



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 07:59 AM EST

PDB ID : 6DHH  
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.2 Angstrom resolution  
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.  
Deposited on : 2018-05-20  
Resolution : 2.20 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](mailto: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>.

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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 : 2.36

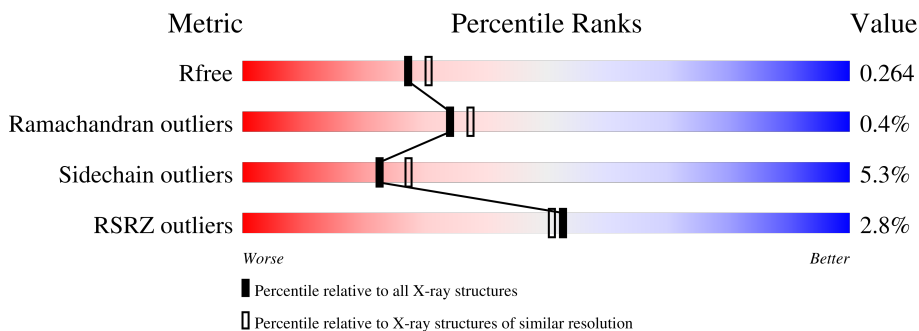
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

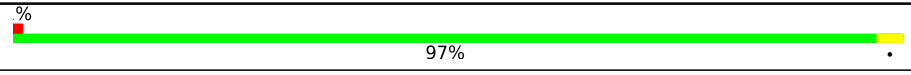
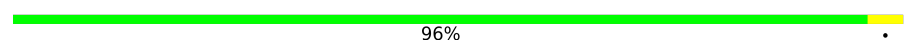
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

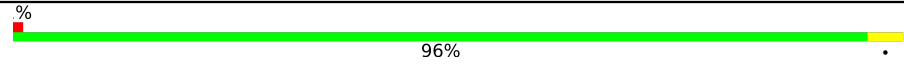
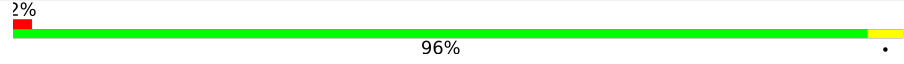
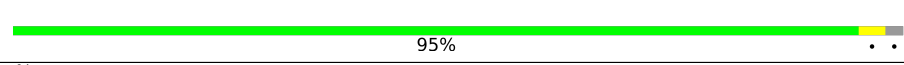
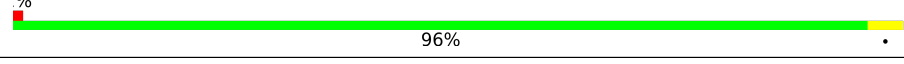
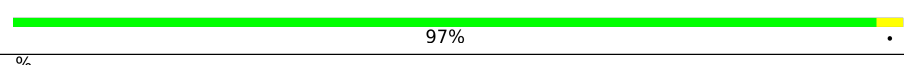
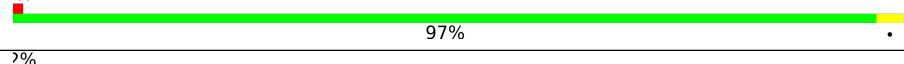
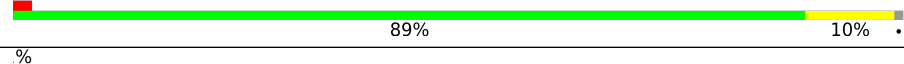
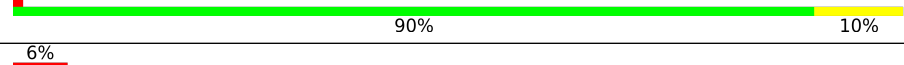
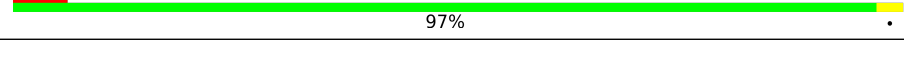
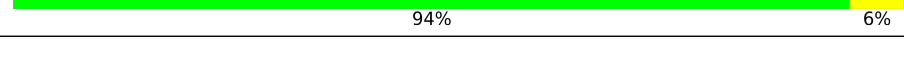
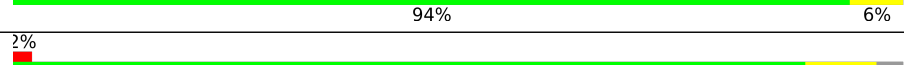
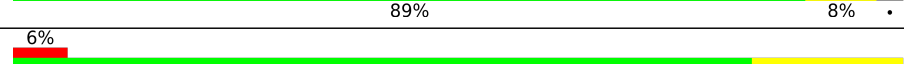
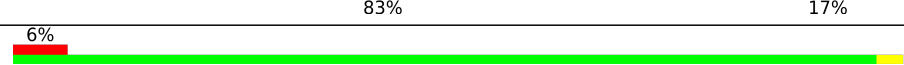
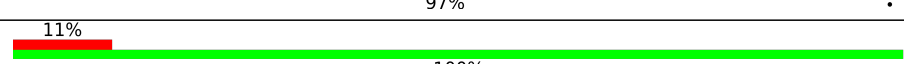
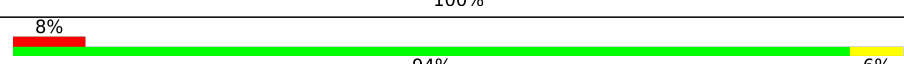
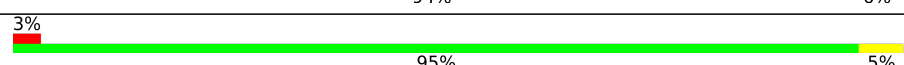
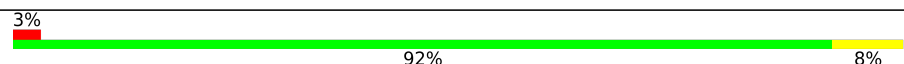
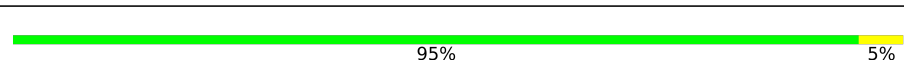
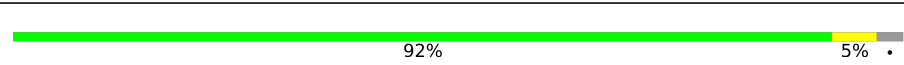
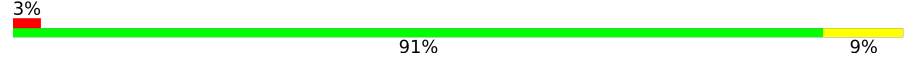
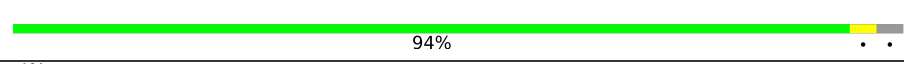
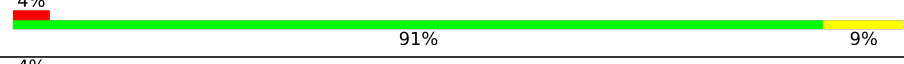
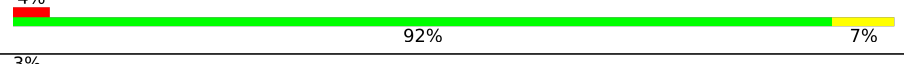
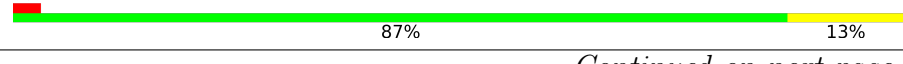

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Mol	Chain	Length	Quality of chain
1	A	334	 97%
1	a	334	 96%

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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) : 2.36

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Mol	Chain	Length	Quality of chain
2	B	505	 96%
2	b	505	 96%
3	C	451	 95%
3	c	451	 96%
4	D	341	 97%
4	d	341	 97%
5	E	82	 89% 10%
5	e	82	 90% 10%
6	F	34	 97%
6	f	34	 94% 6%
7	H	65	 94% 6%
7	h	65	 89% 8%
8	I	36	 83% 17%
8	i	36	 97%
9	J	36	 100%
9	j	36	 94% 6%
10	K	37	 95% 5%
10	k	37	 92% 8%
11	L	37	 95% 5%
11	l	37	 92% 5%
12	M	33	 91% 9%
12	m	33	 94%
13	O	244	 91% 9%
13	o	244	 92% 7%
14	T	30	 87% 13%

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Mol	Chain	Length	Quality of chain
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	h	101	X	-	-	-

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103673 atoms, of which 51476 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	H	N	O				S
1	A	334	5130	1717	2508	431	459	15	0	0	0
1	a	334	5118	1714	2499	431	459	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	H	N	O				S
2	B	505	7849	2631	3845	666	694	13	0	5	0
2	b	505	7789	2610	3811	665	690	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	442	6752	2244	3335	570	590	13	0	0	0
3	c	451	6901	2286	3407	587	608	13	0	1	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
6	F	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	H	65	Total	C	H	N	O	S	0	0	0
			1030	338	523	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	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	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			516	172	261	40	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0	0
			525	171	269	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3730	1174	1850	317	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3718	1170	1844	317	383	4			

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

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

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

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



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
17	Y	27	Total	C	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
20	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			
20	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

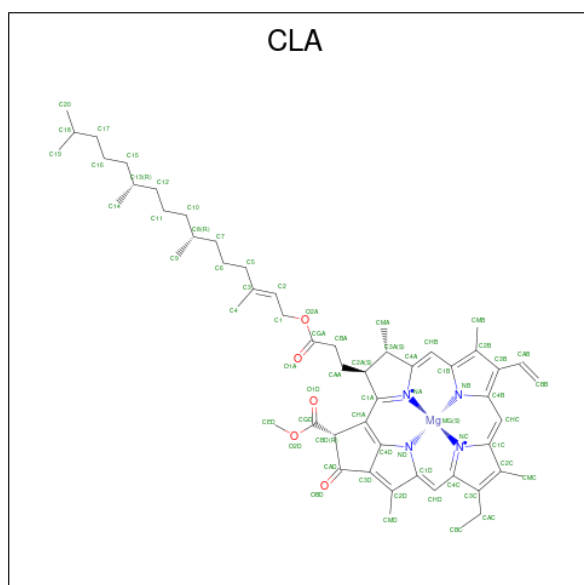
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	A	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	A	1	Total C H Mg N O 102 44 48 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0

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

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

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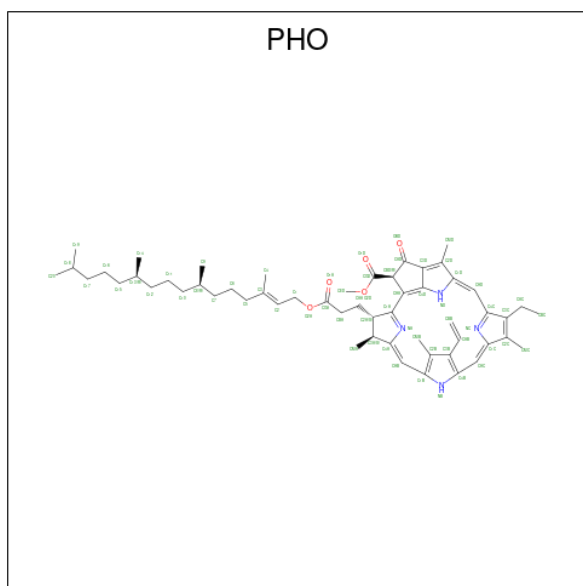
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total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

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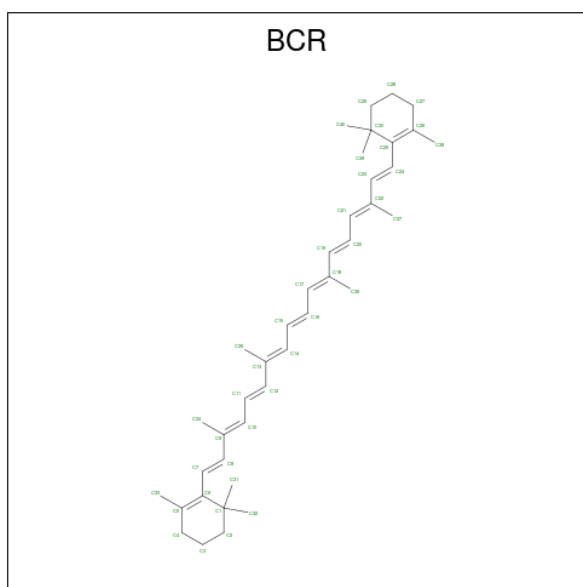
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
23	h	1	137	55	72	1	4	5	0	0

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



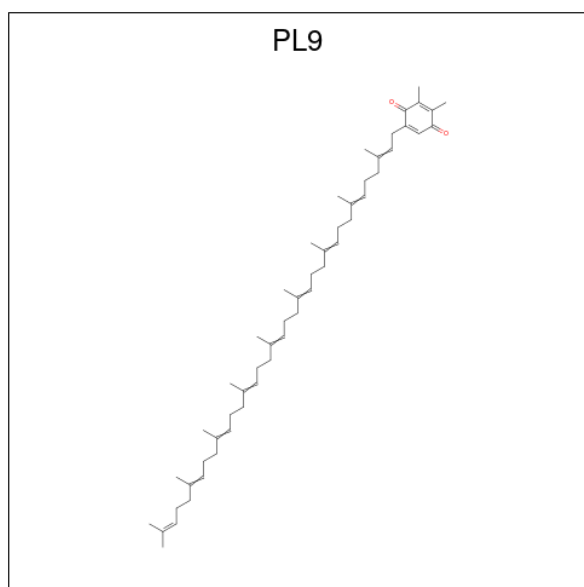
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total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

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

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



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

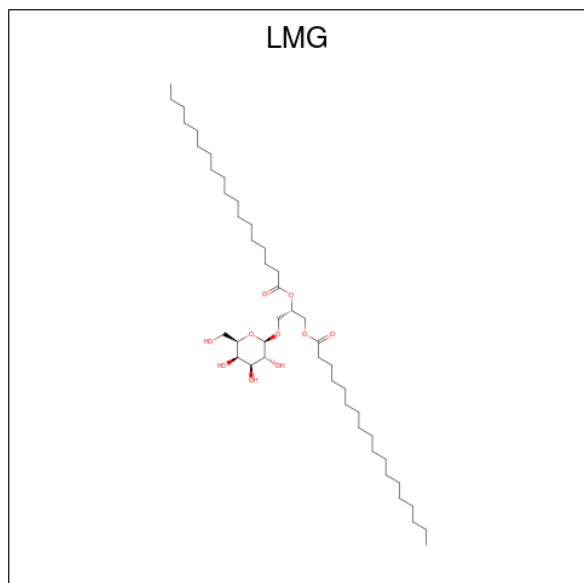
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



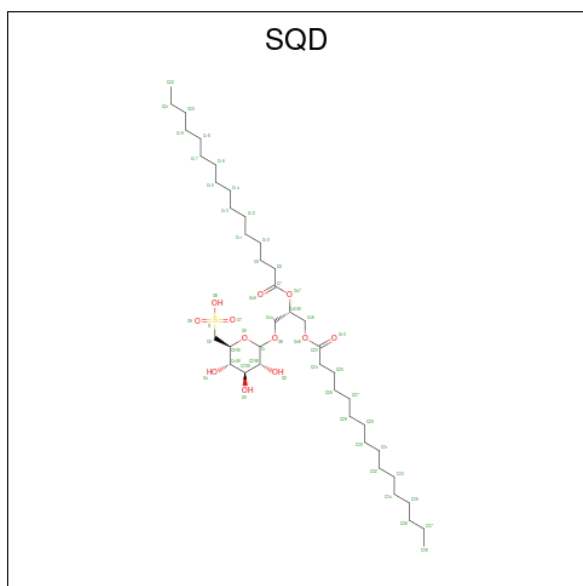
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			123	41	72	10		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			57	21	34	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
27	c	1	81	27	44	10	0	0
27	c	1	117	38	69	10	0	0
27	d	1	102	34	58	10	0	0
27	m	1	123	41	72	10	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



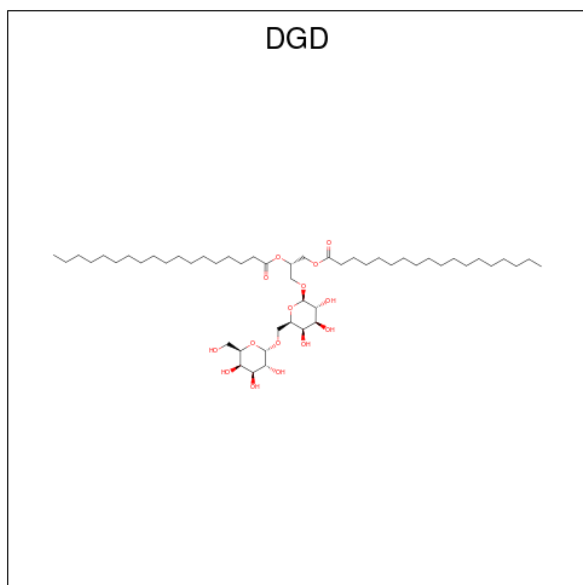
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
28	A	1	122	39	70	12	1	0	0
28	A	1	104	35	65	4	0	0	
28	B	1	132	41	78	12	1	0	0
28	F	1	81	25	45	10	1	0	0
28	a	1	132	41	78	12	1	0	0
28	a	1	92	31	56	5	0	0	
28	b	1	114	36	65	12	1	0	0

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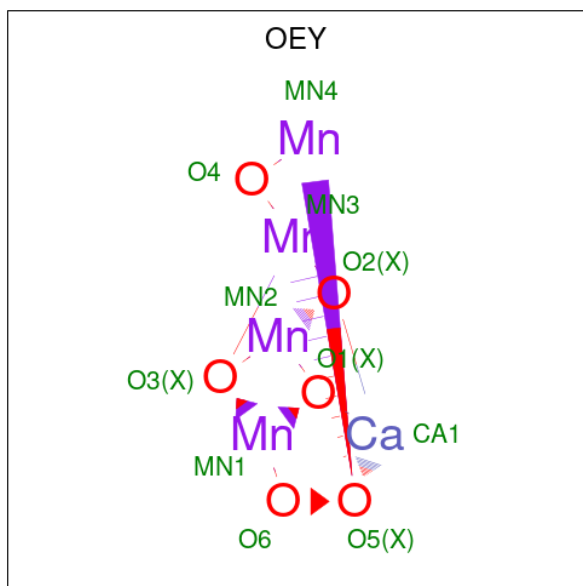
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
28	f	1	90	28	49	12	1	0	0

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



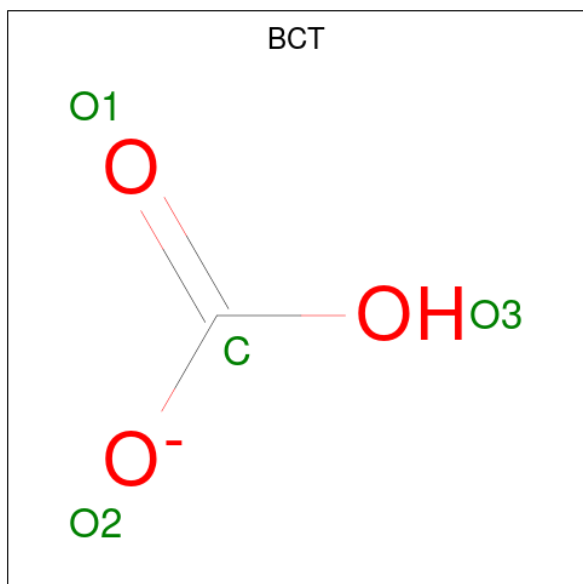
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
29	A	1	162	51	96	15	0	0	
29	C	1	144	47	82	15	0	0	
29	C	1	144	47	82	15	0	0	
29	C	1	144	47	82	15	0	0	
29	H	1	144	47	82	15	0	0	
29	a	1	119	39	75	5	0	0	
29	c	1	144	47	82	15	0	0	
29	c	1	144	47	82	15	0	0	
29	c	1	144	47	82	15	0	0	
29	h	1	144	47	82	15	0	0	

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ).



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

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
31	A	1	5	1	1	3	0	0

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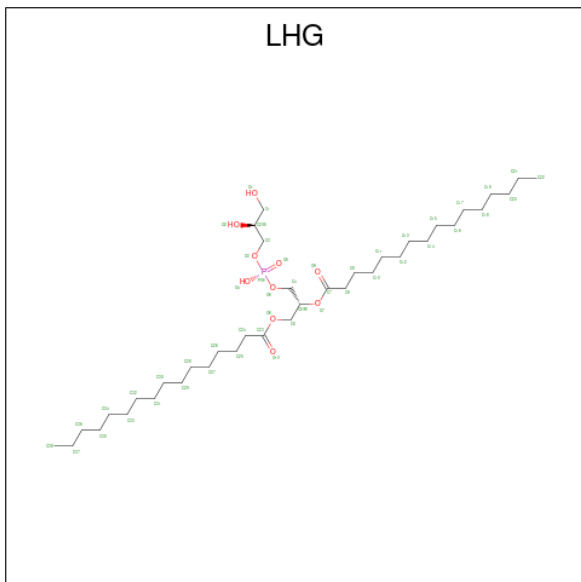
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

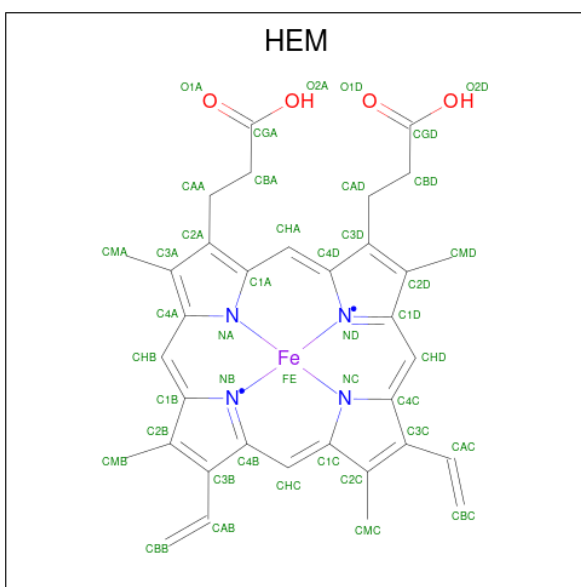
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	5	Total	C	H	O	0	0
			180	63	109	8		
32	C	3	Total	C	H	O	0	0
			103	36	63	4		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	E	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			
32	I	1	Total	C	H		0	0
			41	15	26			
32	J	1	Total	C	H	O	0	0
			28	10	16	2		
32	M	2	Total	C	H	O	0	0
			63	23	38	2		
32	T	1	Total	C	H		0	0
			44	15	29			
32	a	1	Total	C	H	O	0	0
			28	10	16	2		
32	b	5	Total	C	H	O	0	0
			223	76	141	6		
32	c	2	Total	C	H	O	0	0
			83	28	51	4		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	2	Total	C	H	O	0	0
			72	26	44	2		
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



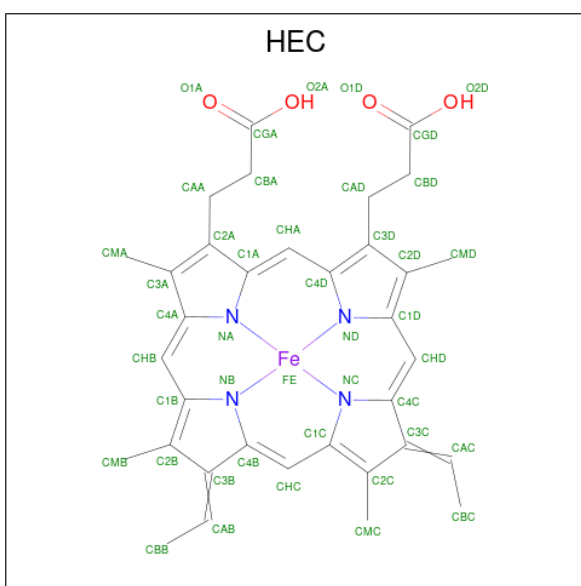
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
33	B	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	D	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	D	1	Total 114	C 36	H 67	O 10	P 1	0	0
33	E	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	L	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	a	1	Total 123	C 38	H 74	O 10	P 1	0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

- 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	
			Total	C	Fe	H	N			O
34	E	1	73	34	1	30	4	4	0	0
34	e	1	73	34	1	30	4	4	0	0

- Molecule 35 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	138	Total O 138 138	0	0
36	B	221	Total O 221 221	0	0
36	C	191	Total O 191 191	0	0
36	D	142	Total O 142 142	0	0
36	E	31	Total O 31 31	0	0
36	F	11	Total O 11 11	0	0
36	H	25	Total O 25 25	0	0
36	I	14	Total O 14 14	0	0
36	J	15	Total O 15 15	0	0
36	K	2	Total O 2 2	0	0
36	L	7	Total O 7 7	0	0
36	M	5	Total O 5 5	0	0
36	O	121	Total O 121 121	0	0
36	T	12	Total O 12 12	0	0
36	U	51	Total O 51 51	0	0
36	V	68	Total O 68 68	0	0
36	Y	5	Total O 5 5	0	0
36	X	8	Total O 8 8	0	0
36	Z	5	Total O 5 5	0	0
36	R	3	Total O 3 3	0	0
36	a	121	Total O 121 121	0	0

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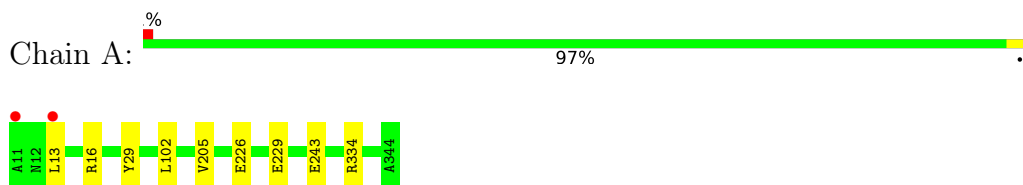
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	b	190	Total O 190 190	0	0
36	c	154	Total O 154 154	0	0
36	d	127	Total O 127 127	0	0
36	e	20	Total O 20 20	0	0
36	f	6	Total O 6 6	0	0
36	h	17	Total O 17 17	0	0
36	i	12	Total O 12 12	0	0
36	j	7	Total O 7 7	0	0
36	k	6	Total O 6 6	0	0
36	l	11	Total O 11 11	0	0
36	m	6	Total O 6 6	0	0
36	o	117	Total O 117 117	0	0
36	t	12	Total O 12 12	0	0
36	u	50	Total O 50 50	0	0
36	v	63	Total O 63 63	0	0
36	y	4	Total O 4 4	0	0
36	x	11	Total O 11 11	0	0
36	z	1	Total O 1 1	0	0
36	r	6	Total O 6 6	0	0

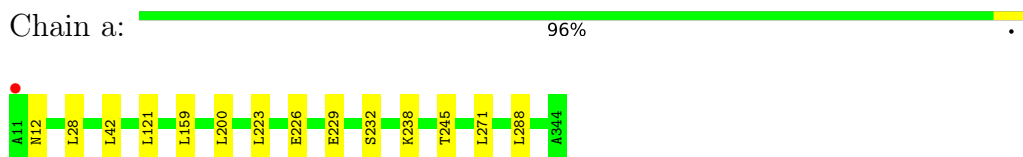
### 3 Residue-property plots [i](#)

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.

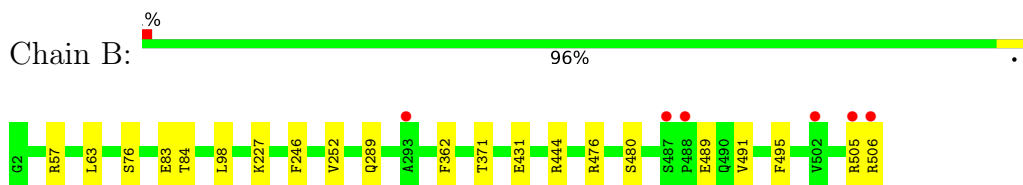
- Molecule 1: Photosystem II protein D1 1



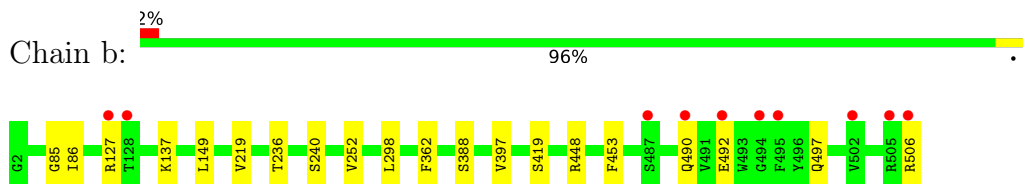
- Molecule 1: Photosystem II protein D1 1



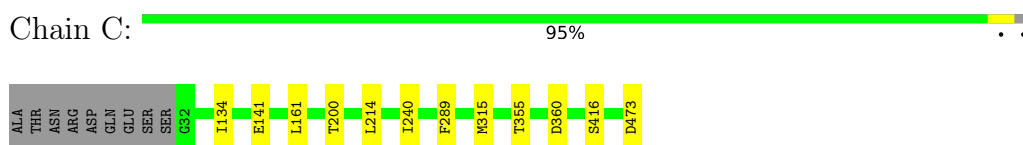
- Molecule 2: Photosystem II CP47 reaction center protein



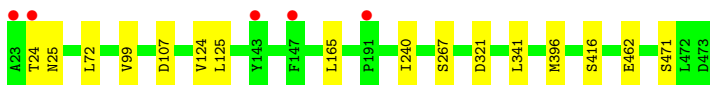
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



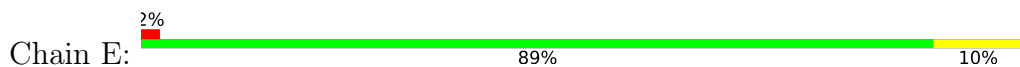
- Molecule 4: Photosystem II D2 protein



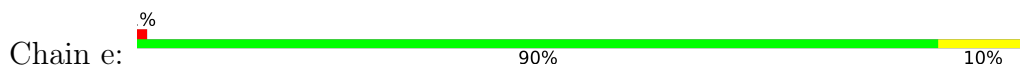
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

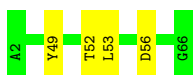


- Molecule 6: Cytochrome b559 subunit beta




- Molecule 7: Photosystem II reaction center protein H

Chain H:  94% 6%




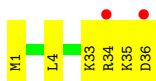
- Molecule 7: Photosystem II reaction center protein H

Chain h:  2% 89% 8%

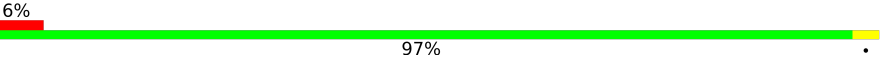


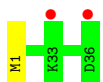
- Molecule 8: Photosystem II reaction center protein I

Chain I:  6% 83% 17%



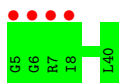
- Molecule 8: Photosystem II reaction center protein I

Chain i:  6% 97%

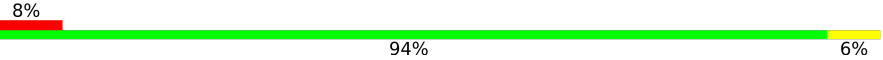


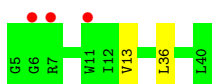
- Molecule 9: Photosystem II reaction center protein J

Chain J:  11% 100%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  8% 94% 6%

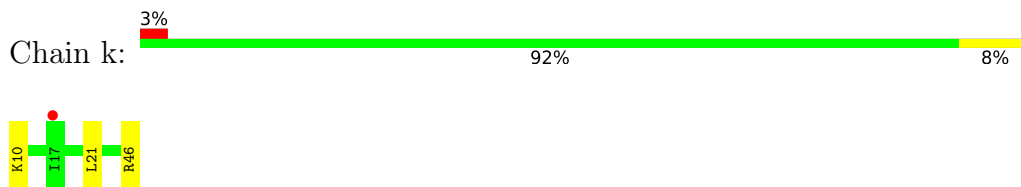


- Molecule 10: Photosystem II reaction center protein K

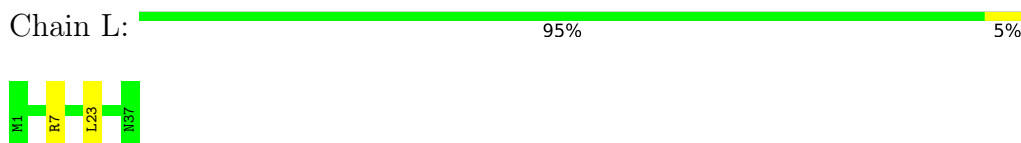
Chain K:  3% 95% 5%



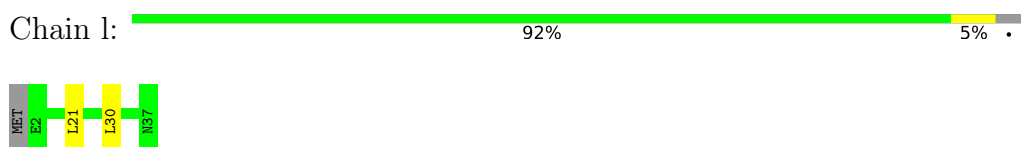
- Molecule 10: Photosystem II reaction center protein K



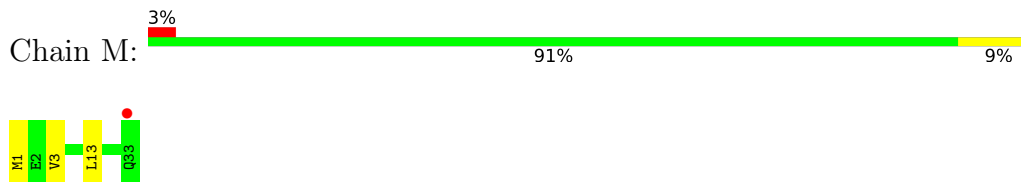
- Molecule 11: Photosystem II reaction center protein L



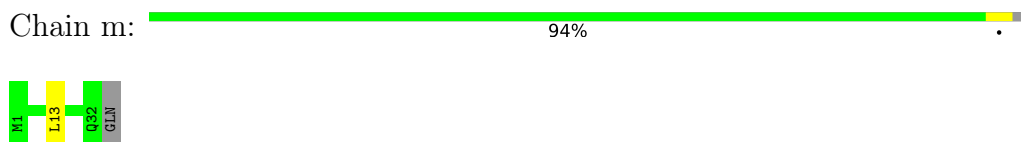
- Molecule 11: Photosystem II reaction center protein L



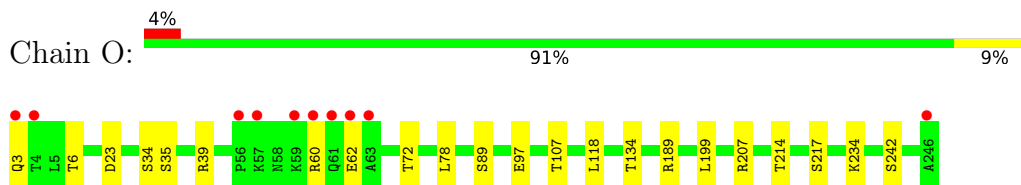
- Molecule 12: Photosystem II reaction center protein M



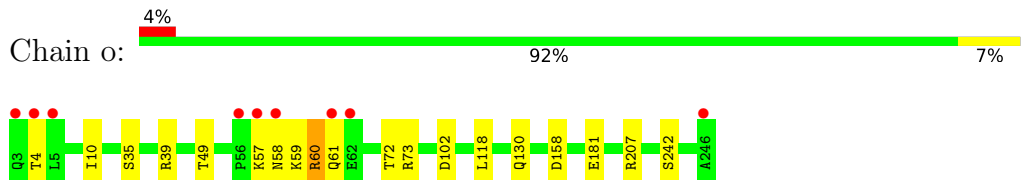
- Molecule 12: Photosystem II reaction center protein M



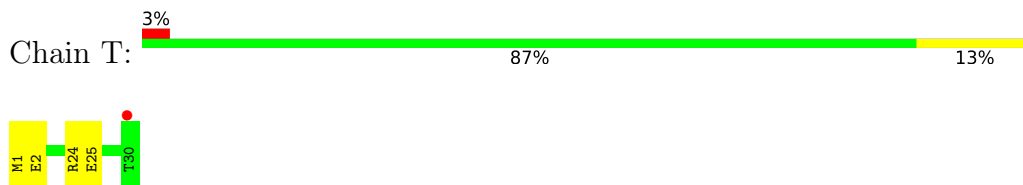
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



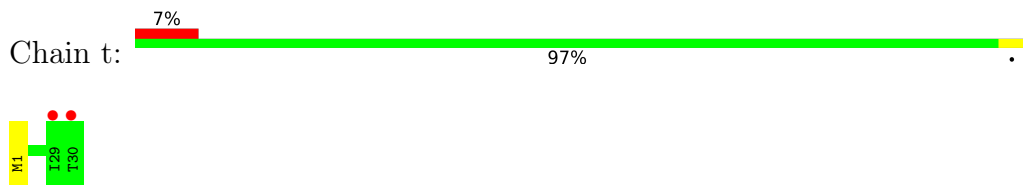
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



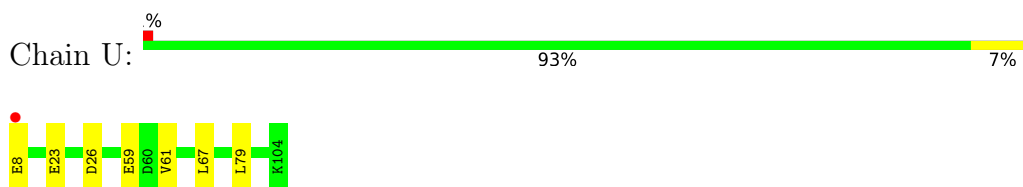
- Molecule 14: Photosystem II reaction center protein T



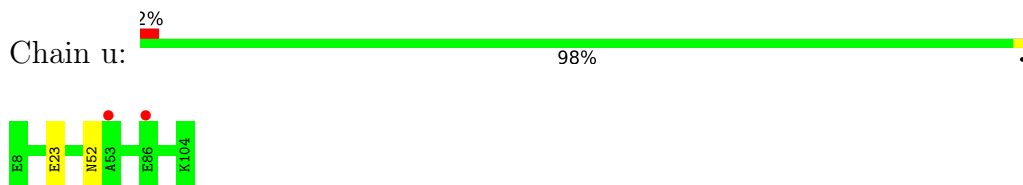
- Molecule 14: Photosystem II reaction center protein T



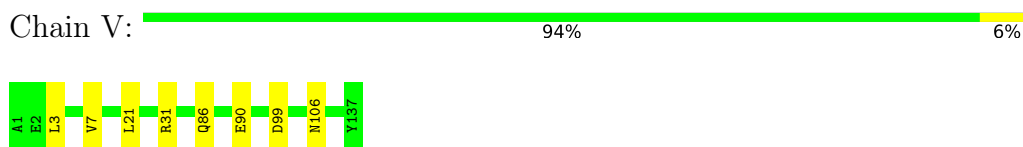
- Molecule 15: Photosystem II 12 kDa extrinsic protein



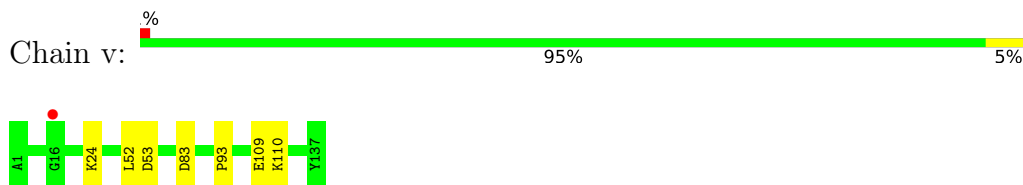
- Molecule 15: Photosystem II 12 kDa extrinsic protein



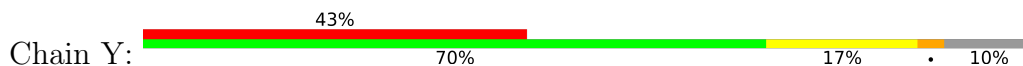
- Molecule 16: Cytochrome c-550

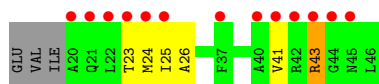


- Molecule 16: Cytochrome c-550

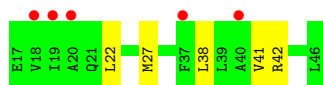
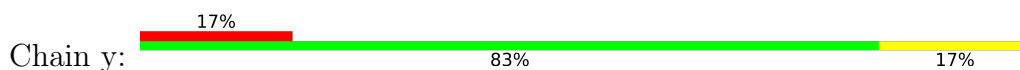


- Molecule 17: Photosystem II reaction center protein Ycf12

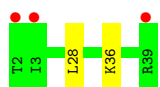




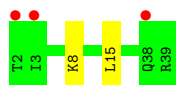
- Molecule 17: Photosystem II reaction center protein Ycf12



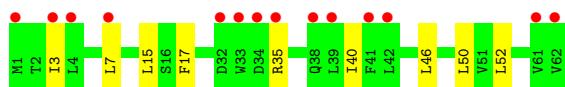
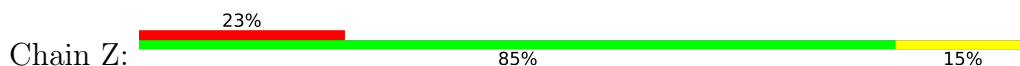
- Molecule 18: Photosystem II reaction center X protein



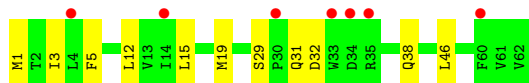
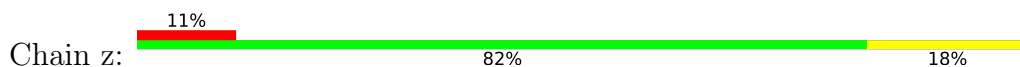
- Molecule 18: Photosystem II reaction center X protein



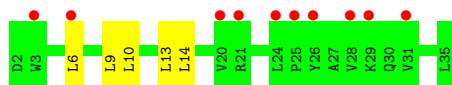
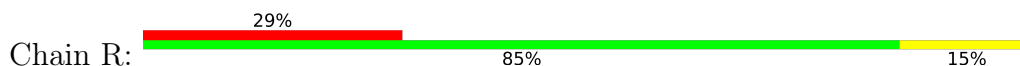
- Molecule 19: Photosystem II reaction center protein Z



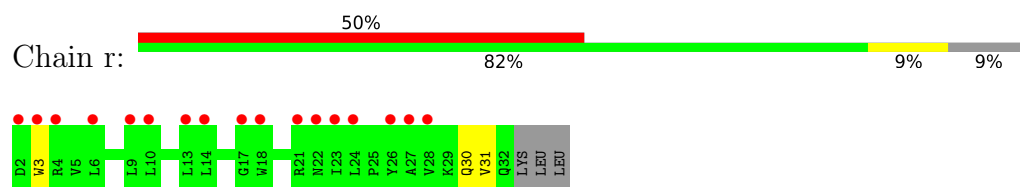
- Molecule 19: Photosystem II reaction center protein Z



- 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, $\alpha$ , $\beta$ , $\gamma$	117.69Å 222.53Å 308.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.85 – 2.20 30.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.85-2.20) 83.7 (30.85-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.75 (at 2.20Å)	Xtrriage
Refinement program	PHENIX dev_svn	Depositor
R, $R_{free}$	0.193 , 0.264 0.193 , 0.264	Depositor DCC
$R_{free}$ test set	3620 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 70.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	103673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.72	1/2707 (0.0%)	0.74	2/3692 (0.1%)
1	a	0.68	0/2704	0.71	1/3688 (0.0%)
2	B	0.69	1/4160 (0.0%)	0.71	1/5668 (0.0%)
2	b	0.67	1/4118 (0.0%)	0.69	1/5611 (0.0%)
3	C	0.65	0/3530	0.69	3/4807 (0.1%)
3	c	0.59	0/3610	0.70	3/4914 (0.1%)
4	D	0.72	1/2812 (0.0%)	0.71	1/3832 (0.0%)
4	d	0.66	0/2821	0.72	1/3844 (0.0%)
5	E	0.59	0/684	0.63	0/935
5	e	0.49	0/683	0.62	0/932
6	F	0.57	0/284	0.60	0/387
6	f	0.44	0/284	0.64	0/387
7	H	0.68	0/520	0.72	0/709
7	h	0.63	0/511	0.72	0/697
8	I	0.60	0/293	0.71	0/396
8	i	0.73	0/293	0.70	0/396
9	J	0.54	0/263	0.67	0/356
9	j	0.54	0/261	0.71	0/353
10	K	0.48	0/314	0.75	0/427
10	k	0.48	0/303	0.67	0/416
11	L	0.70	0/311	0.76	1/422 (0.2%)
11	l	0.64	0/303	0.70	0/412
12	M	0.63	0/249	0.75	0/341
12	m	0.71	0/244	0.70	0/334
13	O	0.62	0/1914	0.74	0/2596
13	o	0.62	0/1905	0.77	3/2583 (0.1%)
14	T	0.71	0/257	0.79	0/349
14	t	0.77	0/255	0.64	0/346
15	U	0.63	0/785	0.74	1/1064 (0.1%)
15	u	0.61	0/785	0.73	0/1064
16	V	0.58	0/1085	0.66	0/1473
16	v	0.55	0/1085	0.70	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.41	0/197	0.64	0/264
17	y	0.37	0/219	0.58	0/294
18	X	0.57	0/284	0.66	0/384
18	x	0.44	0/284	0.60	0/384
19	Z	0.51	0/490	0.62	0/669
19	z	0.46	0/488	0.57	0/666
20	R	0.45	0/277	0.62	0/380
20	r	0.37	0/233	0.54	0/323
All	All	0.64	4/42805 (0.0%)	0.70	19/58268 (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
15	u	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	TYR	CD1-CE1	-5.59	1.30	1.39
4	D	280	TRP	CB-CG	5.36	1.59	1.50
2	B	252	VAL	CB-CG1	5.24	1.63	1.52
2	b	453	PHE	CB-CG	-5.22	1.42	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	334	ARG	NE-CZ-NH1	6.79	123.69	120.30
3	c	107	ASP	CB-CG-OD1	6.72	124.34	118.30
1	a	121	LEU	CB-CG-CD2	-6.53	99.89	111.00
3	C	360	ASP	CB-CG-OD1	-6.42	112.53	118.30
1	A	334	ARG	NE-CZ-NH2	-6.13	117.23	120.30
4	D	110	LEU	CB-CG-CD1	-6.06	100.70	111.00
15	U	26	ASP	CB-CG-OD1	6.03	123.72	118.30
13	o	102	ASP	CB-CG-OD1	5.85	123.56	118.30
11	L	23	LEU	CB-CG-CD2	-5.75	101.22	111.00
13	o	102	ASP	CB-CG-OD2	-5.47	113.38	118.30
3	C	473	ASP	CB-CG-OD1	5.42	123.18	118.30
2	B	57	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	308	ASP	CB-CG-OD2	-5.31	113.53	118.30
3	c	107	ASP	CB-CG-OD2	-5.21	113.61	118.30
3	c	321	ASP	CB-CG-OD1	5.19	122.97	118.30
3	C	214	LEU	CB-CG-CD1	-5.13	102.28	111.00
16	v	83	ASP	CB-CG-OD2	5.08	122.87	118.30
2	b	448	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	52	ASN	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	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
1	a	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
2	B	508/505 (101%)	490 (96%)	18 (4%)	0	100	100
2	b	503/505 (100%)	481 (96%)	20 (4%)	2 (0%)	34	37
3	C	440/451 (98%)	426 (97%)	13 (3%)	1 (0%)	47	55
3	c	450/451 (100%)	431 (96%)	18 (4%)	1 (0%)	47	55
4	D	339/341 (99%)	331 (98%)	7 (2%)	1 (0%)	41	46
4	d	340/341 (100%)	329 (97%)	10 (3%)	1 (0%)	41	46
5	E	80/82 (98%)	79 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
6	f	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
7	H	63/65 (97%)	55 (87%)	8 (13%)	0	100	100
7	h	61/65 (94%)	56 (92%)	5 (8%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	28 (82%)	6 (18%)	0	100	100
9	j	34/36 (94%)	29 (85%)	5 (15%)	0	100	100
10	K	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	4	2
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	222 (91%)	19 (8%)	2 (1%)	19	19
13	o	242/244 (99%)	225 (93%)	14 (6%)	3 (1%)	13	10
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	u	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	17 (68%)	5 (20%)	3 (12%)	0	0
17	y	28/30 (93%)	25 (89%)	1 (4%)	2 (7%)	1	0
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
19	z	60/62 (97%)	51 (85%)	6 (10%)	3 (5%)	2	0
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
20	r	29/34 (85%)	25 (86%)	2 (7%)	2 (7%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5235/5326 (98%)	4988 (95%)	225 (4%)	22 (0%)	34 37

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	60	ARG
13	O	62	GLU
17	Y	41	VAL
3	c	416	SER
13	o	60	ARG
20	r	30	GLN
20	r	31	VAL
17	Y	43	ARG
19	z	15	LEU
19	z	31	GLN
17	Y	26	ALA
2	b	127	ARG
13	o	61	GLN
4	D	338	ASN
13	o	73	ARG
17	y	42	ARG
4	d	65	SER
19	z	5	PHE
2	b	85	GLY
17	y	41	VAL

### 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	270/270 (100%)	263 (97%)	7 (3%)	46 58
1	a	269/270 (100%)	256 (95%)	13 (5%)	25 32
2	B	407/403 (101%)	387 (95%)	20 (5%)	25 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	402/403 (100%)	386 (96%)	16 (4%)	31	40
3	C	344/352 (98%)	336 (98%)	8 (2%)	50	63
3	c	353/352 (100%)	340 (96%)	13 (4%)	34	43
4	D	276/276 (100%)	270 (98%)	6 (2%)	52	65
4	d	277/276 (100%)	270 (98%)	7 (2%)	47	60
5	E	72/72 (100%)	63 (88%)	9 (12%)	4	4
5	e	71/72 (99%)	63 (89%)	8 (11%)	6	5
6	F	28/28 (100%)	27 (96%)	1 (4%)	35	45
6	f	28/28 (100%)	26 (93%)	2 (7%)	14	16
7	H	53/54 (98%)	49 (92%)	4 (8%)	13	14
7	h	53/54 (98%)	48 (91%)	5 (9%)	8	8
8	I	32/32 (100%)	27 (84%)	5 (16%)	2	2
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	24/24 (100%)	24 (100%)	0	100	100
9	j	23/24 (96%)	21 (91%)	2 (9%)	10	10
10	K	31/30 (103%)	30 (97%)	1 (3%)	39	50
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	7
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	54
11	l	34/35 (97%)	32 (94%)	2 (6%)	19	23
12	M	28/29 (97%)	26 (93%)	2 (7%)	14	16
12	m	28/29 (97%)	27 (96%)	1 (4%)	35	45
13	O	208/207 (100%)	188 (90%)	20 (10%)	8	8
13	o	207/207 (100%)	192 (93%)	15 (7%)	14	15
14	T	26/26 (100%)	23 (88%)	3 (12%)	5	5
14	t	25/26 (96%)	25 (100%)	0	100	100
15	U	84/84 (100%)	78 (93%)	6 (7%)	14	16
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	83
16	V	117/117 (100%)	109 (93%)	8 (7%)	16	17
16	v	117/117 (100%)	111 (95%)	6 (5%)	24	29
17	Y	19/23 (83%)	15 (79%)	4 (21%)	1	1
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	31/31 (100%)	29 (94%)	2 (6%)	17	19
18	x	31/31 (100%)	29 (94%)	2 (6%)	17	19
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	1
19	z	51/52 (98%)	43 (84%)	8 (16%)	2	2
20	R	28/29 (97%)	23 (82%)	5 (18%)	2	1
20	r	19/29 (66%)	18 (95%)	1 (5%)	22	27
All	All	4321/4348 (99%)	4092 (95%)	229 (5%)	22	27

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	16	ARG
1	A	102	LEU
1	A	205	VAL
1	A	226	GLU
1	A	229	GLU
1	A	243	GLU
2	B	63	LEU
2	B	76	SER
2	B	83	GLU
2	B	84	THR
2	B	98	LEU
2	B	227	LYS
2	B	246	PHE
2	B	289	GLN
2	B	362	PHE
2	B	371	THR
2	B	431	GLU
2	B	444	ARG
2	B	476	ARG
2	B	480[A]	SER
2	B	480[B]	SER
2	B	489	GLU
2	B	491	VAL
2	B	495	PHE
2	B	505	ARG
2	B	506	ARG
3	C	134	ILE
3	C	141	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	161	LEU
3	C	200	THR
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	12	ARG
4	D	76	VAL
4	D	180	ARG
4	D	241	GLU
4	D	251	ARG
4	D	345	VAL
5	E	4	THR
5	E	11	SER
5	E	12	ASP
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	65	LEU
5	E	71	GLU
5	E	76	VAL
5	E	83	LEU
6	F	12	SER
7	H	49	TYR
7	H	52	THR
7	H	53	LEU
7	H	56	ASP
8	I	4	LEU
8	I	33	LYS
8	I	34	ARG
8	I	35	LYS
8	I	36	ASP
10	K	13	GLU
11	L	7	ARG
12	M	3	VAL
12	M	13	LEU
13	O	3	GLN
13	O	6	THR
13	O	23	ASP
13	O	34	SER
13	O	35	SER
13	O	39	ARG
13	O	72	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	O	78	LEU
13	O	89	SER
13	O	97	GLU
13	O	107	THR
13	O	118	LEU
13	O	134	THR
13	O	189	ARG
13	O	199	LEU
13	O	207	ARG
13	O	214	THR
13	O	217	SER
13	O	234	LYS
13	O	242	SER
14	T	2	GLU
14	T	24	ARG
14	T	25	GLU
15	U	8	GLU
15	U	23	GLU
15	U	59	GLU
15	U	61	VAL
15	U	67	LEU
15	U	79	LEU
16	V	3	LEU
16	V	7	VAL
16	V	21	LEU
16	V	31	ARG
16	V	86	GLN
16	V	90	GLU
16	V	99	ASP
16	V	106	ASN
17	Y	23	THR
17	Y	24	MET
17	Y	25	ILE
17	Y	43	ARG
18	X	28	LEU
18	X	36	LYS
19	Z	3	ILE
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	35	ARG
19	Z	40	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	Z	46	LEU
19	Z	50	LEU
19	Z	52	LEU
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	13	LEU
20	R	14	LEU
1	a	12	ASN
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	232	SER
1	a	238	LYS
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	86	ILE
2	b	137	LYS
2	b	149	LEU
2	b	219	VAL
2	b	236	THR
2	b	240	SER
2	b	252	VAL
2	b	298	LEU
2	b	362	PHE
2	b	388	SER
2	b	397	VAL
2	b	419	SER
2	b	490	GLN
2	b	492	GLU
2	b	497	GLN
2	b	506	ARG
3	c	24	THR
3	c	25	ASN
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	267	SER
3	c	341	LEU
3	c	396	MET
3	c	462	GLU
3	c	471	SER
4	d	180	ARG
4	d	182	LEU
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	16	SER
5	e	39	SER
5	e	54	SER
5	e	61	ARG
5	e	75	GLN
5	e	82	GLN
5	e	83	LEU
5	e	84	LYS
6	f	28	VAL
6	f	44	GLN
7	h	3	ARG
7	h	7	LEU
7	h	37	LEU
7	h	49	TYR
7	h	56	ASP
9	j	13	VAL
9	j	36	LEU
10	k	10	LYS
10	k	21	LEU
10	k	46	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	4	THR
13	o	10	ILE
13	o	35	SER
13	o	39	ARG

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Mol	Chain	Res	Type
13	o	49	THR
13	o	57	LYS
13	o	58	ASN
13	o	59	LYS
13	o	60	ARG
13	o	72	THR
13	o	118	LEU
13	o	130	GLN
13	o	181	GLU
13	o	207	ARG
13	o	242	SER
15	u	23	GLU
16	v	24	LYS
16	v	52	LEU
16	v	53	ASP
16	v	93	PRO
16	v	109	GLU
16	v	110	LYS
17	y	22	LEU
17	y	27	MET
17	y	38	LEU
18	x	8	LYS
18	x	15	LEU
19	z	1	MET
19	z	3	ILE
19	z	12	LEU
19	z	19	MET
19	z	29	SER
19	z	32	ASP
19	z	38	GLN
19	z	46	LEU
20	r	3	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	289	GLN
13	O	82	GLN
13	O	88	ASN
15	U	73	GLN
17	Y	21	GLN
3	c	25	ASN

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Mol	Chain	Res	Type
3	c	28	GLN
13	o	58	ASN
15	u	78	ASN

### 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
14	FME	t	1	14	8,9,10	0.96	0	7,9,11	1.03	1 (14%)
14	FME	T	1	14	8,9,10	1.04	1 (12%)	7,9,11	2.02	2 (28%)
12	FME	M	1	12	8,9,10	1.14	1 (12%)	7,9,11	1.29	1 (14%)
12	FME	m	1	12	8,9,10	0.92	0	7,9,11	0.85	0
8	FME	i	1	8	8,9,10	0.96	0	7,9,11	1.10	1 (14%)
8	FME	I	1	8	8,9,10	0.98	0	7,9,11	1.49	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	4/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	2/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.55	1.42	1.46
14	T	1	FME	CA-N	-2.50	1.42	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	-3.99	116.68	122.82
8	I	1	FME	C-CA-N	3.13	115.38	109.73
12	M	1	FME	C-CA-N	-2.60	105.05	109.73
8	i	1	FME	C-CA-N	2.60	114.42	109.73
14	T	1	FME	O1-CN-N	-2.30	119.20	125.27
14	t	1	FME	CA-N-CN	-2.11	119.58	122.82

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

Of 186 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 149 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	CLA	D	403	-	65,73,73	1.66	12 (18%)	76,113,113	1.61	10 (13%)
23	CLA	c	512	-	65,73,73	1.71	9 (13%)	76,113,113	1.54	10 (13%)
23	CLA	d	404	-	65,73,73	2.06	11 (16%)	76,113,113	1.29	9 (11%)
25	BCR	b	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.41	11 (19%)
23	CLA	A	404	-	65,73,73	1.63	8 (12%)	76,113,113	1.65	13 (17%)
23	CLA	C	507	36	65,73,73	1.47	10 (15%)	76,113,113	1.33	9 (11%)
26	PL9	A	409	-	55,55,55	0.92	1 (1%)	68,69,69	1.66	13 (19%)
29	DGD	c	518	-	63,63,67	1.25	9 (14%)	77,77,81	1.47	14 (18%)
23	CLA	a	407	-	65,73,73	1.56	12 (18%)	76,113,113	1.41	16 (21%)
25	BCR	c	515	-	41,41,41	1.14	4 (9%)	56,56,56	1.47	11 (19%)
25	BCR	h	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.33	9 (16%)
25	BCR	C	520	-	41,41,41	1.01	1 (2%)	56,56,56	1.19	3 (5%)
23	CLA	A	407	-	54,62,73	1.95	15 (27%)	62,99,113	1.98	15 (24%)
31	BCT	A	415	21	2,3,3	1.35	0	2,3,3	2.85	1 (50%)
23	CLA	c	506	-	65,73,73	1.66	10 (15%)	76,113,113	1.66	18 (23%)
23	CLA	b	615	-	65,73,73	1.91	8 (12%)	76,113,113	1.67	11 (14%)
25	BCR	D	405	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	7 (12%)
23	CLA	c	509	-	65,73,73	1.89	9 (13%)	76,113,113	1.78	13 (17%)
23	CLA	b	604	-	65,73,73	1.80	12 (18%)	76,113,113	1.74	13 (17%)
23	CLA	c	507	36	65,73,73	1.45	9 (13%)	76,113,113	1.47	12 (15%)
23	CLA	B	609	-	65,73,73	1.86	12 (18%)	76,113,113	1.24	10 (13%)
23	CLA	b	605	-	65,73,73	1.61	10 (15%)	76,113,113	1.78	15 (19%)
30	OEY	a	416	1,3,36	0,16,16	-	-	-	-	-
23	CLA	D	402	36	65,73,73	1.51	10 (15%)	76,113,113	1.60	13 (17%)
29	DGD	C	516	-	63,63,67	1.40	10 (15%)	77,77,81	1.39	9 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	t	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	8 (14%)
25	BCR	a	408	-	41,41,41	1.15	4 (9%)	56,56,56	1.45	8 (14%)
25	BCR	B	619	-	41,41,41	1.23	3 (7%)	56,56,56	1.36	11 (19%)
23	CLA	b	614	-	65,73,73	1.52	11 (16%)	76,113,113	1.43	14 (18%)
23	CLA	C	501	-	65,73,73	2.26	10 (15%)	76,113,113	1.57	7 (9%)
23	CLA	b	608	36	65,73,73	1.39	8 (12%)	76,113,113	1.35	6 (7%)
23	CLA	C	508	-	65,73,73	1.63	8 (12%)	76,113,113	1.63	11 (14%)
23	CLA	b	611	36	65,73,73	1.41	10 (15%)	76,113,113	1.61	11 (14%)
23	CLA	C	513	-	65,73,73	1.51	9 (13%)	76,113,113	1.66	10 (13%)
23	CLA	c	510	-	65,73,73	1.42	7 (10%)	76,113,113	1.58	14 (18%)
23	CLA	B	604	-	65,73,73	1.52	8 (12%)	76,113,113	1.85	9 (11%)
23	CLA	C	502	-	65,73,73	1.69	8 (12%)	76,113,113	1.37	8 (10%)
23	CLA	h	101	36	65,73,73	1.65	13 (20%)	76,113,113	1.47	11 (14%)
23	CLA	d	403	-	65,73,73	1.56	12 (18%)	76,113,113	1.22	7 (9%)
28	SQD	F	101	-	35,36,54	1.07	3 (8%)	42,45,65	1.88	9 (21%)
31	BCT	a	417	21	2,3,3	1.44	0	2,3,3	2.79	2 (100%)
23	CLA	B	602	-	65,73,73	1.71	8 (12%)	76,113,113	1.78	16 (21%)
25	BCR	d	405	-	41,41,41	1.12	2 (4%)	56,56,56	1.31	7 (12%)
23	CLA	C	509	-	65,73,73	1.55	8 (12%)	76,113,113	1.49	9 (11%)
23	CLA	b	617	-	60,68,73	1.67	12 (20%)	70,107,113	1.74	10 (14%)
28	SQD	f	101	-	40,41,54	1.09	4 (10%)	49,52,65	1.92	9 (18%)
33	LHG	l	101	-	48,48,48	0.83	3 (6%)	51,54,54	1.19	4 (7%)
23	CLA	c	503	-	65,73,73	1.47	7 (10%)	76,113,113	1.57	11 (14%)
27	LMG	A	410	-	48,48,55	1.03	3 (6%)	56,56,63	1.23	5 (8%)
29	DGD	c	517	-	63,63,67	1.28	11 (17%)	77,77,81	1.54	10 (12%)
23	CLA	b	613	-	65,73,73	1.65	12 (18%)	76,113,113	1.61	9 (11%)
23	CLA	b	607	-	65,73,73	1.71	11 (16%)	76,113,113	1.72	9 (11%)
23	CLA	b	609	-	65,73,73	1.43	6 (9%)	76,113,113	1.56	12 (15%)
23	CLA	C	506	-	65,73,73	1.78	11 (16%)	76,113,113	1.29	7 (9%)
23	CLA	b	603	-	65,73,73	1.61	9 (13%)	76,113,113	1.56	15 (19%)
23	CLA	c	501	-	65,73,73	1.61	10 (15%)	76,113,113	1.66	10 (13%)
23	CLA	c	508	-	64,72,73	1.47	8 (12%)	74,111,113	1.43	10 (13%)
23	CLA	B	610	36	65,73,73	1.90	11 (16%)	76,113,113	1.55	13 (17%)
33	LHG	d	408	-	38,38,48	0.89	1 (2%)	41,44,54	1.08	4 (9%)
23	CLA	c	513	-	65,73,73	1.48	9 (13%)	76,113,113	1.31	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	c	521	-	41,41,41	0.90	2 (4%)	56,56,56	1.12	4 (7%)
24	PHO	a	406	-	51,69,69	1.08	4 (7%)	47,99,99	1.29	6 (12%)
23	CLA	B	607	36	65,73,73	1.56	10 (15%)	76,113,113	1.30	8 (10%)
23	CLA	c	502	-	65,73,73	1.67	10 (15%)	76,113,113	1.50	10 (13%)
23	CLA	B	614	-	65,73,73	1.89	10 (15%)	76,113,113	1.33	7 (9%)
27	LMG	B	620	-	51,51,55	0.93	4 (7%)	59,59,63	1.54	12 (20%)
28	SQD	a	411	-	53,54,54	1.02	6 (11%)	62,65,65	1.86	13 (20%)
23	CLA	b	610	-	65,73,73	1.67	10 (15%)	76,113,113	1.41	8 (10%)
26	PL9	a	409	-	55,55,55	1.42	5 (9%)	68,69,69	1.41	10 (14%)
25	BCR	c	514	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	8 (14%)
23	CLA	b	616	-	65,73,73	2.03	12 (18%)	76,113,113	1.56	13 (17%)
27	LMG	c	522	-	48,48,55	1.27	8 (16%)	56,56,63	1.45	7 (12%)
23	CLA	B	616	-	60,68,73	1.84	13 (21%)	70,107,113	1.54	12 (17%)
25	BCR	b	619	-	41,41,41	1.23	2 (4%)	56,56,56	1.35	7 (12%)
25	BCR	C	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.40	10 (17%)
34	HEM	E	102	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.38	6 (13%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.43	11 (19%)
23	CLA	a	405	36	65,73,73	1.63	10 (15%)	76,113,113	1.29	10 (13%)
23	CLA	b	612	-	65,73,73	1.75	9 (13%)	76,113,113	1.65	16 (21%)
29	DGD	a	413	-	43,43,67	1.15	3 (6%)	45,45,81	1.41	6 (13%)
33	LHG	d	407	-	48,48,48	0.87	3 (6%)	51,54,54	1.18	4 (7%)
25	BCR	C	515	-	41,41,41	1.23	4 (9%)	56,56,56	1.38	7 (12%)
23	CLA	B	603	-	65,73,73	1.49	11 (16%)	76,113,113	1.59	12 (15%)
23	CLA	B	612	-	65,73,73	1.32	7 (10%)	76,113,113	1.72	16 (21%)
23	CLA	B	605	-	65,73,73	1.38	11 (16%)	76,113,113	1.59	15 (19%)
25	BCR	B	617	-	41,41,41	1.15	3 (7%)	56,56,56	1.38	7 (12%)
27	LMG	d	409	-	44,44,55	1.14	4 (9%)	52,52,63	1.42	9 (17%)
33	LHG	e	101	-	41,41,48	0.81	2 (4%)	44,47,54	1.28	4 (9%)
25	BCR	A	408	-	41,41,41	1.00	2 (4%)	56,56,56	1.38	8 (14%)
28	SQD	A	411	-	51,52,54	1.06	4 (7%)	60,63,65	2.19	9 (15%)
27	LMG	m	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.56	13 (22%)
33	LHG	a	410	-	48,48,48	0.76	1 (2%)	51,54,54	1.35	6 (11%)
28	SQD	A	412	-	38,38,54	1.14	3 (7%)	40,40,65	1.06	1 (2%)
25	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.20	5 (8%)
23	CLA	B	608	-	65,73,73	1.61	10 (15%)	76,113,113	1.46	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	512	-	65,73,73	1.70	12 (18%)	76,113,113	1.37	9 (11%)
23	CLA	B	615	-	65,73,73	1.79	10 (15%)	76,113,113	1.51	11 (14%)
24	PHO	d	401	-	51,69,69	1.05	4 (7%)	47,99,99	1.48	8 (17%)
33	LHG	D	408	-	48,48,48	1.12	5 (10%)	51,54,54	1.18	4 (7%)
33	LHG	B	622	-	48,48,48	0.88	2 (4%)	51,54,54	1.42	7 (13%)
23	CLA	c	505	-	65,73,73	1.58	8 (12%)	76,113,113	1.44	12 (15%)
28	SQD	a	412	-	35,35,54	1.11	2 (5%)	37,37,65	1.33	4 (10%)
23	CLA	B	611	-	65,73,73	1.39	9 (13%)	76,113,113	1.45	13 (17%)
26	PL9	D	406	-	55,55,55	1.36	5 (9%)	68,69,69	1.51	13 (19%)
27	LMG	c	519	-	37,37,55	1.11	4 (10%)	45,45,63	1.20	3 (6%)
23	CLA	A	405	36	65,73,73	1.41	8 (12%)	76,113,113	1.51	16 (21%)
35	HEC	v	201	16	32,50,50	2.09	4 (12%)	24,82,82	1.84	4 (16%)
23	CLA	D	404	-	65,73,73	1.65	10 (15%)	76,113,113	1.24	10 (13%)
30	OEY	A	414	1,3,36	0,16,16	-	-	-	-	-
27	LMG	b	623	-	21,21,55	0.97	1 (4%)	20,20,63	0.90	0
33	LHG	D	409	-	46,46,48	1.01	4 (8%)	49,52,54	1.32	4 (8%)
23	CLA	C	504	36	59,67,73	1.47	9 (15%)	68,105,113	1.51	11 (16%)
23	CLA	C	511	3	65,73,73	1.84	10 (15%)	76,113,113	1.53	9 (11%)
29	DGD	A	413	-	67,67,67	1.29	10 (14%)	81,81,81	1.36	7 (8%)
23	CLA	C	505	-	65,73,73	1.62	10 (15%)	76,113,113	1.38	9 (11%)
25	BCR	T	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.42	7 (12%)
25	BCR	b	620	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	7 (12%)
33	LHG	L	101	-	48,48,48	0.92	1 (2%)	51,54,54	1.17	3 (5%)
24	PHO	D	401	-	51,69,69	1.07	5 (9%)	47,99,99	1.39	7 (14%)
23	CLA	B	601	36	65,73,73	1.85	11 (16%)	76,113,113	1.70	10 (13%)
29	DGD	H	102	-	63,63,67	1.63	10 (15%)	77,77,81	1.64	15 (19%)
25	BCR	y	101	-	41,41,41	1.10	4 (9%)	56,56,56	1.23	6 (10%)
23	CLA	a	404	-	65,73,73	1.36	8 (12%)	76,113,113	1.72	13 (17%)
23	CLA	b	606	-	65,73,73	1.62	5 (7%)	76,113,113	1.68	16 (21%)
23	CLA	c	511	3	65,73,73	1.81	10 (15%)	76,113,113	1.34	5 (6%)
29	DGD	C	518	-	63,63,67	1.12	6 (9%)	77,77,81	1.49	11 (14%)
27	LMG	D	407	-	51,51,55	1.04	2 (3%)	59,59,63	1.27	5 (8%)
28	SQD	B	623	-	53,54,54	0.91	3 (5%)	62,65,65	1.90	14 (22%)
35	HEC	V	201	16	32,50,50	2.27	4 (12%)	24,82,82	1.02	1 (4%)
28	SQD	b	601	-	48,49,54	1.00	3 (6%)	57,60,65	2.36	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	503	-	65,73,73	1.52	10 (15%)	76,113,113	1.74	14 (18%)
29	DGD	c	516	-	63,63,67	1.28	10 (15%)	77,77,81	1.59	14 (18%)
29	DGD	h	103	-	63,63,67	0.98	4 (6%)	77,77,81	1.60	16 (20%)
27	LMG	a	414	-	49,49,55	0.86	2 (4%)	57,57,63	1.27	3 (5%)
24	PHO	A	406	-	51,69,69	1.19	5 (9%)	47,99,99	1.42	8 (17%)
27	LMG	b	622	-	55,55,55	1.09	4 (7%)	63,63,63	1.45	10 (15%)
29	DGD	C	517	-	63,63,67	1.27	7 (11%)	77,77,81	1.55	10 (12%)
23	CLA	B	606	-	65,73,73	1.92	10 (15%)	76,113,113	1.54	8 (10%)
25	BCR	B	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	7 (12%)
27	LMG	C	519	-	48,48,55	1.11	5 (10%)	56,56,63	1.34	6 (10%)
23	CLA	c	504	36	60,68,73	1.97	10 (16%)	70,107,113	1.64	10 (14%)
33	LHG	E	101	-	48,48,48	1.03	4 (8%)	51,54,54	1.14	3 (5%)
34	HEM	e	102	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.63	8 (17%)
27	LMG	D	411	-	26,26,55	1.01	2 (7%)	26,26,63	1.24	3 (11%)
26	PL9	d	406	-	55,55,55	1.28	6 (10%)	68,69,69	1.68	20 (29%)
23	CLA	B	613	-	65,73,73	1.57	13 (20%)	76,113,113	1.50	14 (18%)
23	CLA	C	510	-	65,73,73	1.74	8 (12%)	76,113,113	1.63	8 (10%)
27	LMG	D	410	-	31,31,55	1.12	3 (9%)	33,33,63	1.12	2 (6%)
23	CLA	d	402	36	65,73,73	1.57	7 (10%)	76,113,113	1.62	8 (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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	403	-	1/1/20/20	12/37/115/115	-
23	CLA	c	512	-	1/1/20/20	21/37/115/115	-
23	CLA	d	404	-	1/1/20/20	9/37/115/115	-
25	BCR	b	618	-	-	4/29/63/63	0/2/2/2
23	CLA	A	404	-	1/1/20/20	5/37/115/115	-
23	CLA	C	507	36	1/1/20/20	12/37/115/115	-
26	PL9	A	409	-	-	21/53/73/73	0/1/1/1
29	DGD	c	518	-	-	20/51/91/95	0/2/2/2
23	CLA	a	407	-	1/1/20/20	10/37/115/115	-
25	BCR	c	515	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	h	102	-	-	6/29/63/63	0/2/2/2
25	BCR	C	520	-	-	12/29/63/63	0/2/2/2
23	CLA	A	407	-	1/1/17/20	2/24/102/115	-
23	CLA	c	506	-	1/1/20/20	21/37/115/115	-
23	CLA	b	615	-	1/1/20/20	16/37/115/115	-
25	BCR	D	405	-	-	13/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/20/20	10/37/115/115	-
23	CLA	b	604	-	1/1/20/20	11/37/115/115	-
23	CLA	c	507	36	1/1/20/20	12/37/115/115	-
23	CLA	B	609	-	-	8/37/115/115	-
23	CLA	b	605	-	1/1/20/20	12/37/115/115	-
23	CLA	D	402	36	1/1/20/20	4/37/115/115	-
29	DGD	C	516	-	-	20/51/91/95	0/2/2/2
25	BCR	t	101	-	-	4/29/63/63	0/2/2/2
25	BCR	a	408	-	-	2/29/63/63	0/2/2/2
25	BCR	B	619	-	-	5/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/20/20	7/37/115/115	-
23	CLA	C	501	-	1/1/20/20	3/37/115/115	-
23	CLA	b	608	36	1/1/20/20	14/37/115/115	-
23	CLA	C	508	-	-	9/37/115/115	-
23	CLA	b	611	36	1/1/20/20	7/37/115/115	-
23	CLA	C	513	-	1/1/20/20	13/37/115/115	-
23	CLA	c	510	-	1/1/20/20	19/37/115/115	-
23	CLA	B	604	-	1/1/20/20	11/37/115/115	-
23	CLA	C	502	-	-	10/37/115/115	-
23	CLA	h	101	36	1/1/20/20	16/37/115/115	-
23	CLA	d	403	-	1/1/20/20	8/37/115/115	-
28	SQD	F	101	-	-	14/28/48/69	0/1/1/1
23	CLA	B	602	-	1/1/20/20	6/37/115/115	-
25	BCR	d	405	-	-	14/29/63/63	0/2/2/2
23	CLA	C	509	-	1/1/20/20	10/37/115/115	-
23	CLA	b	617	-	1/1/19/20	9/31/109/115	-
28	SQD	f	101	-	-	12/36/56/69	0/1/1/1
33	LHG	l	101	-	-	19/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	503	-	-	13/37/115/115	-
27	LMG	A	410	-	-	20/43/63/70	0/1/1/1
29	DGD	c	517	-	-	20/51/91/95	0/2/2/2
23	CLA	b	613	-	1/1/20/20	13/37/115/115	-
23	CLA	b	607	-	1/1/20/20	9/37/115/115	-
23	CLA	b	609	-	-	7/37/115/115	-
23	CLA	C	506	-	1/1/20/20	16/37/115/115	-
23	CLA	b	603	-	1/1/20/20	8/37/115/115	-
23	CLA	c	501	-	1/1/20/20	8/37/115/115	-
23	CLA	c	508	-	-	11/36/114/115	-
23	CLA	B	610	36	1/1/20/20	7/37/115/115	-
33	LHG	d	408	-	-	14/43/43/53	-
23	CLA	c	513	-	1/1/20/20	12/37/115/115	-
25	BCR	c	521	-	-	4/29/63/63	0/2/2/2
24	PHO	a	406	-	-	7/37/103/103	0/5/6/6
23	CLA	B	607	36	1/1/20/20	12/37/115/115	-
23	CLA	c	502	-	-	7/37/115/115	-
23	CLA	B	614	-	1/1/20/20	13/37/115/115	-
27	LMG	B	620	-	-	21/46/66/70	0/1/1/1
28	SQD	a	411	-	-	18/49/69/69	0/1/1/1
23	CLA	b	610	-	-	7/37/115/115	-
26	PL9	a	409	-	-	27/53/73/73	0/1/1/1
25	BCR	c	514	-	-	11/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/20/20	8/37/115/115	-
27	LMG	c	522	-	-	21/43/63/70	0/1/1/1
23	CLA	B	616	-	1/1/19/20	9/31/109/115	-
25	BCR	b	619	-	-	5/29/63/63	0/2/2/2
25	BCR	C	514	-	-	15/29/63/63	0/2/2/2
34	HEM	E	102	6,5	-	1/12/54/54	-
25	BCR	H	101	-	-	7/29/63/63	0/2/2/2
23	CLA	a	405	36	1/1/20/20	10/37/115/115	-
23	CLA	b	612	-	-	11/37/115/115	-
29	DGD	a	413	-	-	21/45/45/95	-
33	LHG	d	407	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	515	-	-	4/29/63/63	0/2/2/2
23	CLA	B	603	-	-	16/37/115/115	-
23	CLA	B	612	-	1/1/20/20	11/37/115/115	-
23	CLA	B	605	-	1/1/20/20	8/37/115/115	-
25	BCR	B	617	-	-	4/29/63/63	0/2/2/2
27	LMG	d	409	-	-	11/39/59/70	0/1/1/1
33	LHG	e	101	-	-	23/46/46/53	-
25	BCR	A	408	-	-	7/29/63/63	0/2/2/2
28	SQD	A	411	-	-	19/47/67/69	0/1/1/1
27	LMG	m	101	-	-	19/46/66/70	0/1/1/1
33	LHG	a	410	-	-	19/53/53/53	-
28	SQD	A	412	-	-	17/39/39/69	-
25	BCR	K	101	-	-	10/29/63/63	0/2/2/2
23	CLA	B	608	-	-	3/37/115/115	-
23	CLA	C	512	-	1/1/20/20	10/37/115/115	-
23	CLA	B	615	-	1/1/20/20	9/37/115/115	-
24	PHO	d	401	-	-	3/37/103/103	0/5/6/6
33	LHG	D	408	-	-	25/53/53/53	-
33	LHG	B	622	-	-	11/53/53/53	-
23	CLA	c	505	-	1/1/20/20	15/37/115/115	-
28	SQD	a	412	-	-	22/37/37/69	-
23	CLA	B	611	-	1/1/20/20	10/37/115/115	-
26	PL9	D	406	-	-	10/53/73/73	0/1/1/1
27	LMG	c	519	-	-	10/31/51/70	0/1/1/1
23	CLA	A	405	36	-	4/37/115/115	-
35	HEC	v	201	16	-	2/10/54/54	-
23	CLA	D	404	-	-	11/37/115/115	-
27	LMG	b	623	-	-	12/17/17/70	-
33	LHG	D	409	-	-	25/51/51/53	-
23	CLA	C	504	36	1/1/18/20	7/30/108/115	-
23	CLA	C	511	3	-	4/37/115/115	-
29	DGD	A	413	-	-	31/55/95/95	0/2/2/2
23	CLA	C	505	-	1/1/20/20	10/37/115/115	-
25	BCR	T	101	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
33	LHG	L	101	-	-	21/53/53/53	-
24	PHO	D	401	-	-	4/37/103/103	0/5/6/6
23	CLA	B	601	36	-	14/37/115/115	-
29	DGD	H	102	-	-	17/51/91/95	0/2/2/2
25	BCR	y	101	-	-	8/29/63/63	0/2/2/2
23	CLA	a	404	-	1/1/20/20	11/37/115/115	-
23	CLA	b	606	-	1/1/20/20	6/37/115/115	-
23	CLA	c	511	3	1/1/20/20	12/37/115/115	-
29	DGD	C	518	-	-	16/51/91/95	0/2/2/2
27	LMG	D	407	-	-	19/46/66/70	0/1/1/1
28	SQD	B	623	-	-	19/49/69/69	0/1/1/1
35	HEC	V	201	16	-	2/10/54/54	-
28	SQD	b	601	-	-	19/44/64/69	0/1/1/1
23	CLA	C	503	-	1/1/20/20	8/37/115/115	-
29	DGD	c	516	-	-	25/51/91/95	0/2/2/2
29	DGD	h	103	-	-	15/51/91/95	0/2/2/2
27	LMG	a	414	-	-	28/44/64/70	0/1/1/1
24	PHO	A	406	-	-	8/37/103/103	0/5/6/6
27	LMG	b	622	-	-	24/50/70/70	0/1/1/1
29	DGD	C	517	-	-	18/51/91/95	0/2/2/2
23	CLA	B	606	-	1/1/20/20	14/37/115/115	-
25	BCR	B	618	-	-	11/29/63/63	0/2/2/2
27	LMG	C	519	-	-	19/43/63/70	0/1/1/1
23	CLA	c	504	36	1/1/19/20	11/31/109/115	-
33	LHG	E	101	-	-	27/53/53/53	-
34	HEM	e	102	6,5	-	3/12/54/54	-
27	LMG	D	411	-	-	13/22/22/70	-
26	PL9	d	406	-	-	21/53/73/73	0/1/1/1
23	CLA	B	613	-	1/1/20/20	9/37/115/115	-
23	CLA	C	510	-	1/1/20/20	11/37/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
23	CLA	d	402	36	1/1/20/20	5/37/115/115	-

