



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 06:31 AM EST

PDB ID : 6DHG
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.5 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 : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36

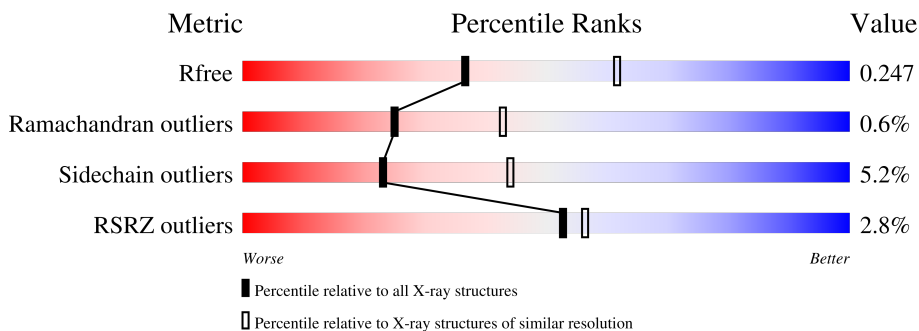
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

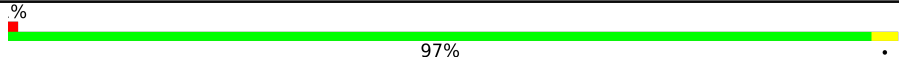
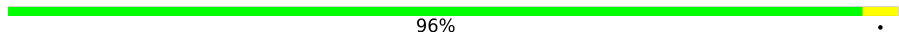
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

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

Continued on next page...

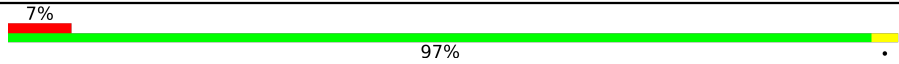
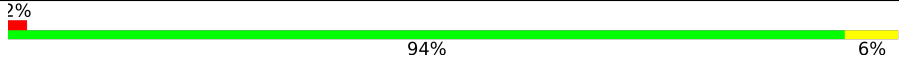
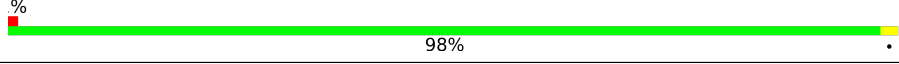
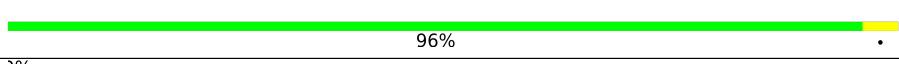
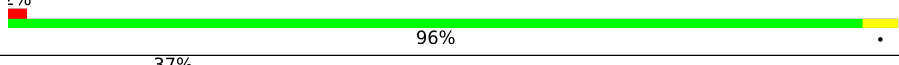
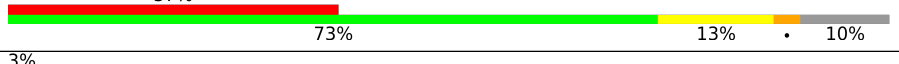
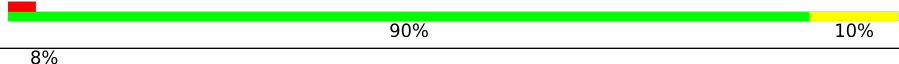
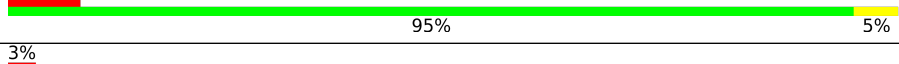
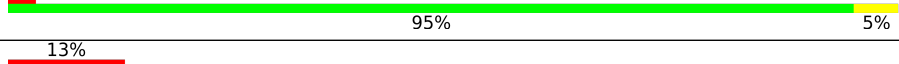




buster-report : 1.1.7 (2018)
 Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
 Refmac : 5.8.0158
 CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	505	96%
2	b	505	97%
3	C	451	96%
3	c	451	96%
4	D	341	98%
4	d	341	98%
5	E	82	88% 11%
5	e	82	93% 7%
6	F	34	100%
6	f	34	94% 6%
7	H	65	91% 9%
7	h	65	91% 6%
8	I	36	86% 14%
8	i	36	94% 6%
9	J	36	94% 6%
9	j	36	94% 6%
10	K	37	86% 14%
10	k	37	89% 11%
11	L	37	100%
11	l	37	89% 5%
12	M	33	88% 12%
12	m	33	88% 9%
13	O	244	90% 10%
13	o	244	92% 7%
14	T	30	87% 13%

Continued on next page...

Continued from previous page...

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	405	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	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	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	508	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	C	514	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	602	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	609	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	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
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	511	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	404	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103658 atoms, of which 51467 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			

Continued on next page...

Continued from previous page...

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
			450	144	232	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			

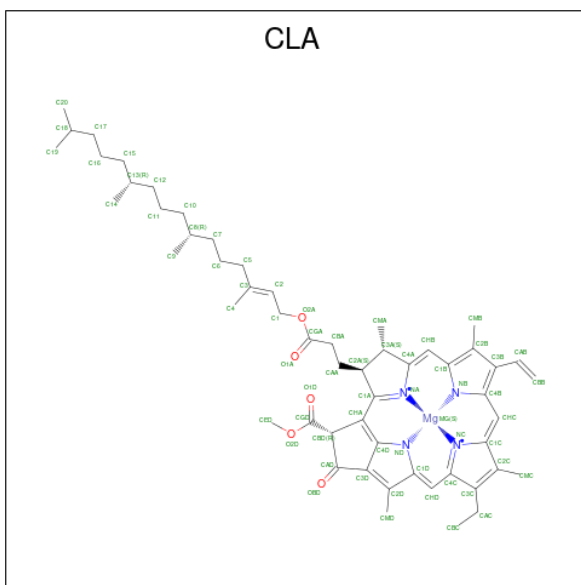
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

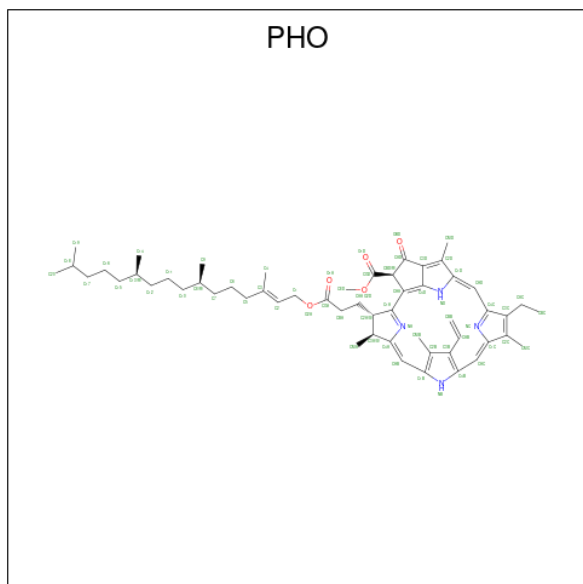
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total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

Continued on next page...

Continued from previous page...

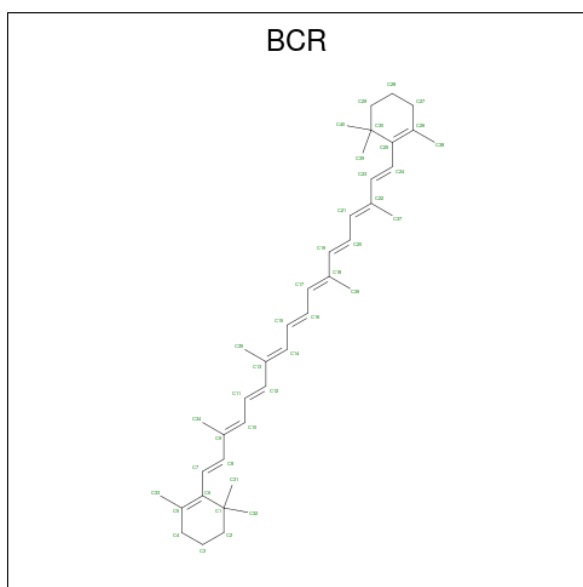
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
23	d	1	137	55	72	1	4	5	0	0

- 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: $C_{40}H_{56}$).



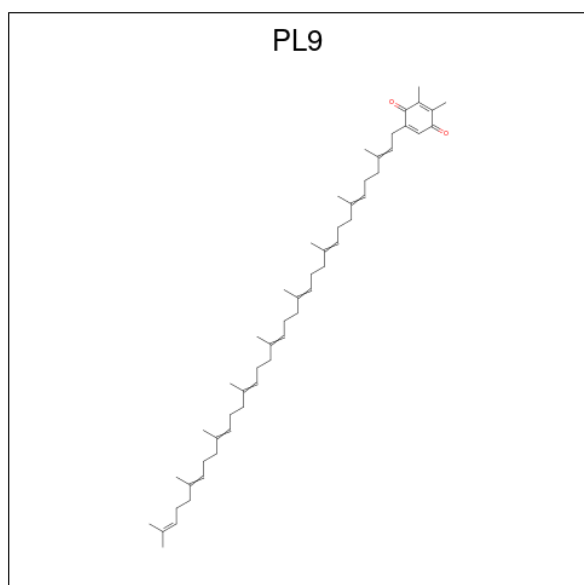
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total	C	H	0	0
			96	40	56		
25	H	1	Total	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	Z	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		

Continued on next page...

Continued from previous page...

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	k	1	96	40	56	0	0
25	t	1	96	40	56	0	0
25	x	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: $C_{53}H_{80}O_2$).



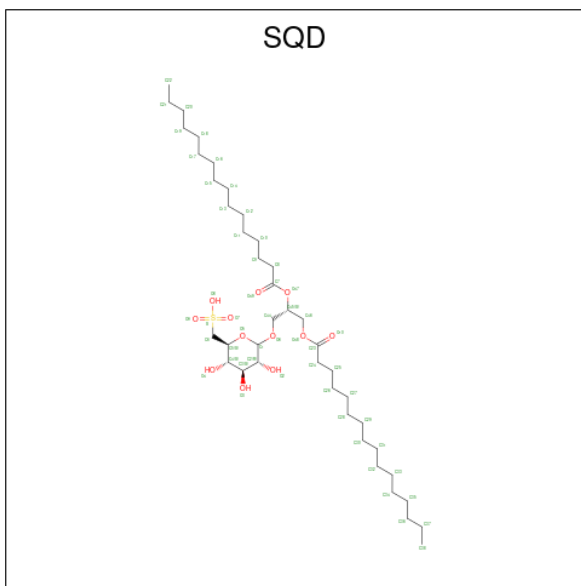
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	A	1	135	53	80	2	0	0
26	D	1	135	53	80	2	0	0

Continued on next page...

Continued from previous page...

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

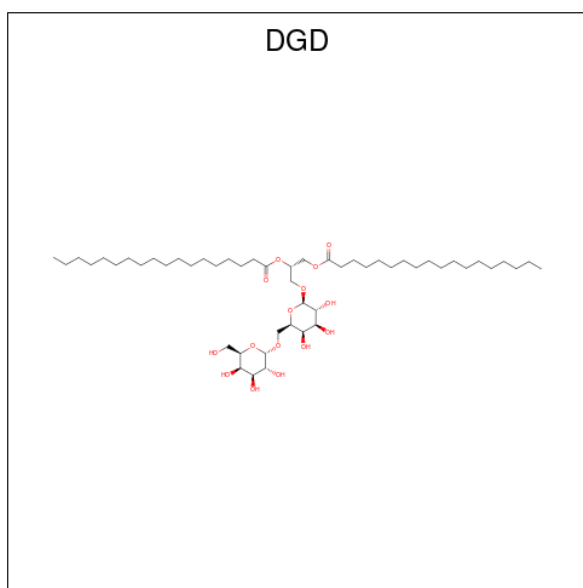
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	a	1	Total	C	H	O		0	0
			92	31	56	5			
27	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

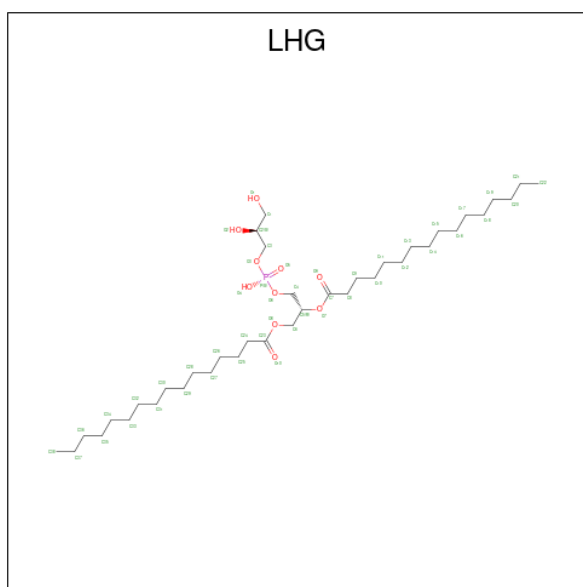
- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: $C_{51}H_{96}O_{15}$).



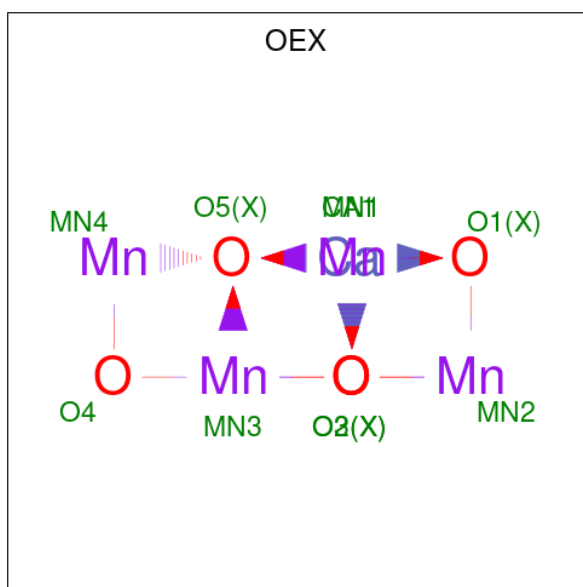
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			162	51	96	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	H	1	Total	C	H	O	0	0
			144	47	82	15		
28	a	1	Total	C	H	O	0	0
			119	39	75	5		
28	c	1	Total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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



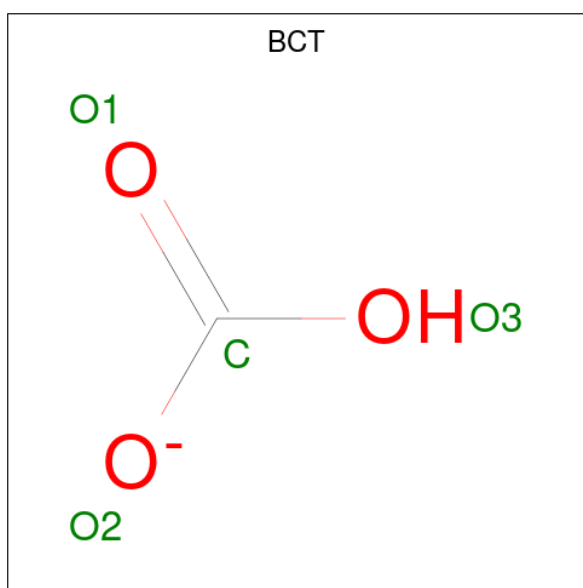
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
29	A	1	Total 123	C 38	H 74	O 10	P 1	0	0
29	D	1	Total 123	C 38	H 74	O 10	P 1	0	0
29	D	1	Total 114	C 36	H 67	O 10	P 1	0	0
29	E	1	Total 123	C 38	H 74	O 10	P 1	0	0
29	L	1	Total 123	C 38	H 74	O 10	P 1	0	0
29	d	1	Total 123	C 38	H 74	O 10	P 1	0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

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

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

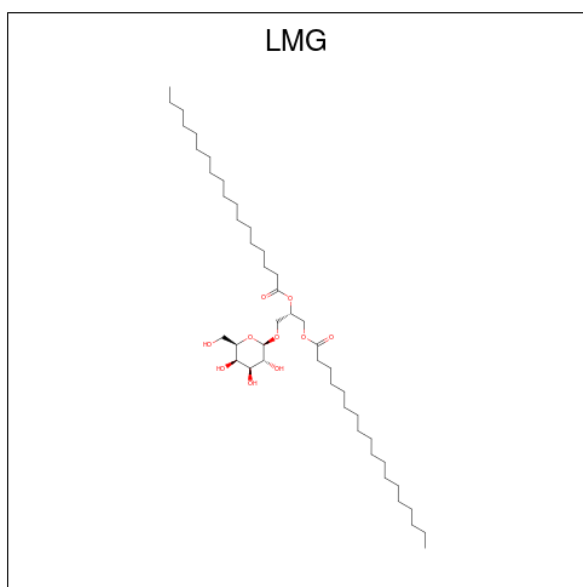


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
31	A	1	5	1	1	3	0	0
31	a	1	5	1	1	3	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	6	Total	C	H	O	0	0
			226	79	137	10		
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
			47	16	31			
32	a	1	Total	C	H	O	0	0
			28	10	16	2		
32	b	5	Total	C	H	O	0	0
			220	75	139	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	1	Total	C	H		0	0
			26	10	16			
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

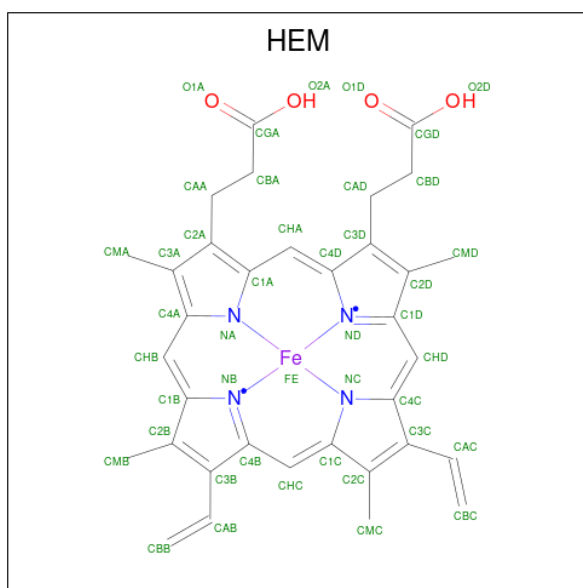
- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
33	C	1	Total 114	C 38	H 66	O 10	0	0
33	C	1	Total 114	C 38	H 66	O 10	0	0
33	D	1	Total 123	C 41	H 72	O 10	0	0
33	D	1	Total 78	C 27	H 45	O 6	0	0
33	D	1	Total 68	C 24	H 40	O 4	0	0
33	M	1	Total 123	C 41	H 72	O 10	0	0
33	b	1	Total 141	C 45	H 86	O 10	0	0
33	c	1	Total 81	C 27	H 44	O 10	0	0
33	c	1	Total 117	C 38	H 69	O 10	0	0
33	c	1	Total 117	C 39	H 68	O 10	0	0
33	d	1	Total 57	C 21	H 34	O 2	0	0
33	d	1	Total 102	C 34	H 58	O 10	0	0
33	m	1	Total 123	C 41	H 72	O 10	0	0

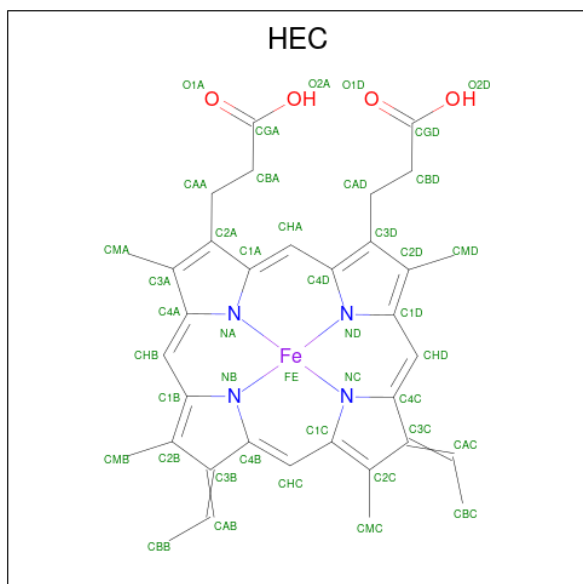
- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



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: C₃₄H₃₄FeN₄O₄).



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

Continued on next page...

Continued from previous page...

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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	136	Total 136	O 136	0	0
36	B	216	Total 216	O 216	0	0
36	C	192	Total 192	O 192	0	0
36	D	138	Total 138	O 138	0	0
36	E	30	Total 30	O 30	0	0
36	F	10	Total 10	O 10	0	0
36	H	25	Total 25	O 25	0	0
36	I	16	Total 16	O 16	0	0
36	J	13	Total 13	O 13	0	0
36	L	7	Total 7	O 7	0	0
36	M	7	Total 7	O 7	0	0
36	O	128	Total 128	O 128	0	0
36	T	11	Total 11	O 11	0	0
36	U	47	Total 47	O 47	0	0
36	V	73	Total 73	O 73	0	0
36	Y	6	Total 6	O 6	0	0
36	X	8	Total 8	O 8	0	0
36	Z	5	Total 5	O 5	0	0

Continued on next page...

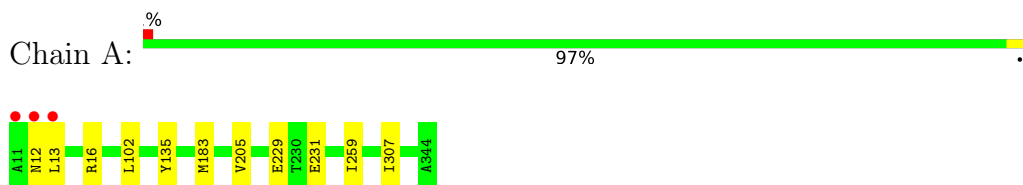
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	R	4	Total O 4 4	0	0
36	a	119	Total O 119 119	0	0
36	b	190	Total O 190 190	0	0
36	c	162	Total O 162 162	0	0
36	d	120	Total O 120 120	0	0
36	e	22	Total O 22 22	0	0
36	f	4	Total O 4 4	0	0
36	h	19	Total O 19 19	0	0
36	i	10	Total O 10 10	0	0
36	j	8	Total O 8 8	0	0
36	k	5	Total O 5 5	0	0
36	l	11	Total O 11 11	0	0
36	m	5	Total O 5 5	0	0
36	o	113	Total O 113 113	0	0
36	t	11	Total O 11 11	0	0
36	u	54	Total O 54 54	0	0
36	v	64	Total O 64 64	0	0
36	y	4	Total O 4 4	0	0
36	x	13	Total O 13 13	0	0
36	z	1	Total O 1 1	0	0
36	r	5	Total O 5 5	0	0

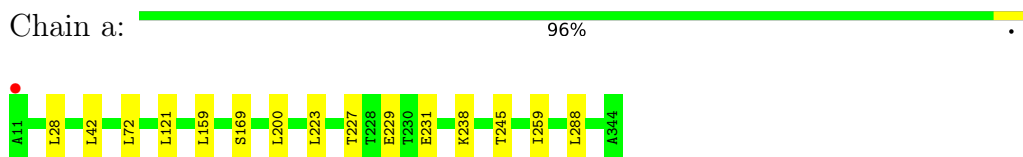
3 Residue-property plots [i](#)

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.

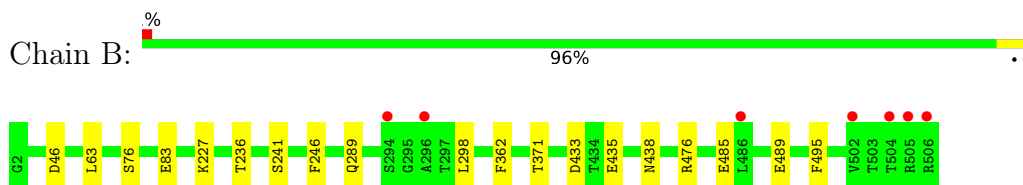
- Molecule 1: Photosystem II protein D1 1



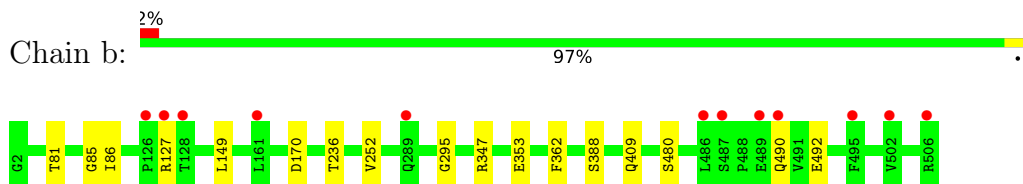
- Molecule 1: Photosystem II protein D1 1



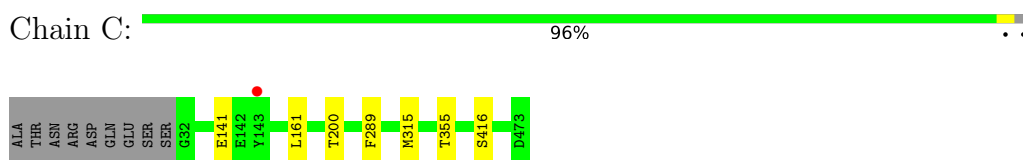
- Molecule 2: Photosystem II CP47 reaction center protein



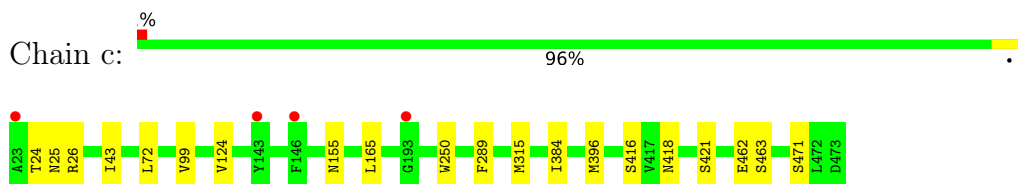
- Molecule 2: Photosystem II CP47 reaction center protein



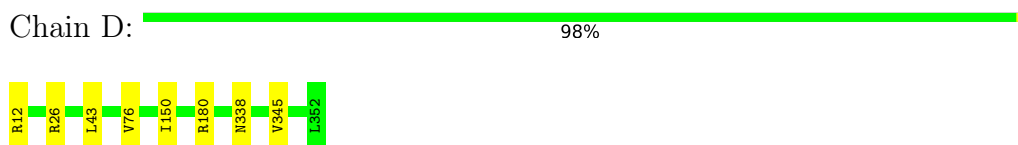
- Molecule 3: Photosystem II CP43 reaction center protein



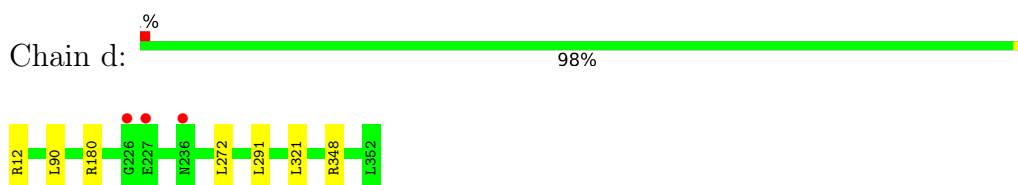
- Molecule 3: Photosystem II CP43 reaction center protein



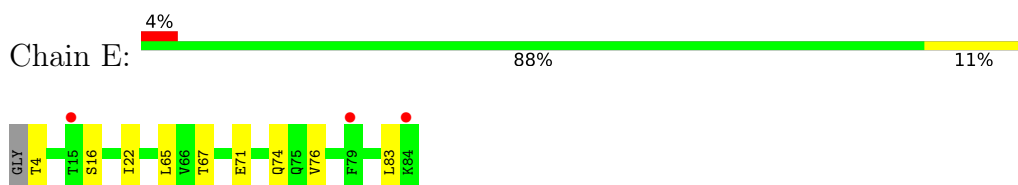
- Molecule 4: Photosystem II D2 protein



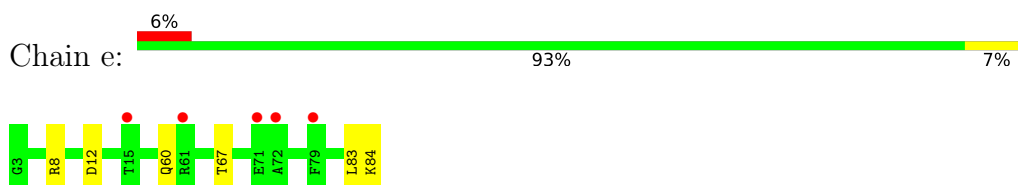
- Molecule 4: Photosystem II D2 protein



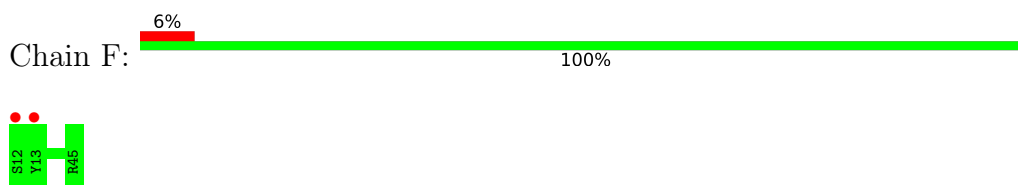
- Molecule 5: Cytochrome b559 subunit alpha



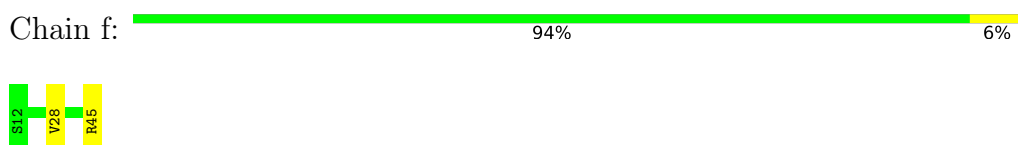
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta

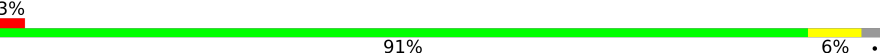


- Molecule 7: Photosystem II reaction center protein H

Chain H:  91% 9%




- Molecule 7: Photosystem II reaction center protein H

Chain h:  3% 91% 6%

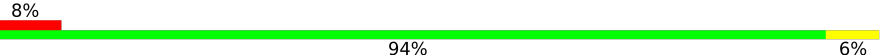


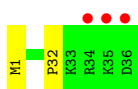
- Molecule 8: Photosystem II reaction center protein I

Chain I:  86% 14%

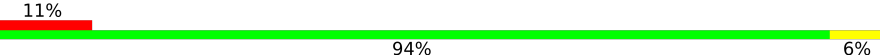


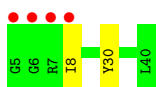
- Molecule 8: Photosystem II reaction center protein I

Chain i:  8% 94% 6%

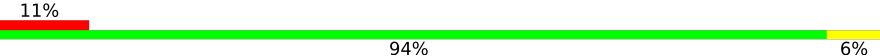


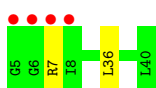
- Molecule 9: Photosystem II reaction center protein J

Chain J:  11% 94% 6%




- Molecule 9: Photosystem II reaction center protein J

Chain j:  11% 94% 6%

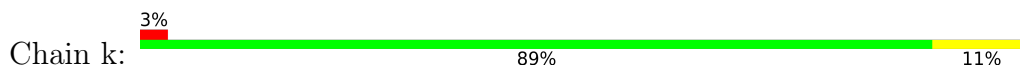


- Molecule 10: Photosystem II reaction center protein K

Chain K:  86% 14%



- Molecule 10: Photosystem II reaction center protein K

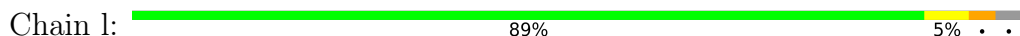


- Molecule 11: Photosystem II reaction center protein L

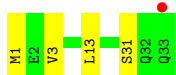
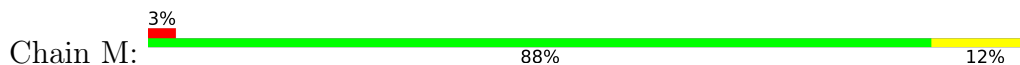


There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein L



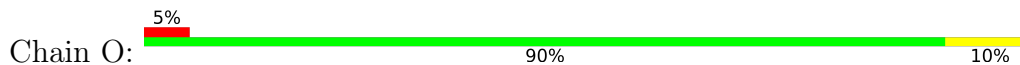
- Molecule 12: Photosystem II reaction center protein M



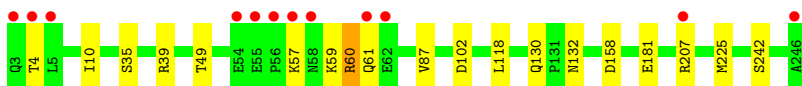
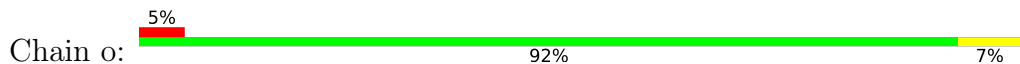
- Molecule 12: Photosystem II reaction center protein M



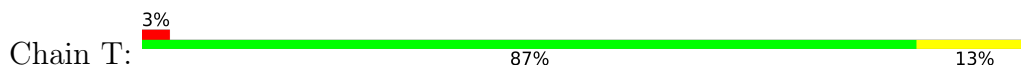
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



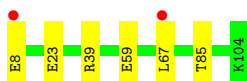
- Molecule 14: Photosystem II reaction center protein T



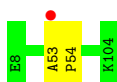
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



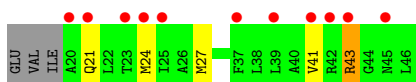
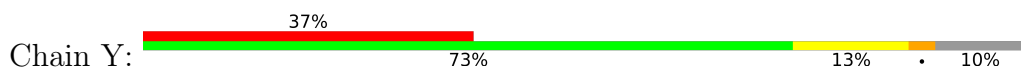
- Molecule 16: Cytochrome c-550



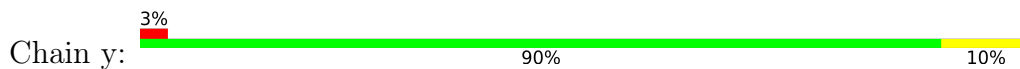
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



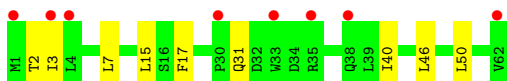
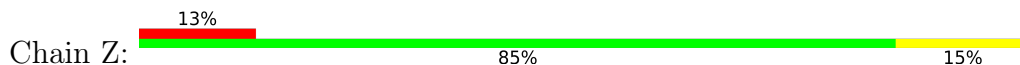
- Molecule 18: Photosystem II reaction center X protein



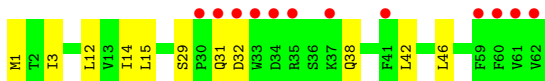
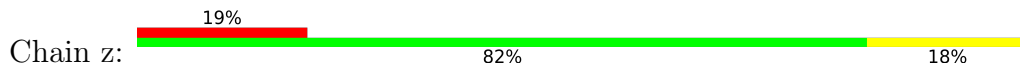
- Molecule 18: Photosystem II reaction center X protein



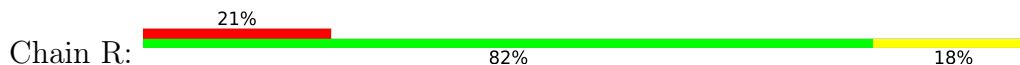
- Molecule 19: Photosystem II reaction center protein Z



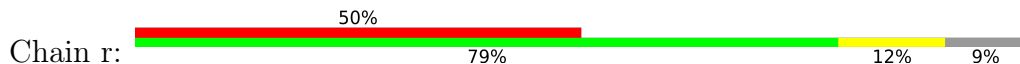
- Molecule 19: Photosystem II reaction center protein Z

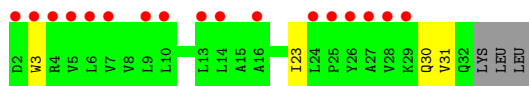


- Molecule 20: Photosystem II protein Y



- 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, α , β , γ	117.55Å 222.69Å 309.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.78 – 2.50 30.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.78-2.50) 87.6 (30.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.51Å)	Xtrriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.167 , 0.246 0.167 , 0.247	Depositor DCC
R_{free} test set	2481 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtrriage
Anisotropy	0.353	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103658	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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%)	0.73	1/3692 (0.0%)
1	a	0.68	0/2704	0.71	1/3688 (0.0%)
2	B	0.68	0/4160	0.71	2/5668 (0.0%)
2	b	0.63	0/4118	0.69	0/5611
3	C	0.64	0/3530	0.68	0/4807
3	c	0.59	0/3610	0.67	0/4914
4	D	0.69	0/2812	0.70	0/3832
4	d	0.63	0/2821	0.69	1/3844 (0.0%)
5	E	0.57	0/684	0.66	0/935
5	e	0.56	0/683	0.63	0/932
6	F	0.57	0/284	0.59	0/387
6	f	0.54	0/284	0.58	0/387
7	H	0.68	1/520 (0.2%)	0.72	0/709
7	h	0.62	0/511	0.74	0/697
8	I	0.67	0/293	0.75	0/396
8	i	0.76	0/293	0.74	0/396
9	J	0.54	0/263	0.70	0/356
9	j	0.54	0/261	0.64	0/353
10	K	0.50	0/314	0.65	0/427
10	k	0.51	0/303	0.72	0/416
11	L	0.69	0/311	0.74	0/422
11	l	0.62	0/303	0.71	0/412
12	M	0.70	0/249	0.71	0/341
12	m	0.75	0/244	0.67	0/334
13	O	0.62	0/1914	0.77	2/2596 (0.1%)
13	o	0.60	0/1905	0.76	3/2583 (0.1%)
14	T	0.79	1/257 (0.4%)	0.77	0/349
14	t	0.71	0/255	0.64	0/346
15	U	0.62	0/785	0.70	0/1064
15	u	0.65	0/785	0.75	0/1064
16	V	0.58	0/1085	0.69	0/1473
16	v	0.62	0/1085	0.69	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.47	0/197	0.69	0/264
17	y	0.39	0/219	0.57	0/294
18	X	0.61	0/284	0.70	0/384
18	x	0.40	0/284	0.62	0/384
19	Z	0.53	0/490	0.64	0/669
19	z	0.48	0/488	0.56	0/666
20	R	0.39	0/277	0.57	0/380
20	r	0.39	0/233	0.55	0/323
All	All	0.64	3/42805 (0.0%)	0.70	10/58268 (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
17	Y	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	6	TYR	CD2-CE2	-5.58	1.30	1.39
1	A	135	TYR	CD1-CE1	-5.56	1.31	1.39
7	H	41	PHE	CB-CG	-5.18	1.42	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	7.76	125.28	118.30
13	O	158	ASP	CB-CG-OD1	6.08	123.78	118.30
4	d	348	ARG	NE-CZ-NH2	-5.81	117.39	120.30
13	o	102	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	183	MET	CA-CB-CG	5.64	122.88	113.30
13	O	223	ASP	CB-CG-OD2	5.60	123.34	118.30
13	o	158	ASP	CB-CG-OD2	-5.46	113.39	118.30
2	B	433	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	a	72	LEU	CB-CG-CD1	-5.31	101.97	111.00
2	B	46	ASP	CB-CG-OD2	-5.14	113.68	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	Y	21	GLN	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%)	9 (3%)	1 (0%)	41	61
1	a	332/334 (99%)	320 (96%)	11 (3%)	1 (0%)	41	61
2	B	508/505 (101%)	488 (96%)	19 (4%)	1 (0%)	47	68
2	b	503/505 (100%)	480 (95%)	20 (4%)	3 (1%)	25	43
3	C	440/451 (98%)	420 (96%)	19 (4%)	1 (0%)	47	68
3	c	450/451 (100%)	433 (96%)	15 (3%)	2 (0%)	34	54
4	D	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	41	61
4	d	340/341 (100%)	323 (95%)	17 (5%)	0	100	100
5	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	j	34/36 (94%)	32 (94%)	2 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4	6
10	k	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	33 (97%)	0	1 (3%)	4	6
12	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	m	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
13	O	243/244 (100%)	225 (93%)	14 (6%)	4 (2%)	9	17
13	o	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	13	24
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
15	u	95/97 (98%)	91 (96%)	3 (3%)	1 (1%)	14	26
16	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	v	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
17	Y	25/30 (83%)	18 (72%)	5 (20%)	2 (8%)	1	1
17	y	28/30 (93%)	23 (82%)	4 (14%)	1 (4%)	3	4
18	X	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	7
18	x	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	47 (78%)	11 (18%)	2 (3%)	4	5
20	R	32/34 (94%)	30 (94%)	1 (3%)	1 (3%)	4	5
20	r	29/34 (85%)	24 (83%)	3 (10%)	2 (7%)	1	1
All	All	5235/5326 (98%)	4963 (95%)	243 (5%)	29 (1%)	25	43

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	62	GLU
17	Y	41	VAL
3	c	416	SER
13	o	60	ARG
13	o	61	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	u	53	ALA
19	z	15	LEU
20	r	30	GLN
17	Y	43	ARG
20	R	34	LEU
2	b	85	GLY
20	r	31	VAL
2	B	438	ASN
18	X	38	GLN
19	z	14	ILE
4	D	338	ASN
2	b	127	ARG
13	O	138	THR
3	c	250	TRP
11	l	7	ARG
13	o	132	ASN
17	y	41	VAL
13	O	57	LYS
2	b	295	GLY
13	O	133	VAL
1	A	259	ILE
1	a	259	ILE

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%)	262 (97%)	8 (3%)	41 68
1	a	269/270 (100%)	256 (95%)	13 (5%)	25 48
2	B	407/403 (101%)	391 (96%)	16 (4%)	32 57
2	b	402/403 (100%)	388 (96%)	14 (4%)	36 62
3	C	344/352 (98%)	338 (98%)	6 (2%)	60 82
3	c	353/352 (100%)	335 (95%)	18 (5%)	24 45
4	D	276/276 (100%)	269 (98%)	7 (2%)	47 73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	277/276 (100%)	271 (98%)	6 (2%)	52	77
5	E	72/72 (100%)	62 (86%)	10 (14%)	3	6
5	e	71/72 (99%)	65 (92%)	6 (8%)	10	21
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	28/28 (100%)	26 (93%)	2 (7%)	14	28
7	H	53/54 (98%)	48 (91%)	5 (9%)	8	17
7	h	53/54 (98%)	49 (92%)	4 (8%)	13	26
8	I	32/32 (100%)	28 (88%)	4 (12%)	4	8
8	i	32/32 (100%)	31 (97%)	1 (3%)	40	67
9	J	24/24 (100%)	22 (92%)	2 (8%)	11	22
9	j	23/24 (96%)	21 (91%)	2 (9%)	10	20
10	K	31/30 (103%)	26 (84%)	5 (16%)	2	4
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	7
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	19
12	M	28/29 (97%)	25 (89%)	3 (11%)	6	13
12	m	28/29 (97%)	26 (93%)	2 (7%)	14	28
13	O	208/207 (100%)	189 (91%)	19 (9%)	9	18
13	o	207/207 (100%)	192 (93%)	15 (7%)	14	28
14	T	26/26 (100%)	24 (92%)	2 (8%)	13	25
14	t	25/26 (96%)	25 (100%)	0	100	100
15	U	84/84 (100%)	78 (93%)	6 (7%)	14	28
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	88
16	V	117/117 (100%)	112 (96%)	5 (4%)	29	53
16	v	117/117 (100%)	111 (95%)	6 (5%)	24	45
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2	4
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	18
18	X	31/31 (100%)	30 (97%)	1 (3%)	39	65
18	x	31/31 (100%)	29 (94%)	2 (6%)	17	33
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	3
19	z	51/52 (98%)	42 (82%)	9 (18%)	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	28/29 (97%)	23 (82%)	5 (18%)	2	3
20	r	19/29 (66%)	17 (90%)	2 (10%)	7	13
All	All	4321/4348 (99%)	4093 (95%)	228 (5%)	23	43

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	16	ARG
1	A	102	LEU
1	A	205	VAL
1	A	229	GLU
1	A	231	GLU
1	A	307	ILE
2	B	63	LEU
2	B	76	SER
2	B	83	GLU
2	B	227	LYS
2	B	236	THR
2	B	241	SER
2	B	246	PHE
2	B	289	GLN
2	B	298	LEU
2	B	362	PHE
2	B	371	THR
2	B	435	GLU
2	B	476	ARG
2	B	485	GLU
2	B	489	GLU
2	B	495	PHE
3	C	141	GLU
3	C	161	LEU
3	C	200	THR
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	12	ARG
4	D	26	ARG
4	D	43	LEU
4	D	76	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	150	ILE
4	D	180	ARG
4	D	345	VAL
5	E	4	THR
5	E	16	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	65	LEU
5	E	67	THR
5	E	71	GLU
5	E	74	GLN
5	E	76	VAL
5	E	83	LEU
7	H	20	LYS
7	H	27	THR
7	H	49	TYR
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	33	LYS
8	I	34	ARG
8	I	35	LYS
9	J	8	ILE
9	J	30	TYR
10	K	10	LYS
10	K	25	LEU
10	K	43	VAL
10	K	46[A]	ARG
10	K	46[B]	ARG
12	M	3	VAL
12	M	13	LEU
12	M	31	SER
13	O	3	GLN
13	O	4	THR
13	O	23	ASP
13	O	24	ASP
13	O	34	SER
13	O	39	ARG
13	O	45	LEU
13	O	72	THR
13	O	78	LEU
13	O	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	O	107	THR
13	O	118	LEU
13	O	134	THR
13	O	135	SER
13	O	182	LEU
13	O	191	SER
13	O	207	ARG
13	O	214	THR
13	O	217	SER
14	T	2	GLU
14	T	24	ARG
15	U	8	GLU
15	U	23	GLU
15	U	39	ARG
15	U	59	GLU
15	U	67	LEU
15	U	85	THR
16	V	3	LEU
16	V	7	VAL
16	V	21	LEU
16	V	31	ARG
16	V	86	GLN
17	Y	24	MET
17	Y	27	MET
17	Y	43	ARG
18	X	39	ARG
19	Z	2	THR
19	Z	3	ILE
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	31	GLN
19	Z	40	ILE
19	Z	46	LEU
19	Z	50	LEU
20	R	2	ASP
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	13	LEU
1	a	28	LEU
1	a	42	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	121	LEU
1	a	159	LEU
1	a	169	SER
1	a	200	LEU
1	a	223	LEU
1	a	227	THR
1	a	229	GLU
1	a	231	GLU
1	a	238	LYS
1	a	245	THR
1	a	288	LEU
2	b	81	THR
2	b	86	ILE
2	b	149	LEU
2	b	170	ASP
2	b	236	THR
2	b	252	VAL
2	b	347	ARG
2	b	353	GLU
2	b	362	PHE
2	b	388	SER
2	b	409	GLN
2	b	480	SER
2	b	490	GLN
2	b	492	GLU
3	c	24	THR
3	c	25	ASN
3	c	26	ARG
3	c	43	ILE
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	155	ASN
3	c	165	LEU
3	c	289	PHE
3	c	315	MET
3	c	384	ILE
3	c	396	MET
3	c	418	ASN
3	c	421	SER
3	c	462	GLU
3	c	463	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	c	471	SER
4	d	12	ARG
4	d	90	LEU
4	d	180	ARG
4	d	272	LEU
4	d	291	LEU
4	d	321	LEU
5	e	8	ARG
5	e	12	ASP
5	e	60	GLN
5	e	67	THR
5	e	83	LEU
5	e	84	LYS
6	f	28	VAL
6	f	45	ARG
7	h	3	ARG
7	h	7	LEU
7	h	21	VAL
7	h	49	TYR
8	i	32	PRO
9	j	7	ARG
9	j	36	LEU
10	k	10	LYS
10	k	21	LEU
10	k	30	VAL
10	k	46	ARG
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	4	THR
13	o	10	ILE
13	o	35	SER
13	o	39	ARG
13	o	49	THR
13	o	57	LYS
13	o	59	LYS
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	o	181	GLU
13	o	207	ARG
13	o	225	MET
13	o	242	SER
15	u	54	PRO
16	v	15	GLU
16	v	24	LYS
16	v	52	LEU
16	v	100	ILE
16	v	106	ASN
16	v	108	THR
17	y	22	LEU
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	29	SER
19	z	31	GLN
19	z	32	ASP
19	z	38	GLN
19	z	42	LEU
19	z	46	LEU
20	r	3	TRP
20	r	23	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	285	ASN
2	B	289	GLN
13	O	82	GLN
13	O	231	HIS
15	U	37	GLN
16	V	86	GLN
19	Z	6	GLN
2	b	179	GLN
2	b	281	GLN
2	b	282	GLN
2	b	497	GLN
3	c	25	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	c	28	GLN
5	e	74	GLN
13	o	58	ASN
19	z	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	m	1	12	8,9,10	1.06	1 (12%)	7,9,11	0.66	0
14	FME	T	1	14	8,9,10	0.96	1 (12%)	7,9,11	1.55	1 (14%)
8	FME	i	1	8	8,9,10	1.25	1 (12%)	7,9,11	1.06	0
8	FME	I	1	8	8,9,10	1.09	1 (12%)	7,9,11	1.33	1 (14%)
14	FME	t	1	14	8,9,10	1.07	1 (12%)	7,9,11	1.04	0
12	FME	M	1	12	8,9,10	1.14	1 (12%)	7,9,11	1.08	0

