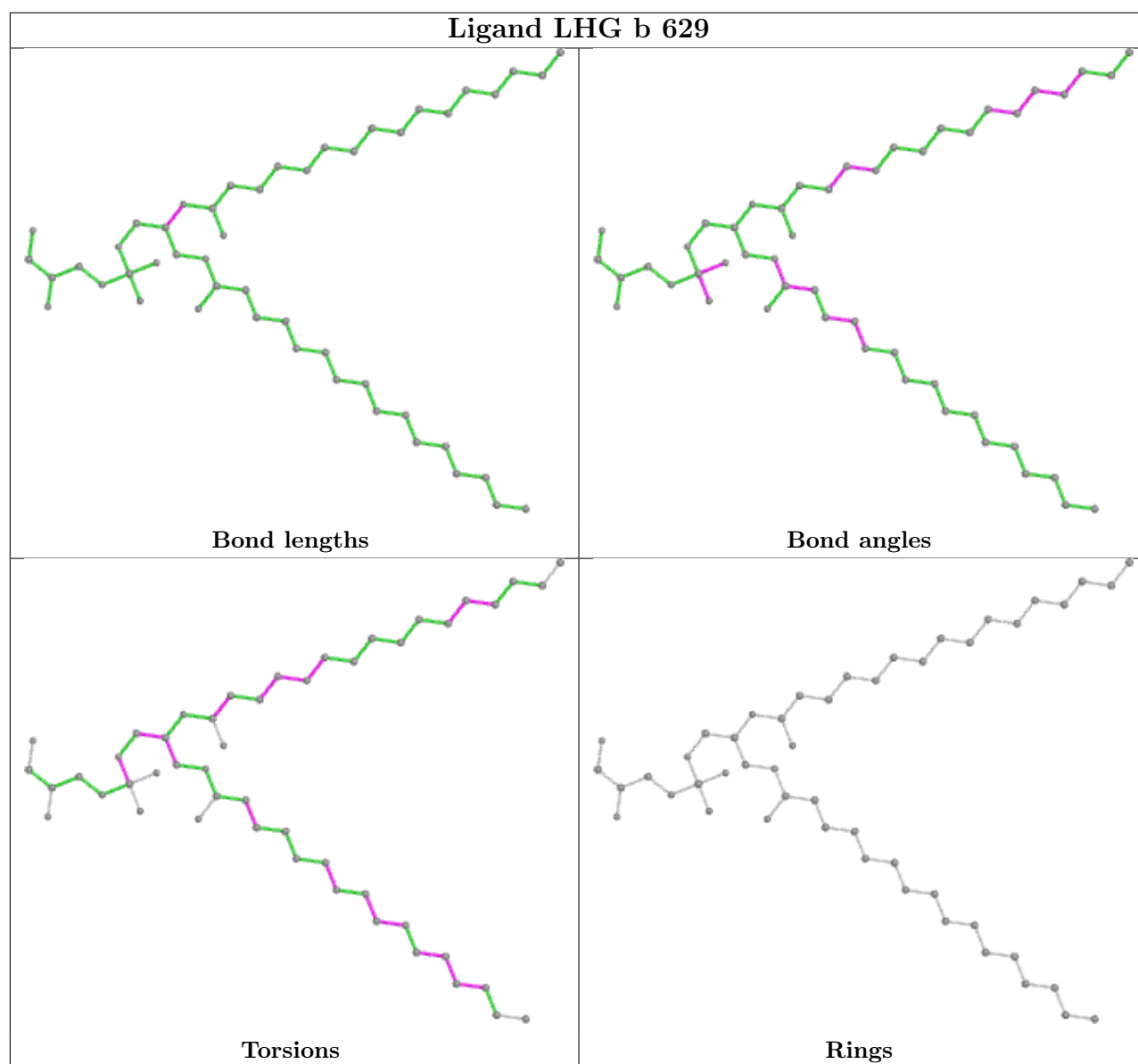


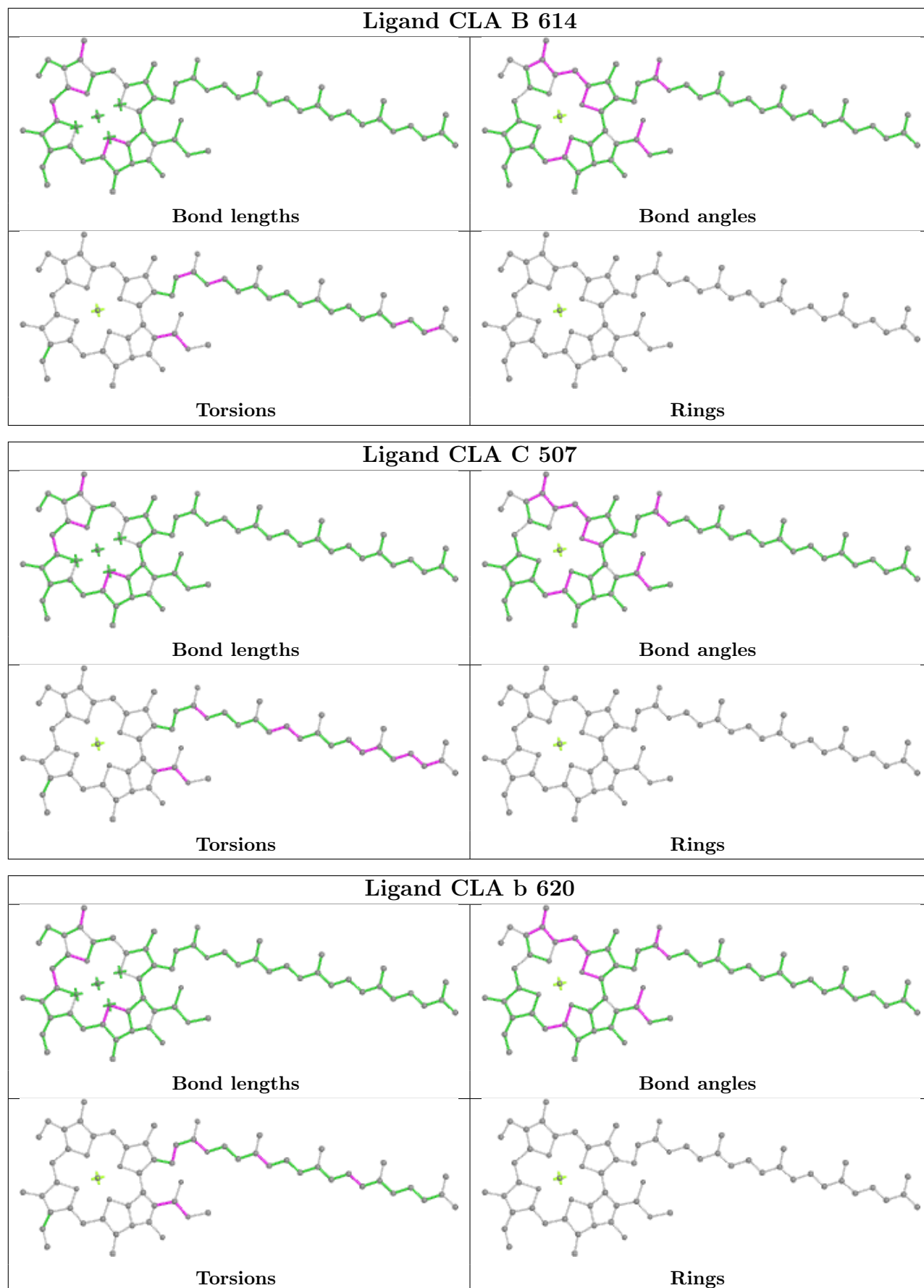


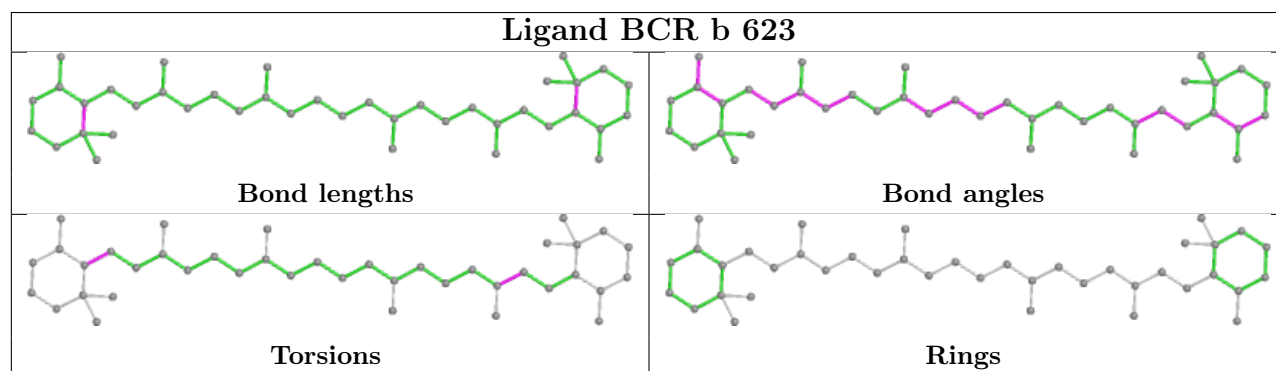
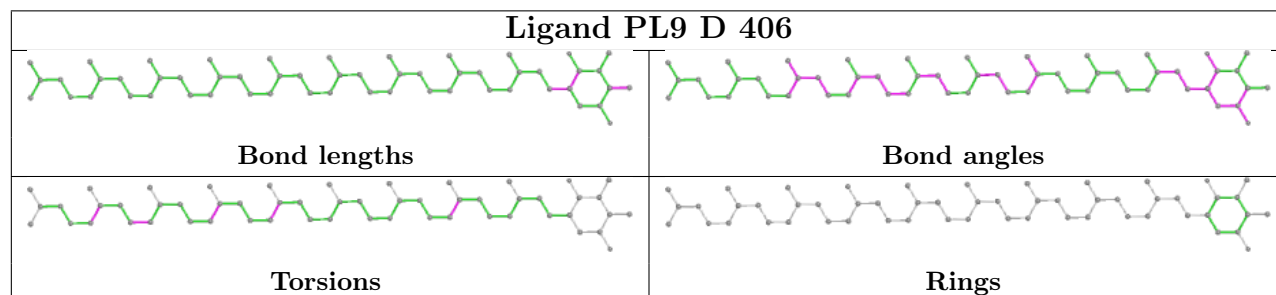
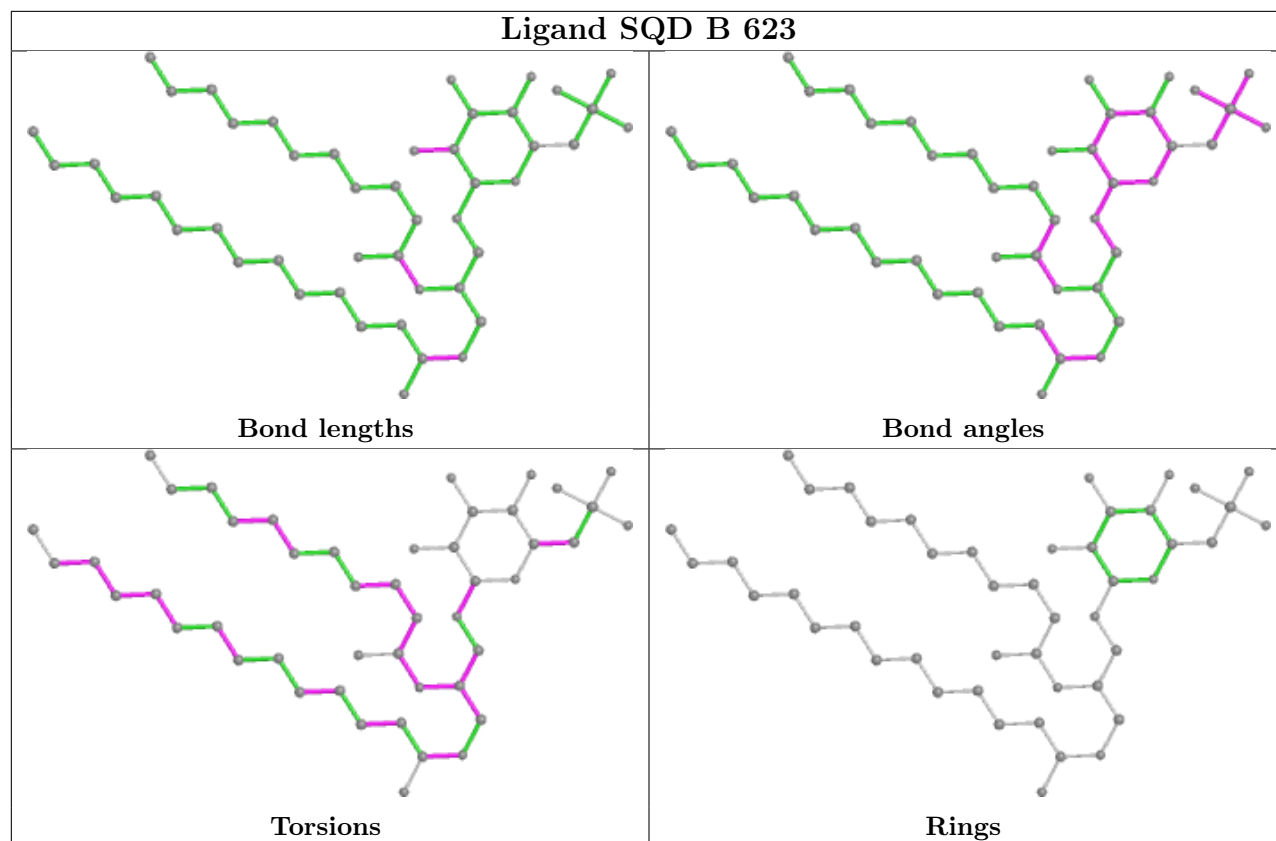