All (967) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	MG-ND	-11.02	1.83	2.05
23	B	614	CLA	C4B-NB	8.90	1.43	1.35
23	b	615	CLA	C4B-NB	8.81	1.43	1.35
23	C	511	CLA	MG-NA	8.53	2.26	2.06
23	C	501	CLA	MG-NA	8.49	2.26	2.06
23	B	610	CLA	C4B-NB	8.39	1.42	1.35
23	c	511	CLA	C4B-NB	8.34	1.42	1.35
23	b	612	CLA	MG-NA	8.32	2.26	2.06
23	B	606	CLA	MG-NA	8.29	2.26	2.06
23	D	404	CLA	C4B-NB	8.18	1.42	1.35
23	d	404	CLA	MG-NA	8.18	2.25	2.06
23	c	509	CLA	C4B-NB	8.14	1.42	1.35
23	B	601	CLA	C4B-NB	8.11	1.42	1.35
23	d	404	CLA	C4B-NB	8.06	1.42	1.35
23	B	616	CLA	C4B-NB	7.97	1.42	1.35
23	B	602	CLA	C4B-NB	7.90	1.42	1.35
23	h	101	CLA	C4B-NB	7.87	1.42	1.35
23	b	616	CLA	MG-NC	-7.87	1.87	2.06
23	c	509	CLA	MG-ND	7.78	2.21	2.05
23	b	610	CLA	C4B-NB	7.77	1.42	1.35
23	C	502	CLA	C4B-NB	7.73	1.42	1.35
23	A	404	CLA	C4B-NB	7.61	1.42	1.35
35	V	201	HEC	C2B-C3B	-7.57	1.32	1.40
23	b	603	CLA	C4B-NB	7.53	1.41	1.35
23	C	505	CLA	C4B-NB	7.50	1.41	1.35
23	B	606	CLA	C4B-NB	7.49	1.41	1.35
23	C	506	CLA	MG-ND	-7.38	1.91	2.05
23	b	617	CLA	C4B-NB	7.32	1.41	1.35
23	C	510	CLA	C4B-NB	7.32	1.41	1.35
23	C	512	CLA	MG-ND	-7.30	1.91	2.05
23	b	606	CLA	C4B-NB	7.26	1.41	1.35
23	b	607	CLA	MG-NA	7.25	2.23	2.06
23	c	504	CLA	C4B-NB	7.24	1.41	1.35
35	v	201	HEC	C2B-C3B	-7.22	1.33	1.40
23	b	616	CLA	C4B-NB	7.17	1.41	1.35
23	c	512	CLA	C4B-NB	7.15	1.41	1.35
23	c	503	CLA	C4B-NB	7.09	1.41	1.35
23	b	604	CLA	C4B-NB	6.96	1.41	1.35
23	B	615	CLA	C4B-NB	6.80	1.41	1.35
23	B	613	CLA	C4B-NB	6.80	1.41	1.35
23	B	601	CLA	MG-NA	6.76	2.22	2.06
23	c	502	CLA	MG-ND	6.72	2.19	2.05
23	C	506	CLA	C4B-NB	6.71	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	MG-NA	6.68	2.22	2.06
23	C	501	CLA	C4B-NB	6.66	1.41	1.35
23	b	609	CLA	C4B-NB	6.66	1.41	1.35
23	B	609	CLA	MG-ND	-6.64	1.92	2.05
23	c	511	CLA	MG-NA	6.58	2.21	2.06
23	b	614	CLA	C4B-NB	6.54	1.41	1.35
23	b	604	CLA	MG-ND	-6.54	1.92	2.05
23	B	610	CLA	MG-ND	-6.52	1.92	2.05
23	A	407	CLA	MG-ND	-6.52	1.92	2.05
23	c	513	CLA	C4B-NB	6.49	1.41	1.35
23	C	510	CLA	MG-NA	6.45	2.21	2.06
23	b	616	CLA	MG-NA	6.43	2.21	2.06
23	B	614	CLA	MG-NA	6.38	2.21	2.06
23	c	501	CLA	C4B-NB	6.35	1.40	1.35
23	C	511	CLA	C4B-NB	6.34	1.40	1.35
23	C	509	CLA	C4B-NB	6.31	1.40	1.35
23	d	403	CLA	C4B-NB	6.29	1.40	1.35
23	c	506	CLA	MG-NA	6.18	2.21	2.06
23	D	403	CLA	C4B-NB	6.18	1.40	1.35
23	c	505	CLA	MG-NC	-6.17	1.91	2.06
23	B	602	CLA	MG-ND	6.16	2.18	2.05
23	C	507	CLA	C4B-NB	6.13	1.40	1.35
23	b	610	CLA	MG-NA	6.11	2.20	2.06
23	b	615	CLA	MG-ND	-6.11	1.93	2.05
23	C	508	CLA	C4B-NB	6.09	1.40	1.35
23	B	607	CLA	C4B-NB	6.07	1.40	1.35
23	C	509	CLA	MG-ND	6.07	2.17	2.05
23	d	404	CLA	MG-NC	-6.07	1.91	2.06
23	b	615	CLA	MG-NA	6.05	2.20	2.06
23	a	405	CLA	C4B-NB	6.02	1.40	1.35
23	C	513	CLA	C4B-NB	6.01	1.40	1.35
23	C	503	CLA	C4B-NB	5.97	1.40	1.35
23	c	504	CLA	MG-NC	5.96	2.20	2.06
23	a	405	CLA	MG-ND	-5.94	1.94	2.05
23	b	607	CLA	C4B-NB	5.92	1.40	1.35
23	c	512	CLA	MG-NC	5.87	2.20	2.06
35	V	201	HEC	C3C-C2C	-5.85	1.34	1.40
23	c	504	CLA	MG-NA	-5.82	1.92	2.06
23	c	502	CLA	C4B-NB	5.81	1.40	1.35
23	A	405	CLA	C4B-NB	5.81	1.40	1.35
23	c	508	CLA	C4B-NB	5.80	1.40	1.35
23	c	505	CLA	C4B-NB	5.76	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C4B-NB	5.75	1.40	1.35
23	C	512	CLA	C4B-NB	5.73	1.40	1.35
23	b	605	CLA	C4B-NB	5.71	1.40	1.35
23	C	504	CLA	C4B-NB	5.69	1.40	1.35
23	B	603	CLA	C4B-NB	5.61	1.40	1.35
23	B	615	CLA	MG-ND	5.59	2.16	2.05
23	B	609	CLA	C4B-NB	5.59	1.40	1.35
23	B	604	CLA	C4B-NB	5.57	1.40	1.35
23	C	513	CLA	MG-ND	5.56	2.16	2.05
23	B	609	CLA	MG-NA	5.54	2.19	2.06
23	b	606	CLA	MG-ND	5.53	2.16	2.05
23	A	407	CLA	C4B-NB	5.46	1.40	1.35
26	a	409	PL9	C7-C3	5.43	1.56	1.51
23	c	506	CLA	C4B-NB	5.43	1.40	1.35
23	C	502	CLA	MG-NC	5.40	2.19	2.06
23	c	501	CLA	MG-NA	5.34	2.19	2.06
23	c	504	CLA	MG-ND	-5.34	1.95	2.05
23	B	611	CLA	C4B-NB	5.30	1.39	1.35
23	D	403	CLA	MG-ND	-5.30	1.95	2.05
29	H	102	DGD	O5D-C1E	5.28	1.49	1.40
23	b	608	CLA	C4B-NB	5.26	1.39	1.35
23	C	508	CLA	MG-NA	5.22	2.18	2.06
23	D	402	CLA	C4B-NB	5.19	1.39	1.35
23	b	613	CLA	C4B-NB	5.17	1.39	1.35
23	b	613	CLA	MG-NA	5.16	2.18	2.06
35	v	201	HEC	C3C-C2C	-5.10	1.35	1.40
23	b	604	CLA	MG-NA	5.09	2.18	2.06
23	B	615	CLA	C4D-ND	-5.04	1.30	1.37
23	B	608	CLA	C4D-ND	-5.03	1.30	1.37
23	b	611	CLA	C4B-NB	4.97	1.39	1.35
23	d	404	CLA	MG-ND	-4.95	1.96	2.05
23	B	612	CLA	C4D-ND	-4.90	1.31	1.37
23	C	508	CLA	MG-ND	4.89	2.15	2.05
23	a	407	CLA	C4B-NB	4.84	1.39	1.35
23	B	604	CLA	MG-NA	4.80	2.17	2.06
26	a	409	PL9	C53-C6	-4.80	1.40	1.50
23	c	507	CLA	C4B-NB	4.77	1.39	1.35
23	b	606	CLA	C4D-ND	-4.74	1.31	1.37
23	d	402	CLA	C4B-NB	4.74	1.39	1.35
23	D	403	CLA	MG-NA	4.72	2.17	2.06
23	c	506	CLA	MG-ND	-4.69	1.96	2.05
23	c	505	CLA	C4D-ND	-4.69	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	102	HEM	C3C-C2C	-4.68	1.33	1.40
33	L	101	LHG	O7-C5	-4.67	1.34	1.46
23	a	404	CLA	MG-NA	4.65	2.17	2.06
34	e	102	HEM	C3C-C2C	-4.64	1.33	1.40
25	b	619	BCR	C30-C25	-4.62	1.47	1.53
23	B	614	CLA	MG-ND	-4.61	1.96	2.05
25	h	102	BCR	C30-C25	-4.59	1.47	1.53
23	b	603	CLA	C1D-ND	4.58	1.43	1.37
23	b	615	CLA	C1D-ND	4.57	1.43	1.37
23	B	605	CLA	C4D-ND	-4.50	1.31	1.37
23	D	402	CLA	C4D-ND	-4.50	1.31	1.37
23	c	501	CLA	C4D-ND	-4.48	1.31	1.37
25	B	619	BCR	C1-C6	-4.45	1.47	1.53
29	C	516	DGD	C4E-C3E	4.44	1.63	1.52
23	b	612	CLA	C4B-NB	4.39	1.39	1.35
23	C	503	CLA	MG-NA	4.38	2.16	2.06
23	b	608	CLA	C4D-ND	-4.38	1.31	1.37
23	d	402	CLA	C1D-ND	4.35	1.43	1.37
23	c	508	CLA	C4D-ND	-4.35	1.31	1.37
23	a	407	CLA	C1D-ND	4.34	1.43	1.37
23	C	505	CLA	MG-NC	4.34	2.16	2.06
23	B	615	CLA	CMB-C2B	-4.31	1.42	1.51
23	c	510	CLA	MG-NC	-4.30	1.96	2.06
23	b	605	CLA	C1D-ND	4.29	1.43	1.37
23	B	612	CLA	C4B-NB	4.25	1.39	1.35
23	C	501	CLA	C1D-ND	4.25	1.43	1.37
23	a	407	CLA	C4D-ND	-4.24	1.31	1.37
23	B	607	CLA	C3B-C2B	-4.24	1.34	1.40
23	C	506	CLA	MG-NA	4.22	2.16	2.06
23	D	404	CLA	C1D-ND	4.19	1.42	1.37
23	B	608	CLA	MG-ND	4.17	2.14	2.05
23	c	507	CLA	MG-NA	-4.14	1.96	2.06
25	K	101	BCR	C30-C25	-4.14	1.48	1.53
23	B	602	CLA	C4D-ND	-4.12	1.32	1.37
25	K	101	BCR	C1-C6	-4.12	1.48	1.53
23	A	407	CLA	MG-NC	-4.10	1.96	2.06
23	B	609	CLA	C1D-ND	4.09	1.42	1.37
23	c	502	CLA	C4D-ND	-4.09	1.32	1.37
26	D	406	PL9	C6-C1	-4.08	1.41	1.48
23	c	510	CLA	C4B-NB	4.08	1.38	1.35
23	c	509	CLA	C1D-ND	4.06	1.42	1.37
23	b	611	CLA	C4D-ND	-4.06	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C1D-ND	4.05	1.42	1.37
23	c	509	CLA	C4D-ND	-4.05	1.32	1.37
29	H	102	DGD	C4D-C5D	4.05	1.61	1.53
23	A	404	CLA	C4D-ND	-4.04	1.32	1.37
29	H	102	DGD	C1E-C2E	4.04	1.64	1.52
23	B	605	CLA	MG-ND	-4.03	1.97	2.05
23	b	609	CLA	CHC-C1C	4.02	1.45	1.35
23	c	512	CLA	C1D-ND	3.99	1.42	1.37
23	b	613	CLA	C1D-ND	3.97	1.42	1.37
23	C	503	CLA	C4D-ND	-3.96	1.32	1.37
23	c	509	CLA	CHC-C1C	3.96	1.45	1.35
23	B	611	CLA	C4D-ND	-3.94	1.32	1.37
23	B	613	CLA	CMD-C2D	-3.94	1.42	1.50
23	h	101	CLA	MG-NA	3.94	2.15	2.06
23	b	605	CLA	C4D-ND	-3.93	1.32	1.37
23	C	511	CLA	C1D-ND	3.92	1.42	1.37
23	A	404	CLA	MG-NA	3.90	2.15	2.06
23	B	610	CLA	C1D-ND	3.90	1.42	1.37
23	B	610	CLA	C3B-C2B	-3.90	1.35	1.40
35	v	201	HEC	CBB-CAB	-3.89	1.34	1.49
29	H	102	DGD	O2G-C2G	-3.88	1.36	1.46
23	d	403	CLA	CMB-C2B	-3.87	1.43	1.51
29	A	413	DGD	O3G-C1D	3.87	1.46	1.40
23	A	404	CLA	MG-NC	-3.86	1.97	2.06
25	C	514	BCR	C1-C6	-3.85	1.48	1.53
25	C	515	BCR	C1-C6	-3.82	1.48	1.53
23	B	616	CLA	C4D-ND	-3.81	1.32	1.37
23	c	510	CLA	MG-NA	3.81	2.15	2.06
23	b	613	CLA	MG-NC	-3.80	1.97	2.06
25	T	101	BCR	C30-C25	-3.80	1.48	1.53
25	B	617	BCR	C1-C6	-3.79	1.48	1.53
23	C	505	CLA	C4D-ND	-3.78	1.32	1.37
23	c	502	CLA	MG-NA	3.78	2.15	2.06
23	b	603	CLA	C4D-ND	-3.78	1.32	1.37
23	B	609	CLA	MG-NC	-3.77	1.97	2.06
23	c	507	CLA	C4D-ND	-3.77	1.32	1.37
23	b	612	CLA	C4D-ND	-3.77	1.32	1.37
35	V	201	HEC	CBB-CAB	-3.75	1.35	1.49
29	A	413	DGD	C4D-C5D	3.74	1.60	1.53
23	B	616	CLA	C1D-ND	3.73	1.42	1.37
23	B	616	CLA	MG-NC	3.73	2.15	2.06
23	b	610	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	CLA	C4B-NB	3.72	1.38	1.35
23	C	508	CLA	C4D-ND	-3.72	1.32	1.37
23	B	604	CLA	CHC-C1C	3.72	1.44	1.35
28	a	411	SQD	O48-C23	3.70	1.44	1.33
23	B	601	CLA	C3B-C2B	-3.69	1.35	1.40
23	a	405	CLA	C4D-ND	-3.69	1.32	1.37
28	A	412	SQD	O48-C23	3.68	1.44	1.33
23	D	402	CLA	MG-NC	-3.67	1.97	2.06
23	C	513	CLA	C4D-ND	-3.66	1.32	1.37
23	B	616	CLA	C3B-C2B	-3.65	1.35	1.40
29	c	518	DGD	C4D-C3D	3.65	1.61	1.52
23	C	510	CLA	C4D-ND	-3.65	1.32	1.37
23	B	606	CLA	MG-NC	-3.64	1.97	2.06
23	B	610	CLA	C4D-ND	-3.64	1.32	1.37
23	c	507	CLA	C3B-C2B	-3.63	1.35	1.40
26	d	406	PL9	C3-C4	-3.62	1.43	1.49
35	V	201	HEC	CBC-CAC	-3.61	1.35	1.49
25	y	101	BCR	C30-C25	-3.61	1.48	1.53
29	C	517	DGD	O5D-C1E	3.61	1.46	1.40
29	C	517	DGD	O2G-C2G	-3.61	1.37	1.46
23	A	407	CLA	CMB-C2B	-3.61	1.44	1.51
23	C	502	CLA	C1D-ND	3.59	1.42	1.37
25	b	618	BCR	C30-C25	-3.59	1.48	1.53
27	b	622	LMG	C4-C3	3.59	1.61	1.52
23	b	605	CLA	CHC-C1C	3.59	1.44	1.35
23	B	601	CLA	C1D-ND	3.59	1.42	1.37
23	c	503	CLA	C4D-ND	-3.58	1.32	1.37
23	B	605	CLA	CHC-C1C	3.58	1.44	1.35
23	a	404	CLA	CHC-C1C	3.58	1.44	1.35
29	A	413	DGD	C1E-C2E	3.57	1.62	1.52
23	d	403	CLA	C4D-ND	-3.57	1.32	1.37
23	B	606	CLA	CHC-C1C	3.57	1.44	1.35
23	b	606	CLA	CHC-C1C	3.56	1.44	1.35
23	c	510	CLA	C4D-ND	-3.56	1.32	1.37
23	B	606	CLA	C1D-ND	3.55	1.42	1.37
29	H	102	DGD	O5D-C6D	-3.55	1.37	1.43
23	B	603	CLA	C4D-ND	-3.55	1.32	1.37
23	b	617	CLA	C1D-ND	3.54	1.42	1.37
23	c	508	CLA	MG-ND	3.54	2.12	2.05
28	a	412	SQD	O48-C23	3.54	1.43	1.33
23	c	512	CLA	C4D-ND	-3.53	1.32	1.37
23	C	513	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	405	BCR	C1-C6	-3.52	1.48	1.53
25	c	514	BCR	C1-C6	-3.52	1.48	1.53
23	A	407	CLA	C4D-ND	-3.52	1.32	1.37
23	B	616	CLA	MG-NA	3.51	2.14	2.06
29	c	518	DGD	C6D-C5D	3.51	1.62	1.51
27	C	519	LMG	O7-C8	-3.50	1.37	1.46
23	a	407	CLA	MG-ND	-3.50	1.98	2.05
28	b	601	SQD	O48-C23	3.48	1.43	1.33
28	b	601	SQD	O47-C7	3.48	1.44	1.34
29	C	517	DGD	C4D-C3D	3.48	1.61	1.52
23	c	508	CLA	CHC-C1C	3.48	1.43	1.35
23	C	510	CLA	CHC-C1C	3.46	1.43	1.35
26	D	406	PL9	C11-C9	-3.46	1.44	1.51
23	b	613	CLA	MG-ND	-3.46	1.98	2.05
23	c	511	CLA	CHC-C1C	3.45	1.43	1.35
23	c	504	CLA	CHC-C1C	3.45	1.43	1.35
23	C	512	CLA	CHC-C1C	3.45	1.43	1.35
23	B	615	CLA	CHC-C1C	3.43	1.43	1.35
27	d	409	LMG	O1-C7	-3.43	1.37	1.43
23	B	608	CLA	CHC-C1C	3.42	1.43	1.35
23	b	607	CLA	C4D-ND	-3.42	1.33	1.37
23	b	614	CLA	MG-NA	3.41	2.14	2.06
23	h	101	CLA	C1D-ND	3.41	1.42	1.37
23	b	617	CLA	C4D-ND	-3.40	1.33	1.37
23	b	605	CLA	MG-NC	3.40	2.14	2.06
23	B	601	CLA	MG-ND	-3.40	1.99	2.05
23	b	605	CLA	MG-ND	-3.40	1.99	2.05
24	A	406	PHO	C3A-C2A	3.38	1.57	1.54
23	b	612	CLA	CMD-C2D	-3.37	1.43	1.50
29	c	518	DGD	O2E-C2E	-3.36	1.35	1.43
29	c	517	DGD	O3G-C1D	-3.36	1.34	1.40
23	B	613	CLA	C1D-ND	3.36	1.41	1.37
23	c	511	CLA	C1D-ND	3.35	1.41	1.37
23	b	616	CLA	CHC-C1C	3.34	1.43	1.35
23	C	509	CLA	C4D-ND	-3.33	1.33	1.37
23	B	606	CLA	C4D-ND	-3.33	1.33	1.37
25	b	618	BCR	C1-C6	-3.33	1.49	1.53
29	C	516	DGD	O2E-C2E	-3.32	1.35	1.43
23	b	609	CLA	C4D-ND	-3.32	1.33	1.37
23	B	604	CLA	C1D-ND	3.32	1.41	1.37
23	B	607	CLA	CMB-C2B	-3.31	1.44	1.51
23	D	404	CLA	C3B-C2B	-3.30	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	409	LHG	P-O6	3.30	1.72	1.59
23	a	405	CLA	MG-NA	3.29	2.14	2.06
23	c	513	CLA	CMB-C2B	-3.29	1.44	1.51
24	d	401	PHO	CAC-C3C	-3.29	1.46	1.52
23	a	407	CLA	CMC-C2C	-3.29	1.43	1.50
23	A	407	CLA	CMD-C2D	-3.28	1.43	1.50
28	a	412	SQD	O47-C7	3.28	1.43	1.34
23	b	611	CLA	MG-NC	3.27	2.14	2.06
29	c	517	DGD	O4E-C4E	-3.26	1.35	1.43
23	b	614	CLA	C4D-ND	-3.25	1.33	1.37
23	D	403	CLA	C1D-ND	3.25	1.41	1.37
34	E	102	HEM	C3C-CAC	3.25	1.54	1.47
29	H	102	DGD	C4E-C5E	3.24	1.59	1.53
23	b	608	CLA	C3B-C2B	-3.24	1.35	1.40
23	c	504	CLA	C4D-ND	-3.24	1.33	1.37
23	b	612	CLA	MG-NC	-3.24	1.98	2.06
23	b	612	CLA	CHC-C1C	3.24	1.43	1.35
23	c	512	CLA	CHC-C1C	3.23	1.43	1.35
23	A	405	CLA	CMB-C2B	-3.23	1.44	1.51
23	b	613	CLA	C1B-NB	3.23	1.38	1.35
23	b	615	CLA	CHC-C1C	3.23	1.43	1.35
25	B	618	BCR	C30-C25	-3.23	1.49	1.53
33	d	408	LHG	P-O6	3.22	1.72	1.59
33	D	408	LHG	O8-C6	-3.21	1.37	1.45
29	a	413	DGD	O2G-C1B	3.20	1.43	1.34
23	C	501	CLA	CHC-C1C	3.19	1.43	1.35
23	B	607	CLA	C4B-CHC	-3.19	1.32	1.41
28	A	412	SQD	O47-C7	3.19	1.43	1.34
23	d	404	CLA	CMB-C2B	-3.19	1.45	1.51
23	c	513	CLA	C4D-ND	-3.18	1.33	1.37
25	B	617	BCR	C30-C25	-3.18	1.49	1.53
23	B	610	CLA	CHC-C1C	3.18	1.43	1.35
23	B	614	CLA	CHC-C1C	3.18	1.43	1.35
27	c	522	LMG	C4-C3	3.18	1.60	1.52
28	A	411	SQD	O48-C23	3.18	1.42	1.33
28	f	101	SQD	O47-C7	3.18	1.43	1.34
23	C	508	CLA	C1D-ND	3.18	1.41	1.37
23	c	513	CLA	CHC-C1C	3.17	1.43	1.35
28	F	101	SQD	O48-C23	3.17	1.42	1.33
29	c	517	DGD	C4E-C3E	3.17	1.60	1.52
29	c	516	DGD	O3G-C3G	-3.16	1.38	1.43
23	B	611	CLA	C1D-ND	3.16	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CMB-C2B	-3.16	1.45	1.51
23	b	617	CLA	CMB-C2B	-3.15	1.45	1.51
23	a	404	CLA	C4D-ND	-3.15	1.33	1.37
35	v	201	HEC	CBC-CAC	-3.15	1.37	1.49
27	d	409	LMG	O7-C8	-3.15	1.38	1.46
23	B	614	CLA	C4D-ND	-3.14	1.33	1.37
26	d	406	PL9	C16-C14	-3.14	1.44	1.51
23	C	507	CLA	C1D-ND	3.14	1.41	1.37
23	A	405	CLA	C4D-ND	-3.14	1.33	1.37
29	H	102	DGD	O2D-C2D	-3.14	1.35	1.43
29	a	413	DGD	O1G-C1A	3.14	1.42	1.33
33	E	101	LHG	O8-C23	3.14	1.42	1.33
23	A	405	CLA	CHC-C1C	3.13	1.43	1.35
27	b	622	LMG	O6-C1	3.12	1.49	1.41
23	C	502	CLA	CHC-C1C	3.10	1.42	1.35
23	B	610	CLA	MG-NA	3.10	2.13	2.06
23	b	607	CLA	C1D-ND	3.09	1.41	1.37
23	b	611	CLA	CMD-C2D	-3.09	1.44	1.50
23	C	502	CLA	C4D-ND	-3.09	1.33	1.37
23	C	504	CLA	MG-NA	3.08	2.13	2.06
23	B	614	CLA	CMB-C2B	-3.08	1.45	1.51
25	h	102	BCR	C1-C6	-3.08	1.49	1.53
23	B	608	CLA	CMD-C2D	-3.08	1.44	1.50
23	d	402	CLA	CMB-C2B	-3.08	1.45	1.51
29	c	516	DGD	C4D-C3D	3.08	1.60	1.52
29	c	516	DGD	O2E-C2E	-3.08	1.35	1.43
23	c	506	CLA	CHC-C1C	3.08	1.42	1.35
23	B	603	CLA	C3B-C2B	-3.07	1.36	1.40
23	C	510	CLA	C1D-ND	3.07	1.41	1.37
23	B	603	CLA	C1D-ND	3.07	1.41	1.37
34	e	102	HEM	C3C-CAC	3.07	1.54	1.47
25	H	101	BCR	C30-C25	-3.05	1.49	1.53
23	D	404	CLA	C4D-ND	-3.04	1.33	1.37
29	C	518	DGD	O4E-C4E	-3.04	1.35	1.43
23	c	513	CLA	MG-NC	-3.04	1.99	2.06
23	C	504	CLA	CMB-C2B	-3.04	1.45	1.51
23	a	407	CLA	CMB-C2B	-3.04	1.45	1.51
25	C	514	BCR	C30-C25	-3.04	1.49	1.53
29	C	517	DGD	C1E-C2E	3.03	1.61	1.52
28	B	623	SQD	O47-C7	3.03	1.42	1.34
23	B	607	CLA	C1D-ND	3.03	1.41	1.37
23	C	502	CLA	CMB-C2B	-3.03	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	CMB-C2B	-3.02	1.45	1.51
28	A	411	SQD	O47-C7	3.02	1.42	1.34
23	b	608	CLA	CHC-C1C	3.02	1.42	1.35
29	H	102	DGD	O1G-C1G	-3.02	1.38	1.45
23	c	511	CLA	MG-NC	3.01	2.13	2.06
23	C	512	CLA	C3B-C2B	-3.01	1.36	1.40
23	D	403	CLA	CHC-C1C	3.01	1.42	1.35
23	c	505	CLA	CHC-C1C	3.01	1.42	1.35
23	c	501	CLA	C1D-ND	3.01	1.41	1.37
23	C	506	CLA	CHC-C1C	3.00	1.42	1.35
23	b	604	CLA	CMB-C2B	-3.00	1.45	1.51
25	a	408	BCR	C1-C6	-3.00	1.49	1.53
29	c	516	DGD	O5D-C6D	-3.00	1.38	1.43
23	c	512	CLA	CMB-C2B	-3.00	1.45	1.51
23	A	407	CLA	C1D-ND	3.00	1.41	1.37
23	B	605	CLA	MG-NC	-3.00	1.99	2.06
23	C	511	CLA	CMB-C2B	-3.00	1.45	1.51
27	B	620	LMG	C1-C2	2.99	1.61	1.52
27	c	522	LMG	O1-C1	2.99	1.45	1.40
23	b	609	CLA	C3B-CAB	-2.98	1.41	1.47
23	b	617	CLA	C3B-CAB	-2.98	1.41	1.47
23	C	508	CLA	CHC-C1C	2.98	1.42	1.35
29	C	516	DGD	C1D-C2D	2.98	1.61	1.52
23	B	602	CLA	C1D-ND	2.97	1.41	1.37
23	B	609	CLA	C3B-C2B	-2.97	1.36	1.40
25	a	408	BCR	C30-C25	-2.97	1.49	1.53
23	C	511	CLA	CHC-C1C	2.96	1.42	1.35
23	b	616	CLA	CAA-C2A	-2.96	1.48	1.54
23	B	606	CLA	C3B-C2B	-2.96	1.36	1.40
23	b	604	CLA	CHC-C1C	2.95	1.42	1.35
27	d	409	LMG	O4-C4	-2.95	1.36	1.43
23	a	405	CLA	CMB-C2B	-2.95	1.45	1.51
23	B	602	CLA	CHC-C1C	2.95	1.42	1.35
23	a	407	CLA	C4B-CHC	-2.93	1.32	1.41
28	A	411	SQD	O2-C2	-2.93	1.36	1.43
25	c	514	BCR	C30-C25	-2.93	1.49	1.53
23	C	512	CLA	C1D-ND	2.92	1.41	1.37
23	c	510	CLA	C1D-ND	2.92	1.41	1.37
25	b	620	BCR	C30-C25	-2.92	1.49	1.53
23	d	403	CLA	CHC-C1C	2.92	1.42	1.35
23	b	605	CLA	CMB-C2B	-2.91	1.45	1.51
23	b	616	CLA	C1D-ND	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	412	SQD	O47-C45	-2.91	1.42	1.47
27	c	522	LMG	C7-C8	2.91	1.59	1.50
23	A	404	CLA	CHC-C1C	2.91	1.42	1.35
23	B	616	CLA	MG-ND	2.91	2.11	2.05
23	d	403	CLA	C3B-CAB	-2.91	1.42	1.47
23	c	503	CLA	C1D-ND	2.91	1.41	1.37
23	B	609	CLA	C4D-ND	-2.91	1.33	1.37
23	C	505	CLA	C3B-C2B	-2.90	1.36	1.40
23	B	607	CLA	MG-NA	2.90	2.13	2.06
23	a	405	CLA	C1D-ND	2.90	1.41	1.37
23	b	613	CLA	C4D-ND	-2.90	1.33	1.37
23	b	616	CLA	CMC-C2C	-2.90	1.44	1.50
23	c	508	CLA	C1D-ND	2.90	1.41	1.37
23	B	603	CLA	CMC-C2C	-2.90	1.44	1.50
23	C	503	CLA	MG-ND	2.89	2.11	2.05
23	B	611	CLA	CHC-C1C	2.89	1.42	1.35
23	b	610	CLA	C4D-ND	-2.89	1.33	1.37
29	a	413	DGD	C2B-C1B	2.89	1.59	1.50
26	d	406	PL9	C30-C29	-2.89	1.43	1.50
25	D	405	BCR	C1-C6	-2.87	1.49	1.53
29	h	103	DGD	O5D-C6D	-2.87	1.38	1.43
23	D	402	CLA	MG-ND	2.86	2.11	2.05
23	b	611	CLA	CMB-C2B	-2.86	1.45	1.51
23	B	601	CLA	CHC-C1C	2.86	1.42	1.35
23	c	503	CLA	CHC-C1C	2.86	1.42	1.35
25	b	619	BCR	C1-C6	-2.86	1.49	1.53
23	b	604	CLA	C4D-ND	-2.86	1.33	1.37
27	c	522	LMG	C3-C2	2.85	1.59	1.52
23	B	615	CLA	C3B-C2B	-2.85	1.36	1.40
23	B	604	CLA	C4D-ND	-2.84	1.33	1.37
23	b	616	CLA	C4D-ND	-2.84	1.33	1.37
27	c	519	LMG	C7-C8	2.83	1.59	1.50
29	C	518	DGD	C1G-C2G	2.83	1.59	1.50
23	b	614	CLA	C3B-C2B	-2.83	1.36	1.40
28	f	101	SQD	O48-C23	2.82	1.41	1.33
23	c	507	CLA	C1D-ND	2.82	1.41	1.37
23	b	608	CLA	C1D-ND	2.81	1.41	1.37
23	c	511	CLA	CMB-C2B	-2.81	1.45	1.51
23	b	614	CLA	MG-ND	-2.81	2.00	2.05
29	C	518	DGD	O2G-C2G	-2.80	1.39	1.46
23	B	610	CLA	CMD-C2D	-2.80	1.44	1.50
33	d	407	LHG	O7-C5	-2.80	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	408	LHG	C24-C23	2.80	1.58	1.50
23	B	605	CLA	CMB-C2B	-2.79	1.45	1.51
23	B	605	CLA	C4B-NB	2.79	1.37	1.35
23	D	404	CLA	CMD-C2D	-2.79	1.44	1.50
23	d	403	CLA	C3B-C2B	-2.78	1.36	1.40
23	a	404	CLA	C1D-ND	2.78	1.41	1.37
23	b	617	CLA	CMD-C2D	-2.78	1.44	1.50
23	c	513	CLA	C1D-ND	2.77	1.41	1.37
23	b	607	CLA	MG-NC	-2.77	1.99	2.06
23	C	507	CLA	C3B-C2B	-2.77	1.36	1.40
23	D	402	CLA	CHC-C1C	2.77	1.42	1.35
29	c	516	DGD	O3D-C3D	-2.77	1.36	1.43
23	c	513	CLA	MG-NA	2.77	2.12	2.06
26	A	409	PL9	C53-C6	-2.75	1.45	1.50
29	C	516	DGD	O2G-C2G	-2.75	1.39	1.46
23	d	404	CLA	CMD-C2D	-2.74	1.45	1.50
23	C	503	CLA	CHC-C1C	2.74	1.42	1.35
23	c	507	CLA	C4B-CHC	-2.74	1.33	1.41
27	m	101	LMG	C4-C3	2.74	1.59	1.52
23	A	404	CLA	C1D-ND	2.74	1.41	1.37
27	A	410	LMG	C7-C8	2.73	1.59	1.50
25	c	515	BCR	C1-C6	-2.73	1.50	1.53
23	b	617	CLA	MG-NC	2.73	2.12	2.06
29	c	517	DGD	O3E-C3E	-2.73	1.36	1.43
23	b	616	CLA	CMB-C2B	-2.72	1.46	1.51
23	h	101	CLA	C1B-NB	2.72	1.37	1.35
23	D	404	CLA	C3B-CAB	-2.72	1.42	1.47
23	C	501	CLA	C4D-ND	-2.72	1.34	1.37
23	C	505	CLA	CMB-C2B	-2.71	1.46	1.51
23	B	610	CLA	CMB-C2B	-2.71	1.46	1.51
23	B	609	CLA	C3B-CAB	-2.71	1.42	1.47
23	B	613	CLA	C4D-ND	-2.71	1.34	1.37
29	c	518	DGD	O1G-C1G	-2.71	1.39	1.45
23	c	503	CLA	MG-NC	2.71	2.12	2.06
25	d	405	BCR	C30-C25	-2.70	1.50	1.53
23	B	605	CLA	C1D-ND	2.70	1.41	1.37
23	A	405	CLA	C1D-ND	2.70	1.41	1.37
23	B	611	CLA	CMB-C2B	-2.70	1.46	1.51
25	B	619	BCR	C30-C25	-2.70	1.50	1.53
23	b	603	CLA	CHC-C1C	2.69	1.41	1.35
33	d	407	LHG	P-O3	2.69	1.70	1.59
23	b	617	CLA	C3B-C2B	-2.69	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	515	BCR	C30-C25	-2.69	1.50	1.53
23	B	611	CLA	CMD-C2D	-2.68	1.45	1.50
25	C	520	BCR	C30-C25	-2.68	1.50	1.53
23	C	501	CLA	C3B-C2B	-2.68	1.36	1.40
23	a	407	CLA	C3B-C2B	-2.68	1.36	1.40
23	B	609	CLA	O2D-CGD	2.68	1.39	1.33
23	c	502	CLA	C3B-C2B	-2.68	1.36	1.40
23	b	616	CLA	MG-ND	-2.68	2.00	2.05
29	C	516	DGD	O2D-C2D	-2.68	1.36	1.43
27	b	622	LMG	C6-C5	2.67	1.60	1.51
23	C	509	CLA	CMB-C2B	-2.67	1.46	1.51
28	F	101	SQD	O3-C3	-2.67	1.36	1.43
23	B	612	CLA	CHC-C1C	2.67	1.41	1.35
24	D	401	PHO	CAC-C3C	-2.66	1.47	1.52
23	C	507	CLA	CHC-C1C	2.66	1.41	1.35
34	E	102	HEM	CAB-C3B	2.66	1.54	1.47
23	b	614	CLA	CMD-C2D	-2.66	1.45	1.50
27	D	410	LMG	C9-C8	2.66	1.58	1.50
23	h	101	CLA	CHC-C1C	2.66	1.41	1.35
23	a	405	CLA	CHC-C1C	2.66	1.41	1.35
29	c	516	DGD	O2G-C2G	-2.66	1.39	1.46
23	c	506	CLA	CAC-C3C	-2.65	1.44	1.51
23	c	501	CLA	CMB-C2B	-2.65	1.46	1.51
23	C	504	CLA	CHC-C1C	2.65	1.41	1.35
25	D	405	BCR	C30-C25	-2.65	1.50	1.53
23	C	507	CLA	C4D-ND	-2.65	1.34	1.37
23	C	507	CLA	CMB-C2B	-2.65	1.46	1.51
27	c	522	LMG	C9-C8	2.65	1.58	1.50
23	B	601	CLA	CMB-C2B	-2.65	1.46	1.51
23	C	506	CLA	C3B-C2B	-2.64	1.36	1.40
23	B	612	CLA	C1D-ND	2.64	1.41	1.37
27	a	414	LMG	O8-C9	-2.64	1.39	1.45
29	c	516	DGD	C2B-C1B	-2.64	1.43	1.50
29	c	518	DGD	O3D-C3D	-2.64	1.36	1.43
33	D	408	LHG	P-O3	2.64	1.70	1.59
23	c	501	CLA	C4B-CHC	-2.64	1.33	1.41
23	b	611	CLA	C3B-C2B	-2.63	1.36	1.40
27	D	410	LMG	C7-C8	2.63	1.57	1.51
29	A	413	DGD	C3E-C2E	2.62	1.59	1.52
29	c	518	DGD	O3G-C3G	-2.62	1.39	1.43
23	B	613	CLA	C3B-CAB	-2.62	1.42	1.47
23	b	616	CLA	CMD-C2D	-2.62	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C4B-CHC	-2.62	1.33	1.41
23	b	613	CLA	CMB-C2B	-2.62	1.46	1.51
34	e	102	HEM	CAB-C3B	2.62	1.54	1.47
23	b	607	CLA	C3B-C2B	-2.61	1.36	1.40
23	h	101	CLA	CMC-C2C	-2.61	1.45	1.50
23	b	604	CLA	CMA-C3A	-2.61	1.47	1.53
26	D	406	PL9	C5-C4	-2.61	1.37	1.47
26	a	409	PL9	C6-C1	-2.61	1.43	1.48
25	B	618	BCR	C1-C6	-2.60	1.50	1.53
23	c	510	CLA	CHC-C1C	2.60	1.41	1.35
25	b	620	BCR	C1-C6	-2.60	1.50	1.53
23	b	606	CLA	C4B-CHC	-2.59	1.33	1.41
23	C	504	CLA	C4D-ND	-2.59	1.34	1.37
25	C	515	BCR	C30-C25	-2.59	1.50	1.53
23	C	512	CLA	C4D-ND	-2.59	1.34	1.37
23	B	616	CLA	CMD-C2D	-2.59	1.45	1.50
29	A	413	DGD	C4E-C5E	2.59	1.58	1.53
23	a	404	CLA	MG-ND	2.59	2.10	2.05
24	a	406	PHO	CAC-C3C	-2.59	1.47	1.52
23	B	608	CLA	CMB-C2B	-2.58	1.46	1.51
23	B	603	CLA	CMA-C3A	-2.58	1.47	1.53
23	b	605	CLA	C3D-C4D	2.58	1.50	1.44
23	d	402	CLA	CHC-C1C	2.58	1.41	1.35
23	c	509	CLA	C3C-C2C	2.58	1.42	1.36
23	B	606	CLA	C3B-CAB	-2.58	1.42	1.47
33	E	101	LHG	C24-C23	2.58	1.58	1.50
26	D	406	PL9	C3-C4	-2.57	1.45	1.49
27	c	519	LMG	C4-C5	2.57	1.58	1.53
23	B	604	CLA	MG-NC	2.57	2.12	2.06
23	c	508	CLA	CMB-C2B	-2.56	1.46	1.51
25	A	408	BCR	C1-C6	-2.56	1.50	1.53
23	c	506	CLA	CMD-C2D	-2.56	1.45	1.50
23	B	613	CLA	OBD-CAD	2.56	1.26	1.22
23	B	616	CLA	CMC-C2C	-2.56	1.45	1.50
23	B	602	CLA	CMB-C2B	-2.56	1.46	1.51
23	d	404	CLA	CHC-C1C	2.55	1.41	1.35
23	D	404	CLA	CHC-C1C	2.55	1.41	1.35
23	c	511	CLA	C4D-ND	-2.55	1.34	1.37
23	c	507	CLA	CMB-C2B	-2.55	1.46	1.51
23	c	512	CLA	CMD-C2D	-2.55	1.45	1.50
23	c	509	CLA	CMB-C2B	-2.55	1.46	1.51
23	B	611	CLA	MG-NC	-2.54	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	C3B-CAB	-2.54	1.42	1.47
23	B	606	CLA	MG-ND	-2.54	2.00	2.05
23	C	511	CLA	C4D-ND	-2.53	1.34	1.37
25	C	515	BCR	C33-C5	-2.53	1.46	1.50
24	A	406	PHO	O2D-CGD	2.53	1.39	1.33
23	D	403	CLA	C1B-NB	2.53	1.37	1.35
23	h	101	CLA	C4D-ND	-2.53	1.34	1.37
23	B	613	CLA	C1C-NC	-2.53	1.34	1.37
25	c	515	BCR	C33-C5	-2.53	1.46	1.50
23	c	506	CLA	CMB-C2B	-2.53	1.46	1.51
26	d	406	PL9	C45-C44	-2.53	1.44	1.50
23	C	511	CLA	C3B-C2B	-2.53	1.36	1.40
23	D	403	CLA	C4D-ND	-2.52	1.34	1.37
27	A	410	LMG	C4-C3	2.52	1.58	1.52
23	B	608	CLA	C3B-CAB	-2.52	1.42	1.47
23	C	502	CLA	C3B-C2B	-2.52	1.36	1.40
23	c	505	CLA	CMB-C2B	-2.52	1.46	1.51
23	b	614	CLA	CHC-C1C	2.52	1.41	1.35
23	B	615	CLA	C3B-CAB	-2.52	1.42	1.47
23	c	506	CLA	C3B-C2B	-2.51	1.36	1.40
23	d	403	CLA	C1D-ND	2.51	1.40	1.37
23	a	405	CLA	C3B-CAB	-2.51	1.42	1.47
27	b	622	LMG	C7-C8	2.51	1.58	1.50
33	D	409	LHG	C4-C5	2.51	1.58	1.50
23	c	506	CLA	C4D-ND	-2.51	1.34	1.37
27	C	519	LMG	C4-C5	2.51	1.58	1.53
28	B	623	SQD	O48-C23	2.50	1.40	1.33
23	B	608	CLA	CMC-C2C	-2.50	1.45	1.50
23	B	609	CLA	CHC-C1C	2.50	1.41	1.35
23	C	510	CLA	C3B-C2B	-2.50	1.36	1.40
23	d	403	CLA	MG-ND	-2.50	2.00	2.05
33	E	101	LHG	P-O6	2.50	1.69	1.59
23	C	510	CLA	O2A-CGA	2.50	1.40	1.33
23	b	611	CLA	C1C-NC	-2.49	1.34	1.37
23	C	513	CLA	CHC-C1C	2.49	1.41	1.35
23	C	505	CLA	C3B-CAB	-2.49	1.42	1.47
29	C	517	DGD	C4E-C5E	2.49	1.58	1.53
23	D	402	CLA	C1D-ND	2.49	1.40	1.37
23	B	610	CLA	C3D-C4D	2.49	1.49	1.44
23	B	607	CLA	C4D-ND	-2.49	1.34	1.37
23	C	506	CLA	C3B-CAB	-2.49	1.42	1.47
29	H	102	DGD	C6D-C5D	2.49	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C1D-ND	2.48	1.40	1.37
23	b	610	CLA	CHC-C1C	2.48	1.41	1.35
29	C	516	DGD	O5D-C1E	2.47	1.44	1.40
23	b	605	CLA	CMC-C2C	-2.46	1.45	1.50
25	t	101	BCR	C30-C25	-2.46	1.50	1.53
29	C	518	DGD	O3G-C3G	-2.46	1.39	1.43
23	b	613	CLA	CMC-C2C	-2.46	1.45	1.50
26	d	406	PL9	C46-C44	-2.46	1.46	1.51
28	a	411	SQD	O2-C2	-2.46	1.37	1.43
23	B	609	CLA	CMC-C2C	-2.45	1.45	1.50
29	A	413	DGD	C3G-C2G	2.45	1.58	1.50
23	c	507	CLA	CMC-C2C	-2.45	1.45	1.50
23	C	512	CLA	C1D-C2D	2.45	1.50	1.45
23	b	604	CLA	CMD-C2D	-2.45	1.45	1.50
25	y	101	BCR	C1-C6	-2.45	1.50	1.53
23	B	607	CLA	CAC-C3C	-2.45	1.44	1.51
23	B	616	CLA	CMB-C2B	-2.44	1.46	1.51
25	T	101	BCR	C1-C6	-2.43	1.50	1.53
27	D	411	LMG	O8-C28	2.43	1.38	1.30
23	c	505	CLA	C3B-C2B	-2.42	1.37	1.40
23	A	405	CLA	C4B-CHC	-2.42	1.34	1.41
23	b	605	CLA	MG-NA	2.42	2.12	2.06
29	C	517	DGD	O3E-C3E	-2.42	1.37	1.43
23	C	503	CLA	CMB-C2B	-2.42	1.46	1.51
23	b	612	CLA	CMB-C2B	-2.42	1.46	1.51
23	C	501	CLA	CMD-C2D	-2.42	1.45	1.50
23	c	511	CLA	C3B-C2B	-2.42	1.37	1.40
23	b	604	CLA	MG-NC	-2.42	2.00	2.06
29	c	517	DGD	C6E-C5E	2.41	1.59	1.51
23	B	601	CLA	MG-NC	2.41	2.12	2.06
29	c	516	DGD	C4E-C3E	2.41	1.58	1.52
23	B	613	CLA	CMB-C2B	-2.41	1.46	1.51
23	B	615	CLA	C1D-ND	2.41	1.40	1.37
33	e	101	LHG	O7-C5	-2.41	1.40	1.46
23	c	509	CLA	C3B-CAB	-2.41	1.43	1.47
25	b	618	BCR	C33-C5	-2.40	1.47	1.50
23	C	507	CLA	C3B-CAB	-2.40	1.43	1.47
27	m	101	LMG	O1-C7	-2.40	1.39	1.43
33	l	101	LHG	C8-C7	-2.40	1.43	1.50
23	B	609	CLA	CMD-C2D	-2.40	1.45	1.50
23	B	607	CLA	O2D-CGD	2.40	1.39	1.33
23	B	613	CLA	CHC-C1C	2.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	O1D-CGD	2.39	1.27	1.21
23	B	603	CLA	O2D-CGD	2.39	1.39	1.33
23	C	502	CLA	MG-NA	-2.39	2.00	2.06
23	c	504	CLA	CMB-C2B	-2.39	1.46	1.51
26	a	409	PL9	C10-C9	-2.39	1.44	1.50
27	C	519	LMG	C3-C2	2.39	1.58	1.52
23	C	506	CLA	C4D-ND	-2.39	1.34	1.37
23	A	407	CLA	CHC-C1C	2.38	1.41	1.35
29	c	518	DGD	C1D-C2D	2.38	1.59	1.52
23	A	405	CLA	CMD-C2D	-2.38	1.45	1.50
28	a	411	SQD	O47-C7	2.38	1.41	1.34
23	c	501	CLA	CMC-C2C	-2.38	1.45	1.50
29	c	517	DGD	O1G-C1A	2.38	1.40	1.33
23	B	603	CLA	C3B-CAB	-2.37	1.43	1.47
29	C	516	DGD	O3E-C3E	-2.37	1.37	1.43
23	d	404	CLA	C3B-CAB	-2.37	1.43	1.47
23	b	608	CLA	C3B-CAB	-2.37	1.43	1.47
27	B	620	LMG	C9-C8	2.36	1.58	1.50
23	A	404	CLA	C5-C3	-2.36	1.46	1.51
23	c	502	CLA	C4B-CHC	-2.36	1.34	1.41
23	B	614	CLA	C3B-C2B	-2.36	1.37	1.40
25	B	619	BCR	C33-C5	-2.36	1.47	1.50
24	D	401	PHO	CHA-CBD	-2.36	1.49	1.52
23	C	505	CLA	C4C-C3C	2.35	1.49	1.45
23	d	402	CLA	C3B-C2B	-2.35	1.37	1.40
23	B	613	CLA	MG-NC	2.35	2.11	2.06
33	D	409	LHG	O3-C3	-2.35	1.35	1.44
23	C	503	CLA	C1D-ND	2.35	1.40	1.37
23	B	612	CLA	CMB-C2B	-2.35	1.46	1.51
23	C	508	CLA	C3B-CAB	-2.35	1.43	1.47
23	D	402	CLA	C1D-C2D	2.35	1.50	1.45
29	h	103	DGD	C3D-C2D	2.35	1.58	1.52
28	f	101	SQD	O3-C3	-2.34	1.37	1.43
25	B	617	BCR	C33-C5	-2.34	1.47	1.50
23	C	507	CLA	MG-NA	2.34	2.11	2.06
23	B	614	CLA	C3B-CAB	-2.34	1.43	1.47
23	b	603	CLA	MG-NA	2.34	2.11	2.06
23	B	606	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	610	CLA	MG-ND	-2.34	2.01	2.05
23	A	404	CLA	MG-ND	2.33	2.10	2.05
27	c	522	LMG	O6-C5	-2.33	1.38	1.44
25	a	408	BCR	C33-C5	-2.33	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	522	LMG	C1-C2	2.33	1.59	1.52
29	A	413	DGD	C6E-C5E	2.32	1.59	1.51
23	A	407	CLA	MG-NA	-2.32	2.00	2.06
23	B	607	CLA	CHC-C1C	2.32	1.40	1.35
23	b	603	CLA	CAC-C3C	-2.32	1.45	1.51
25	t	101	BCR	C33-C5	-2.31	1.47	1.50
23	B	608	CLA	C3B-C2B	-2.31	1.37	1.40
23	B	614	CLA	CMC-C2C	-2.31	1.45	1.50
23	b	610	CLA	CMC-C2C	-2.31	1.45	1.50
23	B	613	CLA	C3B-C2B	-2.31	1.37	1.40
29	h	103	DGD	O2D-C2D	-2.31	1.37	1.43
23	C	504	CLA	C1D-ND	2.30	1.40	1.37
24	d	401	PHO	C3B-CAB	-2.30	1.43	1.47
27	b	623	LMG	O7-C10	2.30	1.38	1.30
29	A	413	DGD	O5D-C1E	2.30	1.44	1.40
23	b	604	CLA	CMC-C2C	-2.30	1.45	1.50
25	c	515	BCR	C36-C18	-2.30	1.46	1.50
23	B	603	CLA	MG-ND	2.29	2.10	2.05
23	d	404	CLA	C3B-C2B	-2.29	1.37	1.40
24	D	401	PHO	CMD-C2D	-2.29	1.46	1.51
23	C	501	CLA	C3B-CAB	-2.29	1.43	1.47
28	a	411	SQD	O5-C5	-2.29	1.38	1.44
23	B	601	CLA	CMD-C2D	-2.29	1.45	1.50
23	h	101	CLA	CMB-C2B	-2.29	1.46	1.51
33	B	622	LHG	O6-C4	-2.29	1.36	1.44
23	b	611	CLA	CHC-C1C	2.29	1.40	1.35
33	l	101	LHG	O8-C23	2.29	1.40	1.33
23	c	504	CLA	C1D-ND	2.28	1.40	1.37
23	C	511	CLA	CMC-C2C	-2.28	1.46	1.50
23	c	505	CLA	MG-ND	2.28	2.10	2.05
23	c	504	CLA	C1B-NB	-2.28	1.33	1.35
23	c	502	CLA	CMB-C2B	-2.28	1.46	1.51
23	D	403	CLA	C1C-NC	-2.28	1.34	1.37
23	C	506	CLA	CMD-C2D	-2.28	1.46	1.50
27	c	522	LMG	C4-C5	2.28	1.57	1.53
24	a	406	PHO	C1A-C2A	2.27	1.54	1.51
24	D	401	PHO	CBD-CGD	-2.27	1.49	1.52
27	C	519	LMG	O8-C9	-2.27	1.40	1.45
29	C	518	DGD	C4D-C5D	2.27	1.57	1.53
34	e	102	HEM	CAA-C2A	2.27	1.55	1.52
23	A	407	CLA	C3B-CAB	-2.27	1.43	1.47
28	F	101	SQD	O2-C2	-2.27	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	CMC-C2C	-2.27	1.46	1.50
23	d	404	CLA	C4D-ND	-2.26	1.34	1.37
23	c	505	CLA	C1D-ND	2.26	1.40	1.37
27	c	519	LMG	C3-C2	2.26	1.58	1.52
23	C	513	CLA	CMB-C2B	-2.26	1.46	1.51
25	c	521	BCR	C30-C25	-2.26	1.50	1.53
23	b	604	CLA	C1D-ND	2.26	1.40	1.37
29	c	517	DGD	C1D-C2D	2.25	1.59	1.52
28	B	623	SQD	O2-C2	-2.25	1.37	1.43
33	d	407	LHG	C3-C2	2.25	1.59	1.51
23	B	605	CLA	CMC-C2C	-2.25	1.46	1.50
23	B	603	CLA	CMB-C2B	-2.25	1.47	1.51
23	B	602	CLA	CAC-C3C	-2.25	1.45	1.51
23	B	611	CLA	C4B-CHC	-2.25	1.34	1.41
27	C	519	LMG	C1-C2	2.25	1.59	1.52
23	c	511	CLA	C3C-C2C	2.25	1.41	1.36
28	f	101	SQD	O2-C2	-2.25	1.37	1.43
23	B	603	CLA	MG-NC	2.24	2.11	2.06
23	B	602	CLA	CMD-C2D	-2.24	1.46	1.50
23	B	605	CLA	O2D-CED	-2.24	1.40	1.45
25	A	408	BCR	C33-C5	-2.24	1.47	1.50
29	c	517	DGD	O1G-C1G	-2.23	1.40	1.45
23	C	511	CLA	C4B-CHC	-2.23	1.34	1.41
23	b	617	CLA	C1B-NB	2.23	1.37	1.35
23	b	612	CLA	C4B-CHC	-2.23	1.34	1.41
23	a	407	CLA	C3B-CAB	-2.23	1.43	1.47
23	C	505	CLA	C1D-ND	2.23	1.40	1.37
29	H	102	DGD	C6E-C5E	2.23	1.59	1.51
23	C	510	CLA	MG-NC	2.23	2.11	2.06
23	b	615	CLA	MG-NC	2.22	2.11	2.06
23	b	614	CLA	C1D-ND	2.22	1.40	1.37
25	C	515	BCR	C38-C26	-2.22	1.47	1.50
23	c	507	CLA	C3B-CAB	-2.22	1.43	1.47
23	c	502	CLA	C1D-ND	2.21	1.40	1.37
23	C	512	CLA	CMB-C2B	-2.21	1.47	1.51
23	b	617	CLA	C4B-CHC	-2.21	1.34	1.41
23	B	613	CLA	C5-C3	-2.21	1.46	1.51
23	b	614	CLA	C5-C3	-2.21	1.46	1.51
23	b	607	CLA	CMB-C2B	-2.21	1.47	1.51
27	D	411	LMG	O7-C10	2.20	1.38	1.30
24	a	406	PHO	CMC-C2C	-2.20	1.46	1.51
23	A	407	CLA	C4B-CHC	-2.20	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C4B-CHC	-2.20	1.34	1.41
23	a	405	CLA	CMD-C2D	-2.20	1.46	1.50
34	E	102	HEM	FE-NB	2.20	2.07	1.96
23	B	605	CLA	CMD-C2D	-2.20	1.46	1.50
27	D	407	LMG	O2-C2	-2.20	1.37	1.43
23	c	502	CLA	O2A-CGA	2.20	1.39	1.33
23	B	615	CLA	CAC-C3C	-2.20	1.45	1.51
23	B	612	CLA	C1C-NC	-2.20	1.34	1.37
23	B	601	CLA	CMC-C2C	-2.19	1.46	1.50
23	A	407	CLA	C1A-CHA	-2.19	1.34	1.43
23	b	609	CLA	C1D-C2D	2.19	1.49	1.45
23	d	403	CLA	MG-NA	2.19	2.11	2.06
33	D	408	LHG	O7-C5	-2.19	1.41	1.46
23	C	507	CLA	C4B-CHC	-2.19	1.34	1.41
23	B	616	CLA	C4B-CHC	-2.19	1.34	1.41
23	C	512	CLA	C1A-CHA	-2.19	1.34	1.43
23	b	611	CLA	C1D-ND	2.19	1.40	1.37
29	c	516	DGD	O1G-C1G	-2.19	1.40	1.45
23	c	513	CLA	CMD-C2D	-2.18	1.46	1.50
29	C	516	DGD	O1G-C1A	2.18	1.39	1.33
29	c	518	DGD	C4E-C5E	-2.18	1.48	1.53
24	a	406	PHO	CMB-C2B	-2.18	1.46	1.51
24	d	401	PHO	CMC-C2C	-2.18	1.46	1.51
23	C	503	CLA	C3B-CAB	-2.18	1.43	1.47
23	B	605	CLA	C3B-C2B	-2.18	1.37	1.40
27	D	410	LMG	O8-C28	2.18	1.39	1.33
23	b	607	CLA	C1B-NB	2.18	1.37	1.35
23	c	503	CLA	CMB-C2B	-2.18	1.47	1.51
29	C	516	DGD	C3D-C2D	2.17	1.57	1.52
26	d	406	PL9	C46-C47	-2.17	1.46	1.53
23	a	407	CLA	MG-NC	-2.17	2.01	2.06
23	D	402	CLA	CMB-C2B	-2.17	1.47	1.51
23	B	604	CLA	CMC-C2C	-2.17	1.46	1.50
23	b	607	CLA	CHC-C1C	2.17	1.40	1.35
23	C	509	CLA	CMD-C2D	-2.17	1.46	1.50
23	b	612	CLA	CMA-C3A	-2.17	1.48	1.53
23	c	501	CLA	CHC-C1C	2.17	1.40	1.35
24	A	406	PHO	C1A-C2A	2.16	1.54	1.51
28	a	411	SQD	O47-C45	-2.16	1.41	1.46
23	C	513	CLA	C4B-CHC	-2.16	1.35	1.41
23	b	608	CLA	CMD-C2D	-2.16	1.46	1.50
23	c	501	CLA	MG-ND	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	CLA	CMB-C2B	-2.16	1.47	1.51
23	C	501	CLA	CMC-C2C	-2.16	1.46	1.50
23	b	615	CLA	CMC-C2C	-2.15	1.46	1.50
23	b	604	CLA	C3B-C2B	-2.15	1.37	1.40
23	D	402	CLA	C3D-C4D	2.15	1.49	1.44
23	B	610	CLA	CMC-C2C	-2.15	1.46	1.50
23	b	607	CLA	C4B-CHC	-2.15	1.35	1.41
29	c	517	DGD	C3E-C2E	2.14	1.57	1.52
23	C	509	CLA	C4B-CHC	-2.14	1.35	1.41
23	A	405	CLA	C3B-C2B	-2.14	1.37	1.40
23	B	608	CLA	C3C-C2C	2.14	1.41	1.36
33	D	408	LHG	C8-C7	-2.14	1.44	1.50
23	b	616	CLA	C3B-CAB	-2.14	1.43	1.47
33	a	410	LHG	O7-C5	-2.14	1.41	1.46
23	d	403	CLA	CMC-C2C	-2.13	1.46	1.50
23	b	608	CLA	C4B-CHC	-2.13	1.35	1.41
23	A	407	CLA	C3B-C2B	-2.13	1.37	1.40
23	D	403	CLA	C4B-CHC	-2.13	1.35	1.41
23	a	407	CLA	CAC-C3C	-2.13	1.45	1.51
23	a	407	CLA	CHC-C1C	2.13	1.40	1.35
23	C	509	CLA	C3B-C2B	-2.13	1.37	1.40
29	A	413	DGD	O2G-C1B	2.13	1.40	1.34
33	e	101	LHG	P-O6	2.12	1.67	1.59
23	b	617	CLA	O2D-CED	-2.12	1.40	1.45
33	l	101	LHG	C6-C5	2.12	1.57	1.50
23	D	403	CLA	CMD-C2D	-2.11	1.46	1.50
23	D	403	CLA	CMB-C2B	-2.11	1.47	1.51
28	b	601	SQD	O3-C3	-2.11	1.38	1.43
24	A	406	PHO	CMC-C2C	-2.11	1.46	1.51
25	y	101	BCR	C33-C5	-2.11	1.47	1.50
23	B	616	CLA	C2-C3	2.11	1.38	1.33
26	D	406	PL9	C27-C28	-2.10	1.43	1.50
29	c	517	DGD	O3G-C3G	-2.10	1.39	1.43
29	c	517	DGD	C1E-C2E	2.10	1.58	1.52
23	A	407	CLA	CHD-C1D	-2.10	1.34	1.38
27	D	407	LMG	C30-C29	2.10	1.59	1.52
23	B	613	CLA	CMC-C2C	-2.10	1.46	1.50
23	B	615	CLA	MG-NC	2.10	2.11	2.06
23	C	512	CLA	CAA-C2A	-2.10	1.50	1.54
23	b	611	CLA	CMC-C2C	-2.10	1.46	1.50
23	c	509	CLA	C3D-C4D	2.10	1.48	1.44
23	D	402	CLA	C4C-C3C	2.09	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	622	LHG	O7-C5	-2.09	1.41	1.46
33	D	409	LHG	C3-C2	2.09	1.58	1.51
27	a	414	LMG	C4-C5	2.09	1.57	1.53
23	c	511	CLA	C1D-C2D	2.09	1.49	1.45
23	b	613	CLA	CMD-C2D	-2.09	1.46	1.50
23	B	614	CLA	C1D-ND	2.09	1.40	1.37
23	c	504	CLA	CAC-C3C	-2.09	1.45	1.51
23	a	405	CLA	C4B-CHC	-2.09	1.35	1.41
26	a	409	PL9	C40-C39	-2.09	1.45	1.50
29	C	518	DGD	C2A-C1A	-2.08	1.44	1.50
27	c	519	LMG	C4-C3	2.08	1.57	1.52
23	d	403	CLA	CMD-C2D	-2.08	1.46	1.50
23	c	503	CLA	C3B-C2B	-2.08	1.37	1.40
23	C	512	CLA	CMD-C2D	-2.08	1.46	1.50
23	c	501	CLA	CAC-C3C	-2.08	1.45	1.51
23	C	508	CLA	C1D-C2D	2.08	1.49	1.45
23	h	101	CLA	O2A-CGA	2.08	1.39	1.33
23	B	616	CLA	C4C-C3C	2.08	1.48	1.45
23	c	512	CLA	CMC-C2C	-2.08	1.46	1.50
29	h	103	DGD	C4D-C5D	2.07	1.57	1.53
23	D	404	CLA	C1A-CHA	-2.07	1.34	1.43
23	C	512	CLA	C5-C3	-2.07	1.47	1.51
34	e	102	HEM	C3B-C2B	-2.07	1.33	1.37
25	c	521	BCR	C38-C26	-2.07	1.47	1.50
23	D	404	CLA	C4B-CHC	-2.07	1.35	1.41
23	h	101	CLA	C3D-C4D	2.07	1.48	1.44
23	d	402	CLA	C1D-C2D	2.07	1.49	1.45
23	C	506	CLA	O2D-CGD	2.06	1.38	1.33
23	h	101	CLA	C3B-CAB	-2.06	1.43	1.47
23	C	503	CLA	C3B-C2B	-2.06	1.37	1.40
23	b	614	CLA	C1C-NC	-2.06	1.34	1.37
23	B	611	CLA	C3B-CAB	-2.06	1.43	1.47
23	b	603	CLA	C1B-NB	2.05	1.37	1.35
23	C	505	CLA	CHC-C1C	2.05	1.40	1.35
23	b	610	CLA	CMB-C2B	-2.05	1.47	1.51
24	A	406	PHO	O2A-CGA	2.05	1.39	1.33
24	D	401	PHO	CMC-C2C	-2.05	1.46	1.51
23	C	511	CLA	C3D-C4D	2.05	1.48	1.44
25	a	408	BCR	C27-C26	-2.05	1.47	1.51
23	b	603	CLA	CMD-C2D	-2.05	1.46	1.50
33	E	101	LHG	P-O3	2.05	1.67	1.59
23	C	504	CLA	CMA-C3A	-2.05	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	413	DGD	C4D-C3D	2.04	1.57	1.52
23	C	506	CLA	CAC-C3C	-2.04	1.45	1.51
23	b	617	CLA	MG-ND	-2.04	2.01	2.05
23	c	502	CLA	CMC-C2C	-2.04	1.46	1.50
23	h	101	CLA	MG-NC	-2.04	2.01	2.06
23	c	508	CLA	C4B-CHC	-2.04	1.35	1.41
27	B	620	LMG	C6-C5	2.04	1.58	1.51
29	c	518	DGD	C6E-C5E	-2.04	1.45	1.51
27	B	620	LMG	C7-C8	2.03	1.56	1.50
23	c	510	CLA	CMB-C2B	-2.03	1.47	1.51
23	b	613	CLA	C4B-CHC	-2.03	1.35	1.41
23	c	513	CLA	C4B-CHC	-2.03	1.35	1.41
23	B	604	CLA	O2A-CGA	2.03	1.39	1.33
23	b	610	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	610	CLA	CAC-C3C	-2.03	1.45	1.51
25	y	101	BCR	C38-C26	-2.03	1.47	1.50
28	A	411	SQD	O47-C45	-2.03	1.41	1.46
23	A	407	CLA	C3D-C4D	2.02	1.48	1.44
23	d	403	CLA	C4B-CHC	-2.02	1.35	1.41
23	C	504	CLA	O2D-CGD	2.02	1.38	1.33
28	a	411	SQD	O3-C3	-2.02	1.38	1.43
23	b	603	CLA	C4B-CHC	-2.02	1.35	1.41
27	A	410	LMG	C1-C2	2.02	1.58	1.52
23	a	404	CLA	CMC-C2C	-2.02	1.46	1.50
23	b	607	CLA	MG-ND	2.02	2.09	2.05
23	d	404	CLA	CMC-C2C	-2.02	1.46	1.50
23	h	101	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	613	CLA	C3D-C4D	2.01	1.48	1.44
23	C	507	CLA	MG-ND	-2.01	2.01	2.05
23	D	403	CLA	CMC-C2C	-2.01	1.46	1.50
23	b	615	CLA	C3D-C4D	2.01	1.48	1.44
23	C	513	CLA	CMD-C2D	-2.01	1.46	1.50
29	c	516	DGD	C6D-C5D	2.01	1.57	1.51
24	d	401	PHO	CMA-C3A	-2.01	1.49	1.53
23	C	504	CLA	C1D-C2D	2.01	1.49	1.45
23	c	512	CLA	C3B-CAB	-2.00	1.43	1.47
29	C	517	DGD	O1G-C1G	-2.00	1.40	1.45
23	C	513	CLA	C1D-C2D	2.00	1.49	1.45
23	b	609	CLA	CMB-C2B	-2.00	1.47	1.51
29	C	516	DGD	O5D-C6D	-2.00	1.40	1.43
23	C	509	CLA	C1B-NB	2.00	1.37	1.35
27	d	409	LMG	C4-C5	2.00	1.57	1.53

All (1361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C4A-NA-C1A	10.58	111.46	106.71
23	d	402	CLA	C4A-NA-C1A	10.17	111.28	106.71
23	C	510	CLA	C4A-NA-C1A	9.94	111.18	106.71
23	b	607	CLA	C4A-NA-C1A	9.94	111.18	106.71
28	b	601	SQD	O6-C1-C2	9.77	123.55	108.30
23	b	605	CLA	C4A-NA-C1A	9.41	110.94	106.71
23	D	403	CLA	C4A-NA-C1A	9.10	110.80	106.71
28	A	411	SQD	O6-C1-C2	9.02	122.38	108.30
28	A	411	SQD	O7-S-C6	8.75	117.34	106.94
23	C	511	CLA	C4A-NA-C1A	8.46	110.51	106.71
23	C	501	CLA	C4A-NA-C1A	8.18	110.39	106.71
23	c	509	CLA	C4A-NA-C1A	8.17	110.38	106.71
23	C	513	CLA	C4A-NA-C1A	7.83	110.23	106.71
23	B	606	CLA	C4A-NA-C1A	7.71	110.17	106.71
23	C	503	CLA	C4A-NA-C1A	7.70	110.17	106.71
23	B	612	CLA	C4A-NA-C1A	7.66	110.15	106.71
23	B	601	CLA	C4A-NA-C1A	7.62	110.13	106.71
28	a	411	SQD	O6-C1-C2	7.58	120.13	108.30
23	b	617	CLA	C4A-NA-C1A	7.48	110.07	106.71
23	c	503	CLA	C4A-NA-C1A	7.46	110.06	106.71
23	b	604	CLA	C4A-NA-C1A	7.31	109.99	106.71
23	c	501	CLA	C4A-NA-C1A	7.22	109.95	106.71
23	b	615	CLA	C4A-NA-C1A	6.96	109.84	106.71
23	a	404	CLA	C4A-NA-C1A	6.95	109.83	106.71
23	b	612	CLA	C4A-NA-C1A	6.88	109.80	106.71
28	f	101	SQD	O9-S-C6	6.88	115.11	106.94
23	c	502	CLA	C4A-NA-C1A	6.80	109.76	106.71
23	C	508	CLA	C4A-NA-C1A	6.67	109.70	106.71
23	c	506	CLA	C4A-NA-C1A	6.60	109.67	106.71
26	A	409	PL9	C7-C3-C4	6.58	122.23	116.88
23	B	615	CLA	C4A-NA-C1A	6.45	109.61	106.71
23	B	616	CLA	C4A-NA-C1A	6.44	109.60	106.71
23	A	404	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	b	611	CLA	C4A-NA-C1A	6.34	109.56	106.71
29	c	517	DGD	O3G-C3G-C2G	-6.33	95.63	110.90
23	c	511	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	c	504	CLA	C4A-NA-C1A	5.95	109.38	106.71
29	H	102	DGD	O3G-C3G-C2G	-5.85	96.77	110.90
23	c	512	CLA	C4A-NA-C1A	5.83	109.33	106.71
28	f	101	SQD	O6-C1-C2	5.80	117.36	108.30
23	C	509	CLA	C4A-NA-C1A	5.80	109.31	106.71
23	b	615	CLA	CMB-C2B-C1B	-5.80	119.55	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	CMB-C2B-C1B	-5.78	119.59	128.46
29	C	517	DGD	O3G-C3G-C2G	-5.77	96.98	110.90
23	B	607	CLA	C4A-NA-C1A	5.71	109.27	106.71
23	B	610	CLA	O2D-CGD-O1D	-5.68	112.73	123.84
23	b	613	CLA	CMB-C2B-C1B	-5.67	119.76	128.46
23	B	601	CLA	O2D-CGD-O1D	-5.65	112.79	123.84
28	B	623	SQD	O7-S-C6	5.64	113.64	106.94
23	B	602	CLA	C4A-NA-C1A	5.64	109.24	106.71
26	a	409	PL9	C7-C3-C4	5.54	121.38	116.88
23	c	508	CLA	C4A-NA-C1A	5.52	109.19	106.71
23	c	501	CLA	O2D-CGD-O1D	-5.47	113.14	123.84
23	B	603	CLA	C4A-NA-C1A	5.47	109.16	106.71
23	B	605	CLA	C4A-NA-C1A	5.46	109.16	106.71
23	B	602	CLA	CHB-C4A-NA	5.45	132.05	124.51
23	A	407	CLA	C1D-ND-C4D	-5.39	102.51	106.33
23	c	505	CLA	CHD-C1D-ND	-5.39	119.50	124.45
23	D	402	CLA	C4A-NA-C1A	5.37	109.12	106.71
35	v	201	HEC	CMC-C2C-C1C	-5.30	120.32	128.46
23	C	507	CLA	C4A-NA-C1A	5.25	109.06	106.71
23	b	610	CLA	C4A-NA-C1A	5.22	109.05	106.71
23	B	614	CLA	O2D-CGD-O1D	-5.15	113.76	123.84
28	F	101	SQD	O6-C1-C2	5.14	116.33	108.30
23	c	504	CLA	CMB-C2B-C1B	-5.13	120.57	128.46
23	b	611	CLA	O2D-CGD-O1D	-5.13	113.80	123.84
27	b	622	LMG	O1-C1-C2	-5.12	100.31	108.30
28	a	411	SQD	O9-S-C6	5.09	112.99	106.94
23	b	613	CLA	CMB-C2B-C3B	5.09	134.19	124.68
28	a	412	SQD	O47-C7-C8	5.07	122.43	111.50
29	a	413	DGD	O3G-C3G-C2G	-5.05	98.40	111.78
23	C	509	CLA	CHD-C1D-ND	-4.98	119.88	124.45
23	b	604	CLA	O2D-CGD-O1D	-4.97	114.11	123.84
23	A	405	CLA	O2D-CGD-O1D	-4.97	114.12	123.84
23	c	512	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
23	b	604	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
28	F	101	SQD	O9-S-C6	4.86	112.72	106.94
23	b	606	CLA	CHD-C1D-ND	-4.79	120.05	124.45
28	b	601	SQD	C45-O47-C7	4.79	129.58	117.79
23	h	101	CLA	C4A-NA-C1A	4.78	108.86	106.71
23	C	503	CLA	CHD-C1D-ND	-4.78	120.06	124.45
23	b	610	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
23	b	609	CLA	CHB-C4A-NA	4.77	131.10	124.51
28	b	601	SQD	C1-C2-C3	-4.74	100.11	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	CHD-C1D-ND	-4.74	120.09	124.45
23	A	407	CLA	CMB-C2B-C3B	4.72	133.51	124.68
23	c	509	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
23	B	601	CLA	O1D-CGD-CBD	4.70	134.10	124.48
29	h	103	DGD	O3G-C3G-C2G	-4.68	99.60	110.90
29	c	516	DGD	O3G-C3G-C2G	-4.68	99.60	110.90
23	C	506	CLA	C4A-NA-C1A	4.66	108.80	106.71
23	C	502	CLA	O2D-CGD-O1D	-4.62	114.80	123.84
29	H	102	DGD	C1D-C2D-C3D	-4.60	100.41	110.00
23	b	608	CLA	O2D-CGD-O1D	-4.59	114.87	123.84
23	B	613	CLA	C1-C2-C3	-4.58	118.12	126.04
23	b	616	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
23	d	403	CLA	C4A-NA-C1A	4.56	108.76	106.71
23	C	508	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
28	A	411	SQD	C1-C2-C3	-4.52	100.59	110.00
24	D	401	PHO	O1D-CGD-CBD	4.51	132.26	124.74
23	b	606	CLA	C4A-NA-C1A	4.51	108.73	106.71
28	B	623	SQD	O6-C1-C2	4.49	115.31	108.30
23	b	615	CLA	CMB-C2B-C3B	4.48	133.06	124.68
34	e	102	HEM	CBA-CAA-C2A	-4.46	105.02	112.62
28	F	101	SQD	O8-S-C6	4.42	112.79	105.74
23	C	505	CLA	CAC-C3C-C4C	4.42	130.55	124.81
33	D	409	LHG	O4-P-O5	4.41	134.05	112.24
23	C	504	CLA	CMB-C2B-C1B	-4.40	121.71	128.46
23	c	512	CLA	CMB-C2B-C3B	4.39	132.89	124.68
23	b	613	CLA	C4A-NA-C1A	4.39	108.68	106.71
33	d	407	LHG	O4-P-O5	4.38	133.89	112.24
35	v	201	HEC	CMC-C2C-C3C	4.34	130.93	125.82
23	C	508	CLA	CHD-C1D-ND	-4.34	120.46	124.45
28	b	601	SQD	O7-S-C6	4.33	112.08	106.94
23	b	617	CLA	O2D-CGD-O1D	-4.33	115.38	123.84
28	b	601	SQD	O9-S-C6	4.32	112.08	106.94
23	c	501	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
23	A	407	CLA	CHD-C1D-ND	-4.30	120.50	124.45
23	B	610	CLA	C4A-NA-C1A	4.30	108.64	106.71
23	c	509	CLA	CMB-C2B-C3B	4.29	132.70	124.68
23	b	609	CLA	C4A-NA-C1A	4.27	108.62	106.71
23	c	508	CLA	CHB-C4A-NA	4.26	130.40	124.51
23	B	602	CLA	O2D-CGD-O1D	-4.25	115.52	123.84
33	a	410	LHG	O4-P-O5	4.24	133.21	112.24
26	D	406	PL9	C7-C3-C4	4.24	120.32	116.88
29	C	517	DGD	O5D-C1E-C2E	4.22	114.89	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	622	LHG	O4-P-O5	4.22	133.09	112.24
29	c	517	DGD	O6D-C1D-O3G	-4.21	100.00	109.97
23	b	609	CLA	O2D-CGD-CBD	4.20	118.72	111.27
23	B	612	CLA	CAC-C3C-C4C	4.19	130.25	124.81
23	c	504	CLA	CMB-C2B-C3B	4.19	132.51	124.68
23	c	507	CLA	CHD-C1D-ND	-4.17	120.63	124.45
23	b	614	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
29	c	516	DGD	O2D-C2D-C1D	-4.15	99.97	110.05
23	b	607	CLA	CHD-C1D-ND	-4.15	120.64	124.45
23	A	405	CLA	CMB-C2B-C1B	-4.14	122.09	128.46
23	b	615	CLA	O2D-CGD-CBD	4.14	118.62	111.27
28	B	623	SQD	O9-S-O7	-4.14	99.63	113.95
34	e	102	HEM	CMC-C2C-C3C	4.12	132.38	124.68
33	d	408	LHG	O4-P-O5	4.11	132.58	112.24
23	B	604	CLA	C2D-C1D-ND	-4.11	107.08	110.10
33	e	101	LHG	O4-P-O5	4.11	132.55	112.24
28	B	623	SQD	C3-C4-C5	4.10	117.56	110.24
23	c	508	CLA	CHD-C1D-ND	-4.10	120.69	124.45
23	b	603	CLA	CHB-C4A-NA	4.08	130.15	124.51
23	B	615	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
29	C	518	DGD	O3E-C3E-C2E	-4.07	100.94	110.35
28	B	623	SQD	O47-C7-C8	4.06	120.26	111.50
23	B	604	CLA	CHB-C4A-NA	4.06	130.12	124.51
23	d	404	CLA	CHD-C1D-ND	-4.05	120.73	124.45
23	B	602	CLA	O2D-CGD-CBD	4.03	118.42	111.27
23	a	405	CLA	C4A-NA-C1A	4.03	108.52	106.71
23	c	513	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
23	D	402	CLA	CHB-C4A-NA	4.02	130.07	124.51
23	b	606	CLA	C4D-CHA-C1A	4.02	126.14	121.25
28	A	411	SQD	O47-C7-C8	4.01	120.15	111.50
23	B	605	CLA	CHD-C1D-ND	-4.01	120.77	124.45
29	C	516	DGD	O3G-C3G-C2G	-4.01	101.23	110.90
23	C	512	CLA	CHB-C4A-NA	4.00	130.04	124.51
23	A	404	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
23	B	611	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
23	c	510	CLA	CHD-C1D-ND	-3.98	120.80	124.45
23	b	604	CLA	O2D-CGD-CBD	3.97	118.33	111.27
23	c	505	CLA	C4A-NA-C1A	3.97	108.49	106.71
28	b	601	SQD	O2-C2-C1	3.97	119.69	110.05
23	a	404	CLA	CHD-C1D-ND	-3.97	120.81	124.45
33	E	101	LHG	O4-P-O5	3.93	131.67	112.24
33	D	408	LHG	O4-P-O5	3.92	131.60	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
23	a	405	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	C	508	CLA	CMB-C2B-C3B	3.91	131.99	124.68
23	A	407	CLA	C1B-CHB-C4A	-3.91	122.38	130.12
23	C	513	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	C	512	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
23	h	101	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
26	d	406	PL9	C37-C38-C39	-3.88	118.31	127.66
23	C	501	CLA	CAC-C3C-C4C	3.87	129.84	124.81
23	c	503	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
23	c	510	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
29	C	518	DGD	O3G-C3G-C2G	-3.83	101.65	110.90
25	b	619	BCR	C35-C13-C14	-3.83	117.56	122.92
23	B	614	CLA	O2D-CGD-CBD	3.82	118.06	111.27
23	b	610	CLA	CMB-C2B-C3B	3.82	131.83	124.68
23	b	611	CLA	CAC-C3C-C4C	3.82	129.76	124.81
23	C	513	CLA	CHD-C1D-ND	-3.82	120.95	124.45
23	B	608	CLA	O2D-CGD-O1D	-3.80	116.40	123.84
23	b	605	CLA	C1-C2-C3	-3.79	119.48	126.04
23	B	610	CLA	O2A-CGA-O1A	-3.79	114.02	123.59
23	c	506	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
23	B	604	CLA	CMB-C2B-C1B	-3.79	122.65	128.46
23	B	602	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
28	A	412	SQD	O47-C7-C8	3.77	119.62	111.50
23	B	608	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
33	l	101	LHG	O4-P-O5	3.76	130.85	112.24
23	C	513	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
23	C	502	CLA	C4A-NA-C1A	3.76	108.39	106.71
23	c	507	CLA	C2C-C1C-NC	3.76	113.49	109.97
23	b	611	CLA	O1D-CGD-CBD	3.75	132.16	124.48
23	b	617	CLA	CHB-C4A-NA	3.75	129.70	124.51
26	A	409	PL9	C7-C3-C2	-3.75	118.37	123.30
25	B	617	BCR	C2-C1-C6	3.74	116.24	110.48
24	d	401	PHO	O1D-CGD-CBD	3.74	130.96	124.74
23	c	513	CLA	C4A-NA-C1A	3.73	108.38	106.71
25	b	618	BCR	C2-C1-C6	3.73	116.22	110.48
23	c	501	CLA	O2D-CGD-CBD	3.73	117.89	111.27
23	c	509	CLA	O2A-CGA-O1A	-3.73	114.19	123.59
23	c	510	CLA	CMB-C2B-C3B	3.72	131.63	124.68
27	c	522	LMG	O6-C1-O1	-3.71	101.19	109.97
29	h	103	DGD	C3D-C4D-C5D	-3.70	103.63	110.24
23	B	606	CLA	CGD-CBD-CAD	-3.70	98.76	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	O2D-CGD-CBD	3.69	117.82	111.27
23	b	615	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
23	C	502	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
28	b	601	SQD	C3-C4-C5	3.68	116.80	110.24
28	a	411	SQD	O7-S-C6	3.68	111.31	106.94
31	A	415	BCT	O2-C-O1	3.67	129.07	119.55
23	b	617	CLA	O2D-CGD-CBD	3.67	117.79	111.27
23	b	616	CLA	CMB-C2B-C3B	3.67	131.54	124.68
23	B	612	CLA	CHB-C4A-NA	3.67	129.58	124.51
23	b	606	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
23	b	613	CLA	C1B-CHB-C4A	-3.66	122.87	130.12
28	b	601	SQD	O8-S-C6	3.66	111.57	105.74
26	D	406	PL9	C37-C38-C39	-3.66	118.85	127.66
23	B	613	CLA	C1D-ND-C4D	-3.65	103.74	106.33
23	b	603	CLA	CHD-C1D-ND	-3.65	121.10	124.45
23	B	613	CLA	C1B-CHB-C4A	-3.65	122.90	130.12
29	c	516	DGD	O3G-C1D-C2D	-3.64	102.62	108.30
23	b	614	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
23	b	614	CLA	C4A-NA-C1A	3.63	108.34	106.71
23	c	506	CLA	CBC-CAC-C3C	-3.62	102.44	112.43
23	b	603	CLA	CMB-C2B-C3B	3.62	131.45	124.68
23	h	101	CLA	O2D-CGD-CBD	3.61	117.68	111.27
28	B	623	SQD	O9-S-C6	3.61	111.23	106.94
28	b	601	SQD	O48-C23-C24	3.60	123.21	111.91
28	b	601	SQD	O9-S-O7	-3.59	101.51	113.95
23	b	603	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	B	603	CLA	O2D-CGD-CBD	3.59	117.65	111.27
23	B	616	CLA	C2C-C1C-NC	3.59	113.34	109.97
23	C	504	CLA	CHD-C1D-ND	-3.59	121.15	124.45
23	b	606	CLA	C4D-C3D-CAD	-3.58	103.88	108.10
23	b	604	CLA	CMB-C2B-C3B	3.58	131.37	124.68
23	b	608	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
23	A	404	CLA	CMB-C2B-C3B	3.57	131.35	124.68
23	d	404	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
23	B	608	CLA	C6-C5-C3	-3.56	104.11	113.45
23	B	602	CLA	CHD-C1D-ND	-3.56	121.18	124.45
23	b	612	CLA	CHD-C1D-ND	-3.55	121.19	124.45
33	B	622	LHG	O8-C23-C24	3.55	123.06	111.91
23	a	404	CLA	O1D-CGD-CBD	3.55	131.75	124.48
28	B	623	SQD	O48-C23-C24	3.54	123.03	111.91
33	B	622	LHG	O8-C23-O10	-3.54	114.66	123.59
23	C	507	CLA	CMB-C2B-C1B	-3.53	123.03	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	CHB-C4A-NA	3.52	129.38	124.51
23	C	513	CLA	CMB-C2B-C3B	3.51	131.25	124.68
23	d	403	CLA	C4-C3-C5	3.51	121.18	115.27
25	b	620	BCR	C38-C26-C25	-3.51	120.58	124.53
23	b	608	CLA	O1D-CGD-CBD	3.51	131.66	124.48
23	b	603	CLA	C3C-C4C-NC	-3.51	106.64	110.57
23	b	608	CLA	CHD-C1D-ND	-3.50	121.23	124.45
23	b	609	CLA	C3B-C4B-NB	-3.50	104.68	109.21
23	b	612	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
23	b	608	CLA	CMB-C2B-C3B	3.50	131.22	124.68
23	b	616	CLA	CHD-C1D-ND	-3.49	121.24	124.45
23	b	612	CLA	C2D-C1D-ND	-3.48	107.54	110.10
33	L	101	LHG	O4-P-O5	3.48	129.46	112.24
33	a	410	LHG	O8-C23-C24	3.47	122.79	111.91
28	a	411	SQD	O47-C7-C8	3.47	118.97	111.50
23	c	507	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
23	B	609	CLA	C4A-NA-C1A	3.46	108.26	106.71
25	T	101	BCR	C7-C8-C9	-3.46	121.00	126.23
29	a	413	DGD	C1G-C2G-C3G	-3.46	103.71	111.80
23	D	404	CLA	CHD-C1D-ND	-3.45	121.28	124.45
23	B	603	CLA	CHB-C4A-NA	3.45	129.28	124.51
23	B	608	CLA	CMB-C2B-C3B	3.44	131.12	124.68
23	c	507	CLA	C4A-NA-C1A	3.44	108.25	106.71
23	c	505	CLA	O2D-CGD-CBD	3.44	117.37	111.27
28	B	623	SQD	C1-O5-C5	-3.43	106.95	113.69
29	c	518	DGD	O3G-C3G-C2G	-3.43	102.62	110.90
23	c	507	CLA	CHB-C4A-NA	3.42	129.24	124.51
23	B	608	CLA	CHD-C1D-ND	-3.42	121.31	124.45
23	B	615	CLA	CHB-C4A-NA	3.42	129.24	124.51
25	a	408	BCR	C35-C13-C14	-3.42	118.13	122.92
23	C	507	CLA	CMB-C2B-C3B	3.41	131.06	124.68
27	c	522	LMG	C4-C3-C2	3.41	116.78	110.82
23	B	603	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
23	B	612	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
23	a	405	CLA	CMB-C2B-C3B	3.40	131.05	124.68
23	B	603	CLA	CMB-C2B-C3B	3.40	131.05	124.68
29	A	413	DGD	O5D-C1E-C2E	3.40	113.60	108.30
23	B	606	CLA	CHD-C1D-ND	-3.39	121.34	124.45
23	b	614	CLA	C7-C6-C5	-3.39	104.15	113.36
25	C	514	BCR	C33-C5-C6	-3.39	120.72	124.53
23	b	613	CLA	CAC-C3C-C4C	3.39	129.20	124.81
23	D	402	CLA	CMB-C2B-C3B	3.39	131.01	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	411	SQD	O9-S-O7	-3.38	102.24	113.95
23	C	501	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
23	b	616	CLA	C1D-ND-C4D	-3.38	103.94	106.33
23	B	608	CLA	C4A-NA-C1A	3.37	108.22	106.71
23	B	605	CLA	C4-C3-C5	3.37	120.93	115.27
23	B	602	CLA	CMB-C2B-C3B	3.36	130.97	124.68
23	b	603	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
23	b	616	CLA	C1B-CHB-C4A	-3.35	123.47	130.12
23	D	403	CLA	CHB-C4A-NA	3.35	129.15	124.51
33	D	409	LHG	O8-C23-C24	3.35	122.42	111.91
23	c	504	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
28	B	623	SQD	O5-C5-C4	3.35	115.78	109.69
25	c	514	BCR	C15-C16-C17	-3.35	116.62	123.47
23	A	404	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
29	H	102	DGD	C3E-C4E-C5E	-3.34	104.28	110.24
23	c	509	CLA	O1D-CGD-CBD	3.34	131.32	124.48
25	T	101	BCR	C27-C26-C25	3.34	127.58	122.73
25	b	618	BCR	C27-C26-C25	3.34	127.58	122.73
25	T	101	BCR	C35-C13-C14	-3.34	118.25	122.92
23	c	508	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
23	c	509	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
24	D	401	PHO	O2D-CGD-CBD	-3.33	106.78	111.00
25	y	101	BCR	C27-C26-C25	3.33	127.56	122.73
23	C	508	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
23	B	614	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
27	D	410	LMG	O1-C7-C8	-3.32	102.98	111.78
28	a	411	SQD	O8-S-C6	3.32	111.03	105.74
28	B	623	SQD	O48-C23-O10	-3.32	115.22	123.59
25	C	515	BCR	C15-C14-C13	-3.31	122.58	127.31
25	B	618	BCR	C37-C22-C21	-3.31	118.28	122.92
23	B	609	CLA	CHA-C1A-NA	-3.31	118.82	126.40
23	D	403	CLA	O2D-CGD-CBD	3.30	117.14	111.27
23	B	601	CLA	CHB-C4A-NA	3.30	129.07	124.51
23	c	512	CLA	CHB-C4A-NA	3.30	129.07	124.51
29	c	518	DGD	O5E-C6E-C5E	-3.30	99.98	111.29
23	B	609	CLA	CMB-C2B-C3B	3.29	130.84	124.68
24	A	406	PHO	CMB-C2B-C3B	3.29	130.84	124.68
25	h	102	BCR	C38-C26-C25	-3.29	120.84	124.53
23	B	604	CLA	CMB-C2B-C3B	3.29	130.83	124.68
23	C	509	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
23	B	612	CLA	CHD-C1D-ND	-3.29	121.44	124.45
27	D	411	LMG	O7-C10-O9	-3.28	115.12	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	617	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
23	b	609	CLA	CMB-C2B-C3B	3.27	130.79	124.68
23	D	404	CLA	C1B-CHB-C4A	-3.27	123.65	130.12
23	B	610	CLA	CHB-C4A-NA	3.26	129.02	124.51
23	c	513	CLA	CHB-C4A-NA	3.26	129.02	124.51
29	h	103	DGD	C3G-C2G-C1G	-3.26	104.08	111.79
23	B	605	CLA	O1D-CGD-CBD	3.26	131.15	124.48
27	m	101	LMG	O7-C10-O9	-3.26	115.83	123.70
26	A	409	PL9	C20-C19-C21	3.25	120.74	115.27
23	c	505	CLA	CHB-C4A-NA	3.25	129.00	124.51
25	c	515	BCR	C35-C13-C14	-3.23	118.39	122.92
23	b	616	CLA	CHD-C4C-C3C	-3.23	120.09	124.84
27	d	409	LMG	O1-C1-C2	-3.23	103.25	108.30
23	a	404	CLA	CMB-C2B-C3B	3.23	130.72	124.68
34	E	102	HEM	CBA-CAA-C2A	-3.22	107.12	112.62
28	f	101	SQD	O47-C7-C8	3.22	119.78	110.80
27	C	519	LMG	O1-C7-C8	-3.20	103.17	110.90
23	b	609	CLA	CHD-C1D-ND	-3.20	121.51	124.45
23	A	407	CLA	C4-C3-C5	3.20	120.66	115.27
31	a	417	BCT	O2-C-O1	3.20	127.83	119.55
27	a	414	LMG	C1-O6-C5	-3.19	107.42	113.69
23	b	613	CLA	C11-C12-C13	-3.19	105.60	115.92
23	b	612	CLA	CMB-C2B-C3B	3.19	130.65	124.68
23	C	504	CLA	CMB-C2B-C3B	3.19	130.64	124.68
25	t	101	BCR	C15-C16-C17	-3.19	116.95	123.47
28	a	412	SQD	O48-C23-C24	3.18	121.89	111.91
23	a	404	CLA	C3A-C2A-C1A	3.18	106.10	101.34
23	B	605	CLA	CHB-C4A-NA	3.18	128.91	124.51
23	b	605	CLA	C4-C3-C5	3.18	120.62	115.27
23	c	502	CLA	CHD-C1D-ND	-3.18	121.54	124.45
25	B	617	BCR	C35-C13-C14	-3.17	118.48	122.92
28	b	601	SQD	O5-C5-C4	3.17	115.45	109.69
26	d	406	PL9	C8-C7-C3	3.17	120.93	111.98
23	B	616	CLA	C1-O2A-CGA	3.17	124.75	116.44
23	A	405	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	C	503	CLA	O2A-C1-C2	-3.16	100.33	108.64
25	c	514	BCR	C27-C26-C25	3.16	127.32	122.73
24	a	406	PHO	C1-C2-C3	-3.15	120.59	126.04
25	c	515	BCR	C27-C26-C25	3.15	127.31	122.73
28	A	411	SQD	O9-S-O7	-3.15	103.06	113.95
24	d	401	PHO	CMB-C2B-C3B	3.14	130.56	124.68
29	A	413	DGD	C3G-C2G-C1G	-3.14	104.36	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	101	BCR	C39-C30-C25	-3.14	105.21	110.30
26	d	406	PL9	C7-C3-C4	3.13	119.42	116.88
23	c	501	CLA	CMB-C2B-C3B	3.13	130.54	124.68
23	B	613	CLA	OBD-CAD-C3D	3.13	136.05	128.52
34	E	102	HEM	CBD-CAD-C3D	-3.12	103.95	112.63
23	c	513	CLA	CMB-C2B-C3B	3.12	130.52	124.68
23	d	402	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
27	B	620	LMG	O6-C1-O1	-3.12	102.59	109.97
25	B	617	BCR	C29-C30-C25	3.11	115.27	110.48
23	a	404	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
23	c	510	CLA	C4A-NA-C1A	3.11	108.10	106.71
23	b	607	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
23	B	603	CLA	CHD-C1D-ND	-3.10	121.61	124.45
25	a	408	BCR	C2-C1-C6	3.10	115.25	110.48
23	B	606	CLA	O2D-CGD-CBD	3.10	116.77	111.27
25	H	101	BCR	C2-C1-C6	3.10	115.25	110.48
23	c	510	CLA	C7-C6-C5	-3.10	104.95	113.36
23	D	402	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
29	h	103	DGD	C1E-O6E-C5E	3.09	119.76	113.69
25	c	521	BCR	C27-C26-C25	3.09	127.22	122.73
29	C	516	DGD	O6D-C1D-O3G	-3.09	102.65	109.97
23	D	402	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
26	d	406	PL9	O1-C4-C3	-3.09	117.31	120.72
23	B	603	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
23	B	602	CLA	CHC-C1C-NC	3.09	128.89	124.20
28	f	101	SQD	O8-S-C6	3.09	110.66	105.74
23	b	617	CLA	CMB-C2B-C3B	3.09	130.45	124.68
23	a	407	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
23	B	611	CLA	C2C-C1C-NC	3.08	112.86	109.97
23	C	503	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
24	A	406	PHO	CMA-C3A-C4A	-3.08	107.64	114.38
25	c	515	BCR	C36-C18-C17	-3.08	118.61	122.92
25	D	405	BCR	C24-C23-C22	-3.08	121.59	126.23
23	D	404	CLA	C1D-ND-C4D	-3.07	104.15	106.33
29	C	518	DGD	O6D-C1D-O3G	-3.07	102.69	109.97
23	C	504	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
28	f	101	SQD	O5-C5-C4	3.07	115.27	109.69
28	F	101	SQD	C1-C2-C3	-3.07	103.61	110.00
29	C	518	DGD	O3G-C1D-C2D	-3.07	103.52	108.30
23	b	609	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	B	614	CLA	CHD-C1D-ND	-3.06	121.64	124.45
23	c	506	CLA	CMB-C2B-C3B	3.06	130.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	v	201	HEC	CBD-CAD-C3D	-3.06	107.40	112.62
25	A	408	BCR	C11-C10-C9	-3.06	122.95	127.31
23	A	405	CLA	O2D-CGD-CBD	3.05	116.69	111.27
23	c	509	CLA	CHD-C1D-ND	-3.05	121.65	124.45
23	D	404	CLA	C4-C3-C5	3.05	120.40	115.27
23	B	602	CLA	C2D-C1D-ND	-3.05	107.86	110.10
23	A	407	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	B	615	CLA	C4-C3-C5	-3.05	110.14	115.27
29	c	517	DGD	C3G-O3G-C1D	3.05	119.69	113.74
28	f	101	SQD	O9-S-O7	-3.05	103.41	113.95
23	c	506	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	A	404	CLA	CAA-CBA-CGA	-3.04	104.36	113.25
27	c	522	LMG	O7-C10-O9	-3.04	116.35	123.70
23	B	608	CLA	CHB-C4A-NA	3.04	128.72	124.51
23	B	601	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
23	C	506	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
29	c	517	DGD	CDB-CCB-CBB	-3.03	99.04	114.42
23	A	405	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
23	b	617	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
27	c	522	LMG	O3-C3-C2	-3.03	103.35	110.35
29	h	103	DGD	C6D-C5D-C4D	3.02	118.40	112.09
23	c	503	CLA	CMB-C2B-C3B	3.02	130.33	124.68
23	b	606	CLA	C1-C2-C3	-3.02	120.83	126.04
26	d	406	PL9	C22-C23-C24	-3.02	120.40	127.66
23	C	512	CLA	CHD-C1D-ND	-3.02	121.68	124.45
23	b	616	CLA	C4A-NA-C1A	3.01	108.06	106.71
27	d	409	LMG	O6-C1-O1	-3.01	102.84	109.97
25	h	102	BCR	C27-C26-C25	3.01	127.10	122.73
29	c	518	DGD	C3G-C2G-C1G	-3.01	104.67	111.79
25	c	515	BCR	C34-C9-C10	-3.01	118.71	122.92
27	m	101	LMG	O8-C28-O10	-3.01	116.00	123.59
23	c	506	CLA	C4-C3-C5	3.00	120.32	115.27
23	C	503	CLA	C4-C3-C5	3.00	120.32	115.27
23	b	617	CLA	C2C-C1C-NC	3.00	112.78	109.97
25	b	619	BCR	C15-C14-C13	-3.00	123.03	127.31
24	a	406	PHO	CMB-C2B-C3B	3.00	130.28	124.68
23	c	506	CLA	O1D-CGD-CBD	2.99	130.61	124.48
23	c	512	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	b	616	CLA	CHC-C1C-NC	2.99	128.74	124.20
23	B	608	CLA	O2D-CGD-CBD	2.99	116.58	111.27
23	b	610	CLA	O1D-CGD-CBD	2.99	130.60	124.48
29	C	516	DGD	O3E-C3E-C2E	-2.99	103.44	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
28	A	411	SQD	O9-S-C6	2.99	110.49	106.94
24	a	406	PHO	O2D-CGD-O1D	-2.98	118.00	123.84
33	E	101	LHG	O8-C23-C24	2.98	121.28	111.91
23	A	407	CLA	C3D-C4D-ND	2.98	115.07	110.24
23	B	614	CLA	CBC-CAC-C3C	-2.98	104.20	112.43
25	H	101	BCR	C27-C26-C25	2.98	127.06	122.73
25	B	617	BCR	C15-C14-C13	-2.98	123.06	127.31
23	C	512	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
23	C	509	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	B	605	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	a	404	CLA	CHC-C1C-NC	2.97	128.71	124.20
34	E	102	HEM	CHC-C4B-NB	2.97	127.65	124.43
25	a	408	BCR	C27-C26-C25	2.96	127.03	122.73
23	D	402	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
23	c	503	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	B	611	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
23	B	611	CLA	O2D-CGD-CBD	2.96	116.52	111.27
23	B	605	CLA	CHD-C4C-C3C	-2.95	120.50	124.84
23	b	605	CLA	CHC-C1C-NC	2.95	128.68	124.20
23	b	603	CLA	O2D-CGD-CBD	2.95	116.50	111.27
26	a	409	PL9	C22-C23-C24	-2.94	120.57	127.66
23	B	603	CLA	O2A-CGA-O1A	-2.94	116.16	123.59
23	B	604	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
23	b	613	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
27	A	410	LMG	O6-C1-O1	-2.93	103.02	109.97
29	C	517	DGD	C1D-C2D-C3D	-2.93	103.89	110.00
23	c	510	CLA	CHB-C4A-NA	2.93	128.56	124.51
23	b	604	CLA	C4-C3-C5	2.93	120.20	115.27
23	b	609	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
23	b	615	CLA	CHD-C1D-ND	-2.92	121.77	124.45
25	d	405	BCR	C38-C26-C25	-2.92	121.25	124.53
29	C	516	DGD	O5D-C6D-C5D	-2.92	103.64	109.05
23	c	510	CLA	CAA-CBA-CGA	-2.92	104.72	113.25
29	H	102	DGD	C6D-C5D-C4D	2.92	118.19	112.09
23	b	603	CLA	C4A-NA-C1A	2.92	108.02	106.71
23	B	609	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
23	A	404	CLA	CHB-C4A-NA	2.91	128.54	124.51
29	c	516	DGD	C3G-C2G-C1G	-2.91	104.91	111.79
23	C	513	CLA	CHB-C4A-NA	2.90	128.53	124.51
23	A	405	CLA	CAC-C3C-C4C	2.90	128.57	124.81
23	A	405	CLA	C3A-C2A-C1A	2.90	105.68	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C35-C13-C14	-2.90	118.86	122.92
25	C	514	BCR	C34-C9-C10	-2.90	118.86	122.92
33	D	409	LHG	O8-C23-O10	-2.90	116.28	123.59
33	a	410	LHG	O8-C23-O10	-2.90	116.28	123.59
25	a	408	BCR	C38-C26-C27	-2.90	108.05	113.62
23	c	510	CLA	O2A-C1-C2	-2.89	101.03	108.64
23	C	501	CLA	O2A-CGA-O1A	-2.89	116.29	123.59
23	b	605	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
23	C	505	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
27	D	407	LMG	O3-C3-C2	-2.89	103.67	110.35
23	b	604	CLA	CHD-C1D-ND	-2.89	121.80	124.45
23	a	407	CLA	C4A-NA-C1A	2.88	108.00	106.71
26	d	406	PL9	C11-C9-C8	-2.88	115.28	121.12
23	B	613	CLA	C4A-NA-C1A	2.88	108.00	106.71
29	h	103	DGD	O3E-C3E-C2E	-2.88	103.69	110.35
25	A	408	BCR	C16-C15-C14	-2.88	117.58	123.47
25	b	620	BCR	C27-C26-C25	2.88	126.91	122.73
23	B	612	CLA	C1-O2A-CGA	2.87	123.98	116.44
28	A	411	SQD	O48-C23-C24	2.87	120.92	111.91
23	B	610	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
29	H	102	DGD	O2D-C2D-C1D	-2.87	103.09	110.05
23	b	611	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
25	y	101	BCR	C30-C25-C26	-2.86	118.58	122.61
23	b	606	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	c	509	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
26	D	406	PL9	C22-C23-C24	-2.85	120.79	127.66
27	m	101	LMG	O3-C3-C2	-2.85	103.75	110.35
23	c	513	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
27	m	101	LMG	O7-C10-C11	2.85	117.64	111.50
27	D	407	LMG	O8-C28-O10	-2.85	116.41	123.59
23	C	512	CLA	O1D-CGD-CBD	2.84	130.30	124.48
23	c	502	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
23	B	601	CLA	CHA-C4D-ND	2.84	138.45	132.50
23	b	607	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
23	c	511	CLA	C2D-C1D-ND	-2.84	108.01	110.10
23	d	404	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
23	h	101	CLA	CHD-C1D-ND	-2.84	121.84	124.45
23	C	505	CLA	C4A-NA-C1A	2.84	107.98	106.71
23	c	511	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
27	d	409	LMG	C6-C5-C4	-2.84	106.36	113.00
25	B	619	BCR	C29-C30-C25	2.84	114.85	110.48
29	c	516	DGD	C3D-C4D-C5D	-2.83	105.18	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C4A-NA-C1A	2.83	107.98	106.71
23	c	508	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
25	c	515	BCR	C30-C25-C26	-2.83	118.63	122.61
26	d	406	PL9	C50-C49-C48	-2.82	114.48	122.65
25	B	618	BCR	C27-C26-C25	2.82	126.83	122.73
23	b	611	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	B	616	CLA	CAC-C3C-C4C	2.81	128.46	124.81
23	b	611	CLA	CAA-CBA-CGA	-2.81	105.03	113.25
29	C	517	DGD	O6D-C1D-O3G	-2.81	103.32	109.97
24	A	406	PHO	C1A-C2A-C3A	-2.80	100.17	102.84
25	d	405	BCR	C16-C15-C14	-2.80	117.73	123.47
23	c	510	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
23	C	511	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	C	503	CLA	CMB-C2B-C3B	2.80	129.91	124.68
26	D	406	PL9	C8-C7-C3	2.80	119.89	111.98
23	c	509	CLA	CHB-C4A-NA	2.79	128.38	124.51
29	A	413	DGD	O5D-C6D-C5D	-2.79	103.88	109.05
27	B	620	LMG	C4-C3-C2	-2.79	105.95	110.82
29	C	518	DGD	CDB-CCB-CBB	-2.79	100.26	114.42
23	c	503	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
23	B	606	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	c	502	CLA	C1-O2A-CGA	2.78	123.74	116.44
29	C	518	DGD	C3G-C2G-C1G	-2.78	105.22	111.79
23	b	604	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
29	h	103	DGD	O6E-C5E-C4E	2.78	114.74	109.69
23	B	612	CLA	CMB-C2B-C3B	2.78	129.87	124.68
23	b	605	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	C	509	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
24	A	406	PHO	CED-O2D-CGD	2.77	122.20	115.94
23	B	616	CLA	C1-C2-C3	2.77	130.83	126.04
23	B	611	CLA	CMB-C2B-C3B	2.76	129.85	124.68
23	c	502	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
28	A	411	SQD	C1-O5-C5	-2.76	108.27	113.69
34	e	102	HEM	CBD-CAD-C3D	-2.76	104.96	112.63
23	c	508	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	D	402	CLA	O2D-CGD-CBD	2.76	116.17	111.27
23	h	101	CLA	O2A-C1-C2	2.76	115.88	108.64
23	a	405	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	c	513	CLA	CHD-C1D-ND	-2.75	121.92	124.45
25	b	620	BCR	C2-C1-C6	2.75	114.72	110.48
23	B	613	CLA	CMB-C2B-C3B	2.75	129.82	124.68
23	c	501	CLA	C2C-C1C-NC	2.75	112.55	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	407	LHG	O8-C23-C24	2.75	120.53	111.91
23	h	101	CLA	O2A-CGA-O1A	-2.75	116.66	123.59
25	H	101	BCR	C38-C26-C25	-2.74	121.45	124.53
23	A	404	CLA	CHD-C1D-ND	-2.74	121.93	124.45
23	c	501	CLA	CED-O2D-CGD	-2.74	109.73	115.94
26	A	409	PL9	C27-C28-C29	-2.74	121.05	127.66
23	b	612	CLA	CHD-C1D-C2D	2.74	131.23	125.48
25	H	101	BCR	C16-C15-C14	-2.74	117.86	123.47
23	b	609	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
29	c	517	DGD	C8B-C7B-C6B	-2.74	100.52	114.42
23	B	605	CLA	C4D-C3D-CAD	-2.74	104.87	108.10
23	D	403	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
23	C	504	CLA	CHD-C4C-NC	2.73	128.51	124.20
27	a	414	LMG	O6-C1-O1	-2.73	103.50	109.97
23	D	402	CLA	CED-O2D-CGD	-2.73	109.76	115.94
26	A	409	PL9	C22-C23-C24	-2.73	121.09	127.66
23	B	615	CLA	C6-C7-C8	-2.73	107.11	115.92
25	C	515	BCR	C15-C16-C17	-2.73	117.89	123.47
26	D	406	PL9	C12-C13-C14	-2.73	121.10	127.66
23	d	403	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
23	B	615	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
23	C	506	CLA	CMB-C2B-C3B	2.72	129.77	124.68
29	h	103	DGD	C1D-O6D-C5D	-2.71	108.37	113.69
23	B	613	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	B	619	BCR	C12-C13-C14	-2.71	114.79	118.94
27	b	622	LMG	C1-O6-C5	-2.71	108.37	113.69
34	E	102	HEM	C4B-CHC-C1C	2.71	126.13	122.56
27	d	409	LMG	O6-C5-C4	2.70	114.61	109.69
23	B	612	CLA	O1D-CGD-CBD	2.70	130.02	124.48
27	C	519	LMG	O7-C10-O9	-2.70	117.17	123.70
28	B	623	SQD	C4-C3-C2	2.70	115.54	110.82
24	D	401	PHO	CMB-C2B-C3B	2.70	129.73	124.68
28	a	411	SQD	C1-C2-C3	-2.70	104.37	110.00
23	C	509	CLA	C1-C2-C3	-2.70	121.38	126.04
25	b	619	BCR	C8-C7-C6	-2.70	119.63	127.20
33	d	407	LHG	C20-C19-C18	-2.70	100.74	114.42
29	C	516	DGD	C6D-O5D-C1E	2.70	119.01	113.74
23	C	503	CLA	C7-C6-C5	-2.70	106.04	113.36
28	A	411	SQD	O48-C23-O10	-2.70	116.79	123.59
23	b	606	CLA	CMB-C2B-C3B	2.69	129.72	124.68
25	H	101	BCR	C8-C9-C10	2.69	123.08	118.94
34	e	102	HEM	CHB-C1B-NB	2.69	127.71	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	O6E-C1E-O5D	-2.69	103.59	109.97
23	B	613	CLA	C3D-C4D-ND	2.69	114.59	110.24
23	d	404	CLA	CHA-C1A-NA	-2.69	120.24	126.40
23	B	612	CLA	C11-C12-C13	-2.69	107.23	115.92
23	D	403	CLA	CED-O2D-CGD	2.68	122.01	115.94
29	H	102	DGD	O2G-C1B-O1B	-2.68	117.22	123.70
23	C	504	CLA	C11-C10-C8	-2.68	107.25	115.92
27	c	519	LMG	O6-C1-O1	-2.68	103.62	109.97
23	B	614	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
25	H	101	BCR	C24-C23-C22	-2.68	122.19	126.23
33	a	410	LHG	C11-C10-C9	-2.68	100.83	114.42
23	B	601	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
23	c	503	CLA	C2D-C1D-ND	-2.67	108.14	110.10
25	b	618	BCR	C32-C1-C6	-2.67	105.97	110.30
27	m	101	LMG	C40-C39-C38	-2.67	100.88	114.42
25	B	619	BCR	C34-C9-C10	-2.67	119.19	122.92
23	b	603	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
25	T	101	BCR	C36-C18-C17	-2.66	119.19	122.92
23	b	604	CLA	O2A-C1-C2	-2.66	101.64	108.64
23	d	403	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
26	d	406	PL9	O2-C1-C6	2.66	125.20	120.59
23	c	503	CLA	CHD-C1D-ND	-2.66	122.01	124.45
27	B	620	LMG	O7-C10-O9	-2.66	117.28	123.70
23	c	508	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
23	c	503	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	B	615	CLA	C1-O2A-CGA	2.65	123.40	116.44
23	A	405	CLA	CED-O2D-CGD	-2.65	109.95	115.94
28	F	101	SQD	O48-C23-O10	-2.65	116.91	123.59
25	A	408	BCR	C40-C30-C25	2.65	114.59	110.30
23	a	407	CLA	CMB-C2B-C3B	2.65	129.63	124.68
23	h	101	CLA	CMB-C2B-C1B	-2.64	124.40	128.46
27	m	101	LMG	O1-C7-C8	-2.64	104.53	110.90
26	a	409	PL9	C7-C3-C2	-2.64	119.83	123.30
33	e	101	LHG	O8-C23-O10	-2.64	116.94	123.59
26	d	406	PL9	C40-C39-C38	-2.63	116.92	123.68
29	c	516	DGD	CDB-CCB-CBB	-2.63	101.06	114.42
25	c	515	BCR	C38-C26-C25	-2.63	121.58	124.53
29	C	518	DGD	CBB-CAB-C9B	-2.63	101.08	114.42
23	c	507	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
23	h	101	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
23	c	505	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
29	H	102	DGD	C4D-C3D-C2D	-2.62	106.25	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C2D-C1D-ND	-2.62	108.17	110.10
33	e	101	LHG	O8-C23-C24	2.62	120.13	111.91
25	a	408	BCR	C15-C14-C13	-2.62	123.57	127.31
23	c	507	CLA	CMB-C2B-C3B	2.62	129.57	124.68
23	B	603	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	c	508	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	A	407	CLA	O2D-CGD-CBD	2.61	115.91	111.27
23	C	503	CLA	CHD-C1D-C2D	2.61	130.96	125.48
25	h	102	BCR	C8-C9-C10	2.61	122.95	118.94
33	L	101	LHG	O8-C23-C24	2.61	120.10	111.91
29	c	518	DGD	C6D-O5D-C1E	2.61	118.83	113.74
23	b	613	CLA	C2C-C1C-NC	2.61	112.41	109.97
23	b	616	CLA	CHD-C4C-NC	2.61	128.31	124.20
28	F	101	SQD	O5-C5-C4	2.61	114.43	109.69
26	D	406	PL9	C42-C43-C44	-2.60	121.39	127.66
27	B	620	LMG	C38-C37-C36	-2.60	101.21	114.42
27	B	620	LMG	C40-C39-C38	-2.60	101.22	114.42
23	B	612	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
28	F	101	SQD	O48-C23-C24	2.60	120.07	111.91
23	b	614	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	d	404	CLA	CMB-C2B-C3B	2.59	129.53	124.68
26	A	409	PL9	C36-C34-C33	-2.59	115.87	121.12
23	B	607	CLA	CHD-C1D-ND	-2.59	122.07	124.45
23	B	602	CLA	C3C-C4C-NC	-2.59	107.66	110.57
25	h	102	BCR	C33-C5-C6	-2.59	121.62	124.53
23	b	608	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
23	b	616	CLA	CAA-CBA-CGA	-2.59	105.68	113.25
23	C	508	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	B	616	CLA	C2D-C1D-ND	-2.59	108.20	110.10
29	H	102	DGD	C3G-C2G-C1G	-2.59	105.67	111.79
23	c	505	CLA	CHC-C1C-NC	2.59	128.13	124.20
23	B	602	CLA	CHD-C1D-C2D	2.58	130.90	125.48
27	m	101	LMG	C9-C8-C7	-2.58	105.68	111.79
23	b	614	CLA	O2D-CGD-CBD	2.58	115.86	111.27
23	C	503	CLA	C5-C3-C2	-2.58	115.89	121.12
33	B	622	LHG	C11-C10-C9	-2.58	101.35	114.42
23	C	511	CLA	CAC-C3C-C4C	2.57	128.15	124.81
23	c	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	b	607	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	C	502	CLA	O2D-CGD-CBD	2.57	115.84	111.27
25	b	618	BCR	C35-C13-C14	-2.57	119.33	122.92
29	C	518	DGD	O3D-C3D-C4D	-2.56	104.42	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	CMD-C2D-C1D	-2.56	120.20	124.71
23	B	616	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
29	a	413	DGD	C2G-O2G-C1B	2.56	124.09	117.79
27	m	101	LMG	C31-C30-C29	-2.56	103.99	113.19
33	D	408	LHG	O8-C23-O10	-2.56	117.14	123.59
29	C	517	DGD	CDB-CCB-CBB	-2.56	101.44	114.42
23	C	505	CLA	C2D-C1D-ND	-2.56	108.22	110.10
23	B	602	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
27	B	620	LMG	C1-C2-C3	-2.55	104.67	110.00
25	d	405	BCR	C33-C5-C6	-2.55	121.66	124.53
26	A	409	PL9	C31-C29-C28	2.55	126.28	121.12
23	b	606	CLA	C1D-ND-C4D	2.55	108.15	106.33
25	A	408	BCR	C27-C26-C25	2.55	126.44	122.73
28	B	623	SQD	O47-C45-C46	2.55	117.64	108.40
26	d	406	PL9	C20-C19-C21	2.55	119.56	115.27
23	C	508	CLA	C3C-C4C-NC	-2.55	107.71	110.57
23	C	506	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	C	510	CLA	C1D-ND-C4D	2.55	108.14	106.33
23	C	505	CLA	O1D-CGD-CBD	2.55	129.70	124.48
29	c	518	DGD	O6E-C5E-C6E	-2.54	100.11	106.44
25	A	408	BCR	C24-C23-C22	-2.54	122.39	126.23
28	B	623	SQD	O47-C7-O49	-2.54	117.57	123.70
25	b	618	BCR	C15-C14-C13	-2.54	123.69	127.31
25	K	101	BCR	C27-C26-C25	2.53	126.41	122.73
23	b	614	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
24	d	401	PHO	CGD-CBD-CAD	2.53	118.94	110.73
23	B	607	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
23	h	101	CLA	CHB-C4A-NA	2.53	128.01	124.51
33	B	622	LHG	O3-P-O5	-2.53	99.18	109.07
25	b	618	BCR	C3-C4-C5	-2.53	109.56	114.08
23	D	404	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
25	c	514	BCR	C39-C30-C25	2.53	114.40	110.30
23	c	512	CLA	C1-C2-C3	-2.52	121.68	126.04
23	C	510	CLA	C2D-C1D-ND	-2.52	108.24	110.10
23	c	502	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
26	D	406	PL9	C7-C3-C2	-2.52	119.98	123.30
23	a	407	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	a	404	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
29	c	518	DGD	C1D-C2D-C3D	-2.52	104.75	110.00
25	B	618	BCR	C38-C26-C27	-2.52	108.78	113.62
23	B	613	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
25	C	514	BCR	C24-C23-C22	-2.52	122.43	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	O2D-CGD-CBD	2.52	115.74	111.27
23	B	615	CLA	CMB-C2B-C3B	2.52	129.38	124.68
25	H	101	BCR	C29-C30-C25	2.51	114.35	110.48
33	l	101	LHG	O8-C23-O10	-2.51	117.25	123.59
23	c	507	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
29	A	413	DGD	CDB-CCB-CBB	-2.51	101.68	114.42
26	a	409	PL9	C37-C38-C39	-2.51	121.62	127.66
23	h	101	CLA	CBA-CAA-C2A	2.51	121.27	113.86
26	A	409	PL9	C36-C37-C38	-2.51	103.64	111.88
23	B	613	CLA	O1D-CGD-CBD	2.51	129.62	124.48
23	B	613	CLA	C7-C6-C5	-2.51	106.55	113.36
23	a	407	CLA	CHA-C1A-NA	-2.51	120.66	126.40
23	C	509	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	C	520	BCR	C29-C30-C25	2.50	114.33	110.48
23	C	504	CLA	C4-C3-C5	2.50	119.48	115.27
23	c	501	CLA	CHD-C1D-ND	-2.50	122.16	124.45
27	A	410	LMG	C38-C37-C36	-2.50	101.74	114.42
29	c	517	DGD	O3D-C3D-C4D	-2.50	104.58	110.35
23	c	512	CLA	C2D-C1D-ND	-2.50	108.27	110.10
23	a	407	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
23	B	605	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
34	e	102	HEM	CHA-C4D-ND	2.49	127.46	124.38
26	A	409	PL9	C21-C19-C18	-2.49	116.08	121.12
29	h	103	DGD	C4D-C3D-C2D	-2.49	106.48	110.82
23	B	604	CLA	O1D-CGD-CBD	2.49	129.58	124.48
24	D	401	PHO	O2A-CGA-O1A	-2.49	117.31	123.59
25	K	101	BCR	C38-C26-C25	-2.49	121.74	124.53
23	B	611	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
33	d	408	LHG	C25-C24-C23	2.49	122.66	113.62
27	d	409	LMG	C40-C39-C38	-2.48	101.81	114.42
23	c	503	CLA	O1D-CGD-CBD	2.48	129.57	124.48
25	C	514	BCR	C2-C1-C6	2.48	114.30	110.48
23	C	503	CLA	C4D-CHA-C1A	2.48	124.27	121.25
27	D	407	LMG	O2-C2-C1	-2.48	104.02	110.05
23	c	504	CLA	O2D-CGD-CBD	2.48	115.68	111.27
23	c	507	CLA	CHD-C4C-NC	2.48	128.11	124.20
26	A	409	PL9	O2-C1-C2	-2.48	116.10	121.78
29	c	517	DGD	O2E-C2E-C1E	-2.48	104.03	110.05
23	d	402	CLA	O2D-CGD-CBD	2.47	115.67	111.27
25	h	102	BCR	C35-C13-C14	-2.47	119.46	122.92
26	d	406	PL9	C40-C39-C41	2.47	119.43	115.27
29	C	516	DGD	CDB-CCB-CBB	-2.47	101.88	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	102	DGD	C1D-O6D-C5D	-2.47	108.84	113.69
25	A	408	BCR	C2-C1-C6	2.47	114.28	110.48
23	c	506	CLA	C3C-C4C-NC	-2.47	107.80	110.57
28	a	412	SQD	O49-C7-C8	-2.47	114.10	123.73
23	C	503	CLA	C6-C7-C8	-2.47	107.94	115.92
25	b	620	BCR	C11-C10-C9	-2.46	123.79	127.31
23	C	506	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
23	A	407	CLA	CHB-C4A-NA	2.46	127.92	124.51
27	B	620	LMG	C3-C4-C5	-2.46	105.85	110.24
25	c	515	BCR	C11-C10-C9	-2.46	123.80	127.31
23	C	513	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
34	E	102	HEM	CMA-C3A-C4A	-2.46	124.69	128.46
23	B	607	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
25	b	619	BCR	C30-C25-C26	-2.46	119.15	122.61
23	B	616	CLA	C5-C3-C2	2.46	126.09	121.12
23	b	604	CLA	CHB-C4A-NA	2.45	127.91	124.51
25	c	515	BCR	C2-C1-C6	2.45	114.26	110.48
23	D	403	CLA	CMB-C2B-C3B	2.45	129.26	124.68
23	b	603	CLA	C1-O2A-CGA	2.45	122.88	116.44
23	C	510	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
24	A	406	PHO	CMC-C2C-C3C	2.45	129.56	124.94
23	b	604	CLA	CED-O2D-CGD	-2.45	110.40	115.94
23	C	507	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	d	401	PHO	CMA-C3A-C4A	-2.44	109.02	114.38
25	t	101	BCR	C27-C26-C25	2.44	126.28	122.73
25	t	101	BCR	C36-C18-C19	2.44	121.92	118.08
25	a	408	BCR	C3-C4-C5	-2.44	109.72	114.08
23	D	403	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
23	c	511	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
26	d	406	PL9	O2-C1-C2	-2.44	116.20	121.78
25	B	618	BCR	C30-C25-C26	-2.44	119.18	122.61
23	b	606	CLA	CMD-C2D-C3D	2.43	133.22	127.61
28	B	623	SQD	C25-C24-C23	-2.43	104.77	113.62
23	c	507	CLA	CHD-C4C-C3C	-2.43	121.26	124.84
25	B	619	BCR	C37-C22-C21	-2.43	119.52	122.92
24	A	406	PHO	C1B-NB-C4B	2.43	112.08	107.09
26	d	406	PL9	C31-C29-C28	2.43	126.03	121.12
23	C	506	CLA	CHD-C1D-ND	-2.43	122.22	124.45
27	d	409	LMG	O3-C3-C2	-2.43	104.73	110.35
33	D	408	LHG	O8-C23-C24	2.43	119.53	111.91
25	c	514	BCR	C15-C14-C13	-2.43	123.85	127.31
23	A	407	CLA	CBC-CAC-C3C	-2.43	105.74	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	O3D-C3D-C4D	-2.42	104.75	110.35
23	B	607	CLA	C2C-C1C-NC	2.42	112.24	109.97
25	H	101	BCR	C1-C6-C5	-2.42	119.20	122.61
25	C	514	BCR	C11-C10-C9	-2.42	123.86	127.31
23	C	511	CLA	CHA-C1A-NA	-2.42	120.86	126.40
25	d	405	BCR	C29-C30-C25	2.42	114.20	110.48
29	c	516	DGD	C5B-C4B-C3B	-2.42	102.16	114.42
23	a	404	CLA	CMA-C3A-C4A	2.42	118.27	111.77
23	b	607	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	C	519	LMG	O1-C1-C2	-2.41	104.54	108.30
24	a	406	PHO	O1D-CGD-CBD	2.41	128.75	124.74
24	a	406	PHO	C5-C3-C2	2.41	125.99	121.12
23	B	610	CLA	O1D-CGD-CBD	2.41	129.41	124.48
23	c	510	CLA	C16-C15-C13	-2.41	108.14	115.92
23	b	614	CLA	C1D-ND-C4D	-2.41	104.62	106.33
23	C	512	CLA	CMB-C2B-C3B	2.41	129.18	124.68
25	D	405	BCR	C38-C26-C25	-2.41	121.83	124.53
25	D	405	BCR	C2-C1-C6	2.41	114.18	110.48
25	C	515	BCR	C29-C30-C25	2.40	114.18	110.48
27	B	620	LMG	O1-C7-C8	-2.40	105.10	110.90
23	b	617	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
23	C	508	CLA	C7-C6-C5	-2.40	106.84	113.36
23	C	510	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
23	c	505	CLA	CHD-C1D-C2D	2.40	130.51	125.48
24	A	406	PHO	O2D-CGD-CBD	2.40	114.03	111.00
25	A	408	BCR	C38-C26-C27	-2.40	109.01	113.62
23	A	405	CLA	O2A-C1-C2	-2.39	102.34	108.64
23	B	605	CLA	CHD-C4C-NC	2.39	127.97	124.20
29	h	103	DGD	O6E-C5E-C6E	-2.39	100.49	106.44
23	C	502	CLA	O1D-CGD-CBD	2.39	129.37	124.48
23	b	605	CLA	CAC-C3C-C4C	2.38	127.90	124.81
24	d	401	PHO	C6-C7-C8	-2.38	108.22	115.92
34	e	102	HEM	C4B-CHC-C1C	2.38	125.70	122.56
25	c	515	BCR	C29-C30-C25	2.38	114.14	110.48
23	b	614	CLA	C2A-C3A-C4A	2.38	105.71	101.87
23	B	612	CLA	C9-C8-C7	-2.38	102.68	111.29
23	b	611	CLA	C4-C3-C5	2.38	119.27	115.27
25	C	515	BCR	C2-C1-C6	2.38	114.14	110.48
23	B	609	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
23	a	405	CLA	O2D-CGD-CBD	2.37	115.48	111.27
23	c	506	CLA	C2D-C1D-ND	-2.37	108.36	110.10
25	b	619	BCR	C11-C10-C9	-2.37	123.93	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CMB-C2B-C1B	-2.37	124.82	128.46
23	b	609	CLA	C6-C7-C8	-2.37	108.27	115.92
26	d	406	PL9	C7-C3-C2	-2.36	120.19	123.30
29	c	518	DGD	O3G-C1D-C2D	-2.36	104.61	108.30
24	D	401	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
23	C	508	CLA	CHD-C1D-C2D	2.36	130.43	125.48
23	C	502	CLA	CMB-C2B-C3B	2.36	129.09	124.68
29	C	516	DGD	O2D-C2D-C1D	-2.36	104.32	110.05
25	d	405	BCR	C27-C26-C25	2.36	126.15	122.73
23	A	405	CLA	CMD-C2D-C3D	2.36	133.03	127.61
26	D	406	PL9	C35-C34-C36	2.36	119.23	115.27
23	c	509	CLA	C3A-C2A-C1A	2.36	104.87	101.34
23	b	603	CLA	CHC-C1C-NC	2.35	127.78	124.20
25	c	514	BCR	C30-C25-C26	-2.35	119.30	122.61
23	b	606	CLA	OBD-CAD-C3D	2.35	134.17	128.52
28	f	101	SQD	O48-C23-O10	-2.35	117.67	123.59
23	C	507	CLA	C2A-C1A-CHA	2.35	127.96	123.86
27	b	622	LMG	C40-C39-C38	-2.34	102.52	114.42
23	a	405	CLA	CED-O2D-CGD	-2.34	110.64	115.94
26	A	409	PL9	C12-C13-C14	-2.34	122.02	127.66
23	c	506	CLA	CHA-C1A-NA	-2.34	121.03	126.40
25	C	514	BCR	C7-C8-C9	-2.34	122.69	126.23
25	C	515	BCR	C36-C18-C17	-2.34	119.64	122.92
25	h	102	BCR	C7-C8-C9	-2.34	122.69	126.23
23	C	511	CLA	C2A-C1A-CHA	2.34	127.95	123.86
27	b	622	LMG	C8-O7-C10	2.34	123.56	117.79
29	c	516	DGD	C4D-C3D-C2D	-2.34	106.74	110.82
29	c	516	DGD	C8B-C7B-C6B	-2.34	102.55	114.42
25	h	102	BCR	C34-C9-C8	-2.34	114.39	118.08
25	b	618	BCR	C33-C5-C6	-2.34	121.91	124.53
29	c	516	DGD	O6E-C5E-C4E	2.33	113.93	109.69
27	b	622	LMG	O7-C10-O9	-2.33	118.06	123.70
23	b	606	CLA	CHD-C1D-C2D	2.33	130.37	125.48
25	D	405	BCR	C35-C13-C14	-2.33	119.66	122.92
29	c	518	DGD	CDB-CCB-CBB	-2.33	102.60	114.42
23	c	505	CLA	C11-C10-C8	-2.33	108.40	115.92
23	C	501	CLA	O2D-CGD-CBD	2.33	115.40	111.27
29	A	413	DGD	C1E-O6E-C5E	2.33	118.25	113.69
25	c	515	BCR	C8-C9-C10	2.32	122.51	118.94
23	c	509	CLA	C3B-C4B-NB	-2.32	106.21	109.21
31	a	417	BCT	O3-C-O1	-2.32	113.52	119.55
23	c	507	CLA	CMB-C2B-C1B	-2.32	124.89	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	409	LMG	O1-C7-C8	-2.32	105.30	110.90
33	e	101	LHG	C11-C10-C9	-2.32	102.64	114.42
23	C	505	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	b	612	CLA	C1-C2-C3	-2.32	122.03	126.04
23	c	506	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
23	A	404	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
27	C	519	LMG	C9-C8-C7	-2.32	106.30	111.79
28	a	411	SQD	C3-C4-C5	2.32	114.38	110.24
23	B	613	CLA	C2C-C1C-NC	2.32	112.14	109.97
23	b	607	CLA	C2C-C1C-NC	2.32	112.14	109.97
23	B	606	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	b	609	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
28	a	411	SQD	O10-C23-C24	-2.32	114.69	123.73
27	c	519	LMG	O2-C2-C1	-2.32	104.42	110.05
23	d	403	CLA	CMB-C2B-C3B	2.31	129.01	124.68
23	B	610	CLA	CED-O2D-CGD	-2.31	110.71	115.94
23	A	404	CLA	CAA-C2A-C1A	-2.31	104.40	111.97
25	B	618	BCR	C15-C16-C17	-2.31	118.74	123.47
25	H	101	BCR	C34-C9-C10	-2.31	119.69	122.92
23	b	615	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	b	606	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
25	B	619	BCR	C30-C25-C26	-2.31	119.36	122.61
25	c	514	BCR	C33-C5-C6	-2.31	121.94	124.53
23	d	404	CLA	CHD-C1D-C2D	2.31	130.31	125.48
23	b	612	CLA	CHB-C4A-NA	2.30	127.70	124.51
23	c	503	CLA	C3A-C2A-C1A	2.30	104.79	101.34
23	B	612	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	D	406	PL9	C31-C32-C33	-2.30	104.31	111.88
25	c	521	BCR	C29-C30-C25	2.30	114.03	110.48
27	b	622	LMG	C42-C41-C40	-2.30	102.74	114.42
23	B	611	CLA	C1-C2-C3	-2.30	122.06	126.04
23	a	407	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
23	A	405	CLA	C1-O2A-CGA	2.30	122.48	116.44
23	A	405	CLA	O1D-CGD-CBD	2.30	129.19	124.48
29	A	413	DGD	C4E-C3E-C2E	-2.30	106.81	110.82
23	B	603	CLA	C6-C7-C8	-2.30	108.49	115.92
25	T	101	BCR	C38-C26-C27	-2.30	109.20	113.62
23	a	407	CLA	C4-C3-C5	2.30	119.14	115.27
23	D	402	CLA	CHD-C1D-C2D	2.30	130.30	125.48
23	B	610	CLA	CGD-CBD-CAD	-2.29	103.30	110.73
23	b	615	CLA	CAC-C3C-C4C	2.29	127.79	124.81
25	b	619	BCR	C27-C26-C25	2.29	126.06	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	406	PL9	C7-C8-C9	-2.29	122.98	126.79
25	b	619	BCR	C2-C1-C6	2.29	114.01	110.48
28	b	601	SQD	O5-C1-C2	-2.29	105.50	110.35
23	c	506	CLA	C4-C3-C2	-2.29	117.80	123.68
23	A	407	CLA	CHD-C4C-NC	2.29	127.81	124.20
23	A	405	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
23	B	609	CLA	CHA-C4D-ND	2.29	137.28	132.50
25	C	515	BCR	C27-C26-C25	2.29	126.05	122.73
25	B	619	BCR	C11-C10-C9	-2.29	124.05	127.31
24	D	401	PHO	C1-C2-C3	-2.29	122.09	126.04
23	d	404	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
23	d	403	CLA	C5-C3-C2	-2.28	116.50	121.12
23	c	505	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	B	601	CLA	C1-C2-C3	-2.28	122.10	126.04
23	A	404	CLA	O1D-CGD-CBD	2.28	129.15	124.48
27	D	411	LMG	O8-C28-O10	-2.28	117.62	123.30
29	C	517	DGD	O4D-C4D-C5D	-2.28	103.64	109.30
29	H	102	DGD	C4E-C3E-C2E	-2.28	106.85	110.82
23	B	602	CLA	C1-O2A-CGA	2.28	122.42	116.44
28	F	101	SQD	O9-S-O7	-2.28	106.07	113.95
25	C	514	BCR	C15-C16-C17	-2.28	118.81	123.47
27	m	101	LMG	C6-C5-C4	-2.28	107.67	113.00
23	c	506	CLA	O2A-C1-C2	-2.27	102.66	108.64
28	a	412	SQD	C45-O47-C7	2.27	123.38	117.79
23	B	605	CLA	C1-O2A-CGA	-2.27	110.48	116.44
25	A	408	BCR	C8-C7-C6	-2.27	120.82	127.20
23	b	612	CLA	C1D-ND-C4D	2.27	107.95	106.33
23	C	505	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
23	B	607	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
23	C	501	CLA	CAC-C3C-C2C	-2.26	123.66	127.53
25	t	101	BCR	C1-C6-C5	-2.26	119.43	122.61
23	d	402	CLA	CHD-C1D-ND	-2.26	122.38	124.45
23	c	512	CLA	CGD-CBD-CAD	2.26	118.04	110.73
23	A	407	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
23	c	504	CLA	C7-C6-C5	-2.25	107.24	113.36
27	m	101	LMG	O1-C1-C2	-2.25	104.79	108.30
25	y	101	BCR	C23-C22-C21	-2.25	115.48	118.94
23	c	511	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
29	C	518	DGD	C4A-C3A-C2A	-2.25	105.10	113.19
23	a	404	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	b	611	CLA	C1-C2-C3	-2.25	122.15	126.04
27	c	519	LMG	C40-C39-C38	-2.25	103.01	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	519	LMG	O6-C1-O1	-2.25	104.65	109.97
23	B	601	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
23	c	505	CLA	CHD-C4C-NC	2.25	127.74	124.20
23	b	605	CLA	CGD-CBD-CAD	-2.25	103.46	110.73
33	B	622	LHG	C18-C17-C16	-2.25	103.02	114.42
29	C	516	DGD	O3D-C3D-C4D	-2.24	105.16	110.35
33	D	408	LHG	C20-C19-C18	-2.24	103.03	114.42
23	c	504	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
27	m	101	LMG	C1-O6-C5	-2.24	109.28	113.69
23	b	612	CLA	C3C-C4C-NC	-2.24	108.06	110.57
25	B	619	BCR	C33-C5-C6	-2.24	122.01	124.53
23	C	509	CLA	CED-O2D-CGD	2.24	121.00	115.94
23	d	402	CLA	C3A-C2A-C1A	2.24	104.69	101.34
25	h	102	BCR	C30-C25-C26	-2.24	119.46	122.61
23	a	407	CLA	CMD-C2D-C3D	2.24	132.76	127.61
27	c	522	LMG	O2-C2-C1	-2.24	104.61	110.05
23	B	609	CLA	C2C-C1C-NC	2.23	112.06	109.97
23	B	605	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
29	C	517	DGD	O5E-C6E-C5E	-2.23	103.63	111.29
28	b	601	SQD	O47-C7-C8	2.23	116.31	111.50
28	F	101	SQD	C44-O6-C1	2.23	117.54	113.84
23	D	403	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
23	C	509	CLA	C4-C3-C5	2.23	119.03	115.27
26	d	406	PL9	C45-C44-C46	-2.23	111.52	115.27
25	T	101	BCR	C8-C9-C10	2.23	122.36	118.94
25	B	619	BCR	C1-C6-C5	-2.23	119.47	122.61
35	V	201	HEC	CMC-C2C-C1C	-2.23	125.03	128.46
23	c	502	CLA	CMB-C2B-C3B	2.23	128.85	124.68
25	c	514	BCR	C34-C9-C10	-2.23	119.80	122.92
23	B	609	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
27	C	519	LMG	O2-C2-C1	-2.23	104.63	110.05
23	d	404	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	b	605	CLA	OBD-CAD-C3D	2.23	133.88	128.52
23	c	510	CLA	O2D-CGD-CBD	2.23	115.23	111.27
23	b	611	CLA	C11-C12-C13	-2.23	108.72	115.92
23	b	603	CLA	CHD-C1D-C2D	2.22	130.15	125.48
23	C	504	CLA	CMC-C2C-C1C	2.22	128.43	125.04
25	C	514	BCR	C35-C13-C14	-2.22	119.81	122.92
23	C	512	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
23	A	405	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	B	615	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	b	618	BCR	C8-C7-C6	-2.22	120.96	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	411	SQD	C10-C9-C8	-2.22	105.21	113.19
23	B	616	CLA	CHA-C1A-NA	-2.22	121.31	126.40
23	B	615	CLA	C2A-C3A-C4A	2.22	105.45	101.87
25	D	405	BCR	C28-C27-C26	-2.22	110.12	114.08
23	C	511	CLA	CHD-C4C-C3C	2.22	128.10	124.84
23	b	616	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	a	407	CLA	CHC-C1C-NC	2.22	127.56	124.20
23	C	504	CLA	C4A-NA-C1A	2.22	107.70	106.71
26	a	409	PL9	C32-C33-C34	-2.21	122.33	127.66
28	a	411	SQD	O47-C7-O49	-2.21	118.36	123.70
23	b	603	CLA	CHD-C4C-NC	2.21	127.69	124.20
23	b	606	CLA	C16-C15-C13	-2.21	108.78	115.92
29	H	102	DGD	C8B-C7B-C6B	-2.21	103.22	114.42
23	C	510	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	B	605	CLA	C16-C15-C13	-2.21	108.78	115.92
29	c	518	DGD	O6D-C1D-O3G	-2.21	104.75	109.97
23	c	509	CLA	CHD-C4C-NC	2.21	127.68	124.20
27	D	407	LMG	O6-C1-O1	-2.21	104.75	109.97
26	a	409	PL9	C35-C34-C36	2.20	118.98	115.27
23	b	610	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
34	e	102	HEM	C3B-C2B-C1B	2.20	108.12	106.49
25	B	619	BCR	C32-C1-C6	-2.20	106.72	110.30
23	C	513	CLA	CHD-C1D-C2D	2.20	130.10	125.48
23	b	605	CLA	CMB-C2B-C3B	2.20	128.80	124.68
23	c	507	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
33	L	101	LHG	C11-C10-C9	-2.20	103.25	114.42
23	C	513	CLA	O1D-CGD-CBD	2.20	128.99	124.48
23	a	407	CLA	CGD-CBD-CAD	-2.20	103.60	110.73
23	c	505	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
25	c	514	BCR	C35-C13-C14	-2.20	119.84	122.92
23	C	505	CLA	C1-C2-C3	-2.20	122.24	126.04
23	B	611	CLA	C9-C8-C10	-2.20	103.32	111.29
27	b	622	LMG	O6-C5-C6	2.20	111.91	106.44
23	b	612	CLA	C5-C3-C2	2.20	125.57	121.12
25	C	515	BCR	C1-C6-C5	-2.20	119.52	122.61
23	B	612	CLA	C16-C15-C13	-2.19	108.83	115.92
34	E	102	HEM	CHD-C1D-ND	2.19	126.81	124.43
27	B	620	LMG	C9-C8-C7	-2.19	106.60	111.79
27	m	101	LMG	C1-C2-C3	-2.19	105.43	110.00
23	C	504	CLA	CHB-C4A-NA	2.19	127.54	124.51
26	d	406	PL9	C30-C29-C28	-2.19	118.06	123.68
26	A	409	PL9	C41-C39-C38	-2.19	116.68	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	410	LHG	C5-O7-C7	-2.19	112.41	117.79
23	B	613	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
27	A	410	LMG	O7-C10-O9	-2.19	118.42	123.70
23	C	502	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	C	510	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	c	501	CLA	C7-C6-C5	-2.18	107.43	113.36
33	E	101	LHG	C27-C26-C25	-2.18	103.34	114.42
23	b	612	CLA	CHD-C4C-NC	2.18	127.64	124.20
25	c	521	BCR	C31-C1-C6	2.18	113.84	110.30
23	c	508	CLA	CHD-C1D-C2D	2.18	130.06	125.48
27	A	410	LMG	O3-C3-C2	-2.18	105.31	110.35
23	b	612	CLA	C11-C12-C13	-2.18	108.88	115.92
25	b	620	BCR	C37-C22-C21	-2.18	119.87	122.92
28	a	411	SQD	O48-C23-C24	2.18	118.74	111.91
23	c	501	CLA	O1D-CGD-CBD	2.18	128.94	124.48
23	a	404	CLA	CAC-C3C-C4C	2.17	127.63	124.81
23	A	405	CLA	CMD-C2D-C1D	-2.17	120.88	124.71
23	d	402	CLA	C3C-C4C-NC	-2.17	108.13	110.57
23	B	606	CLA	CMD-C2D-C1D	2.17	128.54	124.71
28	b	601	SQD	O47-C45-C46	2.17	116.27	108.40
24	D	401	PHO	OBD-CAD-CBD	-2.17	122.64	125.82
25	C	520	BCR	C27-C26-C25	2.17	125.88	122.73
23	a	404	CLA	CHB-C4A-NA	2.17	127.52	124.51
23	B	602	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	a	409	PL9	C11-C9-C8	-2.17	116.72	121.12
23	a	405	CLA	CHA-C1A-NA	-2.17	121.43	126.40
23	b	603	CLA	CMD-C2D-C1D	2.17	128.53	124.71
26	a	409	PL9	C27-C28-C29	-2.17	122.44	127.66
25	b	618	BCR	C16-C15-C14	-2.17	119.03	123.47
23	C	503	CLA	O1D-CGD-CBD	2.17	128.92	124.48
23	c	502	CLA	O2A-C1-C2	-2.17	102.94	108.64
23	b	609	CLA	C11-C10-C8	-2.17	108.92	115.92
29	h	103	DGD	C1D-C2D-C3D	-2.17	105.49	110.00
25	C	514	BCR	C15-C14-C13	-2.17	124.22	127.31
23	c	513	CLA	C2D-C1D-ND	-2.16	108.51	110.10
29	a	413	DGD	CDB-CCB-CBB	-2.16	103.45	114.42
23	a	407	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	b	614	CLA	C1-O2A-CGA	2.16	122.11	116.44
27	B	620	LMG	C8-O7-C10	2.16	123.10	117.79
29	c	516	DGD	C4E-C3E-C2E	-2.16	107.06	110.82
23	B	604	CLA	OBD-CAD-C3D	2.16	133.71	128.52
29	C	517	DGD	C4E-C3E-C2E	-2.16	107.06	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C2C-C1C-NC	2.15	111.99	109.97
23	B	602	CLA	CHC-C1C-C2C	-2.15	120.76	126.72
23	a	404	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
23	d	402	CLA	CHB-C4A-NA	2.15	127.49	124.51
23	c	504	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
23	B	616	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
33	B	622	LHG	C15-C14-C13	-2.15	103.51	114.42
24	d	401	PHO	C1B-NB-C4B	2.15	111.51	107.09
23	d	402	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
25	D	405	BCR	C7-C8-C9	-2.15	122.99	126.23
29	c	516	DGD	O5E-C6E-C5E	-2.15	103.92	111.29
27	b	622	LMG	O2-C2-C1	-2.15	104.83	110.05
29	A	413	DGD	C2G-O2G-C1B	2.15	123.08	117.79
23	B	603	CLA	C14-C13-C15	-2.15	103.52	111.29
29	c	516	DGD	CBB-CAB-C9B	-2.14	103.54	114.42
25	b	620	BCR	C29-C30-C25	2.14	113.78	110.48
29	c	518	DGD	C3E-C4E-C5E	-2.14	106.42	110.24
23	b	612	CLA	C11-C10-C8	-2.14	109.00	115.92
23	A	407	CLA	CED-O2D-CGD	-2.14	111.09	115.94
25	t	101	BCR	C36-C18-C17	-2.14	119.92	122.92
29	c	518	DGD	CAB-C9B-C8B	-2.14	103.56	114.42
23	b	605	CLA	O1A-CGA-CBA	2.14	132.08	123.73
23	a	407	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
25	B	619	BCR	C15-C16-C17	-2.14	119.10	123.47
29	h	103	DGD	CDB-CCB-CBB	-2.14	103.58	114.42
24	d	401	PHO	CMC-C2C-C3C	2.14	128.97	124.94
23	b	614	CLA	CHA-C1A-NA	-2.13	121.51	126.40
24	A	406	PHO	O2D-CGD-O1D	-2.13	119.67	123.84
26	A	409	PL9	C40-C39-C38	-2.13	118.21	123.68
33	d	407	LHG	C11-C10-C9	-2.13	103.60	114.42
23	h	101	CLA	CMB-C2B-C3B	2.13	128.67	124.68
25	b	620	BCR	C15-C16-C17	-2.13	119.11	123.47
25	B	617	BCR	C24-C23-C22	-2.13	123.02	126.23
23	D	403	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	b	605	CLA	O2A-C1-C2	-2.13	103.04	108.64
29	c	517	DGD	C1D-C2D-C3D	-2.13	105.56	110.00
26	D	406	PL9	C15-C14-C13	-2.13	118.22	123.68
34	e	102	HEM	CAB-C3B-C2B	-2.13	121.60	128.60
27	b	622	LMG	C3-C4-C5	-2.13	106.45	110.24
27	c	522	LMG	C17-C16-C15	-2.13	103.64	114.42
23	D	402	CLA	C16-C15-C13	-2.12	109.06	115.92
23	b	614	CLA	CMB-C2B-C3B	2.12	128.65	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	102	DGD	O5D-C1E-C2E	2.12	111.62	108.30
29	C	518	DGD	O6E-C5E-C4E	2.12	113.55	109.69
23	D	404	CLA	C2C-C1C-NC	2.12	111.96	109.97
23	B	615	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	B	617	BCR	C15-C16-C17	-2.12	119.13	123.47
26	D	406	PL9	C11-C9-C8	-2.12	116.83	121.12
23	c	510	CLA	C5-C3-C2	-2.12	116.83	121.12
23	C	510	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	B	612	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
23	b	616	CLA	C4-C3-C5	2.11	118.83	115.27
23	A	404	CLA	C1-O2A-CGA	-2.11	110.90	116.44
23	c	504	CLA	C3D-C4D-ND	2.11	113.66	110.24
23	a	407	CLA	O2D-CGD-CBD	2.11	115.02	111.27
23	B	610	CLA	CBC-CAC-C3C	-2.11	106.60	112.43
23	B	612	CLA	C7-C6-C5	-2.11	107.62	113.36
25	C	520	BCR	C37-C22-C21	-2.11	119.97	122.92
23	c	513	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
25	t	101	BCR	C2-C1-C6	2.11	113.73	110.48
33	a	410	LHG	C20-C19-C18	-2.11	103.71	114.42
25	t	101	BCR	C35-C13-C14	-2.11	119.97	122.92
23	B	611	CLA	C2D-C1D-ND	-2.11	108.55	110.10
25	B	619	BCR	C2-C1-C6	2.11	113.73	110.48
23	B	605	CLA	CHD-C1D-C2D	2.11	129.90	125.48
35	v	201	HEC	CMB-C2B-C1B	-2.11	125.22	128.46
25	c	515	BCR	C33-C5-C6	-2.11	122.16	124.53
23	D	404	CLA	C3D-C4D-ND	2.11	113.65	110.24
23	D	403	CLA	CAC-C3C-C2C	2.11	131.13	127.53
29	h	103	DGD	CCB-CBB-CAB	-2.11	103.73	114.42
23	b	615	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
23	c	512	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
25	H	101	BCR	C34-C9-C8	-2.10	114.76	118.08
23	C	506	CLA	CHB-C4A-NA	2.10	127.42	124.51
25	a	408	BCR	C29-C30-C25	2.10	113.72	110.48
26	d	406	PL9	C46-C47-C48	-2.10	104.97	111.88
25	y	101	BCR	C33-C5-C6	-2.10	122.17	124.53
23	b	617	CLA	C2A-C3A-C4A	2.10	105.27	101.87
23	c	505	CLA	C1-C2-C3	-2.10	122.41	126.04
23	C	507	CLA	C3A-C2A-C1A	2.10	104.48	101.34
23	B	611	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
25	B	618	BCR	C35-C13-C14	-2.10	119.98	122.92
23	b	615	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
29	h	103	DGD	CBB-CAB-C9B	-2.10	103.77	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
23	C	503	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
25	c	521	BCR	C33-C5-C6	-2.10	122.17	124.53
23	c	502	CLA	C4D-CHA-C1A	2.10	123.80	121.25
23	C	511	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
23	B	611	CLA	C4A-NA-C1A	2.09	107.65	106.71
23	A	404	CLA	C3A-C2A-C1A	2.09	104.47	101.34
23	c	512	CLA	CHA-C1A-NA	-2.09	121.61	126.40
24	d	401	PHO	C1-C2-C3	-2.09	122.42	126.04
23	B	611	CLA	CHD-C4C-NC	2.09	127.50	124.20
27	d	409	LMG	O2-C2-C1	-2.09	104.96	110.05
25	t	101	BCR	C11-C10-C9	-2.09	124.32	127.31
23	b	605	CLA	C2A-C1A-CHA	2.09	127.52	123.86
23	C	501	CLA	CHA-C1A-NA	-2.09	121.61	126.40
23	c	506	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
23	c	506	CLA	CHA-C4D-ND	2.09	136.87	132.50
23	C	513	CLA	CHD-C4C-NC	2.09	127.50	124.20
25	y	101	BCR	C38-C26-C27	-2.09	109.60	113.62
25	d	405	BCR	C8-C7-C6	-2.09	121.34	127.20
23	B	616	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
27	c	522	LMG	C9-C8-C7	-2.09	106.85	111.79
29	a	413	DGD	CFB-CEB-CDB	-2.09	103.84	114.42
23	B	607	CLA	CHB-C4A-NA	2.09	127.40	124.51
23	B	610	CLA	C6-C5-C3	2.09	118.92	113.45
23	b	610	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
33	d	408	LHG	O8-C23-O10	-2.08	118.33	123.59
27	D	411	LMG	C38-C37-C36	-2.08	103.85	114.42
29	c	517	DGD	C3G-C2G-C1G	-2.08	106.86	111.79
23	C	507	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
23	b	612	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
26	d	406	PL9	C45-C44-C43	-2.08	118.34	123.68
23	C	508	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
25	b	618	BCR	C30-C25-C26	-2.08	119.69	122.61
27	m	101	LMG	C19-C18-C17	-2.08	103.88	114.42
23	B	606	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	d	406	PL9	C27-C28-C29	-2.08	122.66	127.66
29	c	517	DGD	O2G-C1B-O1B	-2.08	118.68	123.70
29	a	413	DGD	C5B-C4B-C3B	-2.08	103.88	114.42
23	b	603	CLA	CGD-CBD-CAD	-2.08	104.01	110.73
23	b	611	CLA	CHD-C4C-C3C	2.08	127.89	124.84
23	b	606	CLA	O2A-C1-C2	-2.08	103.18	108.64
25	B	617	BCR	C3-C4-C5	-2.08	110.37	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CHA-C1A-NA	-2.07	121.65	126.40
27	D	407	LMG	C3-C4-C5	-2.07	106.54	110.24
23	b	605	CLA	C7-C6-C5	-2.07	107.73	113.36
25	b	618	BCR	C15-C16-C17	-2.07	119.23	123.47
23	D	404	CLA	CHA-C1A-NA	-2.07	121.66	126.40
33	l	101	LHG	C20-C19-C18	-2.07	103.93	114.42
23	b	605	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
28	b	601	SQD	O10-C23-C24	-2.07	115.67	123.73
25	a	408	BCR	C37-C22-C21	-2.07	120.03	122.92
23	b	612	CLA	C4-C3-C5	-2.07	111.80	115.27
23	d	404	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
28	f	101	SQD	C1-C2-C3	-2.06	105.70	110.00
26	a	409	PL9	C8-C7-C3	2.06	117.81	111.98
23	C	503	CLA	CHB-C4A-NA	2.06	127.36	124.51
25	C	514	BCR	C8-C9-C10	2.06	122.10	118.94
23	B	616	CLA	O2D-CGD-CBD	2.06	114.93	111.27
23	B	608	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
23	B	610	CLA	CHA-C1A-NA	-2.06	121.69	126.40
23	b	604	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	b	610	CLA	C16-C15-C13	-2.06	109.27	115.92
27	d	409	LMG	O2-C2-C3	-2.06	105.59	110.35
23	a	405	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
23	B	614	CLA	C3B-C4B-NB	-2.06	106.55	109.21
25	K	101	BCR	C8-C7-C6	-2.06	121.43	127.20
23	c	506	CLA	C9-C8-C7	2.05	118.73	111.29
28	f	101	SQD	C1-O5-C5	-2.05	109.66	113.69
23	B	608	CLA	C6-C7-C8	-2.05	109.28	115.92
27	B	620	LMG	C37-C36-C35	-2.05	104.00	114.42
29	c	518	DGD	C9B-C8B-C7B	-2.05	104.00	114.42
23	c	509	CLA	O2A-CGA-CBA	2.05	118.35	111.91
23	C	504	CLA	C6-C5-C3	2.05	118.84	113.45
23	c	506	CLA	C2A-C1A-CHA	2.05	127.45	123.86
23	B	611	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
29	c	518	DGD	C1E-O6E-C5E	-2.05	109.66	113.69
29	c	516	DGD	C1D-C2D-C3D	-2.05	105.72	110.00
23	C	502	CLA	O2A-C1-C2	2.05	114.03	108.64
23	C	512	CLA	CHA-C4D-ND	2.05	136.79	132.50
23	B	602	CLA	CHD-C4C-NC	2.05	127.43	124.20
25	D	405	BCR	C16-C15-C14	-2.05	119.28	123.47
23	b	616	CLA	C3A-C2A-C1A	2.05	104.41	101.34
23	d	403	CLA	C11-C12-C13	-2.05	109.31	115.92
24	a	406	PHO	O2A-CGA-O1A	-2.04	118.43	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	518	DGD	O5D-C6D-C5D	-2.04	105.27	109.05
23	B	609	CLA	C2A-C1A-CHA	2.04	127.42	123.86
23	c	503	CLA	CHD-C1D-C2D	2.04	129.76	125.48
23	C	507	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
23	B	609	CLA	CHB-C4A-NA	2.04	127.33	124.51
27	a	414	LMG	O2-C2-C3	-2.04	105.64	110.35
29	h	103	DGD	O5E-C6E-C5E	-2.04	104.30	111.29
29	C	516	DGD	C8B-C7B-C6B	-2.04	104.09	114.42
26	d	406	PL9	C11-C12-C13	-2.04	105.19	111.88
27	D	410	LMG	O7-C10-O9	-2.03	118.78	123.70
29	H	102	DGD	C7B-C6B-C5B	-2.03	104.10	114.42
23	D	402	CLA	C7-C6-C5	-2.03	107.83	113.36
23	C	505	CLA	C6-C7-C8	-2.03	109.35	115.92
27	b	622	LMG	C1-C2-C3	-2.03	105.76	110.00
23	A	404	CLA	CHD-C4C-NC	2.03	127.41	124.20
23	D	404	CLA	C1-C2-C3	-2.03	122.53	126.04
27	B	620	LMG	O8-C28-O10	-2.03	118.47	123.59
28	b	601	SQD	O49-C7-C8	-2.03	115.82	123.73
23	c	508	CLA	O2D-CGD-CBD	2.03	114.87	111.27
23	B	612	CLA	CHC-C1C-NC	2.03	127.28	124.20
23	B	613	CLA	C2A-C3A-C4A	2.03	105.14	101.87
23	b	615	CLA	CHA-C4D-ND	2.02	136.73	132.50
25	h	102	BCR	C39-C30-C25	-2.02	107.02	110.30
25	d	405	BCR	C35-C13-C14	-2.02	120.09	122.92
23	b	606	CLA	CAD-C3D-C2D	2.02	150.56	140.80
23	A	405	CLA	O1A-CGA-CBA	2.02	131.62	123.73
23	b	604	CLA	C5-C3-C2	-2.02	117.03	121.12
23	D	402	CLA	CAC-C3C-C4C	2.02	127.43	124.81
33	l	101	LHG	C27-C26-C25	-2.02	104.17	114.42
33	d	408	LHG	O8-C6-C5	-2.02	102.55	108.43
26	D	406	PL9	C27-C28-C29	-2.02	122.80	127.66
26	a	409	PL9	C30-C29-C28	-2.02	118.50	123.68
23	b	607	CLA	O2D-CGD-CBD	2.02	114.85	111.27
23	b	614	CLA	CAA-C2A-C1A	2.02	118.59	111.97
28	a	411	SQD	O8-S-O9	-2.02	106.35	111.27
23	C	511	CLA	CMC-C2C-C1C	-2.02	121.97	125.04
23	b	607	CLA	C3C-C4C-NC	-2.01	108.31	110.57
23	b	613	CLA	C1-C2-C3	-2.01	122.56	126.04
25	B	618	BCR	C15-C14-C13	-2.01	124.44	127.31
23	a	405	CLA	CMD-C2D-C3D	2.01	132.24	127.61
25	y	101	BCR	C2-C1-C6	2.01	113.58	110.48
23	A	407	CLA	OBD-CAD-C3D	2.01	133.36	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	103	DGD	O2D-C2D-C1D	-2.01	105.16	110.05
25	T	101	BCR	C1-C6-C5	-2.01	119.78	122.61
23	C	511	CLA	CMC-C2C-C3C	2.01	131.58	126.12
23	c	502	CLA	CHD-C4C-NC	2.01	127.37	124.20
33	D	409	LHG	C11-C10-C9	-2.01	104.22	114.42
29	H	102	DGD	CAB-C9B-C8B	-2.01	104.23	114.42
23	B	607	CLA	CHA-C1A-NA	-2.01	121.80	126.40
27	A	410	LMG	C36-C35-C34	-2.01	104.23	114.42
23	B	603	CLA	C2A-C1A-CHA	2.01	127.37	123.86
23	a	407	CLA	C2A-C1A-CHA	2.00	127.36	123.86
29	H	102	DGD	O3D-C3D-C4D	-2.00	105.72	110.35
23	B	605	CLA	CMC-C2C-C1C	2.00	128.09	125.04
23	c	510	CLA	O1D-CGD-CBD	2.00	128.58	124.48
23	C	507	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	D	404	CLA	C6-C7-C8	-2.00	109.45	115.92
25	K	101	BCR	C30-C25-C26	-2.00	119.80	122.61
29	c	518	DGD	O1G-C1A-C2A	-2.00	105.63	111.91