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.68	1.42	1.46
14	t	1	FME	CA-N	-2.51	1.42	1.46
14	T	1	FME	CA-N	-2.47	1.42	1.46
12	m	1	FME	CA-N	-2.40	1.42	1.46
8	I	1	FME	CA-N	-2.33	1.43	1.46
12	M	1	FME	CA-N	-2.16	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.37	119.17	122.82
14	T	1	FME	CA-N-CN	-2.36	119.19	122.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
33	LMG	C	501	-	48,48,55	1.17	6 (12%)	56,56,63	1.37	10 (17%)
33	LMG	c	519	-	37,37,55	1.13	4 (10%)	45,45,63	1.30	6 (13%)
28	DGD	C	518	-	63,63,67	1.11	7 (11%)	77,77,81	1.42	11 (14%)
23	CLA	B	601	36	65,73,73	1.78	11 (16%)	76,113,113	1.36	10 (13%)
29	LHG	L	101	-	48,48,48	0.93	4 (8%)	51,54,54	1.08	2 (3%)
23	CLA	b	603	-	65,73,73	1.67	12 (18%)	76,113,113	1.62	17 (22%)
23	CLA	A	407	-	54,62,73	1.82	12 (22%)	62,99,113	1.93	16 (25%)
25	BCR	C	520	-	41,41,41	1.03	3 (7%)	56,56,56	1.36	7 (12%)
34	HEM	e	102	6,5	41,50,50	1.38	4 (9%)	45,82,82	1.59	8 (17%)
35	HEC	V	201	16	32,50,50	2.39	6 (18%)	24,82,82	1.65	3 (12%)
25	BCR	H	101	-	41,41,41	1.26	3 (7%)	56,56,56	1.34	7 (12%)
31	BCT	A	415	21	2,3,3	1.34	0	2,3,3	2.88	1 (50%)
23	CLA	b	614	-	65,73,73	1.57	9 (13%)	76,113,113	1.51	10 (13%)
27	SQD	b	601	-	48,49,54	1.01	2 (4%)	57,60,65	2.23	17 (29%)
25	BCR	D	405	-	41,41,41	1.08	3 (7%)	56,56,56	1.18	5 (8%)
25	BCR	c	515	-	41,41,41	1.21	4 (9%)	56,56,56	1.42	12 (21%)
25	BCR	c	514	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	8 (14%)
23	CLA	b	602	36	65,73,73	1.83	11 (16%)	76,113,113	1.44	13 (17%)
23	CLA	B	602	-	65,73,73	1.56	7 (10%)	76,113,113	1.42	12 (15%)
27	SQD	B	621	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	15 (24%)
23	CLA	A	404	-	65,73,73	1.66	10 (15%)	76,113,113	1.44	8 (10%)
25	BCR	B	618	-	41,41,41	1.37	4 (9%)	56,56,56	1.44	7 (12%)
23	CLA	b	606	-	65,73,73	1.49	8 (12%)	76,113,113	1.85	17 (22%)
23	CLA	b	609	-	65,73,73	1.68	10 (15%)	76,113,113	1.44	13 (17%)
23	CLA	C	503	-	65,73,73	1.44	7 (10%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	507	-	65,73,73	2.11	11 (16%)	76,113,113	1.38	11 (14%)
27	SQD	f	101	-	40,41,54	1.12	5 (12%)	49,52,65	1.80	13 (26%)
29	LHG	d	407	-	48,48,48	0.81	0	51,54,54	1.31	5 (9%)
23	CLA	c	511	3	65,73,73	1.85	8 (12%)	76,113,113	1.33	5 (6%)
23	CLA	b	617	-	60,68,73	1.61	10 (16%)	70,107,113	1.66	12 (17%)
23	CLA	b	607	-	65,73,73	1.58	9 (13%)	76,113,113	1.51	14 (18%)
23	CLA	c	504	36	60,68,73	1.64	8 (13%)	70,107,113	1.39	6 (8%)
31	BCT	a	404	21	2,3,3	1.42	0	2,3,3	3.13	2 (100%)
23	CLA	b	615	-	65,73,73	1.63	10 (15%)	76,113,113	1.66	17 (22%)
23	CLA	B	604	-	65,73,73	1.68	11 (16%)	76,113,113	1.51	10 (13%)
23	CLA	b	611	36	65,73,73	1.51	10 (15%)	76,113,113	1.37	14 (18%)
23	CLA	b	616	-	65,73,73	2.33	10 (15%)	76,113,113	1.55	12 (15%)
25	BCR	b	618	-	41,41,41	1.16	3 (7%)	56,56,56	1.28	6 (10%)
23	CLA	c	503	-	65,73,73	1.83	11 (16%)	76,113,113	1.53	13 (17%)
28	DGD	c	518	-	63,63,67	1.27	9 (14%)	77,77,81	1.53	12 (15%)
25	BCR	x	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.40	11 (19%)
24	PHO	d	401	-	51,69,69	1.08	4 (7%)	47,99,99	1.38	6 (12%)
27	SQD	F	101	-	35,36,54	0.93	1 (2%)	42,45,65	1.95	10 (23%)
25	BCR	Z	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.43	10 (17%)
27	SQD	A	410	-	51,52,54	1.10	6 (11%)	60,63,65	2.10	12 (20%)
28	DGD	C	517	-	63,63,67	1.24	10 (15%)	77,77,81	1.56	12 (15%)
29	LHG	e	101	-	41,41,48	0.87	3 (7%)	44,47,54	1.37	6 (13%)
25	BCR	A	408	-	41,41,41	1.18	3 (7%)	56,56,56	1.51	10 (17%)
33	LMG	D	410	-	31,31,55	1.15	3 (9%)	33,33,63	1.11	2 (6%)
30	OEX	A	414	1,3,36	0,15,15	-	-	-	-	-
26	PL9	d	406	-	55,55,55	1.36	7 (12%)	68,69,69	1.79	19 (27%)
23	CLA	a	405	-	65,73,73	1.60	9 (13%)	76,113,113	1.54	15 (19%)
23	CLA	B	606	-	65,73,73	1.68	12 (18%)	76,113,113	1.70	13 (17%)
26	PL9	D	406	-	55,55,55	1.58	9 (16%)	68,69,69	1.65	14 (20%)
26	PL9	A	409	-	55,55,55	1.34	5 (9%)	68,69,69	1.44	8 (11%)
23	CLA	c	506	-	65,73,73	1.91	13 (20%)	76,113,113	1.54	13 (17%)
23	CLA	B	614	-	65,73,73	1.62	9 (13%)	76,113,113	1.58	8 (10%)
23	CLA	c	513	-	65,73,73	1.47	9 (13%)	76,113,113	1.28	12 (15%)
25	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	7 (12%)
25	BCR	T	101	-	41,41,41	1.19	4 (9%)	56,56,56	1.45	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	510	-	65,73,73	1.41	7 (10%)	76,113,113	1.44	8 (10%)
23	CLA	A	405	36	65,73,73	1.56	9 (13%)	76,113,113	1.54	11 (14%)
23	CLA	B	610	36	65,73,73	1.58	9 (13%)	76,113,113	1.65	12 (15%)
23	CLA	D	402	36	65,73,73	1.43	8 (12%)	76,113,113	1.20	9 (11%)
33	LMG	d	411	-	44,44,55	1.21	4 (9%)	52,52,63	1.49	6 (11%)
23	CLA	b	605	-	65,73,73	1.49	7 (10%)	76,113,113	1.47	14 (18%)
23	CLA	c	510	-	65,73,73	1.42	7 (10%)	76,113,113	1.62	11 (14%)
23	CLA	D	404	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	11 (14%)
23	CLA	c	512	-	65,73,73	1.59	8 (12%)	76,113,113	1.33	8 (10%)
23	CLA	c	507	36	65,73,73	1.63	11 (16%)	76,113,113	1.58	12 (15%)
23	CLA	d	402	36	65,73,73	1.65	10 (15%)	76,113,113	1.85	11 (14%)
27	SQD	a	411	-	53,54,54	0.99	5 (9%)	62,65,65	1.90	9 (14%)
33	LMG	m	101	-	51,51,55	0.96	4 (7%)	59,59,63	1.55	8 (13%)
28	DGD	a	413	-	43,43,67	1.46	4 (9%)	45,45,81	1.22	5 (11%)
23	CLA	D	403	-	65,73,73	1.51	10 (15%)	76,113,113	1.61	10 (13%)
33	LMG	C	519	-	48,48,55	1.03	6 (12%)	56,56,63	1.32	6 (10%)
33	LMG	D	407	-	51,51,55	1.01	5 (9%)	59,59,63	1.20	3 (5%)
33	LMG	d	410	-	21,21,55	0.95	1 (4%)	20,20,63	0.89	1 (5%)
25	BCR	d	405	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	8 (14%)
23	CLA	B	615	-	65,73,73	1.99	11 (16%)	76,113,113	1.35	10 (13%)
23	CLA	C	504	-	65,73,73	1.76	9 (13%)	76,113,113	1.84	17 (22%)
24	PHO	D	401	-	51,69,69	1.15	5 (9%)	47,99,99	1.42	7 (14%)
25	BCR	t	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.44	13 (23%)
28	DGD	c	517	-	63,63,67	1.19	6 (9%)	77,77,81	1.34	8 (10%)
24	PHO	A	406	-	51,69,69	1.17	6 (11%)	47,99,99	1.27	6 (12%)
23	CLA	a	406	36	65,73,73	1.42	8 (12%)	76,113,113	1.74	13 (17%)
25	BCR	B	617	-	41,41,41	1.28	4 (9%)	56,56,56	1.39	9 (16%)
25	BCR	a	409	-	41,41,41	1.11	3 (7%)	56,56,56	1.33	6 (10%)
29	LHG	D	409	-	46,46,48	1.07	3 (6%)	49,52,54	1.28	5 (10%)
33	LMG	c	524	-	49,49,55	1.16	4 (8%)	57,57,63	1.29	4 (7%)
25	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.13	3 (5%)
23	CLA	b	613	-	65,73,73	1.25	8 (12%)	76,113,113	1.88	15 (19%)
33	LMG	M	101	-	51,51,55	0.98	2 (3%)	59,59,63	1.48	9 (15%)
24	PHO	a	407	-	51,69,69	1.10	5 (9%)	47,99,99	1.25	5 (10%)
23	CLA	C	508	36	65,73,73	1.63	12 (18%)	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	B	613	-	65,73,73	1.67	11 (16%)	76,113,113	1.66	14 (18%)
23	CLA	C	512	3	65,73,73	1.88	10 (15%)	76,113,113	1.52	9 (11%)
23	CLA	B	609	-	65,73,73	1.66	12 (18%)	76,113,113	1.57	15 (19%)
23	CLA	a	408	-	65,73,73	1.75	11 (16%)	76,113,113	1.40	11 (14%)
28	DGD	C	516	-	63,63,67	1.38	7 (11%)	77,77,81	1.33	10 (12%)
29	LHG	E	101	-	48,48,48	0.91	3 (6%)	51,54,54	1.21	3 (5%)
33	LMG	c	522	-	48,48,55	1.19	6 (12%)	56,56,63	1.36	5 (8%)
23	CLA	C	506	-	65,73,73	1.40	7 (10%)	76,113,113	1.49	11 (14%)
23	CLA	C	513	-	65,73,73	1.79	11 (16%)	76,113,113	1.42	12 (15%)
25	BCR	b	619	-	41,41,41	1.29	2 (4%)	56,56,56	1.31	7 (12%)
28	DGD	h	101	-	63,63,67	1.20	6 (9%)	77,77,81	1.59	17 (22%)
29	LHG	D	408	-	48,48,48	1.04	3 (6%)	51,54,54	1.26	6 (11%)
28	DGD	A	412	-	67,67,67	1.41	12 (17%)	81,81,81	1.37	6 (7%)
25	BCR	B	619	-	41,41,41	1.18	4 (9%)	56,56,56	1.25	7 (12%)
23	CLA	B	605	-	65,73,73	1.72	10 (15%)	76,113,113	1.47	17 (22%)
28	DGD	c	516	-	63,63,67	1.19	5 (7%)	77,77,81	1.55	15 (19%)
23	CLA	B	612	-	65,73,73	1.41	7 (10%)	76,113,113	1.58	12 (15%)
23	CLA	b	610	-	65,73,73	1.61	11 (16%)	76,113,113	1.41	11 (14%)
27	SQD	A	411	-	38,38,54	1.09	4 (10%)	40,40,65	1.47	4 (10%)
25	BCR	b	620	-	41,41,41	1.07	3 (7%)	56,56,56	1.29	8 (14%)
29	LHG	l	101	-	48,48,48	0.79	2 (4%)	51,54,54	1.16	3 (5%)
35	HEC	v	201	16	32,50,50	2.45	4 (12%)	24,82,82	1.44	3 (12%)
25	BCR	c	521	-	41,41,41	0.97	2 (4%)	56,56,56	1.18	5 (8%)
33	LMG	b	622	-	55,55,55	1.06	4 (7%)	63,63,63	1.56	5 (7%)
23	CLA	C	505	36	59,67,73	2.04	13 (22%)	68,105,113	1.31	9 (13%)
23	CLA	C	514	-	65,73,73	1.58	10 (15%)	76,113,113	1.62	11 (14%)
23	CLA	b	612	-	65,73,73	1.73	10 (15%)	76,113,113	1.55	18 (23%)
25	BCR	C	515	-	41,41,41	1.26	5 (12%)	56,56,56	1.33	8 (14%)
23	CLA	b	604	-	65,73,73	1.60	11 (16%)	76,113,113	1.54	12 (15%)
23	CLA	B	607	36	65,73,73	1.45	12 (18%)	76,113,113	1.39	9 (11%)
23	CLA	c	509	-	65,73,73	1.76	8 (12%)	76,113,113	1.83	13 (17%)
29	LHG	d	409	-	38,38,48	0.86	2 (5%)	41,44,54	1.11	3 (7%)
23	CLA	B	603	-	65,73,73	1.62	12 (18%)	76,113,113	1.53	12 (15%)
23	CLA	B	611	-	65,73,73	1.60	10 (15%)	76,113,113	1.45	10 (13%)
23	CLA	c	502	-	65,73,73	1.43	7 (10%)	76,113,113	1.58	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PL9	a	410	-	55,55,55	1.27	5 (9%)	68,69,69	1.55	16 (23%)
23	CLA	d	403	-	65,73,73	1.51	9 (13%)	76,113,113	1.18	6 (7%)
23	CLA	B	608	-	65,73,73	1.59	13 (20%)	76,113,113	1.35	8 (10%)
29	LHG	d	408	-	48,48,48	0.68	0	51,54,54	1.20	4 (7%)
23	CLA	c	505	-	65,73,73	1.68	8 (12%)	76,113,113	1.27	9 (11%)
23	CLA	C	509	-	65,73,73	1.65	12 (18%)	76,113,113	1.73	17 (22%)
23	CLA	c	501	-	65,73,73	1.59	8 (12%)	76,113,113	2.02	11 (14%)
23	CLA	C	502	-	65,73,73	1.80	9 (13%)	76,113,113	1.77	10 (13%)
23	CLA	b	608	36	65,73,73	1.30	8 (12%)	76,113,113	1.39	11 (14%)
29	LHG	A	413	-	48,48,48	0.86	2 (4%)	51,54,54	1.52	9 (17%)
28	DGD	H	102	-	63,63,67	1.34	13 (20%)	77,77,81	1.50	12 (15%)
30	OEX	a	415	1,3,36	0,15,15	-	-	-	-	-
23	CLA	d	404	-	65,73,73	1.96	10 (15%)	76,113,113	1.48	11 (14%)
23	CLA	B	616	-	60,68,73	1.76	11 (18%)	70,107,113	1.48	9 (12%)
34	HEM	E	103	6,5	41,50,50	1.47	5 (12%)	45,82,82	1.25	5 (11%)
23	CLA	C	511	-	65,73,73	1.52	9 (13%)	76,113,113	1.50	9 (11%)
27	SQD	a	412	-	35,35,54	1.06	2 (5%)	37,37,65	1.44	5 (13%)
23	CLA	c	508	-	64,72,73	1.91	10 (15%)	74,111,113	1.40	11 (14%)
33	LMG	D	411	-	26,26,55	0.80	1 (3%)	26,26,63	1.19	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	501	-	-	21/43/63/70	0/1/1/1
33	LMG	c	519	-	-	12/31/51/70	0/1/1/1
28	DGD	C	518	-	-	15/51/91/95	0/2/2/2
23	CLA	B	601	36	1/1/20/20	12/37/115/115	-
29	LHG	L	101	-	-	23/53/53/53	-
23	CLA	b	603	-	1/1/20/20	10/37/115/115	-
23	CLA	A	407	-	1/1/17/20	6/24/102/115	-
25	BCR	C	520	-	-	11/29/63/63	0/2/2/2
34	HEM	e	102	6,5	-	3/12/54/54	-
35	HEC	V	201	16	-	2/10/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	H	101	-	-	10/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/20/20	10/37/115/115	-
27	SQD	b	601	-	-	21/44/64/69	0/1/1/1
25	BCR	D	405	-	-	3/29/63/63	0/2/2/2
25	BCR	c	515	-	-	5/29/63/63	0/2/2/2
25	BCR	c	514	-	-	15/29/63/63	0/2/2/2
23	CLA	b	602	36	1/1/20/20	16/37/115/115	-
23	CLA	B	602	-	1/1/20/20	7/37/115/115	-
27	SQD	B	621	-	-	23/49/69/69	0/1/1/1
23	CLA	A	404	-	1/1/20/20	4/37/115/115	-
25	BCR	B	618	-	-	3/29/63/63	0/2/2/2
23	CLA	b	606	-	1/1/20/20	8/37/115/115	-
23	CLA	b	609	-	1/1/20/20	6/37/115/115	-
23	CLA	C	503	-	1/1/20/20	12/37/115/115	-
23	CLA	C	507	-	-	19/37/115/115	-
27	SQD	f	101	-	-	16/36/56/69	0/1/1/1
29	LHG	d	407	-	-	21/53/53/53	-
23	CLA	c	511	3	1/1/20/20	10/37/115/115	-
23	CLA	b	617	-	1/1/19/20	6/31/109/115	-
23	CLA	b	607	-	1/1/20/20	11/37/115/115	-
23	CLA	c	504	36	1/1/19/20	9/31/109/115	-
23	CLA	b	615	-	1/1/20/20	15/37/115/115	-
23	CLA	B	604	-	1/1/20/20	13/37/115/115	-
23	CLA	b	611	36	1/1/20/20	1/37/115/115	-
23	CLA	b	616	-	1/1/20/20	8/37/115/115	-
25	BCR	b	618	-	-	5/29/63/63	0/2/2/2
23	CLA	c	503	-	1/1/20/20	9/37/115/115	-
28	DGD	c	518	-	-	22/51/91/95	0/2/2/2
25	BCR	x	102	-	-	11/29/63/63	0/2/2/2
24	PHO	d	401	-	-	3/37/103/103	0/5/6/6
27	SQD	F	101	-	-	13/28/48/69	0/1/1/1
25	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
27	SQD	A	410	-	-	18/47/67/69	0/1/1/1
28	DGD	C	517	-	-	20/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	e	101	-	-	30/46/46/53	-
25	BCR	A	408	-	-	7/29/63/63	0/2/2/2
33	LMG	D	410	-	-	17/33/33/70	-
26	PL9	d	406	-	-	18/53/73/73	0/1/1/1
23	CLA	a	405	-	1/1/20/20	6/37/115/115	-
23	CLA	B	606	-	1/1/20/20	13/37/115/115	-
26	PL9	D	406	-	-	11/53/73/73	0/1/1/1
26	PL9	A	409	-	-	19/53/73/73	0/1/1/1
23	CLA	c	506	-	1/1/20/20	17/37/115/115	-
23	CLA	B	614	-	1/1/20/20	13/37/115/115	-
23	CLA	c	513	-	1/1/20/20	10/37/115/115	-
25	BCR	K	101	-	-	13/29/63/63	0/2/2/2
25	BCR	T	101	-	-	2/29/63/63	0/2/2/2
23	CLA	C	510	-	1/1/20/20	9/37/115/115	-
23	CLA	A	405	36	1/1/20/20	4/37/115/115	-
23	CLA	B	610	36	1/1/20/20	10/37/115/115	-
23	CLA	D	402	36	1/1/20/20	5/37/115/115	-
33	LMG	d	411	-	-	8/39/59/70	0/1/1/1
23	CLA	b	605	-	1/1/20/20	11/37/115/115	-
23	CLA	c	510	-	1/1/20/20	15/37/115/115	-
23	CLA	D	404	-	-	12/37/115/115	-
23	CLA	c	512	-	1/1/20/20	23/37/115/115	-
23	CLA	c	507	36	1/1/20/20	10/37/115/115	-
23	CLA	d	402	36	1/1/20/20	4/37/115/115	-
27	SQD	a	411	-	-	22/49/69/69	0/1/1/1
33	LMG	m	101	-	-	21/46/66/70	0/1/1/1
28	DGD	a	413	-	-	21/45/45/95	-
23	CLA	D	403	-	-	10/37/115/115	-
33	LMG	C	519	-	-	16/43/63/70	0/1/1/1
33	LMG	D	407	-	-	18/46/66/70	0/1/1/1
33	LMG	d	410	-	-	15/17/17/70	-
25	BCR	d	405	-	-	13/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/20/20	7/37/115/115	-
23	CLA	C	504	-	-	7/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	D	401	-	-	0/37/103/103	0/5/6/6
25	BCR	t	101	-	-	7/29/63/63	0/2/2/2
28	DGD	c	517	-	-	19/51/91/95	0/2/2/2
24	PHO	A	406	-	-	9/37/103/103	0/5/6/6
23	CLA	a	406	36	1/1/20/20	12/37/115/115	-
25	BCR	B	617	-	-	11/29/63/63	0/2/2/2
25	BCR	a	409	-	-	2/29/63/63	0/2/2/2
29	LHG	D	409	-	-	23/51/51/53	-
33	LMG	c	524	-	-	16/44/64/70	0/1/1/1
25	BCR	k	101	-	-	13/29/63/63	0/2/2/2
23	CLA	b	613	-	1/1/20/20	11/37/115/115	-
33	LMG	M	101	-	-	19/46/66/70	0/1/1/1
24	PHO	a	407	-	-	6/37/103/103	0/5/6/6
23	CLA	C	508	36	1/1/20/20	7/37/115/115	-
23	CLA	B	613	-	1/1/20/20	6/37/115/115	-
23	CLA	C	512	3	1/1/20/20	7/37/115/115	-
23	CLA	a	408	-	1/1/20/20	8/37/115/115	-
23	CLA	B	609	-	-	6/37/115/115	-
28	DGD	C	516	-	-	24/51/91/95	0/2/2/2
29	LHG	E	101	-	-	27/53/53/53	-
33	LMG	c	522	-	-	21/43/63/70	0/1/1/1
23	CLA	C	506	-	1/1/20/20	13/37/115/115	-
23	CLA	C	513	-	1/1/20/20	11/37/115/115	-
25	BCR	b	619	-	-	13/29/63/63	0/2/2/2
28	DGD	h	101	-	-	17/51/91/95	0/2/2/2
29	LHG	D	408	-	-	26/53/53/53	-
28	DGD	A	412	-	-	28/55/95/95	0/2/2/2
25	BCR	B	619	-	-	5/29/63/63	0/2/2/2
23	CLA	B	605	-	1/1/20/20	12/37/115/115	-
28	DGD	c	516	-	-	23/51/91/95	0/2/2/2
23	CLA	B	612	-	1/1/20/20	19/37/115/115	-
23	CLA	b	610	-	1/1/20/20	13/37/115/115	-
27	SQD	A	411	-	-	14/39/39/69	-
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	l	101	-	-	16/53/53/53	-
35	HEC	v	201	16	-	2/10/54/54	-
25	BCR	c	521	-	-	7/29/63/63	0/2/2/2
33	LMG	b	622	-	-	20/50/70/70	0/1/1/1
23	CLA	C	505	36	1/1/18/20	8/30/108/115	-
23	CLA	C	514	-	1/1/20/20	13/37/115/115	-
23	CLA	b	612	-	1/1/20/20	14/37/115/115	-
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
23	CLA	b	604	-	1/1/20/20	10/37/115/115	-
23	CLA	B	607	36	1/1/20/20	9/37/115/115	-
23	CLA	c	509	-	1/1/20/20	15/37/115/115	-
29	LHG	d	409	-	-	11/43/43/53	-
23	CLA	B	603	-	1/1/20/20	11/37/115/115	-
23	CLA	B	611	-	1/1/20/20	6/37/115/115	-
23	CLA	c	502	-	-	8/37/115/115	-
26	PL9	a	410	-	-	20/53/73/73	0/1/1/1
23	CLA	d	403	-	-	8/37/115/115	-
23	CLA	B	608	-	-	0/37/115/115	-
29	LHG	d	408	-	-	19/53/53/53	-
23	CLA	c	505	-	1/1/20/20	10/37/115/115	-
23	CLA	C	509	-	1/1/20/20	6/37/115/115	-
23	CLA	c	501	-	1/1/20/20	6/37/115/115	-
23	CLA	C	502	-	1/1/20/20	4/37/115/115	-
23	CLA	b	608	36	1/1/20/20	15/37/115/115	-
29	LHG	A	413	-	-	15/53/53/53	-
28	DGD	H	102	-	-	16/51/91/95	0/2/2/2
23	CLA	d	404	-	1/1/20/20	7/37/115/115	-
23	CLA	B	616	-	1/1/19/20	8/31/109/115	-
34	HEM	E	103	6,5	-	2/12/54/54	-
23	CLA	C	511	-	1/1/20/20	14/37/115/115	-
27	SQD	a	412	-	-	19/37/37/69	-
23	CLA	c	508	-	-	15/36/114/115	-
33	LMG	D	411	-	-	15/22/22/70	-

All (990) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	MG-NA	11.51	2.33	2.06
23	C	507	CLA	MG-ND	-11.00	1.84	2.05
23	C	505	CLA	MG-ND	-10.38	1.85	2.05
23	c	508	CLA	MG-ND	9.89	2.25	2.05
23	B	615	CLA	C4B-NB	9.83	1.44	1.35
23	c	506	CLA	MG-ND	-9.43	1.87	2.05
23	c	503	CLA	C4B-NB	9.41	1.43	1.35
23	d	404	CLA	MG-ND	-9.35	1.87	2.05
23	C	512	CLA	MG-NA	8.81	2.27	2.06
35	v	201	HEC	C2B-C3B	-8.55	1.31	1.40
23	c	504	CLA	C4B-NB	8.29	1.42	1.35
23	B	601	CLA	C4B-NB	8.29	1.42	1.35
23	C	504	CLA	MG-NA	8.14	2.25	2.06
23	c	505	CLA	C4B-NB	8.10	1.42	1.35
23	c	511	CLA	C4B-NB	8.10	1.42	1.35
35	V	201	HEC	C2B-C3B	-7.99	1.32	1.40
23	B	614	CLA	C4B-NB	7.95	1.42	1.35
23	B	616	CLA	C4B-NB	7.80	1.42	1.35
23	a	405	CLA	C4B-NB	7.73	1.42	1.35
23	d	404	CLA	C4B-NB	7.72	1.42	1.35
23	C	502	CLA	MG-NA	7.70	2.24	2.06
23	c	512	CLA	C4B-NB	7.69	1.42	1.35
23	b	615	CLA	C4B-NB	7.68	1.42	1.35
23	b	603	CLA	C4B-NB	7.64	1.42	1.35
23	C	502	CLA	C4B-NB	7.60	1.42	1.35
23	b	602	CLA	C4B-NB	7.57	1.42	1.35
23	B	610	CLA	C4B-NB	7.57	1.42	1.35
23	B	604	CLA	MG-NA	7.45	2.24	2.06
23	B	602	CLA	C4B-NB	7.36	1.41	1.35
23	C	513	CLA	MG-ND	-7.35	1.91	2.05
23	b	616	CLA	C4B-NB	7.34	1.41	1.35
23	b	606	CLA	C4B-NB	7.34	1.41	1.35
23	C	512	CLA	C4B-NB	7.33	1.41	1.35
35	V	201	HEC	C3C-C2C	-7.31	1.33	1.40
23	a	408	CLA	MG-NC	-7.30	1.88	2.06
23	d	402	CLA	C4B-NB	7.24	1.41	1.35
23	b	610	CLA	C4B-NB	7.17	1.41	1.35
23	b	604	CLA	C4B-NB	7.16	1.41	1.35
23	b	602	CLA	MG-NA	7.14	2.23	2.06
23	B	605	CLA	C4B-NB	7.11	1.41	1.35
23	c	511	CLA	MG-NA	7.07	2.23	2.06
23	C	504	CLA	C4B-NB	6.95	1.41	1.35
23	b	616	CLA	MG-ND	-6.93	1.92	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C4B-NB	6.92	1.41	1.35
23	c	501	CLA	MG-NA	6.90	2.22	2.06
23	b	609	CLA	MG-ND	-6.86	1.92	2.05
23	C	510	CLA	C4B-NB	6.82	1.41	1.35
23	c	509	CLA	C4B-NB	6.80	1.41	1.35
23	A	404	CLA	C4B-NB	6.79	1.41	1.35
23	C	506	CLA	C4B-NB	6.71	1.41	1.35
35	v	201	HEC	C3C-C2C	-6.66	1.33	1.40
23	C	511	CLA	C4B-NB	6.61	1.41	1.35
23	B	603	CLA	MG-NA	6.61	2.22	2.06
23	b	612	CLA	MG-ND	6.57	2.18	2.05
23	C	514	CLA	C4B-NB	6.50	1.41	1.35
23	c	513	CLA	C4B-NB	6.46	1.41	1.35
23	C	508	CLA	C4B-NB	6.43	1.40	1.35
23	b	607	CLA	C4B-NB	6.41	1.40	1.35
23	C	509	CLA	C4B-NB	6.36	1.40	1.35
23	B	606	CLA	MG-NA	6.30	2.21	2.06
23	B	611	CLA	MG-NA	6.29	2.21	2.06
23	A	407	CLA	MG-ND	-6.24	1.93	2.05
23	b	614	CLA	C4B-NB	6.23	1.40	1.35
23	B	613	CLA	C4B-NB	6.23	1.40	1.35
23	C	507	CLA	C4B-NB	6.22	1.40	1.35
23	B	601	CLA	MG-NA	6.21	2.21	2.06
23	C	505	CLA	C4B-NB	6.18	1.40	1.35
23	A	405	CLA	C4B-NB	6.11	1.40	1.35
23	b	609	CLA	C4B-NB	6.11	1.40	1.35
23	C	503	CLA	C4B-NB	5.92	1.40	1.35
23	c	501	CLA	C4B-NB	5.81	1.40	1.35
23	d	403	CLA	C4B-NB	5.81	1.40	1.35
26	D	406	PL9	C6-C1	-5.79	1.38	1.48
23	A	407	CLA	C4B-NB	5.79	1.40	1.35
23	b	617	CLA	C4B-NB	5.78	1.40	1.35
23	a	408	CLA	C4B-NB	5.76	1.40	1.35
23	c	510	CLA	C4B-NB	5.67	1.40	1.35
23	a	406	CLA	C4B-NB	5.66	1.40	1.35
23	B	615	CLA	MG-NC	5.58	2.19	2.06
23	c	507	CLA	C4B-NB	5.50	1.40	1.35
23	c	509	CLA	MG-ND	5.48	2.16	2.05
23	b	605	CLA	C4B-NB	5.46	1.40	1.35
28	a	413	DGD	O2G-C1B	5.42	1.49	1.34
23	b	616	CLA	MG-NC	-5.41	1.93	2.06
23	d	402	CLA	MG-NA	5.35	2.19	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C4B-NB	5.33	1.40	1.35
23	B	606	CLA	C4B-NB	5.33	1.40	1.35
23	B	603	CLA	C4B-NB	5.28	1.39	1.35
23	c	508	CLA	C4B-NB	5.28	1.39	1.35
26	A	409	PL9	C7-C3	-5.23	1.46	1.51
23	c	502	CLA	C4B-NB	5.23	1.39	1.35
23	b	608	CLA	C4B-NB	5.19	1.39	1.35
23	b	611	CLA	C4B-NB	5.18	1.39	1.35
23	C	513	CLA	C4B-NB	5.14	1.39	1.35
23	A	405	CLA	MG-NC	5.10	2.18	2.06
23	D	402	CLA	C4B-NB	5.10	1.39	1.35
23	B	609	CLA	MG-NC	-5.09	1.94	2.06
23	B	612	CLA	C4D-ND	-5.00	1.30	1.37
28	C	516	DGD	C4E-C3E	4.99	1.65	1.52
23	c	507	CLA	MG-ND	-4.99	1.95	2.05
23	B	613	CLA	MG-ND	-4.99	1.95	2.05
26	d	406	PL9	C7-C3	-4.98	1.46	1.51
23	B	608	CLA	MG-ND	-4.97	1.95	2.05
23	b	612	CLA	C4B-NB	4.94	1.39	1.35
23	b	607	CLA	MG-NA	4.89	2.17	2.06
25	B	618	BCR	C30-C25	-4.86	1.47	1.53
23	b	612	CLA	MG-NA	4.83	2.17	2.06
23	c	505	CLA	C4D-ND	-4.81	1.31	1.37
23	B	616	CLA	MG-ND	4.81	2.15	2.05
23	B	608	CLA	C4D-ND	-4.81	1.31	1.37
23	b	605	CLA	MG-ND	-4.73	1.96	2.05
23	C	507	CLA	MG-NA	4.72	2.17	2.06
23	C	509	CLA	MG-NA	4.70	2.17	2.06
33	d	411	LMG	O1-C7	-4.68	1.35	1.43
23	c	503	CLA	MG-NC	4.67	2.17	2.06
23	B	607	CLA	MG-ND	-4.66	1.96	2.05
23	a	406	CLA	C4D-ND	-4.64	1.31	1.37
34	E	103	HEM	C3C-C2C	-4.64	1.33	1.40
23	c	509	CLA	C1D-ND	4.61	1.43	1.37
23	B	607	CLA	C4B-NB	4.57	1.39	1.35
23	c	509	CLA	MG-NC	4.53	2.17	2.06
23	c	508	CLA	C4D-ND	-4.52	1.31	1.37
23	b	610	CLA	MG-ND	-4.45	1.97	2.05
23	D	403	CLA	C1D-ND	4.42	1.43	1.37
23	B	613	CLA	MG-NA	4.40	2.16	2.06
23	A	405	CLA	MG-NA	-4.39	1.95	2.06
28	A	412	DGD	C4D-C5D	4.38	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	CLA	C4D-ND	-4.37	1.31	1.37
23	b	603	CLA	C1D-ND	4.36	1.43	1.37
23	b	605	CLA	C4D-ND	-4.32	1.31	1.37
23	A	404	CLA	MG-NC	-4.30	1.96	2.06
23	c	509	CLA	C4D-ND	-4.29	1.31	1.37
23	B	606	CLA	C3B-C2B	-4.29	1.34	1.40
23	a	405	CLA	C1D-ND	4.26	1.43	1.37
23	A	407	CLA	C4D-ND	-4.25	1.31	1.37
25	B	617	BCR	C1-C6	-4.23	1.48	1.53
23	B	611	CLA	C4B-NB	4.20	1.39	1.35
25	K	101	BCR	C1-C6	-4.19	1.48	1.53
23	B	612	CLA	C4B-NB	4.18	1.38	1.35
25	b	619	BCR	C30-C25	-4.18	1.48	1.53
23	C	508	CLA	MG-NA	4.18	2.16	2.06
23	D	403	CLA	MG-ND	4.16	2.14	2.05
23	C	514	CLA	C1D-ND	4.16	1.42	1.37
25	H	101	BCR	C1-C6	-4.15	1.48	1.53
23	B	608	CLA	C4B-NB	4.14	1.38	1.35
23	D	404	CLA	C4B-NB	4.14	1.38	1.35
23	C	512	CLA	C1D-ND	4.14	1.42	1.37
23	c	505	CLA	CHC-C1C	4.13	1.45	1.35
29	D	409	LHG	P-O6	4.11	1.76	1.59
23	C	514	CLA	MG-NC	4.11	2.16	2.06
23	D	403	CLA	C4B-NB	4.11	1.38	1.35
23	D	402	CLA	C1D-ND	4.10	1.42	1.37
23	c	506	CLA	C1D-ND	4.08	1.42	1.37
23	B	615	CLA	C4D-ND	-4.06	1.32	1.37
35	V	201	HEC	CBB-CAB	-4.05	1.34	1.49
23	c	507	CLA	C3B-C2B	-4.01	1.34	1.40
23	b	610	CLA	C1D-ND	4.00	1.42	1.37
23	B	605	CLA	MG-NC	-3.99	1.96	2.06
23	C	503	CLA	C4D-ND	-3.99	1.32	1.37
23	c	512	CLA	C1D-ND	3.97	1.42	1.37
35	v	201	HEC	CBB-CAB	-3.97	1.34	1.49
33	D	410	LMG	C7-C8	3.95	1.61	1.51
23	D	404	CLA	C1D-ND	3.94	1.42	1.37
25	H	101	BCR	C30-C25	-3.94	1.48	1.53
23	B	611	CLA	C4D-ND	-3.94	1.32	1.37
35	v	201	HEC	CBC-CAC	-3.93	1.34	1.49
23	b	617	CLA	MG-NC	3.92	2.15	2.06
23	c	511	CLA	CHC-C1C	3.91	1.45	1.35
26	D	406	PL9	C52-C5	-3.90	1.42	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	CHC-C1C	3.89	1.44	1.35
25	b	618	BCR	C1-C6	-3.89	1.48	1.53
23	b	613	CLA	C4B-NB	3.88	1.38	1.35
25	K	101	BCR	C30-C25	-3.87	1.48	1.53
25	B	619	BCR	C1-C6	-3.87	1.48	1.53
35	V	201	HEC	CBC-CAC	-3.87	1.35	1.49
23	b	614	CLA	MG-NA	3.86	2.15	2.06
23	A	404	CLA	C4D-ND	-3.86	1.32	1.37
25	x	102	BCR	C30-C25	-3.84	1.48	1.53
23	B	605	CLA	CHC-C1C	3.83	1.44	1.35
23	b	609	CLA	CHC-C1C	3.83	1.44	1.35
23	C	507	CLA	C4D-ND	-3.83	1.32	1.37
23	c	504	CLA	CHC-C1C	3.82	1.44	1.35
28	a	413	DGD	C3G-C2G	3.82	1.60	1.51
23	b	614	CLA	MG-ND	-3.79	1.98	2.05
23	b	615	CLA	C4D-ND	-3.78	1.32	1.37
23	A	405	CLA	C4D-ND	-3.78	1.32	1.37
23	C	513	CLA	C4D-ND	-3.77	1.32	1.37
23	D	404	CLA	C3B-C2B	-3.76	1.35	1.40
27	b	601	SQD	O48-C23	3.76	1.44	1.33
34	e	102	HEM	C3C-C2C	-3.75	1.35	1.40
23	B	611	CLA	MG-NC	-3.74	1.97	2.06
23	C	511	CLA	CHC-C1C	3.73	1.44	1.35
23	b	611	CLA	C4D-ND	-3.73	1.32	1.37
23	b	607	CLA	C1D-ND	3.72	1.42	1.37
23	A	404	CLA	C1D-ND	3.72	1.42	1.37
23	D	403	CLA	C4D-ND	-3.71	1.32	1.37
25	C	515	BCR	C1-C6	-3.71	1.48	1.53
23	b	612	CLA	C4D-ND	-3.70	1.32	1.37
33	c	524	LMG	C4-C5	3.70	1.60	1.53
23	B	606	CLA	MG-ND	-3.69	1.98	2.05
23	d	402	CLA	CHC-C1C	3.69	1.44	1.35
23	B	613	CLA	C1D-ND	3.68	1.42	1.37
23	B	615	CLA	CMB-C2B	-3.67	1.44	1.51
23	b	616	CLA	C1D-ND	3.67	1.42	1.37
23	B	616	CLA	C4D-ND	-3.66	1.32	1.37
28	c	517	DGD	C6E-C5E	3.66	1.64	1.51
23	d	403	CLA	C4D-ND	-3.65	1.32	1.37
23	a	405	CLA	C1B-NB	3.64	1.38	1.35
23	B	610	CLA	CHC-C1C	3.64	1.44	1.35
23	D	402	CLA	C4D-ND	-3.64	1.32	1.37
25	b	619	BCR	C1-C6	-3.62	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C4D-ND	-3.61	1.32	1.37
23	d	403	CLA	C1D-ND	3.60	1.42	1.37
28	A	412	DGD	C4E-C5E	3.59	1.60	1.53
23	B	605	CLA	MG-ND	-3.59	1.98	2.05
23	b	615	CLA	CMB-C2B	-3.58	1.44	1.51
28	H	102	DGD	O1G-C1G	-3.58	1.37	1.45
28	h	101	DGD	O2D-C2D	-3.57	1.34	1.43
23	c	510	CLA	C1D-ND	3.57	1.42	1.37
23	B	604	CLA	C4D-ND	-3.56	1.32	1.37
23	c	513	CLA	MG-NA	3.56	2.14	2.06
23	b	602	CLA	CHC-C1C	3.56	1.44	1.35
23	c	501	CLA	MG-ND	-3.55	1.98	2.05
23	B	605	CLA	C4D-ND	-3.55	1.32	1.37
23	c	507	CLA	C4D-ND	-3.54	1.32	1.37
27	a	412	SQD	O48-C23	3.54	1.43	1.33
23	b	607	CLA	C4D-ND	-3.53	1.32	1.37
23	B	610	CLA	C4D-ND	-3.53	1.32	1.37
23	b	611	CLA	MG-NA	3.53	2.14	2.06
23	b	605	CLA	C1D-ND	3.52	1.42	1.37
23	C	506	CLA	CHC-C1C	3.52	1.44	1.35
23	B	604	CLA	C4B-NB	3.52	1.38	1.35
23	b	606	CLA	C4D-ND	-3.52	1.32	1.37
23	c	511	CLA	MG-ND	3.52	2.12	2.05
23	C	513	CLA	CHC-C1C	3.52	1.44	1.35
23	B	615	CLA	C1D-ND	3.51	1.42	1.37
23	b	617	CLA	C4D-ND	-3.51	1.32	1.37
25	A	408	BCR	C1-C6	-3.51	1.48	1.53
23	c	512	CLA	CHC-C1C	3.51	1.44	1.35
25	Z	101	BCR	C30-C25	-3.51	1.49	1.53
23	C	507	CLA	C1D-ND	3.50	1.42	1.37
23	c	504	CLA	C4D-ND	-3.50	1.32	1.37
26	D	406	PL9	C11-C9	-3.50	1.44	1.51
23	B	616	CLA	MG-NC	3.50	2.14	2.06
23	d	403	CLA	MG-NA	3.50	2.14	2.06
23	A	407	CLA	MG-NA	-3.49	1.98	2.06
23	A	404	CLA	CHC-C1C	3.49	1.43	1.35
23	C	505	CLA	MG-NA	3.49	2.14	2.06
23	C	511	CLA	C1D-ND	3.49	1.42	1.37
23	C	508	CLA	MG-ND	-3.48	1.98	2.05
25	d	405	BCR	C1-C6	-3.47	1.49	1.53
29	D	408	LHG	O8-C6	-3.47	1.37	1.45
23	A	404	CLA	MG-NA	3.47	2.14	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C1D-ND	3.46	1.42	1.37
23	C	502	CLA	CHC-C1C	3.46	1.43	1.35
23	b	604	CLA	C1D-ND	3.45	1.42	1.37
23	B	602	CLA	C1D-ND	3.44	1.42	1.37
23	C	514	CLA	C4D-ND	-3.44	1.33	1.37
23	b	602	CLA	C1D-ND	3.43	1.42	1.37
23	B	612	CLA	C1D-ND	3.43	1.42	1.37
23	B	614	CLA	MG-NA	3.43	2.14	2.06
23	c	503	CLA	C4D-ND	-3.42	1.33	1.37
23	B	605	CLA	C3B-C2B	-3.42	1.35	1.40
23	a	408	CLA	CMD-C2D	-3.42	1.43	1.50
23	B	601	CLA	C3B-C2B	-3.41	1.35	1.40
23	b	615	CLA	MG-ND	3.40	2.12	2.05
23	b	614	CLA	C4D-ND	-3.40	1.33	1.37
23	B	605	CLA	MG-NA	3.39	2.14	2.06
23	b	606	CLA	MG-NC	-3.39	1.98	2.06
23	B	616	CLA	C1D-ND	3.39	1.42	1.37
23	B	603	CLA	C1D-ND	3.39	1.41	1.37
23	b	617	CLA	C1D-ND	3.39	1.41	1.37
23	C	503	CLA	C1D-ND	3.38	1.41	1.37
23	C	508	CLA	MG-NC	-3.38	1.98	2.06
24	A	406	PHO	C3B-C2B	-3.37	1.35	1.40
23	B	604	CLA	CHC-C1C	3.36	1.43	1.35
23	c	506	CLA	C4D-ND	-3.36	1.33	1.37
23	B	608	CLA	C1D-ND	3.35	1.41	1.37
23	c	507	CLA	C1D-ND	3.35	1.41	1.37
23	B	601	CLA	CMB-C2B	-3.35	1.44	1.51
23	b	602	CLA	C1B-NB	3.35	1.38	1.35
28	c	518	DGD	C6D-C5D	3.34	1.62	1.51
23	b	603	CLA	CHC-C1C	3.34	1.43	1.35
23	B	605	CLA	CMB-C2B	-3.33	1.44	1.51
24	D	401	PHO	CAC-C3C	-3.33	1.46	1.52
27	A	411	SQD	O48-C23	3.33	1.43	1.33
23	b	604	CLA	MG-NC	3.33	2.14	2.06
23	B	614	CLA	MG-ND	-3.32	1.99	2.05
23	b	608	CLA	C4D-ND	-3.32	1.33	1.37
23	C	513	CLA	MG-NA	3.31	2.14	2.06
23	c	508	CLA	C1D-ND	3.31	1.41	1.37
23	C	513	CLA	C1D-ND	3.31	1.41	1.37
27	f	101	SQD	O47-C7	3.31	1.43	1.34
28	c	517	DGD	C3E-C2E	3.30	1.60	1.52
23	b	611	CLA	C1D-ND	3.29	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	MG-NA	3.29	2.14	2.06
23	C	509	CLA	CMB-C2B	-3.29	1.44	1.51
27	A	411	SQD	O47-C7	3.29	1.43	1.34
23	B	613	CLA	C4D-ND	-3.29	1.33	1.37
23	c	505	CLA	MG-NA	3.28	2.14	2.06
23	C	502	CLA	C1D-ND	3.28	1.41	1.37
23	b	614	CLA	C1D-ND	3.28	1.41	1.37
23	a	406	CLA	C3B-C2B	-3.28	1.35	1.40
26	d	406	PL9	C3-C4	-3.27	1.44	1.49
23	D	402	CLA	CHC-C1C	3.27	1.43	1.35
23	c	511	CLA	C1D-ND	3.26	1.41	1.37
25	T	101	BCR	C30-C25	-3.26	1.49	1.53
23	d	404	CLA	C4D-ND	-3.25	1.33	1.37
23	B	608	CLA	C1B-NB	-3.25	1.32	1.35
23	C	513	CLA	MG-NC	3.25	2.14	2.06
23	c	503	CLA	C1D-ND	3.25	1.41	1.37
23	B	610	CLA	CMB-C2B	-3.24	1.44	1.51
23	B	615	CLA	C3B-C2B	-3.24	1.35	1.40
23	c	510	CLA	CHC-C1C	3.24	1.43	1.35
23	c	511	CLA	C4D-ND	-3.23	1.33	1.37
28	c	516	DGD	O3G-C3G	-3.23	1.37	1.43
28	c	518	DGD	O2G-C1B	3.22	1.43	1.34
23	C	505	CLA	CHC-C1C	3.21	1.43	1.35
23	b	612	CLA	CHC-C1C	3.21	1.43	1.35
23	a	405	CLA	CHC-C1C	3.21	1.43	1.35
27	B	621	SQD	O47-C7	3.21	1.43	1.34
23	a	405	CLA	C4D-ND	-3.21	1.33	1.37
23	C	507	CLA	C3B-CAB	-3.21	1.41	1.47
23	a	408	CLA	C4B-CHC	-3.20	1.32	1.41
27	a	412	SQD	O47-C7	3.19	1.43	1.34
23	b	617	CLA	MG-NA	-3.19	1.98	2.06
23	d	402	CLA	C1D-ND	3.19	1.41	1.37
27	a	411	SQD	O48-C23	3.18	1.42	1.33
33	C	501	LMG	C4-C5	3.18	1.59	1.53
23	B	609	CLA	MG-NA	3.18	2.13	2.06
23	B	610	CLA	C3B-C2B	-3.18	1.36	1.40
23	B	614	CLA	CHC-C1C	3.18	1.43	1.35
23	d	403	CLA	CHC-C1C	3.18	1.43	1.35
23	C	510	CLA	CHC-C1C	3.18	1.43	1.35
23	b	603	CLA	C4D-ND	-3.17	1.33	1.37
23	c	502	CLA	CHC-C1C	3.17	1.43	1.35
27	B	621	SQD	O48-C23	3.17	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	520	BCR	C30-C25	-3.17	1.49	1.53
23	C	513	CLA	CMB-C2B	-3.17	1.45	1.51
23	b	613	CLA	MG-NA	-3.16	1.98	2.06
27	b	601	SQD	O47-C7	3.15	1.43	1.34
25	k	101	BCR	C30-C25	-3.14	1.49	1.53
23	b	604	CLA	C4D-ND	-3.14	1.33	1.37
23	B	601	CLA	C1D-ND	3.14	1.41	1.37
28	A	412	DGD	C3G-C2G	3.14	1.60	1.50
23	B	602	CLA	MG-NA	3.14	2.13	2.06
25	b	618	BCR	C30-C25	-3.13	1.49	1.53
23	c	505	CLA	CMB-C2B	-3.13	1.45	1.51
23	C	511	CLA	MG-NA	3.13	2.13	2.06
33	c	522	LMG	C7-C8	3.13	1.60	1.50
23	C	505	CLA	C1D-ND	3.12	1.41	1.37
23	c	508	CLA	CHC-C1C	3.12	1.43	1.35
23	C	504	CLA	C1D-ND	3.11	1.41	1.37
23	c	513	CLA	C1D-ND	3.11	1.41	1.37
27	A	410	SQD	O48-C23	3.11	1.42	1.33
27	f	101	SQD	O48-C23	3.11	1.42	1.33
23	B	609	CLA	C3B-C2B	-3.10	1.36	1.40
23	D	404	CLA	MG-NA	-3.10	1.98	2.06
23	D	404	CLA	CMD-C2D	-3.10	1.44	1.50
23	a	406	CLA	CMB-C2B	-3.10	1.45	1.51
23	c	507	CLA	CMB-C2B	-3.09	1.45	1.51
23	B	609	CLA	C4D-ND	-3.09	1.33	1.37
24	A	406	PHO	O2D-CGD	3.09	1.40	1.33
26	A	409	PL9	C37-C38	3.09	1.60	1.50
23	b	614	CLA	CHC-C1C	3.09	1.42	1.35
23	C	512	CLA	C4D-ND	-3.08	1.33	1.37
28	h	101	DGD	C1E-C2E	3.08	1.61	1.52
33	D	410	LMG	C9-C8	3.08	1.60	1.50
23	b	617	CLA	C3B-CAB	-3.07	1.41	1.47
23	C	509	CLA	C1D-ND	3.07	1.41	1.37
23	B	602	CLA	CHC-C1C	3.07	1.42	1.35
33	C	501	LMG	C4-C3	3.07	1.60	1.52
23	c	506	CLA	CHC-C1C	3.07	1.42	1.35
28	A	412	DGD	C6E-C5E	3.06	1.62	1.51
23	c	503	CLA	CHC-C1C	3.06	1.42	1.35
23	c	507	CLA	C3B-CAB	-3.06	1.41	1.47
33	d	411	LMG	O7-C8	-3.06	1.38	1.46
23	B	603	CLA	C4D-ND	-3.05	1.33	1.37
23	B	603	CLA	C3B-C2B	-3.05	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	412	DGD	C1E-C2E	3.04	1.61	1.52
25	c	515	BCR	C1-C6	-3.04	1.49	1.53
23	B	605	CLA	C1D-ND	3.04	1.41	1.37
28	c	518	DGD	C4E-C5E	3.04	1.59	1.53
27	A	411	SQD	O47-C45	-3.04	1.41	1.47
23	B	604	CLA	C1B-NB	3.04	1.37	1.35
23	B	606	CLA	CMB-C2B	-3.03	1.45	1.51
33	b	622	LMG	C4-C3	3.03	1.60	1.52
23	b	604	CLA	CHC-C1C	3.03	1.42	1.35
28	C	517	DGD	C4D-C3D	3.03	1.60	1.52
23	c	508	CLA	MG-NA	3.03	2.13	2.06
23	C	504	CLA	CMB-C2B	-3.03	1.45	1.51
23	C	512	CLA	CHC-C1C	3.03	1.42	1.35
33	C	519	LMG	O7-C8	-3.03	1.39	1.46
23	b	609	CLA	C4D-ND	-3.02	1.33	1.37
23	C	503	CLA	CHC-C1C	3.02	1.42	1.35
28	C	516	DGD	C3D-C2D	3.02	1.60	1.52
28	c	516	DGD	C4D-C3D	3.02	1.60	1.52
25	D	405	BCR	C1-C6	-3.01	1.49	1.53
23	B	612	CLA	CMC-C2C	-3.01	1.44	1.50
23	C	502	CLA	C4D-ND	-3.01	1.33	1.37
26	d	406	PL9	C6-C1	-3.00	1.43	1.48
23	b	609	CLA	C3B-CAB	-3.00	1.41	1.47
25	b	620	BCR	C1-C6	-3.00	1.49	1.53
23	c	512	CLA	C4D-ND	-3.00	1.33	1.37
23	B	611	CLA	CMB-C2B	-3.00	1.45	1.51
25	a	409	BCR	C30-C25	-2.99	1.49	1.53
23	b	610	CLA	MG-NA	2.99	2.13	2.06
25	T	101	BCR	C38-C26	-2.98	1.46	1.50
23	d	404	CLA	MG-NA	2.98	2.13	2.06
23	c	502	CLA	MG-NA	2.98	2.13	2.06
29	A	413	LHG	O7-C5	-2.97	1.39	1.46
23	D	403	CLA	MG-NA	2.97	2.13	2.06
23	B	615	CLA	C3B-CAB	-2.97	1.41	1.47
23	b	611	CLA	C3B-C2B	-2.96	1.36	1.40
23	c	506	CLA	C3B-C2B	-2.95	1.36	1.40
23	c	502	CLA	C4D-ND	-2.95	1.33	1.37
33	m	101	LMG	O7-C8	-2.95	1.39	1.46
23	d	402	CLA	C3B-C2B	-2.95	1.36	1.40
23	b	605	CLA	CHC-C1C	2.95	1.42	1.35
23	B	607	CLA	C4D-ND	-2.94	1.33	1.37
26	a	410	PL9	C53-C6	-2.94	1.44	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	CMB-C2B	-2.94	1.45	1.51
26	a	410	PL9	C3-C4	-2.94	1.44	1.49
26	d	406	PL9	C30-C29	-2.93	1.43	1.50
23	b	615	CLA	CMC-C2C	-2.93	1.44	1.50
33	c	524	LMG	O6-C5	-2.92	1.37	1.44
23	C	509	CLA	C4D-ND	-2.92	1.33	1.37
23	b	607	CLA	CHC-C1C	2.92	1.42	1.35
23	C	507	CLA	CHC-C1C	2.92	1.42	1.35
33	c	522	LMG	C1-C2	2.91	1.60	1.52
23	B	614	CLA	MG-NC	2.90	2.13	2.06
23	c	501	CLA	C1D-ND	2.90	1.41	1.37
27	A	410	SQD	O47-C7	2.89	1.42	1.34
23	B	608	CLA	C3B-C2B	-2.89	1.36	1.40
25	a	409	BCR	C1-C6	-2.89	1.49	1.53
23	b	609	CLA	C1D-ND	2.89	1.41	1.37
28	c	517	DGD	O4E-C4E	-2.89	1.36	1.43
23	c	506	CLA	CAC-C3C	-2.89	1.43	1.51
23	c	513	CLA	CHC-C1C	2.89	1.42	1.35
28	c	518	DGD	C2A-C1A	-2.88	1.42	1.50
23	C	509	CLA	MG-NC	2.88	2.13	2.06
23	A	407	CLA	C4B-CHC	-2.88	1.33	1.41
23	A	407	CLA	C1D-ND	2.87	1.41	1.37
23	b	615	CLA	CHC-C1C	2.87	1.42	1.35
23	B	612	CLA	CHC-C1C	2.87	1.42	1.35
23	c	503	CLA	CMB-C2B	-2.87	1.45	1.51
23	C	508	CLA	CHC-C1C	2.86	1.42	1.35
25	c	515	BCR	C30-C25	-2.85	1.49	1.53
24	a	407	PHO	C3B-C2B	-2.85	1.36	1.40
23	b	604	CLA	MG-ND	-2.85	2.00	2.05
23	c	503	CLA	C3B-CAB	-2.85	1.42	1.47
33	D	407	LMG	C6-C5	2.85	1.61	1.51
23	b	607	CLA	C3B-C2B	-2.84	1.36	1.40
23	B	615	CLA	MG-NA	2.84	2.13	2.06
27	F	101	SQD	O48-C23	2.84	1.41	1.33
26	a	410	PL9	C11-C9	-2.83	1.45	1.51
28	H	102	DGD	O3D-C3D	-2.83	1.36	1.43
23	D	403	CLA	CHC-C1C	2.83	1.42	1.35
23	b	613	CLA	CHC-C1C	2.82	1.42	1.35
23	b	615	CLA	C1D-ND	2.82	1.41	1.37
23	b	617	CLA	C3B-C2B	-2.82	1.36	1.40
23	B	603	CLA	CMA-C3A	-2.82	1.47	1.53
23	c	513	CLA	C4D-ND	-2.82	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	O2A-CGA	2.82	1.41	1.33
23	C	510	CLA	C4D-ND	-2.82	1.33	1.37
23	c	510	CLA	C4D-ND	-2.81	1.33	1.37
25	D	405	BCR	C30-C25	-2.81	1.49	1.53
28	A	412	DGD	O5D-C1E	2.81	1.45	1.40
23	D	404	CLA	C3B-CAB	-2.80	1.42	1.47
23	c	503	CLA	C3B-C2B	-2.80	1.36	1.40
25	c	521	BCR	C1-C6	-2.80	1.49	1.53
23	D	403	CLA	C1C-NC	-2.79	1.33	1.37
23	b	616	CLA	CHC-C1C	2.79	1.42	1.35
33	c	522	LMG	O1-C1	2.79	1.44	1.40
28	C	518	DGD	C1G-C2G	2.79	1.59	1.50
27	A	410	SQD	O2-C2	-2.78	1.36	1.43
23	C	506	CLA	CMB-C2B	-2.78	1.45	1.51
27	a	411	SQD	O47-C7	2.78	1.42	1.34
23	D	404	CLA	MG-NC	2.77	2.12	2.06
23	C	511	CLA	C4D-ND	-2.77	1.33	1.37
23	d	404	CLA	CMB-C2B	-2.77	1.45	1.51
23	b	612	CLA	CMB-C2B	-2.77	1.45	1.51
23	C	508	CLA	C1D-ND	2.77	1.41	1.37
23	B	616	CLA	CMC-C2C	-2.77	1.44	1.50
23	D	404	CLA	C4D-ND	-2.76	1.33	1.37
23	b	608	CLA	CMB-C2B	-2.76	1.45	1.51
23	A	404	CLA	MG-ND	-2.76	2.00	2.05
25	c	515	BCR	C33-C5	-2.76	1.46	1.50
23	B	607	CLA	C3B-C2B	-2.76	1.36	1.40
23	B	609	CLA	C4B-CHC	-2.76	1.33	1.41
23	B	609	CLA	CMD-C2D	-2.76	1.45	1.50
23	D	404	CLA	CHC-C1C	2.76	1.42	1.35
23	C	508	CLA	C3B-C2B	-2.76	1.36	1.40
23	B	615	CLA	CHC-C1C	2.76	1.42	1.35
23	B	607	CLA	C1D-ND	2.76	1.41	1.37
23	B	607	CLA	CHC-C1C	2.76	1.42	1.35
23	B	611	CLA	CMD-C2D	-2.76	1.45	1.50
33	c	519	LMG	C4-C5	2.75	1.58	1.53
28	h	101	DGD	O1G-C1G	-2.75	1.38	1.45
23	B	612	CLA	MG-ND	-2.75	2.00	2.05
23	b	606	CLA	CMB-C2B	-2.75	1.45	1.51
23	c	511	CLA	MG-NC	2.75	2.12	2.06
23	B	613	CLA	C3B-CAB	-2.75	1.42	1.47
24	a	407	PHO	CAC-C3C	-2.74	1.47	1.52
26	D	406	PL9	C30-C29	-2.74	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CMB-C2B	-2.74	1.45	1.51
23	c	512	CLA	MG-NC	2.74	2.12	2.06
23	b	617	CLA	CMD-C2D	-2.74	1.45	1.50
23	a	406	CLA	CHC-C1C	2.73	1.42	1.35
25	k	101	BCR	C1-C6	-2.73	1.50	1.53
23	B	606	CLA	C4D-ND	-2.73	1.33	1.37
33	d	411	LMG	O2-C2	-2.73	1.36	1.43
23	d	404	CLA	C3B-CAB	-2.73	1.42	1.47
23	b	603	CLA	CMD-C2D	-2.73	1.45	1.50
23	B	611	CLA	C1B-NB	2.73	1.37	1.35
23	B	613	CLA	C4B-CHC	-2.72	1.33	1.41
23	a	408	CLA	CMB-C2B	-2.72	1.46	1.51
23	d	404	CLA	C3B-C2B	-2.72	1.36	1.40
23	d	404	CLA	CMD-C2D	-2.72	1.45	1.50
34	e	102	HEM	C3C-CAC	2.71	1.53	1.47
23	c	503	CLA	MG-NA	2.71	2.12	2.06
23	b	611	CLA	CMB-C2B	-2.71	1.46	1.51
28	H	102	DGD	C1E-C2E	2.71	1.60	1.52
25	Z	101	BCR	C1-C6	-2.71	1.50	1.53
24	D	401	PHO	CMC-C2C	-2.71	1.45	1.51
23	A	407	CLA	MG-NC	-2.71	1.99	2.06
23	C	506	CLA	C4D-ND	-2.70	1.34	1.37
28	H	102	DGD	O2D-C2D	-2.70	1.36	1.43
23	B	609	CLA	CMC-C2C	-2.70	1.45	1.50
23	A	405	CLA	CHC-C1C	2.70	1.41	1.35
23	C	509	CLA	MG-ND	-2.70	2.00	2.05
23	d	402	CLA	C4D-ND	-2.69	1.34	1.37
25	B	618	BCR	C1-C6	-2.69	1.50	1.53
23	C	504	CLA	C4B-CHC	-2.69	1.33	1.41
23	C	507	CLA	C3B-C2B	-2.69	1.36	1.40
28	C	516	DGD	O1G-C1A	2.69	1.41	1.33
23	C	506	CLA	C3B-C2B	-2.68	1.36	1.40
23	c	501	CLA	CAC-C3C	-2.68	1.44	1.51
28	c	516	DGD	C3D-C2D	2.67	1.59	1.52
23	B	606	CLA	C1D-ND	2.66	1.41	1.37
23	b	612	CLA	C3B-C2B	-2.66	1.36	1.40
23	a	408	CLA	CMC-C2C	-2.66	1.45	1.50
28	H	102	DGD	C4D-C5D	2.66	1.58	1.53
29	e	101	LHG	O7-C5	-2.66	1.39	1.46
23	B	609	CLA	CMB-C2B	-2.66	1.46	1.51
25	T	101	BCR	C1-C6	-2.65	1.50	1.53
29	E	101	LHG	O7-C5	-2.65	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402	CLA	CMB-C2B	-2.65	1.46	1.51
33	c	522	LMG	C4-C3	2.65	1.59	1.52
23	B	608	CLA	CMD-C2D	-2.65	1.45	1.50
28	A	412	DGD	O2G-C1B	2.65	1.41	1.34
23	C	509	CLA	C3B-C2B	-2.64	1.36	1.40
23	C	509	CLA	CHC-C1C	2.64	1.41	1.35
23	B	616	CLA	CMD-C2D	-2.64	1.45	1.50
24	d	401	PHO	CAC-C3C	-2.64	1.47	1.52
23	B	610	CLA	MG-ND	2.64	2.11	2.05
25	C	515	BCR	C33-C5	-2.64	1.46	1.50
24	A	406	PHO	CMD-C2D	-2.64	1.45	1.51
23	C	513	CLA	C3B-C2B	-2.63	1.36	1.40
28	C	518	DGD	O2G-C2G	-2.63	1.40	1.46
23	B	601	CLA	C3B-CAB	-2.63	1.42	1.47
23	B	604	CLA	C1D-C2D	2.63	1.50	1.45
23	c	504	CLA	MG-NC	2.63	2.12	2.06
23	c	507	CLA	MG-NA	-2.63	2.00	2.06
23	b	610	CLA	C4D-ND	-2.63	1.34	1.37
23	C	503	CLA	CMB-C2B	-2.62	1.46	1.51
23	c	512	CLA	C3B-CAB	-2.62	1.42	1.47
25	d	405	BCR	C30-C25	-2.62	1.50	1.53
23	c	507	CLA	C4B-CHC	-2.62	1.33	1.41
23	C	514	CLA	CHC-C1C	2.62	1.41	1.35
23	b	614	CLA	CMB-C2B	-2.62	1.46	1.51
23	B	613	CLA	C1C-NC	-2.61	1.33	1.37
23	c	503	CLA	CMC-C2C	-2.61	1.45	1.50
23	C	508	CLA	CMB-C2B	-2.61	1.46	1.51
23	b	604	CLA	C3B-C2B	-2.61	1.36	1.40
23	a	405	CLA	MG-NA	2.61	2.12	2.06
23	b	608	CLA	C1C-NC	-2.60	1.33	1.37
23	b	610	CLA	CMB-C2B	-2.60	1.46	1.51
23	B	609	CLA	C3B-CAB	-2.59	1.42	1.47
28	H	102	DGD	O5D-C6D	-2.59	1.39	1.43
24	d	401	PHO	CMC-C2C	-2.59	1.45	1.51
23	B	611	CLA	C1D-ND	2.59	1.41	1.37
25	c	514	BCR	C1-C6	-2.59	1.50	1.53
23	D	403	CLA	CMD-C2D	-2.59	1.45	1.50
25	B	617	BCR	C33-C5	-2.58	1.46	1.50
23	A	407	CLA	CMC-C2C	-2.58	1.45	1.50
23	C	514	CLA	MG-NA	2.58	2.12	2.06
23	B	616	CLA	C3B-C2B	-2.58	1.36	1.40
23	B	606	CLA	CHC-C1C	2.58	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	CMB-C2B	-2.58	1.46	1.51
23	B	611	CLA	CHC-C1C	2.57	1.41	1.35
23	C	503	CLA	C3B-C2B	-2.57	1.36	1.40
23	C	514	CLA	CMB-C2B	-2.57	1.46	1.51
28	h	101	DGD	C4E-C3E	2.57	1.58	1.52
23	b	603	CLA	MG-NA	2.57	2.12	2.06
23	C	502	CLA	C3B-C2B	-2.57	1.36	1.40
23	d	402	CLA	CMB-C2B	-2.57	1.46	1.51
23	b	616	CLA	CMB-C2B	-2.56	1.46	1.51
29	L	101	LHG	O8-C23	2.56	1.40	1.33
29	l	101	LHG	O8-C23	2.56	1.40	1.33
23	a	405	CLA	CMD-C2D	-2.55	1.45	1.50
28	C	518	DGD	O3E-C3E	-2.55	1.37	1.43
23	b	612	CLA	MG-NC	-2.55	2.00	2.06
28	A	412	DGD	C4D-C3D	2.55	1.58	1.52
28	H	102	DGD	O5D-C1E	2.55	1.44	1.40
28	C	518	DGD	C4E-C3E	2.54	1.58	1.52
23	c	513	CLA	CMB-C2B	-2.54	1.46	1.51
23	A	404	CLA	C3B-CAB	-2.53	1.42	1.47
23	A	405	CLA	CMB-C2B	-2.53	1.46	1.51
23	C	508	CLA	C4D-ND	-2.53	1.34	1.37
23	b	603	CLA	MG-ND	-2.53	2.00	2.05
23	C	505	CLA	CMB-C2B	-2.53	1.46	1.51
26	a	410	PL9	C6-C1	-2.53	1.44	1.48
23	A	404	CLA	C1B-NB	2.53	1.37	1.35
28	C	516	DGD	O2G-C2G	-2.53	1.40	1.46
23	B	604	CLA	MG-ND	2.52	2.10	2.05
23	B	604	CLA	C1D-ND	2.52	1.40	1.37
33	C	519	LMG	O3-C3	-2.52	1.37	1.43
23	A	407	CLA	CMB-C2B	-2.52	1.46	1.51
33	M	101	LMG	C1-C2	2.51	1.59	1.52
23	a	408	CLA	CMA-C3A	-2.51	1.47	1.53
23	B	608	CLA	CMB-C2B	-2.51	1.46	1.51
23	C	513	CLA	CMD-C2D	-2.51	1.45	1.50
27	A	410	SQD	O3-C3	-2.51	1.37	1.43
33	d	410	LMG	O7-C10	2.51	1.39	1.30
26	a	410	PL9	C7-C3	-2.51	1.48	1.51
34	E	103	HEM	CAB-C3B	2.51	1.54	1.47
29	E	101	LHG	O8-C23	2.50	1.40	1.33
33	C	519	LMG	O4-C4	-2.50	1.37	1.43
23	b	604	CLA	CMC-C2C	-2.50	1.45	1.50
23	B	603	CLA	C3B-CAB	-2.50	1.42	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	CMB-C2B	-2.49	1.46	1.51
23	d	403	CLA	CAA-C2A	-2.49	1.49	1.54
23	a	408	CLA	C3B-C2B	-2.49	1.36	1.40
26	d	406	PL9	C53-C6	-2.49	1.45	1.50
23	B	616	CLA	C3B-CAB	-2.49	1.42	1.47
23	c	502	CLA	MG-ND	2.49	2.10	2.05
23	C	510	CLA	CMB-C2B	-2.49	1.46	1.51
23	b	611	CLA	CHC-C1C	2.49	1.41	1.35
23	b	608	CLA	C3B-C2B	-2.48	1.36	1.40
23	b	606	CLA	CHC-C1C	2.48	1.41	1.35
28	C	517	DGD	C3E-C2E	2.48	1.58	1.52
23	B	607	CLA	C3B-CAB	-2.47	1.42	1.47
23	c	508	CLA	CMC-C2C	-2.47	1.45	1.50
23	B	601	CLA	CHC-C1C	2.47	1.41	1.35
34	E	103	HEM	C3C-CAC	2.47	1.52	1.47
23	b	603	CLA	CAC-C3C	-2.46	1.44	1.51
23	b	611	CLA	CMD-C2D	-2.46	1.45	1.50
23	b	605	CLA	CMB-C2B	-2.46	1.46	1.51
23	c	504	CLA	C1D-ND	2.46	1.40	1.37
23	b	604	CLA	CMD-C2D	-2.46	1.45	1.50
27	f	101	SQD	O2-C2	-2.46	1.37	1.43
23	a	405	CLA	CMB-C2B	-2.45	1.46	1.51
23	B	602	CLA	C4D-ND	-2.45	1.34	1.37
23	c	507	CLA	CMC-C2C	-2.44	1.45	1.50
29	D	408	LHG	C24-C23	2.44	1.57	1.50
23	c	505	CLA	C3B-CAB	-2.44	1.43	1.47
23	C	504	CLA	CHC-C1C	2.44	1.41	1.35
23	c	506	CLA	MG-NC	2.44	2.12	2.06
33	c	519	LMG	O2-C2	-2.44	1.37	1.43
28	C	517	DGD	O4E-C4E	-2.44	1.37	1.43
23	C	502	CLA	C3D-C4D	2.43	1.49	1.44
23	b	605	CLA	MG-NC	2.43	2.12	2.06
33	m	101	LMG	O6-C5	-2.43	1.38	1.44
23	B	607	CLA	MG-NC	2.43	2.12	2.06
23	b	608	CLA	CMD-C2D	-2.43	1.45	1.50
33	c	522	LMG	C3-C2	2.43	1.58	1.52
25	c	515	BCR	C38-C26	-2.42	1.47	1.50
23	C	512	CLA	C1D-C2D	2.42	1.50	1.45
28	h	101	DGD	C4D-C5D	2.42	1.58	1.53
23	B	602	CLA	CMB-C2B	-2.42	1.46	1.51
23	C	504	CLA	C3B-C2B	-2.42	1.37	1.40
23	C	510	CLA	MG-ND	2.42	2.10	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	C3B-CAB	-2.42	1.42	1.47
24	a	407	PHO	CBD-CGD	-2.42	1.49	1.52
33	c	522	LMG	O6-C5	-2.42	1.38	1.44
33	D	407	LMG	O2-C2	-2.41	1.37	1.43
24	A	406	PHO	C3B-CAB	-2.41	1.42	1.47
23	C	508	CLA	CMC-C2C	-2.41	1.45	1.50
28	A	412	DGD	C3E-C2E	2.41	1.58	1.52
23	a	406	CLA	C3B-CAB	-2.40	1.43	1.47
28	C	517	DGD	O3G-C3G	-2.40	1.39	1.43
23	c	512	CLA	CMD-C2D	-2.40	1.45	1.50
23	b	607	CLA	C4B-CHC	-2.39	1.34	1.41
25	C	515	BCR	C30-C25	-2.39	1.50	1.53
23	B	601	CLA	C1D-C2D	2.39	1.50	1.45
28	C	517	DGD	C1E-C2E	2.38	1.59	1.52
24	A	406	PHO	CBD-CGD	-2.38	1.49	1.52
28	a	413	DGD	C1G-C2G	2.38	1.58	1.50
28	C	516	DGD	O2D-C2D	-2.38	1.37	1.43
23	A	405	CLA	CMD-C2D	-2.38	1.45	1.50
23	d	403	CLA	CMB-C2B	-2.38	1.46	1.51
23	B	613	CLA	CMC-C2C	-2.38	1.45	1.50
33	d	411	LMG	C4-C5	2.38	1.58	1.53
25	c	521	BCR	C38-C26	-2.38	1.47	1.50
23	b	616	CLA	C4D-ND	-2.37	1.34	1.37
33	b	622	LMG	O1-C7	-2.37	1.39	1.43
23	B	604	CLA	O2A-CGA	2.37	1.40	1.33
23	b	612	CLA	C3B-CAB	-2.37	1.43	1.47
23	D	403	CLA	C3B-C2B	-2.37	1.37	1.40
23	B	607	CLA	CMB-C2B	-2.37	1.46	1.51
23	C	511	CLA	O2A-CGA	2.37	1.40	1.33
25	B	617	BCR	C30-C25	-2.37	1.50	1.53
23	B	606	CLA	C3B-CAB	-2.37	1.43	1.47
23	C	503	CLA	MG-NA	2.37	2.11	2.06
28	C	516	DGD	C4D-C3D	2.36	1.58	1.52
25	b	618	BCR	C33-C5	-2.36	1.47	1.50
33	C	501	LMG	C7-C8	2.36	1.57	1.50
33	b	622	LMG	C4-C5	2.36	1.58	1.53
23	a	408	CLA	C1D-ND	2.36	1.40	1.37
23	b	609	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	602	CLA	CMB-C2B	-2.36	1.46	1.51
23	c	506	CLA	C3B-CAB	-2.35	1.43	1.47
23	b	613	CLA	C1B-NB	-2.35	1.33	1.35
28	A	412	DGD	O6D-C1D	2.35	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	CMD-C2D	-2.35	1.45	1.50
23	B	603	CLA	CMB-C2B	-2.35	1.46	1.51
26	A	409	PL9	C10-C9	-2.34	1.44	1.50
29	L	101	LHG	O7-C5	-2.34	1.40	1.46
23	c	505	CLA	C1D-ND	2.34	1.40	1.37
23	B	613	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	615	CLA	C1D-C2D	2.34	1.49	1.45
35	V	201	HEC	C2A-C3A	-2.34	1.30	1.37
23	c	501	CLA	MG-NC	2.34	2.11	2.06
23	b	603	CLA	C4B-CHC	-2.33	1.34	1.41
33	D	410	LMG	O8-C28	2.33	1.40	1.33
33	m	101	LMG	O1-C7	-2.33	1.39	1.43
23	C	507	CLA	CMB-C2B	-2.33	1.46	1.51
28	c	518	DGD	O6E-C1E	-2.33	1.35	1.41
29	L	101	LHG	P-O6	2.33	1.68	1.59
23	B	614	CLA	C1B-NB	2.32	1.37	1.35
27	f	101	SQD	O3-C3	-2.32	1.37	1.43
28	c	518	DGD	O2D-C2D	-2.32	1.37	1.43
23	A	407	CLA	CMD-C2D	-2.32	1.45	1.50
23	C	502	CLA	CMD-C2D	-2.32	1.45	1.50
23	c	512	CLA	C3D-C4D	2.32	1.49	1.44
23	D	403	CLA	CMB-C2B	-2.32	1.46	1.51
23	B	614	CLA	CMB-C2B	-2.31	1.46	1.51
23	c	501	CLA	CMD-C2D	-2.31	1.45	1.50
23	b	616	CLA	CMC-C2C	-2.31	1.45	1.50
29	D	409	LHG	O7-C7	2.31	1.40	1.34
23	B	601	CLA	CMD-C2D	-2.31	1.45	1.50
23	d	404	CLA	C1D-ND	2.31	1.40	1.37
33	D	407	LMG	O8-C28	2.30	1.40	1.33
33	C	519	LMG	C3-C2	2.30	1.58	1.52
23	B	608	CLA	CHC-C1C	2.29	1.40	1.35
23	b	609	CLA	C3B-C2B	-2.29	1.37	1.40
27	A	410	SQD	O4-C4	-2.29	1.37	1.43
29	D	408	LHG	O7-C5	-2.29	1.40	1.46
23	B	616	CLA	CMB-C2B	-2.29	1.46	1.51
33	C	501	LMG	O7-C8	-2.29	1.40	1.46
23	c	513	CLA	CMD-C2D	-2.29	1.46	1.50
23	b	614	CLA	C5-C3	-2.29	1.46	1.51
28	c	517	DGD	C4E-C5E	2.28	1.57	1.53
23	B	609	CLA	CAC-C3C	-2.28	1.45	1.51
28	H	102	DGD	C4E-C3E	2.28	1.58	1.52
29	e	101	LHG	P-O6	2.28	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	411	LMG	O8-C28	2.28	1.38	1.30
23	B	614	CLA	C4D-ND	-2.28	1.34	1.37
27	a	411	SQD	O3-C3	-2.27	1.37	1.43
23	a	408	CLA	C1C-NC	-2.27	1.34	1.37
23	B	604	CLA	MG-NC	-2.27	2.00	2.06
23	D	402	CLA	C3B-C2B	-2.27	1.37	1.40
29	e	101	LHG	O8-C23	2.27	1.40	1.33
29	d	409	LHG	P-O6	2.27	1.68	1.59
33	b	622	LMG	C7-C8	2.27	1.57	1.50
25	B	619	BCR	C30-C25	-2.26	1.50	1.53
23	b	610	CLA	CHC-C1C	2.26	1.40	1.35
26	D	406	PL9	C41-C39	-2.26	1.46	1.51
28	C	517	DGD	O3D-C3D	-2.26	1.37	1.43
23	B	605	CLA	CMC-C2C	-2.26	1.46	1.50
25	T	101	BCR	C27-C26	-2.26	1.46	1.51
26	A	409	PL9	C21-C19	2.26	1.56	1.51
23	B	603	CLA	C1A-CHA	-2.26	1.33	1.43
23	D	404	CLA	C4B-CHC	-2.26	1.34	1.41
28	C	517	DGD	O6D-C5D	-2.25	1.38	1.44
26	d	406	PL9	C7-C8	-2.25	1.47	1.50
23	C	512	CLA	CMB-C2B	-2.25	1.47	1.51
23	b	603	CLA	C1B-NB	2.25	1.37	1.35
23	c	506	CLA	C4B-CHC	-2.25	1.34	1.41
28	A	412	DGD	O1G-C1A	2.25	1.39	1.33
23	B	606	CLA	C4B-CHC	-2.24	1.34	1.41
28	H	102	DGD	C6D-C5D	2.24	1.58	1.51
29	D	409	LHG	O3-C3	-2.24	1.36	1.44
25	A	408	BCR	C33-C5	-2.24	1.47	1.50
23	b	614	CLA	C3B-CAB	-2.24	1.43	1.47
23	B	603	CLA	CHC-C1C	2.24	1.40	1.35
33	D	407	LMG	O6-C5	-2.24	1.38	1.44
23	a	406	CLA	MG-ND	-2.23	2.01	2.05
25	t	101	BCR	C30-C25	-2.23	1.50	1.53
23	c	513	CLA	CMC-C2C	-2.22	1.46	1.50
28	H	102	DGD	C4E-C5E	2.22	1.57	1.53
23	d	402	CLA	C3D-C4D	2.22	1.49	1.44
24	d	401	PHO	CMD-C2D	-2.22	1.46	1.51
35	V	201	HEC	CMD-C2D	2.22	1.56	1.51
28	c	518	DGD	C1E-C2E	2.22	1.58	1.52
23	C	505	CLA	MG-NC	2.21	2.11	2.06
23	B	614	CLA	C3B-CAB	-2.21	1.43	1.47
23	B	606	CLA	CMD-C2D	-2.21	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	518	DGD	O2E-C2E	-2.21	1.37	1.43
23	b	604	CLA	C3B-CAB	-2.21	1.43	1.47
28	a	413	DGD	O1G-C1A	2.21	1.39	1.33
23	c	508	CLA	CMD-C2D	-2.20	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.20	1.46	1.50
33	C	501	LMG	O1-C1	2.20	1.43	1.40
26	D	406	PL9	C27-C28	-2.20	1.43	1.50
27	B	621	SQD	O2-C2	-2.20	1.37	1.43
25	C	515	BCR	C38-C26	-2.20	1.47	1.50
34	e	102	HEM	C3B-C2B	-2.20	1.32	1.37
25	C	515	BCR	C34-C9	-2.20	1.46	1.50
23	A	407	CLA	C3B-CAB	-2.19	1.43	1.47
25	b	620	BCR	C30-C25	-2.19	1.50	1.53
23	C	510	CLA	MG-NA	2.19	2.11	2.06
23	b	617	CLA	CHC-C1C	2.19	1.40	1.35
23	C	511	CLA	CMD-C2D	-2.18	1.46	1.50
27	a	411	SQD	O2-C2	-2.18	1.37	1.43
29	E	101	LHG	P-O6	2.18	1.68	1.59
28	C	517	DGD	C1G-C2G	2.18	1.57	1.50
28	c	516	DGD	O3E-C3E	-2.18	1.37	1.43
23	C	511	CLA	MG-NC	2.18	2.11	2.06
28	h	101	DGD	C3G-C2G	2.18	1.57	1.50
23	C	504	CLA	CMC-C2C	-2.18	1.46	1.50
23	C	505	CLA	CMD-C2D	-2.17	1.46	1.50
29	A	413	LHG	O6-C4	-2.17	1.36	1.44
23	b	606	CLA	MG-NA	2.17	2.11	2.06
28	C	516	DGD	C2B-C1B	-2.17	1.44	1.50
27	A	410	SQD	O47-C45	-2.17	1.41	1.46
25	D	405	BCR	C27-C26	-2.17	1.46	1.51
23	b	603	CLA	CMB-C2B	-2.17	1.47	1.51
33	m	101	LMG	O4-C4	-2.17	1.37	1.43
23	c	506	CLA	CMB-C2B	-2.17	1.47	1.51
28	c	518	DGD	C3G-C2G	2.17	1.57	1.50
23	B	608	CLA	MG-NA	-2.17	2.01	2.06
23	b	615	CLA	C1A-CHA	-2.16	1.34	1.43
23	c	504	CLA	C1C-C2C	2.16	1.48	1.44
28	c	518	DGD	O1G-C1G	-2.16	1.40	1.45
23	B	610	CLA	CMA-C3A	-2.16	1.48	1.53
23	B	615	CLA	C5-C3	-2.16	1.46	1.51
23	B	607	CLA	CAC-C3C	-2.16	1.45	1.51
28	C	518	DGD	C2A-C1A	-2.16	1.44	1.50
23	b	608	CLA	CHC-C1C	2.16	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	520	BCR	C38-C26	-2.15	1.47	1.50
23	B	609	CLA	C1D-ND	2.15	1.40	1.37
23	b	615	CLA	C3B-C2B	-2.15	1.37	1.40
25	C	520	BCR	C1-C6	-2.15	1.50	1.53
24	a	407	PHO	CMB-C2B	-2.15	1.46	1.51
26	D	406	PL9	C5-C4	-2.15	1.39	1.47
26	d	406	PL9	C46-C44	-2.14	1.46	1.51
23	C	508	CLA	C1B-NB	-2.14	1.33	1.35
23	B	608	CLA	C4B-CHC	-2.14	1.35	1.41
23	b	607	CLA	CMB-C2B	-2.14	1.47	1.51
23	b	611	CLA	C1C-NC	-2.14	1.34	1.37
23	B	612	CLA	CMD-C2D	-2.14	1.46	1.50
23	B	603	CLA	C3C-C2C	2.14	1.41	1.36
26	A	409	PL9	C3-C4	-2.14	1.46	1.49
23	b	613	CLA	CMC-C2C	-2.13	1.46	1.50
28	c	516	DGD	O5D-C1E	2.13	1.43	1.40
23	c	509	CLA	C3C-C2C	2.13	1.41	1.36
25	B	619	BCR	C38-C26	-2.13	1.47	1.50
29	l	101	LHG	P-O6	2.13	1.67	1.59
23	C	505	CLA	C3B-C2B	-2.13	1.37	1.40
24	D	401	PHO	C3B-C2B	-2.13	1.37	1.40
23	c	505	CLA	CMD-C2D	-2.13	1.46	1.50
28	A	412	DGD	O1G-C1G	-2.13	1.40	1.45
23	c	502	CLA	CMC-C2C	-2.13	1.46	1.50
23	b	613	CLA	O2D-CED	-2.13	1.40	1.45
25	B	618	BCR	C39-C30	-2.13	1.49	1.53
23	C	506	CLA	C4C-C3C	2.13	1.48	1.45
23	C	507	CLA	C1A-CHA	-2.12	1.34	1.43
23	B	607	CLA	C4B-CHC	-2.12	1.35	1.41
27	a	411	SQD	O4-C4	-2.12	1.38	1.43
23	B	606	CLA	CMC-C2C	-2.12	1.46	1.50
23	a	405	CLA	CMC-C2C	-2.12	1.46	1.50
23	b	606	CLA	CMD-C2D	-2.12	1.46	1.50
23	C	504	CLA	C4D-ND	-2.12	1.34	1.37
23	C	511	CLA	CAA-C2A	-2.12	1.50	1.54
29	d	409	LHG	C3-C2	2.12	1.58	1.51
27	A	411	SQD	C46-C45	2.12	1.55	1.50
23	B	608	CLA	C3D-C4D	2.12	1.49	1.44
23	b	603	CLA	C3B-CAB	-2.12	1.43	1.47
25	A	408	BCR	C27-C26	-2.12	1.46	1.51
23	C	509	CLA	C1D-C2D	2.11	1.49	1.45
33	D	407	LMG	C4-C3	2.11	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	CMD-C2D	-2.11	1.46	1.50
23	d	403	CLA	CMC-C2C	-2.11	1.46	1.50
23	b	613	CLA	CMB-C2B	-2.11	1.47	1.51
23	D	402	CLA	C4B-CHC	-2.11	1.35	1.41
23	C	512	CLA	C1B-NB	2.11	1.37	1.35
23	B	604	CLA	C3B-C2B	-2.11	1.37	1.40
33	c	519	LMG	O8-C9	-2.10	1.40	1.45
33	C	519	LMG	C4-C3	2.10	1.57	1.52
23	C	507	CLA	CMA-C3A	-2.10	1.48	1.53
23	b	610	CLA	CMC-C2C	-2.10	1.46	1.50
29	L	101	LHG	C4-C5	2.10	1.57	1.50
24	D	401	PHO	CMD-C2D	-2.10	1.46	1.51
23	b	606	CLA	C4B-CHC	-2.10	1.35	1.41
23	b	616	CLA	CMD-C2D	-2.10	1.46	1.50
23	B	615	CLA	CMD-C2D	-2.10	1.46	1.50
34	e	102	HEM	CAB-C3B	2.10	1.53	1.47
23	C	514	CLA	C3B-CAB	-2.09	1.43	1.47
23	c	510	CLA	C5-C3	-2.09	1.46	1.51
25	x	102	BCR	C1-C6	-2.09	1.50	1.53
23	B	602	CLA	CMC-C2C	-2.09	1.46	1.50
23	b	608	CLA	C3B-CAB	-2.09	1.43	1.47
28	H	102	DGD	O2G-C2G	-2.09	1.41	1.46
23	C	512	CLA	C3B-C2B	-2.09	1.37	1.40
28	C	517	DGD	O2G-C2G	-2.09	1.41	1.46
23	B	603	CLA	MG-ND	2.09	2.09	2.05
23	b	602	CLA	CMD-C2D	-2.09	1.46	1.50
23	B	610	CLA	CMC-C2C	-2.09	1.46	1.50
26	D	406	PL9	C7-C8	-2.08	1.47	1.50
23	b	607	CLA	CMC-C2C	-2.08	1.46	1.50
23	c	511	CLA	C3C-C2C	2.08	1.41	1.36
23	D	402	CLA	CMC-C2C	-2.08	1.46	1.50
23	d	403	CLA	MG-NC	2.08	2.11	2.06
24	A	406	PHO	CMC-C2C	-2.08	1.46	1.51
23	c	501	CLA	C4B-CHC	-2.08	1.35	1.41
34	E	103	HEM	CMB-C2B	2.08	1.55	1.50
25	B	617	BCR	C38-C26	-2.08	1.47	1.50
28	H	102	DGD	O2G-C1B	2.08	1.40	1.34
33	C	519	LMG	C4-C5	2.07	1.57	1.53
25	a	409	BCR	C35-C13	-2.07	1.46	1.50
23	C	509	CLA	CMD-C2D	-2.07	1.46	1.50
23	d	404	CLA	CHC-C1C	2.07	1.40	1.35
25	b	620	BCR	C38-C26	-2.07	1.47	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	524	LMG	C1-C2	2.07	1.58	1.52
25	k	101	BCR	C33-C5	-2.07	1.47	1.50
26	D	406	PL9	C21-C19	-2.06	1.47	1.51
27	f	101	SQD	O4-C4	-2.06	1.38	1.43
23	C	510	CLA	C1D-ND	2.06	1.40	1.37
33	C	501	LMG	C1-C2	2.06	1.58	1.52
23	b	602	CLA	C3B-CAB	-2.06	1.43	1.47
23	A	407	CLA	CAC-C3C	-2.06	1.45	1.51
23	C	505	CLA	C4D-ND	-2.05	1.34	1.37
23	C	505	CLA	C4B-CHC	-2.05	1.35	1.41
28	c	517	DGD	O1G-C1A	2.05	1.39	1.33
28	C	517	DGD	C4E-C5E	2.05	1.57	1.53
23	C	514	CLA	C4B-CHC	-2.05	1.35	1.41
25	t	101	BCR	C1-C6	-2.05	1.50	1.53
23	b	602	CLA	C3D-C4D	2.05	1.48	1.44
23	B	608	CLA	O2D-CED	-2.05	1.40	1.45
33	c	519	LMG	O7-C8	-2.05	1.41	1.46
23	c	503	CLA	C1D-C2D	2.04	1.49	1.45
28	C	518	DGD	O1G-C1G	-2.04	1.40	1.45
23	c	509	CLA	O1D-CGD	2.04	1.26	1.21
23	C	512	CLA	C3D-C4D	2.04	1.48	1.44
23	c	506	CLA	CMC-C2C	-2.04	1.46	1.50
23	b	611	CLA	CMA-C3A	-2.04	1.48	1.53
25	t	101	BCR	C33-C5	-2.04	1.47	1.50
23	c	508	CLA	C4B-CHC	-2.03	1.35	1.41
23	B	607	CLA	C1C-NC	-2.03	1.34	1.37
23	c	510	CLA	CMD-C2D	-2.03	1.46	1.50
33	c	524	LMG	O8-C28	2.03	1.39	1.33
33	M	101	LMG	C9-C8	2.03	1.56	1.50
23	B	601	CLA	C4D-ND	-2.03	1.34	1.37
23	C	505	CLA	C3D-C4D	2.03	1.48	1.44
23	b	602	CLA	CMC-C2C	-2.03	1.46	1.50
23	C	513	CLA	C1A-CHA	-2.03	1.34	1.43
23	b	610	CLA	C1A-CHA	-2.03	1.34	1.43
23	C	506	CLA	C4B-CHC	-2.03	1.35	1.41
23	B	610	CLA	C1D-ND	2.03	1.40	1.37
23	b	609	CLA	C1D-C2D	2.03	1.49	1.45
28	H	102	DGD	O3E-C3E	-2.03	1.38	1.43
23	C	509	CLA	C3B-CAB	-2.02	1.43	1.47
23	b	610	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	610	CLA	CMA-C3A	-2.02	1.48	1.53
23	C	514	CLA	CMD-C2D	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	CHC-C1C	2.02	1.40	1.35
23	c	507	CLA	CHC-C1C	2.02	1.40	1.35
23	B	601	CLA	CAA-C2A	-2.02	1.50	1.54
23	A	405	CLA	C1D-ND	2.02	1.40	1.37
23	b	609	CLA	CBD-CGD	-2.02	1.46	1.52
23	d	402	CLA	C1C-C2C	2.02	1.48	1.44
23	c	510	CLA	CMC-C2C	-2.02	1.46	1.50
25	H	101	BCR	C33-C5	-2.02	1.47	1.50
28	c	517	DGD	O2G-C2G	-2.01	1.41	1.46
23	B	611	CLA	C4B-CHC	-2.01	1.35	1.41
23	C	502	CLA	CMB-C2B	-2.01	1.47	1.51
23	A	404	CLA	O2D-CGD	2.01	1.38	1.33
24	d	401	PHO	C3B-CAB	-2.01	1.43	1.47
23	C	505	CLA	C4D-CHA	2.01	1.45	1.38
23	A	405	CLA	CAA-C2A	-2.01	1.50	1.54
25	B	618	BCR	C33-C5	-2.01	1.47	1.50
34	E	103	HEM	C4A-CHB	-2.01	1.35	1.41
23	d	402	CLA	C1B-NB	2.00	1.37	1.35
23	a	406	CLA	C4B-CHC	-2.00	1.35	1.41
24	D	401	PHO	C1C-NC	-2.00	1.32	1.38
23	c	513	CLA	C3B-C2B	-2.00	1.37	1.40
25	B	619	BCR	C33-C5	-2.00	1.47	1.50
23	c	504	CLA	CMD-C2D	-2.00	1.46	1.50