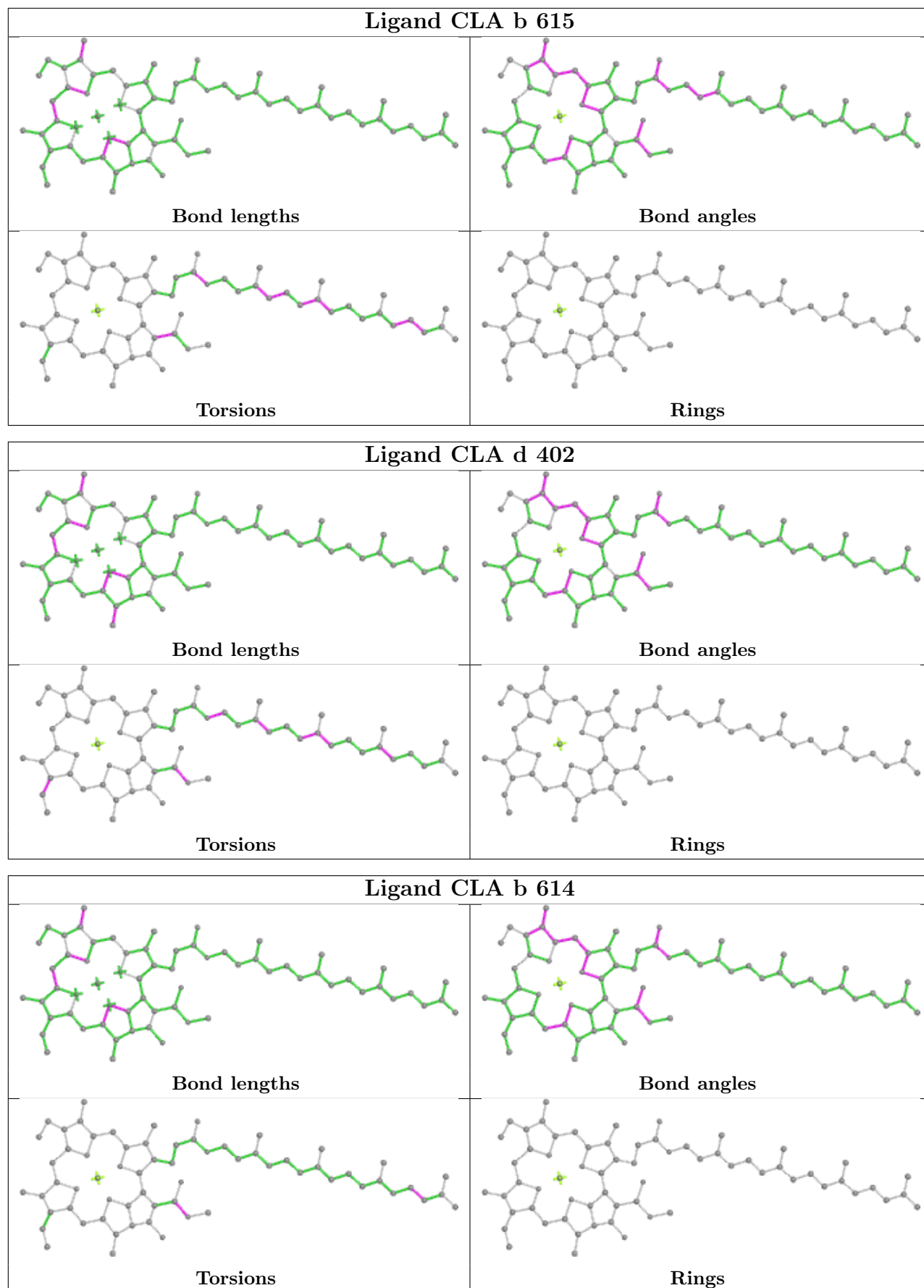


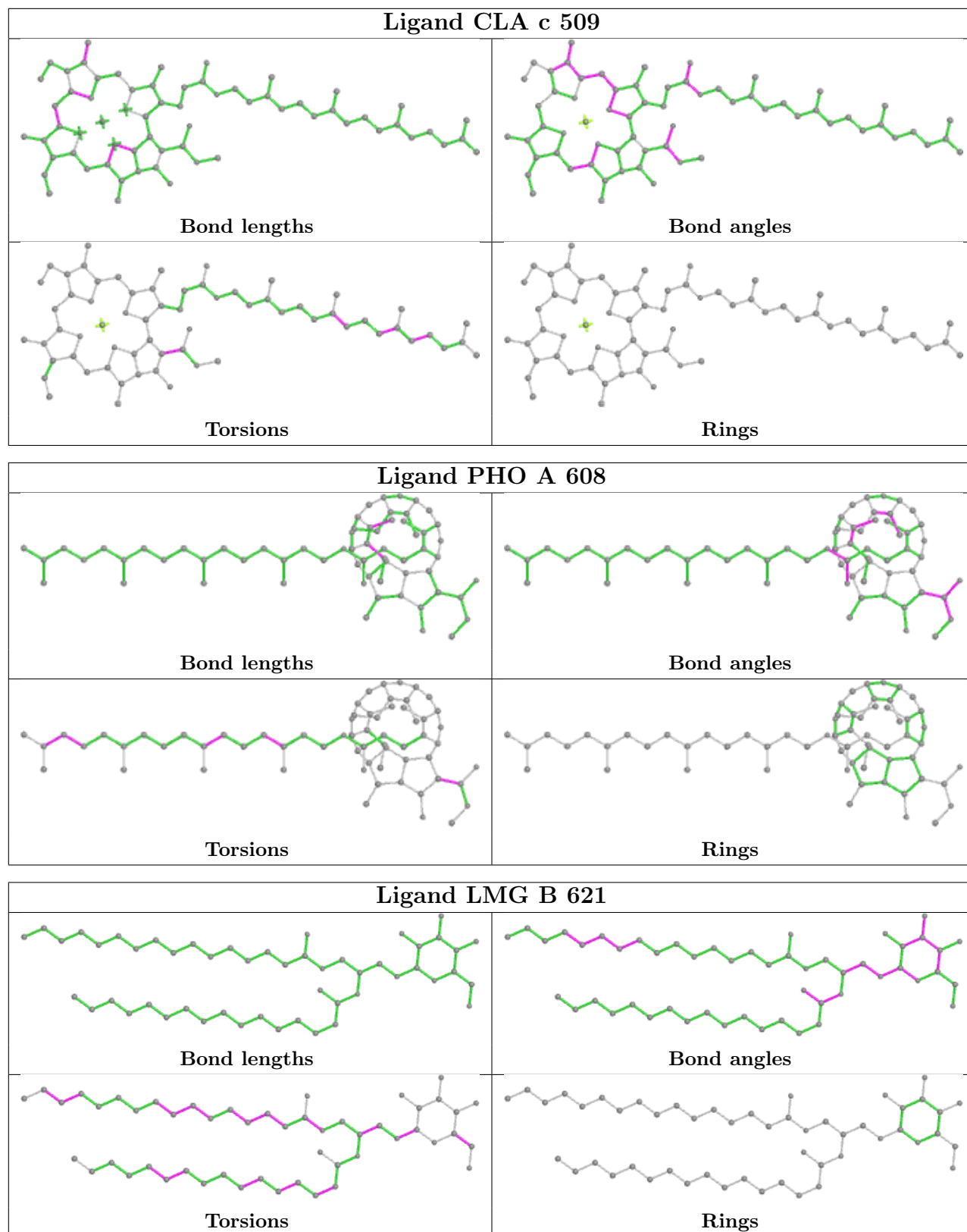


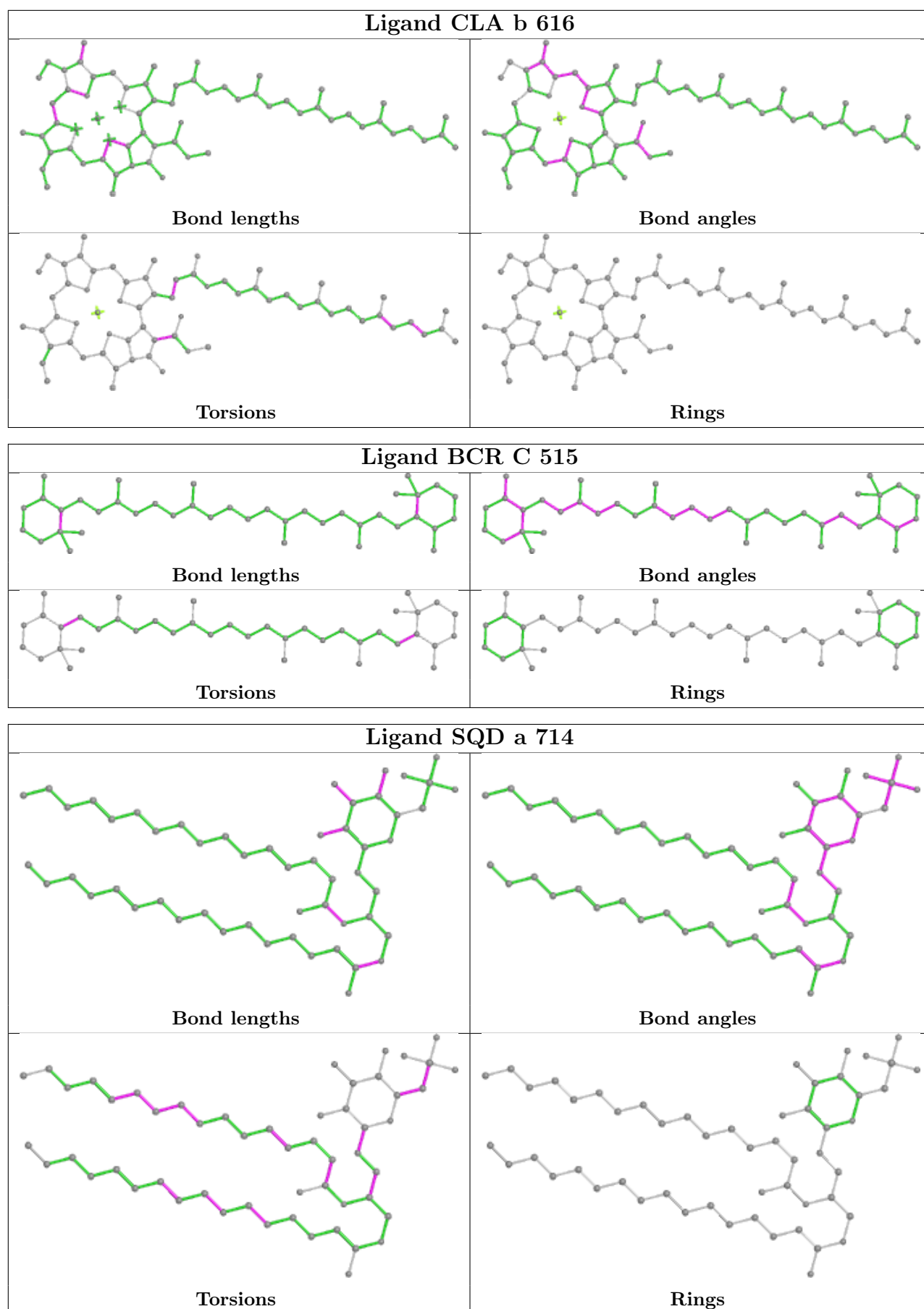


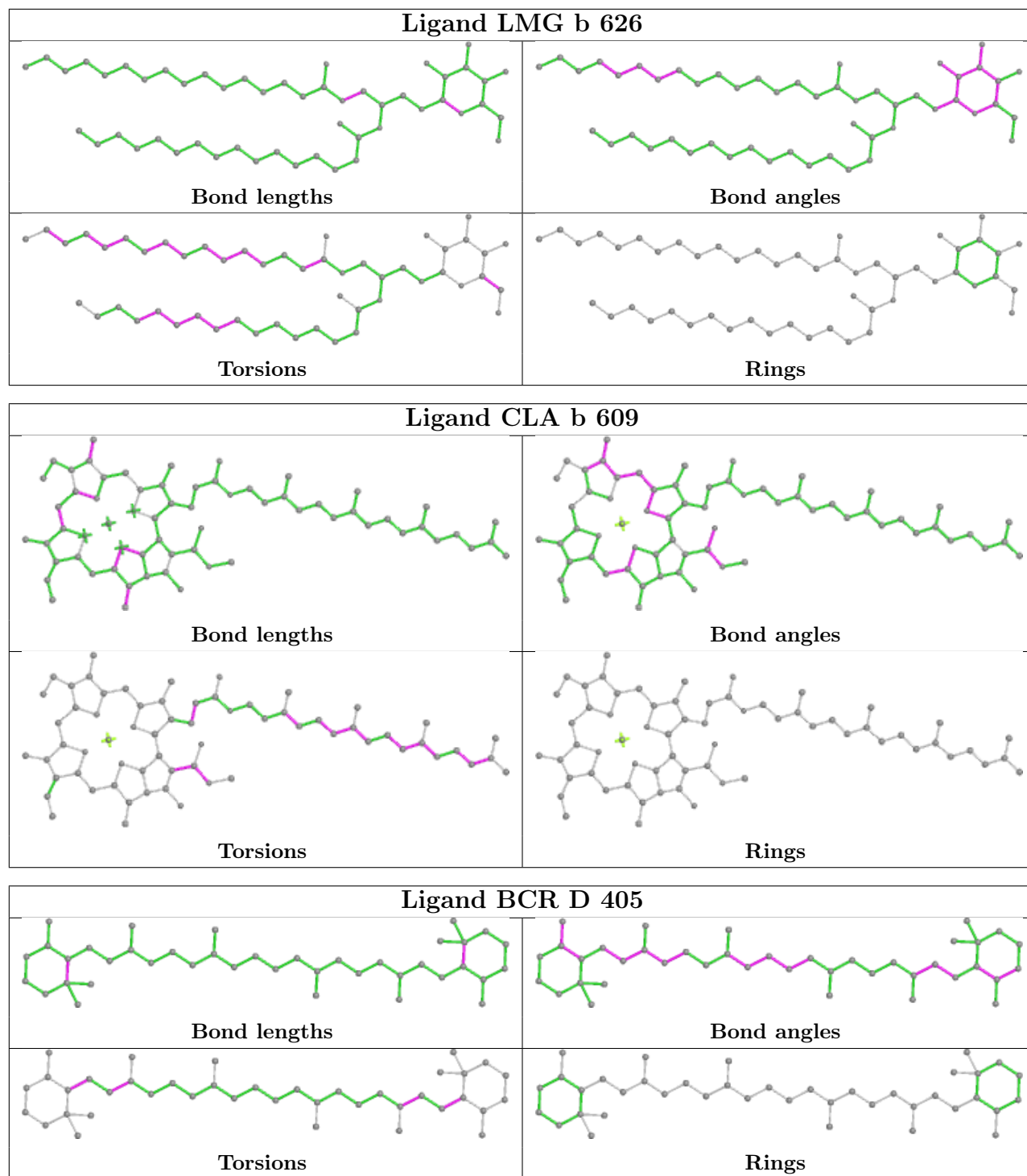


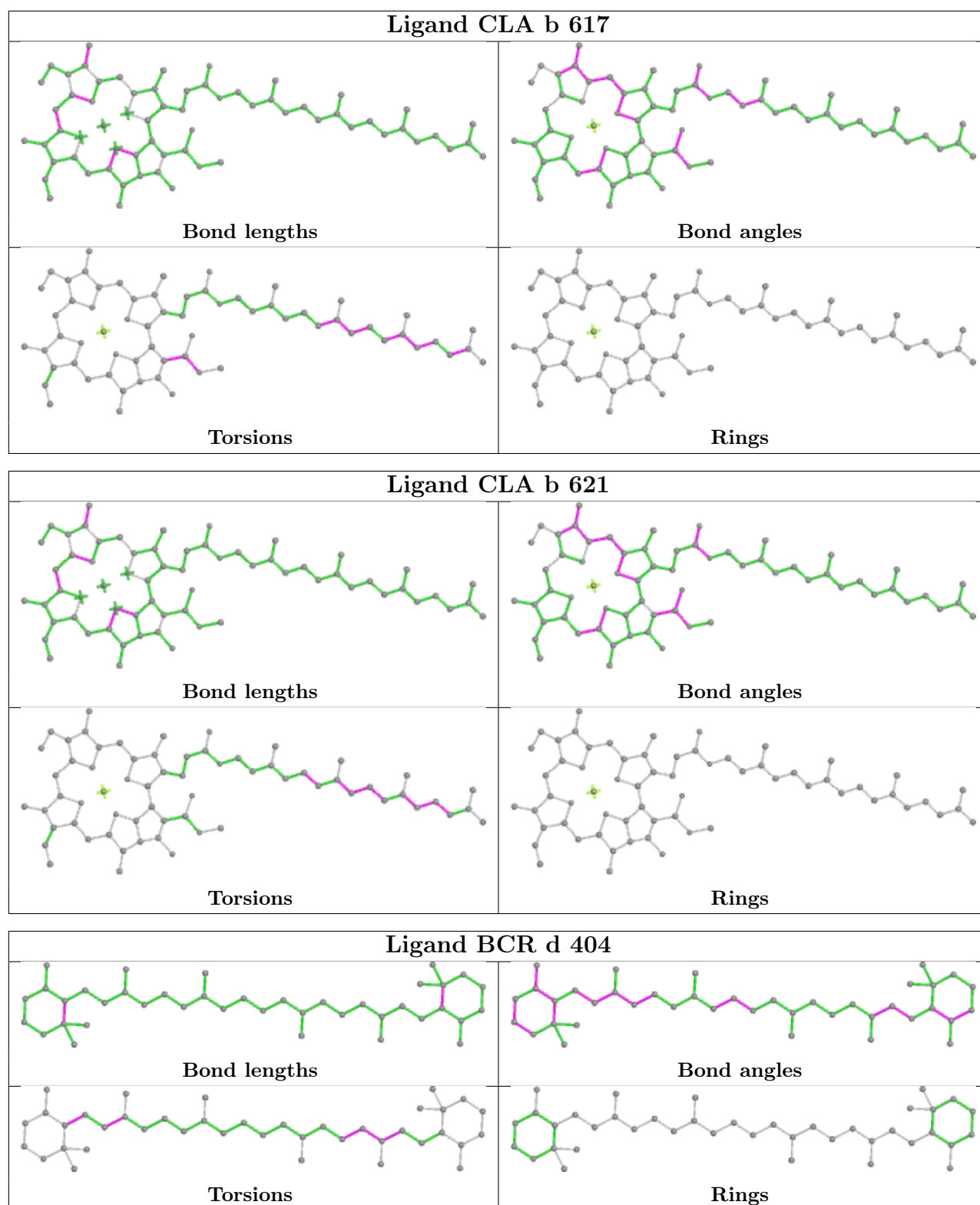


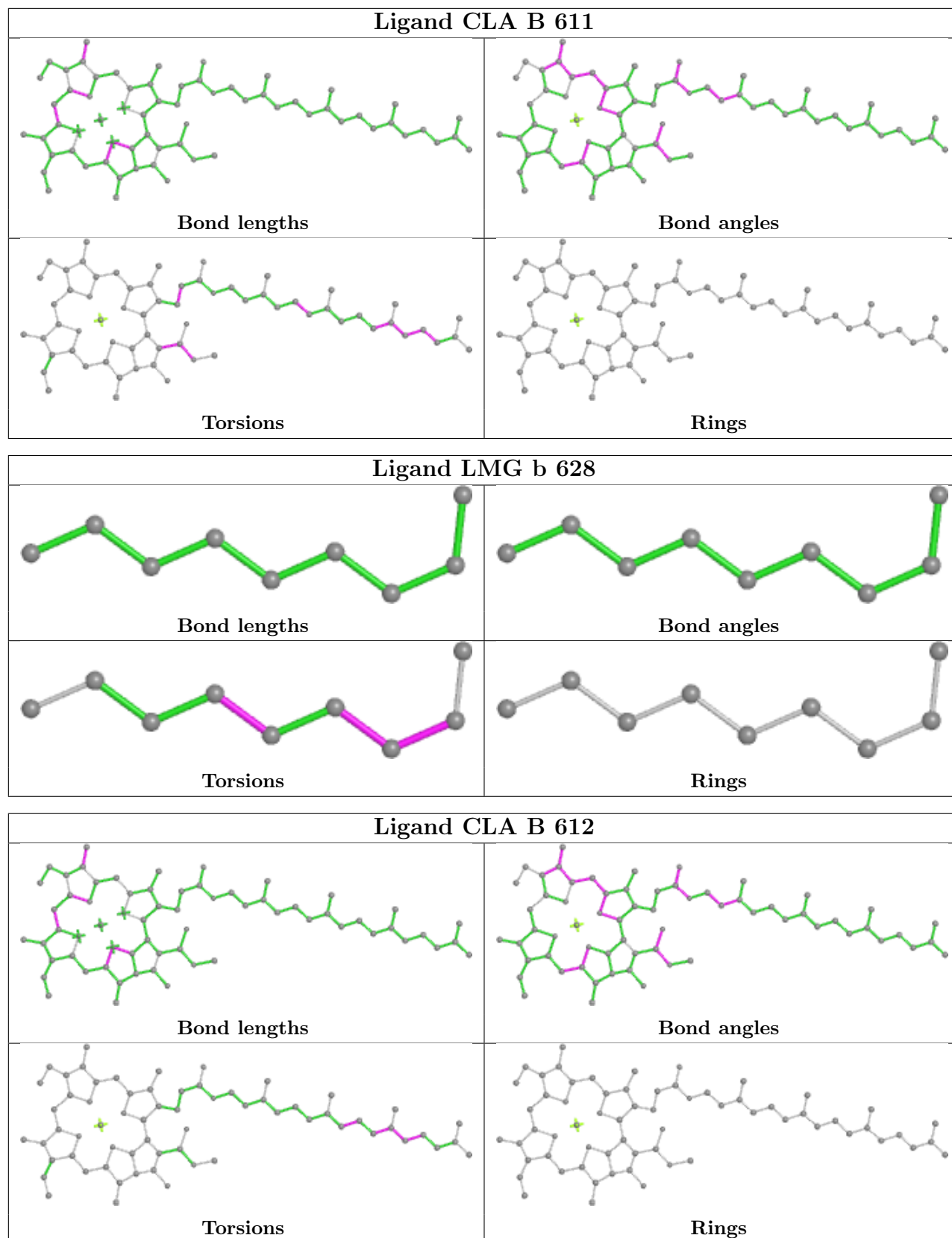


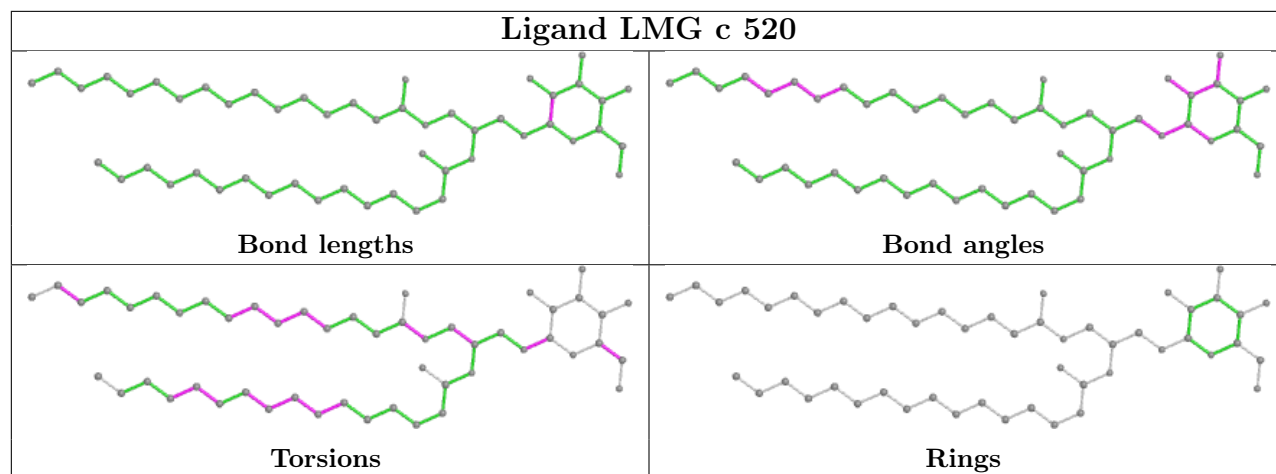












5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.32	2 (0%) 89 86	38, 46, 69, 82	0
1	a	334/344 (97%)	-0.21	4 (1%) 79 73	35, 48, 71, 82	0
2	B	504/510 (98%)	-0.11	9 (1%) 68 61	38, 50, 74, 98	0
2	b	504/510 (98%)	-0.11	24 (4%) 30 21	38, 50, 76, 94	0
3	C	451/461 (97%)	-0.14	3 (0%) 87 84	41, 54, 71, 90	0
3	c	451/461 (97%)	-0.10	3 (0%) 87 84	39, 55, 74, 90	0
4	D	341/352 (96%)	-0.35	1 (0%) 94 93	37, 48, 63, 82	0
4	d	341/352 (96%)	-0.21	2 (0%) 89 86	40, 50, 67, 85	0
5	E	81/84 (96%)	0.29	8 (9%) 7 4	47, 67, 79, 85	0
5	e	82/84 (97%)	0.71	12 (14%) 2 1	52, 70, 85, 87	0
6	F	34/45 (75%)	-0.17	0 100 100	54, 64, 78, 84	0
6	f	34/45 (75%)	-0.35	0 100 100	56, 63, 77, 80	0
7	H	63/63 (100%)	0.13	2 (3%) 47 37	43, 55, 68, 73	0
7	h	63/63 (100%)	0.02	0 100 100	48, 56, 64, 68	0
8	I	35/38 (92%)	0.14	2 (5%) 23 15	43, 53, 83, 94	0
8	i	35/38 (92%)	0.13	3 (8%) 10 5	44, 51, 82, 89	0
9	J	36/40 (90%)	-0.01	2 (5%) 24 16	56, 64, 86, 99	0
9	j	36/40 (90%)	0.12	2 (5%) 24 16	55, 66, 85, 89	0
10	K	37/46 (80%)	0.34	4 (10%) 5 3	62, 68, 83, 89	0
10	k	37/46 (80%)	0.19	0 100 100	60, 70, 84, 89	0
11	L	37/37 (100%)	-0.32	0 100 100	34, 45, 82, 93	0
11	l	37/37 (100%)	-0.43	1 (2%) 54 44	36, 47, 81, 90	0
12	M	32/36 (88%)	-0.40	1 (3%) 49 39	38, 47, 71, 83	0
12	m	32/36 (88%)	-0.31	1 (3%) 49 39	36, 47, 71, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.03	10 (4%) 37 27	42, 57, 87, 106	0
13	o	244/272 (89%)	-0.06	9 (3%) 41 31	43, 56, 89, 116	0
14	T	29/32 (90%)	-0.08	1 (3%) 45 35	37, 46, 69, 87	0
14	t	29/32 (90%)	-0.52	0 100 100	38, 48, 70, 79	0
15	U	97/134 (72%)	0.04	3 (3%) 49 39	45, 58, 75, 86	0
15	u	97/134 (72%)	-0.20	0 100 100	47, 55, 69, 84	0
16	V	137/163 (84%)	-0.13	0 100 100	45, 55, 67, 85	0
16	v	137/163 (84%)	0.17	4 (2%) 51 41	49, 63, 79, 100	0
17	Y	27/46 (58%)	0.34	1 (3%) 41 31	68, 75, 87, 95	0
17	y	30/46 (65%)	0.39	1 (3%) 46 36	69, 79, 89, 90	0
18	X	38/41 (92%)	0.25	2 (5%) 26 17	52, 60, 82, 93	0
18	x	38/41 (92%)	0.25	4 (10%) 6 3	54, 63, 80, 92	0
19	Z	62/62 (100%)	0.87	18 (29%) 0 0	62, 76, 100, 113	0
19	z	62/62 (100%)	0.64	9 (14%) 2 1	67, 82, 101, 112	0
20	R	34/41 (82%)	1.69	14 (41%) 0 0	70, 82, 94, 95	0
20	r	34/41 (82%)	1.58	12 (35%) 0 0	70, 84, 94, 101	0
All	All	5310/5694 (93%)	-0.06	174 (3%) 46 36	34, 53, 81, 116	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	28	VAL	5.5
13	o	56	PRO	5.4
14	T	30	THR	5.3
16	v	18	THR	5.3
3	C	142	GLU	5.1
19	Z	7	LEU	4.7
13	O	35	SER	4.7
9	J	5	GLY	4.6
2	b	487	SER	4.5
19	Z	2	THR	4.5
13	o	58	ASN	4.4
2	B	488	PRO	4.3
13	o	61	GLN	4.2
13	O	63	ALA	4.2
19	Z	8	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	4.1
19	Z	62	VAL	4.1
20	R	23	ILE	4.0
19	z	34	ASP	3.9
2	b	496	TYR	3.9
20	R	25	PRO	3.8
20	r	25	PRO	3.8
12	M	33	GLN	3.7
19	z	32	ASP	3.7
15	U	8	GLU	3.7
20	r	3	TRP	3.7
9	j	6	GLY	3.6
2	b	504	THR	3.6
8	i	36	ASP	3.6
8	I	34	ARG	3.6
8	I	36	ASP	3.6
13	o	4	THR	3.5
2	b	293	ALA	3.5
3	c	454	GLY	3.4
1	a	13	LEU	3.4
2	b	294	SER	3.4
20	R	18	TRP	3.4
13	O	61	GLN	3.4
20	r	32	GLN	3.3
2	B	128	THR	3.3
10	K	14	ALA	3.3
7	H	2	ALA	3.3
13	o	3	GLN	3.3
19	z	1	MET	3.2
19	z	31	GLN	3.2
2	b	482	ILE	3.2
2	b	503	THR	3.2
18	X	2	THR	3.2
2	b	485	GLU	3.2
13	O	4	THR	3.2
2	b	500	GLY	3.2
19	Z	9	LEU	3.1
16	v	19	ILE	3.1
15	U	73	GLN	3.1
1	a	12	ASN	3.1
19	Z	1	MET	3.1
13	o	5	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
20	r	26	TYR	3.1
16	v	16	GLY	3.1
20	R	24	LEU	3.0
20	R	26	TYR	3.0
5	E	15	THR	3.0
18	x	2	THR	3.0
19	z	62	VAL	3.0
13	O	245	PRO	3.0
20	r	18	TRP	3.0
20	r	2	ASP	3.0
2	b	497	GLN	3.0
19	z	29	SER	2.9
19	z	56	VAL	2.9
20	R	27	ALA	2.9
19	Z	3	ILE	2.9
19	Z	61	VAL	2.9
3	c	453	ALA	2.9
20	R	5	VAL	2.8
20	R	21	ARG	2.8
9	J	7	ARG	2.8
13	o	62	GLU	2.8
5	e	79	PHE	2.8
2	B	487	SER	2.8
19	Z	32	ASP	2.8
20	r	22	ASN	2.8
17	y	20	ALA	2.8
19	Z	6	GLN	2.8
20	R	29	LYS	2.8
2	b	486	LEU	2.8
2	b	502	VAL	2.8
5	E	60	GLN	2.8
5	e	16	SER	2.8
5	e	82	GLN	2.8
5	e	4	THR	2.7
2	B	126	PRO	2.7
1	a	243	GLU	2.7
13	o	60	ARG	2.7
2	B	292	LEU	2.6
12	m	33	GLN	2.6
9	j	5	GLY	2.6
13	O	62	GLU	2.6
19	Z	30	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
4	d	240	ALA	2.6
20	r	34	LEU	2.6
2	B	127	ARG	2.6
2	b	127	ARG	2.6
5	E	13	ILE	2.5
5	e	83	LEU	2.5
2	b	295	GLY	2.5
5	e	5	THR	2.5
20	r	20	VAL	2.5
20	R	31	VAL	2.5
20	R	3	TRP	2.5
1	a	225	ARG	2.5
19	Z	4	LEU	2.4
11	l	1	MET	2.4
2	b	85	GLY	2.4
5	e	60	GLN	2.4
19	z	35	ARG	2.4
2	b	489	GLU	2.4
2	B	484	PRO	2.4
10	K	17	ILE	2.4
19	Z	60	PHE	2.4
20	R	30	GLN	2.4
2	b	505	ARG	2.4
20	r	35	LEU	2.4
13	O	180	GLU	2.3
20	r	19	ALA	2.3
17	Y	43	ARG	2.3
5	E	20	TRP	2.3
20	r	14	LEU	2.3
4	D	238	THR	2.3
1	A	12	ASN	2.3
3	c	23	ALA	2.3
13	o	6	THR	2.2
19	z	2	THR	2.2
13	O	246	ALA	2.2
16	v	106	ASN	2.2
2	b	501	ASP	2.2
19	Z	59	PHE	2.2
5	E	17	VAL	2.2
18	x	37	VAL	2.2
2	B	489	GLU	2.2
5	E	16	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	84	THR	2.2
2	b	129	GLY	2.2
19	Z	33	TRP	2.2
19	Z	57	LEU	2.1
10	K	20	PRO	2.1
18	x	36	LYS	2.1
20	R	33	LYS	2.1
3	C	192	GLY	2.1
5	e	78	THR	2.1
10	K	13	GLU	2.1
8	i	31	ASN	2.1
5	e	77	GLU	2.1
15	U	53	ALA	2.1
2	b	478	VAL	2.1
2	b	239[A]	SER	2.1
18	x	38	GLN	2.1
5	e	81	GLU	2.1
2	b	477	ASP	2.1
4	d	17	ILE	2.1
5	E	61	ARG	2.1
19	Z	52	LEU	2.0
5	e	11	SER	2.0
18	X	34	ILE	2.0
2	B	485	GLU	2.0
7	H	23	PRO	2.0
1	A	228	THR	2.0
3	C	191	PRO	2.0
8	i	34	ARG	2.0
13	O	3	GLN	2.0
5	e	6	GLY	2.0
13	O	37	THR	2.0
5	E	14	ILE	2.0
19	Z	10	ALA	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(\AA^2)	Q<0.9
8	FME	I	1	10/11	0.90	0.28	50,60,70,76	0
8	FME	i	1	10/11	0.90	0.34	49,61,69,69	0
14	FME	T	1	10/11	0.92	0.15	51,58,70,77	0
12	FME	M	1	10/11	0.92	0.29	54,63,77,87	0
12	FME	m	1	10/11	0.94	0.12	52,59,74,79	0
14	FME	t	1	10/11	0.94	0.12	42,56,71,77	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
29	SQD	I	102	40/54	0.65	0.48	44,69,94,102	0
29	SQD	B	623	47/54	0.74	0.27	44,61,109,124	0
32	LHG	e	101	42/49	0.76	0.31	57,76,98,101	0
23	LMG	C	501	51/55	0.77	0.31	46,67,81,88	0
23	LMG	C	520	51/55	0.78	0.28	43,74,86,89	0
23	LMG	d	408	40/55	0.79	0.25	47,61,84,89	0
23	LMG	B	621	51/55	0.80	0.24	52,70,78,88	0
30	UNL	b	606	13/-	0.80	0.24	45,51,57,59	0
32	LHG	E	101	49/49	0.80	0.28	48,77,92,95	0
23	LMG	b	626	51/55	0.80	0.30	38,56,72,77	0
30	UNL	d	401	22/-	0.81	0.23	39,54,63,66	0
30	UNL	z	101	11/-	0.81	0.29	48,65,72,72	0
23	LMG	C	521	51/55	0.81	0.34	49,71,81,91	0
23	LMG	A	603	51/55	0.81	0.26	40,62,77,83	0
30	UNL	b	603	11/-	0.82	0.24	44,54,62,62	0
23	LMG	a	715	51/55	0.82	0.24	47,65,85,91	0
28	PL9	A	611	55/55	0.82	0.29	46,68,78,83	0
23	LMG	c	519	51/55	0.82	0.30	42,75,90,91	0
23	LMG	c	520	51/55	0.82	0.40	61,75,95,100	0
30	UNL	a	716	4/-	0.82	0.31	31,46,50,51	0
29	SQD	b	601	54/54	0.83	0.24	45,66,94,105	0
27	BCR	H	102	40/40	0.84	0.25	41,54,62,62	0
27	BCR	k	101	40/40	0.84	0.24	53,69,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	LMG	b	627	51/55	0.84	0.31	51,70,80,82	0
30	UNL	I	101	9/-	0.84	0.20	44,52,61,61	0
29	SQD	A	614	40/54	0.84	0.22	47,59,68,72	0
30	UNL	a	717	7/-	0.84	0.26	48,53,61,67	0
30	UNL	B	601	12/-	0.85	0.18	31,49,56,56	0
30	UNL	B	622	6/-	0.85	0.26	40,51,56,56	0
30	UNL	i	101	22/-	0.85	0.22	36,50,58,62	0
30	UNL	j	101	9/-	0.85	0.24	52,61,65,65	0
30	UNL	a	718	13/-	0.85	0.21	45,54,61,62	0
23	LMG	a	701	51/55	0.85	0.23	42,64,87,90	0
30	UNL	b	604	11/-	0.85	0.26	38,48,57,59	0
28	PL9	a	713	55/55	0.86	0.25	57,68,77,84	0
25	CLA	C	514	65/65	0.86	0.24	44,73,81,89	0
25	CLA	b	607	65/65	0.86	0.26	48,63,81,91	0
27	BCR	k	102	40/40	0.86	0.26	53,65,81,84	0
25	CLA	c	513	65/65	0.86	0.24	57,68,82,96	0
27	BCR	D	405	40/40	0.87	0.24	48,61,77,81	0
25	CLA	B	602	65/65	0.87	0.22	44,62,75,80	0
29	SQD	f	102	41/54	0.87	0.30	54,73,85,89	0
25	CLA	c	512	65/65	0.87	0.26	60,67,89,91	0
30	UNL	m	101	5/-	0.87	0.24	36,39,42,45	0
23	LMG	b	628	9/55	0.87	0.22	36,50,54,54	0
30	UNL	H	101	8/-	0.87	0.18	43,53,58,64	0
30	UNL	b	605	13/-	0.87	0.21	42,54,62,62	0
27	BCR	C	515	40/40	0.88	0.23	53,63,72,76	0
27	BCR	t	103	40/40	0.88	0.23	36,47,60,63	0
23	LMG	M	101	51/55	0.88	0.20	34,58,74,77	0
25	CLA	C	513	65/65	0.88	0.23	52,66,80,86	0
27	BCR	b	602	40/40	0.88	0.22	45,53,70,76	0
27	BCR	h	101	40/40	0.88	0.22	40,54,68,71	0
30	UNL	M	102	6/-	0.88	0.31	45,51,51,53	0
30	UNL	M	103	16/-	0.88	0.21	41,51,57,58	0
29	SQD	B	626	54/54	0.88	0.25	46,67,90,99	0
29	SQD	D	410	43/54	0.88	0.29	56,75,87,96	0
25	CLA	d	403	65/65	0.88	0.20	45,54,65,66	0
30	UNL	A	613	7/-	0.89	0.18	34,49,53,55	0
25	CLA	D	404	65/65	0.89	0.22	34,44,80,84	0
25	CLA	C	508	65/65	0.89	0.20	41,50,57,66	0
25	CLA	C	511	65/65	0.89	0.24	44,57,64,70	0
25	CLA	B	617	65/65	0.89	0.20	39,52,80,84	0
27	BCR	c	514	40/40	0.89	0.25	61,67,74,75	0
25	CLA	C	505	65/65	0.89	0.22	48,63,71,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	DGD	c	517	62/66	0.89	0.22	54,61,81,92	0
25	CLA	c	511	65/65	0.90	0.18	50,62,71,74	0
27	BCR	K	101	40/40	0.90	0.20	51,60,70,75	0
25	CLA	B	610	65/65	0.90	0.19	36,51,58,63	0
23	LMG	f	101	51/55	0.90	0.20	48,58,84,93	0
27	BCR	d	404	40/40	0.90	0.23	45,59,70,77	0
25	CLA	B	607	65/65	0.90	0.20	41,50,64,75	0
25	CLA	c	503	65/65	0.90	0.21	48,61,68,73	0
25	CLA	c	504	58/65	0.90	0.19	52,59,66,67	0
33	DGD	h	102	62/66	0.90	0.23	41,55,63,66	0
25	CLA	b	612	65/65	0.91	0.17	32,46,56,69	0
23	LMG	D	409	51/55	0.91	0.20	39,61,82,88	0
27	BCR	Y	101	40/40	0.91	0.20	46,66,71,72	0
25	CLA	C	512	65/65	0.91	0.19	52,60,69,71	0
27	BCR	b	624	40/40	0.91	0.20	38,49,58,59	0
25	CLA	c	506	65/65	0.91	0.21	47,57,79,92	0
27	BCR	c	515	40/40	0.91	0.18	38,53,64,72	0
25	CLA	C	506	65/65	0.91	0.19	41,51,57,60	0
25	CLA	C	507	65/65	0.91	0.19	44,55,75,88	0
25	CLA	A	606	65/65	0.91	0.19	29,43,48,53	0
30	UNL	m	102	12/-	0.91	0.19	41,47,50,52	0
25	CLA	a	707	65/65	0.91	0.18	33,47,51,53	0
25	CLA	C	509	65/65	0.91	0.21	46,55,91,100	0
27	BCR	C	516	40/40	0.91	0.20	42,51,58,58	0
33	DGD	C	518	62/66	0.91	0.19	51,62,81,88	0
33	DGD	H	103	62/66	0.91	0.21	39,49,59,62	0
28	PL9	D	406	55/55	0.91	0.21	31,43,52,55	0
25	CLA	b	610	65/65	0.91	0.22	37,47,59,62	0
25	CLA	b	616	65/65	0.92	0.20	34,42,50,56	0
25	CLA	b	621	65/65	0.92	0.17	38,49,55,60	0
29	SQD	A	612	52/54	0.92	0.21	45,67,80,92	0
25	CLA	D	402	65/65	0.92	0.18	31,41,47,51	0
25	CLA	C	510	65/65	0.92	0.20	45,57,64,68	0
25	CLA	c	505	65/65	0.92	0.19	41,52,60,69	0
27	BCR	b	623	40/40	0.92	0.19	42,53,60,61	0
25	CLA	B	616	65/65	0.92	0.16	42,51,60,64	0
29	SQD	a	714	54/54	0.92	0.22	48,68,83,90	0
27	BCR	b	625	40/40	0.92	0.16	36,49,55,58	0
25	CLA	c	510	65/65	0.92	0.21	43,54,63,68	0
25	CLA	a	711	65/65	0.92	0.19	34,46,79,87	0
30	UNL	t	101	10/-	0.92	0.17	26,44,49,50	0
25	CLA	B	605	65/65	0.92	0.22	35,47,62,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	LHG	D	408	49/49	0.92	0.21	42,59,72,84	0
25	CLA	C	503	65/65	0.92	0.23	43,56,62,68	0
32	LHG	a	720	39/49	0.92	0.20	41,54,65,66	0
30	UNL	B	624	11/-	0.92	0.20	34,49,52,53	0
33	DGD	C	517	62/66	0.92	0.20	36,46,65,71	0
25	CLA	B	615	65/65	0.92	0.17	38,48,67,73	0
27	BCR	B	620	40/40	0.92	0.18	39,48,56,71	0
33	DGD	c	516	62/66	0.92	0.20	34,50,68,76	0
25	CLA	b	613	65/65	0.92	0.19	37,44,55,58	0
33	DGD	c	518	62/66	0.92	0.19	44,57,76,81	0
25	CLA	b	615	65/65	0.92	0.17	42,50,55,60	0
25	CLA	B	608	65/65	0.93	0.17	30,42,52,56	0
25	CLA	B	609	65/65	0.93	0.25	32,45,51,59	0
25	CLA	b	608	65/65	0.93	0.19	39,49,60,64	0
24	CL	a	704	1/1	0.93	0.12	59,59,59,59	0
25	CLA	d	402	65/65	0.93	0.16	35,45,51,55	0
25	CLA	B	612	65/65	0.93	0.19	32,42,49,54	0
26	PHO	a	710	64/64	0.93	0.22	38,46,55,62	0
28	PL9	d	405	55/55	0.93	0.20	32,41,53,56	0
27	BCR	B	618	40/40	0.93	0.18	37,52,60,63	0
27	BCR	B	619	40/40	0.93	0.20	35,47,51,52	0
25	CLA	B	614	65/65	0.93	0.20	34,43,57,69	0
25	CLA	B	603	65/65	0.93	0.21	42,52,59,62	0
25	CLA	B	604	65/65	0.93	0.20	33,44,54,57	0
30	UNL	t	102	5/-	0.93	0.20	32,38,43,47	0
25	CLA	b	620	65/65	0.93	0.17	35,52,61,64	0
32	LHG	B	625	49/49	0.93	0.20	41,51,58,61	0
24	CL	A	605	1/1	0.93	0.14	51,51,51,51	0
25	CLA	b	622	47/65	0.93	0.16	40,48,58,64	0
25	CLA	c	502	65/65	0.93	0.21	45,55,67,81	0
27	BCR	a	712	40/40	0.93	0.17	26,44,53,54	0
25	CLA	C	502	65/65	0.93	0.21	38,50,57,64	0
25	CLA	B	606	65/65	0.93	0.18	37,45,52,53	0
33	DGD	C	519	62/66	0.93	0.17	43,56,67,76	0
25	CLA	C	504	65/65	0.93	0.20	43,57,62,68	0
25	CLA	A	607	65/65	0.93	0.19	31,46,91,99	0
25	CLA	c	507	65/65	0.93	0.17	41,50,61,67	0
25	CLA	c	508	65/65	0.93	0.19	46,57,72,82	0
25	CLA	c	509	65/65	0.93	0.19	49,57,70,73	0
34	HEM	E	102	43/43	0.93	0.22	52,66,76,80	0
34	HEM	e	102	43/43	0.93	0.20	60,71,81,91	0
27	BCR	A	610	40/40	0.94	0.15	31,44,52,56	0

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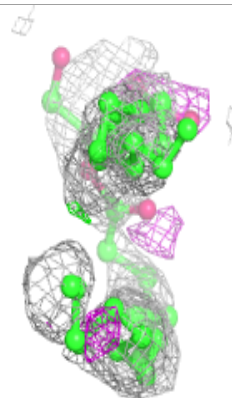
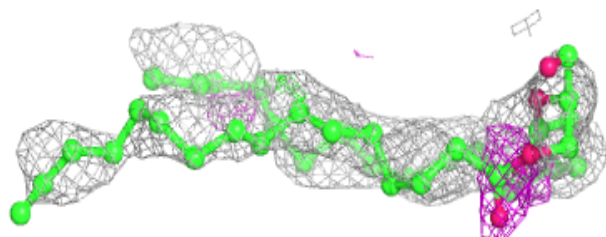
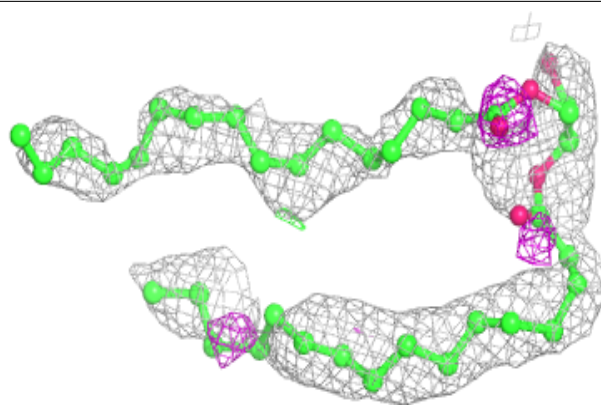
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	LHG	L	101	49/49	0.94	0.17	39,50,57,64	0
25	CLA	b	619	65/65	0.94	0.20	31,42,59,67	0
32	LHG	b	629	49/49	0.94	0.16	36,50,57,64	0
32	LHG	d	406	49/49	0.94	0.19	32,53,61,65	0
32	LHG	d	407	49/49	0.94	0.18	36,46,54,61	0
25	CLA	b	609	65/65	0.94	0.19	34,45,55,61	0
25	CLA	A	609	54/65	0.94	0.16	34,43,60,71	0
25	CLA	B	613	65/65	0.94	0.19	36,43,55,59	0
25	CLA	c	501	65/65	0.94	0.19	37,49,55,59	0
25	CLA	a	719	65/65	0.94	0.16	32,43,49,54	0
25	CLA	b	614	65/65	0.94	0.22	39,48,58,60	0
25	CLA	D	403	65/65	0.94	0.16	33,42,54,61	0
25	CLA	B	611	65/65	0.94	0.20	40,47,55,60	0
26	PHO	D	401	64/64	0.94	0.20	37,46,55,59	0
32	LHG	D	407	49/49	0.94	0.23	34,49,59,60	0
25	CLA	b	617	65/65	0.94	0.19	36,45,50,57	0
25	CLA	a	708	65/65	0.95	0.16	37,47,89,101	0
25	CLA	b	611	65/65	0.95	0.16	30,46,52,56	0
26	PHO	A	608	64/64	0.95	0.18	32,40,46,50	0
25	CLA	b	618	65/65	0.95	0.20	32,43,50,52	0
26	PHO	a	709	64/64	0.95	0.19	26,41,47,50	0
22	FE2	a	703	1/1	0.95	0.03	60,60,60,60	0
35	HEC	V	201	43/43	0.95	0.16	41,51,57,63	0
35	HEC	v	201	43/43	0.95	0.15	46,58,64,72	0
24	CL	a	705	1/1	0.97	0.12	50,50,50,50	0
31	BCT	A	615	4/4	0.97	0.10	46,49,51,54	0
22	FE2	A	602	1/1	0.97	0.03	60,60,60,60	0
21	OEX	a	702	10/10	0.97	0.11	44,52,59,60	0
21	OEX	A	601	10/10	0.98	0.11	42,54,59,60	0
31	BCT	a	706	4/4	0.98	0.09	50,56,56,59	0
24	CL	A	604	1/1	0.99	0.06	39,39,39,39	0

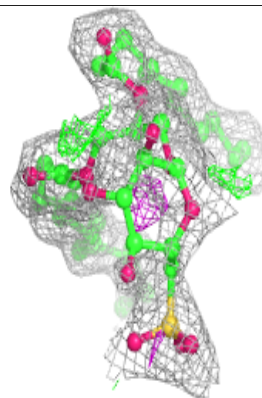
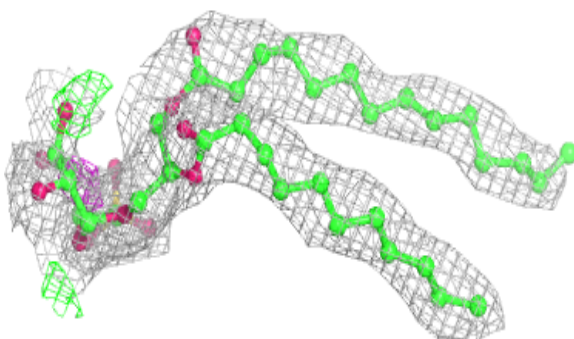
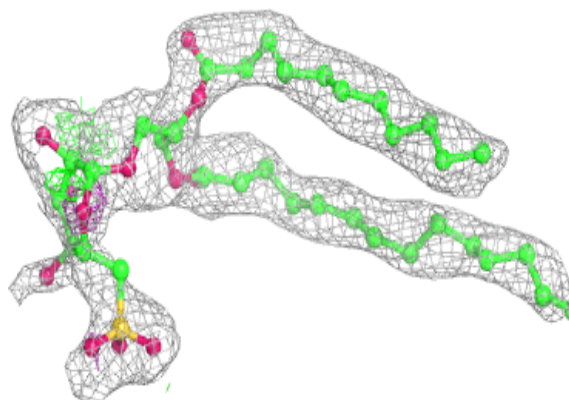
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SQD I 102:

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

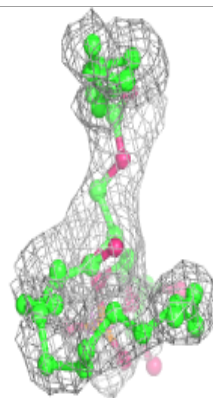
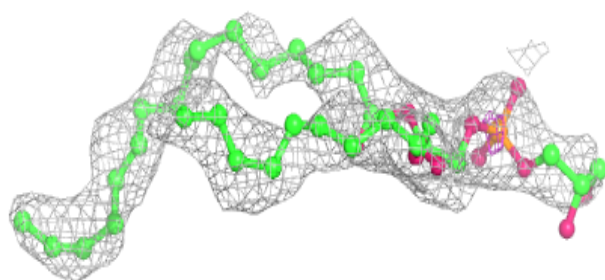
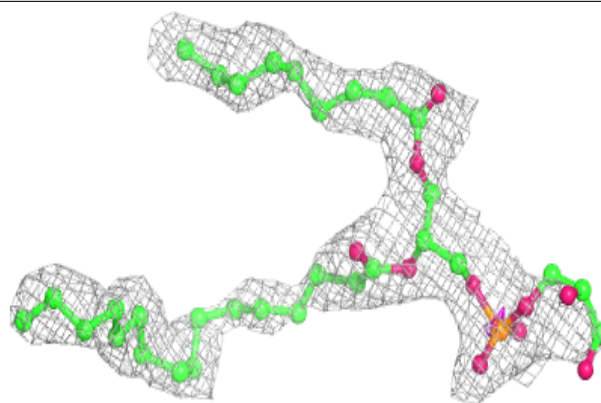
**Electron density around SQD B 623:**

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

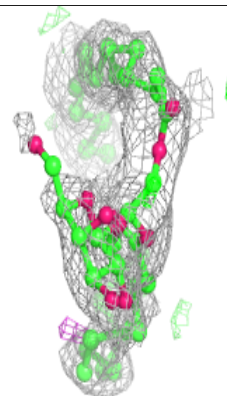
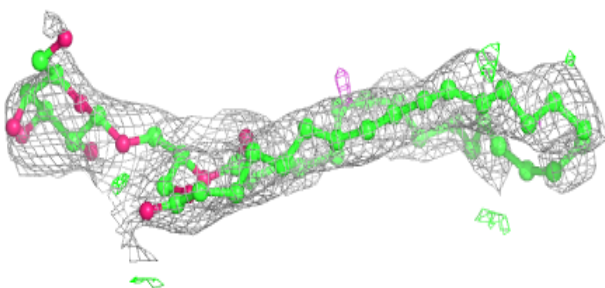
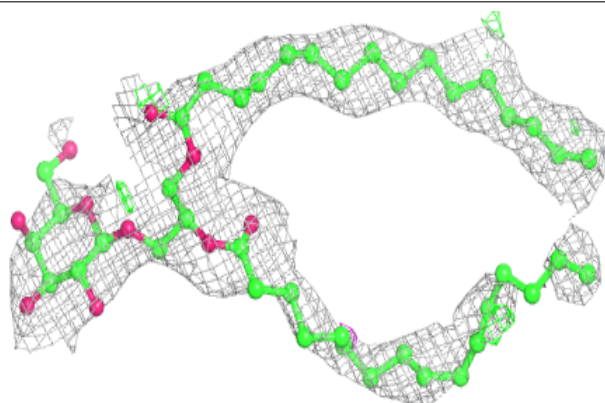


Electron density around LHG e 101:

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

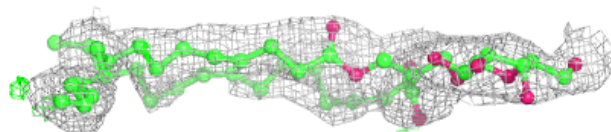
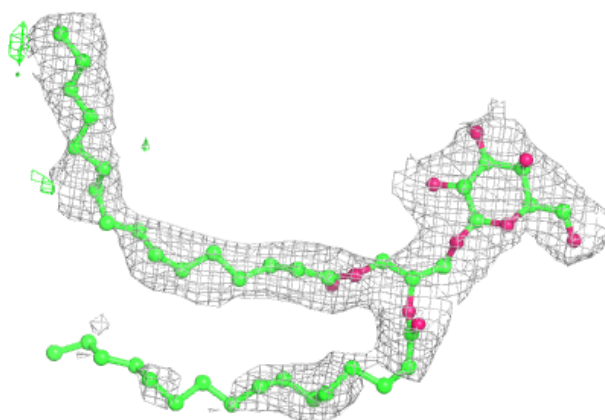
**Electron density around LMG C 501:**

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

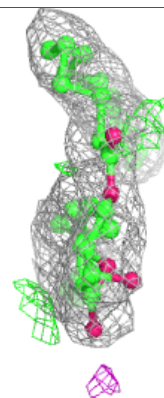
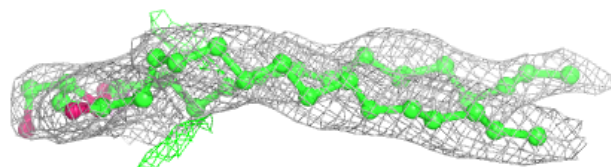
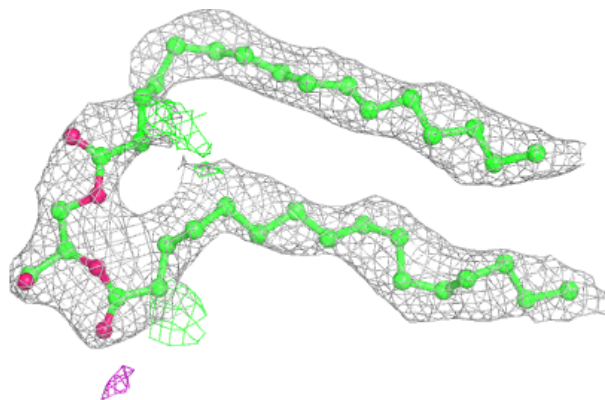


Electron density around LMG C 520:

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

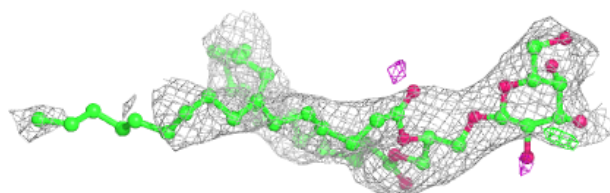
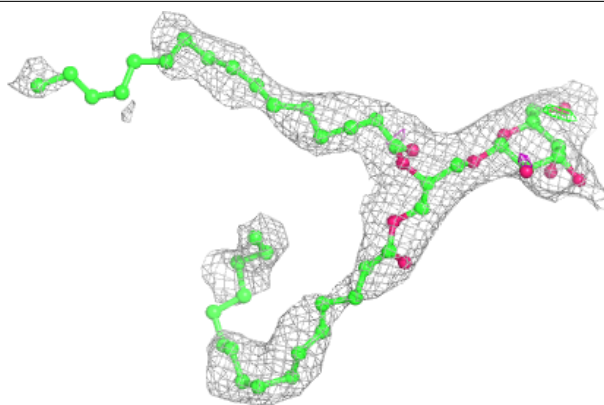
**Electron density around LMG d 408:**

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

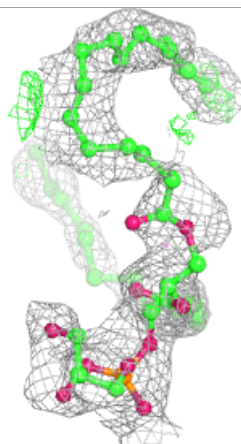
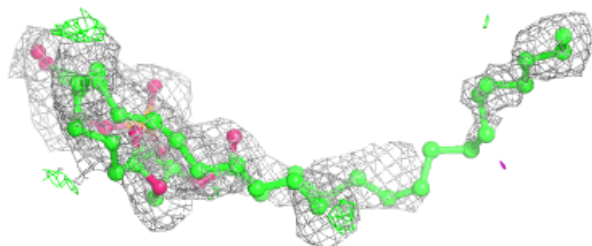
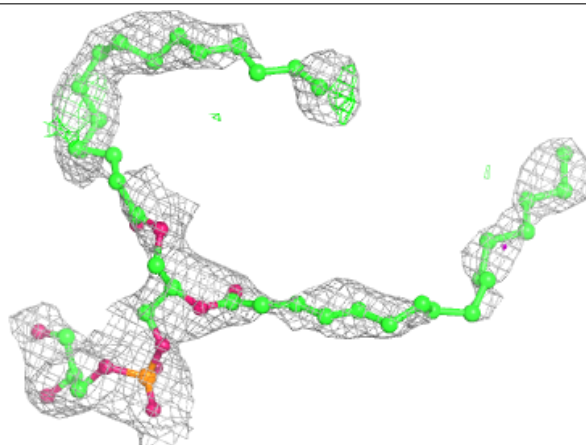


Electron density around LMG B 621:

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

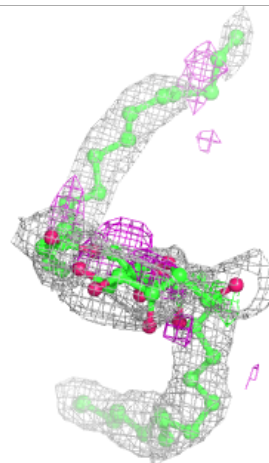
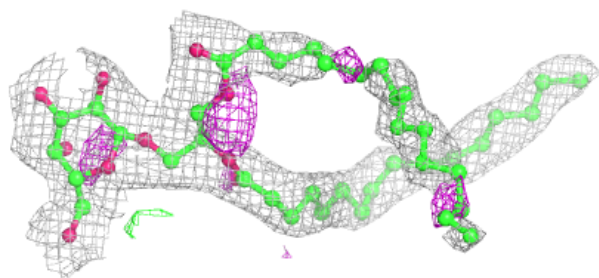
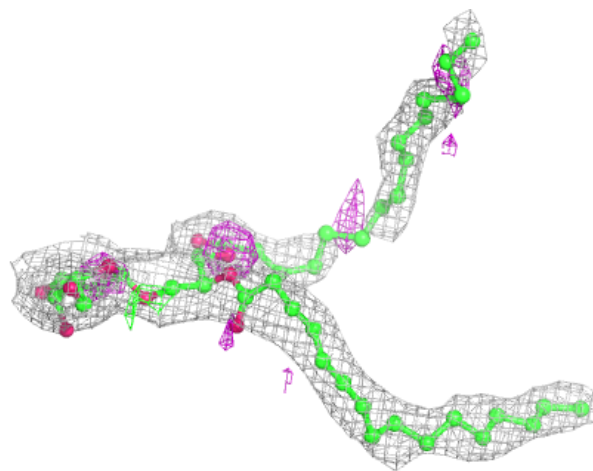
**Electron density around LHG E 101:**

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



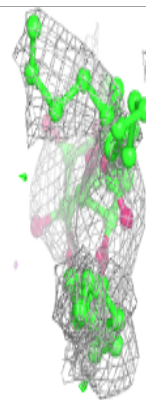
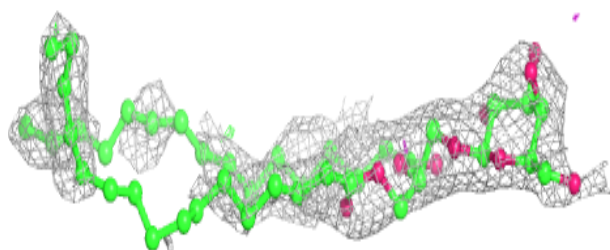
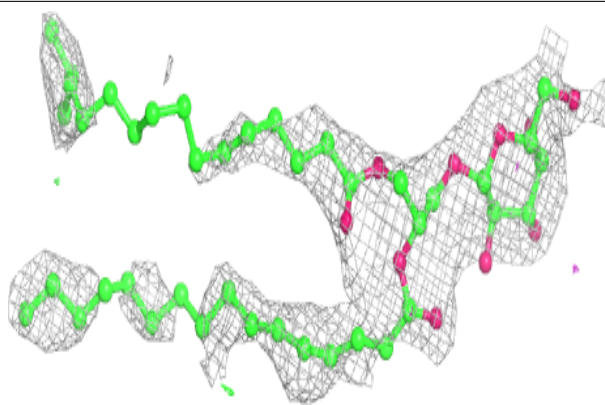
Electron density around LMG b 626:

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

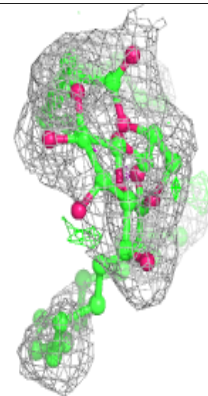
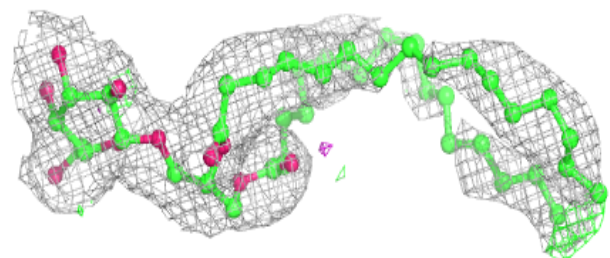
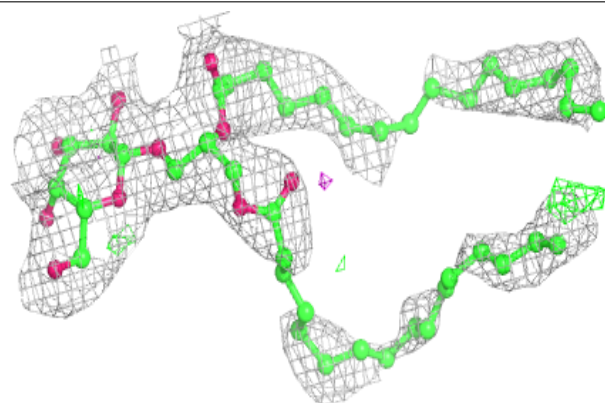


Electron density around LMG C 521:

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

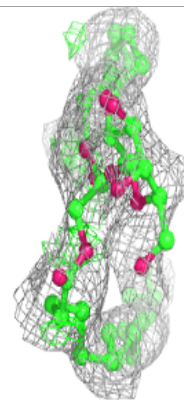
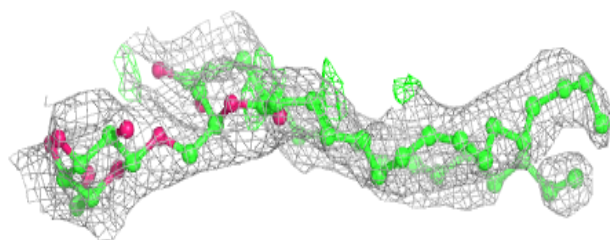
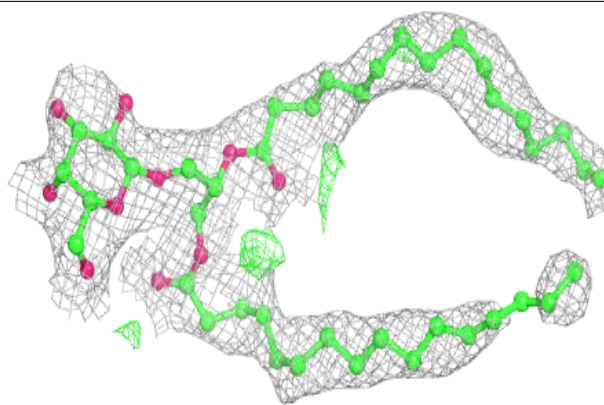
**Electron density around LMG A 603:**

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

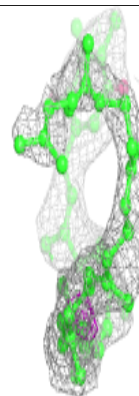
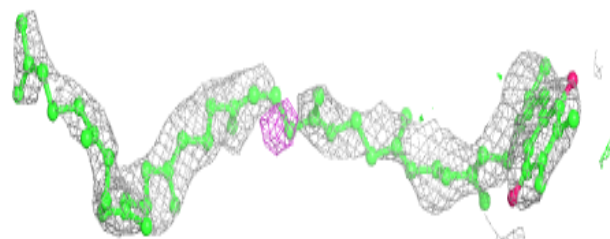
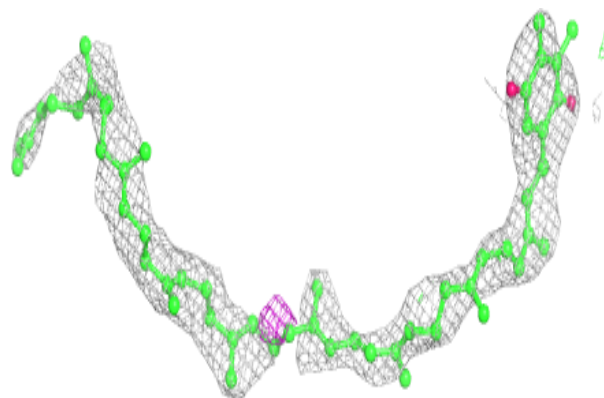


Electron density around LMG a 715:

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

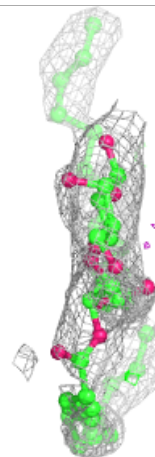
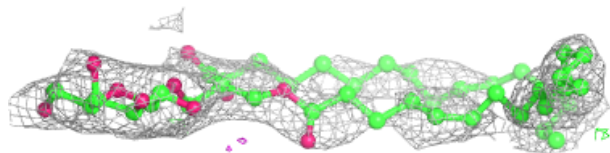
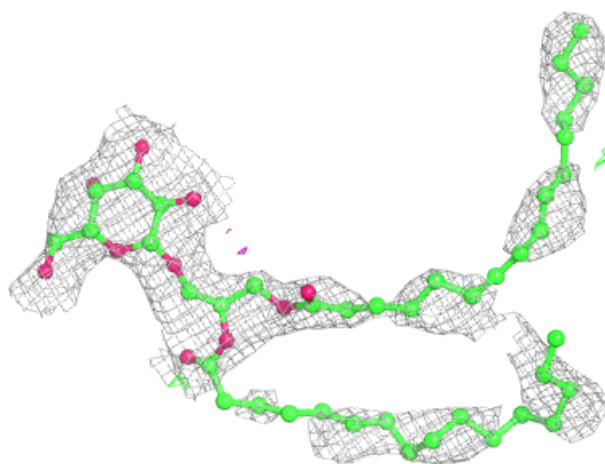
**Electron density around PL9 A 611:**