All (55) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	602	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	509	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	510	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	402	CLA	ND
23	D	403	CLA	ND
23	a	404	CLA	ND
23	a	405	CLA	ND
23	a	407	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	611	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	c	501	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND
23	d	404	CLA	ND
23	h	101	CLA	ND

All (1775) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	407	CLA	C2-C3-C5-C6
23	A	407	CLA	C4-C3-C5-C6
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	B	616	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	C2-C3-C5-C6
23	C	504	CLA	C4-C3-C5-C6
23	C	506	CLA	C1A-C2A-CAA-CBA
23	C	506	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C14-C13-C15-C16
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	C11-C10-C8-C9
23	C	512	CLA	O2A-C1-C2-C3
23	a	405	CLA	CHA-CBD-CGD-O1D
23	a	405	CLA	CHA-CBD-CGD-O2D
23	a	407	CLA	C1A-C2A-CAA-CBA
23	b	603	CLA	CHA-CBD-CGD-O1D
23	b	603	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	C2-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	b	615	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	C11-C10-C8-C9
23	c	507	CLA	C2-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C10-C8-C9
23	c	511	CLA	C14-C13-C15-C16
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	CBD-CGD-O2D-CED
23	h	101	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	C3A-C2A-CAA-CBA
23	h	101	CLA	C2A-CAA-CBA-CGA
23	h	101	CLA	CBD-CGD-O2D-CED
23	h	101	CLA	C11-C10-C8-C9
25	B	617	BCR	C11-C12-C13-C35
25	B	617	BCR	C12-C13-C14-C15
25	B	617	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	B	618	BCR	C7-C8-C9-C34
25	B	618	BCR	C17-C18-C19-C20
25	B	618	BCR	C18-C19-C20-C21
25	B	618	BCR	C20-C21-C22-C37
25	B	618	BCR	C22-C23-C24-C25
25	B	619	BCR	C11-C10-C9-C8
25	C	514	BCR	C11-C10-C9-C8
25	C	514	BCR	C11-C12-C13-C14
25	C	514	BCR	C16-C17-C18-C36
25	C	514	BCR	C20-C21-C22-C37
25	C	515	BCR	C23-C24-C25-C30
25	C	520	BCR	C7-C8-C9-C34
25	C	520	BCR	C11-C10-C9-C8
25	C	520	BCR	C11-C10-C9-C34
25	C	520	BCR	C10-C11-C12-C13
25	C	520	BCR	C37-C22-C23-C24
25	D	405	BCR	C35-C13-C14-C15
25	D	405	BCR	C14-C15-C16-C17
25	D	405	BCR	C16-C17-C18-C19
25	D	405	BCR	C16-C17-C18-C36
25	H	101	BCR	C11-C12-C13-C35
25	H	101	BCR	C37-C22-C23-C24
25	H	101	BCR	C23-C24-C25-C26
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C21-C22-C23-C24
25	T	101	BCR	C1-C6-C7-C8
25	T	101	BCR	C5-C6-C7-C8
25	T	101	BCR	C7-C8-C9-C10
25	T	101	BCR	C7-C8-C9-C34
25	T	101	BCR	C11-C12-C13-C35
25	T	101	BCR	C16-C17-C18-C36
25	T	101	BCR	C20-C21-C22-C23
25	T	101	BCR	C37-C22-C23-C24
25	b	620	BCR	C37-C22-C23-C24
25	c	514	BCR	C11-C10-C9-C34
25	c	514	BCR	C11-C12-C13-C35
25	c	514	BCR	C35-C13-C14-C15
25	c	514	BCR	C18-C19-C20-C21
25	c	514	BCR	C37-C22-C23-C24
25	c	515	BCR	C11-C12-C13-C35
25	c	515	BCR	C35-C13-C14-C15
25	c	515	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
25	c	515	BCR	C17-C18-C19-C20
25	d	405	BCR	C7-C8-C9-C34
25	d	405	BCR	C11-C12-C13-C35
25	d	405	BCR	C16-C17-C18-C19
25	d	405	BCR	C16-C17-C18-C36
25	d	405	BCR	C37-C22-C23-C24
25	h	102	BCR	C18-C19-C20-C21
25	h	102	BCR	C23-C24-C25-C30
25	t	101	BCR	C11-C10-C9-C34
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C7-C8-C9-C34
25	y	101	BCR	C11-C10-C9-C34
25	y	101	BCR	C20-C21-C22-C37
26	A	409	PL9	C9-C11-C12-C13
26	A	409	PL9	C12-C13-C14-C15
26	A	409	PL9	C12-C13-C14-C16
26	A	409	PL9	C18-C19-C21-C22
26	A	409	PL9	C22-C23-C24-C25
26	A	409	PL9	C22-C23-C24-C26
26	A	409	PL9	C32-C33-C34-C36
26	A	409	PL9	C37-C38-C39-C40
26	A	409	PL9	C37-C38-C39-C41
26	D	406	PL9	C12-C13-C14-C16
26	D	406	PL9	C32-C33-C34-C35
26	D	406	PL9	C32-C33-C34-C36
26	a	409	PL9	C7-C8-C9-C10
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C28-C29-C31-C32
26	a	409	PL9	C30-C29-C31-C32
26	a	409	PL9	C32-C33-C34-C35
26	a	409	PL9	C33-C34-C36-C37
26	a	409	PL9	C37-C38-C39-C41
26	d	406	PL9	C27-C28-C29-C31
26	d	406	PL9	C32-C33-C34-C35
26	d	406	PL9	C38-C39-C41-C42
26	d	406	PL9	C42-C43-C44-C46
26	d	406	PL9	C47-C48-C49-C50
27	A	410	LMG	O9-C10-O7-C8
27	C	519	LMG	C11-C10-O7-C8
27	D	410	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	D	410	LMG	O1-C7-C8-O7
27	a	414	LMG	O6-C1-O1-C7
27	b	622	LMG	C2-C1-O1-C7
27	b	622	LMG	O6-C1-O1-C7
27	b	622	LMG	O9-C10-O7-C8
27	b	622	LMG	C11-C10-O7-C8
28	B	623	SQD	C2-C1-O6-C44
28	B	623	SQD	O5-C1-O6-C44
28	B	623	SQD	O6-C44-C45-O47
28	B	623	SQD	O49-C7-O47-C45
28	B	623	SQD	C8-C7-O47-C45
28	F	101	SQD	O10-C23-O48-C46
28	a	411	SQD	O47-C45-C46-O48
28	a	412	SQD	O6-C44-C45-C46
28	a	412	SQD	O6-C44-C45-O47
28	a	412	SQD	C8-C7-O47-C45
28	b	601	SQD	O10-C23-O48-C46
28	b	601	SQD	C5-C6-S-O7
28	b	601	SQD	C5-C6-S-O8
28	b	601	SQD	C5-C6-S-O9
28	f	101	SQD	C2-C1-O6-C44
28	f	101	SQD	O5-C1-O6-C44
29	A	413	DGD	O1B-C1B-O2G-C2G
33	D	408	LHG	O1-C1-C2-C3
33	D	408	LHG	C3-O3-P-O4
33	D	408	LHG	C3-O3-P-O6
33	D	408	LHG	C4-O6-P-O4
33	D	409	LHG	O2-C2-C3-O3
33	D	409	LHG	C3-O3-P-O5
33	D	409	LHG	C3-O3-P-O6
33	D	409	LHG	C4-O6-P-O4
33	E	101	LHG	C4-O6-P-O3
33	E	101	LHG	O10-C23-O8-C6
33	E	101	LHG	C24-C23-O8-C6
33	L	101	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O5
33	a	410	LHG	O1-C1-C2-C3
33	a	410	LHG	C1-C2-C3-O3
33	d	407	LHG	O1-C1-C2-C3
33	d	407	LHG	C3-O3-P-O4
33	d	407	LHG	C4-O6-P-O4
33	e	101	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
33	e	101	LHG	C4-O6-P-O4
33	e	101	LHG	O10-C23-O8-C6
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O5
23	b	617	CLA	O1D-CGD-O2D-CED
23	h	101	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	O1D-CGD-O2D-CED
23	B	614	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
24	a	406	PHO	CBD-CGD-O2D-CED
27	a	414	LMG	O10-C28-O8-C9
23	B	601	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
27	a	414	LMG	C29-C28-O8-C9
28	b	601	SQD	C24-C23-O48-C46
33	e	101	LHG	C24-C23-O8-C6
26	d	406	PL9	C47-C48-C49-C51
23	B	610	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	CBD-CGD-O2D-CED
27	c	522	LMG	O10-C28-O8-C9
28	a	412	SQD	O10-C23-O48-C46
29	a	413	DGD	O1A-C1A-O1G-C1G
23	B	606	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
27	C	519	LMG	O9-C10-O7-C8
27	D	410	LMG	O9-C10-O7-C8
27	c	522	LMG	O9-C10-O7-C8
28	a	412	SQD	O49-C7-O47-C45
29	a	413	DGD	O1B-C1B-O2G-C2G
33	e	101	LHG	O9-C7-O7-C5
23	B	616	CLA	C3-C5-C6-C7
23	b	605	CLA	C3-C5-C6-C7
28	a	412	SQD	C24-C23-O48-C46
29	a	413	DGD	C2A-C1A-O1G-C1G
23	B	604	CLA	C13-C15-C16-C17
27	A	410	LMG	C11-C10-O7-C8
29	A	413	DGD	C2B-C1B-O2G-C2G
24	a	406	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	607	CLA	CBD-CGD-O2D-CED
23	b	615	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
23	c	512	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA
23	b	611	CLA	C2A-CAA-CBA-CGA
27	c	522	LMG	C29-C28-O8-C9
28	F	101	SQD	C24-C23-O48-C46
23	C	505	CLA	C2C-C3C-CAC-CBC
26	A	409	PL9	C42-C43-C44-C45
26	a	409	PL9	C42-C43-C44-C45
26	d	406	PL9	C42-C43-C44-C45
23	c	511	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	O1D-CGD-O2D-CED
26	a	409	PL9	C32-C33-C34-C36
26	d	406	PL9	C32-C33-C34-C36
29	A	413	DGD	O6E-C5E-C6E-O5E
29	C	516	DGD	O6E-C5E-C6E-O5E
28	F	101	SQD	C44-C45-C46-O48
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	614	CLA	CBD-CGD-O2D-CED
33	a	410	LHG	O2-C2-C3-O3
23	C	512	CLA	C3-C5-C6-C7
23	b	603	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
23	B	601	CLA	CBA-CGA-O2A-C1
27	D	410	LMG	C11-C10-O7-C8
33	e	101	LHG	C8-C7-O7-C5
23	C	502	CLA	CBD-CGD-O2D-CED
27	c	522	LMG	O6-C5-C6-O5
23	c	503	CLA	CBD-CGD-O2D-CED
27	c	519	LMG	O6-C5-C6-O5
27	B	620	LMG	O10-C28-O8-C9
27	a	414	LMG	O6-C5-C6-O5
29	C	516	DGD	C4E-C5E-C6E-O5E
29	A	413	DGD	C4E-C5E-C6E-O5E
27	A	410	LMG	O6-C1-O1-C7
26	A	409	PL9	C34-C36-C37-C38
26	A	409	PL9	C44-C46-C47-C48
26	a	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	a	409	PL9	C34-C36-C37-C38
26	d	406	PL9	C44-C46-C47-C48
28	a	411	SQD	C12-C13-C14-C15
23	B	601	CLA	C3-C5-C6-C7
23	D	403	CLA	C3-C5-C6-C7
28	f	101	SQD	C24-C23-O48-C46
23	C	508	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	O1A-CGA-O2A-C1
27	c	522	LMG	C11-C10-O7-C8
29	h	103	DGD	C4E-C5E-C6E-O5E
23	b	604	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	C15-C16-C17-C18
27	a	414	LMG	C4-C5-C6-O5
23	C	505	CLA	C5-C6-C7-C8
23	C	510	CLA	C15-C16-C17-C18
33	D	408	LHG	O2-C2-C3-O3
28	A	411	SQD	C23-C24-C25-C26
33	E	101	LHG	C23-C24-C25-C26
27	a	414	LMG	C2-C1-O1-C7
29	c	517	DGD	C2E-C1E-O5D-C6D
23	b	615	CLA	C2-C3-C5-C6
23	B	603	CLA	C11-C10-C8-C9
23	B	605	CLA	C11-C10-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	C	503	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	C	512	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	607	CLA	C14-C13-C15-C16
23	b	611	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C12-C13-C14
23	c	510	CLA	C11-C12-C13-C14
23	c	512	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C12-C13-C14
23	D	403	CLA	CBD-CGD-O2D-CED
25	B	618	BCR	C37-C22-C23-C24
25	B	619	BCR	C7-C8-C9-C34
25	C	514	BCR	C7-C8-C9-C34
25	C	514	BCR	C11-C12-C13-C35
25	C	514	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	K	101	BCR	C37-C22-C23-C24
25	b	618	BCR	C11-C12-C13-C35
25	y	101	BCR	C7-C8-C9-C10
29	C	518	DGD	C4E-C5E-C6E-O5E
29	c	516	DGD	C1B-C2B-C3B-C4B
33	E	101	LHG	C7-C8-C9-C10
26	a	409	PL9	C47-C48-C49-C50
23	B	601	CLA	C10-C11-C12-C13
23	b	610	CLA	C15-C16-C17-C18
23	b	604	CLA	C8-C10-C11-C12
23	b	612	CLA	C15-C16-C17-C18
23	b	617	CLA	C10-C11-C12-C13
27	D	410	LMG	C10-C11-C12-C13
27	c	522	LMG	C10-C11-C12-C13
29	a	413	DGD	C1A-C2A-C3A-C4A
25	c	515	BCR	C14-C15-C16-C17
29	C	517	DGD	O6E-C5E-C6E-O5E
23	B	602	CLA	C8-C10-C11-C12
23	B	606	CLA	C15-C16-C17-C18
23	B	611	CLA	C13-C15-C16-C17
23	C	503	CLA	C5-C6-C7-C8
23	C	512	CLA	C8-C10-C11-C12
23	C	512	CLA	C15-C16-C17-C18
23	a	407	CLA	C10-C11-C12-C13
23	b	605	CLA	C10-C11-C12-C13
23	c	506	CLA	C5-C6-C7-C8
23	c	507	CLA	C8-C10-C11-C12
33	D	408	LHG	O1-C1-C2-O2
27	D	411	LMG	C28-C29-C30-C31
27	d	409	LMG	C28-C29-C30-C31
27	m	101	LMG	C10-C11-C12-C13
28	A	411	SQD	C7-C8-C9-C10
28	A	412	SQD	C7-C8-C9-C10
29	c	516	DGD	C1A-C2A-C3A-C4A
29	c	518	DGD	C1A-C2A-C3A-C4A
33	a	410	LHG	C7-C8-C9-C10
33	a	410	LHG	C23-C24-C25-C26
33	e	101	LHG	C7-C8-C9-C10
33	l	101	LHG	C23-C24-C25-C26
29	h	103	DGD	O6E-C5E-C6E-O5E
24	d	401	PHO	CBD-CGD-O2D-CED
23	B	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	b	608	CLA	C10-C11-C12-C13
23	b	612	CLA	C13-C15-C16-C17
23	B	607	CLA	C5-C6-C7-C8
23	c	505	CLA	C15-C16-C17-C18
28	B	623	SQD	C23-C24-C25-C26
24	D	401	PHO	CBD-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
29	H	102	DGD	C4E-C5E-C6E-O5E
23	B	606	CLA	C6-C7-C8-C10
23	B	606	CLA	C12-C13-C15-C16
23	a	404	CLA	C11-C10-C8-C7
23	b	605	CLA	C11-C10-C8-C7
23	b	607	CLA	C12-C13-C15-C16
23	b	613	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C7
28	a	411	SQD	O10-C23-O48-C46
33	D	409	LHG	C7-C8-C9-C10
23	B	601	CLA	C5-C6-C7-C8
23	D	404	CLA	C5-C6-C7-C8
23	a	407	CLA	C13-C15-C16-C17
23	c	513	CLA	C8-C10-C11-C12
23	h	101	CLA	C13-C15-C16-C17
23	C	505	CLA	C4C-C3C-CAC-CBC
29	c	518	DGD	O1A-C1A-O1G-C1G
29	c	517	DGD	O6E-C1E-O5D-C6D
23	B	603	CLA	C10-C11-C12-C13
23	B	616	CLA	C5-C6-C7-C8
23	b	609	CLA	C13-C15-C16-C17
26	A	409	PL9	C29-C31-C32-C33
26	a	409	PL9	C44-C46-C47-C48
26	d	406	PL9	C29-C31-C32-C33
25	B	618	BCR	C10-C11-C12-C13
25	D	405	BCR	C10-C11-C12-C13
25	D	405	BCR	C18-C19-C20-C21
25	d	405	BCR	C10-C11-C12-C13
29	H	102	DGD	O6E-C5E-C6E-O5E
29	c	517	DGD	O6E-C5E-C6E-O5E
23	B	602	CLA	C13-C15-C16-C17
23	C	512	CLA	C10-C11-C12-C13
23	b	603	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
23	b	615	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C13-C15-C16-C17
33	d	408	LHG	C24-C25-C26-C27
29	c	517	DGD	C4E-C5E-C6E-O5E
23	B	607	CLA	C13-C15-C16-C17
23	B	611	CLA	C15-C16-C17-C18
23	B	614	CLA	C13-C15-C16-C17
23	a	407	CLA	C5-C6-C7-C8
23	b	606	CLA	C15-C16-C17-C18
23	b	612	CLA	C8-C10-C11-C12
23	c	509	CLA	C10-C11-C12-C13
23	C	511	CLA	CBD-CGD-O2D-CED
29	a	413	DGD	C2B-C1B-O2G-C2G
23	A	404	CLA	C15-C16-C17-C18
23	C	509	CLA	C13-C15-C16-C17
23	c	506	CLA	C13-C15-C16-C17
23	c	509	CLA	C15-C16-C17-C18
23	c	512	CLA	C13-C15-C16-C17
23	h	101	CLA	C15-C16-C17-C18
33	L	101	LHG	C4-O6-P-O3
33	d	407	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O3
29	A	413	DGD	C1A-C2A-C3A-C4A
23	B	609	CLA	C3-C5-C6-C7
27	C	519	LMG	C4-C5-C6-O5
23	b	608	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
26	d	406	PL9	C22-C23-C24-C25
23	b	607	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
23	c	510	CLA	C8-C10-C11-C12
23	c	510	CLA	C15-C16-C17-C18
23	B	609	CLA	C13-C15-C16-C17
23	b	614	CLA	C10-C11-C12-C13
27	A	410	LMG	C29-C28-O8-C9
27	B	620	LMG	C29-C28-O8-C9
23	b	605	CLA	C8-C10-C11-C12
23	B	607	CLA	O1D-CGD-O2D-CED
27	D	407	LMG	C19-C20-C21-C22
28	A	411	SQD	C30-C31-C32-C33
28	a	412	SQD	C12-C13-C14-C15
28	a	412	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	b	601	SQD	C16-C17-C18-C19
23	b	616	CLA	C5-C6-C7-C8
25	B	618	BCR	C16-C17-C18-C36
25	C	514	BCR	C35-C13-C14-C15
25	C	520	BCR	C20-C21-C22-C37
25	D	405	BCR	C20-C21-C22-C37
25	H	101	BCR	C16-C17-C18-C36
25	K	101	BCR	C11-C10-C9-C34
25	a	408	BCR	C16-C17-C18-C36
25	d	405	BCR	C35-C13-C14-C15
25	h	102	BCR	C11-C10-C9-C34
25	t	101	BCR	C16-C17-C18-C36
27	A	410	LMG	C16-C17-C18-C19
27	D	411	LMG	C32-C33-C34-C35
27	a	414	LMG	C29-C30-C31-C32
27	c	519	LMG	C11-C10-O7-C8
28	A	411	SQD	C28-C29-C30-C31
29	H	102	DGD	C3B-C4B-C5B-C6B
29	h	103	DGD	C5B-C6B-C7B-C8B
33	L	101	LHG	C14-C15-C16-C17
33	d	407	LHG	C29-C30-C31-C32
33	e	101	LHG	C17-C18-C19-C20
23	b	608	CLA	O1A-CGA-O2A-C1
23	B	615	CLA	C16-C17-C18-C20
23	b	608	CLA	C16-C17-C18-C20
23	c	502	CLA	C16-C17-C18-C19
27	B	620	LMG	C12-C13-C14-C15
27	a	414	LMG	C12-C13-C14-C15
28	A	411	SQD	C11-C12-C13-C14
27	D	411	LMG	C33-C34-C35-C36
27	b	622	LMG	C19-C20-C21-C22
27	c	519	LMG	C36-C37-C38-C39
28	a	412	SQD	C11-C12-C13-C14
29	H	102	DGD	C4B-C5B-C6B-C7B
33	D	409	LHG	C27-C28-C29-C30
33	a	410	LHG	C25-C26-C27-C28
23	b	614	CLA	O1D-CGD-O2D-CED
29	A	413	DGD	C5B-C6B-C7B-C8B
29	c	518	DGD	CCA-CDA-CEA-CFA
33	E	101	LHG	C28-C29-C30-C31
27	D	407	LMG	C14-C15-C16-C17
27	b	622	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	C9A-CAA-CBA-CCA
29	C	517	DGD	C5B-C6B-C7B-C8B
29	a	413	DGD	C2A-C3A-C4A-C5A
29	c	516	DGD	C4A-C5A-C6A-C7A
33	D	409	LHG	C32-C33-C34-C35
33	L	101	LHG	C18-C19-C20-C21
33	d	407	LHG	C32-C33-C34-C35
33	d	408	LHG	C26-C27-C28-C29
25	B	618	BCR	C11-C10-C9-C8
25	C	514	BCR	C16-C17-C18-C19
25	H	101	BCR	C11-C10-C9-C8
25	H	101	BCR	C16-C17-C18-C19
25	K	101	BCR	C11-C10-C9-C8
25	K	101	BCR	C20-C21-C22-C23
25	T	101	BCR	C16-C17-C18-C19
25	b	620	BCR	C11-C10-C9-C8
25	c	514	BCR	C16-C17-C18-C19
25	c	514	BCR	C20-C21-C22-C23
25	c	515	BCR	C12-C13-C14-C15
25	d	405	BCR	C11-C10-C9-C8
25	h	102	BCR	C11-C10-C9-C8
25	t	101	BCR	C16-C17-C18-C19
29	C	517	DGD	C2E-C1E-O5D-C6D
29	c	517	DGD	C2D-C1D-O3G-C3G
27	C	519	LMG	C30-C31-C32-C33
27	D	407	LMG	C11-C12-C13-C14
28	A	412	SQD	C32-C33-C34-C35
28	a	412	SQD	C10-C11-C12-C13
29	c	516	DGD	C8B-C9B-CAB-CBB
29	c	518	DGD	C5B-C6B-C7B-C8B
33	D	408	LHG	C15-C16-C17-C18
33	e	101	LHG	C14-C15-C16-C17
23	B	601	CLA	C16-C17-C18-C20
23	B	613	CLA	C16-C17-C18-C20
23	c	507	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
23	c	511	CLA	O1D-CGD-O2D-CED
23	C	505	CLA	C4-C3-C5-C6
23	C	510	CLA	C4-C3-C5-C6
29	C	517	DGD	CAB-CBB-CCB-CDB
29	H	102	DGD	C7B-C8B-C9B-CAB
29	a	413	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
29	a	413	DGD	C7B-C8B-C9B-CAB
33	E	101	LHG	C11-C10-C9-C8
33	E	101	LHG	C33-C34-C35-C36
33	L	101	LHG	C32-C33-C34-C35
33	a	410	LHG	C16-C17-C18-C19
33	d	407	LHG	C11-C12-C13-C14
23	B	606	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C14
23	a	404	CLA	C14-C13-C15-C16
23	a	405	CLA	C6-C7-C8-C9
23	b	607	CLA	C6-C7-C8-C9
23	d	402	CLA	C14-C13-C15-C16
27	D	410	LMG	C33-C34-C35-C36
27	D	411	LMG	C16-C17-C18-C19
27	b	622	LMG	C15-C16-C17-C18
27	b	623	LMG	C11-C12-C13-C14
28	B	623	SQD	C28-C29-C30-C31
28	B	623	SQD	C34-C35-C36-C37
29	A	413	DGD	C2A-C3A-C4A-C5A
29	c	516	DGD	C4B-C5B-C6B-C7B
33	D	409	LHG	C9-C10-C11-C12
27	m	101	LMG	C29-C30-C31-C32
28	A	411	SQD	C11-C10-C9-C8
29	A	413	DGD	CAA-CBA-CCA-CDA
29	C	518	DGD	C3A-C4A-C5A-C6A
33	B	622	LHG	C25-C26-C27-C28
33	E	101	LHG	O1-C1-C2-C3
33	d	408	LHG	O1-C1-C2-C3
25	A	408	BCR	C17-C18-C19-C20
27	D	407	LMG	O6-C5-C6-O5
27	A	410	LMG	C14-C15-C16-C17
27	D	407	LMG	C30-C31-C32-C33
27	c	522	LMG	C38-C39-C40-C41
33	B	622	LHG	C9-C10-C11-C12
33	B	622	LHG	C31-C32-C33-C34
33	D	408	LHG	C11-C10-C9-C8
33	L	101	LHG	C30-C31-C32-C33
33	e	101	LHG	C23-C24-C25-C26
27	B	620	LMG	C14-C15-C16-C17
27	B	620	LMG	C36-C37-C38-C39
27	D	411	LMG	C14-C15-C16-C17
27	D	411	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	a	414	LMG	C32-C33-C34-C35
27	b	622	LMG	C18-C19-C20-C21
27	b	623	LMG	C32-C33-C34-C35
28	A	411	SQD	C14-C15-C16-C17
28	b	601	SQD	C26-C27-C28-C29
29	c	518	DGD	C4B-C5B-C6B-C7B
33	D	409	LHG	C30-C31-C32-C33
33	e	101	LHG	C26-C27-C28-C29
29	C	517	DGD	O6E-C1E-O5D-C6D
29	c	517	DGD	O6D-C1D-O3G-C3G
23	B	605	CLA	C15-C16-C17-C18
23	B	612	CLA	C10-C11-C12-C13
23	C	507	CLA	C10-C11-C12-C13
27	D	407	LMG	C38-C39-C40-C41
27	b	623	LMG	C37-C38-C39-C40
28	A	412	SQD	C12-C13-C14-C15
29	C	518	DGD	C5A-C6A-C7A-C8A
33	D	408	LHG	C30-C31-C32-C33
29	c	516	DGD	C4D-C5D-C6D-O5D
28	a	412	SQD	C15-C16-C17-C18
28	f	101	SQD	C31-C32-C33-C34
33	L	101	LHG	C27-C28-C29-C30
33	a	410	LHG	C30-C31-C32-C33
23	c	505	CLA	C5-C6-C7-C8
27	A	410	LMG	O10-C28-O8-C9
28	f	101	SQD	O10-C23-O48-C46
27	B	620	LMG	C19-C20-C21-C22
27	b	622	LMG	C23-C24-C25-C26
33	D	408	LHG	C32-C33-C34-C35
29	c	516	DGD	O6D-C5D-C6D-O5D
27	D	407	LMG	C20-C21-C22-C23
27	m	101	LMG	C31-C32-C33-C34
28	A	412	SQD	C14-C15-C16-C17
33	E	101	LHG	C15-C16-C17-C18
23	a	407	CLA	C3A-C2A-CAA-CBA
23	c	512	CLA	C3A-C2A-CAA-CBA
27	a	414	LMG	C16-C17-C18-C19
27	c	519	LMG	C31-C32-C33-C34
28	F	101	SQD	C25-C26-C27-C28
29	A	413	DGD	CDB-CEB-CFB-CGB
23	D	403	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	b	608	CLA	C16-C17-C18-C19
23	c	502	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
33	l	101	LHG	C27-C28-C29-C30
27	D	407	LMG	C35-C36-C37-C38
29	A	413	DGD	C2B-C3B-C4B-C5B
23	B	604	CLA	O2A-C1-C2-C3
25	d	405	BCR	C14-C15-C16-C17
29	C	516	DGD	C1B-C2B-C3B-C4B
33	d	408	LHG	C23-C24-C25-C26
23	b	612	CLA	C4-C3-C5-C6
26	d	406	PL9	C30-C29-C31-C32
23	C	510	CLA	C2-C3-C5-C6
23	b	612	CLA	C2-C3-C5-C6
26	A	409	PL9	C28-C29-C31-C32
26	D	406	PL9	C13-C14-C16-C17
26	d	406	PL9	C13-C14-C16-C17
33	E	101	LHG	C8-C7-O7-C5
28	A	411	SQD	C12-C13-C14-C15
28	a	411	SQD	C10-C11-C12-C13
28	f	101	SQD	C25-C26-C27-C28
27	c	519	LMG	C4-C5-C6-O5
33	d	407	LHG	O1-C1-C2-O2
27	C	519	LMG	C11-C12-C13-C14
27	d	409	LMG	C14-C15-C16-C17
28	A	412	SQD	C30-C31-C32-C33
28	F	101	SQD	C27-C28-C29-C30
29	c	517	DGD	C7B-C8B-C9B-CAB
33	D	408	LHG	C12-C13-C14-C15
23	c	513	CLA	C16-C17-C18-C20
23	b	611	CLA	C15-C16-C17-C18
28	A	412	SQD	C15-C16-C17-C18
29	A	413	DGD	C8B-C9B-CAB-CBB
23	c	511	CLA	O1A-CGA-O2A-C1
27	D	407	LMG	C16-C17-C18-C19
27	d	409	LMG	C32-C33-C34-C35
28	B	623	SQD	C11-C12-C13-C14
23	b	617	CLA	C2-C1-O2A-CGA
27	c	522	LMG	C36-C37-C38-C39
23	B	613	CLA	C8-C10-C11-C12
27	a	414	LMG	C39-C40-C41-C42
29	a	413	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	l	101	LHG	C9-C10-C11-C12
23	B	609	CLA	C16-C17-C18-C19
23	B	609	CLA	C16-C17-C18-C20
29	c	517	DGD	C1A-C2A-C3A-C4A
25	C	515	BCR	C23-C24-C25-C26
25	D	405	BCR	C23-C24-C25-C26
25	D	405	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C30
25	K	101	BCR	C1-C6-C7-C8
25	b	618	BCR	C1-C6-C7-C8
25	b	618	BCR	C5-C6-C7-C8
25	h	102	BCR	C23-C24-C25-C26
29	C	518	DGD	C6B-C7B-C8B-C9B
33	B	622	LHG	C12-C13-C14-C15
23	C	503	CLA	CBA-CGA-O2A-C1
23	b	615	CLA	CBA-CGA-O2A-C1
33	l	101	LHG	C24-C23-O8-C6
23	c	501	CLA	C8-C10-C11-C12
23	c	512	CLA	C5-C6-C7-C8
27	D	407	LMG	C34-C35-C36-C37
33	e	101	LHG	C16-C17-C18-C19
28	A	411	SQD	C33-C34-C35-C36
29	h	103	DGD	CAB-CBB-CCB-CDB
23	D	403	CLA	C15-C16-C17-C18
27	c	522	LMG	C37-C38-C39-C40
29	A	413	DGD	C6B-C7B-C8B-C9B
29	h	103	DGD	C2B-C3B-C4B-C5B
33	d	408	LHG	C29-C30-C31-C32
23	B	615	CLA	C4-C3-C5-C6
26	d	406	PL9	C15-C14-C16-C17
23	B	609	CLA	C2-C3-C5-C6
23	B	615	CLA	C11-C12-C13-C15
23	C	503	CLA	C11-C10-C8-C7
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C11-C12-C13-C15
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C11-C10-C8-C7
23	D	403	CLA	C12-C13-C15-C16
23	a	405	CLA	C6-C7-C8-C10
23	a	407	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C12-C13-C15
23	b	611	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	C6-C7-C8-C10
23	c	509	CLA	C12-C13-C15-C16
23	d	404	CLA	C11-C12-C13-C15
25	c	514	BCR	C13-C14-C15-C16
24	d	401	PHO	O1D-CGD-O2D-CED
29	c	516	DGD	O1B-C1B-O2G-C2G
33	E	101	LHG	O9-C7-O7-C5
33	D	409	LHG	C23-C24-C25-C26
23	c	506	CLA	CBA-CGA-O2A-C1
27	C	519	LMG	C31-C32-C33-C34
27	b	622	LMG	C11-C12-C13-C14
33	D	408	LHG	C33-C34-C35-C36
33	a	410	LHG	C10-C11-C12-C13
33	e	101	LHG	C13-C14-C15-C16
23	B	605	CLA	C5-C6-C7-C8
23	C	506	CLA	C15-C16-C17-C18
23	a	405	CLA	C8-C10-C11-C12
27	B	620	LMG	O6-C5-C6-O5
27	B	620	LMG	C17-C18-C19-C20
29	C	516	DGD	C4A-C5A-C6A-C7A
33	a	410	LHG	C17-C18-C19-C20
27	a	414	LMG	C28-C29-C30-C31
23	C	502	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	C14-C15-C16-C17
28	A	412	SQD	C28-C29-C30-C31
29	A	413	DGD	CBB-CCB-CDB-CEB
29	C	518	DGD	CAA-CBA-CCA-CDA
29	H	102	DGD	CBA-CCA-CDA-CEA
29	c	517	DGD	CAA-CBA-CCA-CDA
29	h	103	DGD	C3B-C4B-C5B-C6B
33	E	101	LHG	C25-C26-C27-C28
33	a	410	LHG	C32-C33-C34-C35
26	a	409	PL9	C17-C18-C19-C20
29	h	103	DGD	C7A-C8A-C9A-CAA
25	D	405	BCR	C22-C23-C24-C25
23	C	503	CLA	O1A-CGA-O2A-C1
29	c	518	DGD	C2A-C1A-O1G-C1G
23	C	513	CLA	C5-C6-C7-C8
27	A	410	LMG	C38-C39-C40-C41
27	C	519	LMG	C18-C19-C20-C21
29	C	517	DGD	CCB-CDB-CEB-CFB
29	c	518	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	c	522	LMG	C16-C17-C18-C19
29	c	518	DGD	CBB-CCB-CDB-CEB
33	d	407	LHG	C28-C29-C30-C31
23	a	404	CLA	C15-C16-C17-C18
23	B	603	CLA	CBD-CGD-O2D-CED
27	a	414	LMG	C38-C39-C40-C41
23	h	101	CLA	C3-C5-C6-C7
27	m	101	LMG	C19-C20-C21-C22
28	B	623	SQD	C9-C10-C11-C12
33	l	101	LHG	C16-C17-C18-C19
27	A	410	LMG	O1-C7-C8-O7
28	A	411	SQD	O6-C44-C45-O47
29	A	413	DGD	O2G-C2G-C3G-O3G
28	f	101	SQD	C28-C29-C30-C31
29	A	413	DGD	C8A-C9A-CAA-CBA
33	B	622	LHG	C32-C33-C34-C35
33	d	408	LHG	C27-C28-C29-C30
33	e	101	LHG	C11-C10-C9-C8
33	e	101	LHG	C18-C19-C20-C21
33	l	101	LHG	C24-C25-C26-C27
23	B	610	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	B	609	CLA	C4-C3-C5-C6
24	A	406	PHO	C4-C3-C5-C6
28	a	411	SQD	C23-C24-C25-C26
33	d	407	LHG	C7-C8-C9-C10
23	B	615	CLA	C2-C3-C5-C6
26	d	406	PL9	C28-C29-C31-C32
26	D	406	PL9	C4-C3-C7-C8
23	C	504	CLA	C11-C12-C13-C14
23	B	604	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C12-C13-C14
23	C	508	CLA	C6-C7-C8-C9
23	C	509	CLA	C14-C13-C15-C16
23	a	404	CLA	C11-C10-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C12-C13-C14
23	b	613	CLA	C6-C7-C8-C9
23	b	613	CLA	C14-C13-C15-C16
23	c	504	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C10-C8-C9
23	c	509	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	CBD-CGD-O2D-CED
27	D	410	LMG	C11-C12-C13-C14
29	c	516	DGD	O6E-C5E-C6E-O5E
27	c	522	LMG	C12-C13-C14-C15
29	C	516	DGD	C9B-CAB-CBB-CCB
29	c	517	DGD	C6A-C7A-C8A-C9A
33	B	622	LHG	C29-C30-C31-C32
23	b	615	CLA	O1A-CGA-O2A-C1
23	C	503	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C19
28	f	101	SQD	C24-C25-C26-C27
33	e	101	LHG	C25-C26-C27-C28
23	c	511	CLA	C13-C15-C16-C17
33	D	408	LHG	C4-O6-P-O3
33	D	409	LHG	C4-O6-P-O3
27	A	410	LMG	C12-C13-C14-C15
28	A	411	SQD	C26-C27-C28-C29
33	L	101	LHG	C17-C18-C19-C20
27	d	409	LMG	C34-C35-C36-C37
23	C	513	CLA	C13-C15-C16-C17
23	C	513	CLA	CBA-CGA-O2A-C1
27	C	519	LMG	O6-C5-C6-O5
27	c	522	LMG	C34-C35-C36-C37
27	c	519	LMG	C35-C36-C37-C38
27	d	409	LMG	C39-C40-C41-C42
28	F	101	SQD	C30-C31-C32-C33
28	F	101	SQD	C33-C34-C35-C36
28	a	412	SQD	C24-C25-C26-C27
29	A	413	DGD	CEB-CFB-CGB-CHB
33	d	407	LHG	C14-C15-C16-C17
33	d	407	LHG	C30-C31-C32-C33
28	A	412	SQD	C23-C24-C25-C26
28	A	412	SQD	C10-C11-C12-C13
33	D	409	LHG	C1-C2-C3-O3
33	d	407	LHG	C1-C2-C3-O3
26	a	409	PL9	C40-C39-C41-C42
23	c	506	CLA	C2-C3-C5-C6
26	d	406	PL9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
28	b	601	SQD	C25-C26-C27-C28
29	c	517	DGD	CCB-CDB-CEB-CFB
33	D	409	LHG	C25-C26-C27-C28
28	b	601	SQD	C14-C15-C16-C17
29	C	516	DGD	CCB-CDB-CEB-CFB
29	C	518	DGD	CBB-CCB-CDB-CEB
33	D	409	LHG	C11-C12-C13-C14
23	c	506	CLA	O1A-CGA-O2A-C1
28	a	411	SQD	C25-C26-C27-C28
33	d	407	LHG	C15-C16-C17-C18
23	a	404	CLA	C16-C17-C18-C20
27	C	519	LMG	C19-C20-C21-C22
27	b	622	LMG	C16-C17-C18-C19
28	A	411	SQD	O6-C44-C45-C46
28	B	623	SQD	O6-C44-C45-C46
28	a	411	SQD	C44-C45-C46-O48
28	b	601	SQD	C44-C45-C46-O48
29	A	413	DGD	C1G-C2G-C3G-O3G
23	B	612	CLA	C13-C15-C16-C17
23	b	606	CLA	C5-C6-C7-C8
29	C	517	DGD	C2G-C3G-O3G-C1D
29	C	517	DGD	C5D-C6D-O5D-C1E
29	c	517	DGD	C5D-C6D-O5D-C1E
23	C	511	CLA	O1D-CGD-O2D-CED
27	m	101	LMG	C32-C33-C34-C35
33	D	408	LHG	C35-C36-C37-C38
33	a	410	LHG	C19-C20-C21-C22
29	C	518	DGD	O6E-C5E-C6E-O5E
29	c	518	DGD	C3A-C4A-C5A-C6A
33	E	101	LHG	C35-C36-C37-C38
29	h	103	DGD	O2G-C1B-C2B-C3B
27	D	410	LMG	C28-C29-C30-C31
29	h	103	DGD	CCB-CDB-CEB-CFB
33	D	409	LHG	C17-C18-C19-C20
33	E	101	LHG	C16-C17-C18-C19
27	D	407	LMG	C18-C19-C20-C21
33	d	408	LHG	C25-C26-C27-C28
33	d	408	LHG	C33-C34-C35-C36
33	E	101	LHG	O1-C1-C2-O2
33	a	410	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
28	a	412	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	a	414	LMG	C11-C12-C13-C14
27	a	414	LMG	C35-C36-C37-C38
23	b	611	CLA	C2C-C3C-CAC-CBC
29	c	517	DGD	CAB-CBB-CCB-CDB
29	c	518	DGD	C7A-C8A-C9A-CAA
33	L	101	LHG	C19-C20-C21-C22
25	T	101	BCR	C35-C13-C14-C15
25	b	619	BCR	C20-C21-C22-C37
25	c	521	BCR	C20-C21-C22-C37
27	A	410	LMG	O6-C5-C6-O5
27	d	409	LMG	O6-C5-C6-O5
26	D	406	PL9	C30-C29-C31-C32
28	a	412	SQD	C31-C32-C33-C34
23	c	503	CLA	CBA-CGA-O2A-C1
29	c	516	DGD	C2A-C1A-O1G-C1G
33	d	408	LHG	C24-C23-O8-C6
27	D	407	LMG	C40-C41-C42-C43
27	b	623	LMG	C38-C39-C40-C41
28	A	411	SQD	C10-C11-C12-C13
29	c	517	DGD	CDA-CEA-CFA-CGA
33	B	622	LHG	C18-C19-C20-C21
33	L	101	LHG	C15-C16-C17-C18
33	e	101	LHG	C28-C29-C30-C31
28	f	101	SQD	C46-C45-O47-C7
27	b	622	LMG	O6-C5-C6-O5
23	c	506	CLA	C2-C1-O2A-CGA
28	A	412	SQD	C46-C45-O47-C7
28	a	412	SQD	C11-C10-C9-C8
29	h	103	DGD	C6A-C7A-C8A-C9A
33	E	101	LHG	C19-C20-C21-C22
27	m	101	LMG	C33-C34-C35-C36
28	b	601	SQD	C19-C20-C21-C22
29	c	516	DGD	C2A-C3A-C4A-C5A
33	l	101	LHG	C33-C34-C35-C36
23	b	608	CLA	O1D-CGD-O2D-CED
27	b	623	LMG	C30-C31-C32-C33
27	m	101	LMG	C22-C23-C24-C25
33	D	409	LHG	C31-C32-C33-C34
23	B	614	CLA	CBA-CGA-O2A-C1
27	C	519	LMG	C29-C28-O8-C9
23	B	603	CLA	C16-C17-C18-C20
27	D	411	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
27	D	407	LMG	C31-C32-C33-C34
33	d	407	LHG	O2-C2-C3-O3
23	C	508	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	C15-C16-C17-C18
33	B	622	LHG	C16-C17-C18-C19
33	E	101	LHG	C13-C14-C15-C16
23	b	607	CLA	C10-C11-C12-C13
25	y	101	BCR	C11-C10-C9-C8
29	c	518	DGD	CDB-CEB-CFB-CGB
27	a	414	LMG	O7-C8-C9-O8
27	a	414	LMG	C34-C35-C36-C37
27	B	620	LMG	O9-C10-O7-C8
29	H	102	DGD	O1B-C1B-O2G-C2G
28	B	623	SQD	C13-C14-C15-C16
28	a	412	SQD	C18-C19-C20-C21
33	D	408	LHG	C29-C30-C31-C32
33	E	101	LHG	C10-C11-C12-C13
33	E	101	LHG	C26-C27-C28-C29
23	B	604	CLA	C11-C10-C8-C7
23	B	604	CLA	C11-C12-C13-C15
23	B	604	CLA	C12-C13-C15-C16
23	B	606	CLA	C11-C12-C13-C15
23	C	506	CLA	C12-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C7
23	C	509	CLA	C12-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	608	CLA	C6-C7-C8-C10
23	b	608	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C12-C13-C15
23	c	504	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C12-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C10
23	h	101	CLA	C11-C10-C8-C7
24	a	406	PHO	C6-C7-C8-C10
29	C	516	DGD	O1G-C1A-C2A-C3A
27	m	101	LMG	C30-C31-C32-C33
29	A	413	DGD	C3B-C4B-C5B-C6B
29	C	518	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	C11-C10-C8-C9
23	B	615	CLA	C6-C7-C8-C9
23	B	615	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C10-C8-C9
23	b	605	CLA	C11-C12-C13-C14
23	b	607	CLA	C11-C10-C8-C9
23	b	608	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	b	615	CLA	C11-C12-C13-C14
23	c	501	CLA	C11-C12-C13-C14
23	c	505	CLA	C11-C10-C8-C9
23	c	508	CLA	C14-C13-C15-C16
24	D	401	PHO	C6-C7-C8-C9
24	a	406	PHO	C6-C7-C8-C9
27	b	623	LMG	C33-C34-C35-C36
33	D	409	LHG	C15-C16-C17-C18
23	C	506	CLA	CBA-CGA-O2A-C1
23	B	611	CLA	C16-C17-C18-C20
23	a	404	CLA	C16-C17-C18-C19
23	c	504	CLA	C11-C12-C13-C14
27	b	623	LMG	C36-C37-C38-C39
28	A	411	SQD	C24-C25-C26-C27
27	B	620	LMG	C33-C34-C35-C36
33	E	101	LHG	C27-C28-C29-C30
23	b	615	CLA	C8-C10-C11-C12
27	C	519	LMG	C37-C38-C39-C40
28	a	411	SQD	C26-C27-C28-C29
33	D	409	LHG	C24-C25-C26-C27
26	A	409	PL9	C17-C18-C19-C21
27	c	522	LMG	C4-C5-C6-O5
23	B	607	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	C8-C10-C11-C12
23	c	511	CLA	C15-C16-C17-C18
23	d	403	CLA	C16-C17-C18-C20
27	B	620	LMG	C39-C40-C41-C42
33	e	101	LHG	C27-C28-C29-C30
28	F	101	SQD	C26-C27-C28-C29
23	c	507	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	C8-C10-C11-C12
29	H	102	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
27	c	522	LMG	C28-C29-C30-C31
23	C	502	CLA	C16-C17-C18-C19
28	a	412	SQD	C17-C18-C19-C20
28	a	412	SQD	C29-C30-C31-C32
29	A	413	DGD	CCB-CDB-CEB-CFB
23	c	505	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	C15-C16-C17-C18
28	a	411	SQD	C27-C28-C29-C30
29	H	102	DGD	CCB-CDB-CEB-CFB
28	F	101	SQD	C45-C44-O6-C1
23	B	613	CLA	C2C-C3C-CAC-CBC
27	D	411	LMG	C11-C12-C13-C14
23	C	513	CLA	O1A-CGA-O2A-C1
27	D	411	LMG	C13-C14-C15-C16
29	A	413	DGD	CFA-CGA-CHA-CIA
24	A	406	PHO	C16-C17-C18-C19
23	B	616	CLA	CBA-CGA-O2A-C1
23	c	504	CLA	CBA-CGA-O2A-C1
28	B	623	SQD	C24-C23-O48-C46
29	A	413	DGD	C2A-C1A-O1G-C1G
27	B	620	LMG	C7-C8-C9-O8
27	c	522	LMG	O1-C7-C8-C9
33	d	408	LHG	C4-C5-C6-O8
29	H	102	DGD	CDB-CEB-CFB-CGB
29	c	517	DGD	C3B-C4B-C5B-C6B
29	C	518	DGD	CDB-CEB-CFB-CGB
33	L	101	LHG	C9-C10-C11-C12
23	C	513	CLA	O2A-C1-C2-C3
23	h	101	CLA	O2A-C1-C2-C3
23	B	616	CLA	O1A-CGA-O2A-C1
23	b	608	CLA	C8-C10-C11-C12
26	a	409	PL9	C35-C34-C36-C37
23	d	404	CLA	C16-C17-C18-C20
24	A	406	PHO	C2-C3-C5-C6
27	A	410	LMG	C17-C18-C19-C20
27	A	410	LMG	C30-C31-C32-C33
23	B	614	CLA	O1A-CGA-O2A-C1
29	A	413	DGD	CBA-CCA-CDA-CEA
23	c	502	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	CBA-CGA-O2A-C1
27	m	101	LMG	C29-C28-O8-C9
33	L	101	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C16-C17-C18-C19
23	c	503	CLA	O1A-CGA-O2A-C1
23	B	611	CLA	C16-C17-C18-C19
23	c	507	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C19
29	C	518	DGD	C3B-C4B-C5B-C6B
27	c	522	LMG	C32-C33-C34-C35
28	A	412	SQD	C27-C28-C29-C30
33	E	101	LHG	C30-C31-C32-C33
33	l	101	LHG	C35-C36-C37-C38
27	B	620	LMG	C28-C29-C30-C31
27	a	414	LMG	C33-C34-C35-C36
29	a	413	DGD	C5A-C6A-C7A-C8A
27	c	522	LMG	O1-C7-C8-O7
28	a	411	SQD	O6-C44-C45-O47
23	b	614	CLA	C13-C15-C16-C17
28	a	411	SQD	C19-C20-C21-C22
29	H	102	DGD	CDA-CEA-CFA-CGA
28	b	601	SQD	C8-C7-O47-C45
23	c	513	CLA	C16-C17-C18-C19
24	A	406	PHO	C16-C17-C18-C20
29	C	516	DGD	CDA-CEA-CFA-CGA
33	d	407	LHG	C33-C34-C35-C36
29	A	413	DGD	O6D-C1D-O3G-C3G
33	D	408	LHG	C1-C2-C3-O3
27	D	410	LMG	C36-C37-C38-C39
29	C	517	DGD	C6A-C7A-C8A-C9A
33	l	101	LHG	C13-C14-C15-C16
23	A	404	CLA	C2-C1-O2A-CGA
23	c	512	CLA	C2-C1-O2A-CGA
23	d	403	CLA	C2-C1-O2A-CGA
26	a	409	PL9	C38-C39-C41-C42
23	B	613	CLA	C6-C7-C8-C9
23	B	614	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	C	510	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C9
23	a	405	CLA	C14-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	c	510	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	h	101	CLA	C14-C13-C15-C16
23	c	507	CLA	C5-C6-C7-C8
23	c	509	CLA	C8-C10-C11-C12
33	E	101	LHG	C2-C3-O3-P
27	b	623	LMG	C34-C35-C36-C37
29	C	517	DGD	C7B-C8B-C9B-CAB
33	d	407	LHG	C12-C13-C14-C15
33	d	407	LHG	C34-C35-C36-C37
23	B	603	CLA	C16-C17-C18-C19
23	c	506	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	b	613	CLA	C3-C5-C6-C7
25	B	618	BCR	C23-C24-C25-C26
25	B	619	BCR	C5-C6-C7-C8
25	C	520	BCR	C23-C24-C25-C30
25	y	101	BCR	C5-C6-C7-C8
29	C	518	DGD	CBA-CCA-CDA-CEA
25	T	101	BCR	C21-C22-C23-C24
25	d	405	BCR	C21-C22-C23-C24
27	m	101	LMG	C15-C16-C17-C18
23	C	506	CLA	O1A-CGA-O2A-C1
23	D	404	CLA	C16-C17-C18-C20
23	c	504	CLA	C11-C12-C13-C15
23	b	608	CLA	C5-C6-C7-C8
33	l	101	LHG	O6-C4-C5-C6
29	A	413	DGD	C9B-CAB-CBB-CCB
33	D	409	LHG	C11-C10-C9-C8
23	B	611	CLA	C11-C12-C13-C15
23	B	613	CLA	C6-C7-C8-C10
23	B	615	CLA	C6-C7-C8-C10
23	B	616	CLA	C6-C7-C8-C10
23	C	507	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
23	C	510	CLA	C11-C10-C8-C7
23	C	510	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	a	404	CLA	C12-C13-C15-C16
23	a	405	CLA	C11-C10-C8-C7
23	a	405	CLA	C12-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C15
23	b	617	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C12-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C10
23	c	509	CLA	C11-C12-C13-C15
23	c	510	CLA	C12-C13-C15-C16
23	d	402	CLA	C12-C13-C15-C16
23	d	403	CLA	C6-C7-C8-C10
23	h	101	CLA	C12-C13-C15-C16
25	C	520	BCR	C15-C16-C17-C18
25	T	101	BCR	C9-C10-C11-C12
29	c	516	DGD	C3B-C4B-C5B-C6B
23	b	604	CLA	O1A-CGA-O2A-C1
23	c	505	CLA	CBD-CGD-O2D-CED
27	c	519	LMG	C34-C35-C36-C37
27	d	409	LMG	C12-C13-C14-C15
23	b	605	CLA	C13-C15-C16-C17
25	A	408	BCR	C20-C21-C22-C37
25	a	408	BCR	C20-C21-C22-C37
25	c	514	BCR	C16-C17-C18-C36
25	d	405	BCR	C20-C21-C22-C37
25	h	102	BCR	C16-C17-C18-C36
23	C	504	CLA	C3-C5-C6-C7
23	C	506	CLA	C3-C5-C6-C7
27	B	620	LMG	C38-C39-C40-C41
29	c	518	DGD	C8B-C9B-CAB-CBB
23	c	505	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	C10-C11-C12-C13
23	b	604	CLA	CBA-CGA-O2A-C1
29	H	102	DGD	O2G-C1B-C2B-C3B
28	b	601	SQD	C13-C14-C15-C16
29	C	517	DGD	CDA-CEA-CFA-CGA
29	c	516	DGD	C6A-C7A-C8A-C9A
28	A	411	SQD	C32-C33-C34-C35
28	A	412	SQD	C26-C27-C28-C29
28	a	411	SQD	C18-C19-C20-C21
29	c	518	DGD	C6B-C7B-C8B-C9B
23	b	612	CLA	C10-C11-C12-C13
23	h	101	CLA	C10-C11-C12-C13
27	a	414	LMG	C18-C19-C20-C21
29	A	413	DGD	CDA-CEA-CFA-CGA
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	C	501	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
27	A	410	LMG	C9-C8-O7-C10
27	A	410	LMG	C11-C12-C13-C14
29	c	518	DGD	CBA-CCA-CDA-CEA
25	K	101	BCR	C22-C23-C24-C25
25	d	405	BCR	C22-C23-C24-C25
28	a	411	SQD	C24-C23-O48-C46
26	d	406	PL9	C45-C44-C46-C47
23	C	502	CLA	C16-C17-C18-C20
23	c	510	CLA	C2-C3-C5-C6
27	d	409	LMG	C35-C36-C37-C38
27	c	522	LMG	C7-C8-C9-O8
28	a	412	SQD	C44-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-C3G
33	l	101	LHG	O6-C4-C5-O7
23	C	506	CLA	C13-C15-C16-C17
24	D	401	PHO	O1D-CGD-O2D-CED
28	A	412	SQD	C16-C17-C18-C19
34	e	102	HEM	C4B-C3B-CAB-CBB
25	C	514	BCR	C14-C15-C16-C17
28	A	411	SQD	C25-C26-C27-C28
29	a	413	DGD	C6B-C7B-C8B-C9B
29	c	516	DGD	O1A-C1A-O1G-C1G
33	L	101	LHG	C11-C12-C13-C14
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	612	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
29	c	518	DGD	C9A-CAA-CBA-CCA
23	B	607	CLA	O1A-CGA-O2A-C1
23	c	504	CLA	O1A-CGA-O2A-C1
27	C	519	LMG	O10-C28-O8-C9
29	a	413	DGD	CEB-CFB-CGB-CHB
29	c	516	DGD	CBA-CCA-CDA-CEA
28	b	601	SQD	O6-C44-C45-O47
28	b	601	SQD	O47-C45-C46-O48
28	f	101	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
23	c	502	CLA	O1A-CGA-O2A-C1
23	c	508	CLA	O1A-CGA-O2A-C1
29	h	103	DGD	C6B-C7B-C8B-C9B
23	c	510	CLA	C4-C3-C5-C6
27	c	519	LMG	C39-C40-C41-C42
27	m	101	LMG	C37-C38-C39-C40
26	a	409	PL9	C4-C3-C7-C8
23	C	513	CLA	C14-C13-C15-C16
23	b	616	CLA	C14-C13-C15-C16
23	B	603	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	C16-C17-C18-C20
25	A	408	BCR	C7-C8-C9-C34
25	c	514	BCR	C7-C8-C9-C34
27	m	101	LMG	C13-C14-C15-C16
33	D	409	LHG	C10-C11-C12-C13
29	a	413	DGD	CFA-CGA-CHA-CIA
27	A	410	LMG	C37-C38-C39-C40
23	b	605	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	b	612	CLA	C5-C6-C7-C8
33	d	407	LHG	C26-C27-C28-C29
23	B	601	CLA	C2-C1-O2A-CGA
33	D	408	LHG	C16-C17-C18-C19
25	T	101	BCR	C13-C14-C15-C16
28	B	623	SQD	C25-C26-C27-C28
28	F	101	SQD	C29-C30-C31-C32
33	D	408	LHG	C34-C35-C36-C37
33	B	622	LHG	C24-C25-C26-C27
27	c	522	LMG	C11-C12-C13-C14
29	H	102	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C4-O6-P-O5
33	d	407	LHG	C4-O6-P-O5
23	A	405	CLA	C16-C17-C18-C20
33	L	101	LHG	C31-C32-C33-C34
27	c	519	LMG	C29-C28-O8-C9
29	C	517	DGD	C5A-C6A-C7A-C8A
29	c	518	DGD	C4A-C5A-C6A-C7A
23	a	404	CLA	O1D-CGD-O2D-CED
27	c	519	LMG	C32-C33-C34-C35
29	c	516	DGD	CAA-CBA-CCA-CDA
23	C	508	CLA	C16-C17-C18-C19
29	C	516	DGD	C7B-C8B-C9B-CAB
33	L	101	LHG	C11-C10-C9-C8
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	513	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	c	509	CLA	CAA-CBA-CGA-O2A
23	c	513	CLA	C5-C6-C7-C8
29	c	517	DGD	C8B-C9B-CAB-CBB
27	D	410	LMG	C31-C32-C33-C34
27	a	414	LMG	C19-C20-C21-C22
28	B	623	SQD	C33-C34-C35-C36
28	A	412	SQD	O49-C7-O47-C45
23	D	403	CLA	C2C-C3C-CAC-CBC
23	C	509	CLA	C16-C17-C18-C19
23	c	511	CLA	C16-C17-C18-C19
23	B	603	CLA	C12-C13-C15-C16
23	C	504	CLA	C11-C10-C8-C7
23	C	507	CLA	C6-C7-C8-C10
23	D	403	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C12-C13-C15
23	D	404	CLA	C12-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C15
23	b	605	CLA	C12-C13-C15-C16
23	b	610	CLA	C12-C13-C15-C16
23	b	613	CLA	C11-C10-C8-C7
23	b	616	CLA	C11-C10-C8-C7
23	c	501	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	C6-C7-C8-C10
23	c	503	CLA	C11-C10-C8-C7
23	c	505	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
24	A	406	PHO	C6-C7-C8-C10
33	d	407	LHG	C16-C17-C18-C19
23	B	606	CLA	C8-C10-C11-C12
27	D	407	LMG	C28-C29-C30-C31
33	D	408	LHG	C13-C14-C15-C16
23	C	512	CLA	C2A-CAA-CBA-CGA
28	B	623	SQD	C26-C27-C28-C29
28	f	101	SQD	C44-C45-C46-O48
29	a	413	DGD	C4B-C5B-C6B-C7B
27	B	620	LMG	O7-C8-C9-O8
27	b	622	LMG	O1-C7-C8-O7
27	c	522	LMG	O7-C8-C9-O8
28	a	412	SQD	O47-C45-C46-O48
33	d	408	LHG	O7-C5-C6-O8
29	C	518	DGD	CCA-CDA-CEA-CFA
29	a	413	DGD	C3A-C4A-C5A-C6A
23	B	605	CLA	C16-C17-C18-C20
23	C	509	CLA	C5-C6-C7-C8
23	B	606	CLA	C6-C7-C8-C9
23	C	504	CLA	C11-C10-C8-C9
23	D	404	CLA	C14-C13-C15-C16
23	a	405	CLA	C11-C10-C8-C9
23	b	609	CLA	C11-C12-C13-C14
23	b	613	CLA	C11-C10-C8-C9
23	c	503	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C12-C13-C14
25	b	618	BCR	C22-C23-C24-C25
25	b	620	BCR	C6-C7-C8-C9
23	C	513	CLA	C2C-C3C-CAC-CBC
23	b	612	CLA	C16-C17-C18-C19
29	C	516	DGD	C6A-C7A-C8A-C9A
33	a	410	LHG	C31-C32-C33-C34
23	B	608	CLA	C13-C15-C16-C17
23	B	606	CLA	C2C-C3C-CAC-CBC
29	C	518	DGD	CDA-CEA-CFA-CGA
26	a	409	PL9	C12-C13-C14-C15
23	C	505	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	c	505	CLA	C16-C17-C18-C20
33	D	408	LHG	C10-C11-C12-C13
33	a	410	LHG	C11-C10-C9-C8
33	B	622	LHG	C30-C31-C32-C33
23	B	608	CLA	C10-C11-C12-C13
25	b	620	BCR	C35-C13-C14-C15
23	c	513	CLA	C3-C5-C6-C7
23	c	512	CLA	C4-C3-C5-C6
23	A	405	CLA	C16-C17-C18-C19
29	A	413	DGD	O6D-C5D-C6D-O5D
29	C	516	DGD	C5B-C6B-C7B-C8B
27	D	410	LMG	C9-C8-O7-C10
28	b	601	SQD	C46-C45-O47-C7
29	a	413	DGD	C3G-C2G-O2G-C1B
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
23	C	506	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
29	C	517	DGD	C8B-C9B-CAB-CBB
29	H	102	DGD	CCA-CDA-CEA-CFA
27	m	101	LMG	C17-C18-C19-C20
27	D	410	LMG	C12-C13-C14-C15
29	C	517	DGD	C8A-C9A-CAA-CBA
23	c	501	CLA	CBD-CGD-O2D-CED
33	d	408	LHG	C2-C3-O3-P
29	h	103	DGD	CDA-CEA-CFA-CGA
25	C	520	BCR	C13-C14-C15-C16
25	C	520	BCR	C19-C20-C21-C22
27	C	519	LMG	C39-C40-C41-C42
27	b	622	LMG	C35-C36-C37-C38
23	C	509	CLA	C16-C17-C18-C20
23	c	507	CLA	O1D-CGD-O2D-CED
25	A	408	BCR	C5-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C30
25	C	520	BCR	C23-C24-C25-C26
26	D	406	PL9	C28-C29-C31-C32
27	m	101	LMG	C11-C12-C13-C14
33	l	101	LHG	O2-C2-C3-O3
29	C	516	DGD	C4B-C5B-C6B-C7B
33	E	101	LHG	C29-C30-C31-C32
23	c	506	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	O6D-C1D-O3G-C3G
29	c	516	DGD	O6E-C1E-O5D-C6D
23	B	613	CLA	C4C-C3C-CAC-CBC
28	a	412	SQD	C13-C14-C15-C16
33	E	101	LHG	C18-C19-C20-C21
33	D	409	LHG	C12-C13-C14-C15
23	b	604	CLA	C16-C17-C18-C20
23	B	609	CLA	O1D-CGD-O2D-CED
28	F	101	SQD	C32-C33-C34-C35
33	L	101	LHG	C10-C11-C12-C13
29	a	413	DGD	C6A-C7A-C8A-C9A
27	A	410	LMG	O1-C7-C8-C9
27	b	622	LMG	O1-C7-C8-C9
27	b	622	LMG	C7-C8-C9-O8
29	C	516	DGD	C1G-C2G-C3G-O3G
23	B	605	CLA	C10-C11-C12-C13
23	c	510	CLA	C10-C11-C12-C13
23	B	607	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C12-C13-C15
23	c	506	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	B	603	CLA	C14-C13-C15-C16
23	B	604	CLA	C14-C13-C15-C16
23	B	606	CLA	C11-C12-C13-C14
23	B	616	CLA	C6-C7-C8-C9
23	C	502	CLA	C6-C7-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	b	605	CLA	C14-C13-C15-C16
23	b	610	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C9
23	b	616	CLA	C11-C12-C13-C14
23	c	503	CLA	C6-C7-C8-C9
23	c	505	CLA	C6-C7-C8-C9
23	d	404	CLA	C14-C13-C15-C16
25	C	514	BCR	C15-C16-C17-C18
25	b	619	BCR	C9-C10-C11-C12
25	t	101	BCR	C13-C14-C15-C16
27	a	414	LMG	C30-C31-C32-C33
23	B	610	CLA	C2C-C3C-CAC-CBC
27	C	519	LMG	C33-C34-C35-C36
27	D	407	LMG	C13-C14-C15-C16
27	d	409	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C31-C32-C33-C34
27	D	411	LMG	O10-C28-C29-C30
27	m	101	LMG	C40-C41-C42-C43
23	C	502	CLA	C15-C16-C17-C18
23	b	612	CLA	C16-C17-C18-C20
27	D	410	LMG	C16-C17-C18-C19
27	b	622	LMG	C10-C11-C12-C13
27	b	623	LMG	C35-C36-C37-C38
23	a	404	CLA	CBD-CGD-O2D-CED
26	d	406	PL9	C18-C19-C21-C22
33	a	410	LHG	C24-C23-O8-C6
29	c	516	DGD	C7B-C8B-C9B-CAB
29	C	518	DGD	C2A-C3A-C4A-C5A
29	a	413	DGD	O2G-C1B-C2B-C3B
23	B	612	CLA	O1A-CGA-O2A-C1
25	C	514	BCR	C9-C10-C11-C12
25	c	521	BCR	C9-C10-C11-C12
26	D	406	PL9	C14-C16-C17-C18
23	B	601	CLA	C8-C10-C11-C12
27	C	519	LMG	C40-C41-C42-C43
25	c	521	BCR	C18-C19-C20-C21
33	D	408	LHG	C9-C10-C11-C12
27	c	522	LMG	C35-C36-C37-C38
29	A	413	DGD	CEA-CFA-CGA-CHA
26	A	409	PL9	C20-C19-C21-C22
23	C	506	CLA	C2-C3-C5-C6
27	A	410	LMG	C32-C33-C34-C35
29	h	103	DGD	C9A-CAA-CBA-CCA
27	d	409	LMG	C38-C39-C40-C41
28	f	101	SQD	C29-C30-C31-C32
23	B	603	CLA	C13-C15-C16-C17
23	d	404	CLA	C3A-C2A-CAA-CBA
33	L	101	LHG	C33-C34-C35-C36
23	B	603	CLA	CBA-CGA-O2A-C1
27	C	519	LMG	C14-C15-C16-C17
26	A	409	PL9	C30-C29-C31-C32
29	c	518	DGD	C2A-C3A-C4A-C5A
23	b	613	CLA	C8-C10-C11-C12
26	A	409	PL9	C4-C3-C7-C8
23	B	607	CLA	C11-C10-C8-C9
23	b	608	CLA	C11-C10-C8-C9
23	c	503	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	a	406	PHO	C11-C10-C8-C9
23	d	403	CLA	C2C-C3C-CAC-CBC
34	e	102	HEM	CAD-CBD-CGD-O1D
23	c	504	CLA	C5-C6-C7-C8
27	a	414	LMG	C40-C41-C42-C43
23	C	503	CLA	C15-C16-C17-C18
23	a	405	CLA	C10-C11-C12-C13
25	A	408	BCR	C16-C17-C18-C36
25	D	405	BCR	C11-C10-C9-C34
25	b	620	BCR	C11-C10-C9-C34
23	B	604	CLA	C3-C5-C6-C7
23	c	512	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C8-C10-C11-C12
23	h	101	CLA	C8-C10-C11-C12
27	D	407	LMG	C32-C33-C34-C35
28	F	101	SQD	C31-C32-C33-C34
29	C	516	DGD	CAA-CBA-CCA-CDA
23	B	607	CLA	C16-C17-C18-C19
34	e	102	HEM	CAD-CBD-CGD-O2D
29	c	517	DGD	C9A-CAA-CBA-CCA
23	c	503	CLA	C5-C6-C7-C8
29	H	102	DGD	C5A-C6A-C7A-C8A
27	D	411	LMG	O9-C10-C11-C12
27	a	414	LMG	C9-C8-O7-C10
23	c	505	CLA	C4-C3-C5-C6
23	B	602	CLA	C1A-C2A-CAA-CBA
23	D	403	CLA	C1A-C2A-CAA-CBA
23	c	503	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C6-C7-C8-C10
23	C	512	CLA	C12-C13-C15-C16
23	b	609	CLA	C11-C10-C8-C7
23	b	616	CLA	C12-C13-C15-C16
23	c	507	CLA	C12-C13-C15-C16
23	c	512	CLA	C11-C10-C8-C7
23	d	402	CLA	C2C-C3C-CAC-CBC
29	C	518	DGD	C4B-C5B-C6B-C7B
33	d	407	LHG	C17-C18-C19-C20
33	l	101	LHG	C30-C31-C32-C33
33	e	101	LHG	C3-O3-P-O6
33	e	101	LHG	O6-C4-C5-O7
35	V	201	HEC	CAD-CBD-CGD-O1D
35	v	201	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	C8-C10-C11-C12
29	H	102	DGD	C9B-CAB-CBB-CCB
27	m	101	LMG	C18-C19-C20-C21
23	C	502	CLA	C3-C5-C6-C7
27	D	407	LMG	C39-C40-C41-C42
33	a	410	LHG	C33-C34-C35-C36
27	D	411	LMG	O8-C28-C29-C30
35	v	201	HEC	CAD-CBD-CGD-O1D
23	b	611	CLA	C8-C10-C11-C12
29	C	518	DGD	O1A-C1A-O1G-C1G
28	A	411	SQD	O49-C7-O47-C45
23	b	617	CLA	C11-C12-C13-C15
23	c	505	CLA	C16-C17-C18-C19
29	A	413	DGD	C2E-C1E-O5D-C6D
29	h	103	DGD	C7B-C8B-C9B-CAB
28	A	412	SQD	C44-C45-O47-C7
25	C	515	BCR	C13-C14-C15-C16
25	C	515	BCR	C15-C16-C17-C18
25	D	405	BCR	C19-C20-C21-C22
25	c	521	BCR	C15-C16-C17-C18
23	d	403	CLA	C3-C5-C6-C7
27	b	622	LMG	C14-C15-C16-C17
33	l	101	LHG	C32-C33-C34-C35
26	d	406	PL9	C9-C11-C12-C13
26	d	406	PL9	C39-C41-C42-C43
33	d	408	LHG	C30-C31-C32-C33
23	B	601	CLA	C4-C3-C5-C6
23	D	403	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C13-C15-C16-C17
23	b	603	CLA	C6-C7-C8-C9
23	c	506	CLA	C14-C13-C15-C16
27	b	623	LMG	C39-C40-C41-C42
23	c	505	CLA	O1D-CGD-O2D-CED
33	D	409	LHG	C2-C3-O3-P
28	B	623	SQD	C45-C46-O48-C23
23	c	510	CLA	C2A-CAA-CBA-CGA
35	V	201	HEC	CAD-CBD-CGD-O2D
23	B	612	CLA	C2C-C3C-CAC-CBC
27	B	620	LMG	C30-C31-C32-C33
27	D	407	LMG	C15-C16-C17-C18
23	B	611	CLA	O1A-CGA-O2A-C1
25	A	408	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	B	617	BCR	C1-C6-C7-C8
25	B	619	BCR	C1-C6-C7-C8
25	K	101	BCR	C23-C24-C25-C30
25	b	619	BCR	C23-C24-C25-C26
25	b	619	BCR	C23-C24-C25-C30
25	c	515	BCR	C23-C24-C25-C30
25	d	405	BCR	C23-C24-C25-C30
33	D	408	LHG	C19-C20-C21-C22
28	F	101	SQD	O10-C23-C24-C25
25	c	514	BCR	C15-C16-C17-C18
25	c	515	BCR	C9-C10-C11-C12
27	m	101	LMG	C36-C37-C38-C39
28	A	412	SQD	C31-C32-C33-C34
33	L	101	LHG	C29-C30-C31-C32
23	C	513	CLA	C8-C10-C11-C12
23	b	610	CLA	C2-C3-C5-C6
23	c	512	CLA	C2-C3-C5-C6
27	D	411	LMG	O7-C10-C11-C12
33	l	101	LHG	C29-C30-C31-C32
23	b	616	CLA	C8-C10-C11-C12
23	c	504	CLA	C8-C10-C11-C12
29	C	516	DGD	C5D-C6D-O5D-C1E
23	B	610	CLA	C4C-C3C-CAC-CBC
23	c	512	CLA	C15-C16-C17-C18
23	B	610	CLA	C16-C17-C18-C19
28	A	412	SQD	C34-C35-C36-C37
29	c	517	DGD	C5B-C6B-C7B-C8B
23	a	404	CLA	C3-C5-C6-C7
29	A	413	DGD	C3A-C4A-C5A-C6A
23	D	402	CLA	C11-C12-C13-C15
23	B	611	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	CBA-CGA-O2A-C1
33	D	409	LHG	C24-C23-O8-C6
27	C	519	LMG	C32-C33-C34-C35
33	D	408	LHG	C25-C26-C27-C28
23	B	613	CLA	C10-C11-C12-C13
28	a	411	SQD	C17-C18-C19-C20
33	E	101	LHG	C32-C33-C34-C35
23	C	501	CLA	C3-C5-C6-C7
25	C	514	BCR	C11-C10-C9-C34
25	b	619	BCR	C11-C10-C9-C34
28	A	411	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C4-C3-C5-C6
28	a	411	SQD	C13-C14-C15-C16
23	c	505	CLA	C2-C3-C5-C6
23	B	612	CLA	CAA-CBA-CGA-O2A
28	a	411	SQD	O47-C7-C8-C9
27	D	410	LMG	C37-C38-C39-C40
23	B	603	CLA	C6-C7-C8-C9
23	B	614	CLA	C11-C12-C13-C14
23	D	403	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C12-C13-C14
23	b	605	CLA	C6-C7-C8-C9
23	b	609	CLA	C11-C10-C8-C9
23	c	501	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	d	403	CLA	C11-C10-C8-C9
24	A	406	PHO	C6-C7-C8-C9
23	D	403	CLA	C3A-C2A-CAA-CBA
23	D	404	CLA	C3A-C2A-CAA-CBA
24	A	406	PHO	O1A-CGA-O2A-C1
27	b	622	LMG	O7-C10-C11-C12
29	C	516	DGD	O2G-C1B-C2B-C3B
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	607	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	b	611	CLA	CAD-CBD-CGD-O2D
23	b	613	CLA	CAD-CBD-CGD-O2D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
24	a	406	PHO	CAD-CBD-CGD-O2D
27	B	620	LMG	C9-C8-O7-C10
28	B	623	SQD	C46-C45-O47-C7
29	c	516	DGD	CAB-CBB-CCB-CDB
23	B	608	CLA	C15-C16-C17-C18
23	b	609	CLA	C4C-C3C-CAC-CBC
23	A	404	CLA	C2C-C3C-CAC-CBC
27	b	622	LMG	C38-C39-C40-C41
23	b	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	F	101	SQD	O48-C23-C24-C25
28	b	601	SQD	O47-C7-C8-C9
33	l	101	LHG	C15-C16-C17-C18
25	K	101	BCR	C7-C8-C9-C10
25	T	101	BCR	C11-C12-C13-C14
24	d	401	PHO	C2C-C3C-CAC-CBC
27	C	519	LMG	O1-C7-C8-C9
28	b	601	SQD	O6-C44-C45-C46
28	a	411	SQD	C34-C35-C36-C37
29	C	516	DGD	O6D-C5D-C6D-O5D
23	d	404	CLA	C10-C11-C12-C13
23	b	613	CLA	CAA-CBA-CGA-O2A
28	b	601	SQD	C30-C31-C32-C33
23	C	509	CLA	O2A-C1-C2-C3
23	D	404	CLA	O2A-C1-C2-C3
24	a	406	PHO	O2A-C1-C2-C3
23	C	509	CLA	C2A-CAA-CBA-CGA
27	a	414	LMG	C13-C14-C15-C16
27	B	620	LMG	C16-C17-C18-C19
33	D	408	LHG	O9-C7-O7-C5
29	c	518	DGD	C6A-C7A-C8A-C9A
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O2D
23	D	402	CLA	CHA-CBD-CGD-O1D
23	D	402	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	d	402	CLA	CHA-CBD-CGD-O2D
25	A	408	BCR	C15-C16-C17-C18
25	C	514	BCR	C20-C21-C22-C23
25	y	101	BCR	C20-C21-C22-C23
28	B	623	SQD	C30-C31-C32-C33
27	m	101	LMG	O7-C10-C11-C12
27	d	409	LMG	C11-C12-C13-C14
27	b	622	LMG	O7-C8-C9-O8
29	C	516	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
28	a	411	SQD	O48-C23-C24-C25
29	h	103	DGD	C4A-C5A-C6A-C7A
23	B	603	CLA	C2A-CAA-CBA-CGA
33	a	410	LHG	C15-C16-C17-C18
27	b	623	LMG	C29-C30-C31-C32
33	a	410	LHG	C28-C29-C30-C31
23	b	614	CLA	CAA-CBA-CGA-O2A
27	B	620	LMG	C11-C12-C13-C14
33	B	622	LHG	C19-C20-C21-C22
23	A	404	CLA	C4C-C3C-CAC-CBC
23	B	611	CLA	C6-C7-C8-C10
23	C	507	CLA	C11-C12-C13-C15
23	C	510	CLA	C6-C7-C8-C10
23	c	512	CLA	C11-C12-C13-C15
26	d	406	PL9	C4-C3-C7-C8
29	c	518	DGD	CCB-CDB-CEB-CFB
23	a	407	CLA	CAA-CBA-CGA-O2A
33	L	101	LHG	O7-C7-C8-C9
23	B	611	CLA	C6-C7-C8-C9
23	B	612	CLA	C11-C10-C8-C9
23	B	615	CLA	C11-C10-C8-C9
23	C	507	CLA	C6-C7-C8-C9
23	b	612	CLA	C11-C10-C8-C9
23	c	507	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C10-C8-C9
23	d	403	CLA	C6-C7-C8-C9
29	A	413	DGD	C1B-C2B-C3B-C4B
25	C	514	BCR	C13-C14-C15-C16
23	d	402	CLA	C4C-C3C-CAC-CBC
23	C	511	CLA	C8-C10-C11-C12
29	a	413	DGD	CDB-CEB-CFB-CGB
27	b	622	LMG	O8-C28-C29-C30
26	A	409	PL9	C11-C12-C13-C14
29	c	516	DGD	C2B-C3B-C4B-C5B
26	A	409	PL9	C40-C39-C41-C42
27	D	410	LMG	C34-C35-C36-C37
29	H	102	DGD	C8B-C9B-CAB-CBB
24	A	406	PHO	CBA-CGA-O2A-C1
23	D	404	CLA	C1A-C2A-CAA-CBA
23	b	613	CLA	C1A-C2A-CAA-CBA
23	b	616	CLA	C1A-C2A-CAA-CBA
23	d	404	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C5-C6-C7-C8
23	b	613	CLA	CAA-CBA-CGA-O1A
27	C	519	LMG	O9-C10-C11-C12
29	c	516	DGD	O1B-C1B-C2B-C3B
27	B	620	LMG	C32-C33-C34-C35
27	b	622	LMG	C12-C13-C14-C15
28	A	411	SQD	C31-C32-C33-C34
27	a	414	LMG	C7-C8-C9-O8
29	c	516	DGD	C1G-C2G-C3G-O3G
23	B	603	CLA	O1A-CGA-O2A-C1
23	c	501	CLA	CAA-CBA-CGA-O2A
23	C	501	CLA	C16-C17-C18-C20
23	B	612	CLA	CAA-CBA-CGA-O1A
33	D	409	LHG	O10-C23-C24-C25
23	C	513	CLA	C4C-C3C-CAC-CBC
29	C	517	DGD	C6B-C7B-C8B-C9B
29	c	517	DGD	C4A-C5A-C6A-C7A
23	a	407	CLA	CAA-CBA-CGA-O1A
27	m	101	LMG	O9-C10-C11-C12
33	e	101	LHG	O10-C23-C24-C25
26	a	409	PL9	C12-C11-C9-C8
29	c	516	DGD	C2E-C1E-O5D-C6D
23	C	506	CLA	C10-C11-C12-C13
27	b	622	LMG	C32-C33-C34-C35
26	a	409	PL9	C3-C7-C8-C9
33	D	408	LHG	C4-O6-P-O5
33	D	409	LHG	C4-O6-P-O5
23	b	617	CLA	C11-C12-C13-C14
27	a	414	LMG	C15-C16-C17-C18
23	d	404	CLA	C8-C10-C11-C12
29	C	517	DGD	C3A-C4A-C5A-C6A
29	c	516	DGD	CDB-CEB-CFB-CGB
25	c	515	BCR	C23-C24-C25-C26
23	C	507	CLA	C15-C16-C17-C18
29	a	413	DGD	C9B-CAB-CBB-CCB
29	c	516	DGD	O2G-C1B-C2B-C3B
23	a	407	CLA	C15-C16-C17-C18
34	E	102	HEM	CAD-CBD-CGD-O2D
33	L	101	LHG	C24-C25-C26-C27
26	a	409	PL9	C47-C48-C49-C51
25	B	619	BCR	C10-C11-C12-C13
26	D	406	PL9	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C33-C34-C36-C37
26	a	409	PL9	C13-C14-C16-C17
23	B	614	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
29	a	413	DGD	C1G-C2G-O2G-C1B
27	b	623	LMG	C28-C29-C30-C31
23	C	510	CLA	C6-C7-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	C	512	CLA	C14-C13-C15-C16
23	D	402	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C12-C13-C14
23	c	513	CLA	C14-C13-C15-C16
29	c	518	DGD	O1B-C1B-C2B-C3B
23	h	101	CLA	CAA-CBA-CGA-O2A
27	a	414	LMG	O8-C28-C29-C30
27	D	407	LMG	O7-C10-C11-C12
29	A	413	DGD	O2G-C1B-C2B-C3B
33	e	101	LHG	O8-C23-C24-C25
26	D	406	PL9	C41-C42-C43-C44
33	l	101	LHG	C12-C13-C14-C15
27	B	620	LMG	C10-C11-C12-C13
26	a	409	PL9	C17-C18-C19-C21
23	A	404	CLA	C11-C10-C8-C7
23	B	601	CLA	C2-C3-C5-C6
23	B	602	CLA	C3A-C2A-CAA-CBA
23	B	603	CLA	C11-C10-C8-C7
23	C	508	CLA	C12-C13-C15-C16
23	b	603	CLA	C6-C7-C8-C10
23	b	609	CLA	C6-C7-C8-C10
23	c	513	CLA	C12-C13-C15-C16
23	c	510	CLA	CAA-CBA-CGA-O2A
25	C	520	BCR	C7-C8-C9-C10
25	D	405	BCR	C17-C18-C19-C20
25	d	405	BCR	C13-C14-C15-C16
27	a	414	LMG	C31-C32-C33-C34
23	B	607	CLA	C15-C16-C17-C18
23	b	606	CLA	C10-C11-C12-C13
24	D	401	PHO	C8-C10-C11-C12
29	c	517	DGD	C2B-C3B-C4B-C5B
23	b	614	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

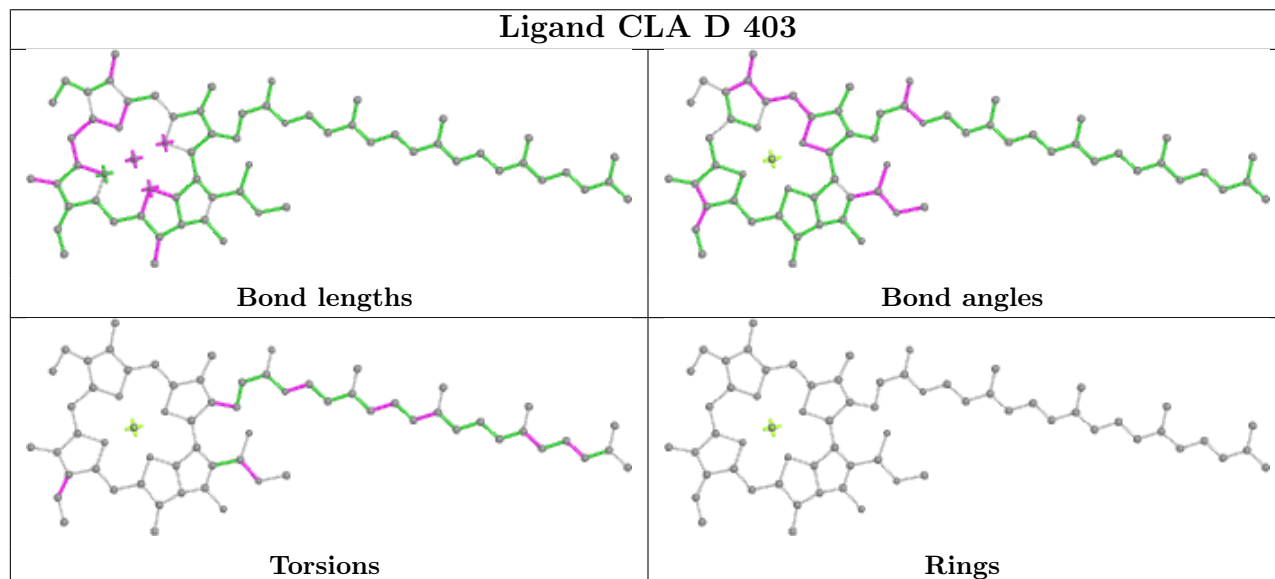
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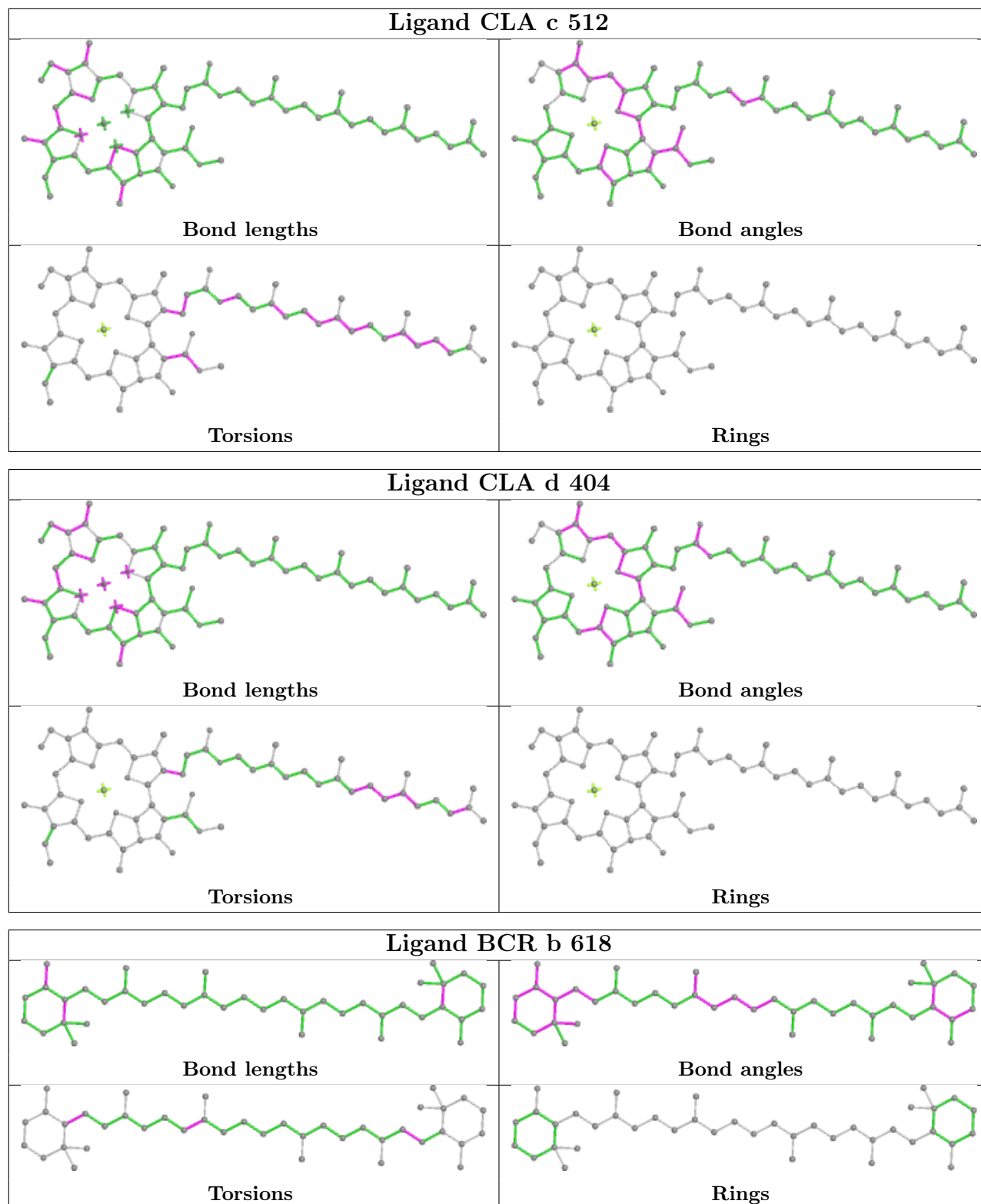
Mol	Chain	Res	Type	Atoms
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23	c	508	CLA	C10-C11-C12-C13
23	c	501	CLA	CAA-CBA-CGA-O1A
23	c	510	CLA	CAA-CBA-CGA-O1A
33	d	407	LHG	O9-C7-C8-C9
28	a	412	SQD	C25-C26-C27-C28
27	A	410	LMG	C8-C9-O8-C28

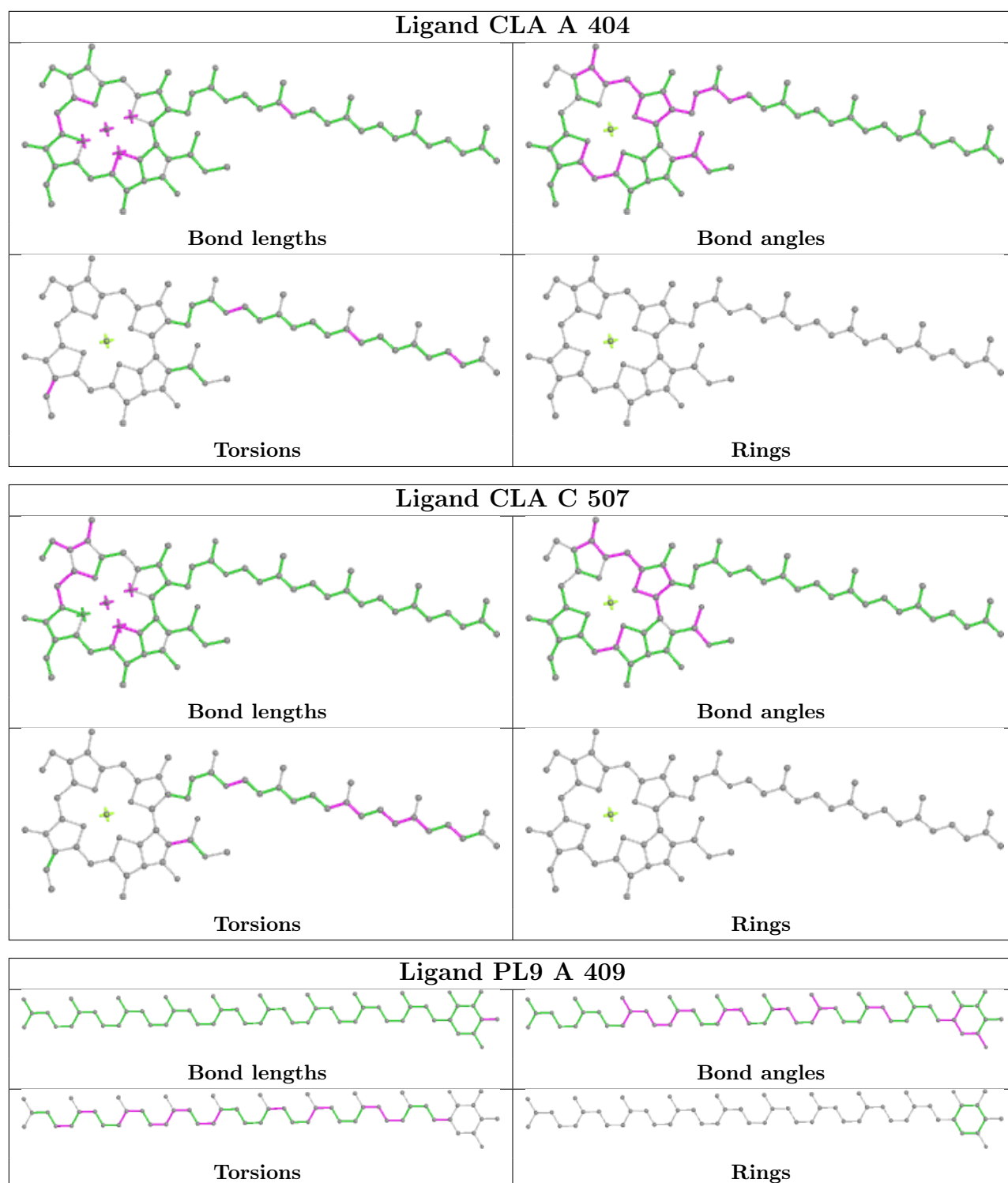
There are no ring outliers.

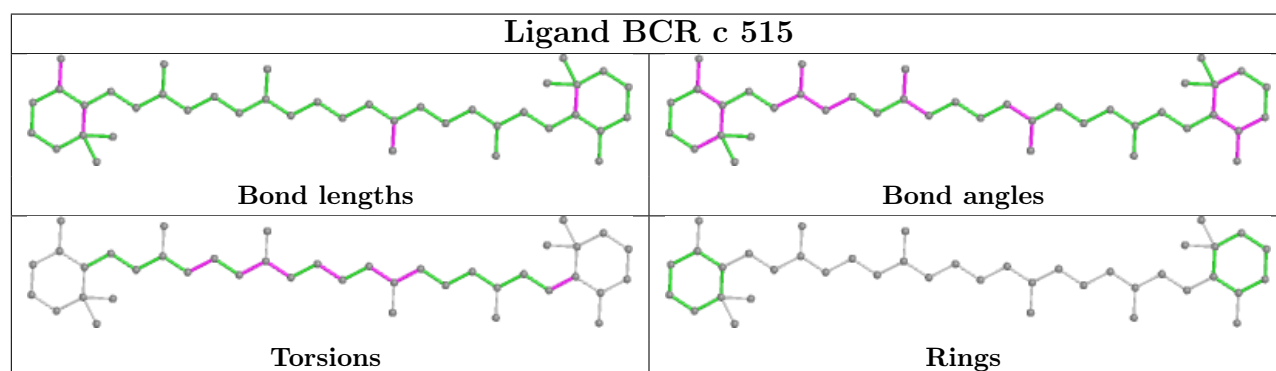
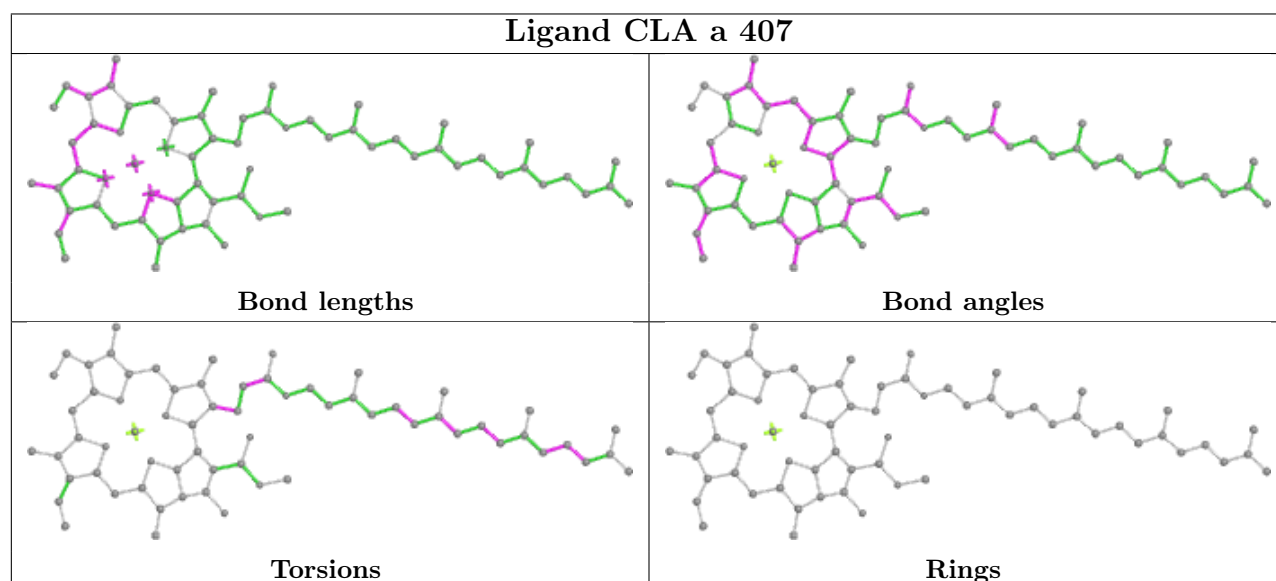
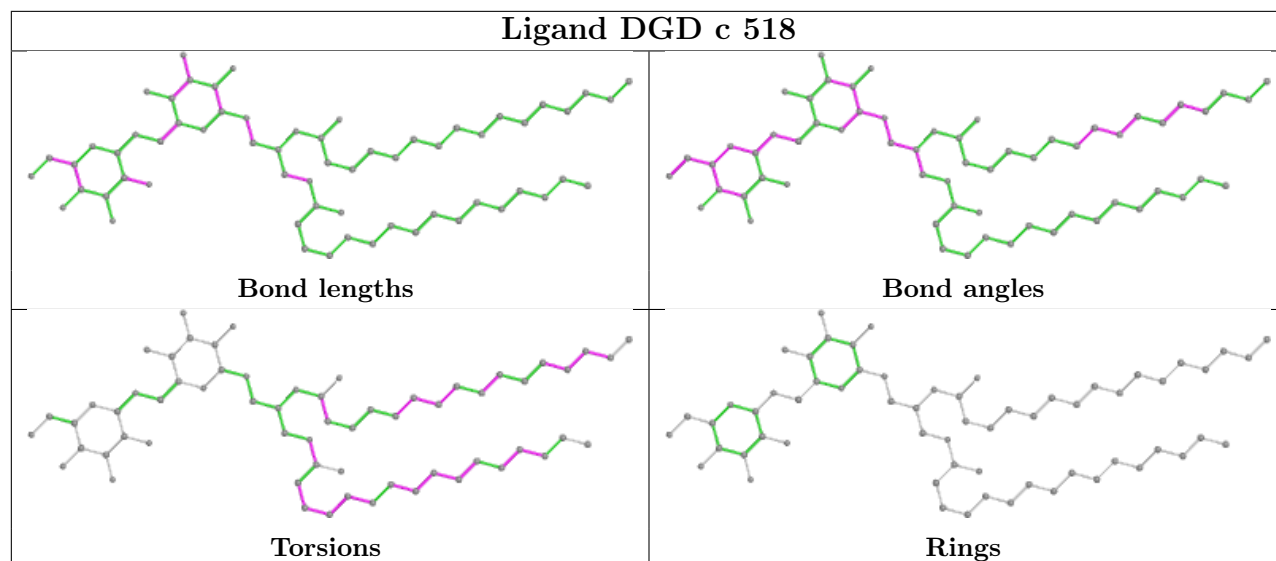
No monomer is involved in short contacts.