All (1390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C4A-NA-C1A	11.10	111.69	106.71
23	c	501	CLA	C4A-NA-C1A	10.59	111.47	106.71
23	C	502	CLA	C4A-NA-C1A	10.55	111.45	106.71
23	d	402	CLA	C4A-NA-C1A	10.41	111.38	106.71
27	A	410	SQD	O6-C1-C2	10.12	124.11	108.30
23	C	504	CLA	C4A-NA-C1A	9.22	110.85	106.71
23	D	403	CLA	C4A-NA-C1A	8.97	110.74	106.71
23	B	606	CLA	C4A-NA-C1A	8.58	110.56	106.71
23	C	514	CLA	C4A-NA-C1A	8.41	110.49	106.71
27	b	601	SQD	O6-C1-C2	8.37	121.37	108.30
23	C	509	CLA	C4A-NA-C1A	8.10	110.35	106.71
23	C	512	CLA	C4A-NA-C1A	7.99	110.30	106.71
27	a	411	SQD	O6-C1-C2	7.93	120.69	108.30
23	C	511	CLA	C4A-NA-C1A	7.75	110.19	106.71
23	B	612	CLA	C4A-NA-C1A	7.69	110.16	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C4A-NA-C1A	7.45	110.06	106.71
23	c	511	CLA	C4A-NA-C1A	7.35	110.01	106.71
23	B	610	CLA	C4A-NA-C1A	7.33	110.00	106.71
23	b	613	CLA	C4A-NA-C1A	6.93	109.82	106.71
23	b	606	CLA	C4A-NA-C1A	6.81	109.77	106.71
33	b	622	LMG	O1-C1-C2	-6.79	97.70	108.30
23	c	502	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	b	616	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	c	507	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	c	504	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	C	510	CLA	C4A-NA-C1A	6.31	109.54	106.71
27	b	601	SQD	O7-S-C6	6.14	114.24	106.94
27	A	410	SQD	O7-S-C6	6.12	114.22	106.94
23	a	405	CLA	C4A-NA-C1A	6.09	109.45	106.71
23	A	407	CLA	O2D-CGD-O1D	-5.97	112.16	123.84
27	a	411	SQD	O9-S-C6	5.95	114.01	106.94
23	A	404	CLA	C4A-NA-C1A	5.95	109.38	106.71
23	B	604	CLA	C4A-NA-C1A	5.94	109.38	106.71
23	B	616	CLA	C4A-NA-C1A	5.84	109.33	106.71
27	F	101	SQD	O8-S-C6	5.84	115.05	105.74
23	B	603	CLA	O2D-CGD-O1D	-5.84	112.42	123.84
23	B	614	CLA	C4A-NA-C1A	5.84	109.33	106.71
27	B	621	SQD	O6-C1-C2	5.78	117.33	108.30
23	c	503	CLA	C4A-NA-C1A	5.76	109.30	106.71
26	D	406	PL9	C7-C3-C4	5.75	121.55	116.88
23	c	501	CLA	O2D-CGD-O1D	-5.70	112.69	123.84
23	B	614	CLA	O2D-CGD-O1D	-5.70	112.70	123.84
23	B	611	CLA	C4A-NA-C1A	5.59	109.22	106.71
27	B	621	SQD	O47-C7-C8	5.56	123.48	111.50
27	F	101	SQD	O6-C1-C2	5.54	116.96	108.30
23	b	617	CLA	O2D-CGD-O1D	-5.54	113.01	123.84
23	c	506	CLA	C4A-NA-C1A	5.53	109.19	106.71
23	b	607	CLA	C4A-NA-C1A	5.52	109.19	106.71
23	b	606	CLA	CHD-C1D-ND	-5.50	119.40	124.45
27	f	101	SQD	O6-C1-C2	5.50	116.89	108.30
23	a	406	CLA	CHB-C4A-NA	5.48	132.09	124.51
28	H	102	DGD	O3G-C3G-C2G	-5.47	97.71	110.90
23	b	613	CLA	CMB-C2B-C1B	-5.42	120.13	128.46
26	a	410	PL9	C7-C3-C4	5.39	121.26	116.88
27	F	101	SQD	O9-S-C6	5.35	113.30	106.94
23	B	614	CLA	CMB-C2B-C1B	-5.18	120.51	128.46
23	b	615	CLA	C4A-NA-C1A	5.17	109.03	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CMB-C2B-C3B	5.16	134.33	124.68
23	c	512	CLA	C4A-NA-C1A	5.13	109.01	106.71
23	b	615	CLA	CHD-C1D-ND	-5.10	119.77	124.45
27	a	412	SQD	O47-C7-C8	5.10	122.49	111.50
26	A	409	PL9	C7-C3-C4	5.07	121.00	116.88
23	c	501	CLA	CMB-C2B-C1B	-5.04	120.72	128.46
23	A	407	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
23	b	612	CLA	CHD-C1D-ND	-4.87	119.98	124.45
26	d	406	PL9	C40-C39-C41	4.84	123.42	115.27
23	b	614	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
23	b	616	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
23	b	614	CLA	C4A-NA-C1A	4.80	108.86	106.71
23	B	607	CLA	CHD-C1D-ND	-4.78	120.06	124.45
23	D	404	CLA	O2D-CGD-O1D	-4.77	114.51	123.84
23	C	502	CLA	O2D-CGD-CBD	4.75	119.71	111.27
23	c	501	CLA	O2D-CGD-CBD	4.71	119.64	111.27
23	c	508	CLA	CHD-C1D-ND	-4.70	120.13	124.45
23	B	605	CLA	CHD-C1D-ND	-4.66	120.17	124.45
23	b	617	CLA	C4A-NA-C1A	4.66	108.80	106.71
23	a	406	CLA	O2D-CGD-CBD	4.64	119.51	111.27
23	B	609	CLA	C4A-NA-C1A	4.63	108.79	106.71
23	b	603	CLA	O2D-CGD-O1D	-4.63	114.79	123.84
23	b	615	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
23	B	608	CLA	C4A-NA-C1A	4.61	108.78	106.71
23	B	609	CLA	CMB-C2B-C1B	-4.61	121.39	128.46
34	e	102	HEM	CBA-CAA-C2A	-4.60	104.77	112.62
23	b	608	CLA	C4A-NA-C1A	4.60	108.77	106.71
23	b	604	CLA	C4A-NA-C1A	4.59	108.77	106.71
23	c	504	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
29	A	413	LHG	O4-P-O5	4.56	134.81	112.24
23	a	406	CLA	C4A-NA-C1A	4.55	108.75	106.71
23	C	508	CLA	CHD-C1D-ND	-4.55	120.28	124.45
33	c	522	LMG	O6-C1-O1	-4.51	99.30	109.97
23	C	508	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
23	B	601	CLA	C4A-NA-C1A	4.48	108.72	106.71
23	A	404	CLA	CHB-C4A-NA	4.47	130.69	124.51
23	b	606	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
28	C	518	DGD	O3G-C3G-C2G	-4.44	100.19	110.90
23	b	606	CLA	O2D-CGD-O1D	-4.43	115.17	123.84
23	C	509	CLA	O2D-CGD-O1D	-4.41	115.22	123.84
23	A	405	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
23	b	613	CLA	CHD-C1D-ND	-4.37	120.43	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	411	SQD	O47-C7-C8	4.37	120.93	111.50
23	A	405	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
23	b	603	CLA	O2D-CGD-CBD	4.37	119.03	111.27
23	A	405	CLA	O2D-CGD-CBD	4.35	119.00	111.27
23	B	610	CLA	O2D-CGD-O1D	-4.35	115.34	123.84
28	C	517	DGD	O3G-C3G-C2G	-4.35	100.41	110.90
23	C	505	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
25	B	618	BCR	C35-C13-C14	-4.33	116.85	122.92
23	b	604	CLA	O2D-CGD-O1D	-4.31	115.42	123.84
23	d	402	CLA	O2D-CGD-O1D	-4.29	115.45	123.84
28	A	412	DGD	C3G-C2G-C1G	-4.27	101.70	111.79
24	D	401	PHO	O1D-CGD-CBD	4.26	131.83	124.74
27	f	101	SQD	O8-S-C6	4.26	112.52	105.74
27	b	601	SQD	O8-S-C6	4.24	112.50	105.74
23	D	404	CLA	C2D-C1D-ND	-4.23	106.99	110.10
23	c	506	CLA	CBC-CAC-C3C	-4.23	100.78	112.43
23	c	510	CLA	O2D-CGD-O1D	-4.23	115.58	123.84
23	b	604	CLA	O2D-CGD-CBD	4.22	118.77	111.27
29	e	101	LHG	O4-P-O5	4.22	133.09	112.24
23	c	513	CLA	C4A-NA-C1A	4.21	108.60	106.71
29	d	407	LHG	O4-P-O5	4.20	133.00	112.24
23	c	510	CLA	CMB-C2B-C3B	4.20	132.53	124.68
23	b	610	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
23	C	504	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
29	E	101	LHG	O4-P-O5	4.17	132.87	112.24
23	A	407	CLA	CMB-C2B-C3B	4.17	132.47	124.68
29	D	408	LHG	O4-P-O5	4.16	132.83	112.24
29	d	409	LHG	O4-P-O5	4.15	132.74	112.24
27	b	601	SQD	O5-C5-C4	4.14	117.22	109.69
23	B	612	CLA	CHB-C4A-NA	4.14	130.23	124.51
23	B	601	CLA	O2D-CGD-O1D	-4.13	115.76	123.84
27	b	601	SQD	C1-C2-C3	-4.11	101.43	110.00
23	B	608	CLA	CHD-C1D-ND	-4.11	120.68	124.45
33	d	411	LMG	O6-C5-C4	4.11	117.15	109.69
23	c	501	CLA	CMB-C2B-C3B	4.08	132.31	124.68
33	d	411	LMG	O1-C1-C2	-4.07	101.94	108.30
23	a	406	CLA	CMA-C3A-C4A	-4.07	100.84	111.77
28	c	516	DGD	O3G-C3G-C2G	-4.07	101.09	110.90
23	b	613	CLA	CHB-C4A-NA	4.04	130.09	124.51
23	c	502	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
23	c	510	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
28	c	516	DGD	C3G-C2G-C1G	-4.02	102.29	111.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	408	LHG	O4-P-O5	4.02	132.09	112.24
23	b	603	CLA	CHB-C4A-NA	4.01	130.06	124.51
23	b	609	CLA	CHD-C1D-ND	-4.01	120.77	124.45
29	D	409	LHG	O4-P-O5	4.01	132.04	112.24
23	C	513	CLA	CHB-C4A-NA	4.00	130.05	124.51
23	B	614	CLA	CMB-C2B-C3B	4.00	132.16	124.68
23	c	508	CLA	CMB-C2B-C1B	-3.99	122.32	128.46
23	c	507	CLA	C1B-CHB-C4A	-3.97	122.25	130.12
23	c	502	CLA	CMB-C2B-C3B	3.97	132.11	124.68
23	c	510	CLA	C4A-NA-C1A	3.96	108.49	106.71
23	d	403	CLA	C4A-NA-C1A	3.96	108.49	106.71
23	a	406	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
27	A	410	SQD	C1-C2-C3	-3.95	101.78	110.00
28	c	518	DGD	C3G-C2G-C1G	-3.94	102.47	111.79
27	B	621	SQD	O8-S-C6	3.92	111.99	105.74
23	d	404	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
23	A	405	CLA	CMB-C2B-C3B	3.91	131.99	124.68
23	b	609	CLA	C1B-CHB-C4A	-3.89	122.42	130.12
28	H	102	DGD	C1D-O6D-C5D	-3.88	106.08	113.69
23	B	607	CLA	C4A-NA-C1A	3.88	108.45	106.71
29	l	101	LHG	O4-P-O5	3.88	131.40	112.24
24	D	401	PHO	O2D-CGD-CBD	-3.87	106.09	111.00
33	m	101	LMG	O7-C10-O9	-3.86	114.38	123.70
23	A	407	CLA	C1B-CHB-C4A	-3.86	122.48	130.12
23	b	617	CLA	CHB-C4A-NA	3.86	129.84	124.51
28	C	517	DGD	C1D-C2D-C3D	-3.85	101.98	110.00
31	A	415	BCT	O2-C-O1	3.83	129.49	119.55
23	B	615	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
23	C	506	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
23	C	505	CLA	C4A-NA-C1A	3.81	108.42	106.71
23	c	510	CLA	CHB-C4A-NA	3.81	129.78	124.51
23	b	603	CLA	CHC-C1C-NC	3.81	129.98	124.20
23	B	615	CLA	C4A-NA-C1A	3.80	108.42	106.71
23	b	603	CLA	CHD-C1D-ND	-3.80	120.96	124.45
23	B	603	CLA	C4A-NA-C1A	3.79	108.41	106.71
23	C	508	CLA	CMB-C2B-C3B	3.78	131.75	124.68
27	B	621	SQD	C1-O5-C5	-3.77	106.29	113.69
23	A	407	CLA	CHD-C1D-ND	-3.77	120.99	124.45
23	b	606	CLA	C1-C2-C3	-3.76	119.54	126.04
23	C	510	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
25	T	101	BCR	C27-C26-C25	3.76	128.19	122.73
23	C	502	CLA	O2D-CGD-O1D	-3.76	116.50	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	410	SQD	O47-C7-C8	3.75	119.58	111.50
27	a	411	SQD	O9-S-O7	-3.74	101.00	113.95
25	b	618	BCR	C33-C5-C6	-3.74	120.33	124.53
25	b	618	BCR	C2-C1-C6	3.73	116.22	110.48
23	b	614	CLA	CMB-C2B-C3B	3.73	131.65	124.68
23	b	617	CLA	O1D-CGD-CBD	3.73	132.11	124.48
23	B	610	CLA	CHD-C1D-ND	-3.72	121.03	124.45
35	V	201	HEC	CMC-C2C-C1C	-3.72	122.75	128.46
23	c	508	CLA	C4A-NA-C1A	3.72	108.38	106.71
23	C	513	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
23	c	509	CLA	CHB-C4A-NA	3.70	129.63	124.51
24	a	407	PHO	CMB-C2B-C3B	3.70	131.61	124.68
26	d	406	PL9	C30-C29-C31	-3.70	109.05	115.27
23	A	407	CLA	O2D-CGD-CBD	3.69	117.83	111.27
25	A	408	BCR	C37-C22-C21	-3.69	117.75	122.92
27	f	101	SQD	O9-S-C6	3.69	111.32	106.94
23	b	603	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
33	b	622	LMG	O2-C2-C1	-3.68	101.12	110.05
34	e	102	HEM	CBD-CAD-C3D	-3.67	102.44	112.63
33	m	101	LMG	O1-C7-C8	-3.66	102.06	110.90
28	h	101	DGD	C4E-C3E-C2E	-3.66	104.43	110.82
23	B	604	CLA	CHD-C1D-ND	-3.66	121.09	124.45
23	d	404	CLA	O2A-CGA-O1A	-3.65	114.37	123.59
23	B	603	CLA	O2D-CGD-CBD	3.64	117.74	111.27
23	C	503	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
26	a	410	PL9	C7-C3-C2	-3.63	118.52	123.30
23	b	607	CLA	CHD-C1D-ND	-3.63	121.12	124.45
23	C	507	CLA	C4A-NA-C1A	3.63	108.34	106.71
23	a	405	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
28	C	518	DGD	O6D-C1D-O3G	-3.62	101.39	109.97
23	C	508	CLA	O2D-CGD-CBD	3.61	117.69	111.27
23	B	602	CLA	CMB-C2B-C3B	3.61	131.42	124.68
23	d	404	CLA	CMB-C2B-C3B	3.61	131.42	124.68
23	B	614	CLA	O1D-CGD-CBD	3.59	131.83	124.48
23	B	616	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
23	c	505	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
26	d	406	PL9	C45-C44-C46	-3.58	109.25	115.27
28	A	412	DGD	O5D-C1E-C2E	3.57	113.88	108.30
25	B	618	BCR	C15-C16-C17	-3.57	116.16	123.47
23	C	503	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
23	b	602	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
23	b	604	CLA	C7-C6-C5	-3.56	103.69	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	O2A-CGA-O1A	-3.56	114.61	123.59
23	B	602	CLA	CHB-C4A-NA	3.55	129.43	124.51
27	A	411	SQD	C45-O47-C7	3.55	122.45	117.88
23	a	406	CLA	CED-O2D-CGD	-3.55	107.91	115.94
23	b	605	CLA	C4A-NA-C1A	3.55	108.30	106.71
33	c	524	LMG	C1-O6-C5	-3.55	106.72	113.69
26	d	406	PL9	C7-C3-C4	3.54	119.76	116.88
23	C	507	CLA	CMB-C2B-C3B	3.54	131.29	124.68
28	c	516	DGD	C3E-C4E-C5E	-3.54	103.93	110.24
31	a	404	BCT	O2-C-O1	3.53	128.71	119.55
27	a	411	SQD	C1-C2-C3	-3.53	102.65	110.00
23	C	507	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
27	A	410	SQD	O9-S-O7	-3.53	101.75	113.95
23	b	609	CLA	CMA-C3A-C4A	-3.52	102.30	111.77
23	B	616	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	B	602	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
23	c	507	CLA	CHB-C4A-NA	3.52	129.38	124.51
23	B	606	CLA	C2A-C1A-CHA	3.51	130.00	123.86
26	A	409	PL9	C7-C3-C2	-3.51	118.68	123.30
23	b	610	CLA	CMB-C2B-C3B	3.50	131.23	124.68
23	B	602	CLA	O2D-CGD-CBD	3.50	117.49	111.27
23	b	616	CLA	CMB-C2B-C3B	3.50	131.22	124.68
23	C	503	CLA	CHD-C1D-ND	-3.49	121.25	124.45
23	b	611	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
23	B	616	CLA	C1-O2A-CGA	3.49	125.60	116.44
23	c	502	CLA	CHD-C1D-ND	-3.49	121.25	124.45
33	d	411	LMG	O2-C2-C1	-3.48	101.59	110.05
29	A	413	LHG	O8-C23-C24	3.48	122.83	111.91
23	B	602	CLA	C2D-C1D-ND	-3.48	107.54	110.10
24	d	401	PHO	O1D-CGD-CBD	3.48	130.53	124.74
29	L	101	LHG	O4-P-O5	3.47	129.41	112.24
23	A	404	CLA	CHD-C1D-ND	-3.47	121.26	124.45
28	h	101	DGD	O3G-C3G-C2G	-3.46	102.54	110.90
26	d	406	PL9	C22-C23-C24	-3.46	119.33	127.66
23	b	602	CLA	O2A-C1-C2	3.45	117.72	108.64
35	V	201	HEC	CMB-C2B-C1B	-3.45	123.16	128.46
29	d	407	LHG	O8-C23-C24	3.44	122.70	111.91
23	B	609	CLA	CMB-C2B-C3B	3.44	131.11	124.68
23	c	509	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
23	C	506	CLA	CAC-C3C-C4C	3.43	129.26	124.81
26	D	406	PL9	C37-C38-C39	-3.43	119.40	127.66
23	b	611	CLA	CAA-CBA-CGA	-3.43	103.24	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	101	BCR	C15-C16-C17	-3.42	116.46	123.47
23	c	503	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
35	v	201	HEC	CBD-CAD-C3D	-3.42	106.79	112.62
34	e	102	HEM	CMC-C2C-C3C	3.41	131.07	124.68
23	b	608	CLA	CHB-C4A-NA	3.41	129.22	124.51
27	f	101	SQD	O47-C7-C8	3.40	120.29	110.80
23	B	613	CLA	C4-C3-C5	3.40	120.99	115.27
23	A	405	CLA	CAC-C3C-C4C	3.40	129.22	124.81
23	b	610	CLA	CHD-C1D-ND	-3.40	121.33	124.45
23	b	602	CLA	C4A-NA-C1A	3.40	108.23	106.71
28	c	518	DGD	O6E-C5E-C4E	3.39	115.85	109.69
23	d	404	CLA	CHA-C1A-NA	-3.39	118.64	126.40
25	b	619	BCR	C8-C7-C6	-3.39	117.69	127.20
27	F	101	SQD	O5-C5-C4	3.38	115.84	109.69
23	b	615	CLA	CMB-C2B-C3B	3.38	131.00	124.68
23	b	609	CLA	CMB-C2B-C3B	3.38	131.00	124.68
28	h	101	DGD	C1E-O6E-C5E	3.38	120.32	113.69
23	C	504	CLA	O2A-C1-C2	-3.37	99.77	108.64
27	a	412	SQD	O48-C23-C24	3.37	122.49	111.91
23	B	604	CLA	O2A-C1-C2	3.36	117.48	108.64
25	b	619	BCR	C30-C25-C26	-3.36	117.88	122.61
23	B	611	CLA	C1-C2-C3	-3.36	120.22	126.04
26	A	409	PL9	C20-C19-C21	3.36	120.92	115.27
25	C	520	BCR	C37-C22-C21	-3.36	118.22	122.92
28	c	517	DGD	O6D-C1D-O3G	-3.36	102.03	109.97
26	d	406	PL9	C7-C8-C9	-3.35	121.21	126.79
27	A	410	SQD	O47-C7-O49	-3.35	115.60	123.70
23	B	604	CLA	O2A-CGA-O1A	-3.34	115.15	123.59
23	A	407	CLA	C4-C3-C5	3.34	120.89	115.27
23	a	408	CLA	CHD-C1D-ND	-3.34	121.39	124.45
23	c	503	CLA	C2D-C1D-ND	-3.32	107.65	110.10
33	m	101	LMG	O6-C1-O1	-3.32	102.12	109.97
23	C	506	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	A	407	CLA	C2C-C1C-NC	3.31	113.07	109.97
23	C	508	CLA	C4A-NA-C1A	3.31	108.19	106.71
23	b	602	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
23	D	403	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
23	C	511	CLA	CHB-C4A-NA	3.31	129.08	124.51
23	b	617	CLA	CMB-C2B-C3B	3.30	130.84	124.68
23	B	613	CLA	CHB-C4A-NA	3.29	129.07	124.51
23	b	608	CLA	C2D-C1D-ND	-3.29	107.68	110.10
23	c	507	CLA	CHD-C1D-ND	-3.29	121.43	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	621	SQD	O7-S-C6	3.29	110.85	106.94
25	B	618	BCR	C15-C14-C13	-3.29	122.62	127.31
29	A	413	LHG	O3-P-O5	-3.29	96.22	109.07
23	B	609	CLA	CHD-C1D-ND	-3.29	121.44	124.45
25	C	520	BCR	C15-C16-C17	-3.28	116.75	123.47
24	d	401	PHO	CMB-C2B-C3B	3.28	130.82	124.68
23	a	406	CLA	CHD-C1D-ND	-3.28	121.44	124.45
23	C	509	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
23	d	402	CLA	CHB-C4A-NA	3.28	129.04	124.51
23	B	607	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
33	C	519	LMG	O1-C7-C8	-3.28	103.00	110.90
28	C	517	DGD	O5D-C1E-C2E	3.27	113.42	108.30
27	b	601	SQD	O9-S-O7	-3.27	102.62	113.95
25	Z	101	BCR	C35-C13-C14	-3.27	118.34	122.92
25	c	515	BCR	C33-C5-C6	-3.27	120.86	124.53
23	b	608	CLA	O1D-CGD-CBD	3.27	131.17	124.48
23	B	609	CLA	C2C-C1C-NC	3.26	113.03	109.97
27	a	411	SQD	O47-C7-O49	-3.26	115.82	123.70
23	B	615	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
25	b	620	BCR	C37-C22-C21	-3.26	118.36	122.92
33	d	411	LMG	C6-C5-C4	-3.25	105.38	113.00
25	A	408	BCR	C38-C26-C27	-3.25	107.36	113.62
23	b	607	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
23	C	510	CLA	CHD-C1D-ND	-3.25	121.47	124.45
23	C	510	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
25	x	102	BCR	C27-C26-C25	3.25	127.44	122.73
23	b	605	CLA	OBD-CAD-C3D	3.24	136.33	128.52
25	c	521	BCR	C11-C10-C9	-3.24	122.68	127.31
23	b	613	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
26	D	406	PL9	C31-C32-C33	-3.24	101.25	111.88
23	B	611	CLA	O2D-CGD-CBD	3.24	117.02	111.27
33	c	519	LMG	O6-C1-O1	-3.23	102.32	109.97
23	C	509	CLA	O2D-CGD-CBD	3.23	117.01	111.27
23	C	504	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
23	b	615	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
23	c	513	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
23	B	608	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
23	B	609	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
28	A	412	DGD	C1D-C2D-C3D	-3.21	103.31	110.00
23	C	505	CLA	CMB-C2B-C3B	3.21	130.68	124.68
25	T	101	BCR	C7-C8-C9	-3.21	121.39	126.23
33	c	524	LMG	O6-C1-O1	-3.21	102.37	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	518	DGD	O3G-C3G-C2G	-3.20	103.17	110.90
23	c	504	CLA	CMB-C2B-C3B	3.20	130.66	124.68
23	d	404	CLA	O2A-C1-C2	-3.20	100.23	108.64
23	c	513	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	c	509	CLA	CMB-C2B-C3B	3.19	130.65	124.68
25	t	101	BCR	C29-C30-C25	3.19	115.39	110.48
23	A	405	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
27	F	101	SQD	O9-S-O7	-3.18	102.94	113.95
23	c	506	CLA	C4-C3-C5	3.18	120.61	115.27
23	B	606	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
28	C	517	DGD	C1D-O6D-C5D	-3.17	107.47	113.69
23	B	605	CLA	C4-C3-C5	3.17	120.60	115.27
28	h	101	DGD	C4D-C3D-C2D	-3.16	105.31	110.82
23	b	606	CLA	CHB-C4A-NA	3.16	128.88	124.51
33	m	101	LMG	O3-C3-C2	-3.16	103.05	110.35
23	D	403	CLA	CHB-C4A-NA	3.16	128.88	124.51
23	B	610	CLA	CHB-C4A-NA	3.15	128.87	124.51
23	B	611	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	c	501	CLA	C2C-C1C-NC	3.15	112.92	109.97
24	A	406	PHO	C1A-C2A-C3A	-3.15	99.85	102.84
23	C	506	CLA	O1D-CGD-CBD	3.14	130.92	124.48
25	H	101	BCR	C29-C30-C25	3.14	115.32	110.48
23	b	614	CLA	C7-C6-C5	-3.14	104.83	113.36
23	c	511	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
23	d	402	CLA	CHD-C1D-ND	-3.14	121.57	124.45
23	B	604	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	Z	101	BCR	C2-C1-C6	3.14	115.31	110.48
23	b	609	CLA	CHB-C4A-NA	3.14	128.85	124.51
25	c	515	BCR	C27-C26-C25	3.14	127.28	122.73
23	C	513	CLA	C2D-C1D-ND	-3.14	107.79	110.10
29	d	408	LHG	O8-C23-C24	3.13	121.73	111.91
23	C	506	CLA	CHB-C4A-NA	3.13	128.84	124.51
23	C	514	CLA	CHB-C4A-NA	3.13	128.84	124.51
23	b	605	CLA	CHB-C4A-NA	3.13	128.84	124.51
25	H	101	BCR	C30-C25-C26	-3.12	118.21	122.61
25	c	514	BCR	C27-C26-C25	3.12	127.27	122.73
23	C	510	CLA	O1D-CGD-CBD	3.12	130.88	124.48
23	c	503	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
28	h	101	DGD	O3E-C3E-C4E	3.12	117.56	110.35
23	b	612	CLA	CHD-C1D-C2D	3.12	132.02	125.48
25	c	521	BCR	C27-C26-C25	3.12	127.26	122.73
29	A	413	LHG	O8-C23-O10	-3.11	115.74	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	O1D-CGD-CBD	3.11	130.84	124.48
23	c	512	CLA	C1-C2-C3	-3.11	120.67	126.04
23	a	408	CLA	CHB-C4A-NA	3.10	128.80	124.51
23	b	614	CLA	CED-O2D-CGD	3.10	122.94	115.94
23	b	606	CLA	O1D-CGD-CBD	3.09	130.81	124.48
23	b	607	CLA	CHD-C4C-NC	3.09	129.07	124.20
27	B	621	SQD	O9-S-O7	-3.09	103.25	113.95
23	B	613	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
23	b	616	CLA	C1-O2A-CGA	3.08	124.53	116.44
23	d	402	CLA	C2A-C1A-CHA	3.08	129.25	123.86
23	d	402	CLA	CMC-C2C-C1C	3.08	129.73	125.04
23	B	605	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	b	604	CLA	C2D-C1D-ND	-3.07	107.84	110.10
34	e	102	HEM	C3B-C2B-C1B	3.07	108.76	106.49
23	c	502	CLA	C3A-C2A-C1A	3.07	105.93	101.34
23	B	615	CLA	C7-C6-C5	-3.06	105.05	113.36
23	c	502	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
25	K	101	BCR	C23-C22-C21	-3.06	114.25	118.94
23	c	505	CLA	CMB-C2B-C3B	3.05	130.38	124.68
27	a	411	SQD	O47-C7-C8	3.05	118.07	111.50
23	b	611	CLA	C4A-NA-C1A	3.05	108.08	106.71
23	C	514	CLA	C2D-C1D-ND	-3.05	107.86	110.10
29	E	101	LHG	O8-C23-C24	3.04	121.45	111.91
28	H	102	DGD	O3E-C3E-C2E	-3.04	103.32	110.35
23	B	616	CLA	CMB-C2B-C3B	3.04	130.37	124.68
23	b	617	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
23	A	407	CLA	C1D-ND-C4D	-3.04	104.18	106.33
23	B	608	CLA	CHB-C4A-NA	3.04	128.71	124.51
26	D	406	PL9	C7-C3-C2	-3.03	119.31	123.30
23	B	606	CLA	CHD-C1D-ND	-3.03	121.67	124.45
23	d	404	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
26	a	410	PL9	C22-C23-C24	-3.03	120.37	127.66
27	a	412	SQD	O48-C23-O10	-3.03	115.95	123.59
28	C	516	DGD	O2D-C2D-C1D	-3.02	102.71	110.05
23	C	510	CLA	CHB-C4A-NA	3.02	128.69	124.51
23	b	606	CLA	CHD-C4C-NC	3.02	128.96	124.20
23	d	403	CLA	O2A-CGA-O1A	-3.02	115.98	123.59
25	C	520	BCR	C27-C26-C25	3.02	127.11	122.73
27	A	411	SQD	O48-C23-O10	-3.01	115.99	123.59
28	h	101	DGD	C3G-C2G-C1G	-3.01	104.67	111.79
23	c	501	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
25	B	618	BCR	C27-C26-C25	3.00	127.09	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	407	LMG	O3-C3-C2	-3.00	103.41	110.35
33	D	407	LMG	O6-C1-O1	-3.00	102.86	109.97
23	a	405	CLA	C3A-C2A-C1A	3.00	105.83	101.34
23	B	613	CLA	C1-C2-C3	-3.00	120.86	126.04
23	C	514	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
23	C	506	CLA	CMB-C2B-C3B	3.00	130.28	124.68
23	c	510	CLA	CHD-C1D-ND	-3.00	121.70	124.45
28	C	517	DGD	O6E-C1E-O5D	-3.00	102.88	109.97
23	a	408	CLA	CAA-CBA-CGA	-2.99	104.52	113.25
23	C	513	CLA	CMB-C2B-C3B	2.99	130.27	124.68
25	B	617	BCR	C30-C25-C26	-2.99	118.41	122.61
35	v	201	HEC	CBA-CAA-C2A	-2.99	107.57	112.60
23	b	611	CLA	O2A-C1-C2	2.99	116.48	108.64
23	b	603	CLA	CMB-C2B-C3B	2.99	130.26	124.68
23	b	613	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
23	A	407	CLA	CHB-C4A-NA	2.98	128.63	124.51
23	B	612	CLA	O2A-CGA-O1A	-2.98	116.07	123.59
25	D	405	BCR	C28-C27-C26	-2.97	108.77	114.08
23	a	408	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
26	D	406	PL9	C11-C12-C13	-2.96	102.15	111.88
23	b	612	CLA	CHD-C4C-NC	2.96	128.87	124.20
23	D	402	CLA	C16-C15-C13	-2.96	106.36	115.92
25	c	515	BCR	C35-C13-C14	-2.96	118.78	122.92
23	b	613	CLA	C11-C12-C13	-2.96	106.36	115.92
33	C	501	LMG	O6-C1-C2	-2.96	104.09	110.35
33	C	501	LMG	C38-C37-C36	-2.95	99.42	114.42
23	a	406	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
29	D	409	LHG	O8-C23-O10	-2.95	116.14	123.59
23	b	602	CLA	CHD-C1D-ND	-2.95	121.74	124.45
23	C	503	CLA	C4A-NA-C1A	2.95	108.03	106.71
33	M	101	LMG	O1-C1-C2	-2.94	103.71	108.30
23	b	610	CLA	C4A-NA-C1A	2.94	108.03	106.71
28	C	517	DGD	O2D-C2D-C1D	-2.94	102.90	110.05
23	b	605	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
27	B	621	SQD	O5-C5-C4	2.94	115.03	109.69
23	B	605	CLA	C16-C15-C13	-2.94	106.43	115.92
23	c	512	CLA	CHB-C4A-NA	2.93	128.57	124.51
28	C	516	DGD	C4E-C3E-C2E	-2.93	105.70	110.82
23	D	404	CLA	O1D-CGD-CBD	2.93	130.48	124.48
25	x	102	BCR	C35-C13-C14	-2.93	118.82	122.92
23	c	505	CLA	C6-C7-C8	-2.93	106.45	115.92
23	B	604	CLA	CMB-C2B-C3B	2.93	130.16	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C4A-NA-C1A	2.92	108.02	106.71
23	D	404	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
23	C	504	CLA	C7-C6-C5	-2.92	105.42	113.36
25	H	101	BCR	C27-C26-C25	2.92	126.97	122.73
27	b	601	SQD	O47-C45-C46	2.92	118.98	108.40
23	B	613	CLA	CMB-C2B-C3B	2.92	130.15	124.68
23	B	616	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
27	A	410	SQD	O2-C2-C1	2.92	117.14	110.05
23	B	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
23	b	612	CLA	C2D-C1D-ND	-2.91	107.96	110.10
25	b	620	BCR	C29-C30-C25	2.91	114.96	110.48
29	d	407	LHG	C11-C10-C9	-2.91	99.67	114.42
23	a	405	CLA	CHD-C1D-ND	-2.91	121.78	124.45
23	c	502	CLA	C1-C2-C3	-2.90	121.02	126.04
33	m	101	LMG	O1-C1-C2	-2.90	103.78	108.30
28	H	102	DGD	O3D-C3D-C4D	-2.89	103.66	110.35
23	b	612	CLA	O2D-CGD-CBD	2.89	116.41	111.27
25	C	515	BCR	C27-C26-C25	2.89	126.93	122.73
23	c	503	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
23	b	617	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
23	C	506	CLA	C4A-NA-C1A	2.88	108.00	106.71
23	a	406	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
23	b	609	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
25	K	101	BCR	C33-C5-C6	-2.88	121.29	124.53
26	D	406	PL9	C36-C34-C33	-2.88	115.29	121.12
25	t	101	BCR	C35-C13-C14	-2.88	118.89	122.92
27	b	601	SQD	O47-C7-C8	2.88	117.70	111.50
28	c	518	DGD	O5E-C6E-C5E	-2.87	101.44	111.29
23	c	501	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
23	b	609	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
23	b	611	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
23	b	604	CLA	CHD-C1D-ND	-2.87	121.82	124.45
23	b	617	CLA	CGD-CBD-CAD	-2.86	101.46	110.73
25	a	409	BCR	C35-C13-C14	-2.86	118.91	122.92
25	T	101	BCR	C38-C26-C27	-2.86	108.12	113.62
26	D	406	PL9	C20-C19-C21	2.86	120.08	115.27
29	D	408	LHG	O8-C23-C24	2.86	120.89	111.91
27	b	601	SQD	O2-C2-C1	2.86	116.99	110.05
23	C	504	CLA	C6-C5-C3	2.86	120.95	113.45
23	b	602	CLA	O2D-CGD-CBD	2.85	116.34	111.27
25	B	617	BCR	C2-C1-C6	2.85	114.87	110.48
28	H	102	DGD	C8B-C7B-C6B	-2.85	99.95	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	514	BCR	C30-C25-C26	-2.85	118.60	122.61
25	H	101	BCR	C2-C1-C6	2.85	114.86	110.48
23	d	402	CLA	O2D-CGD-CBD	2.85	116.33	111.27
23	A	404	CLA	CMB-C2B-C3B	2.85	130.00	124.68
33	b	622	LMG	C8-O7-C10	2.84	124.79	117.79
23	C	507	CLA	CHB-C4A-NA	2.84	128.44	124.51
27	b	601	SQD	C1-O5-C5	2.84	119.27	113.69
25	Z	101	BCR	C7-C8-C9	-2.84	121.94	126.23
23	b	606	CLA	CMB-C2B-C3B	2.84	129.99	124.68
23	b	608	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
23	b	605	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
23	b	605	CLA	CMB-C2B-C3B	2.84	129.98	124.68
23	b	606	CLA	C11-C12-C13	-2.83	106.76	115.92
23	b	615	CLA	CHD-C1D-C2D	2.83	131.42	125.48
27	F	101	SQD	O48-C23-C24	2.83	120.80	111.91
25	B	617	BCR	C27-C26-C25	2.83	126.84	122.73
23	b	602	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
23	b	612	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
33	M	101	LMG	O3-C3-C2	-2.83	103.82	110.35
23	D	402	CLA	C4A-NA-C1A	2.82	107.98	106.71
27	a	411	SQD	O8-S-C6	2.82	110.24	105.74
23	B	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
28	C	517	DGD	C6D-O5D-C1E	2.82	119.24	113.74
23	c	513	CLA	CMB-C2B-C3B	2.82	129.95	124.68
25	A	408	BCR	C29-C30-C25	2.82	114.82	110.48
25	c	515	BCR	C30-C25-C26	-2.82	118.65	122.61
23	b	604	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
23	C	513	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
23	b	612	CLA	C4A-NA-C1A	2.81	107.97	106.71
28	c	516	DGD	O3E-C3E-C2E	-2.81	103.86	110.35
23	b	602	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	b	615	CLA	O1D-CGD-CBD	2.80	130.22	124.48
23	B	606	CLA	CHA-C1A-NA	-2.80	120.00	126.40
25	a	409	BCR	C33-C5-C6	-2.79	121.39	124.53
23	d	404	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	C	511	CLA	CHD-C1D-ND	-2.79	121.89	124.45
27	a	411	SQD	C1-O5-C5	-2.79	108.22	113.69
29	D	408	LHG	O8-C23-O10	-2.79	116.56	123.59
23	D	402	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	c	510	CLA	O1D-CGD-CBD	2.78	130.18	124.48
28	c	516	DGD	CDB-CCB-CBB	-2.78	100.30	114.42
25	k	101	BCR	C27-C26-C25	2.78	126.77	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
23	B	609	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
29	e	101	LHG	O8-C23-C24	2.78	120.63	111.91
27	f	101	SQD	O5-C5-C4	2.77	114.73	109.69
23	b	614	CLA	CHB-C4A-NA	2.77	128.35	124.51
23	B	607	CLA	CMB-C2B-C3B	2.77	129.86	124.68
23	B	613	CLA	C2C-C1C-NC	2.77	112.56	109.97
23	b	602	CLA	CMB-C2B-C3B	2.77	129.86	124.68
23	c	503	CLA	CHD-C1D-ND	-2.76	121.92	124.45
23	b	605	CLA	C1-C2-C3	-2.76	121.27	126.04
28	h	101	DGD	C6D-O5D-C1E	2.76	119.13	113.74
23	B	613	CLA	CED-O2D-CGD	2.76	122.18	115.94
28	C	518	DGD	CDB-CCB-CBB	-2.75	100.45	114.42
23	c	508	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
24	a	407	PHO	O1D-CGD-CBD	2.75	129.32	124.74
23	c	509	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
28	C	516	DGD	C3D-C4D-C5D	-2.75	105.34	110.24
23	B	610	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
23	B	610	CLA	C2D-C1D-ND	2.75	112.13	110.10
27	A	411	SQD	O48-C46-C45	2.75	116.29	108.38
23	b	612	CLA	C11-C10-C8	-2.74	107.05	115.92
29	e	101	LHG	O8-C23-O10	-2.74	116.67	123.59
25	b	618	BCR	C27-C26-C25	2.74	126.71	122.73
23	c	508	CLA	CMB-C2B-C3B	2.74	129.80	124.68
23	D	404	CLA	CHB-C4A-NA	2.74	128.30	124.51
27	B	621	SQD	O47-C7-O49	-2.74	117.09	123.70
23	C	505	CLA	CHA-C1A-NA	-2.74	120.13	126.40
33	C	501	LMG	C1-O6-C5	-2.73	108.32	113.69
25	c	515	BCR	C2-C1-C6	2.73	114.69	110.48
25	C	515	BCR	C15-C16-C17	-2.73	117.88	123.47
23	C	504	CLA	O1D-CGD-CBD	2.73	130.07	124.48
25	c	514	BCR	C15-C14-C13	-2.73	123.42	127.31
23	C	510	CLA	CMB-C2B-C3B	2.73	129.78	124.68
23	b	615	CLA	C4D-CHA-C1A	2.72	124.56	121.25
23	c	507	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
23	d	404	CLA	CBC-CAC-C3C	-2.72	104.94	112.43
33	D	411	LMG	O8-C28-O10	-2.72	116.53	123.30
25	C	515	BCR	C2-C1-C6	2.71	114.66	110.48
23	b	609	CLA	C3B-C4B-NB	-2.71	105.70	109.21
28	H	102	DGD	C1D-C2D-C3D	-2.71	104.36	110.00
27	B	621	SQD	C45-O47-C7	2.71	124.46	117.79
23	B	606	CLA	CMB-C2B-C1B	-2.71	124.31	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CHD-C1D-C2D	2.70	131.15	125.48
26	A	409	PL9	O1-C4-C3	-2.70	117.75	120.72
23	C	511	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	a	406	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
23	C	508	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	C	512	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
23	a	405	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
23	B	612	CLA	CED-O2D-CGD	-2.69	109.84	115.94
23	c	506	CLA	CGD-CBD-CAD	-2.69	102.01	110.73
23	b	605	CLA	C11-C10-C8	-2.69	107.22	115.92
28	h	101	DGD	C3D-C4D-C5D	-2.69	105.44	110.24
23	b	607	CLA	O2D-CGD-CBD	2.69	116.04	111.27
23	B	613	CLA	CAC-C3C-C4C	2.69	128.29	124.81
26	d	406	PL9	C46-C47-C48	-2.68	103.06	111.88
23	C	503	CLA	CMB-C2B-C3B	2.68	129.70	124.68
23	D	404	CLA	C1-C2-C3	-2.68	121.41	126.04
25	A	408	BCR	C27-C26-C25	2.68	126.62	122.73
23	c	507	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
23	C	514	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
31	a	404	BCT	O3-C-O1	-2.68	112.60	119.55
25	c	515	BCR	C29-C30-C25	2.68	114.60	110.48
25	k	101	BCR	C30-C25-C26	-2.67	118.85	122.61
23	c	508	CLA	CHD-C4C-NC	2.67	128.41	124.20
23	B	610	CLA	C1D-ND-C4D	-2.67	104.44	106.33
23	C	509	CLA	CHB-C4A-NA	2.67	128.20	124.51
25	Z	101	BCR	C15-C14-C13	-2.67	123.50	127.31
28	a	413	DGD	O2G-C1B-C2B	2.66	117.24	111.50
23	c	506	CLA	C1D-ND-C4D	2.66	108.23	106.33
23	C	514	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	b	615	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
27	A	410	SQD	O5-C1-C2	-2.66	104.72	110.35
23	b	613	CLA	C1-C2-C3	-2.66	121.44	126.04
23	C	507	CLA	C2A-C3A-C4A	2.66	106.17	101.87
26	a	410	PL9	C37-C38-C39	-2.66	121.26	127.66
23	c	513	CLA	O1D-CGD-CBD	2.66	129.92	124.48
23	C	505	CLA	O2A-CGA-O1A	-2.66	116.89	123.59
23	b	611	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	H	101	BCR	C16-C15-C14	-2.66	118.03	123.47
23	b	612	CLA	CMD-C2D-C1D	2.66	129.39	124.71
27	B	621	SQD	C1-C2-C3	-2.66	104.47	110.00
23	B	605	CLA	CHD-C4C-NC	2.65	128.39	124.20
33	M	101	LMG	C40-C39-C38	-2.65	100.95	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	514	BCR	C15-C16-C17	-2.65	118.04	123.47
25	A	408	BCR	C40-C30-C25	2.65	114.60	110.30
23	b	606	CLA	C16-C15-C13	-2.65	107.35	115.92
26	a	410	PL9	C35-C34-C36	2.65	119.73	115.27
25	H	101	BCR	C35-C13-C14	-2.65	119.21	122.92
23	B	601	CLA	C2D-C1D-ND	-2.65	108.15	110.10
29	e	101	LHG	C5-O7-C7	-2.65	111.27	117.79
23	b	602	CLA	CBA-CAA-C2A	2.65	121.67	113.86
25	a	409	BCR	C29-C30-C25	2.64	114.55	110.48
27	a	411	SQD	O48-C23-C24	2.64	120.20	111.91
23	d	404	CLA	C1-C2-C3	-2.64	121.48	126.04
27	f	101	SQD	C1-O5-C5	-2.64	108.51	113.69
27	f	101	SQD	O9-S-O7	-2.64	104.82	113.95
23	c	507	CLA	CMB-C2B-C3B	2.64	129.61	124.68
23	b	617	CLA	C2D-C1D-ND	-2.64	108.16	110.10
25	B	619	BCR	C33-C5-C6	-2.64	121.57	124.53
23	d	403	CLA	CMB-C2B-C3B	2.63	129.60	124.68
28	c	517	DGD	C3G-O3G-C1D	2.63	118.88	113.74
23	A	407	CLA	O1D-CGD-CBD	2.63	129.87	124.48
27	f	101	SQD	O48-C23-O10	-2.63	116.95	123.59
25	x	102	BCR	C34-C9-C8	-2.63	113.93	118.08
24	D	401	PHO	CMB-C2B-C3B	2.63	129.60	124.68
25	b	619	BCR	C27-C26-C25	2.63	126.55	122.73
27	B	621	SQD	C3-C4-C5	2.62	114.92	110.24
23	B	603	CLA	CMB-C2B-C3B	2.62	129.58	124.68
23	d	402	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
28	c	518	DGD	O3G-C1D-C2D	-2.62	104.21	108.30
33	C	501	LMG	O3-C3-C2	-2.62	104.29	110.35
23	b	612	CLA	CGD-CBD-CAD	-2.62	102.25	110.73
23	c	505	CLA	CED-O2D-CGD	-2.62	110.02	115.94
26	d	406	PL9	C50-C49-C48	-2.62	115.08	122.65
23	D	402	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
23	B	603	CLA	O1D-CGD-CBD	2.62	129.84	124.48
33	c	522	LMG	C9-C8-C7	-2.62	105.60	111.79
29	d	409	LHG	O8-C6-C5	-2.62	100.82	108.43
23	b	606	CLA	CHC-C1C-NC	2.61	128.17	124.20
23	C	514	CLA	C3A-C2A-C1A	2.61	105.25	101.34
23	C	503	CLA	CHA-C1A-NA	-2.61	120.42	126.40
33	C	501	LMG	O8-C28-O10	-2.61	117.00	123.59
25	x	102	BCR	C30-C25-C26	-2.61	118.94	122.61
23	B	604	CLA	CGD-CBD-CAD	-2.61	102.28	110.73
23	b	613	CLA	C6-C5-C3	-2.61	106.62	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	c	514	BCR	C39-C30-C25	2.60	114.52	110.30
28	a	413	DGD	C5B-C4B-C3B	-2.60	101.21	114.42
23	A	405	CLA	C4A-NA-C1A	2.60	107.88	106.71
23	b	608	CLA	C2C-C1C-NC	2.60	112.41	109.97
23	b	616	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
23	b	612	CLA	C3C-C4C-NC	-2.60	107.65	110.57
26	d	406	PL9	C37-C38-C39	-2.60	121.40	127.66
23	B	606	CLA	CGD-CBD-CAD	-2.60	102.31	110.73
23	c	503	CLA	CAC-C3C-C4C	2.60	128.18	124.81
28	c	516	DGD	O2D-C2D-C1D	-2.60	103.74	110.05
25	d	405	BCR	C8-C7-C6	-2.59	119.91	127.20
23	A	404	CLA	C7-C6-C5	-2.59	106.32	113.36