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



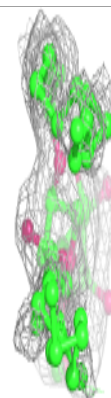
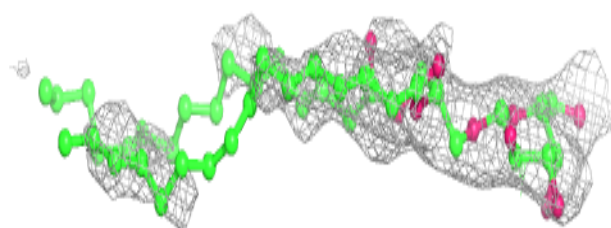
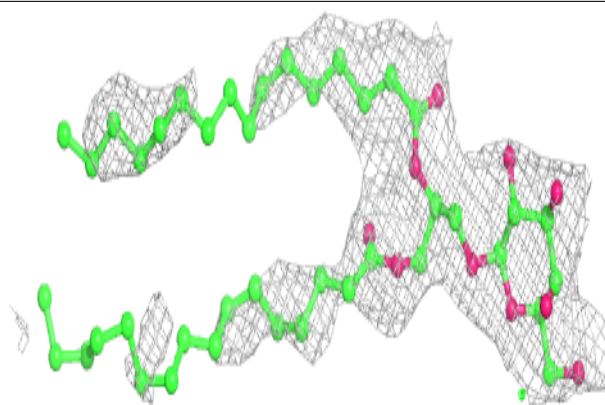
Electron density around LMG c 519:

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

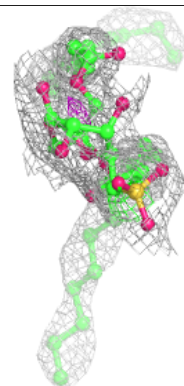
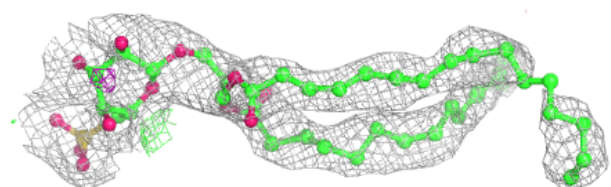
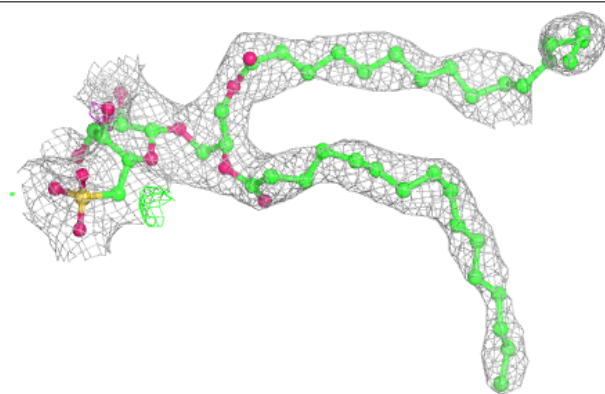


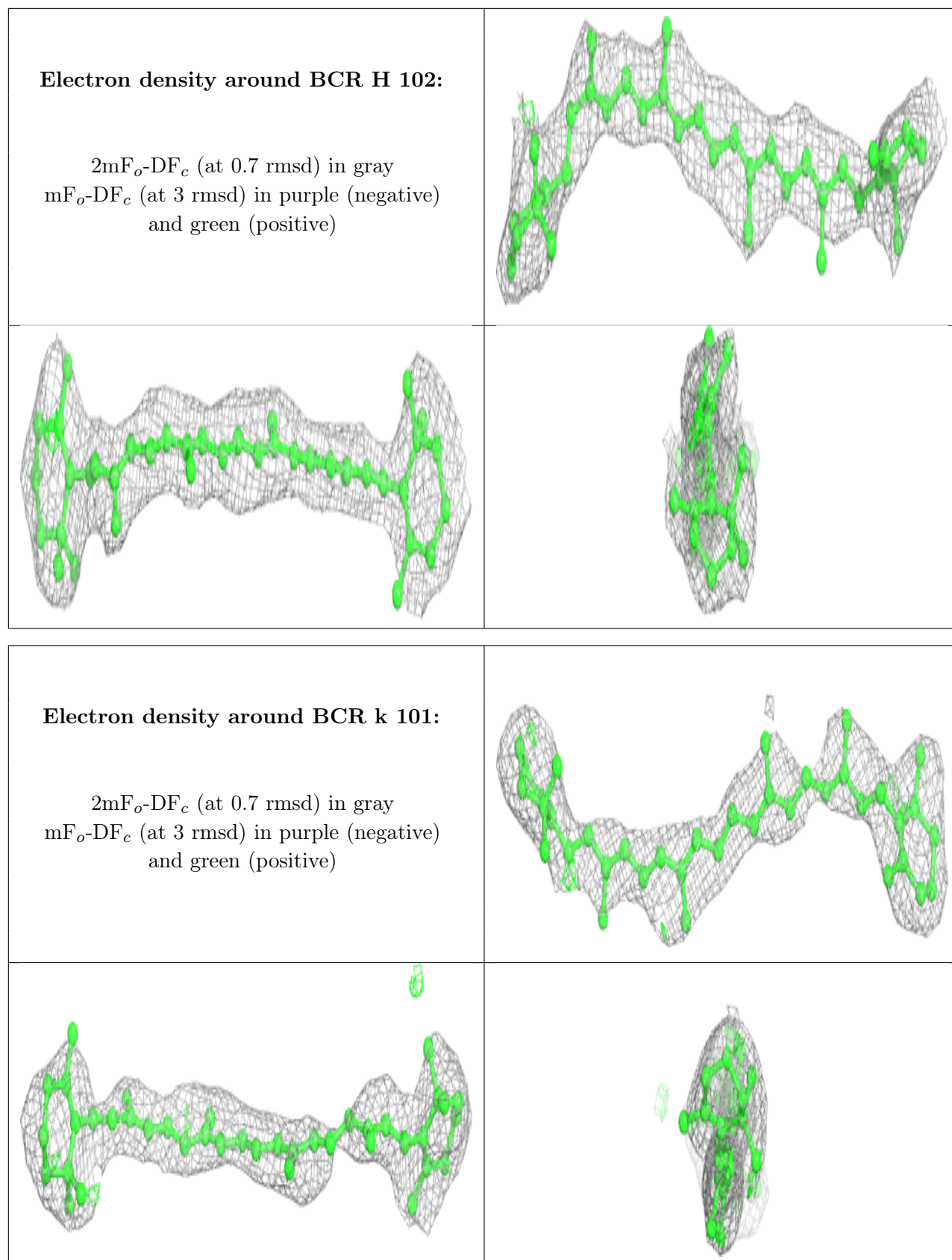
Electron density around LMG c 520:

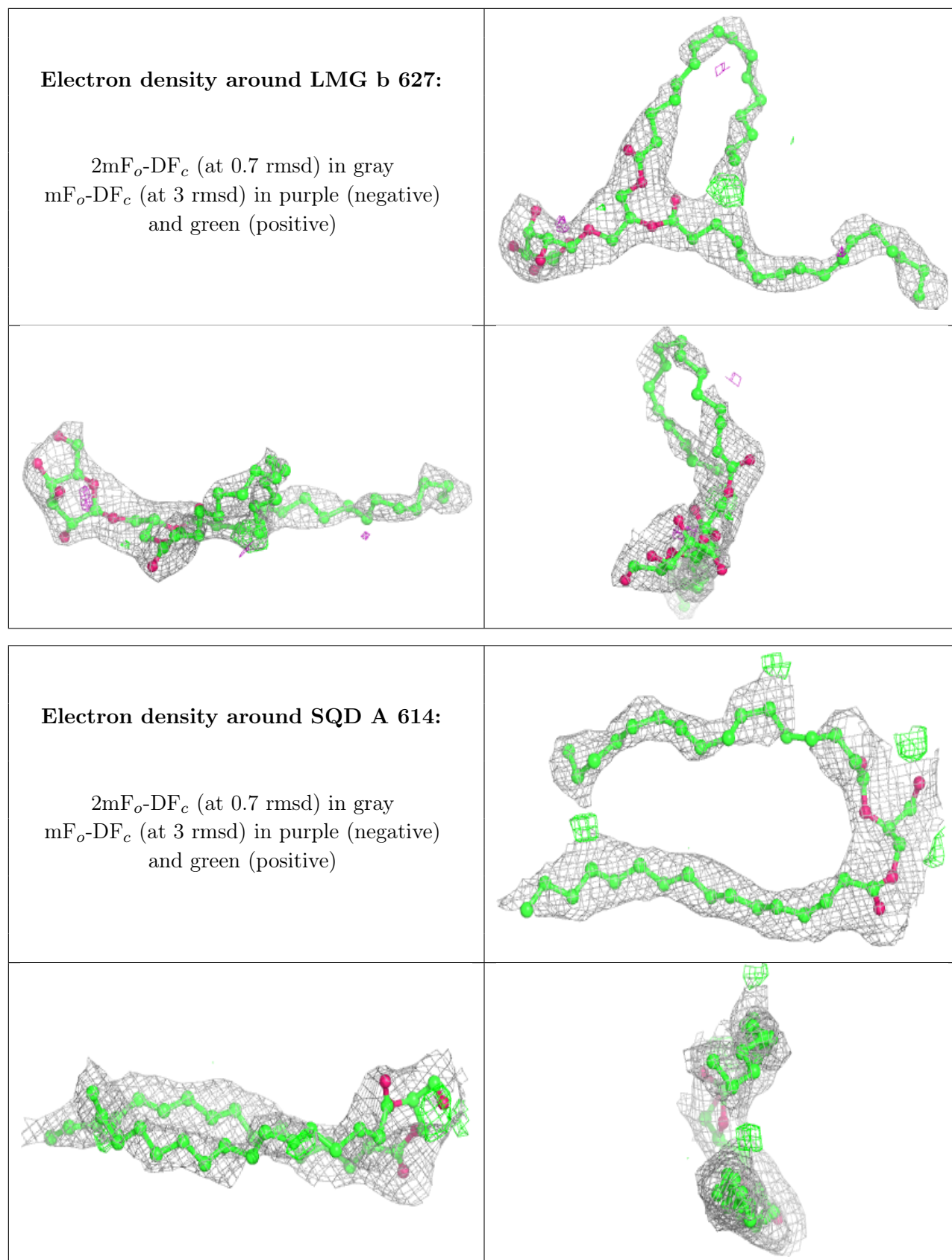
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SQD b 601:**

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

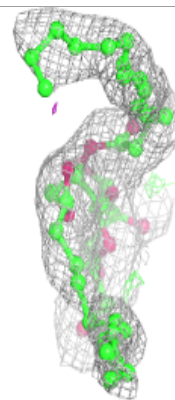
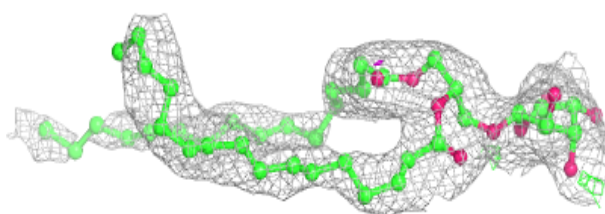
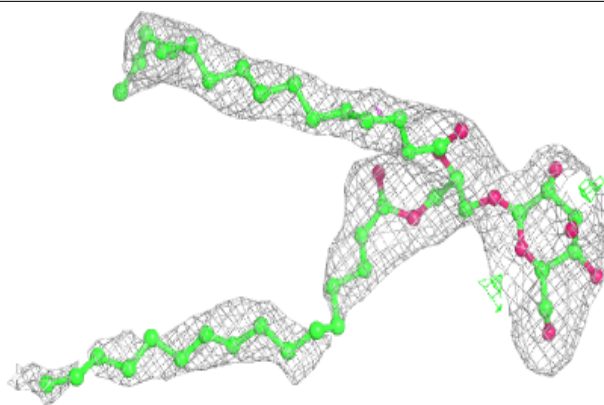




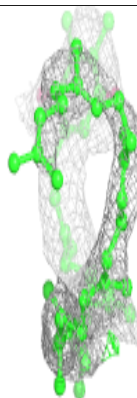
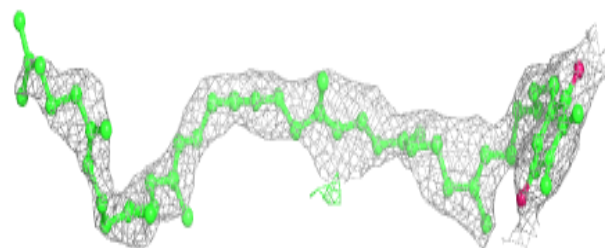
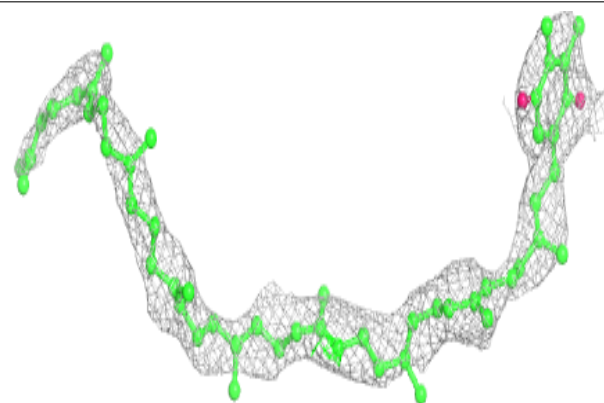


Electron density around LMG a 701:

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

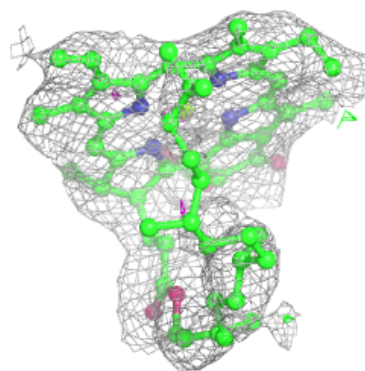
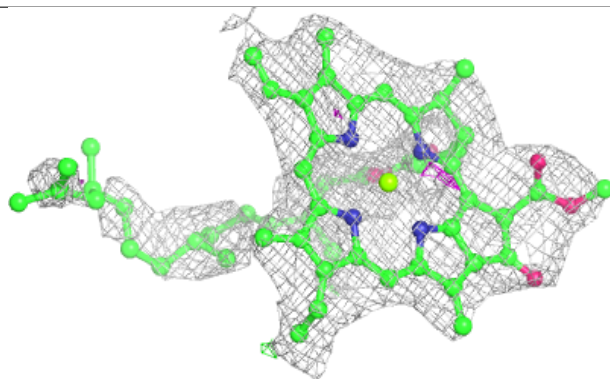
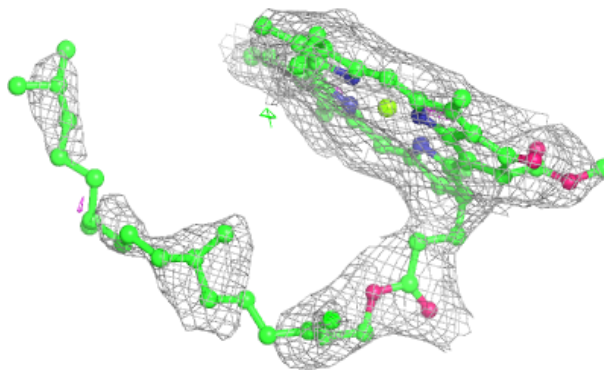
**Electron density around PL9 a 713:**

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



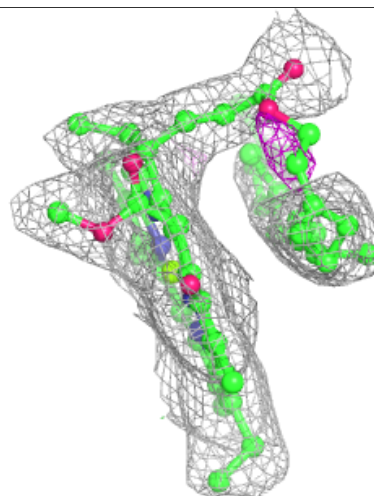
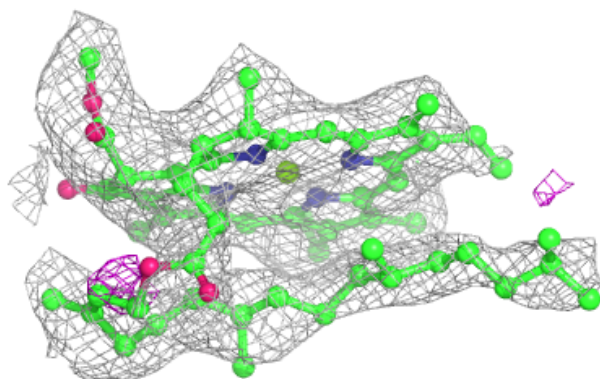
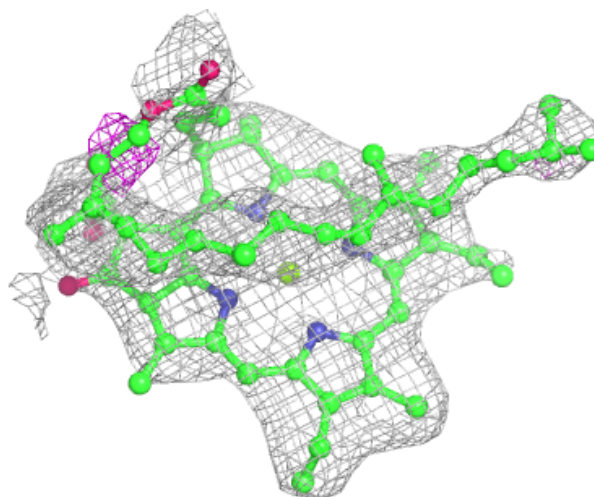
Electron density around CLA C 514:

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



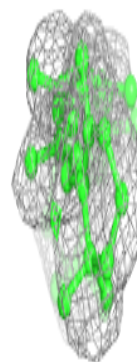
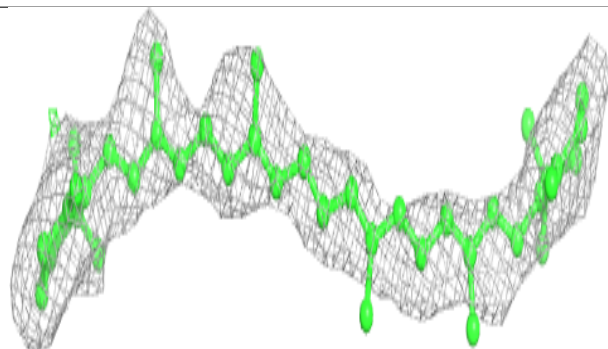
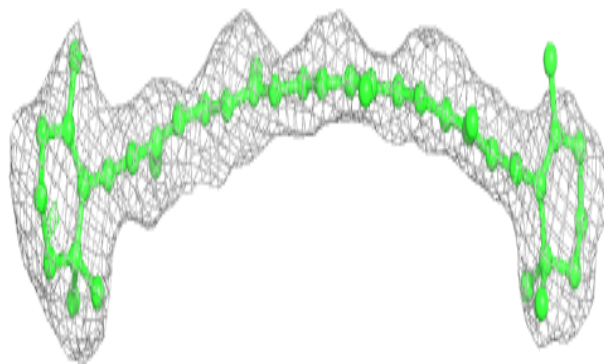
Electron density around CLA b 607:

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

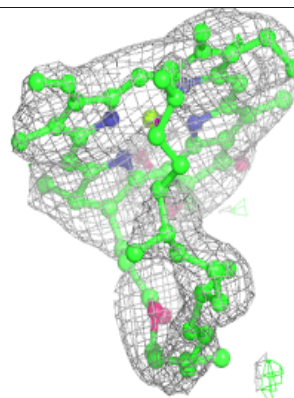
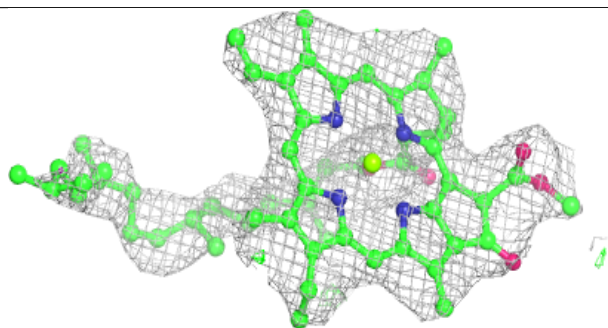
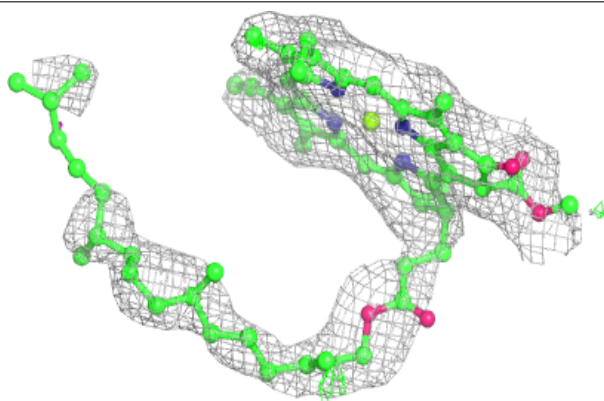


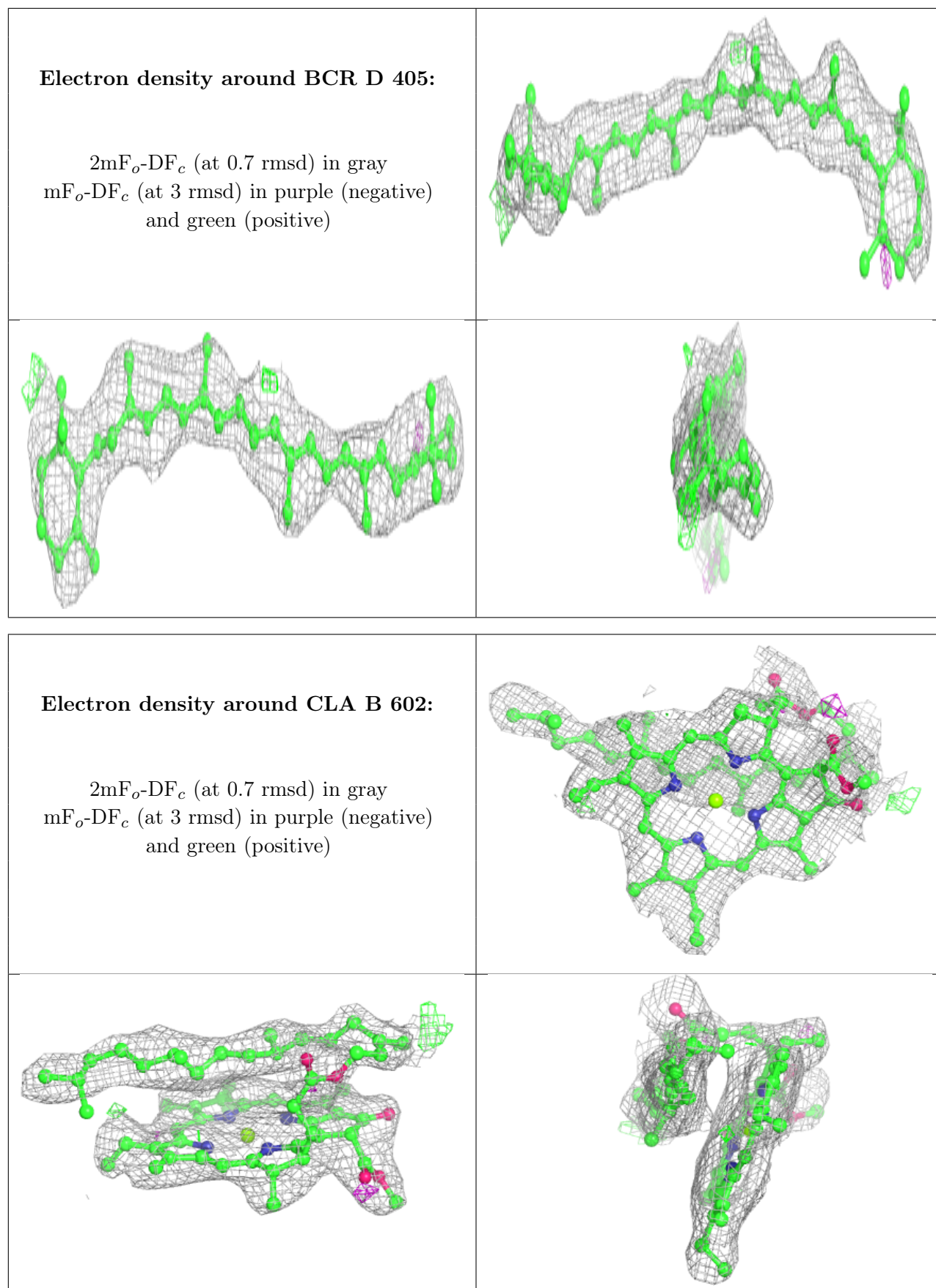
Electron density around BCR k 102:

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

**Electron density around CLA c 513:**

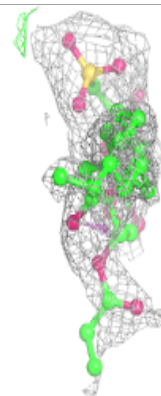
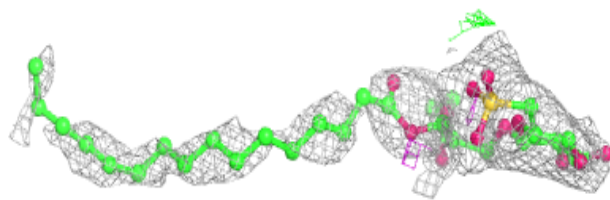
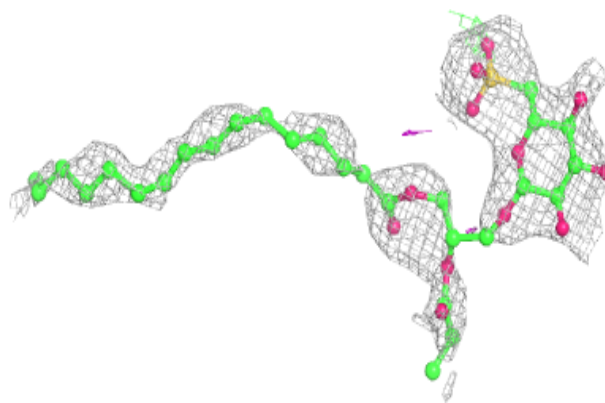
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





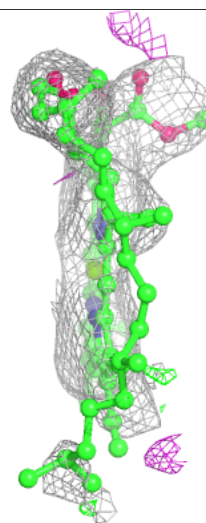
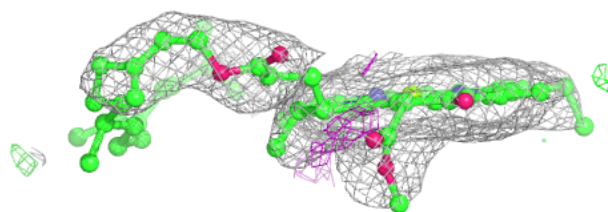
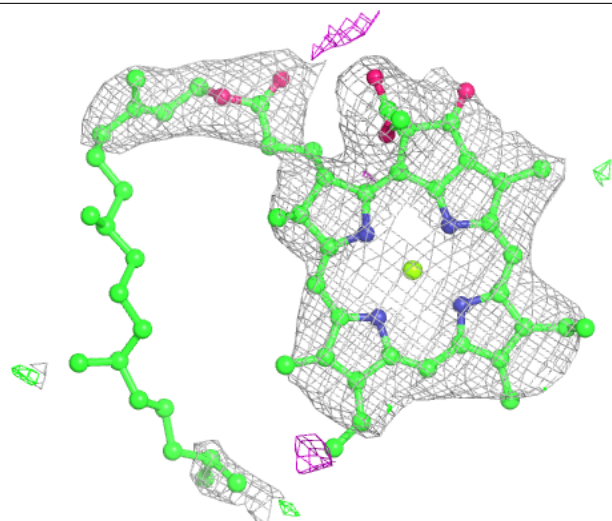
Electron density around SQD f 102:

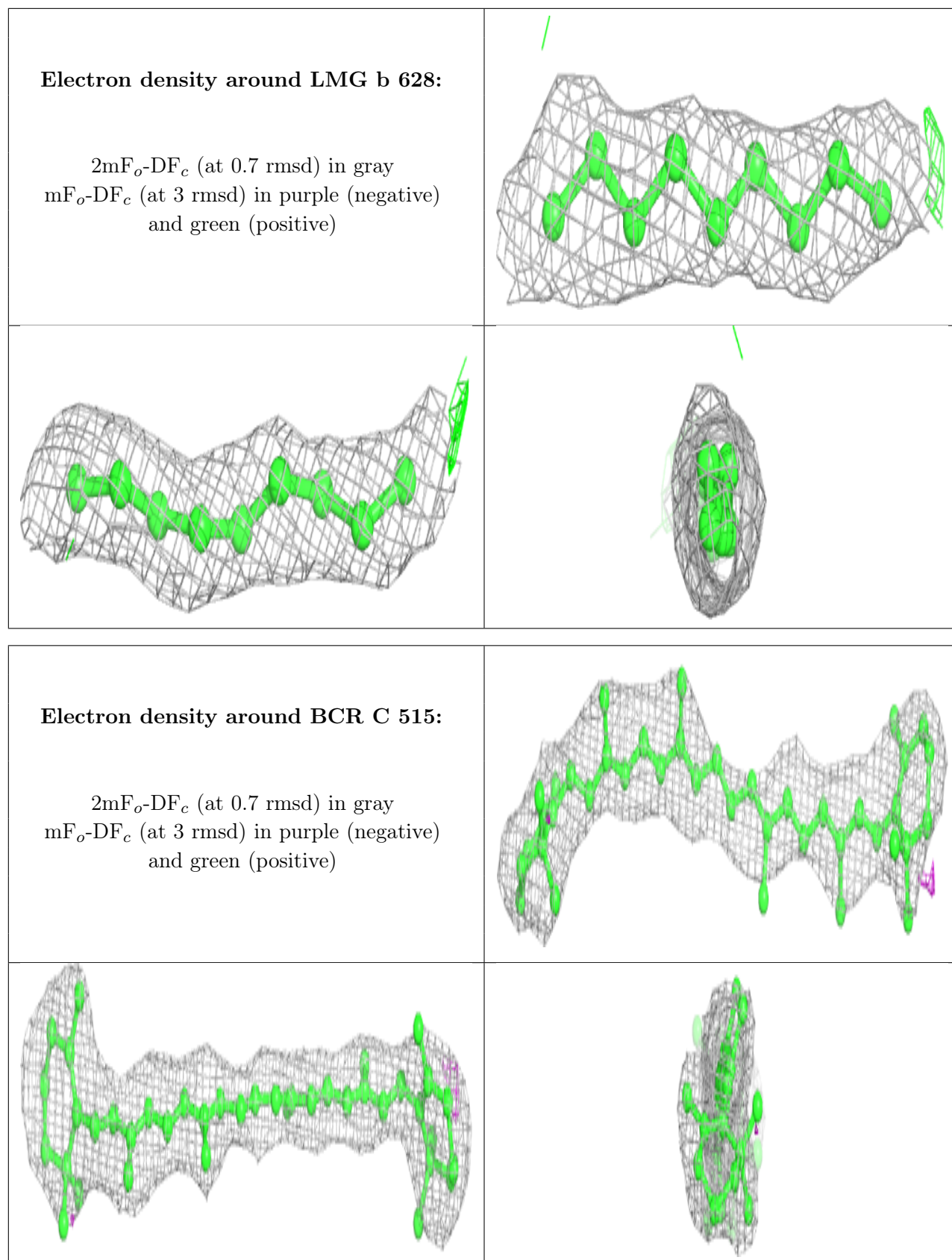
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 512:

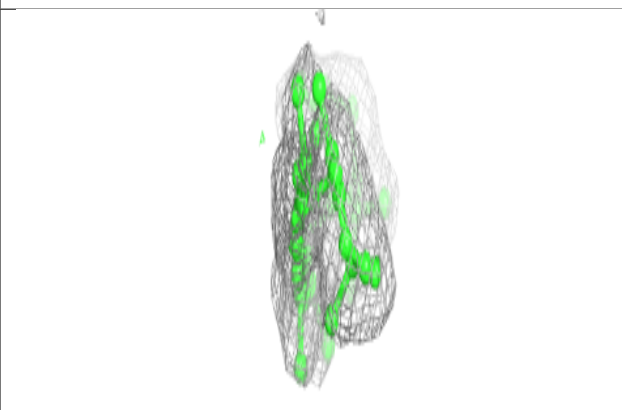
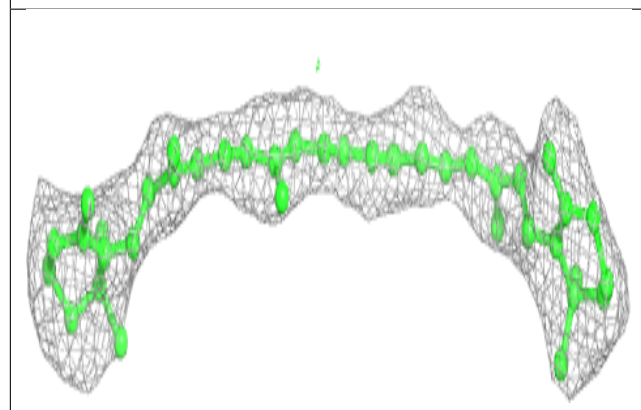
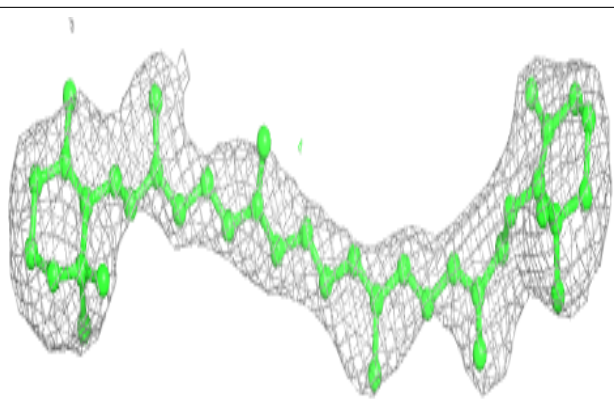
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



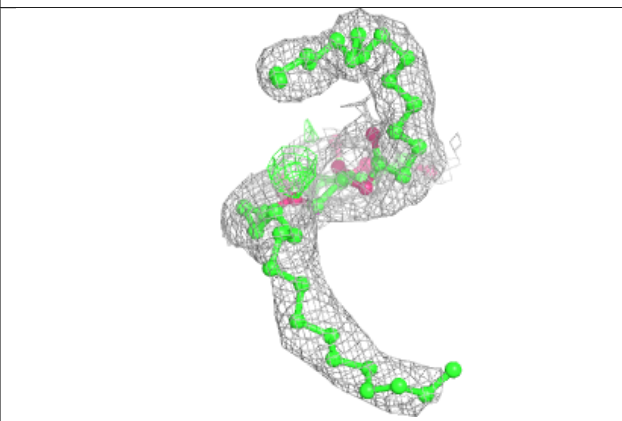
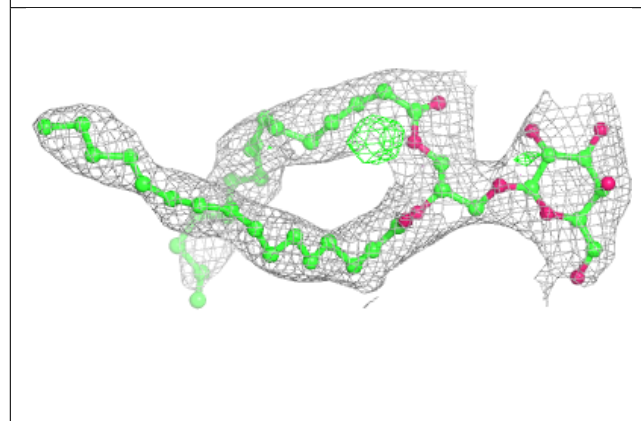
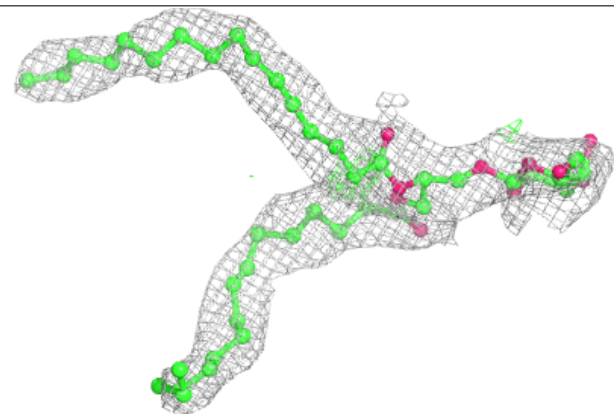


Electron density around BCR t 103:

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

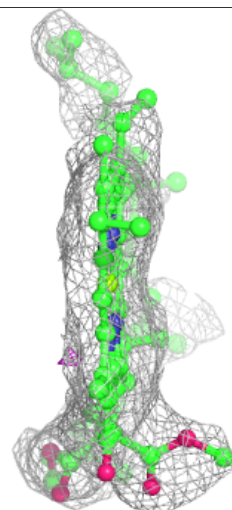
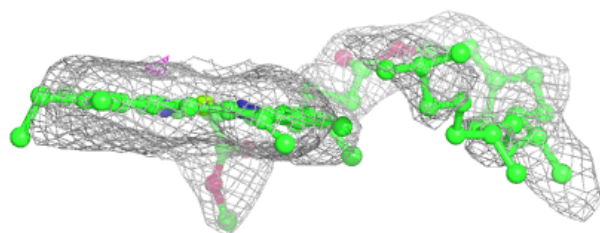
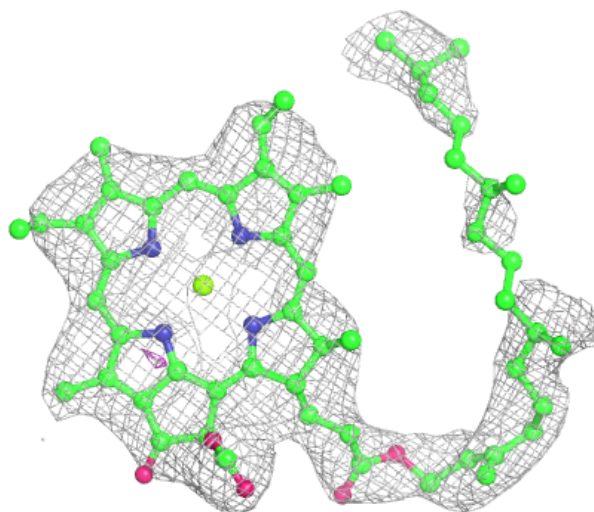
**Electron density around LMG M 101:**

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



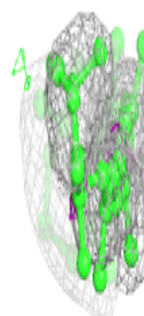
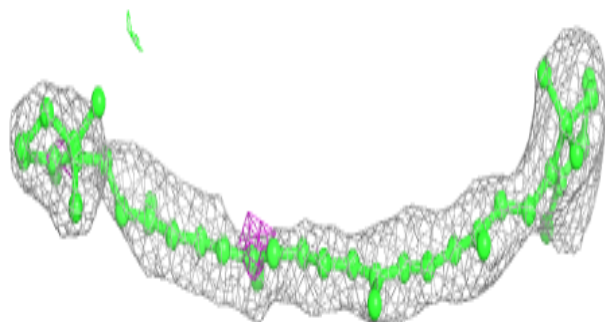
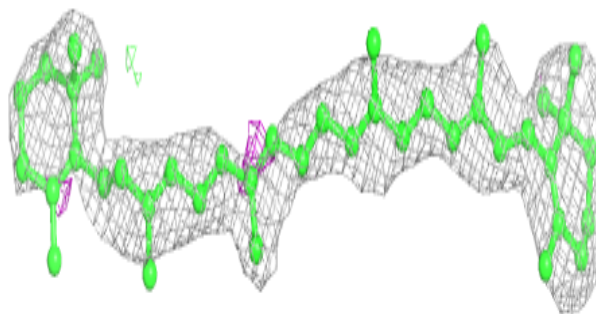
Electron density around CLA C 513:

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

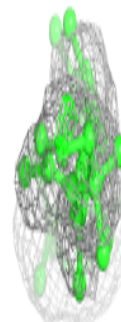
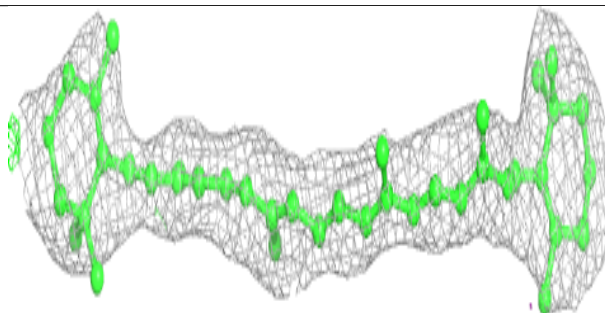
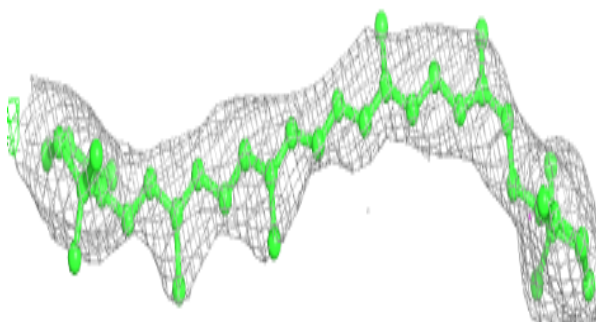


Electron density around BCR b 602:

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

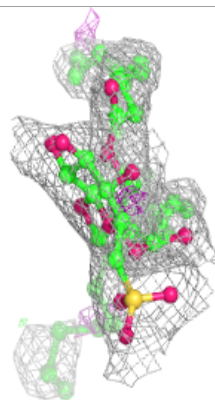
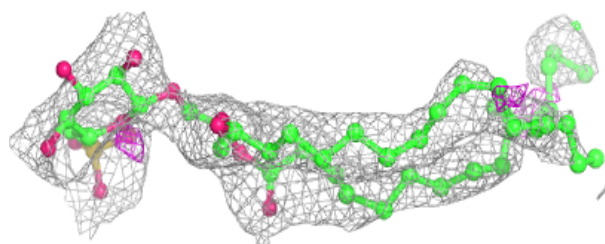
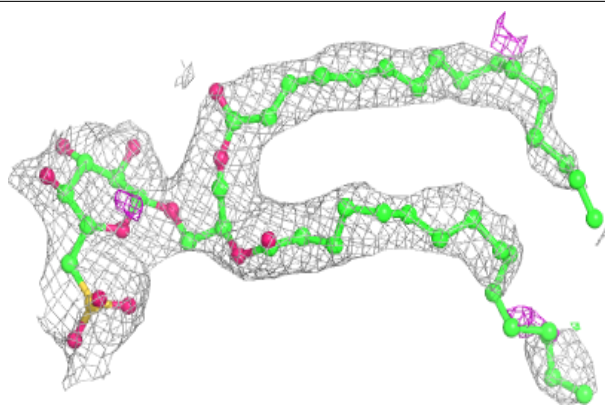
**Electron density around BCR h 101:**

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

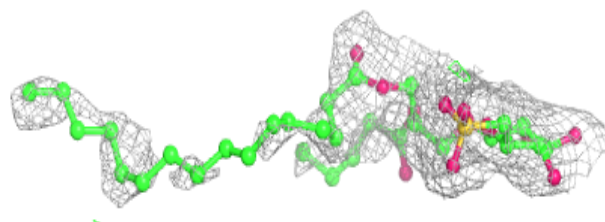
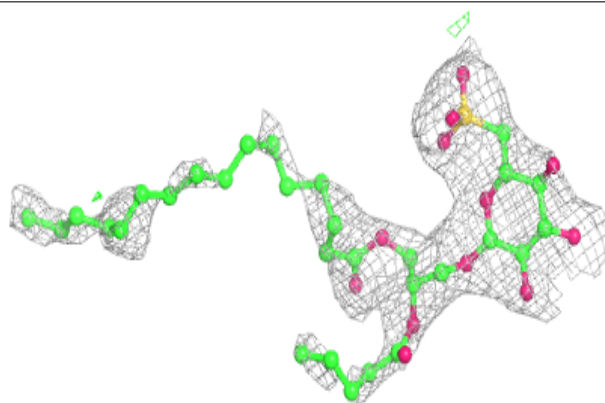


Electron density around SQD B 626:

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

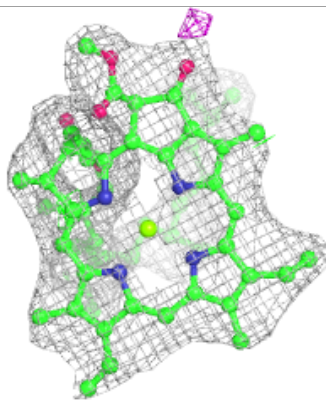
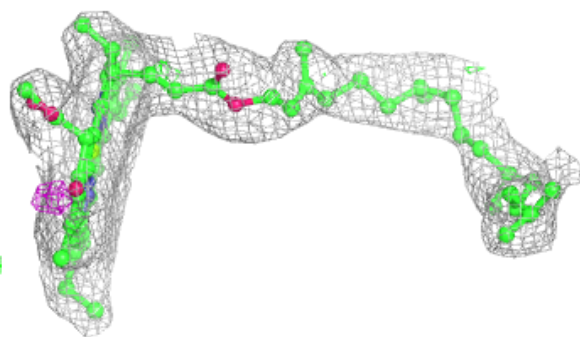
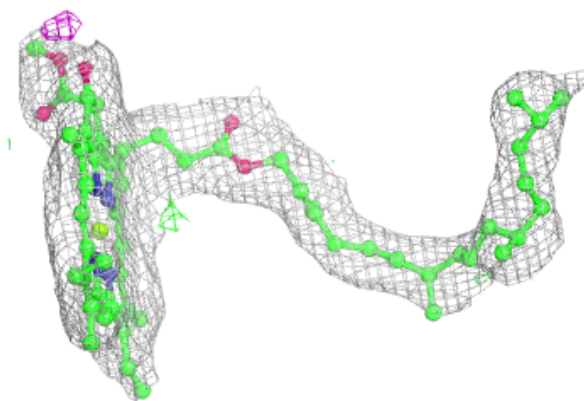
**Electron density around SQD D 410:**

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

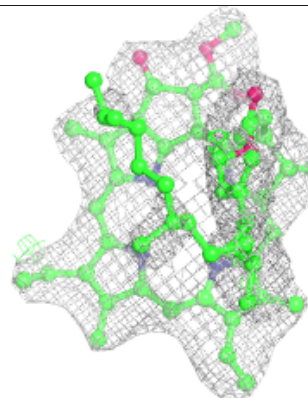
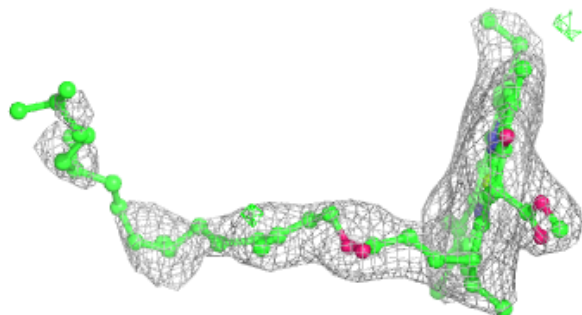
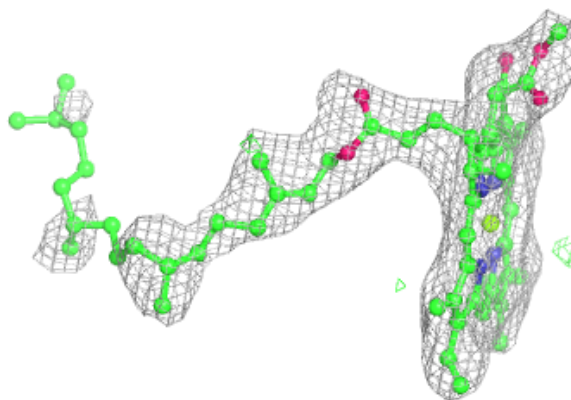


Electron density around CLA d 403:

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

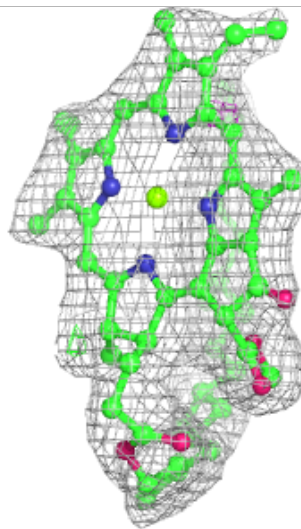
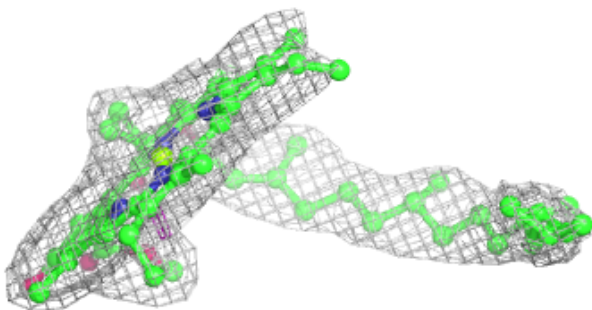
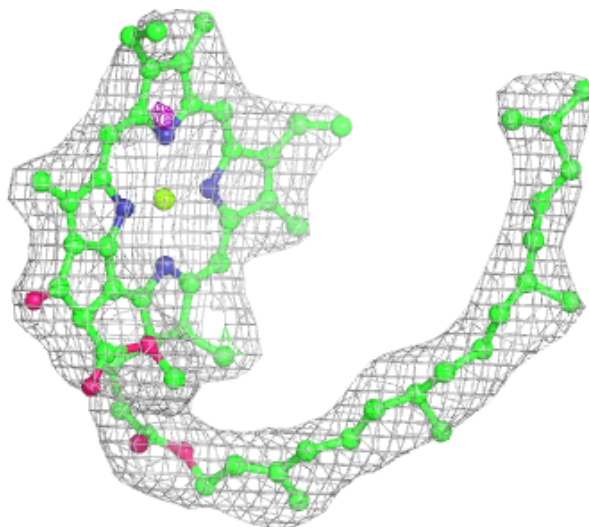
**Electron density around CLA D 404:**

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



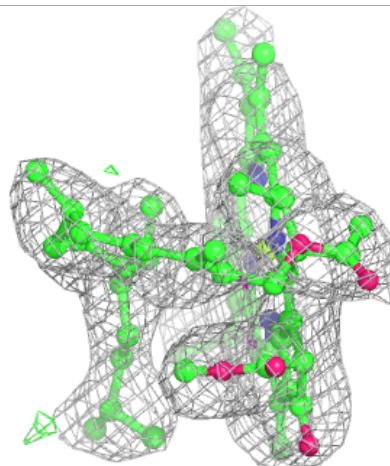
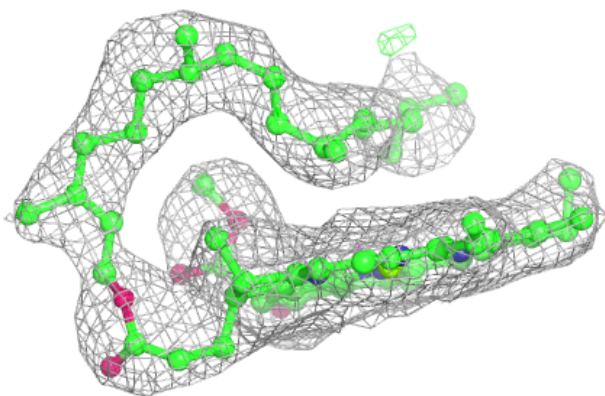
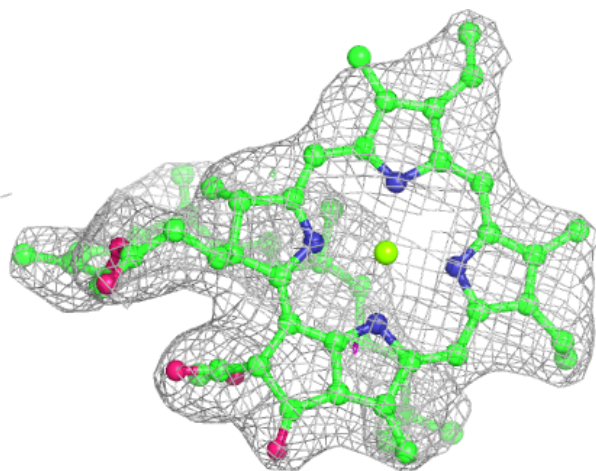
Electron density around CLA C 508:

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



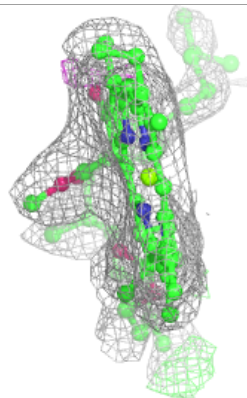
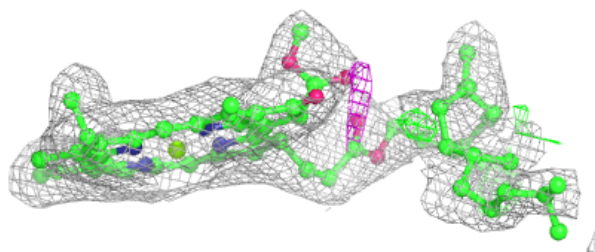
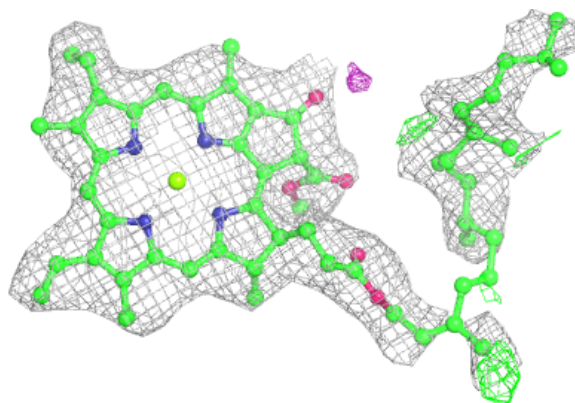
Electron density around CLA C 511:

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

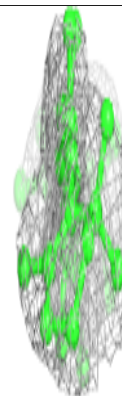
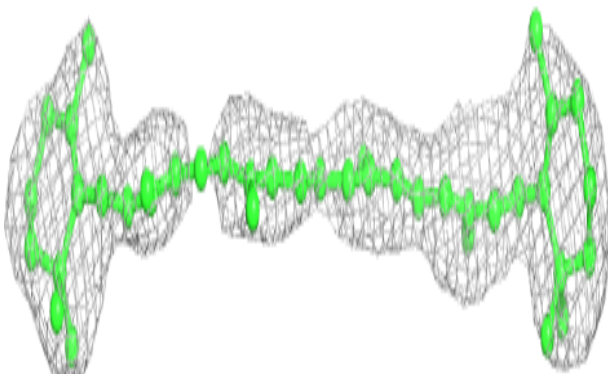
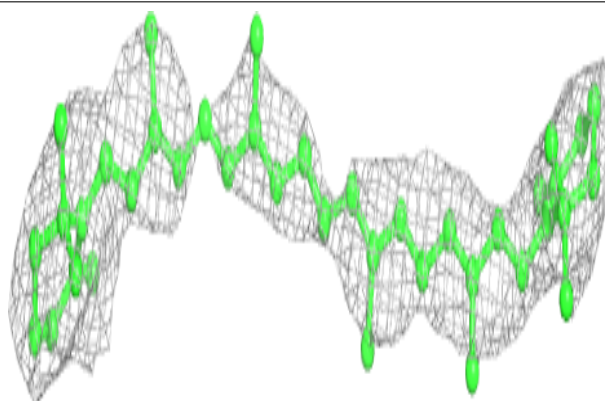


Electron density around CLA B 617:

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

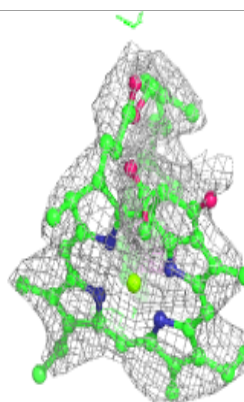
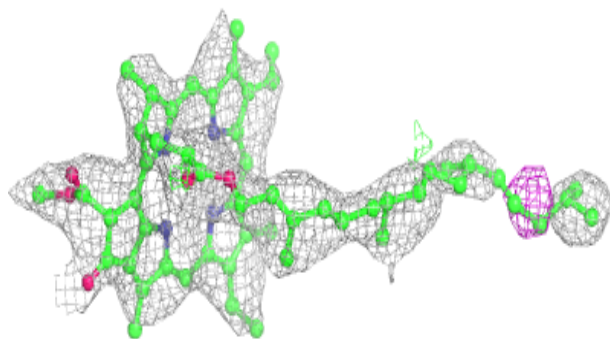
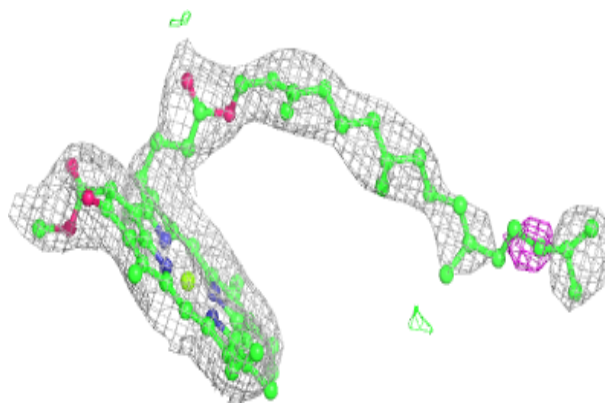
**Electron density around BCR c 514:**

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

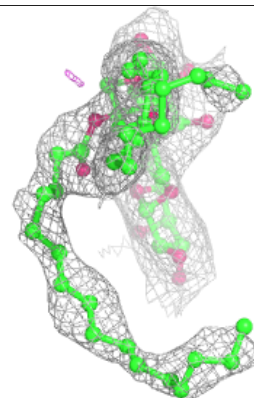
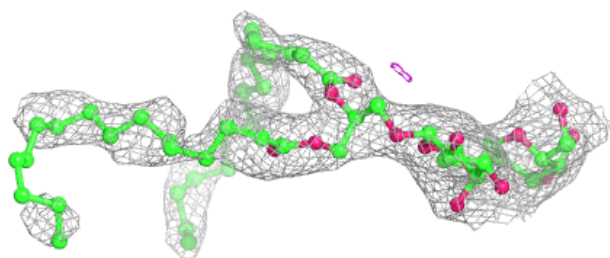
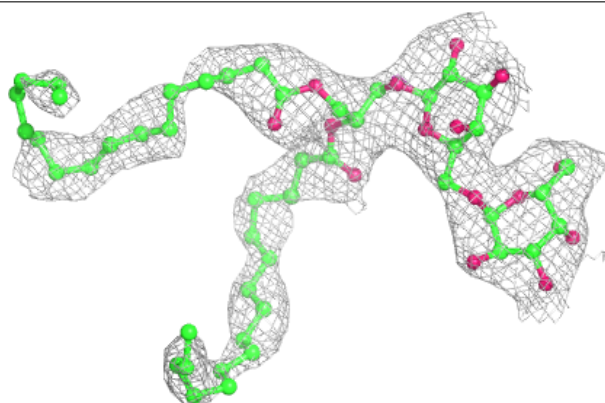


Electron density around CLA C 505:

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

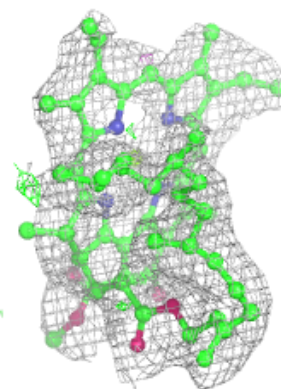
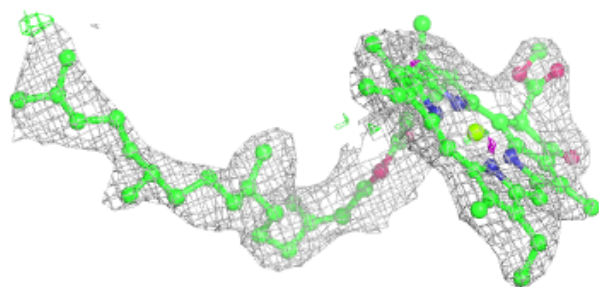
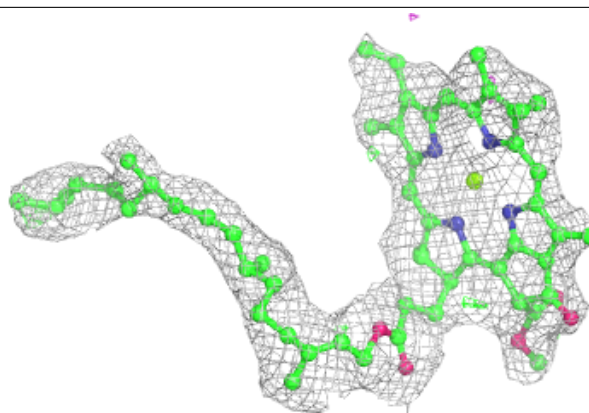
**Electron density around DGD c 517:**

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

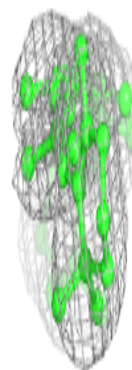
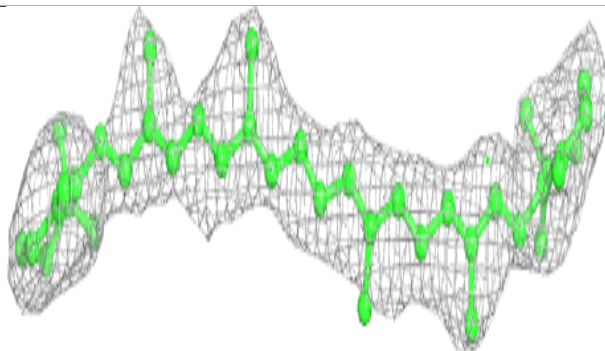
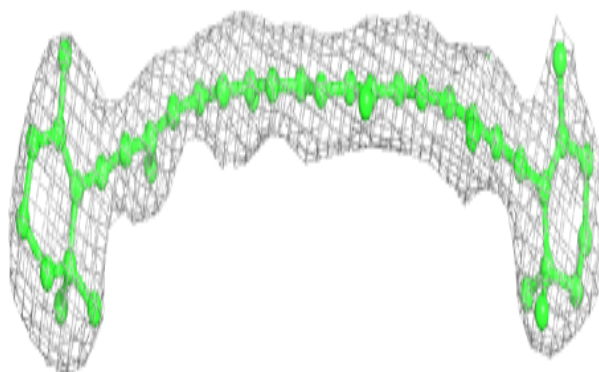


Electron density around CLA c 511:

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

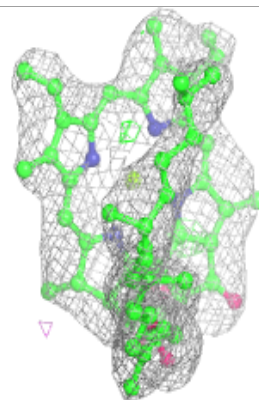
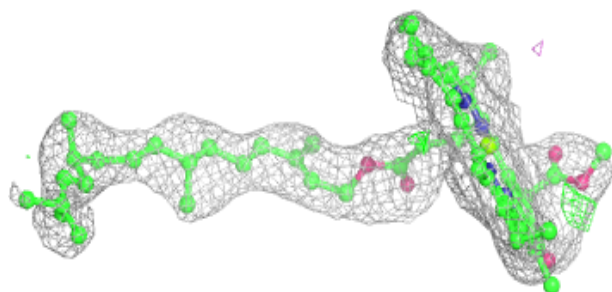
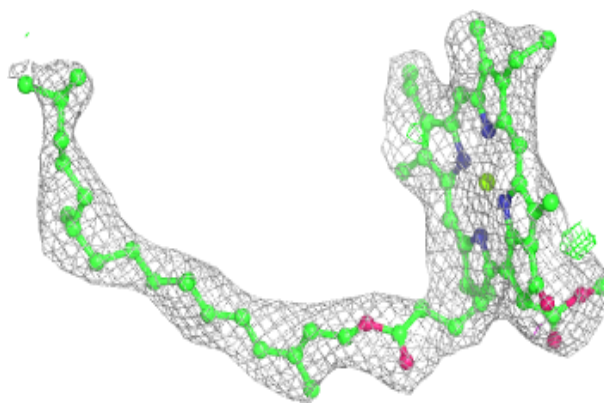
**Electron density around BCR K 101:**

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

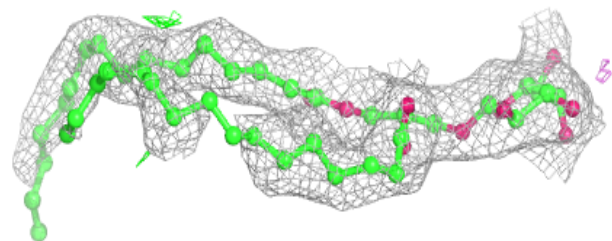
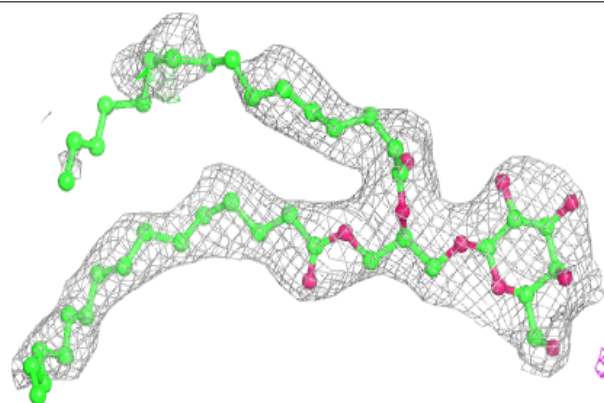


Electron density around CLA B 610:

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

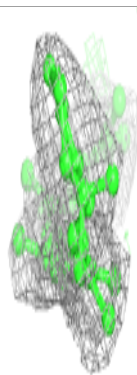
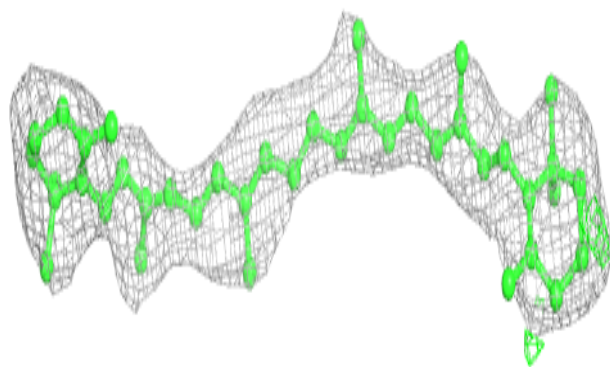
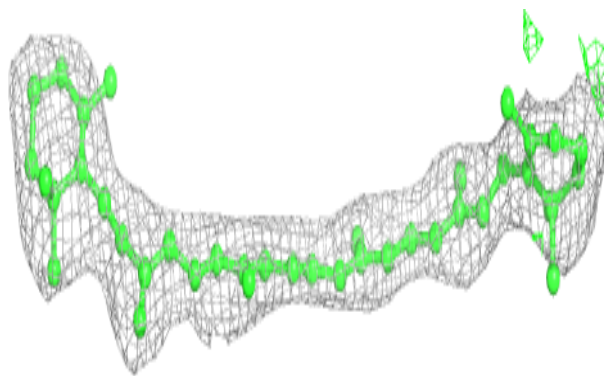
**Electron density around LMG f 101:**

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

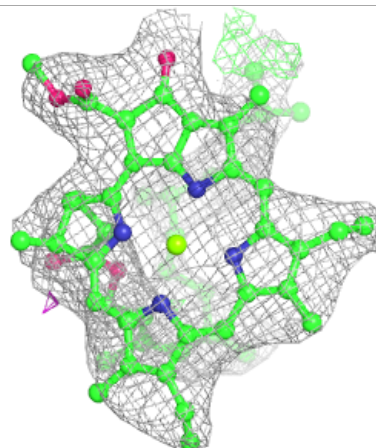
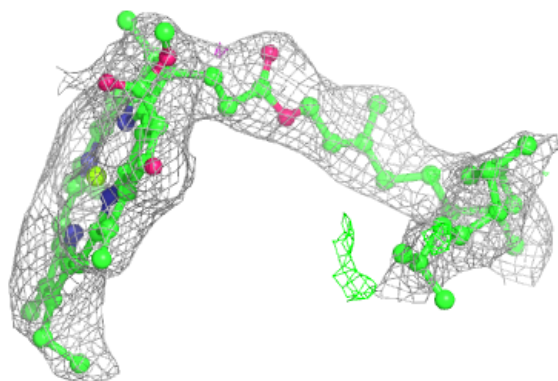
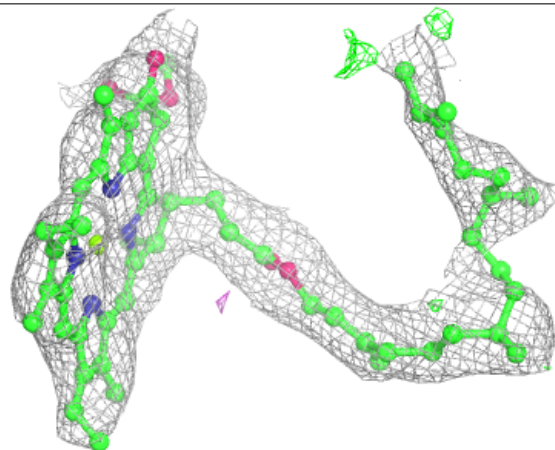


Electron density around BCR d 404:

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

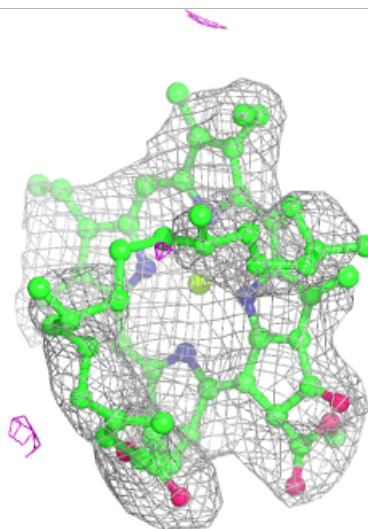
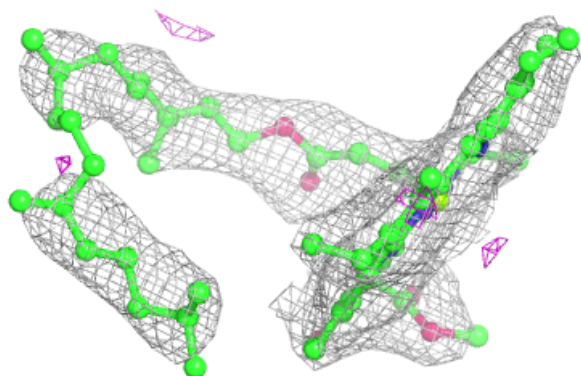
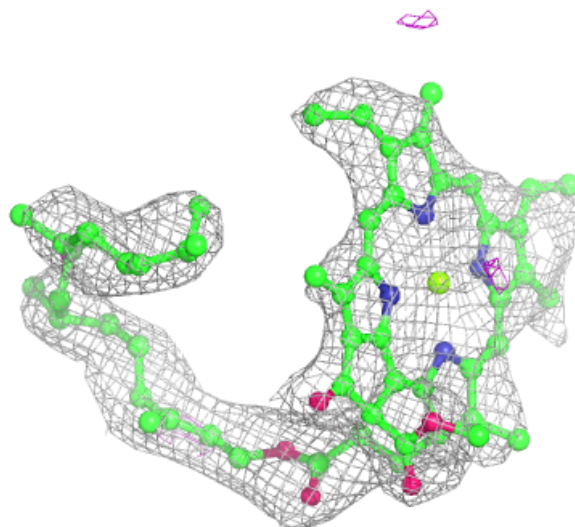
**Electron density around CLA B 607:**

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



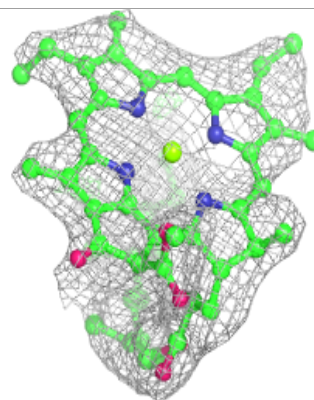
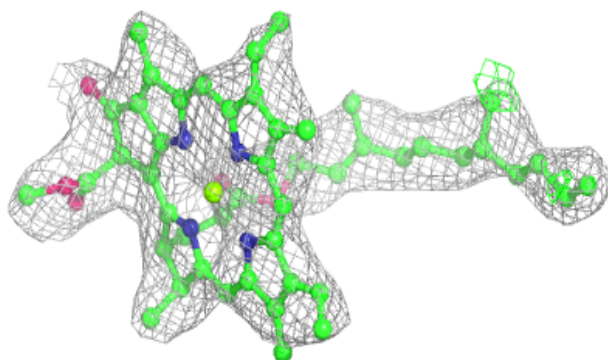
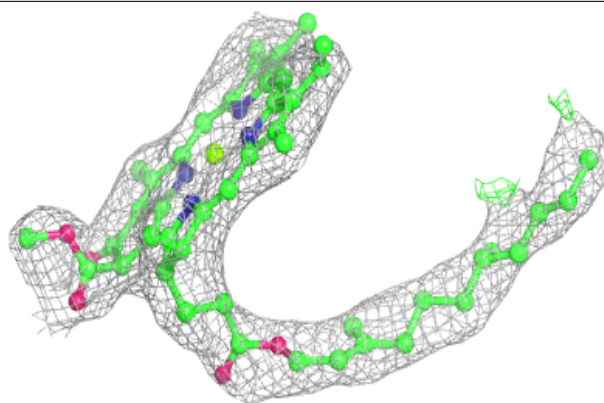
Electron density around CLA c 503:

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

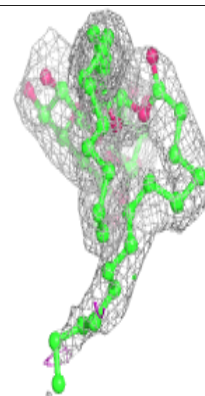
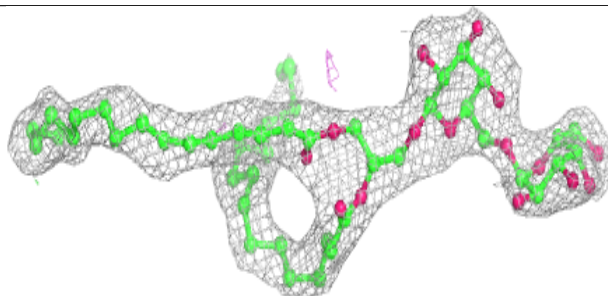
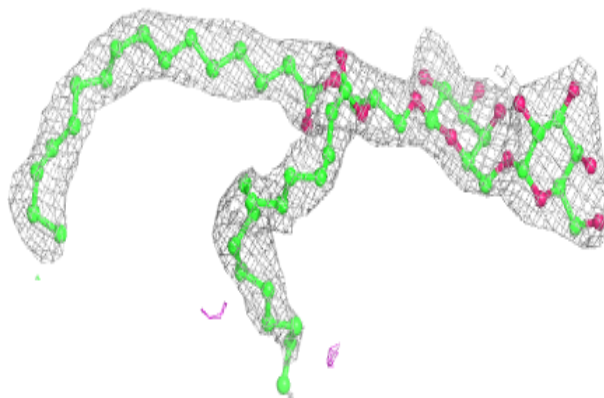


Electron density around CLA c 504:

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

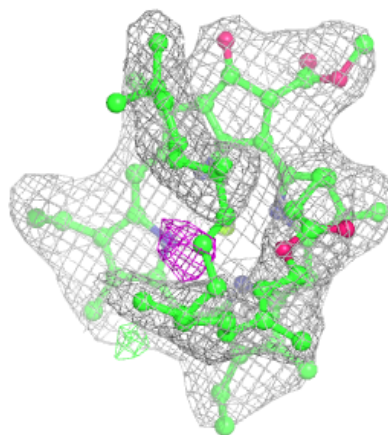
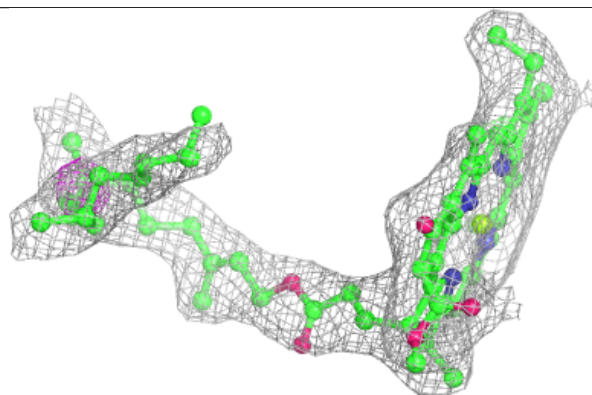
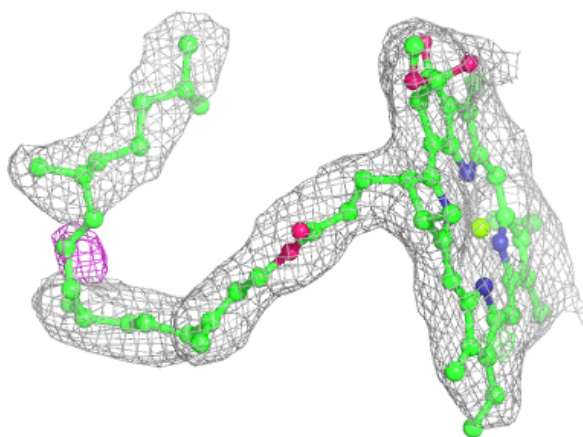
**Electron density around DGD h 102:**

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

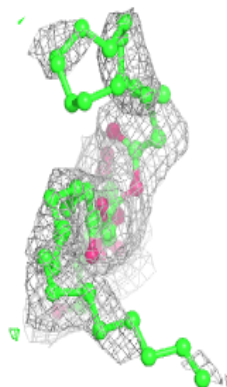
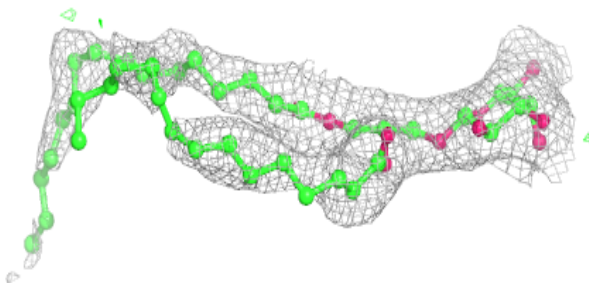
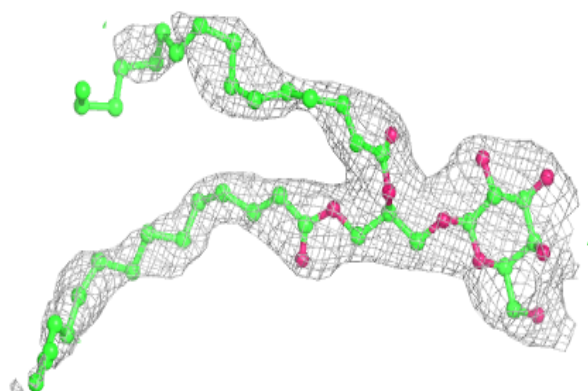


Electron density around CLA b 612:

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

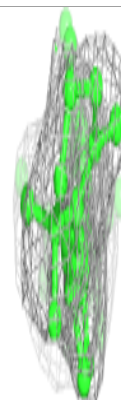
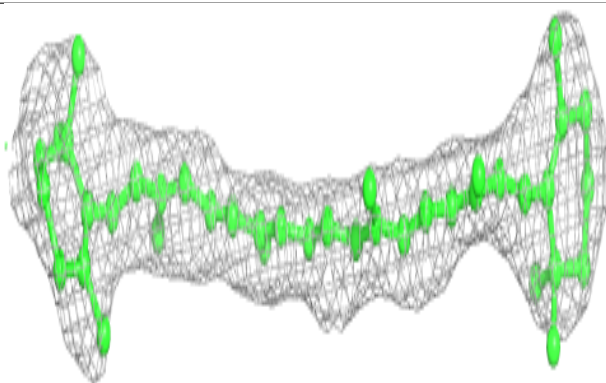
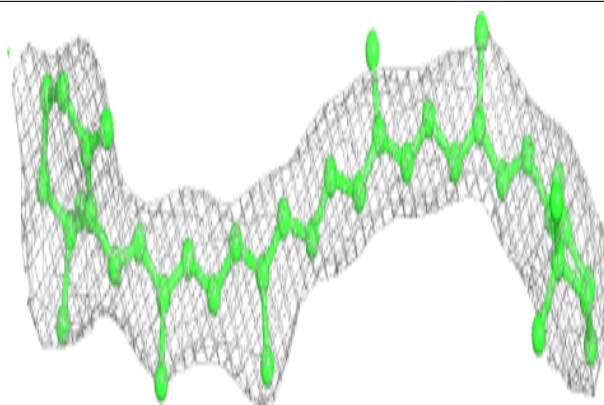
**Electron density around LMG D 409:**

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

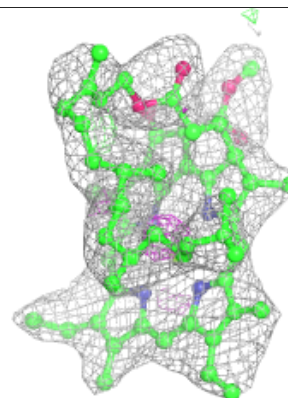
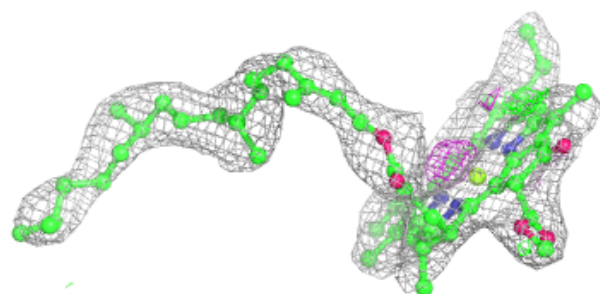
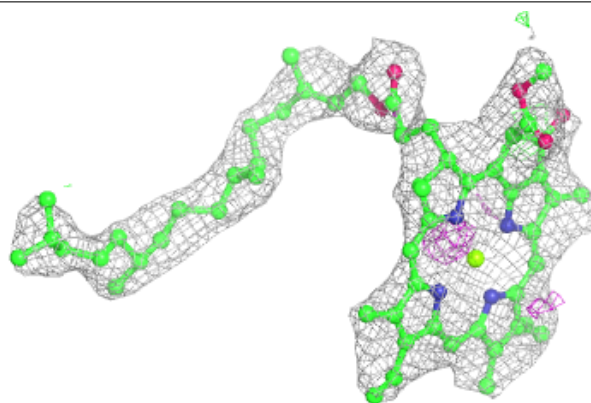


Electron density around BCR Y 101:

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

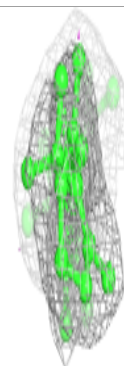
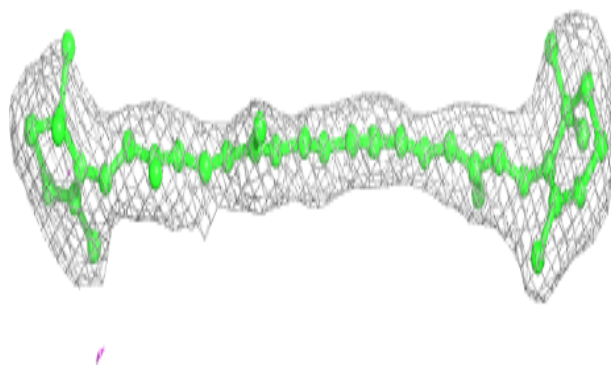
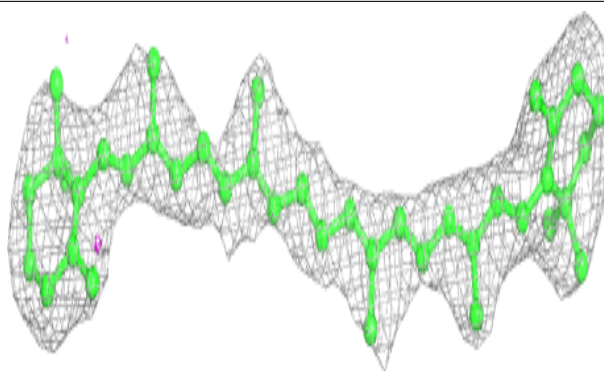
**Electron density around CLA C 512:**