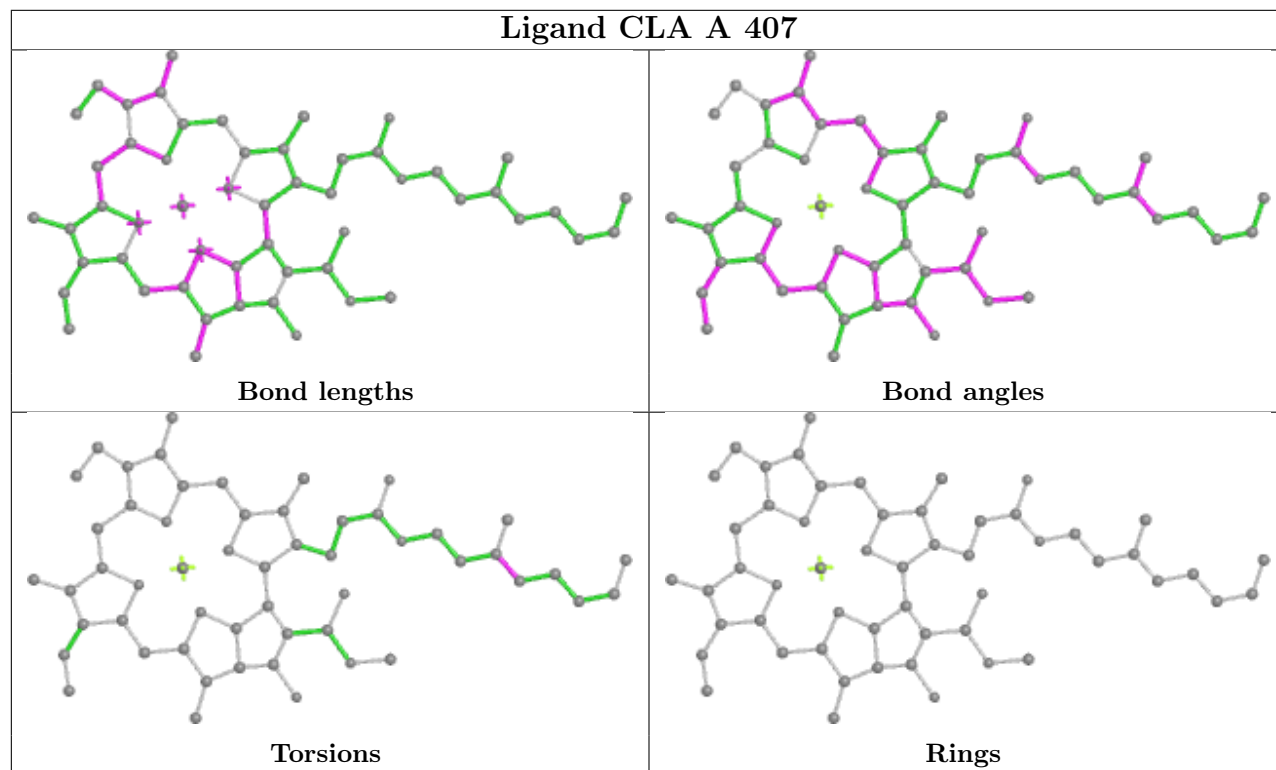
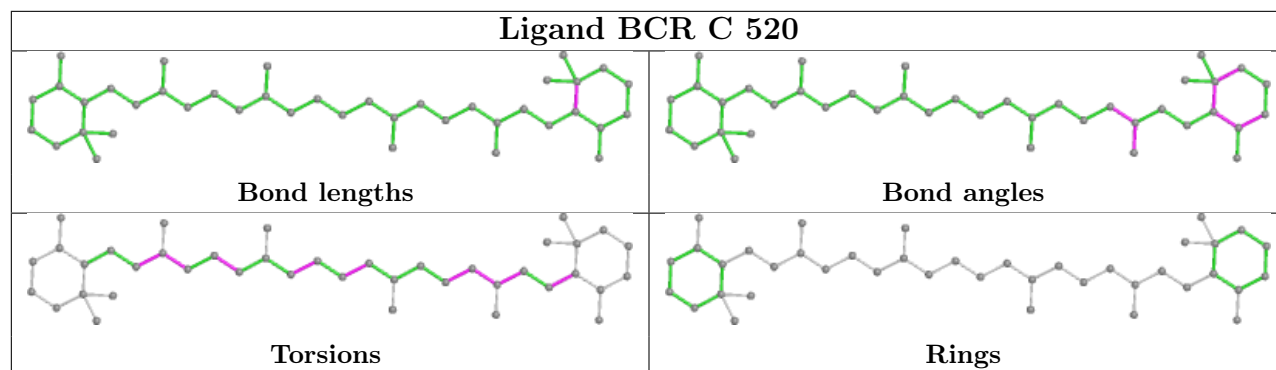
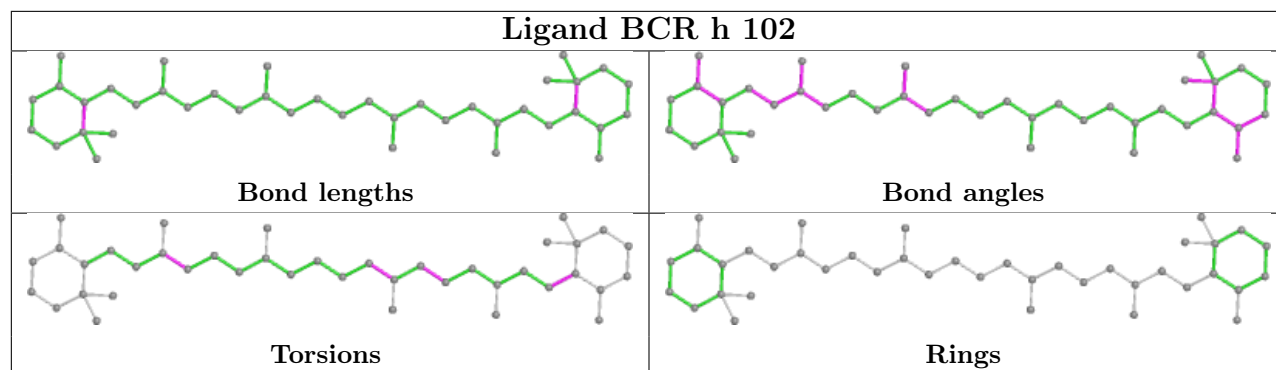
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



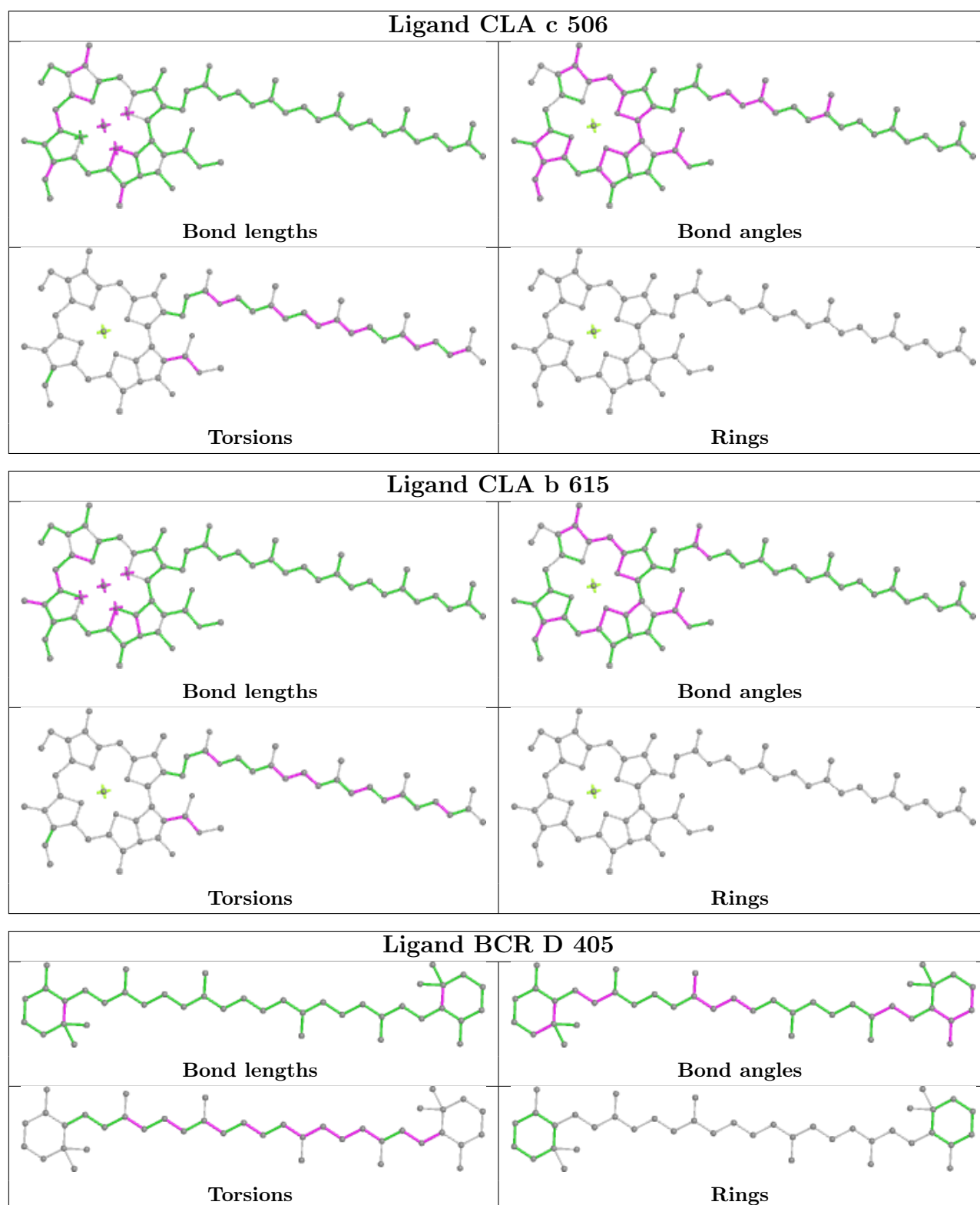


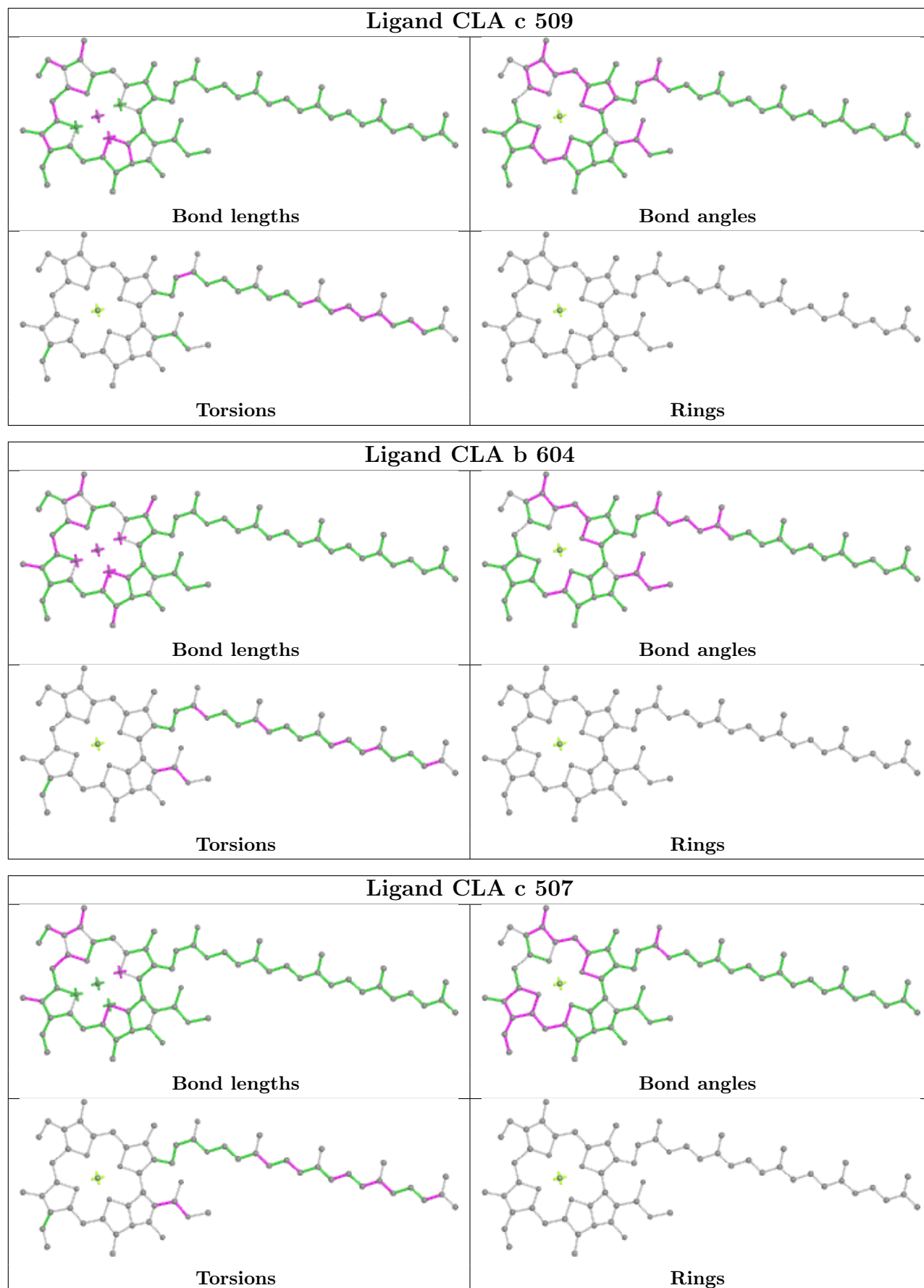


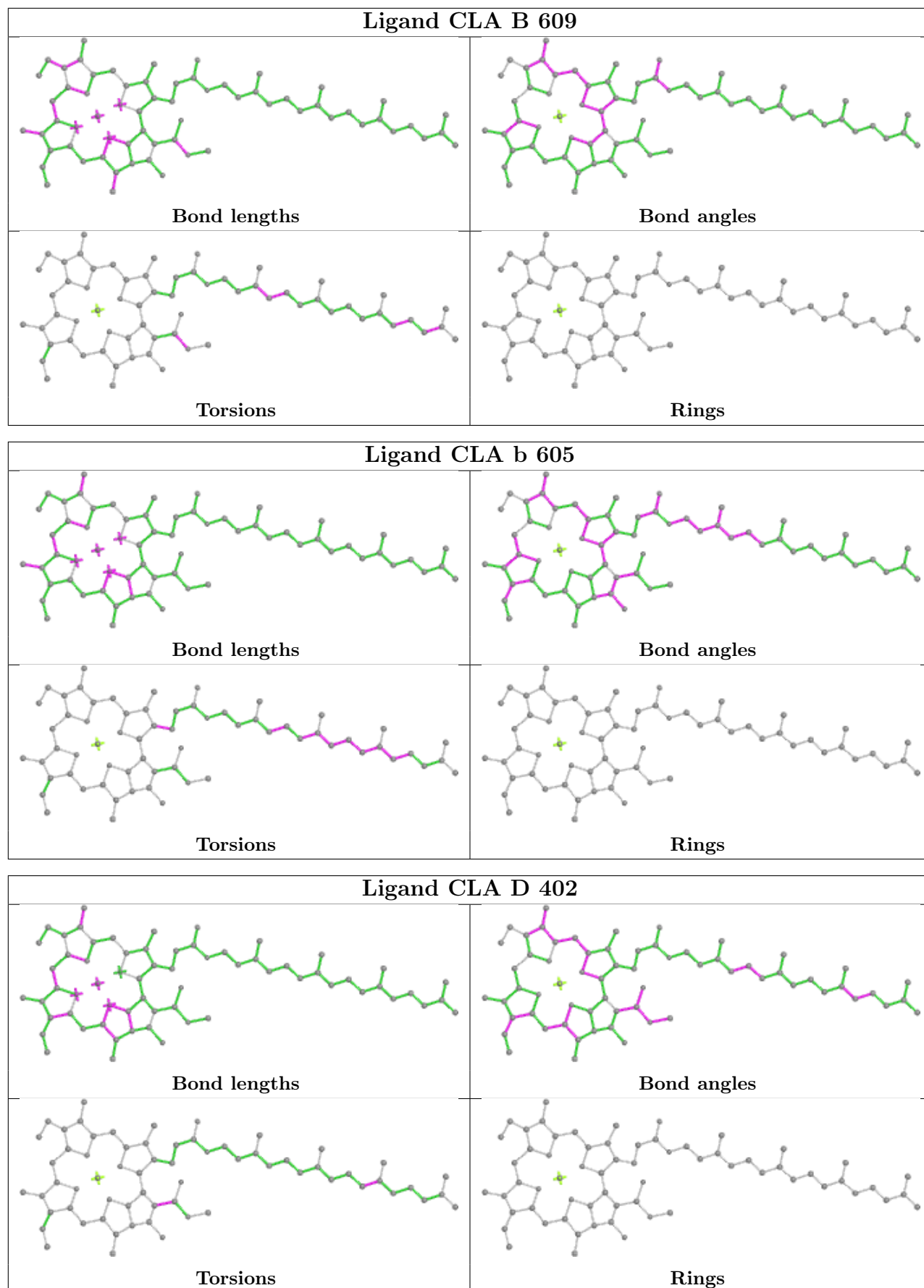


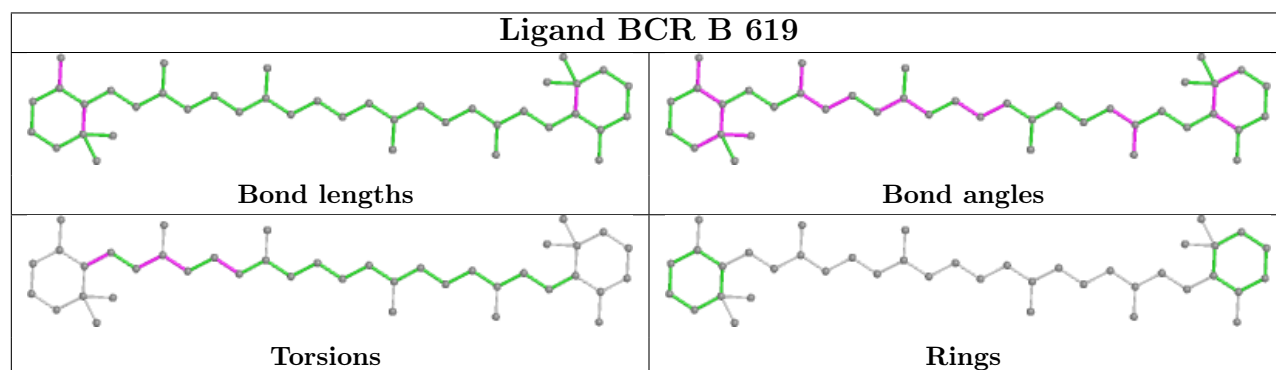
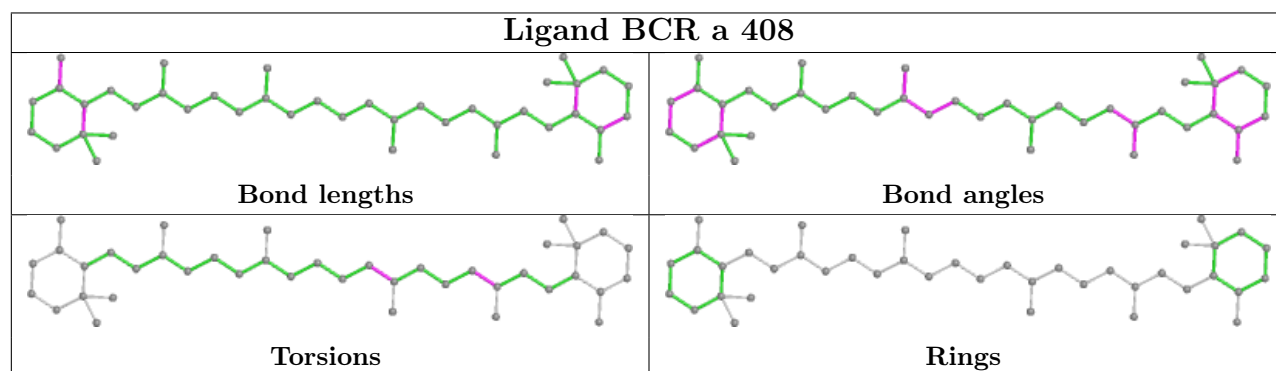
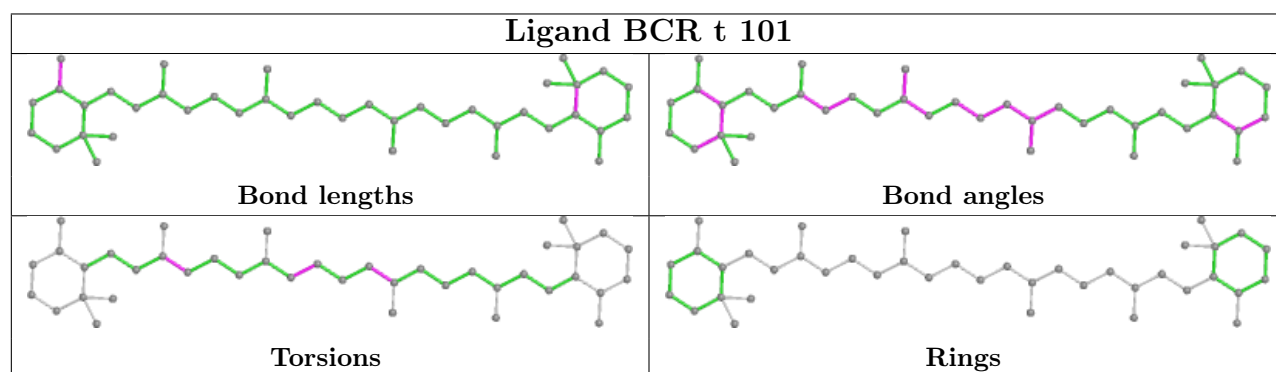
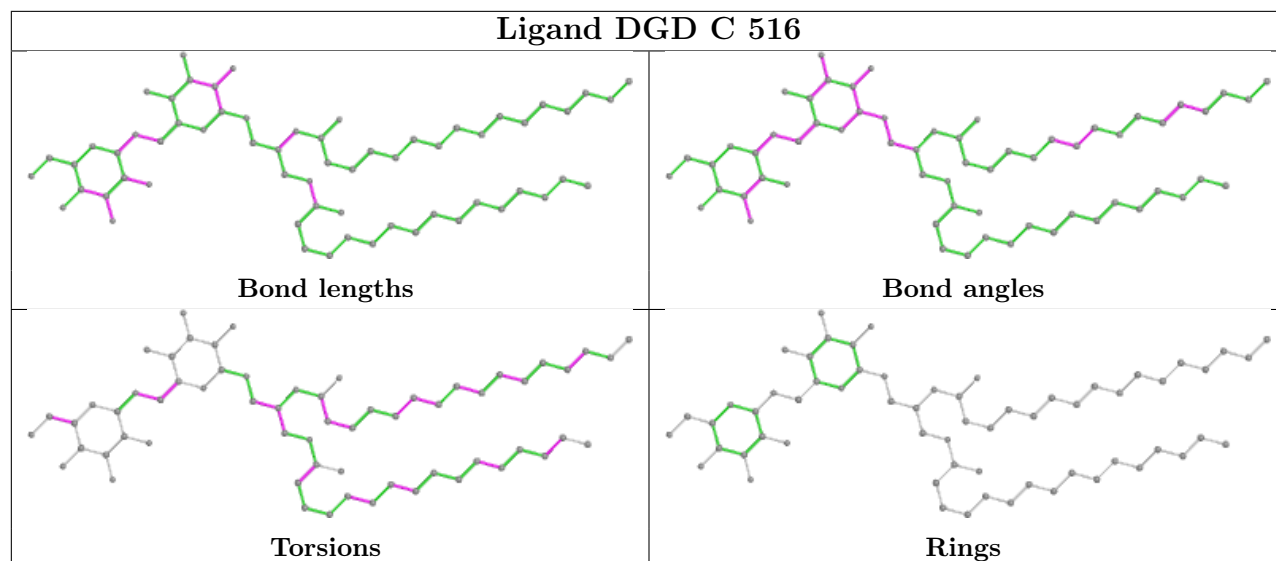


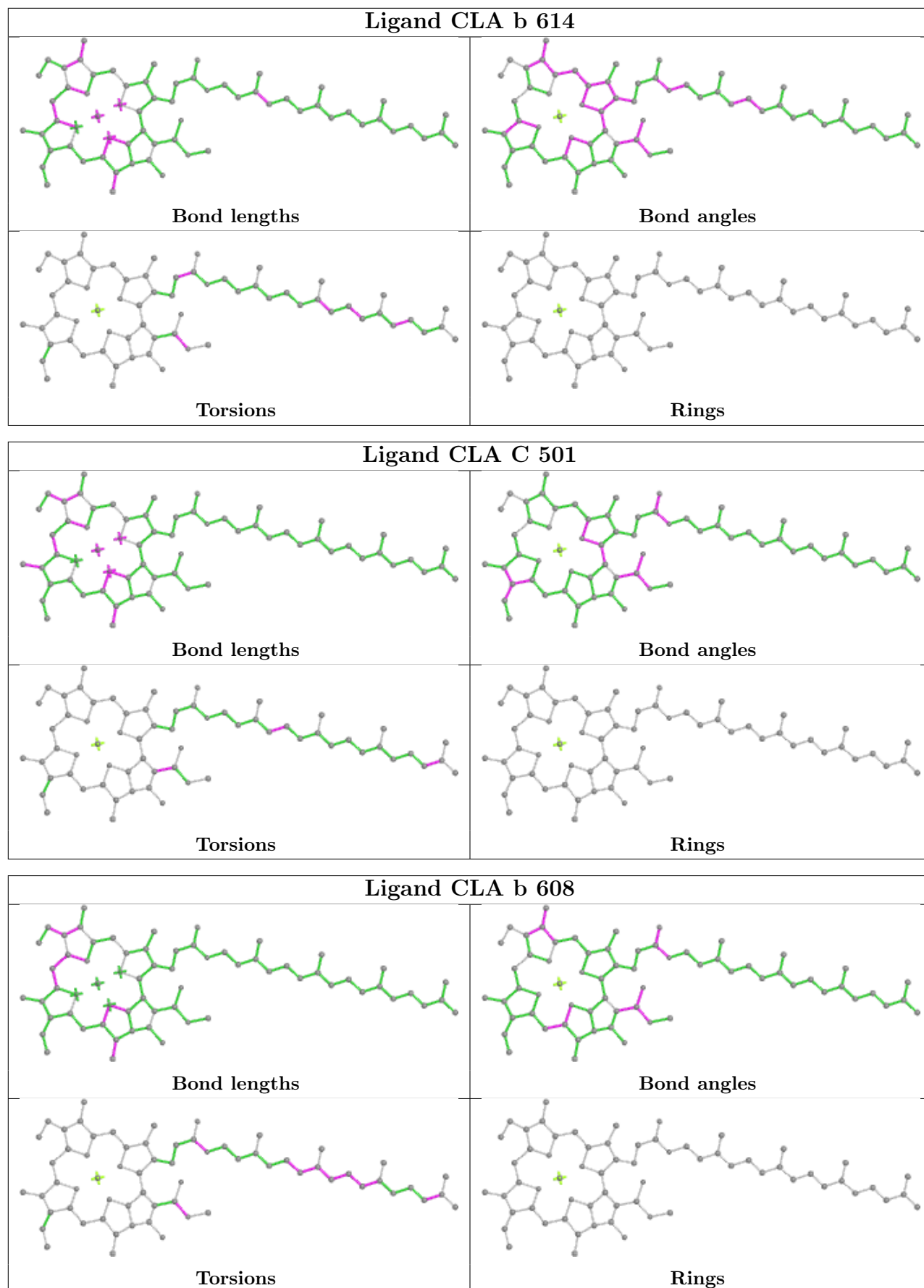


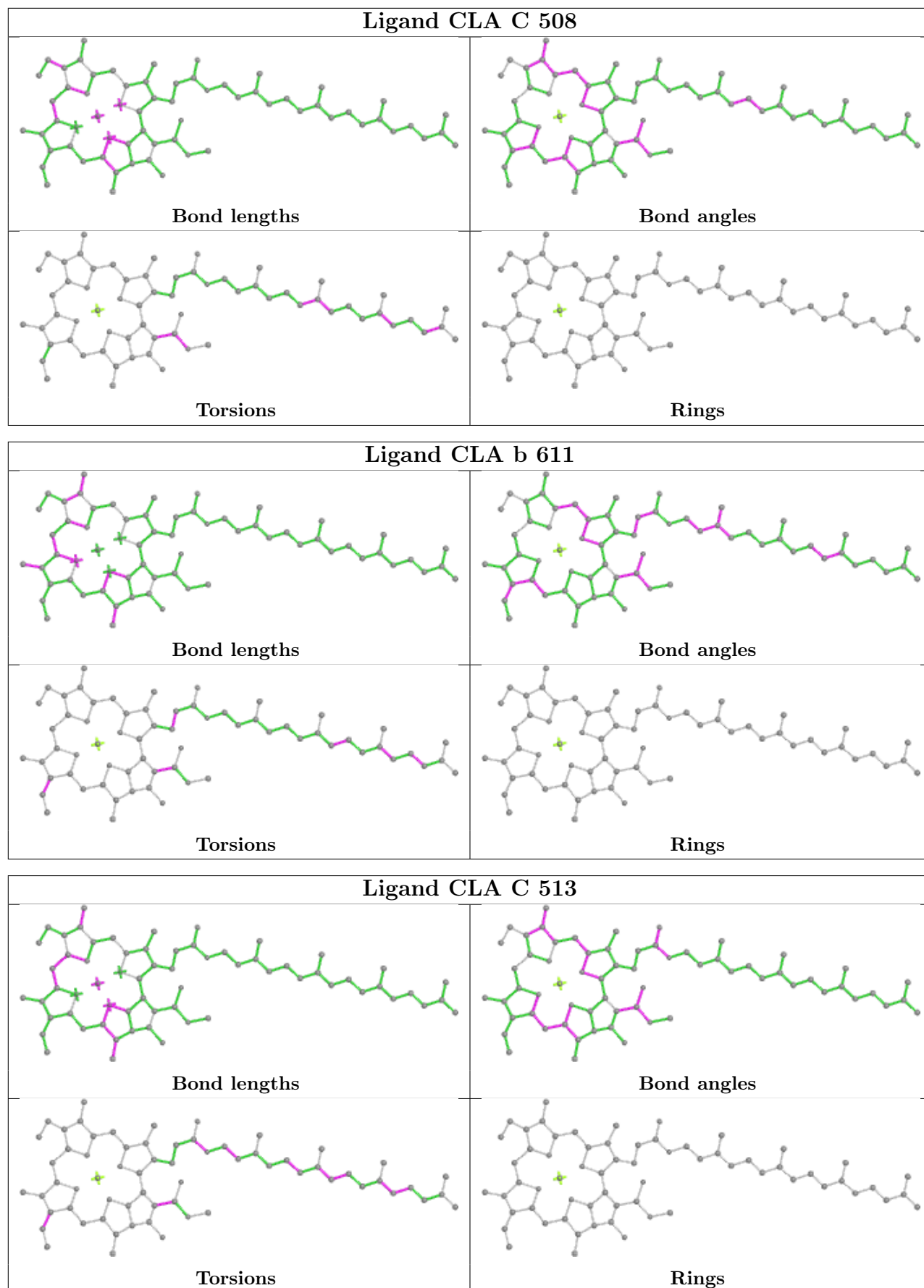


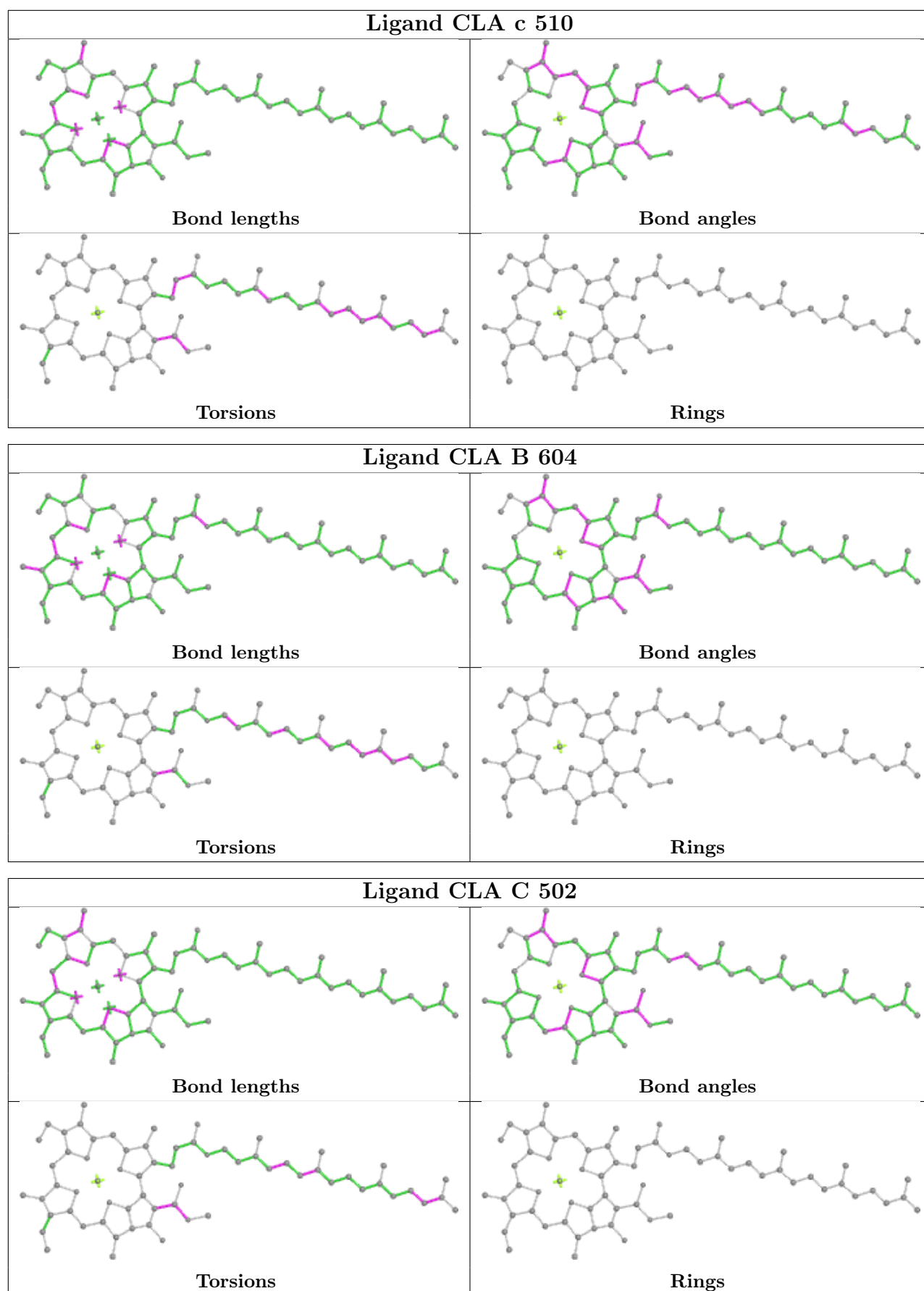


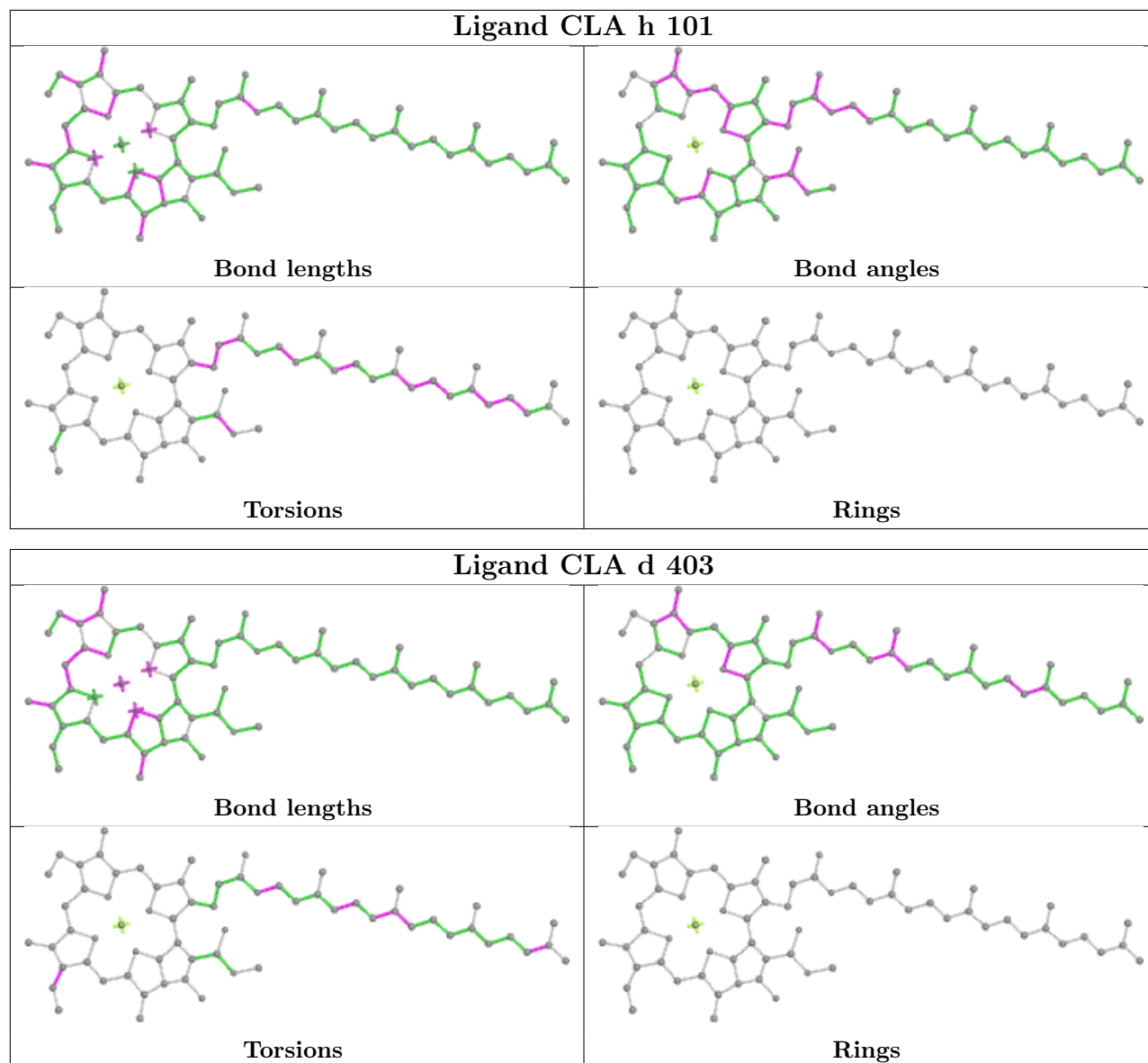




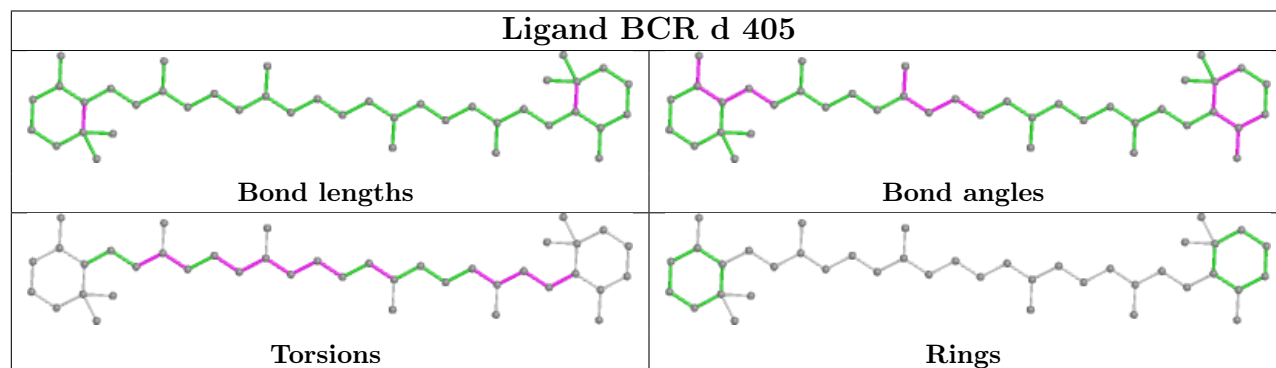
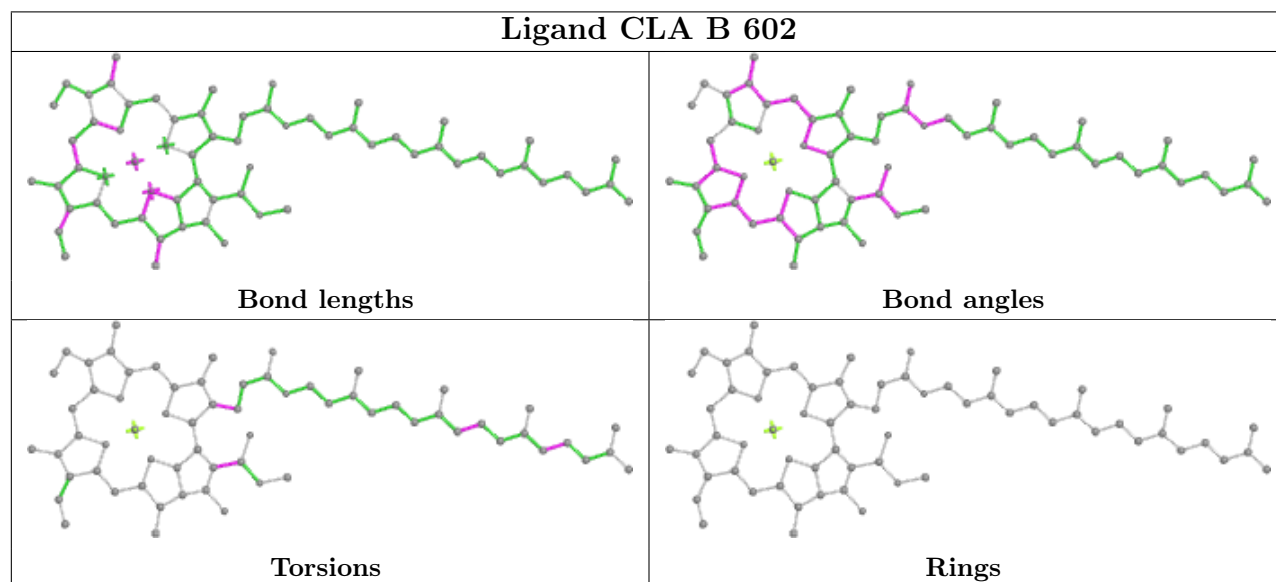
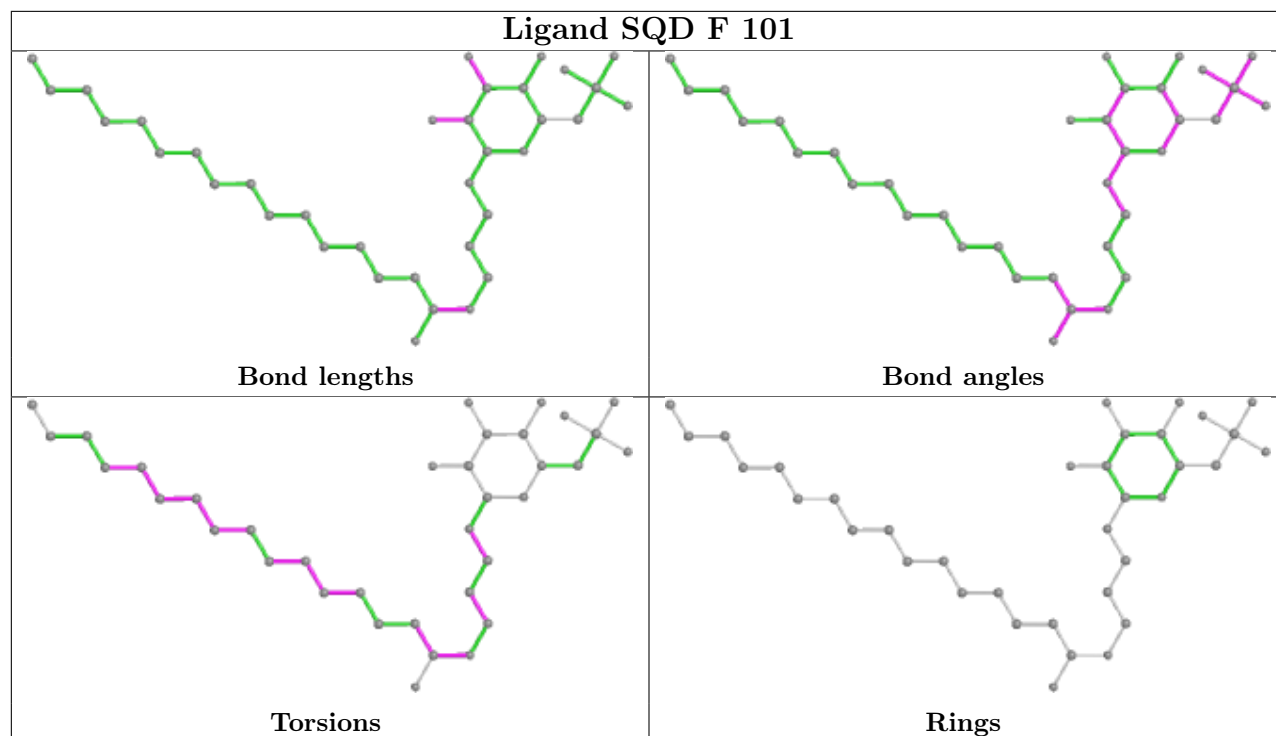


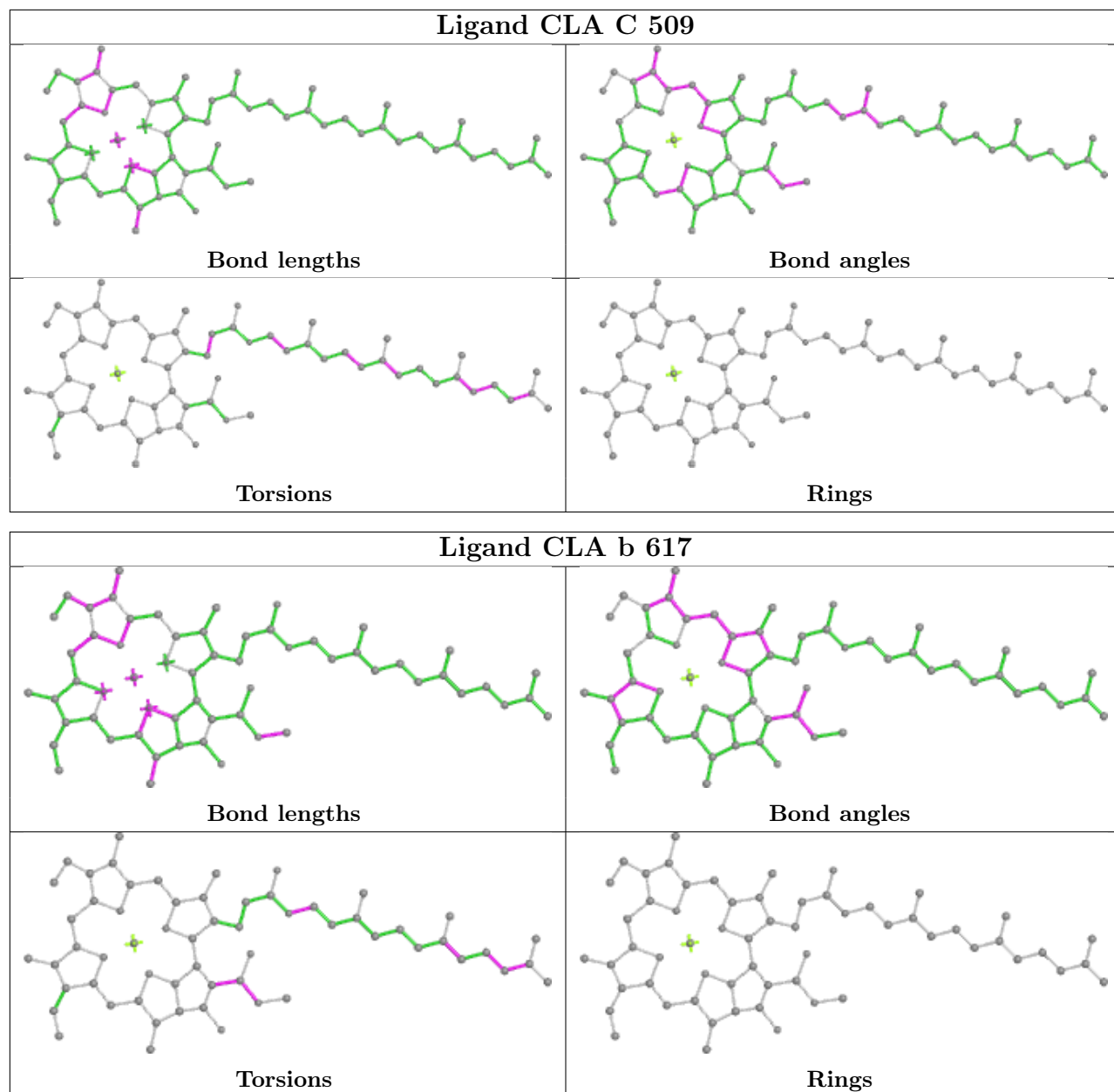


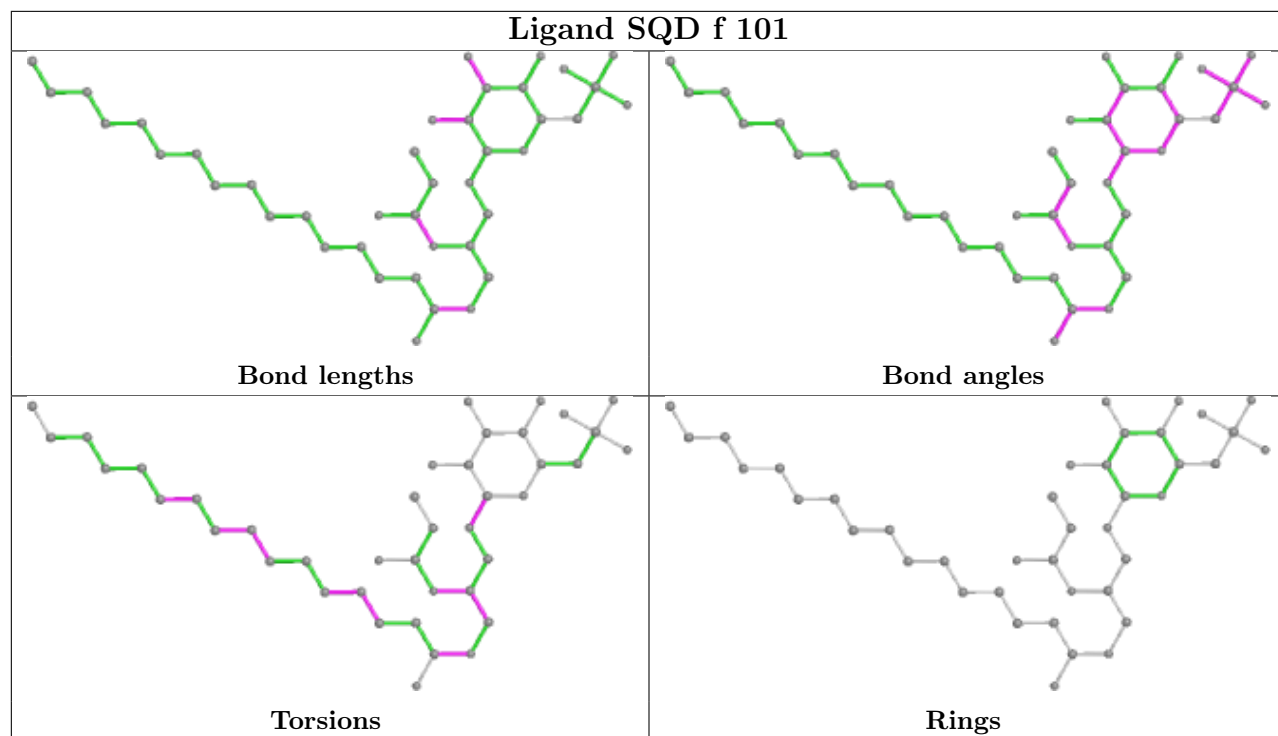


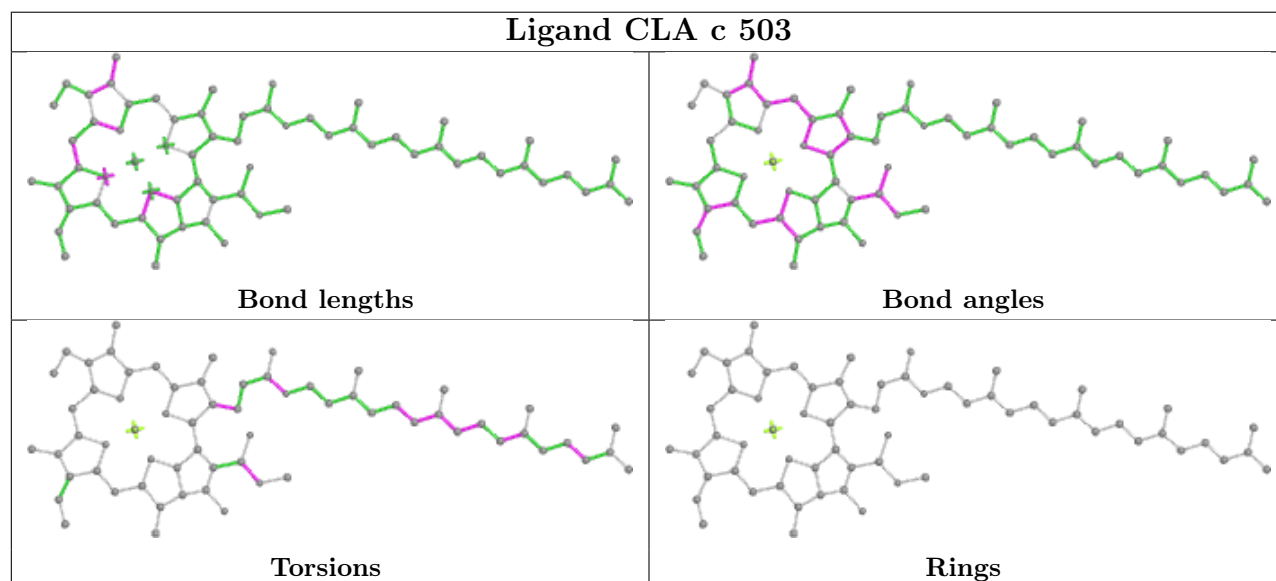
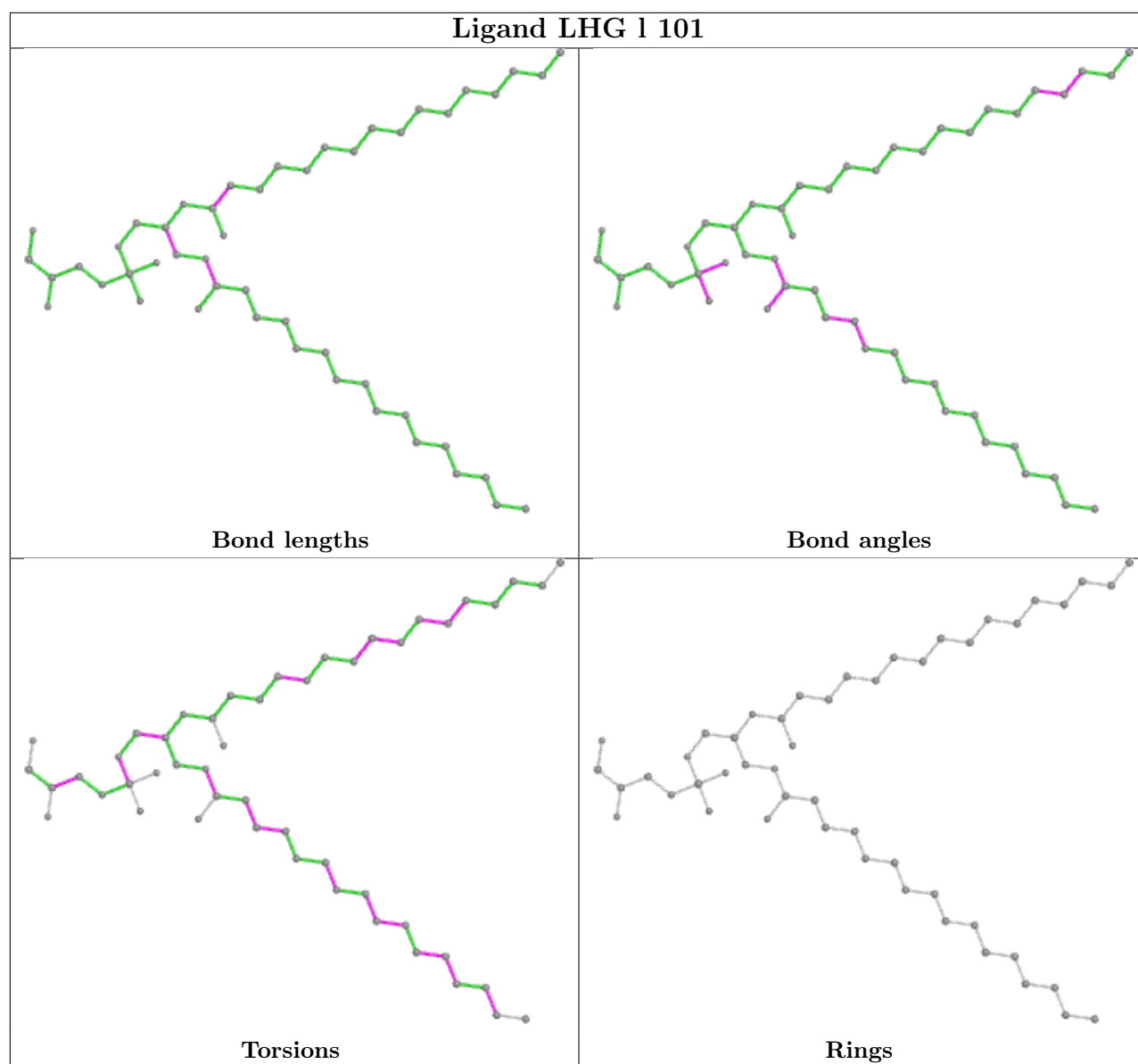


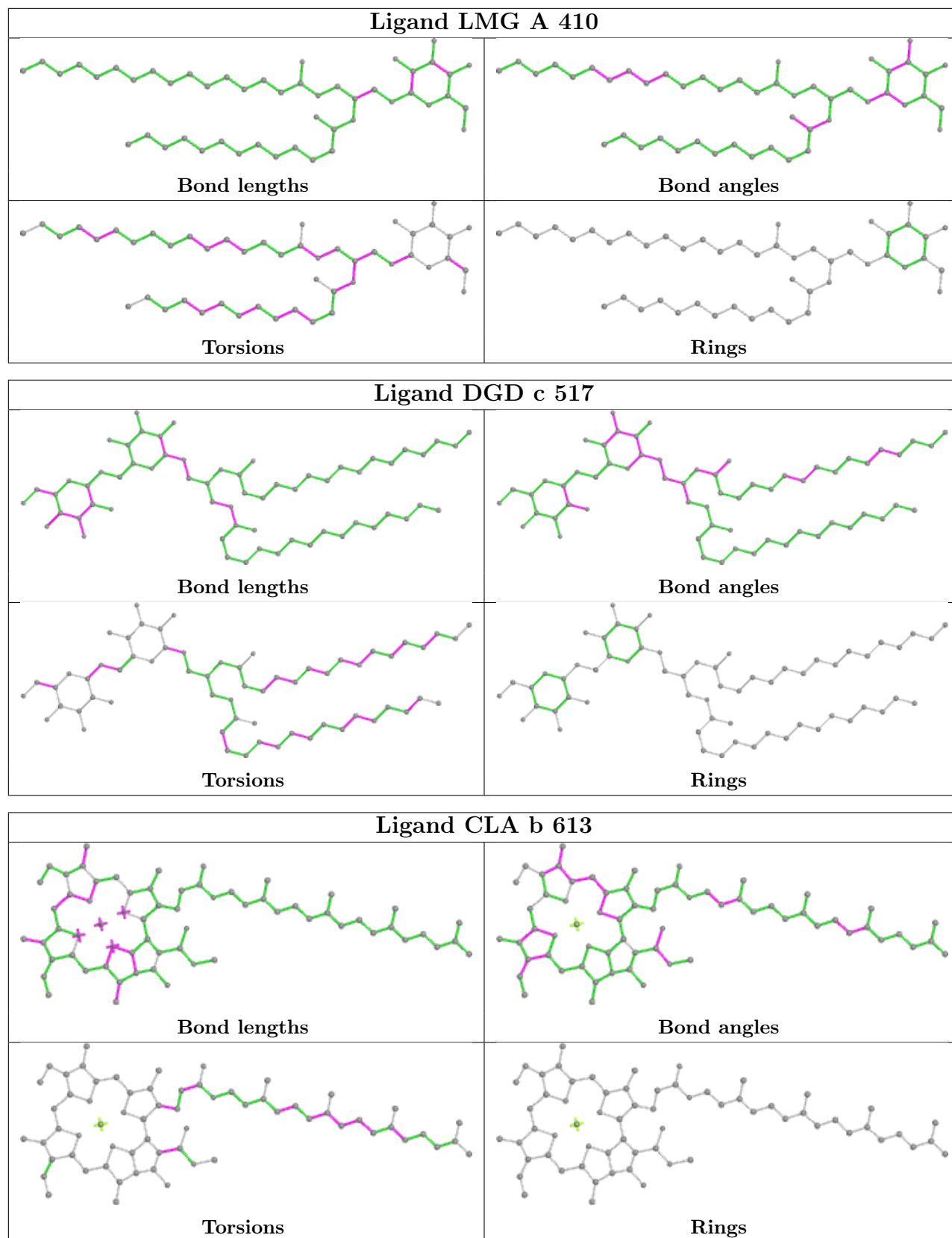


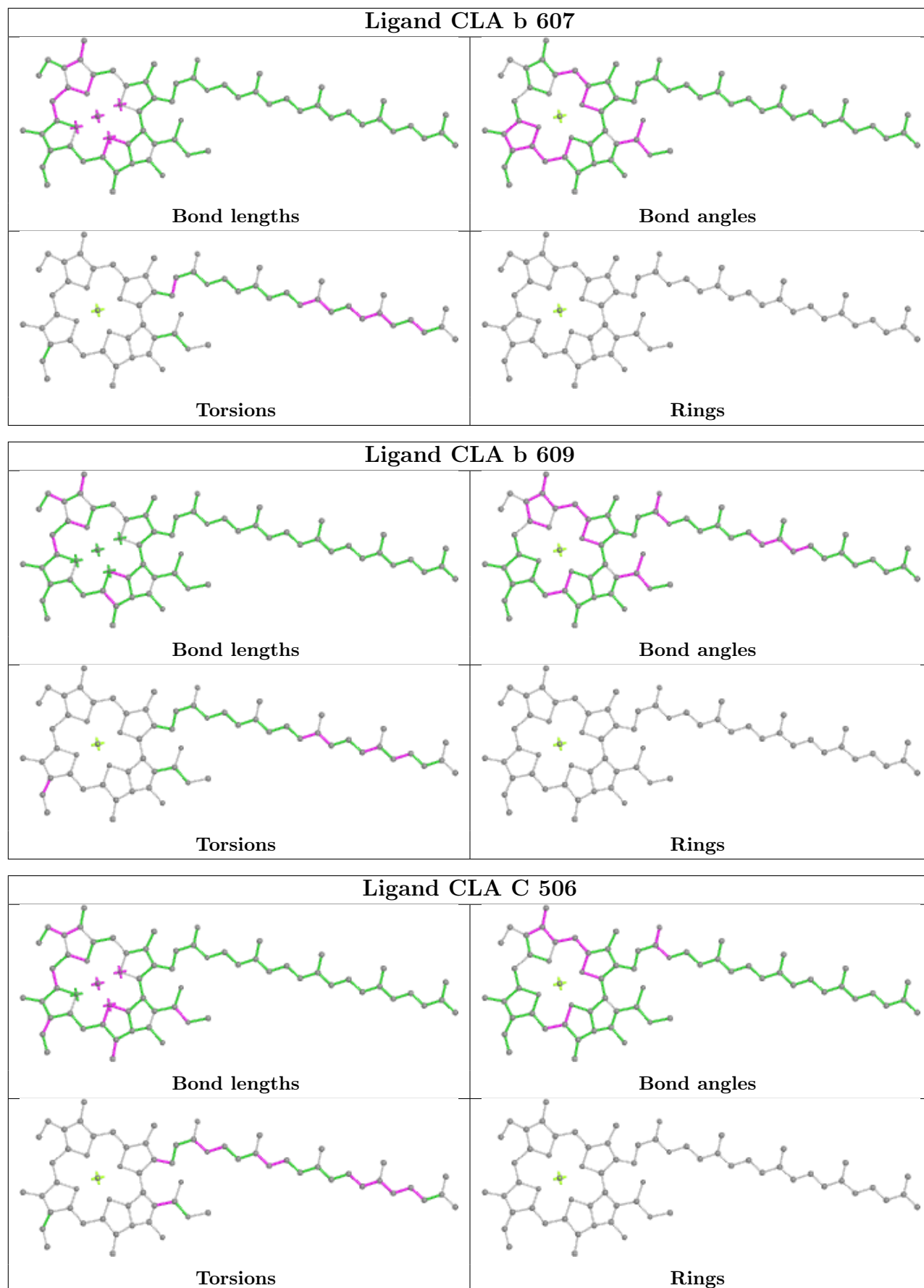


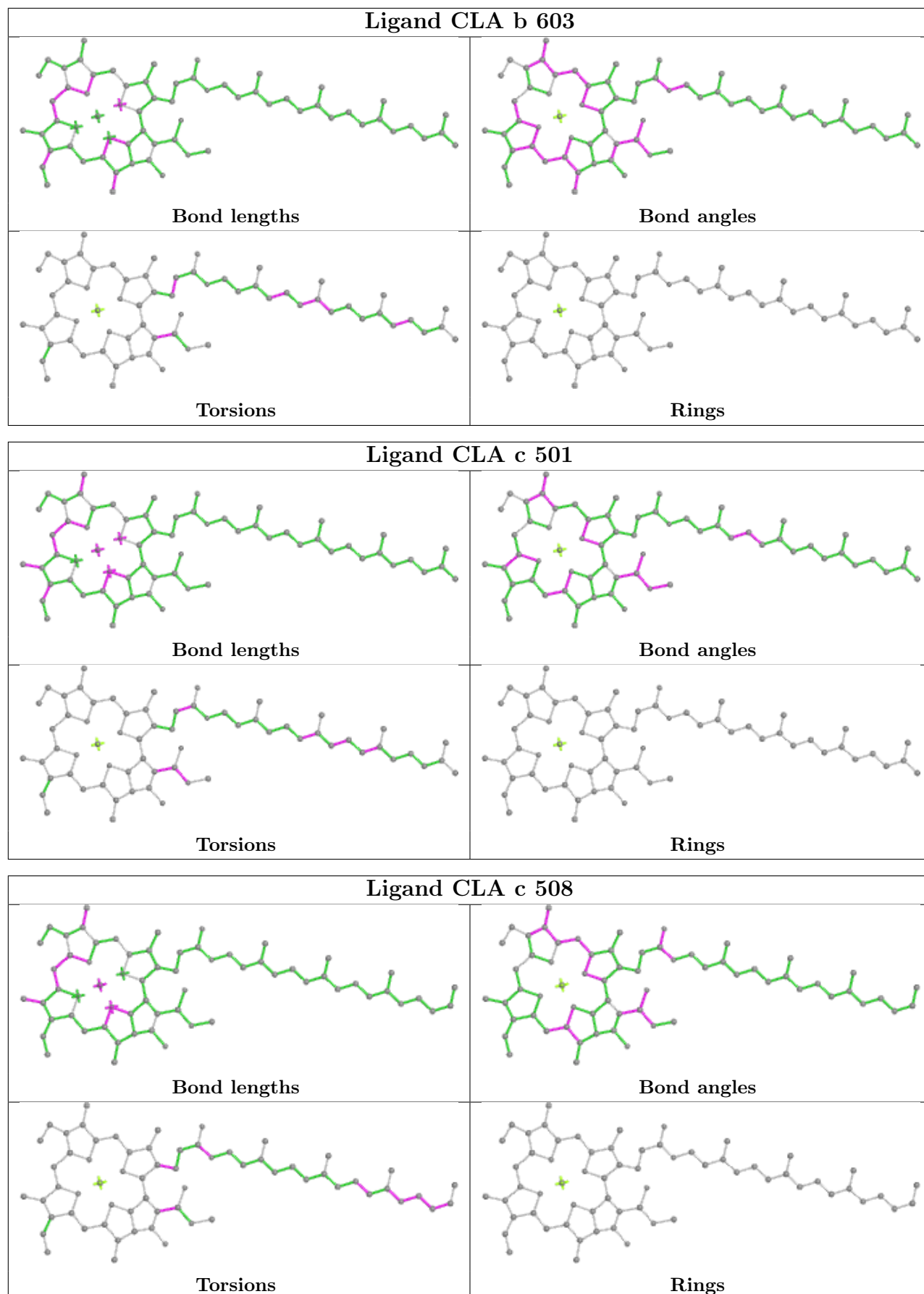


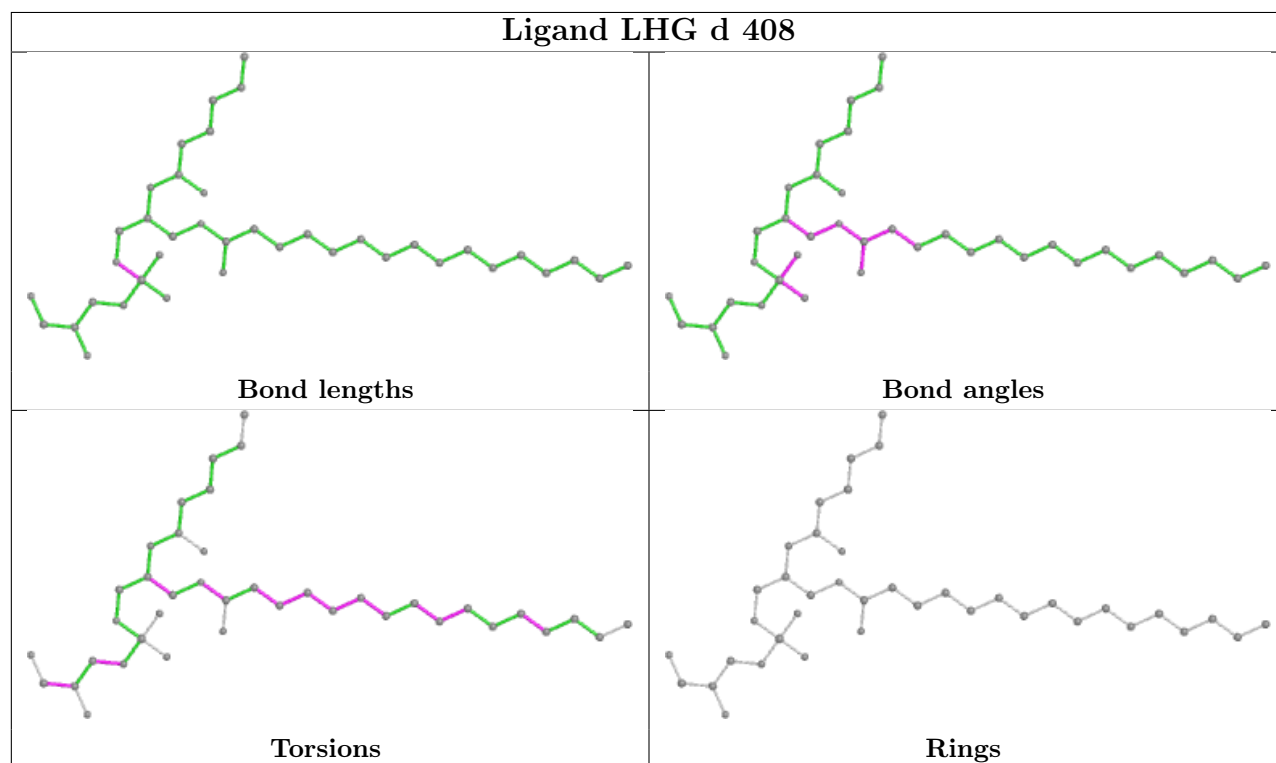
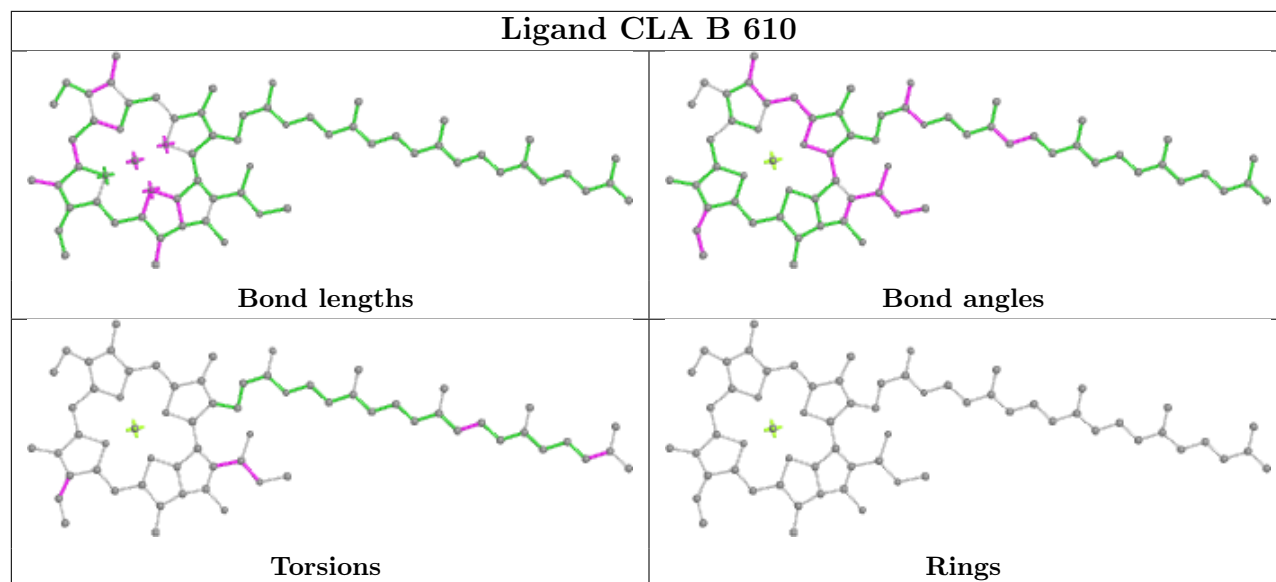




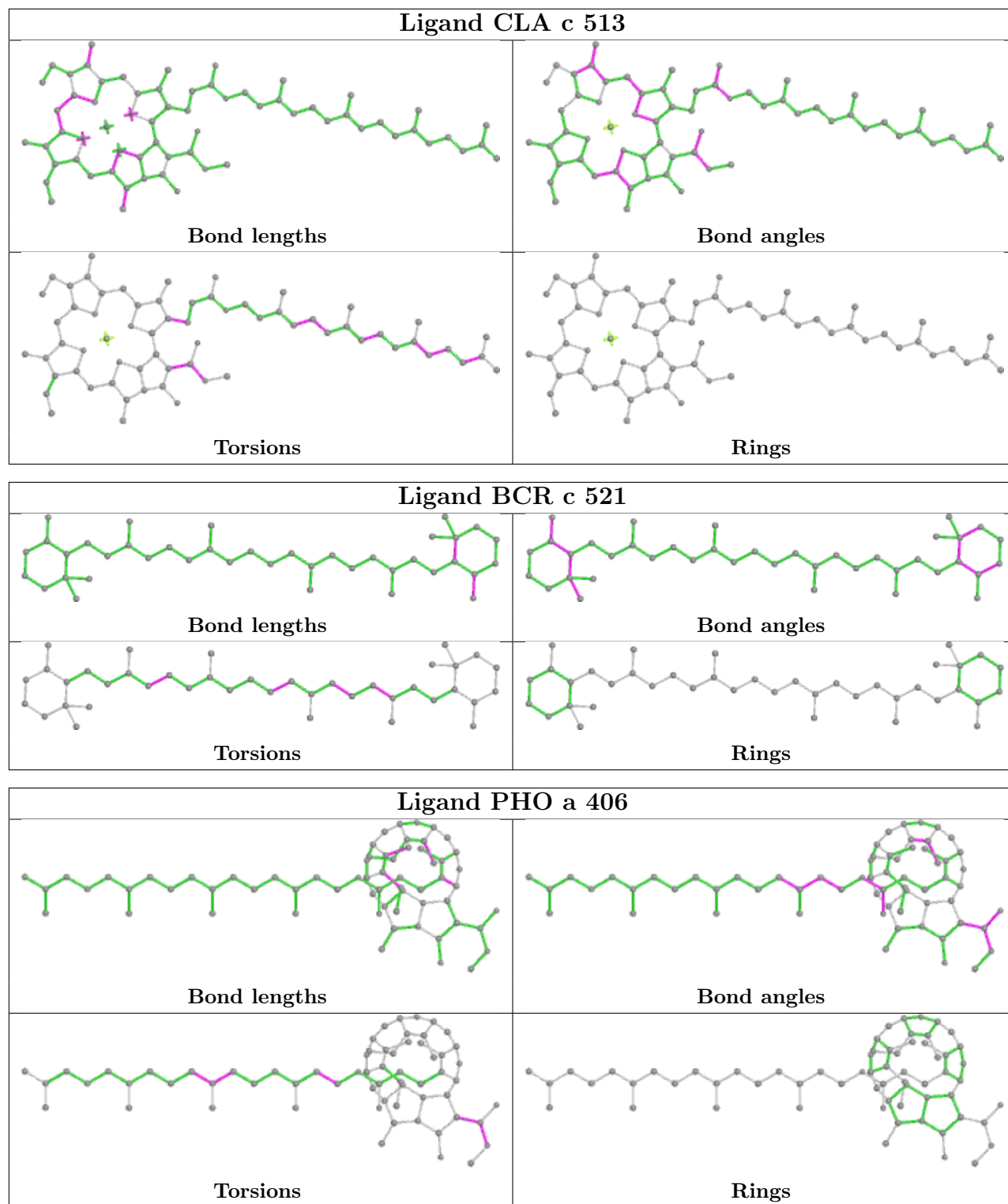


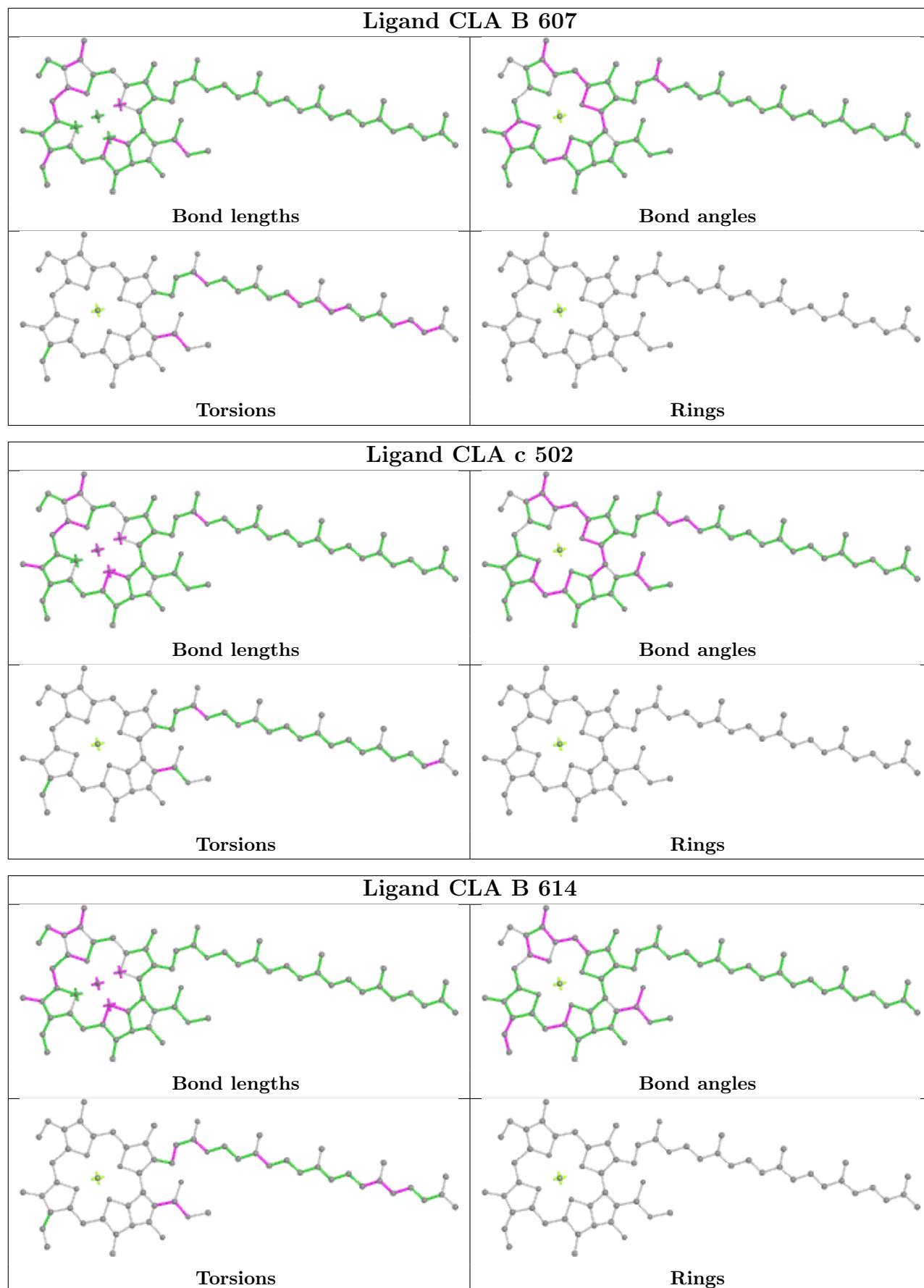


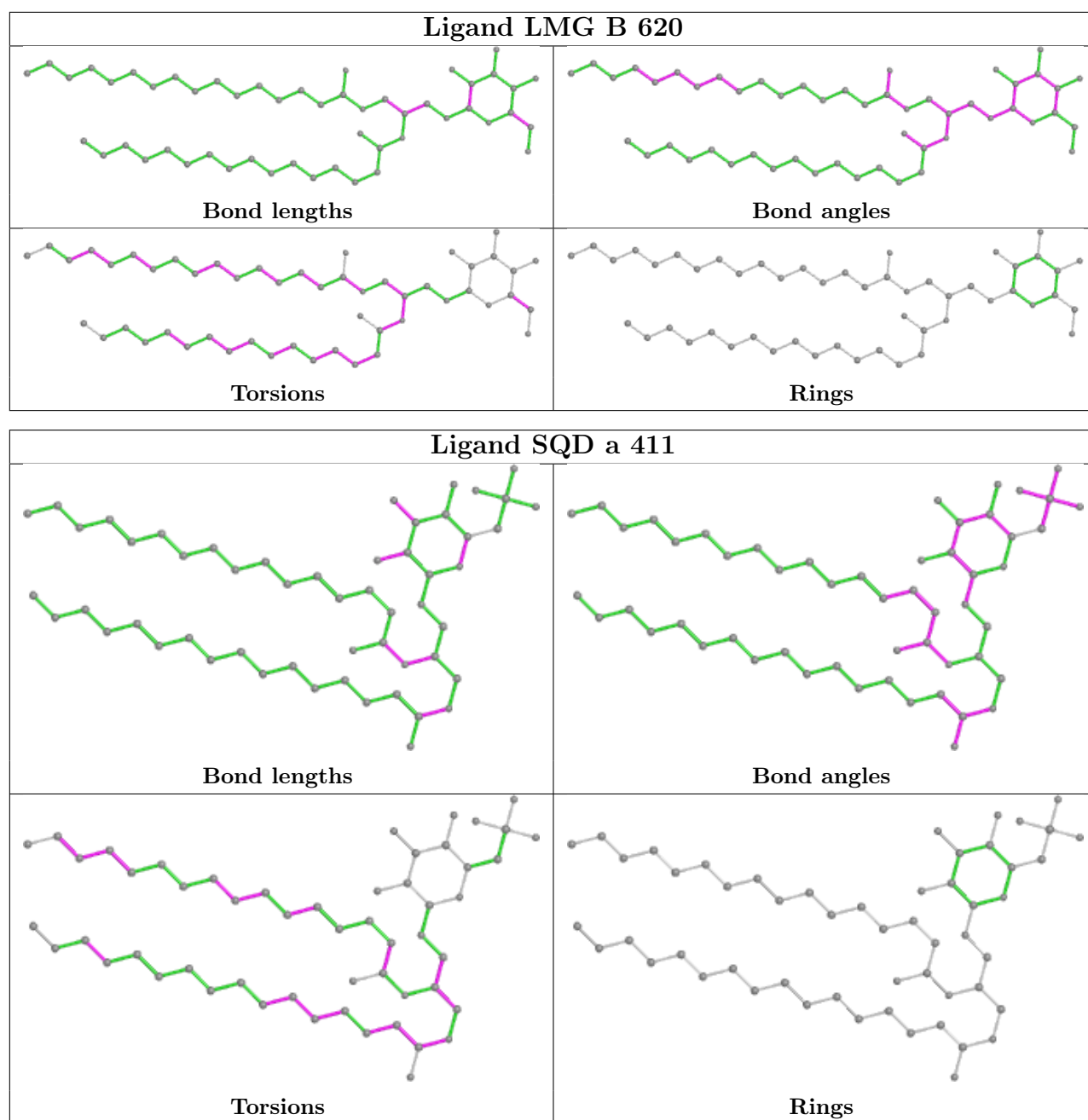


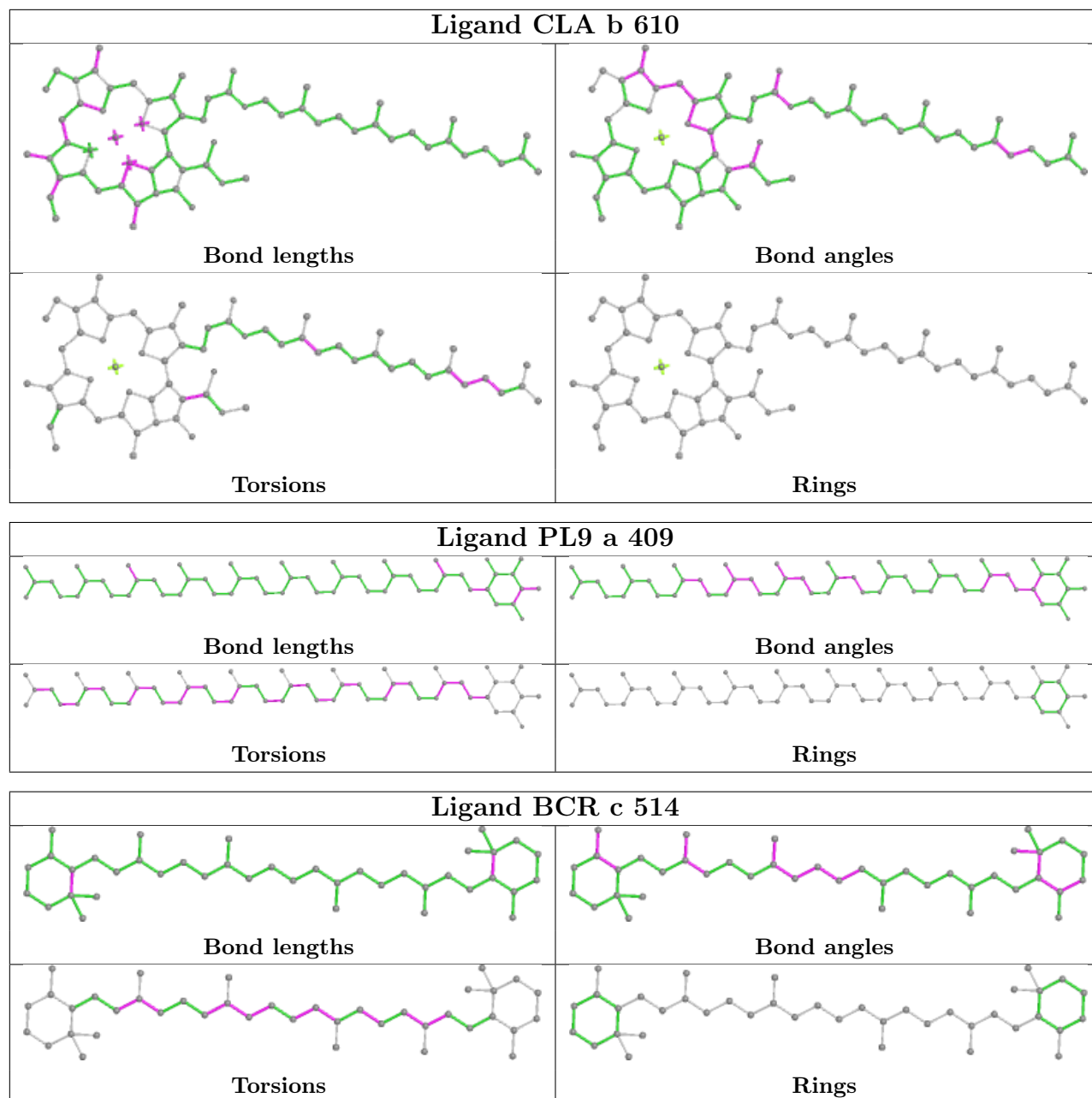


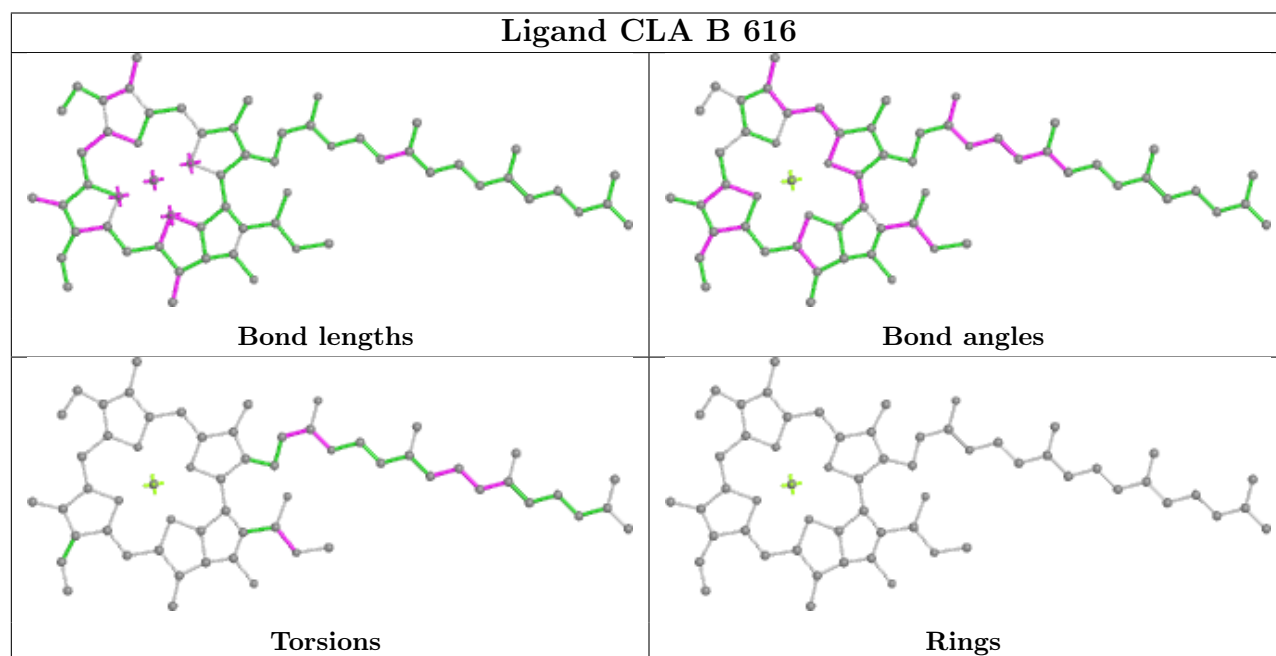
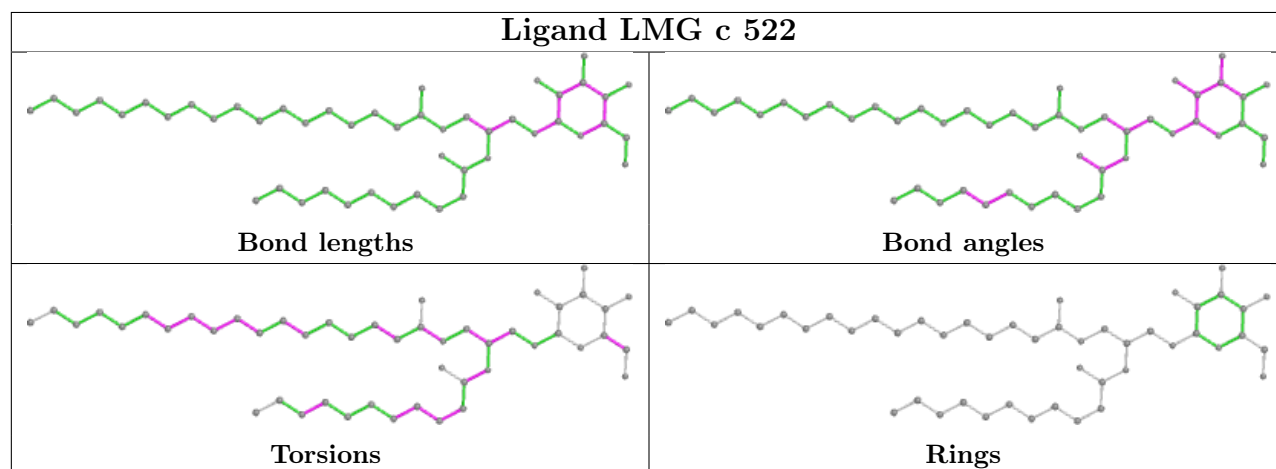
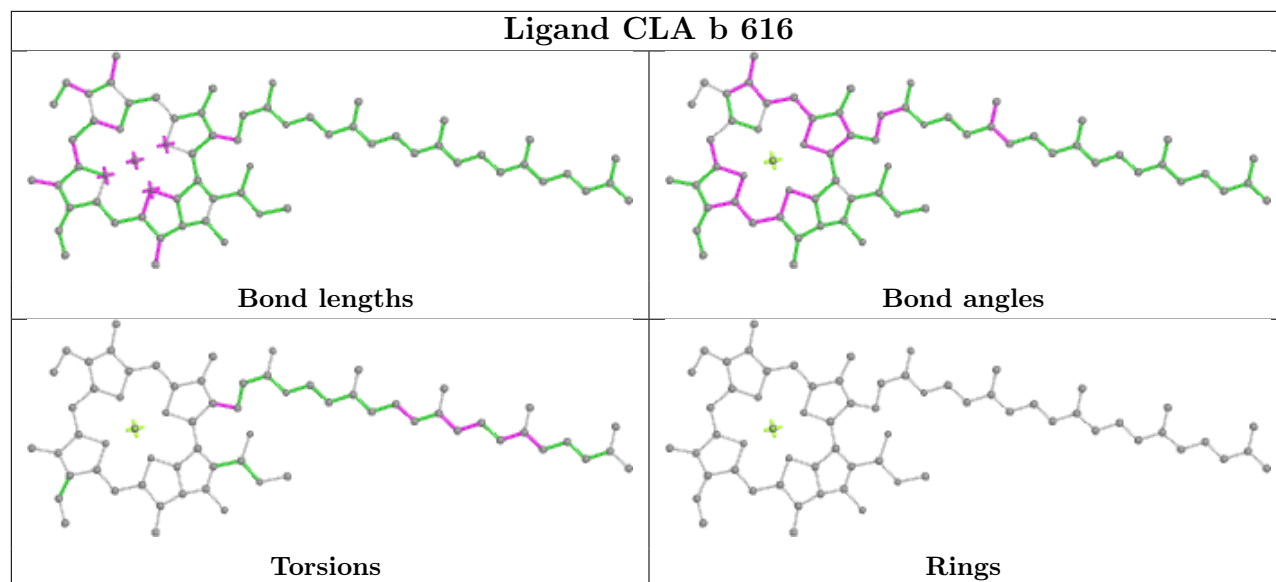


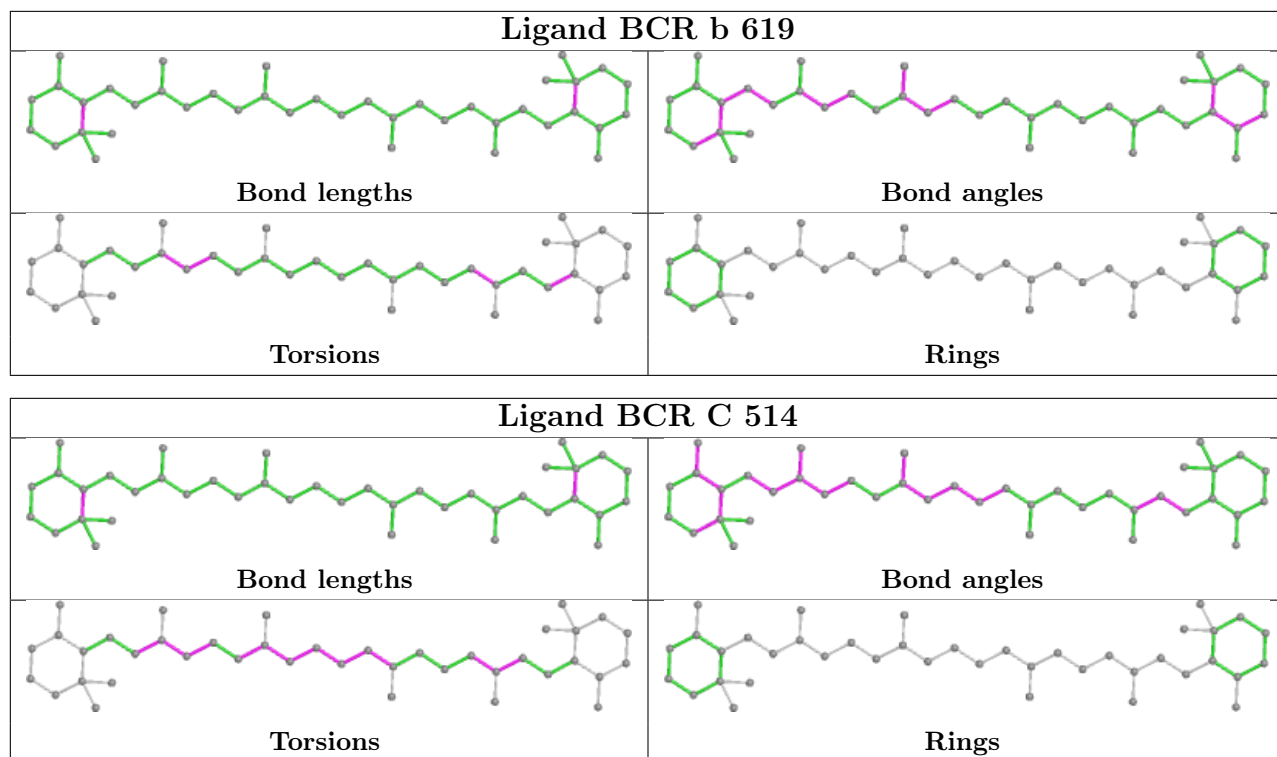


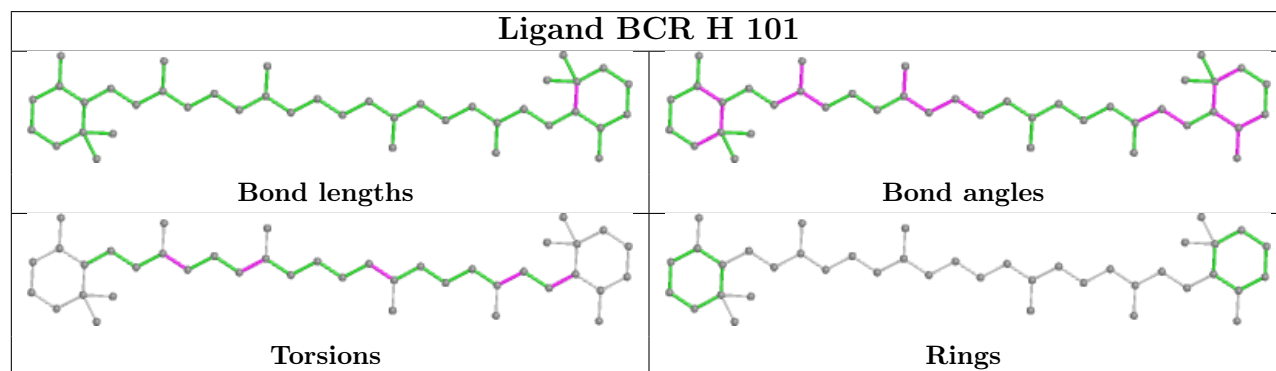
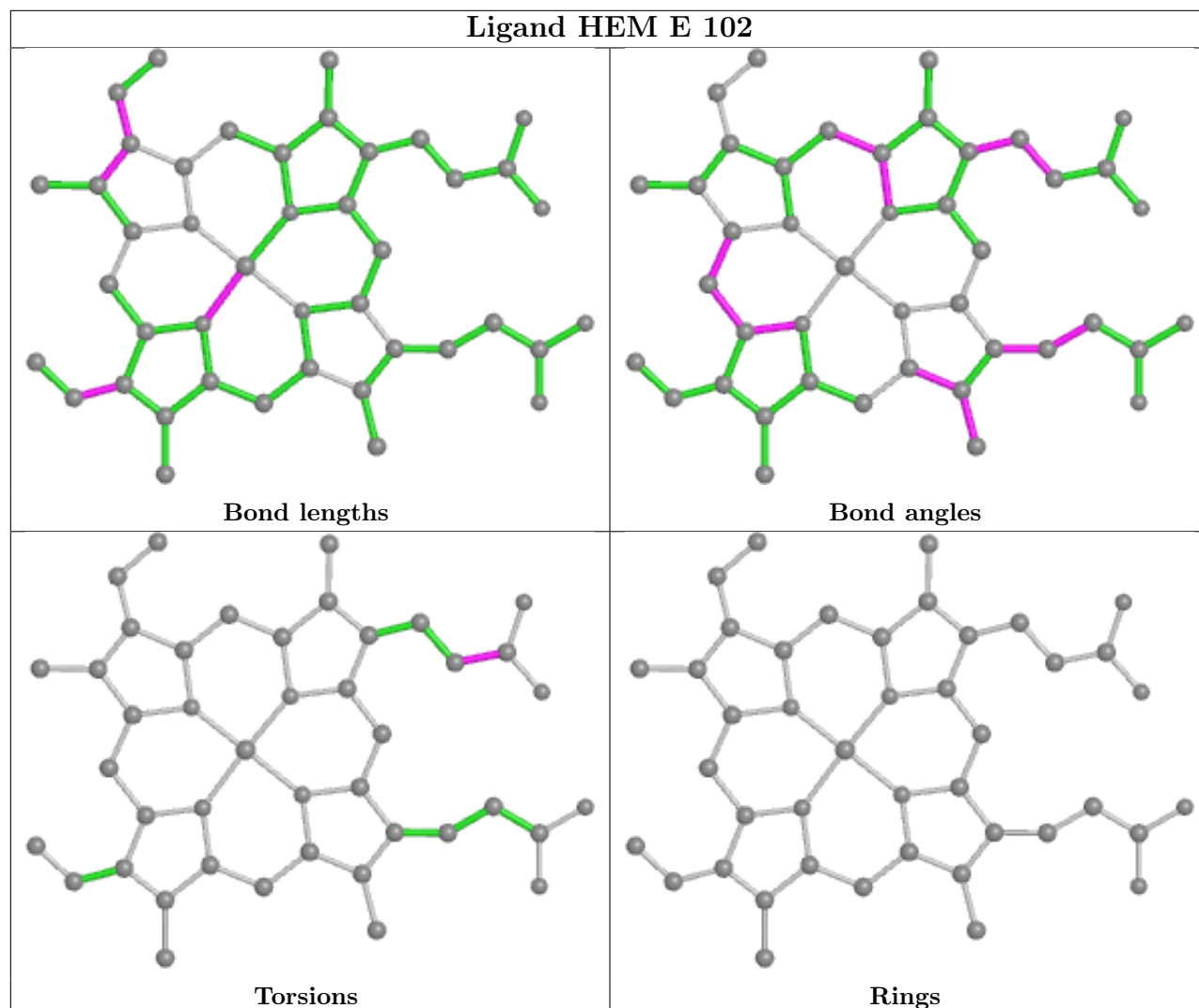


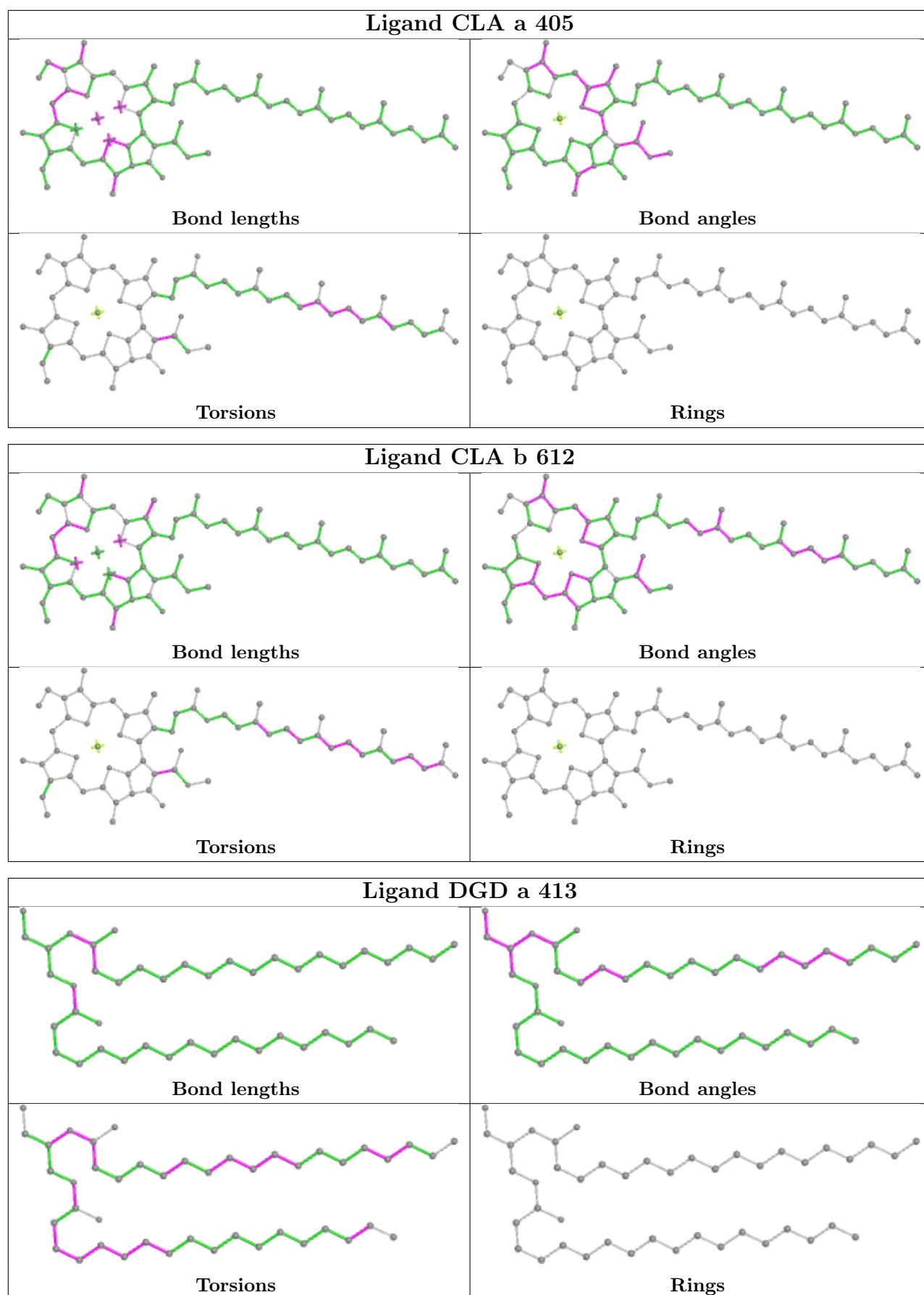




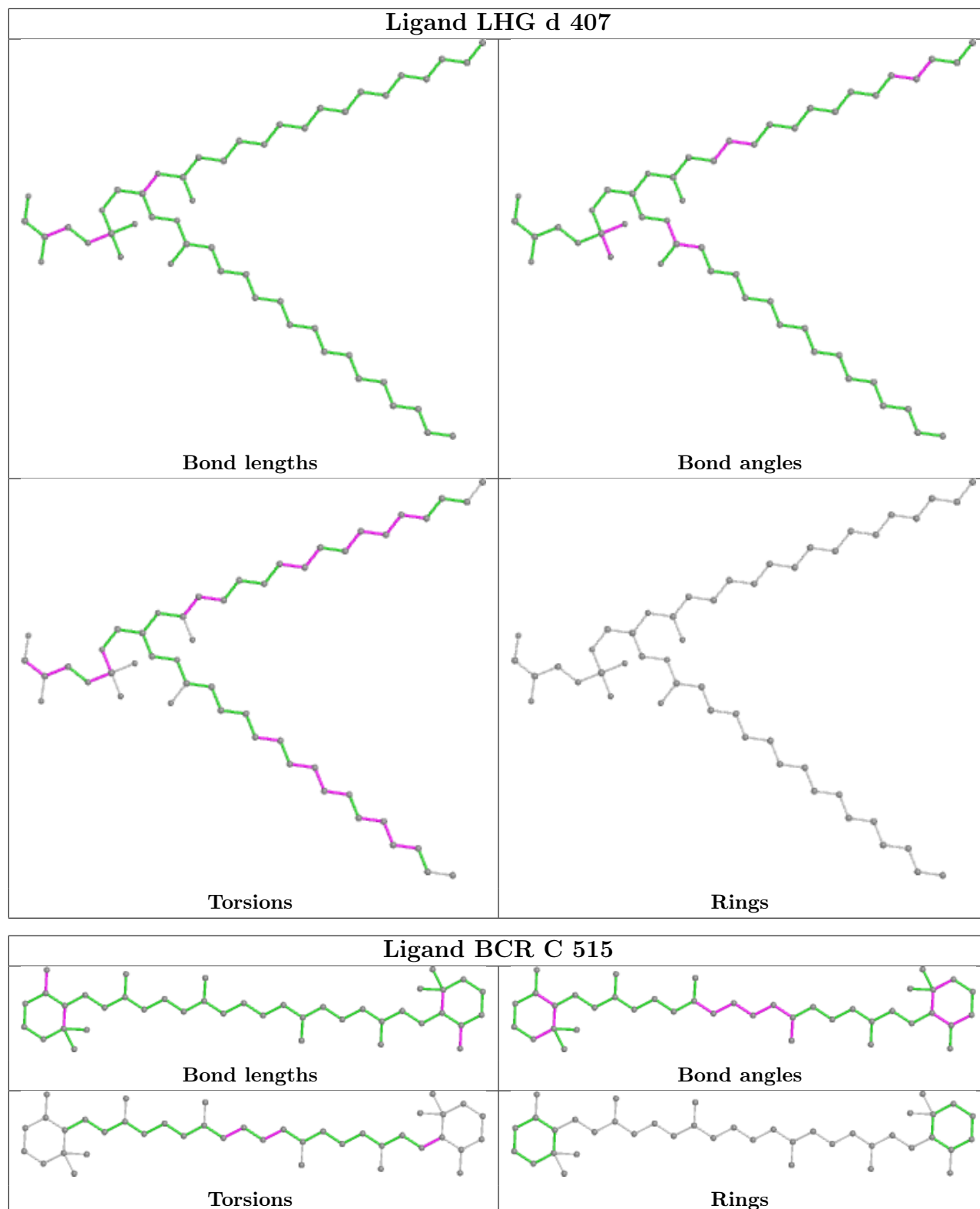


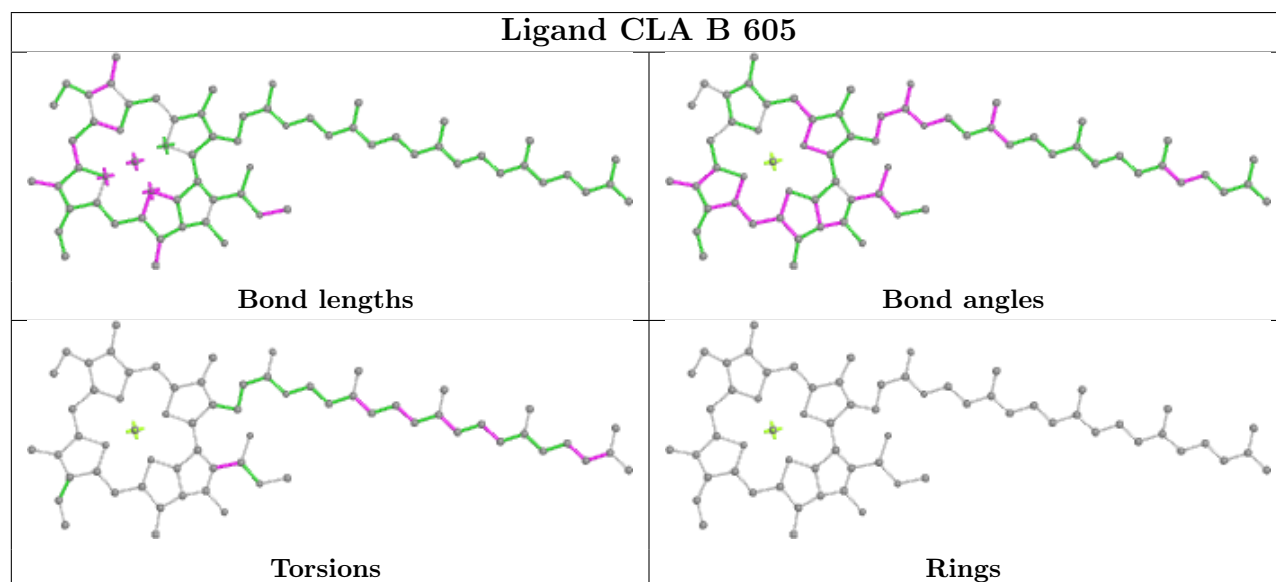
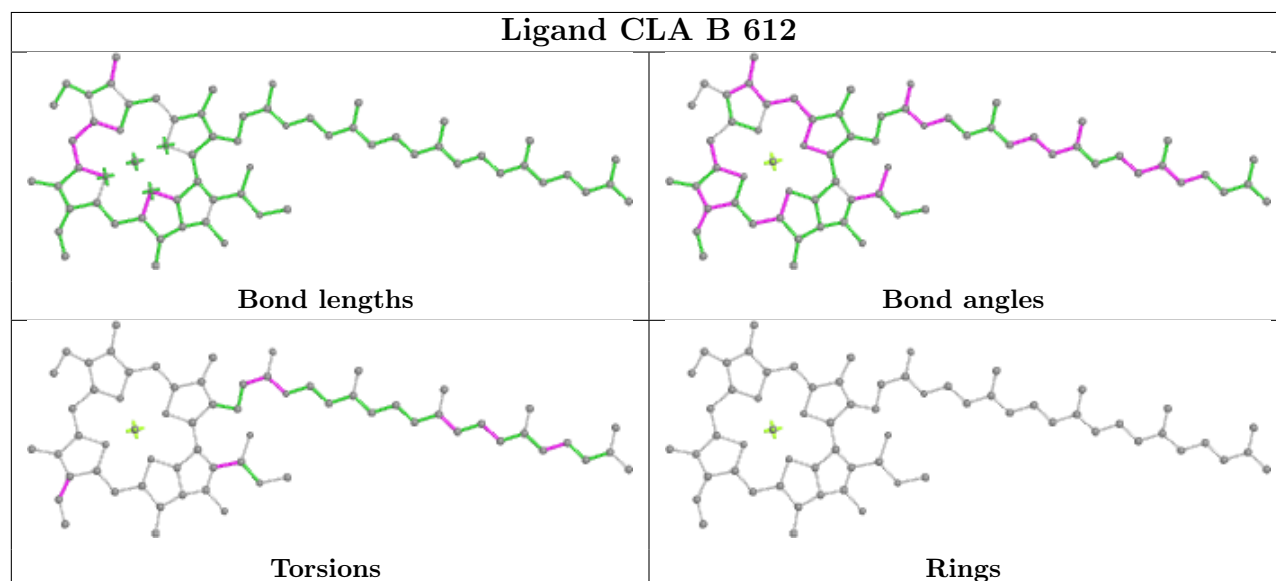
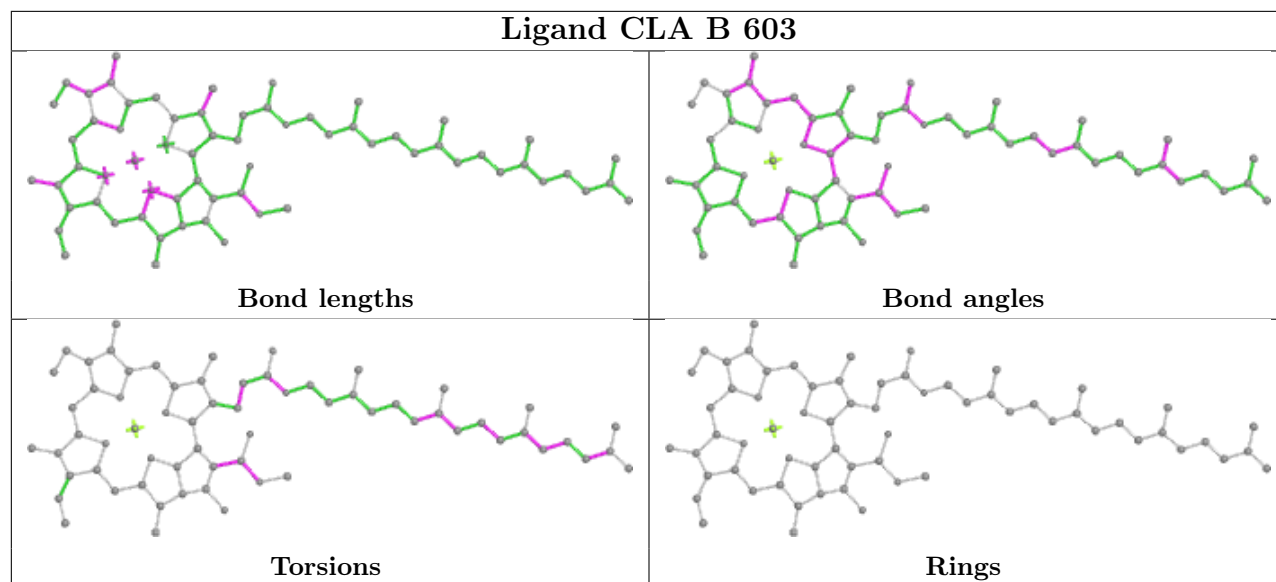