28	a	413	DGD	O1G-C1A-O1A	-2.59	117.05	123.59
23	B	605	CLA	O1D-CGD-CBD	2.59	129.79	124.48
23	C	511	CLA	C16-C15-C13	-2.59	107.55	115.92
25	T	101	BCR	C37-C22-C21	-2.59	119.30	122.92
26	d	406	PL9	C8-C7-C3	2.59	119.29	111.98
29	D	408	LHG	C20-C19-C18	-2.58	101.31	114.42
24	A	406	PHO	OBD-CAD-CBD	-2.58	122.03	125.82
28	c	517	DGD	C8B-C7B-C6B	-2.58	101.31	114.42
23	B	613	CLA	CHA-C1A-NA	-2.58	120.49	126.40
35	v	201	HEC	CMC-C2C-C1C	-2.58	124.50	128.46
23	c	505	CLA	C11-C10-C8	-2.58	107.58	115.92
23	b	603	CLA	C2D-C1D-ND	-2.58	108.20	110.10
23	B	605	CLA	CHD-C4C-C3C	-2.58	121.05	124.84
25	A	408	BCR	C33-C5-C6	-2.58	121.63	124.53
23	B	615	CLA	C6-C5-C3	-2.58	106.70	113.45
25	T	101	BCR	C15-C16-C17	-2.58	118.20	123.47
23	B	608	CLA	CMB-C2B-C3B	2.58	129.50	124.68
26	A	409	PL9	C36-C34-C33	-2.57	115.91	121.12
23	b	605	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
27	b	601	SQD	C3-C4-C5	2.57	114.83	110.24
27	f	101	SQD	O5-C1-C2	-2.57	104.91	110.35
23	D	402	CLA	CHB-C4A-NA	2.57	128.06	124.51
28	H	102	DGD	C3E-C4E-C5E	-2.56	105.66	110.24
24	d	401	PHO	CBA-CAA-C2A	-2.56	106.33	113.81
24	d	401	PHO	C1B-NB-C4B	2.56	112.35	107.09
23	D	402	CLA	CHD-C1D-ND	-2.56	122.10	124.45
23	a	406	CLA	CAC-C3C-C4C	2.56	128.13	124.81
26	a	410	PL9	C27-C28-C29	-2.56	121.50	127.66
23	c	512	CLA	CMB-C2B-C3B	2.56	129.46	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405	CLA	C4D-CHA-C1A	2.56	124.36	121.25
23	B	605	CLA	C4A-NA-C1A	2.56	107.86	106.71
25	B	618	BCR	C2-C1-C6	2.55	114.41	110.48
25	B	619	BCR	C30-C25-C26	-2.55	119.02	122.61
29	d	409	LHG	C25-C24-C23	2.55	122.90	113.62
28	c	516	DGD	O3D-C3D-C4D	-2.55	104.45	110.35
23	C	508	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
24	A	406	PHO	CED-O2D-CGD	2.55	121.71	115.94
23	A	405	CLA	CED-O2D-CGD	-2.55	110.17	115.94
23	c	513	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	b	610	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	b	603	CLA	CHD-C1D-C2D	2.55	130.82	125.48
23	C	506	CLA	O2A-CGA-O1A	-2.55	117.17	123.59
33	M	101	LMG	C3-C4-C5	-2.55	105.70	110.24
23	c	510	CLA	C7-C6-C5	-2.54	106.45	113.36
23	A	405	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	c	506	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
24	a	407	PHO	C1-C2-C3	-2.54	121.65	126.04
23	d	403	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
23	c	502	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
23	C	506	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
25	b	619	BCR	C39-C30-C25	-2.54	106.19	110.30
28	c	518	DGD	O6D-C1D-O3G	-2.53	103.98	109.97
23	C	509	CLA	CED-O2D-CGD	-2.53	110.21	115.94
23	B	603	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
28	C	518	DGD	O3E-C3E-C2E	-2.53	104.51	110.35
25	C	520	BCR	C35-C13-C12	2.53	122.06	118.08
26	D	406	PL9	C22-C23-C24	-2.53	121.58	127.66
23	C	509	CLA	C2D-C1D-ND	-2.53	108.24	110.10
23	d	403	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
25	t	101	BCR	C1-C6-C5	-2.52	119.06	122.61
23	C	504	CLA	CMC-C2C-C1C	-2.52	121.20	125.04
23	c	508	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
28	C	517	DGD	O6E-C5E-C4E	2.52	114.27	109.69
23	b	608	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
29	d	408	LHG	C20-C19-C18	-2.52	101.65	114.42
23	a	408	CLA	O2A-C1-C2	-2.52	102.02	108.64
23	b	615	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
33	b	622	LMG	C1-O6-C5	-2.51	108.76	113.69
28	A	412	DGD	CDB-CCB-CBB	-2.51	101.67	114.42
23	a	408	CLA	CMB-C2B-C3B	2.51	129.37	124.68
29	D	409	LHG	O8-C23-C24	2.51	119.78	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	B	613	CLA	C2A-C1A-CHA	2.50	128.24	123.86
34	e	102	HEM	CHA-C4D-ND	2.50	127.47	124.38
34	E	103	HEM	C2C-C3C-C4C	2.50	108.64	106.90
27	F	101	SQD	C3-C4-C5	2.50	114.70	110.24
25	B	618	BCR	C3-C4-C5	-2.50	109.61	114.08
23	b	610	CLA	CHA-C1A-NA	-2.50	120.68	126.40
23	b	602	CLA	C3C-C4C-NC	-2.50	107.77	110.57
24	A	406	PHO	CMB-C2B-C3B	2.50	129.35	124.68
23	B	607	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
23	b	603	CLA	C4A-NA-C1A	2.50	107.83	106.71
23	c	511	CLA	CMB-C2B-C3B	2.50	129.35	124.68
25	x	102	BCR	C2-C1-C6	2.50	114.32	110.48
23	B	609	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
28	C	516	DGD	C1E-O6E-C5E	2.49	118.58	113.69
23	C	507	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
28	C	516	DGD	O3G-C3G-C2G	-2.49	104.89	110.90
23	B	610	CLA	O2D-CGD-CBD	2.49	115.69	111.27
28	h	101	DGD	C3E-C4E-C5E	-2.49	105.80	110.24
23	a	406	CLA	CMB-C2B-C3B	2.49	129.33	124.68
23	C	507	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
28	c	518	DGD	CAB-C9B-C8B	-2.49	101.80	114.42
23	B	603	CLA	CHD-C1D-ND	-2.49	122.17	124.45
28	C	518	DGD	O3G-C1D-C2D	-2.48	104.43	108.30
23	C	513	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
25	c	521	BCR	C33-C5-C6	-2.48	121.75	124.53
25	c	514	BCR	C2-C1-C6	2.48	114.29	110.48
23	B	604	CLA	O2A-CGA-CBA	2.48	119.68	111.91
25	Z	101	BCR	C33-C5-C6	-2.48	121.75	124.53
28	c	516	DGD	C3D-C4D-C5D	-2.48	105.82	110.24
33	c	522	LMG	O7-C10-O9	-2.47	117.72	123.70
23	C	502	CLA	C3B-C4B-NB	-2.47	106.01	109.21
27	b	601	SQD	O48-C23-C24	2.47	119.67	111.91
24	A	406	PHO	C1B-NB-C4B	2.47	112.17	107.09
27	a	412	SQD	O49-C7-C8	-2.47	114.10	123.73
25	d	405	BCR	C38-C26-C25	-2.46	121.76	124.53
25	B	619	BCR	C27-C26-C25	2.46	126.31	122.73
25	H	101	BCR	C33-C5-C6	-2.46	121.76	124.53
23	b	609	CLA	C6-C7-C8	-2.46	107.96	115.92
23	b	610	CLA	O2D-CGD-CBD	-2.46	106.89	111.27
34	E	103	HEM	CBD-CAD-C3D	-2.46	105.79	112.63
25	a	409	BCR	C2-C1-C6	2.46	114.27	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CHA-C1A-NA	-2.46	120.77	126.40
25	T	101	BCR	C37-C22-C23	2.46	121.95	118.08
23	D	403	CLA	C1-C2-C3	-2.46	121.79	126.04
25	b	618	BCR	C29-C30-C25	2.46	114.26	110.48
27	f	101	SQD	C1-C2-C3	-2.46	104.88	110.00
23	a	405	CLA	CAC-C3C-C4C	2.45	128.00	124.81
28	c	517	DGD	O5D-C6D-C5D	-2.45	104.51	109.05
28	c	516	DGD	O2G-C1B-C2B	-2.45	106.21	111.50
23	C	509	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
23	B	606	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	A	407	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
26	D	406	PL9	C30-C29-C31	-2.45	111.15	115.27
23	C	504	CLA	C6-C7-C8	-2.45	108.01	115.92
33	c	524	LMG	O8-C28-O10	-2.45	117.42	123.59
23	c	512	CLA	CHD-C1D-ND	-2.45	122.21	124.45
26	a	410	PL9	C40-C39-C38	-2.44	117.41	123.68
23	B	611	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
23	C	513	CLA	C16-C15-C13	-2.44	108.02	115.92
23	B	601	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
27	B	621	SQD	O10-C23-C24	-2.44	114.20	123.73
23	C	506	CLA	C2D-C1D-ND	-2.44	108.30	110.10
23	a	408	CLA	CHD-C4C-NC	2.44	128.05	124.20
33	c	522	LMG	O3-C3-C2	-2.44	104.72	110.35
28	h	101	DGD	C1D-C2D-C3D	-2.44	104.92	110.00
23	B	605	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	Z	101	BCR	C27-C26-C25	2.43	126.26	122.73
23	b	617	CLA	C2A-C3A-C4A	2.43	105.80	101.87
28	H	102	DGD	C3G-C2G-C1G	-2.43	106.04	111.79
26	a	410	PL9	C11-C12-C13	-2.43	103.89	111.88
23	b	615	CLA	CHD-C4C-NC	2.43	128.03	124.20
23	b	605	CLA	CGD-CBD-CAD	-2.43	102.87	110.73
26	d	406	PL9	C7-C3-C2	-2.43	120.11	123.30
25	d	405	BCR	C27-C26-C25	2.43	126.26	122.73
23	C	512	CLA	C3C-C4C-NC	-2.43	107.85	110.57
23	c	510	CLA	C16-C15-C13	-2.43	108.08	115.92
28	c	517	DGD	O2E-C2E-C1E	-2.42	104.16	110.05
23	C	507	CLA	CHA-C1A-NA	-2.42	120.85	126.40
23	b	614	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	b	609	CLA	CHA-C1A-NA	-2.42	120.85	126.40
23	c	506	CLA	C2D-C1D-ND	-2.42	108.32	110.10
25	b	620	BCR	C27-C26-C25	2.42	126.24	122.73
23	b	611	CLA	C11-C10-C8	-2.42	108.10	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C4-C5-C6	2.41	126.23	122.73
23	c	505	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	b	601	SQD	C45-O47-C7	2.41	123.73	117.79
23	b	614	CLA	CHA-C1A-NA	-2.41	120.88	126.40
33	M	101	LMG	C38-C37-C36	-2.41	102.19	114.42
26	a	410	PL9	O2-C1-C2	-2.41	116.27	121.78
33	C	501	LMG	O5-C6-C5	-2.41	103.04	111.29
25	C	515	BCR	C40-C30-C25	2.40	114.20	110.30
23	c	513	CLA	CAC-C3C-C4C	2.40	127.92	124.81
25	C	515	BCR	C34-C9-C10	-2.40	119.56	122.92
28	C	517	DGD	CDB-CCB-CBB	-2.40	102.25	114.42
25	B	619	BCR	C34-C9-C10	-2.40	119.56	122.92
23	B	602	CLA	CHD-C1D-ND	-2.40	122.25	124.45
23	b	606	CLA	O1A-CGA-CBA	2.40	133.08	123.73
28	c	517	DGD	CDB-CCB-CBB	-2.39	102.27	114.42
28	c	517	DGD	O3G-C3G-C2G	-2.39	105.12	110.90
23	a	408	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
28	h	101	DGD	O6D-C1D-O3G	-2.39	104.31	109.97
25	b	620	BCR	C16-C15-C14	-2.39	118.58	123.47
24	D	401	PHO	C1-C2-C3	-2.39	121.91	126.04
23	B	613	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
28	H	102	DGD	O6D-C1D-O3G	-2.39	104.32	109.97
23	B	601	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	C	512	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	b	612	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
23	D	403	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
23	a	405	CLA	C4-C3-C5	2.39	119.29	115.27
33	m	101	LMG	C40-C39-C38	-2.39	102.31	114.42
23	b	606	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
23	A	404	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
34	E	103	HEM	CHC-C4B-NB	2.38	127.02	124.43
25	c	515	BCR	C36-C18-C17	-2.38	119.58	122.92
23	c	504	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
25	A	408	BCR	C31-C1-C6	-2.38	106.44	110.30
23	D	403	CLA	CMB-C2B-C3B	2.38	129.13	124.68
23	C	509	CLA	CHA-C1A-NA	-2.38	120.95	126.40
23	c	503	CLA	CMD-C2D-C1D	2.38	128.90	124.71
25	t	101	BCR	C15-C14-C13	-2.38	123.92	127.31
23	a	408	CLA	CHD-C4C-C3C	-2.38	121.35	124.84
23	b	607	CLA	CMB-C2B-C1B	-2.37	124.81	128.46
23	A	407	CLA	CHC-C1C-C2C	-2.37	120.16	126.72
23	C	506	CLA	CMD-C2D-C1D	-2.37	120.53	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	619	BCR	C29-C30-C25	2.37	114.13	110.48
23	B	607	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
28	C	516	DGD	O6D-C1D-O3G	-2.37	104.36	109.97
23	b	610	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	b	619	BCR	C3-C4-C5	-2.37	109.84	114.08
23	C	512	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	c	503	CLA	CMB-C2B-C3B	2.37	129.11	124.68
26	a	410	PL9	C31-C29-C28	2.37	125.91	121.12
23	B	615	CLA	CHA-C1A-NA	-2.37	120.98	126.40
23	c	502	CLA	O1D-CGD-CBD	2.37	129.32	124.48
23	B	614	CLA	O2D-CGD-CBD	2.37	115.47	111.27
23	B	615	CLA	C6-C7-C8	-2.36	108.28	115.92
23	B	601	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
23	b	613	CLA	C11-C10-C8	-2.36	108.28	115.92
23	B	606	CLA	C7-C6-C5	-2.36	106.94	113.36
23	B	602	CLA	CHA-C1A-NA	-2.36	120.99	126.40
35	V	201	HEC	CMD-C2D-C1D	-2.36	124.83	128.46
25	D	405	BCR	C1-C6-C5	-2.36	119.30	122.61
27	b	601	SQD	O9-S-C6	2.36	109.74	106.94
23	C	504	CLA	CMC-C2C-C3C	2.35	132.50	126.12
23	B	609	CLA	CHC-C1C-C2C	-2.35	120.22	126.72
25	b	620	BCR	C11-C10-C9	-2.35	123.95	127.31
23	a	405	CLA	CMB-C2B-C3B	2.35	129.08	124.68
23	D	404	CLA	C6-C7-C8	-2.35	108.32	115.92
25	K	101	BCR	C8-C7-C6	-2.35	120.60	127.20
28	h	101	DGD	CDB-CCB-CBB	-2.35	102.50	114.42
23	b	603	CLA	CGD-CBD-CAD	-2.35	103.13	110.73
28	c	516	DGD	O4D-C4D-C3D	2.35	115.78	110.35
25	t	101	BCR	C36-C18-C19	2.35	121.78	118.08
26	d	406	PL9	C40-C39-C38	-2.35	117.66	123.68
29	A	413	LHG	C18-C17-C16	-2.35	102.52	114.42
23	D	403	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
27	b	601	SQD	O48-C23-O10	-2.35	117.67	123.59
28	h	101	DGD	O3E-C3E-C2E	-2.35	104.93	110.35
23	c	504	CLA	CMC-C2C-C1C	2.34	128.60	125.04
23	B	601	CLA	O1D-CGD-CBD	2.34	129.27	124.48
23	a	405	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	t	101	BCR	C37-C22-C21	-2.34	119.64	122.92
25	c	514	BCR	C35-C13-C14	-2.34	119.65	122.92
33	d	410	LMG	O7-C10-O9	-2.34	117.47	123.30
23	b	607	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	C	512	CLA	CAC-C3C-C4C	2.34	127.84	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	516	DGD	CBB-CAB-C9B	-2.34	102.56	114.42
23	b	616	CLA	CHA-C4D-ND	2.34	137.39	132.50
23	b	607	CLA	CHC-C1C-NC	2.34	127.75	124.20
23	b	612	CLA	CHB-C4A-NA	2.34	127.74	124.51
23	b	602	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
28	C	518	DGD	O3D-C3D-C4D	-2.33	104.96	110.35
26	d	406	PL9	C42-C43-C44	-2.33	122.05	127.66
26	D	406	PL9	C35-C34-C36	2.33	119.18	115.27
23	C	514	CLA	C3C-C4C-NC	-2.33	107.96	110.57
23	C	502	CLA	CAC-C3C-C4C	2.32	127.83	124.81
28	c	518	DGD	O1G-C1A-C2A	-2.32	104.61	111.91
23	c	508	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	c	501	CLA	CHA-C4D-ND	2.32	137.36	132.50
23	b	615	CLA	C3C-C4C-NC	-2.32	107.97	110.57
25	d	405	BCR	C30-C25-C26	-2.32	119.35	122.61
23	B	603	CLA	O1A-CGA-CBA	2.32	132.78	123.73
23	b	614	CLA	CGD-CBD-CAD	-2.32	103.22	110.73
23	c	507	CLA	CHD-C4C-NC	2.32	127.86	124.20
26	d	406	PL9	C36-C34-C33	-2.32	116.43	121.12
33	M	101	LMG	O6-C1-O1	-2.31	104.49	109.97
25	k	101	BCR	C2-C1-C6	2.31	114.04	110.48
23	B	616	CLA	C2C-C1C-NC	2.31	112.14	109.97
23	c	506	CLA	C4-C3-C2	-2.31	117.75	123.68
23	B	608	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	B	615	CLA	C4-C3-C2	2.31	129.60	123.68
23	b	604	CLA	CHD-C1D-C2D	2.31	130.32	125.48
23	c	508	CLA	CHD-C1D-C2D	2.31	130.32	125.48
23	b	603	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
25	Z	101	BCR	C24-C23-C22	-2.31	122.75	126.23
28	h	101	DGD	CBB-CAB-C9B	-2.31	102.72	114.42
26	a	410	PL9	O2-C1-C6	2.31	124.58	120.59
33	b	622	LMG	O7-C10-O9	-2.31	118.13	123.70
23	c	502	CLA	C1-O2A-CGA	2.30	122.49	116.44
23	b	613	CLA	CHD-C4C-C3C	-2.30	121.45	124.84
23	b	616	CLA	C2D-C1D-ND	2.30	111.80	110.10
23	b	604	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
23	C	511	CLA	C3A-C2A-C1A	2.30	104.78	101.34
25	B	618	BCR	C30-C25-C26	-2.30	119.37	122.61
34	E	103	HEM	C1D-C2D-C3D	2.30	109.37	106.96
28	C	516	DGD	O1G-C1A-C2A	-2.30	104.70	111.91
23	b	605	CLA	C4D-C3D-CAD	-2.30	105.39	108.10
23	B	603	CLA	C1B-CHB-C4A	-2.30	125.57	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	CAA-CBA-CGA	-2.30	106.54	113.25
23	D	403	CLA	CHD-C1D-ND	-2.29	122.35	124.45
23	d	402	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
27	A	410	SQD	O48-C23-C24	2.29	119.10	111.91
23	b	608	CLA	C1-C2-C3	-2.29	122.08	126.04
25	b	620	BCR	C2-C1-C6	2.29	114.01	110.48
23	D	403	CLA	O2D-CGD-CBD	2.29	115.34	111.27
23	C	513	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
23	C	507	CLA	O1D-CGD-CBD	2.29	129.16	124.48
26	D	406	PL9	C11-C9-C8	-2.29	116.49	121.12
27	f	101	SQD	O48-C23-C24	2.29	119.08	111.91
23	a	405	CLA	CAA-C2A-C1A	-2.29	104.48	111.97
26	A	409	PL9	C22-C23-C24	-2.29	122.16	127.66
23	C	509	CLA	CMB-C2B-C3B	2.28	128.95	124.68
23	B	605	CLA	C3A-C2A-C1A	2.28	104.76	101.34
23	c	507	CLA	C3A-C2A-C1A	2.28	104.75	101.34
33	c	519	LMG	O7-C10-O9	-2.28	118.44	122.96
28	H	102	DGD	CDB-CCB-CBB	-2.28	102.86	114.42
25	C	515	BCR	C3-C4-C5	-2.27	110.02	114.08
27	A	410	SQD	C1-O5-C5	-2.27	109.22	113.69
25	t	101	BCR	C2-C1-C6	2.27	113.98	110.48
33	M	101	LMG	C8-O7-C10	2.27	123.39	117.79
25	b	620	BCR	C36-C18-C17	-2.27	119.74	122.92
23	b	613	CLA	C3D-C4D-ND	2.27	113.91	110.24
23	B	612	CLA	CMC-C2C-C1C	-2.27	121.58	125.04
28	h	101	DGD	C6D-C5D-C4D	2.27	116.83	112.09
25	B	617	BCR	C16-C15-C14	-2.27	118.83	123.47
23	c	510	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
26	a	410	PL9	C21-C19-C18	-2.27	116.53	121.12
33	d	411	LMG	C40-C39-C38	-2.27	102.92	114.42
23	a	405	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
23	b	612	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
23	b	616	CLA	CED-O2D-CGD	2.27	121.06	115.94
25	C	520	BCR	C38-C26-C25	-2.27	121.98	124.53
23	a	408	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
23	d	404	CLA	C2C-C1C-NC	2.26	112.09	109.97
24	A	406	PHO	O2A-CGA-O1A	-2.26	117.88	123.59
25	a	409	BCR	C16-C15-C14	-2.26	118.84	123.47
25	B	617	BCR	C16-C17-C18	-2.26	124.08	127.31
23	c	503	CLA	CHD-C1D-C2D	2.26	130.22	125.48
23	B	605	CLA	C3D-C4D-ND	2.26	113.89	110.24
23	c	512	CLA	C1B-CHB-C4A	-2.26	125.64	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	621	SQD	O5-C1-O6	2.26	115.33	109.97
23	B	603	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
23	b	603	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
25	b	620	BCR	C30-C25-C26	-2.26	119.44	122.61
23	b	615	CLA	CMD-C2D-C1D	2.26	128.69	124.71
23	B	611	CLA	CGD-CBD-CAD	-2.26	103.43	110.73
23	C	511	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
33	c	519	LMG	C9-C8-C7	-2.25	106.46	111.79
23	b	607	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	B	616	CLA	O2D-CGD-CBD	2.25	115.27	111.27
25	K	101	BCR	C27-C26-C25	2.25	126.00	122.73
29	d	408	LHG	C18-C17-C16	-2.25	103.00	114.42
34	e	102	HEM	CHB-C1B-NB	2.25	127.16	124.38
29	A	413	LHG	C20-C19-C18	-2.25	103.01	114.42
23	C	505	CLA	C2A-C1A-CHA	2.25	127.79	123.86
33	c	524	LMG	O7-C10-O9	-2.25	118.28	123.70
23	D	402	CLA	CMB-C2B-C3B	2.24	128.88	124.68
23	A	407	CLA	C6-C5-C3	2.24	119.34	113.45
23	B	605	CLA	O1A-CGA-CBA	2.24	132.49	123.73
33	D	410	LMG	O1-C7-C8	-2.24	105.83	111.78
23	B	602	CLA	CHD-C1D-C2D	2.24	130.19	125.48
23	B	604	CLA	CHB-C4A-NA	2.24	127.61	124.51
25	A	408	BCR	C15-C16-C17	-2.24	118.88	123.47
25	B	619	BCR	C1-C6-C5	-2.24	119.46	122.61
23	C	513	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	C	507	CLA	C6-C7-C8	-2.24	108.68	115.92
33	C	501	LMG	O6-C1-O1	-2.24	104.67	109.97
23	B	612	CLA	C11-C12-C13	-2.23	108.70	115.92
23	C	509	CLA	C7-C6-C5	-2.23	107.29	113.36
33	d	411	LMG	O5-C6-C5	-2.23	103.63	111.29
26	a	410	PL9	C12-C13-C14	-2.23	122.28	127.66
23	b	606	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
28	A	412	DGD	C4E-C3E-C2E	-2.23	106.93	110.82
23	b	613	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	B	615	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	c	503	CLA	O1D-CGD-CBD	2.22	129.03	124.48
23	D	404	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
23	B	604	CLA	CMD-C2D-C1D	2.22	128.63	124.71
23	b	615	CLA	C6-C5-C3	-2.22	107.63	113.45
23	B	615	CLA	CMB-C2B-C3B	2.22	128.83	124.68
23	C	505	CLA	C6-C5-C3	2.22	119.28	113.45
23	C	504	CLA	C2C-C1C-NC	2.22	112.05	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	101	BCR	C11-C10-C9	-2.22	124.14	127.31
23	d	402	CLA	C3B-C4B-NB	-2.22	106.34	109.21
25	D	405	BCR	C7-C8-C9	-2.22	122.89	126.23
33	M	101	LMG	O8-C28-O10	-2.22	118.00	123.59
28	c	516	DGD	C4B-C3B-C2B	-2.21	105.23	113.19
28	a	413	DGD	C1G-O1G-C1A	2.21	125.32	117.12
23	B	609	CLA	CHD-C4C-NC	2.21	127.69	124.20
23	B	607	CLA	CMC-C2C-C1C	2.21	128.41	125.04
23	B	601	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	b	611	CLA	CHA-C1A-NA	-2.21	121.33	126.40
23	b	607	CLA	C4-C3-C5	2.21	118.99	115.27
25	A	408	BCR	C8-C7-C6	-2.21	120.99	127.20
27	A	410	SQD	C3-C4-C5	2.21	114.18	110.24
23	B	612	CLA	C2A-C3A-C4A	2.21	105.44	101.87
23	c	503	CLA	C1D-ND-C4D	2.21	107.91	106.33
23	b	605	CLA	O2D-CGD-CBD	2.21	115.19	111.27
25	d	405	BCR	C29-C30-C25	2.21	113.88	110.48
25	B	619	BCR	C40-C30-C25	2.21	113.88	110.30
28	H	102	DGD	C6D-C5D-C4D	2.21	116.70	112.09
25	x	102	BCR	C35-C13-C12	2.21	121.55	118.08
27	F	101	SQD	O48-C23-O10	-2.21	118.03	123.59
23	b	605	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
23	B	612	CLA	CHC-C1C-NC	2.20	127.55	124.20
23	C	508	CLA	CHA-C1A-NA	-2.20	121.35	126.40
23	c	507	CLA	O2D-CGD-CBD	2.20	115.18	111.27
25	C	520	BCR	C15-C14-C13	-2.20	124.17	127.31
23	C	502	CLA	C4-C3-C5	2.20	118.97	115.27
23	C	514	CLA	C6-C7-C8	-2.20	108.81	115.92
27	A	410	SQD	O48-C46-C45	2.20	114.83	108.43
23	C	509	CLA	C2A-C1A-CHA	2.20	127.70	123.86
27	f	101	SQD	O5-C1-O6	2.19	115.17	109.97
23	c	507	CLA	C2C-C1C-NC	2.19	112.03	109.97
23	c	512	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
26	d	406	PL9	C32-C33-C34	-2.19	122.39	127.66
33	C	501	LMG	O7-C10-O9	-2.19	118.41	123.70
23	C	509	CLA	CHA-C4D-ND	2.19	137.08	132.50
23	B	613	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
25	d	405	BCR	C1-C6-C5	-2.19	119.53	122.61
23	B	611	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	b	609	CLA	C11-C10-C8	-2.19	108.85	115.92
23	B	610	CLA	O1D-CGD-CBD	2.19	128.96	124.48
23	b	607	CLA	CHA-C1A-NA	-2.19	121.39	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	101	BCR	C34-C9-C8	-2.18	114.64	118.08
23	B	608	CLA	CHD-C4C-NC	2.18	127.64	124.20
23	b	605	CLA	C7-C6-C5	-2.18	107.44	113.36
28	h	101	DGD	O5D-C6D-C5D	-2.18	105.01	109.05
23	A	407	CLA	C4A-NA-C1A	2.18	107.69	106.71
29	E	101	LHG	O8-C23-O10	-2.18	118.10	123.59
28	C	518	DGD	O5D-C6D-C5D	-2.18	105.02	109.05
23	b	607	CLA	CHD-C4C-C3C	-2.18	121.64	124.84
23	a	405	CLA	C2D-C1D-ND	-2.18	108.50	110.10
23	B	616	CLA	C1-C2-C3	2.18	129.81	126.04
23	c	513	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	c	508	CLA	CHB-C4A-NA	2.17	127.51	124.51
28	c	518	DGD	O6E-C1E-O5D	-2.17	104.84	109.97
24	a	407	PHO	O2A-CGA-O1A	-2.17	118.12	123.59
33	D	407	LMG	O8-C28-O10	-2.17	118.12	123.59
27	b	601	SQD	O8-S-O7	-2.17	105.98	111.27
23	c	506	CLA	C3C-C4C-NC	-2.16	108.14	110.57
23	b	602	CLA	C3B-C4B-NB	-2.16	106.41	109.21
23	b	611	CLA	C11-C12-C13	-2.16	108.93	115.92
23	B	611	CLA	CHD-C4C-NC	2.16	127.61	124.20
23	c	507	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
23	B	611	CLA	O1A-CGA-CBA	2.16	132.16	123.73
23	b	604	CLA	C4-C3-C5	2.16	118.91	115.27
23	B	612	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
23	C	503	CLA	CHD-C4C-NC	2.16	127.61	124.20
28	C	517	DGD	O5E-C6E-C5E	-2.16	103.88	111.29
26	a	410	PL9	O1-C4-C3	-2.16	118.34	120.72
29	A	413	LHG	O4-P-O6	-2.16	97.73	107.75
23	B	607	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
25	d	405	BCR	C11-C10-C9	-2.15	124.23	127.31
25	a	409	BCR	C27-C26-C25	2.15	125.86	122.73
23	b	612	CLA	CHA-C1A-NA	-2.15	121.46	126.40
23	A	405	CLA	C11-C12-C13	-2.15	108.96	115.92
25	c	514	BCR	C38-C26-C27	-2.15	109.48	113.62
23	b	603	CLA	CMD-C2D-C1D	2.15	128.51	124.71
23	c	501	CLA	C2A-C1A-CHA	2.15	127.62	123.86
23	C	502	CLA	CMC-C2C-C1C	2.15	128.32	125.04
25	c	521	BCR	C30-C25-C26	-2.15	119.58	122.61
33	C	519	LMG	O3-C3-C2	-2.15	105.38	110.35
23	B	606	CLA	C1-C2-C3	-2.15	122.33	126.04
23	B	612	CLA	C16-C15-C13	-2.15	108.98	115.92
26	d	406	PL9	C11-C9-C8	-2.14	116.78	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405	CLA	O1D-CGD-CBD	2.14	128.87	124.48
23	b	603	CLA	C3C-C4C-NC	-2.14	108.17	110.57
27	F	101	SQD	C1-C2-C3	-2.14	105.53	110.00
25	T	101	BCR	C1-C6-C5	-2.14	119.60	122.61
23	b	607	CLA	C2A-C1A-CHA	2.14	127.60	123.86
25	T	101	BCR	C33-C5-C6	-2.14	122.12	124.53
25	t	101	BCR	C3-C4-C5	-2.14	110.26	114.08
29	A	413	LHG	C5-O7-C7	-2.14	112.53	117.79
23	C	502	CLA	CGD-CBD-CAD	-2.14	103.81	110.73
33	c	519	LMG	O8-C28-O10	-2.14	118.20	123.59
23	b	612	CLA	C11-C12-C13	-2.14	109.01	115.92
23	C	514	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
23	c	513	CLA	C2D-C1D-ND	-2.14	108.53	110.10
25	c	515	BCR	C15-C16-C17	-2.14	119.10	123.47
23	B	611	CLA	C11-C10-C8	-2.13	109.02	115.92
28	C	516	DGD	C3E-C4E-C5E	-2.13	106.43	110.24
33	C	501	LMG	C36-C35-C34	-2.13	103.60	114.42
23	b	616	CLA	CHA-C1A-NA	-2.13	121.52	126.40
23	B	614	CLA	C3B-C4B-NB	-2.13	106.45	109.21
28	c	517	DGD	C3D-C4D-C5D	-2.13	106.44	110.24
23	D	404	CLA	C3D-C2D-C1D	2.13	108.74	105.83
23	B	609	CLA	CHD-C4C-C3C	-2.13	121.71	124.84
23	B	609	CLA	O1D-CGD-CBD	2.13	128.84	124.48
23	c	513	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
29	L	101	LHG	C20-C19-C18	-2.12	103.64	114.42
28	C	516	DGD	O3D-C3D-C4D	-2.12	105.44	110.35
26	a	410	PL9	C7-C8-C9	-2.12	123.26	126.79
25	B	617	BCR	C3-C4-C5	-2.12	110.28	114.08
29	d	407	LHG	C18-C17-C16	-2.12	103.64	114.42
25	K	101	BCR	C24-C23-C22	-2.12	123.03	126.23
23	C	513	CLA	C11-C12-C13	-2.12	109.06	115.92
29	l	101	LHG	C27-C26-C25	-2.12	103.66	114.42
23	B	605	CLA	C1-O2A-CGA	-2.12	110.88	116.44
23	C	512	CLA	C4-C3-C5	2.12	118.84	115.27
23	b	613	CLA	C1D-ND-C4D	-2.12	104.83	106.33
25	c	515	BCR	C8-C9-C10	2.12	122.19	118.94
25	C	520	BCR	C2-C1-C6	2.12	113.74	110.48
23	C	512	CLA	O2D-CGD-CBD	2.12	115.03	111.27
25	x	102	BCR	C37-C22-C21	-2.12	119.96	122.92
23	b	616	CLA	C2A-C1A-CHA	2.12	127.56	123.86
23	c	509	CLA	C2C-C1C-NC	-2.12	107.99	109.97
23	c	506	CLA	CHA-C4D-ND	2.11	136.92	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	406	PL9	C31-C32-C33	-2.11	104.94	111.88
25	c	515	BCR	C38-C26-C27	-2.11	109.56	113.62
23	B	602	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
25	t	101	BCR	C31-C1-C6	2.11	113.72	110.30
23	C	504	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
28	A	412	DGD	O5D-C6D-C5D	-2.11	105.14	109.05
28	a	413	DGD	C2G-O2G-C1B	2.11	122.99	117.79
28	C	517	DGD	CBB-CAB-C9B	-2.11	103.71	114.42
23	C	508	CLA	CHD-C4C-NC	2.11	127.53	124.20
23	b	610	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	b	608	CLA	CMB-C2B-C3B	2.11	128.63	124.68
23	A	404	CLA	C1D-ND-C4D	-2.11	104.84	106.33
23	c	510	CLA	C9-C8-C10	2.11	118.93	111.29
23	c	509	CLA	C4D-CHA-C1A	2.11	123.82	121.25
25	b	619	BCR	C11-C10-C9	-2.11	124.30	127.31
23	B	602	CLA	CHA-C4D-ND	2.11	136.91	132.50
25	x	102	BCR	C33-C5-C6	-2.11	122.16	124.53
23	c	506	CLA	CMC-C2C-C1C	2.11	128.25	125.04
25	c	515	BCR	C1-C6-C5	-2.11	119.64	122.61
24	d	401	PHO	C1-C2-C3	-2.11	122.40	126.04
23	A	405	CLA	CAC-C3C-C2C	-2.10	123.93	127.53
23	B	605	CLA	CHD-C1D-C2D	2.10	129.89	125.48
23	b	607	CLA	CHD-C1D-C2D	2.10	129.89	125.48
23	b	603	CLA	CHA-C4D-ND	2.10	136.89	132.50
23	C	504	CLA	C2D-C1D-ND	-2.10	108.56	110.10
23	B	606	CLA	CMA-C3A-C4A	-2.10	106.14	111.77
23	c	509	CLA	CHD-C1D-ND	-2.10	122.53	124.45
23	B	605	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
26	D	406	PL9	C42-C43-C44	-2.09	122.62	127.66
23	d	402	CLA	C1D-ND-C4D	2.09	107.82	106.33
23	B	605	CLA	C1D-ND-C4D	-2.09	104.85	106.33
26	A	409	PL9	C40-C39-C41	2.09	118.79	115.27
23	B	612	CLA	CMB-C2B-C3B	2.09	128.59	124.68
23	D	404	CLA	CHD-C1D-C2D	2.09	129.86	125.48
25	B	617	BCR	C35-C13-C14	-2.09	120.00	122.92
23	c	506	CLA	CHA-C1A-NA	-2.09	121.61	126.40
33	m	101	LMG	O8-C28-O10	-2.09	118.32	123.59
27	f	101	SQD	C46-C45-C44	-2.09	106.85	111.79
23	C	511	CLA	CMB-C2B-C3B	2.09	128.58	124.68
25	C	515	BCR	C38-C26-C27	-2.09	109.61	113.62
33	C	501	LMG	C9-C8-C7	-2.09	106.85	111.79
33	c	522	LMG	O8-C28-O10	-2.09	118.33	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C38-C26-C25	-2.08	122.19	124.53
23	c	501	CLA	CMC-C2C-C1C	2.08	128.21	125.04
24	D	401	PHO	C1A-C2A-C3A	-2.08	100.86	102.84
23	C	505	CLA	CMC-C2C-C1C	2.08	128.21	125.04
23	B	601	CLA	CHA-C4D-ND	2.08	136.85	132.50
23	b	606	CLA	CHD-C4C-C3C	-2.08	121.78	124.84
29	l	101	LHG	C11-C10-C9	-2.08	103.86	114.42
28	c	516	DGD	C1D-C2D-C3D	-2.08	105.66	110.00
28	c	518	DGD	C7A-C6A-C5A	-2.08	103.87	114.42
25	t	101	BCR	C15-C16-C17	-2.08	119.22	123.47
33	C	519	LMG	O6-C1-O1	-2.08	105.05	109.97
33	c	519	LMG	C4-C3-C2	-2.08	107.19	110.82
28	h	101	DGD	O6E-C5E-C4E	2.08	113.47	109.69
27	F	101	SQD	C46-C45-C44	-2.08	106.79	113.70
23	C	512	CLA	C2D-C1D-ND	-2.08	108.57	110.10
23	C	509	CLA	CMD-C2D-C1D	2.08	128.37	124.71
26	D	406	PL9	C7-C8-C9	-2.08	123.34	126.79
25	t	101	BCR	C35-C13-C12	2.08	121.35	118.08
25	x	102	BCR	C16-C15-C14	-2.07	119.23	123.47
33	m	101	LMG	C9-C8-C7	-2.07	106.89	111.79
28	C	518	DGD	C1D-C2D-C3D	-2.07	105.68	110.00
27	B	621	SQD	O47-C45-C46	2.07	115.90	108.40
23	C	504	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
25	C	515	BCR	C30-C25-C26	-2.07	119.70	122.61
23	C	504	CLA	C5-C3-C2	-2.07	116.93	121.12
23	b	611	CLA	CMB-C2B-C3B	2.07	128.55	124.68
27	B	621	SQD	O48-C23-C24	2.07	118.40	111.91
25	c	521	BCR	C38-C26-C27	-2.07	109.64	113.62
23	C	504	CLA	CHA-C4D-ND	2.07	136.83	132.50
23	b	604	CLA	O2A-C1-C2	-2.07	103.20	108.64
24	a	407	PHO	C1A-C2A-C3A	-2.07	100.87	102.84
23	b	614	CLA	C5-C3-C2	-2.07	116.94	121.12
23	B	603	CLA	C4-C3-C2	-2.07	118.38	123.68
23	D	402	CLA	CMB-C2B-C1B	-2.07	125.29	128.46
25	t	101	BCR	C30-C25-C26	-2.07	119.70	122.61
23	C	513	CLA	CHA-C1A-NA	-2.06	121.67	126.40
24	D	401	PHO	OBD-CAD-CBD	-2.06	122.79	125.82
23	d	404	CLA	CHD-C1D-ND	-2.06	122.56	124.45
29	D	408	LHG	C11-C10-C9	-2.06	103.95	114.42
23	D	404	CLA	O2D-CGD-CBD	2.06	114.93	111.27
23	c	509	CLA	C3B-C4B-NB	-2.06	106.55	109.21
23	B	610	CLA	CHD-C4C-NC	2.06	127.45	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
23	C	504	CLA	CMB-C2B-C3B	2.06	128.53	124.68
23	b	608	CLA	O2A-C1-C2	-2.06	103.22	108.64
23	b	611	CLA	O1D-CGD-CBD	2.06	128.70	124.48
33	M	101	LMG	O7-C10-O9	-2.06	118.72	123.70
26	A	409	PL9	C31-C32-C33	-2.06	105.11	111.88
23	c	511	CLA	CHA-C1A-NA	-2.06	121.68	126.40
27	a	412	SQD	O6-C44-C45	-2.06	106.32	111.78
34	e	102	HEM	CAB-C3B-C2B	-2.06	121.82	128.60
28	c	518	DGD	O6E-C5E-C6E	-2.06	101.32	106.44
23	c	513	CLA	C16-C15-C13	-2.06	109.27	115.92
25	D	405	BCR	C16-C15-C14	-2.06	119.26	123.47
23	B	606	CLA	C2C-C1C-NC	2.06	111.90	109.97
23	b	612	CLA	C5-C3-C2	2.06	125.28	121.12
23	b	612	CLA	CMB-C2B-C3B	2.06	128.52	124.68
25	A	408	BCR	C11-C10-C9	-2.05	124.38	127.31
23	b	611	CLA	CHA-C4D-ND	2.05	136.79	132.50
23	b	609	CLA	C4D-CHA-C1A	2.05	123.75	121.25
29	D	409	LHG	O8-C6-C5	-2.05	102.46	108.43
28	C	518	DGD	C5B-C4B-C3B	-2.05	104.01	114.42
23	b	616	CLA	CHD-C4C-C3C	-2.05	121.83	124.84
23	B	601	CLA	O2D-CGD-CBD	2.05	114.91	111.27
23	b	615	CLA	C2D-C1D-ND	-2.05	108.59	110.10
23	B	607	CLA	C2A-C1A-CHA	2.05	127.44	123.86
23	c	504	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
25	b	618	BCR	C32-C1-C6	-2.05	106.98	110.30
29	d	407	LHG	O8-C23-O10	-2.05	118.42	123.59
23	B	609	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	B	610	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
23	B	612	CLA	CGD-CBD-CAD	2.05	117.36	110.73
25	d	405	BCR	C2-C1-C6	2.05	113.63	110.48
28	C	517	DGD	O3D-C3D-C4D	-2.05	105.62	110.35
25	B	617	BCR	C15-C14-C13	-2.04	124.39	127.31
23	c	512	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
23	D	402	CLA	C7-C6-C5	-2.04	107.81	113.36
23	b	617	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	b	604	CLA	CHB-C4A-NA	2.04	127.34	124.51
23	C	513	CLA	C4A-NA-C1A	2.04	107.62	106.71
24	d	401	PHO	CAA-C2A-C3A	-2.04	107.19	112.78
23	b	615	CLA	CHC-C1C-NC	2.04	127.30	124.20
23	b	610	CLA	CHD-C4C-NC	2.04	127.42	124.20
23	B	606	CLA	O2A-CGA-O1A	-2.04	118.45	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
25	B	617	BCR	C33-C5-C6	-2.04	122.24	124.53
26	a	410	PL9	C36-C34-C33	-2.04	117.00	121.12
25	c	515	BCR	C4-C5-C6	2.04	125.69	122.73
23	C	505	CLA	CHA-C4D-ND	2.04	136.76	132.50
23	a	406	CLA	CHD-C1D-C2D	2.04	129.75	125.48
23	c	509	CLA	C3A-C2A-C1A	2.03	104.39	101.34
29	D	409	LHG	C6-C5-C4	2.03	116.60	111.79
23	b	611	CLA	CAC-C3C-C4C	2.03	127.45	124.81
28	C	518	DGD	C8B-C7B-C6B	-2.03	104.10	114.42
23	c	511	CLA	C3B-C4B-NB	-2.03	106.58	109.21
23	b	617	CLA	O2D-CGD-CBD	2.03	114.88	111.27
25	b	619	BCR	C37-C22-C21	-2.03	120.08	122.92
23	C	509	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
23	b	615	CLA	CHB-C4A-NA	2.03	127.32	124.51
28	C	518	DGD	C3G-C2G-C1G	-2.03	106.98	111.79
23	B	605	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
23	c	509	CLA	O2A-CGA-CBA	2.03	118.28	111.91
23	b	611	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
23	B	609	CLA	OBD-CAD-C3D	2.03	133.40	128.52
23	C	509	CLA	CHD-C1D-ND	-2.03	122.59	124.45
28	C	516	DGD	CCB-CBB-CAB	-2.03	104.13	114.42
26	d	406	PL9	C41-C39-C38	-2.03	117.02	121.12
23	c	509	CLA	C1D-ND-C4D	2.02	107.77	106.33
23	C	508	CLA	CHB-C4A-NA	2.02	127.31	124.51
34	e	102	HEM	C1B-NB-C4B	2.02	107.16	105.07
23	C	511	CLA	O2D-CGD-CBD	2.02	114.86	111.27
23	B	608	CLA	C6-C7-C8	-2.02	109.38	115.92
25	K	101	BCR	C15-C16-C17	-2.02	119.33	123.47
33	C	519	LMG	O2-C2-C1	-2.02	105.14	110.05
27	b	601	SQD	O4-C4-C3	-2.02	105.68	110.35
23	b	603	CLA	CMC-C2C-C3C	2.02	131.60	126.12
28	c	516	DGD	O3G-C1D-C2D	-2.02	105.15	108.30
25	x	102	BCR	C7-C8-C9	-2.02	123.19	126.23
23	C	502	CLA	OBD-CAD-C3D	2.02	133.38	128.52
33	C	519	LMG	C38-C37-C36	-2.02	104.18	114.42
25	x	102	BCR	C38-C26-C27	-2.02	109.74	113.62
23	C	507	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
23	c	506	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
29	A	413	LHG	C11-C10-C9	-2.02	104.19	114.42
23	B	613	CLA	C16-C15-C13	-2.02	109.41	115.92
23	c	513	CLA	O2A-CGA-O1A	-2.01	118.51	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CMC-C2C-C3C	2.01	131.58	126.12
23	C	502	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
23	a	408	CLA	CHA-C1A-NA	-2.01	121.79	126.40
23	c	508	CLA	O2D-CGD-CBD	2.01	114.84	111.27
28	c	516	DGD	O1G-C1A-C2A	-2.01	105.59	111.91
23	a	405	CLA	CHD-C1D-C2D	2.01	129.70	125.48
25	Z	101	BCR	C8-C9-C10	2.01	122.03	118.94
26	d	406	PL9	C30-C29-C28	-2.01	118.52	123.68
23	B	603	CLA	CHA-C4D-ND	2.01	136.70	132.50
23	d	403	CLA	C4D-CHA-C1A	2.01	123.69	121.25
23	c	505	CLA	CMD-C2D-C3D	2.01	132.24	127.61
23	c	503	CLA	C3C-C4C-NC	-2.01	108.32	110.57
29	D	408	LHG	C27-C26-C25	-2.01	104.23	114.42
26	D	406	PL9	C31-C29-C28	2.01	125.18	121.12
23	A	404	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
29	e	101	LHG	O10-C23-C24	-2.01	115.90	123.73
23	c	502	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
28	H	102	DGD	C5B-C4B-C3B	-2.01	104.24	114.42
24	D	401	PHO	C1B-NB-C4B	2.01	111.21	107.09
28	c	518	DGD	CBB-CAB-C9B	-2.00	104.25	114.42
25	D	405	BCR	C2-C1-C6	2.00	113.56	110.48
25	K	101	BCR	C32-C1-C6	-2.00	107.05	110.30
23	B	614	CLA	CHB-C4A-NA	2.00	127.28	124.51
23	C	514	CLA	CAC-C3C-C4C	2.00	127.41	124.81
29	e	101	LHG	C18-C17-C16	-2.00	104.26	114.42
23	A	407	CLA	C3D-C4D-ND	2.00	113.48	110.24
33	c	519	LMG	C31-C30-C29	-2.00	105.99	113.19
33	D	410	LMG	C35-C34-C33	-2.00	104.26	114.42
34	E	103	HEM	CAD-CBD-CGD	2.00	117.91	113.60
33	C	519	LMG	C33-C32-C31	-2.00	104.27	114.42
23	b	609	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (61) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
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	502	CLA	ND
23	C	503	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	508	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	C	514	CLA	ND
23	D	402	CLA	ND
23	a	405	CLA	ND
23	a	406	CLA	ND
23	a	408	CLA	ND
23	b	602	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	609	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	b	617	CLA	ND
23	c	501	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
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
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	404	CLA	ND