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

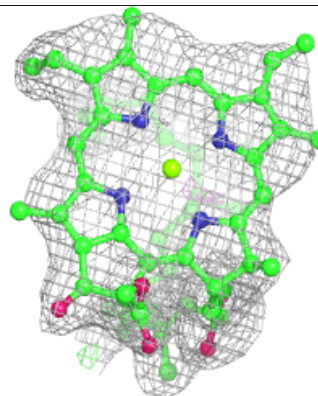
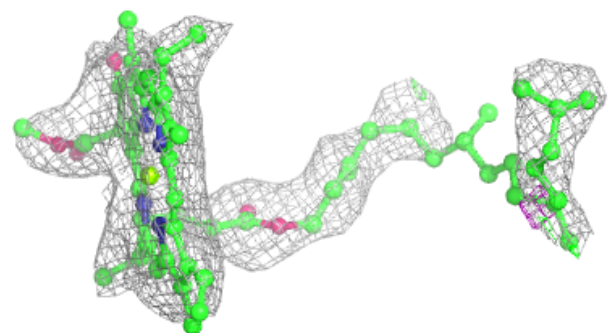
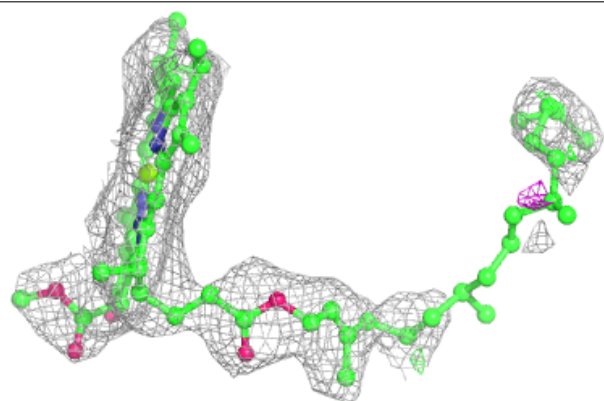


Electron density around BCR b 624:

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

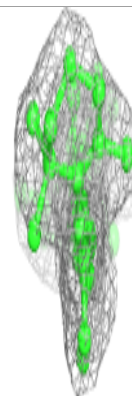
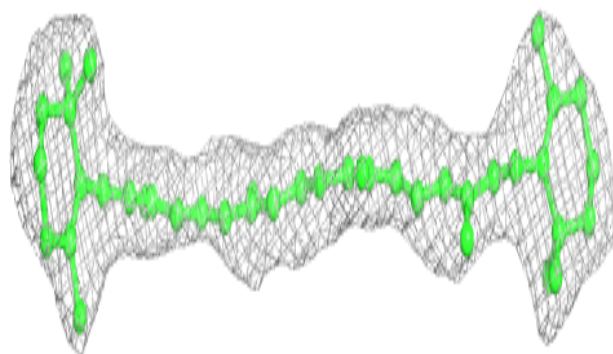
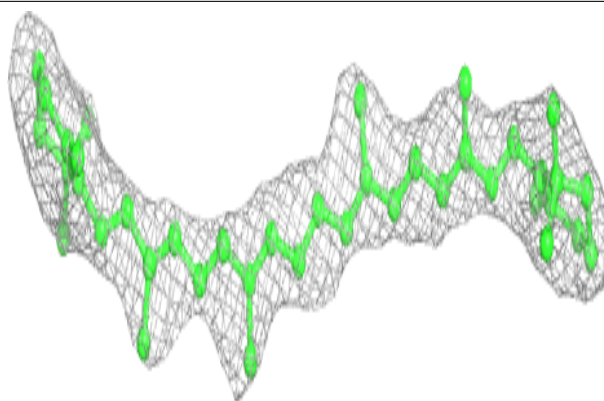
**Electron density around CLA c 506:**

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

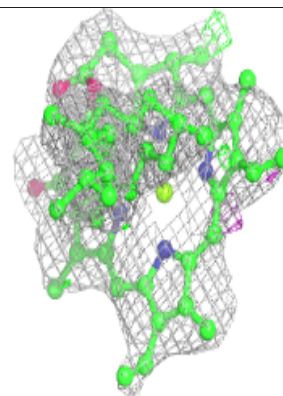
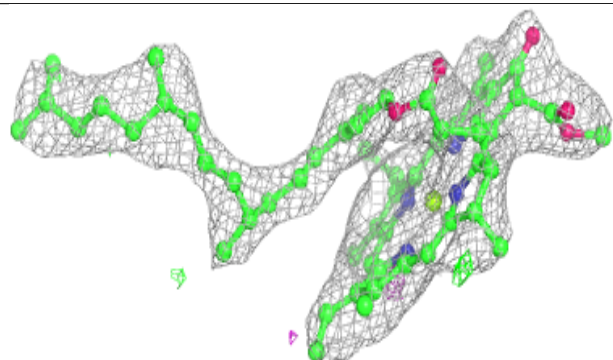
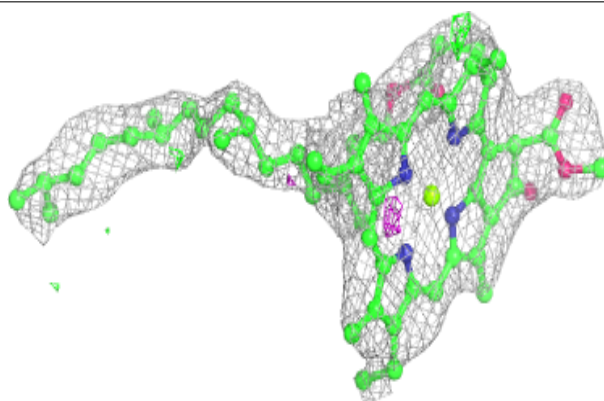


Electron density around BCR c 515:

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

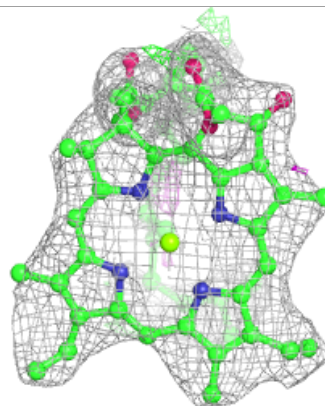
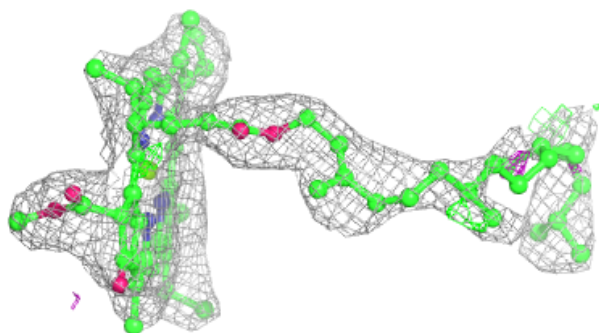
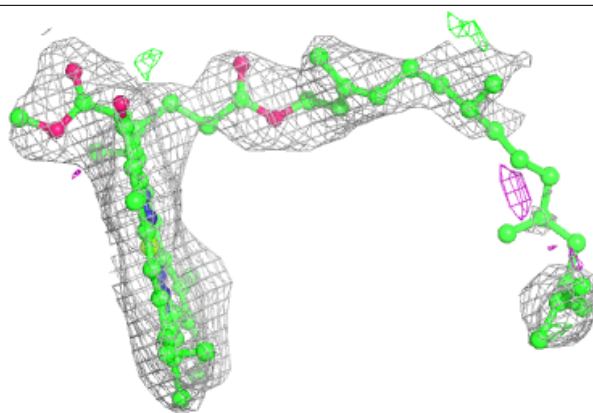
**Electron density around CLA C 506:**

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

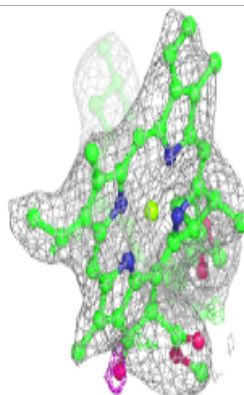
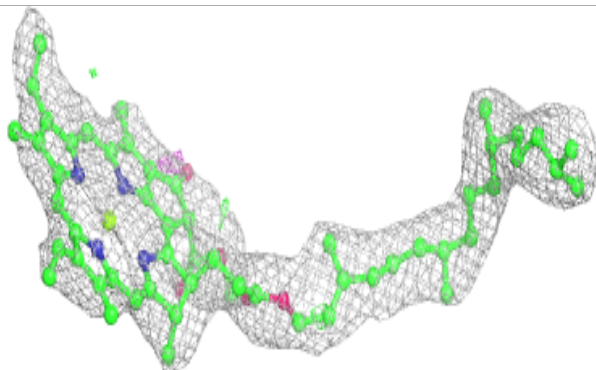
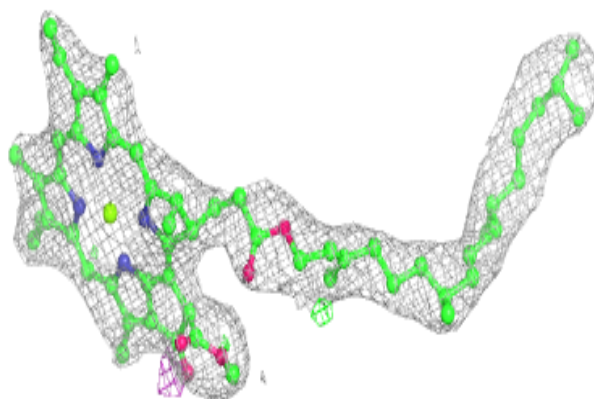


Electron density around CLA C 507:

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

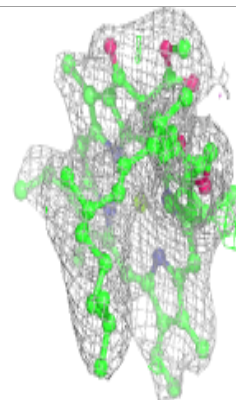
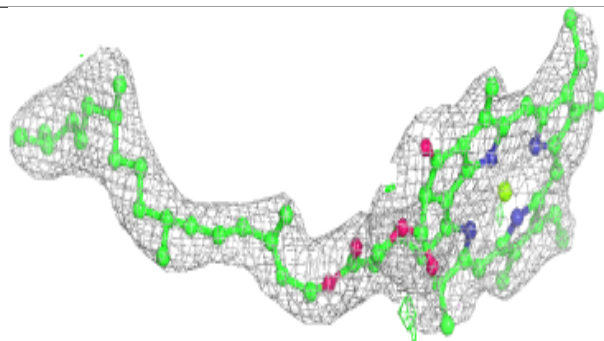
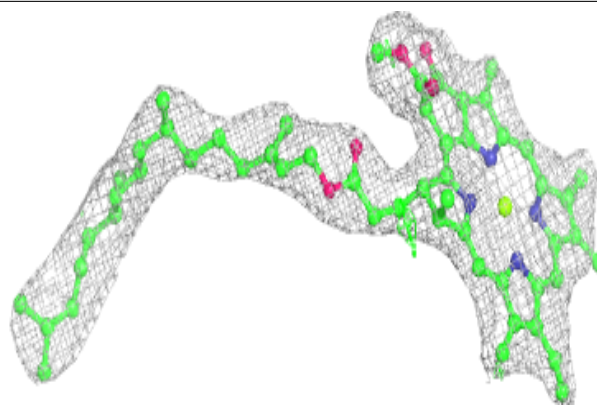
**Electron density around CLA A 606:**

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

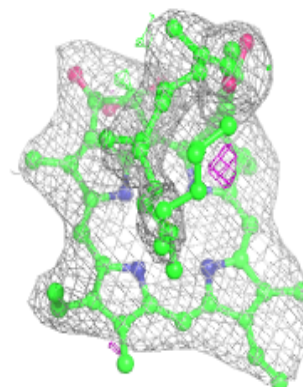
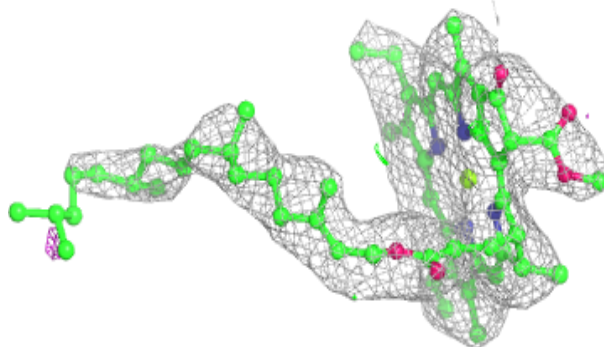
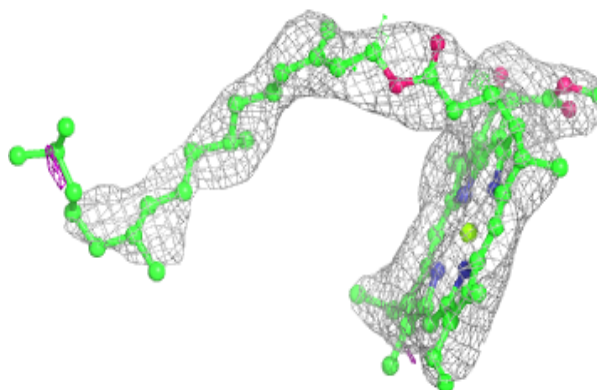


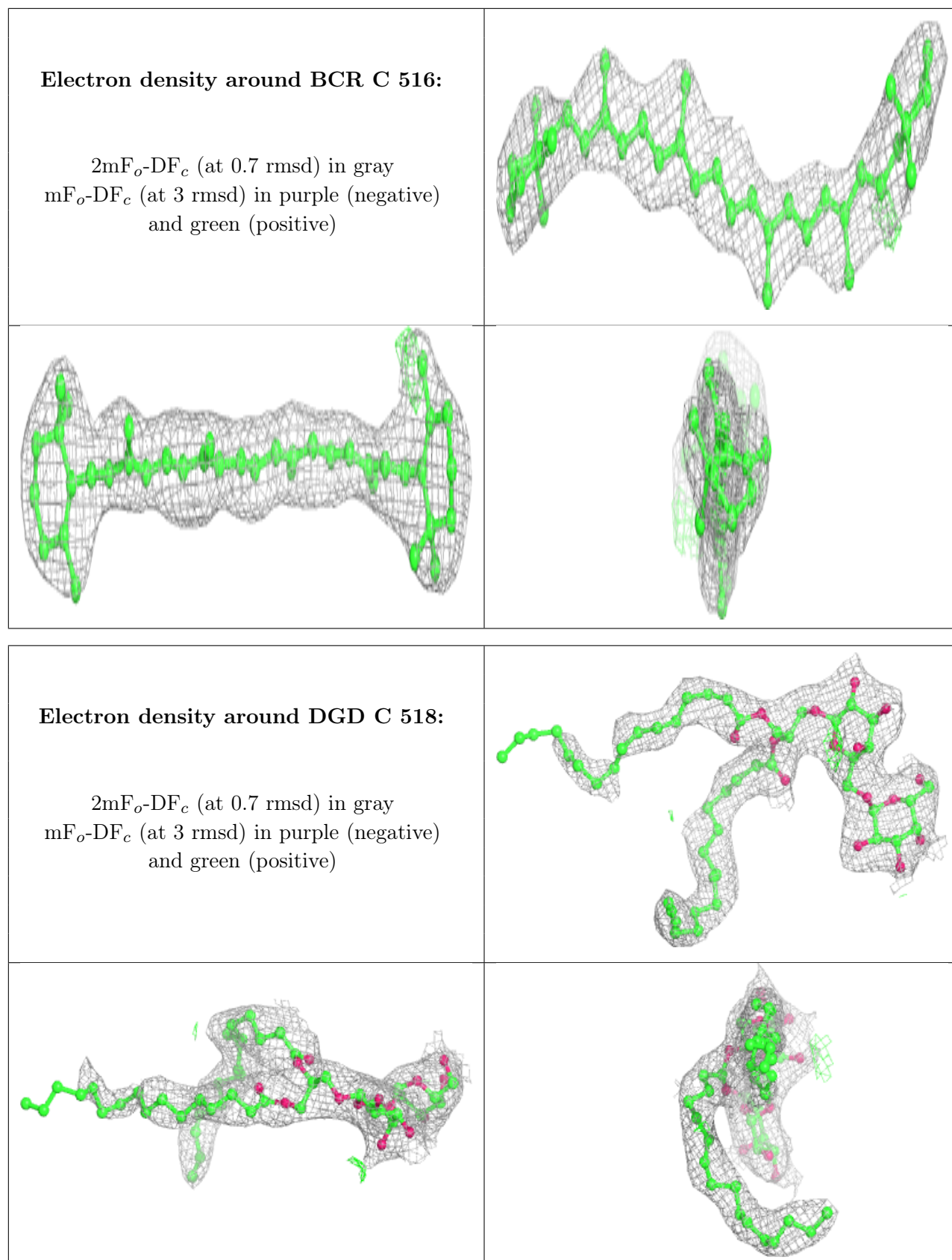
Electron density around CLA a 707:

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

**Electron density around CLA C 509:**

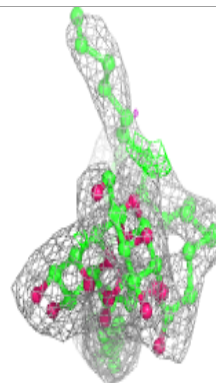
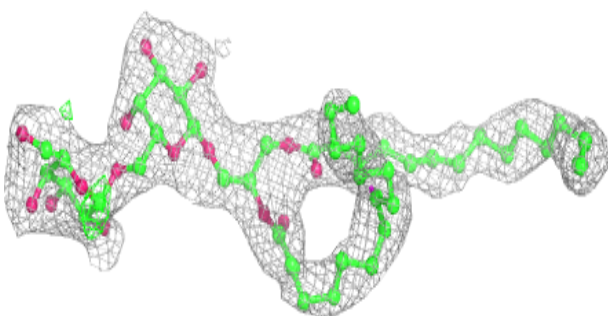
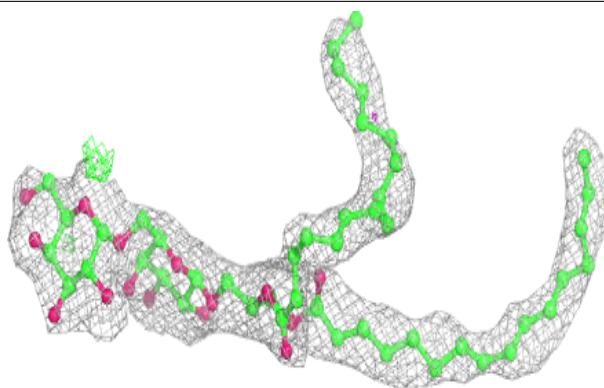
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



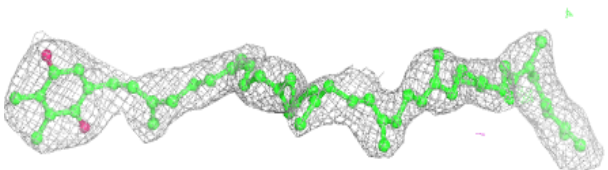
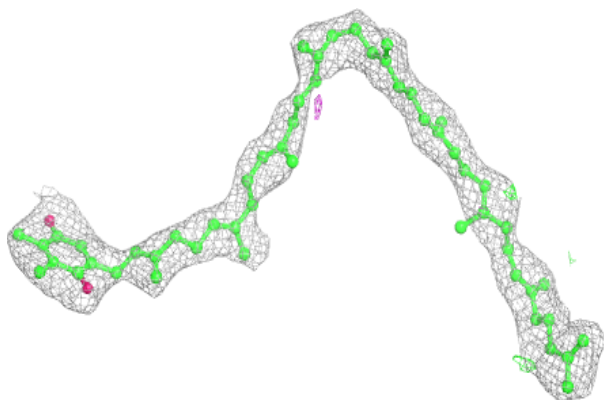


Electron density around DGD H 103:

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

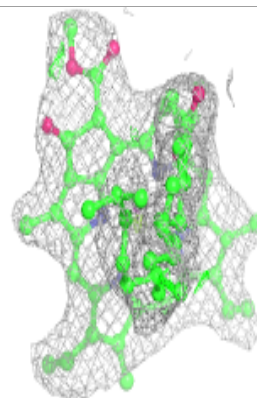
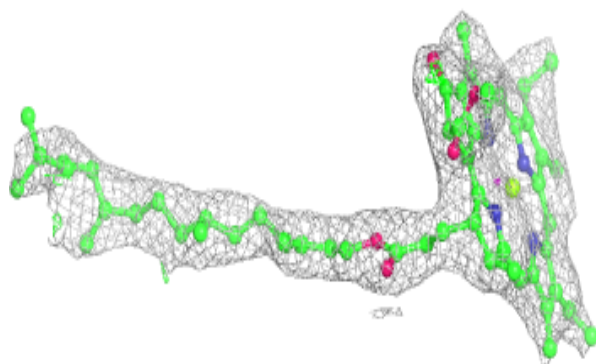
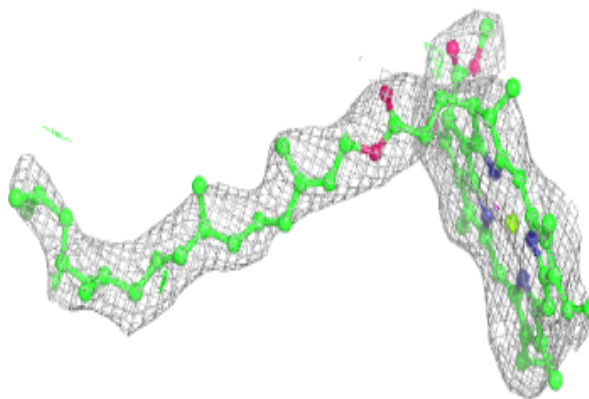
**Electron density around PL9 D 406:**

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

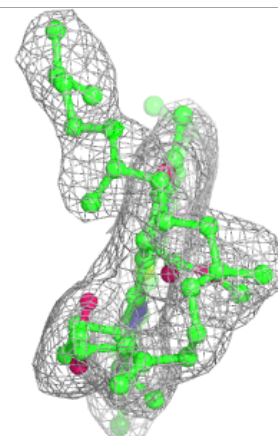
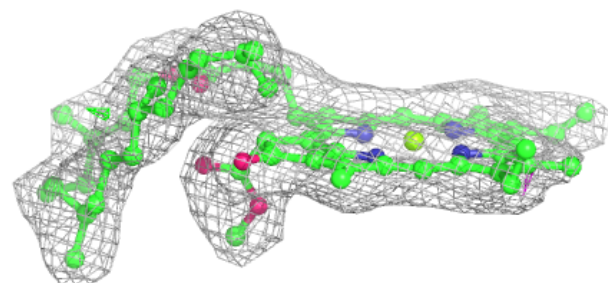
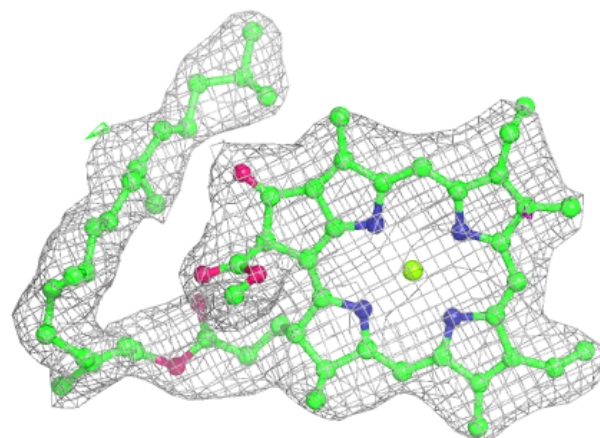


Electron density around CLA b 610:

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

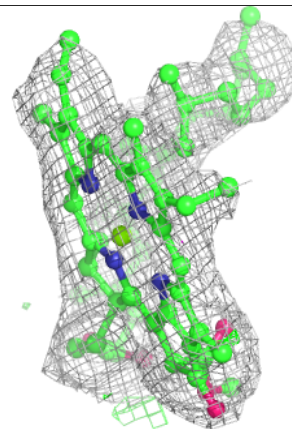
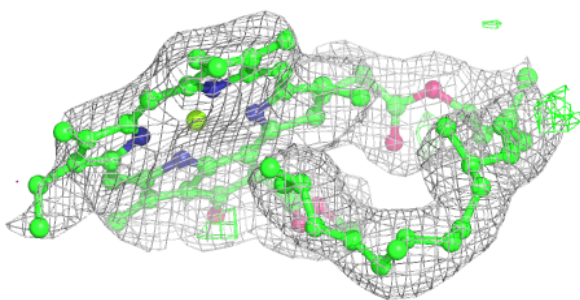
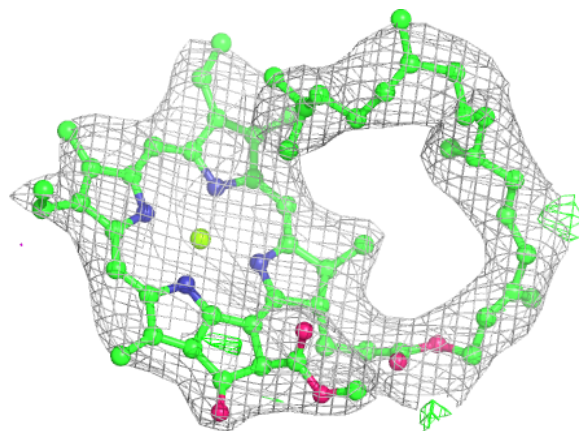
**Electron density around CLA b 616:**

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



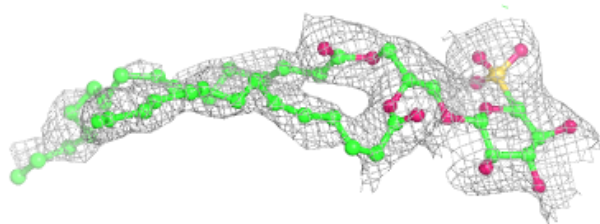
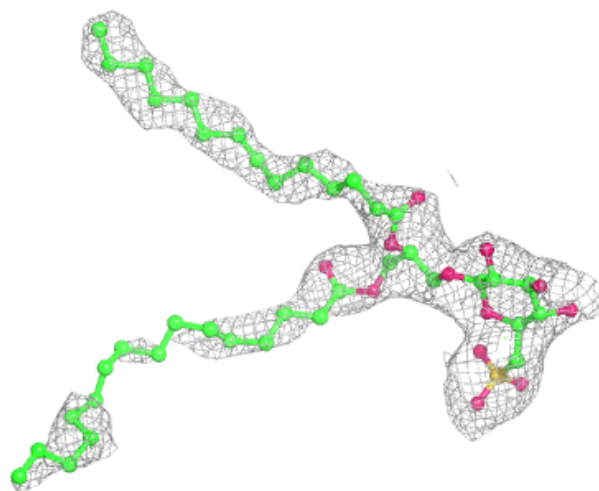
Electron density around CLA b 621:

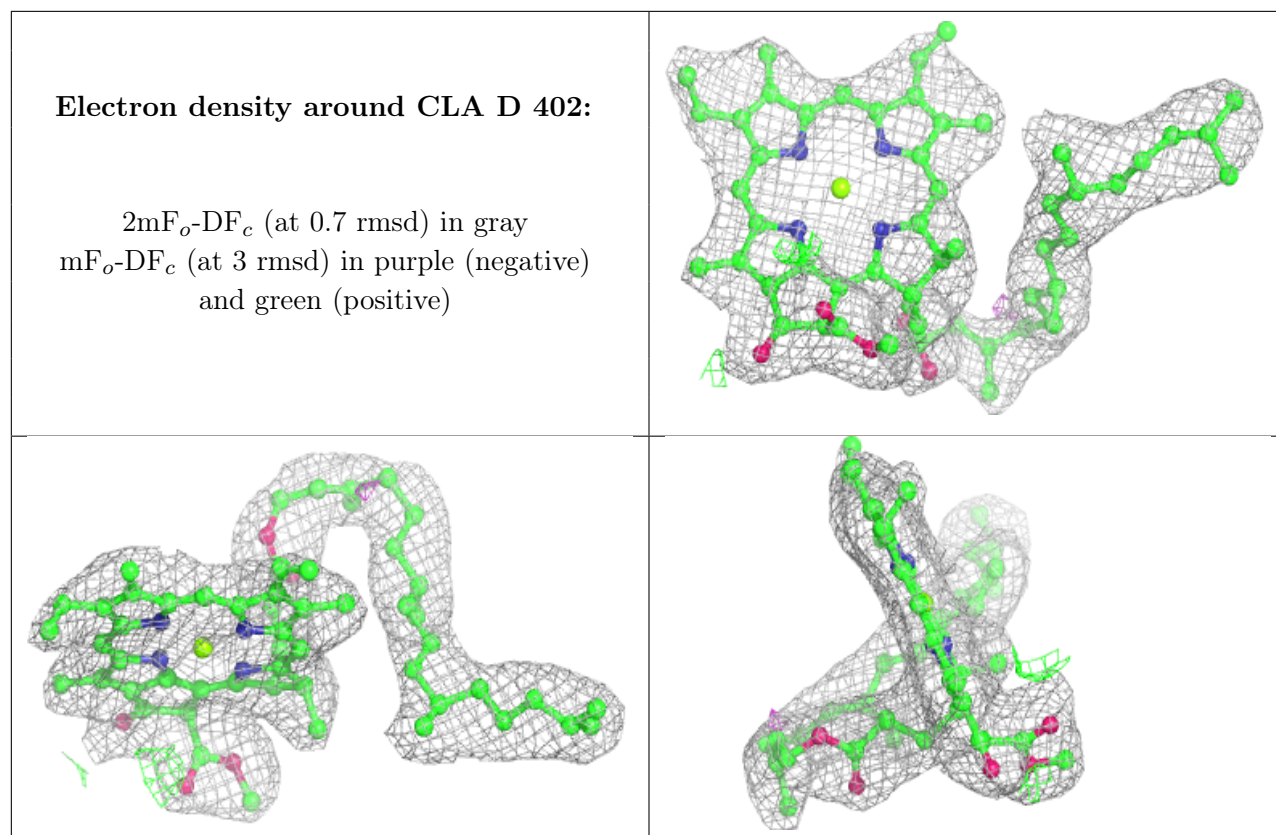
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD A 612:

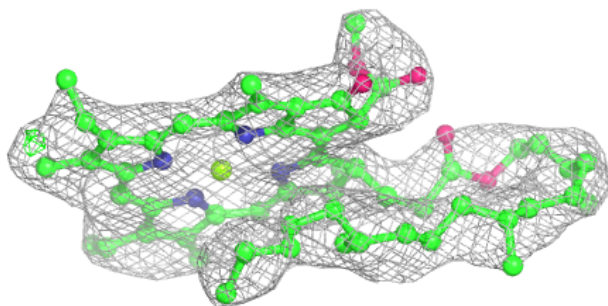
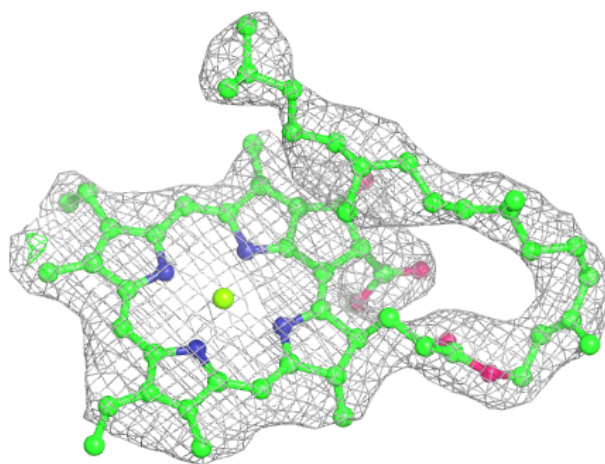
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





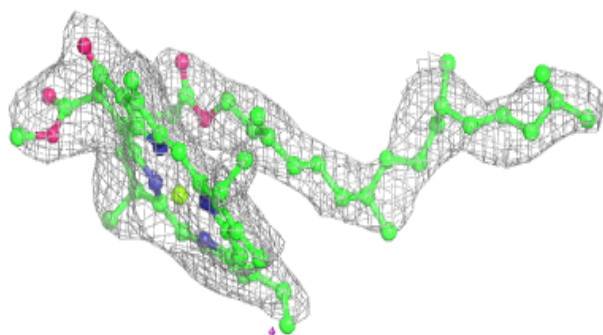
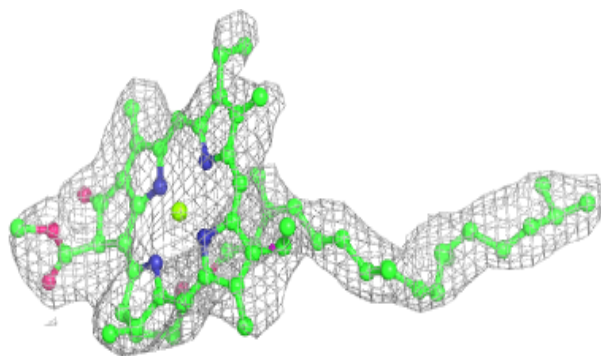
Electron density around CLA C 510:

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

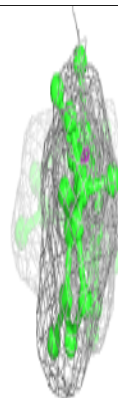
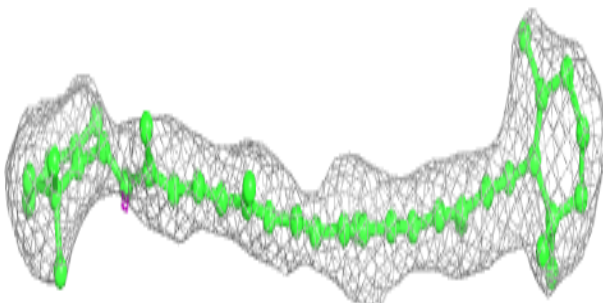
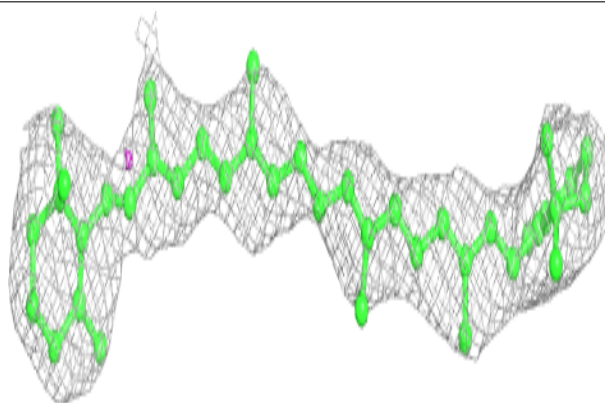


Electron density around CLA c 505:

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

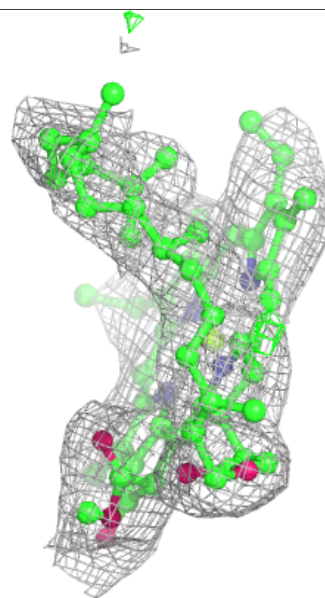
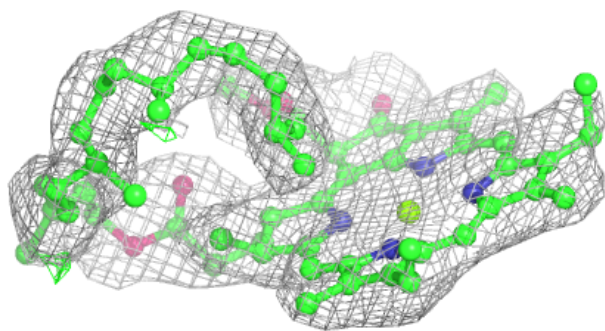
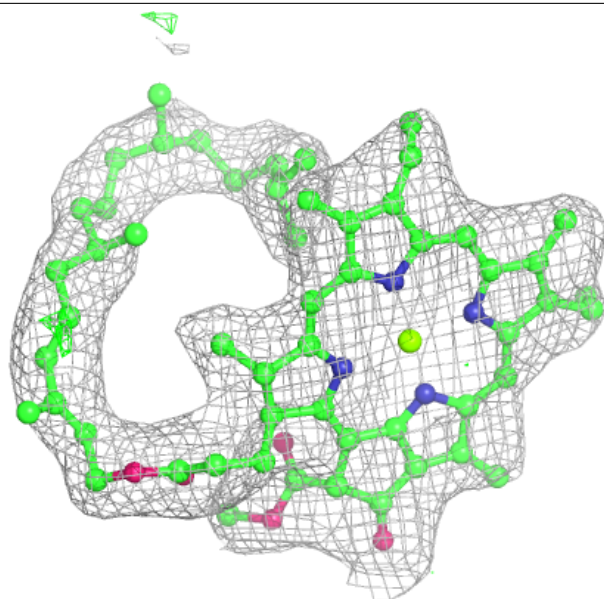
**Electron density around BCR b 623:**

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



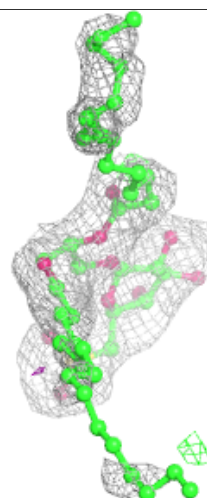
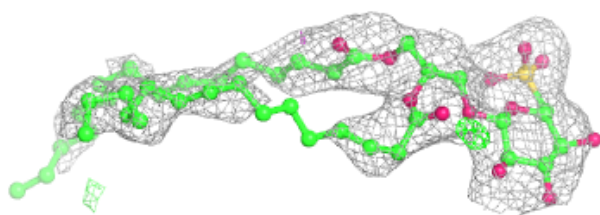
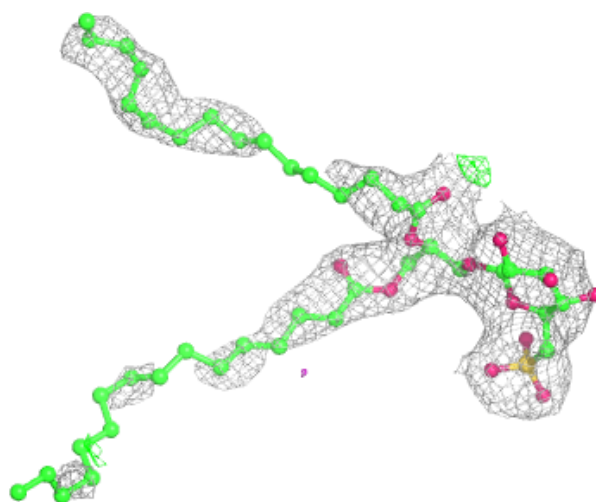
Electron density around CLA B 616:

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



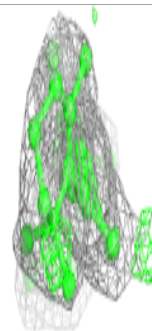
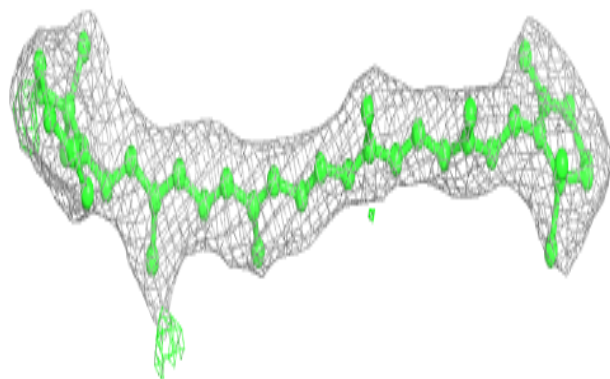
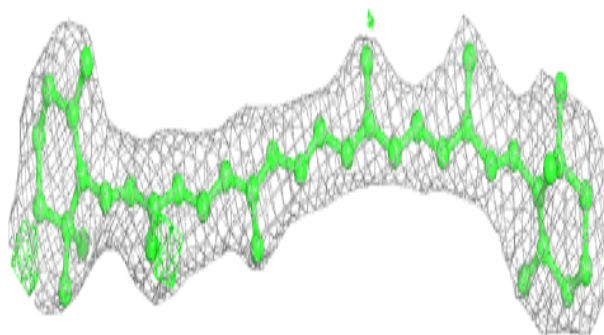
Electron density around SQD a 714:

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

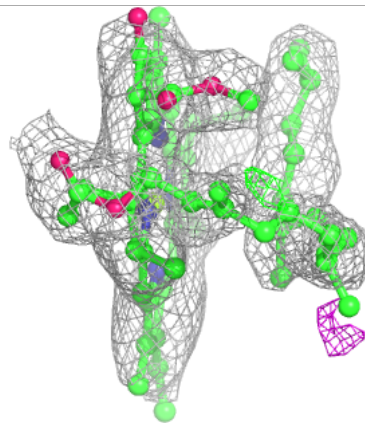
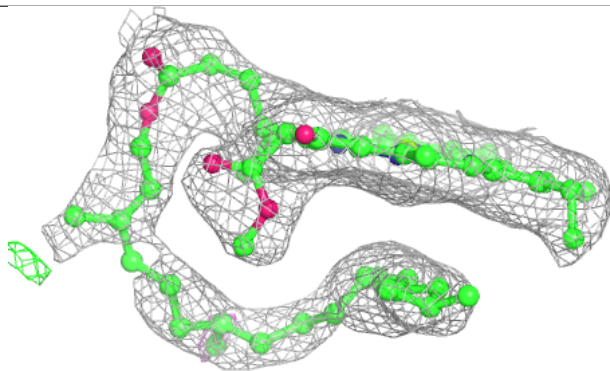
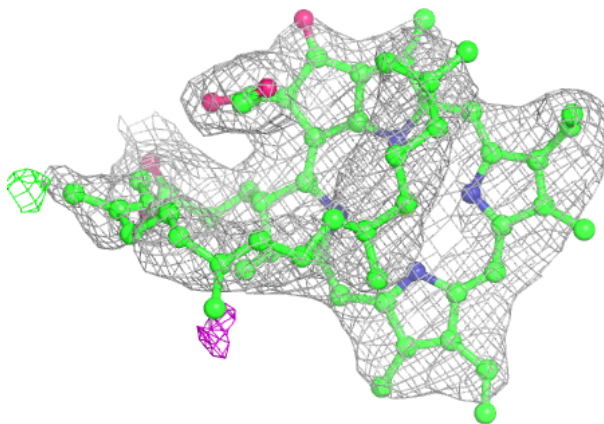


Electron density around BCR b 625:

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

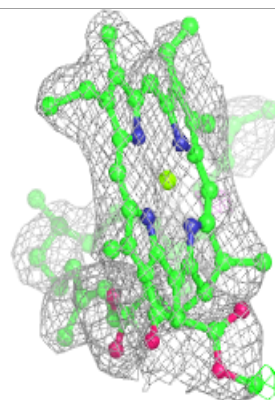
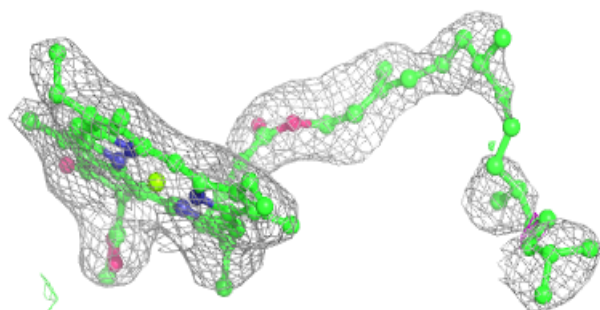
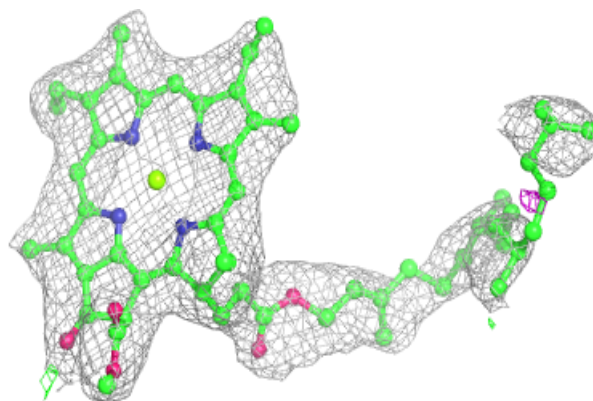
**Electron density around CLA c 510:**

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

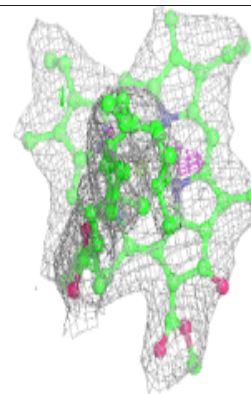
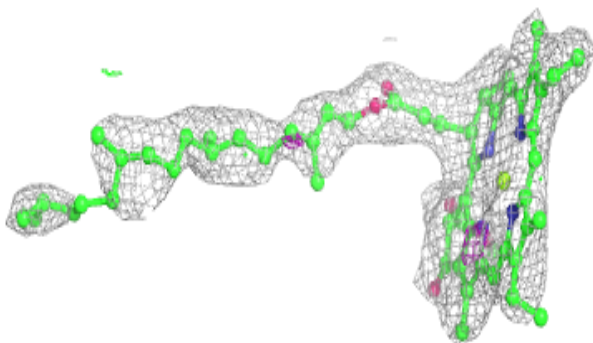
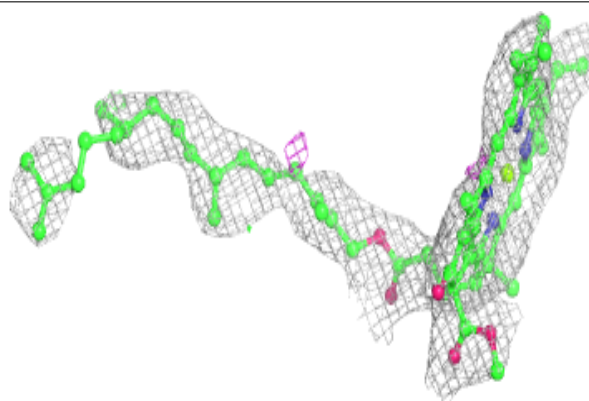


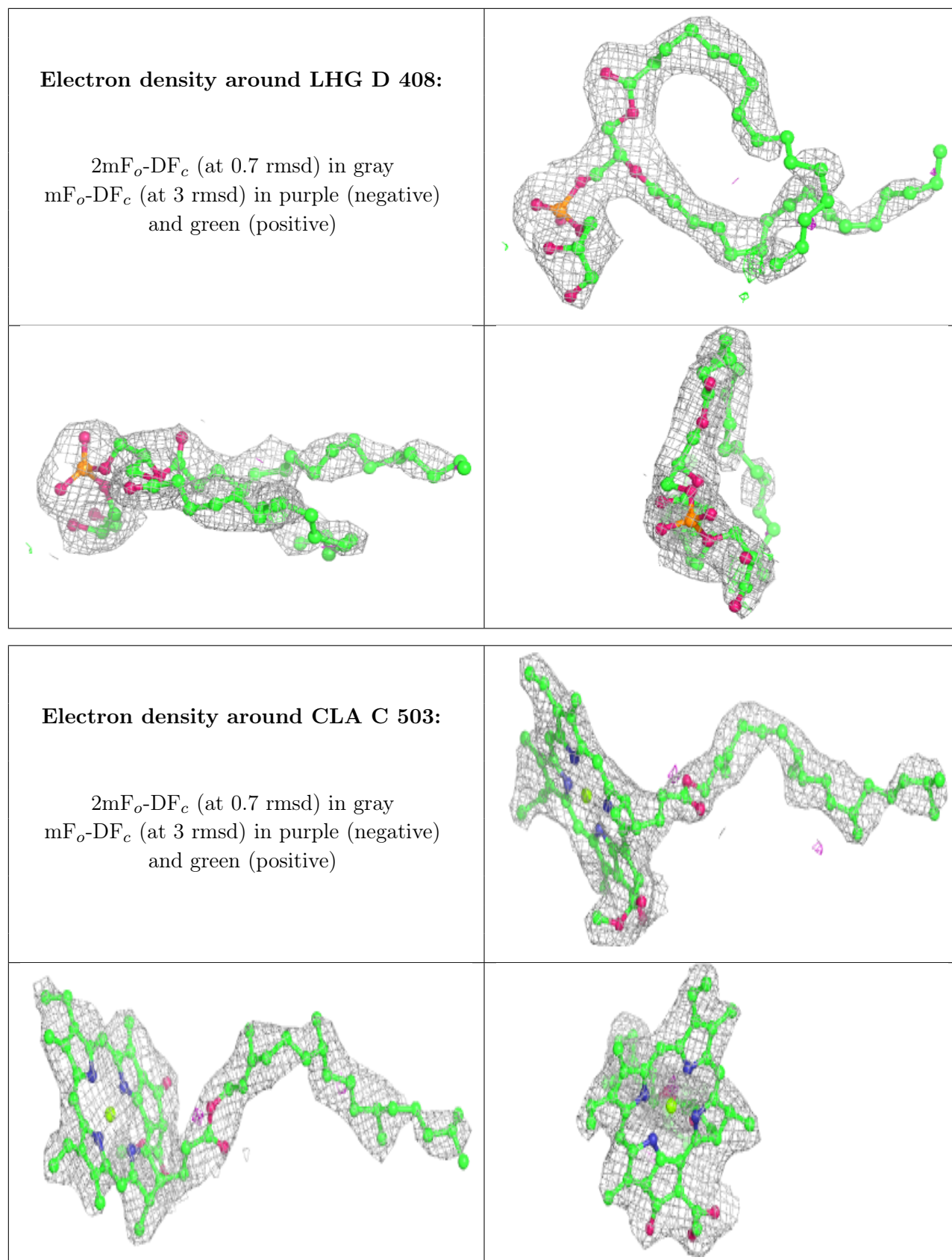
Electron density around CLA a 711:

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

**Electron density around CLA B 605:**

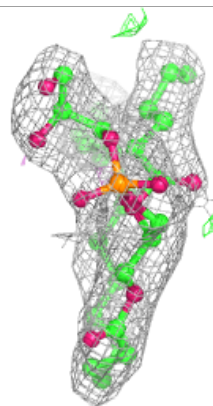
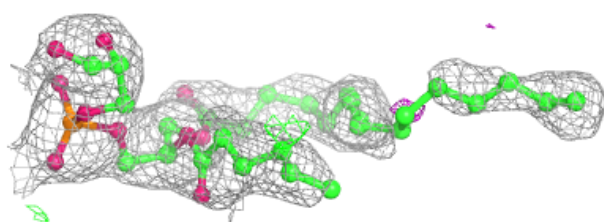
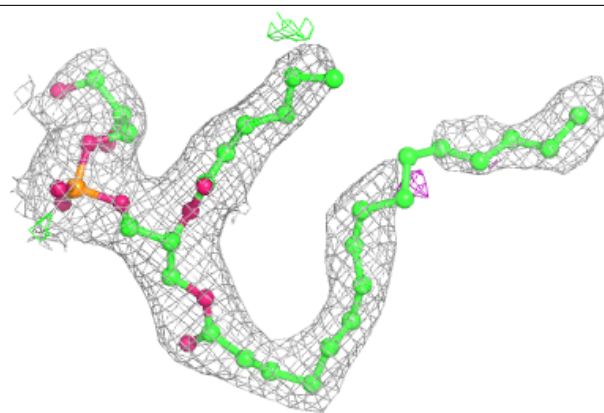
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



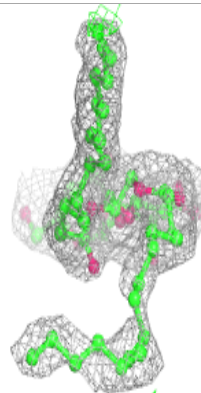
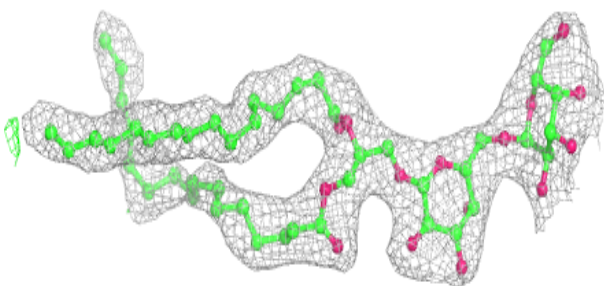
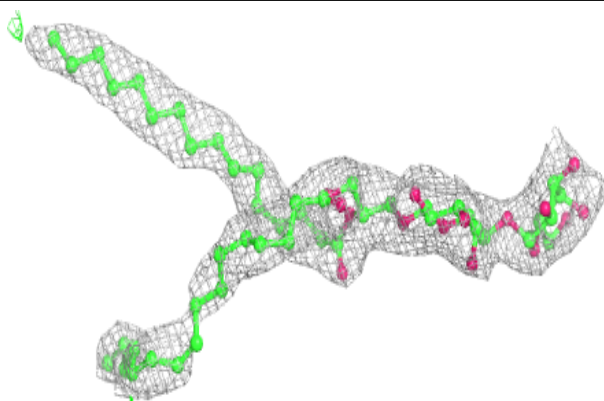


Electron density around LHG a 720:

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

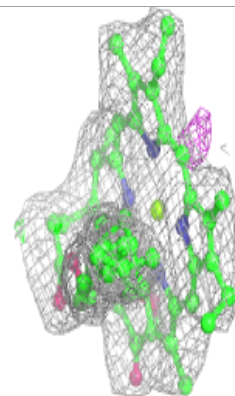
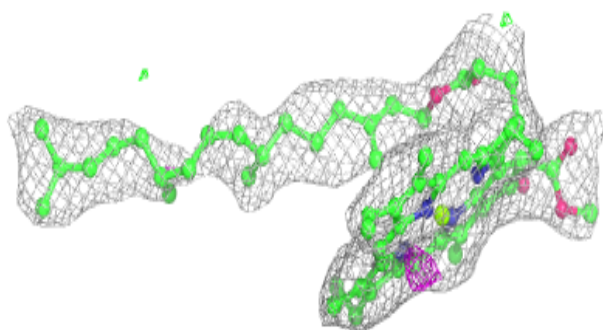
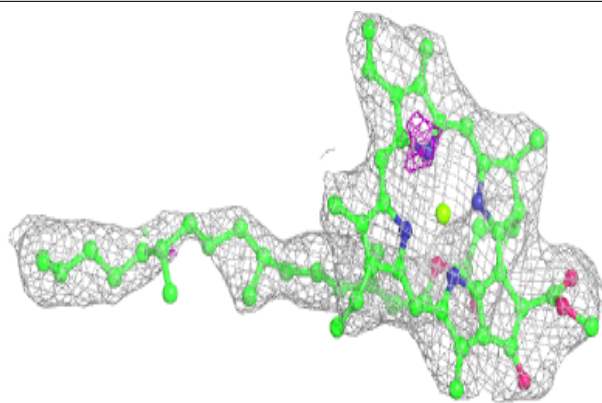
**Electron density around DGD C 517:**

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

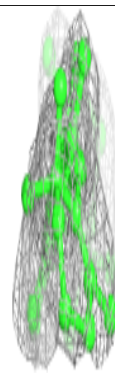
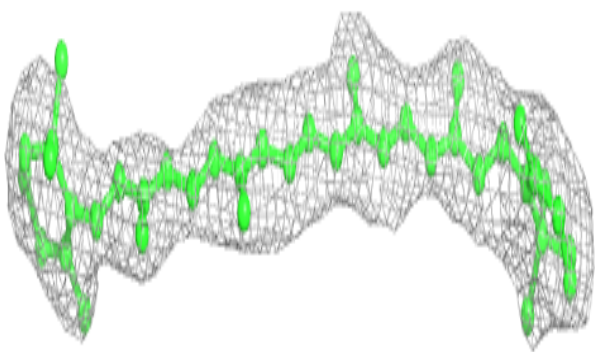
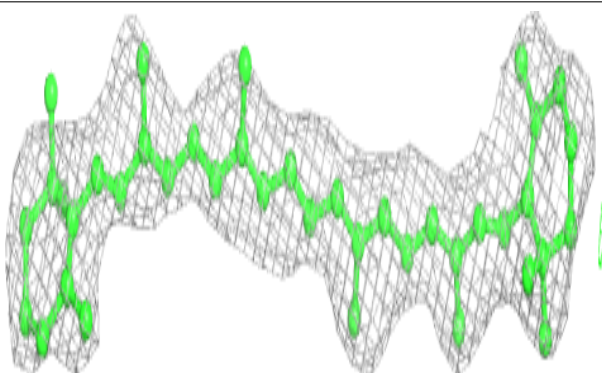


Electron density around CLA B 615:

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

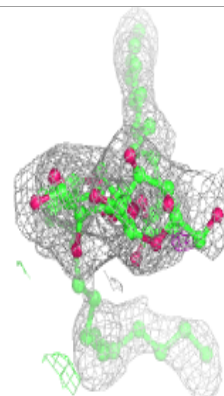
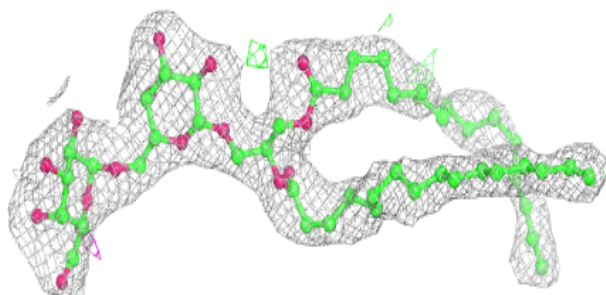
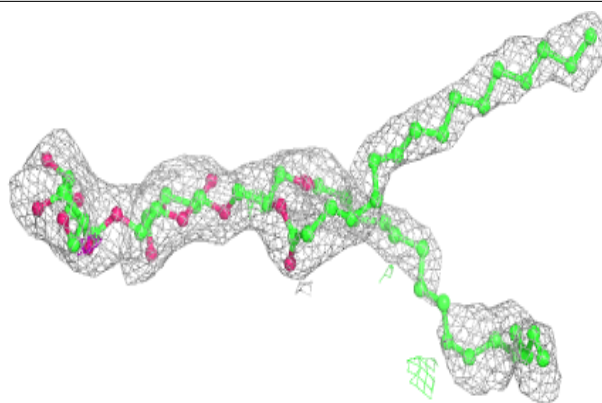
**Electron density around BCR B 620:**

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

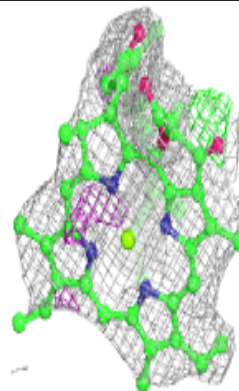
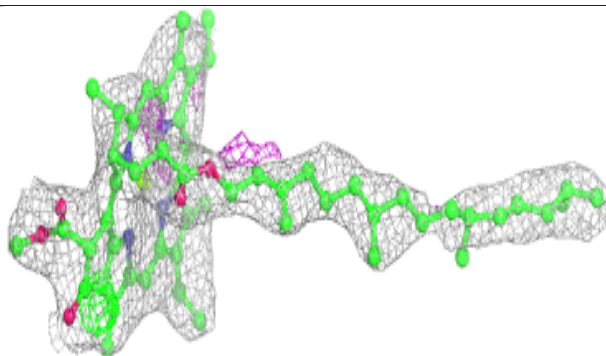
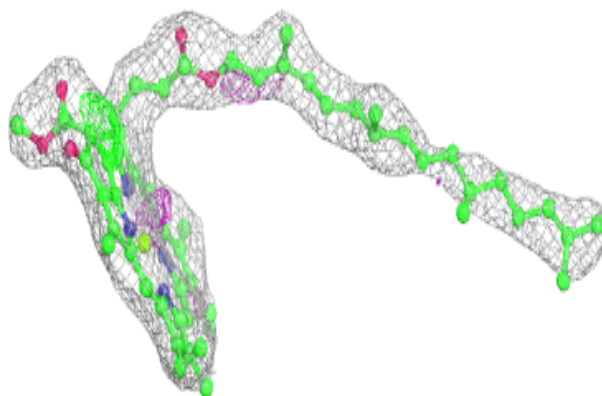


Electron density around DGD c 516:

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

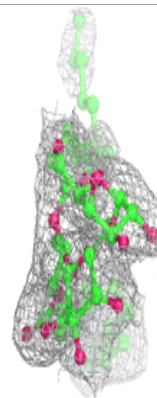
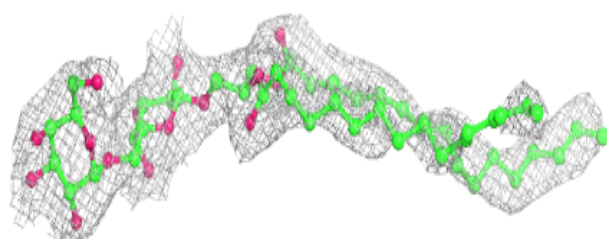
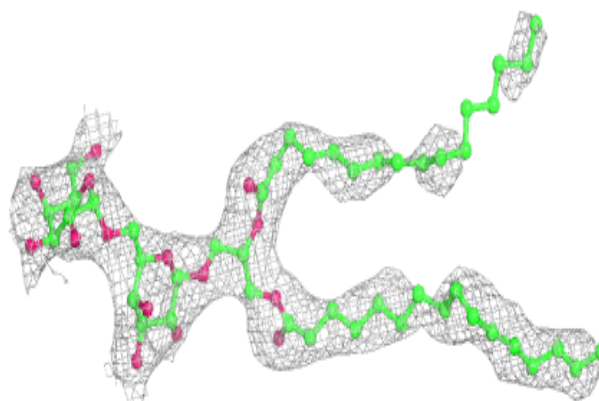
**Electron density around CLA b 613:**

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

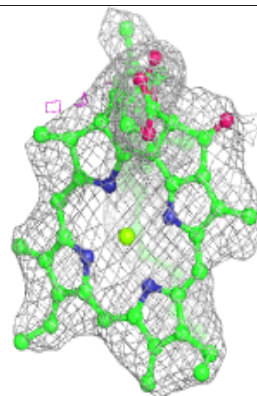
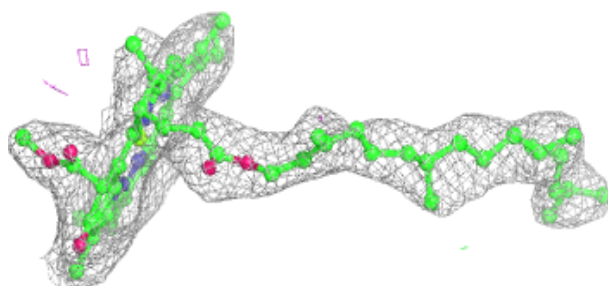
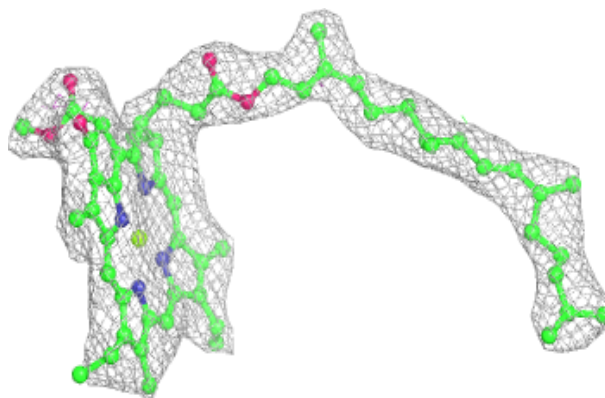


Electron density around DGD c 518:

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

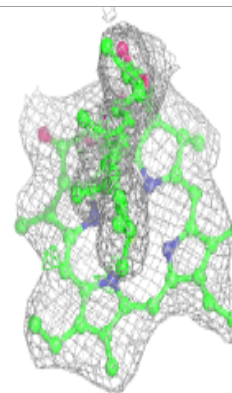
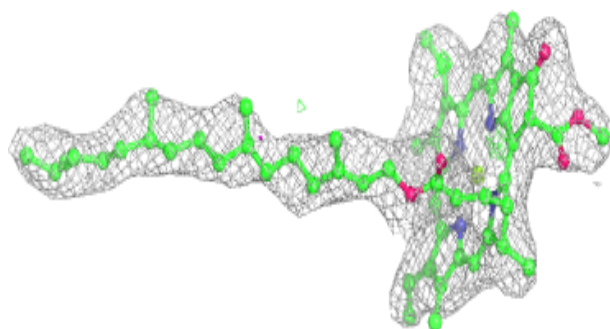
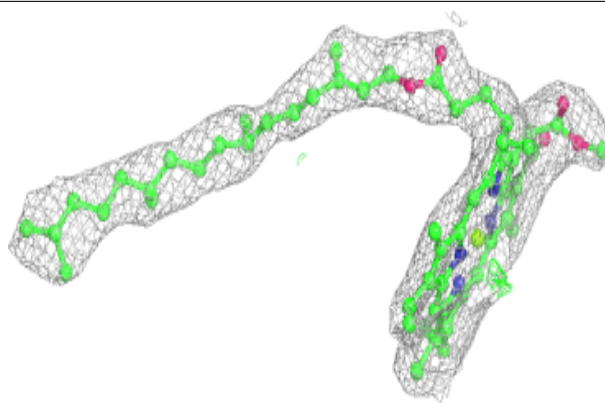
**Electron density around CLA b 615:**

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

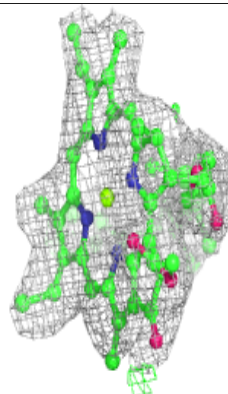
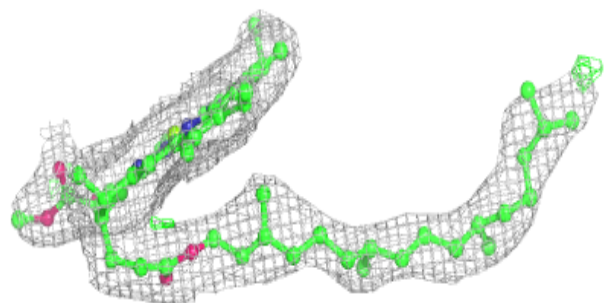
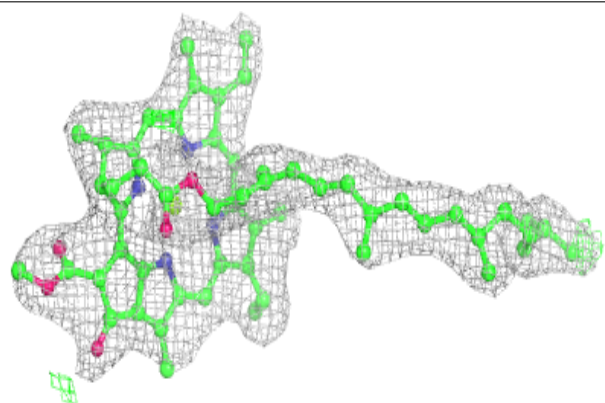


Electron density around CLA B 608:

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

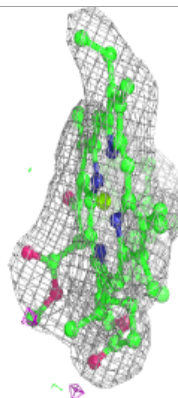
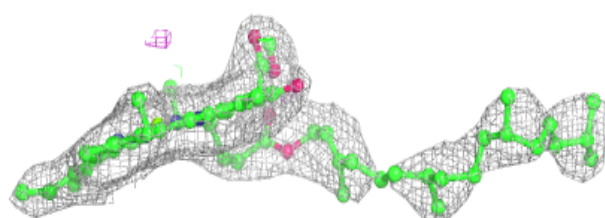
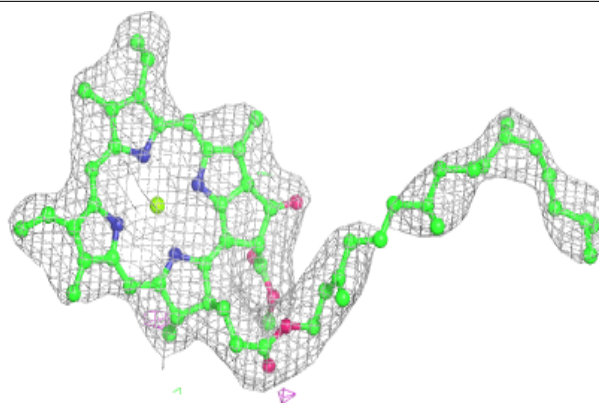
**Electron density around CLA B 609:**

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

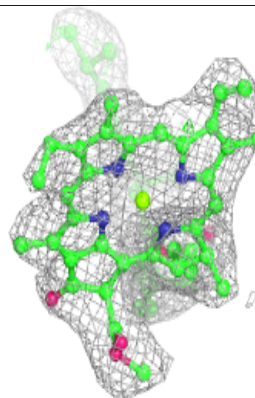
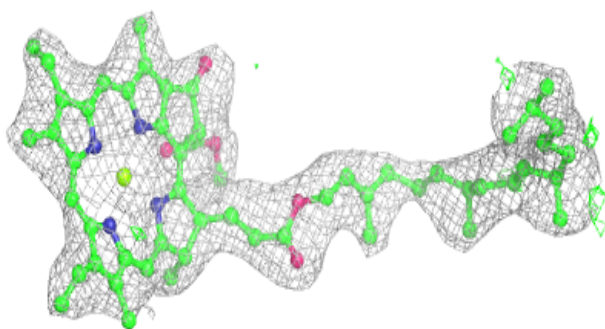
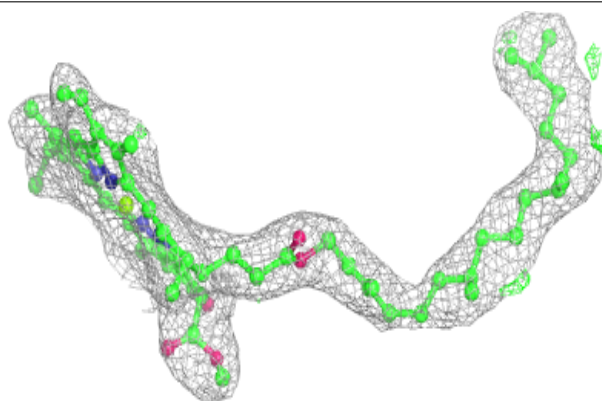


Electron density around CLA b 608:

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

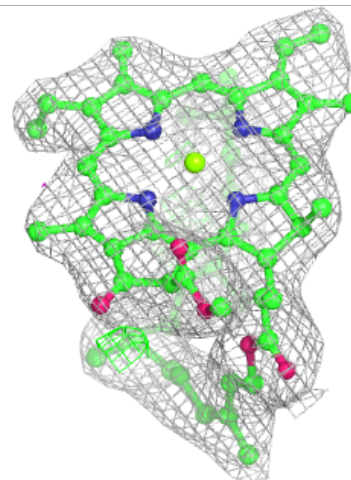
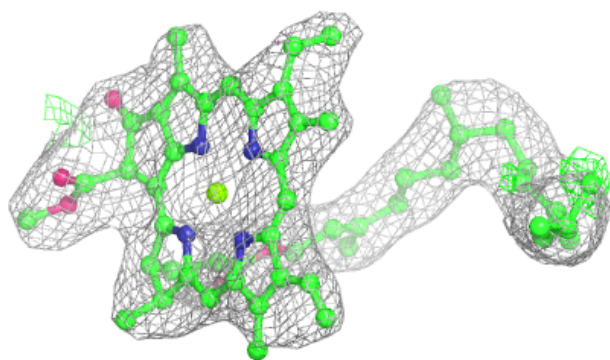
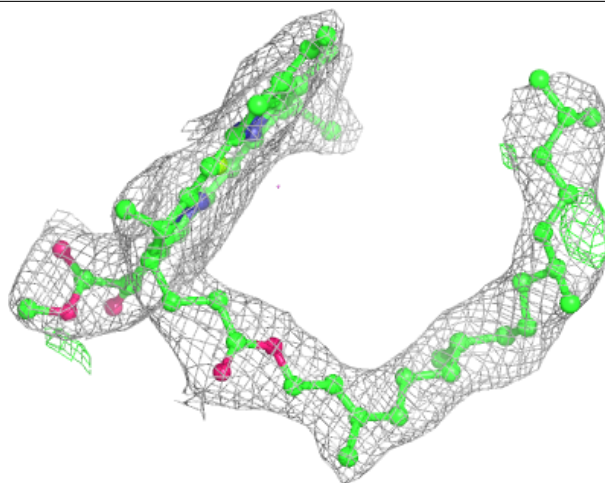
**Electron density around CLA d 402:**

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



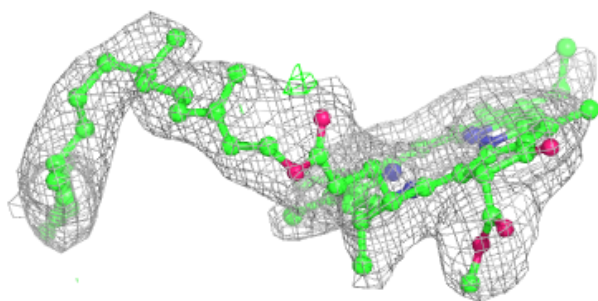
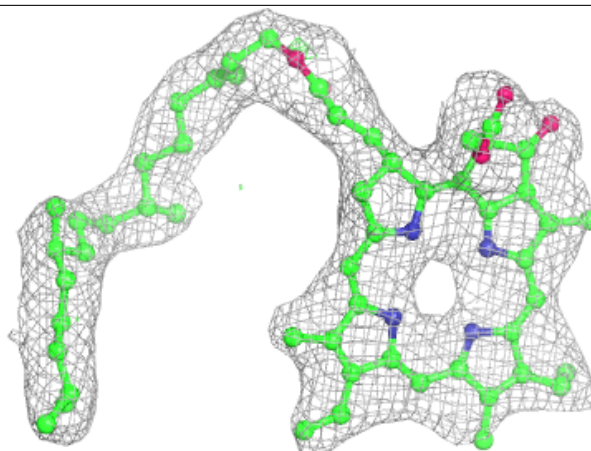
Electron density around CLA B 612:

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

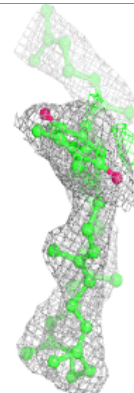
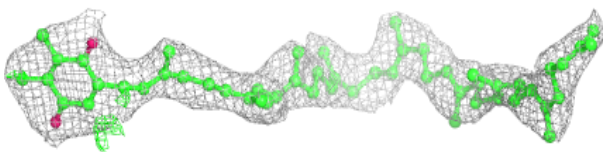
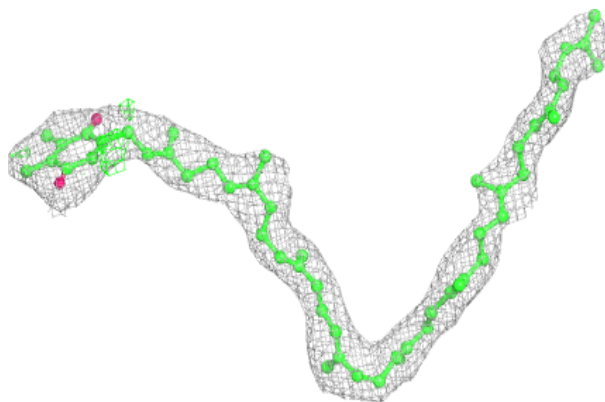


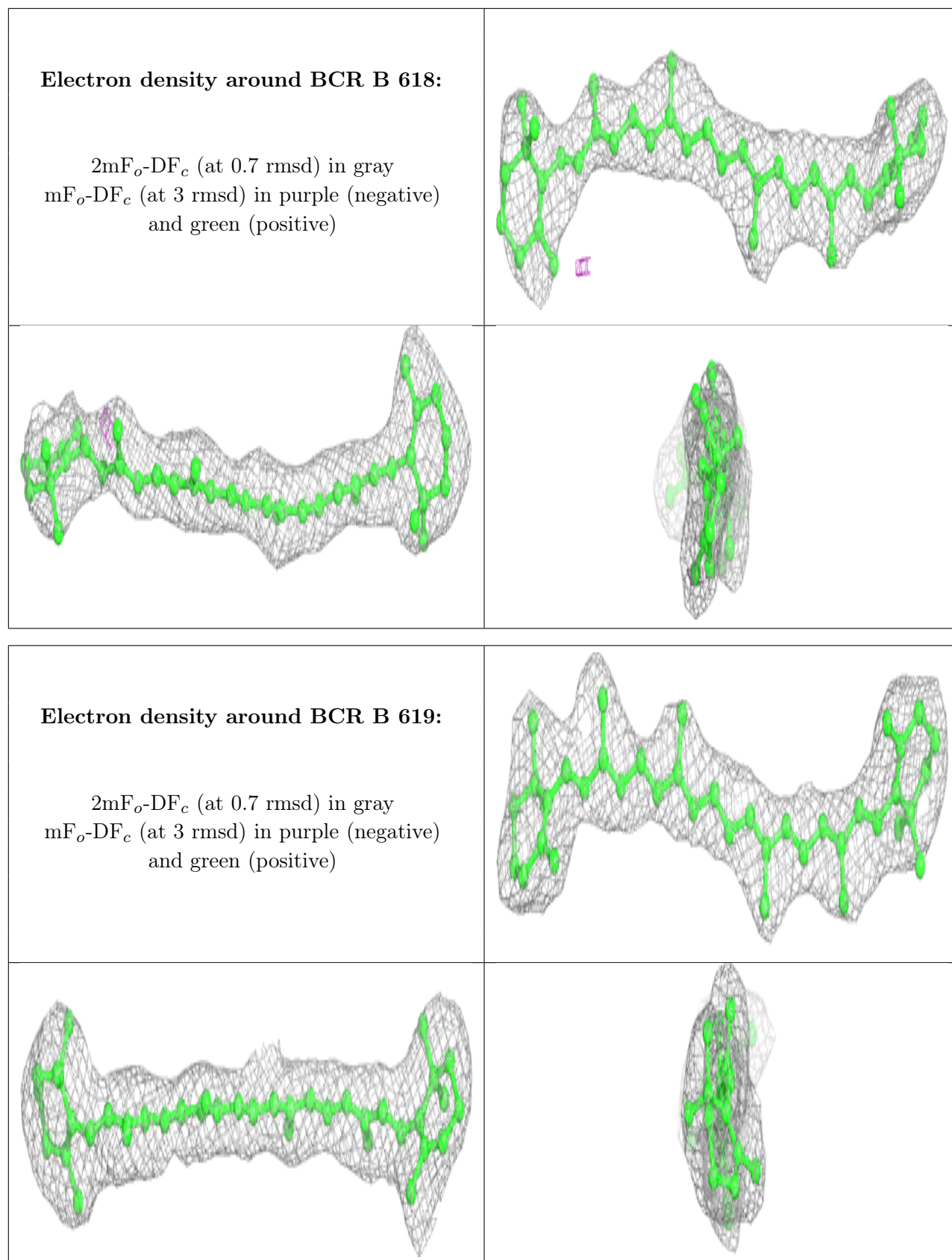
Electron density around PHO a 710:

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

**Electron density around PL9 d 405:**

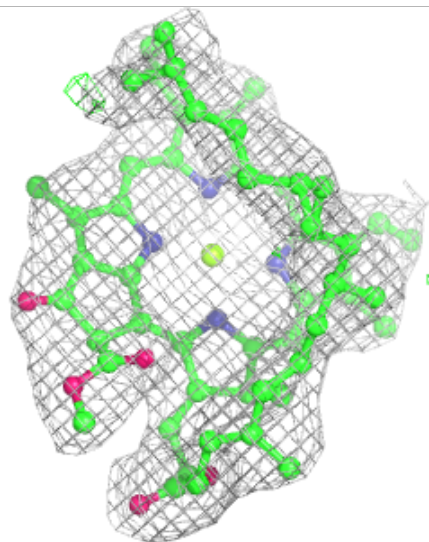
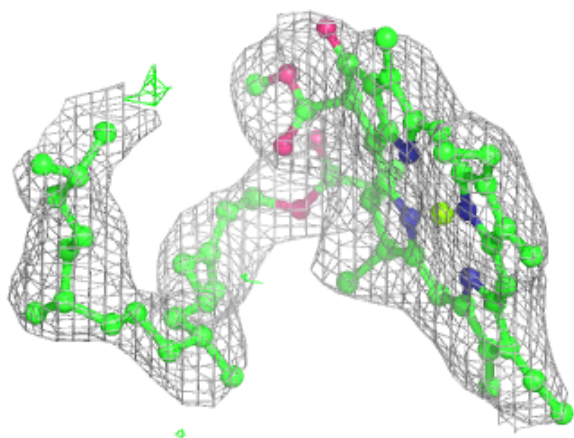
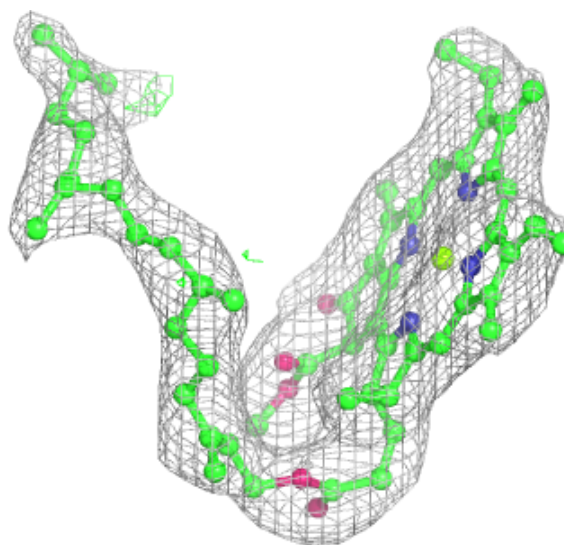
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





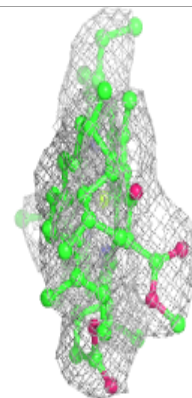
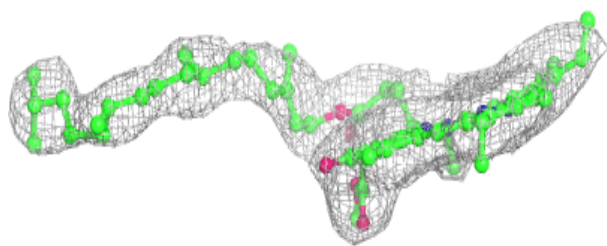
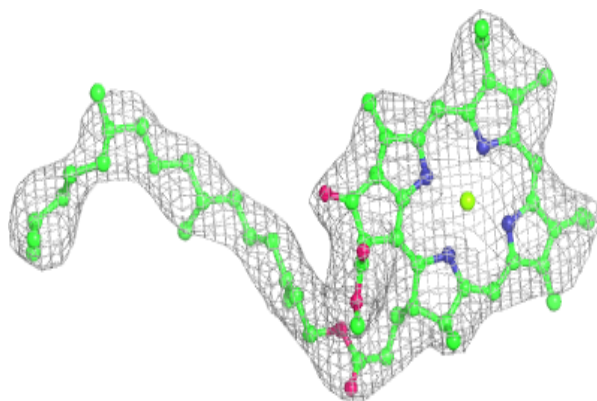
Electron density around CLA B 614:

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

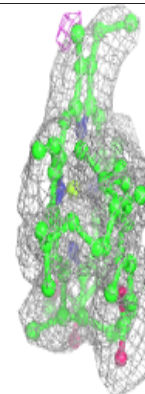
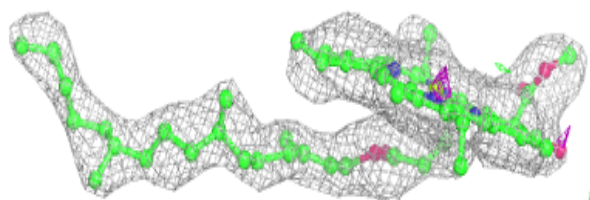
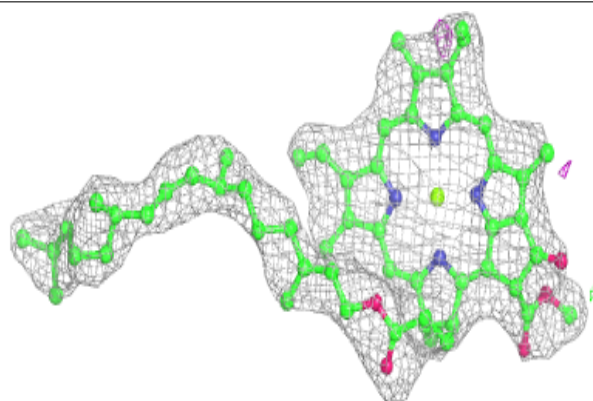


Electron density around CLA B 603:

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

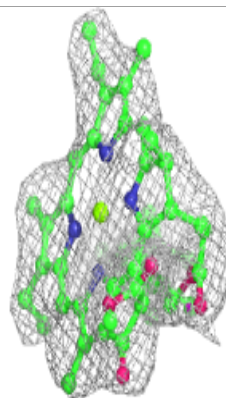
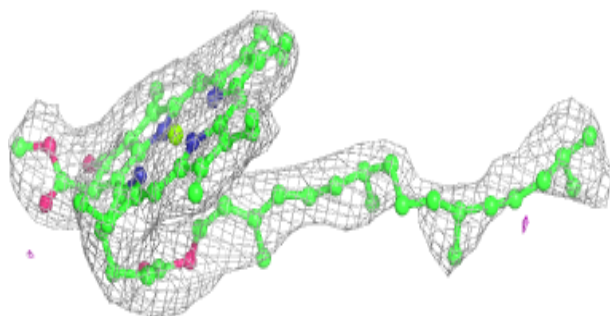
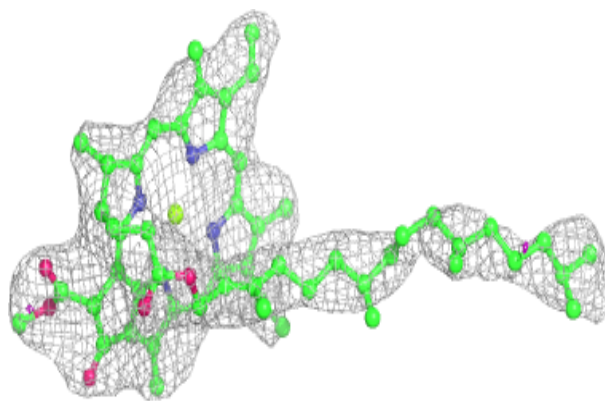
**Electron density around CLA B 604:**

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

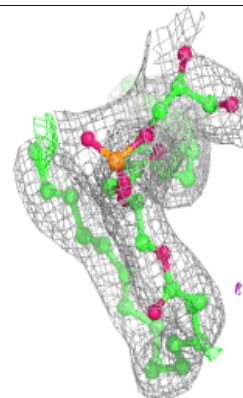
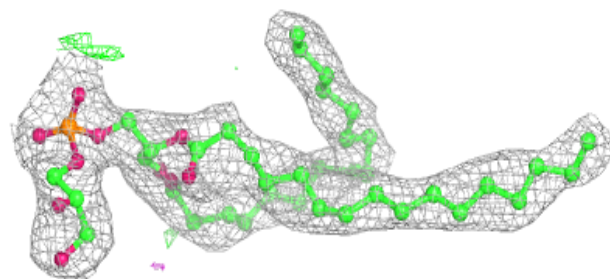
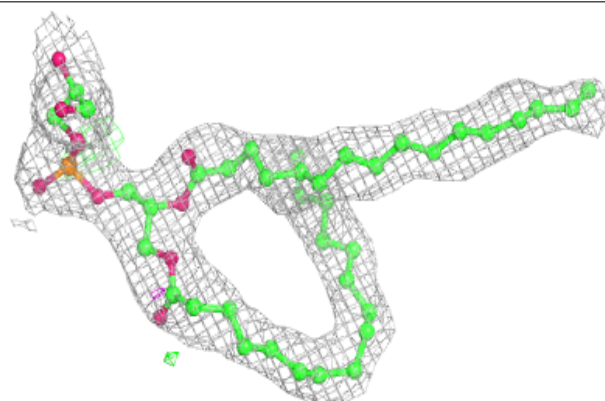


Electron density around CLA b 620:

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

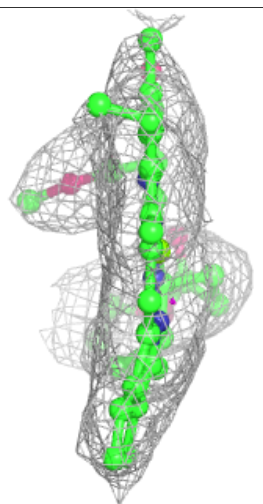
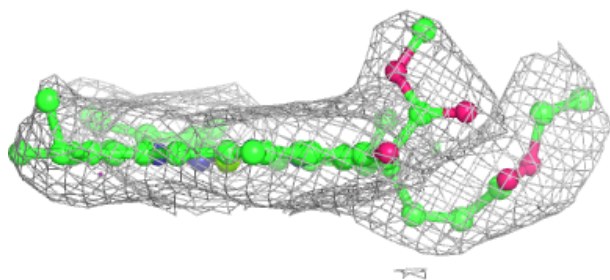
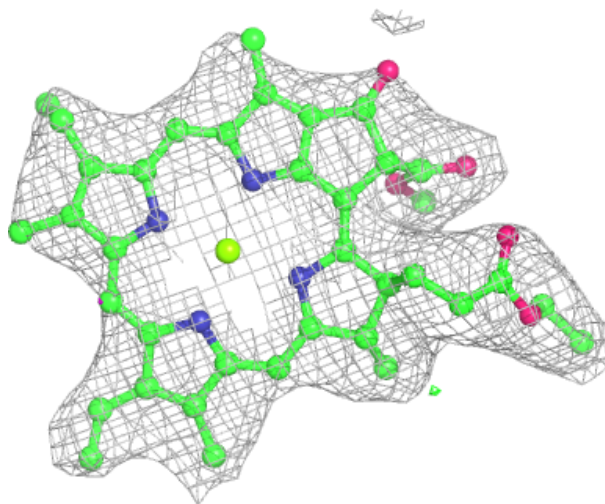
**Electron density around LHG B 625:**

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



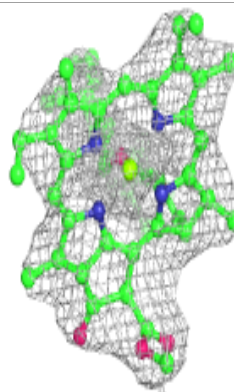
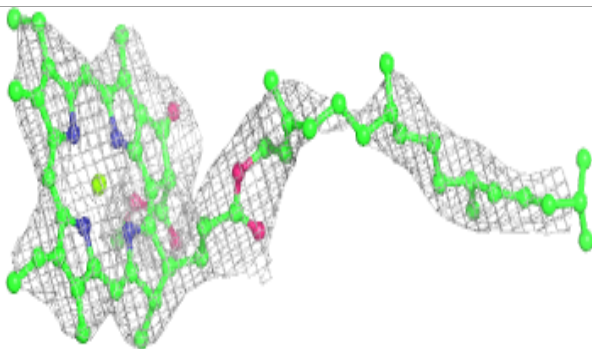
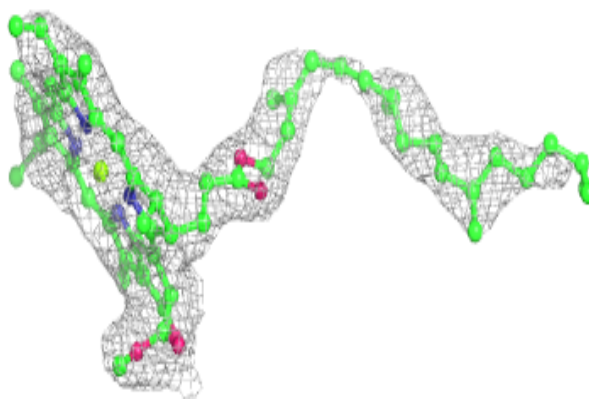
Electron density around CLA b 622:

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

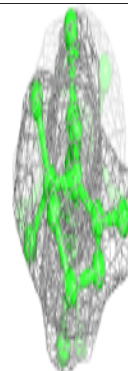
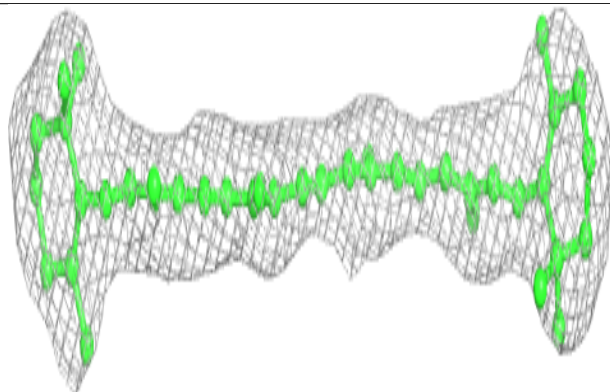
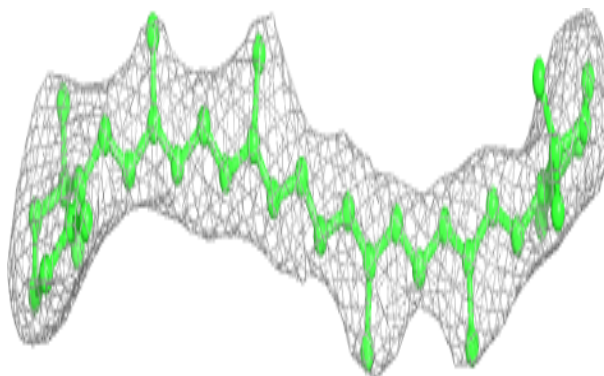


Electron density around CLA c 502:

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

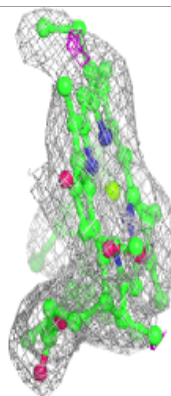
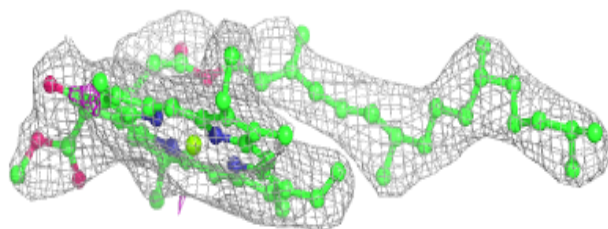
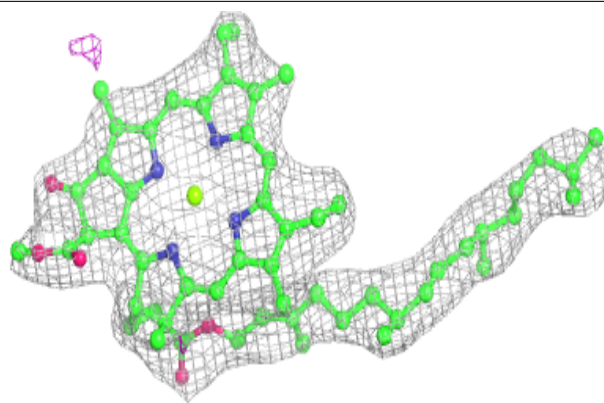
**Electron density around BCR a 712:**

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

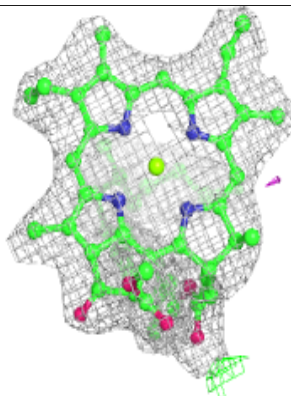
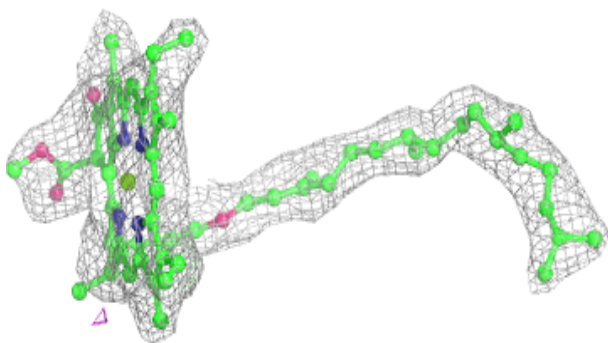
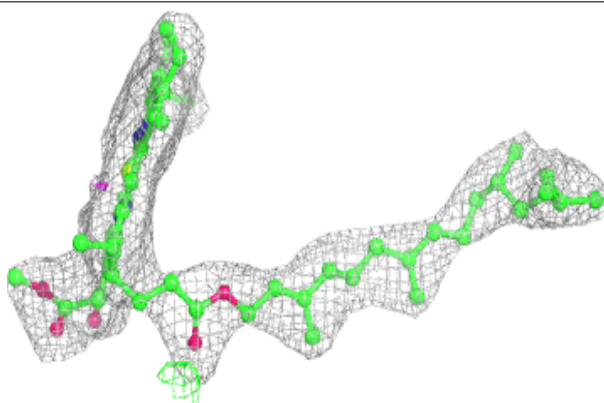


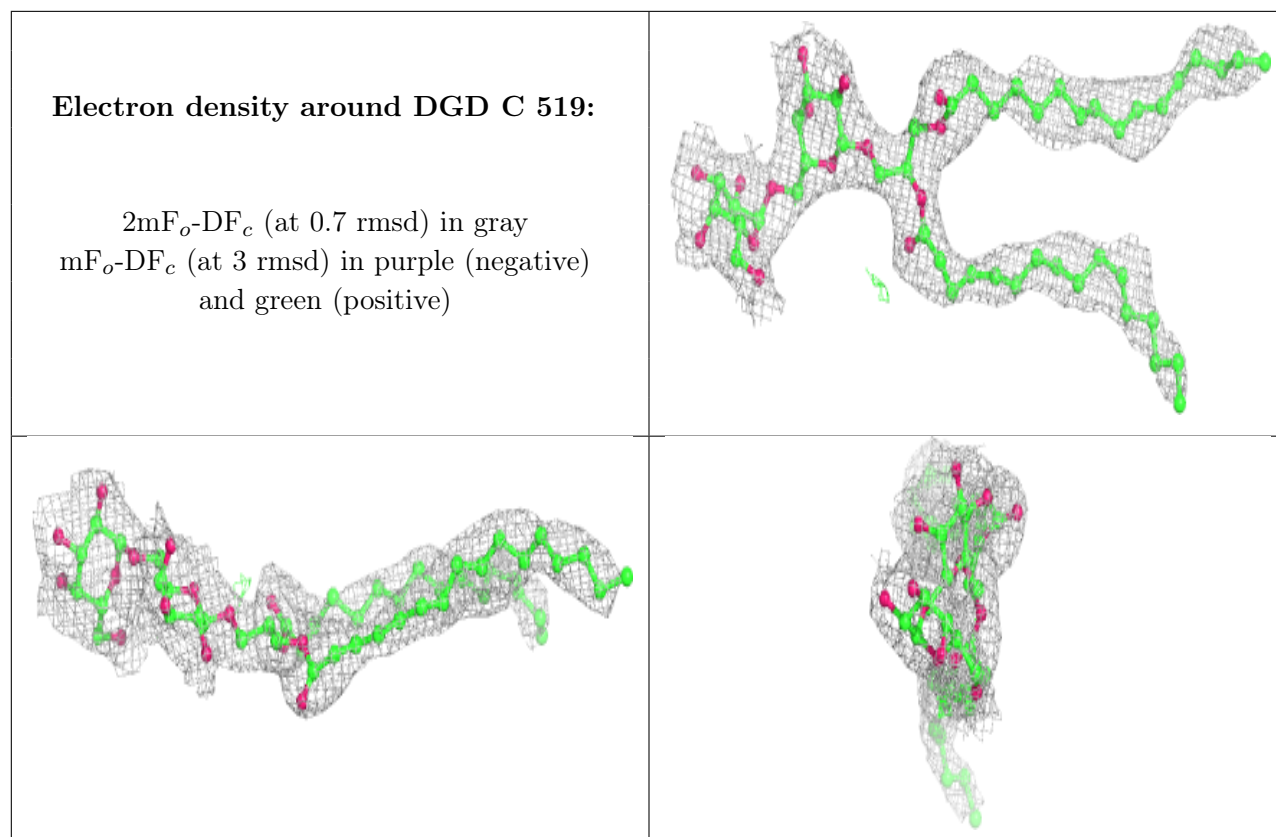
Electron density around CLA C 502:

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

**Electron density around CLA B 606:**

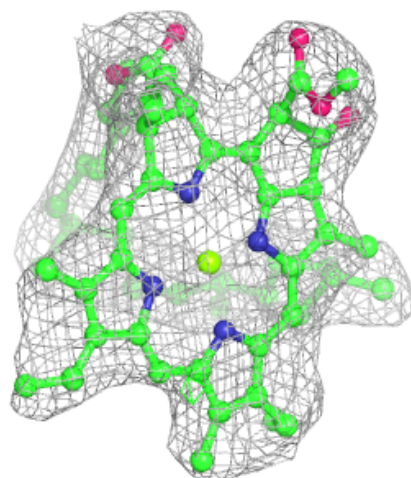
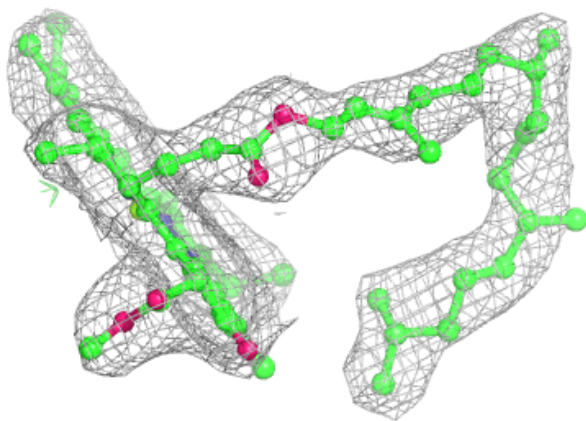
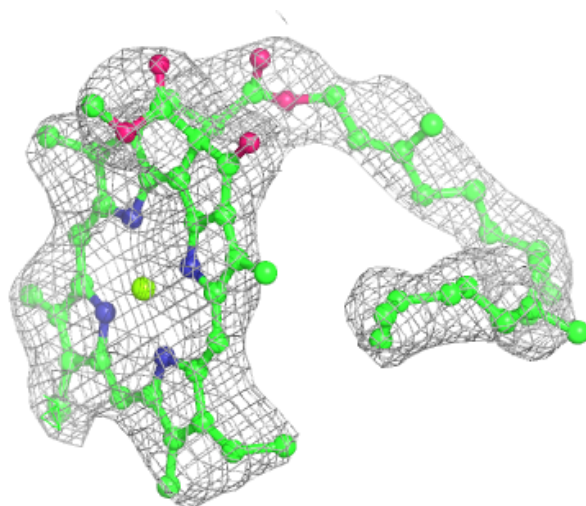
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

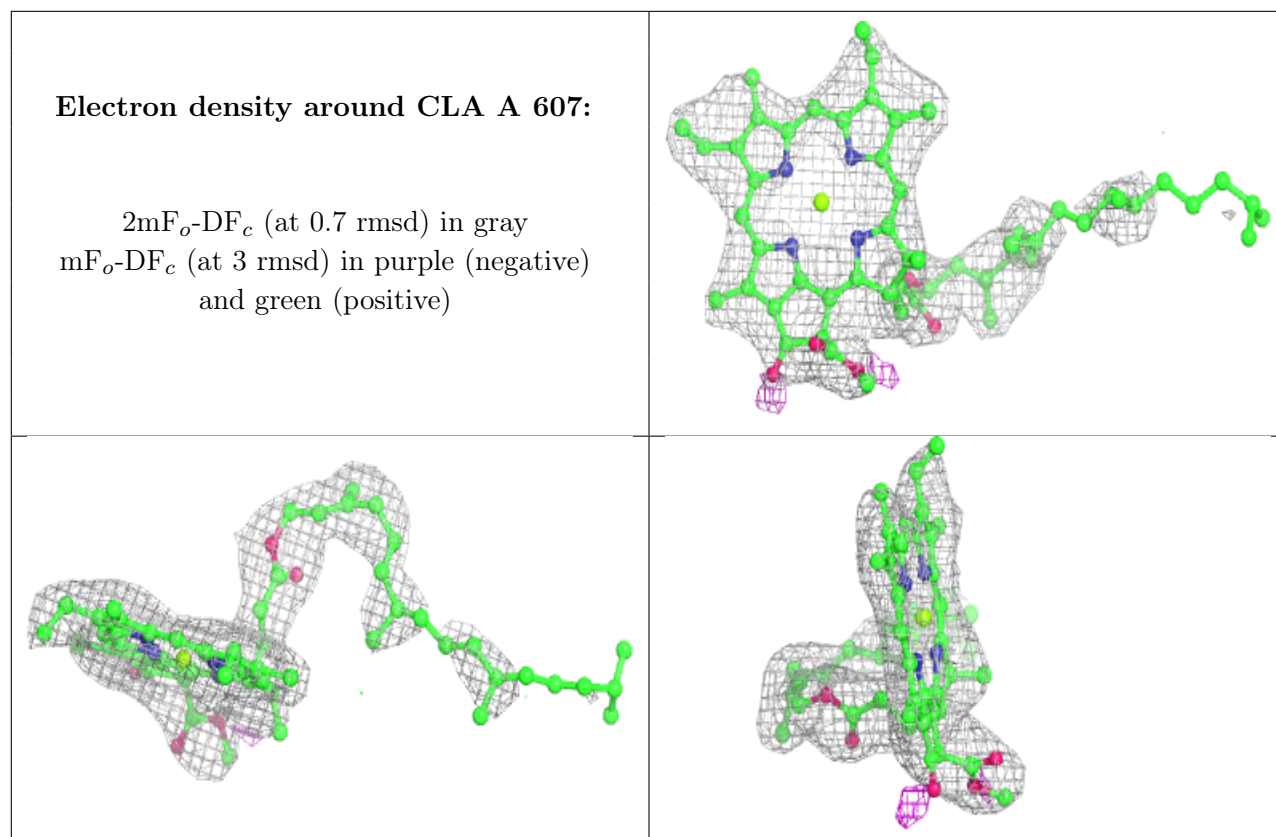




Electron density around CLA C 504:

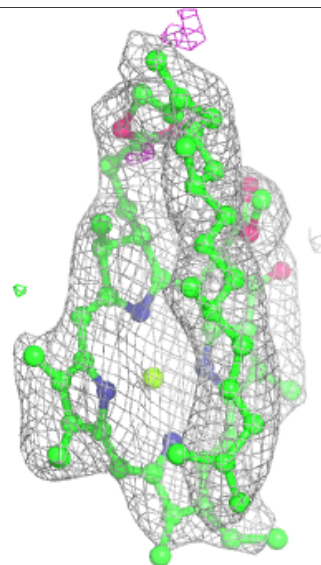
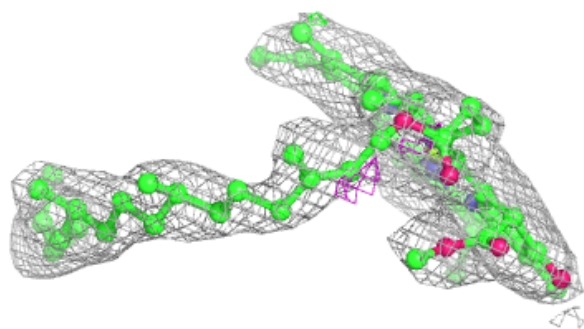
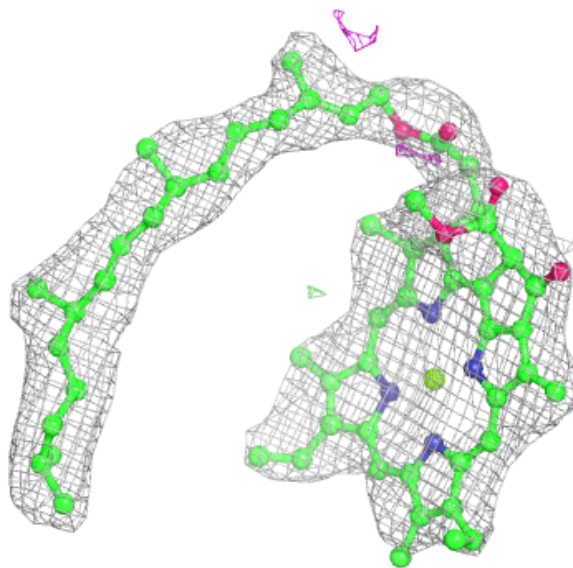
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





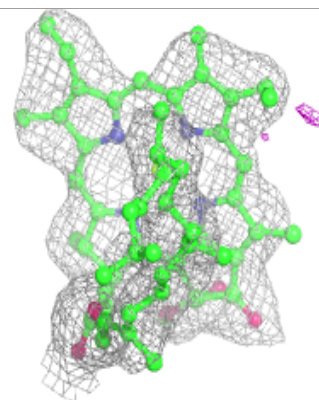
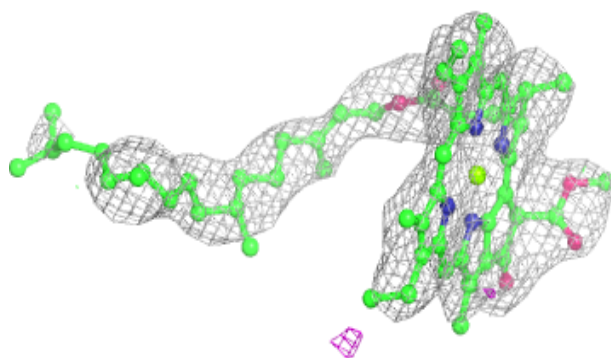
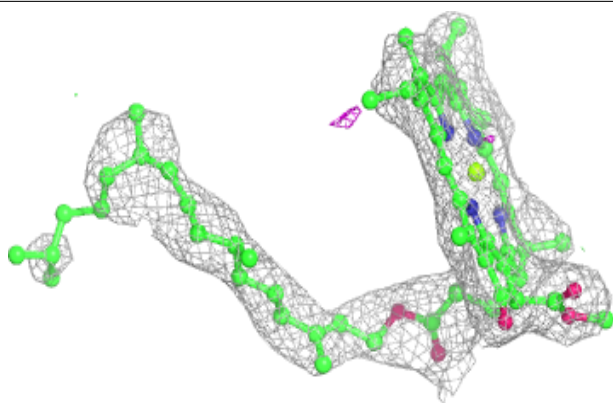
Electron density around CLA c 507:

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



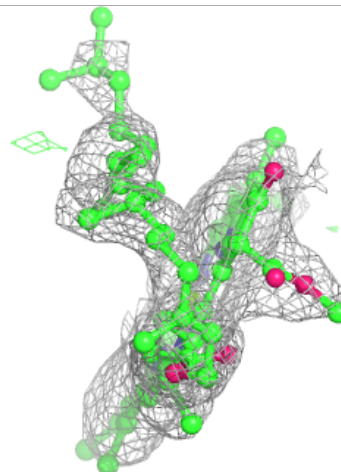
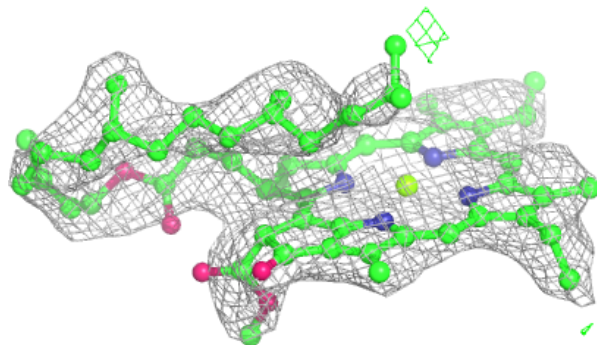
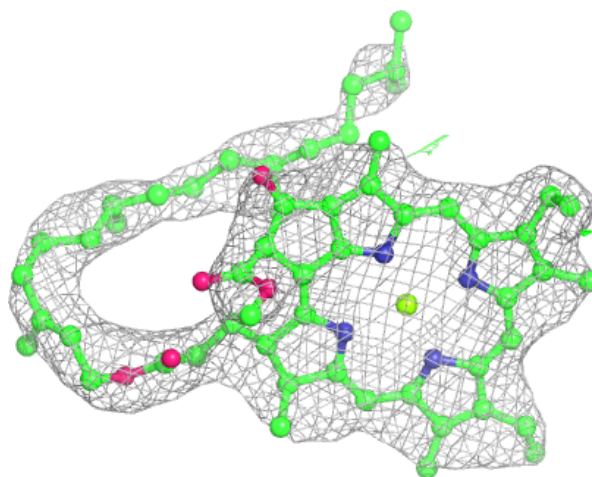
Electron density around CLA c 508:

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



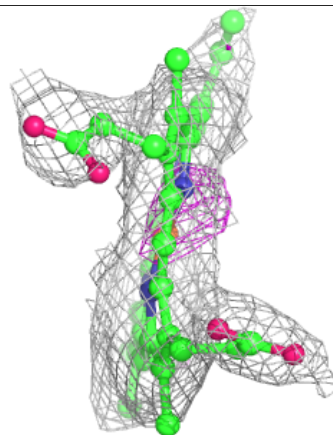
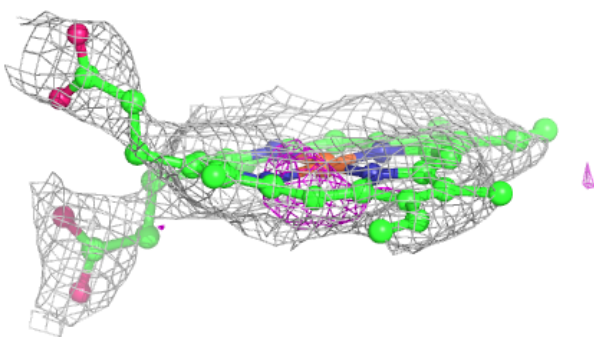
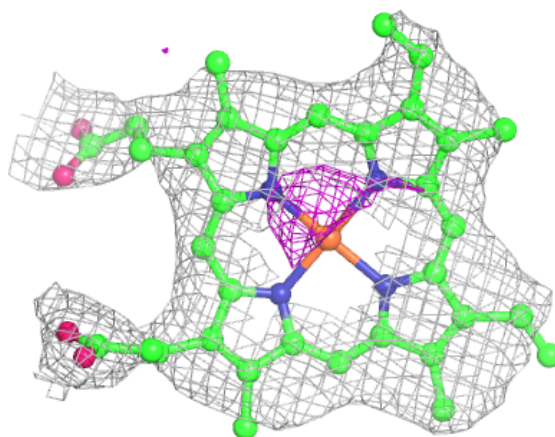
Electron density around CLA c 509:

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



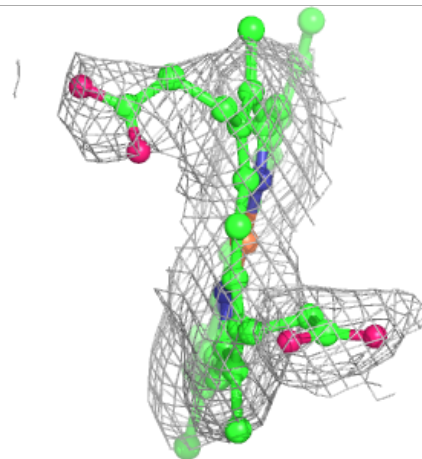
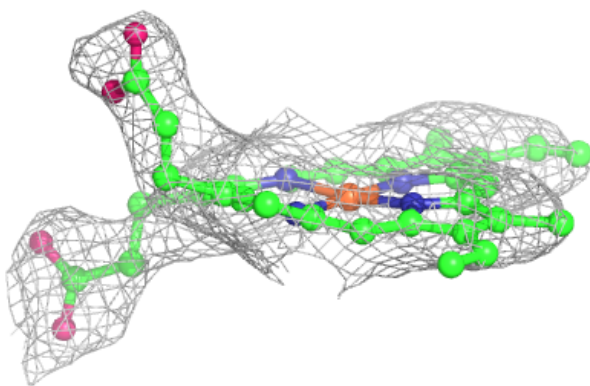
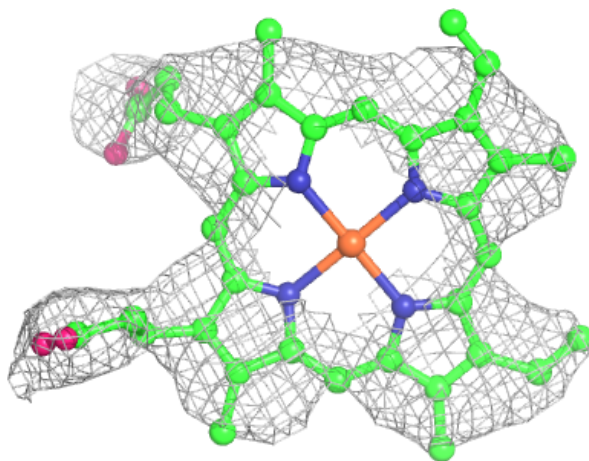
Electron density around HEM E 102:

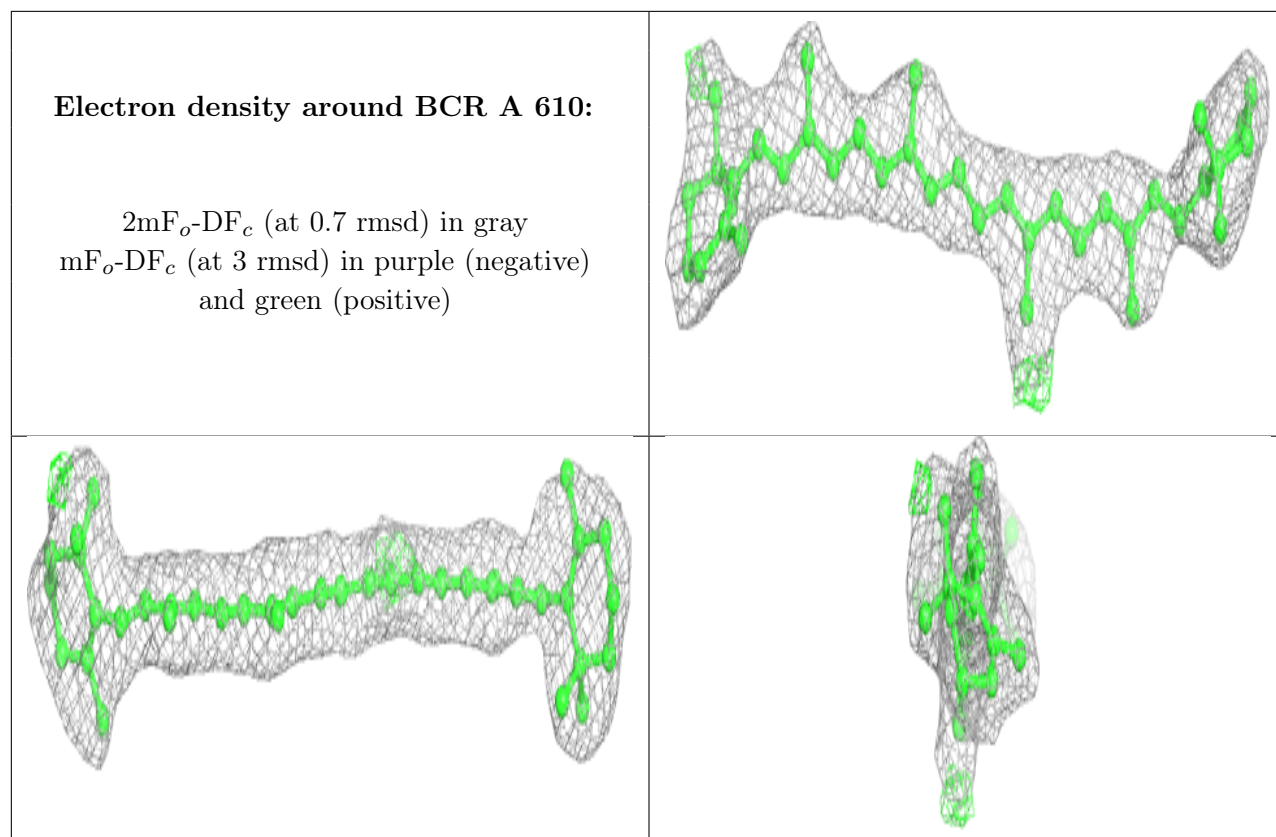
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM e 102:

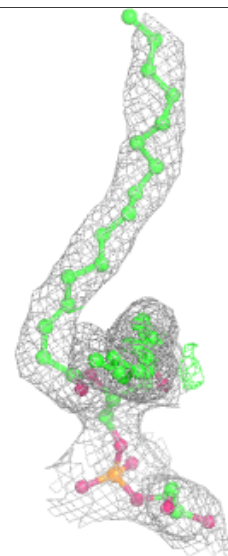
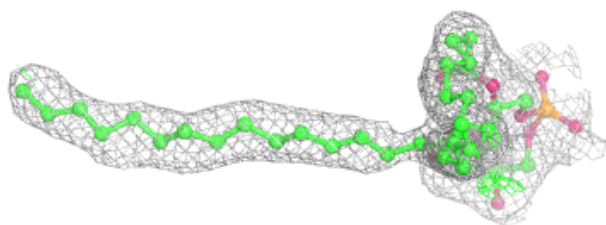
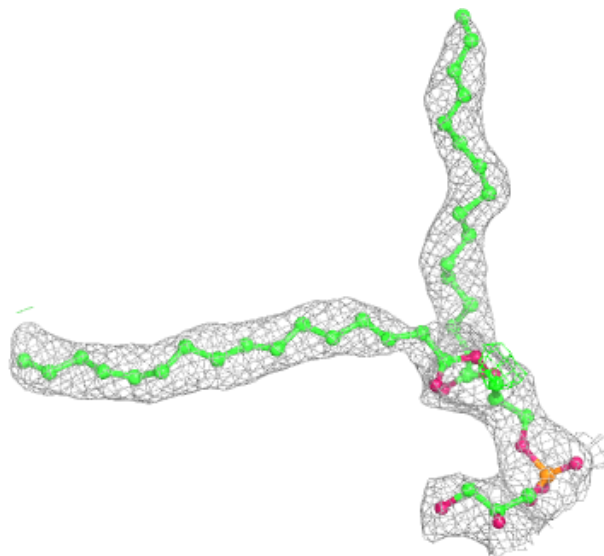
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





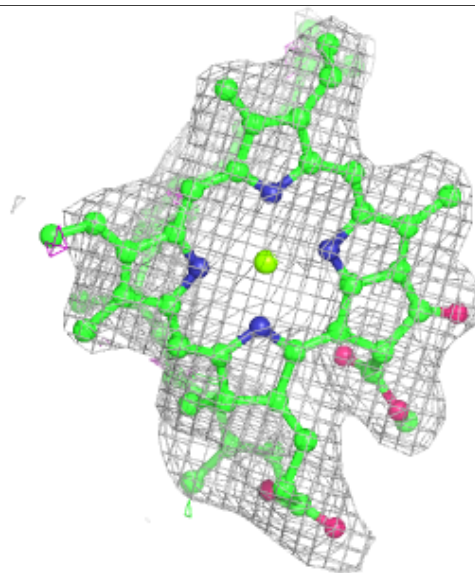
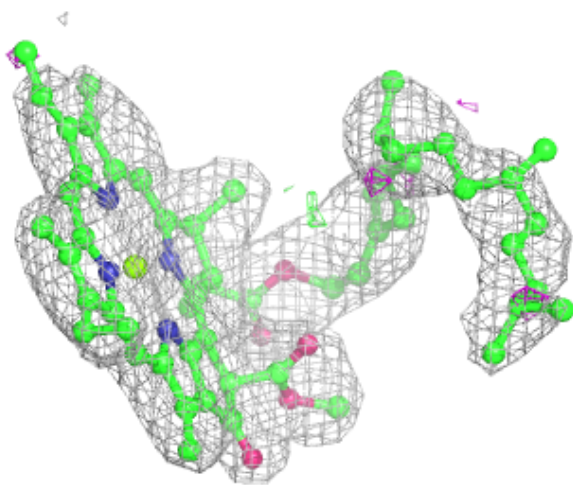
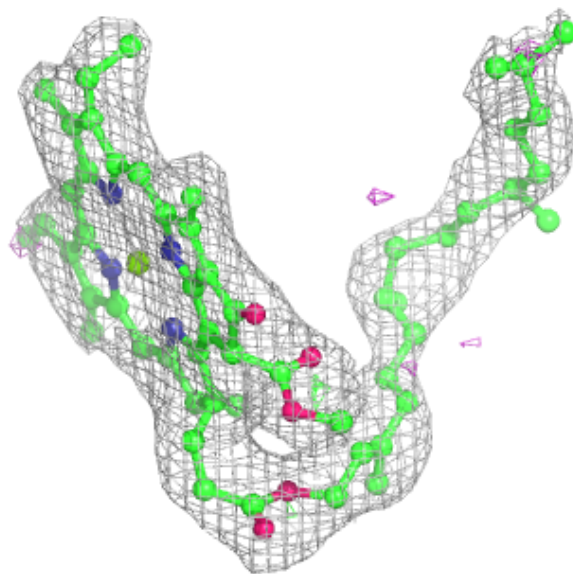
Electron density around LHG L 101:

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



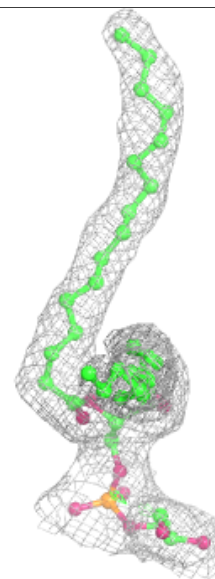
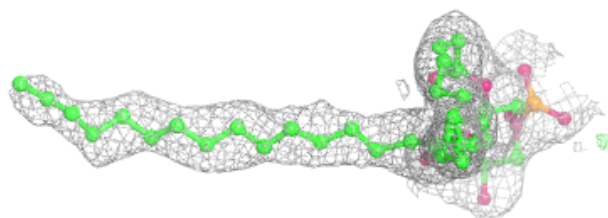
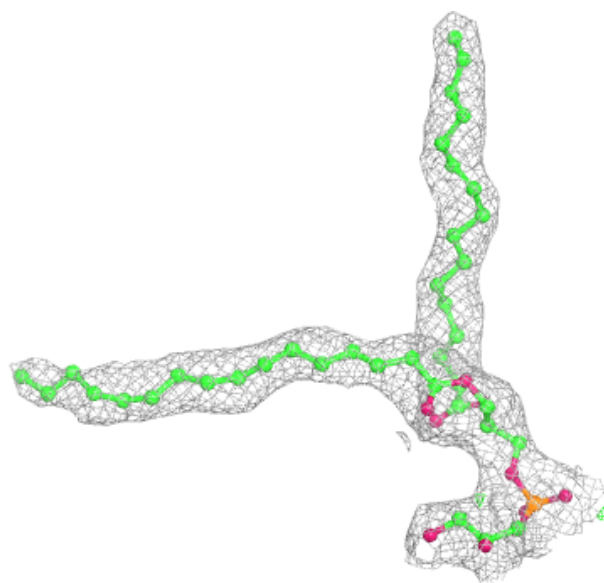
Electron density around CLA b 619:

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



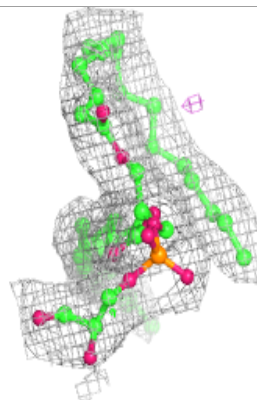
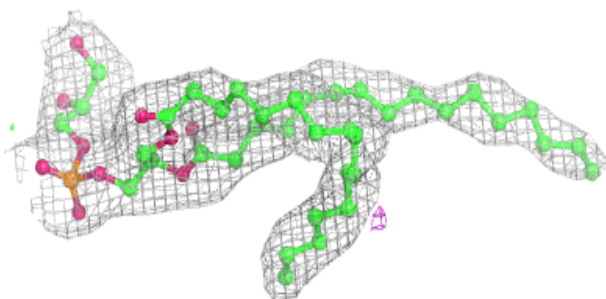
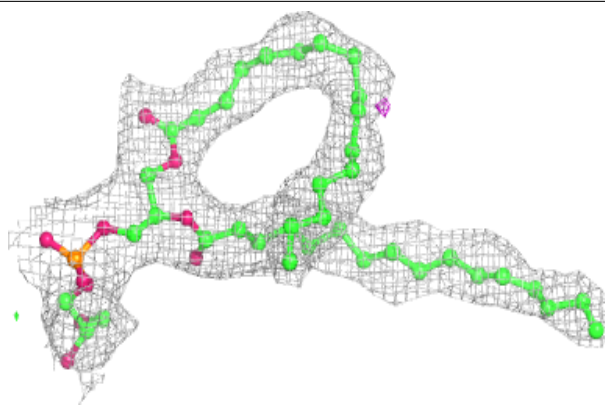
Electron density around LHG b 629:

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

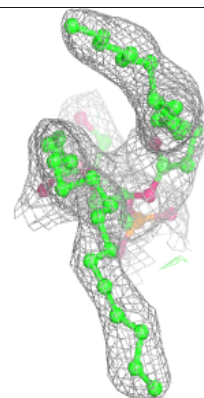
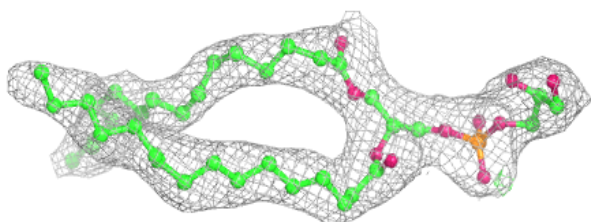
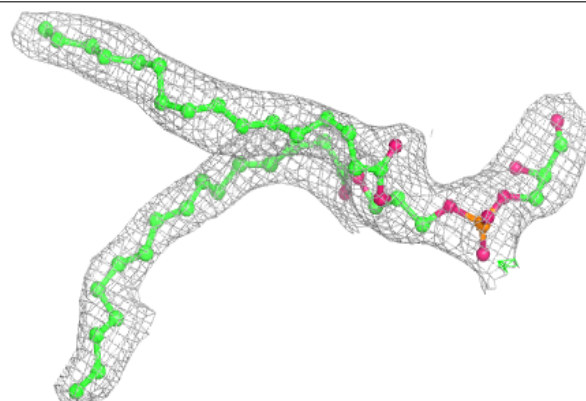


Electron density around LHG d 406:

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

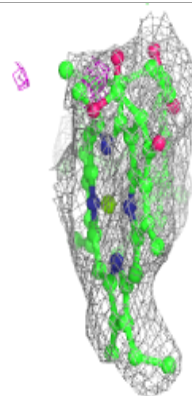
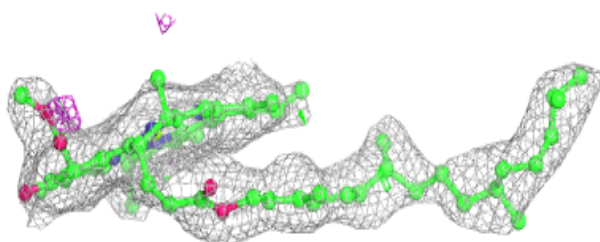
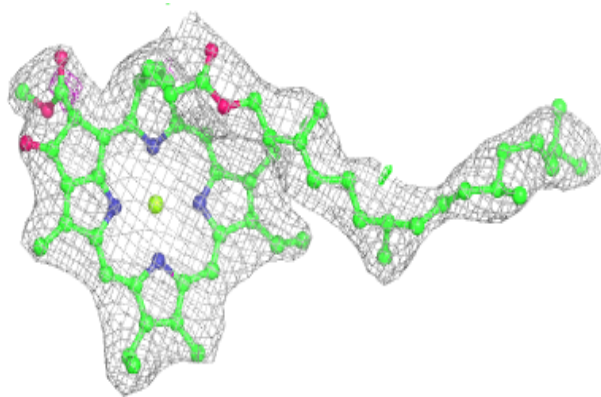
**Electron density around LHG d 407:**

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



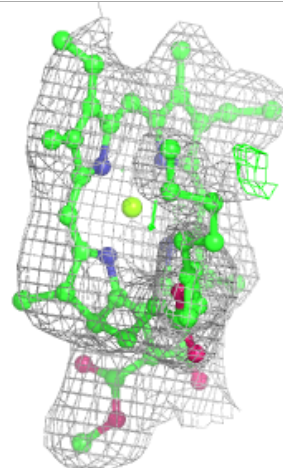
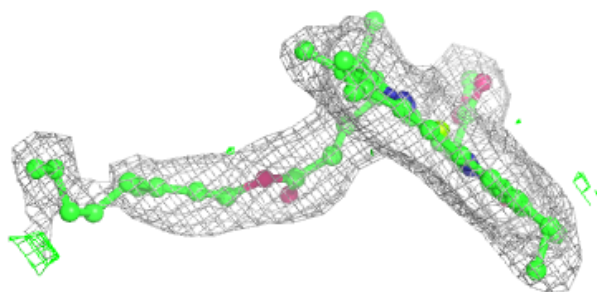
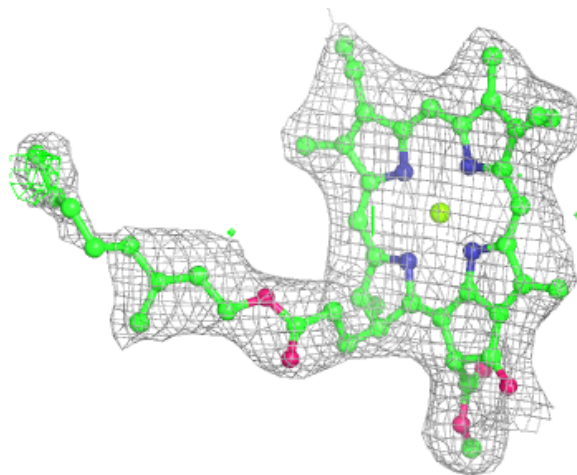
Electron density around CLA b 609:

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



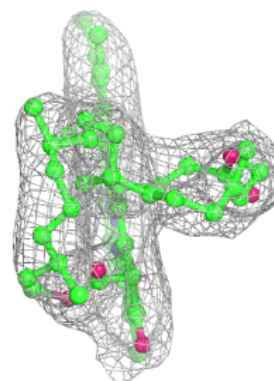
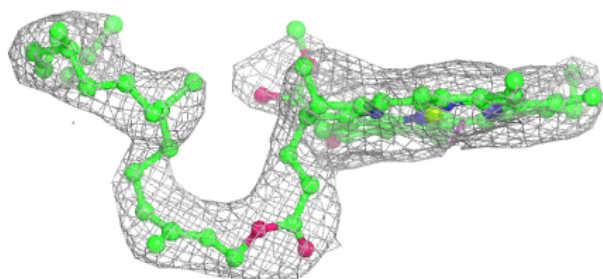
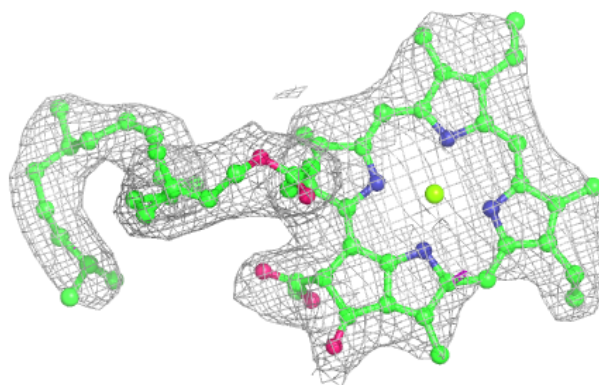
Electron density around CLA A 609:

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

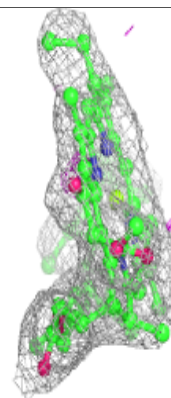
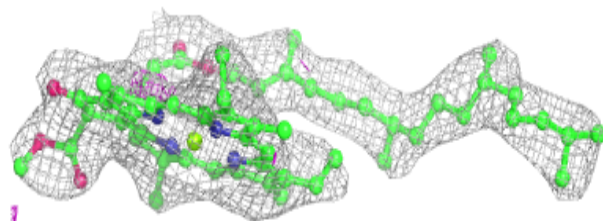
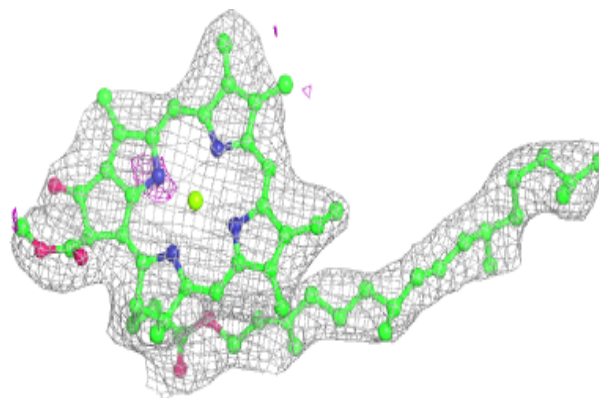


Electron density around CLA B 613:

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

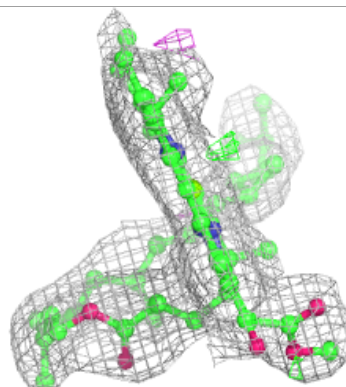
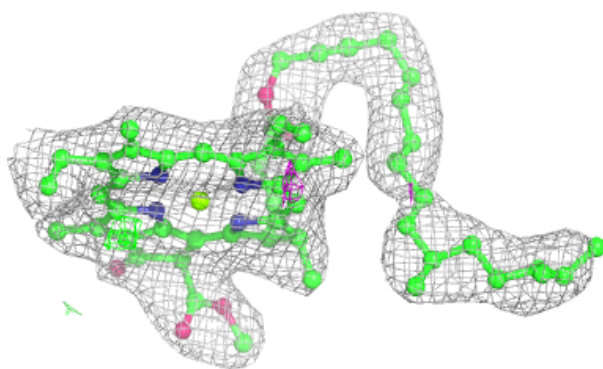
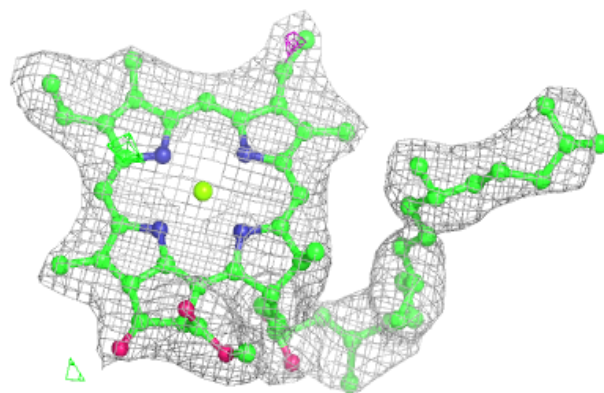
**Electron density around CLA c 501:**

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

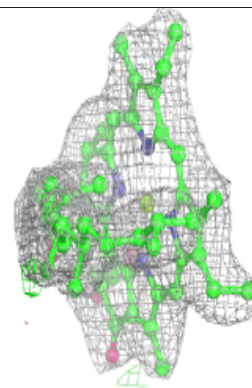
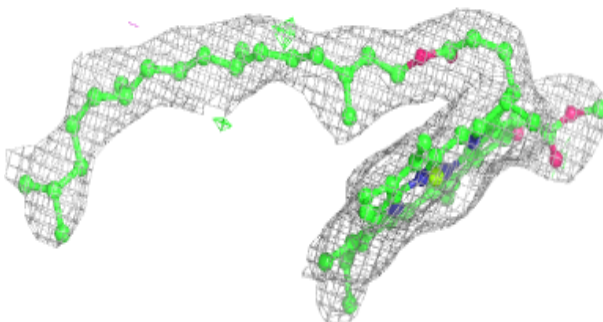
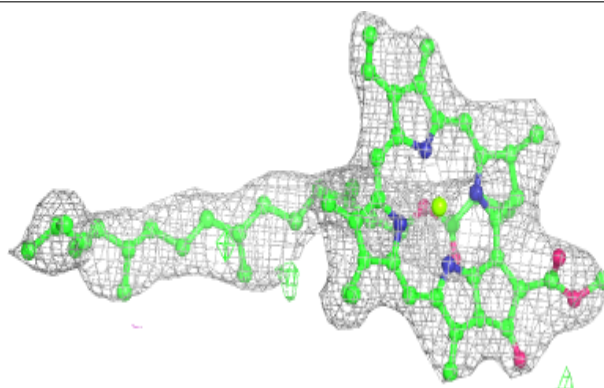


Electron density around CLA a 719:

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

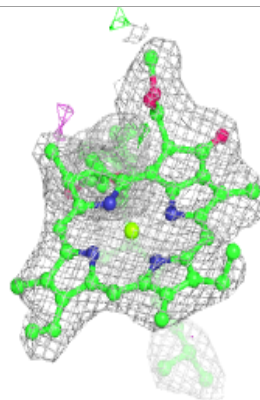
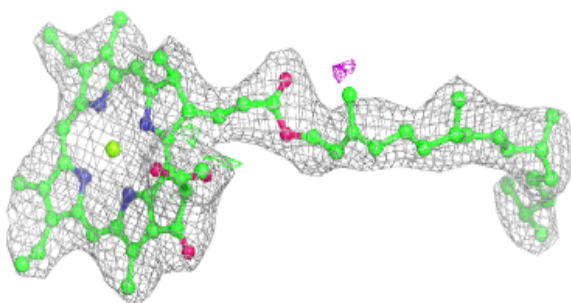
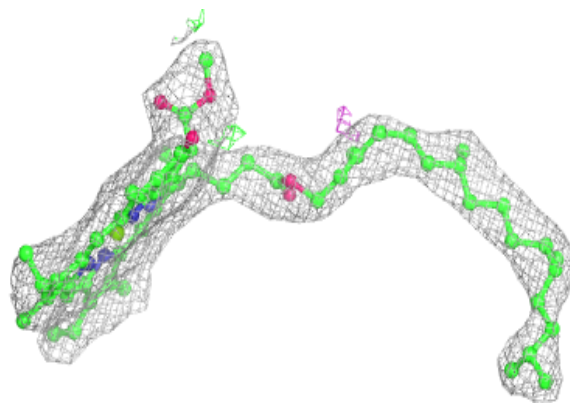
**Electron density around CLA b 614:**

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

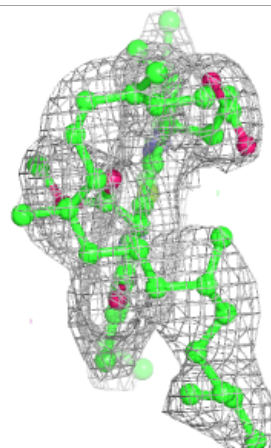
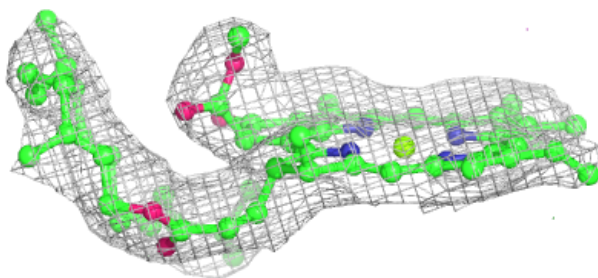
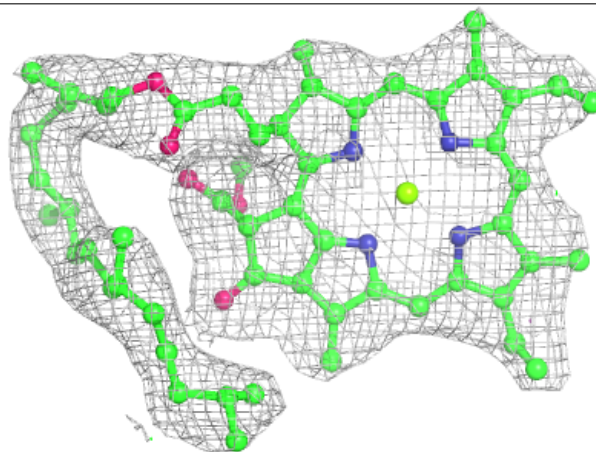


Electron density around CLA D 403:

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

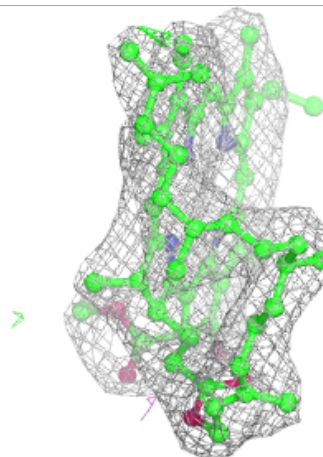
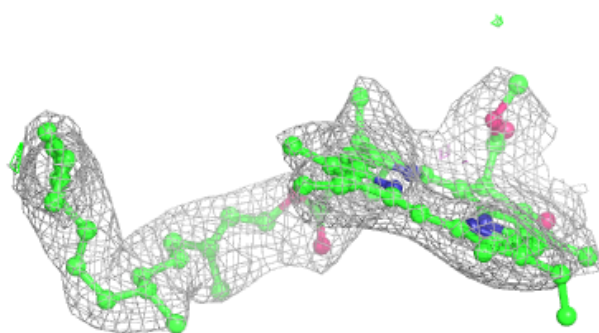
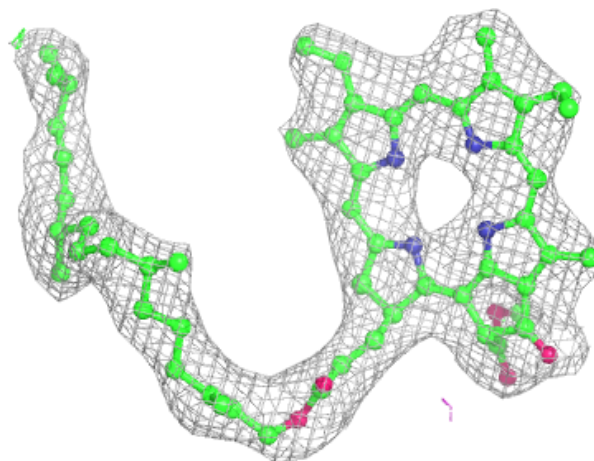
**Electron density around CLA B 611:**

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



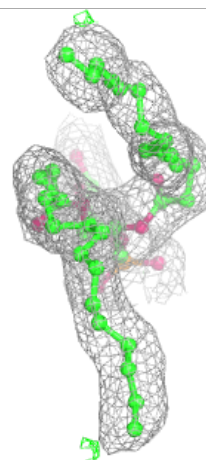
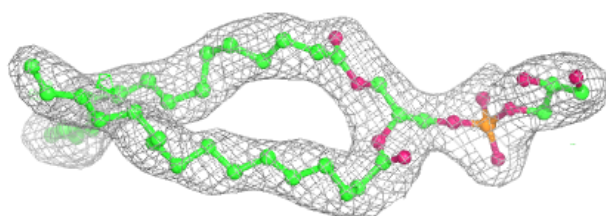
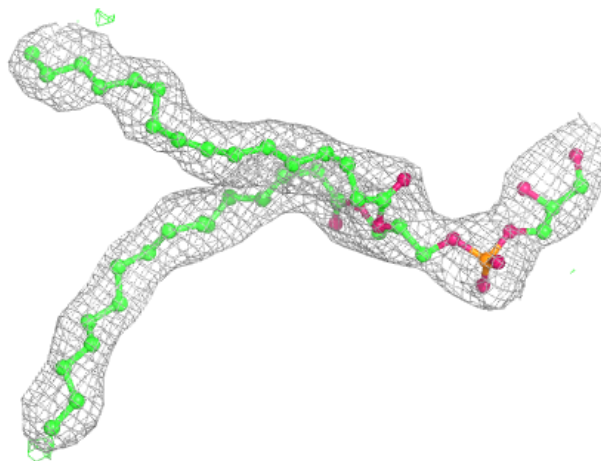
Electron density around PHO D 401:

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



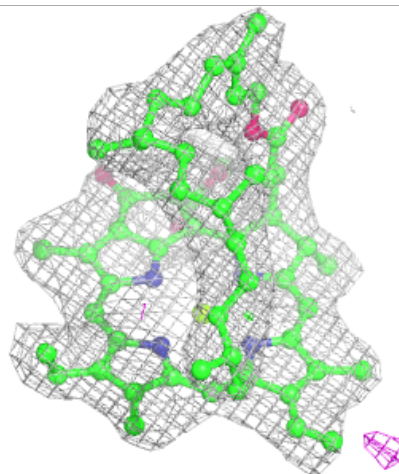
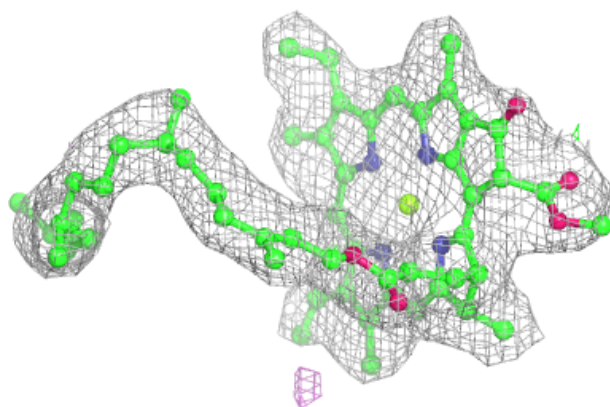
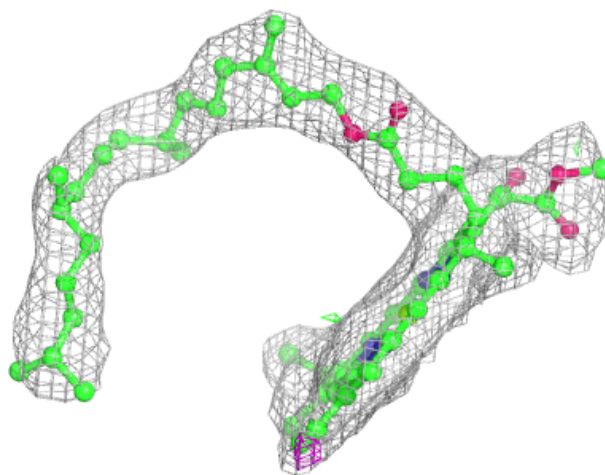
Electron density around LHG D 407:

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



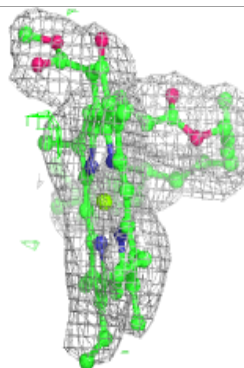
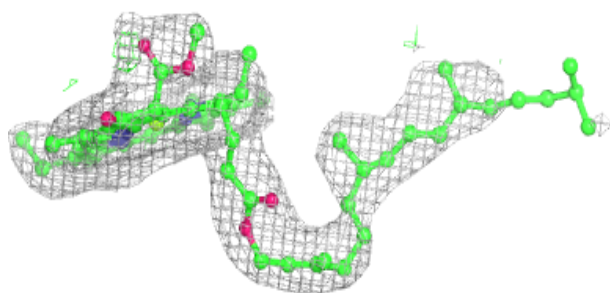
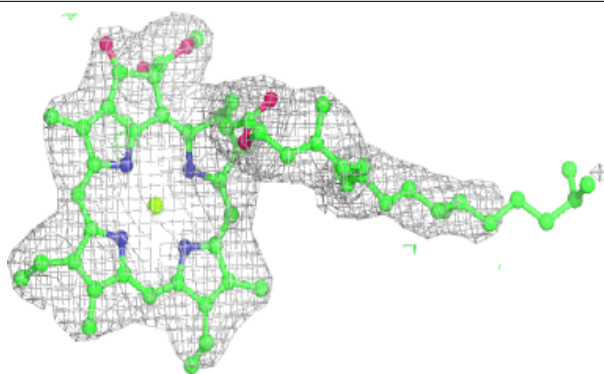
Electron density around CLA b 617:

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

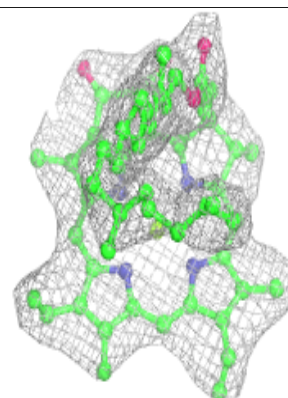
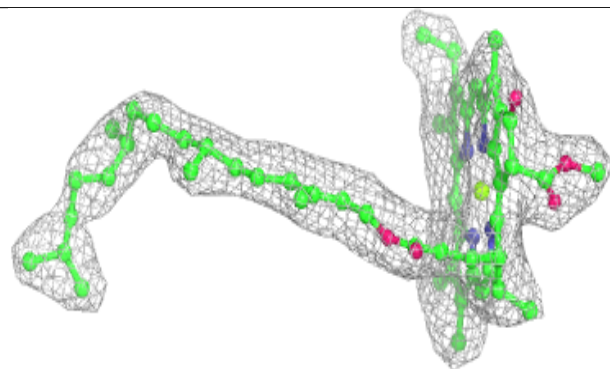
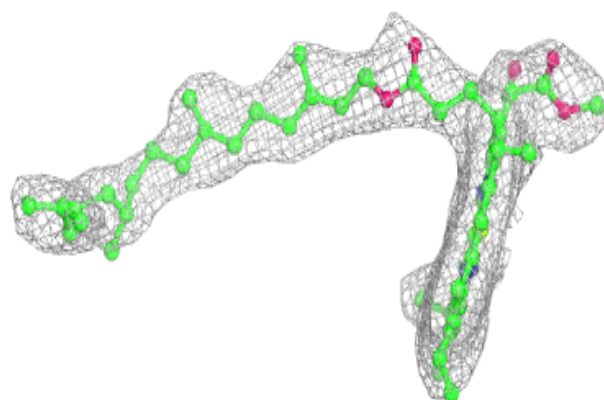


Electron density around CLA a 708:

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

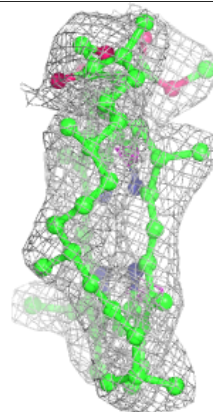
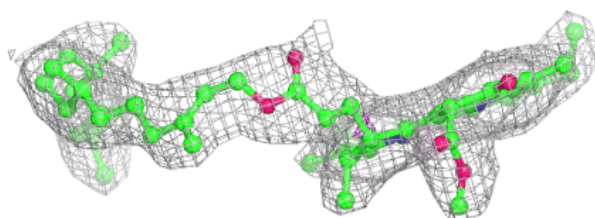
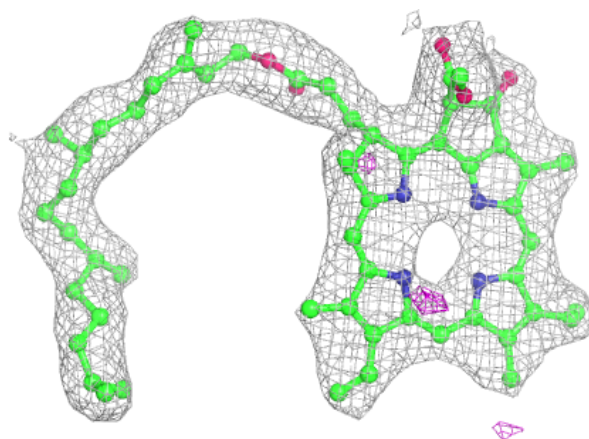
**Electron density around CLA b 611:**

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

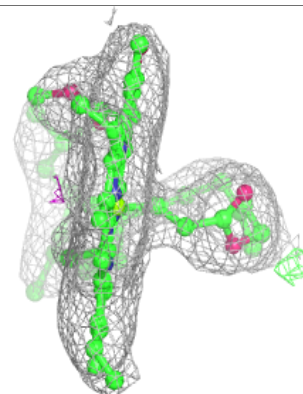
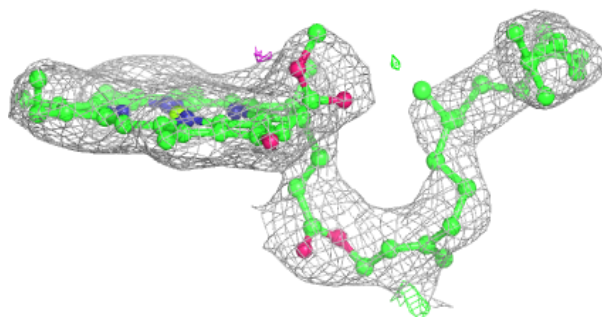
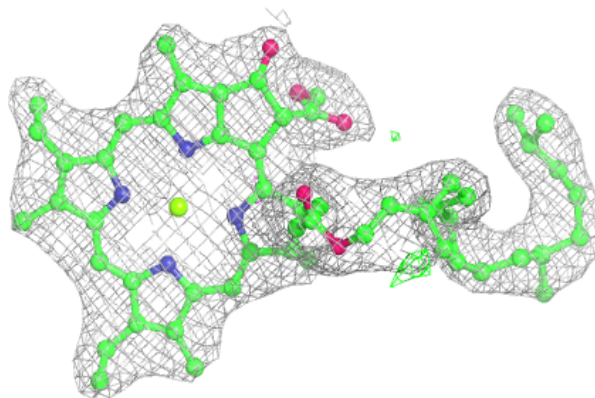


Electron density around PHO A 608:

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

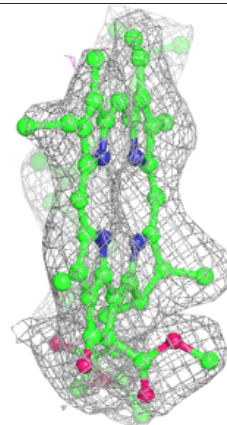
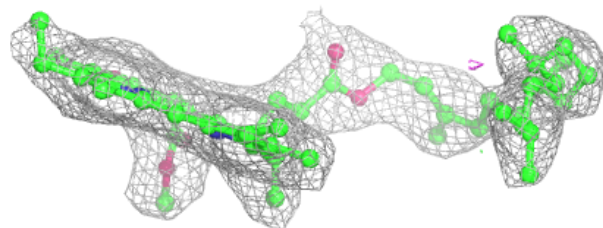
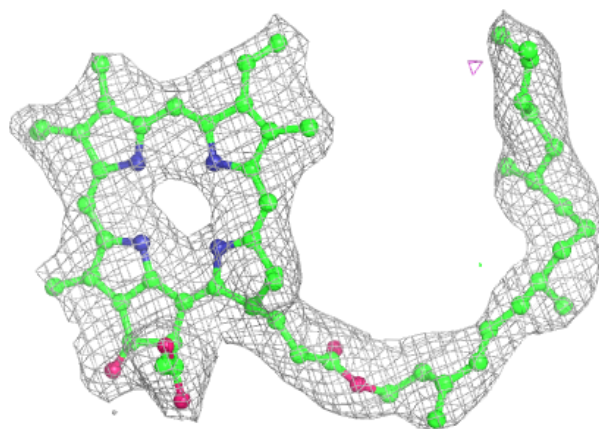
**Electron density around CLA b 618:**

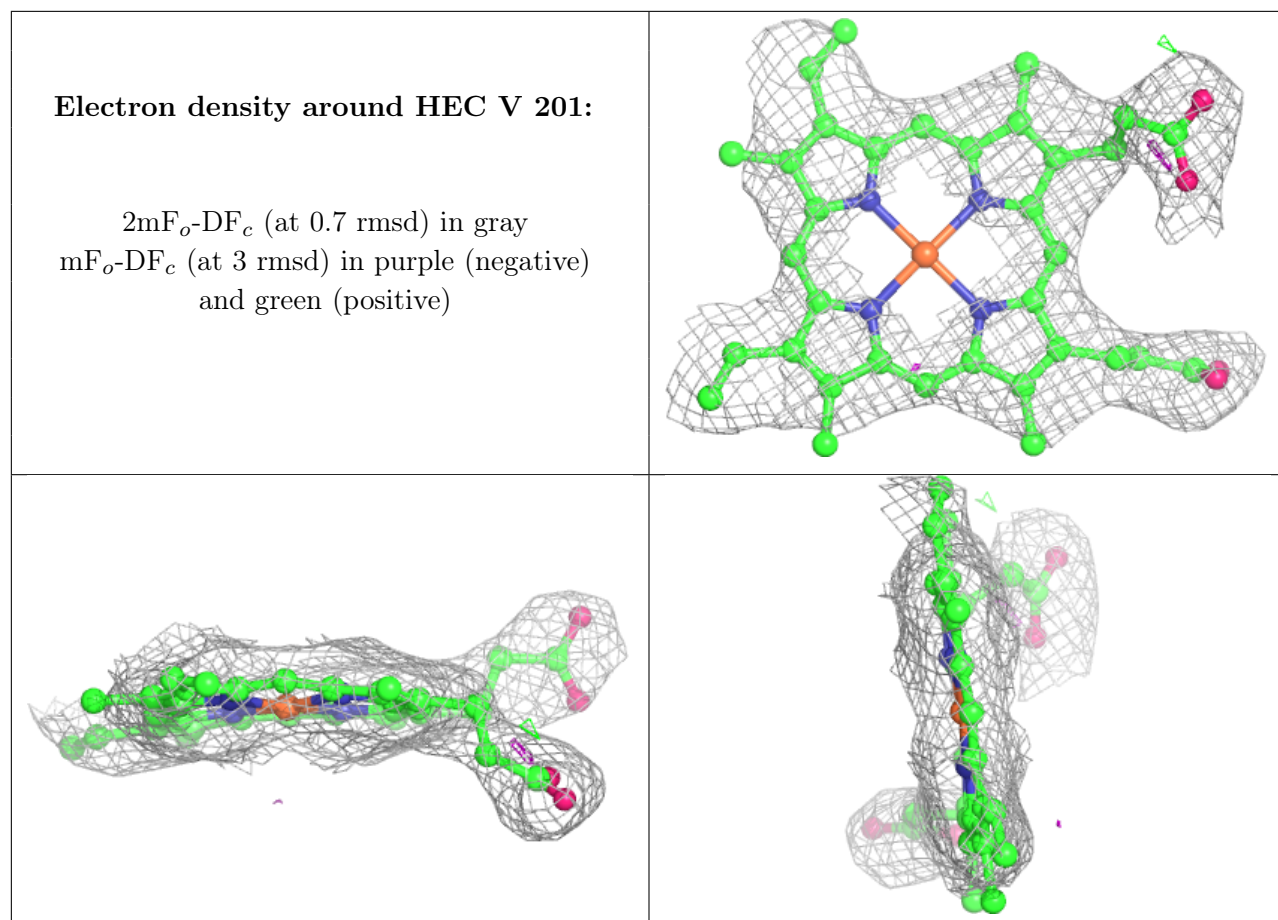
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

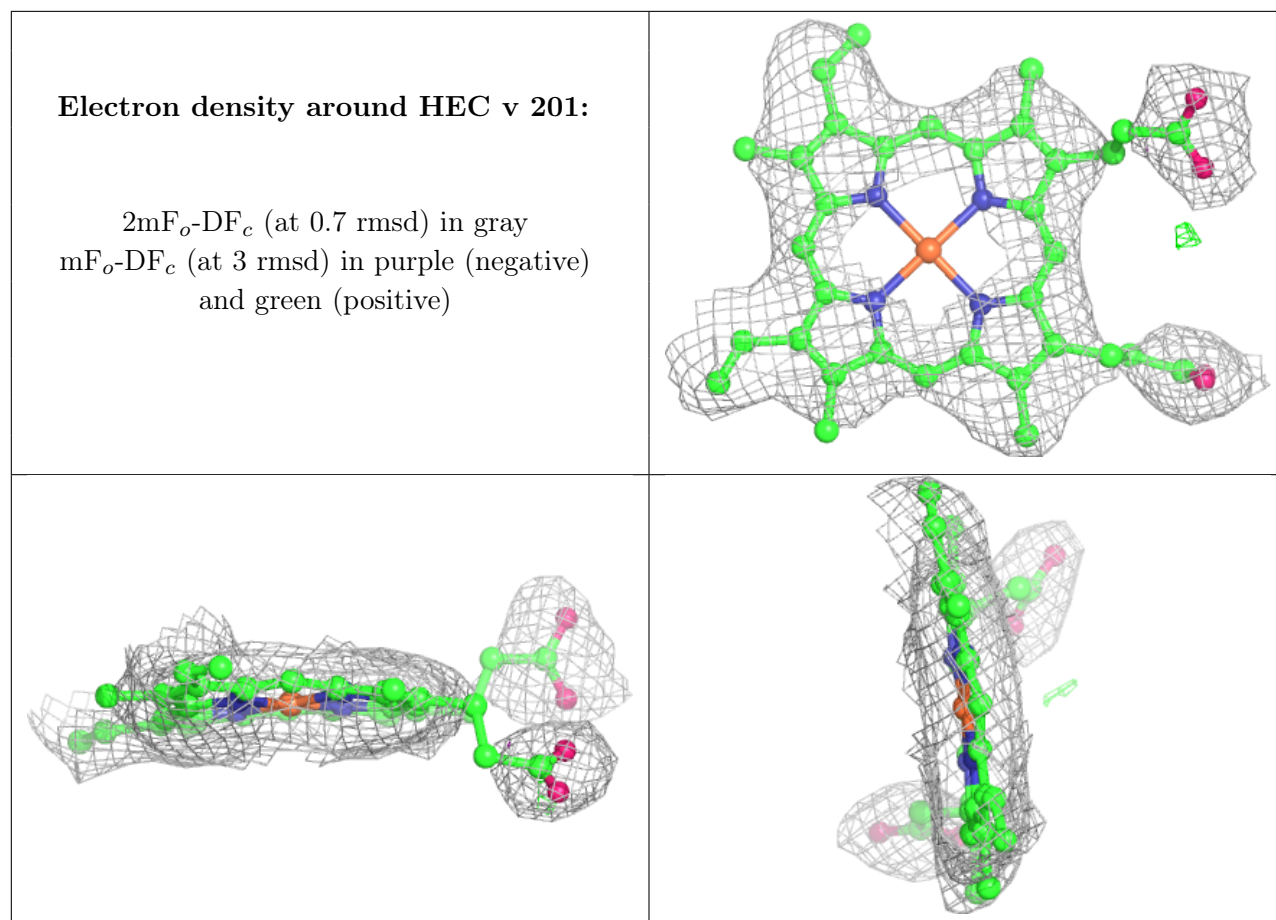


Electron density around PHO a 709:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.