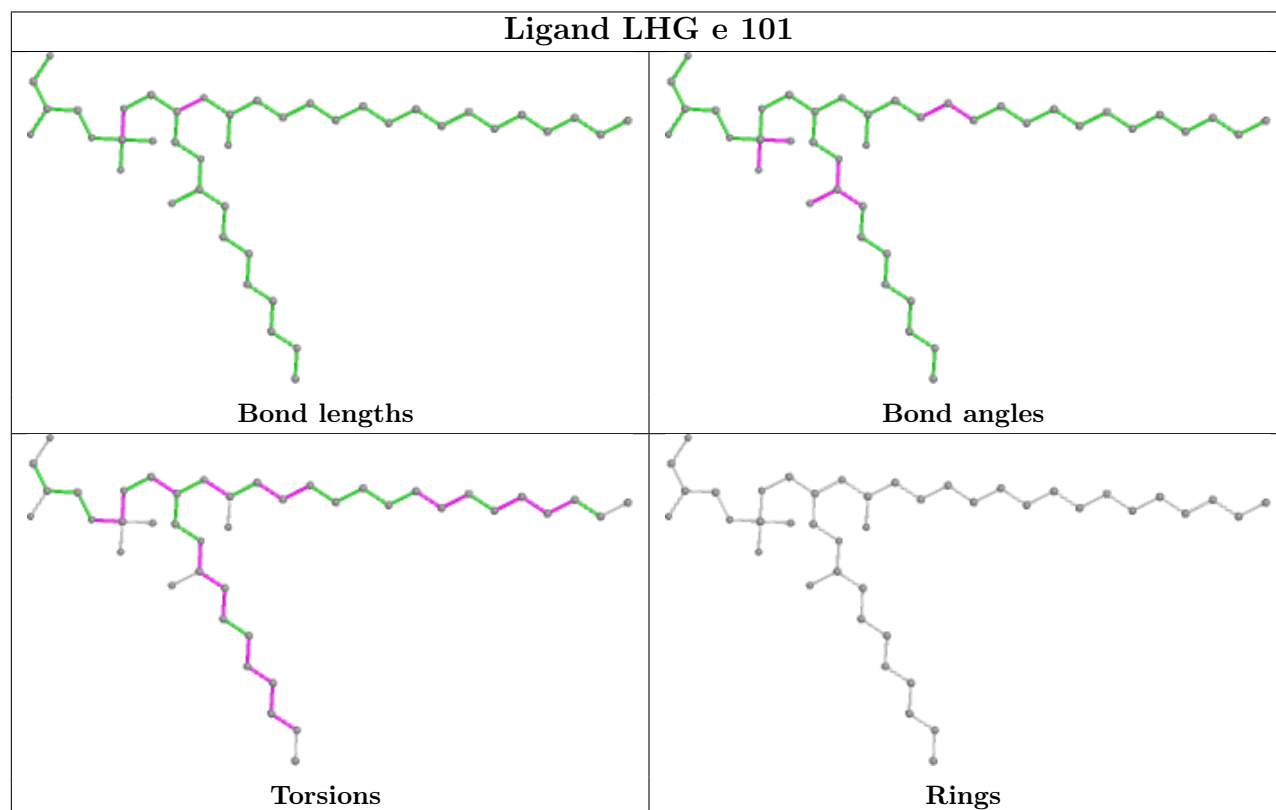
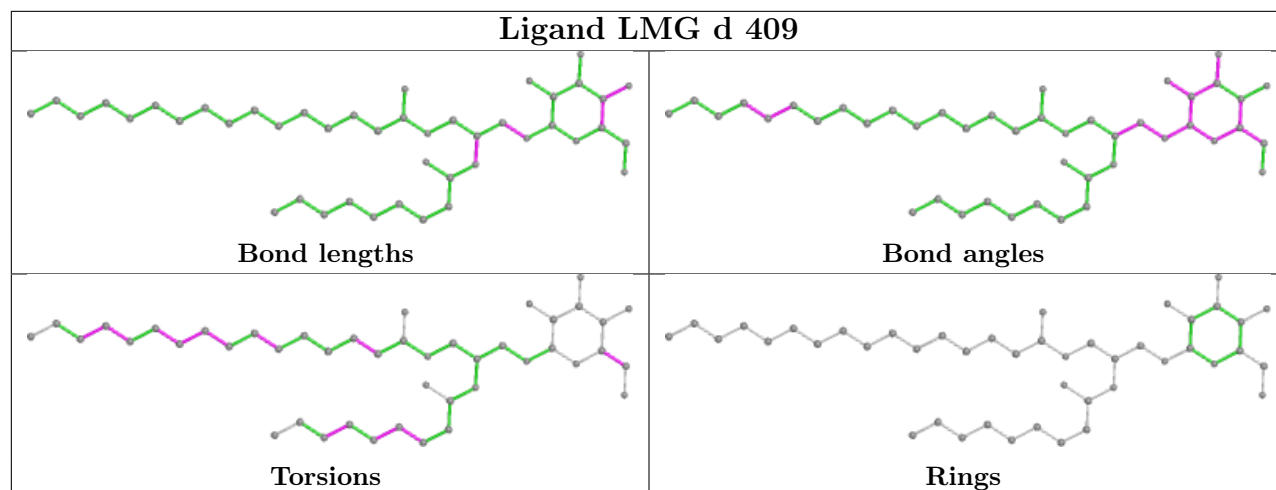
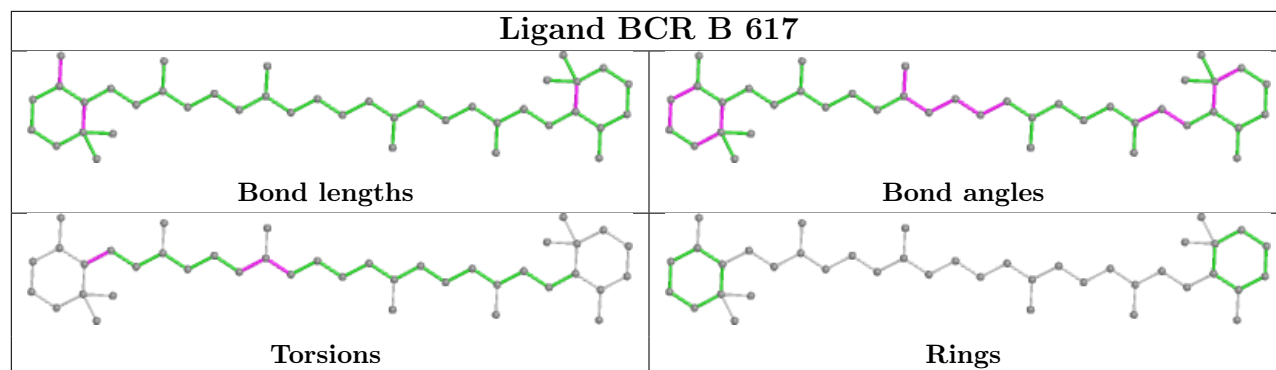


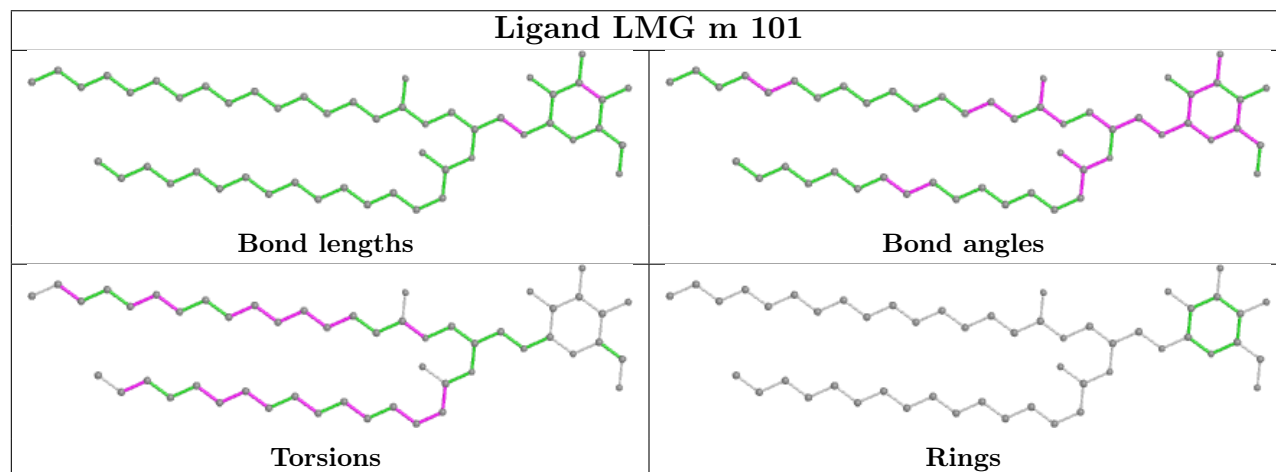
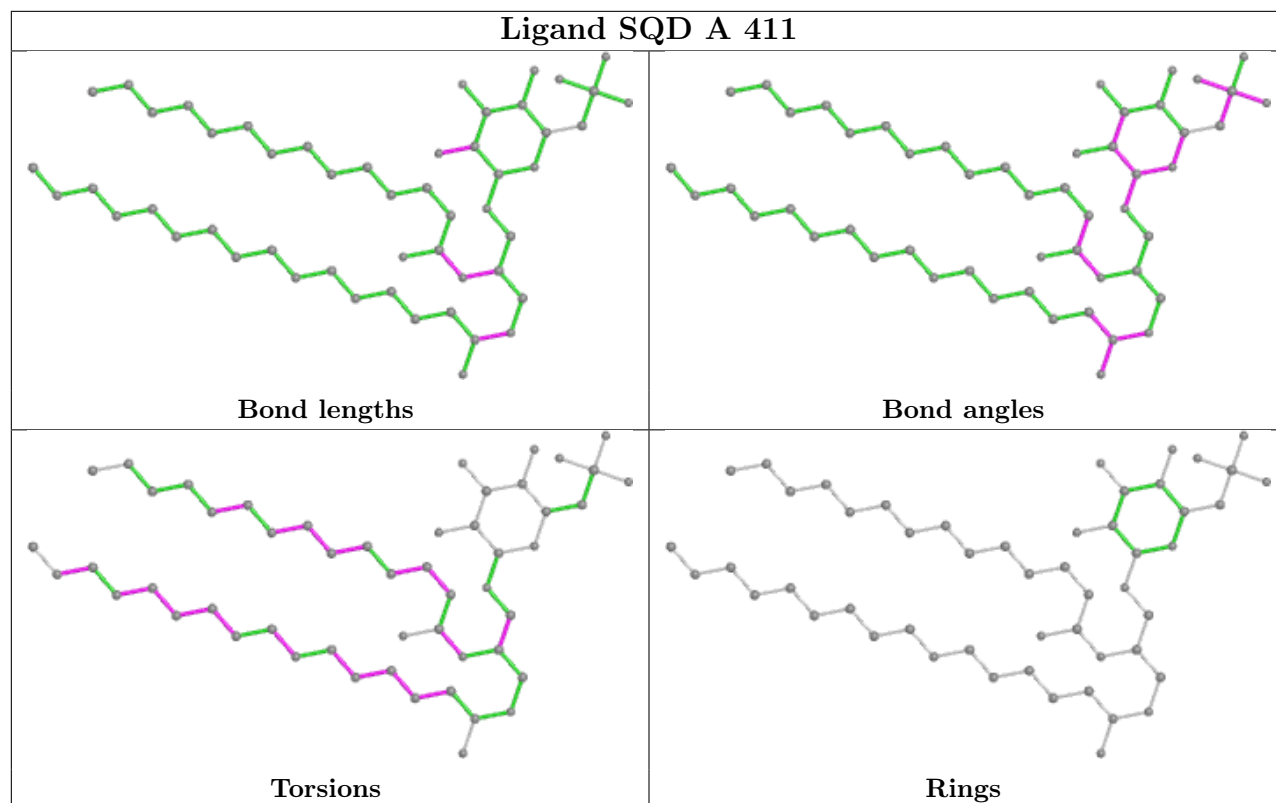
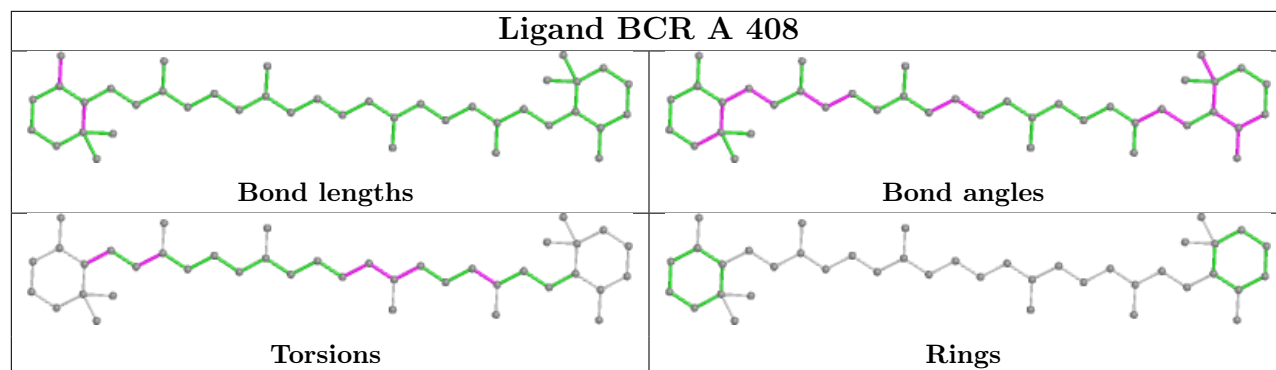


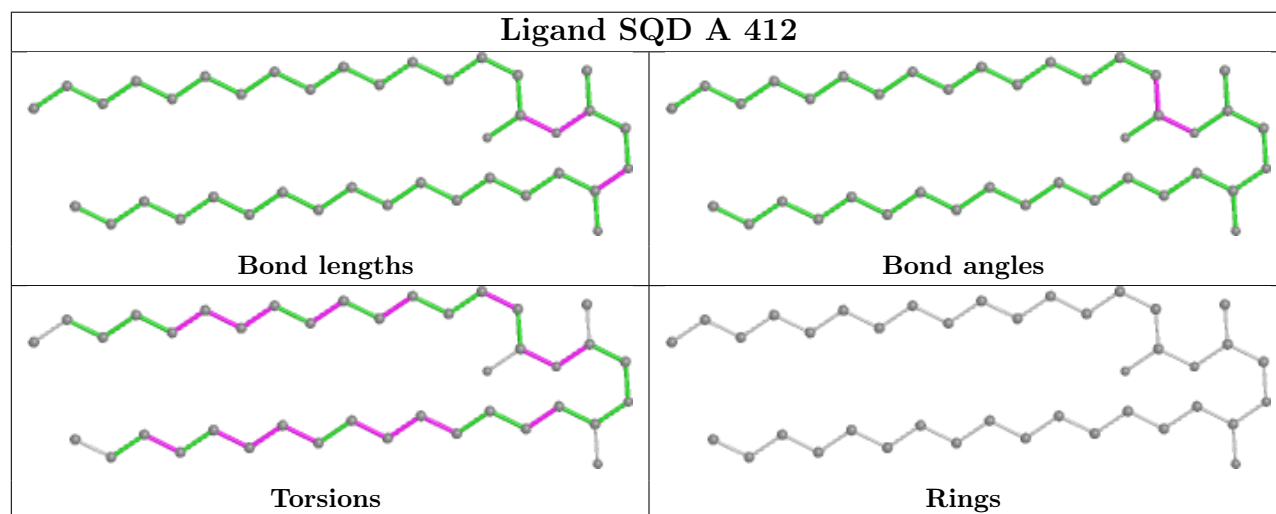
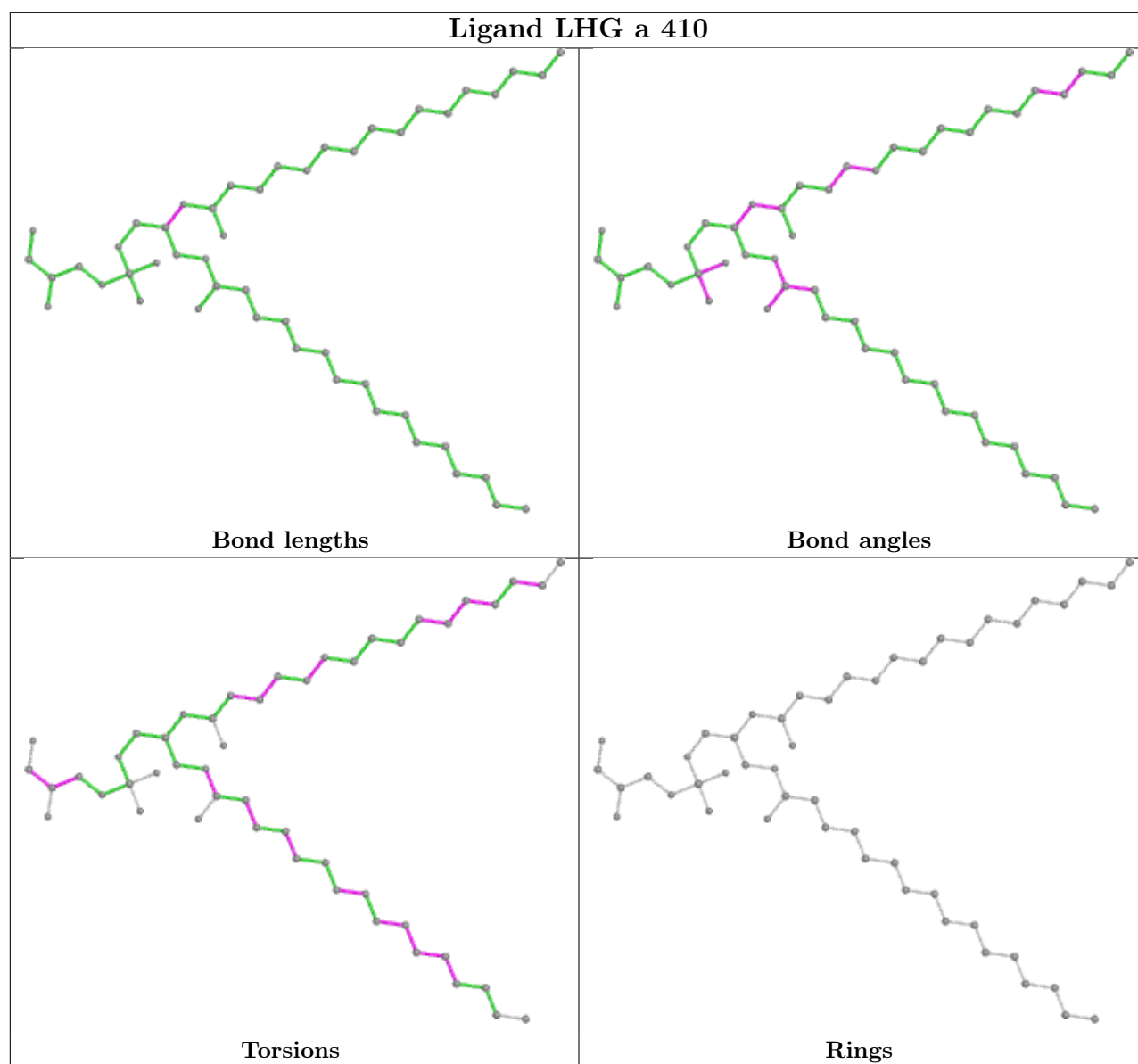


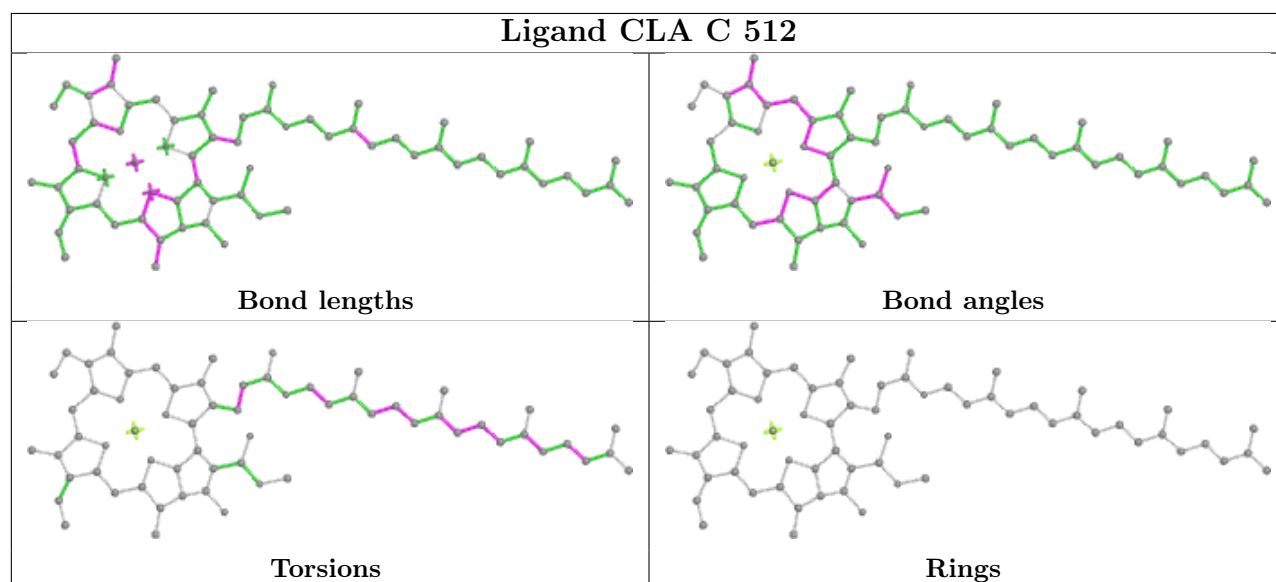
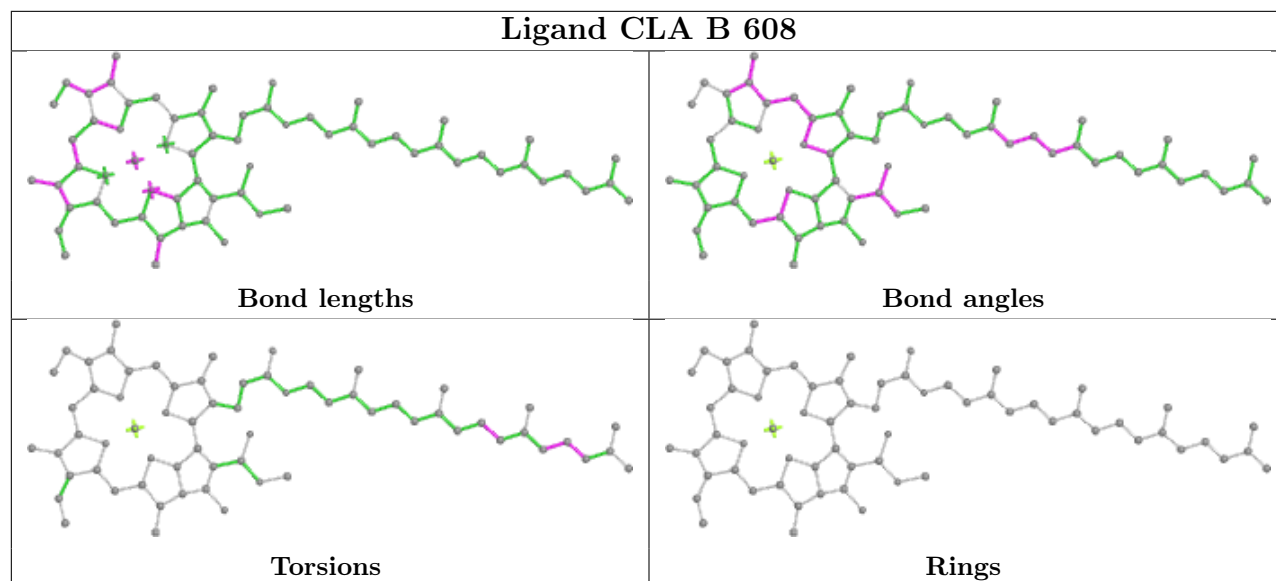
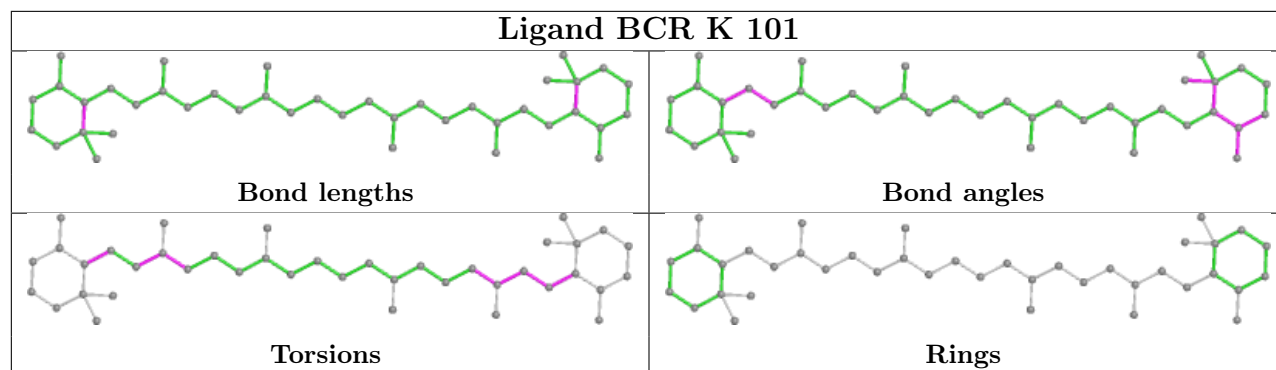


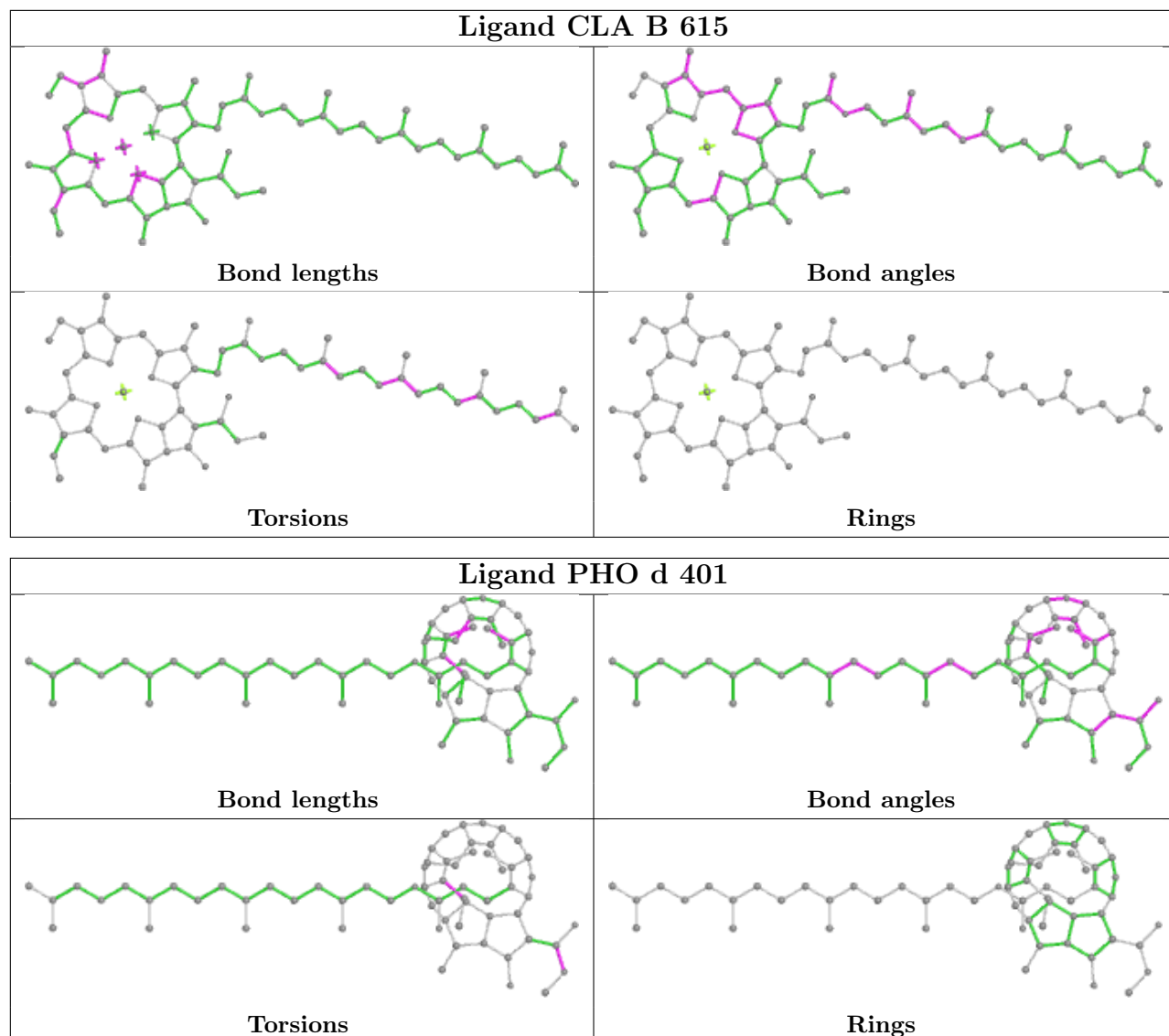


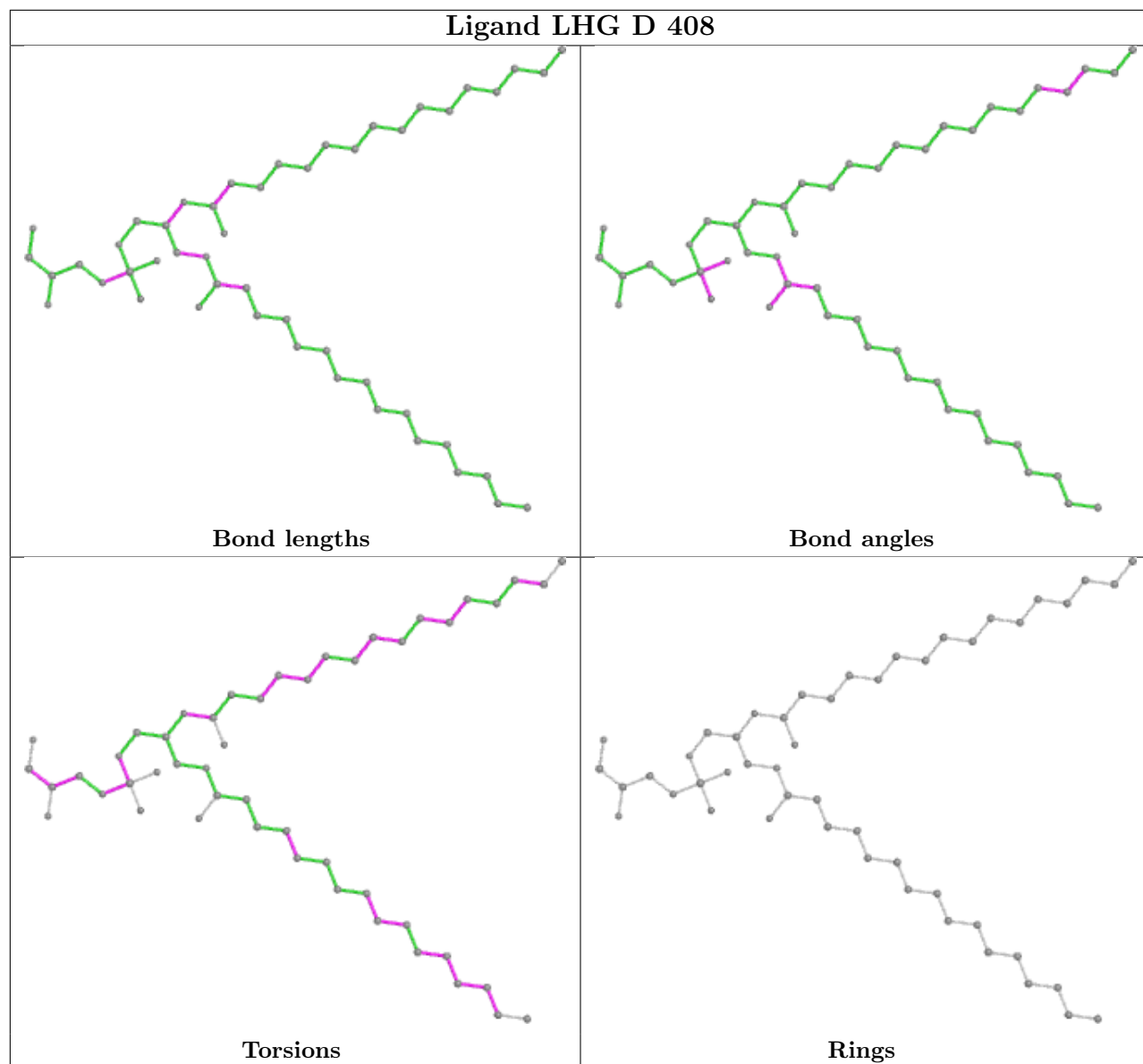




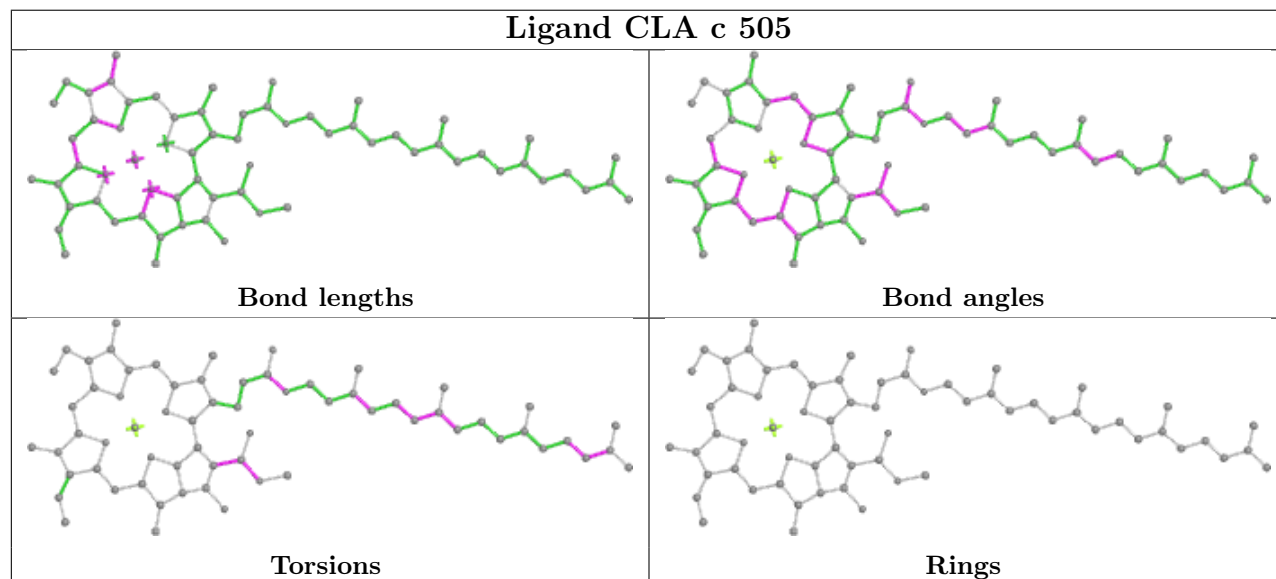
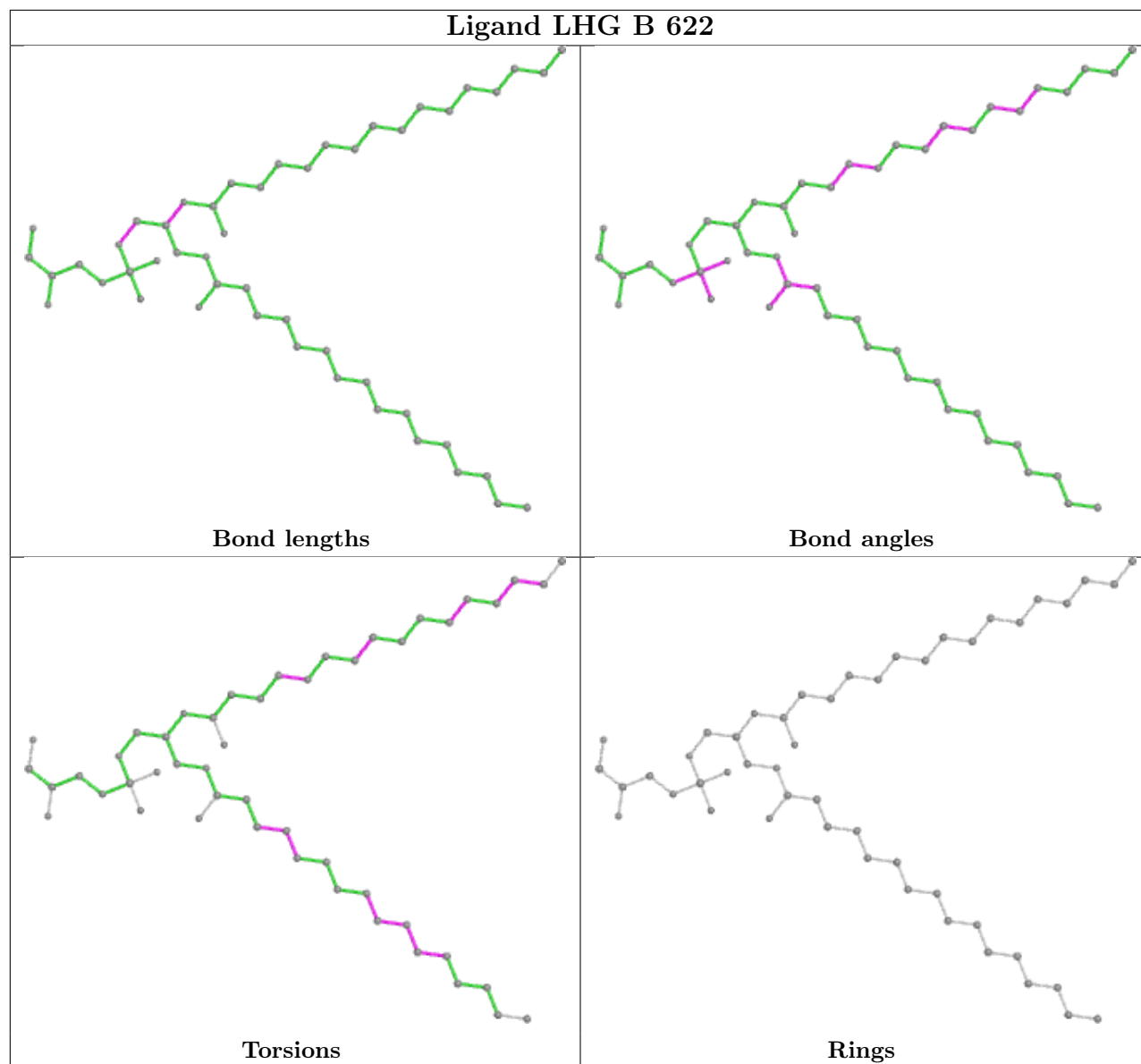


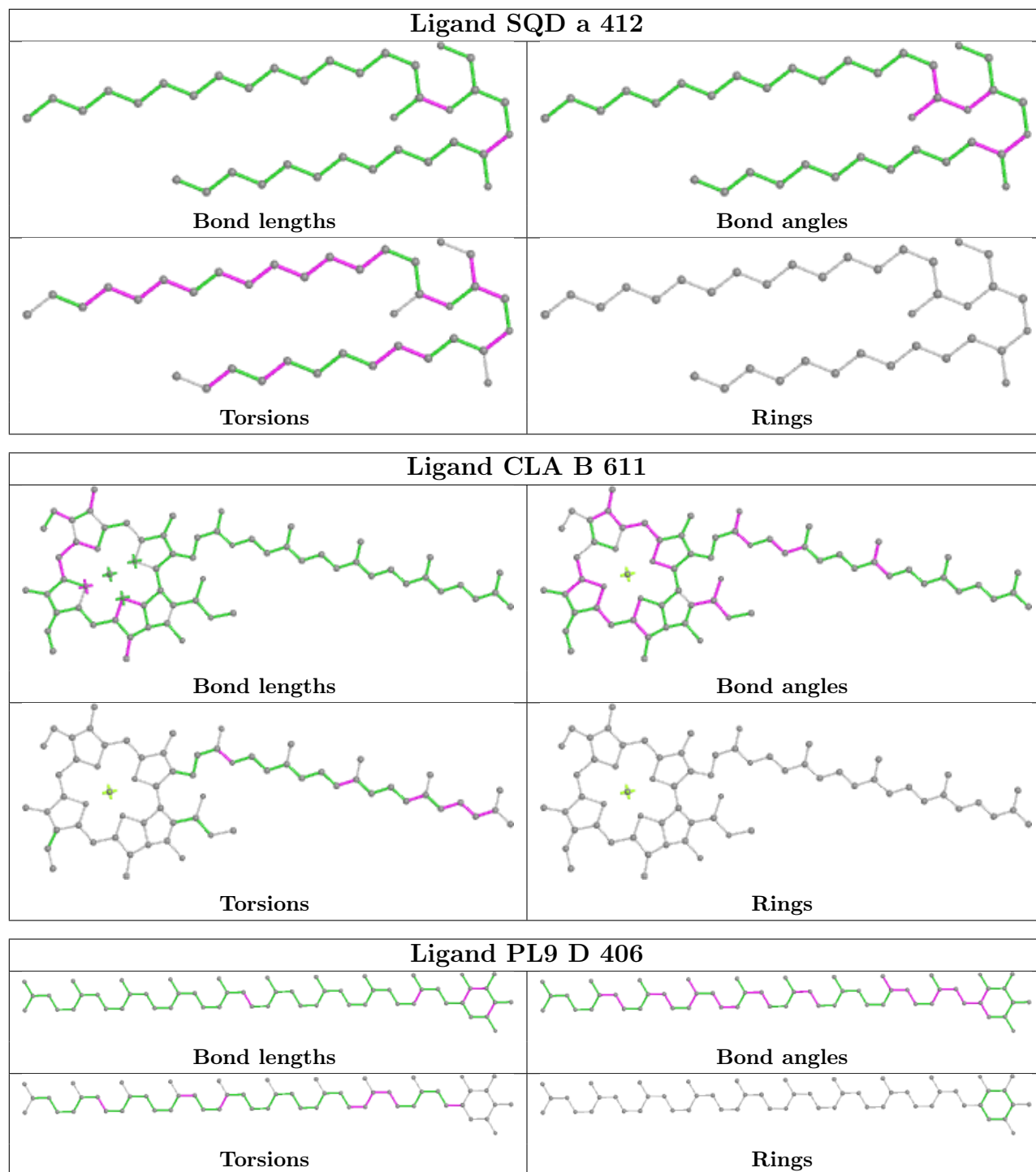


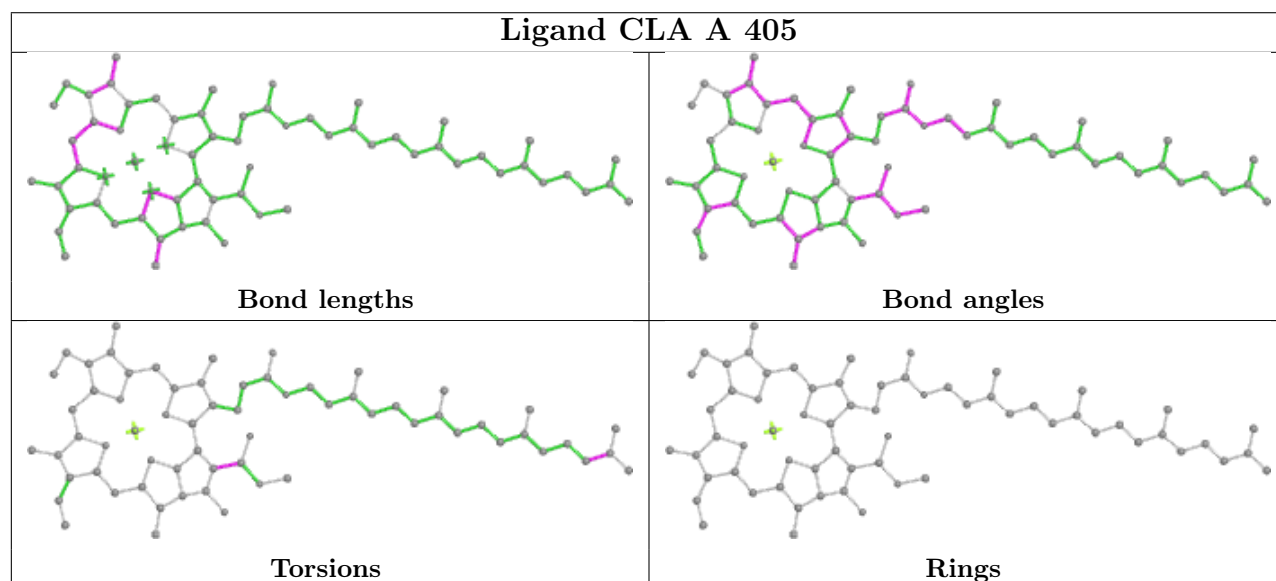
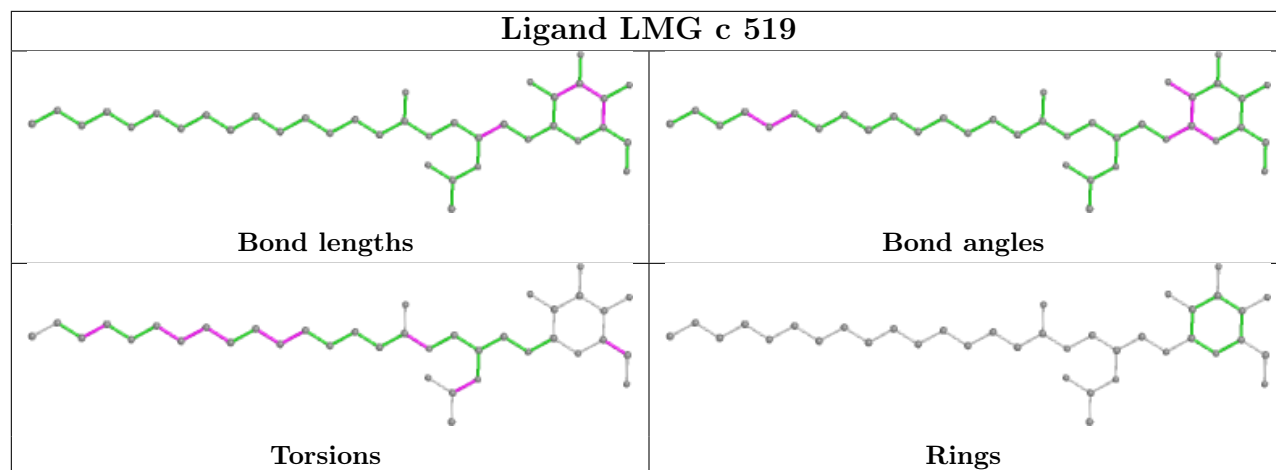


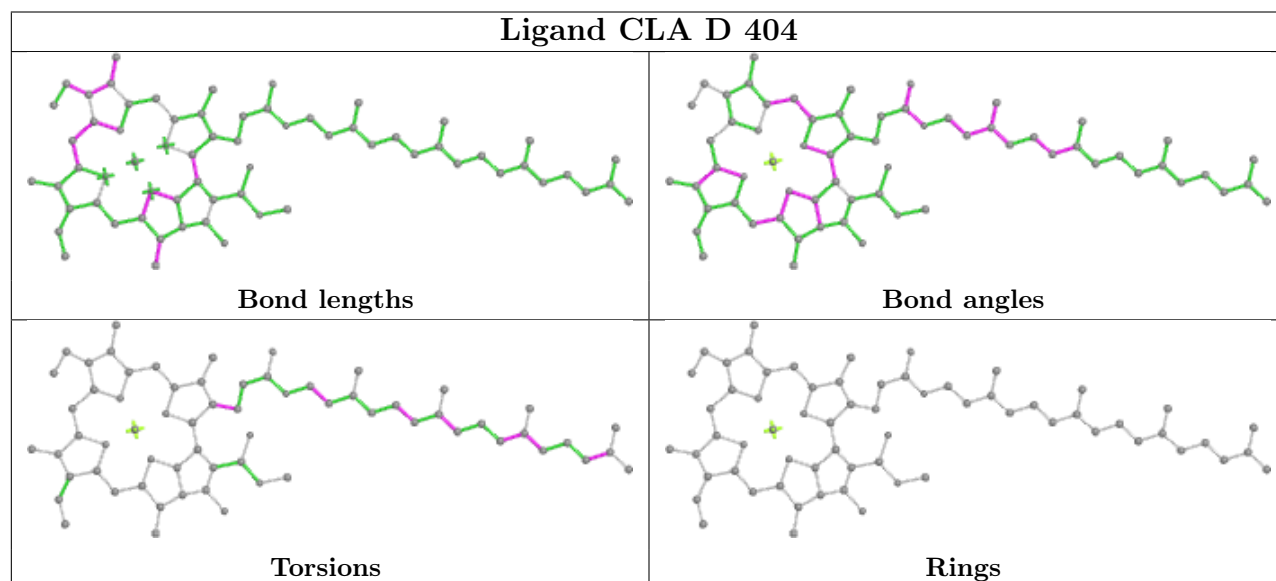
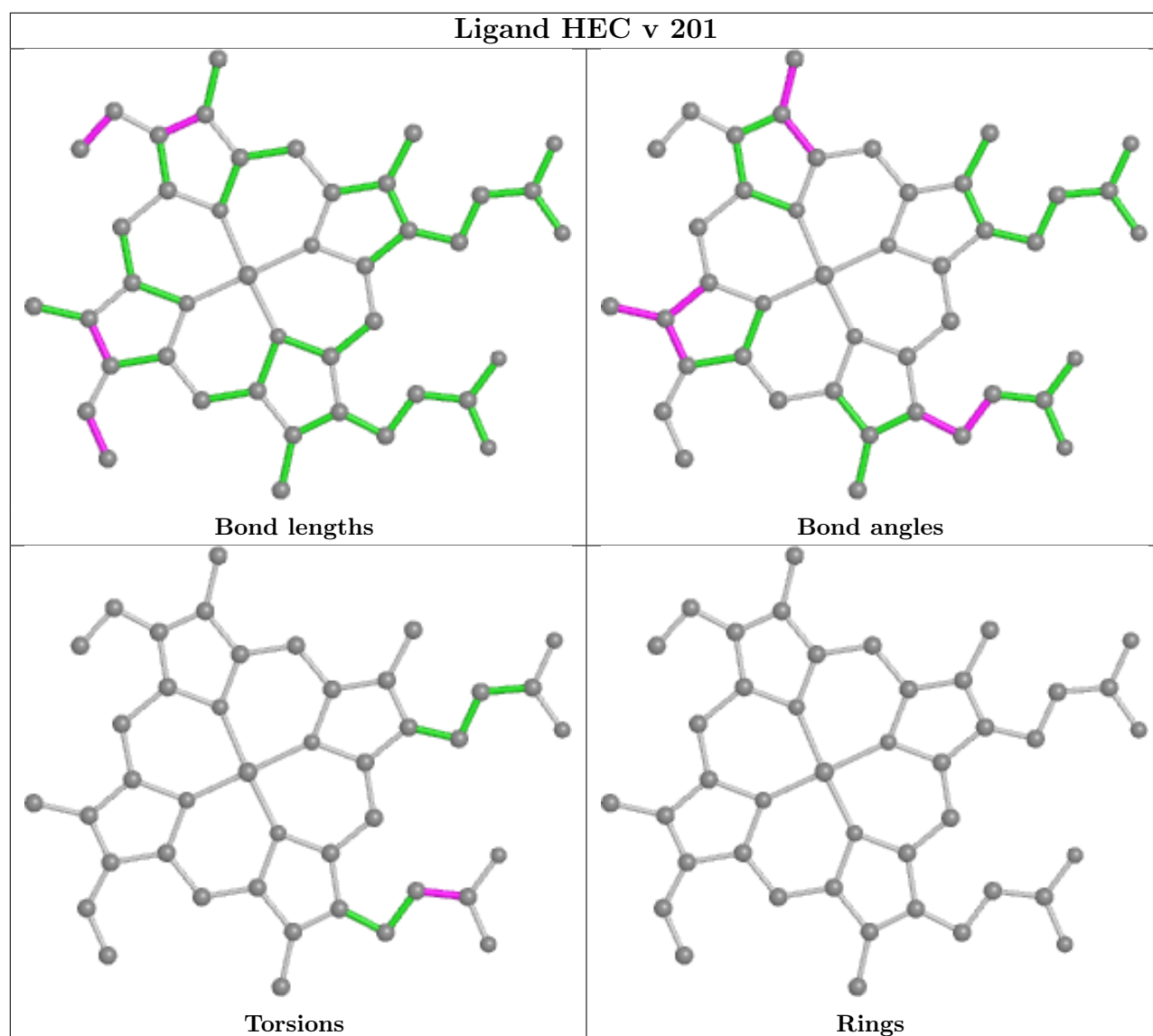


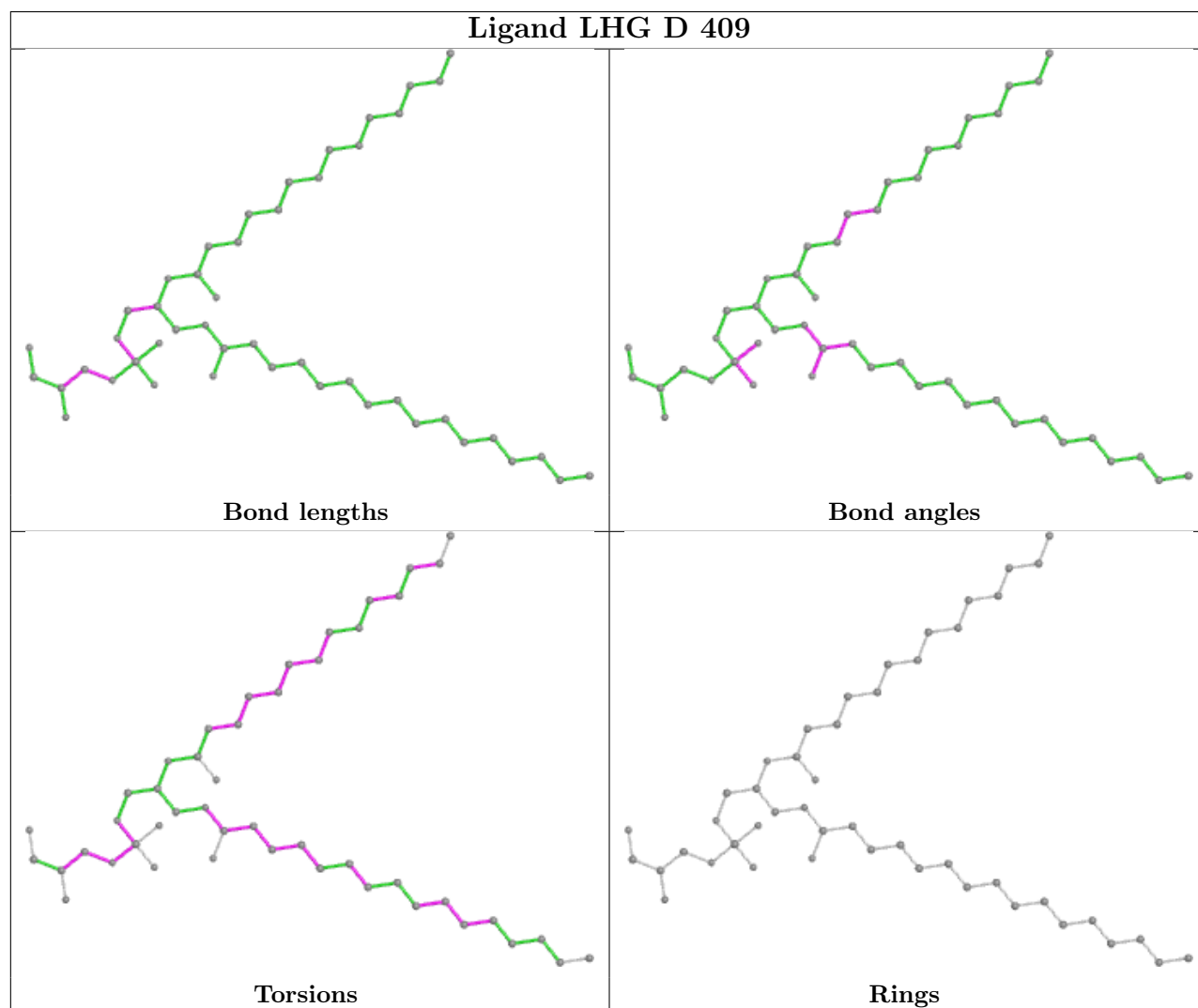
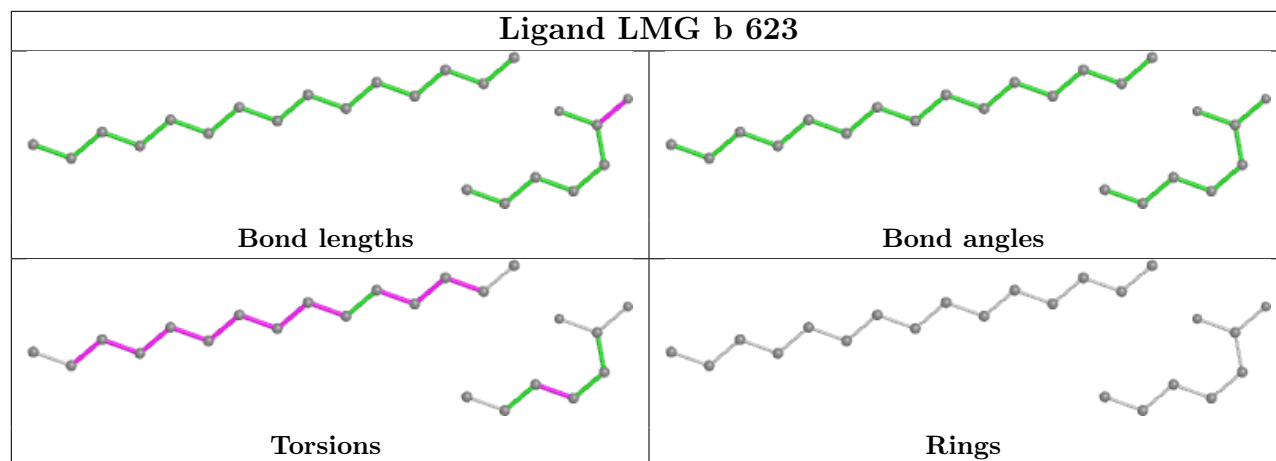


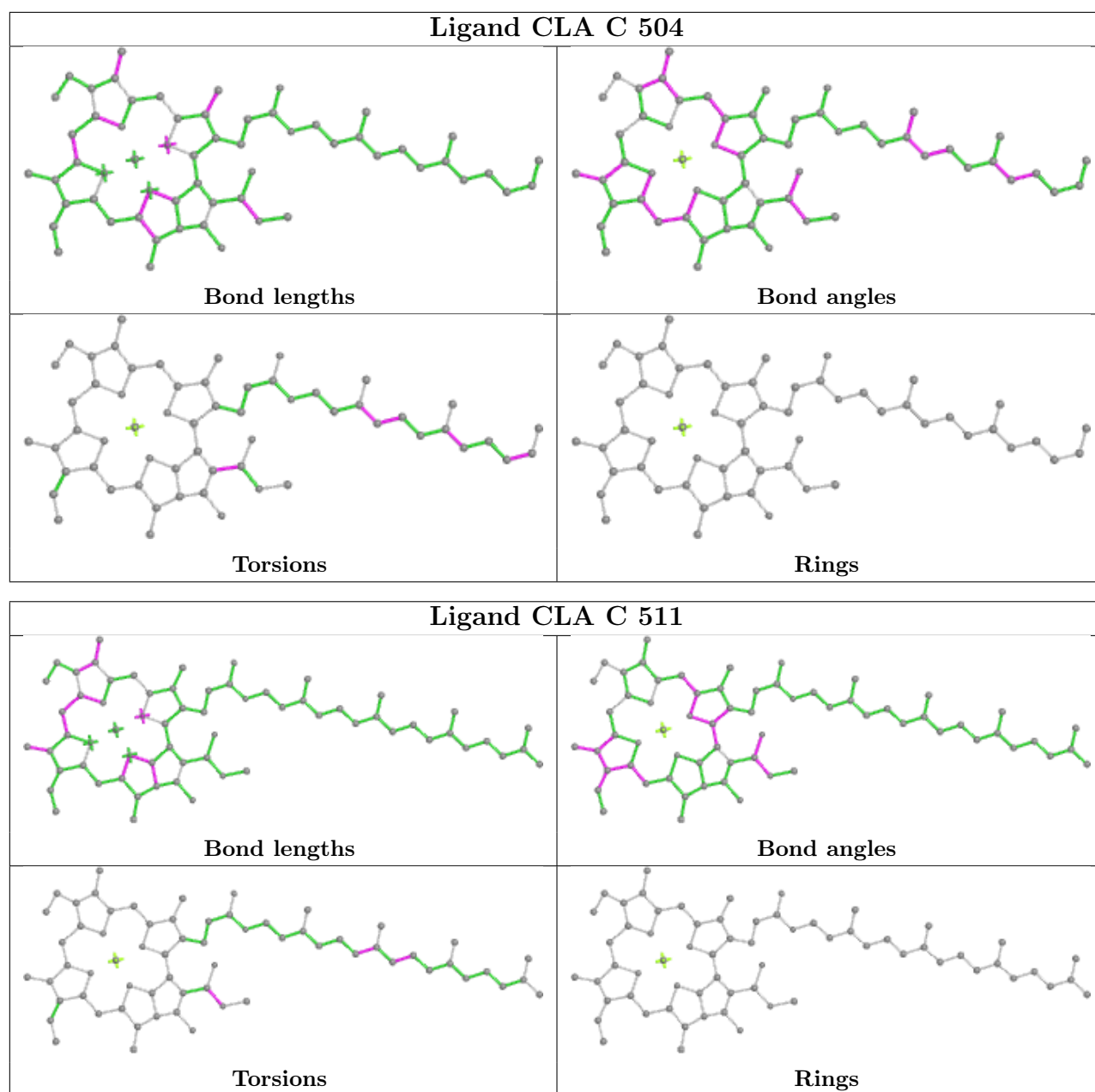


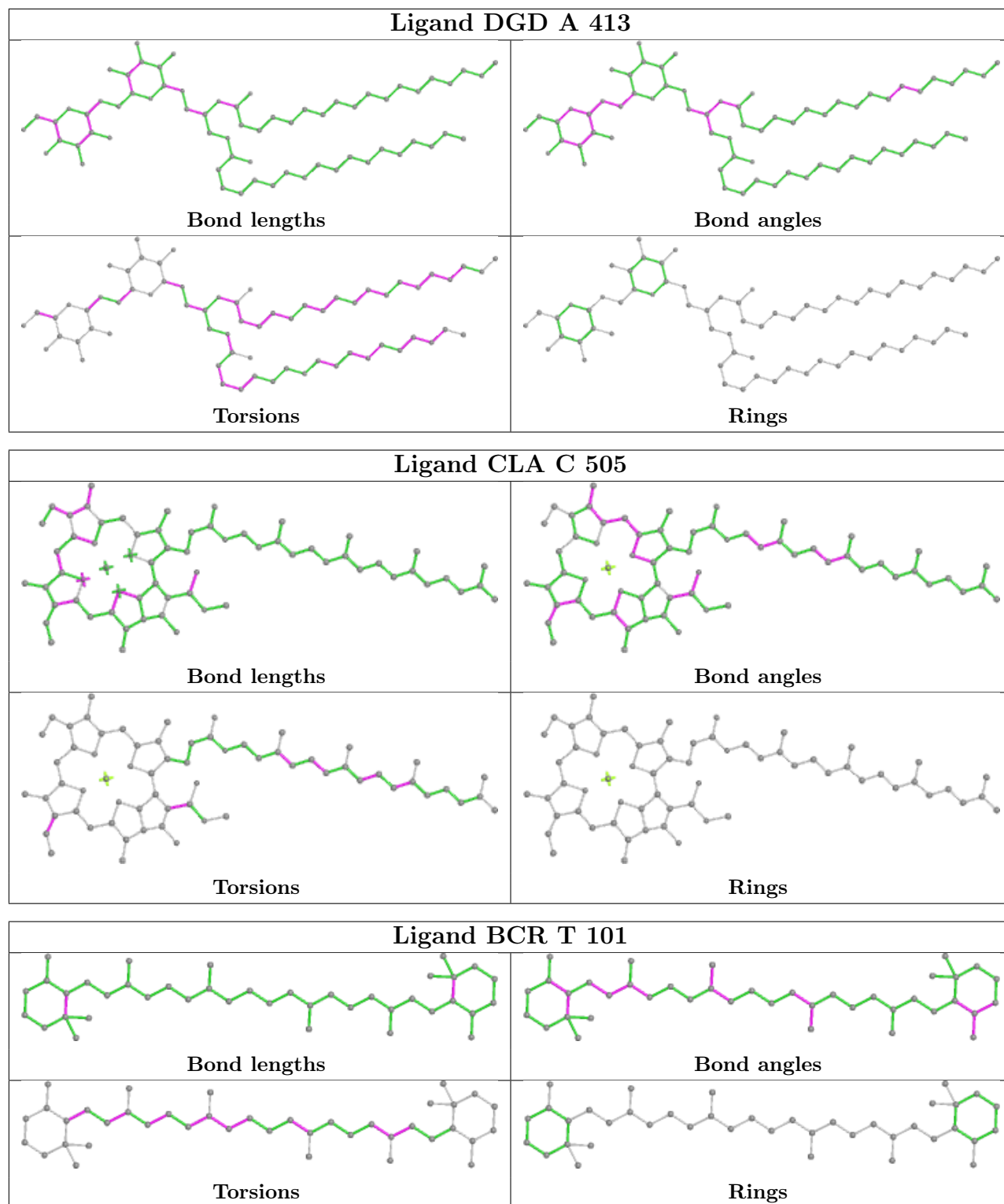


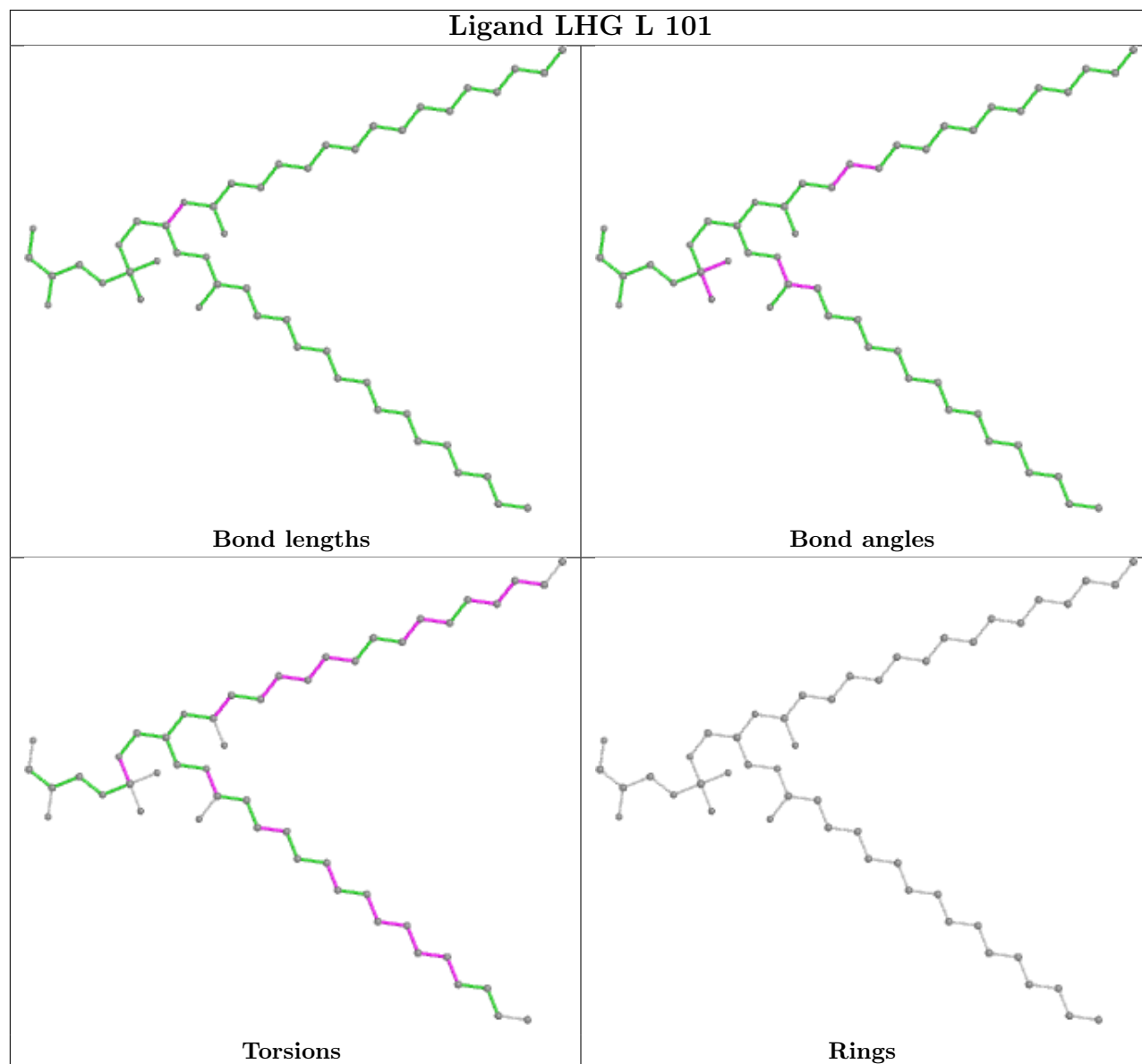
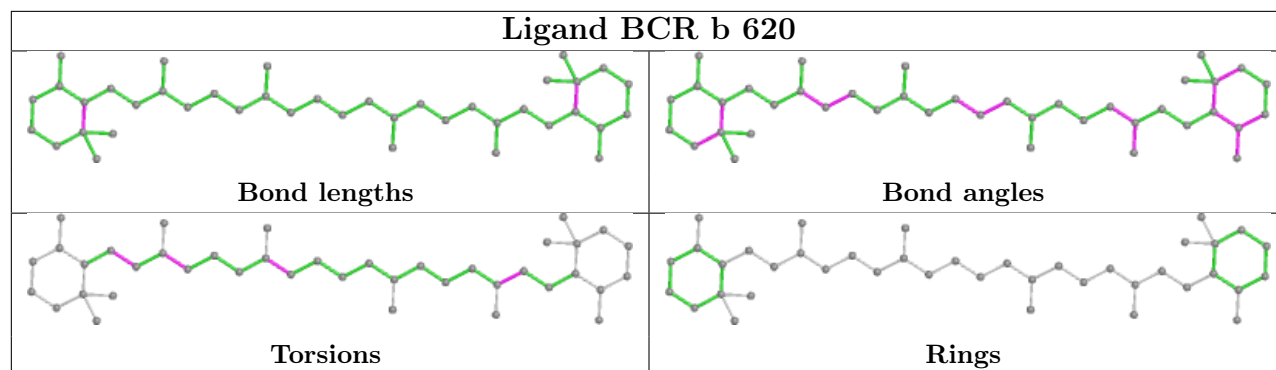




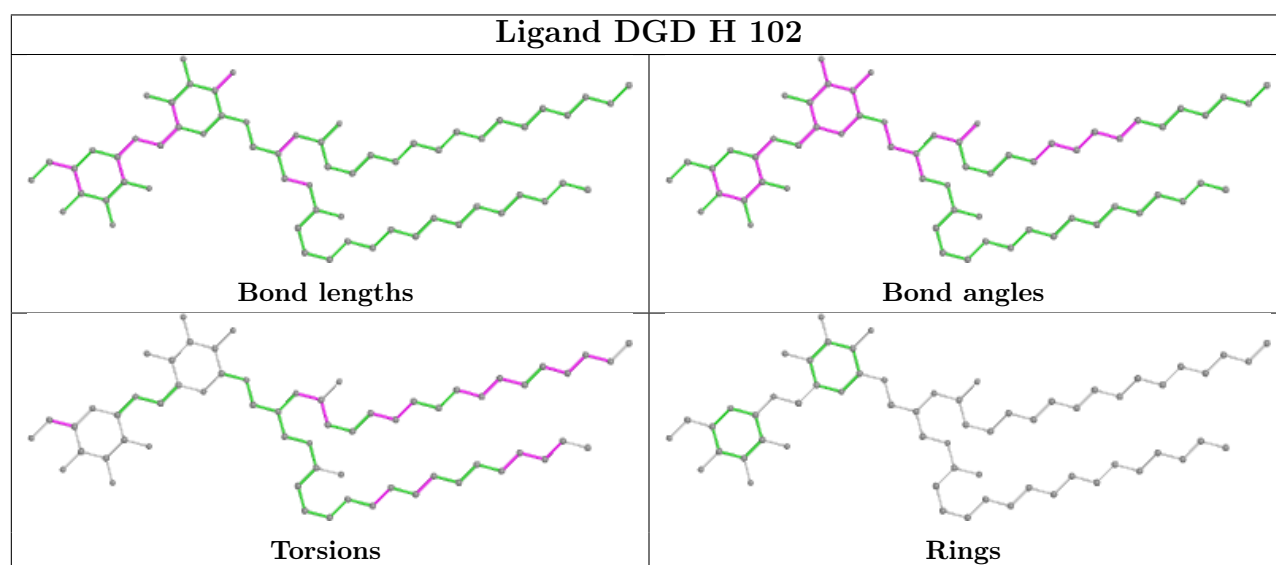
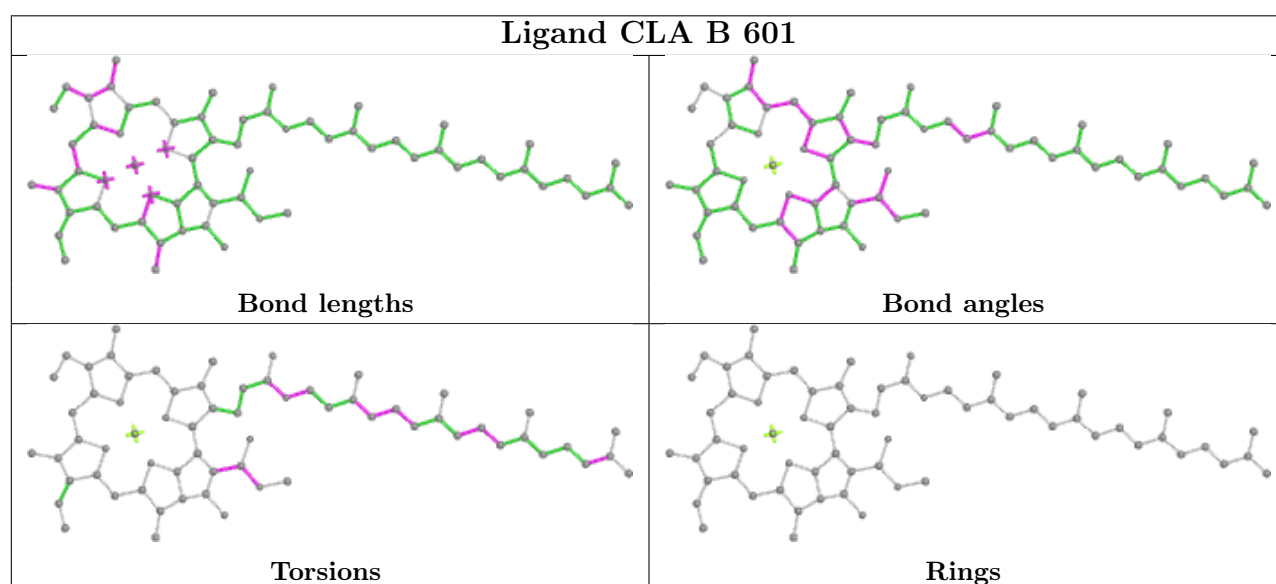
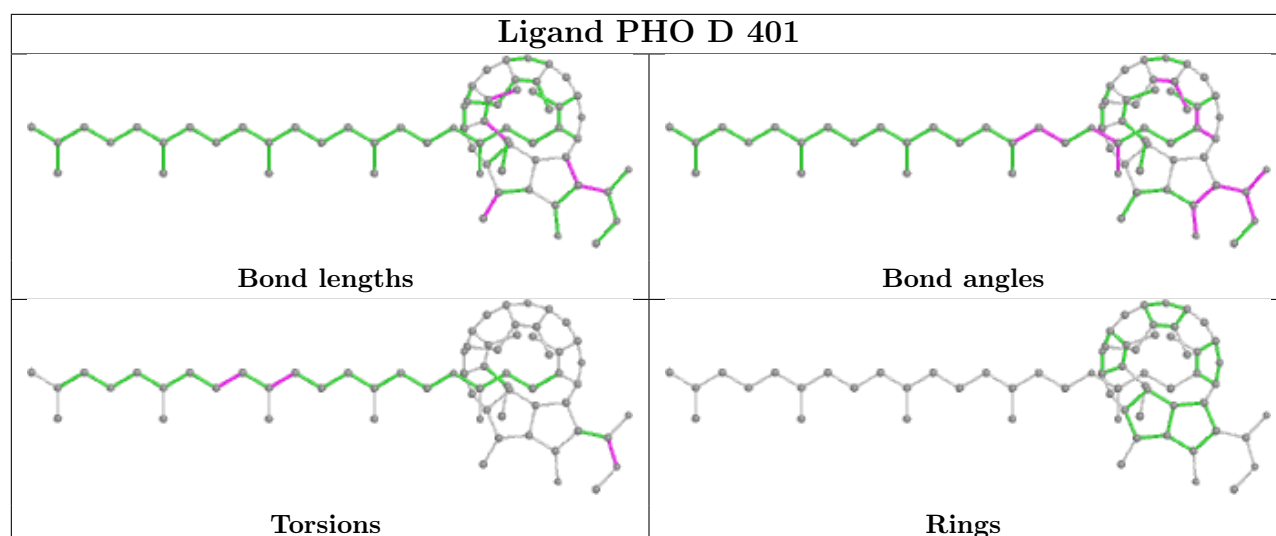


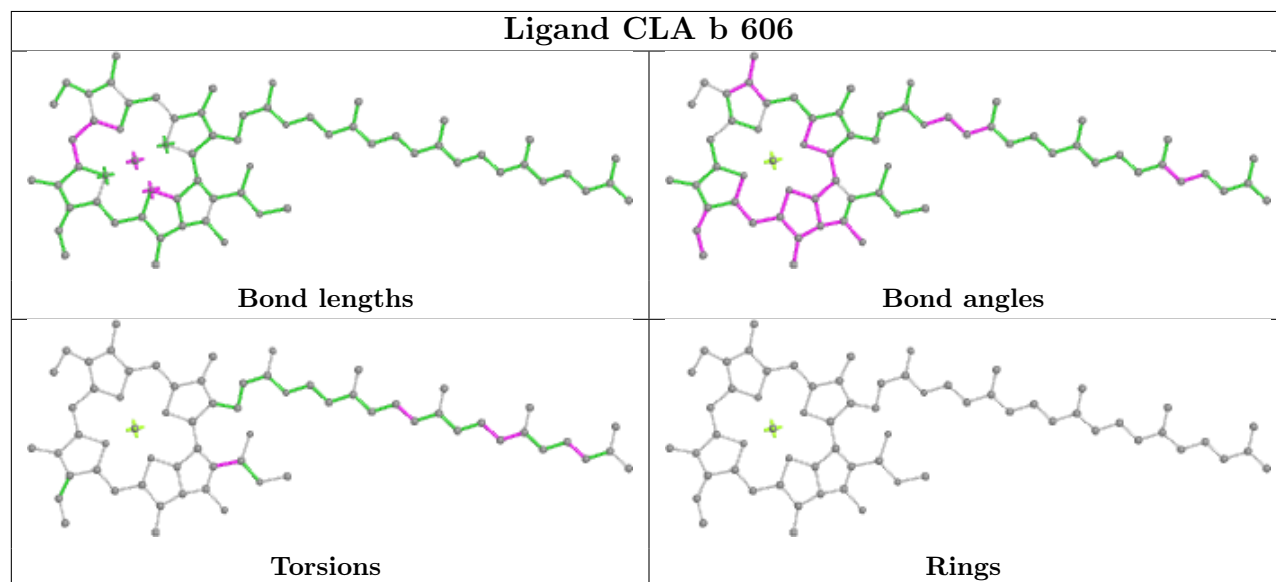
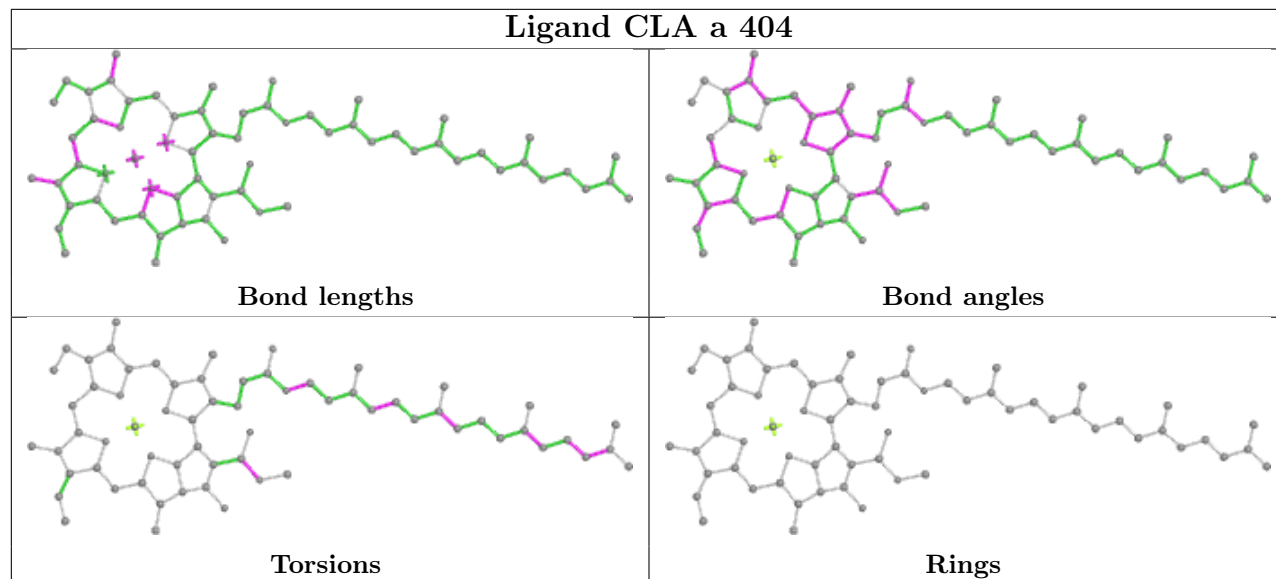
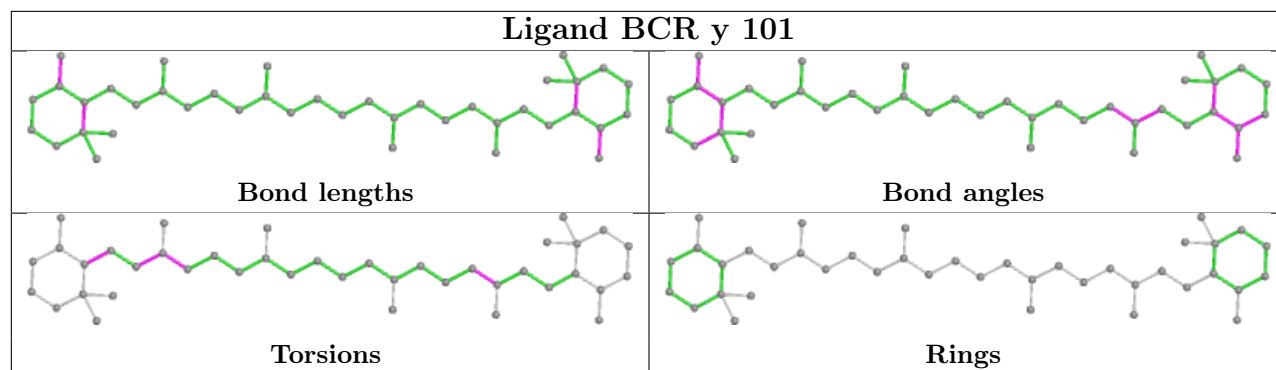


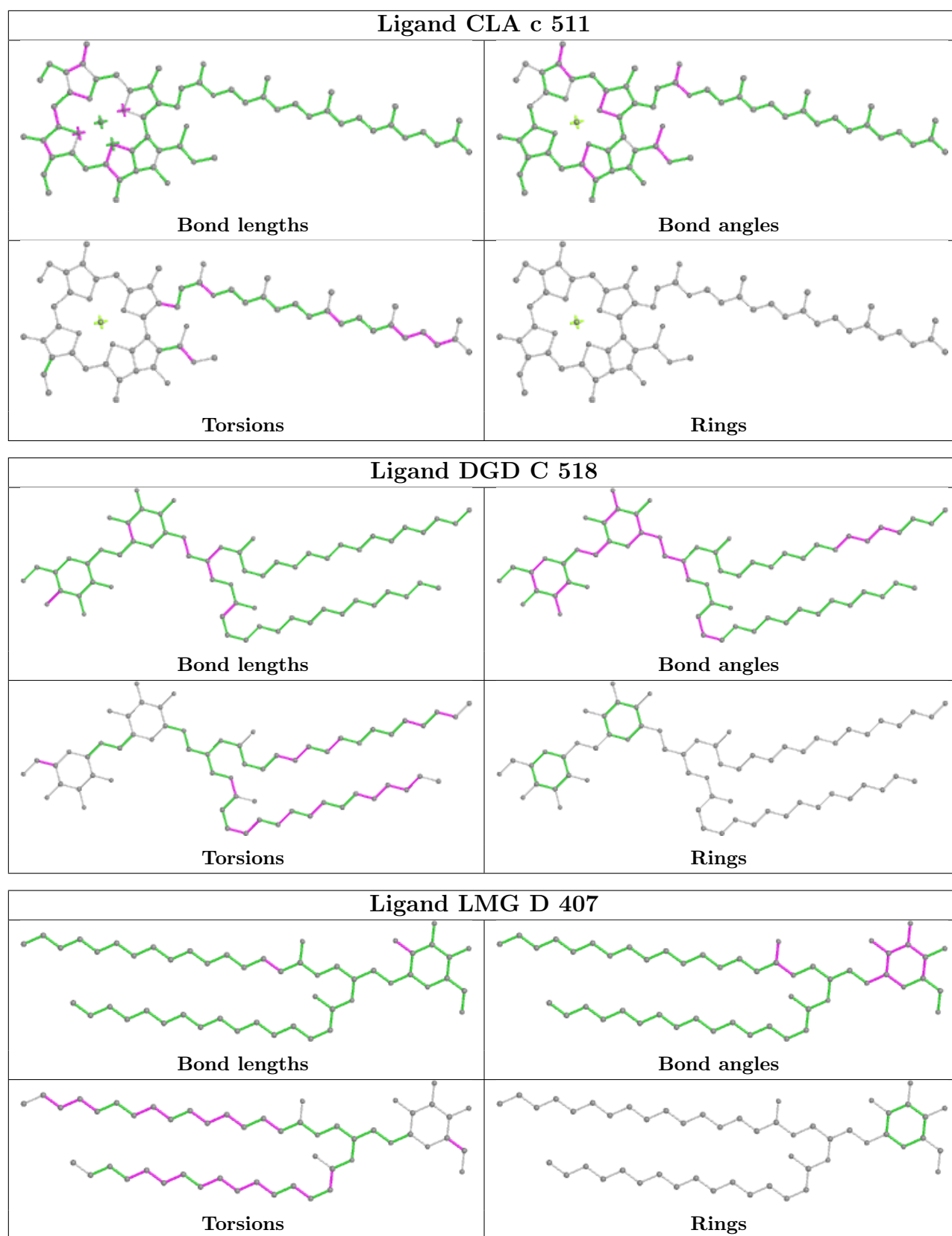


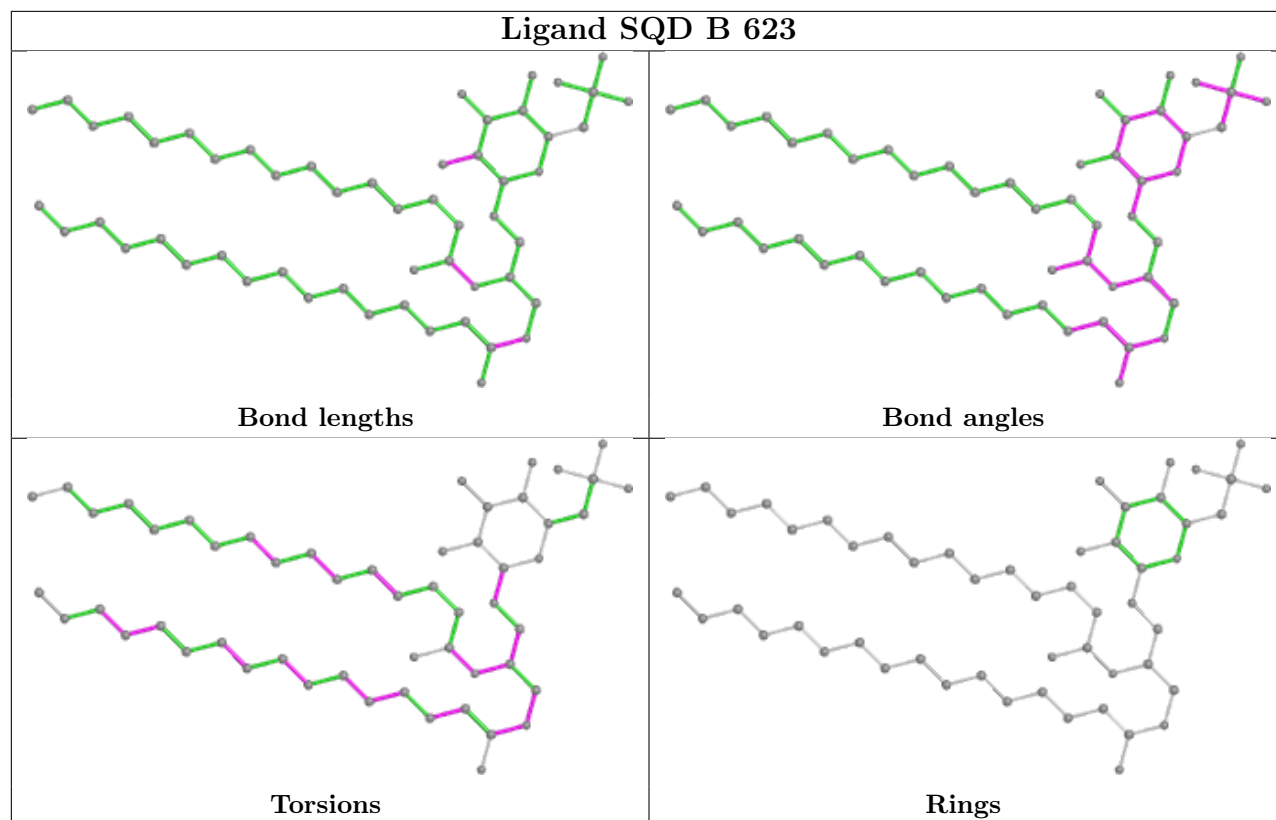


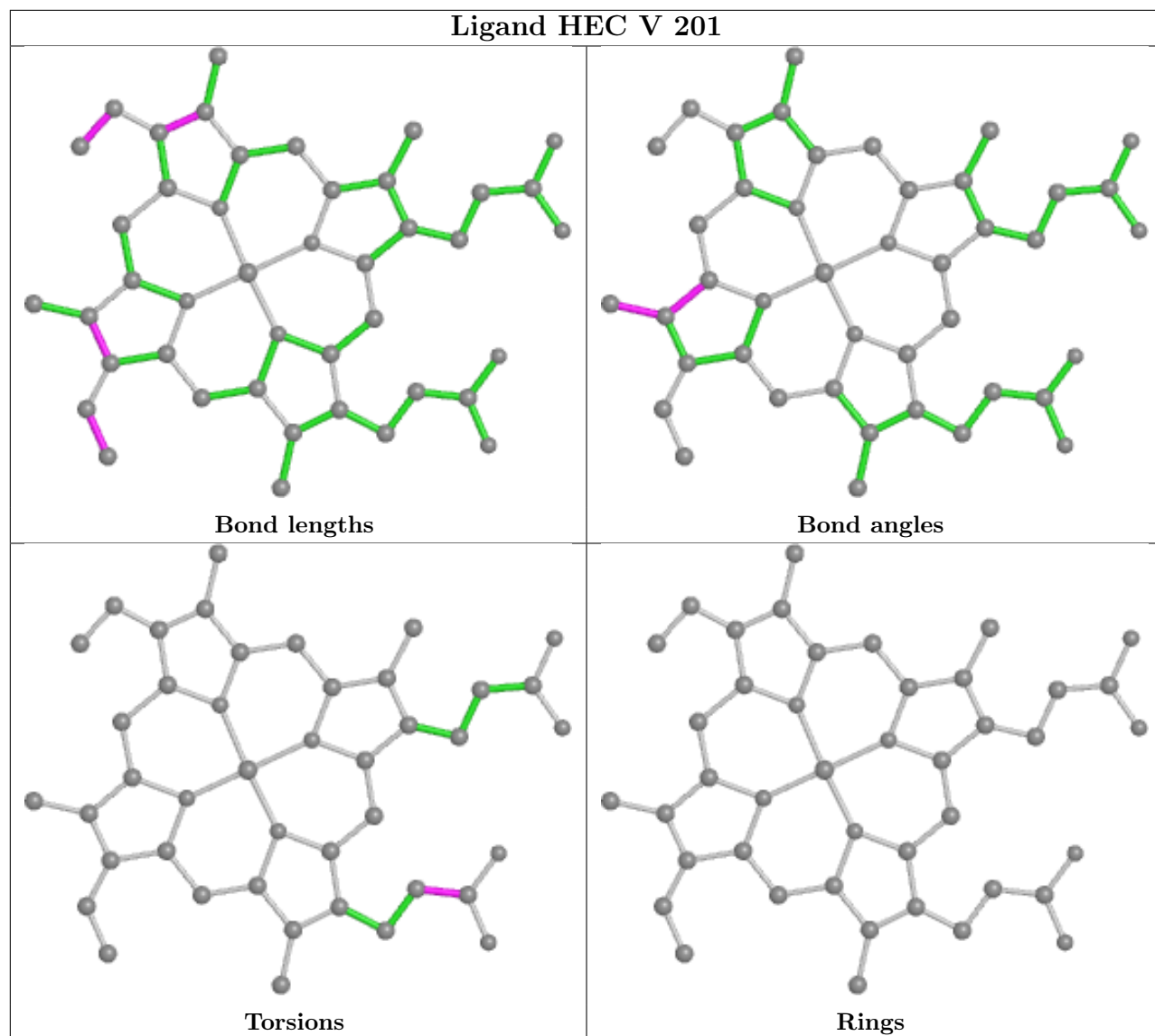


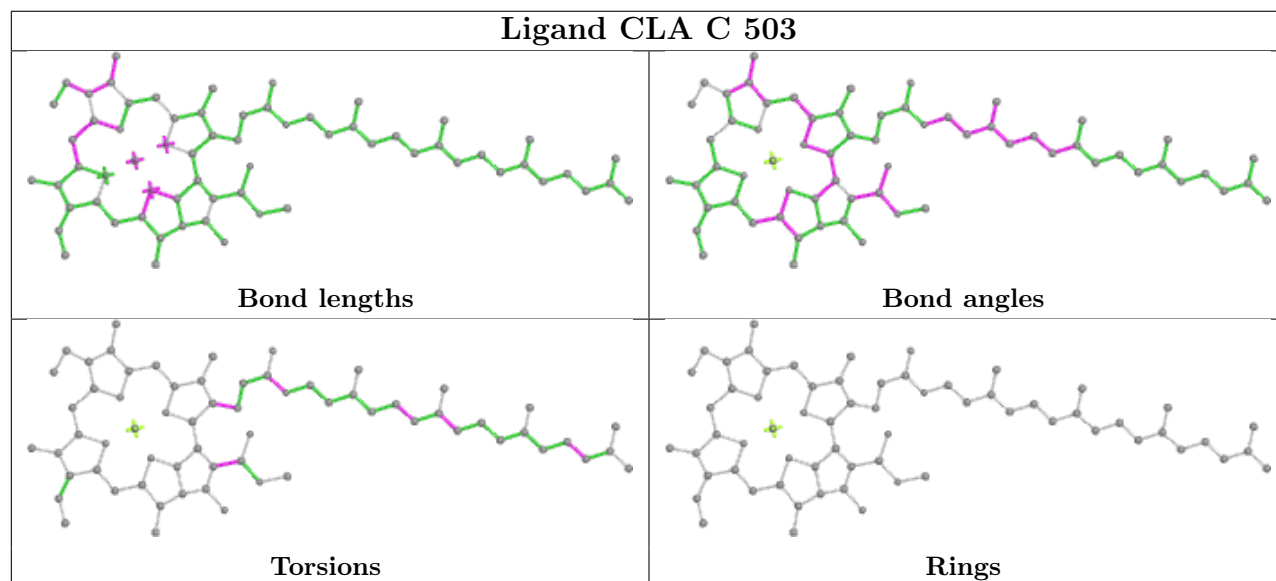
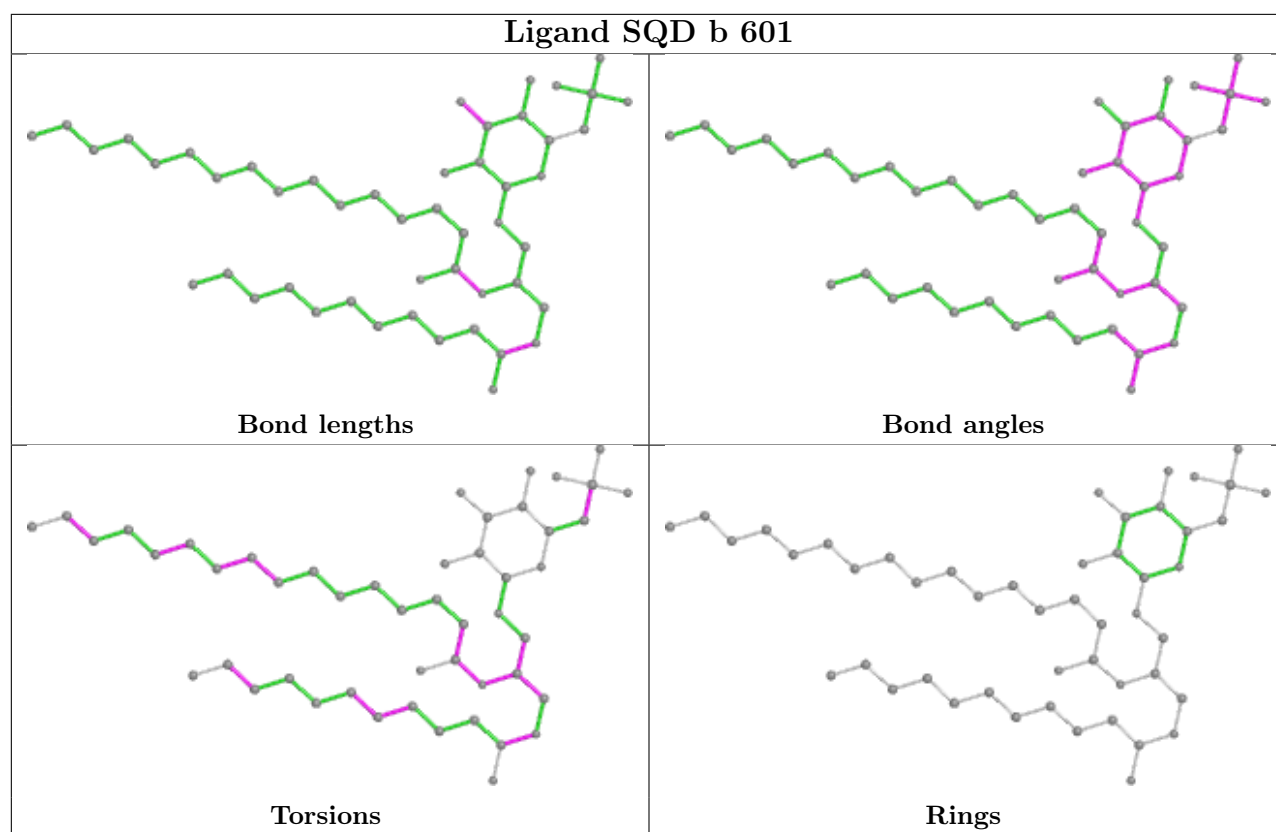