All (1744) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
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
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	505	CLA	C4-C3-C5-C6
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	D	402	CLA	CHA-CBD-CGD-O1D
23	D	402	CLA	CHA-CBD-CGD-O2D
23	D	403	CLA	C12-C13-C15-C16
23	b	602	CLA	C1A-C2A-CAA-CBA
23	b	602	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	615	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	C2-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C11-C10-C8-C9
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C6-C7-C8-C9
24	a	407	PHO	O2A-C1-C2-C3
25	A	408	BCR	C7-C8-C9-C34
25	A	408	BCR	C20-C21-C22-C37
25	B	617	BCR	C16-C17-C18-C36
25	B	618	BCR	C35-C13-C14-C15
25	B	618	BCR	C16-C17-C18-C36
25	B	619	BCR	C11-C10-C9-C8
25	C	515	BCR	C11-C10-C9-C34
25	C	515	BCR	C11-C12-C13-C14
25	C	515	BCR	C11-C12-C13-C35
25	C	520	BCR	C16-C17-C18-C36
25	C	520	BCR	C18-C19-C20-C21
25	C	520	BCR	C20-C21-C22-C37
25	D	405	BCR	C37-C22-C23-C24
25	D	405	BCR	C23-C24-C25-C26
25	H	101	BCR	C11-C12-C13-C35
25	K	101	BCR	C7-C8-C9-C34
25	K	101	BCR	C11-C12-C13-C35
25	K	101	BCR	C17-C18-C19-C20
25	K	101	BCR	C21-C22-C23-C24
25	T	101	BCR	C20-C21-C22-C23
25	T	101	BCR	C20-C21-C22-C37
25	Z	101	BCR	C7-C8-C9-C34
25	Z	101	BCR	C10-C11-C12-C13
25	Z	101	BCR	C11-C12-C13-C35
25	Z	101	BCR	C16-C17-C18-C19
25	Z	101	BCR	C16-C17-C18-C36
25	b	619	BCR	C7-C8-C9-C34
25	b	619	BCR	C11-C10-C9-C8
25	b	619	BCR	C11-C12-C13-C14
25	b	619	BCR	C11-C12-C13-C35
25	b	619	BCR	C20-C21-C22-C37
25	b	619	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	620	BCR	C11-C12-C13-C14
25	b	620	BCR	C11-C12-C13-C35
25	b	620	BCR	C37-C22-C23-C24
25	c	514	BCR	C7-C8-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	C20-C21-C22-C37
25	c	515	BCR	C35-C13-C14-C15
25	c	515	BCR	C20-C21-C22-C37
25	c	521	BCR	C11-C12-C13-C35
25	c	521	BCR	C17-C18-C19-C20
25	c	521	BCR	C36-C18-C19-C20
25	d	405	BCR	C6-C7-C8-C9
25	d	405	BCR	C7-C8-C9-C34
25	d	405	BCR	C11-C12-C13-C35
25	d	405	BCR	C20-C21-C22-C37
25	d	405	BCR	C37-C22-C23-C24
25	d	405	BCR	C22-C23-C24-C25
25	k	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C11-C10-C9-C8
25	k	101	BCR	C11-C12-C13-C35
25	t	101	BCR	C12-C13-C14-C15
25	t	101	BCR	C35-C13-C14-C15
25	t	101	BCR	C14-C15-C16-C17
25	t	101	BCR	C20-C21-C22-C37
25	x	102	BCR	C7-C8-C9-C34
25	x	102	BCR	C11-C12-C13-C35
25	x	102	BCR	C37-C22-C23-C24
25	x	102	BCR	C23-C24-C25-C26
26	A	409	PL9	C9-C11-C12-C13
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	C32-C33-C34-C35
26	D	406	PL9	C32-C33-C34-C36
26	D	406	PL9	C47-C48-C49-C50
26	a	410	PL9	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C24-C26-C27-C28
26	a	410	PL9	C32-C33-C34-C36
26	a	410	PL9	C33-C34-C36-C37
26	a	410	PL9	C34-C36-C37-C38
26	a	410	PL9	C42-C43-C44-C46
26	d	406	PL9	C32-C33-C34-C35
26	d	406	PL9	C37-C38-C39-C40
26	d	406	PL9	C38-C39-C41-C42
26	d	406	PL9	C42-C43-C44-C45
26	d	406	PL9	C44-C46-C47-C48
27	A	410	SQD	C5-C6-S-O7
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O6-C44-C45-O47
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	a	411	SQD	O47-C45-C46-O48
27	a	412	SQD	O49-C7-O47-C45
27	a	412	SQD	O10-C23-O48-C46
27	f	101	SQD	O5-C1-O6-C44
28	A	412	DGD	C2B-C1B-O2G-C2G
28	A	412	DGD	O1B-C1B-O2G-C2G
28	A	412	DGD	O2G-C2G-C3G-O3G
28	a	413	DGD	O1A-C1A-O1G-C1G
28	a	413	DGD	O2G-C2G-C3G-O3G
29	A	413	LHG	O1-C1-C2-C3
29	A	413	LHG	C3-O3-P-O5
29	A	413	LHG	C3-O3-P-O6
29	D	408	LHG	O1-C1-C2-C3
29	D	408	LHG	O2-C2-C3-O3
29	D	408	LHG	C3-O3-P-O5
29	D	408	LHG	C4-O6-P-O4
29	D	409	LHG	C3-O3-P-O5
29	D	409	LHG	C3-O3-P-O6
29	E	101	LHG	O1-C1-C2-C3
29	E	101	LHG	C4-O6-P-O4
29	E	101	LHG	O10-C23-O8-C6
29	L	101	LHG	C4-O6-P-O4
29	L	101	LHG	C4-O6-P-O5
29	d	407	LHG	O1-C1-C2-C3
29	d	407	LHG	C3-O3-P-O4
29	d	407	LHG	C3-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	d	407	LHG	C3-O3-P-O6
29	d	408	LHG	C4-O6-P-O4
29	d	408	LHG	C4-O6-P-O5
29	e	101	LHG	O1-C1-C2-C3
29	e	101	LHG	C3-O3-P-O5
29	e	101	LHG	C4-O6-P-O3
29	e	101	LHG	C4-O6-P-O4
29	e	101	LHG	C4-O6-P-O5
29	e	101	LHG	O10-C23-O8-C6
29	l	101	LHG	C4-O6-P-O3
29	l	101	LHG	C4-O6-P-O5
33	C	501	LMG	O6-C1-O1-C7
33	C	501	LMG	O9-C10-O7-C8
33	C	519	LMG	C11-C10-O7-C8
33	D	410	LMG	O1-C7-C8-C9
33	D	410	LMG	O1-C7-C8-O7
33	D	410	LMG	C11-C10-O7-C8
33	b	622	LMG	O9-C10-O7-C8
33	b	622	LMG	C11-C10-O7-C8
33	c	524	LMG	O6-C1-O1-C7
33	c	524	LMG	O10-C28-O8-C9
33	c	524	LMG	C29-C28-O8-C9
23	C	504	CLA	O1D-CGD-O2D-CED
23	b	602	CLA	O1D-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
24	d	401	PHO	CBD-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
27	a	412	SQD	C24-C23-O48-C46
29	E	101	LHG	C24-C23-O8-C6
29	e	101	LHG	C24-C23-O8-C6
23	B	606	CLA	CBD-CGD-O2D-CED
23	C	502	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
27	F	101	SQD	O10-C23-O48-C46
33	c	522	LMG	O10-C28-O8-C9
23	B	601	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	503	CLA	O1D-CGD-O2D-CED
23	b	604	CLA	CBD-CGD-O2D-CED
28	a	413	DGD	O1B-C1B-O2G-C2G
33	C	519	LMG	O9-C10-O7-C8
33	D	410	LMG	O9-C10-O7-C8
33	c	522	LMG	O9-C10-O7-C8
27	b	601	SQD	O10-C23-O48-C46
23	b	602	CLA	C3-C5-C6-C7
23	b	605	CLA	C3-C5-C6-C7
27	b	601	SQD	C24-C23-O48-C46
28	a	413	DGD	C2A-C1A-O1G-C1G
33	c	522	LMG	C29-C28-O8-C9
27	a	412	SQD	C8-C7-O47-C45
33	C	501	LMG	C11-C10-O7-C8
23	b	607	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	CBD-CGD-O2D-CED
26	a	410	PL9	C30-C29-C31-C32
26	d	406	PL9	C40-C39-C41-C42
23	C	505	CLA	C2-C3-C5-C6
23	b	612	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
23	b	602	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C3-C5-C6-C7
27	F	101	SQD	C24-C23-O48-C46
26	d	406	PL9	C47-C48-C49-C51
26	A	409	PL9	C12-C13-C14-C15
26	a	410	PL9	C42-C43-C44-C45
23	b	603	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	O1D-CGD-O2D-CED
26	A	409	PL9	C17-C18-C19-C21
26	d	406	PL9	C32-C33-C34-C36
26	d	406	PL9	C42-C43-C44-C46
25	c	514	BCR	C9-C10-C11-C12
27	F	101	SQD	C44-C45-C46-O48
23	C	512	CLA	CBD-CGD-O2D-CED
23	b	616	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	CBD-CGD-O2D-CED
29	D	409	LHG	O2-C2-C3-O3
28	c	518	DGD	O1A-C1A-O1G-C1G
24	d	401	PHO	O1D-CGD-O2D-CED
33	C	501	LMG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	612	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
28	h	101	DGD	O6E-C5E-C6E-O5E
33	C	501	LMG	O10-C28-O8-C9
26	A	409	PL9	C47-C48-C49-C50
26	a	410	PL9	C47-C48-C49-C50
33	c	524	LMG	O6-C5-C6-O5
23	c	507	CLA	C4-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	617	CLA	O1D-CGD-O2D-CED
33	c	519	LMG	C11-C10-O7-C8
33	C	501	LMG	O6-C5-C6-O5
33	c	522	LMG	C4-C5-C6-O5
26	A	409	PL9	C34-C36-C37-C38
26	A	409	PL9	C44-C46-C47-C48
26	a	410	PL9	C19-C21-C22-C23
26	d	406	PL9	C34-C36-C37-C38
23	b	613	CLA	O1D-CGD-O2D-CED
33	C	519	LMG	C4-C5-C6-O5
23	c	511	CLA	O1D-CGD-O2D-CED
29	D	408	LHG	C1-C2-C3-O3
23	B	601	CLA	CBA-CGA-O2A-C1
27	A	411	SQD	C24-C23-O48-C46
27	f	101	SQD	C24-C23-O48-C46
33	c	519	LMG	C29-C28-O8-C9
33	c	524	LMG	C4-C5-C6-O5
29	d	407	LHG	C7-C8-C9-C10
23	c	509	CLA	C10-C11-C12-C13
23	b	607	CLA	C15-C16-C17-C18
23	c	503	CLA	C5-C6-C7-C8
27	B	621	SQD	C2-C1-O6-C44
27	f	101	SQD	C2-C1-O6-C44
33	c	524	LMG	C2-C1-O1-C7
27	a	411	SQD	C12-C13-C14-C15
29	D	409	LHG	C29-C30-C31-C32
33	C	501	LMG	C4-C5-C6-O5
23	B	605	CLA	C11-C10-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	B	614	CLA	C11-C12-C13-C14
23	B	614	CLA	C14-C13-C15-C16
23	C	503	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	b	602	CLA	C11-C10-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	b	607	CLA	C14-C13-C15-C16
23	c	502	CLA	C6-C7-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	c	509	CLA	C11-C12-C13-C14
23	d	404	CLA	C11-C12-C13-C14
24	A	406	PHO	C14-C13-C15-C16
23	c	507	CLA	CBD-CGD-O2D-CED
25	K	101	BCR	C37-C22-C23-C24
25	b	620	BCR	C36-C18-C19-C20
25	c	515	BCR	C37-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C34
25	d	405	BCR	C21-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C10
33	m	101	LMG	C10-C11-C12-C13
23	B	601	CLA	O1A-CGA-O2A-C1
23	b	615	CLA	C8-C10-C11-C12
23	c	512	CLA	C13-C15-C16-C17
23	B	606	CLA	O1D-CGD-O2D-CED
29	E	101	LHG	C32-C33-C34-C35
23	C	507	CLA	C3-C5-C6-C7
23	b	604	CLA	C5-C6-C7-C8
27	F	101	SQD	C23-C24-C25-C26
28	c	517	DGD	C1B-C2B-C3B-C4B
29	e	101	LHG	C23-C24-C25-C26
27	a	411	SQD	O10-C23-O48-C46
25	B	618	BCR	C14-C15-C16-C17
23	B	606	CLA	C15-C16-C17-C18
23	B	607	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	C	513	CLA	C10-C11-C12-C13
23	b	606	CLA	C5-C6-C7-C8
23	b	606	CLA	C15-C16-C17-C18
23	b	608	CLA	C10-C11-C12-C13
23	b	612	CLA	C10-C11-C12-C13
23	b	612	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	612	CLA	C15-C16-C17-C18
23	b	615	CLA	C5-C6-C7-C8
23	c	510	CLA	C15-C16-C17-C18
28	h	101	DGD	C4E-C5E-C6E-O5E
29	A	413	LHG	O1-C1-C2-O2
27	A	410	SQD	C7-C8-C9-C10
28	c	518	DGD	C1A-C2A-C3A-C4A
29	E	101	LHG	C7-C8-C9-C10
33	D	411	LMG	C28-C29-C30-C31
33	c	519	LMG	O6-C5-C6-O5
23	C	502	CLA	O1D-CGD-O2D-CED
23	c	508	CLA	C13-C15-C16-C17
27	b	601	SQD	C11-C10-C9-C8
28	c	516	DGD	O6E-C5E-C6E-O5E
23	c	506	CLA	C2-C1-O2A-CGA
26	d	406	PL9	C37-C38-C39-C41
23	b	602	CLA	C15-C16-C17-C18
23	b	607	CLA	C10-C11-C12-C13
23	c	511	CLA	C13-C15-C16-C17
27	A	411	SQD	C7-C8-C9-C10
23	d	403	CLA	CBD-CGD-O2D-CED
27	b	601	SQD	C8-C7-O47-C45
23	B	604	CLA	C10-C11-C12-C13
23	B	605	CLA	C5-C6-C7-C8
23	b	602	CLA	C8-C10-C11-C12
23	b	603	CLA	C13-C15-C16-C17
23	B	612	CLA	C6-C7-C8-C10
23	C	507	CLA	C12-C13-C15-C16
23	b	613	CLA	C6-C7-C8-C10
23	c	502	CLA	C11-C12-C13-C15
23	c	512	CLA	C11-C12-C13-C15
25	B	619	BCR	C13-C14-C15-C16
23	c	512	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	C13-C15-C16-C17
23	B	615	CLA	C10-C11-C12-C13
23	C	508	CLA	C10-C11-C12-C13
23	b	610	CLA	C15-C16-C17-C18
23	c	505	CLA	C15-C16-C17-C18
33	C	519	LMG	O6-C5-C6-O5
23	c	510	CLA	C8-C10-C11-C12
33	c	522	LMG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	617	BCR	C18-C19-C20-C21
25	C	515	BCR	C10-C11-C12-C13
25	Z	101	BCR	C18-C19-C20-C21
25	b	619	BCR	C10-C11-C12-C13
25	b	619	BCR	C18-C19-C20-C21
25	x	102	BCR	C18-C19-C20-C21
29	A	413	LHG	O2-C2-C3-O3
29	d	407	LHG	O2-C2-C3-O3
29	e	101	LHG	O2-C2-C3-O3
23	A	404	CLA	C15-C16-C17-C18
23	a	406	CLA	C10-C11-C12-C13
23	c	503	CLA	C8-C10-C11-C12
28	c	518	DGD	C2A-C1A-O1G-C1G
23	a	408	CLA	C10-C11-C12-C13
33	M	101	LMG	O10-C28-O8-C9
23	B	607	CLA	C13-C15-C16-C17
23	B	611	CLA	C13-C15-C16-C17
23	C	510	CLA	C13-C15-C16-C17
23	C	511	CLA	C15-C16-C17-C18
23	c	509	CLA	C15-C16-C17-C18
29	D	408	LHG	C3-O3-P-O6
29	L	101	LHG	C4-O6-P-O3
29	d	408	LHG	C4-O6-P-O3
27	A	410	SQD	C23-C24-C25-C26
23	C	503	CLA	C3-C5-C6-C7
23	B	613	CLA	C8-C10-C11-C12
23	C	506	CLA	C5-C6-C7-C8
23	c	508	CLA	C10-C11-C12-C13
23	c	512	CLA	O1D-CGD-O2D-CED
28	A	412	DGD	O6D-C5D-C6D-O5D
28	c	516	DGD	C1A-C2A-C3A-C4A
33	M	101	LMG	C10-C11-C12-C13
33	d	411	LMG	C28-C29-C30-C31
29	A	413	LHG	C1-C2-C3-O3
29	d	407	LHG	C1-C2-C3-O3
29	e	101	LHG	C1-C2-C3-O3
23	C	508	CLA	C13-C15-C16-C17
23	B	616	CLA	C11-C12-C13-C14
23	c	506	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
26	d	406	PL9	C47-C48-C49-C50
23	b	608	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	C	501	LMG	C29-C28-O8-C9
33	C	519	LMG	C29-C28-O8-C9
23	B	602	CLA	C13-C15-C16-C17
33	d	410	LMG	C35-C36-C37-C38
23	b	616	CLA	O1D-CGD-O2D-CED
28	a	413	DGD	C2B-C1B-O2G-C2G
25	A	408	BCR	C35-C13-C14-C15
25	B	617	BCR	C35-C13-C14-C15
25	B	617	BCR	C20-C21-C22-C37
25	C	515	BCR	C16-C17-C18-C36
25	C	520	BCR	C11-C10-C9-C34
25	H	101	BCR	C20-C21-C22-C37
25	K	101	BCR	C20-C21-C22-C37
25	Z	101	BCR	C20-C21-C22-C37
25	a	409	BCR	C20-C21-C22-C37
25	b	618	BCR	C20-C21-C22-C37
25	b	620	BCR	C20-C21-C22-C37
25	c	514	BCR	C16-C17-C18-C36
25	c	515	BCR	C16-C17-C18-C36
25	c	521	BCR	C16-C17-C18-C36
25	d	405	BCR	C16-C17-C18-C36
25	k	101	BCR	C11-C10-C9-C34
25	k	101	BCR	C16-C17-C18-C36
25	k	101	BCR	C20-C21-C22-C37
25	x	102	BCR	C16-C17-C18-C36
27	A	410	SQD	C11-C12-C13-C14
27	A	410	SQD	C33-C34-C35-C36
27	a	411	SQD	C34-C35-C36-C37
27	a	412	SQD	C15-C16-C17-C18
28	A	412	DGD	C5B-C6B-C7B-C8B
28	C	518	DGD	CAA-CBA-CCA-CDA
28	a	413	DGD	C5A-C6A-C7A-C8A
28	a	413	DGD	C8B-C9B-CAB-CBB
28	c	516	DGD	C3B-C4B-C5B-C6B
29	L	101	LHG	C32-C33-C34-C35
29	d	408	LHG	C11-C12-C13-C14
29	e	101	LHG	C11-C10-C9-C8
29	e	101	LHG	C17-C18-C19-C20
29	e	101	LHG	C26-C27-C28-C29
33	M	101	LMG	C39-C40-C41-C42
33	d	411	LMG	C34-C35-C36-C37
23	b	604	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	503	CLA	C16-C17-C18-C19
27	a	411	SQD	C26-C27-C28-C29
28	A	412	DGD	C4A-C5A-C6A-C7A
28	C	517	DGD	C8B-C9B-CAB-CBB
28	C	517	DGD	CCB-CDB-CEB-CFB
28	h	101	DGD	CBA-CCA-CDA-CEA
33	D	407	LMG	C39-C40-C41-C42
33	c	522	LMG	C16-C17-C18-C19
23	B	614	CLA	C5-C6-C7-C8
28	A	412	DGD	CAA-CBA-CCA-CDA
28	C	518	DGD	C5A-C6A-C7A-C8A
28	H	102	DGD	C4B-C5B-C6B-C7B
33	D	407	LMG	C35-C36-C37-C38
27	A	411	SQD	C14-C15-C16-C17
27	F	101	SQD	C33-C34-C35-C36
29	D	409	LHG	C32-C33-C34-C35
29	d	409	LHG	C30-C31-C32-C33
33	c	524	LMG	C12-C13-C14-C15
27	b	601	SQD	C18-C19-C20-C21
28	A	412	DGD	C6B-C7B-C8B-C9B
28	C	517	DGD	C6A-C7A-C8A-C9A
28	H	102	DGD	CCA-CDA-CEA-CFA
23	b	603	CLA	O1D-CGD-O2D-CED
25	B	617	BCR	C12-C13-C14-C15
25	B	617	BCR	C20-C21-C22-C23
25	C	515	BCR	C11-C10-C9-C8
25	C	520	BCR	C16-C17-C18-C19
25	C	520	BCR	C20-C21-C22-C23
25	H	101	BCR	C11-C10-C9-C8
25	H	101	BCR	C20-C21-C22-C23
25	c	514	BCR	C12-C13-C14-C15
25	c	514	BCR	C20-C21-C22-C23
25	c	521	BCR	C16-C17-C18-C19
25	d	405	BCR	C11-C10-C9-C8
25	k	101	BCR	C20-C21-C22-C23
25	t	101	BCR	C16-C17-C18-C19
28	A	412	DGD	C2E-C1E-O5D-C6D
28	C	517	DGD	C2E-C1E-O5D-C6D
28	c	517	DGD	C2E-C1E-O5D-C6D
27	B	621	SQD	C24-C23-O48-C46
27	a	411	SQD	C11-C12-C13-C14
28	c	517	DGD	C8B-C9B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	h	101	DGD	C2B-C3B-C4B-C5B
29	A	413	LHG	C14-C15-C16-C17
29	D	409	LHG	C27-C28-C29-C30
29	d	408	LHG	C14-C15-C16-C17
29	d	409	LHG	C27-C28-C29-C30
33	b	622	LMG	C11-C12-C13-C14
33	c	522	LMG	C34-C35-C36-C37
33	d	411	LMG	C39-C40-C41-C42
33	m	101	LMG	C11-C12-C13-C14
23	A	405	CLA	C16-C17-C18-C20
23	D	404	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	b	612	CLA	O1D-CGD-O2D-CED
28	C	517	DGD	C9A-CAA-CBA-CCA
33	C	501	LMG	C16-C17-C18-C19
33	D	407	LMG	C20-C21-C22-C23
33	M	101	LMG	C38-C39-C40-C41
33	d	410	LMG	C37-C38-C39-C40
23	C	504	CLA	C6-C7-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	b	612	CLA	C11-C10-C8-C9
23	b	616	CLA	C14-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C9
23	c	504	CLA	C11-C10-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
27	B	621	SQD	C9-C10-C11-C12
27	B	621	SQD	C11-C12-C13-C14
27	a	412	SQD	C10-C11-C12-C13
27	a	412	SQD	C12-C13-C14-C15
28	C	516	DGD	C4A-C5A-C6A-C7A
28	C	517	DGD	C5B-C6B-C7B-C8B
28	a	413	DGD	C5B-C6B-C7B-C8B
29	E	101	LHG	C11-C10-C9-C8
29	d	408	LHG	C29-C30-C31-C32
33	c	519	LMG	C31-C32-C33-C34
33	d	410	LMG	C38-C39-C40-C41
23	B	604	CLA	C13-C15-C16-C17
27	b	601	SQD	C16-C17-C18-C19
33	c	524	LMG	C38-C39-C40-C41
29	d	408	LHG	O1-C1-C2-C3
29	d	409	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	617	BCR	C17-C18-C19-C20
33	c	522	LMG	C11-C10-O7-C8
27	B	621	SQD	C17-C18-C19-C20
28	A	412	DGD	CEA-CFA-CGA-CHA
28	h	101	DGD	C5B-C6B-C7B-C8B
29	D	409	LHG	C25-C26-C27-C28
33	D	407	LMG	C34-C35-C36-C37
33	b	622	LMG	C18-C19-C20-C21
28	c	517	DGD	C1A-C2A-C3A-C4A
27	a	411	SQD	C30-C31-C32-C33
28	A	412	DGD	CCA-CDA-CEA-CFA
28	A	412	DGD	C2B-C3B-C4B-C5B
28	a	413	DGD	C4A-C5A-C6A-C7A
28	h	101	DGD	CCB-CDB-CEB-CFB
29	D	409	LHG	C11-C12-C13-C14
29	L	101	LHG	C27-C28-C29-C30
29	d	407	LHG	C17-C18-C19-C20
29	d	408	LHG	C32-C33-C34-C35
29	e	101	LHG	C12-C13-C14-C15
29	e	101	LHG	C18-C19-C20-C21
29	l	101	LHG	C13-C14-C15-C16
33	D	407	LMG	C14-C15-C16-C17
33	D	411	LMG	C33-C34-C35-C36
33	b	622	LMG	C15-C16-C17-C18
33	b	622	LMG	C19-C20-C21-C22
33	c	524	LMG	C34-C35-C36-C37
28	C	516	DGD	O6E-C5E-C6E-O5E
23	B	611	CLA	C16-C17-C18-C20
23	c	506	CLA	C16-C17-C18-C19
28	C	517	DGD	O6E-C1E-O5D-C6D
28	c	517	DGD	O6E-C1E-O5D-C6D
23	B	611	CLA	C15-C16-C17-C18
23	B	612	CLA	C13-C15-C16-C17
27	F	101	SQD	C25-C26-C27-C28
28	A	412	DGD	CEB-CFB-CGB-CHB
28	c	518	DGD	CBB-CCB-CDB-CEB
28	h	101	DGD	C3A-C4A-C5A-C6A
28	h	101	DGD	CAB-CBB-CCB-CDB
29	D	409	LHG	C9-C10-C11-C12
29	D	409	LHG	C34-C35-C36-C37
29	E	101	LHG	C15-C16-C17-C18
29	l	101	LHG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	D	407	LMG	C11-C12-C13-C14
33	D	407	LMG	C19-C20-C21-C22
33	M	101	LMG	C36-C37-C38-C39
28	A	412	DGD	C4D-C5D-C6D-O5D
27	f	101	SQD	C29-C30-C31-C32
27	f	101	SQD	C31-C32-C33-C34
28	c	518	DGD	C4B-C5B-C6B-C7B
29	D	408	LHG	C10-C11-C12-C13
33	D	411	LMG	C11-C12-C13-C14
29	d	408	LHG	C7-C8-C9-C10
23	b	615	CLA	C13-C15-C16-C17
27	A	411	SQD	C12-C13-C14-C15
27	a	412	SQD	C18-C19-C20-C21
28	c	516	DGD	C9A-CAA-CBA-CCA
29	D	408	LHG	C15-C16-C17-C18
29	L	101	LHG	C30-C31-C32-C33
33	m	101	LMG	C17-C18-C19-C20
23	c	512	CLA	CBA-CGA-O2A-C1
27	a	411	SQD	C24-C23-O48-C46
28	c	516	DGD	O6D-C5D-C6D-O5D
29	l	101	LHG	C16-C17-C18-C19
33	d	410	LMG	C33-C34-C35-C36
23	b	602	CLA	C3A-C2A-CAA-CBA
23	c	512	CLA	C3A-C2A-CAA-CBA
25	c	514	BCR	C13-C14-C15-C16
27	f	101	SQD	C28-C29-C30-C31
28	a	413	DGD	C3B-C4B-C5B-C6B
33	D	411	LMG	C32-C33-C34-C35
23	b	608	CLA	O1A-CGA-O2A-C1
23	A	405	CLA	C16-C17-C18-C19
23	C	503	CLA	C16-C17-C18-C20
23	a	405	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C20
27	B	621	SQD	C13-C14-C15-C16
27	b	601	SQD	C10-C11-C12-C13
29	d	407	LHG	C30-C31-C32-C33
29	d	409	LHG	C26-C27-C28-C29
29	l	101	LHG	C9-C10-C11-C12
33	b	622	LMG	C31-C32-C33-C34
23	C	512	CLA	O1D-CGD-O2D-CED
33	c	522	LMG	O6-C5-C6-O5
29	d	407	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	l	101	LHG	C27-C28-C29-C30
25	b	619	BCR	C14-C15-C16-C17
23	C	513	CLA	C3-C5-C6-C7
27	a	412	SQD	C11-C12-C13-C14
33	c	524	LMG	C16-C17-C18-C19
23	C	511	CLA	C4-C3-C5-C6
24	A	406	PHO	C4-C3-C5-C6
26	D	406	PL9	C30-C29-C31-C32
24	A	406	PHO	C2-C3-C5-C6
26	d	406	PL9	C28-C29-C31-C32
23	c	505	CLA	O1D-CGD-O2D-CED
28	A	412	DGD	CBA-CCA-CDA-CEA
33	D	407	LMG	C30-C31-C32-C33
33	m	101	LMG	C31-C32-C33-C34
26	D	406	PL9	C47-C48-C49-C51
29	D	408	LHG	O1-C1-C2-O2
29	d	407	LHG	O1-C1-C2-O2
29	e	101	LHG	O1-C1-C2-O2
28	C	518	DGD	C3A-C4A-C5A-C6A
28	c	516	DGD	C4B-C5B-C6B-C7B
29	D	408	LHG	C11-C10-C9-C8
29	d	407	LHG	C32-C33-C34-C35
29	d	408	LHG	C30-C31-C32-C33
23	B	616	CLA	C11-C12-C13-C15
23	c	507	CLA	C16-C17-C18-C20
29	D	408	LHG	C11-C12-C13-C14
29	e	101	LHG	C10-C11-C12-C13
33	C	501	LMG	C14-C15-C16-C17
27	B	621	SQD	C29-C30-C31-C32
28	A	412	DGD	CDB-CEB-CFB-CGB
28	c	517	DGD	C6A-C7A-C8A-C9A
29	A	413	LHG	C27-C28-C29-C30
29	e	101	LHG	C14-C15-C16-C17
33	M	101	LMG	C12-C13-C14-C15
33	c	522	LMG	C36-C37-C38-C39
33	d	410	LMG	C31-C32-C33-C34
26	a	410	PL9	C47-C48-C49-C51
29	A	413	LHG	C12-C13-C14-C15
29	D	408	LHG	C30-C31-C32-C33
29	d	409	LHG	C29-C30-C31-C32
33	c	519	LMG	C39-C40-C41-C42
23	a	408	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	602	CLA	C10-C11-C12-C13
28	c	516	DGD	C4D-C5D-C6D-O5D
23	c	512	CLA	O1A-CGA-O2A-C1
27	A	411	SQD	C10-C11-C12-C13
23	b	607	CLA	C3-C5-C6-C7
25	A	408	BCR	C1-C6-C7-C8
25	A	408	BCR	C5-C6-C7-C8
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	C	520	BCR	C1-C6-C7-C8
25	C	520	BCR	C5-C6-C7-C8
25	D	405	BCR	C23-C24-C25-C30
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C26
25	x	102	BCR	C23-C24-C25-C30
28	A	412	DGD	C9B-CAB-CBB-CCB
28	c	517	DGD	CAA-CBA-CCA-CDA
33	c	519	LMG	C36-C37-C38-C39
23	B	605	CLA	C10-C11-C12-C13
23	B	611	CLA	C8-C10-C11-C12
23	B	612	CLA	C10-C11-C12-C13
23	C	504	CLA	C8-C10-C11-C12
23	c	504	CLA	C5-C6-C7-C8
28	c	516	DGD	C8B-C9B-CAB-CBB
33	c	524	LMG	C13-C14-C15-C16
33	c	522	LMG	C32-C33-C34-C35
26	A	409	PL9	C47-C48-C49-C51
27	F	101	SQD	C26-C27-C28-C29
29	D	408	LHG	C32-C33-C34-C35
29	D	409	LHG	C30-C31-C32-C33
23	B	614	CLA	C4-C3-C5-C6
23	B	605	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C12-C13-C15
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C11-C12-C13-C15
23	C	509	CLA	C12-C13-C15-C16
23	C	511	CLA	C2-C3-C5-C6
23	C	512	CLA	C6-C7-C8-C10
23	C	514	CLA	C11-C10-C8-C7
23	D	402	CLA	C11-C12-C13-C15
23	a	406	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	605	CLA	C6-C7-C8-C10
23	b	607	CLA	C12-C13-C15-C16
23	b	616	CLA	C12-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C7
23	c	504	CLA	C11-C10-C8-C7
23	c	506	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	c	509	CLA	C12-C13-C15-C16
23	c	511	CLA	C12-C13-C15-C16
26	D	406	PL9	C13-C14-C16-C17
26	D	406	PL9	C28-C29-C31-C32
27	a	411	SQD	C14-C15-C16-C17
29	E	101	LHG	O9-C7-O7-C5
29	L	101	LHG	C23-C24-C25-C26
23	c	503	CLA	CBA-CGA-O2A-C1
33	m	101	LMG	C29-C28-O8-C9
29	D	408	LHG	C29-C30-C31-C32
23	b	611	CLA	C2A-CAA-CBA-CGA
23	D	404	CLA	C5-C6-C7-C8
28	H	102	DGD	C8B-C9B-CAB-CBB
33	c	522	LMG	C38-C39-C40-C41
28	C	518	DGD	CCA-CDA-CEA-CFA
28	c	518	DGD	C8A-C9A-CAA-CBA
29	D	409	LHG	C24-C25-C26-C27
33	b	622	LMG	C16-C17-C18-C19
33	c	522	LMG	C11-C12-C13-C14
29	A	413	LHG	C7-C8-C9-C10
33	c	524	LMG	C28-C29-C30-C31
23	D	403	CLA	C15-C16-C17-C18
28	A	412	DGD	C4B-C5B-C6B-C7B
29	D	408	LHG	C34-C35-C36-C37
29	L	101	LHG	C18-C19-C20-C21
33	D	407	LMG	C13-C14-C15-C16
26	D	406	PL9	C7-C8-C9-C10
28	C	517	DGD	C5A-C6A-C7A-C8A
33	D	410	LMG	C33-C34-C35-C36
28	C	518	DGD	O1A-C1A-O1G-C1G
28	A	412	DGD	C2A-C1A-O1G-C1G
28	A	412	DGD	O6E-C1E-O5D-C6D
23	b	615	CLA	C15-C16-C17-C18
23	c	506	CLA	C5-C6-C7-C8
23	c	507	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	D	406	PL9	C44-C46-C47-C48
27	F	101	SQD	C31-C32-C33-C34
28	a	413	DGD	C7B-C8B-C9B-CAB
29	D	408	LHG	C25-C26-C27-C28
29	d	408	LHG	C34-C35-C36-C37
29	l	101	LHG	C32-C33-C34-C35
33	b	622	LMG	C23-C24-C25-C26
33	d	410	LMG	C32-C33-C34-C35
33	d	411	LMG	C14-C15-C16-C17
33	c	519	LMG	C35-C36-C37-C38
23	C	506	CLA	CBD-CGD-O2D-CED
29	d	407	LHG	C33-C34-C35-C36
27	B	621	SQD	C10-C11-C12-C13
33	b	622	LMG	O6-C5-C6-O5
28	C	517	DGD	C3A-C4A-C5A-C6A
33	M	101	LMG	C17-C18-C19-C20
23	B	607	CLA	C16-C17-C18-C20
29	e	101	LHG	C27-C28-C29-C30
33	D	411	LMG	C31-C32-C33-C34
33	b	622	LMG	C34-C35-C36-C37
23	B	612	CLA	C5-C6-C7-C8
26	a	410	PL9	C40-C39-C41-C42
26	d	406	PL9	C15-C14-C16-C17
26	d	406	PL9	C4-C3-C7-C8
27	B	621	SQD	C34-C35-C36-C37
23	B	615	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	507	CLA	C11-C12-C13-C14
23	C	507	CLA	C14-C13-C15-C16
23	C	512	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	a	406	CLA	C6-C7-C8-C9
23	a	408	CLA	C11-C10-C8-C9
23	b	613	CLA	C6-C7-C8-C9
23	c	502	CLA	C11-C12-C13-C14
23	c	509	CLA	C14-C13-C15-C16
23	c	511	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C14
33	d	411	LMG	O6-C5-C6-O5
28	c	516	DGD	C4A-C5A-C6A-C7A
33	C	501	LMG	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	609	CLA	C5-C6-C7-C8
23	B	607	CLA	C1A-C2A-CAA-CBA
23	a	408	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	C16-C17-C18-C19
23	b	608	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
27	a	411	SQD	C8-C7-O47-C45
29	E	101	LHG	C8-C7-O7-C5
33	M	101	LMG	C11-C10-O7-C8
27	A	410	SQD	C31-C32-C33-C34
27	b	601	SQD	C13-C14-C15-C16
28	C	518	DGD	C7A-C8A-C9A-CAA
29	L	101	LHG	C33-C34-C35-C36
29	e	101	LHG	C16-C17-C18-C19
33	D	411	LMG	C16-C17-C18-C19
33	d	410	LMG	C34-C35-C36-C37
25	B	619	BCR	C15-C16-C17-C18
23	C	513	CLA	C8-C10-C11-C12
23	b	604	CLA	C8-C10-C11-C12
29	D	408	LHG	C4-O6-P-O3
29	e	101	LHG	C3-O3-P-O6
28	a	413	DGD	C2A-C3A-C4A-C5A
23	a	408	CLA	C5-C6-C7-C8
29	E	101	LHG	O6-C4-C5-C6
29	l	101	LHG	O6-C4-C5-C6
28	a	413	DGD	CBA-CCA-CDA-CEA
33	D	411	LMG	C34-C35-C36-C37
29	d	409	LHG	C23-C24-C25-C26
23	c	511	CLA	C16-C17-C18-C20
28	h	101	DGD	C7A-C8A-C9A-CAA
29	d	407	LHG	C16-C17-C18-C19
27	A	410	SQD	C24-C25-C26-C27
28	C	516	DGD	C2B-C3B-C4B-C5B
28	C	517	DGD	C2B-C3B-C4B-C5B
28	c	518	DGD	CCA-CDA-CEA-CFA
33	m	101	LMG	C37-C38-C39-C40
23	B	601	CLA	C10-C11-C12-C13
23	c	507	CLA	C5-C6-C7-C8
29	E	101	LHG	C24-C25-C26-C27
33	c	522	LMG	C40-C41-C42-C43
27	a	411	SQD	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	516	DGD	C4B-C5B-C6B-C7B
29	d	407	LHG	C25-C26-C27-C28
23	B	603	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C19
23	A	407	CLA	C6-C7-C8-C9
27	B	621	SQD	O6-C44-C45-C46
27	a	411	SQD	C44-C45-C46-O48
27	a	412	SQD	C44-C45-C46-O48
27	b	601	SQD	C44-C45-C46-O48
28	C	516	DGD	O1G-C1G-C2G-C3G
28	C	517	DGD	O6E-C5E-C6E-O5E
28	c	518	DGD	C6B-C7B-C8B-C9B
23	c	503	CLA	O1A-CGA-O2A-C1
27	B	621	SQD	C45-C44-O6-C1
28	C	517	DGD	C2G-C3G-O3G-C1D
28	C	517	DGD	C5D-C6D-O5D-C1E
28	c	517	DGD	C5D-C6D-O5D-C1E
29	L	101	LHG	C12-C13-C14-C15
28	h	101	DGD	C6A-C7A-C8A-C9A
33	M	101	LMG	C13-C14-C15-C16
33	D	410	LMG	C10-C11-C12-C13
26	A	409	PL9	C24-C26-C27-C28
29	e	101	LHG	C28-C29-C30-C31
33	C	519	LMG	C11-C12-C13-C14
27	a	411	SQD	C18-C19-C20-C21
33	b	622	LMG	C38-C39-C40-C41
23	d	404	CLA	C8-C10-C11-C12
23	B	609	CLA	C4-C3-C5-C6
23	b	612	CLA	C4-C3-C5-C6
27	A	410	SQD	C15-C16-C17-C18
28	a	413	DGD	CFA-CGA-CHA-CIA
28	c	517	DGD	C4A-C5A-C6A-C7A
29	E	101	LHG	C13-C14-C15-C16
23	C	507	CLA	C2-C3-C5-C6
33	D	410	LMG	C28-C29-C30-C31
23	B	603	CLA	C16-C17-C18-C19
23	b	612	CLA	C8-C10-C11-C12
23	c	506	CLA	C8-C10-C11-C12
27	A	411	SQD	C27-C28-C29-C30
29	D	409	LHG	C17-C18-C19-C20
33	C	519	LMG	C40-C41-C42-C43
33	d	410	LMG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	b	601	SQD	C46-C45-O47-C7
27	F	101	SQD	C30-C31-C32-C33
28	c	518	DGD	C2A-C3A-C4A-C5A
29	e	101	LHG	C11-C12-C13-C14
33	D	407	LMG	O6-C5-C6-O5
29	A	413	LHG	C25-C26-C27-C28
28	c	518	DGD	CDB-CEB-CFB-CGB
33	D	407	LMG	C38-C39-C40-C41
33	D	411	LMG	C37-C38-C39-C40
28	C	518	DGD	C6B-C7B-C8B-C9B
23	C	507	CLA	C13-C15-C16-C17
33	m	101	LMG	C19-C20-C21-C22
23	B	616	CLA	C5-C6-C7-C8
23	C	507	CLA	C8-C10-C11-C12
23	a	405	CLA	C15-C16-C17-C18
25	c	514	BCR	C16-C17-C18-C19
25	d	405	BCR	C20-C21-C22-C23
29	A	413	LHG	C18-C19-C20-C21
27	A	410	SQD	O6-C44-C45-O47
33	C	501	LMG	O1-C7-C8-O7
23	C	505	CLA	C11-C12-C13-C14
28	C	517	DGD	CCA-CDA-CEA-CFA
28	c	518	DGD	C5B-C6B-C7B-C8B
33	D	410	LMG	C37-C38-C39-C40
29	e	101	LHG	O9-C7-O7-C5
23	b	614	CLA	C8-C10-C11-C12
23	b	616	CLA	C5-C6-C7-C8
28	H	102	DGD	O1A-C1A-O1G-C1G
23	D	404	CLA	C16-C17-C18-C20
23	b	608	CLA	C16-C17-C18-C19
28	C	518	DGD	CBA-CCA-CDA-CEA
33	m	101	LMG	C29-C30-C31-C32
23	C	507	CLA	C4-C3-C5-C6
26	d	406	PL9	C45-C44-C46-C47
27	f	101	SQD	C25-C26-C27-C28
23	B	605	CLA	C12-C13-C15-C16
23	B	609	CLA	C2-C3-C5-C6
23	B	614	CLA	C11-C12-C13-C15
23	B	614	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C10-C8-C7
23	C	507	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	406	CLA	C12-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C7
23	b	602	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C12-C13-C15
23	b	608	CLA	C6-C7-C8-C10
23	b	613	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	508	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
24	a	407	PHO	C6-C7-C8-C10
23	B	604	CLA	C11-C10-C8-C9
23	B	605	CLA	C11-C12-C13-C14
23	B	612	CLA	C6-C7-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	D	402	CLA	C11-C12-C13-C14
23	D	404	CLA	C11-C10-C8-C9
23	a	406	CLA	C14-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C14
23	b	605	CLA	C11-C12-C13-C14
23	b	605	CLA	C14-C13-C15-C16
23	b	608	CLA	C6-C7-C8-C9
23	b	609	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
23	c	508	CLA	C14-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C9
33	C	501	LMG	C30-C31-C32-C33
33	D	411	LMG	C14-C15-C16-C17
27	a	412	SQD	C26-C27-C28-C29
33	C	519	LMG	C18-C19-C20-C21
25	C	520	BCR	C37-C22-C23-C24
23	c	504	CLA	C11-C12-C13-C14
27	a	412	SQD	C31-C32-C33-C34
29	d	407	LHG	C19-C20-C21-C22
33	M	101	LMG	C19-C20-C21-C22
28	H	102	DGD	C3B-C4B-C5B-C6B
33	m	101	LMG	C32-C33-C34-C35
29	l	101	LHG	C35-C36-C37-C38
23	C	514	CLA	C10-C11-C12-C13
23	b	608	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C5-C6-C7-C8
27	a	412	SQD	C17-C18-C19-C20
27	a	412	SQD	C29-C30-C31-C32
33	C	519	LMG	C31-C32-C33-C34
28	C	516	DGD	O6D-C5D-C6D-O5D
28	c	517	DGD	CAB-CBB-CCB-CDB
27	B	621	SQD	C23-C24-C25-C26
28	H	102	DGD	C1A-C2A-C3A-C4A
27	A	410	SQD	C32-C33-C34-C35
29	d	407	LHG	C10-C11-C12-C13
26	A	409	PL9	C25-C24-C26-C27
23	b	612	CLA	C2-C3-C5-C6
29	d	409	LHG	C7-C8-C9-C10
23	B	604	CLA	C2C-C3C-CAC-CBC
27	b	601	SQD	C25-C26-C27-C28
29	D	408	LHG	C16-C17-C18-C19
28	C	518	DGD	CDB-CEB-CFB-CGB
23	A	404	CLA	C4C-C3C-CAC-CBC
28	c	518	DGD	C3A-C4A-C5A-C6A
29	d	409	LHG	C32-C33-C34-C35
27	F	101	SQD	C45-C44-O6-C1
27	a	412	SQD	C11-C10-C9-C8
28	C	517	DGD	C8A-C9A-CAA-CBA
29	l	101	LHG	C24-C25-C26-C27
33	D	407	LMG	C40-C41-C42-C43
33	c	522	LMG	C12-C13-C14-C15
23	C	506	CLA	C16-C17-C18-C19
29	l	101	LHG	C24-C23-O8-C6
29	L	101	LHG	C25-C26-C27-C28
23	B	614	CLA	C8-C10-C11-C12
27	A	410	SQD	O6-C44-C45-C46
33	b	622	LMG	C7-C8-C9-O8
33	c	522	LMG	O1-C7-C8-C9
27	A	410	SQD	C26-C27-C28-C29
27	b	601	SQD	C15-C16-C17-C18
33	D	407	LMG	C16-C17-C18-C19
33	d	411	LMG	C35-C36-C37-C38
23	C	513	CLA	O2A-C1-C2-C3
33	C	501	LMG	C33-C34-C35-C36
27	b	601	SQD	C26-C27-C28-C29
27	b	601	SQD	C30-C31-C32-C33
24	a	407	PHO	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	D	410	LMG	C12-C13-C14-C15
27	A	411	SQD	C28-C29-C30-C31
33	c	524	LMG	C29-C30-C31-C32
33	m	101	LMG	C14-C15-C16-C17
29	d	409	LHG	O1-C1-C2-O2
23	C	511	CLA	C10-C11-C12-C13
23	C	514	CLA	C13-C15-C16-C17
23	D	403	CLA	C10-C11-C12-C13
29	D	408	LHG	C12-C13-C14-C15
29	l	101	LHG	O6-C4-C5-O7
27	A	411	SQD	C24-C25-C26-C27
26	a	410	PL9	C32-C33-C34-C35
29	D	409	LHG	C23-C24-C25-C26
23	B	611	CLA	C16-C17-C18-C19
23	c	509	CLA	C2C-C3C-CAC-CBC
28	C	516	DGD	C6B-C7B-C8B-C9B
23	A	404	CLA	C2C-C3C-CAC-CBC
27	A	411	SQD	C19-C20-C21-C22
29	d	409	LHG	C25-C26-C27-C28
33	d	411	LMG	C13-C14-C15-C16
29	D	408	LHG	C33-C34-C35-C36
29	E	101	LHG	C9-C10-C11-C12
28	A	412	DGD	CFA-CGA-CHA-CIA
28	A	412	DGD	C8B-C9B-CAB-CBB
27	a	411	SQD	O6-C44-C45-O47
27	a	412	SQD	O47-C45-C46-O48
33	M	101	LMG	O7-C8-C9-O8
23	B	603	CLA	CBA-CGA-O2A-C1
29	d	408	LHG	C15-C16-C17-C18
23	B	607	CLA	C16-C17-C18-C19
28	c	517	DGD	C8A-C9A-CAA-CBA
23	B	613	CLA	C5-C6-C7-C8
23	c	513	CLA	C13-C15-C16-C17
28	a	413	DGD	C1G-C2G-C3G-O3G
29	E	101	LHG	C16-C17-C18-C19
28	c	516	DGD	O1B-C1B-O2G-C2G
23	B	604	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C10-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	c	510	CLA	C11-C12-C13-C14
27	F	101	SQD	C27-C28-C29-C30
28	a	413	DGD	CAB-CBB-CCB-CDB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	516	DGD	C2A-C3A-C4A-C5A
29	D	408	LHG	C28-C29-C30-C31
27	a	411	SQD	C28-C29-C30-C31
29	E	101	LHG	C33-C34-C35-C36
33	D	410	LMG	C34-C35-C36-C37
23	c	507	CLA	C16-C17-C18-C19
25	H	101	BCR	C23-C24-C25-C26
25	k	101	BCR	C5-C6-C7-C8
23	c	501	CLA	C8-C10-C11-C12
29	D	408	LHG	C18-C19-C20-C21
33	m	101	LMG	C40-C41-C42-C43
25	K	101	BCR	C7-C8-C9-C10
25	x	102	BCR	C11-C12-C13-C14
25	x	102	BCR	C17-C18-C19-C20
23	d	403	CLA	O1D-CGD-O2D-CED
25	k	101	BCR	C14-C15-C16-C17
23	b	616	CLA	C8-C10-C11-C12
29	E	101	LHG	C29-C30-C31-C32
29	L	101	LHG	C35-C36-C37-C38
23	C	506	CLA	C16-C17-C18-C20
23	c	508	CLA	C16-C17-C18-C19
33	D	410	LMG	C15-C16-C17-C18
33	c	519	LMG	O10-C28-O8-C9
28	c	516	DGD	C2B-C3B-C4B-C5B
23	B	605	CLA	C15-C16-C17-C18
23	C	512	CLA	C8-C10-C11-C12
29	D	409	LHG	O6-C4-C5-C6
33	C	501	LMG	C17-C18-C19-C20
23	B	604	CLA	C11-C10-C8-C7
23	B	604	CLA	C12-C13-C15-C16
23	B	605	CLA	C11-C12-C13-C15
23	B	614	CLA	C2-C3-C5-C6
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
23	C	509	CLA	C11-C10-C8-C7
23	C	510	CLA	C12-C13-C15-C16
23	C	511	CLA	C12-C13-C15-C16
23	C	514	CLA	C12-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C7
23	D	404	CLA	C12-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C15
23	b	605	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	605	CLA	C11-C12-C13-C15
23	b	605	CLA	C12-C13-C15-C16
23	b	609	CLA	C11-C10-C8-C7
23	b	609	CLA	C11-C12-C13-C15
23	b	610	CLA	C12-C13-C15-C16
23	b	612	CLA	C11-C10-C8-C7
23	c	501	CLA	C11-C12-C13-C15
23	c	505	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C10-C8-C7
23	c	509	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7
23	d	404	CLA	C11-C12-C13-C15
27	F	101	SQD	C32-C33-C34-C35
27	a	412	SQD	O6-C44-C45-O47
23	B	601	CLA	C15-C16-C17-C18
23	c	504	CLA	C8-C10-C11-C12
23	B	615	CLA	C16-C17-C18-C20
23	c	504	CLA	C11-C12-C13-C15
33	c	519	LMG	C28-C29-C30-C31
23	B	612	CLA	C15-C16-C17-C18
28	C	516	DGD	CBA-CCA-CDA-CEA
25	H	101	BCR	C11-C10-C9-C34
25	H	101	BCR	C35-C13-C14-C15
25	H	101	BCR	C16-C17-C18-C36
25	K	101	BCR	C16-C17-C18-C36
25	a	409	BCR	C11-C10-C9-C34
25	b	618	BCR	C11-C10-C9-C34
25	t	101	BCR	C16-C17-C18-C36
23	C	511	CLA	C16-C17-C18-C20
28	c	518	DGD	C2B-C3B-C4B-C5B
33	M	101	LMG	C33-C34-C35-C36
28	C	518	DGD	CBB-CCB-CDB-CEB
33	c	519	LMG	C38-C39-C40-C41
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	C	511	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D
29	L	101	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	411	SQD	C23-C24-C25-C26
33	d	410	LMG	C36-C37-C38-C39
23	B	612	CLA	CBA-CGA-O2A-C1
33	C	501	LMG	C39-C40-C41-C42
33	d	410	LMG	C39-C40-C41-C42
33	c	522	LMG	C7-C8-C9-O8
27	f	101	SQD	O10-C23-O48-C46
29	D	409	LHG	O6-C4-C5-O7
23	b	608	CLA	C5-C6-C7-C8
28	H	102	DGD	CBA-CCA-CDA-CEA
34	e	102	HEM	C4B-C3B-CAB-CBB
23	c	509	CLA	CBA-CGA-O2A-C1
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C16-C17-C18-C19
28	C	516	DGD	O1B-C1B-O2G-C2G
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	612	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	C	505	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	b	606	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
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O1D
23	B	612	CLA	O1A-CGA-O2A-C1
28	c	517	DGD	O1A-C1A-O1G-C1G
33	C	519	LMG	O10-C28-O8-C9
25	B	617	BCR	C16-C17-C18-C19
25	c	515	BCR	C12-C13-C14-C15
25	x	102	BCR	C11-C10-C9-C8
27	b	601	SQD	O6-C44-C45-O47
28	C	516	DGD	O2G-C2G-C3G-O3G
33	c	522	LMG	O7-C8-C9-O8
23	B	610	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C10-C11-C12-C13
29	E	101	LHG	O1-C1-C2-O2
29	d	408	LHG	O1-C1-C2-O2
29	d	408	LHG	C26-C27-C28-C29
33	M	101	LMG	C14-C15-C16-C17
23	b	610	CLA	C3-C5-C6-C7
23	C	506	CLA	C4-C3-C5-C6
23	B	603	CLA	O1A-CGA-O2A-C1
29	D	408	LHG	O10-C23-O8-C6
26	A	409	PL9	C13-C14-C16-C17
26	A	409	PL9	C4-C3-C7-C8
28	C	516	DGD	O1G-C1A-C2A-C3A
23	C	511	CLA	C11-C10-C8-C9
23	b	609	CLA	C11-C10-C8-C9
29	L	101	LHG	C14-C15-C16-C17
23	b	603	CLA	C8-C10-C11-C12
27	A	410	SQD	C5-C6-S-O8
27	b	601	SQD	C5-C6-S-O8
29	D	409	LHG	C31-C32-C33-C34
33	m	101	LMG	C30-C31-C32-C33
29	E	101	LHG	C10-C11-C12-C13
27	f	101	SQD	C35-C36-C37-C38
25	k	101	BCR	C17-C18-C19-C20
28	H	102	DGD	C5A-C6A-C7A-C8A
23	c	513	CLA	C1A-C2A-CAA-CBA
23	b	614	CLA	C13-C15-C16-C17
28	C	516	DGD	C4D-C5D-C6D-O5D
28	c	518	DGD	CCB-CDB-CEB-CFB
29	A	413	LHG	C24-C25-C26-C27
25	K	101	BCR	C19-C20-C21-C22
23	b	614	CLA	O1D-CGD-O2D-CED
33	D	410	LMG	C11-C12-C13-C14
33	d	411	LMG	C38-C39-C40-C41
33	C	519	LMG	C30-C31-C32-C33
33	m	101	LMG	C36-C37-C38-C39
29	D	408	LHG	C3-O3-P-O4
29	D	408	LHG	C4-O6-P-O5
23	B	610	CLA	C16-C17-C18-C19
28	C	517	DGD	O6D-C1D-O3G-C3G
23	C	512	CLA	CBA-CGA-O2A-C1
28	H	102	DGD	O2G-C1B-C2B-C3B
28	C	518	DGD	C3B-C4B-C5B-C6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	b	622	LMG	C42-C43-C44-C45
23	c	502	CLA	C3-C5-C6-C7
23	a	406	CLA	C15-C16-C17-C18
23	C	513	CLA	C16-C17-C18-C19
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	514	CLA	CAD-CBD-CGD-O1D
23	b	606	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	503	CLA	C10-C11-C12-C13
27	A	410	SQD	C25-C26-C27-C28
28	c	518	DGD	CAA-CBA-CCA-CDA
29	L	101	LHG	C19-C20-C21-C22
33	d	410	LMG	C11-C12-C13-C14
23	c	507	CLA	C8-C10-C11-C12
33	b	622	LMG	C35-C36-C37-C38
29	E	101	LHG	C18-C19-C20-C21
23	D	404	CLA	CBA-CGA-O2A-C1
23	B	606	CLA	C11-C12-C13-C15
23	B	612	CLA	C11-C10-C8-C7
23	B	616	CLA	C6-C7-C8-C10
23	C	503	CLA	C6-C7-C8-C10
23	C	504	CLA	C6-C7-C8-C10
23	C	507	CLA	C3A-C2A-CAA-CBA
23	C	511	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	b	603	CLA	C6-C7-C8-C10
23	b	608	CLA	C11-C12-C13-C15
23	b	616	CLA	C11-C10-C8-C7
23	c	503	CLA	C11-C10-C8-C7
23	c	509	CLA	C11-C12-C13-C15
23	c	512	CLA	C11-C10-C8-C7
23	d	403	CLA	C6-C7-C8-C10
24	A	406	PHO	C12-C13-C15-C16
27	f	101	SQD	C24-C25-C26-C27
28	H	102	DGD	C9B-CAB-CBB-CCB
27	B	621	SQD	C25-C26-C27-C28
28	c	516	DGD	C5B-C6B-C7B-C8B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	C8-C10-C11-C12
27	A	411	SQD	C32-C33-C34-C35
23	D	404	CLA	O1A-CGA-O2A-C1
28	c	518	DGD	C4A-C5A-C6A-C7A
28	A	412	DGD	C1G-C2G-C3G-O3G
28	C	516	DGD	C1G-C2G-C3G-O3G
33	M	101	LMG	C7-C8-C9-O8
29	L	101	LHG	O9-C7-O7-C5
28	C	516	DGD	O1G-C1G-C2G-O2G
33	c	522	LMG	O1-C7-C8-O7
28	C	518	DGD	C4B-C5B-C6B-C7B
28	h	101	DGD	C5A-C6A-C7A-C8A
29	A	413	LHG	C29-C30-C31-C32
28	c	517	DGD	C2G-C3G-O3G-C1D
23	B	612	CLA	C8-C10-C11-C12
23	b	614	CLA	C5-C6-C7-C8
28	C	518	DGD	C2A-C3A-C4A-C5A
23	c	509	CLA	O1A-CGA-O2A-C1
23	b	612	CLA	C5-C6-C7-C8
23	B	601	CLA	C4-C3-C5-C6
28	c	517	DGD	C7B-C8B-C9B-CAB
29	L	101	LHG	C31-C32-C33-C34
29	l	101	LHG	C19-C20-C21-C22
23	D	403	CLA	C14-C13-C15-C16
23	c	513	CLA	C14-C13-C15-C16
25	b	618	BCR	C6-C7-C8-C9
25	c	514	BCR	C22-C23-C24-C25
33	C	519	LMG	C14-C15-C16-C17
23	C	513	CLA	C16-C17-C18-C20
27	A	410	SQD	C30-C31-C32-C33
29	A	413	LHG	C19-C20-C21-C22
29	d	408	LHG	C13-C14-C15-C16
23	C	512	CLA	O1A-CGA-O2A-C1
23	c	506	CLA	O1A-CGA-O2A-C1
29	e	101	LHG	C7-C8-C9-C10
33	D	407	LMG	C28-C29-C30-C31
23	b	610	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C19
29	L	101	LHG	C29-C30-C31-C32
28	H	102	DGD	CCB-CDB-CEB-CFB
29	d	407	LHG	C31-C32-C33-C34
23	C	506	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	d	407	LHG	C27-C28-C29-C30
27	B	621	SQD	C11-C10-C9-C8
28	c	517	DGD	CDA-CEA-CFA-CGA
28	c	516	DGD	C8A-C9A-CAA-CBA
28	a	413	DGD	C1G-C2G-O2G-C1B
33	C	501	LMG	C9-C8-O7-C10
33	D	410	LMG	C9-C8-O7-C10
29	D	409	LHG	C1-C2-C3-O3
23	b	615	CLA	C2A-CAA-CBA-CGA
23	A	404	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	c	512	CLA	C2-C1-O2A-CGA
33	m	101	LMG	C15-C16-C17-C18
29	D	408	LHG	C23-C24-C25-C26
28	c	518	DGD	C5A-C6A-C7A-C8A
33	b	622	LMG	C30-C31-C32-C33
33	c	524	LMG	C19-C20-C21-C22
33	d	410	LMG	C29-C30-C31-C32
29	E	101	LHG	O6-C4-C5-O7
23	c	511	CLA	C15-C16-C17-C18
26	A	409	PL9	C20-C19-C21-C22
25	b	618	BCR	C1-C6-C7-C8
27	A	411	SQD	C30-C31-C32-C33
23	C	503	CLA	C15-C16-C17-C18
28	c	516	DGD	CAB-CBB-CCB-CDB
23	c	512	CLA	C16-C17-C18-C19
28	C	516	DGD	O6E-C1E-O5D-C6D
28	c	516	DGD	O6E-C1E-O5D-C6D
33	C	519	LMG	O6-C1-O1-C7
27	b	601	SQD	O47-C45-C46-O48
33	c	524	LMG	C32-C33-C34-C35
29	E	101	LHG	C4-O6-P-O3
29	d	408	LHG	C3-O3-P-O6
28	C	516	DGD	CAA-CBA-CCA-CDA
33	c	522	LMG	C37-C38-C39-C40
29	D	409	LHG	C16-C17-C18-C19
23	d	403	CLA	C3-C5-C6-C7
23	c	512	CLA	C4-C3-C5-C6
28	H	102	DGD	C6B-C7B-C8B-C9B
33	C	501	LMG	C11-C12-C13-C14
23	B	604	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C11-C10-C8-C7
23	C	511	CLA	C6-C7-C8-C10
23	a	405	CLA	C11-C10-C8-C7
24	a	407	PHO	C2-C3-C5-C6
29	E	101	LHG	C30-C31-C32-C33
23	B	604	CLA	C11-C12-C13-C14
23	B	605	CLA	C14-C13-C15-C16
23	B	606	CLA	C11-C12-C13-C14
23	B	612	CLA	C11-C10-C8-C9
23	C	506	CLA	C14-C13-C15-C16
23	C	510	CLA	C14-C13-C15-C16
23	D	404	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C12-C13-C14
23	b	608	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C9
23	c	503	CLA	C11-C10-C8-C9
23	c	513	CLA	C6-C7-C8-C9
24	a	407	PHO	C6-C7-C8-C9
25	b	619	BCR	C9-C10-C11-C12
25	d	405	BCR	C9-C10-C11-C12
33	D	407	LMG	C15-C16-C17-C18
33	D	407	LMG	C21-C22-C23-C24
23	C	504	CLA	C10-C11-C12-C13
29	L	101	LHG	C24-C25-C26-C27
28	H	102	DGD	C1B-C2B-C3B-C4B
23	b	610	CLA	C16-C17-C18-C20
29	l	101	LHG	C14-C15-C16-C17
29	E	101	LHG	C2-C3-O3-P
29	d	409	LHG	C2-C3-O3-P
28	c	517	DGD	C3A-C4A-C5A-C6A
25	k	101	BCR	C11-C12-C13-C14
28	H	102	DGD	CAA-CBA-CCA-CDA
28	a	413	DGD	C1A-C2A-C3A-C4A
33	c	522	LMG	C28-C29-C30-C31
23	B	609	CLA	C16-C17-C18-C19
23	C	511	CLA	C16-C17-C18-C19
23	A	407	CLA	CBA-CGA-O2A-C1
23	b	615	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	CBA-CGA-O2A-C1
28	c	518	DGD	C9A-CAA-CBA-CCA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	516	DGD	C7B-C8B-C9B-CAB
24	A	406	PHO	CBA-CGA-O2A-C1
27	a	412	SQD	C27-C28-C29-C30
23	C	502	CLA	C2A-CAA-CBA-CGA
23	B	602	CLA	C16-C17-C18-C19
33	D	411	LMG	O10-C28-C29-C30
25	K	101	BCR	C13-C14-C15-C16
25	c	514	BCR	C15-C16-C17-C18
25	c	521	BCR	C9-C10-C11-C12
33	c	519	LMG	C4-C5-C6-O5
27	a	411	SQD	C24-C25-C26-C27
25	A	408	BCR	C18-C19-C20-C21
34	E	103	HEM	CAD-CBD-CGD-O2D
23	a	406	CLA	C8-C10-C11-C12
23	a	406	CLA	C13-C15-C16-C17
33	M	101	LMG	C40-C41-C42-C43
23	C	503	CLA	O1A-CGA-O2A-C1
28	A	412	DGD	CCB-CDB-CEB-CFB
23	B	609	CLA	C5-C6-C7-C8
29	l	101	LHG	C34-C35-C36-C37
35	v	201	HEC	CAD-CBD-CGD-O1D
23	B	613	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	B	602	CLA	C8-C10-C11-C12
28	C	516	DGD	CAB-CBB-CCB-CDB
28	c	517	DGD	CCA-CDA-CEA-CFA
28	h	101	DGD	C7B-C8B-C9B-CAB
28	c	517	DGD	O1G-C1G-C2G-O2G
33	b	622	LMG	O7-C8-C9-O8
34	e	102	HEM	CAD-CBD-CGD-O1D
28	C	518	DGD	CDA-CEA-CFA-CGA
33	M	101	LMG	C32-C33-C34-C35
27	b	601	SQD	O49-C7-O47-C45
27	A	410	SQD	C35-C36-C37-C38
26	a	410	PL9	C4-C3-C7-C8
27	F	101	SQD	O48-C23-C24-C25
23	b	603	CLA	C14-C13-C15-C16
23	b	615	CLA	C6-C7-C8-C9
28	A	412	DGD	C3B-C4B-C5B-C6B
33	D	411	LMG	O8-C28-C29-C30
23	C	507	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	503	CLA	C15-C16-C17-C18
25	B	619	BCR	C20-C21-C22-C37
25	C	515	BCR	C35-C13-C14-C15
35	v	201	HEC	CAD-CBD-CGD-O2D
23	b	615	CLA	O1A-CGA-O2A-C1
27	A	410	SQD	C17-C18-C19-C20
29	e	101	LHG	C13-C14-C15-C16
23	D	404	CLA	O2A-C1-C2-C3
23	b	602	CLA	O2A-C1-C2-C3
33	D	410	LMG	C29-C30-C31-C32
23	c	508	CLA	C15-C16-C17-C18
27	f	101	SQD	C44-C45-O47-C7
27	f	101	SQD	C46-C45-O47-C7
28	a	413	DGD	O2G-C1B-C2B-C3B
23	B	606	CLA	C6-C7-C8-C10
23	a	406	CLA	C11-C10-C8-C7
23	c	502	CLA	C6-C7-C8-C10
23	c	511	CLA	C6-C7-C8-C10
23	c	512	CLA	C6-C7-C8-C10
23	c	512	CLA	C12-C13-C15-C16
26	a	410	PL9	C38-C39-C41-C42
23	B	610	CLA	C2C-C3C-CAC-CBC
23	A	407	CLA	O1A-CGA-O2A-C1
25	d	405	BCR	C19-C20-C21-C22
33	M	101	LMG	O6-C5-C6-O5
27	B	621	SQD	C35-C36-C37-C38
33	b	622	LMG	C12-C13-C14-C15
23	B	610	CLA	C16-C17-C18-C20
23	c	501	CLA	C2A-CAA-CBA-CGA
33	D	410	LMG	C31-C32-C33-C34
24	A	406	PHO	O1A-CGA-O2A-C1
34	E	103	HEM	CAD-CBD-CGD-O1D
23	C	506	CLA	C8-C10-C11-C12
28	A	412	DGD	CBB-CCB-CDB-CEB
23	B	602	CLA	C16-C17-C18-C20
33	D	411	LMG	C29-C30-C31-C32
23	c	510	CLA	C4-C3-C5-C6
28	c	516	DGD	CCA-CDA-CEA-CFA
33	d	410	LMG	O9-C10-C11-C12
34	e	102	HEM	CAD-CBD-CGD-O2D
23	B	604	CLA	C15-C16-C17-C18
23	D	402	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	d	408	LHG	C23-C24-C25-C26
25	A	408	BCR	C20-C21-C22-C23
27	A	411	SQD	O47-C45-C46-O48
28	a	413	DGD	O1G-C1G-C2G-O2G
29	e	101	LHG	O7-C5-C6-O8
33	m	101	LMG	C39-C40-C41-C42
33	M	101	LMG	C29-C30-C31-C32
33	b	622	LMG	O8-C28-C29-C30
29	d	407	LHG	C24-C25-C26-C27
23	b	610	CLA	O1D-CGD-O2D-CED
26	a	410	PL9	C7-C8-C9-C10
23	C	507	CLA	C2-C1-O2A-CGA
23	B	601	CLA	C2-C3-C5-C6
28	A	412	DGD	CAB-CBB-CCB-CDB
23	B	606	CLA	C14-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	c	510	CLA	C14-C13-C15-C16
27	A	411	SQD	C26-C27-C28-C29
23	b	610	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	O1A-CGA-O2A-C1
27	a	411	SQD	C16-C17-C18-C19
29	D	409	LHG	C15-C16-C17-C18
28	C	517	DGD	C3B-C4B-C5B-C6B
33	c	519	LMG	C40-C41-C42-C43
23	D	403	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
23	c	509	CLA	C4C-C3C-CAC-CBC
28	C	517	DGD	O1A-C1A-O1G-C1G
25	C	520	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C30
25	K	101	BCR	C23-C24-C25-C30
25	b	618	BCR	C5-C6-C7-C8
25	d	405	BCR	C23-C24-C25-C30
28	h	101	DGD	O2G-C1B-C2B-C3B
28	c	516	DGD	O1G-C1G-C2G-C3G
33	C	519	LMG	O1-C7-C8-C9
23	b	609	CLA	C13-C15-C16-C17
33	d	410	LMG	C12-C13-C14-C15
27	a	412	SQD	C19-C20-C21-C22
29	E	101	LHG	C28-C29-C30-C31
23	B	613	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C4-C3-C5-C6
23	d	404	CLA	C13-C15-C16-C17
23	c	512	CLA	C2-C3-C5-C6
28	c	516	DGD	C5D-C6D-O5D-C1E
33	m	101	LMG	C8-C7-O1-C1
28	c	518	DGD	C7A-C8A-C9A-CAA
33	m	101	LMG	C33-C34-C35-C36
23	C	502	CLA	C16-C17-C18-C20
23	c	512	CLA	C16-C17-C18-C20
23	c	508	CLA	CBA-CGA-O2A-C1
28	h	101	DGD	O6E-C1E-O5D-C6D
26	a	410	PL9	C35-C34-C36-C37
23	b	603	CLA	C12-C13-C15-C16
23	b	610	CLA	C2-C3-C5-C6
33	d	410	LMG	O7-C10-C11-C12
27	B	621	SQD	C33-C34-C35-C36
28	c	516	DGD	CDB-CEB-CFB-CGB
33	D	410	LMG	C14-C15-C16-C17
23	C	514	CLA	C4C-C3C-CAC-CBC
28	C	516	DGD	C5A-C6A-C7A-C8A
28	C	516	DGD	C2E-C1E-O5D-C6D
28	C	517	DGD	C2D-C1D-O3G-C3G
23	b	614	CLA	CAA-CBA-CGA-O2A
26	d	406	PL9	C2-C3-C7-C8
23	C	503	CLA	CBA-CGA-O2A-C1
23	d	402	CLA	CBA-CGA-O2A-C1
24	A	406	PHO	C4C-C3C-CAC-CBC
33	D	411	LMG	C30-C31-C32-C33
23	b	606	CLA	C8-C10-C11-C12
26	d	406	PL9	C33-C34-C36-C37
23	B	604	CLA	C4C-C3C-CAC-CBC
33	c	524	LMG	O8-C28-C29-C30
23	B	610	CLA	C4C-C3C-CAC-CBC
23	B	603	CLA	C11-C10-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	C	513	CLA	C14-C13-C15-C16
23	C	514	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C10-C8-C9
33	D	411	LMG	O7-C10-C11-C12
23	B	616	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	A	407	CLA	CAD-CBD-CGD-O2D
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	609	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	602	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
26	a	410	PL9	C37-C38-C39-C40
29	L	101	LHG	C13-C14-C15-C16
23	C	510	CLA	C5-C6-C7-C8
23	b	613	CLA	CAA-CBA-CGA-O2A
27	A	410	SQD	O47-C7-C8-C9
28	C	516	DGD	CDA-CEA-CFA-CGA
25	b	619	BCR	C22-C23-C24-C25
23	B	602	CLA	C15-C16-C17-C18
28	H	102	DGD	C5B-C6B-C7B-C8B
33	D	411	LMG	O9-C10-C11-C12
23	c	510	CLA	C2-C3-C5-C6
23	c	509	CLA	CAA-CBA-CGA-O2A
27	B	621	SQD	O47-C7-C8-C9
25	B	619	BCR	C11-C12-C13-C14
25	Z	101	BCR	C7-C8-C9-C10
25	Z	101	BCR	C11-C12-C13-C14
25	t	101	BCR	C17-C18-C19-C20
29	e	101	LHG	C25-C26-C27-C28
24	A	406	PHO	C2C-C3C-CAC-CBC
24	d	401	PHO	C2C-C3C-CAC-CBC
27	b	601	SQD	O6-C44-C45-C46
29	e	101	LHG	C4-C5-C6-O8
33	C	501	LMG	O1-C7-C8-C9
23	C	504	CLA	C15-C16-C17-C18
23	b	617	CLA	C10-C11-C12-C13
33	m	101	LMG	O8-C28-C29-C30
35	V	201	HEC	CAD-CBD-CGD-O1D
23	B	603	CLA	C15-C16-C17-C18
23	B	604	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	403	CLA	O2A-C1-C2-C3
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C13-C15-C16-C17
33	C	519	LMG	C32-C33-C34-C35
35	V	201	HEC	CAD-CBD-CGD-O2D
29	d	407	LHG	C11-C10-C9-C8
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	CHA-CBD-CGD-O2D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	608	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O1D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	b	617	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	d	402	CLA	CHA-CBD-CGD-O1D
23	d	402	CLA	CHA-CBD-CGD-O2D
25	c	521	BCR	C13-C14-C15-C16
27	a	411	SQD	O47-C7-C8-C9
28	c	516	DGD	CBB-CCB-CDB-CEB
33	D	407	LMG	C31-C32-C33-C34
25	B	617	BCR	C11-C10-C9-C8
29	L	101	LHG	O7-C7-C8-C9
23	B	613	CLA	CAA-CBA-CGA-O2A
23	c	501	CLA	CAA-CBA-CGA-O2A
27	a	411	SQD	O48-C23-C24-C25
23	B	602	CLA	C2A-CAA-CBA-CGA
23	C	509	CLA	C16-C17-C18-C19
23	C	514	CLA	CBA-CGA-O2A-C1
23	d	404	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C12-C13-C15
27	a	411	SQD	C25-C26-C27-C28
29	d	408	LHG	C31-C32-C33-C34
33	C	501	LMG	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	616	CLA	C6-C7-C8-C9
23	a	406	CLA	C11-C10-C8-C9
23	a	408	CLA	C6-C7-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	d	403	CLA	C6-C7-C8-C9
27	B	621	SQD	C7-C8-C9-C10
29	D	409	LHG	C28-C29-C30-C31
23	B	606	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	c	513	CLA	C3-C5-C6-C7
23	c	508	CLA	O1A-CGA-O2A-C1
28	H	102	DGD	CDB-CEB-CFB-CGB
26	D	406	PL9	C21-C22-C23-C24
23	c	510	CLA	CAA-CBA-CGA-O2A
23	b	604	CLA	C4-C3-C5-C6
23	B	610	CLA	CBD-CGD-O2D-CED
29	e	101	LHG	O10-C23-C24-C25
25	H	101	BCR	C17-C18-C19-C20
25	c	514	BCR	C7-C8-C9-C10
29	D	409	LHG	C24-C23-O8-C6
28	C	516	DGD	C3B-C4B-C5B-C6B
33	m	101	LMG	C21-C22-C23-C24
23	B	602	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
23	C	514	CLA	C1A-C2A-CAA-CBA
27	a	411	SQD	C29-C30-C31-C32
28	c	518	DGD	C9B-CAB-CBB-CCB
23	c	506	CLA	C10-C11-C12-C13
23	D	403	CLA	C2-C1-O2A-CGA
23	B	607	CLA	C15-C16-C17-C18
23	B	612	CLA	CAA-CBA-CGA-O1A
28	c	518	DGD	O1B-C1B-C2B-C3B
28	h	101	DGD	C3B-C4B-C5B-C6B
27	f	101	SQD	C44-C45-C46-O48
28	h	101	DGD	C1G-C2G-C3G-O3G
23	C	510	CLA	C8-C10-C11-C12
23	b	602	CLA	C13-C15-C16-C17
23	B	610	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	CBD-CGD-O2D-CED
27	B	621	SQD	O49-C7-C8-C9
23	b	613	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C4-C3-C5-C6
23	b	613	CLA	CAA-CBA-CGA-O1A
23	b	614	CLA	CAA-CBA-CGA-O1A
29	D	409	LHG	O10-C23-C24-C25
23	b	604	CLA	C2-C3-C5-C6
25	Z	101	BCR	C6-C7-C8-C9
27	A	411	SQD	C16-C17-C18-C19
29	E	101	LHG	C4-O6-P-O5
29	d	408	LHG	C3-O3-P-O5
28	a	413	DGD	C7A-C8A-C9A-CAA
23	c	501	CLA	CAA-CBA-CGA-O1A
28	c	517	DGD	C9A-CAA-CBA-CCA
29	E	101	LHG	C14-C15-C16-C17
23	b	614	CLA	C15-C16-C17-C18
23	C	514	CLA	C2C-C3C-CAC-CBC
27	b	601	SQD	C14-C15-C16-C17
23	C	514	CLA	O1A-CGA-O2A-C1
23	C	506	CLA	CAA-CBA-CGA-O2A
28	A	412	DGD	C7A-C8A-C9A-CAA
27	f	101	SQD	C27-C28-C29-C30
23	B	603	CLA	C10-C11-C12-C13
23	c	509	CLA	C8-C10-C11-C12
23	C	513	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	C4-C3-C5-C6
23	B	603	CLA	C5-C6-C7-C8
23	B	607	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
28	C	516	DGD	O1B-C1B-C2B-C3B
28	h	101	DGD	C6B-C7B-C8B-C9B
29	L	101	LHG	C11-C12-C13-C14
33	D	407	LMG	O7-C10-C11-C12
23	a	405	CLA	C11-C10-C8-C9
23	b	603	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
33	C	519	LMG	C39-C40-C41-C42
23	B	601	CLA	CAA-CBA-CGA-O2A
27	b	601	SQD	O47-C7-C8-C9
33	m	101	LMG	O7-C10-C11-C12
28	C	516	DGD	C6A-C7A-C8A-C9A
27	f	101	SQD	C30-C31-C32-C33
28	c	516	DGD	O2G-C1B-C2B-C3B

Continued on next page...

Continued from previous page...

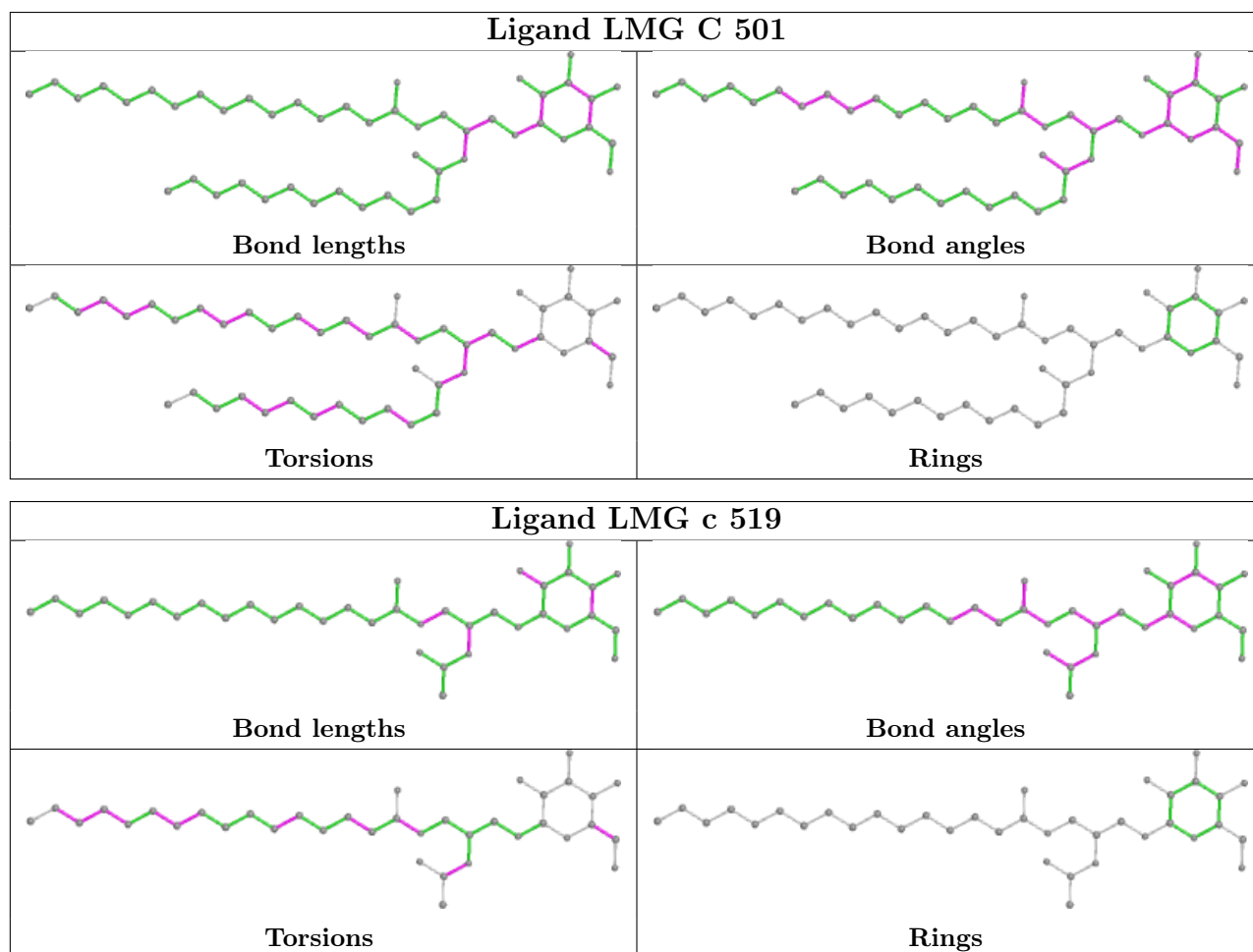
Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C21-C22-C23-C24
23	b	605	CLA	C13-C15-C16-C17
23	d	402	CLA	C2C-C3C-CAC-CBC
27	f	101	SQD	C26-C27-C28-C29
33	C	501	LMG	C37-C38-C39-C40
23	c	505	CLA	C4-C3-C5-C6
23	C	508	CLA	C5-C6-C7-C8
33	D	410	LMG	C16-C17-C18-C19
23	B	606	CLA	C12-C13-C15-C16
23	D	403	CLA	C6-C7-C8-C10
23	D	403	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	612	CLA	C6-C7-C8-C10
23	c	505	CLA	C2-C3-C5-C6
23	c	513	CLA	C6-C7-C8-C10
23	d	403	CLA	C11-C12-C13-C15
23	a	408	CLA	CAA-CBA-CGA-O2A
28	C	517	DGD	O1G-C1A-C2A-C3A
28	c	518	DGD	O1G-C1A-C2A-C3A
25	b	619	BCR	C21-C22-C23-C24
25	c	514	BCR	C11-C12-C13-C14
25	x	102	BCR	C7-C8-C9-C10
33	M	101	LMG	O10-C28-C29-C30
25	C	520	BCR	C19-C20-C21-C22
33	b	622	LMG	O6-C1-O1-C7
23	B	612	CLA	C2C-C3C-CAC-CBC
23	B	601	CLA	CAA-CBA-CGA-O1A
23	B	613	CLA	CAA-CBA-CGA-O1A
23	b	613	CLA	C3-C5-C6-C7
28	C	518	DGD	C8A-C9A-CAA-CBA
23	c	505	CLA	C10-C11-C12-C13
26	D	406	PL9	C36-C37-C38-C39
23	d	404	CLA	O1A-CGA-O2A-C1
28	C	516	DGD	O2G-C1B-C2B-C3B
29	L	101	LHG	C15-C16-C17-C18
23	c	510	CLA	CAA-CBA-CGA-O1A
33	m	101	LMG	O9-C10-C11-C12
23	B	606	CLA	C13-C15-C16-C17

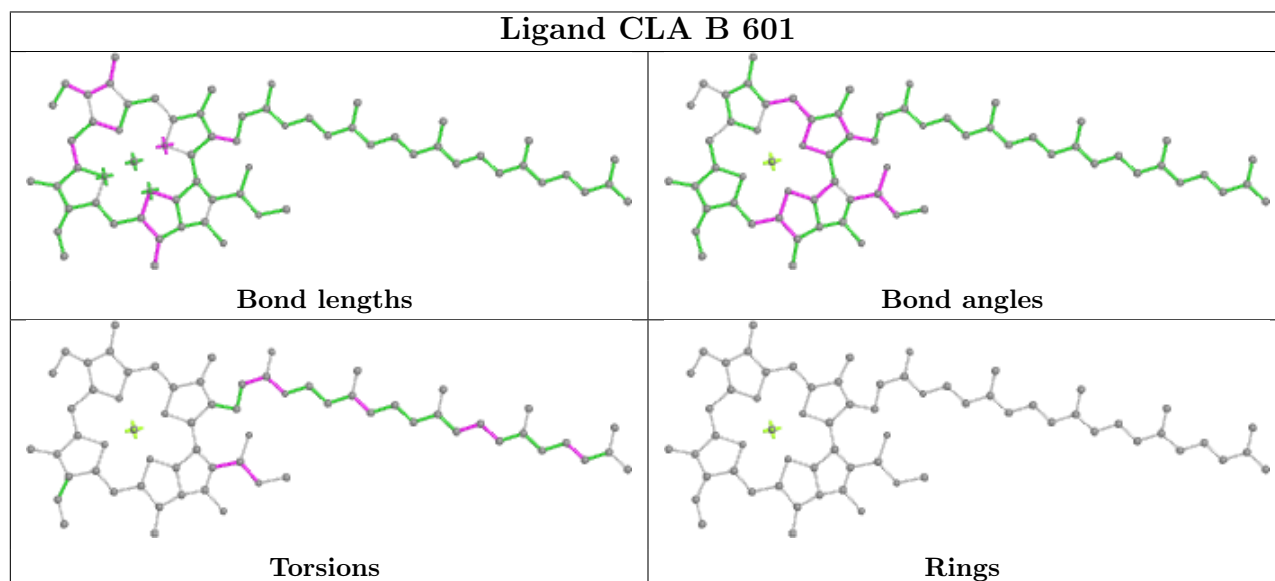
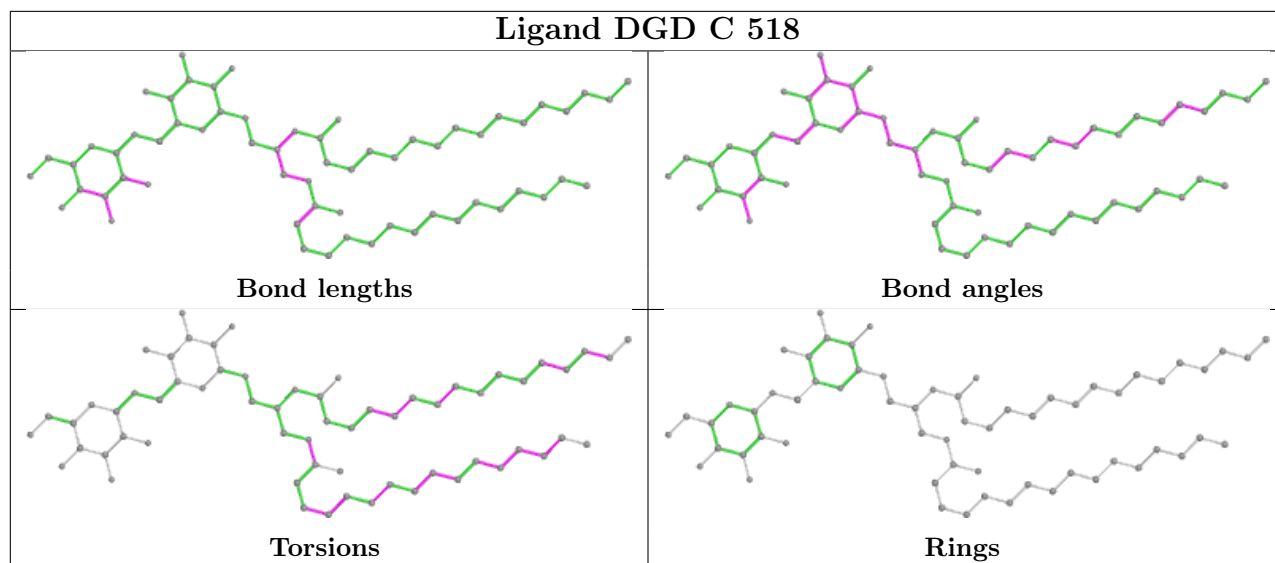
There are no ring outliers.

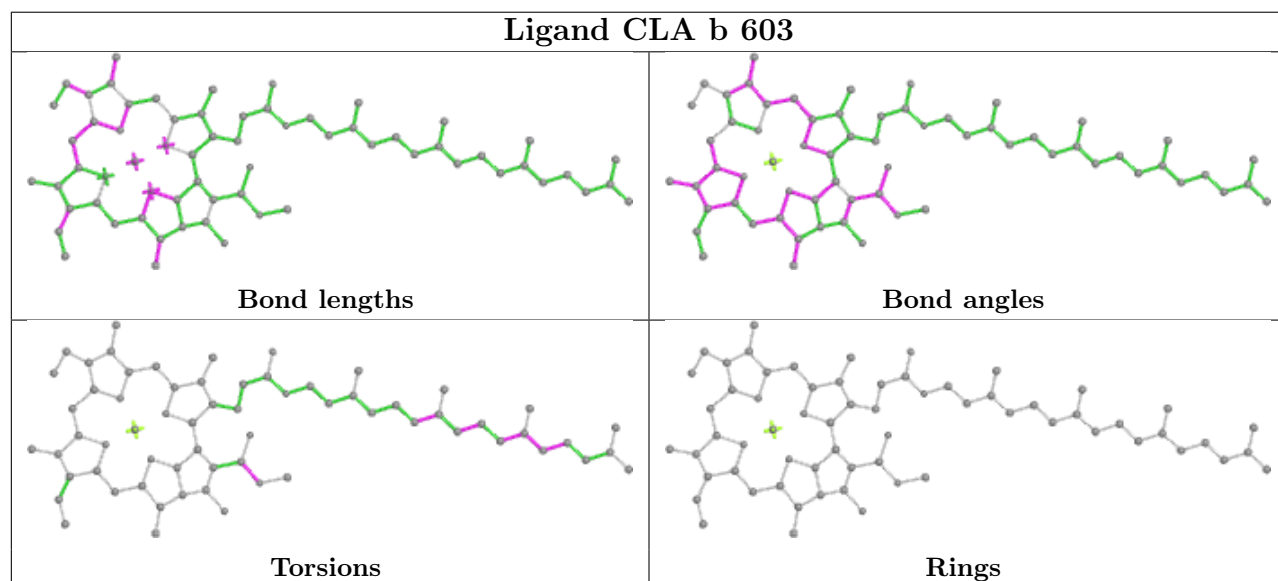
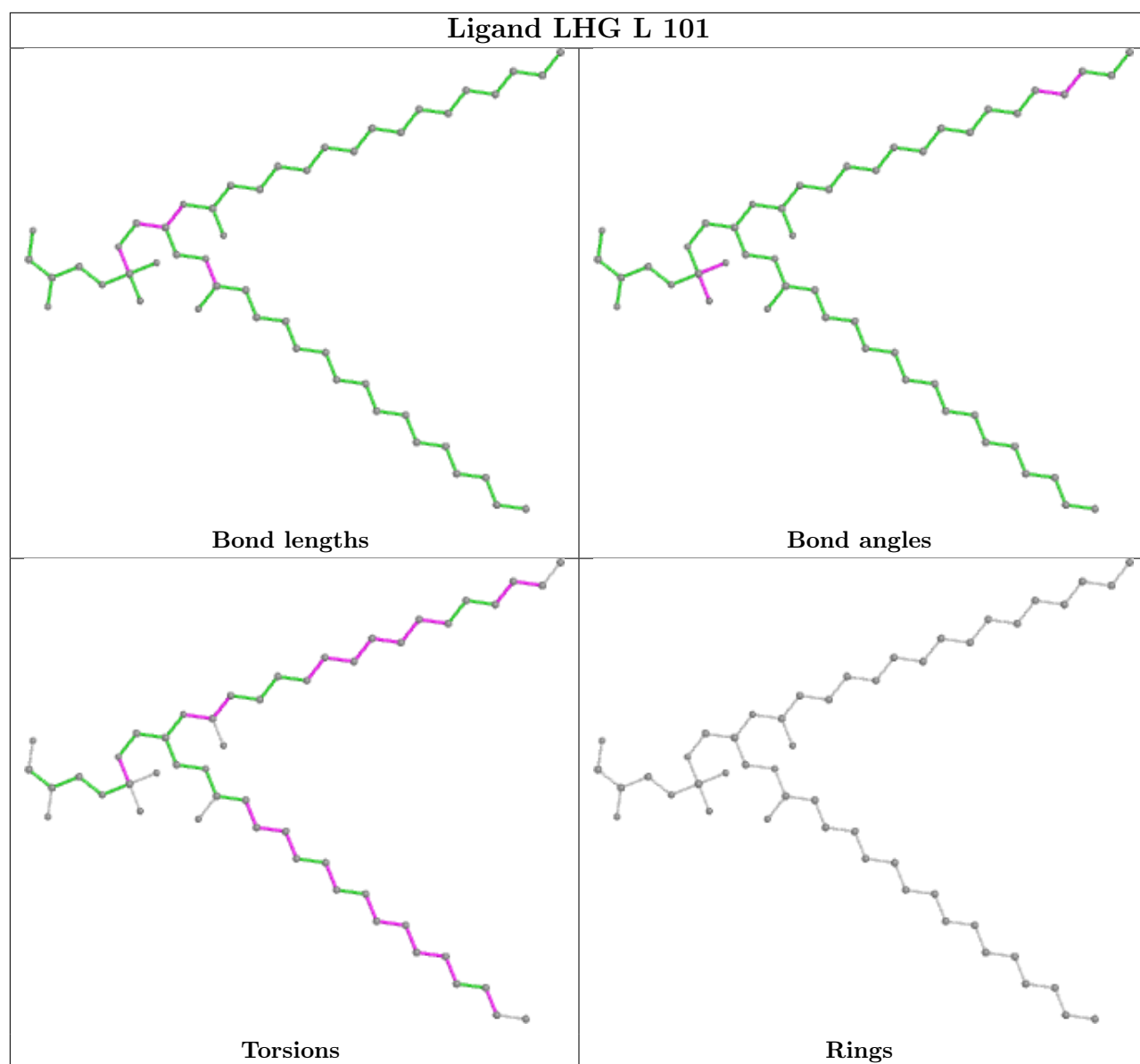
No monomer is involved in short contacts.

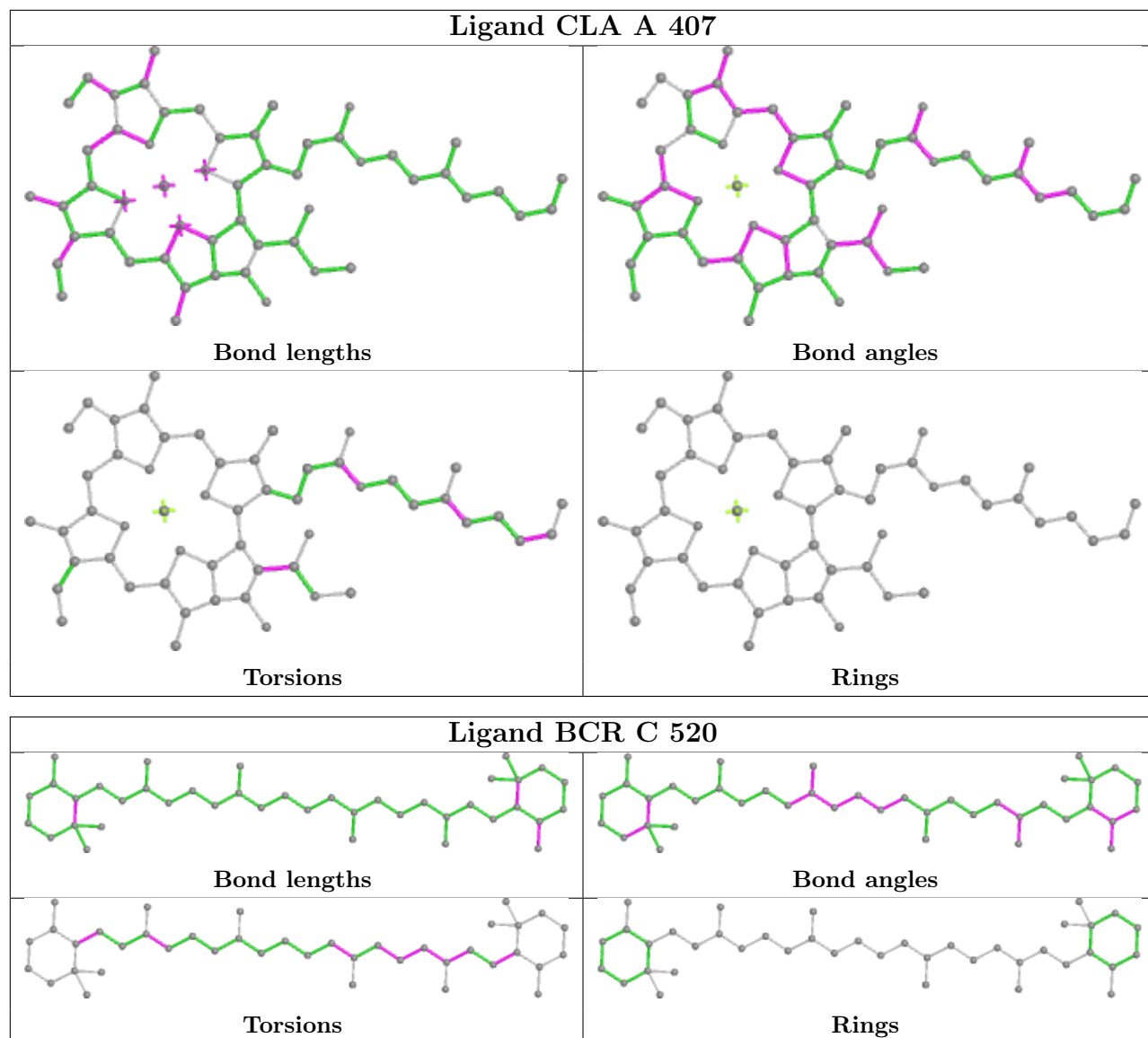
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

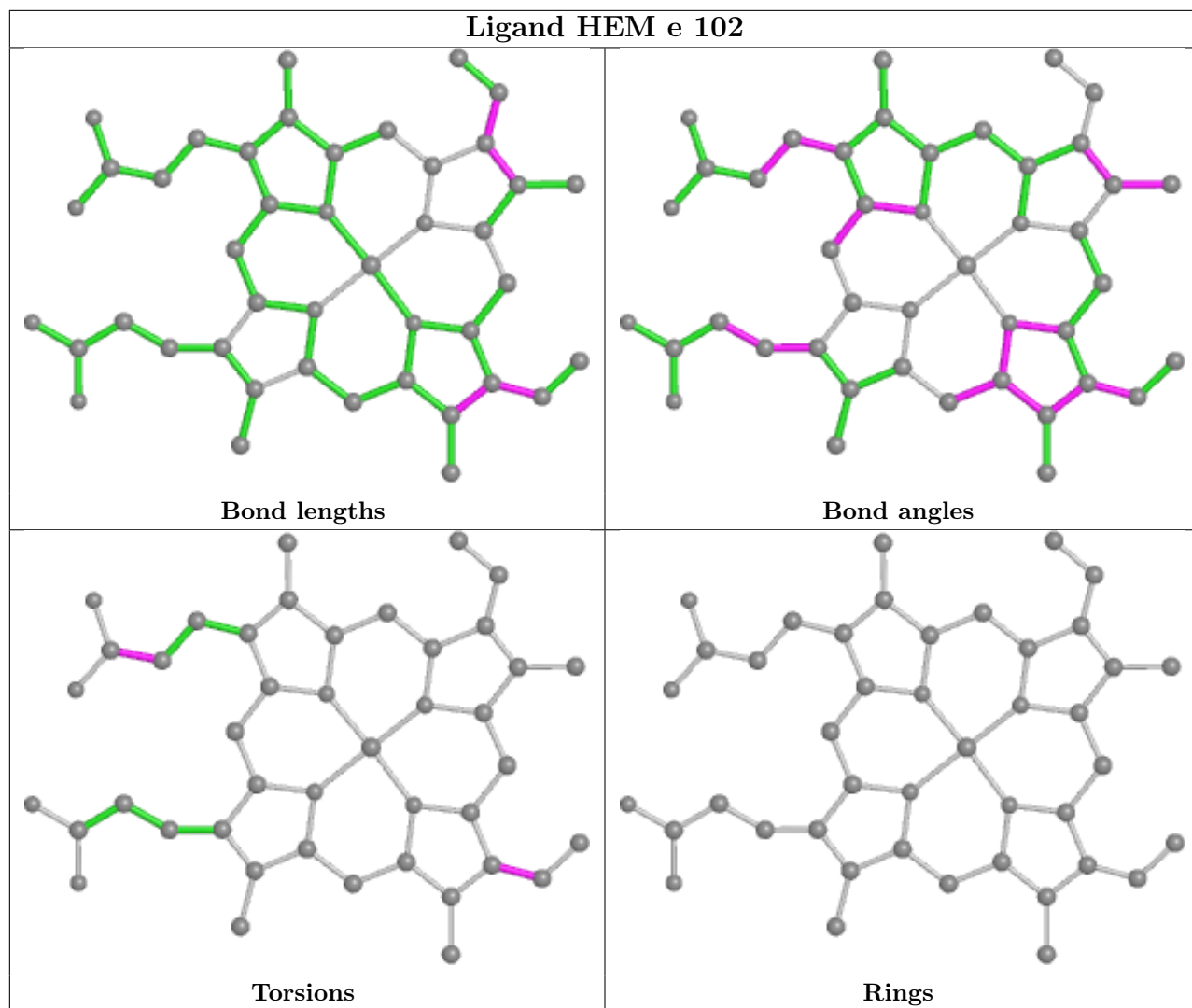
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

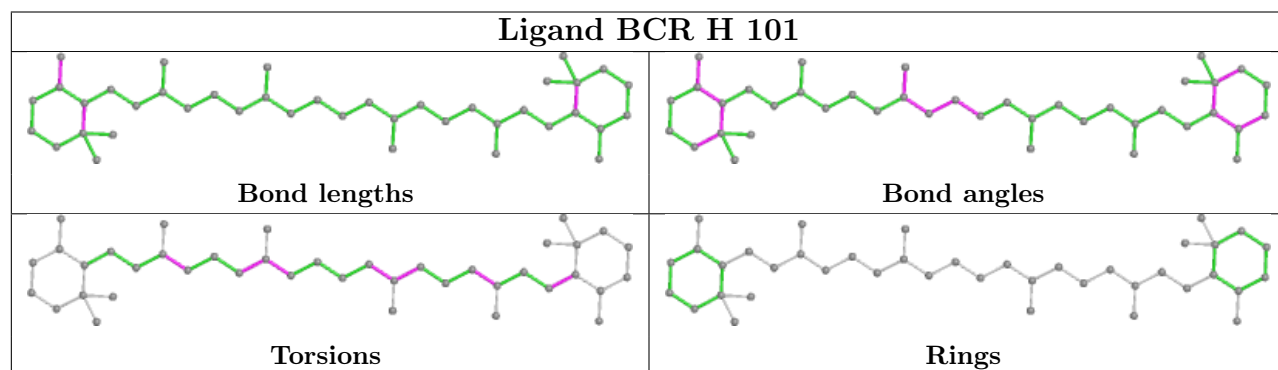
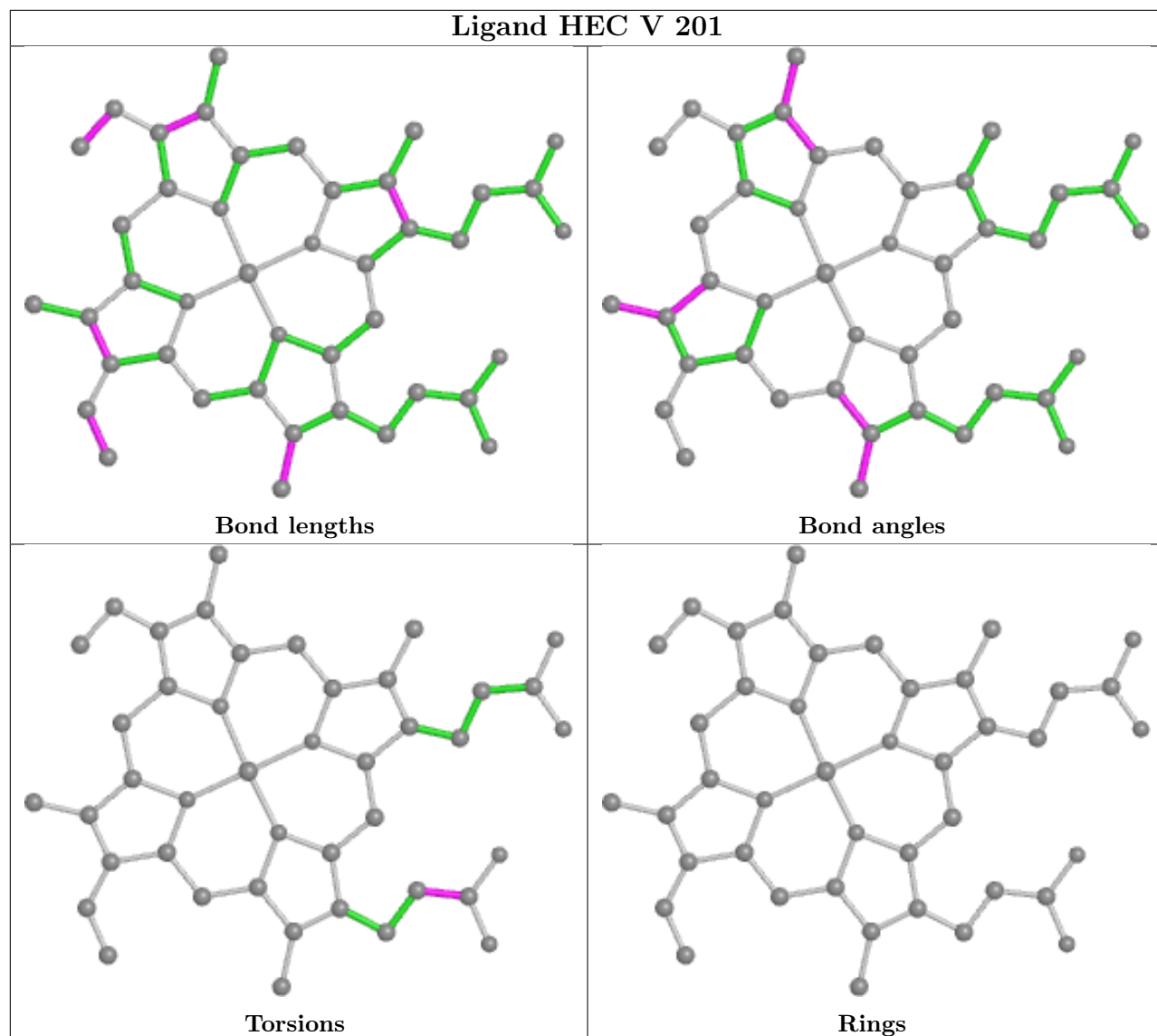


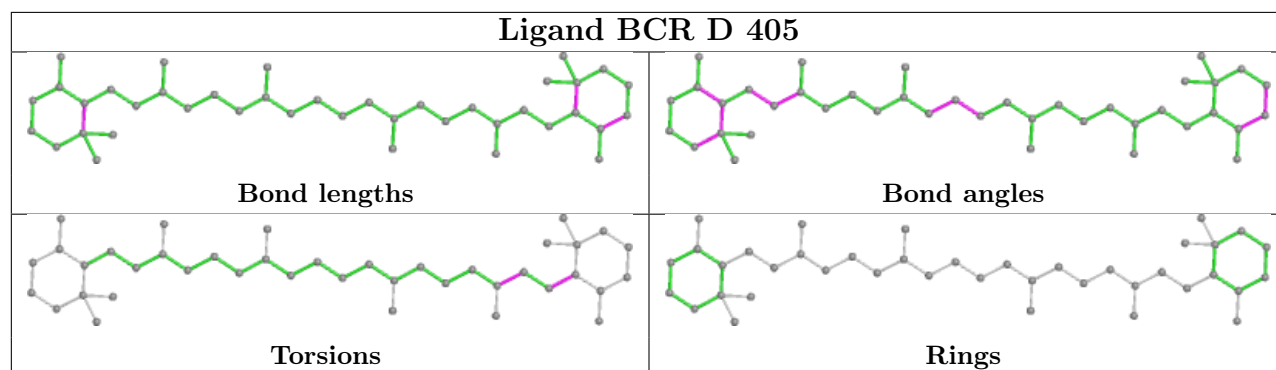
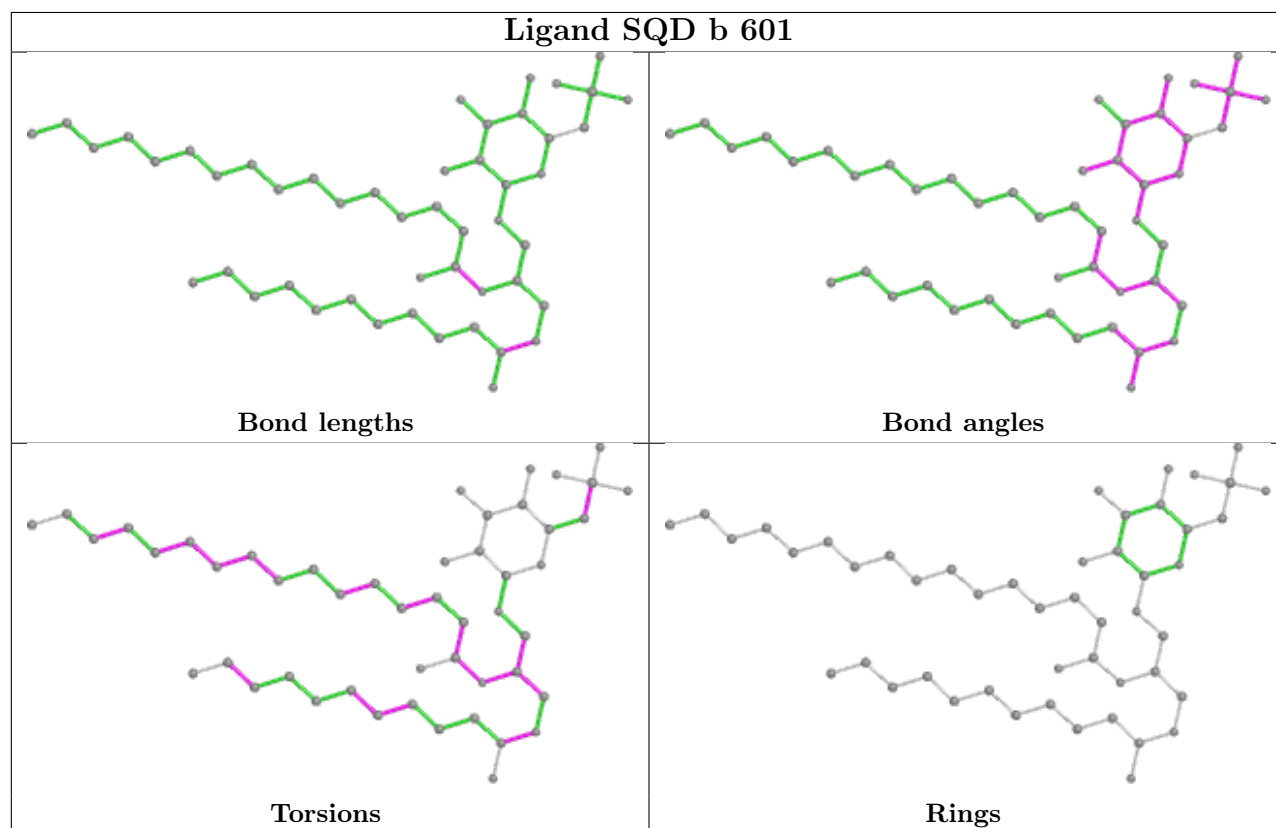
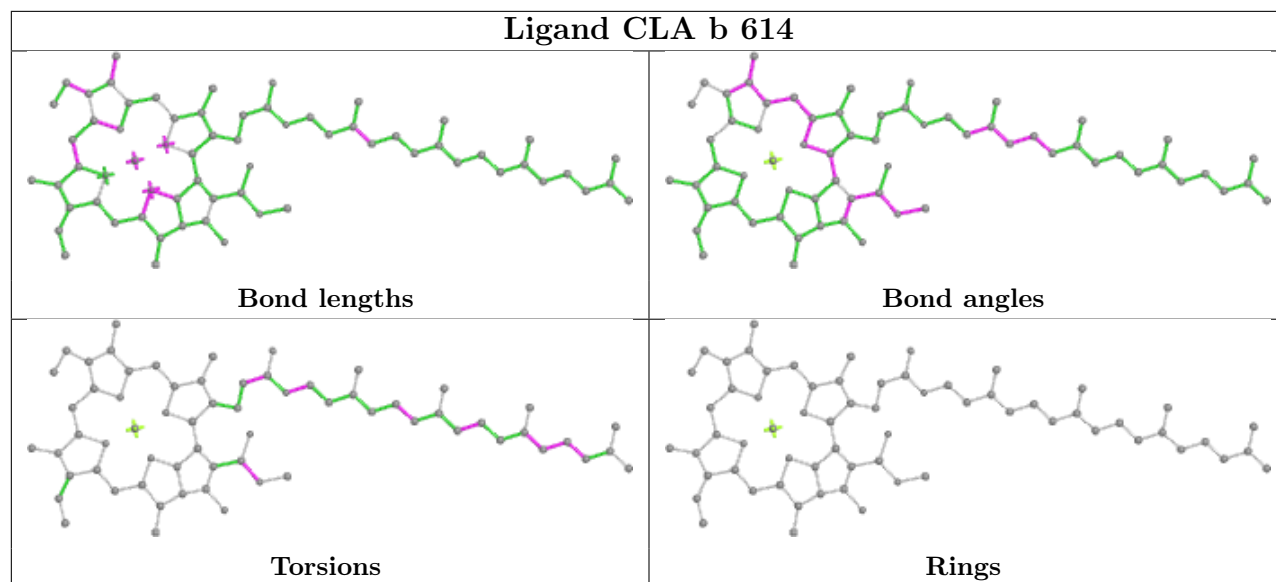


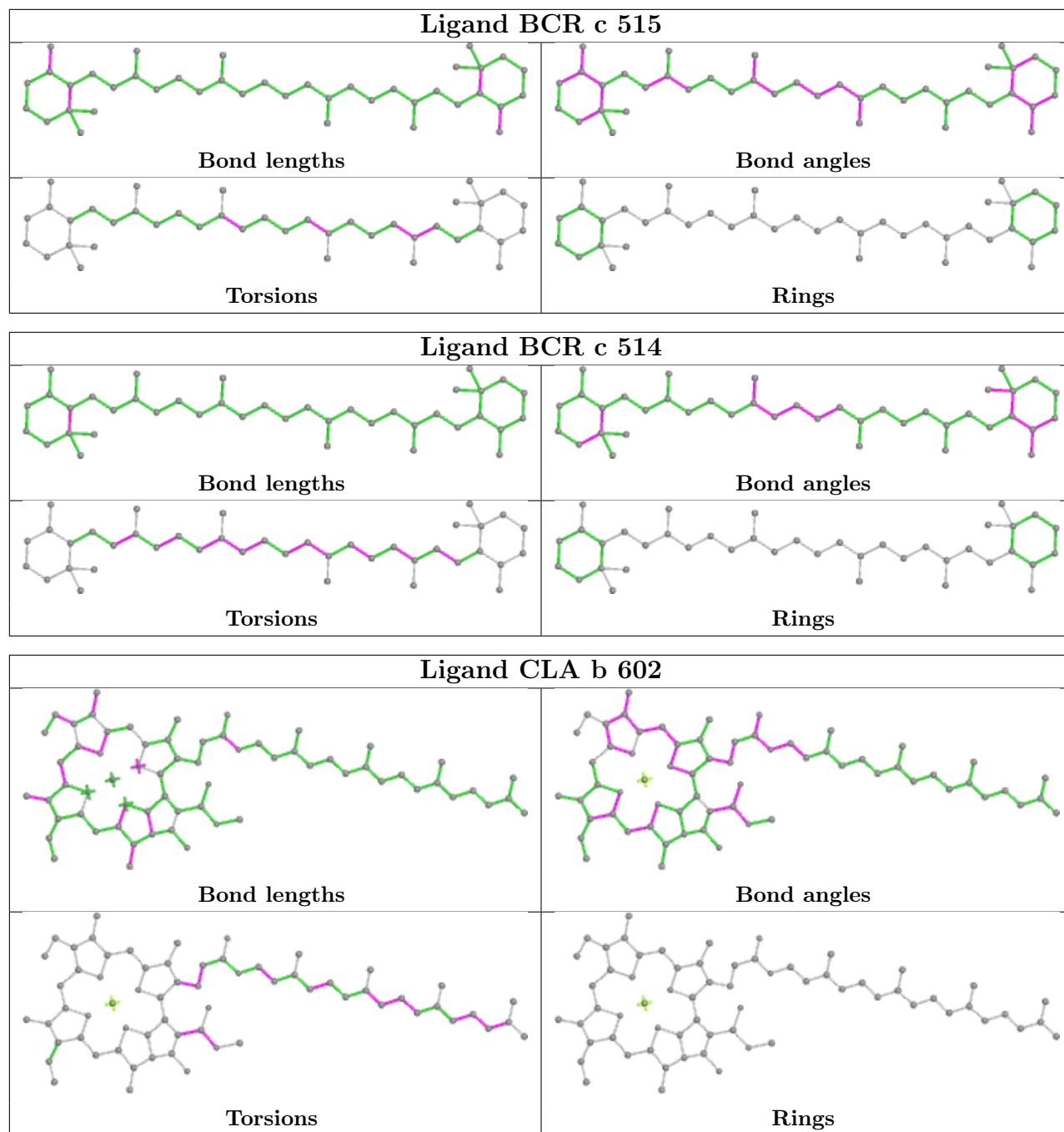


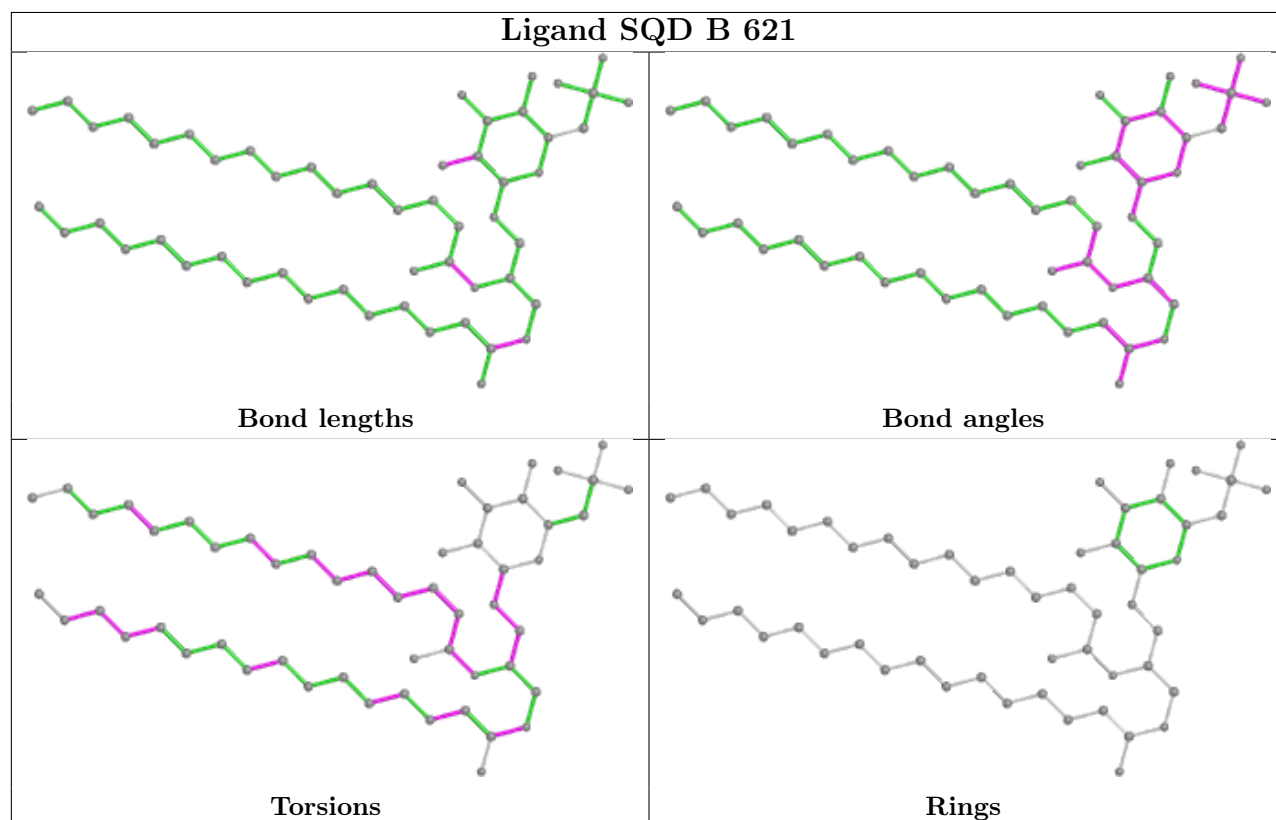
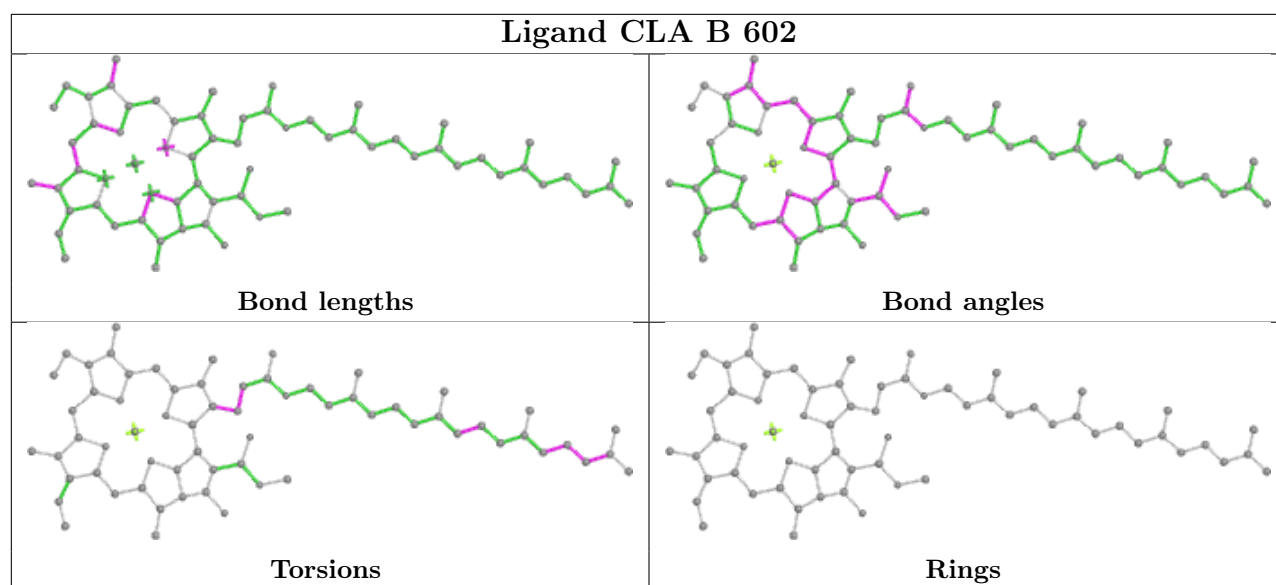