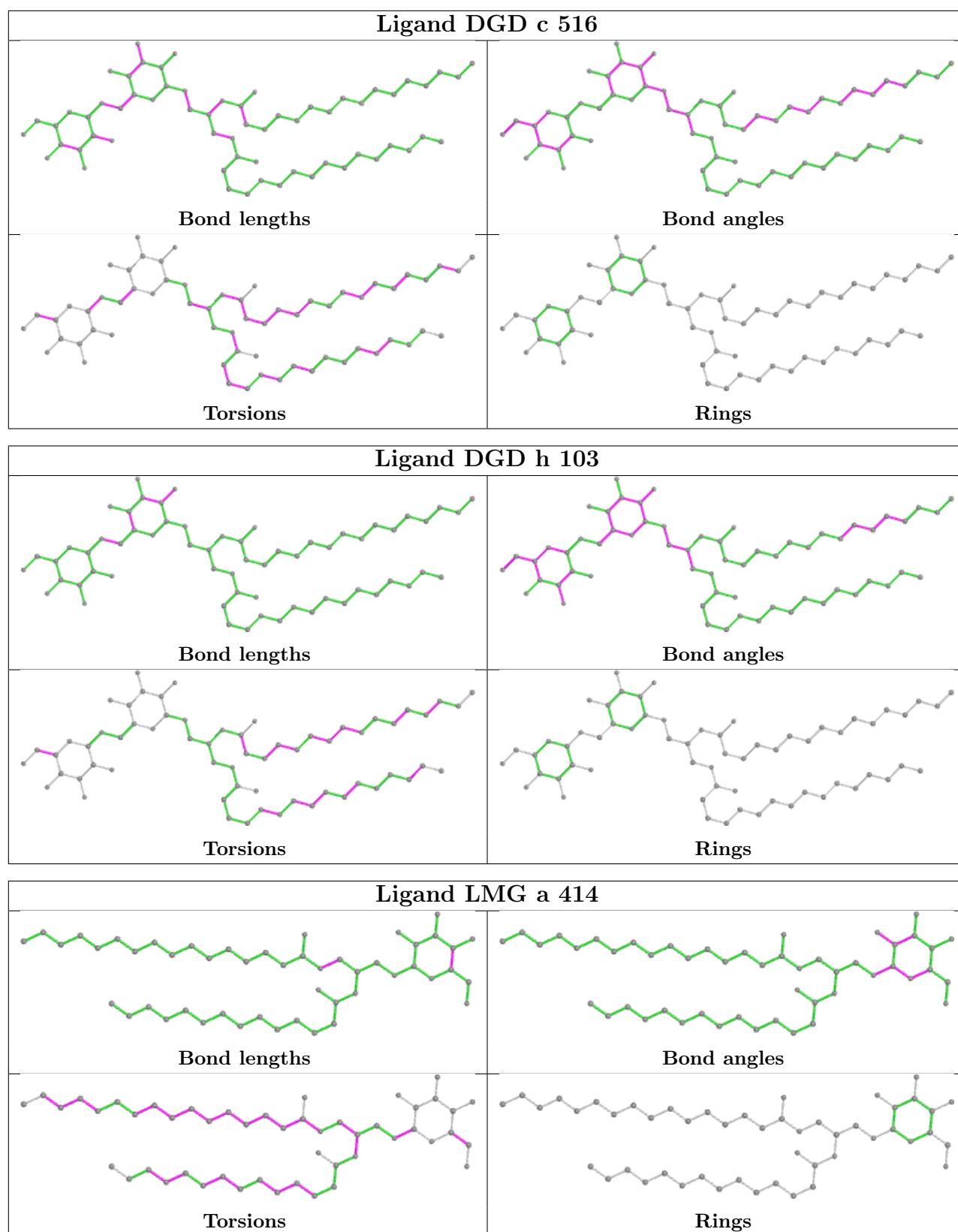


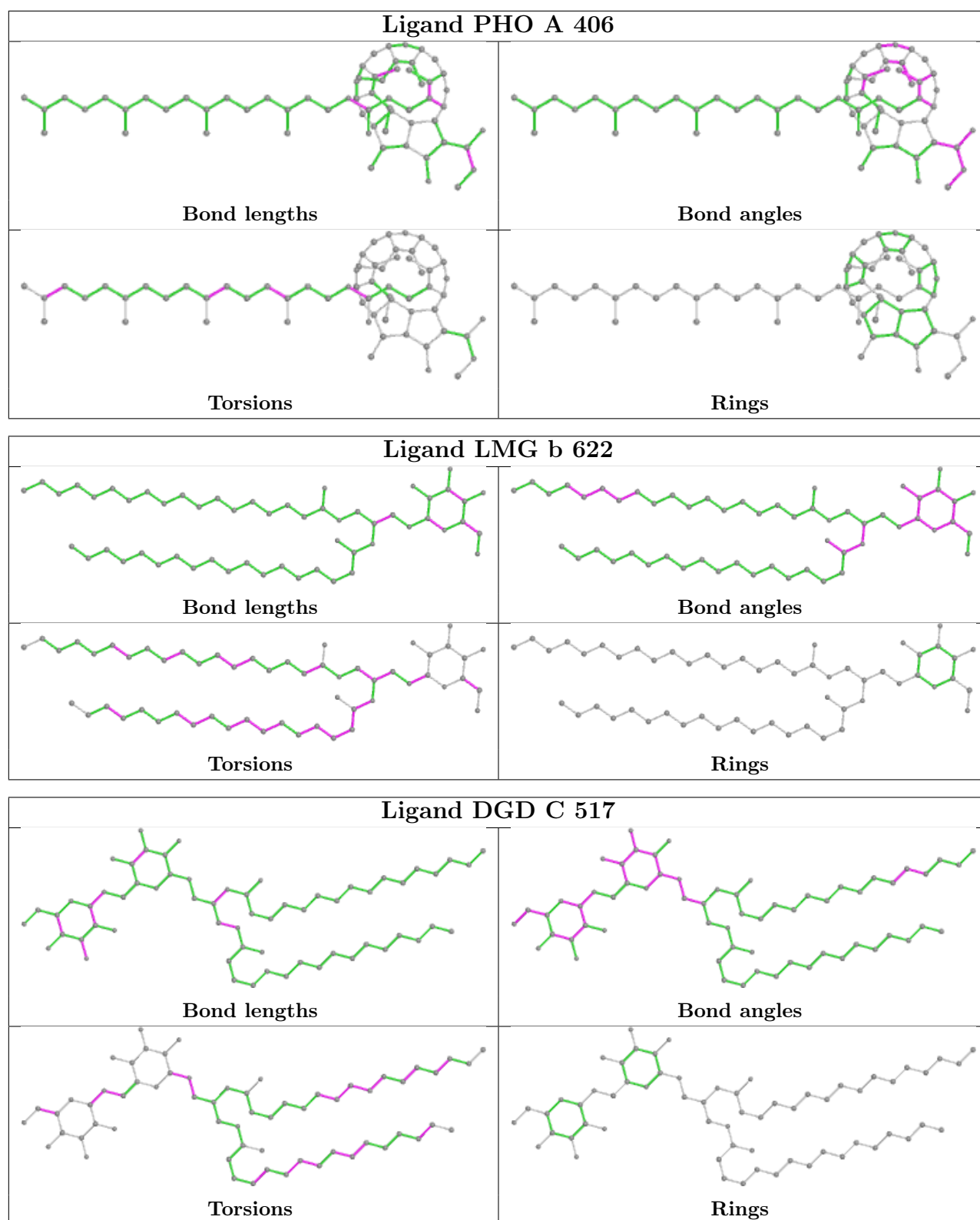




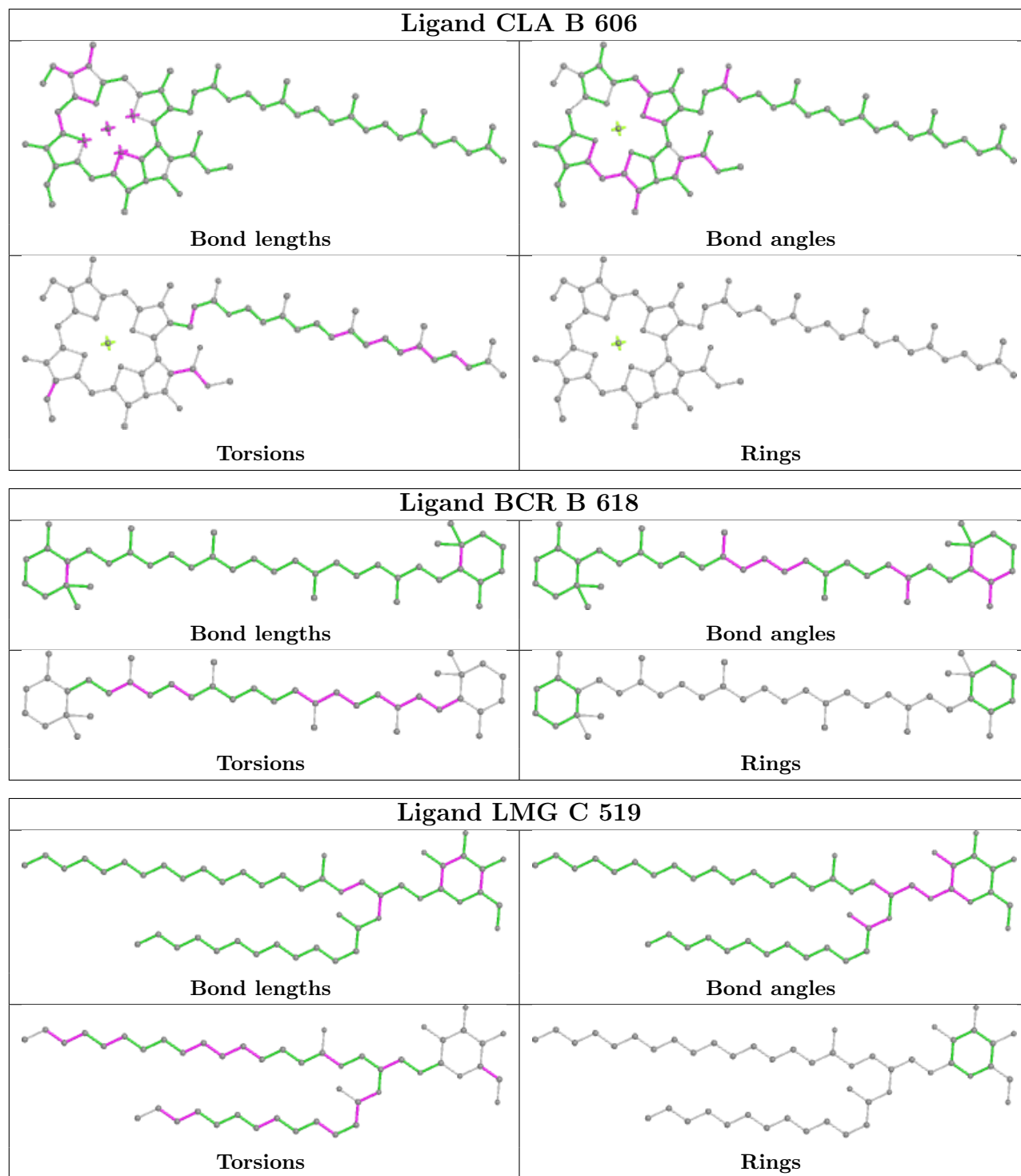


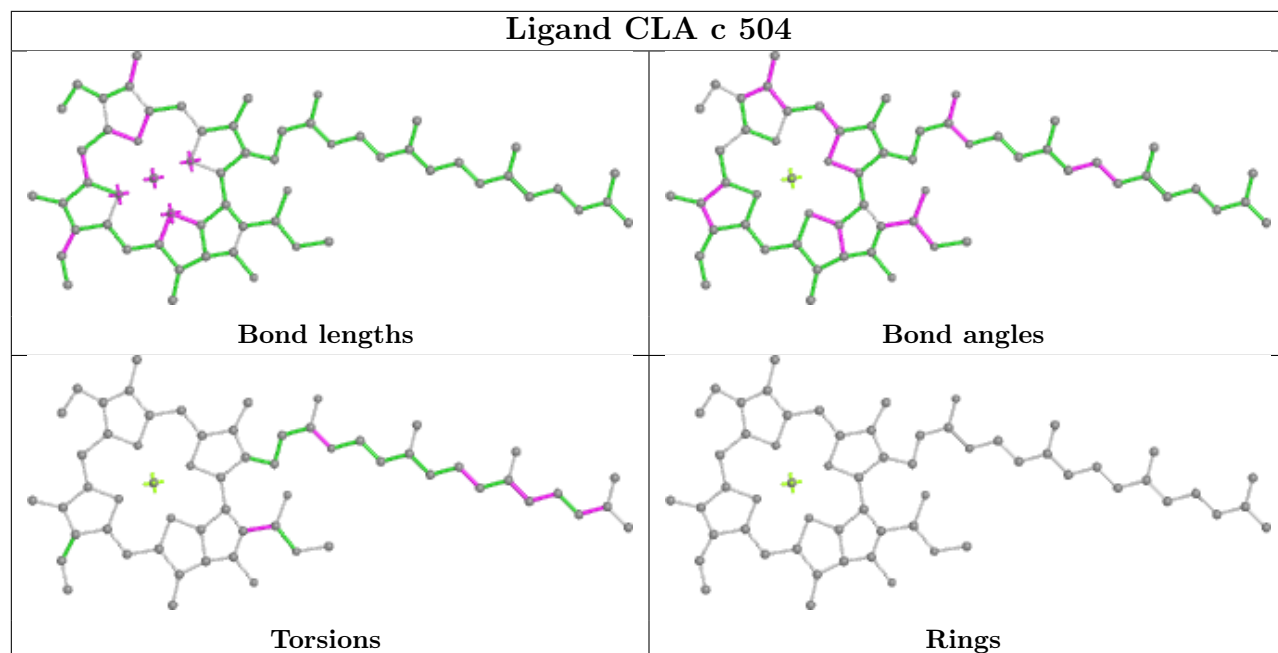


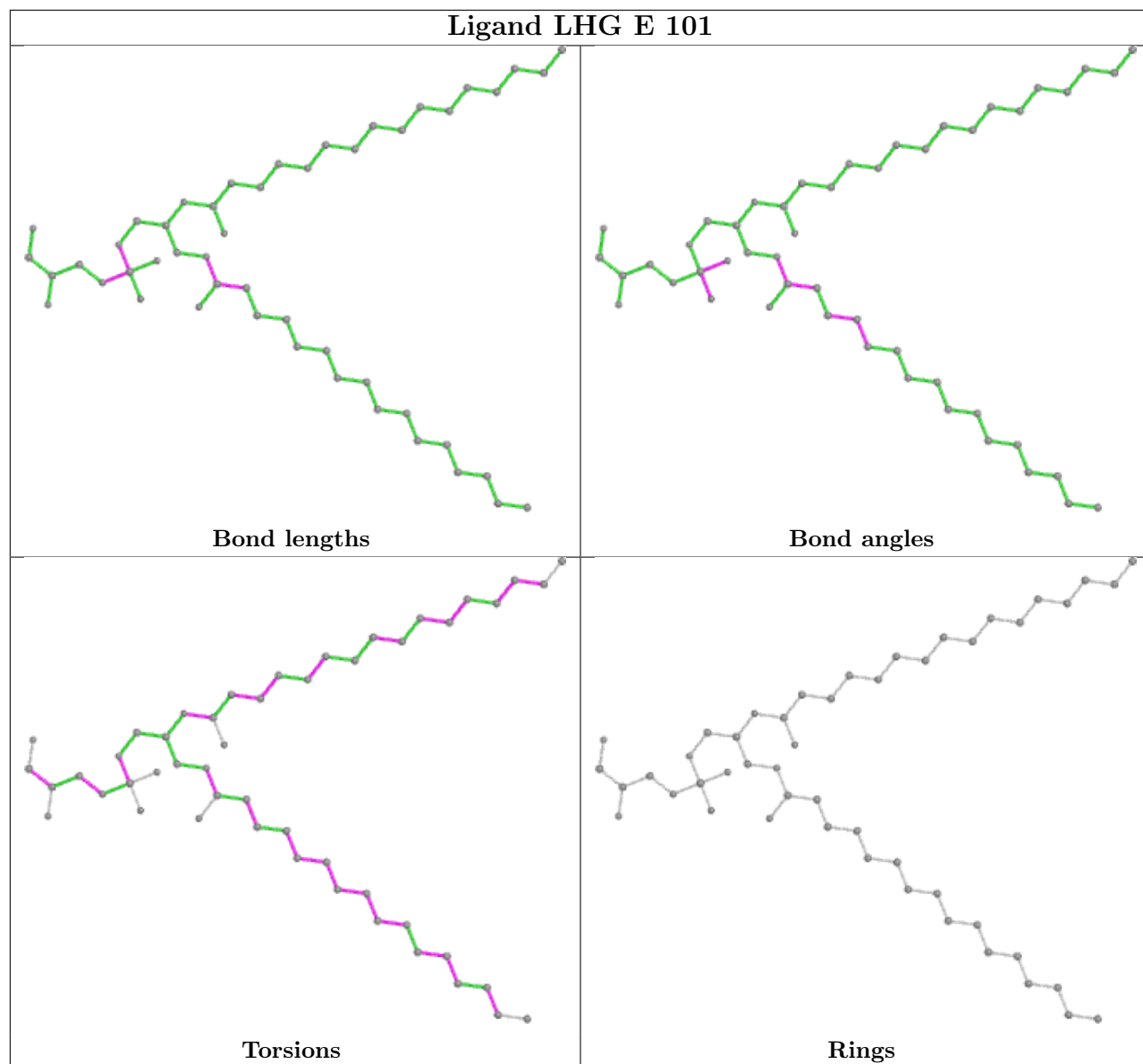


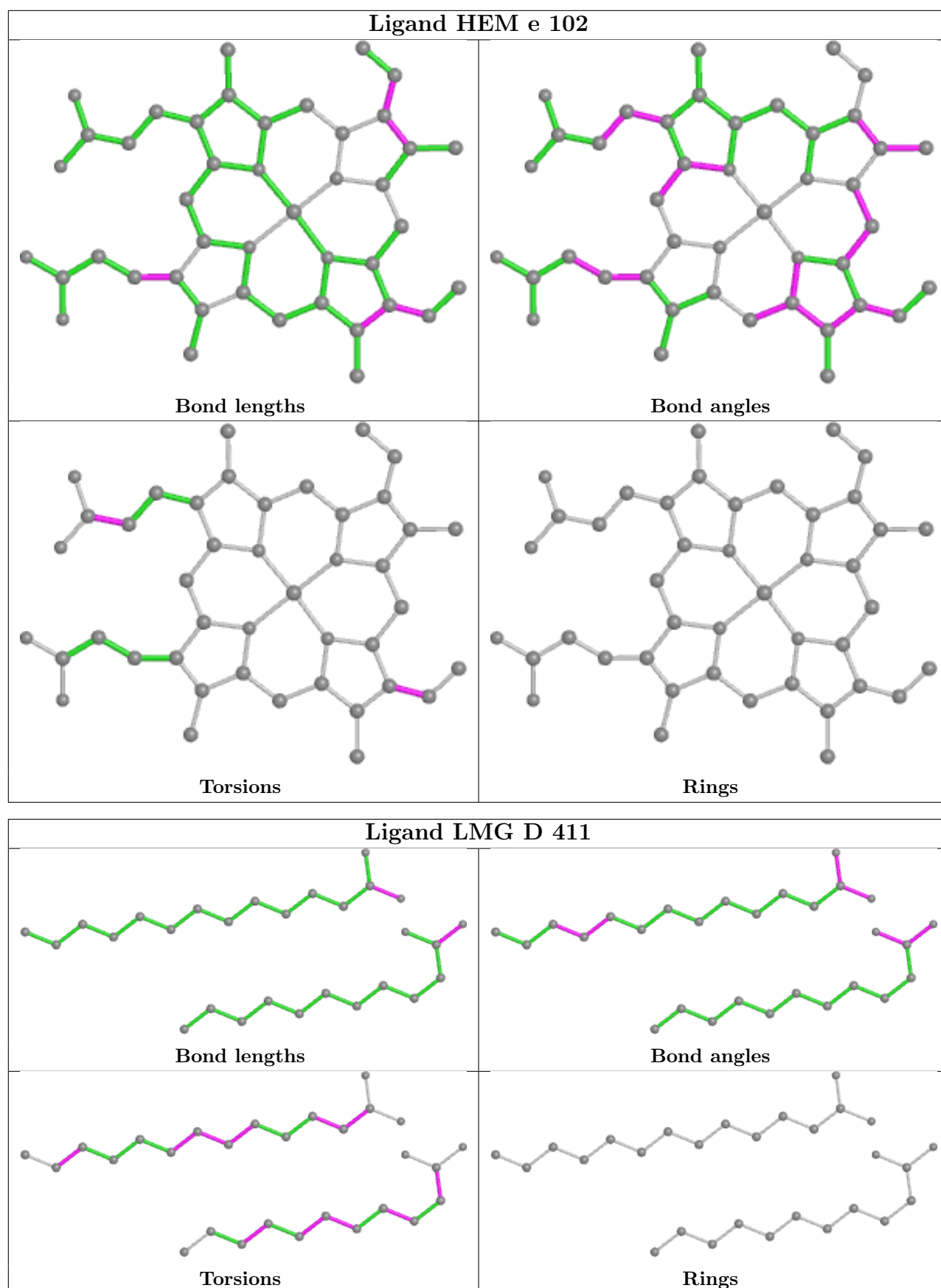


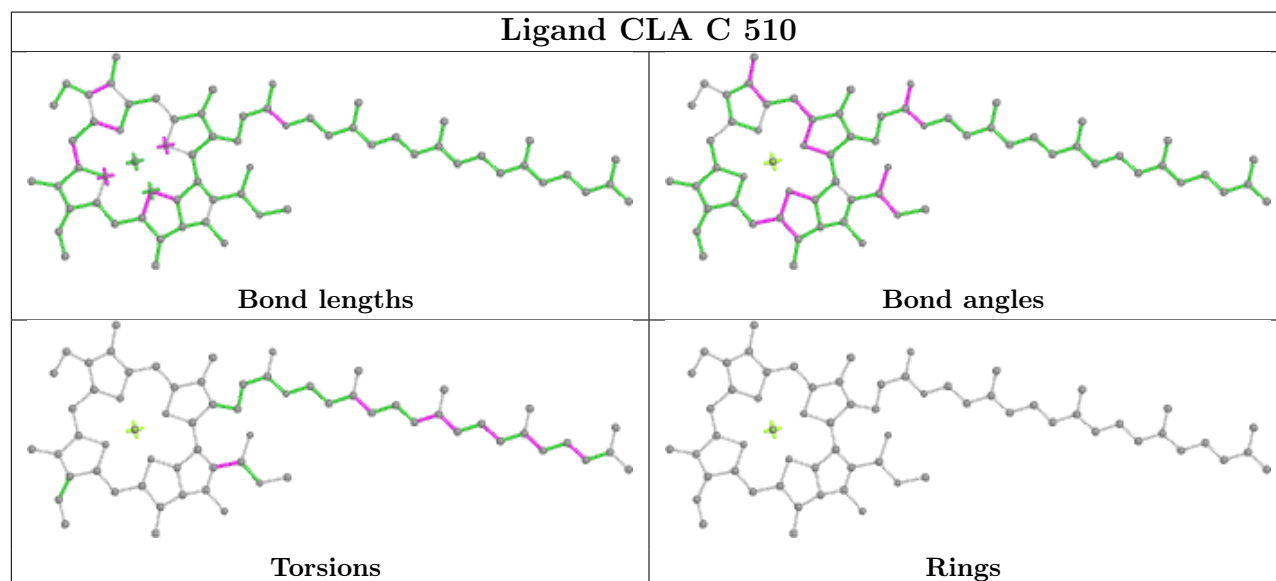
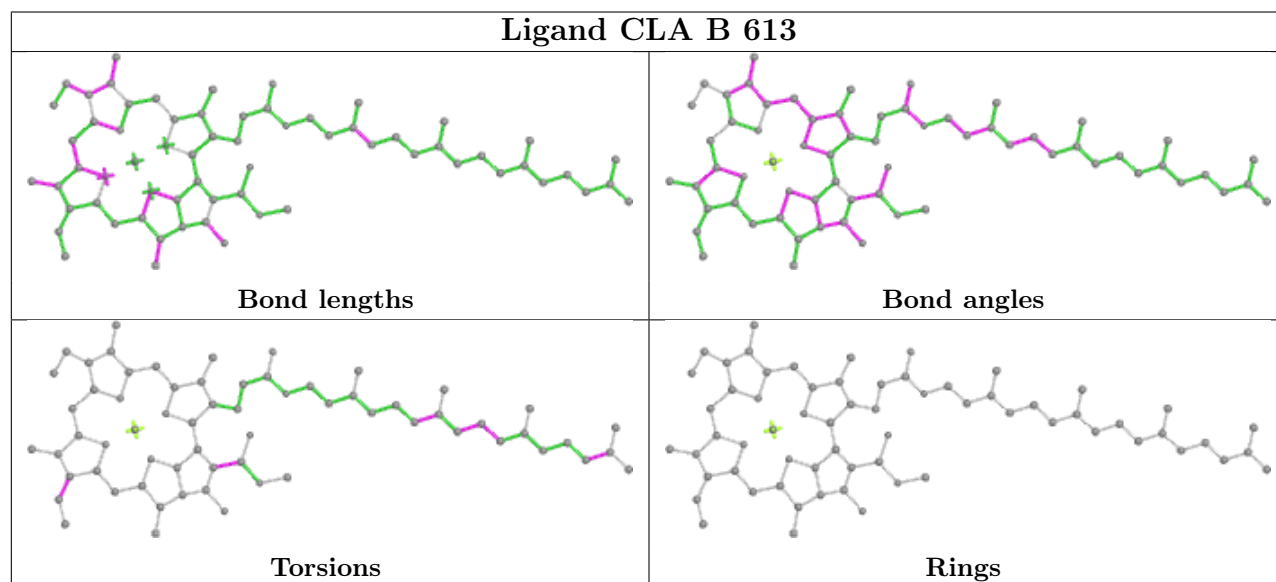
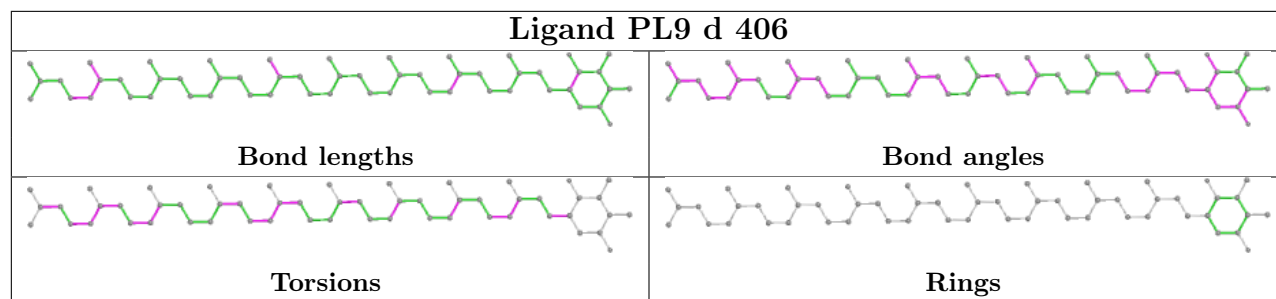


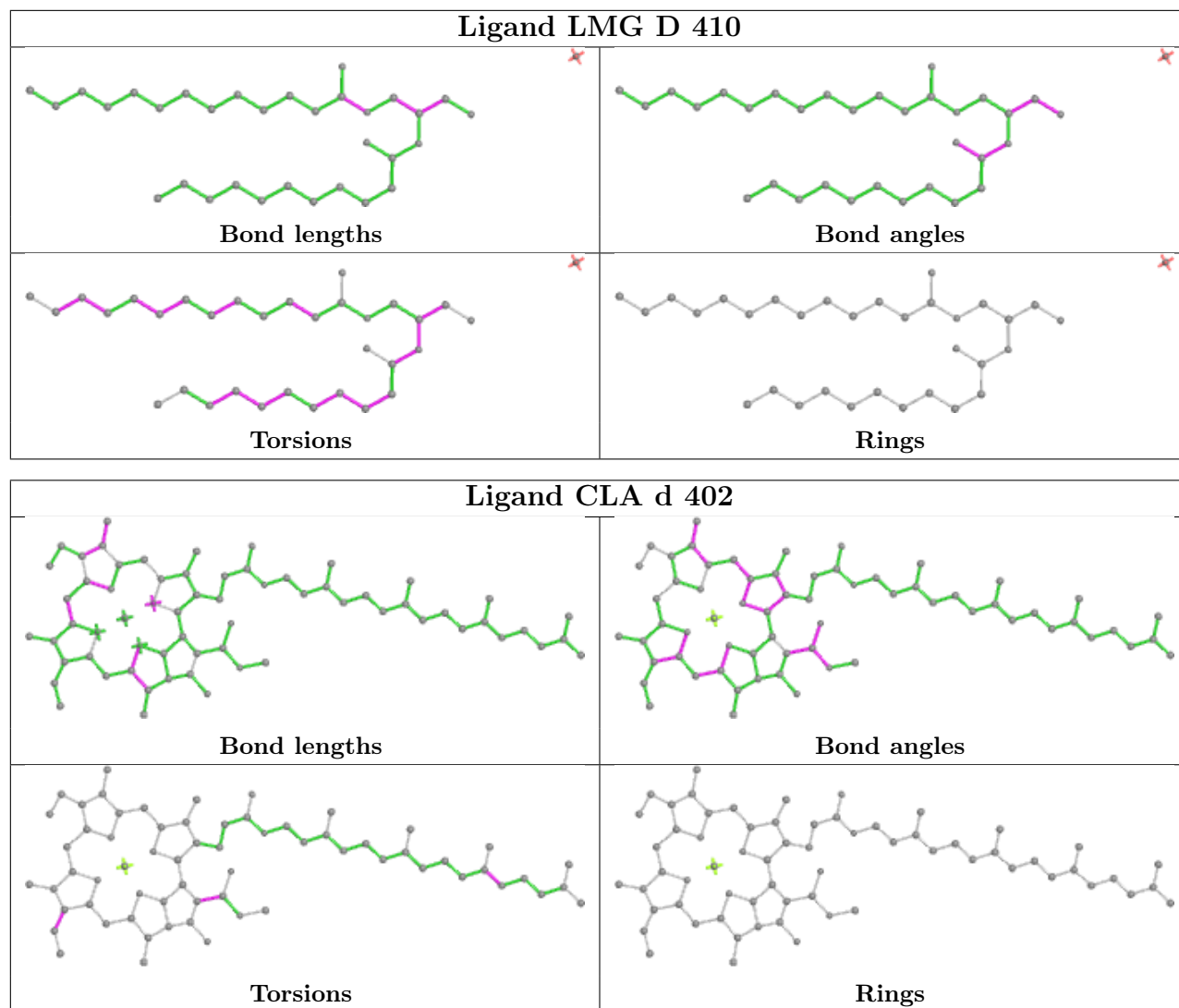












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	-0.53	2 (0%) 89 88	22, 30, 52, 77	0
1	a	334/334 (100%)	-0.49	1 (0%) 94 93	22, 32, 61, 86	0
2	B	505/505 (100%)	-0.45	6 (1%) 79 77	22, 34, 64, 101	0
2	b	505/505 (100%)	-0.34	10 (1%) 65 63	24, 38, 74, 107	0
3	C	442/451 (98%)	-0.40	0 100 100	24, 38, 56, 78	0
3	c	451/451 (100%)	-0.30	5 (1%) 80 79	26, 42, 62, 108	0
4	D	341/341 (100%)	-0.46	0 100 100	23, 32, 51, 87	0
4	d	341/341 (100%)	-0.39	4 (1%) 79 77	23, 36, 60, 85	0
5	E	81/82 (98%)	-0.06	2 (2%) 57 55	32, 50, 70, 76	0
5	e	82/82 (100%)	0.06	1 (1%) 79 77	40, 60, 79, 90	0
6	F	34/34 (100%)	-0.30	2 (5%) 22 21	36, 45, 67, 93	0
6	f	34/34 (100%)	-0.20	0 100 100	42, 51, 81, 88	0
7	H	65/65 (100%)	-0.13	0 100 100	33, 42, 60, 67	0
7	h	63/65 (96%)	0.05	1 (1%) 72 70	39, 51, 62, 74	0
8	I	35/36 (97%)	-0.29	2 (5%) 23 22	32, 39, 71, 79	0
8	i	35/36 (97%)	-0.22	2 (5%) 23 22	33, 42, 72, 86	0
9	J	36/36 (100%)	0.00	4 (11%) 5 4	35, 51, 75, 96	0
9	j	36/36 (100%)	0.05	3 (8%) 11 10	38, 55, 79, 88	0
10	K	37/37 (100%)	-0.20	1 (2%) 54 52	41, 54, 68, 74	0
10	k	37/37 (100%)	0.02	1 (2%) 54 52	45, 59, 72, 85	0
11	L	37/37 (100%)	-0.31	0 100 100	25, 32, 67, 78	0
11	l	36/37 (97%)	-0.43	0 100 100	26, 33, 74, 77	0
12	M	32/33 (96%)	-0.36	1 (3%) 49 47	28, 35, 62, 76	0
12	m	31/33 (93%)	-0.27	0 100 100	26, 35, 52, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/244 (100%)	-0.14	10 (4%) 37 35	23, 43, 79, 137	0
13	o	244/244 (100%)	-0.24	9 (3%) 41 39	24, 42, 82, 122	0
14	T	29/30 (96%)	-0.69	1 (3%) 45 43	26, 32, 62, 79	0
14	t	29/30 (96%)	-0.37	2 (6%) 16 15	28, 33, 81, 93	0
15	U	97/97 (100%)	-0.39	1 (1%) 82 81	29, 44, 68, 93	0
15	u	97/97 (100%)	-0.48	2 (2%) 63 61	30, 42, 61, 83	0
16	V	137/137 (100%)	-0.62	0 100 100	29, 41, 56, 84	0
16	v	137/137 (100%)	-0.28	1 (0%) 87 86	33, 49, 70, 81	0
17	Y	27/30 (90%)	1.70	13 (48%) 0 0	55, 78, 107, 116	0
17	y	30/30 (100%)	0.40	5 (16%) 1 1	58, 70, 87, 102	0
18	X	38/38 (100%)	-0.13	3 (7%) 12 11	35, 49, 79, 87	0
18	x	38/38 (100%)	0.00	3 (7%) 12 11	46, 57, 75, 103	0
19	Z	62/62 (100%)	0.64	14 (22%) 0 0	47, 64, 110, 120	0
19	z	62/62 (100%)	0.70	7 (11%) 5 4	55, 71, 110, 125	0
20	R	34/34 (100%)	1.28	10 (29%) 0 0	56, 70, 89, 97	0
20	r	31/34 (91%)	2.02	17 (54%) 0 0	65, 84, 101, 108	0
All	All	5300/5326 (99%)	-0.29	146 (2%) 53 51	22, 39, 75, 137	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	59	LYS	8.3
19	z	33	TRP	7.8
13	o	3	GLN	7.3
1	A	13	LEU	6.4
13	O	60	ARG	5.9
13	O	61	GLN	5.7
13	O	4	THR	5.6
13	O	3	GLN	5.5
3	c	23	ALA	5.4
18	X	2	THR	5.3
6	F	12	SER	5.2
17	Y	41	VAL	5.2
13	o	58	ASN	5.1
20	r	26	TYR	4.9
9	J	6	GLY	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	b	127	ARG	4.6
17	Y	20	ALA	4.5
13	o	56	PRO	4.3
19	z	35	ARG	4.3
2	b	128	THR	4.2
19	Z	1	MET	4.2
17	Y	23	THR	4.1
9	J	5	GLY	4.1
20	r	14	LEU	4.1
2	B	502	VAL	4.0
4	d	227[A]	GLU	4.0
17	Y	24	MET	4.0
20	R	3	TRP	4.0
5	e	79	PHE	4.0
3	c	24	THR	3.9
9	J	7	ARG	3.9
8	i	36	ASP	3.9
20	r	24	LEU	3.8
17	Y	42	ARG	3.8
15	U	8	GLU	3.7
17	Y	45	ASN	3.6
7	h	6	TRP	3.6
20	r	13	LEU	3.6
13	O	56	PRO	3.6
20	r	27	ALA	3.5
14	t	29	ILE	3.5
19	Z	33	TRP	3.5
17	y	40	ALA	3.5
14	t	30	THR	3.4
17	Y	37	PHE	3.4
13	o	4	THR	3.4
19	Z	62	VAL	3.4
8	I	36	ASP	3.4
2	B	505	ARG	3.4
20	r	3	TRP	3.3
20	R	21	ARG	3.2
17	Y	40	ALA	3.2
19	z	30	PRO	3.2
1	a	11	ALA	3.2
13	O	246	ALA	3.1
20	r	22	ASN	3.1
20	r	6	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	d	226	GLY	3.1
10	k	17	ILE	3.0
17	Y	25	ILE	3.0
2	b	490	GLN	3.0
19	Z	39	LEU	3.0
14	T	30	THR	3.0
17	Y	43	ARG	3.0
17	Y	21	GLN	2.9
19	Z	3	ILE	2.9
20	r	21	ARG	2.9
19	z	34	ASP	2.9
9	j	6	GLY	2.9
2	B	506	ARG	2.9
19	Z	7	LEU	2.9
20	r	10	LEU	2.9
9	J	8	ILE	2.9
20	R	31	VAL	2.9
5	E	79	PHE	2.8
2	b	495	PHE	2.8
20	r	17	GLY	2.8
18	X	3	ILE	2.8
13	o	5	LEU	2.7
2	b	506	ARG	2.7
19	Z	38	GLN	2.7
20	R	25	PRO	2.7
13	o	62	GLU	2.6
17	Y	22	LEU	2.6
19	Z	32	ASP	2.6
6	F	13	TYR	2.6
18	x	3	ILE	2.6
19	Z	42	LEU	2.6
2	b	494	GLY	2.6
20	r	18	TRP	2.6
19	z	60	PHE	2.6
3	c	143	TYR	2.6
19	Z	34	ASP	2.6
13	O	62	GLU	2.5
20	R	29	LYS	2.5
2	b	487	SER	2.5
20	r	4	ARG	2.4
17	Y	44	GLY	2.4
13	o	61	GLN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	o	57	LYS	2.4
20	r	23	ILE	2.4
20	R	20	VAL	2.4
19	Z	4	LEU	2.4
20	r	9	LEU	2.4
9	j	7	ARG	2.4
18	x	38	GLN	2.4
20	r	2	ASP	2.3
2	B	487	SER	2.3
20	r	28	VAL	2.3
18	X	39	ARG	2.3
17	y	19	ILE	2.3
8	I	34	ARG	2.3
1	A	11	ALA	2.3
13	O	63	ALA	2.3
12	M	33	GLN	2.3
2	b	505	ARG	2.3
19	z	14	ILE	2.3
3	c	191	PRO	2.3
19	z	4	LEU	2.2
20	R	6	LEU	2.2
2	b	492	GLU	2.2
16	v	16	GLY	2.2
2	B	293	ALA	2.2
2	B	488	PRO	2.2
4	d	64	ALA	2.2
20	R	26	TYR	2.2
17	y	37	PHE	2.2
18	x	2	THR	2.2
5	E	83	LEU	2.2
2	b	502	VAL	2.2
17	y	20	ALA	2.1
10	K	10	LYS	2.1
9	j	11	TRP	2.1
13	o	246	ALA	2.1
20	R	28	VAL	2.1
20	R	24	LEU	2.1
15	u	53	ALA	2.1
17	y	18	VAL	2.1
19	Z	35	ARG	2.1
8	i	33	LYS	2.1
4	d	51	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
19	Z	61	VAL	2.1
19	Z	41	PHE	2.1
15	u	86	GLU	2.0
13	O	57	LYS	2.0
3	c	147	PHE	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	M	1	10/11	0.90	0.18	40,50,73,76	0
14	FME	t	1	10/11	0.90	0.12	33,48,73,78	0
14	FME	T	1	10/11	0.91	0.14	32,46,75,75	0
8	FME	i	1	10/11	0.94	0.12	37,52,72,72	0
8	FME	I	1	10/11	0.94	0.16	39,53,74,74	0
12	FME	m	1	10/11	0.96	0.14	34,58,78,84	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
32	UNL	a	415	28/-	0.70	0.37	43,71,87,94	0
27	LMG	b	623	23/55	0.76	0.22	35,66,90,91	0
32	UNL	E	103	28/-	0.78	0.31	58,81,95,97	0
27	LMG	b	622	55/55	0.79	0.26	41,78,99,111	0
33	LHG	E	101	49/49	0.80	0.23	51,82,112,120	0
32	UNL	H	103	53/-	0.81	0.23	35,77,97,101	0
32	UNL	B	626	28/-	0.81	0.36	50,75,87,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	UNL	b	621	55/-	0.81	0.19	40,62,91,109	0
28	SQD	a	412	36/54	0.81	0.18	29,68,100,110	0
32	UNL	I	101	41/-	0.82	0.16	40,55,77,82	0
32	UNL	b	625	55/-	0.82	0.21	44,66,86,91	0
32	UNL	c	523	28/-	0.82	0.20	43,69,80,82	0
27	LMG	c	522	48/55	0.82	0.26	50,82,110,114	0
32	UNL	b	626	26/-	0.83	0.24	33,59,66,67	0
26	PL9	a	409	55/55	0.83	0.27	34,67,89,101	0
32	UNL	B	627	47/-	0.83	0.27	41,65,89,89	0
29	DGD	a	413	44/66	0.84	0.16	33,59,88,94	0
32	UNL	C	521	28/-	0.84	0.13	36,50,61,62	0
32	UNL	J	101	28/-	0.84	0.12	49,62,72,75	0
32	UNL	T	102	44/-	0.84	0.19	41,55,68,72	0
32	UNL	x	101	55/-	0.84	0.20	47,62,78,78	0
27	LMG	D	410	33/55	0.84	0.16	29,57,87,90	0
25	BCR	h	102	40/40	0.85	0.15	33,56,73,81	0
32	UNL	d	410	43/-	0.85	0.20	33,57,72,73	0
23	CLA	h	101	65/65	0.85	0.17	44,72,93,100	0
32	UNL	c	520	55/-	0.85	0.20	42,61,79,90	0
26	PL9	A	409	55/55	0.86	0.26	37,62,89,101	0
32	UNL	b	624	40/-	0.86	0.16	38,64,80,83	0
32	UNL	C	522	28/-	0.86	0.14	42,59,72,78	0
28	SQD	b	601	49/54	0.86	0.15	44,64,103,114	0
29	DGD	A	413	66/66	0.86	0.19	43,68,93,121	0
23	CLA	c	512	65/65	0.86	0.14	39,60,93,109	0
32	UNL	B	624	34/-	0.86	0.20	39,55,71,72	0
23	CLA	c	513	65/65	0.86	0.22	42,75,107,123	0
28	SQD	A	412	39/54	0.86	0.23	40,69,102,121	0
25	BCR	y	101	40/40	0.87	0.14	41,63,77,84	0
23	CLA	C	512	65/65	0.87	0.18	36,61,111,127	0
32	UNL	l	102	53/-	0.87	0.16	30,48,99,103	0
32	UNL	t	103	46/-	0.87	0.13	38,61,81,82	0
23	CLA	C	513	65/65	0.87	0.17	40,70,102,114	0
23	CLA	B	616	60/65	0.87	0.16	27,44,87,103	0
33	LHG	e	101	42/49	0.87	0.27	63,88,113,120	0
27	LMG	D	411	28/55	0.88	0.16	30,51,68,74	0
28	SQD	f	101	41/54	0.88	0.22	49,85,120,123	0
25	BCR	D	405	40/40	0.88	0.14	29,46,100,116	0
25	BCR	H	101	40/40	0.88	0.12	32,46,59,66	0
32	UNL	B	621	43/-	0.88	0.14	38,54,69,73	0
32	UNL	M	102	26/-	0.88	0.19	30,53,63,67	0
32	UNL	m	102	28/-	0.88	0.15	40,55,69,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMG	c	519	37/55	0.88	0.18	34,70,93,96	0
25	BCR	d	405	40/40	0.88	0.14	36,57,95,108	0
27	LMG	C	519	48/55	0.88	0.15	43,68,88,96	0
23	CLA	B	601	65/65	0.88	0.15	31,63,100,113	0
32	UNL	j	101	28/-	0.89	0.10	42,60,71,74	0
27	LMG	a	414	49/55	0.89	0.16	36,60,94,101	0
32	UNL	D	412	55/-	0.89	0.20	32,51,79,101	0
32	UNL	t	102	26/-	0.89	0.21	42,56,67,68	0
25	BCR	K	101	40/40	0.89	0.13	41,56,68,75	0
27	LMG	A	410	48/55	0.89	0.18	30,61,81,105	0
32	UNL	b	602	47/-	0.89	0.21	36,59,74,79	0
27	LMG	B	620	51/55	0.89	0.12	29,51,72,81	0
23	CLA	b	617	60/65	0.90	0.15	26,49,99,106	0
32	UNL	B	625	28/-	0.90	0.11	29,46,67,72	0
28	SQD	B	623	54/54	0.90	0.13	37,62,88,98	0
23	CLA	D	404	65/65	0.90	0.15	19,42,114,122	0
27	LMG	m	101	51/55	0.90	0.13	29,52,83,98	0
23	CLA	c	508	64/65	0.91	0.14	32,51,98,118	0
23	CLA	b	616	65/65	0.91	0.13	20,40,63,68	0
27	LMG	D	407	51/55	0.91	0.16	27,59,79,87	0
29	DGD	C	517	62/66	0.91	0.14	31,56,95,117	0
23	CLA	a	407	65/65	0.91	0.14	15,37,99,110	0
23	CLA	d	404	65/65	0.91	0.15	25,53,100,107	0
25	BCR	c	514	40/40	0.91	0.16	37,58,73,75	0
28	SQD	a	411	54/54	0.91	0.13	36,71,94,110	0
25	BCR	c	521	40/40	0.91	0.17	34,57,70,77	0
25	BCR	B	617	40/40	0.92	0.12	26,43,57,60	0
29	DGD	c	518	62/66	0.92	0.12	26,54,77,93	0
29	DGD	h	103	62/66	0.92	0.13	35,54,73,79	0
25	BCR	C	514	40/40	0.92	0.14	34,59,76,77	0
25	BCR	C	515	40/40	0.92	0.12	21,38,53,67	0
25	BCR	C	520	40/40	0.92	0.18	38,55,67,74	0
23	CLA	c	506	65/65	0.92	0.14	32,53,112,129	0
23	CLA	B	615	65/65	0.92	0.14	20,41,67,95	0
23	CLA	b	605	65/65	0.92	0.15	20,39,87,103	0
25	BCR	b	619	40/40	0.92	0.10	25,42,59,66	0
32	UNL	C	523	47/-	0.92	0.10	39,52,63,69	0
25	BCR	b	620	40/40	0.92	0.12	30,50,66,69	0
23	CLA	B	606	65/65	0.92	0.13	21,41,75,98	0
23	CLA	C	505	65/65	0.92	0.18	24,42,75,88	0
29	DGD	C	516	62/66	0.92	0.14	21,40,76,98	0
23	CLA	c	503	65/65	0.92	0.16	31,48,61,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	UNL	M	101	37/-	0.92	0.13	30,49,71,75	0
29	DGD	H	102	62/66	0.92	0.13	28,49,67,77	0
29	DGD	c	517	62/66	0.93	0.12	32,52,81,95	0
23	CLA	B	604	65/65	0.93	0.13	21,36,84,94	0
23	CLA	c	502	65/65	0.93	0.13	24,46,76,85	0
25	BCR	A	408	40/40	0.93	0.10	24,34,42,56	0
27	LMG	d	409	44/55	0.93	0.13	31,53,84,107	0
23	CLA	a	405	65/65	0.93	0.13	25,42,98,111	0
25	BCR	B	618	40/40	0.93	0.11	25,43,58,64	0
25	BCR	B	619	40/40	0.93	0.12	33,47,58,62	0
28	SQD	F	101	36/54	0.93	0.14	43,66,89,96	0
23	CLA	c	504	60/65	0.93	0.13	24,47,79,81	0
23	CLA	C	506	65/65	0.93	0.13	28,45,95,114	0
23	CLA	c	507	65/65	0.93	0.14	28,45,63,74	0
23	CLA	A	405	65/65	0.93	0.13	23,36,106,121	0
23	CLA	c	510	65/65	0.93	0.14	30,51,72,79	0
23	CLA	c	511	65/65	0.93	0.15	34,62,79,87	0
25	BCR	T	101	40/40	0.93	0.10	29,43,58,68	0
23	CLA	b	607	65/65	0.93	0.11	25,46,80,86	0
33	LHG	d	408	39/49	0.93	0.12	36,50,75,78	0
23	CLA	C	502	65/65	0.93	0.12	25,42,62,68	0
23	CLA	B	613	65/65	0.94	0.13	17,34,63,74	0
23	CLA	C	507	65/65	0.94	0.13	22,39,51,59	0
23	CLA	b	603	65/65	0.94	0.16	29,47,74,80	0
23	CLA	c	509	65/65	0.94	0.16	28,49,74,79	0
23	CLA	C	508	65/65	0.94	0.12	27,46,102,120	0
23	CLA	C	509	65/65	0.94	0.15	27,46,61,74	0
25	BCR	a	408	40/40	0.94	0.09	25,35,50,55	0
25	BCR	b	618	40/40	0.94	0.11	25,46,57,65	0
23	CLA	b	610	65/65	0.94	0.12	28,46,65,77	0
23	CLA	b	613	65/65	0.94	0.15	17,35,49,56	0
23	CLA	b	615	65/65	0.94	0.15	23,44,73,79	0
23	CLA	C	510	65/65	0.94	0.13	31,51,78,88	0
24	PHO	a	406	64/64	0.94	0.12	22,34,46,48	0
24	PHO	d	401	64/64	0.94	0.11	27,42,52,57	0
23	CLA	C	511	65/65	0.94	0.12	33,57,78,85	0
23	CLA	B	614	65/65	0.94	0.13	22,41,85,96	0
26	PL9	D	406	55/55	0.94	0.12	22,36,51,54	0
23	CLA	C	504	59/65	0.94	0.14	22,44,81,96	0
33	LHG	a	410	49/49	0.94	0.13	38,53,87,104	0
23	CLA	B	609	65/65	0.94	0.11	23,37,52,63	0
23	CLA	c	505	65/65	0.94	0.14	26,44,62,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	LHG	l	101	49/49	0.94	0.14	31,49,66,78	0
28	SQD	A	411	52/54	0.95	0.14	30,64,88,97	0
23	CLA	d	403	65/65	0.95	0.11	20,38,63,75	0
25	BCR	c	515	40/40	0.95	0.12	32,49,69,77	0
23	CLA	b	612	65/65	0.95	0.11	18,36,51,56	0
23	CLA	C	501	65/65	0.95	0.12	24,37,54,64	0
24	PHO	A	406	64/64	0.95	0.11	17,30,42,53	0
25	BCR	t	101	40/40	0.95	0.09	27,42,57,61	0
23	CLA	b	614	65/65	0.95	0.14	19,33,86,94	0
23	CLA	B	607	65/65	0.95	0.12	18,35,71,85	0
23	CLA	C	503	65/65	0.95	0.11	27,44,56,69	0
23	CLA	D	402	65/65	0.95	0.11	17,29,54,61	0
29	DGD	C	518	62/66	0.95	0.10	28,47,84,98	0
26	PL9	d	406	55/55	0.95	0.11	23,37,48,48	0
23	CLA	c	501	65/65	0.95	0.13	25,42,59,68	0
29	DGD	c	516	62/66	0.95	0.12	20,45,71,80	0
23	CLA	D	403	65/65	0.95	0.11	15,34,60,62	0
23	CLA	B	602	65/65	0.95	0.12	24,39,68,80	0
23	CLA	a	404	65/65	0.95	0.11	20,32,45,53	0
23	CLA	B	610	65/65	0.95	0.15	18,33,48,50	0
23	CLA	B	611	65/65	0.95	0.10	19,32,49,53	0
23	CLA	B	603	65/65	0.95	0.14	18,34,60,70	0
23	CLA	b	604	65/65	0.95	0.14	24,41,67,69	0
33	LHG	B	622	49/49	0.95	0.12	26,46,73,77	0
33	LHG	D	409	47/49	0.95	0.11	25,51,82,101	0
23	CLA	A	407	54/65	0.95	0.13	12,31,68,79	0
23	CLA	B	605	65/65	0.95	0.14	18,33,47,57	0
33	LHG	d	407	49/49	0.95	0.11	26,45,64,80	0
23	CLA	b	609	65/65	0.95	0.12	26,43,65,70	0
23	CLA	A	404	65/65	0.95	0.10	16,29,43,51	0
23	CLA	b	611	65/65	0.95	0.14	25,39,59,60	0
34	HEM	E	102	43/43	0.95	0.13	33,52,67,72	0
23	CLA	b	608	65/65	0.96	0.11	19,37,78,96	0
33	LHG	L	101	49/49	0.96	0.12	28,45,61,67	0
23	CLA	B	612	65/65	0.96	0.14	17,32,57,69	0
23	CLA	b	606	65/65	0.96	0.12	21,36,53,59	0
24	PHO	D	401	64/64	0.96	0.09	23,35,46,51	0
23	CLA	d	402	65/65	0.96	0.10	22,34,43,51	0
33	LHG	D	408	49/49	0.96	0.11	22,43,59,74	0
23	CLA	B	608	65/65	0.96	0.10	19,37,56,61	0
34	HEM	e	102	43/43	0.96	0.13	39,56,79,91	0
31	BCT	A	415	4/4	0.97	0.16	31,36,37,44	0

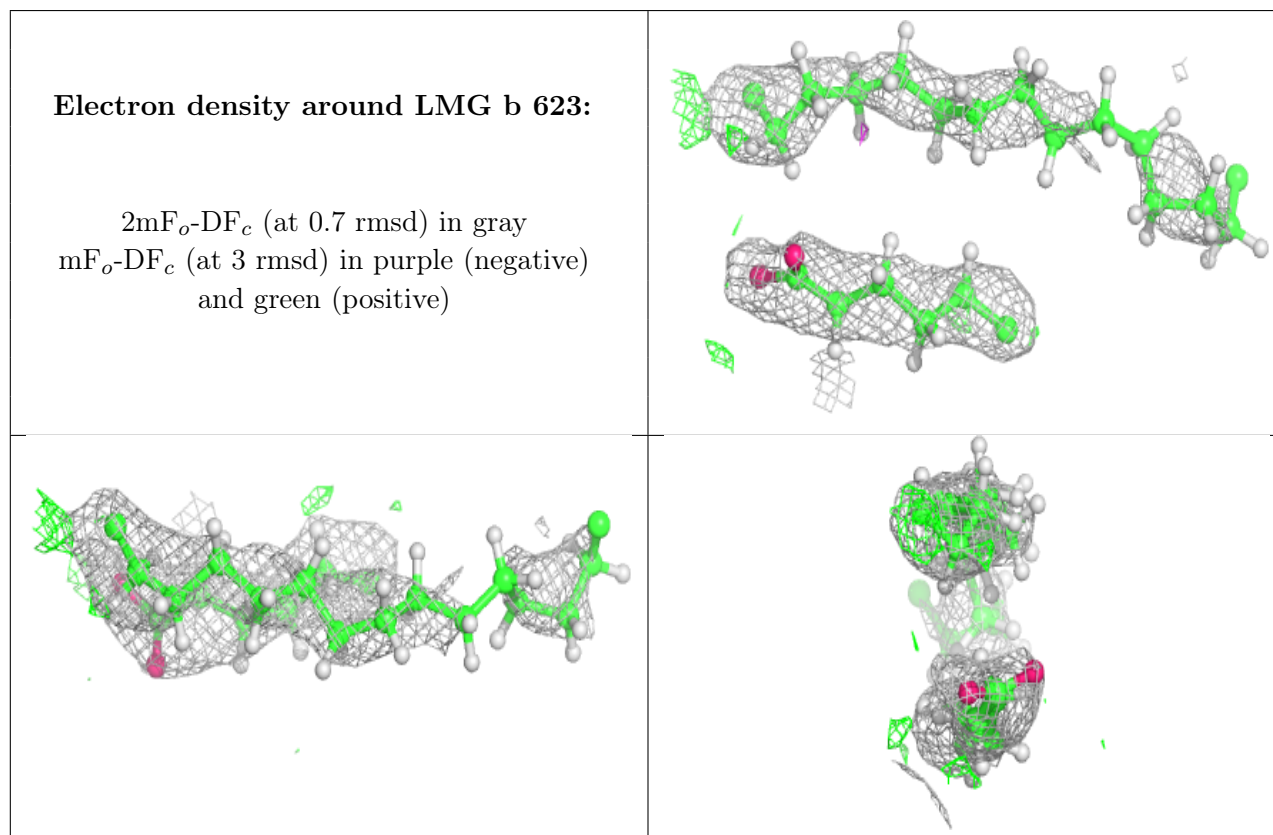
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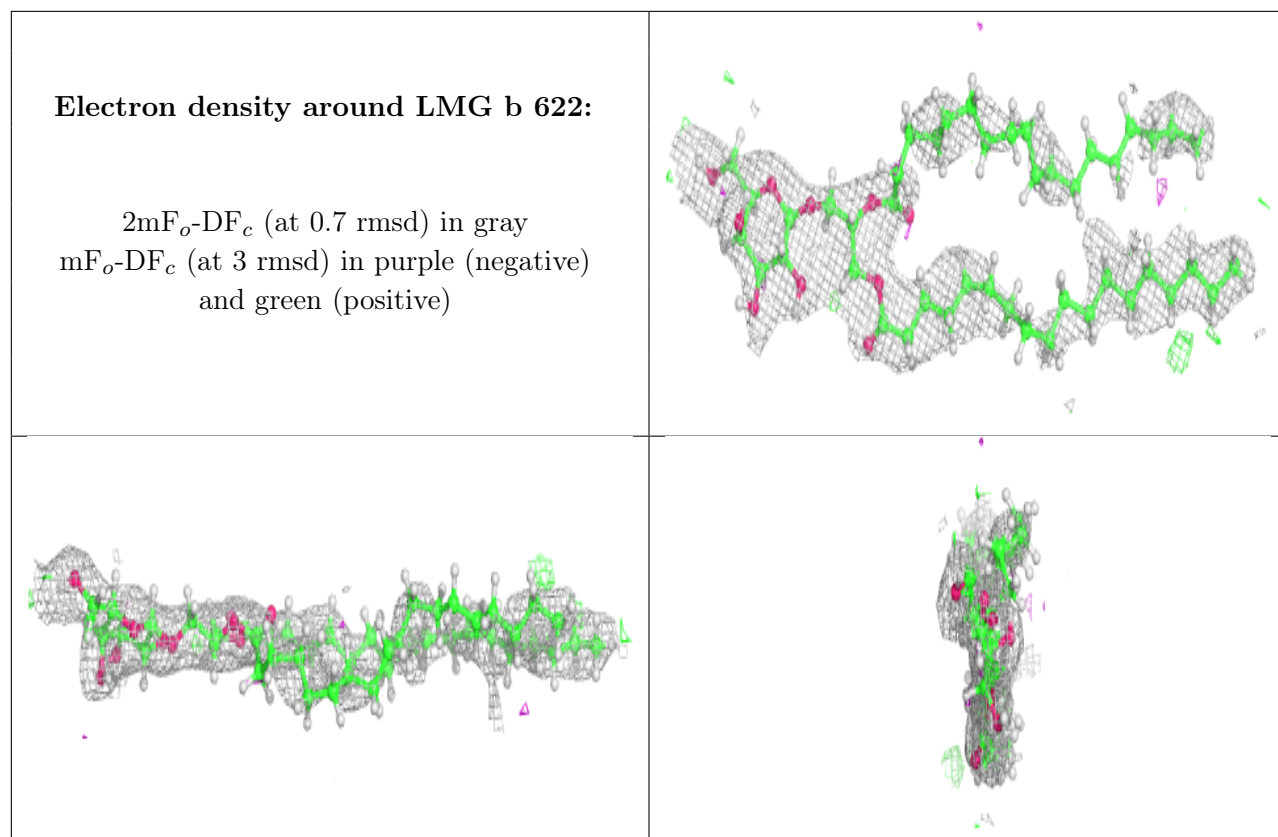


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	HEC	V	201	43/43	0.97	0.13	25,34,45,49	0
35	HEC	v	201	43/43	0.97	0.14	26,38,52,54	0
31	BCT	a	417	4/4	0.98	0.15	30,37,42,45	0
22	CL	a	403	1/1	0.98	0.05	29,29,29,29	0
30	OEY	A	414	11/11	0.99	0.10	28,31,39,43	1
30	OEY	a	416	11/11	0.99	0.11	24,30,34,35	0
22	CL	A	402	1/1	0.99	0.08	26,26,26,26	0
22	CL	A	403	1/1	0.99	0.02	25,25,25,25	0
22	CL	a	402	1/1	0.99	0.02	31,31,31,31	0
21	FE2	A	401	1/1	0.99	0.08	33,33,33,33	0
21	FE2	a	401	1/1	0.99	0.06	37,37,37,37	0

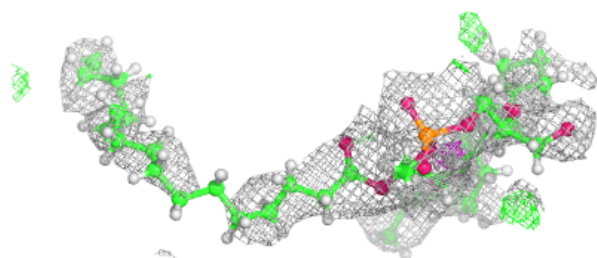
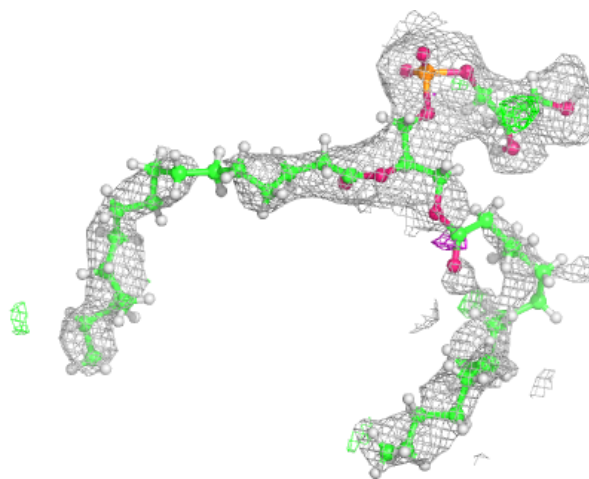
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





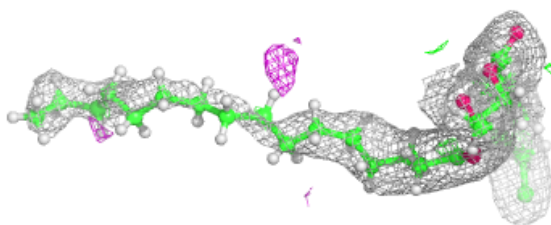
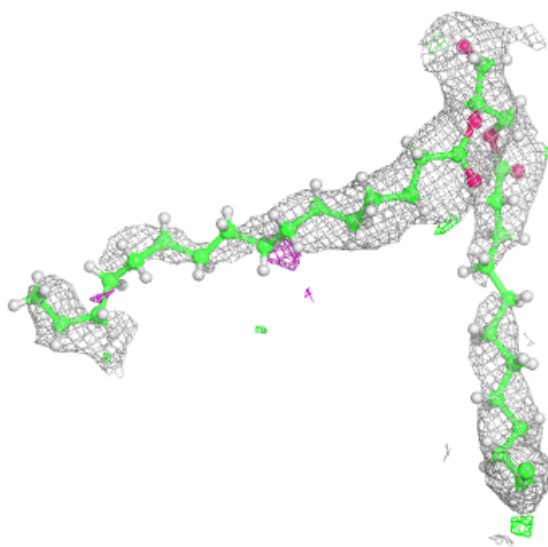
**Electron density around LHG E 101:**

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



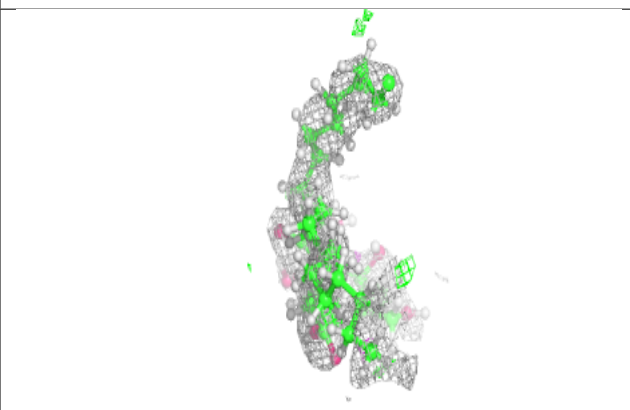
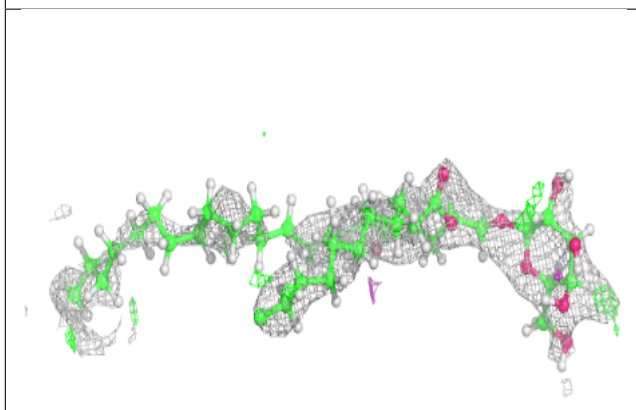
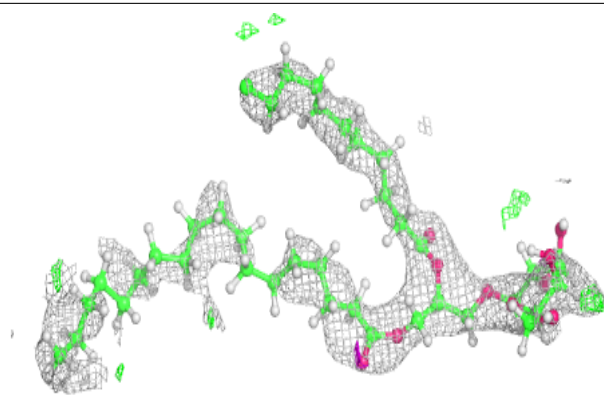
**Electron density around SQD a 412:**

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

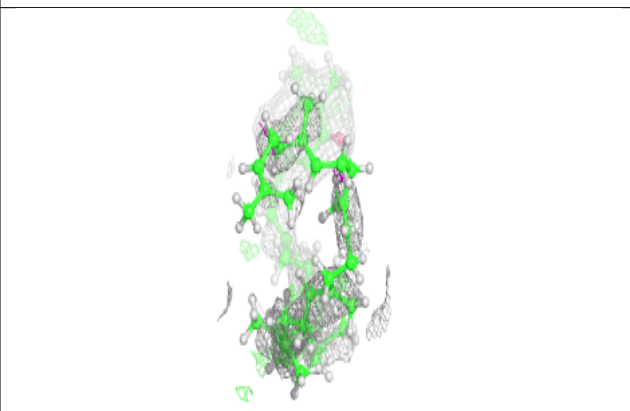
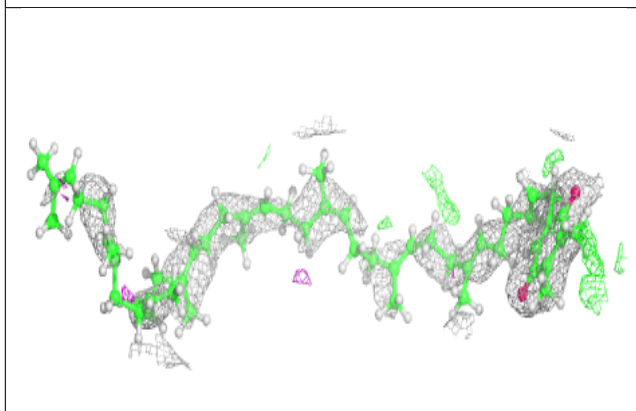
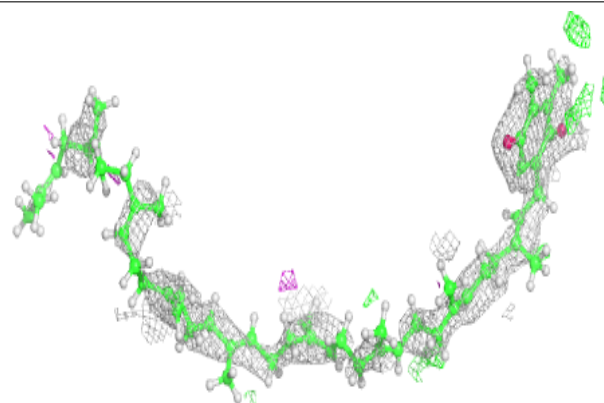


**Electron density around LMG c 522:**

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

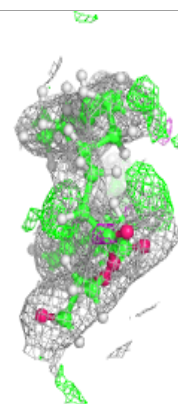
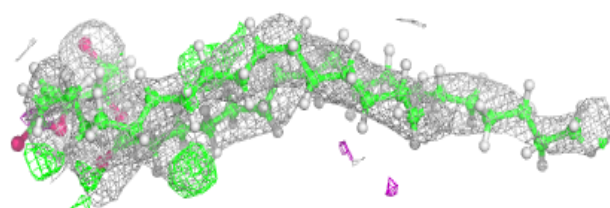
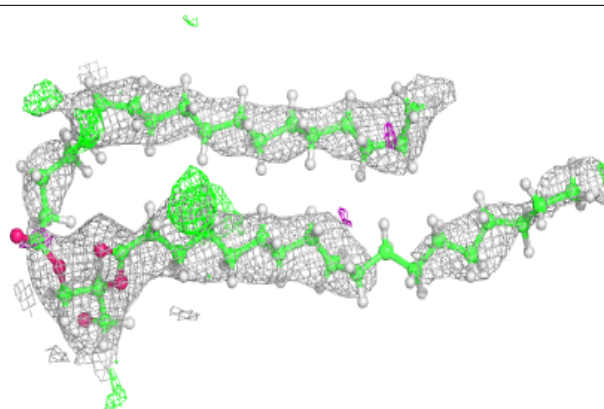
**Electron density around PL9 a 409:**

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

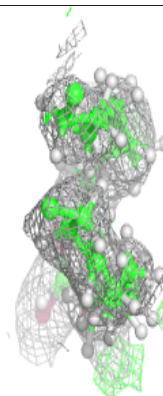
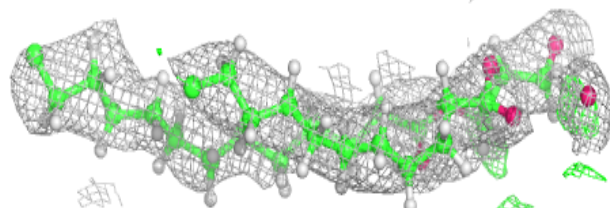
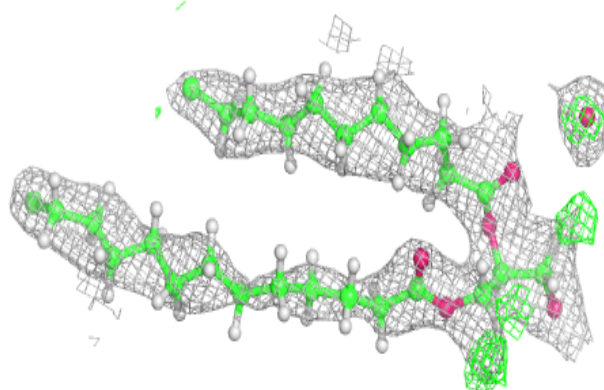


**Electron density around DGD a 413:**

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

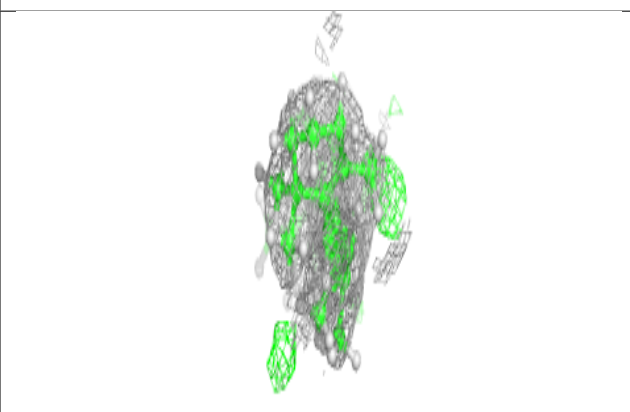
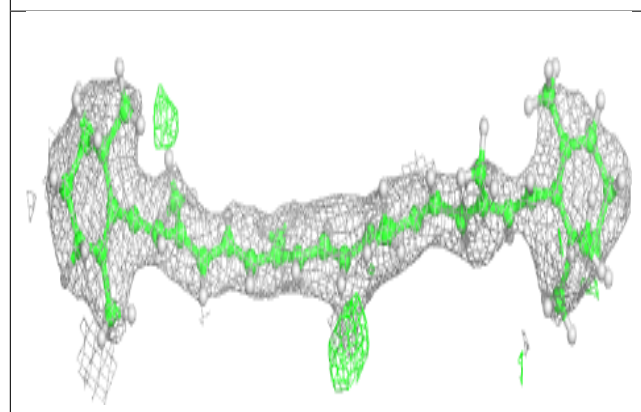
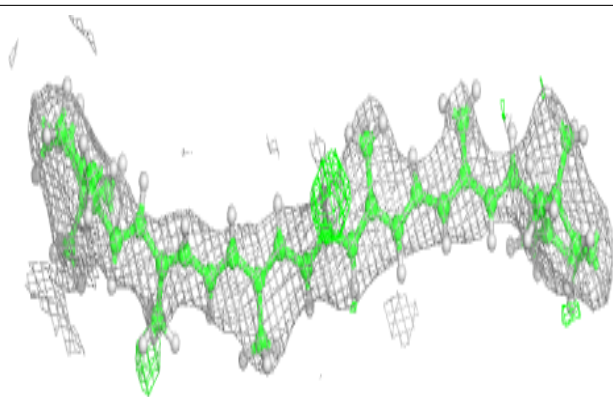
**Electron density around LMG D 410:**

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

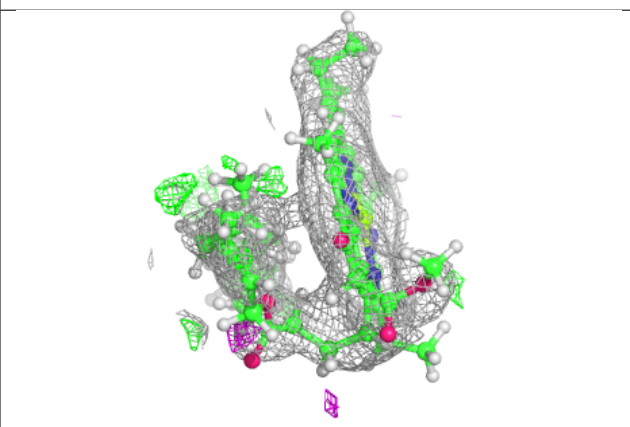
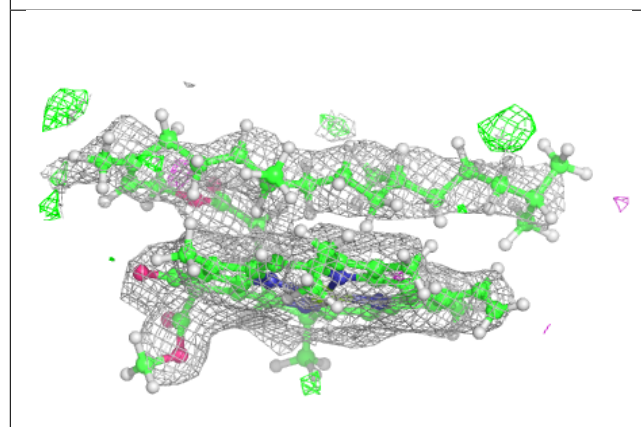
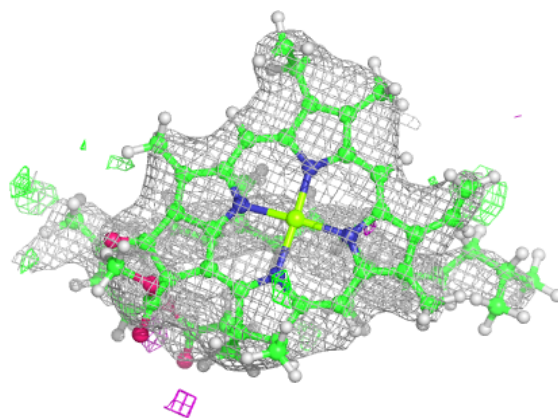


**Electron density around BCR h 102:**

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

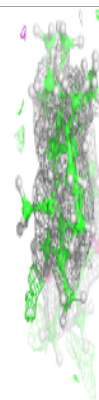
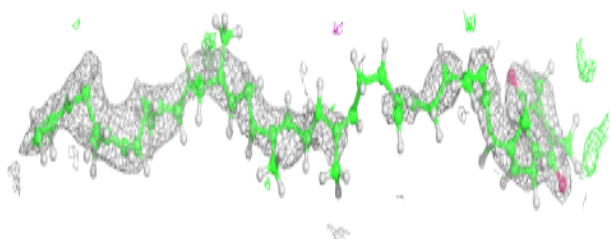
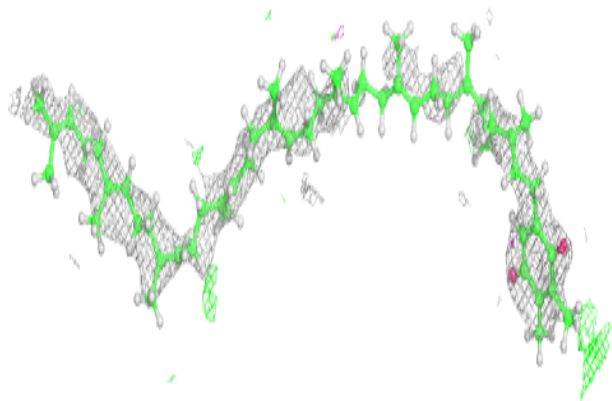
**Electron density around CLA h 101:**

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

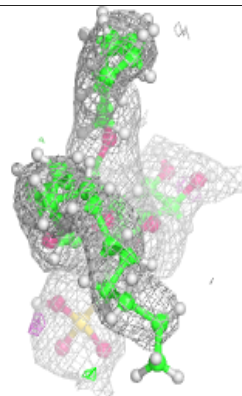
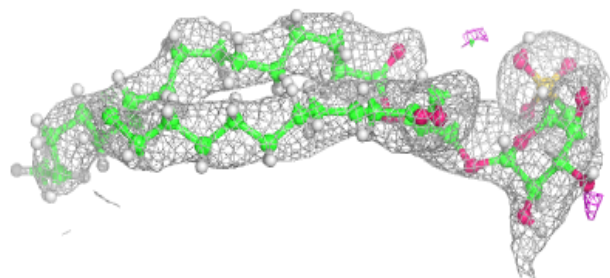
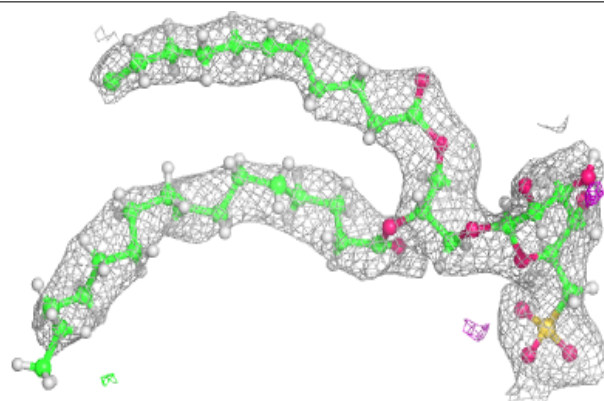


**Electron density around PL9 A 409:**

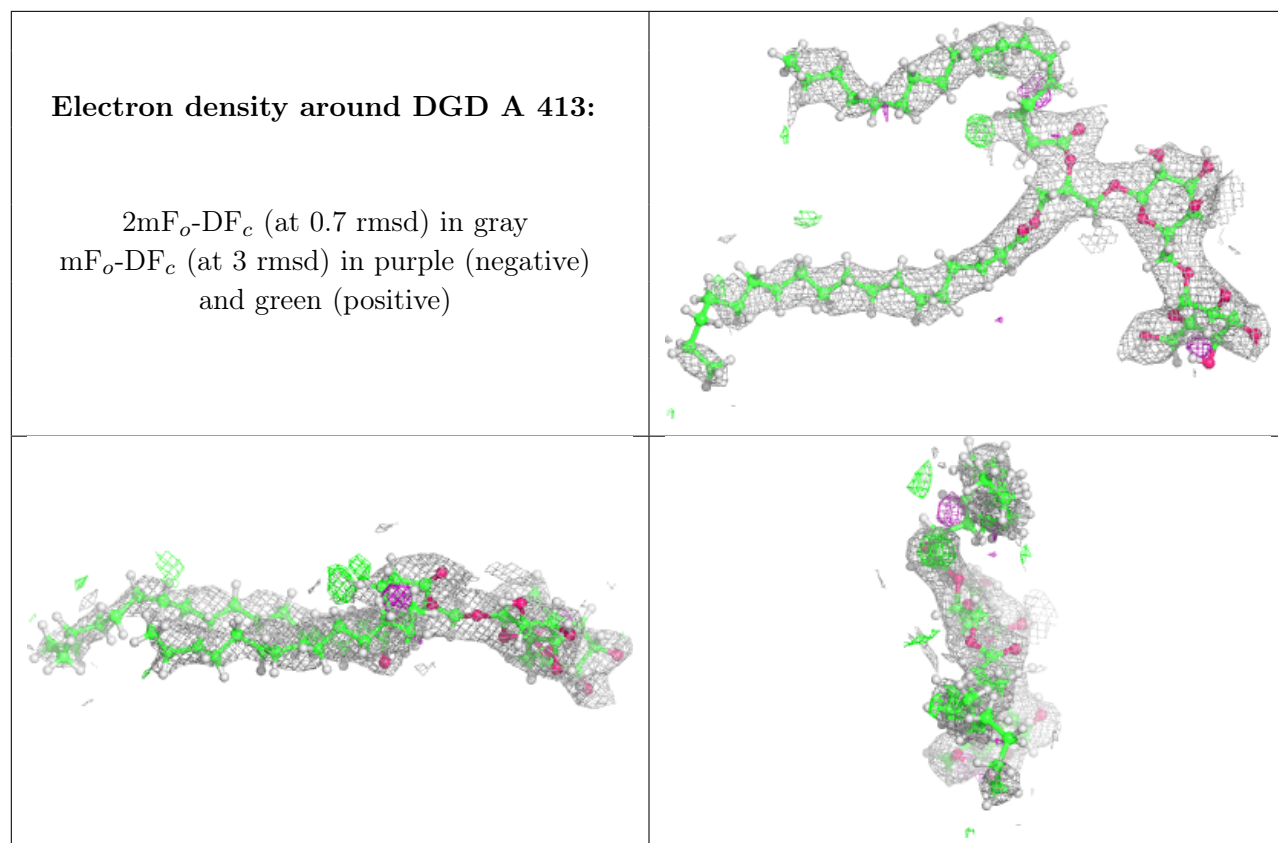
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around SQD b 601:**

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

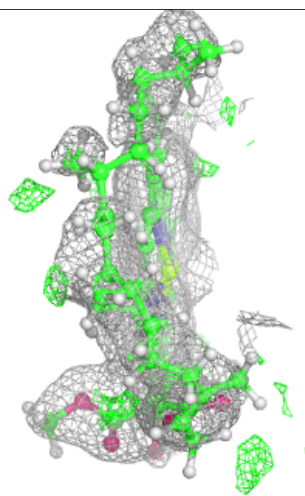
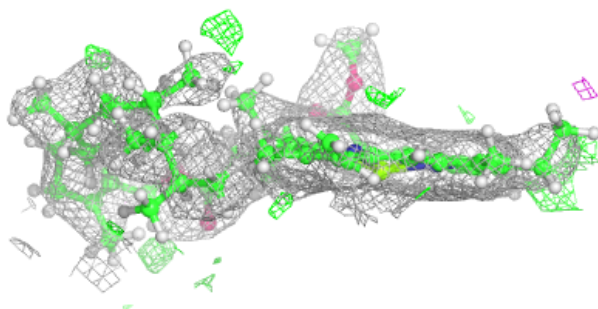
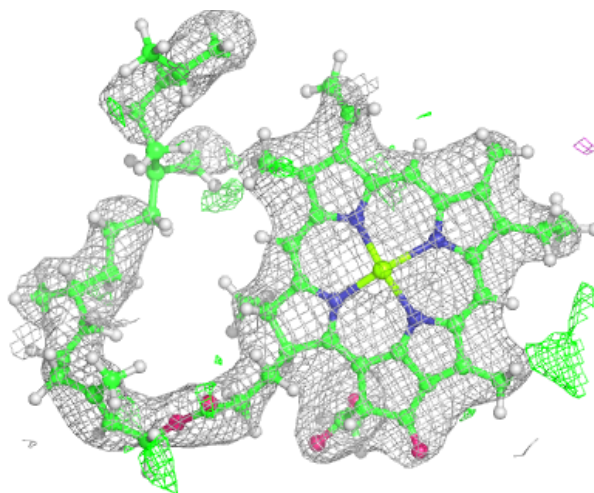






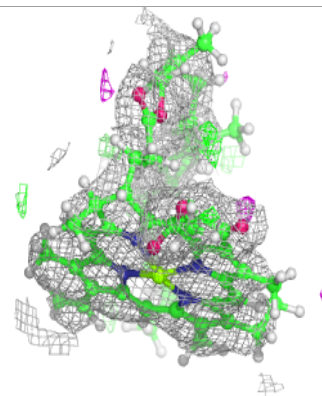
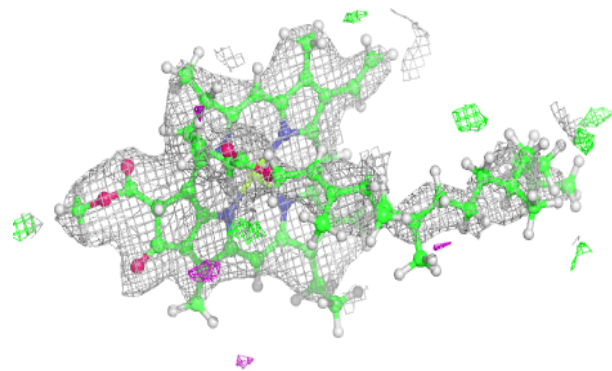
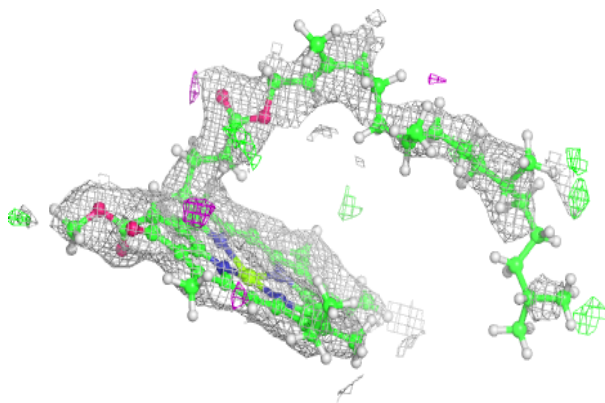
**Electron density around CLA c 512:**

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



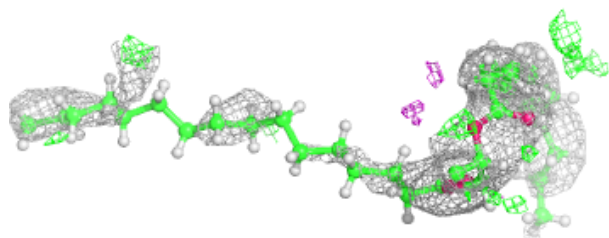
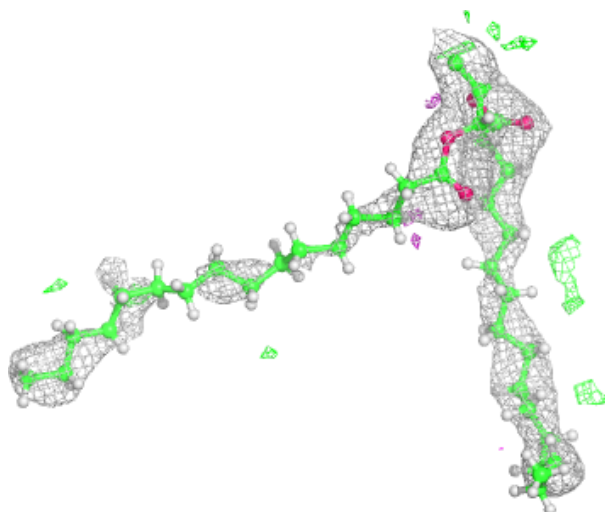
**Electron density around CLA c 513:**

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



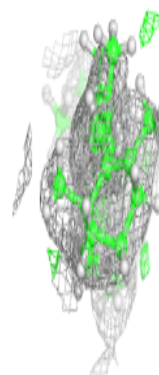
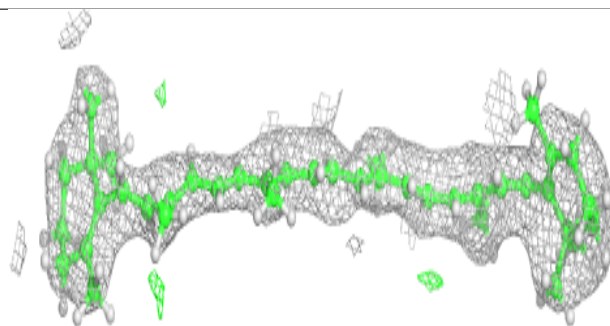
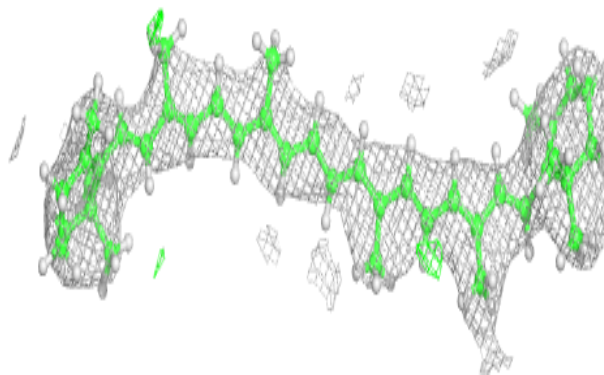
**Electron density around SQD A 412:**

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



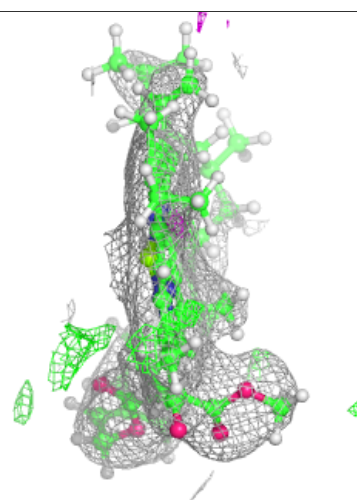
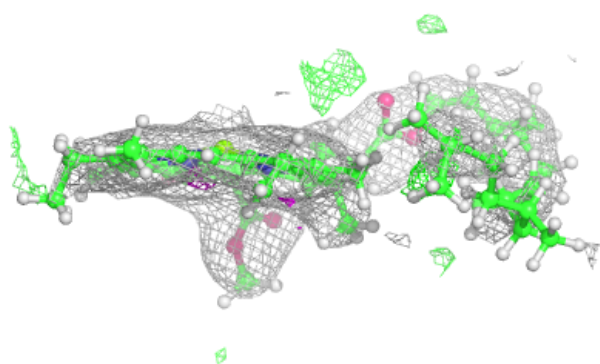
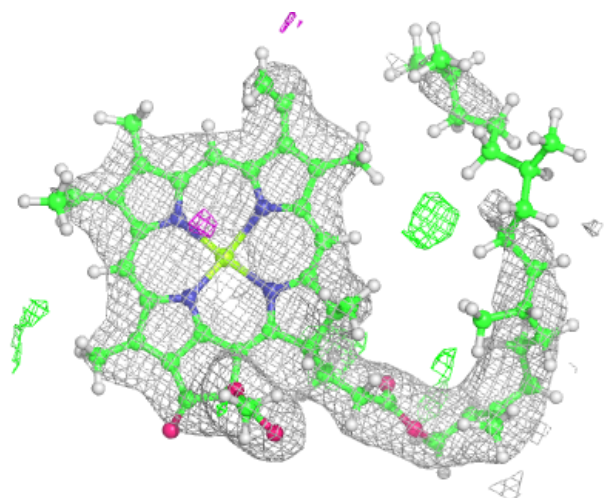
**Electron density around BCR y 101:**

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



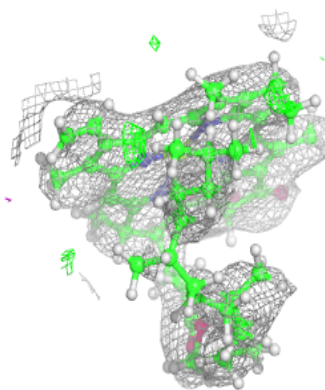
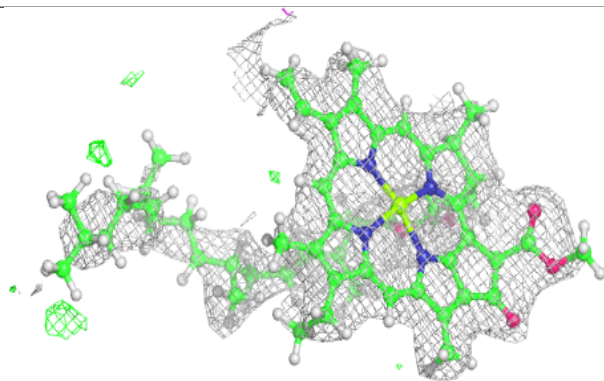
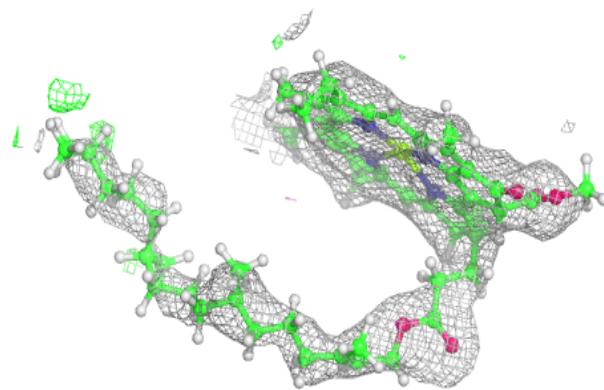
**Electron density around CLA C 512:**

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



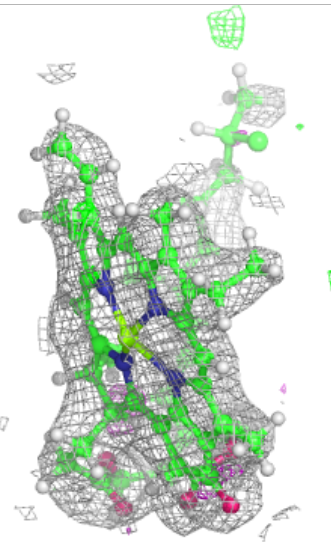
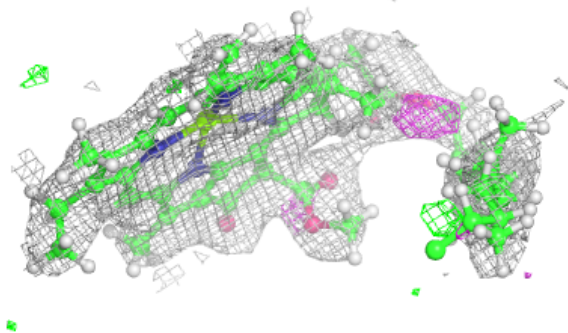
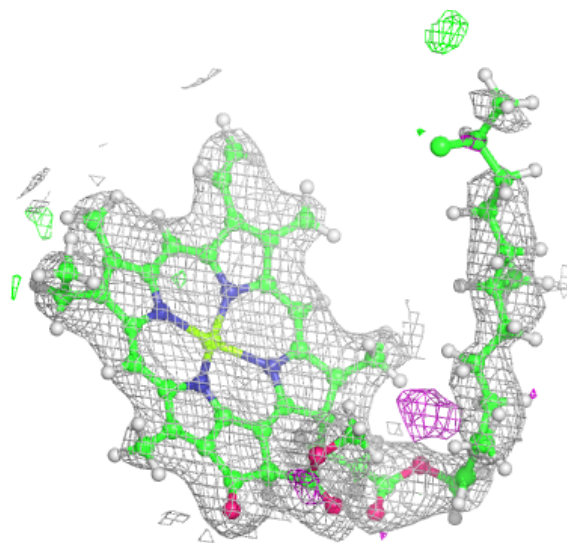
**Electron density around CLA C 513:**

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



**Electron density around CLA B 616:**

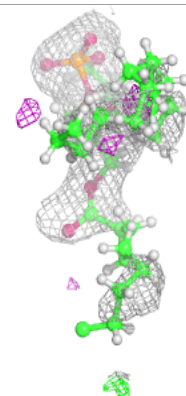
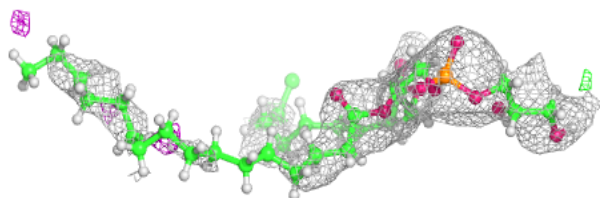
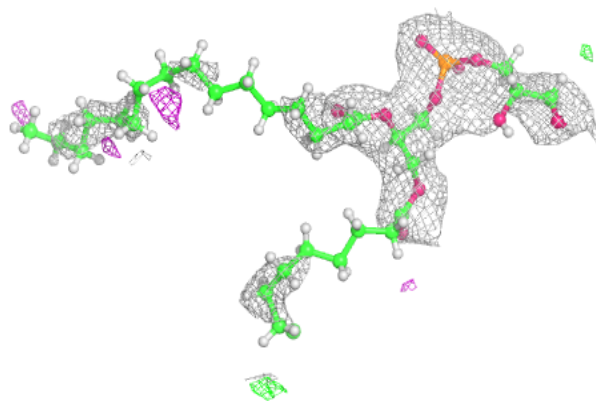
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



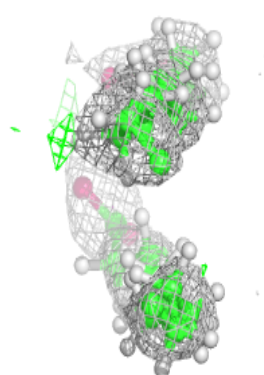
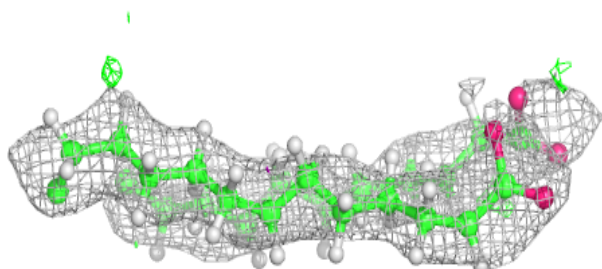
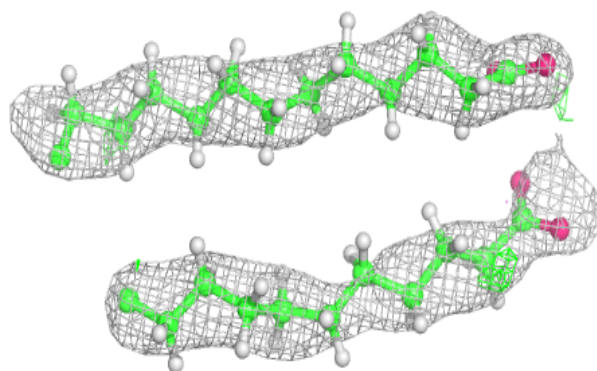


**Electron density around LHG e 101:**

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

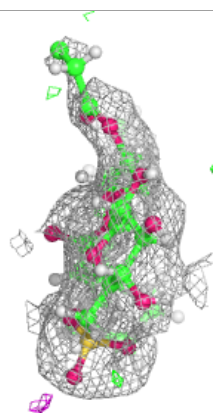
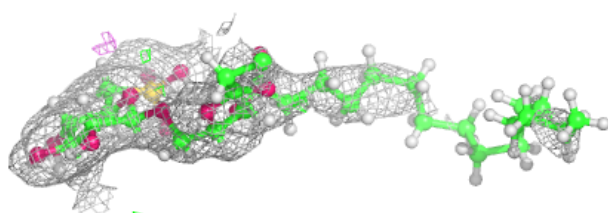
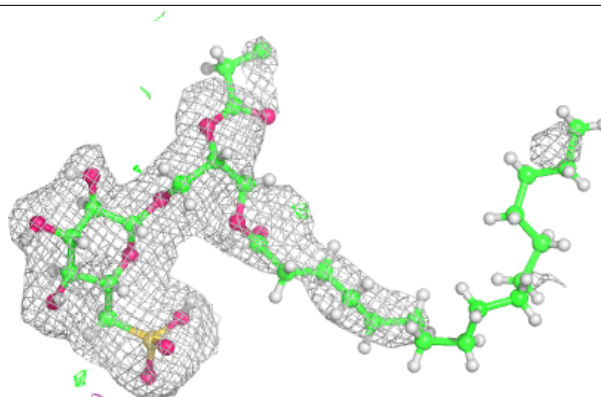
**Electron density around LMG D 411:**

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

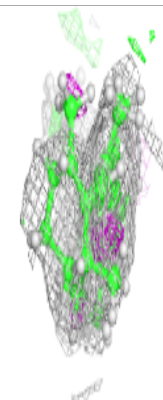
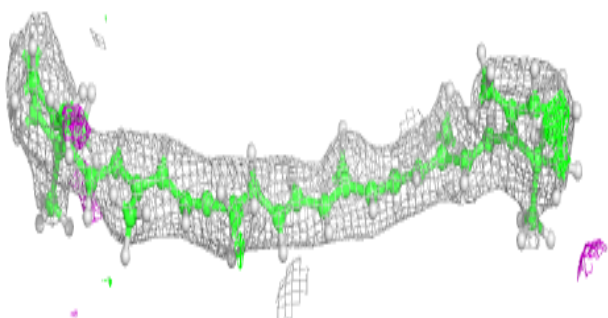
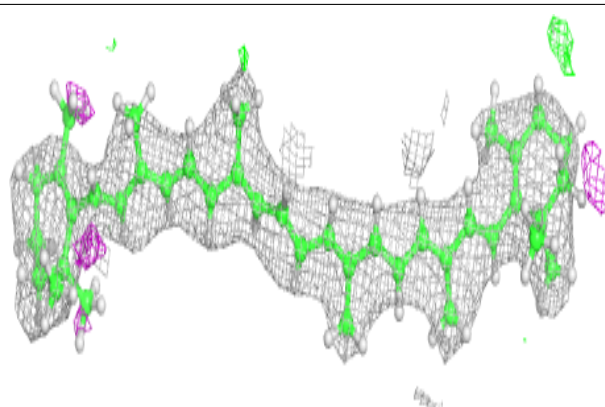


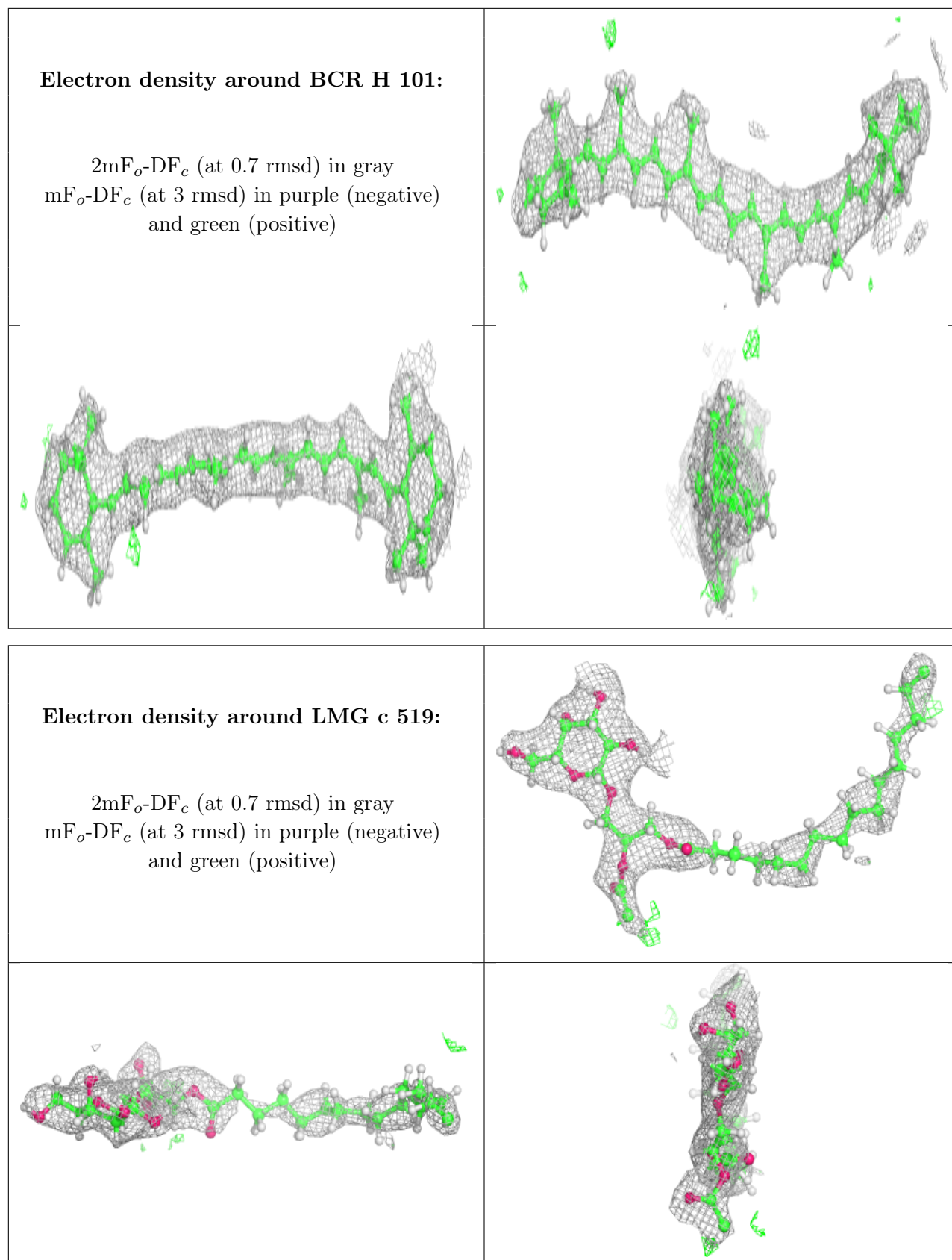
**Electron density around SQD f 101:**

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

**Electron density around BCR D 405:**

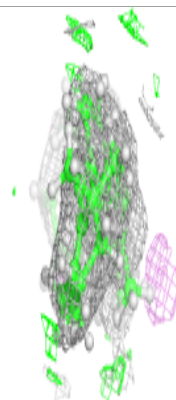
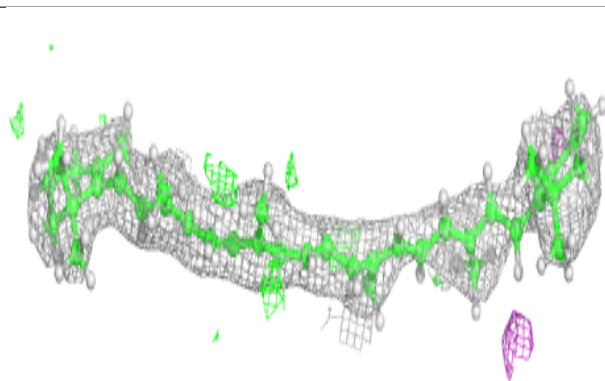
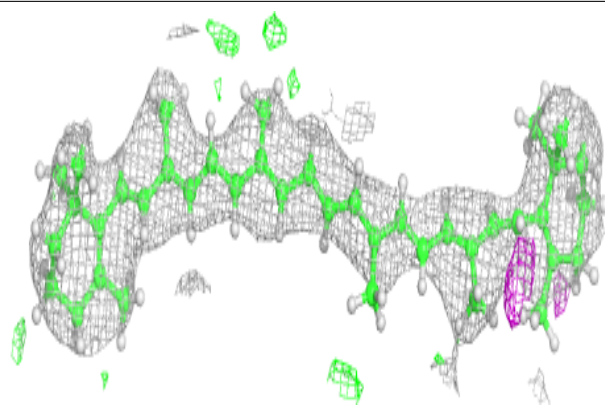
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





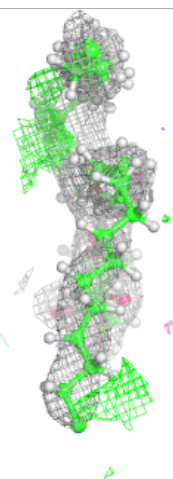
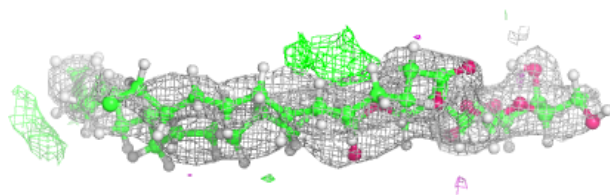
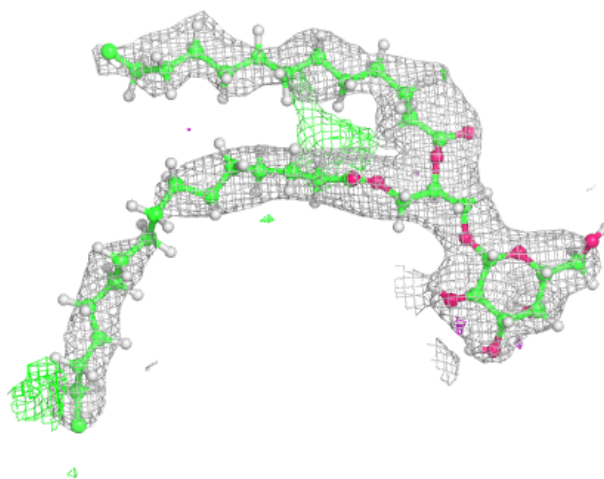
**Electron density around BCR d 405:**

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



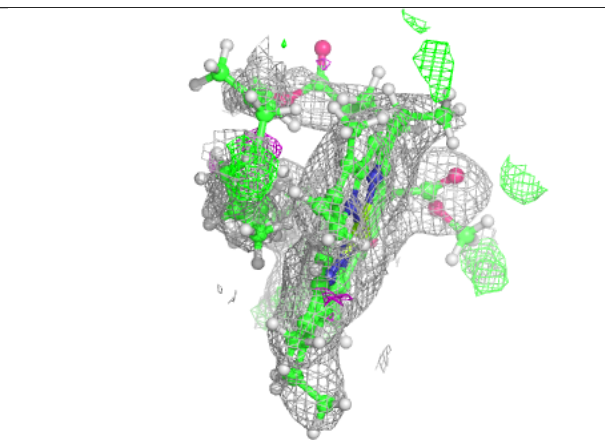
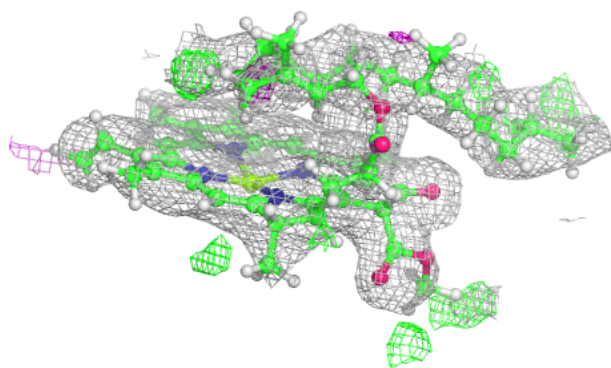
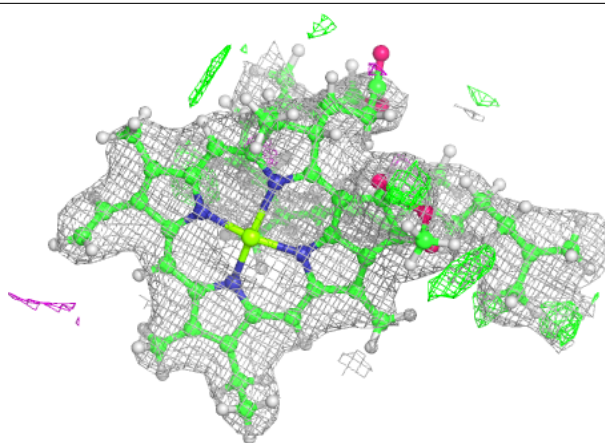
**Electron density around LMG C 519:**

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

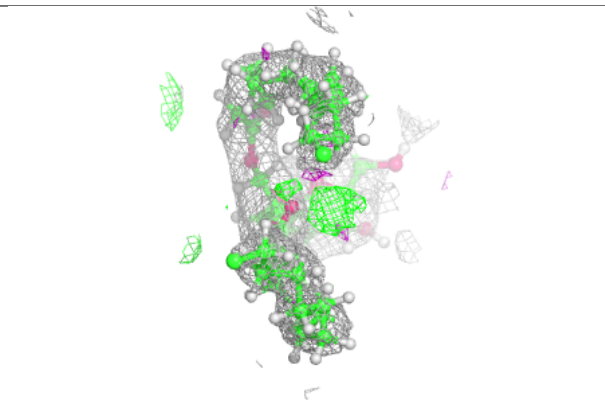
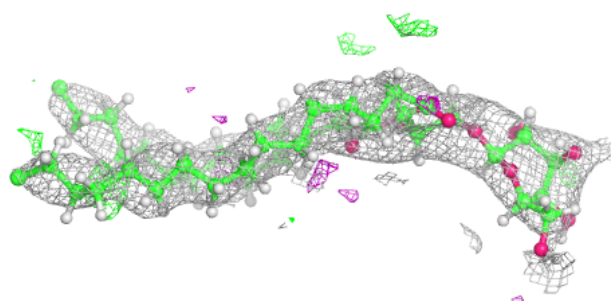
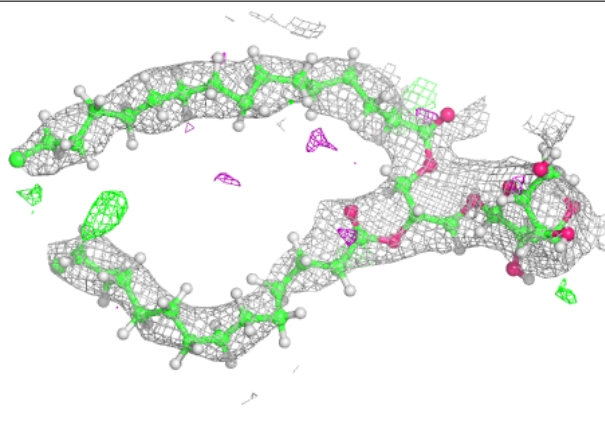


**Electron density around CLA B 601:**

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

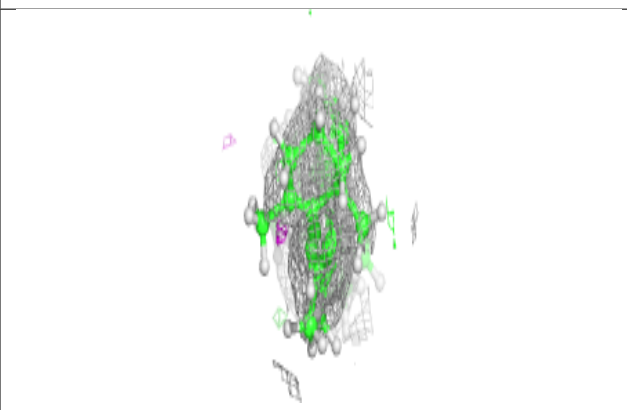
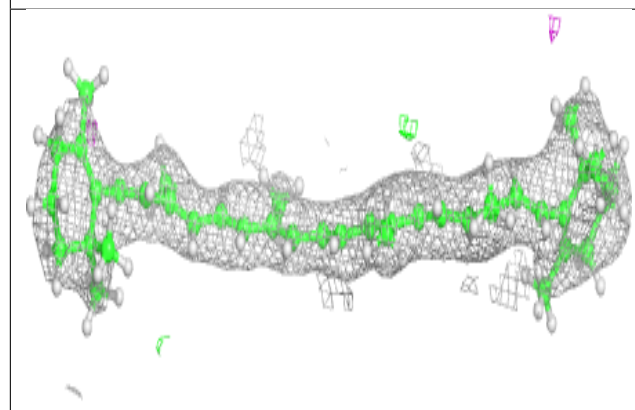
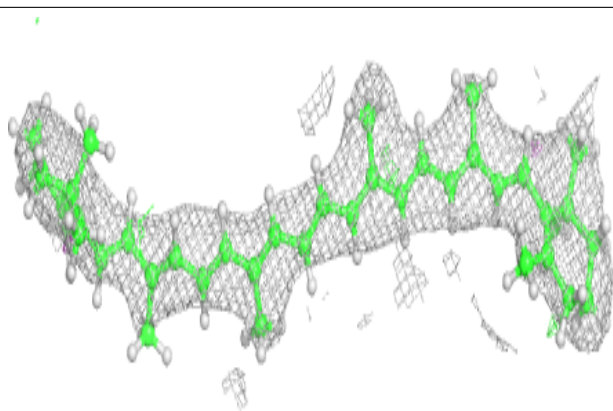
**Electron density around LMG a 414:**

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

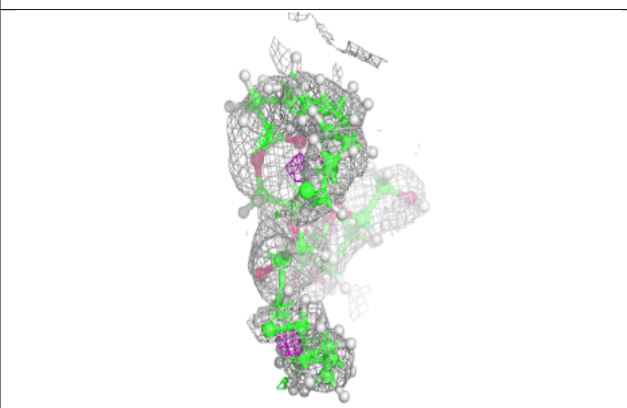
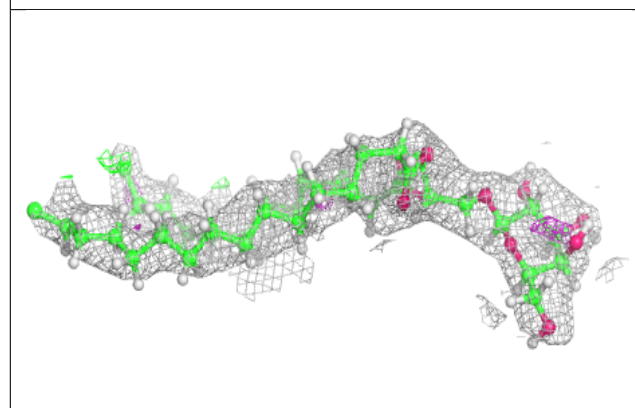
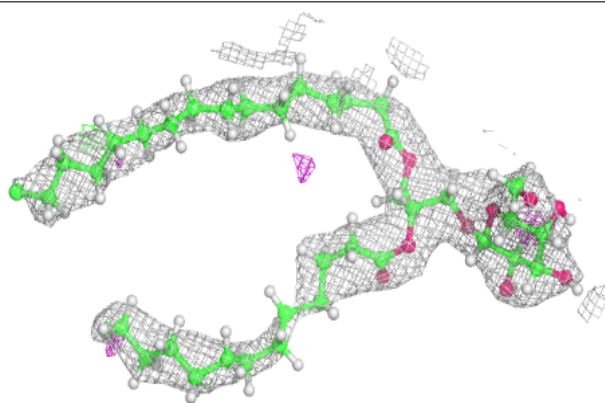


**Electron density around BCR K 101:**

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

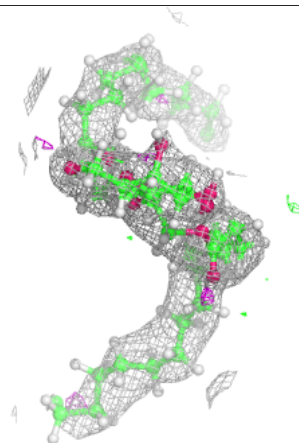
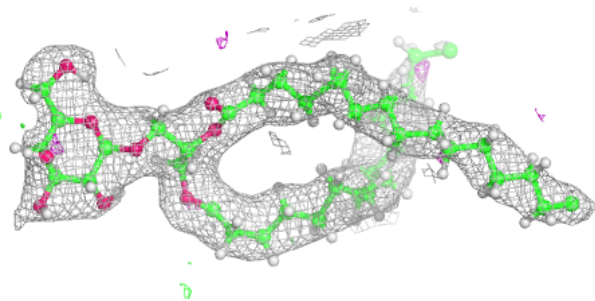
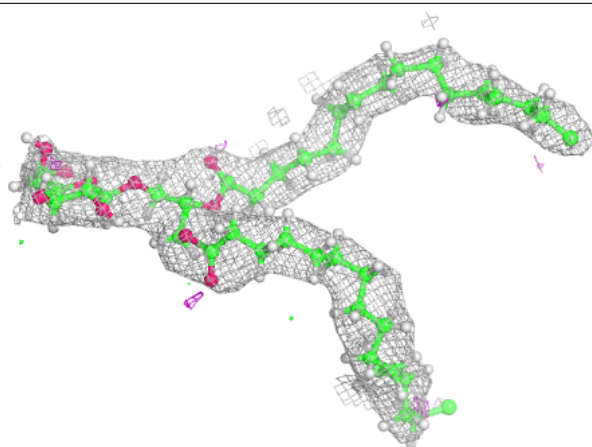
**Electron density around LMG A 410:**

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



**Electron density around LMG B 620:**

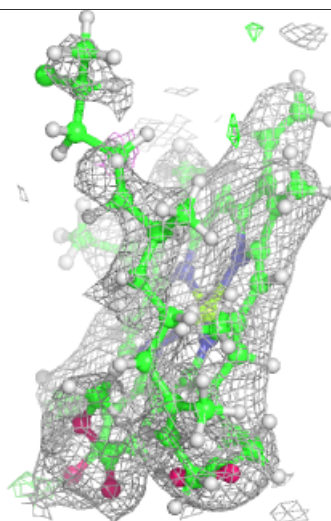
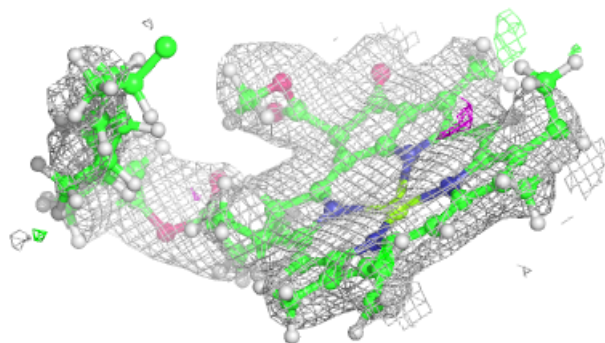
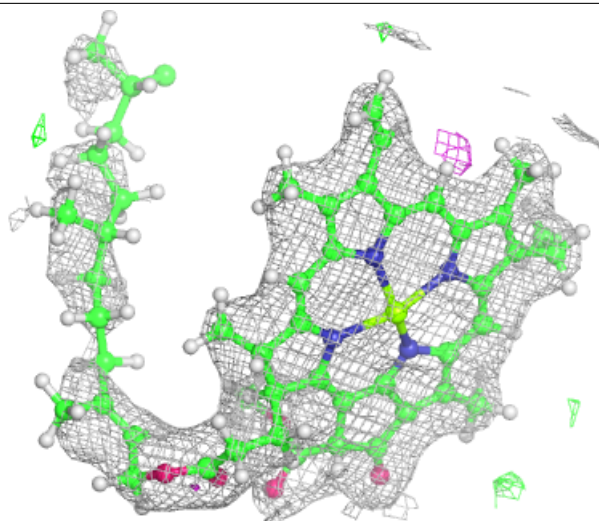
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





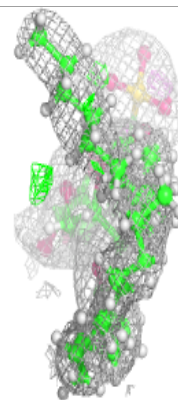
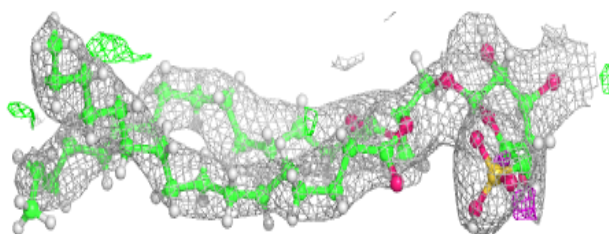
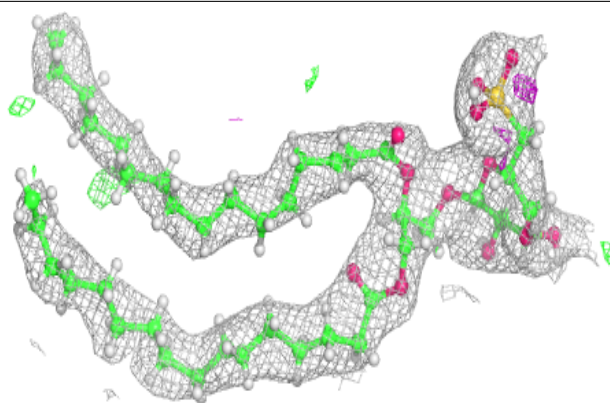
**Electron density around CLA b 617:**

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

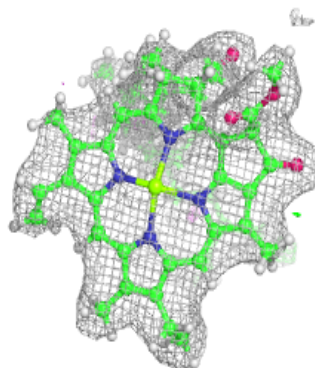
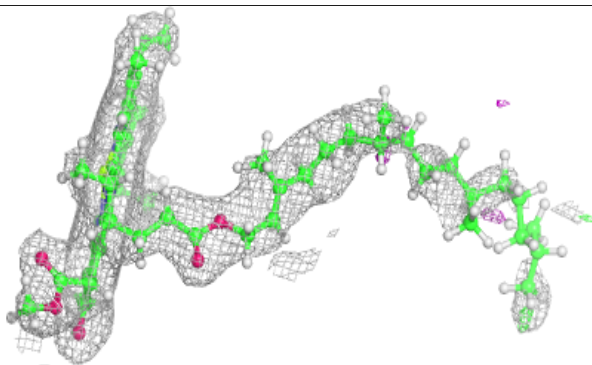
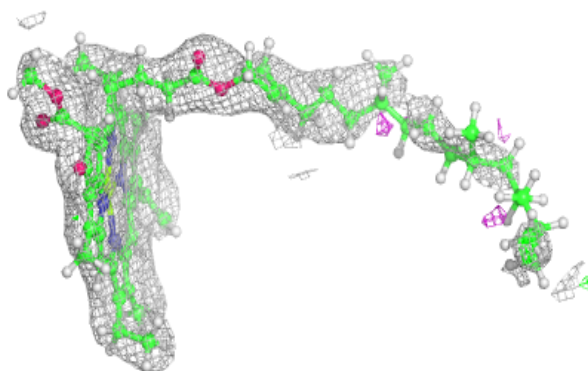


**Electron density around SQD B 623:**

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

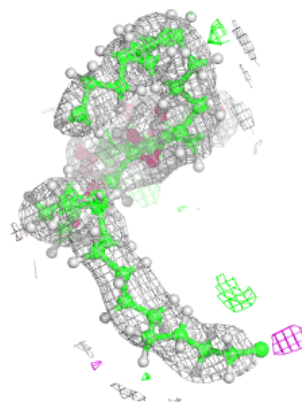
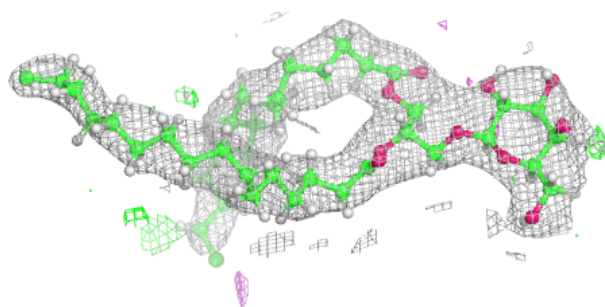
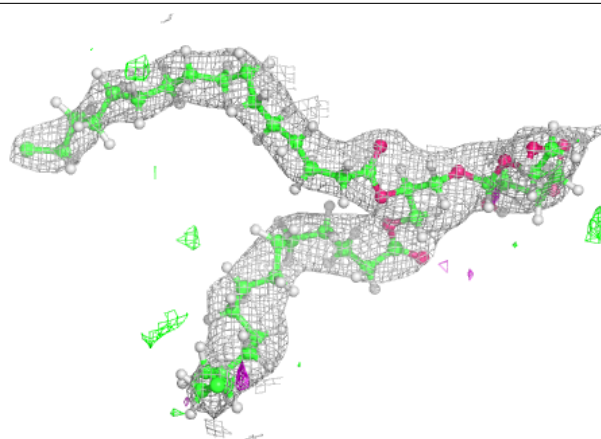
**Electron density around CLA D 404:**

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

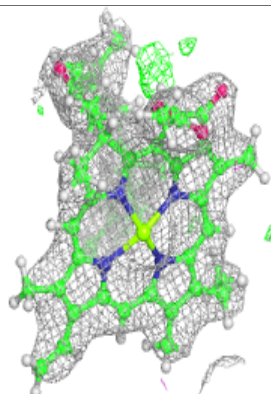
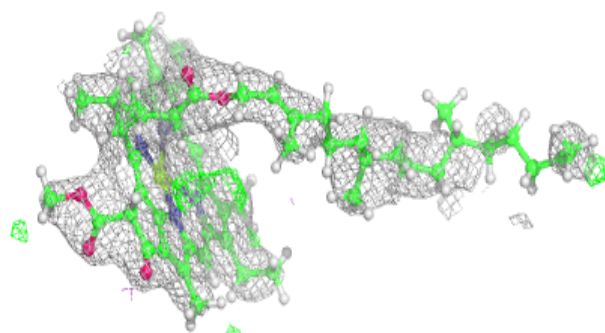
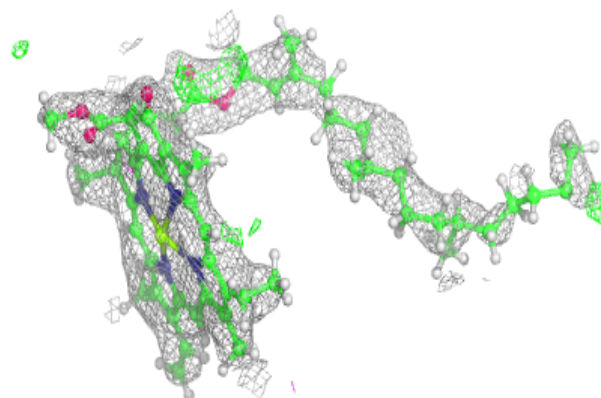


**Electron density around LMG m 101:**

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

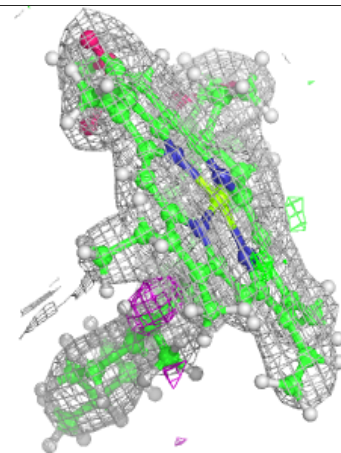
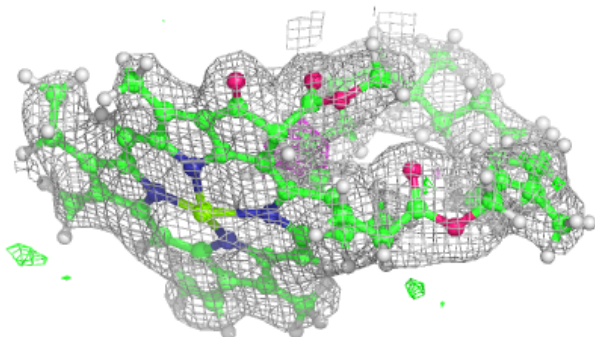
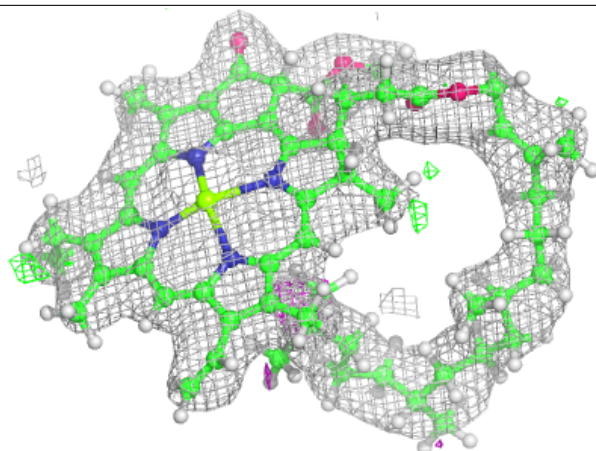
**Electron density around CLA c 508:**

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

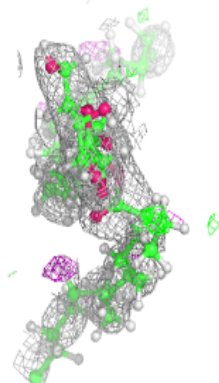
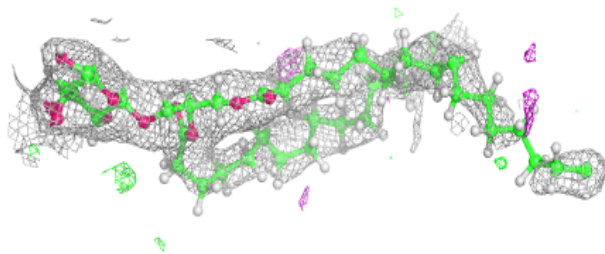
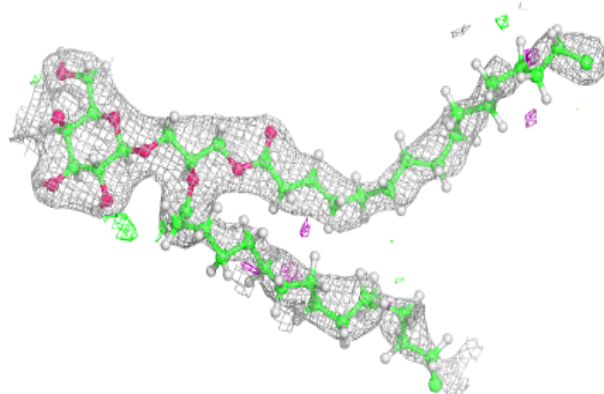


**Electron density around CLA b 616:**

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

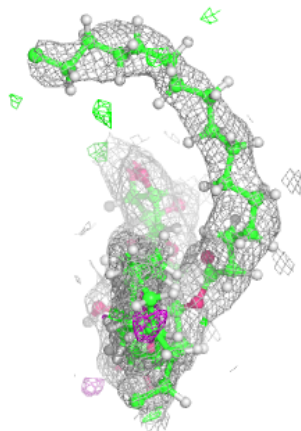
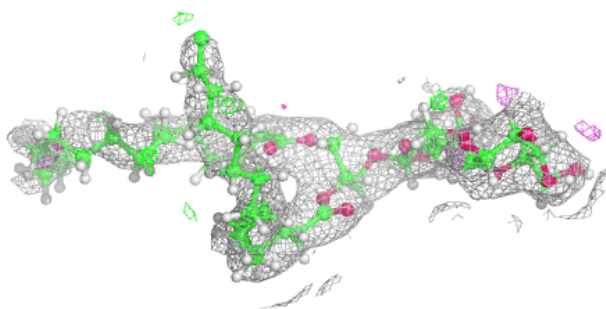
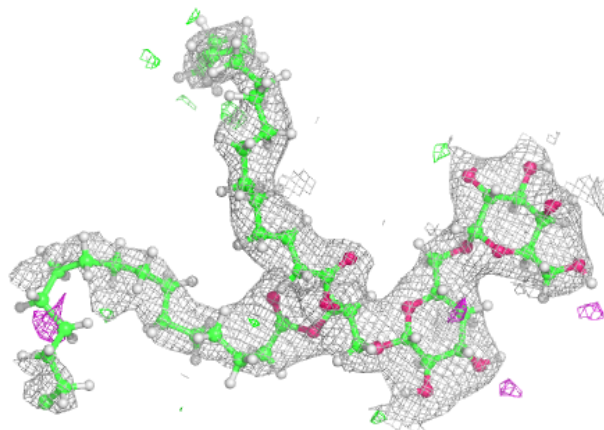
**Electron density around LMG D 407:**

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



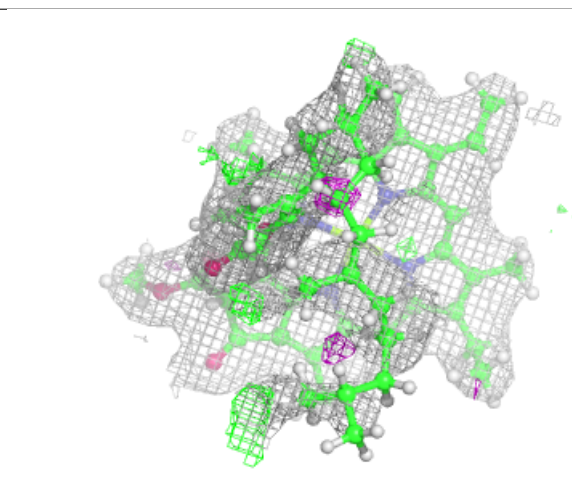
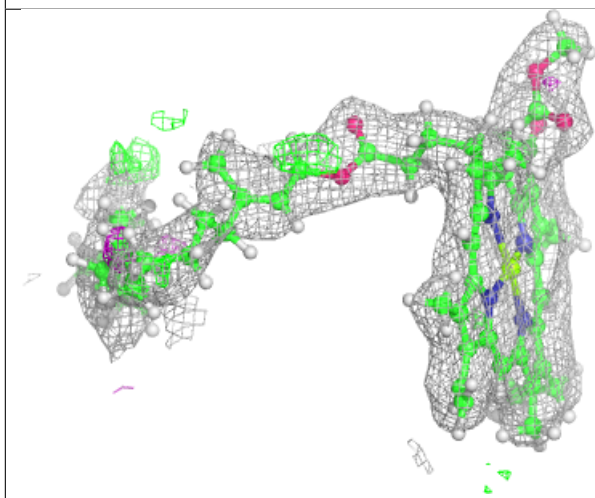
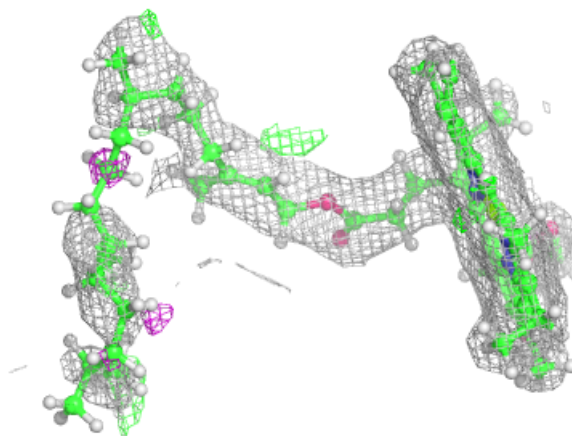
**Electron density around DGD C 517:**

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



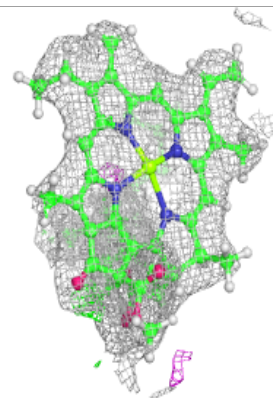
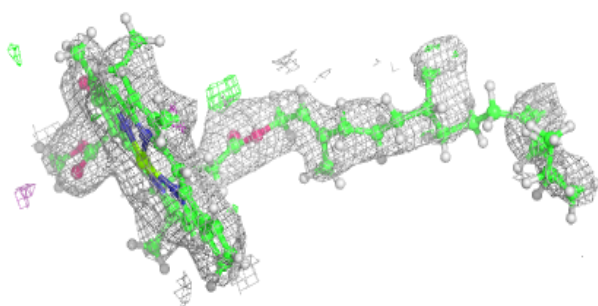
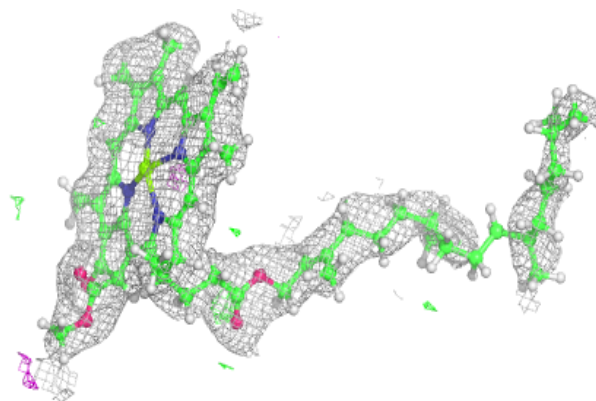
**Electron density around CLA a 407:**

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

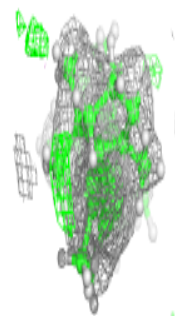
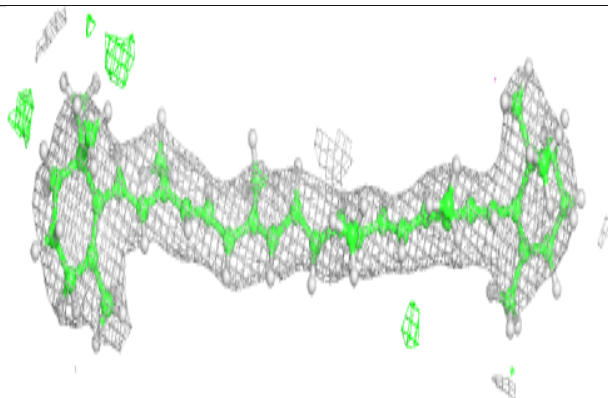
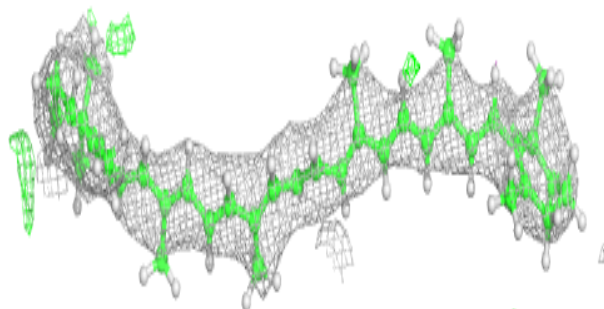


**Electron density around CLA d 404:**

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

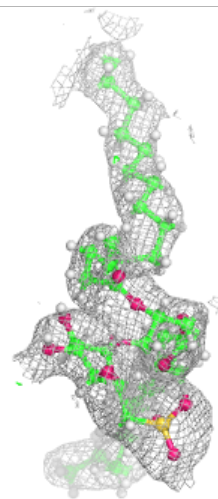
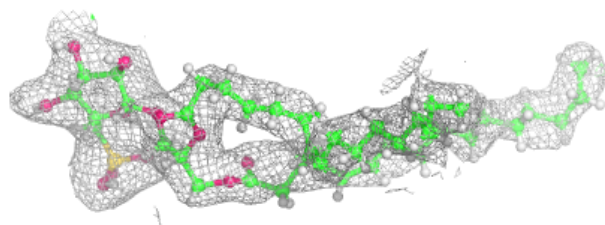
**Electron density around BCR c 514:**

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



**Electron density around SQD a 411:**

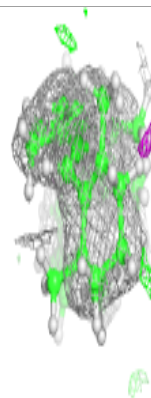
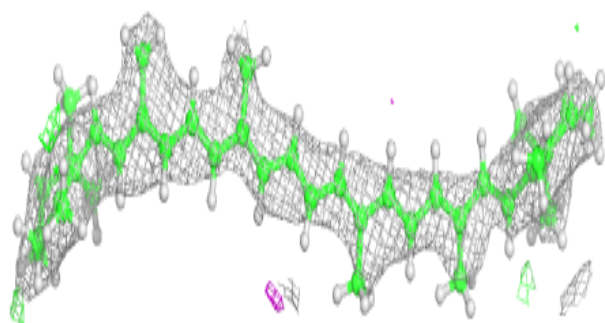
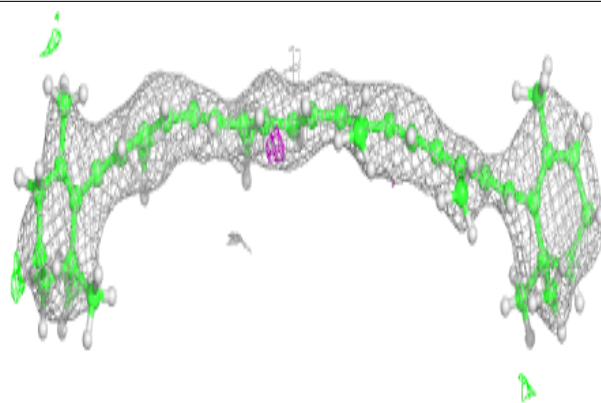
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



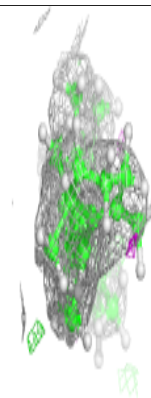
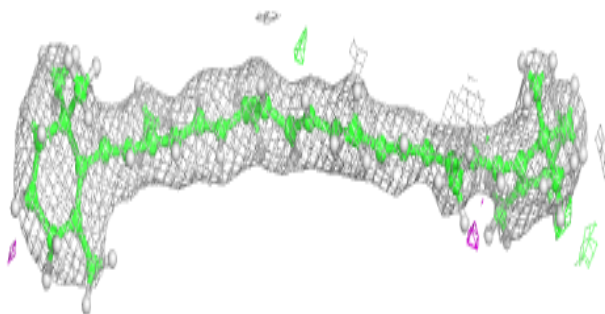
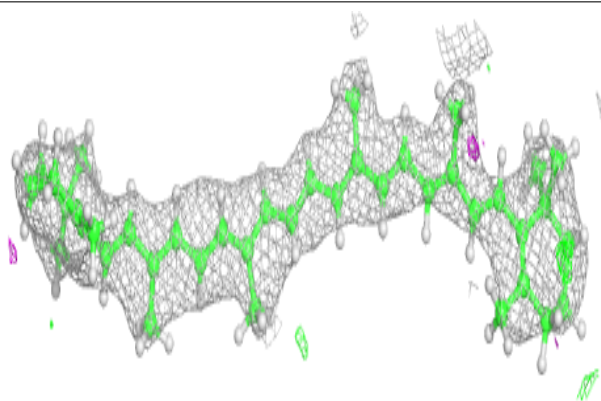


**Electron density around BCR c 521:**

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

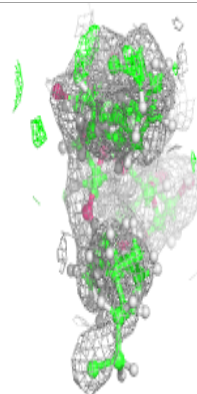
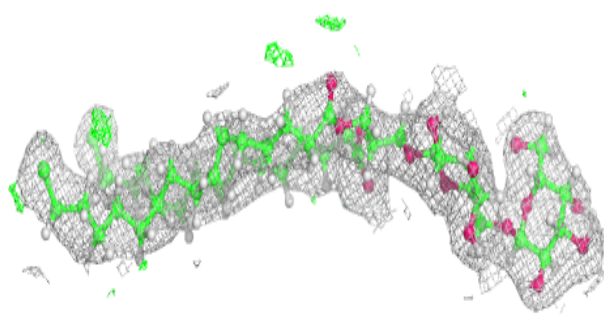
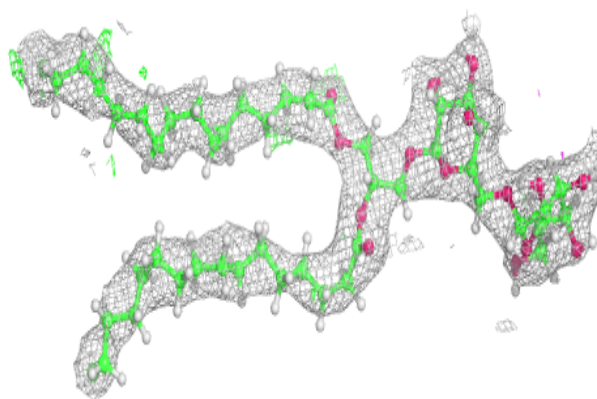
**Electron density around BCR B 617:**

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

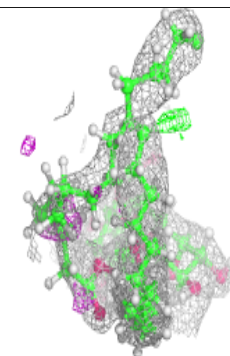
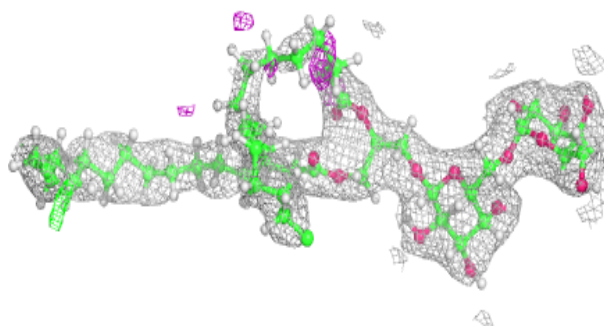
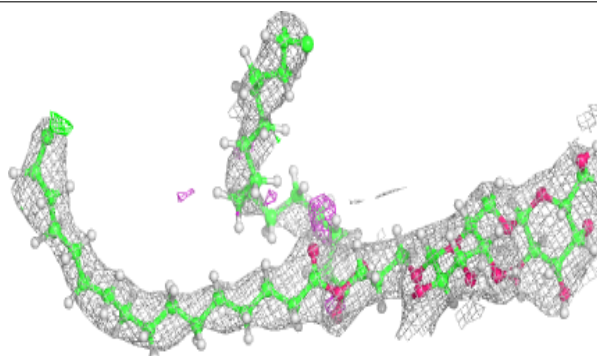


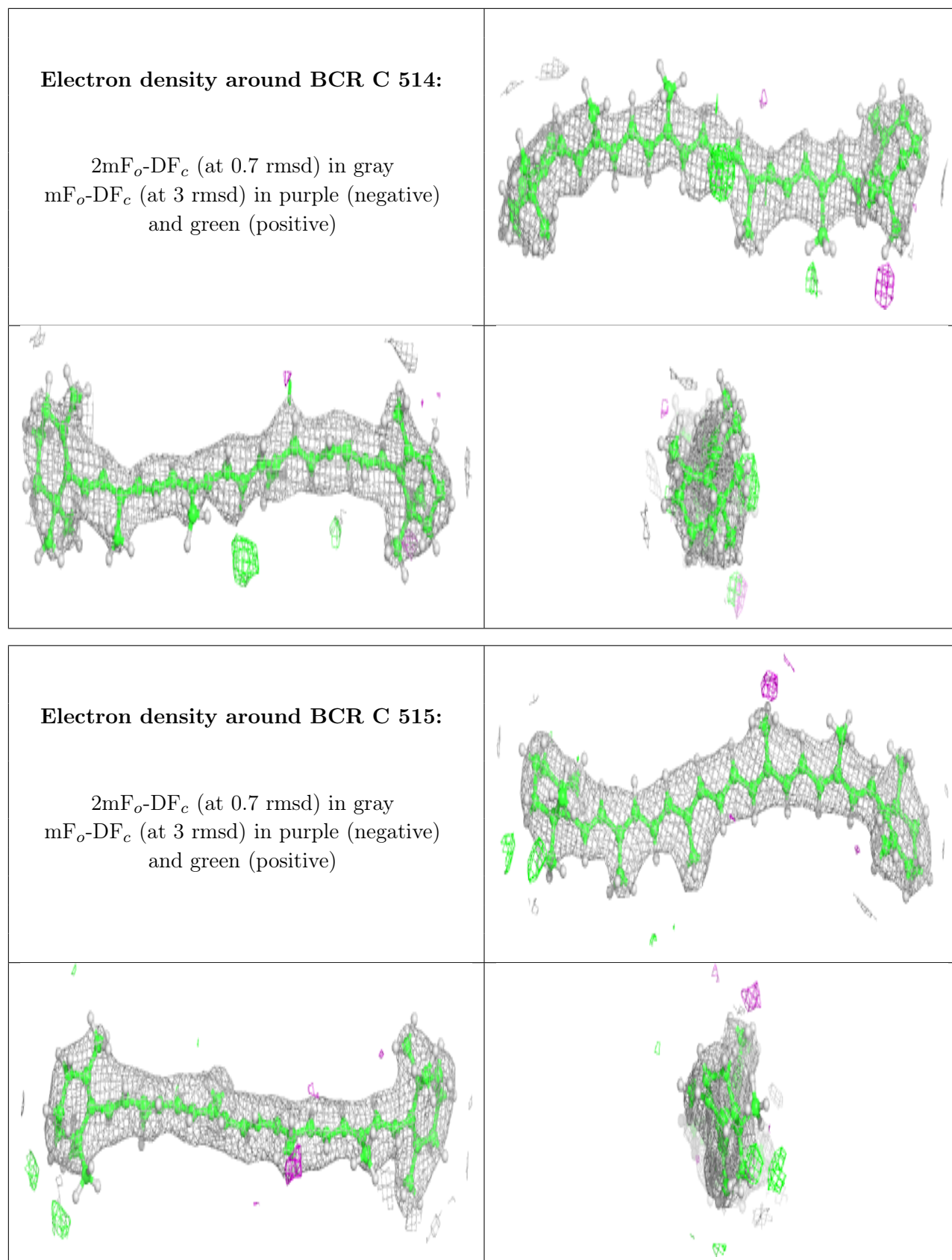
**Electron density around DGD c 518:**

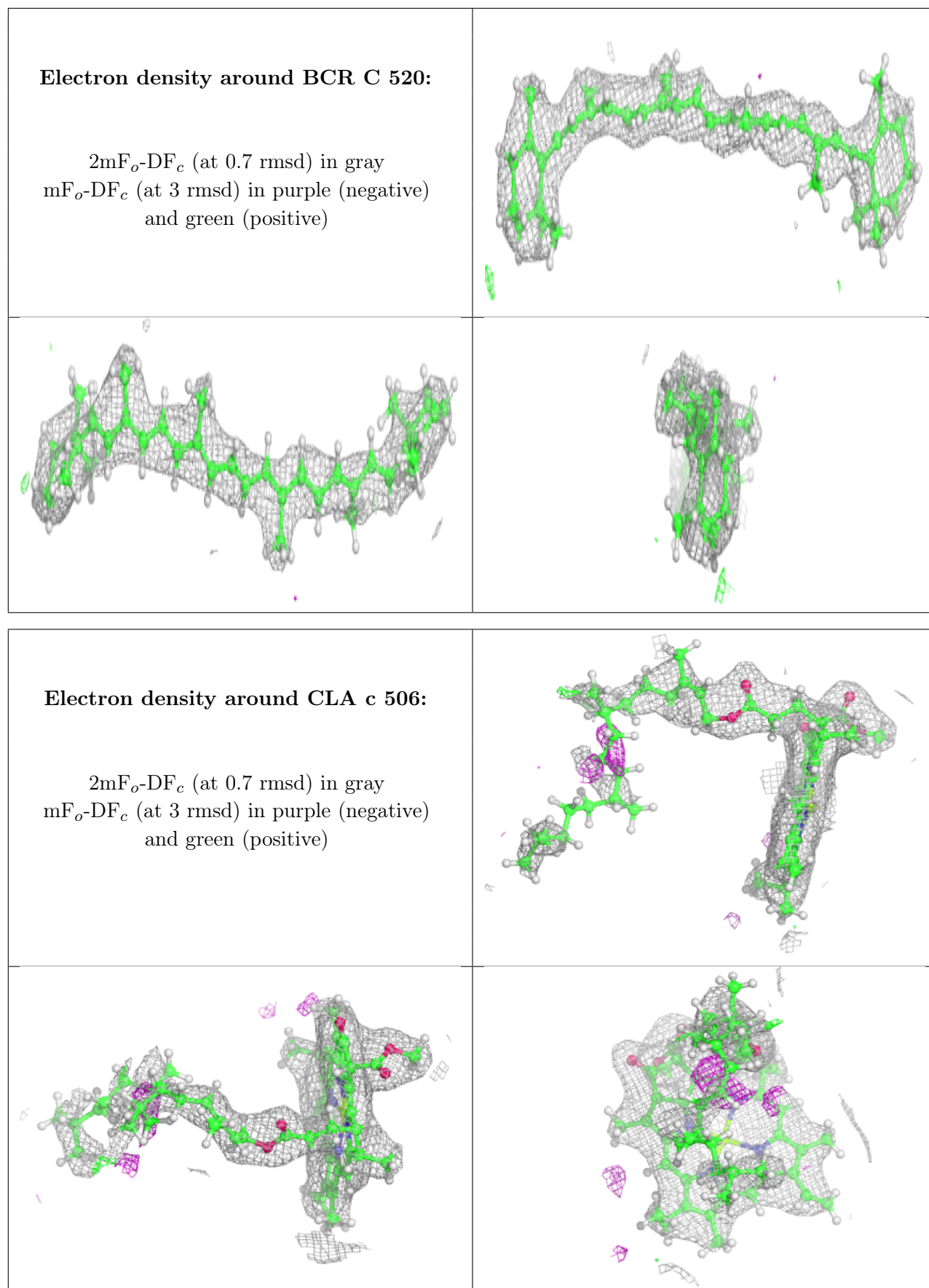
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

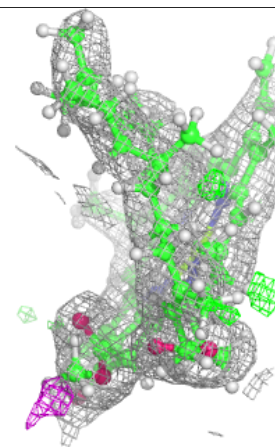
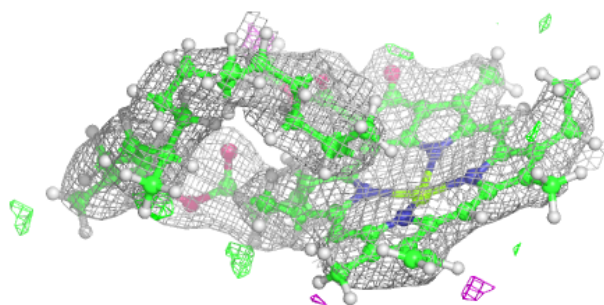
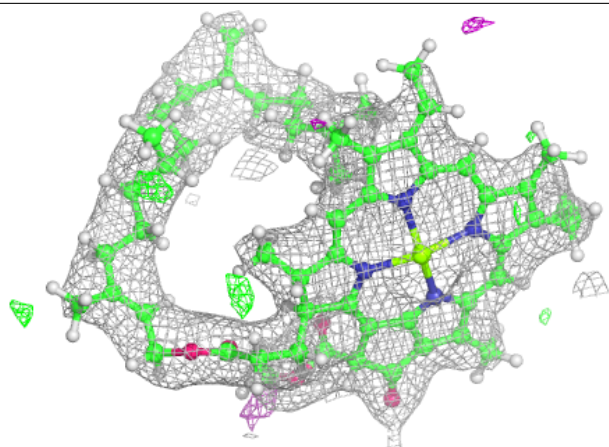




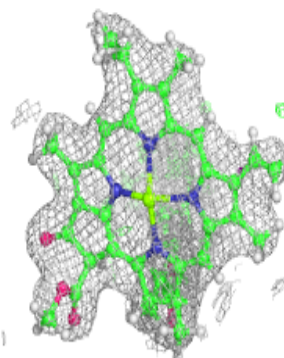
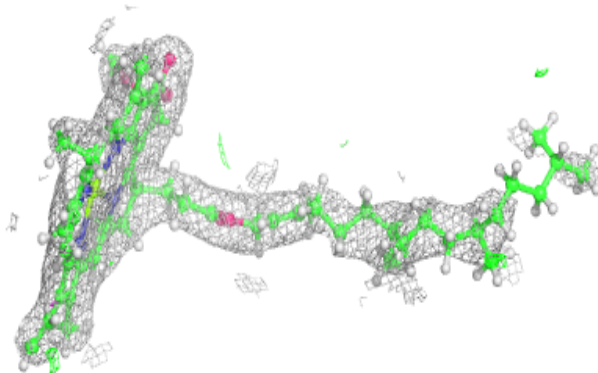
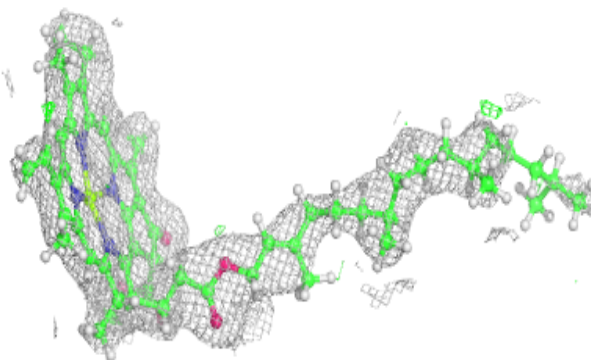


**Electron density around CLA B 615:**

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

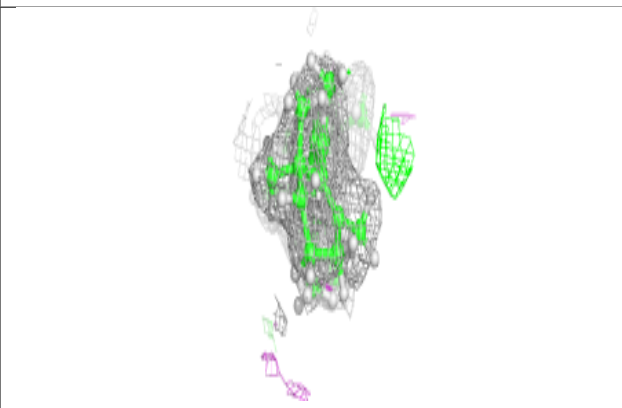
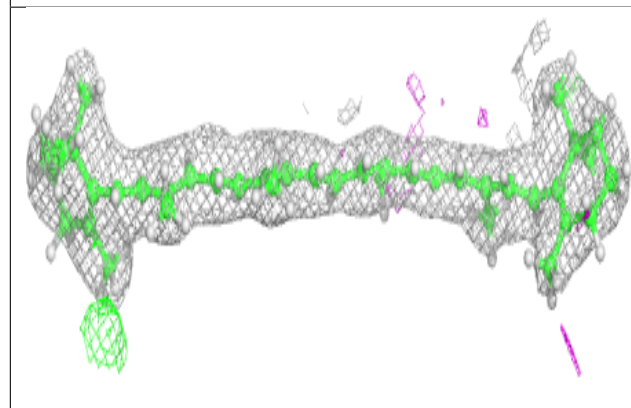
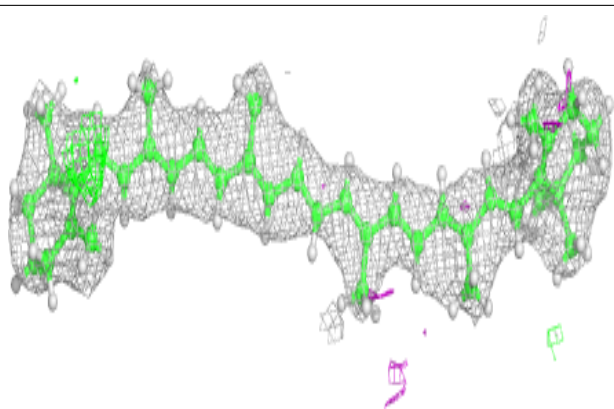
**Electron density around CLA b 605:**

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

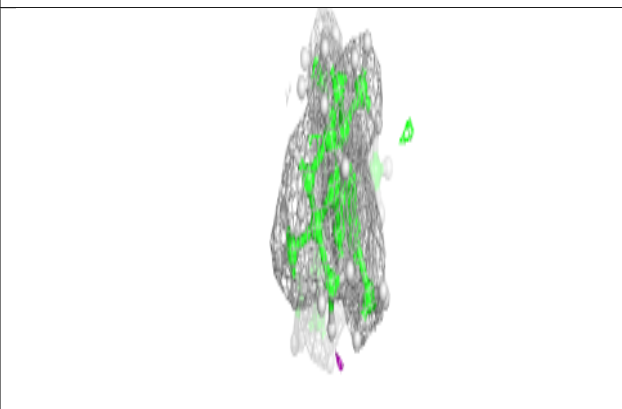
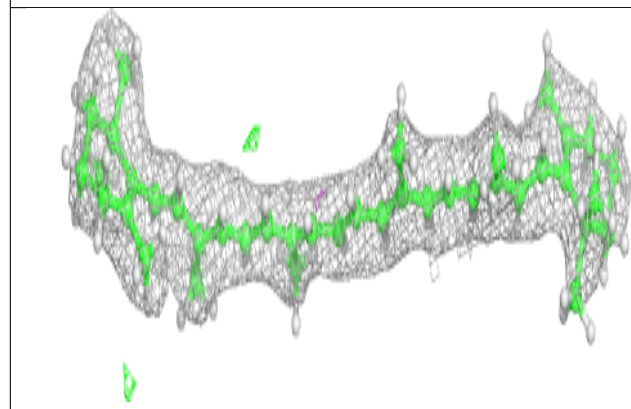
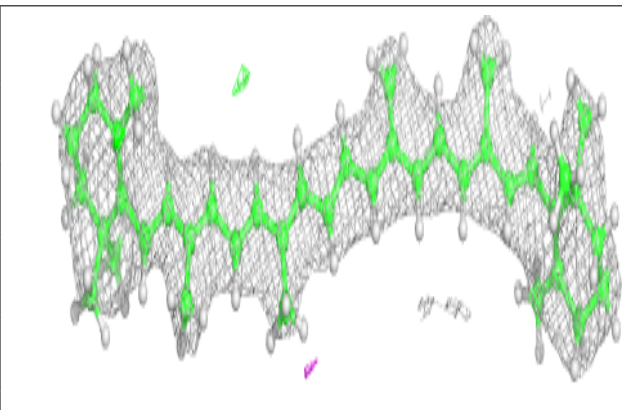


**Electron density around BCR b 619:**

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

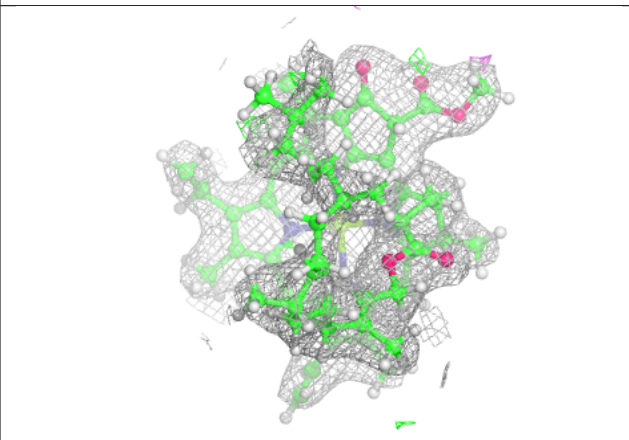
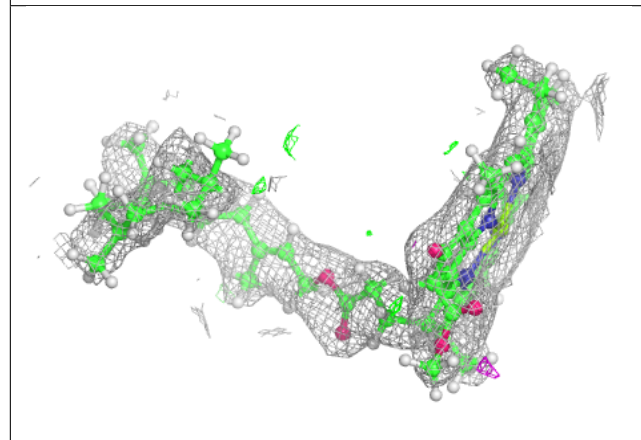
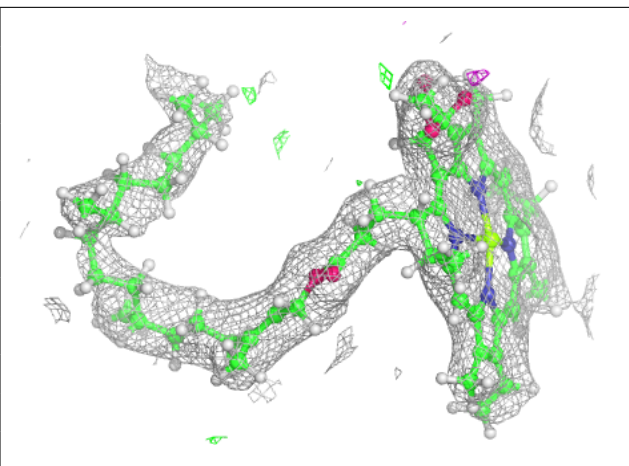
**Electron density around BCR b 620:**

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

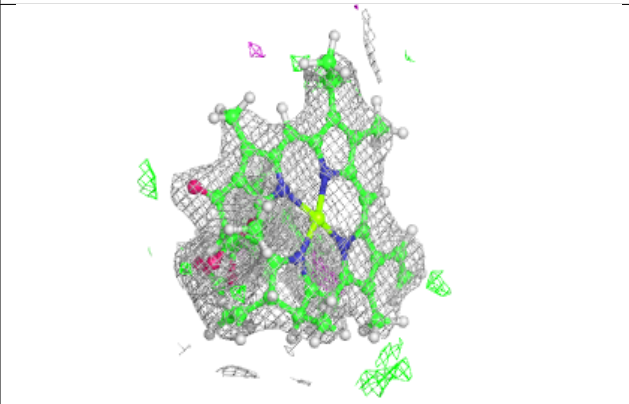
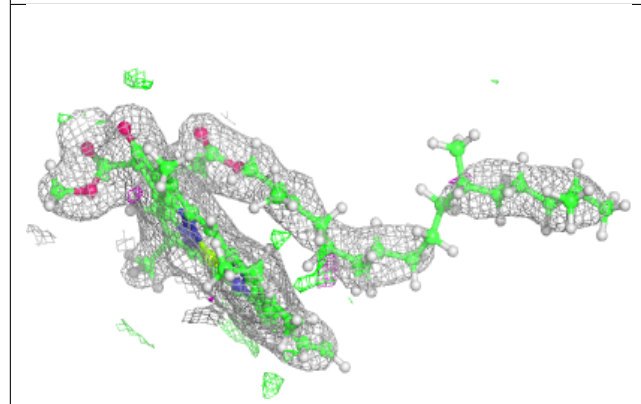
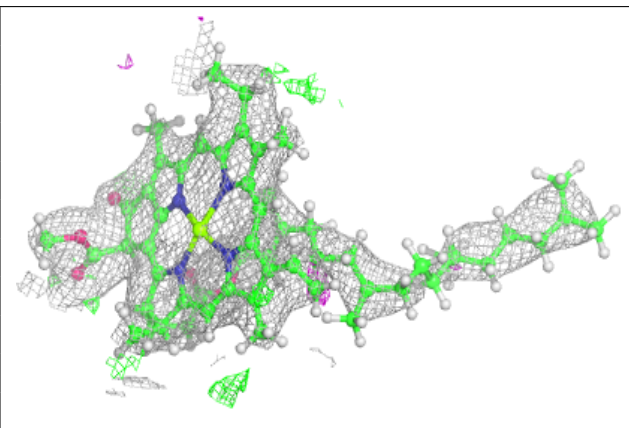


**Electron density around CLA B 606:**

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

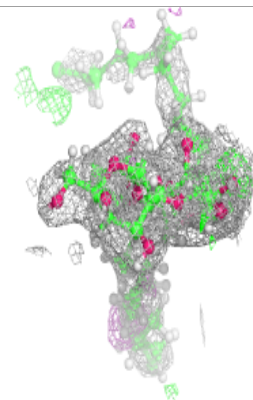
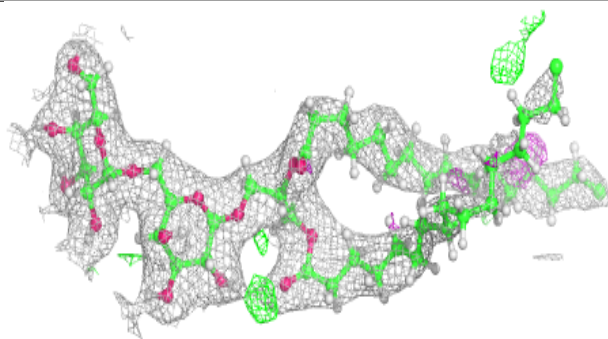
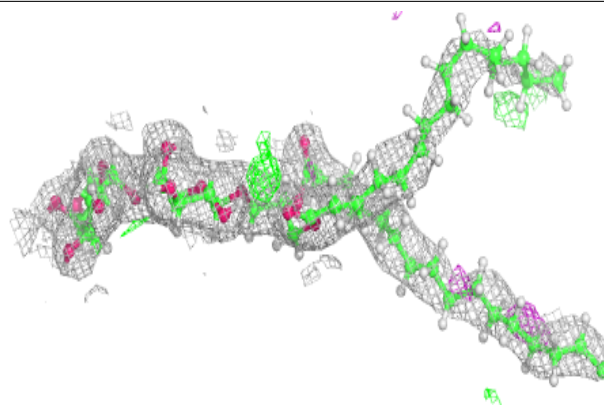
**Electron density around CLA C 505:**

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

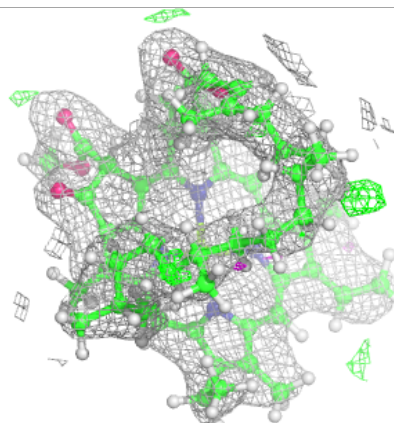
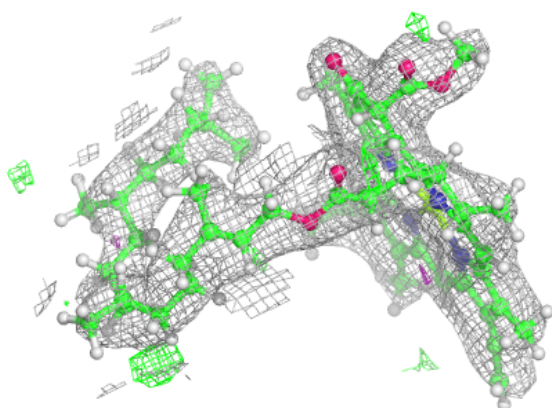
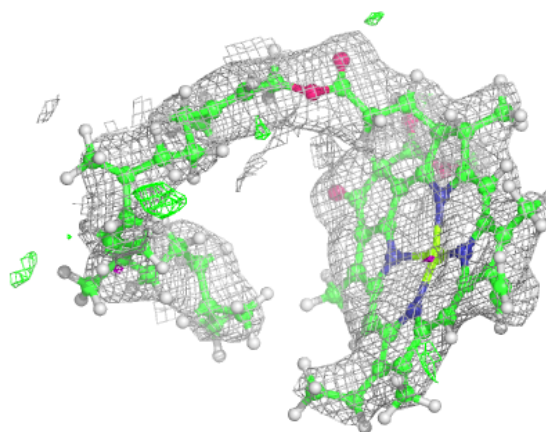


**Electron density around DGD C 516:**

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

**Electron density around CLA c 503:**

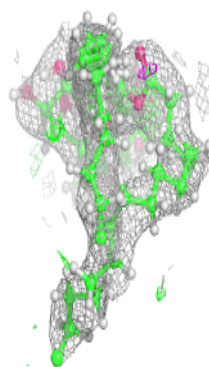
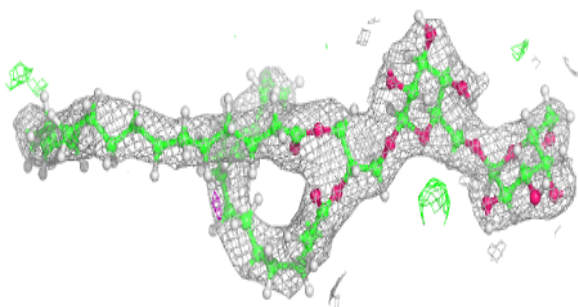
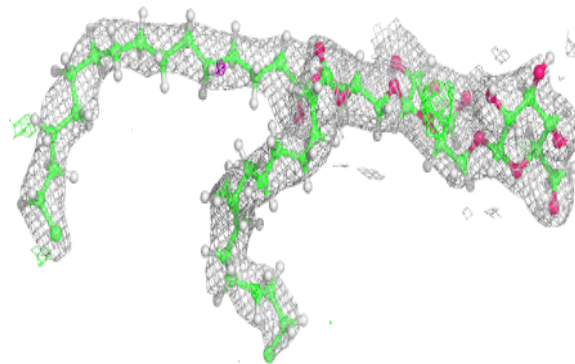
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



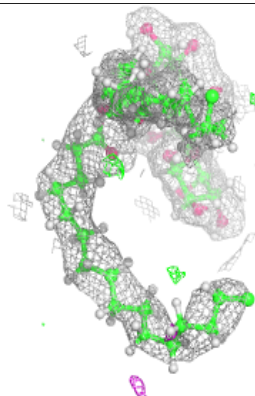
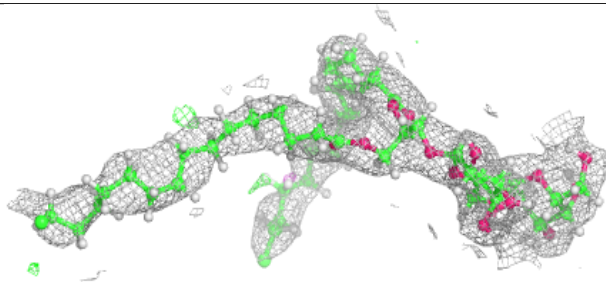
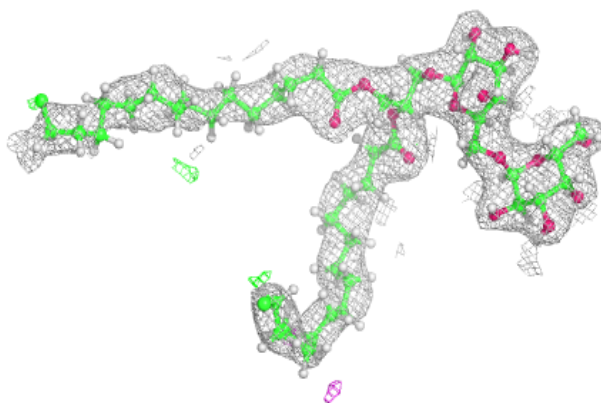


**Electron density around DGD H 102:**

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

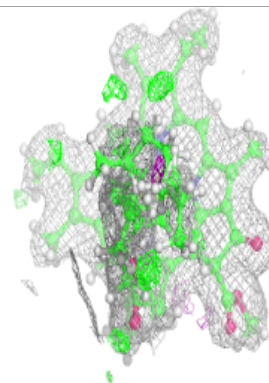
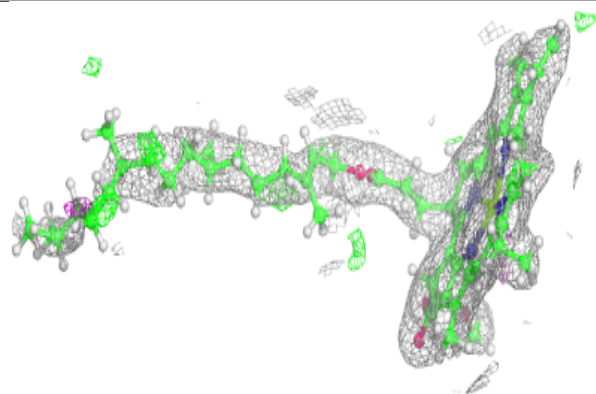
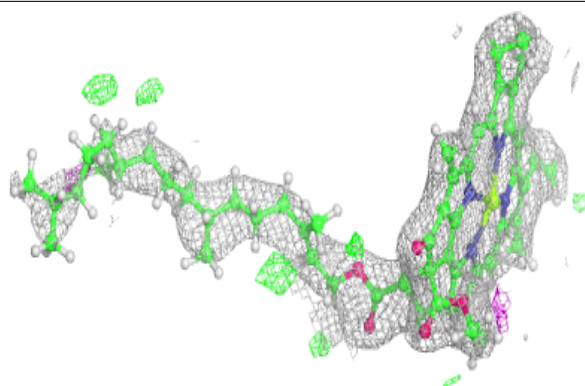
**Electron density around DGD c 517:**

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

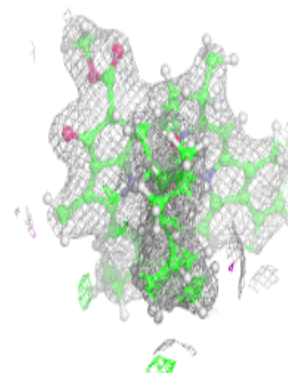
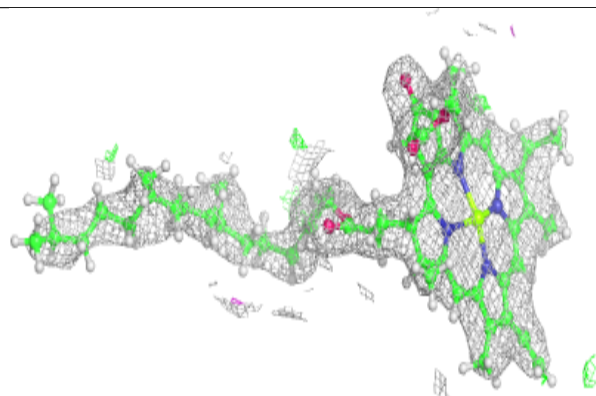
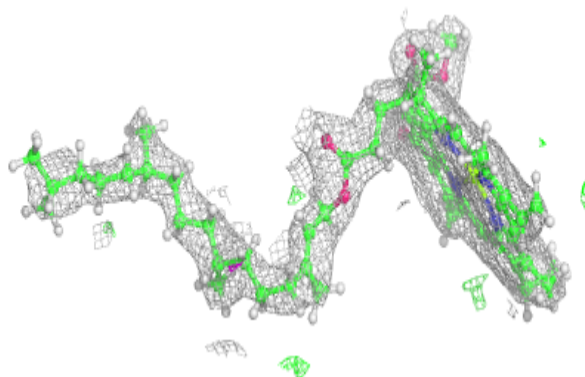


**Electron density around CLA B 604:**

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

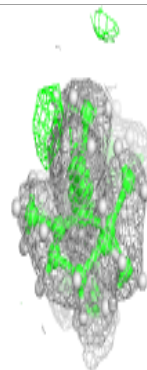
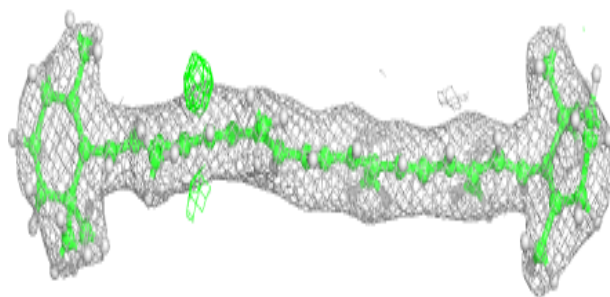
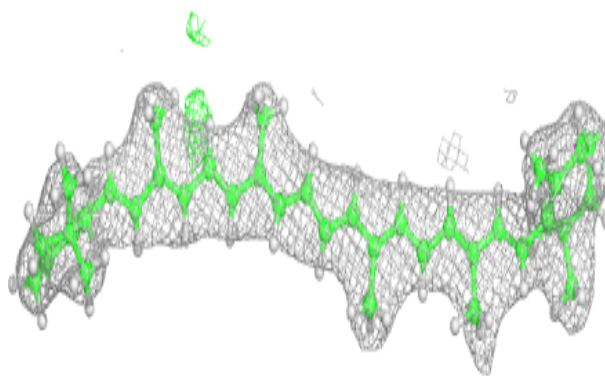
**Electron density around CLA c 502:**

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

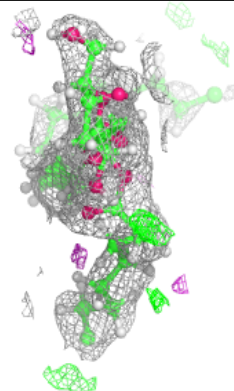
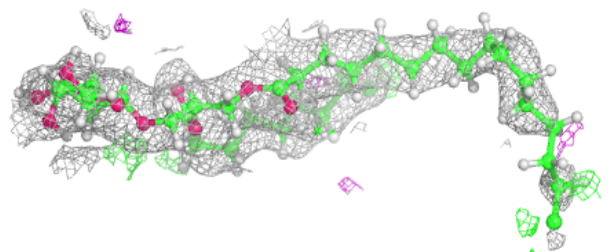
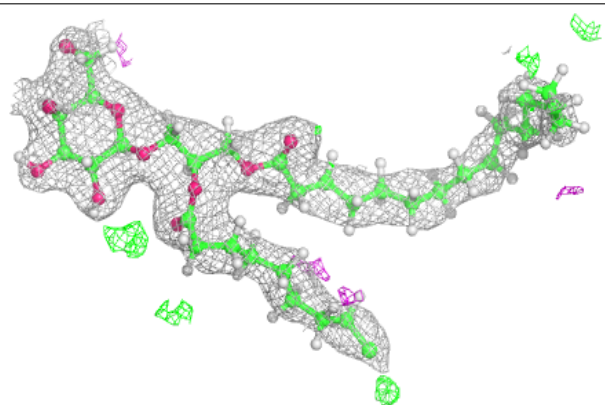


**Electron density around BCR A 408:**

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

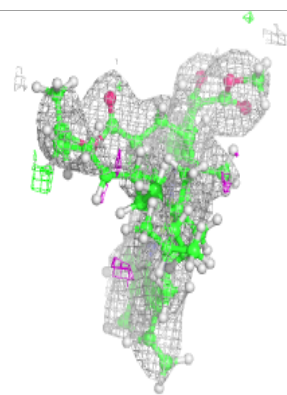
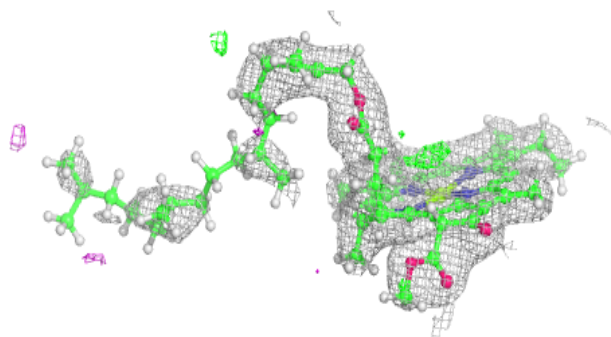
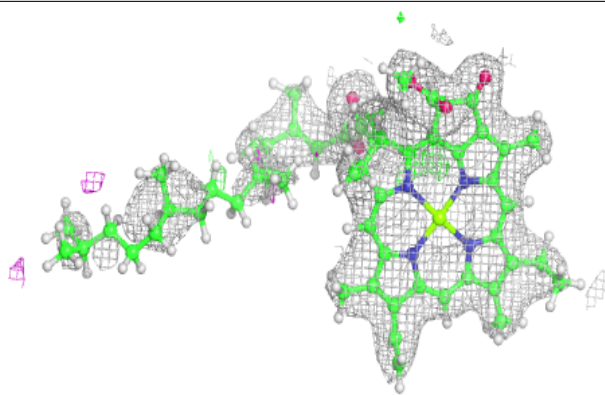
**Electron density around LMG d 409:**

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

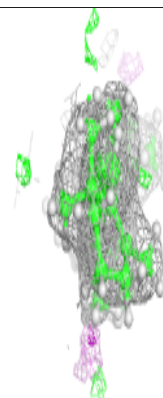
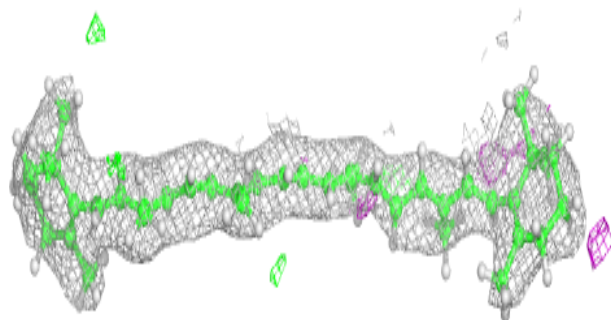
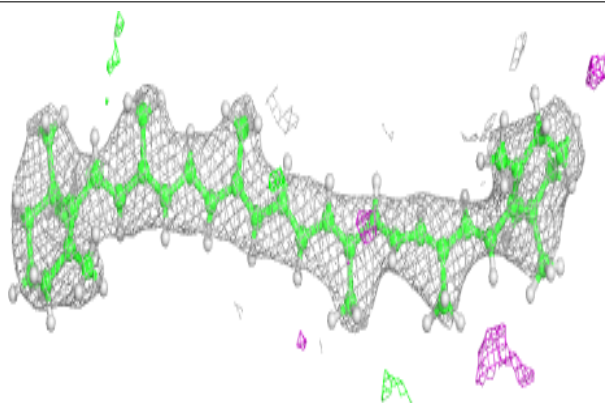


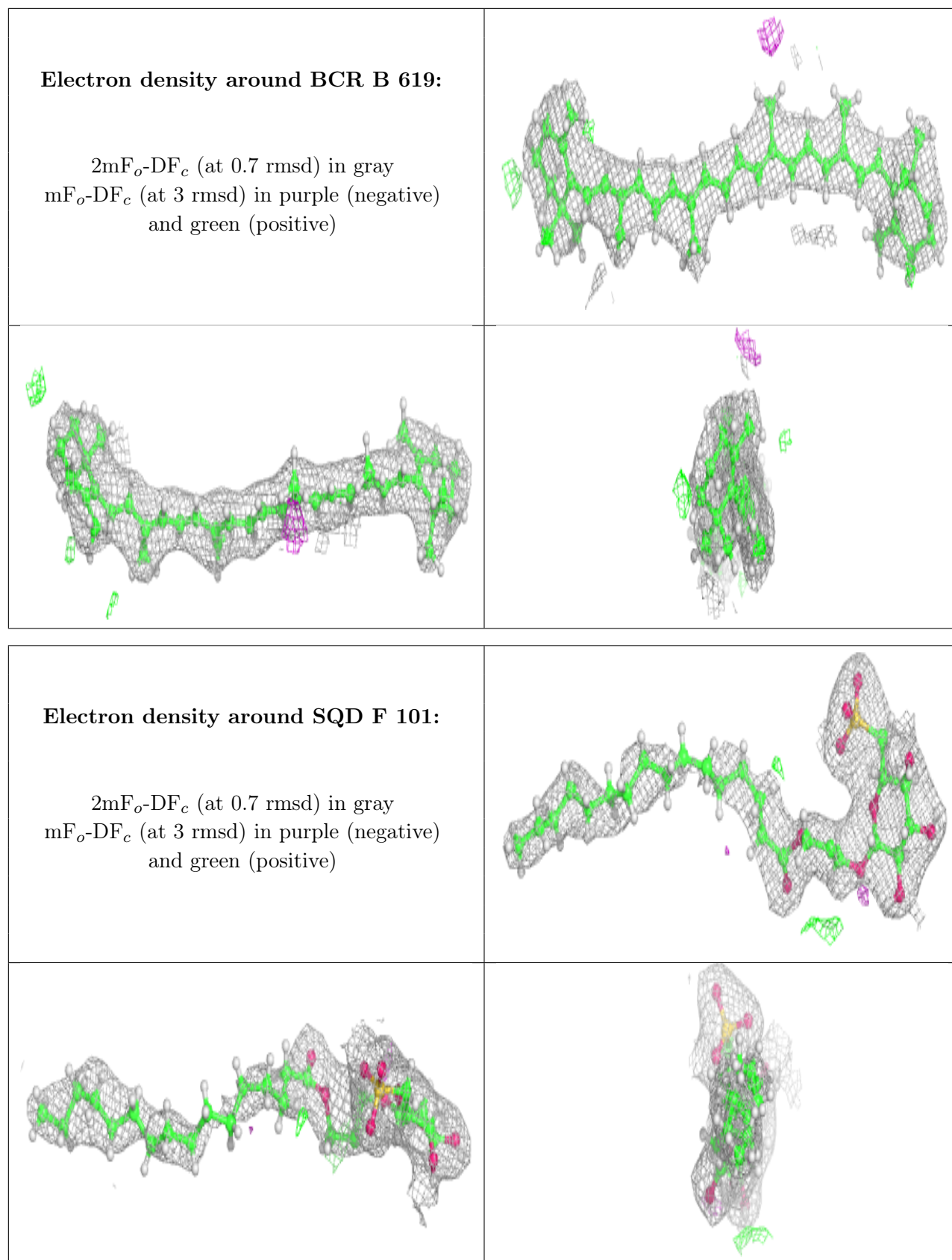
**Electron density around CLA a 405:**

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

**Electron density around BCR B 618:**

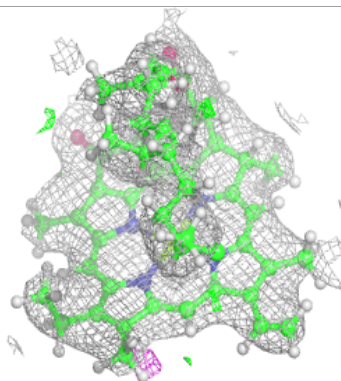
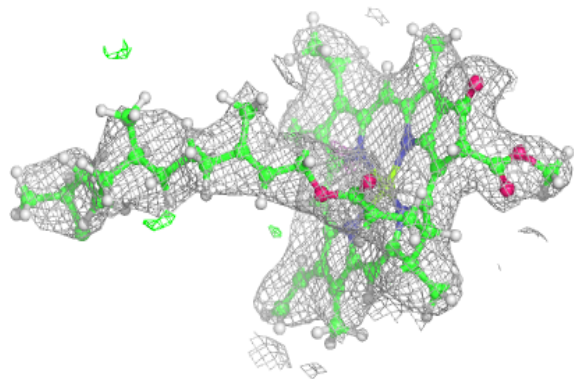
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



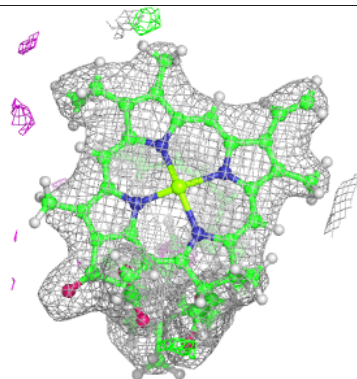
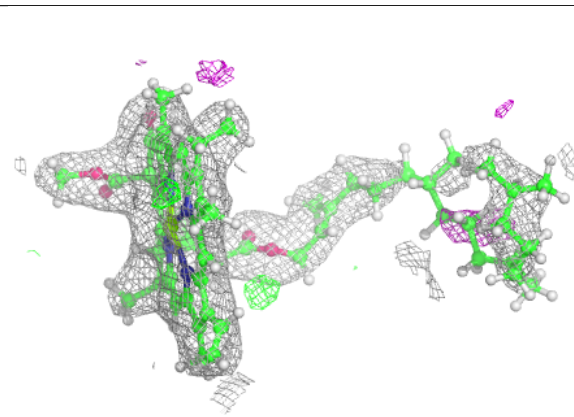
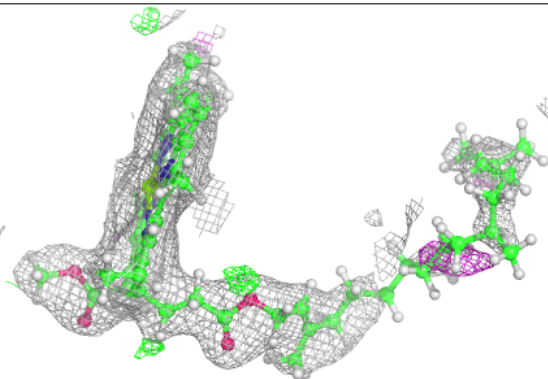


**Electron density around CLA c 504:**

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

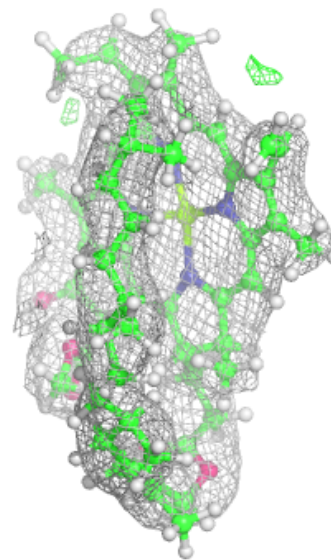
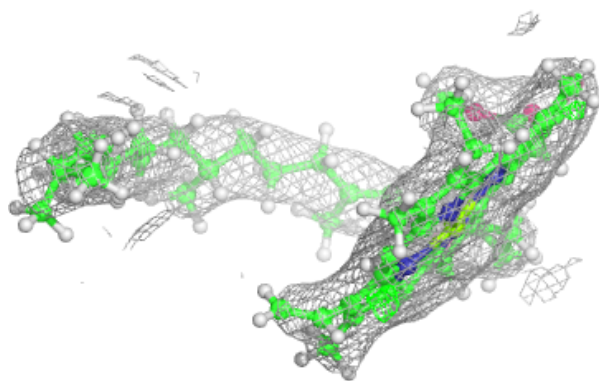
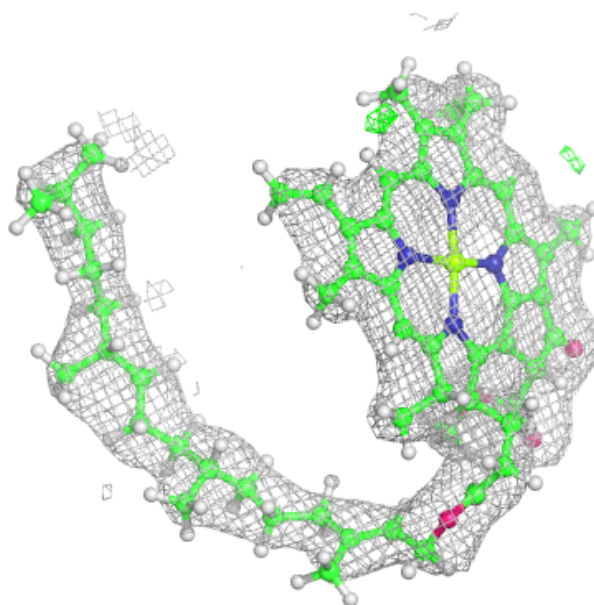
**Electron density around CLA C 506:**

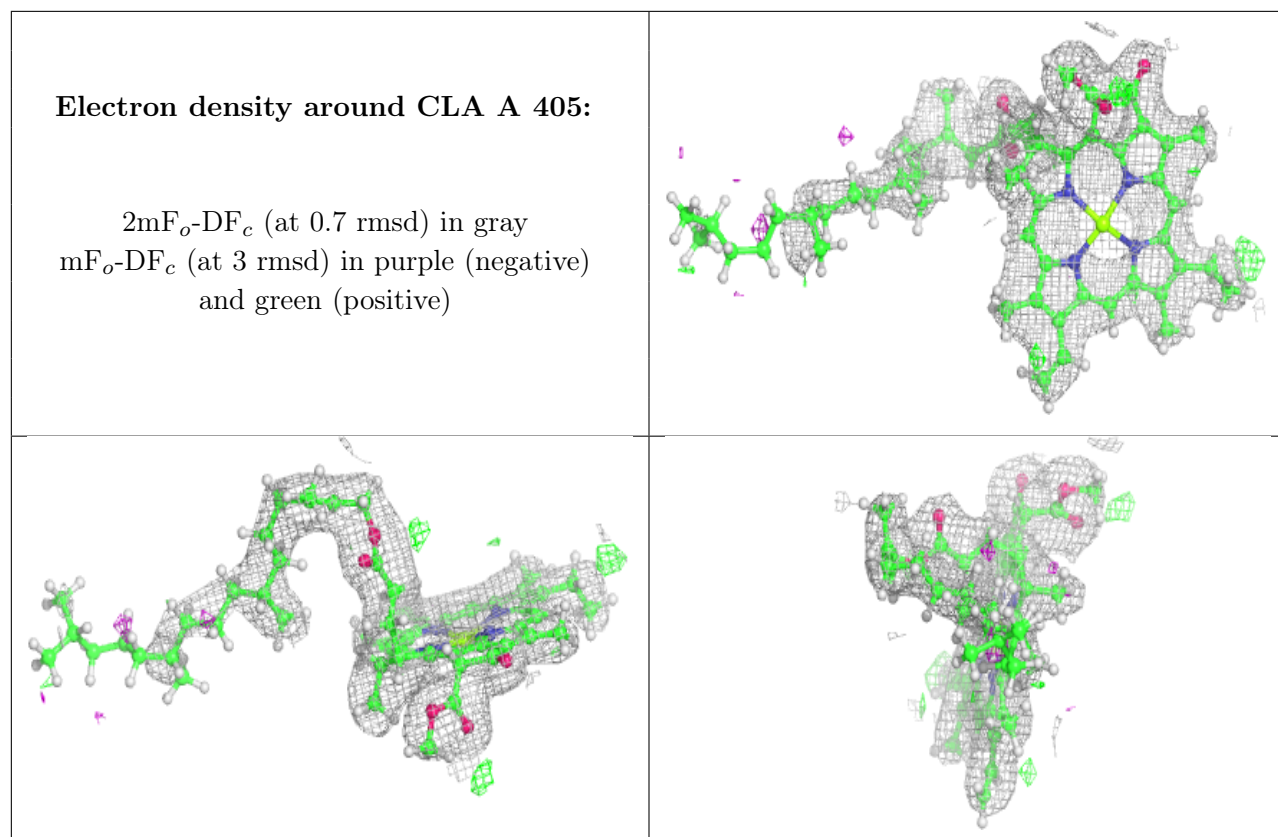
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 507:**

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

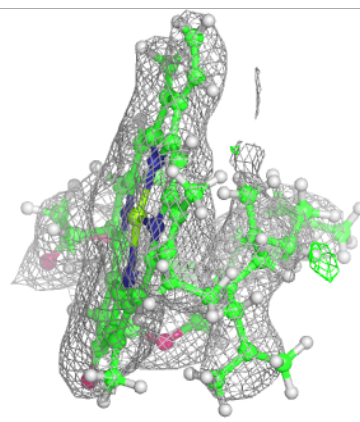
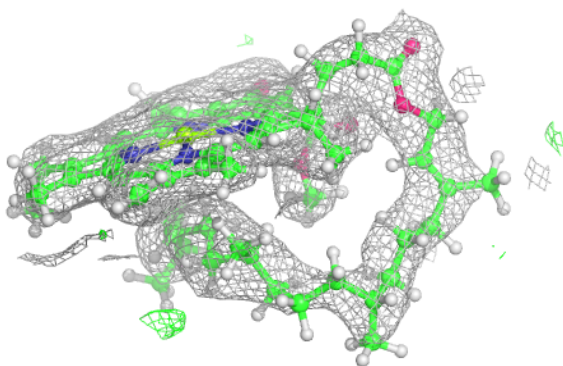
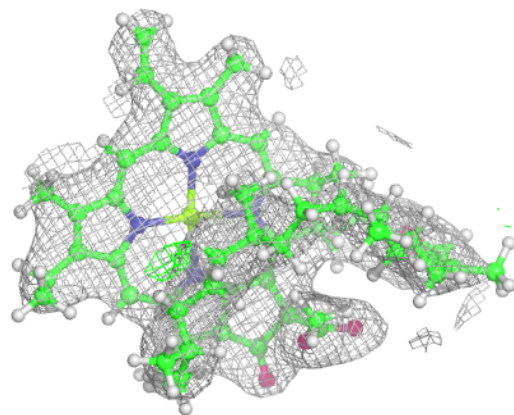






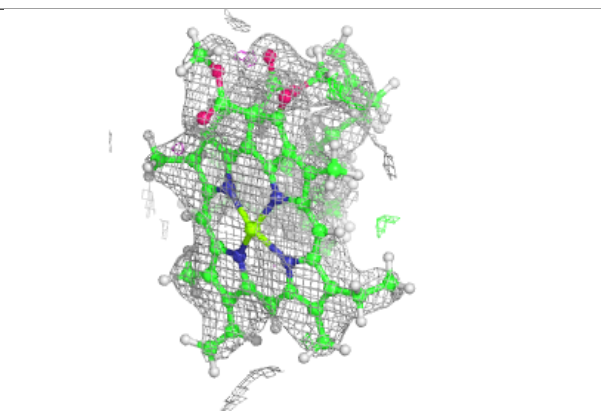
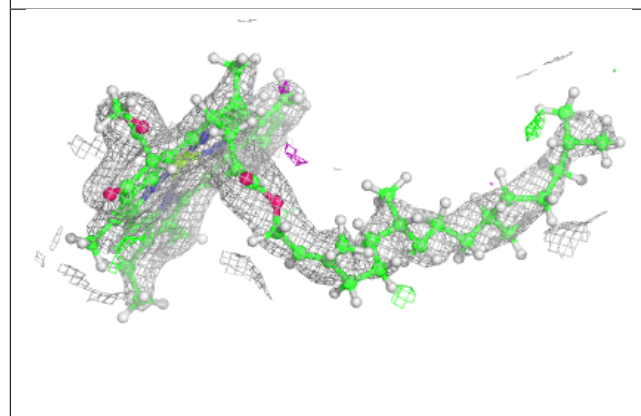
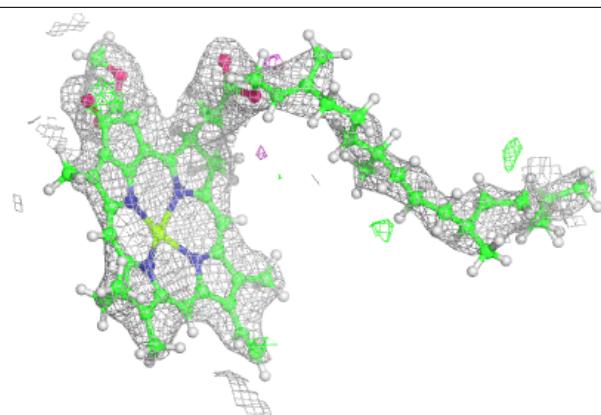
**Electron density around CLA c 510:**

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

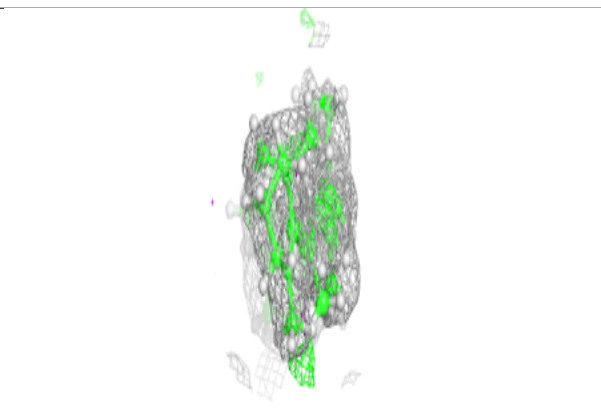
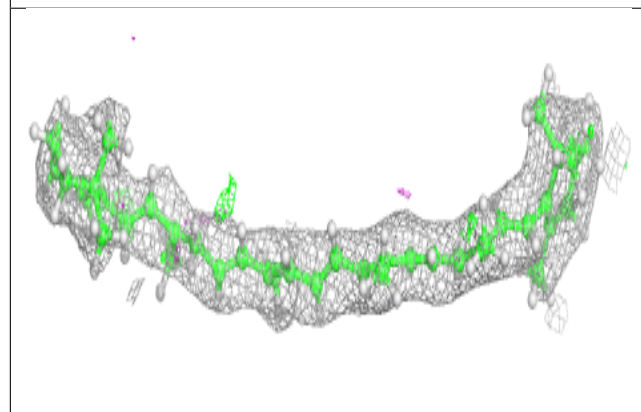
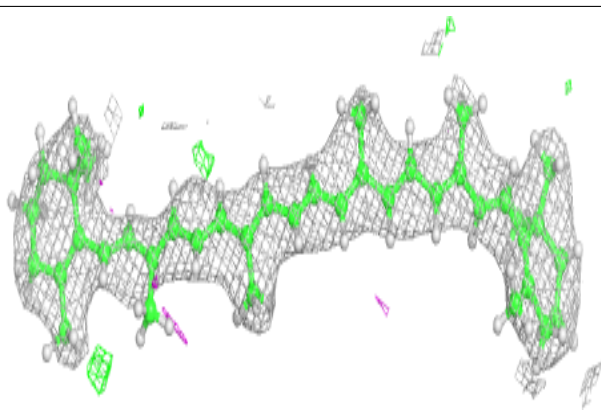


**Electron density around CLA c 511:**

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

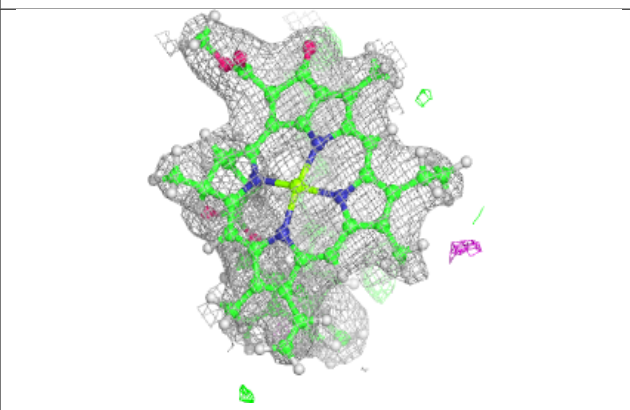
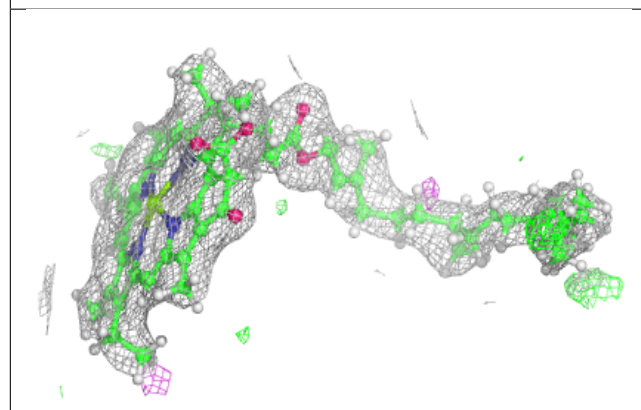
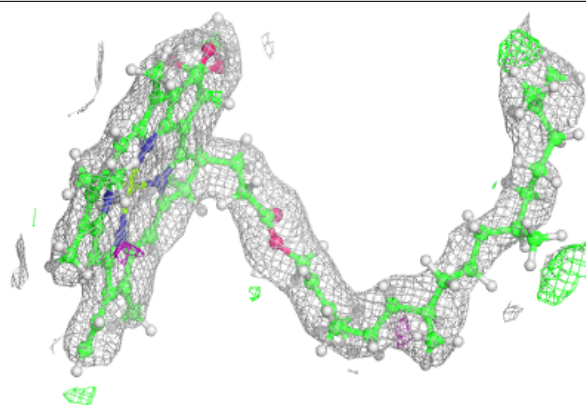
**Electron density around BCR T 101:**

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

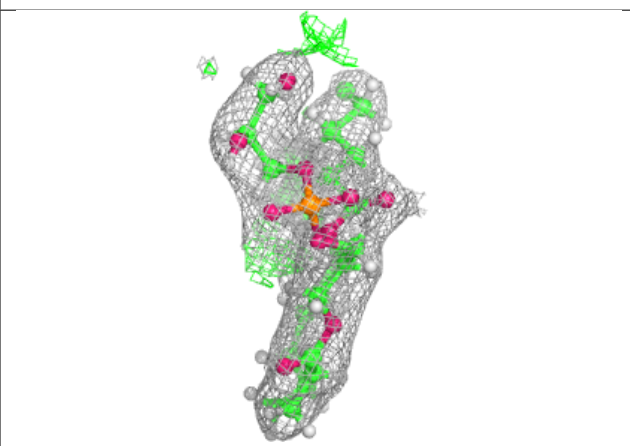
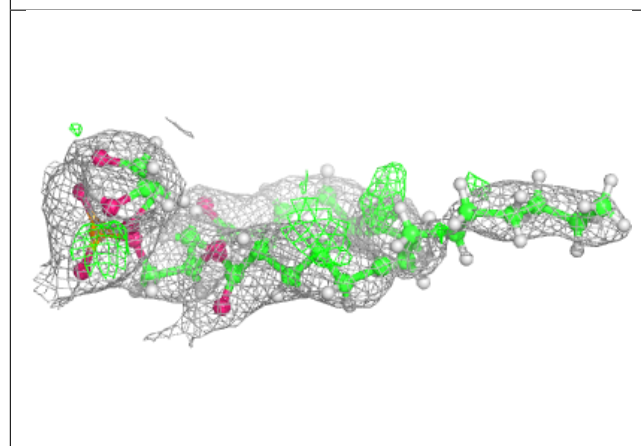
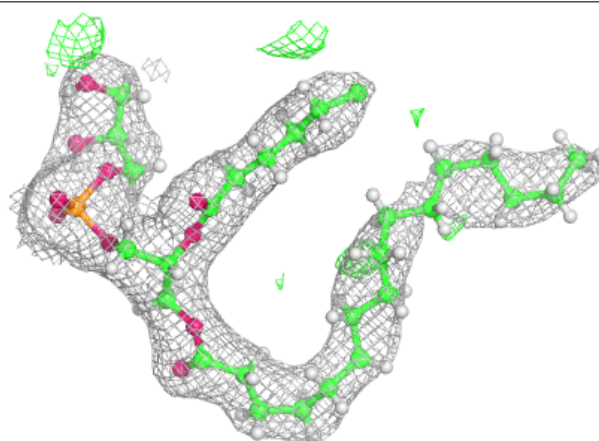


**Electron density around CLA b 607:**

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

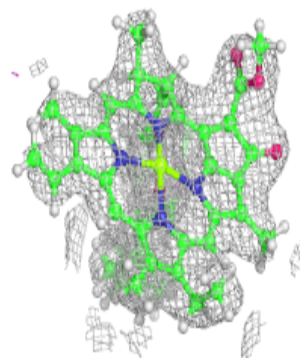
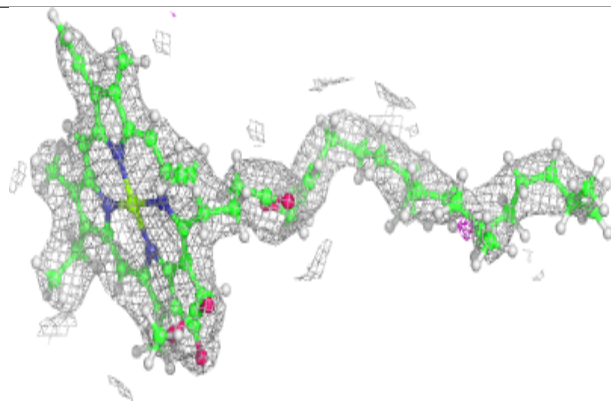
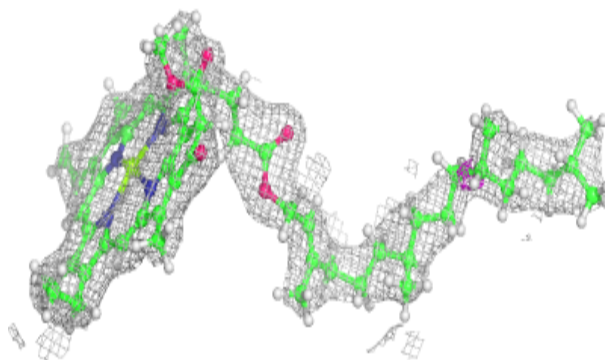
**Electron density around LHG d 408:**

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



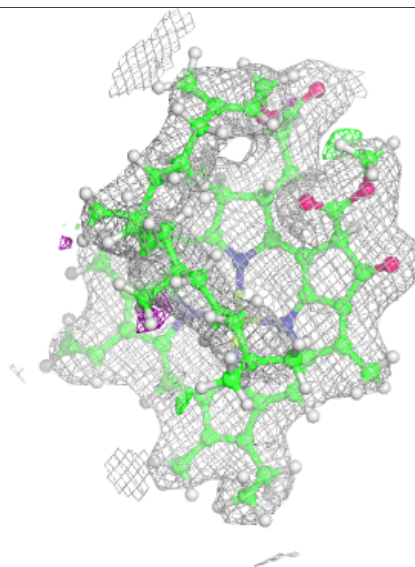
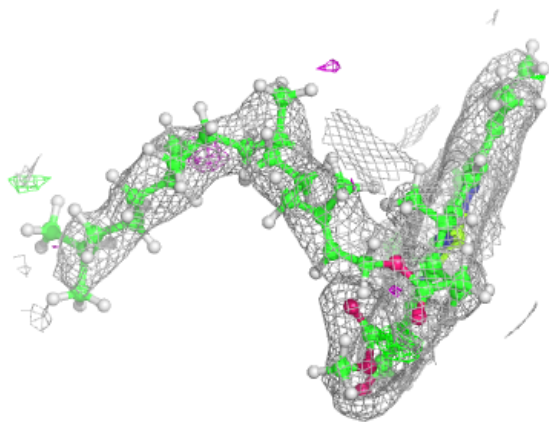
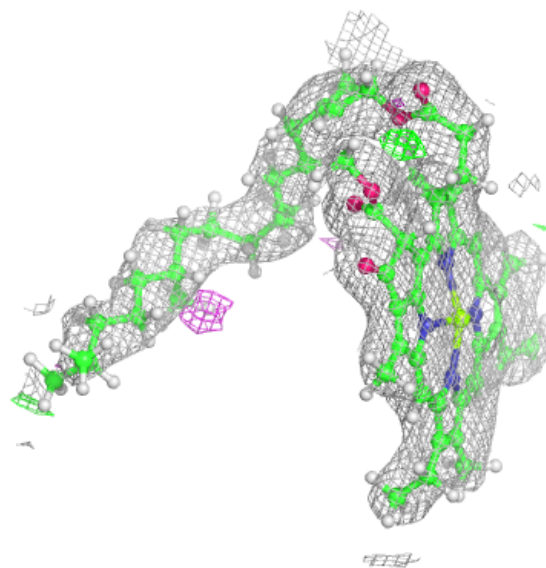
**Electron density around CLA C 502:**

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



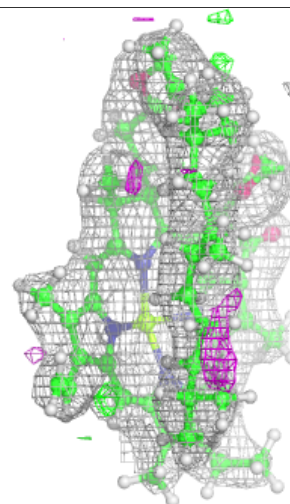
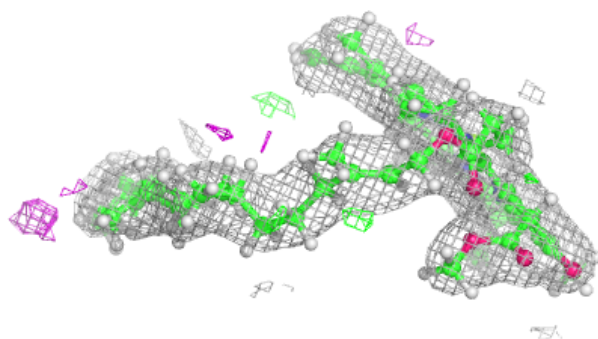
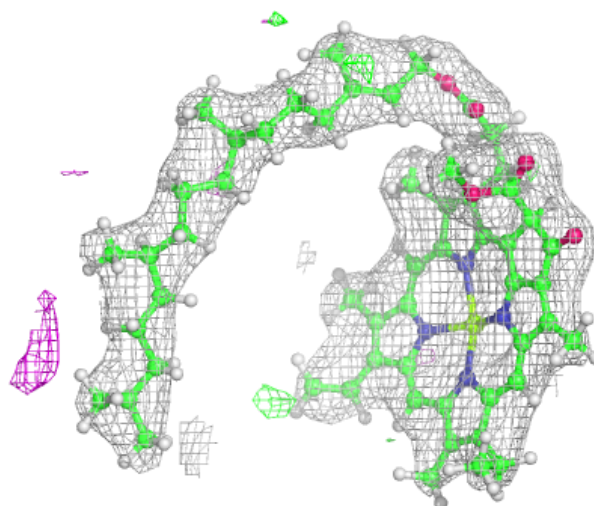
**Electron density around CLA B 613:**

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



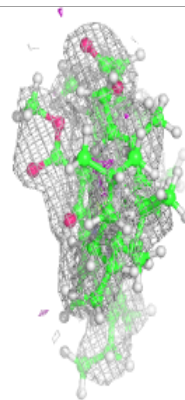
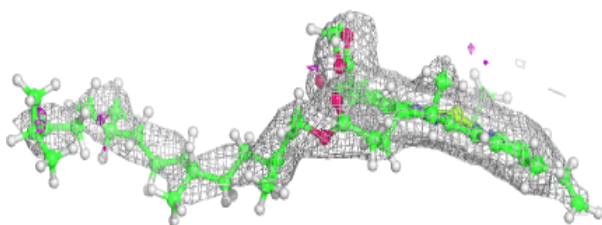
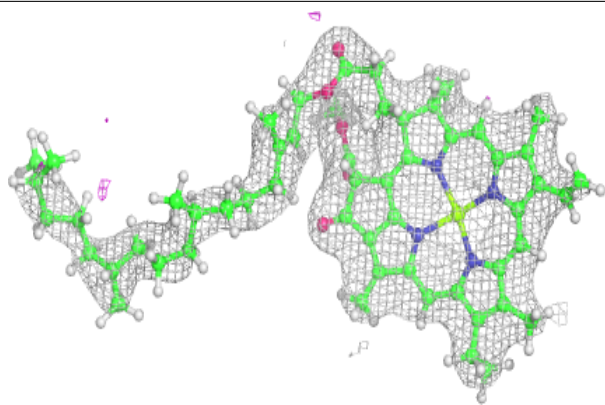
**Electron density around CLA C 507:**

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



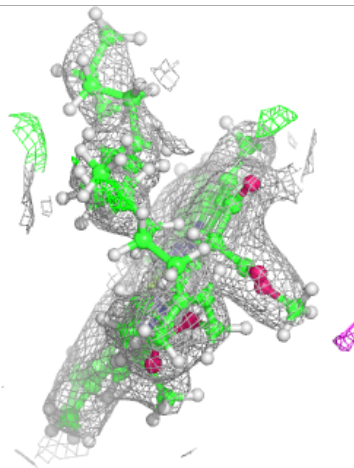
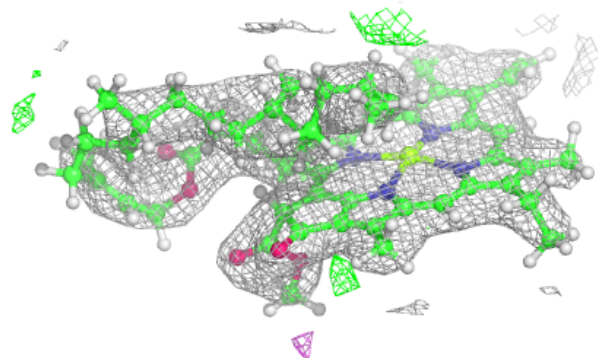
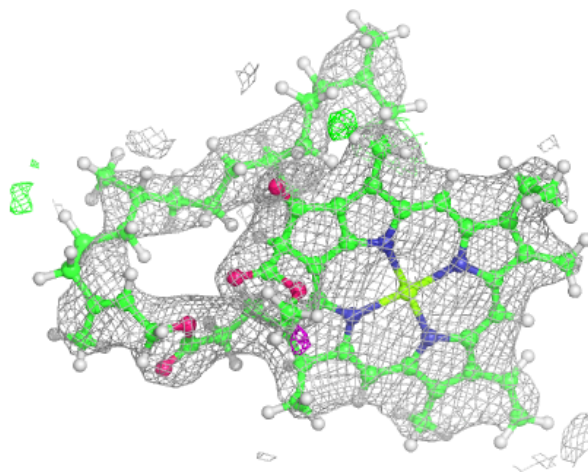
**Electron density around CLA b 603:**

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

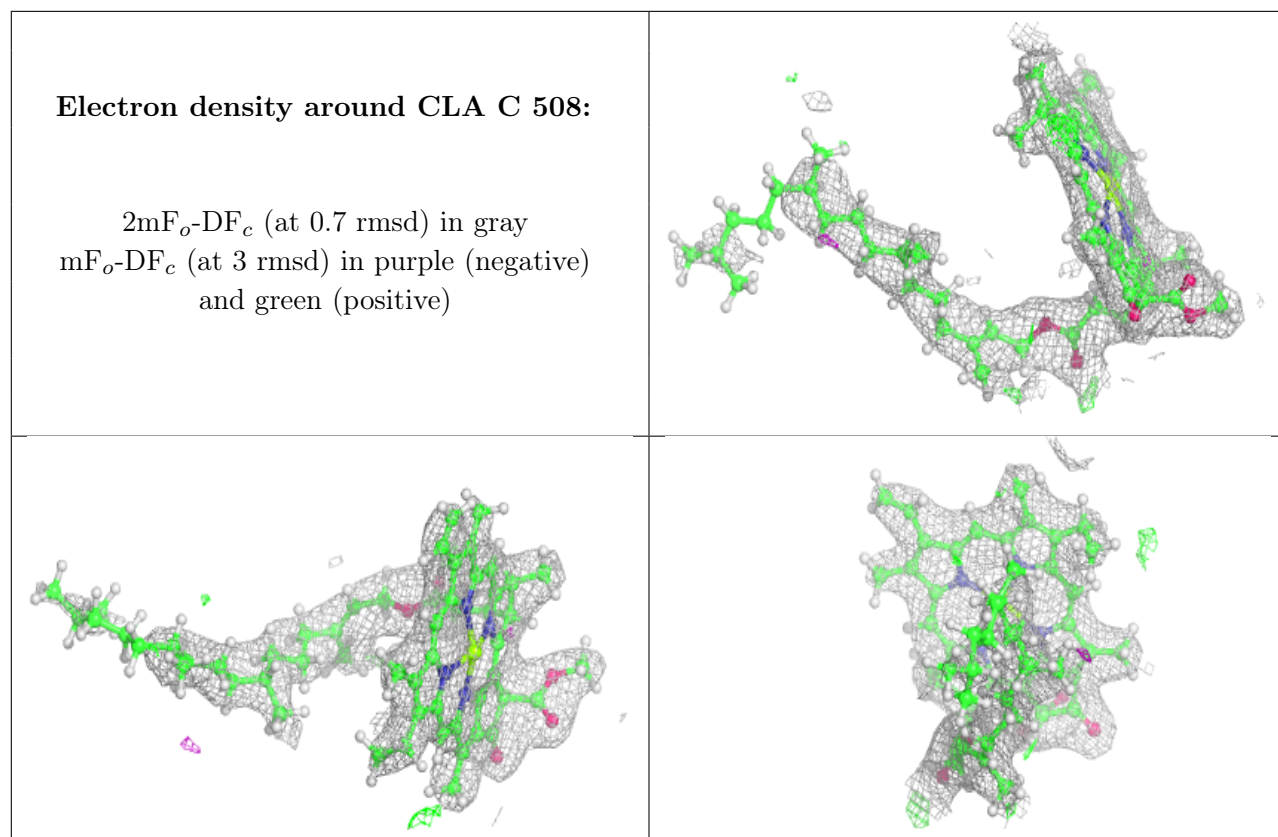


**Electron density around CLA c 509:**

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

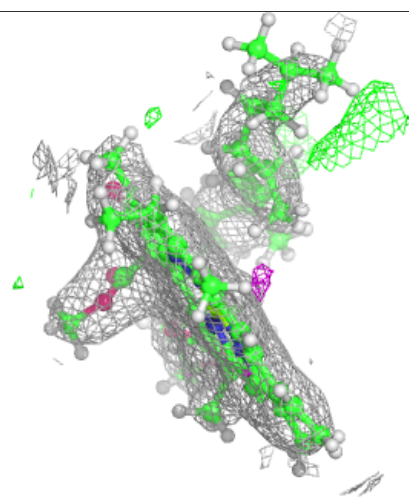
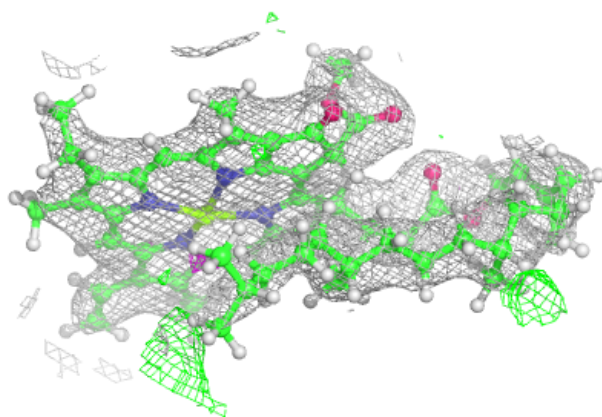
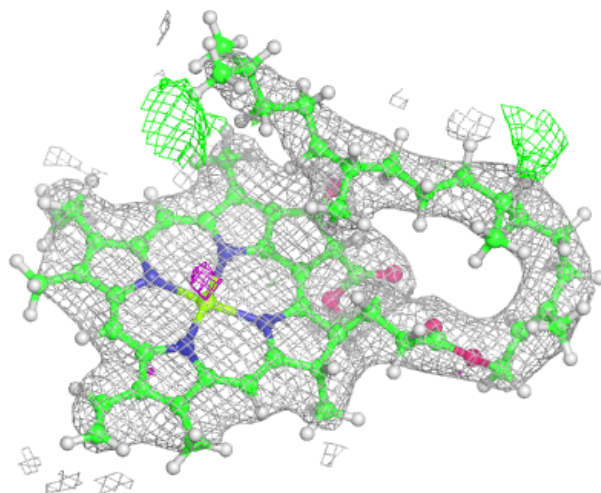






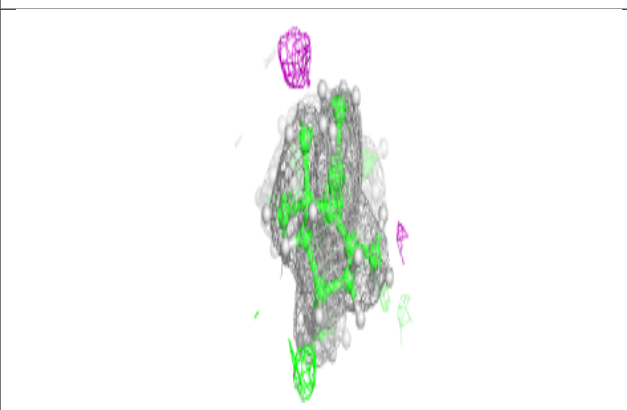
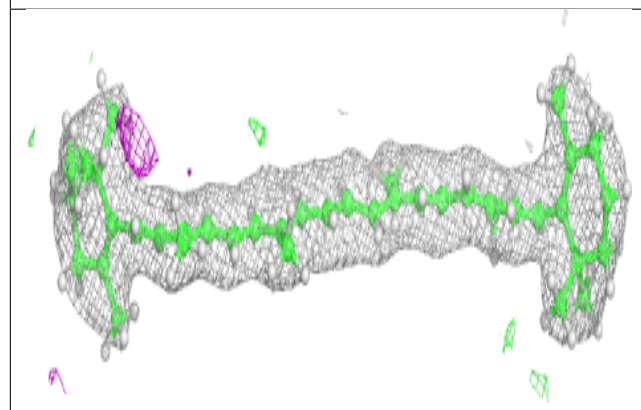
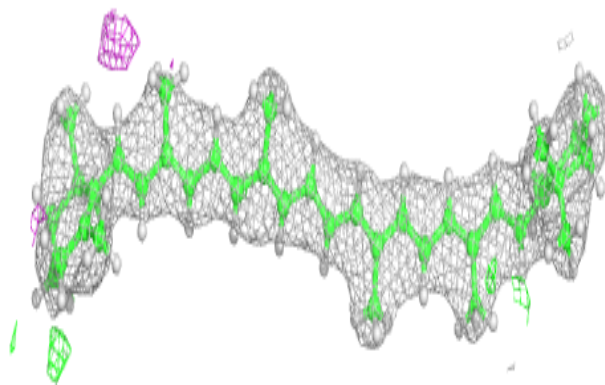
**Electron density around CLA C 509:**

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

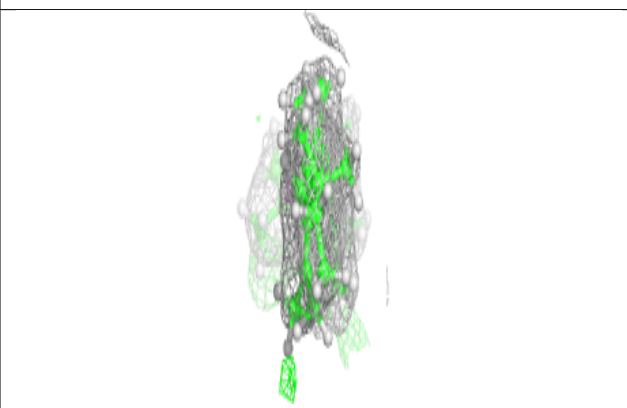
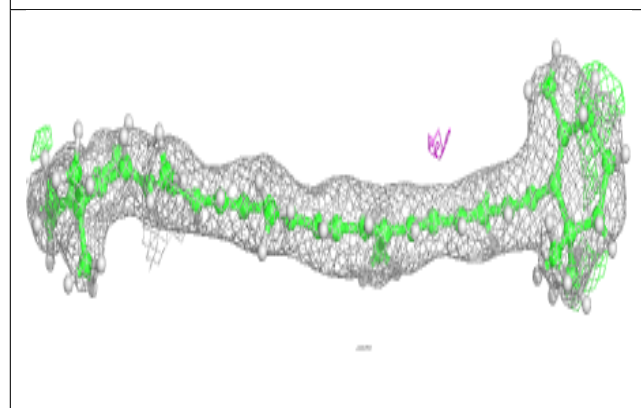
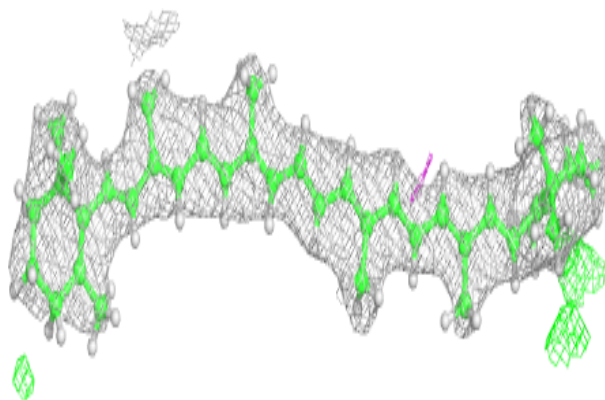


**Electron density around BCR a 408:**

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

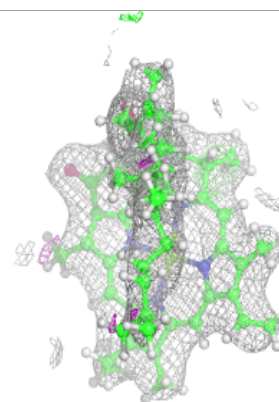
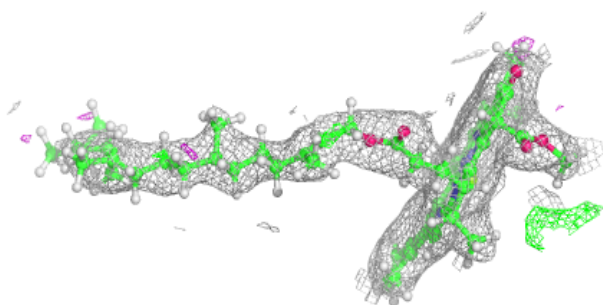
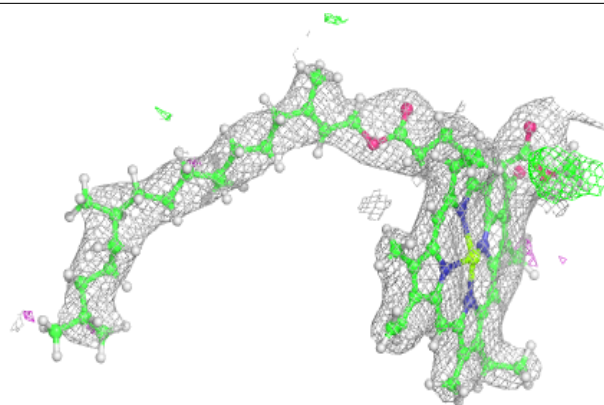
**Electron density around BCR b 618:**

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

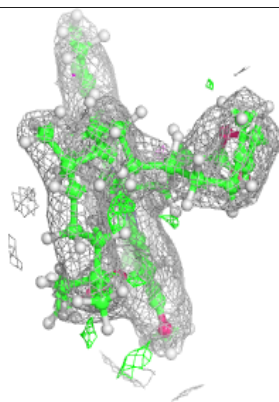
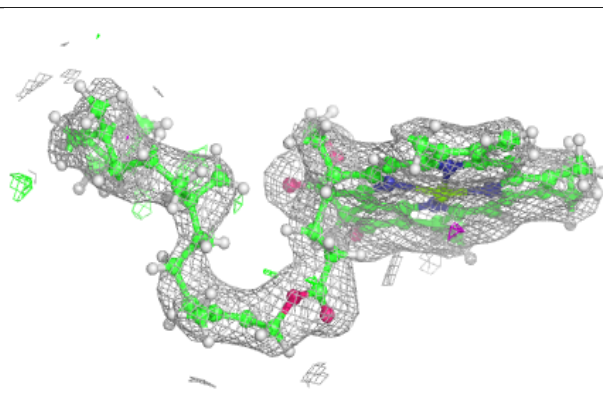
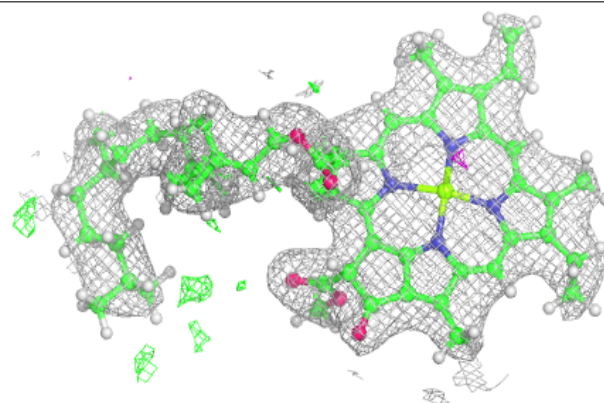