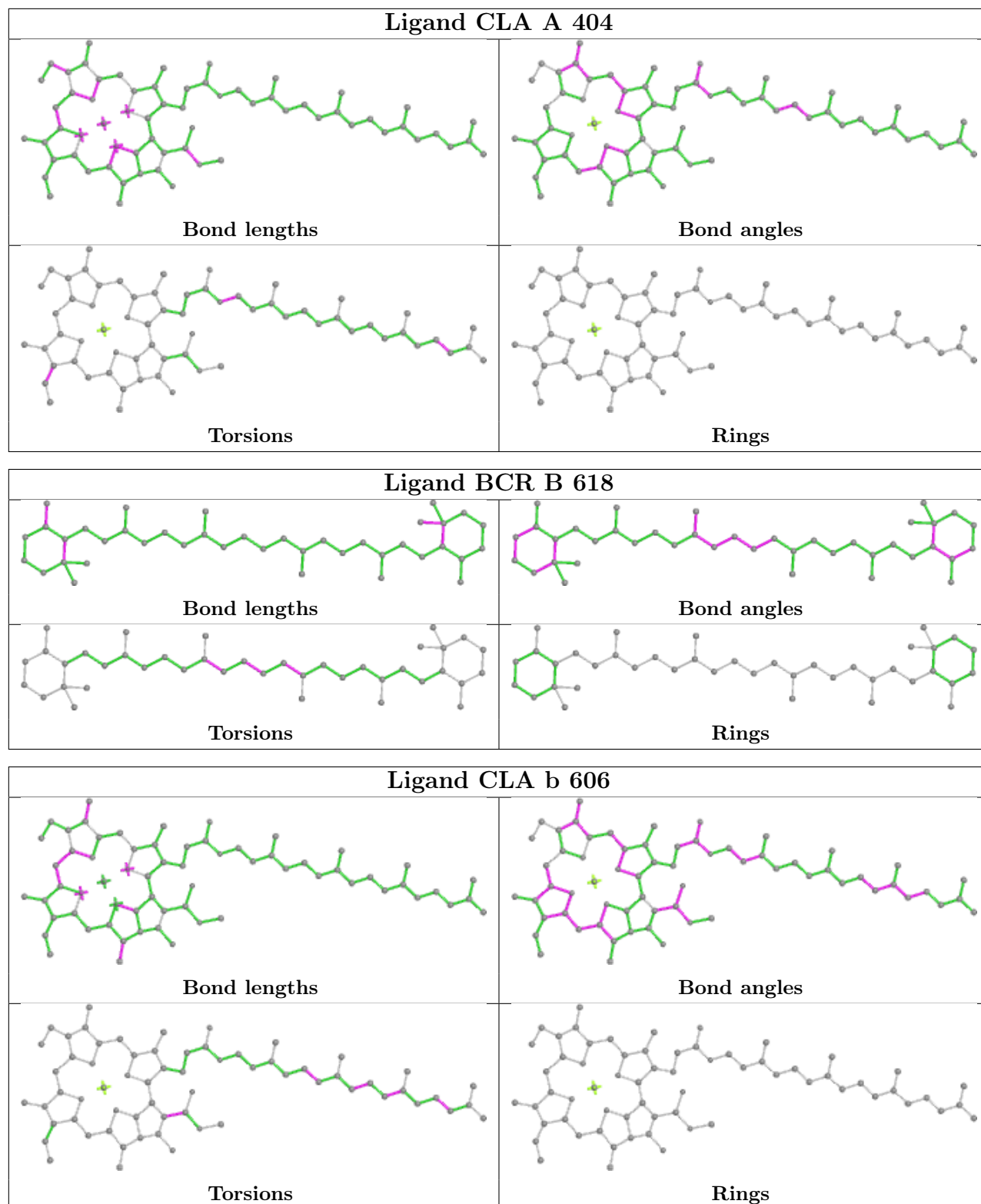


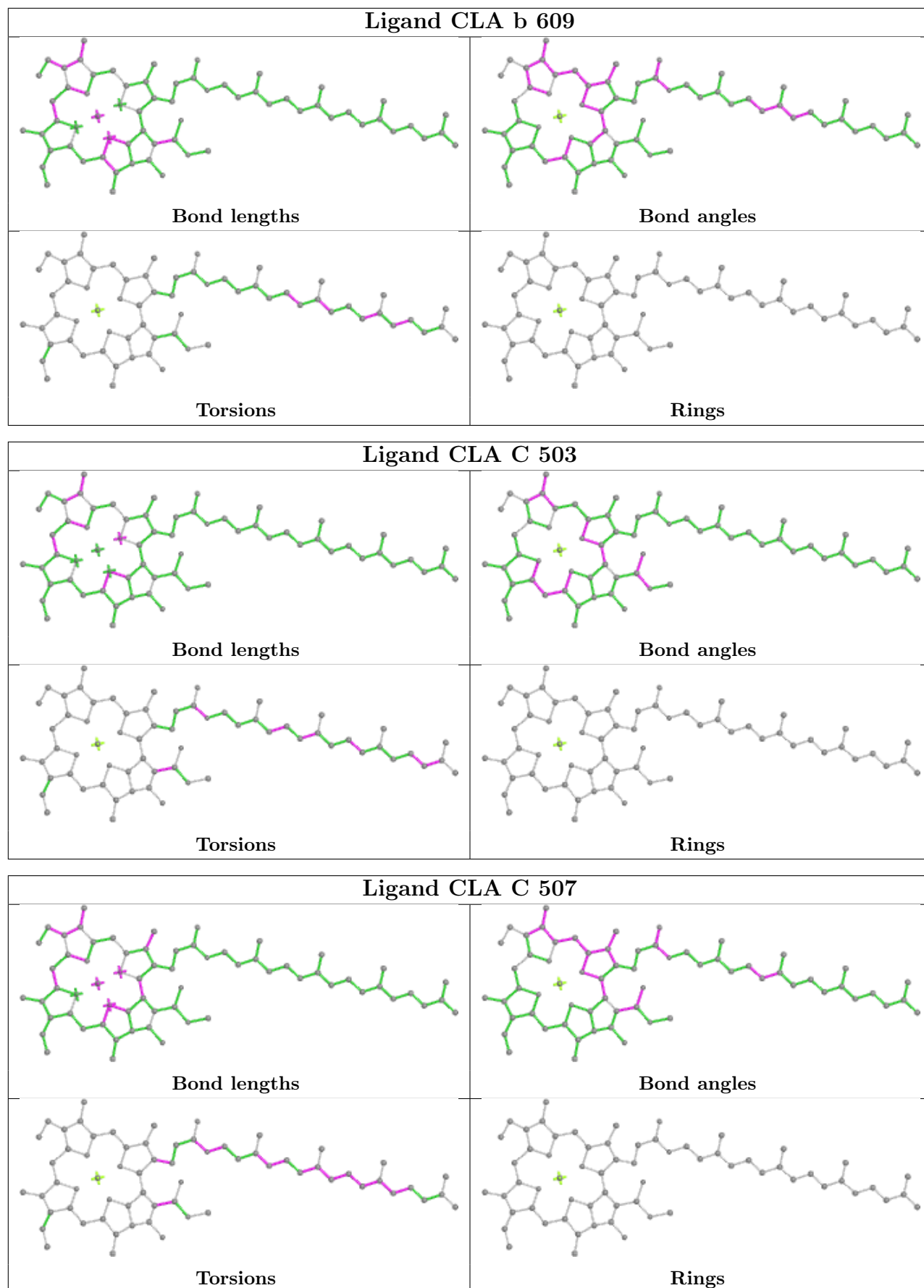


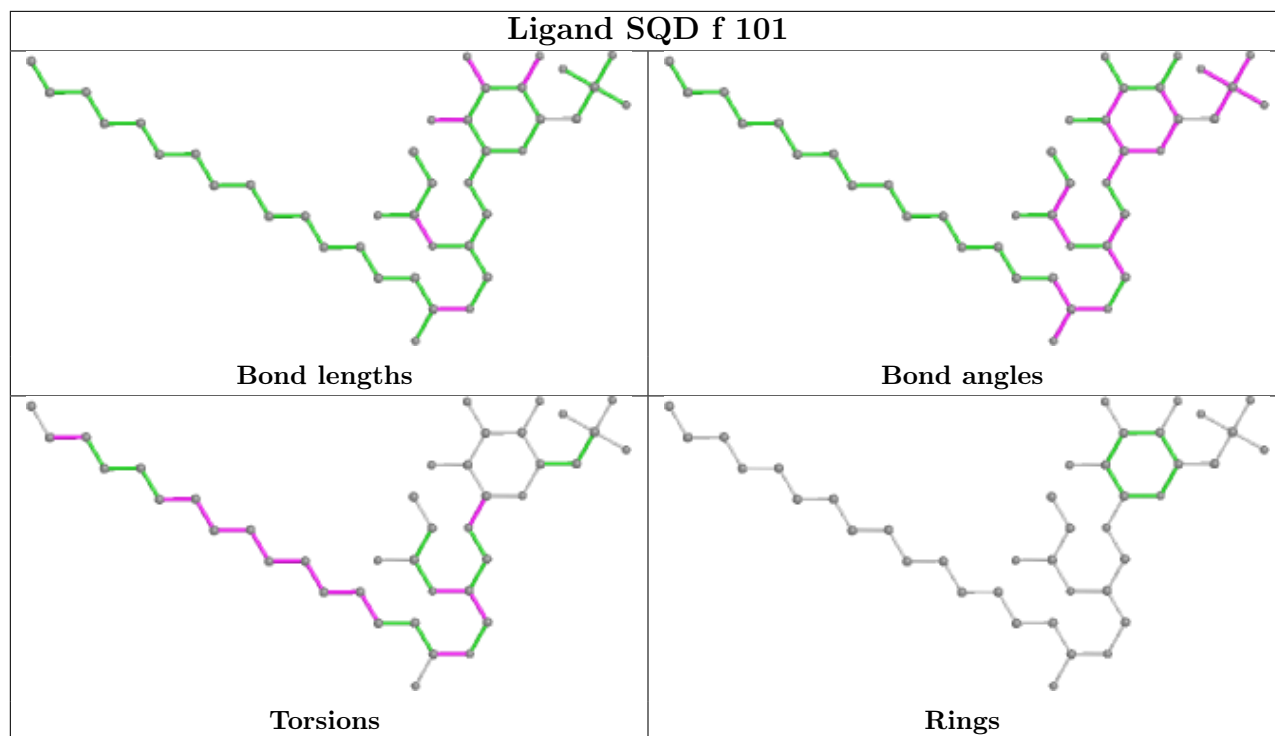


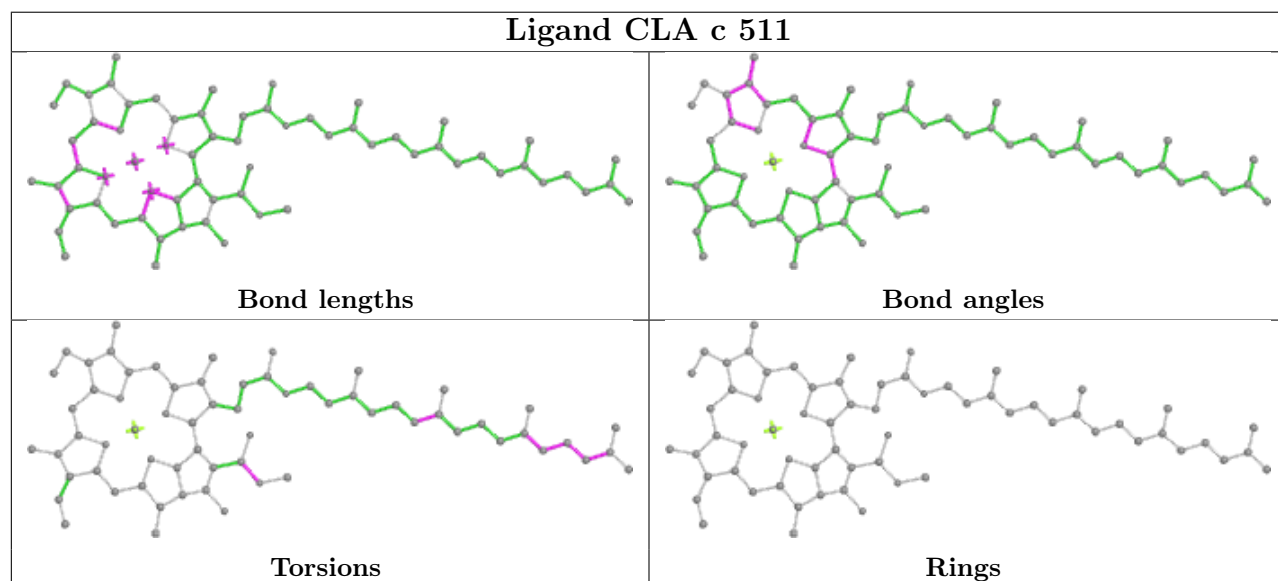
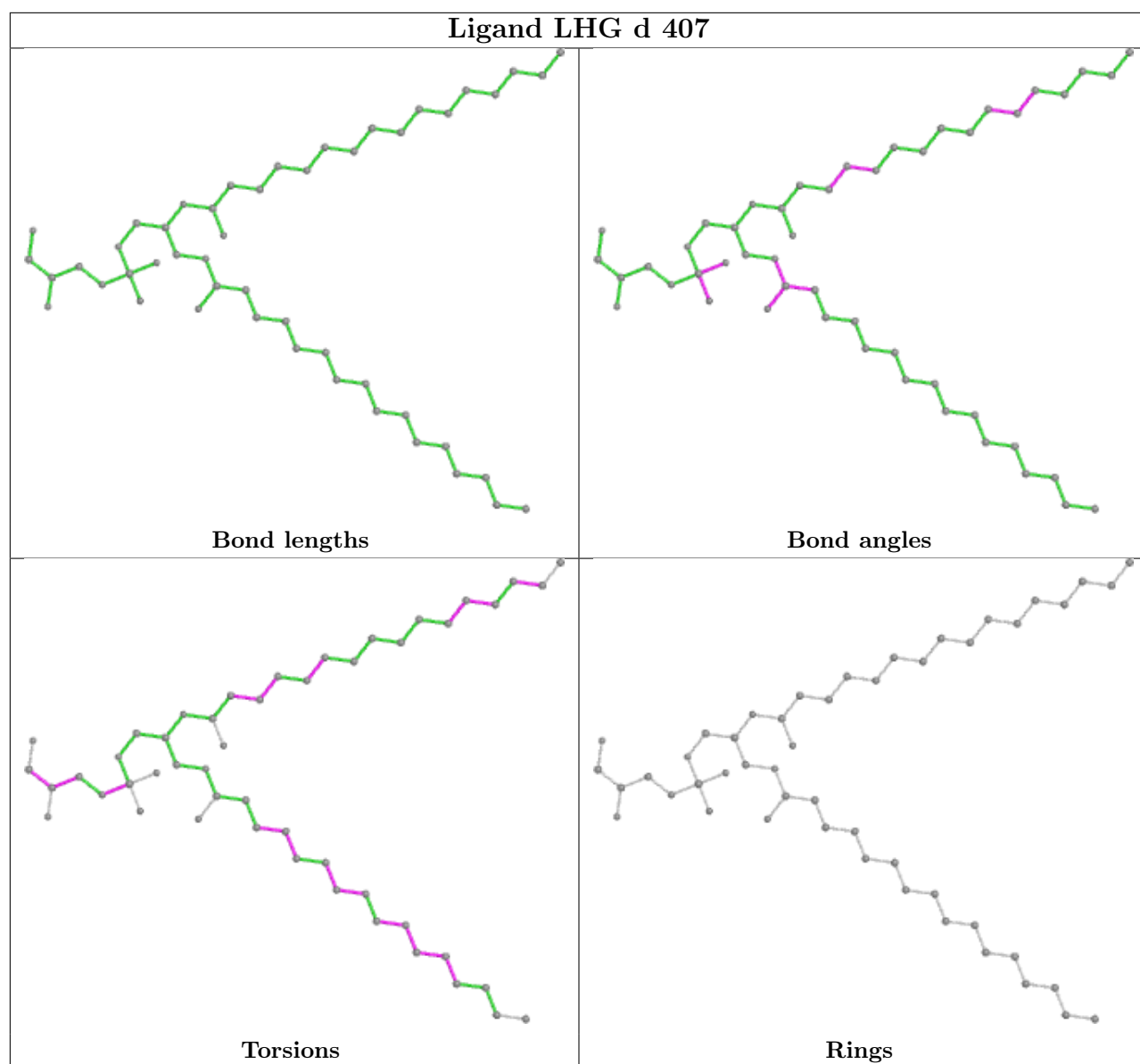


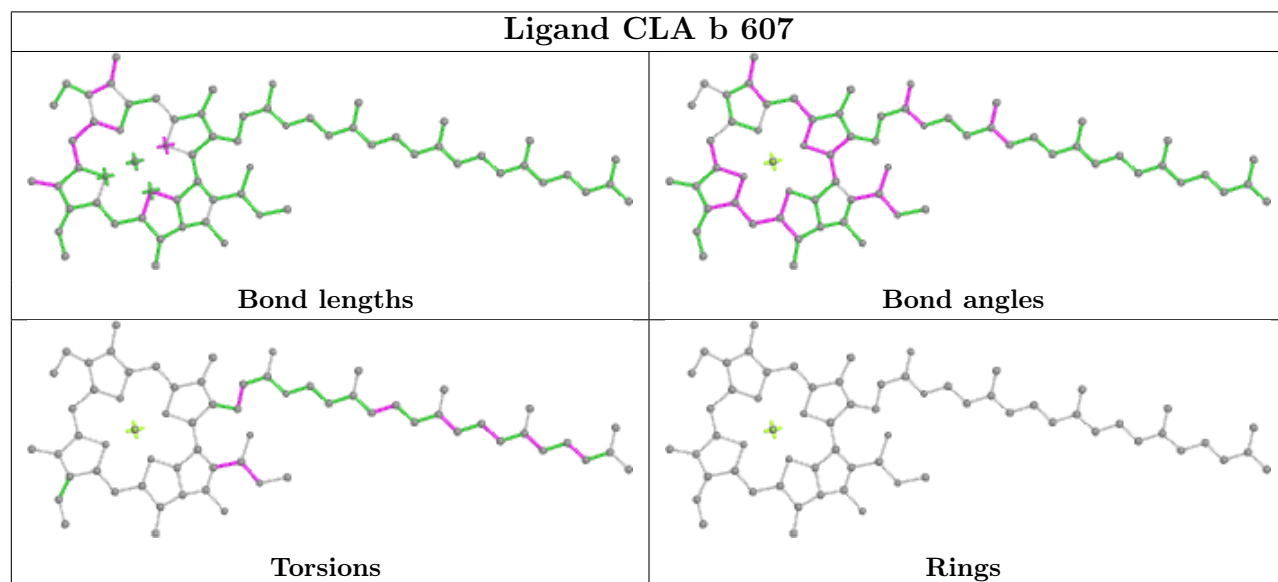
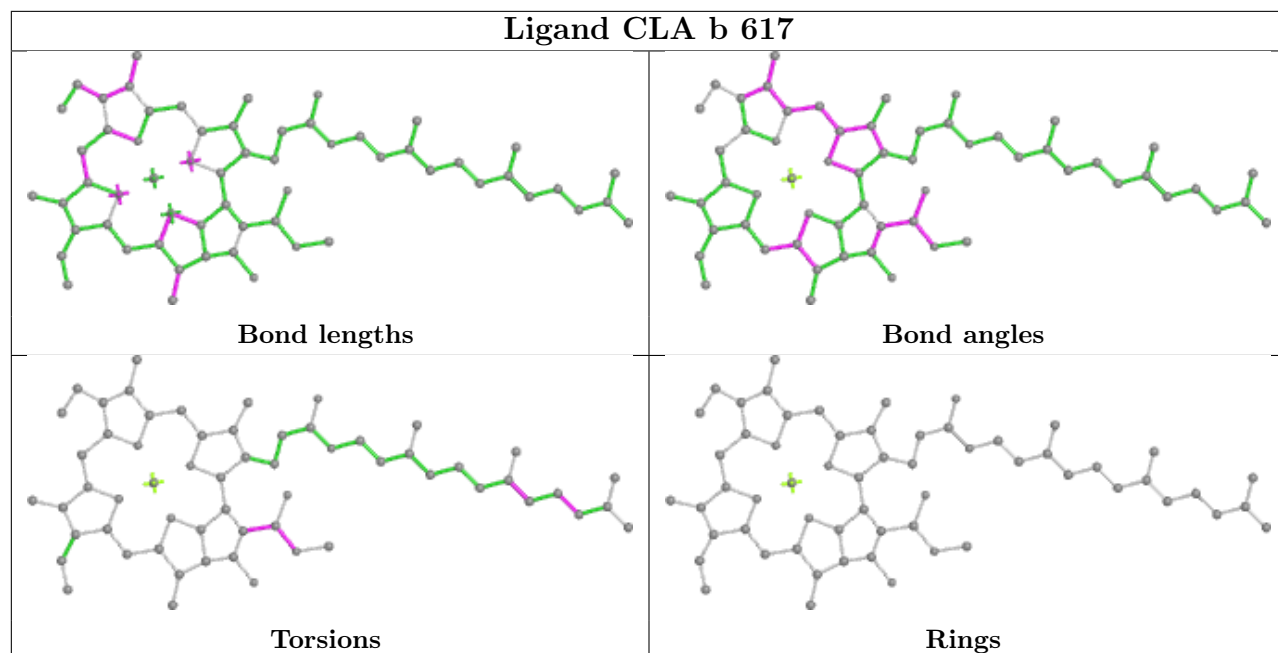


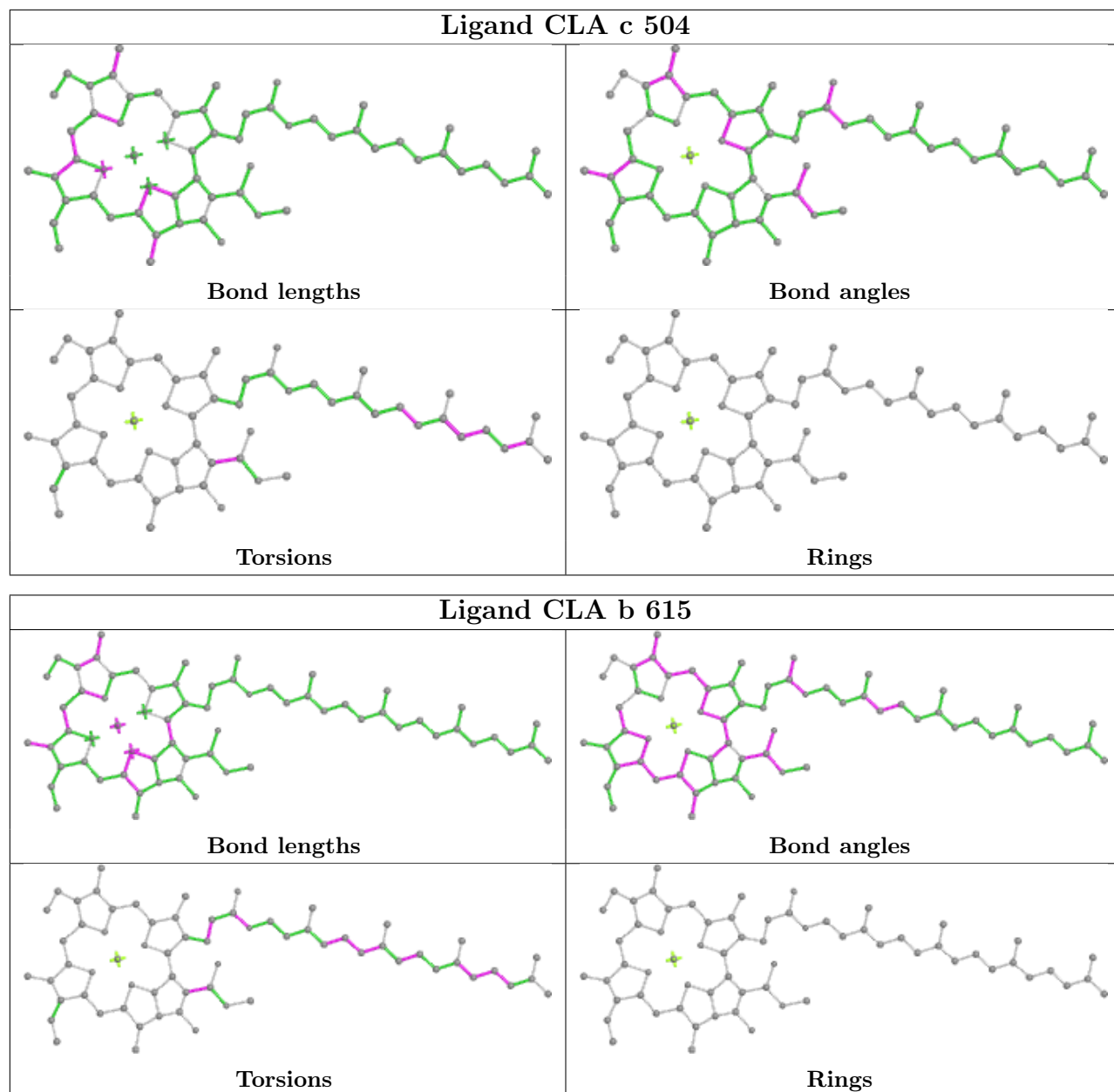


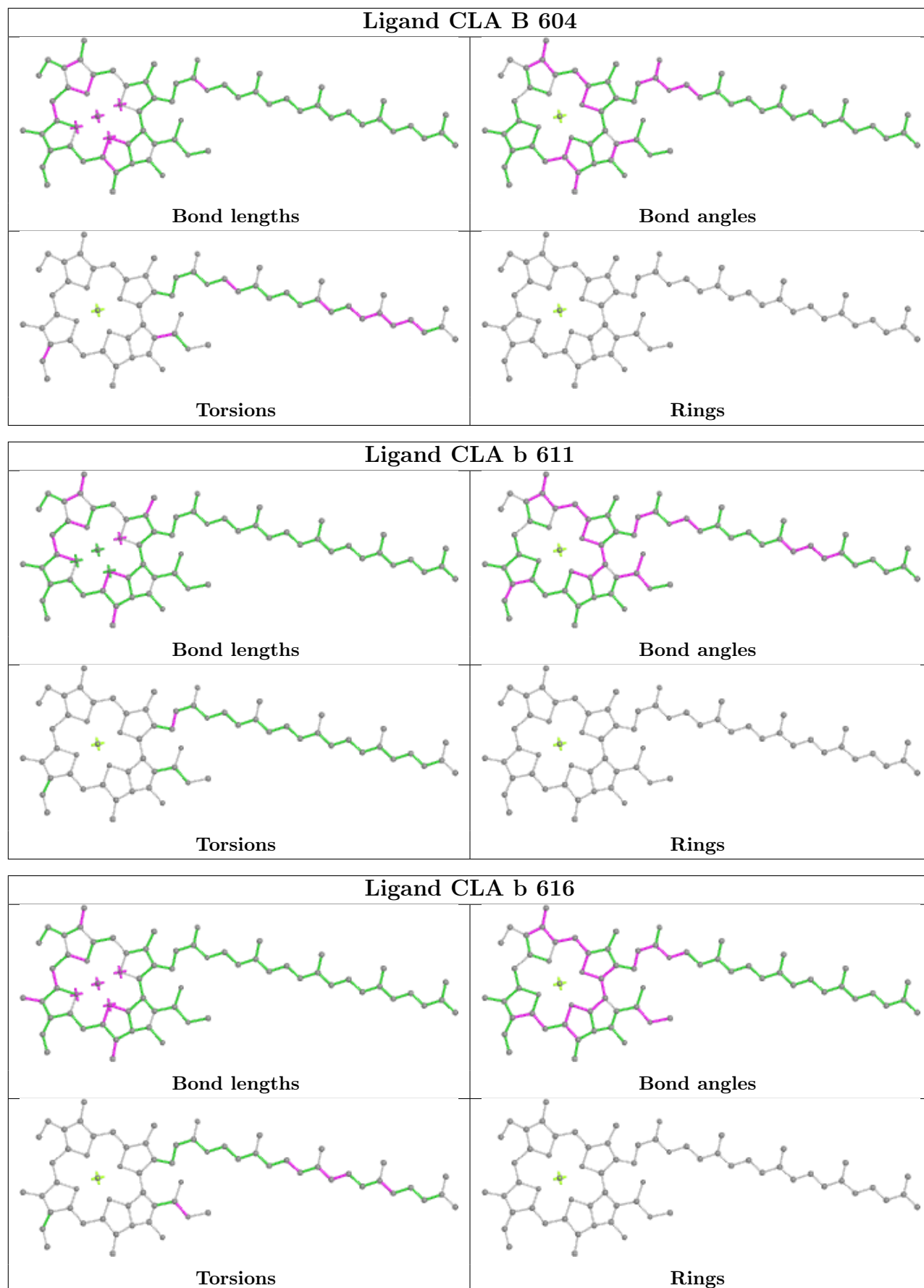


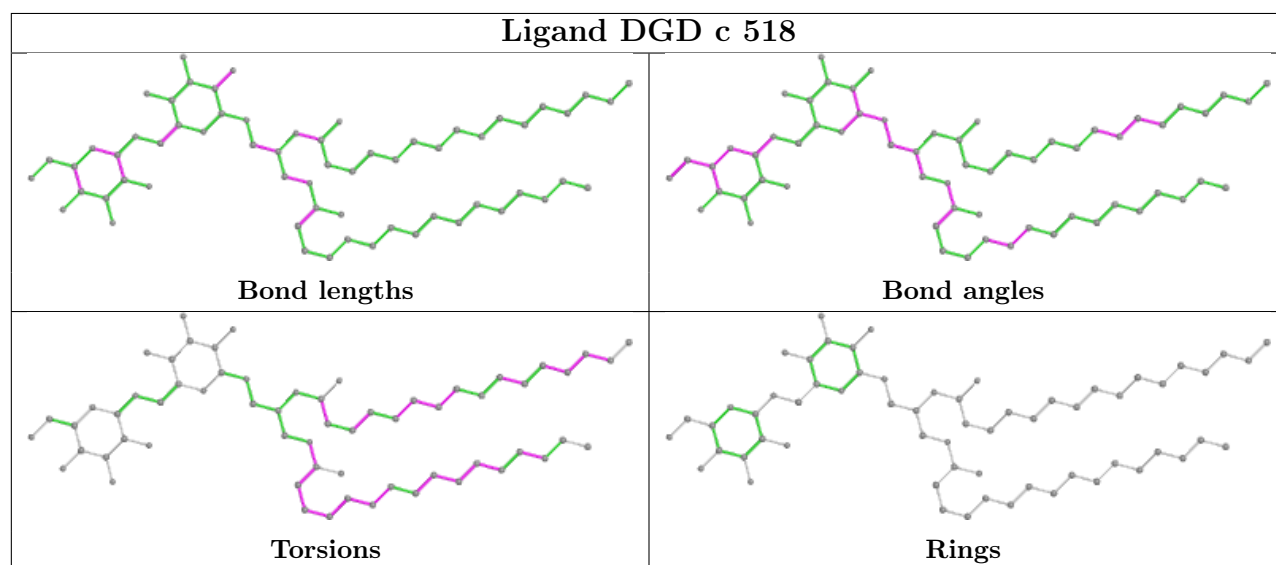
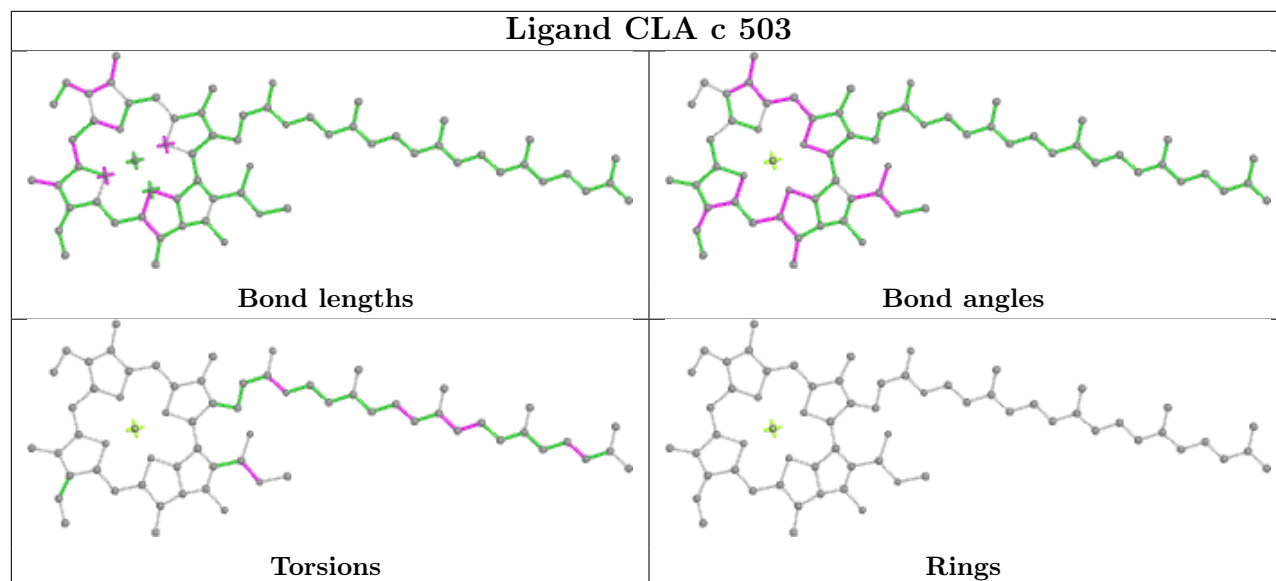
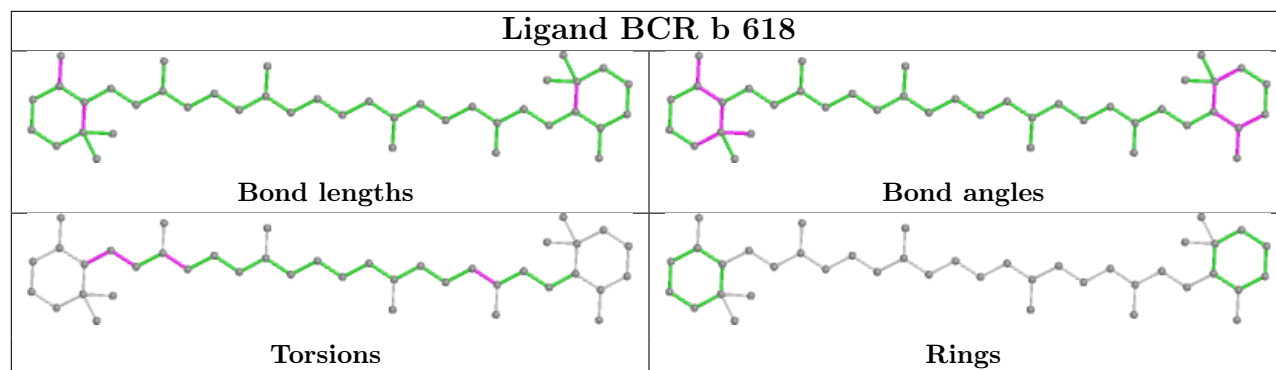


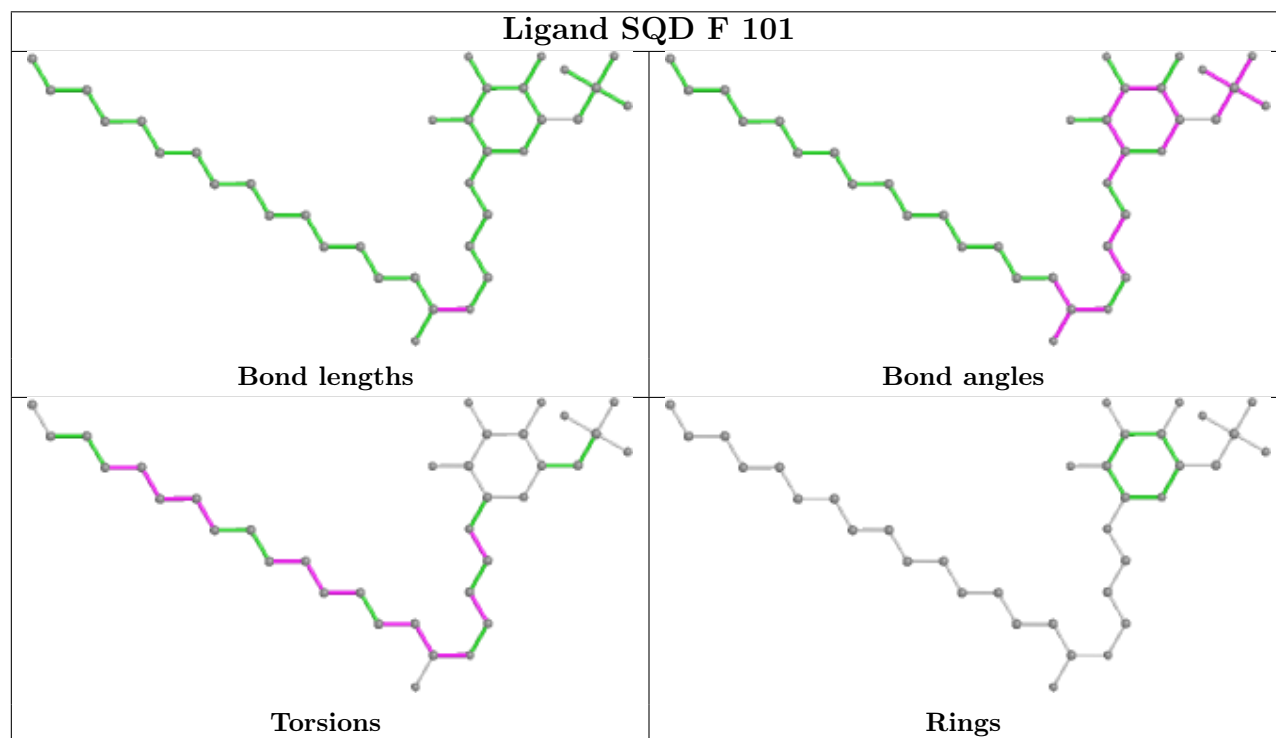
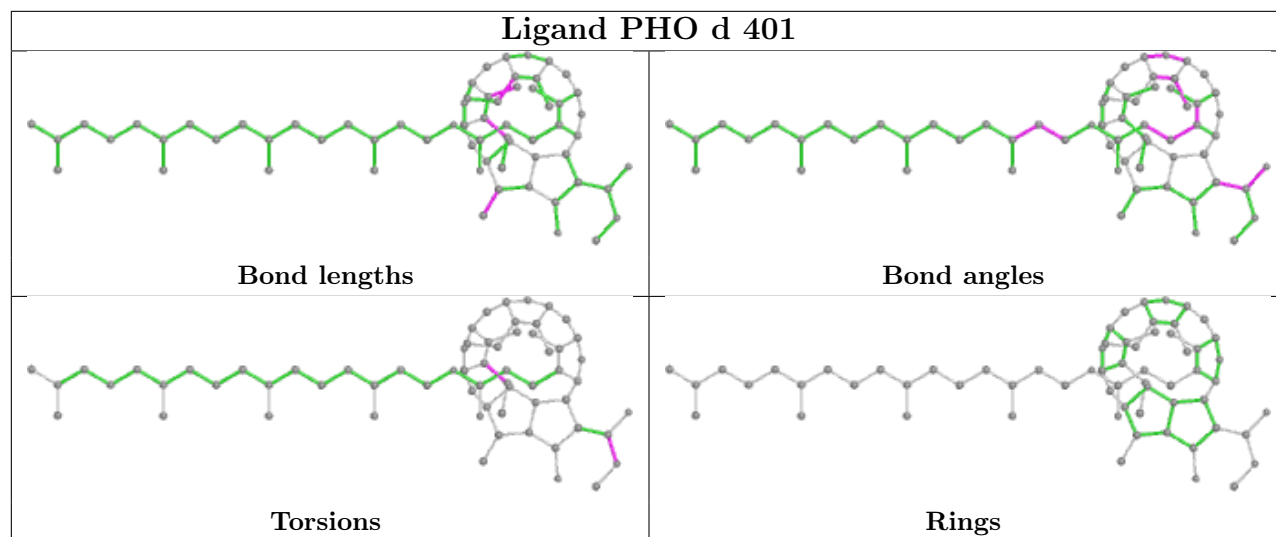
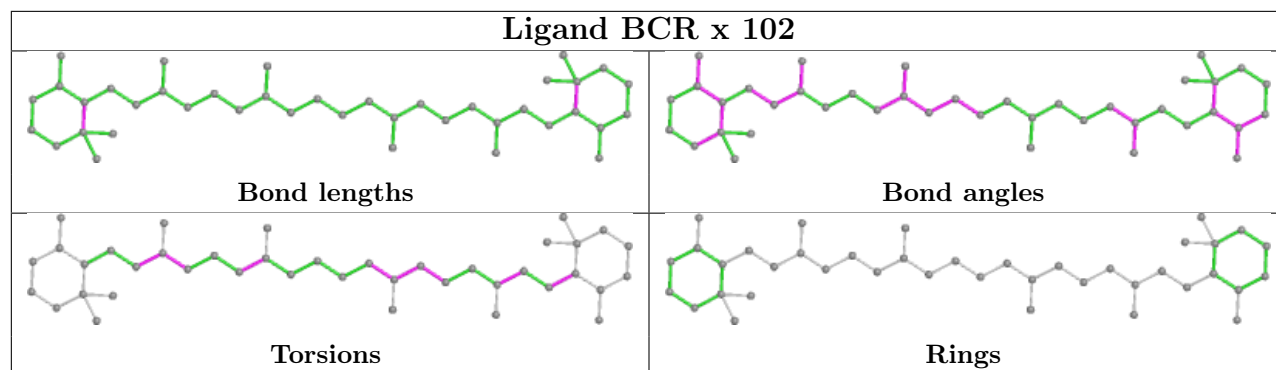


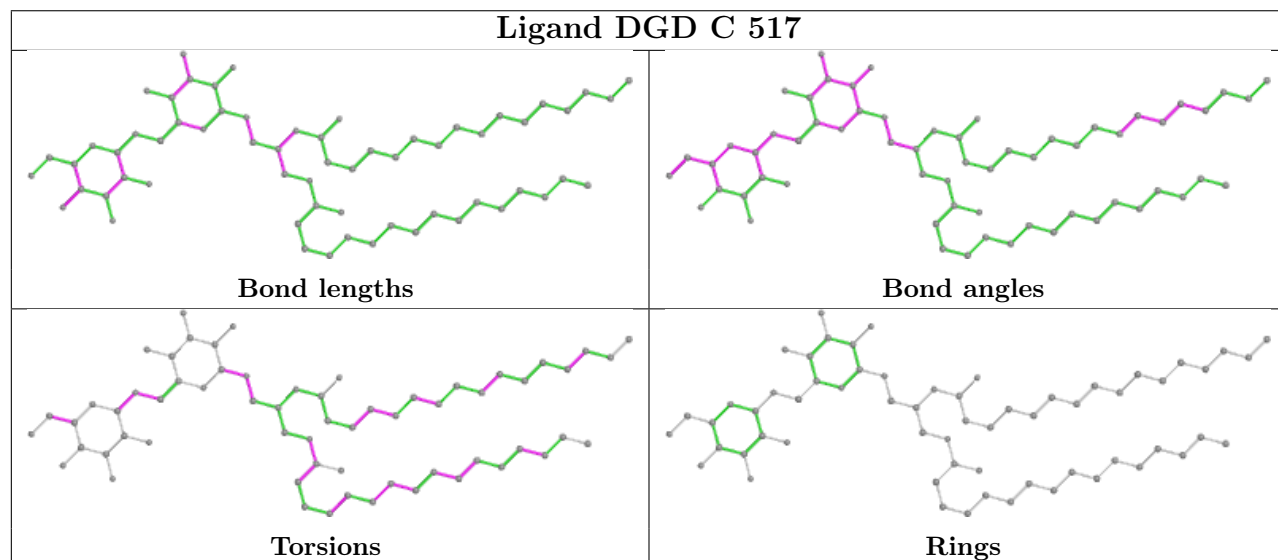
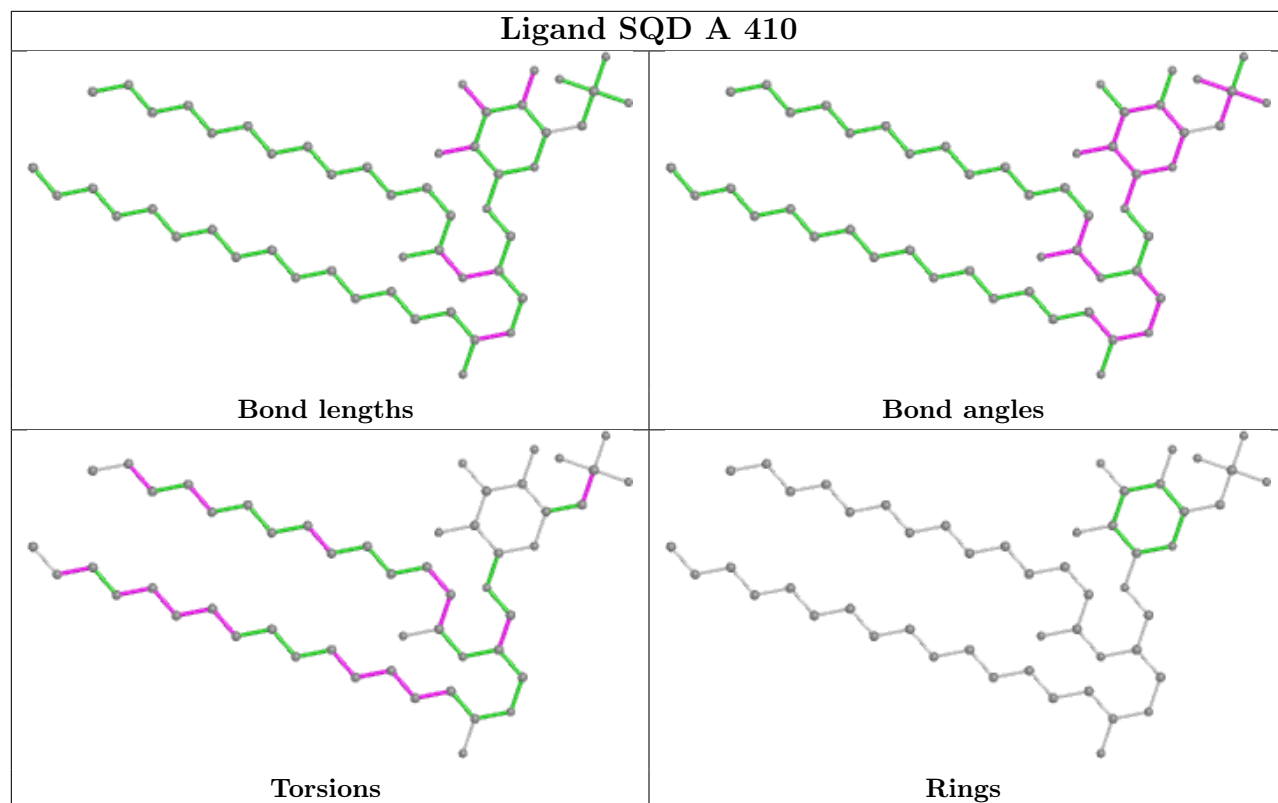
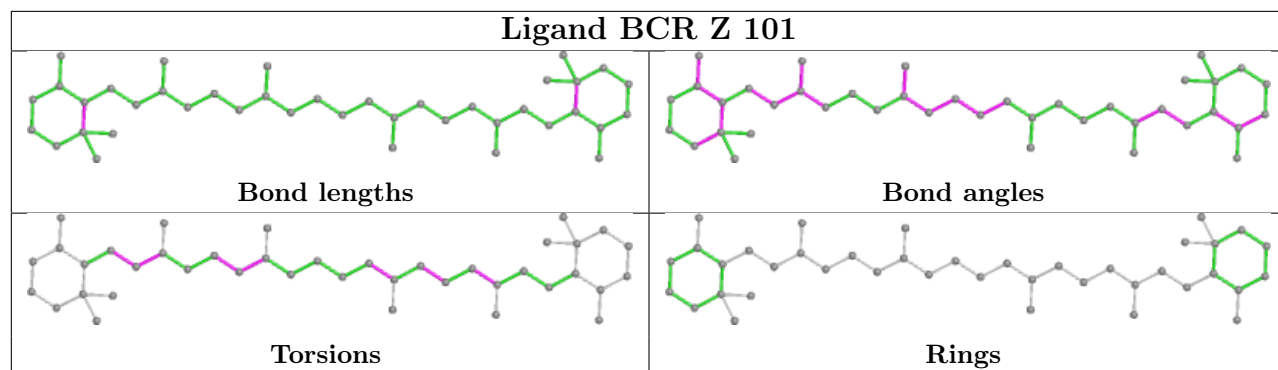


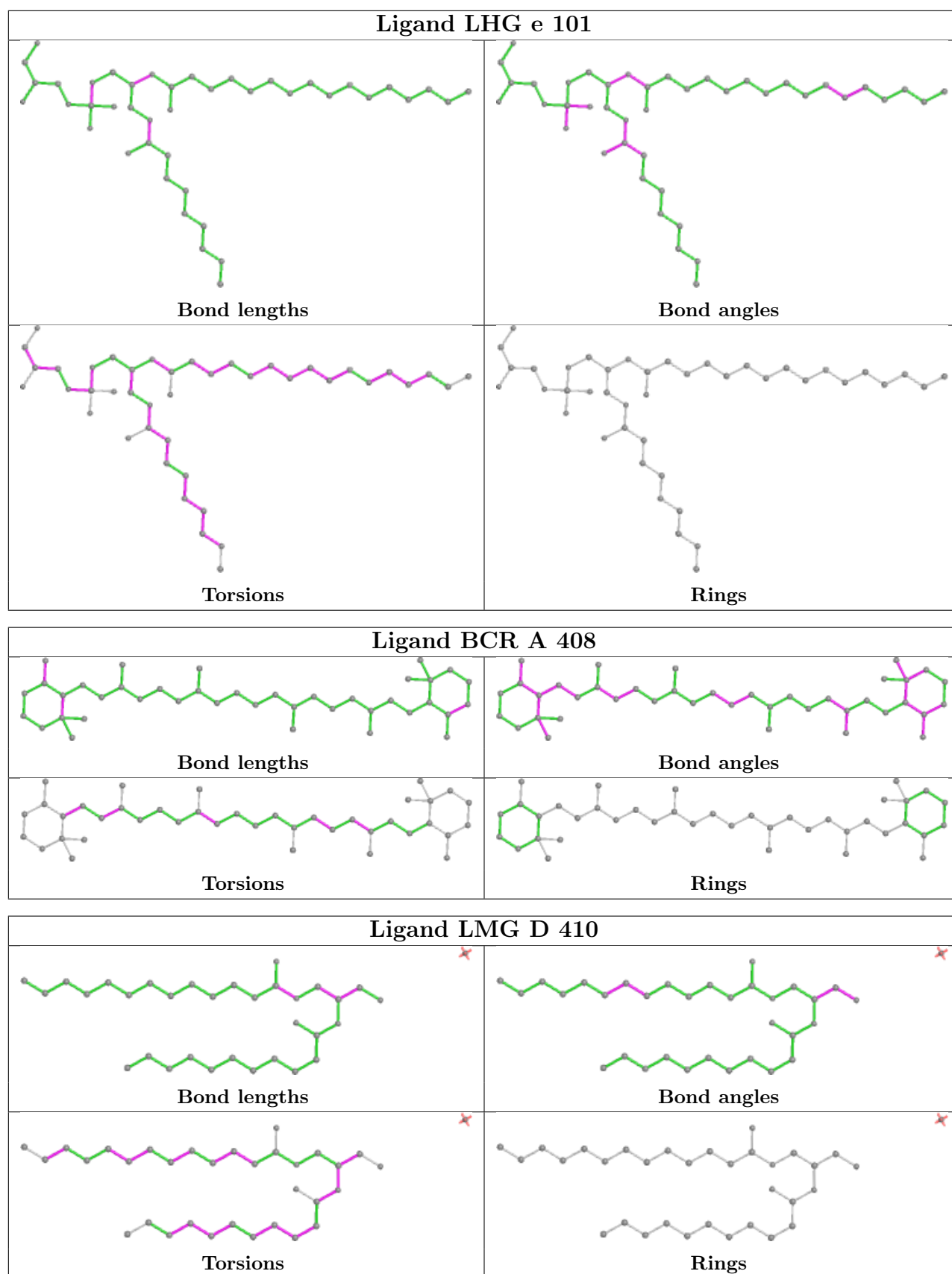


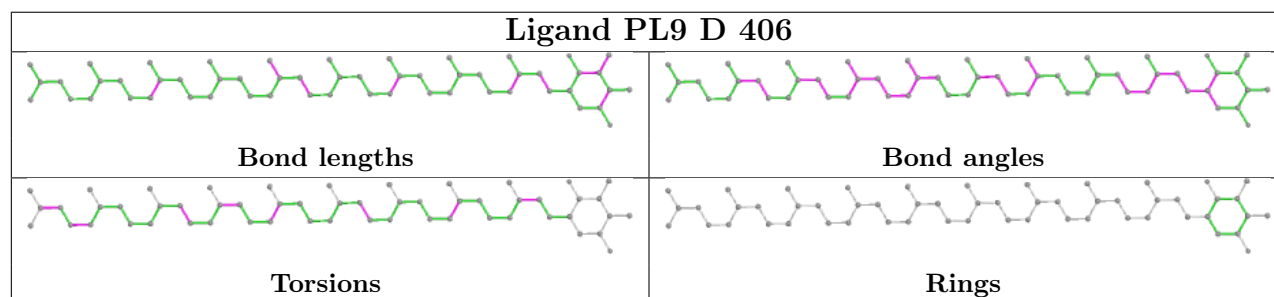
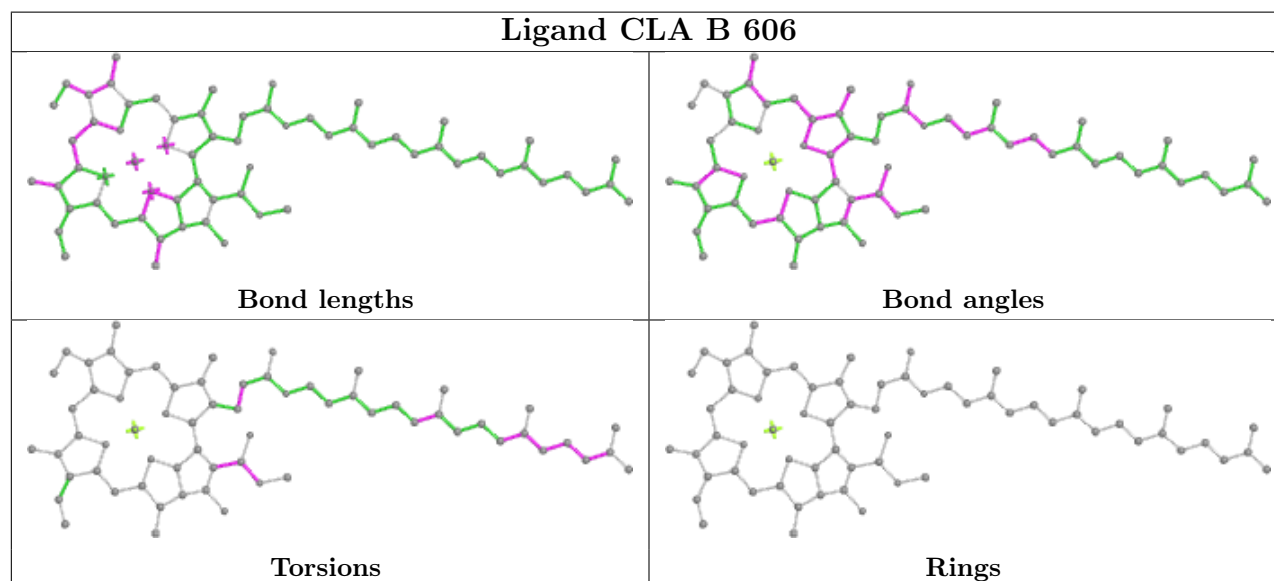
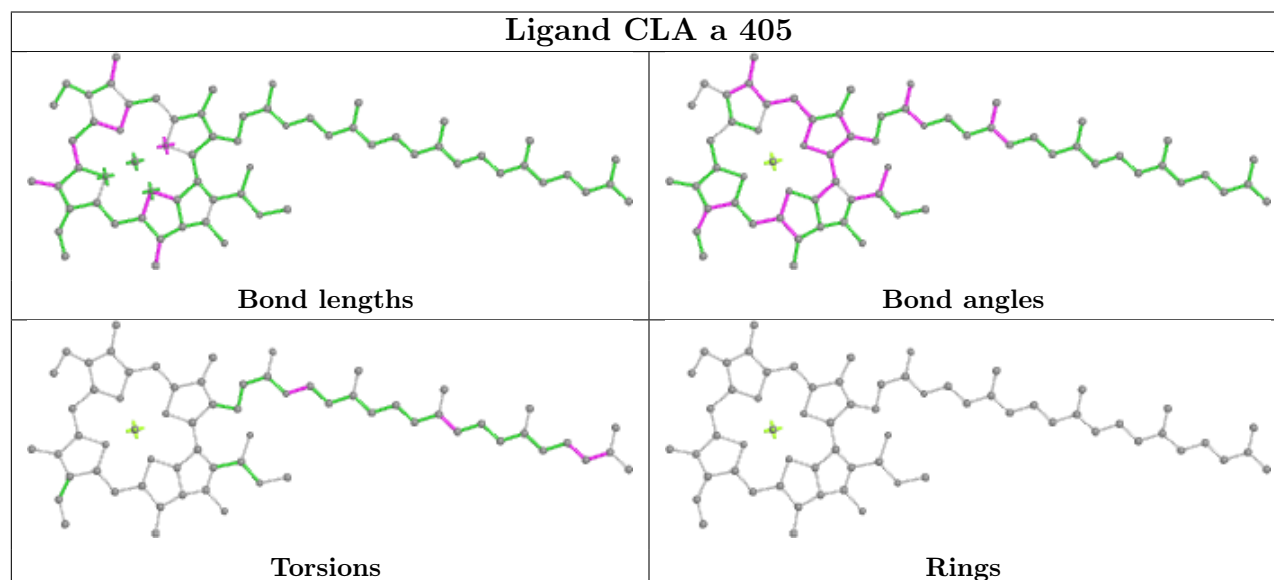
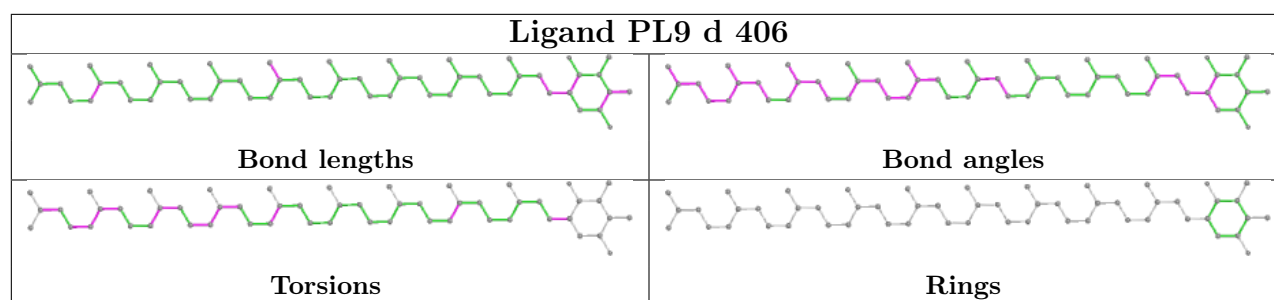