**Electron density around CLA b 610:**

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

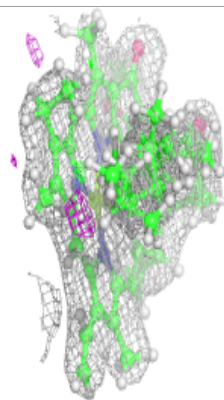
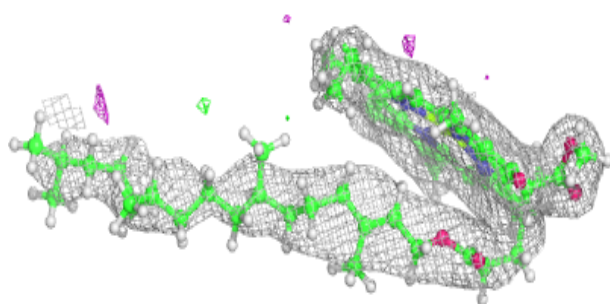
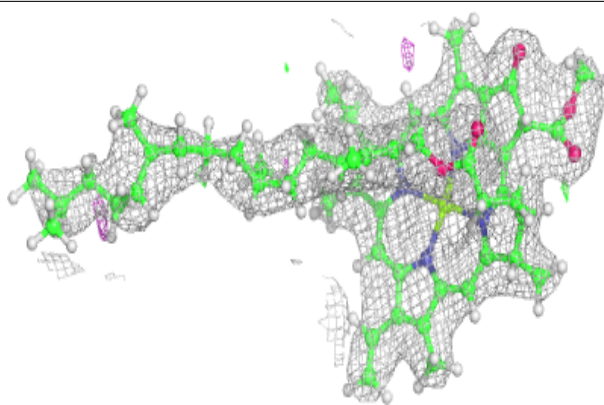
**Electron density around CLA b 613:**

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



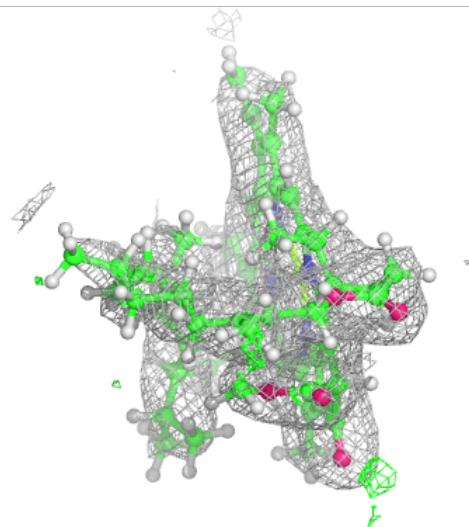
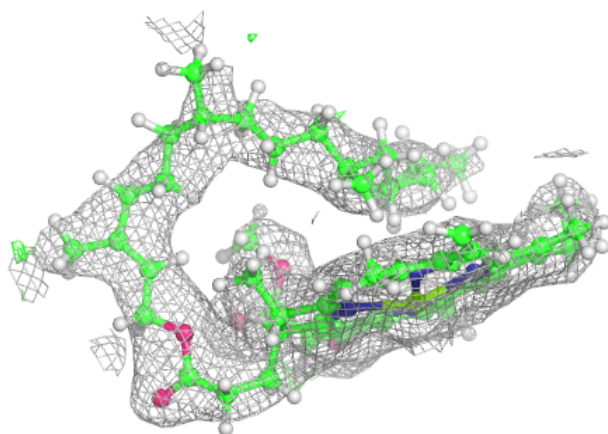
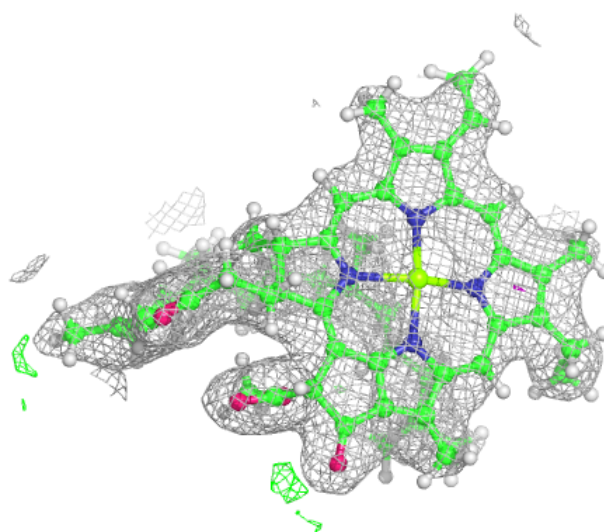
**Electron density around CLA b 615:**

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



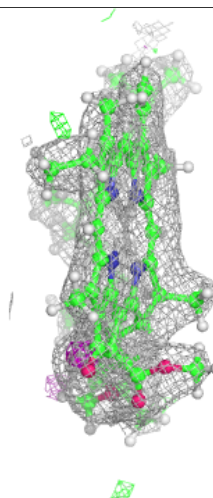
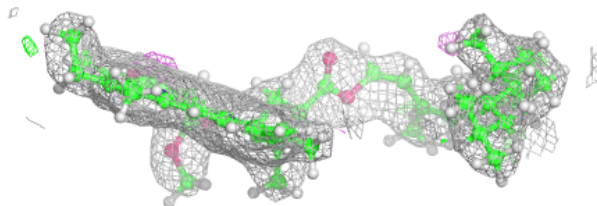
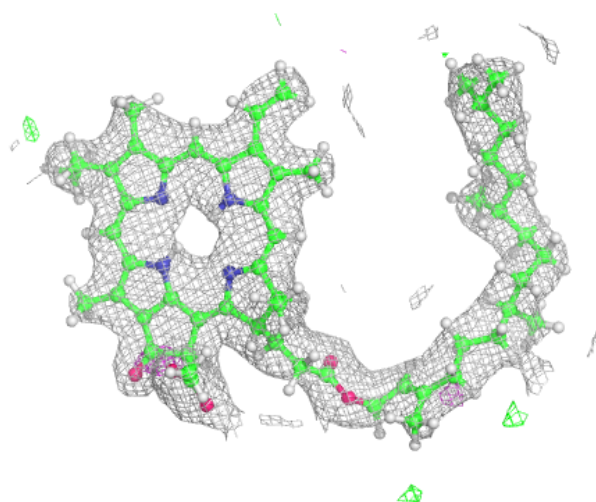
**Electron density around CLA C 510:**

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



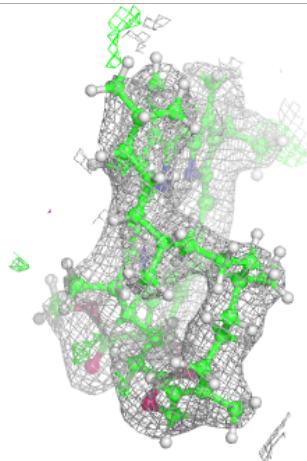
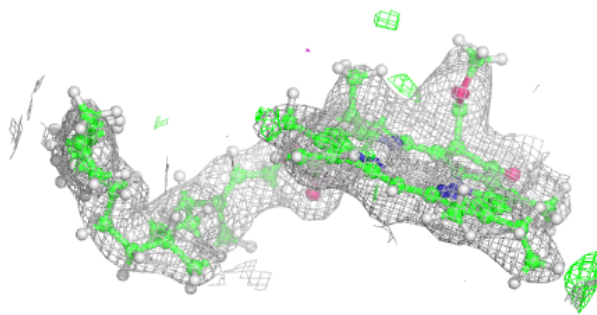
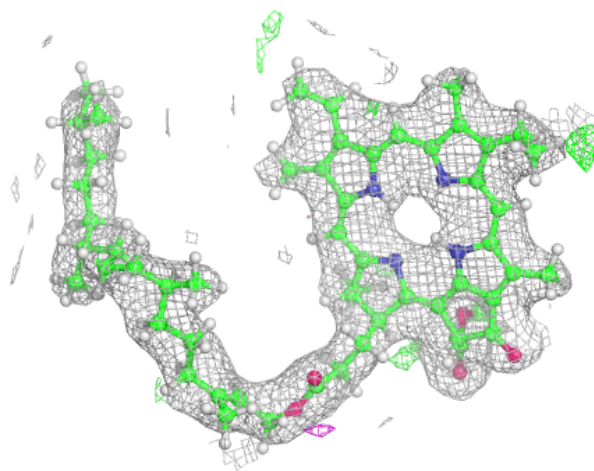
**Electron density around PHO a 406:**

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



**Electron density around PHO d 401:**

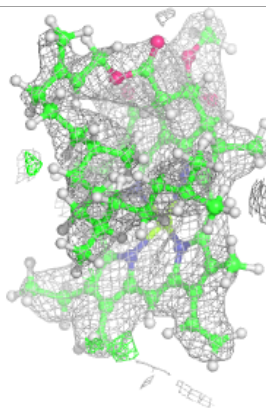
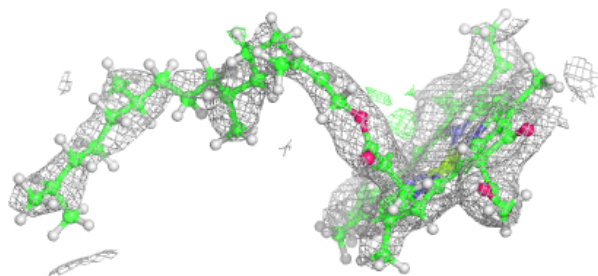
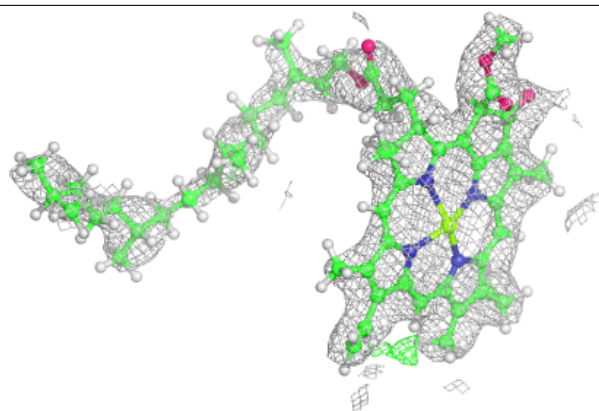
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



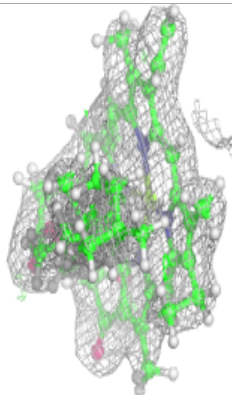
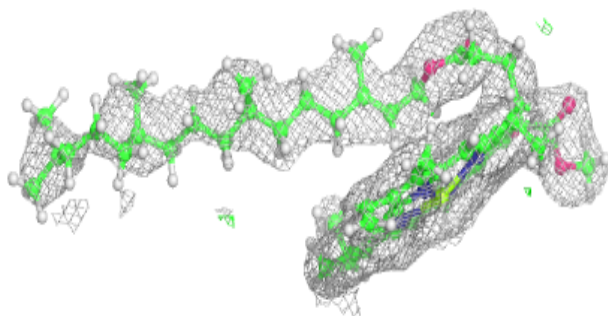
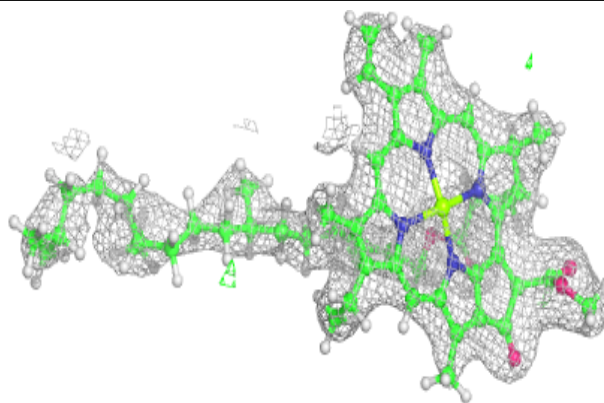


**Electron density around CLA C 511:**

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

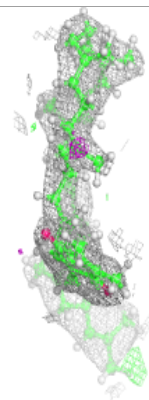
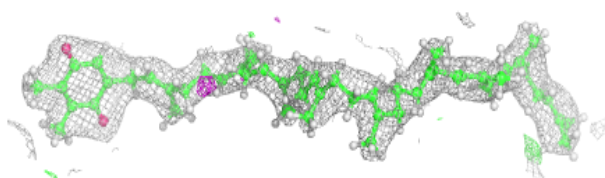
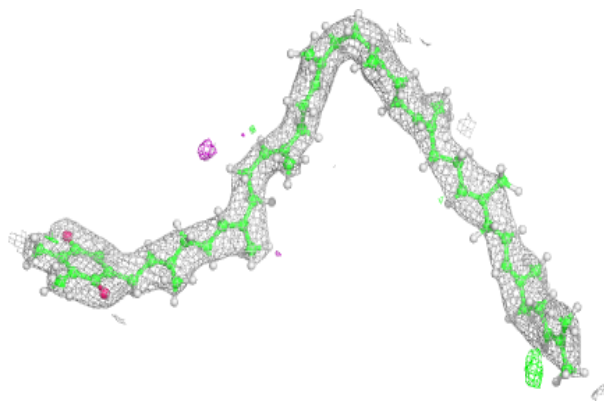
**Electron density around CLA B 614:**

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

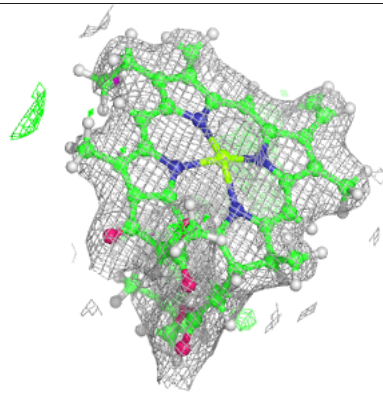
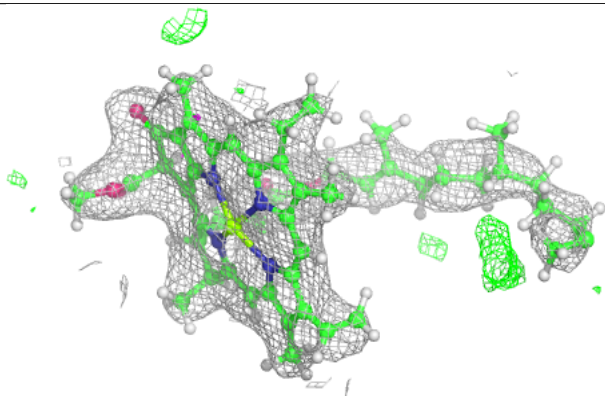
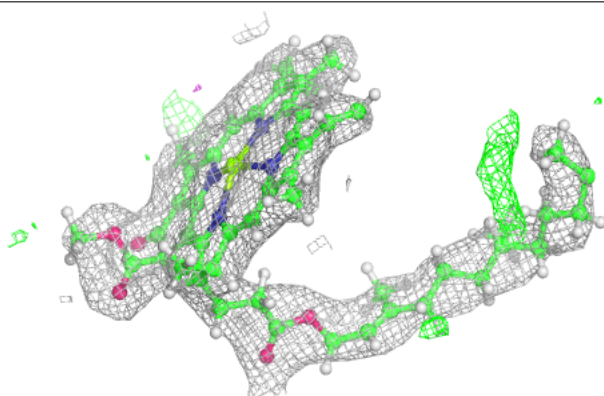


**Electron density around PL9 D 406:**

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

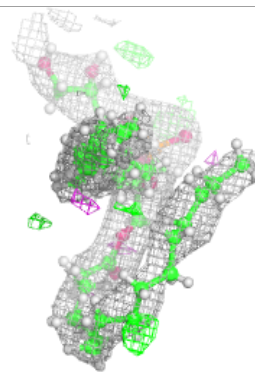
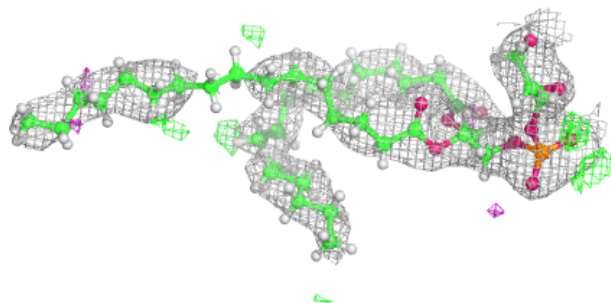
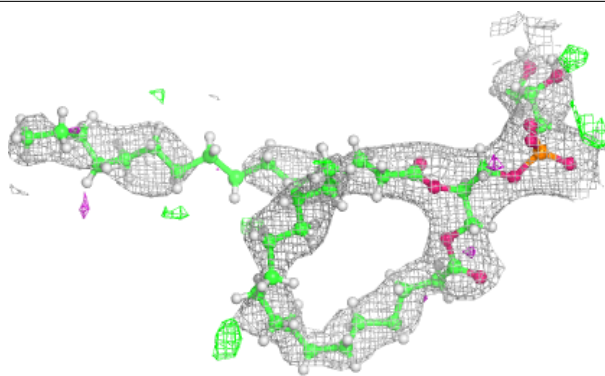
**Electron density around CLA C 504:**

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

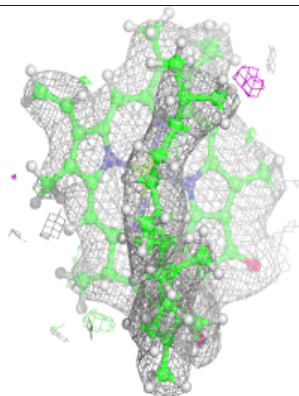
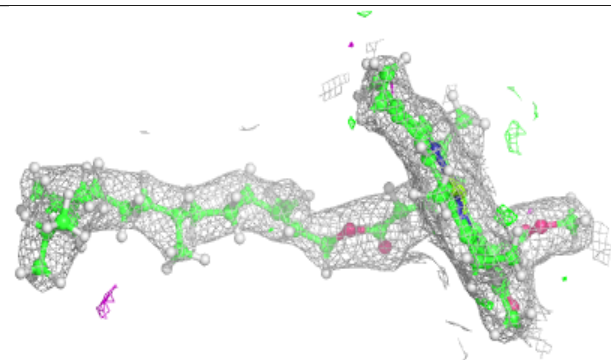
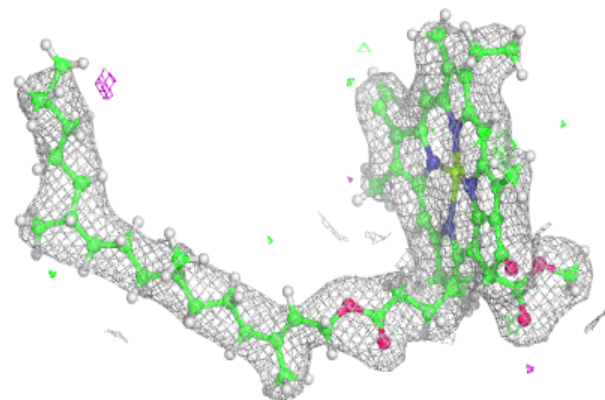


**Electron density around LHG a 410:**

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

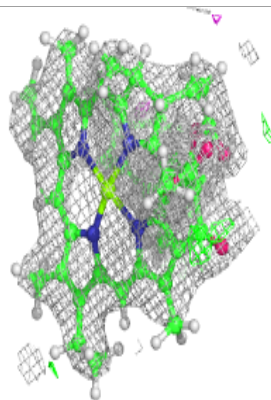
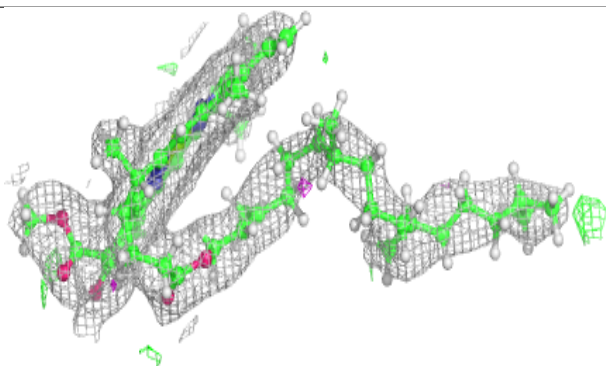
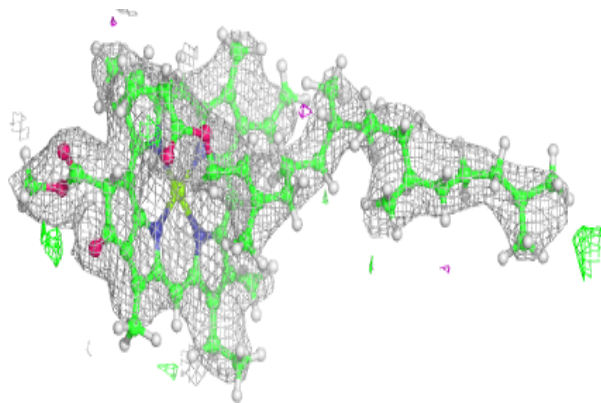
**Electron density around CLA B 609:**

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



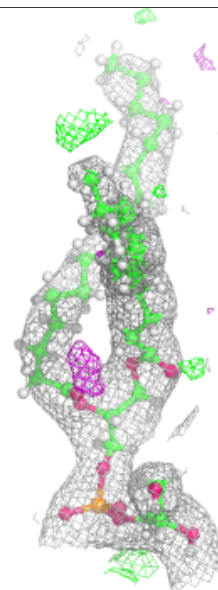
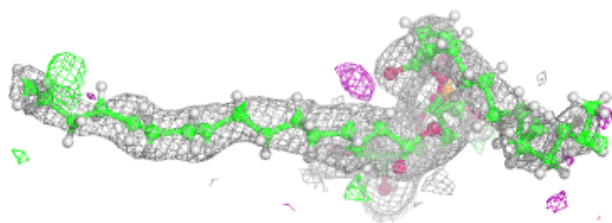
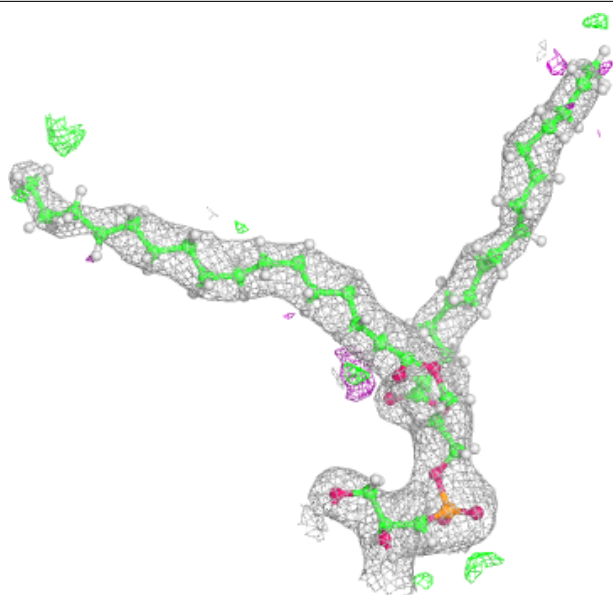
**Electron density around CLA c 505:**

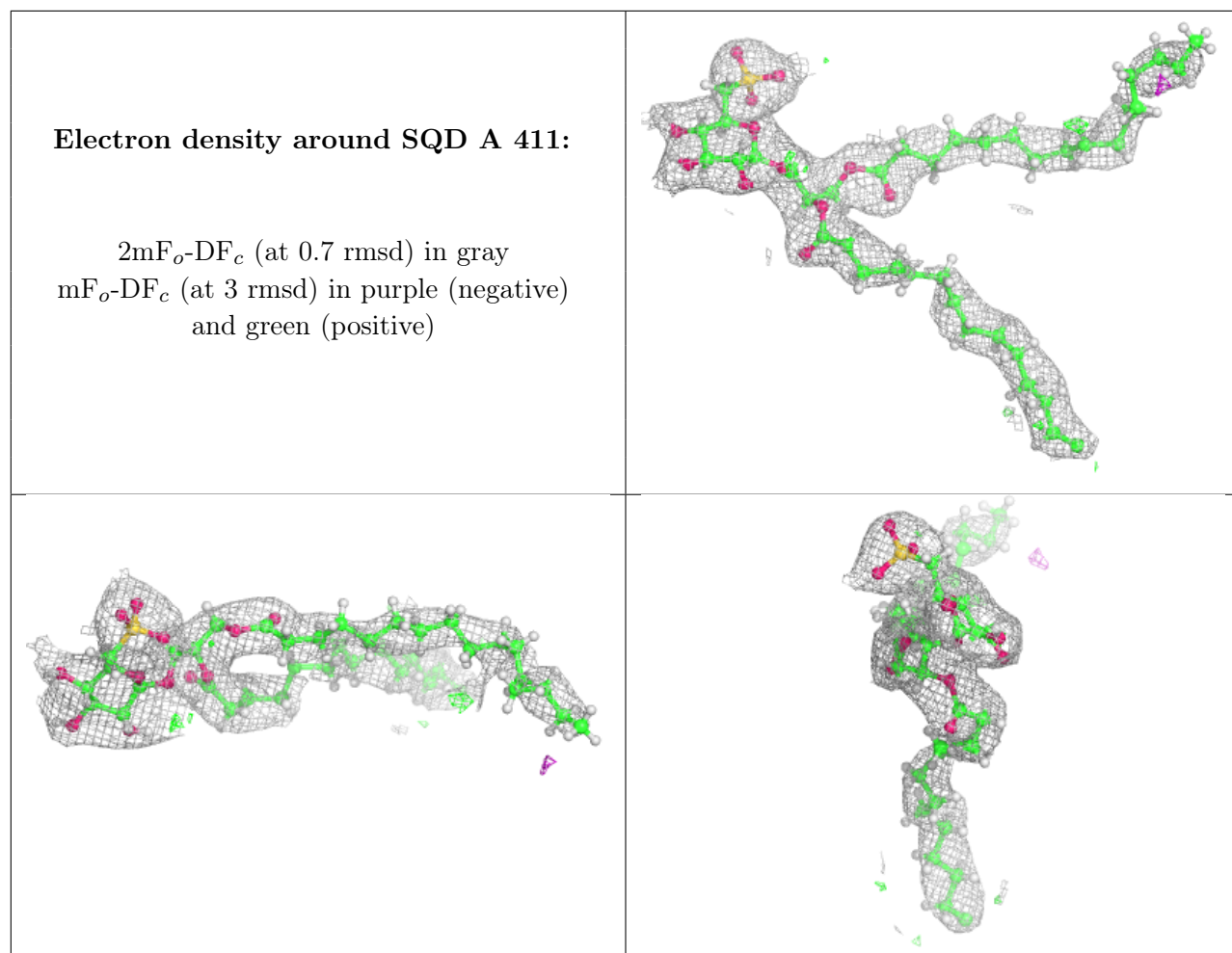
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)



**Electron density around LHG 1 101:**

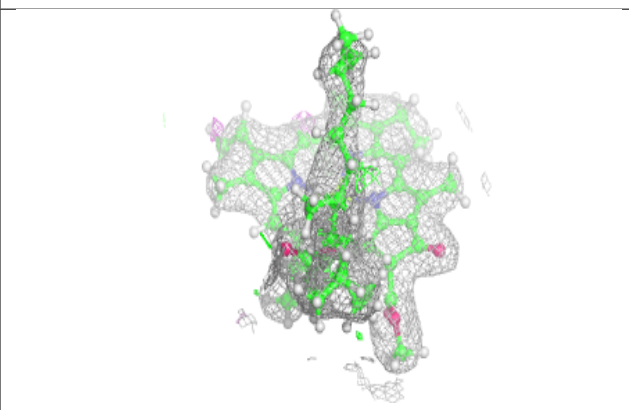
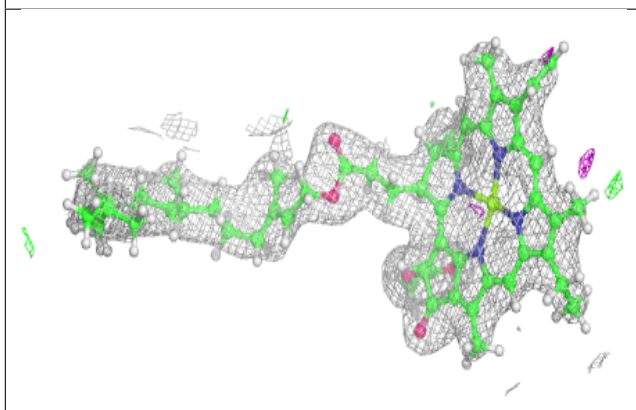
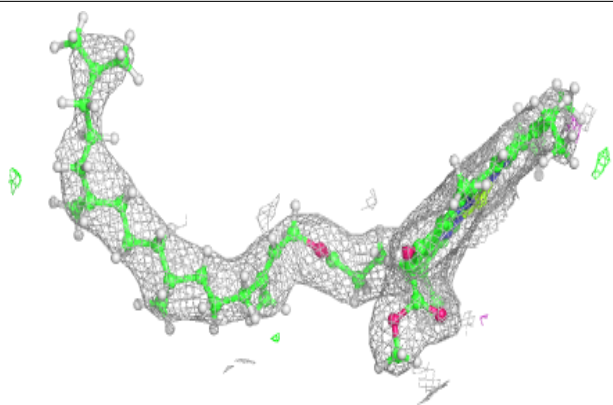
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



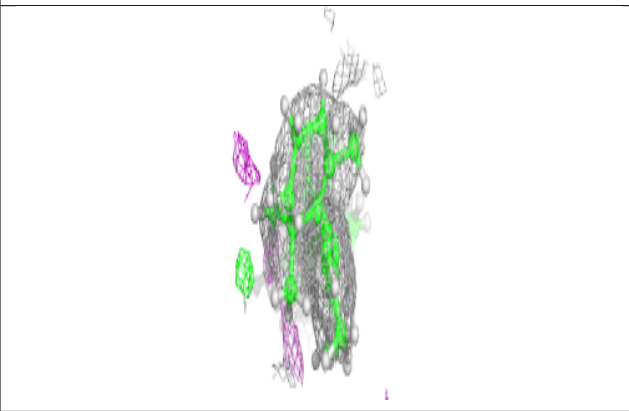
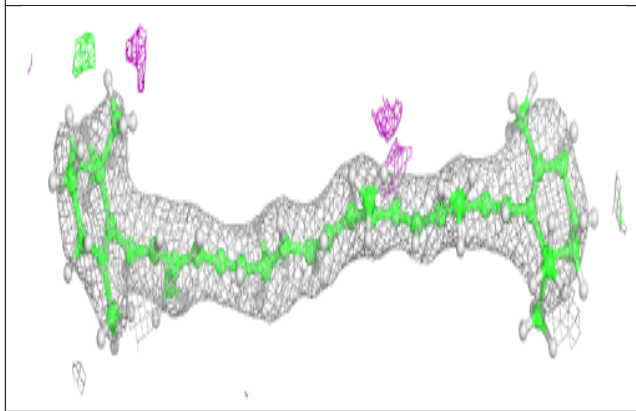
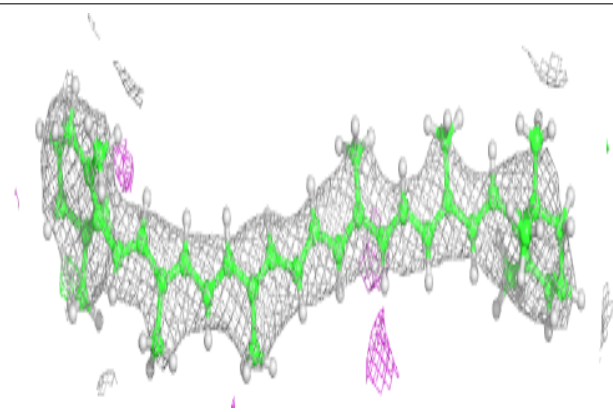


**Electron density around CLA d 403:**

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

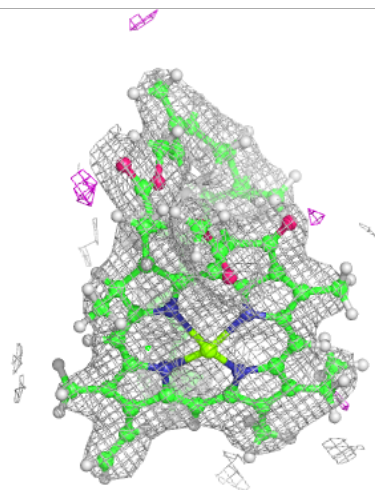
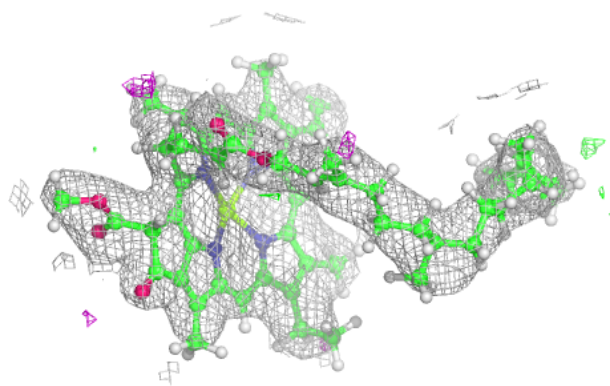
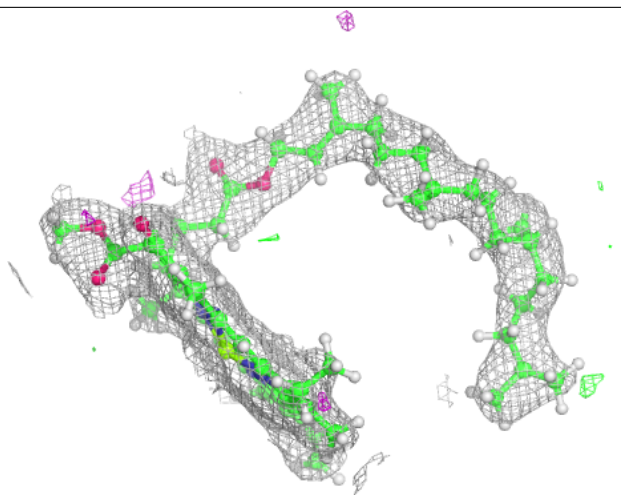
**Electron density around BCR c 515:**

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



**Electron density around CLA b 612:**

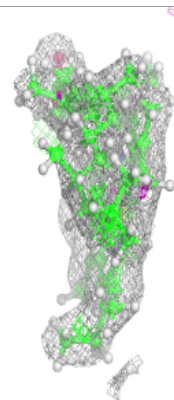
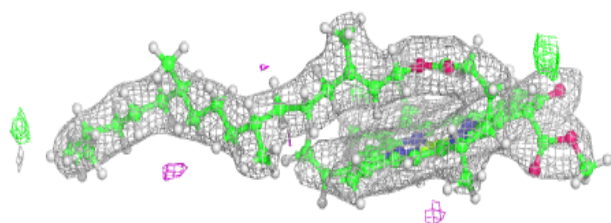
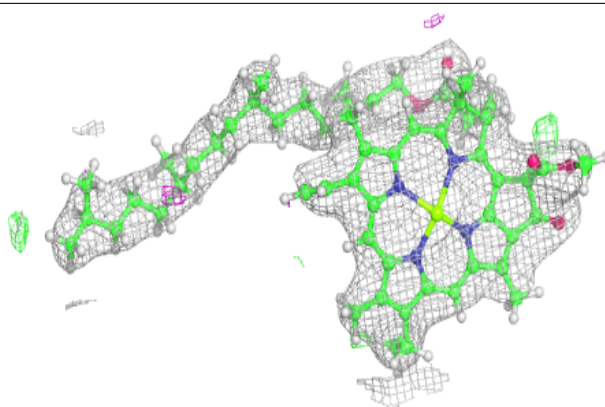
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



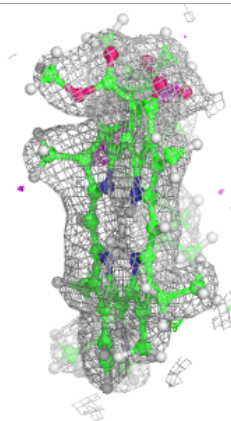
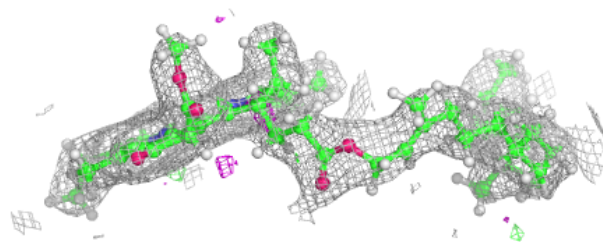
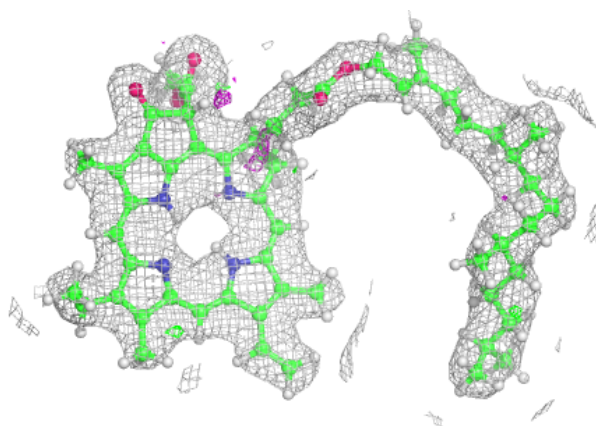


**Electron density around CLA C 501:**

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

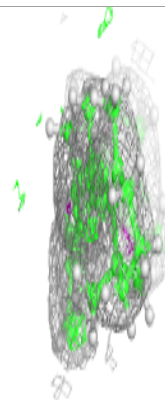
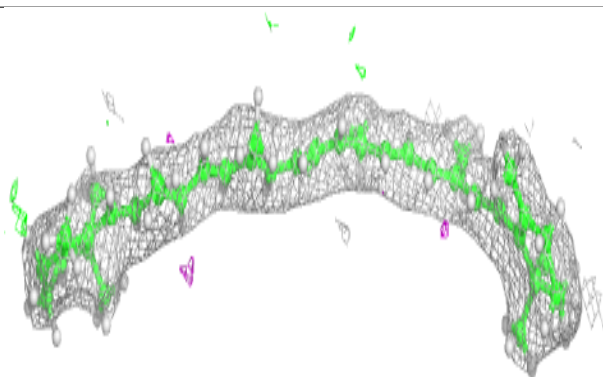
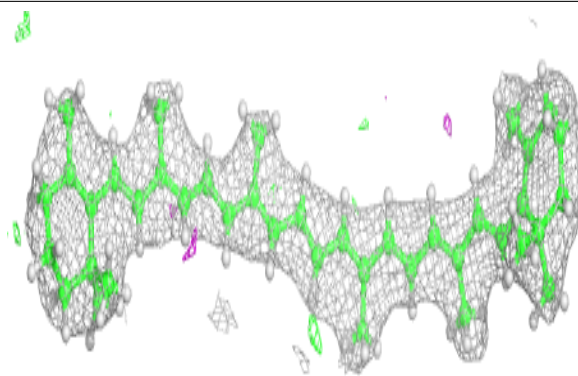
**Electron density around PHO A 406:**

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



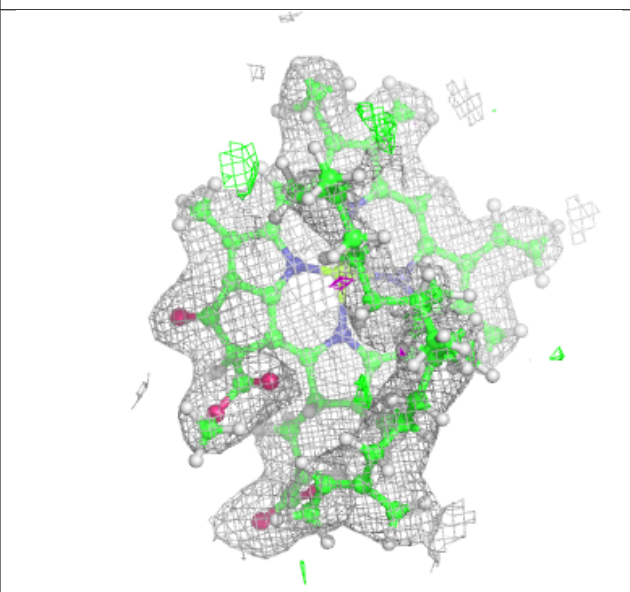
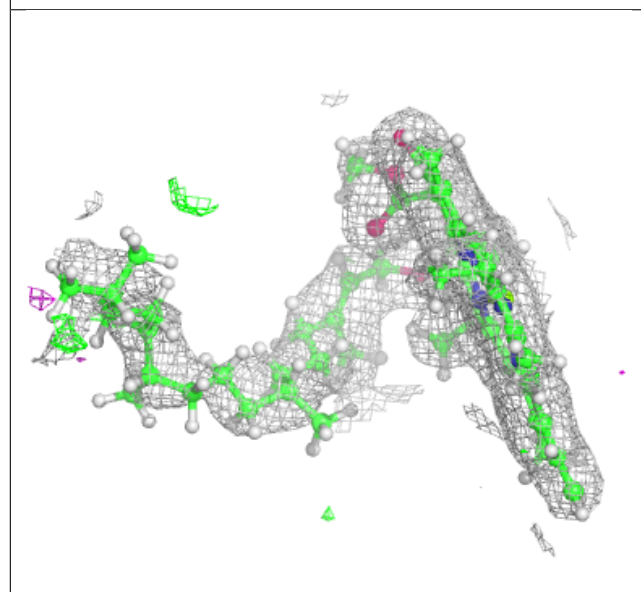
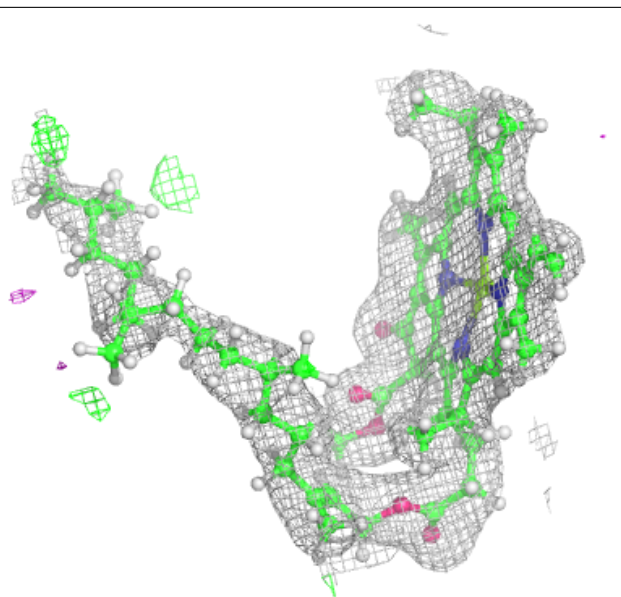
**Electron density around BCR t 101:**

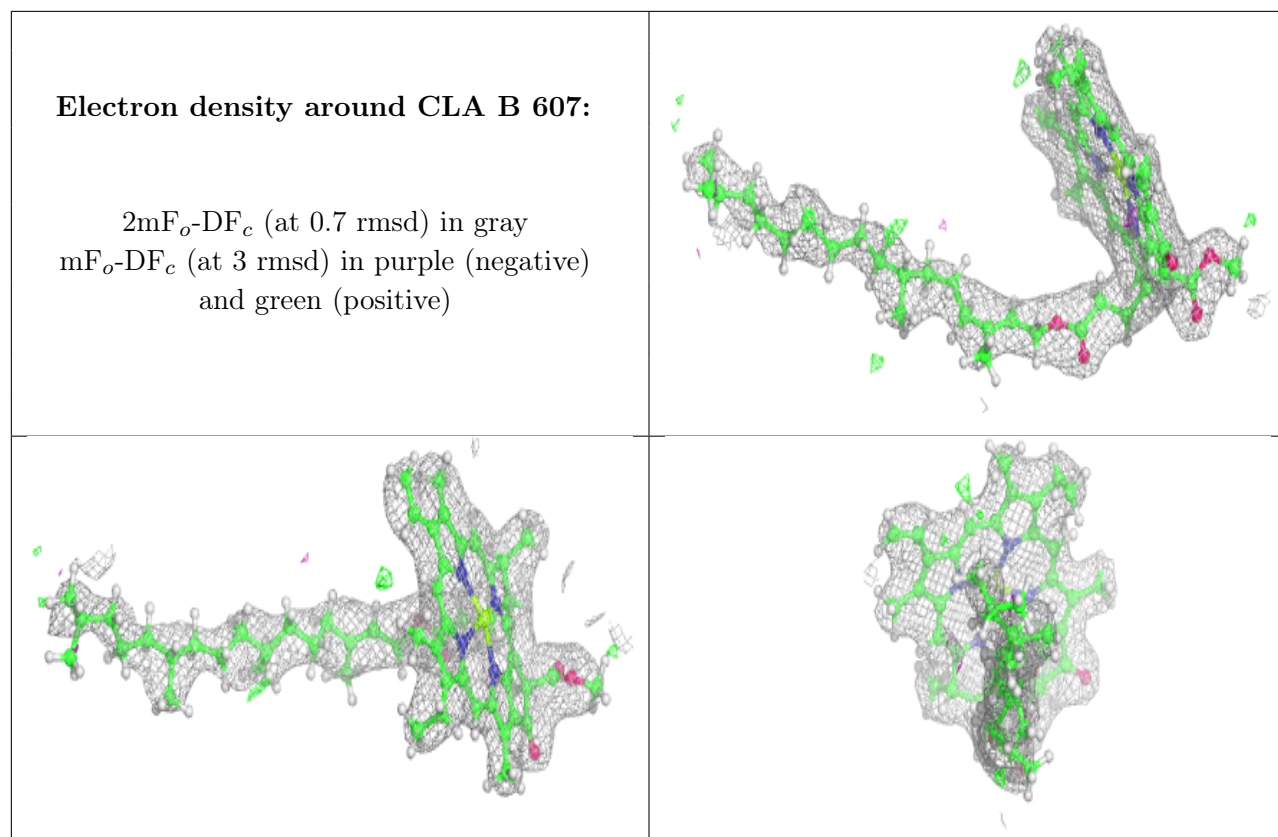
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA b 614:**

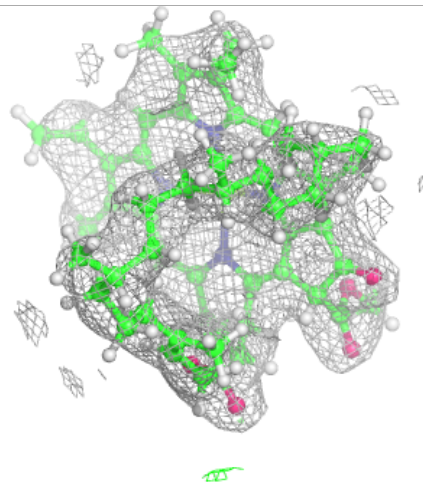
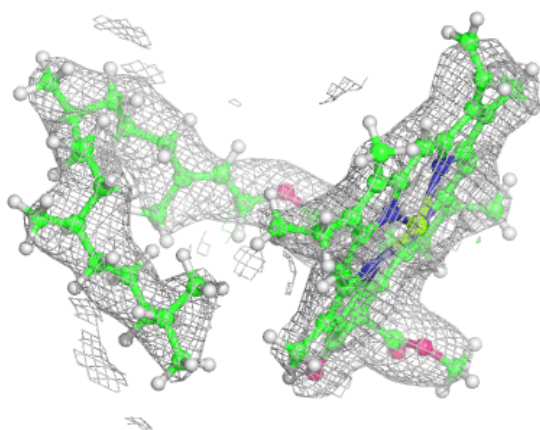
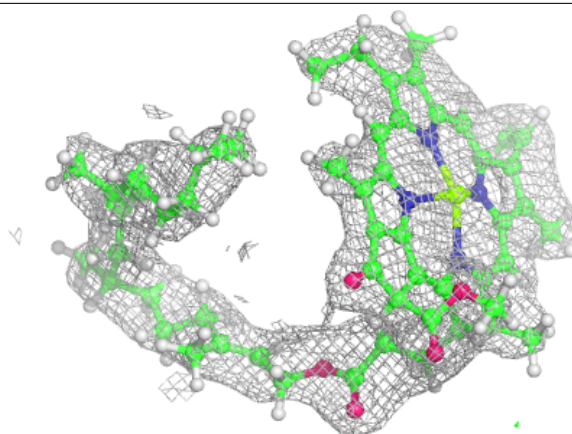
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





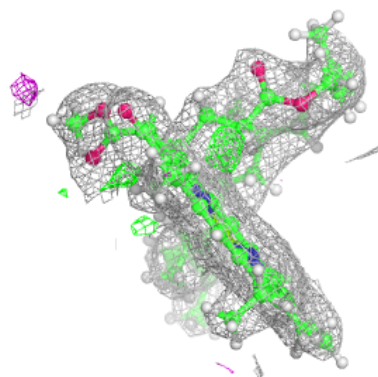
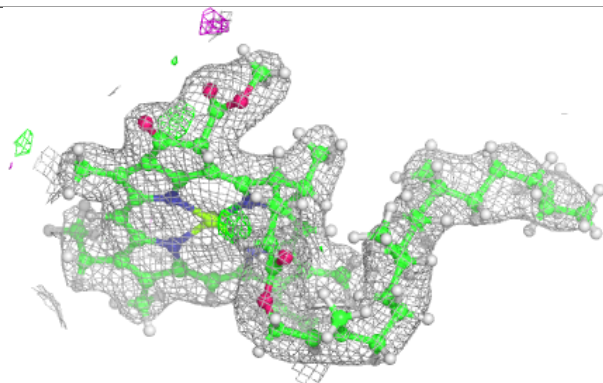
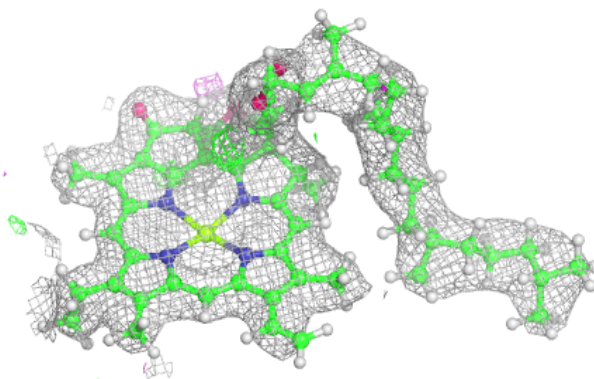
**Electron density around CLA C 503:**

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

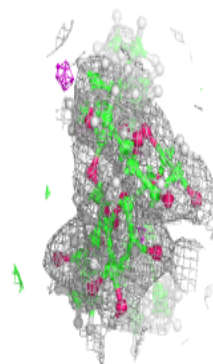
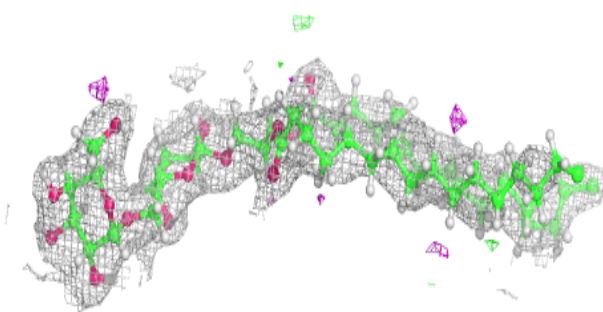
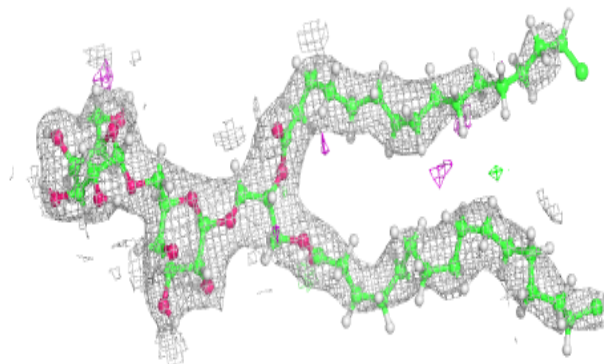


**Electron density around CLA D 402:**

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

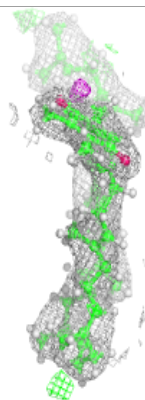
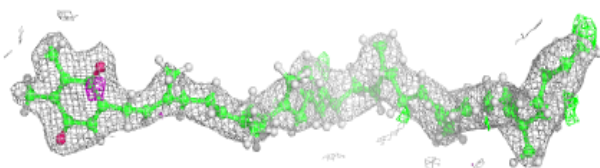
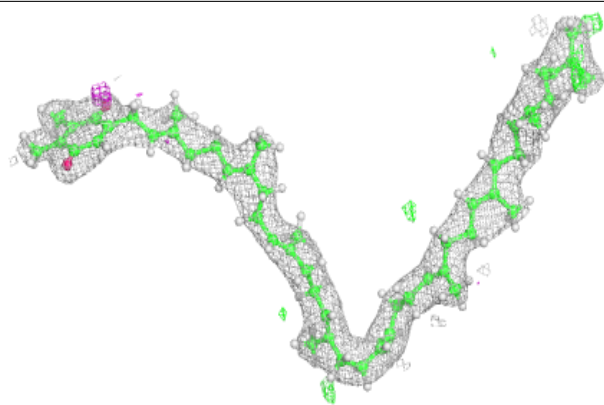
**Electron density around DGD C 518:**

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

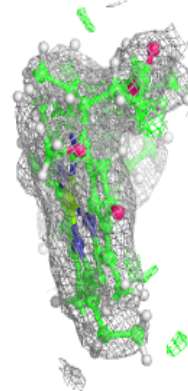
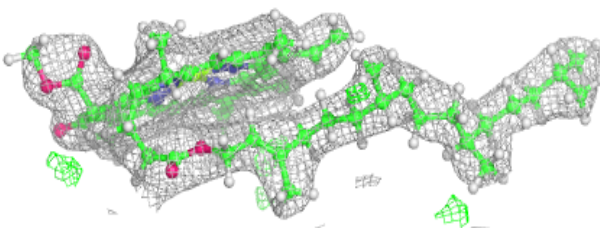
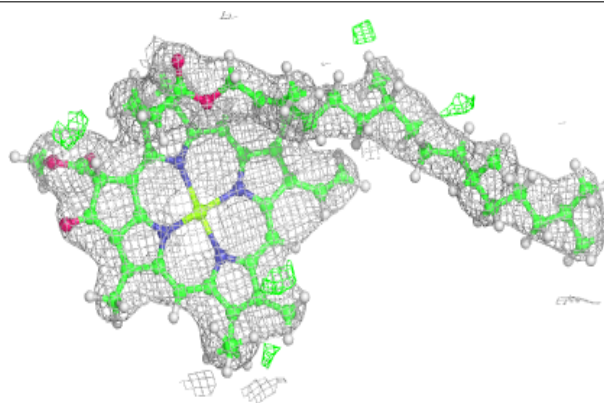


**Electron density around PL9 d 406:**

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

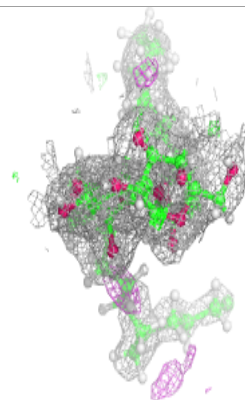
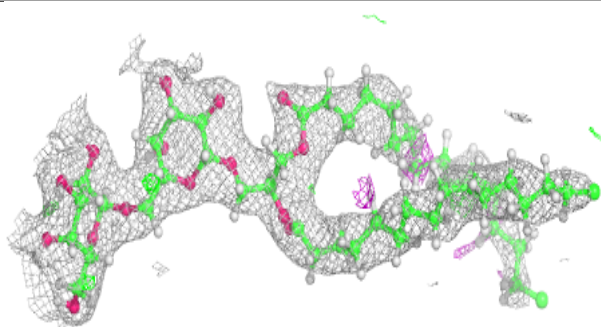
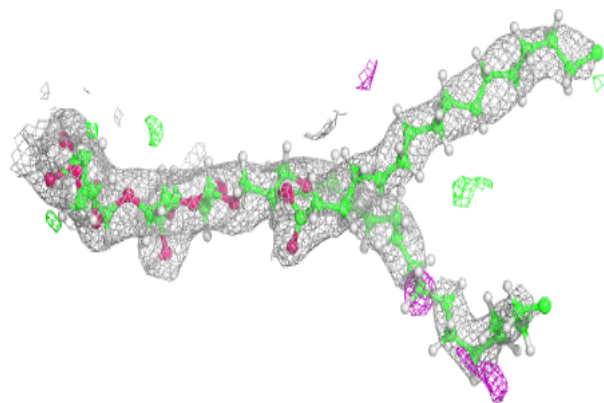
**Electron density around CLA c 501:**

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

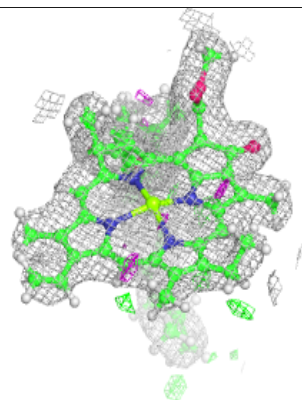
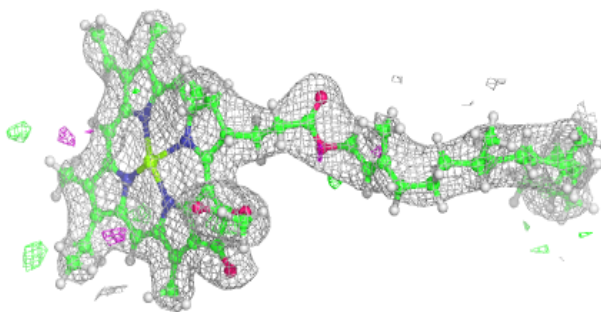
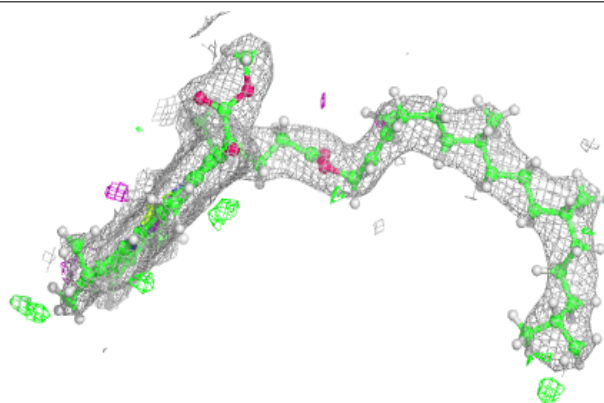


**Electron density around DGD c 516:**

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

**Electron density around CLA D 403:**

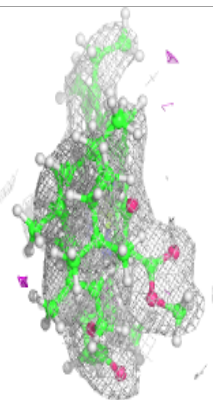
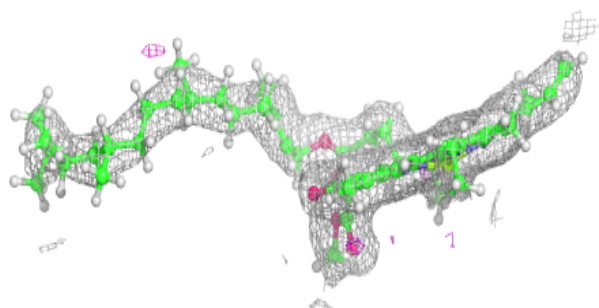
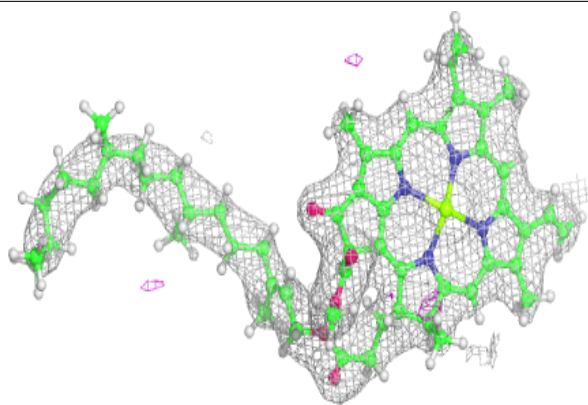
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



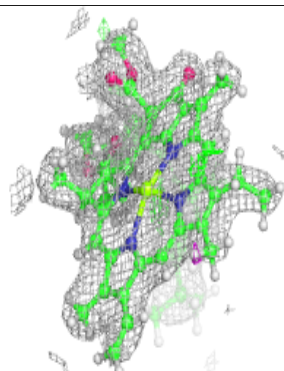
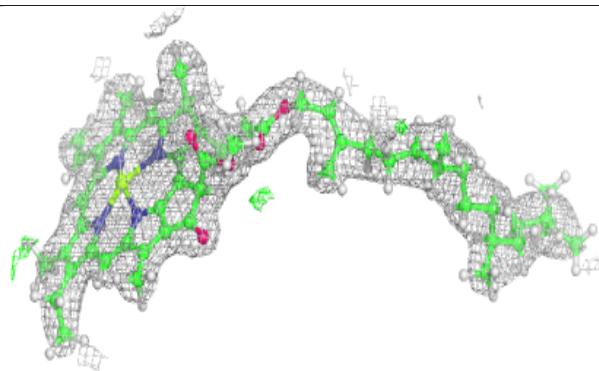
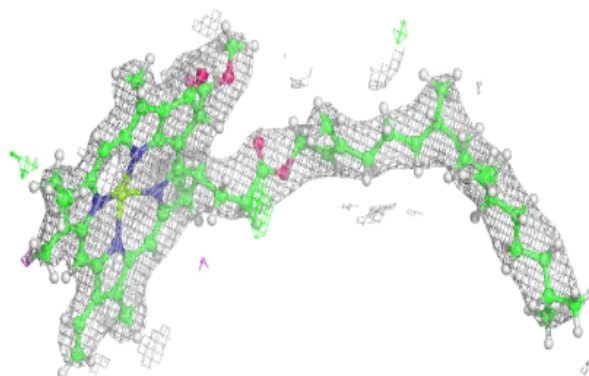


**Electron density around CLA B 602:**

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

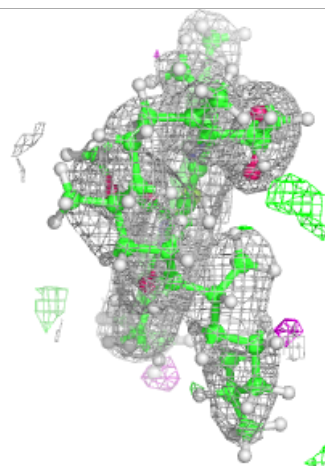
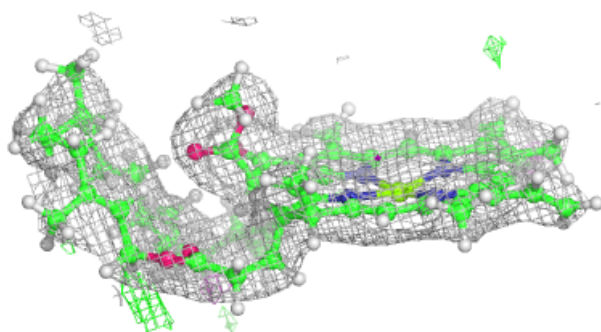
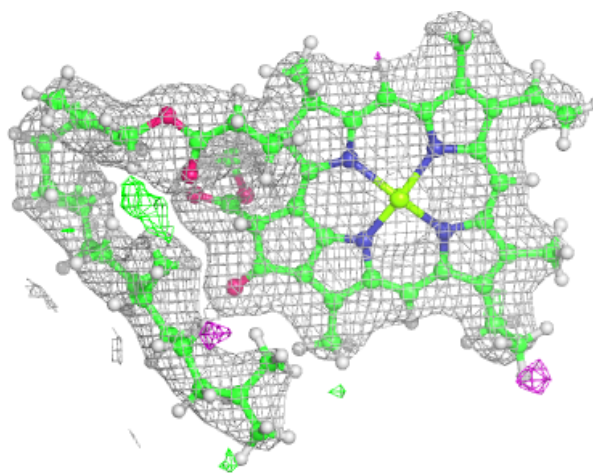
**Electron density around CLA a 404:**

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



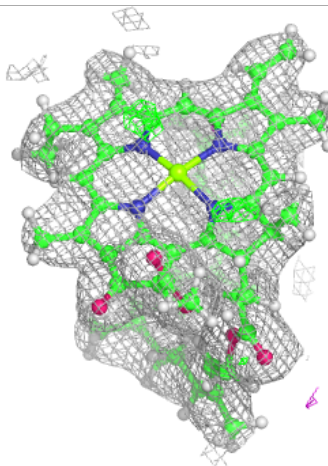
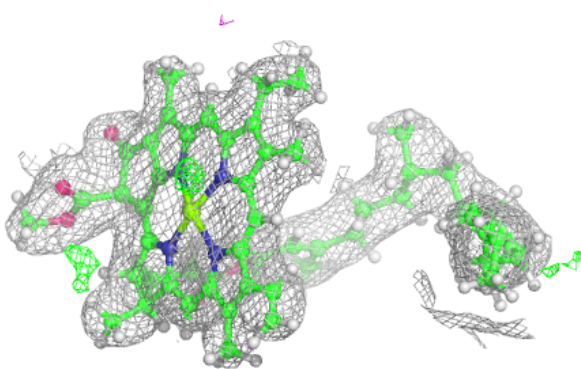
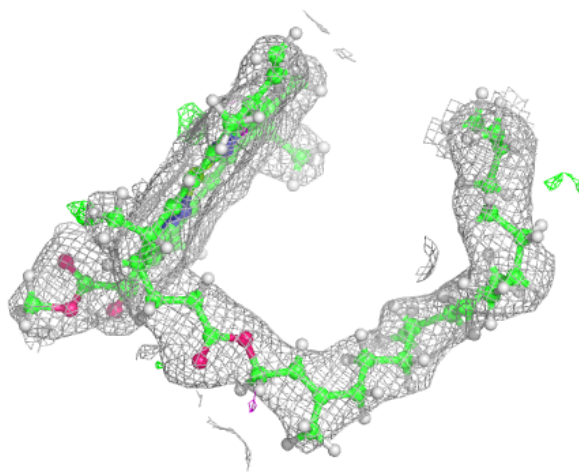
**Electron density around CLA B 610:**

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



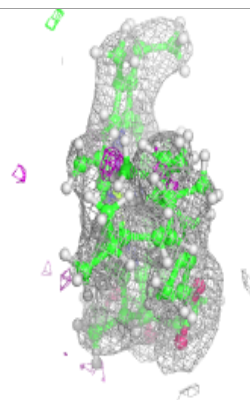
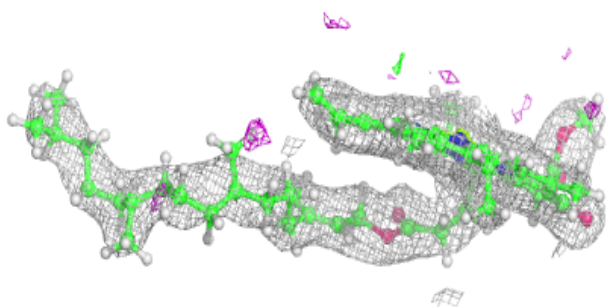
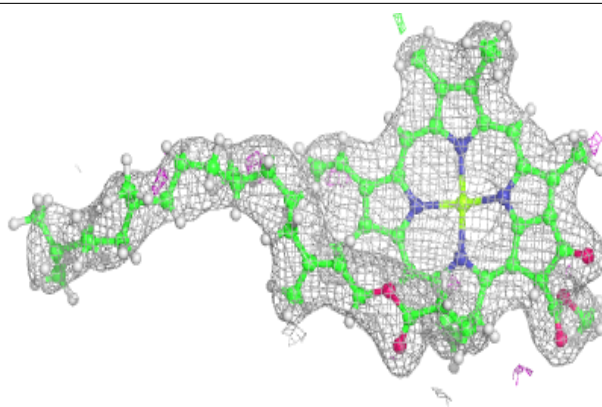
**Electron density around CLA B 611:**

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

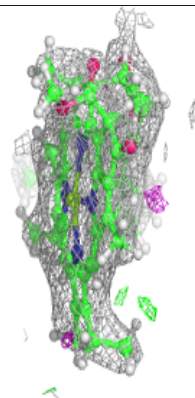
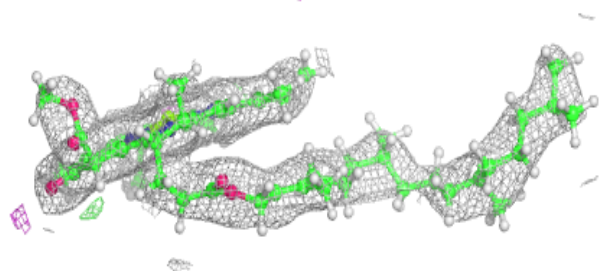
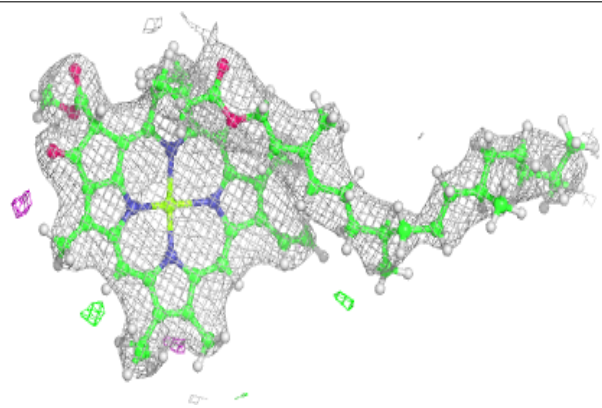


**Electron density around CLA B 603:**

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

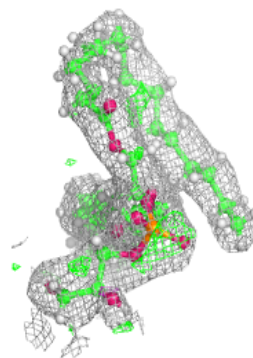
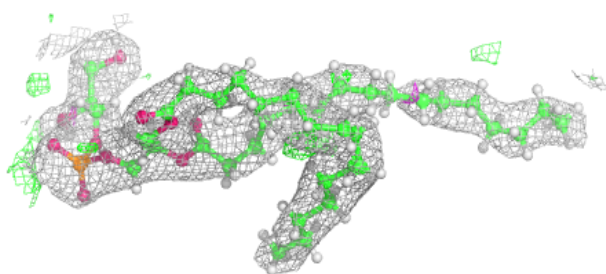
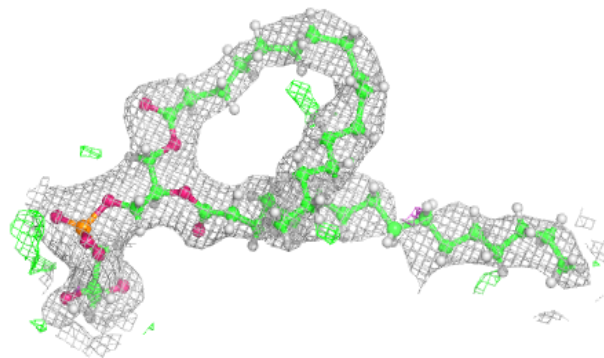
**Electron density around CLA b 604:**

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

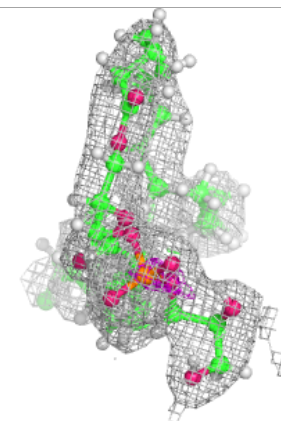
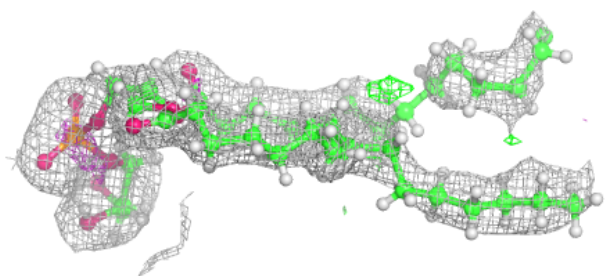
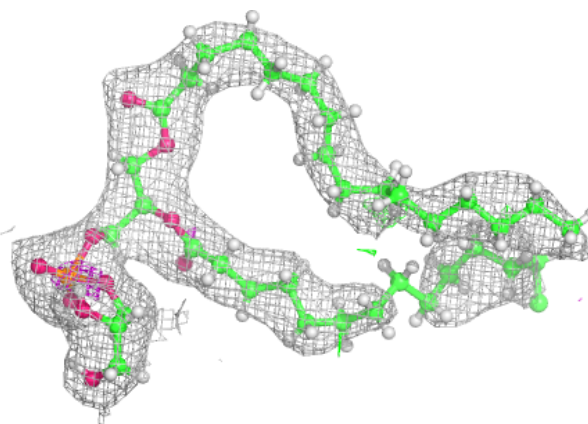


**Electron density around LHG B 622:**

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

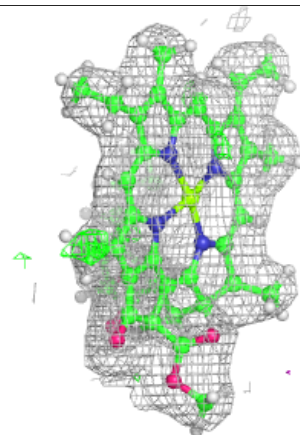
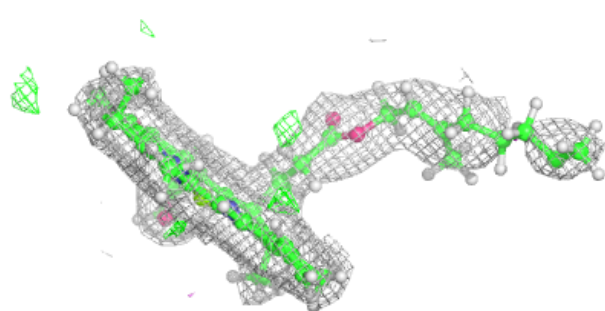
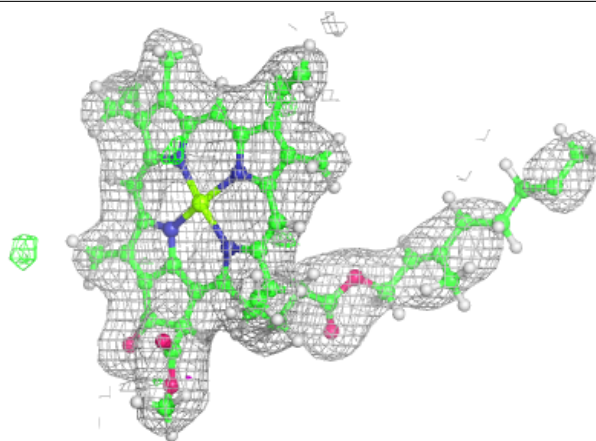
**Electron density around LHG D 409:**

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

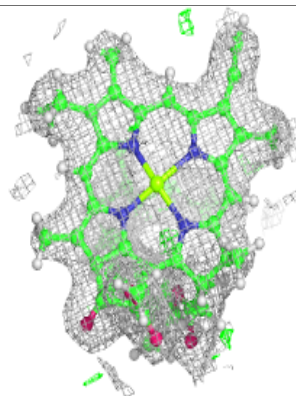
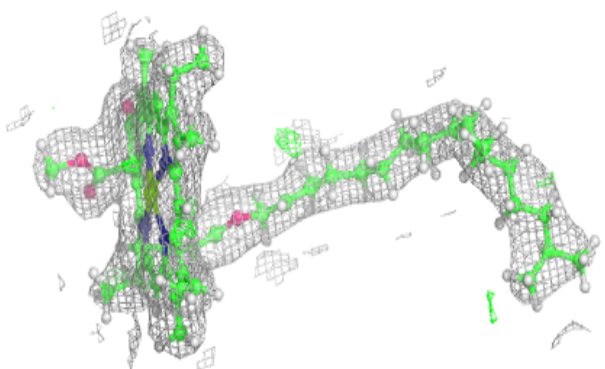
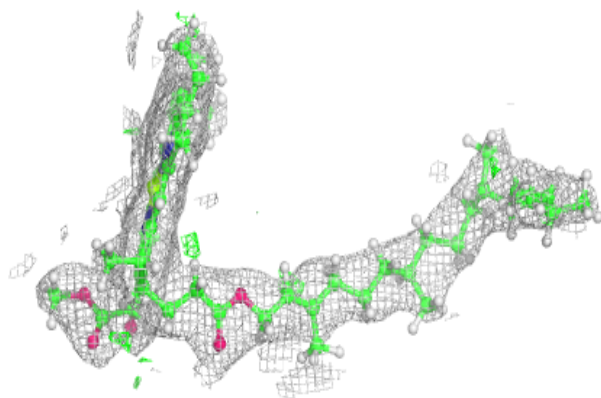


**Electron density around CLA A 407:**

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

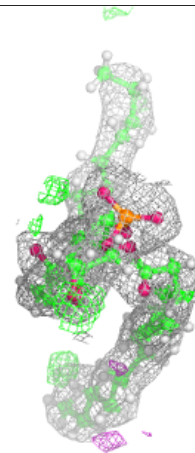
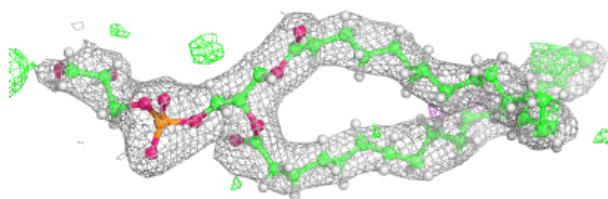
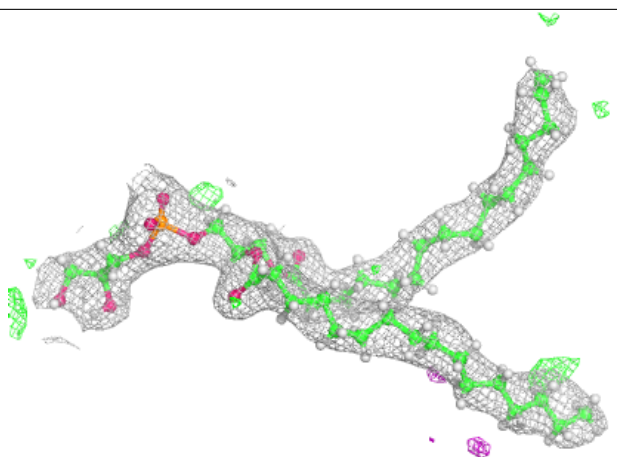
**Electron density around CLA B 605:**

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

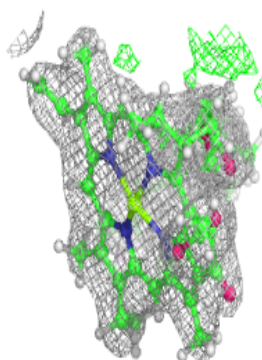
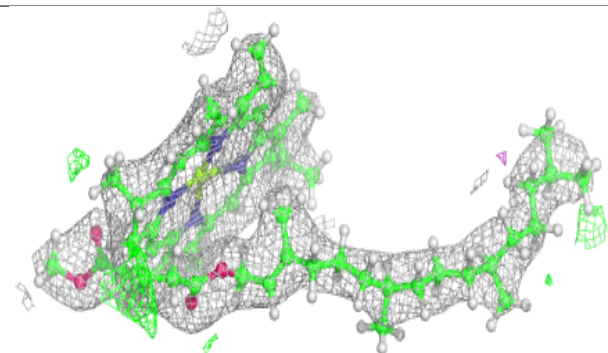
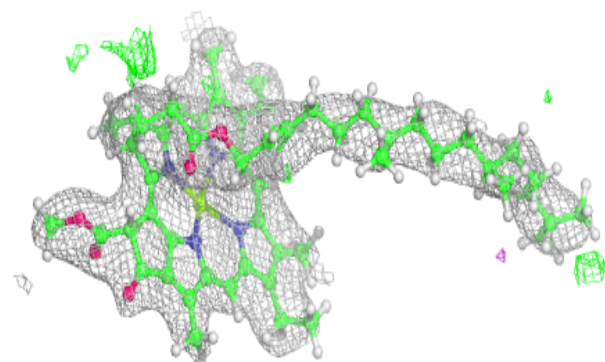


**Electron density around LHG d 407:**

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

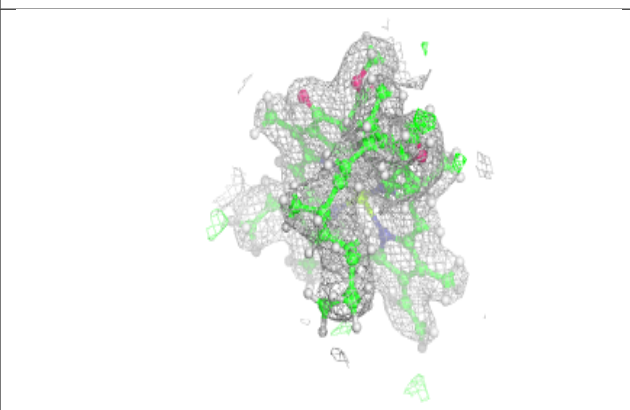
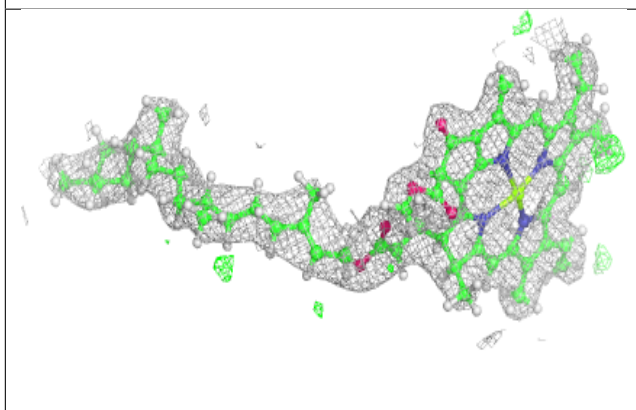
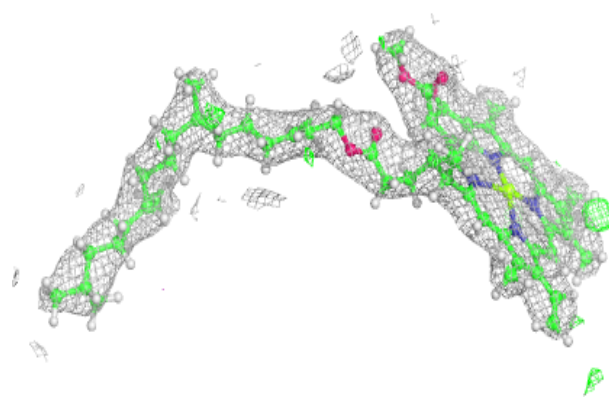
**Electron density around CLA b 609:**

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

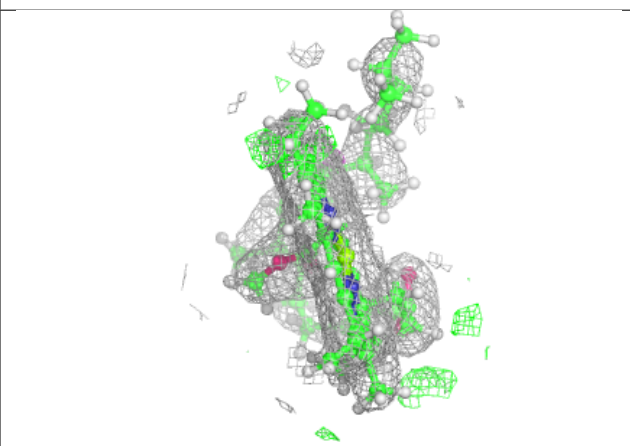
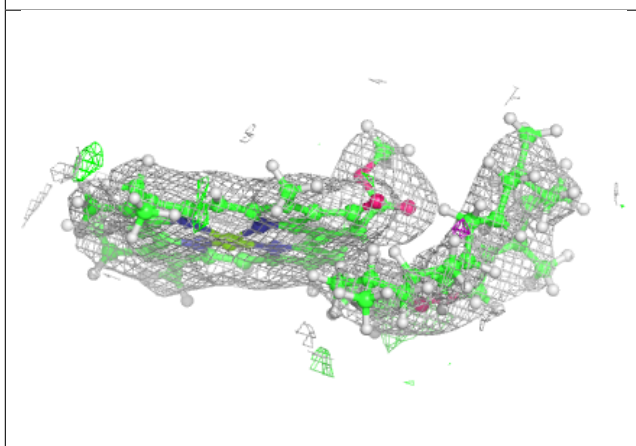
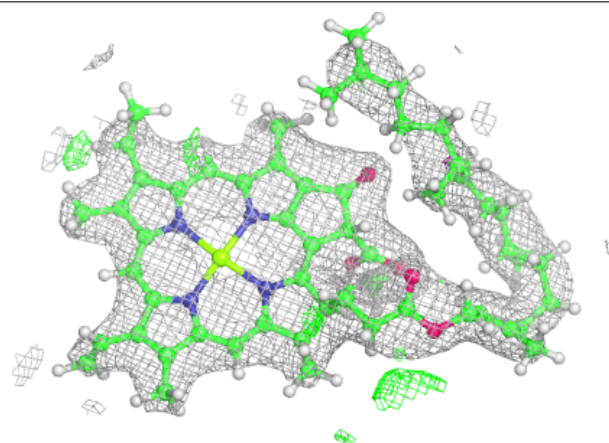


**Electron density around CLA A 404:**

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

**Electron density around CLA b 611:**

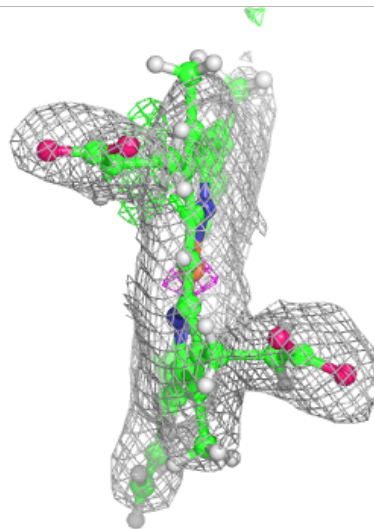
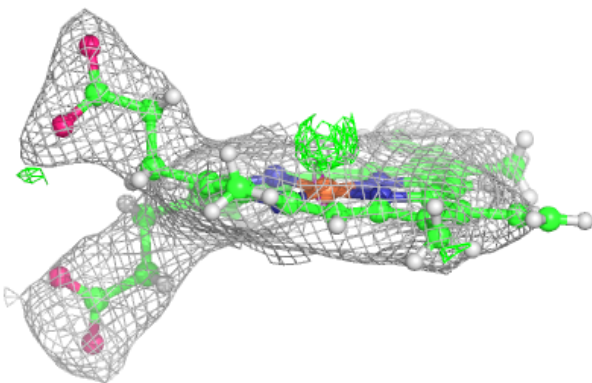
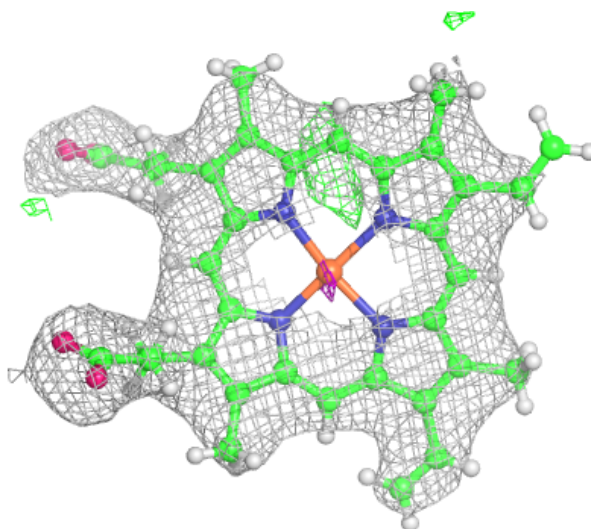
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





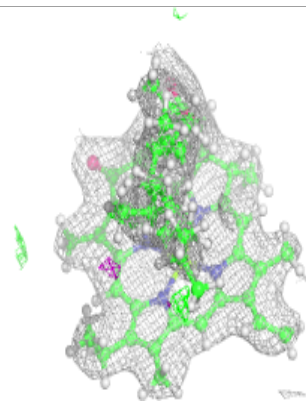
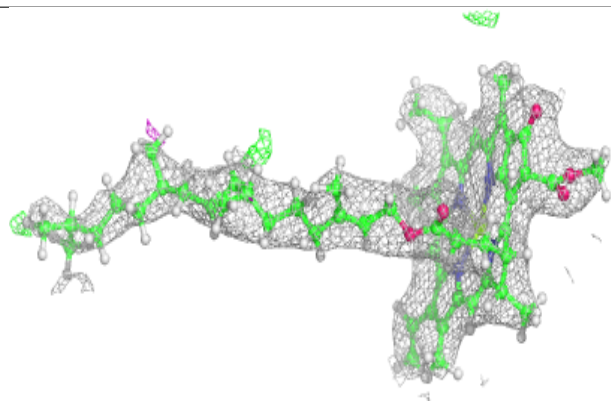
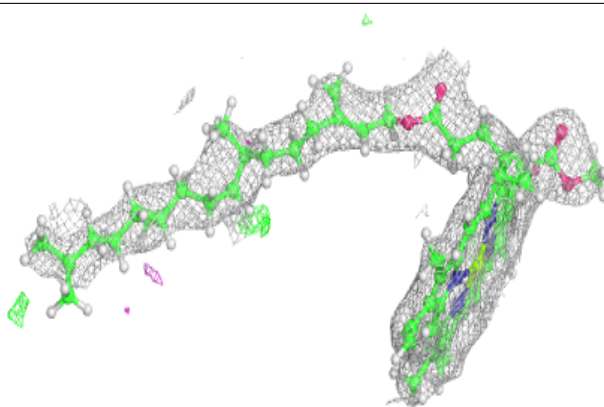
**Electron density around HEM E 102:**

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



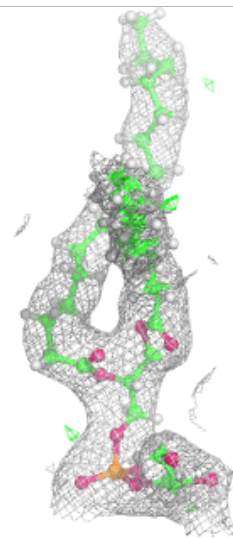
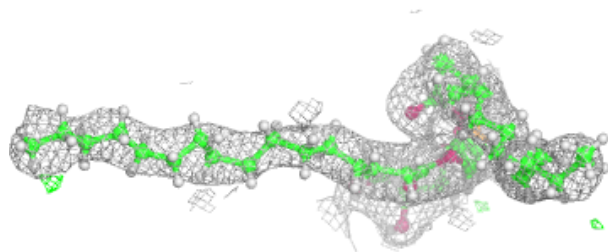
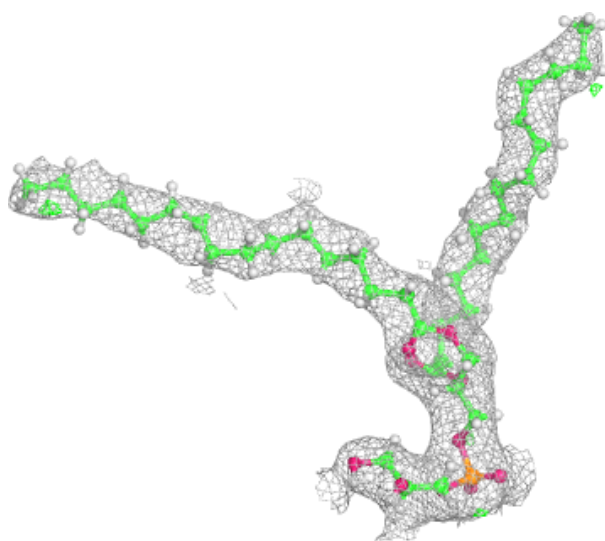
**Electron density around CLA b 608:**

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



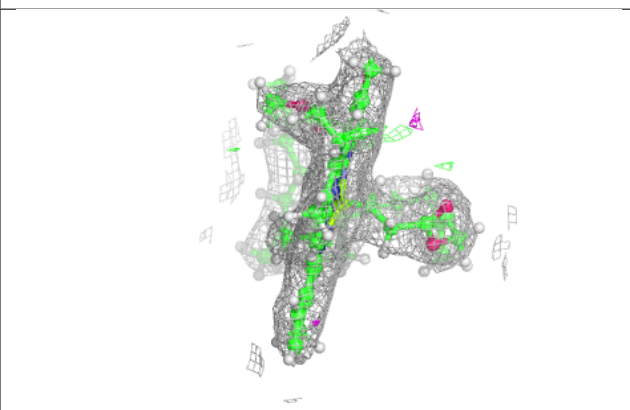
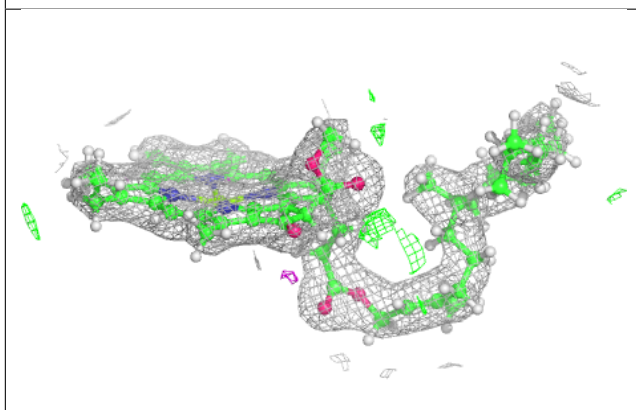
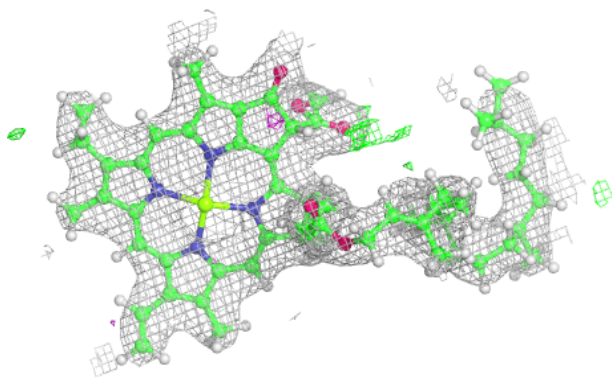
**Electron density around LHG L 101:**

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

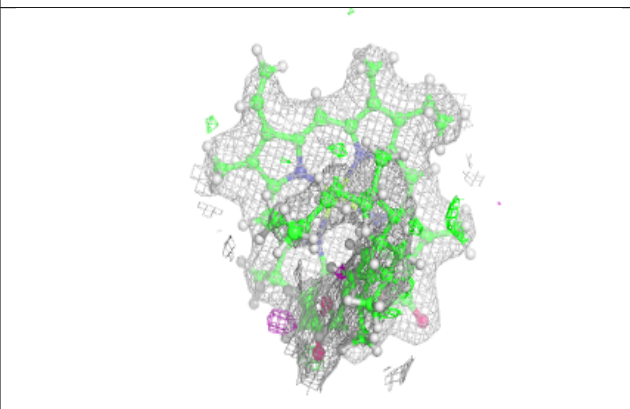
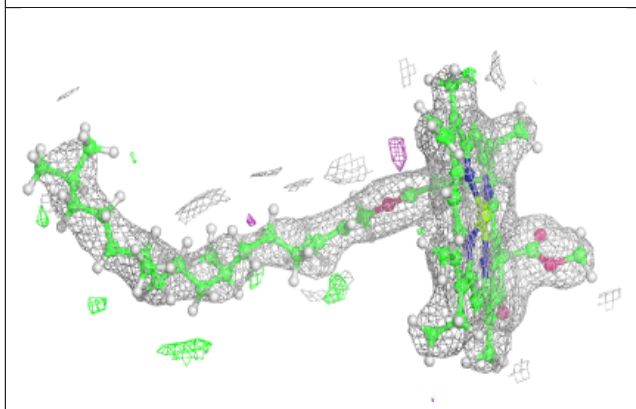
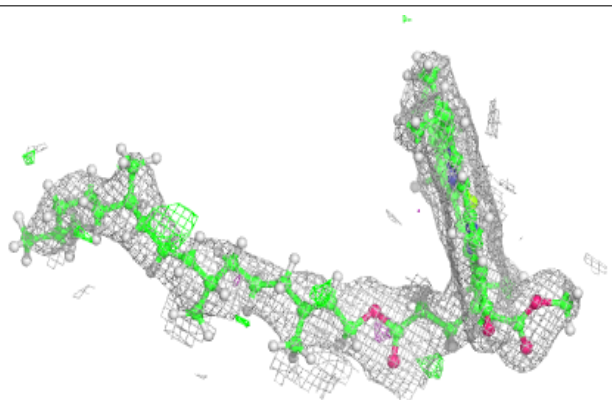


**Electron density around CLA B 612:**

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

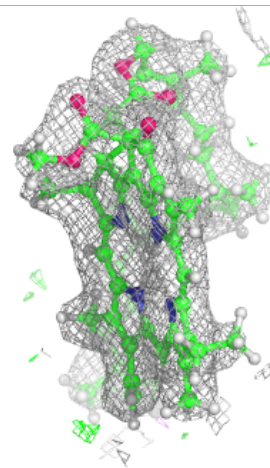
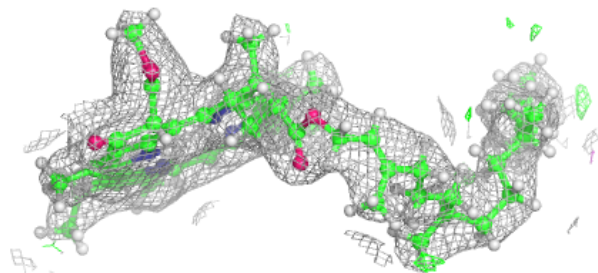
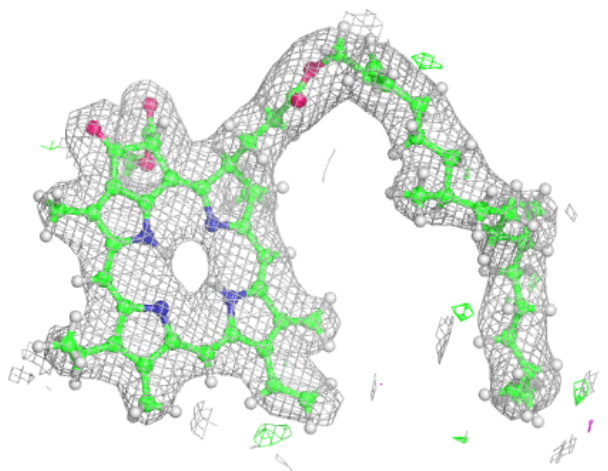
**Electron density around CLA b 606:**

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



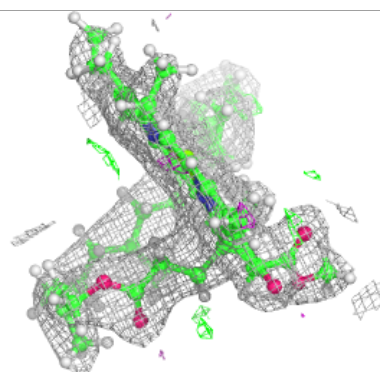
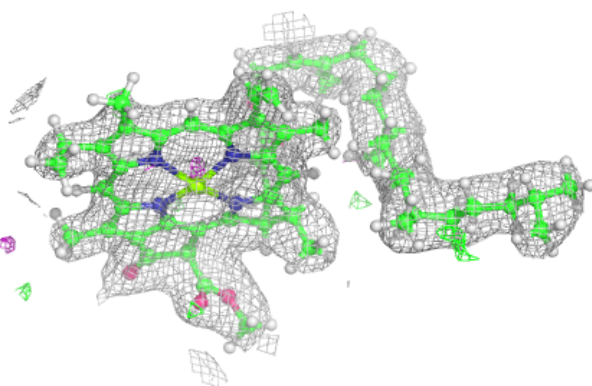
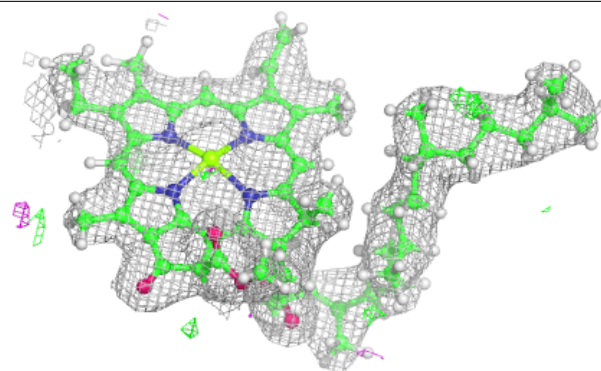
**Electron density around PHO D 401:**

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

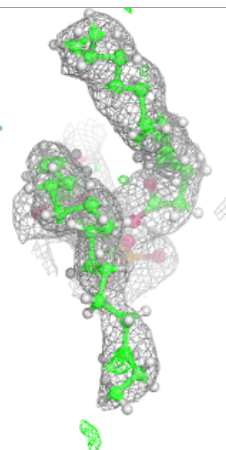
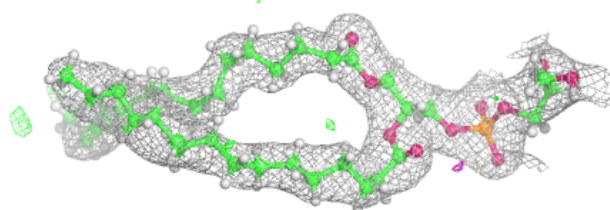
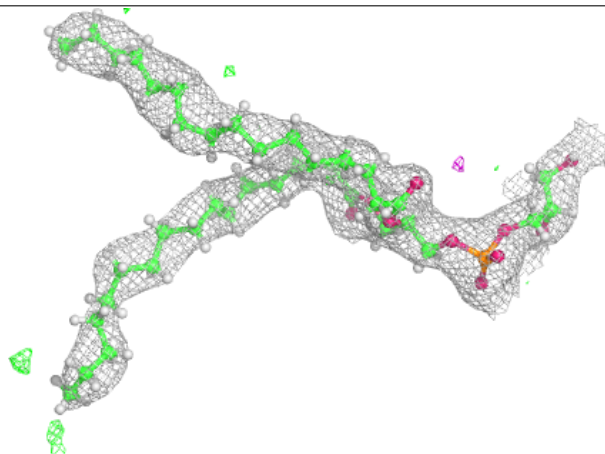


**Electron density around CLA d 402:**

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

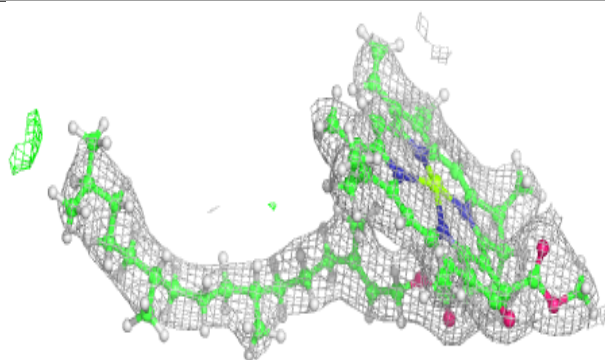
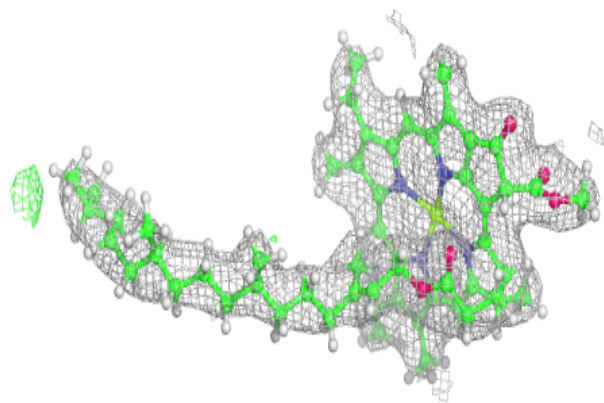
**Electron density around LHG D 408:**

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



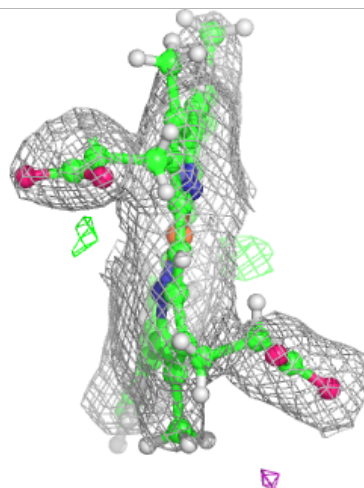
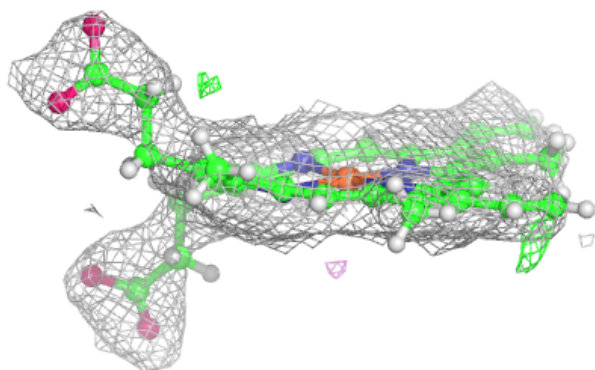
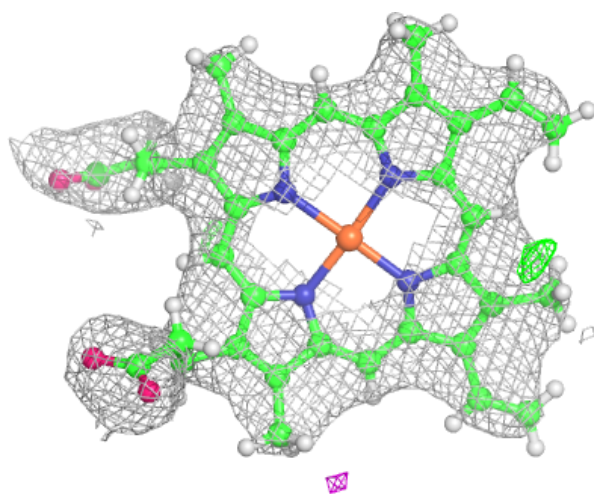
**Electron density around CLA B 608:**

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

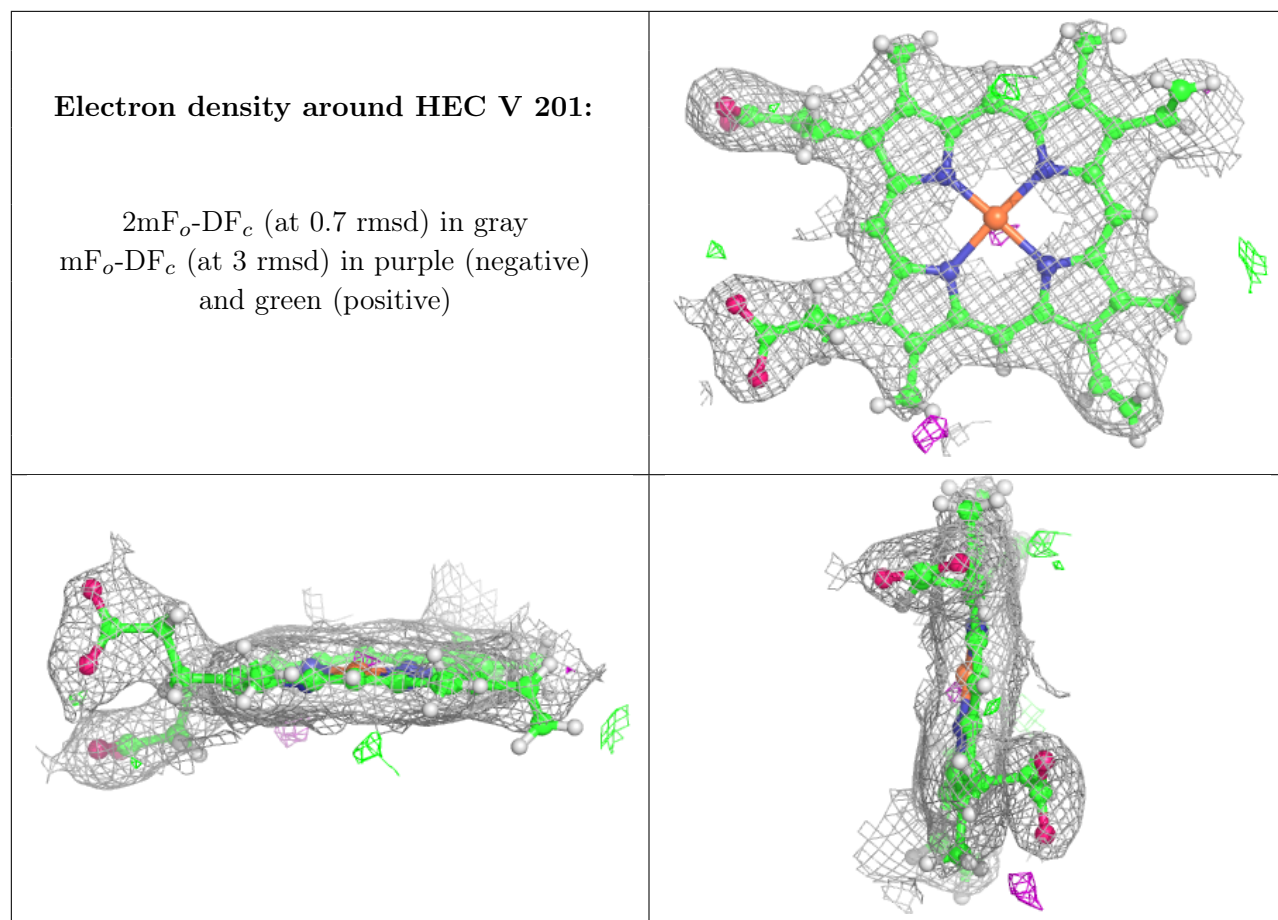


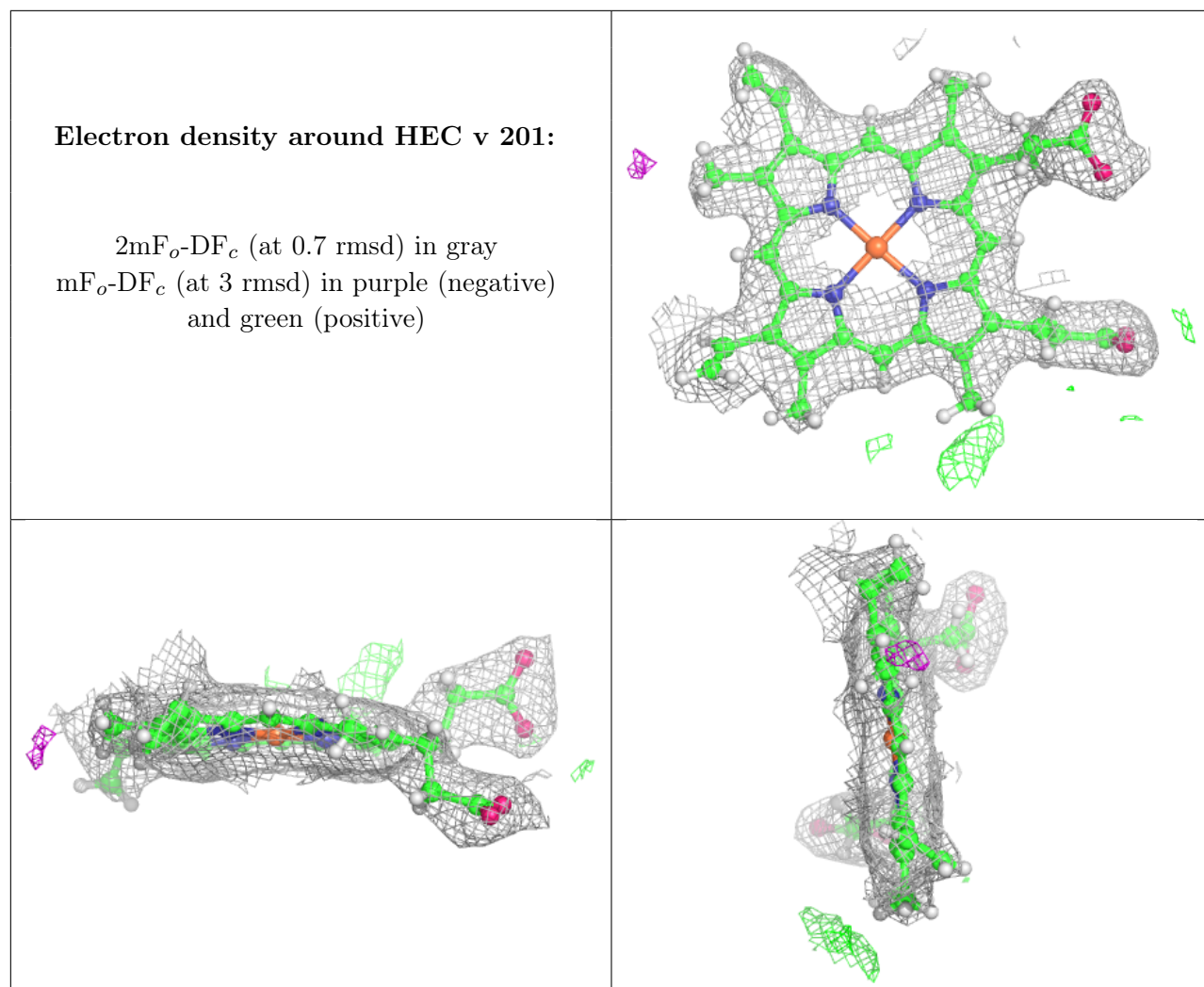
**Electron density around HEM e 102:**

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









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

There are no such residues in this entry.