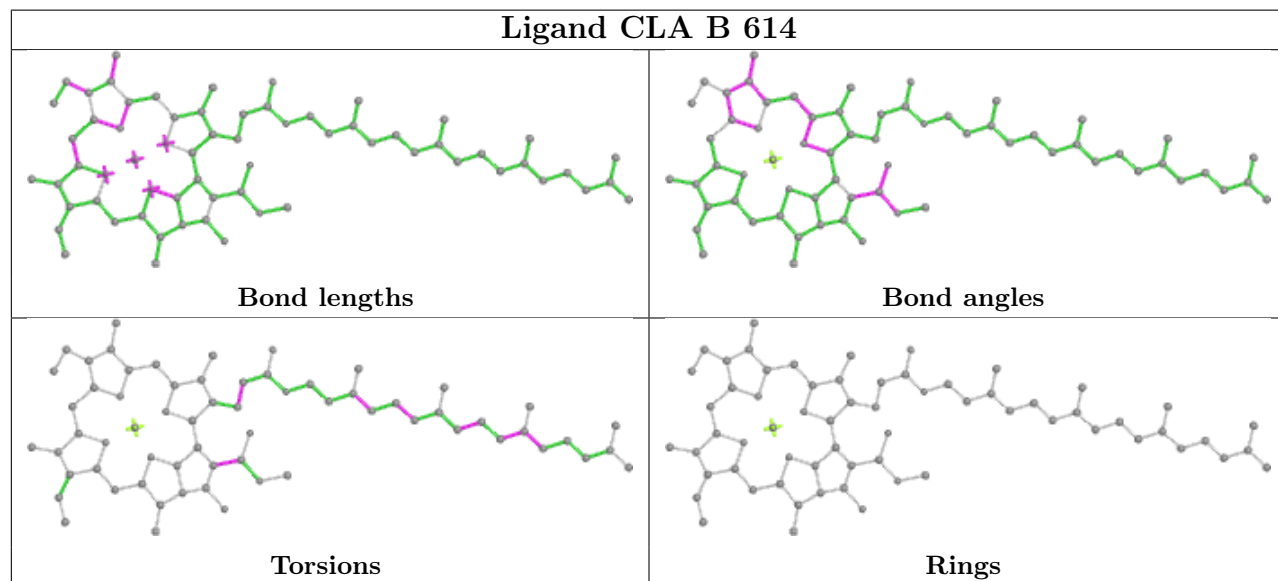
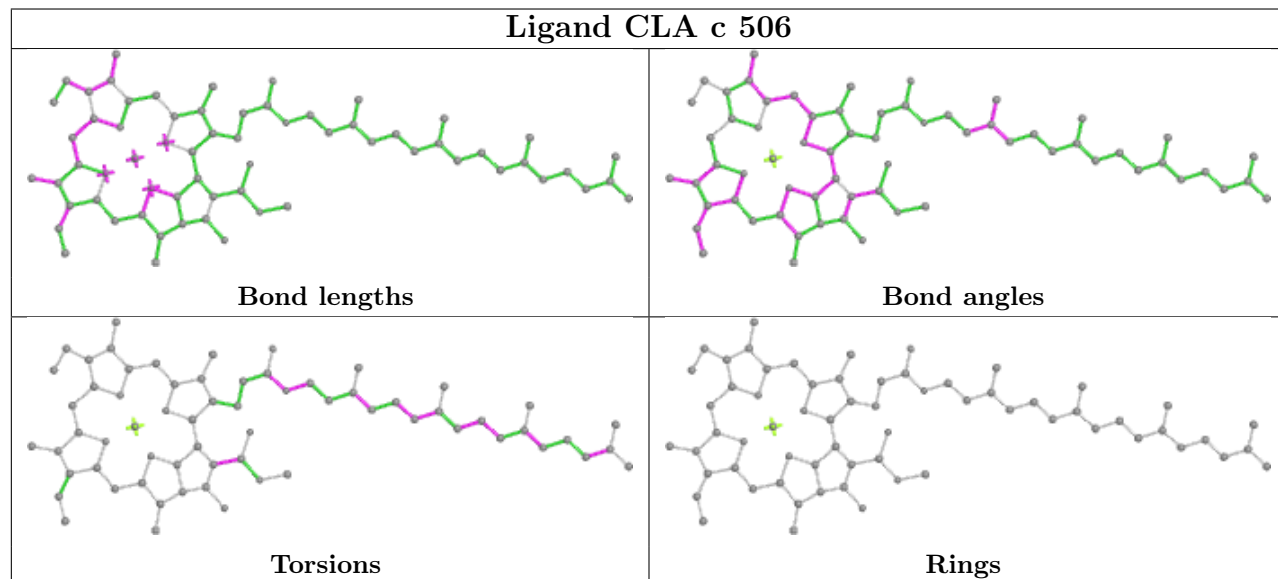
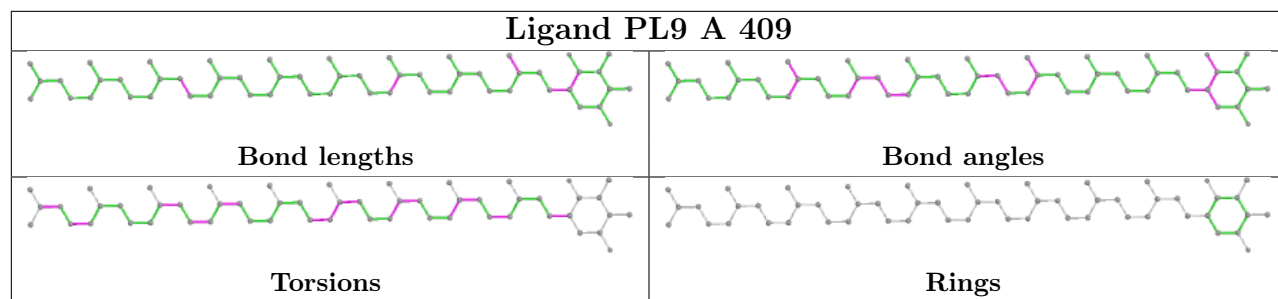


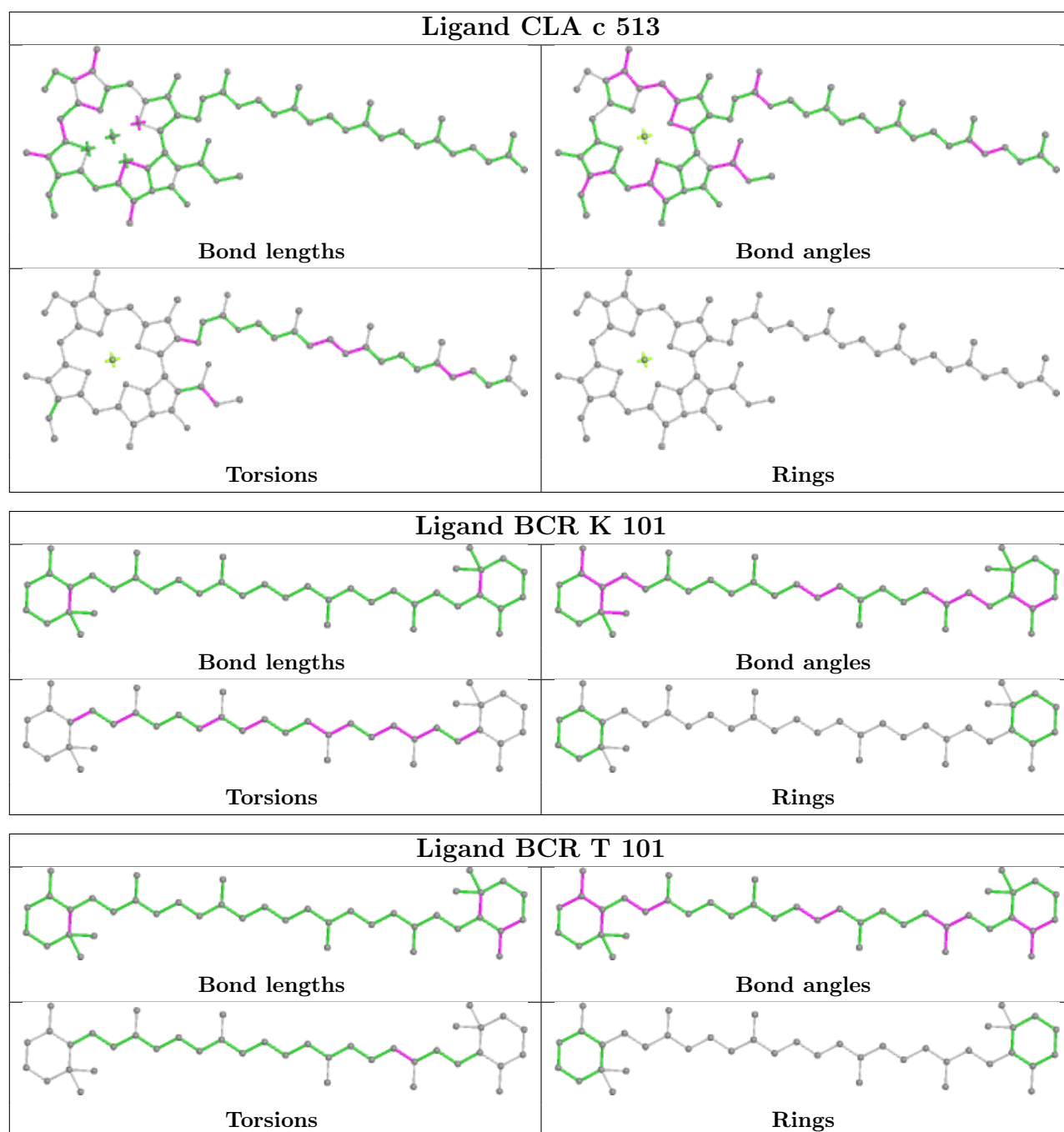


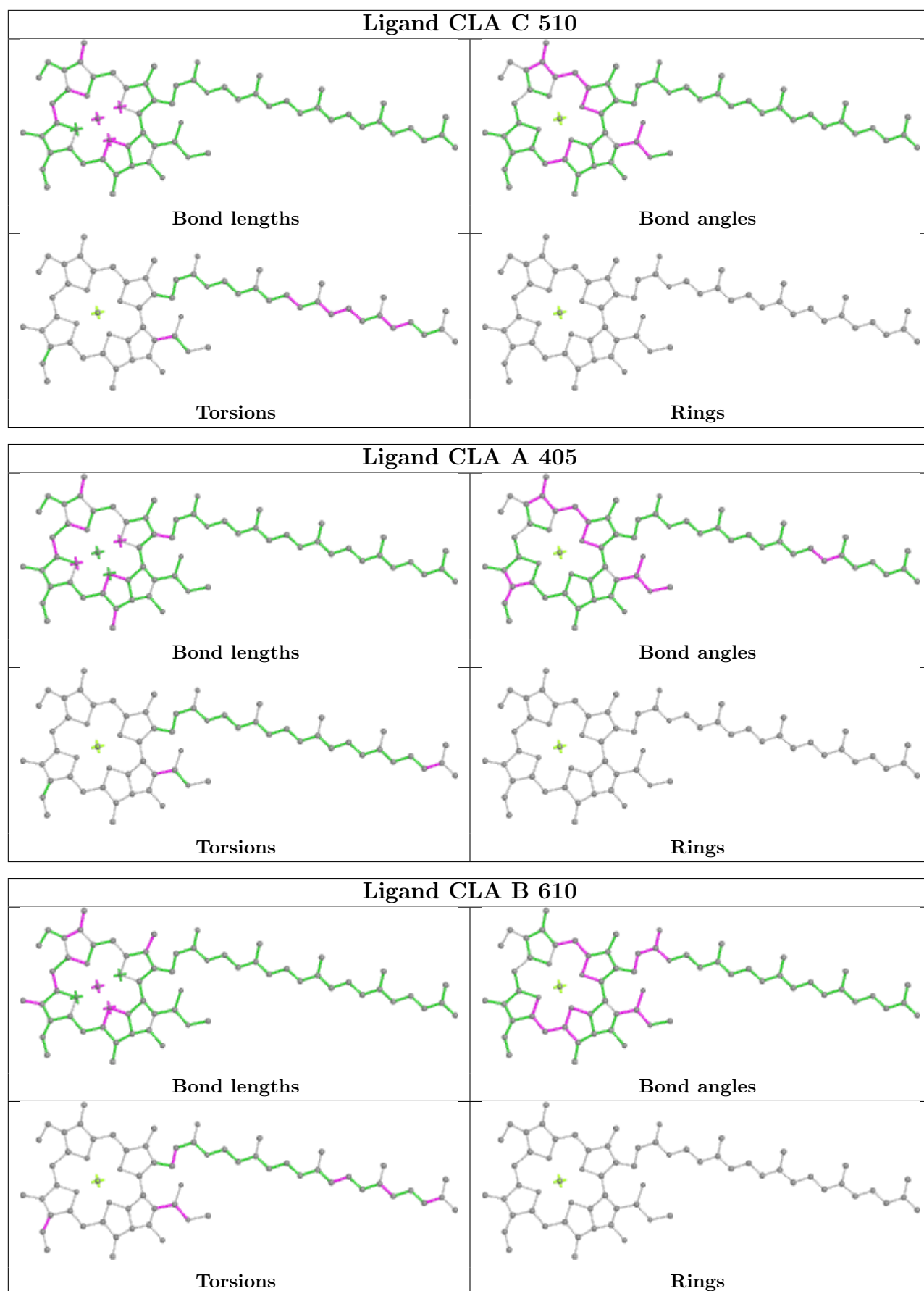


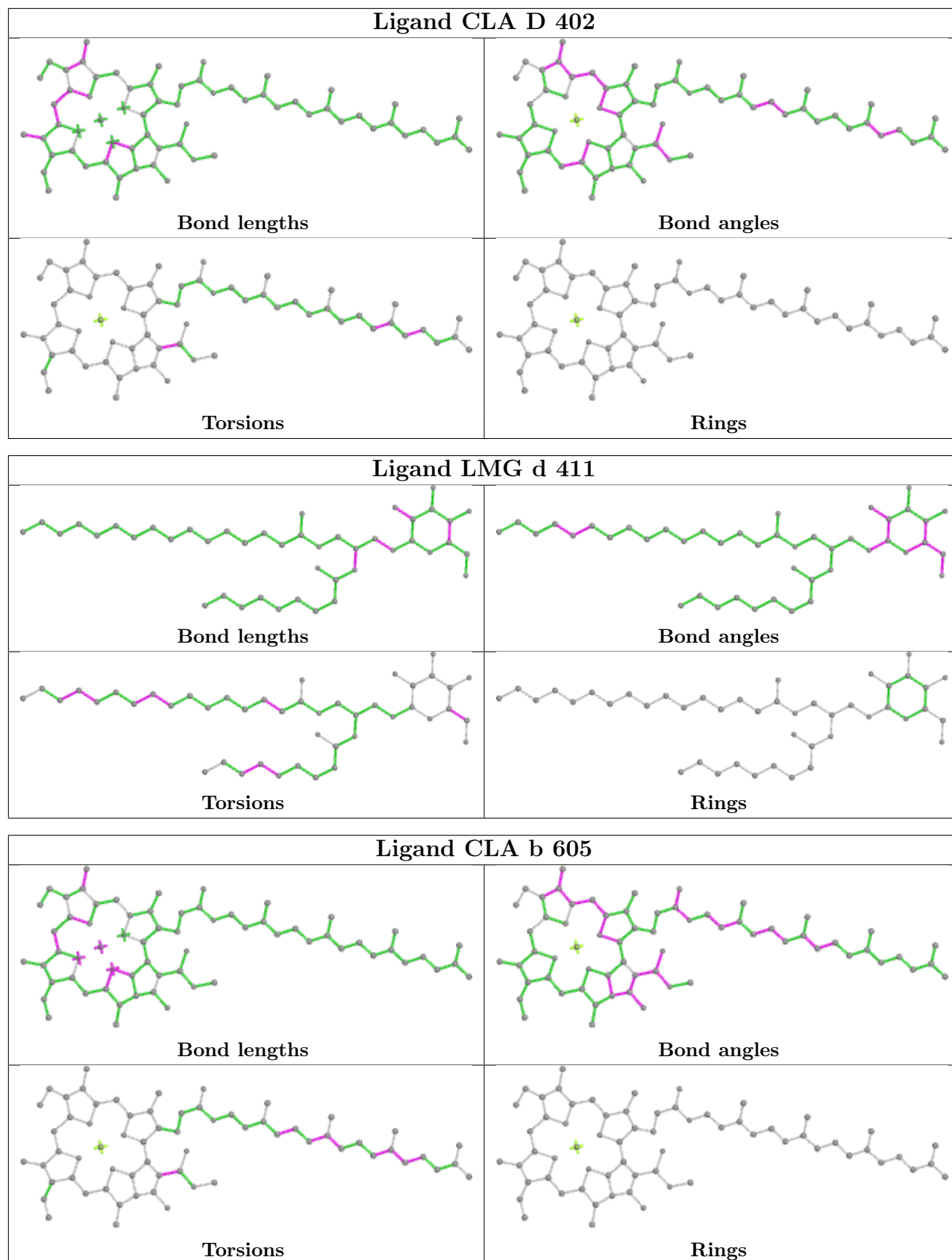


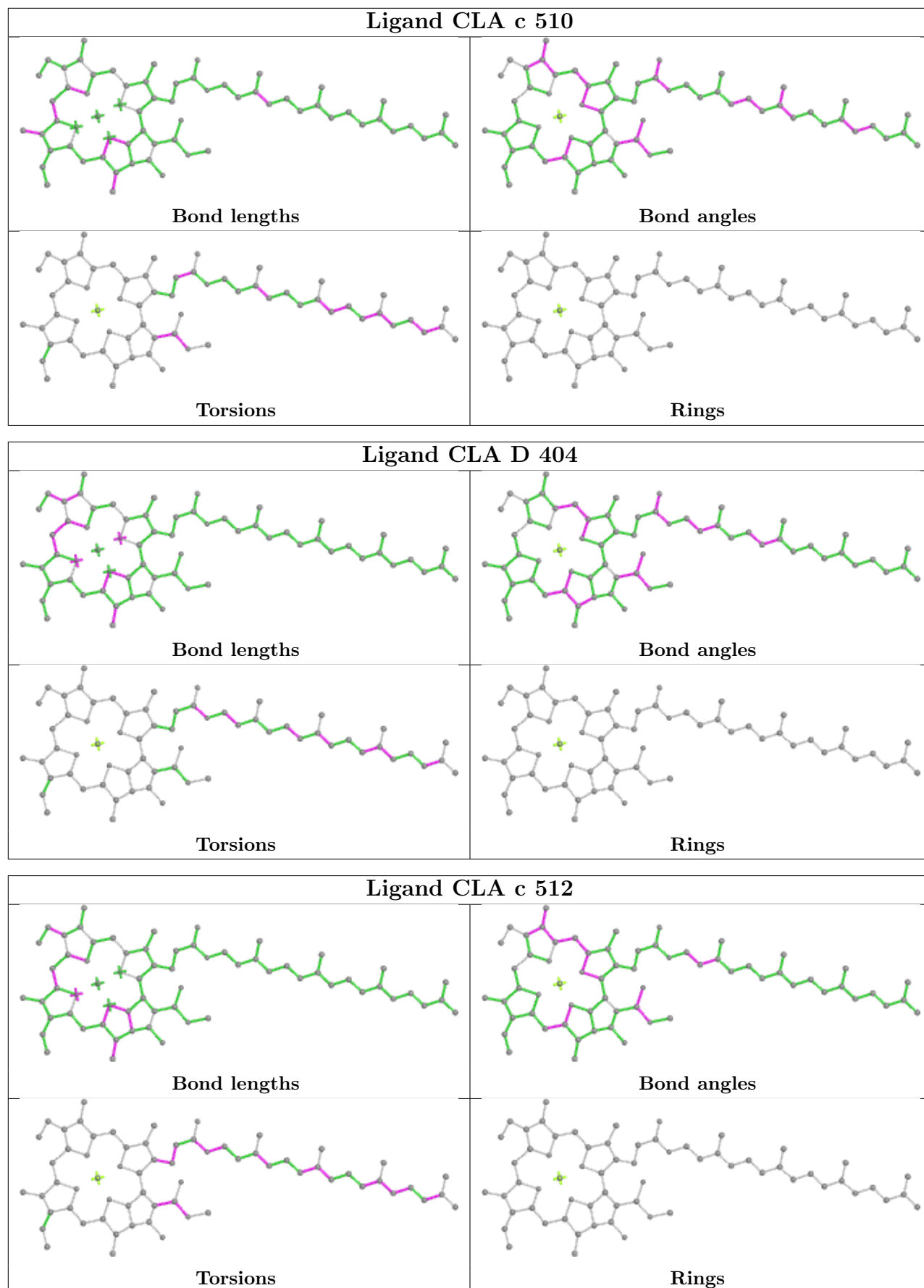


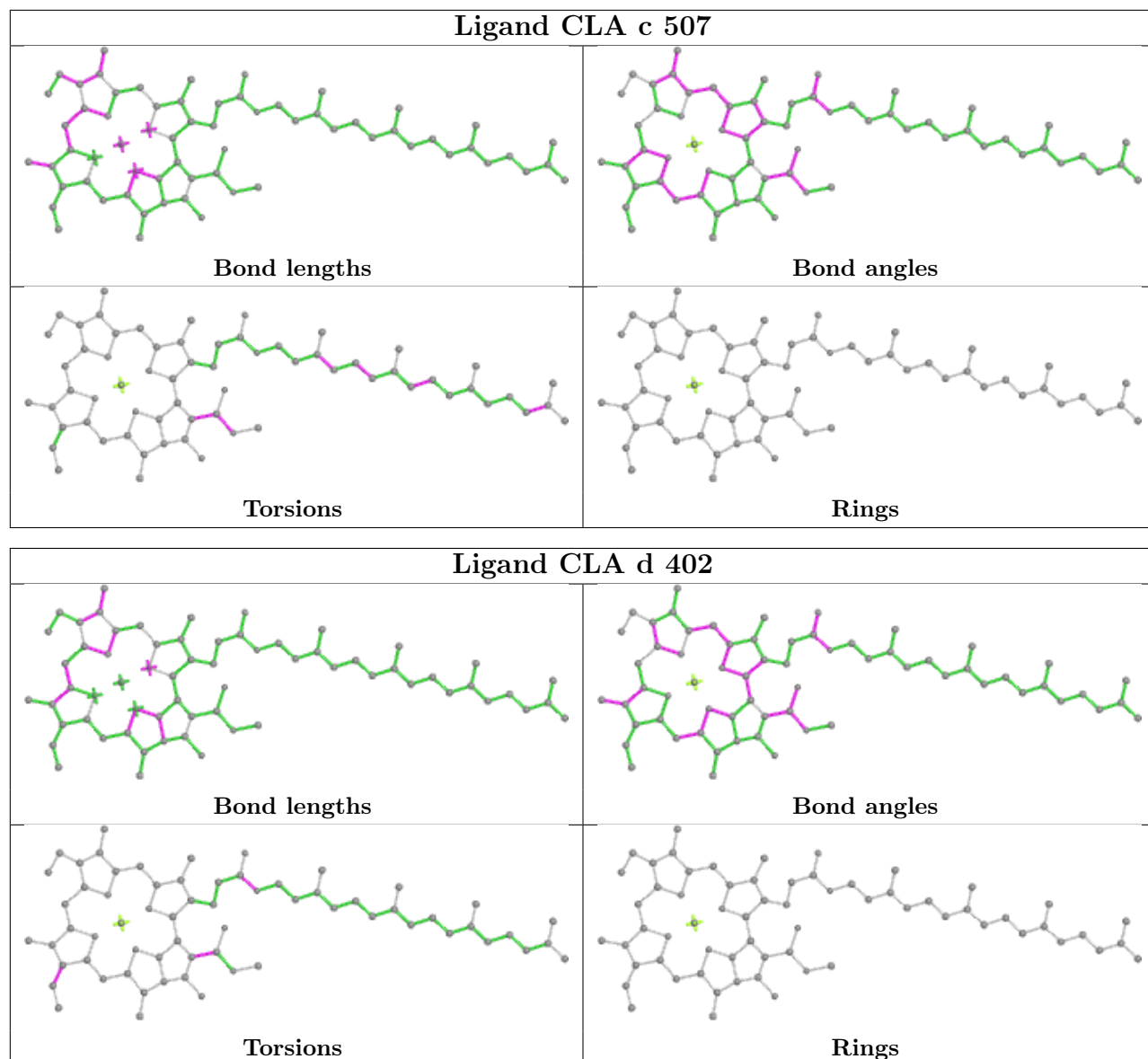


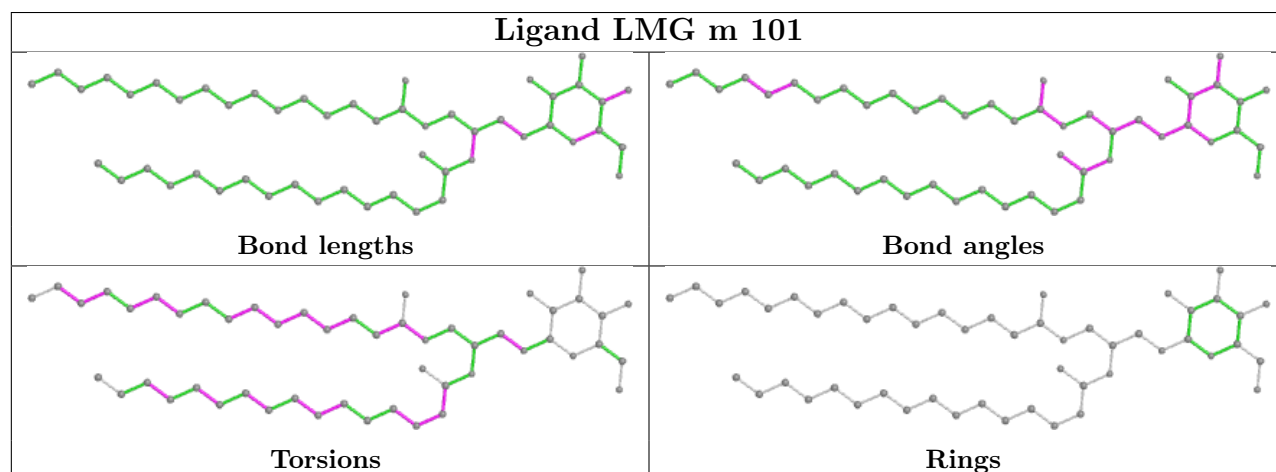
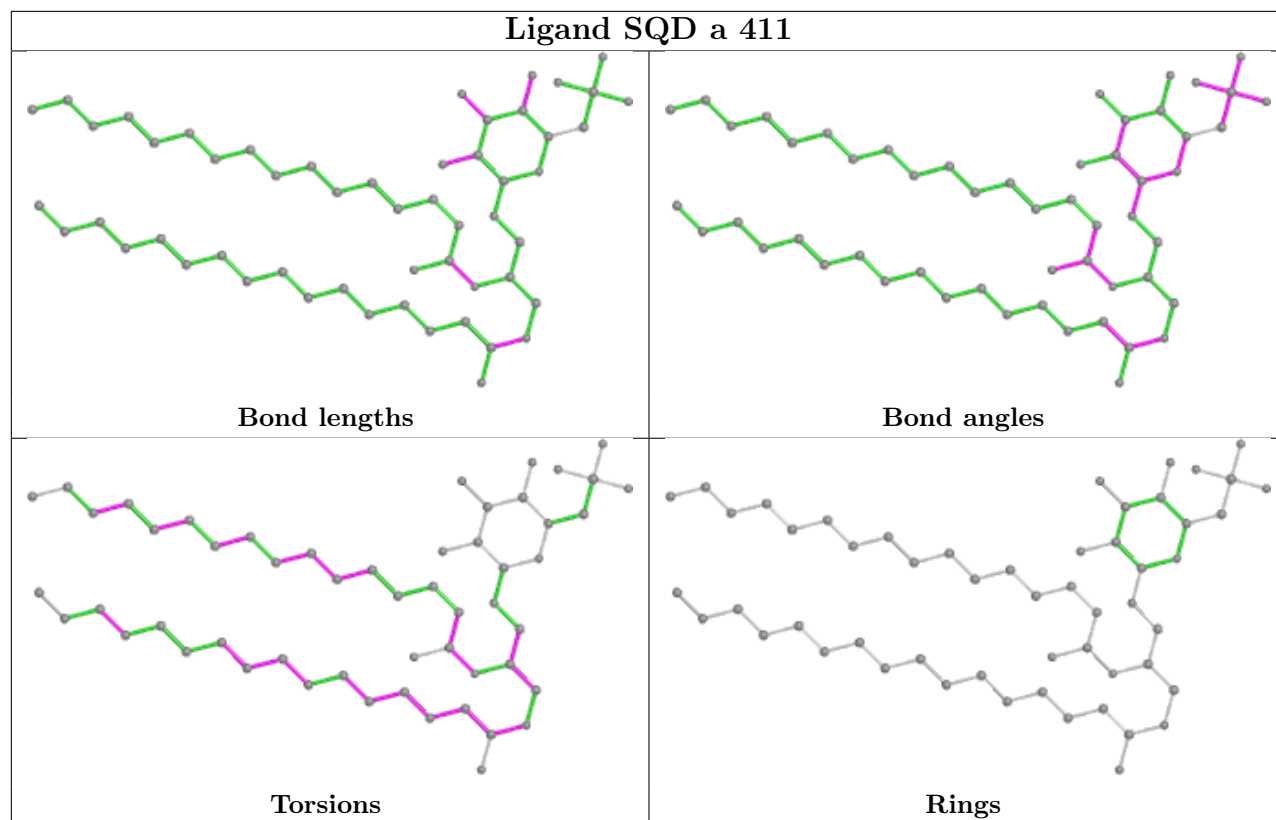


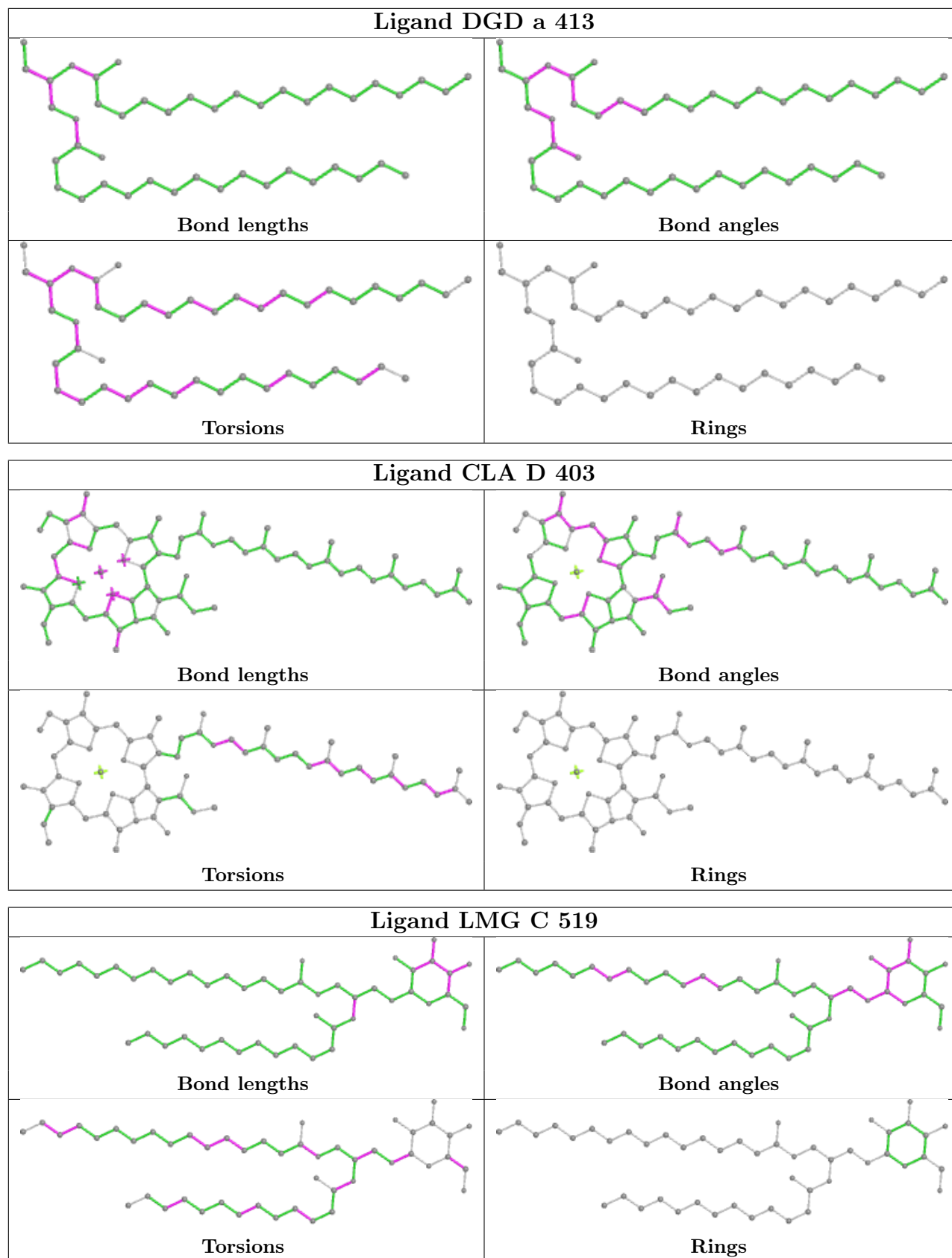


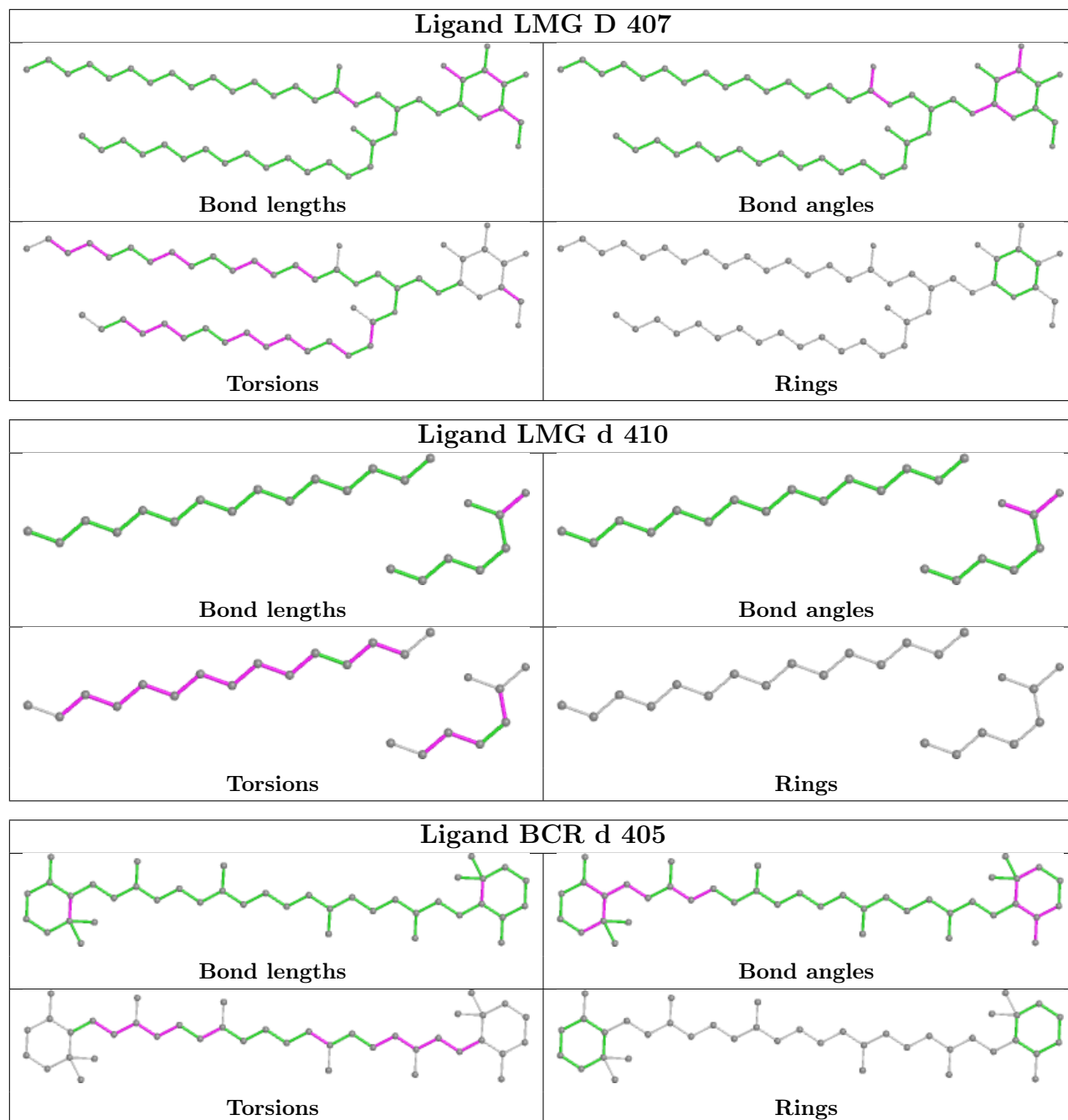


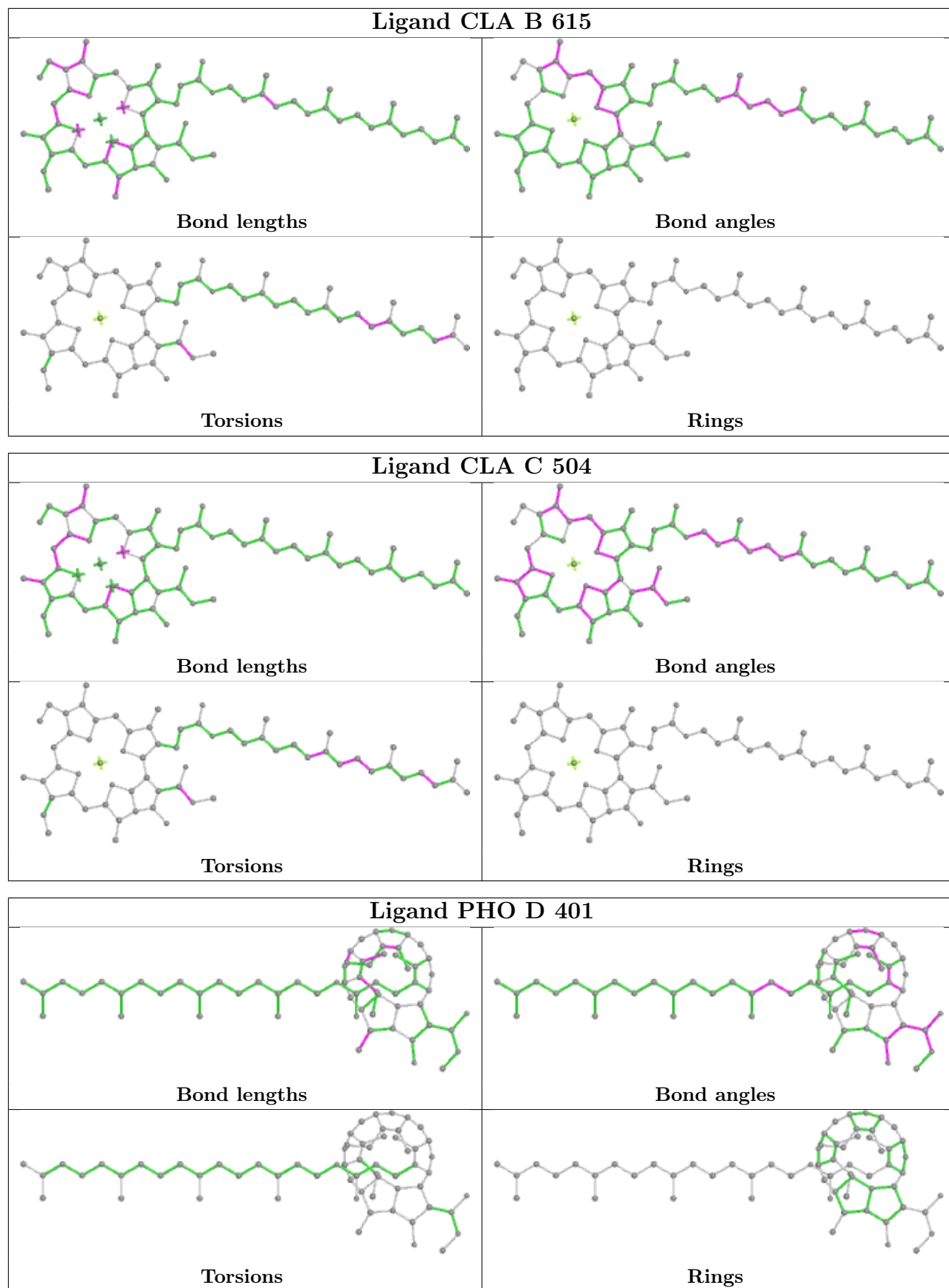


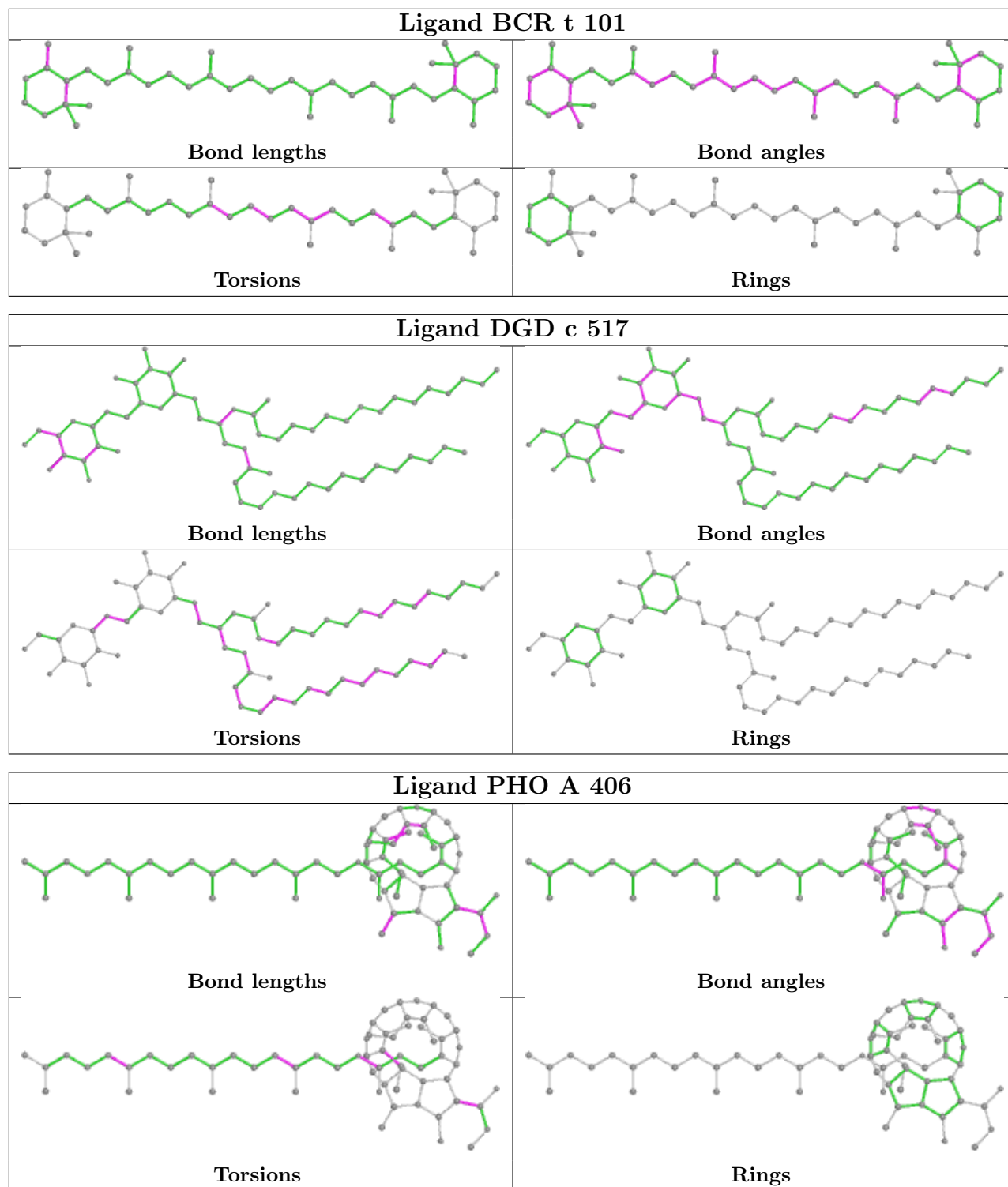


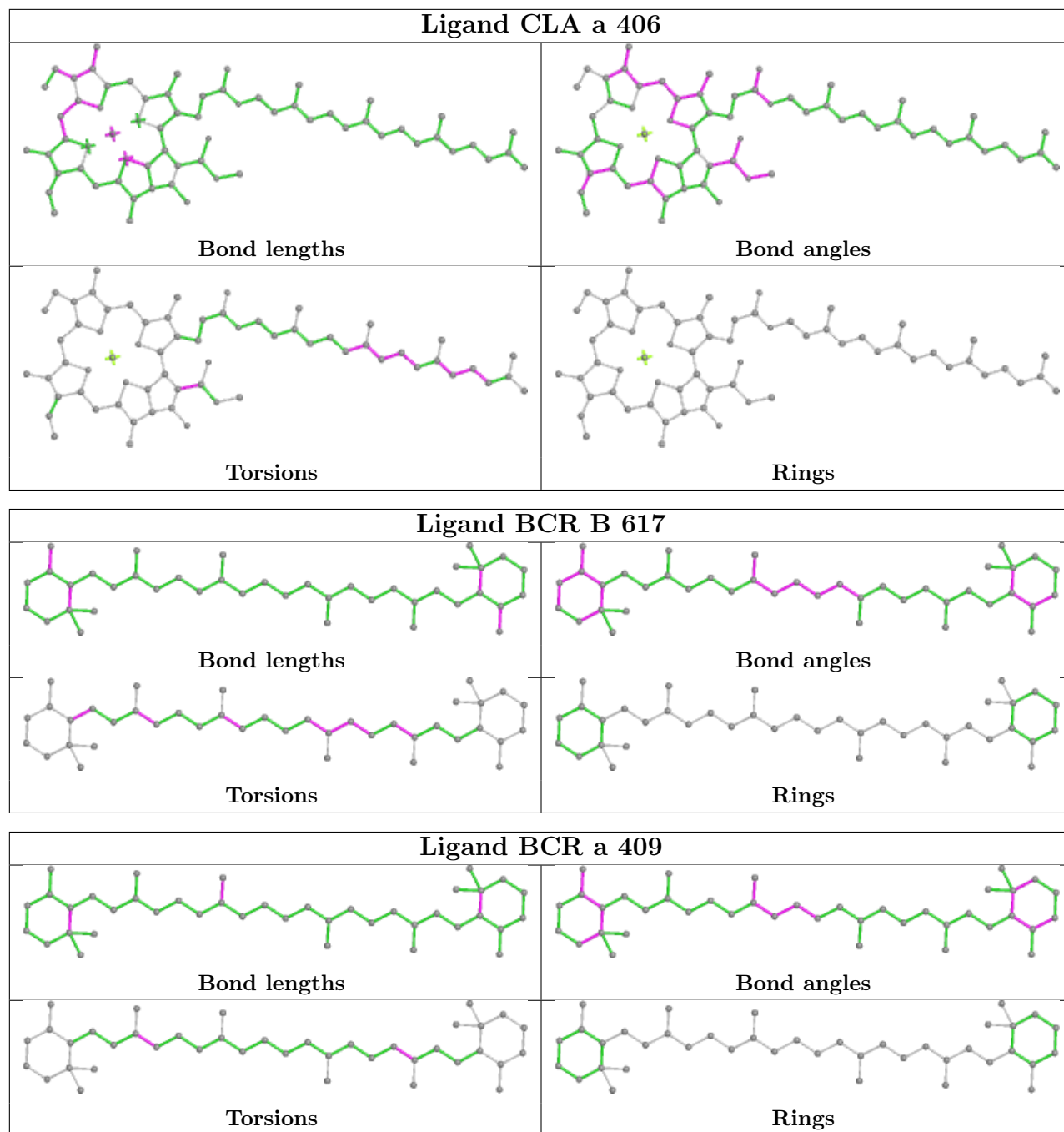


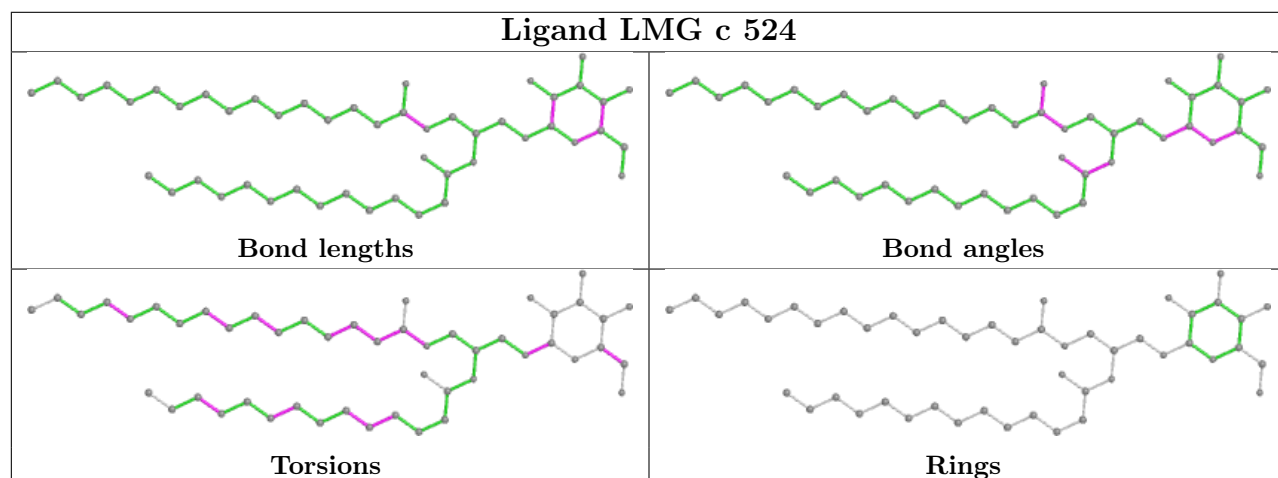
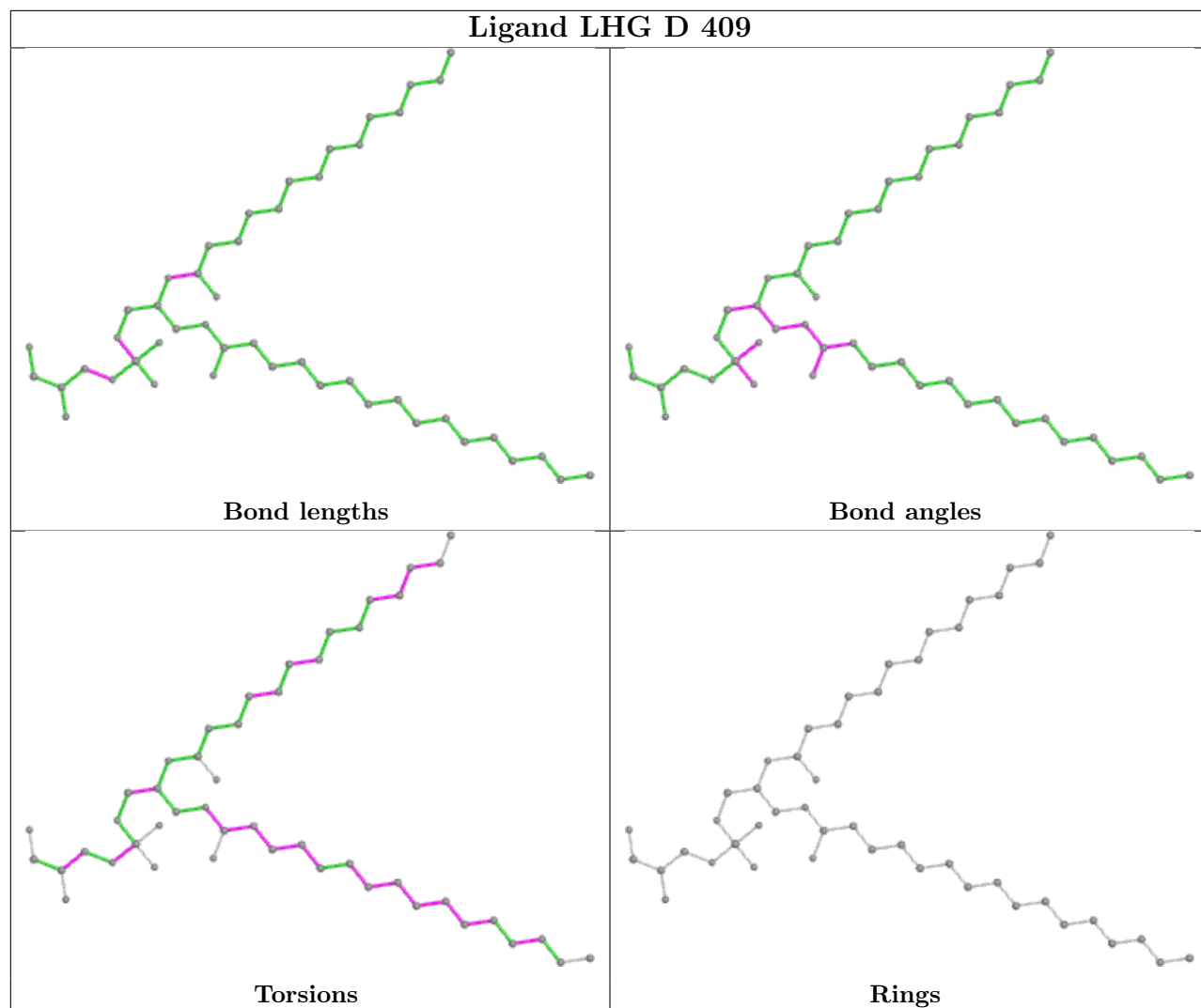


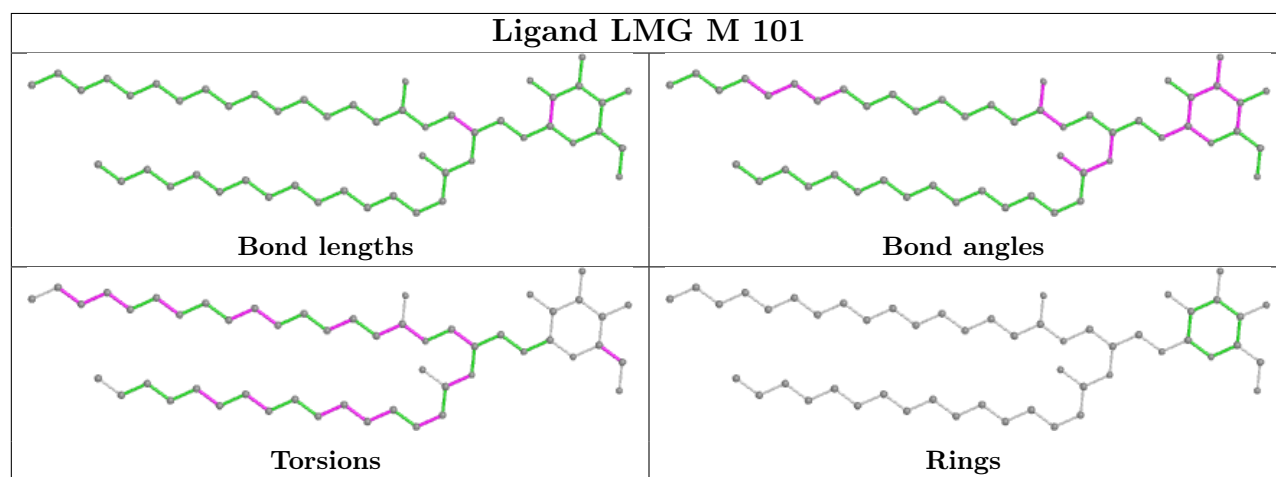
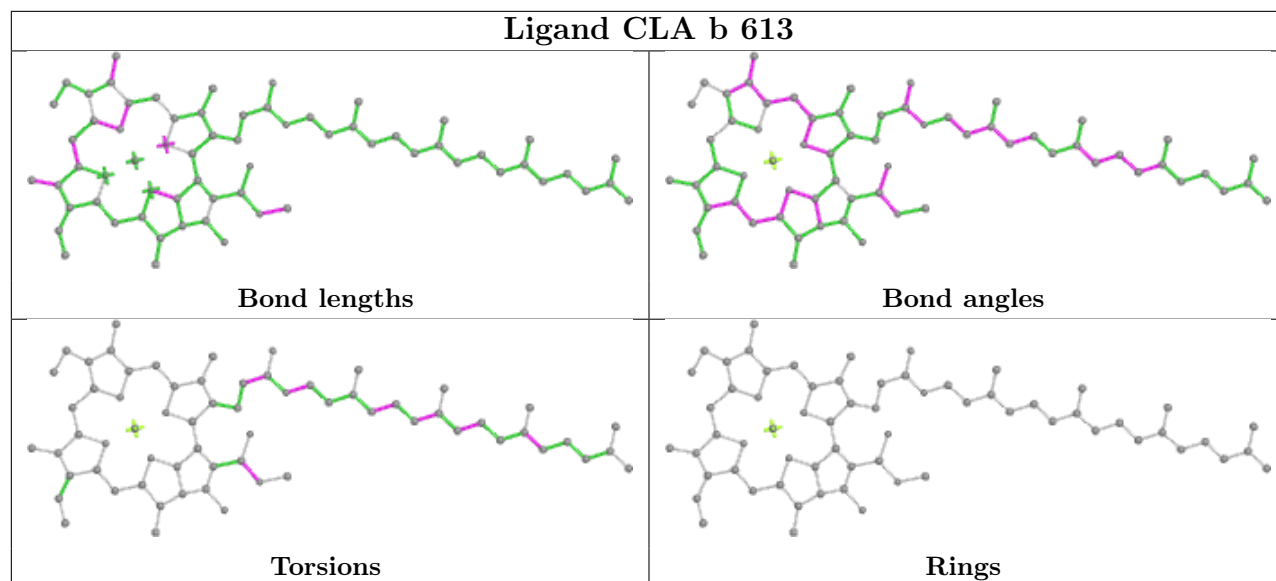
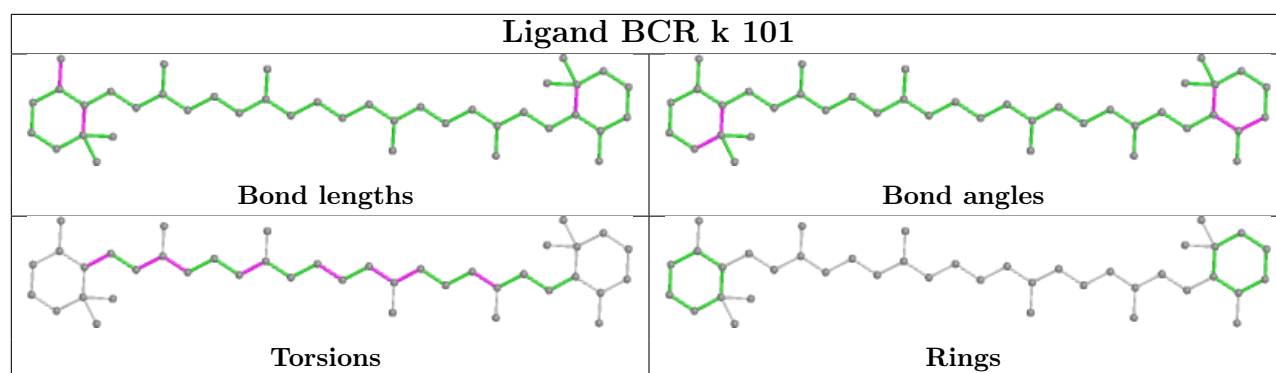


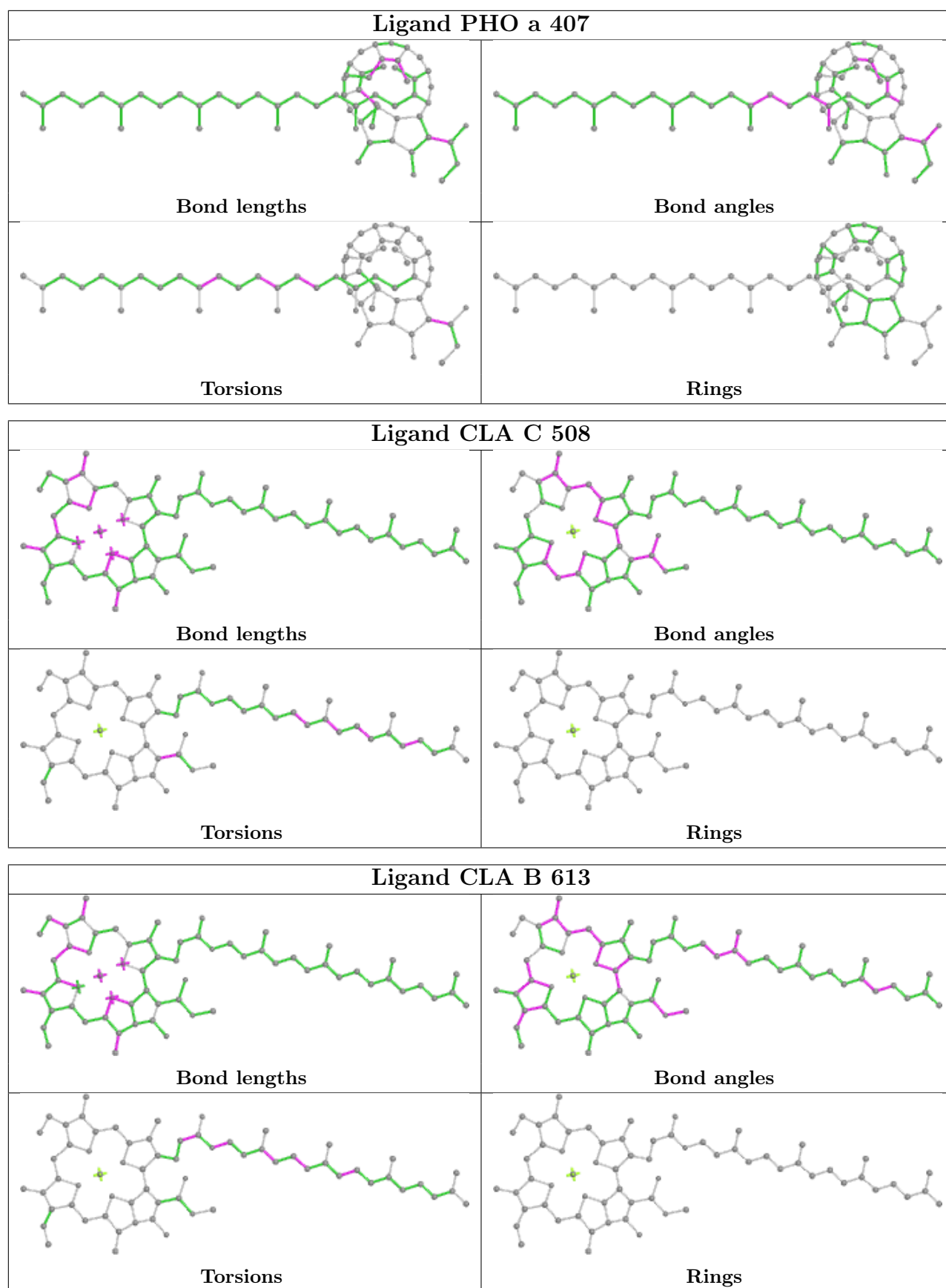


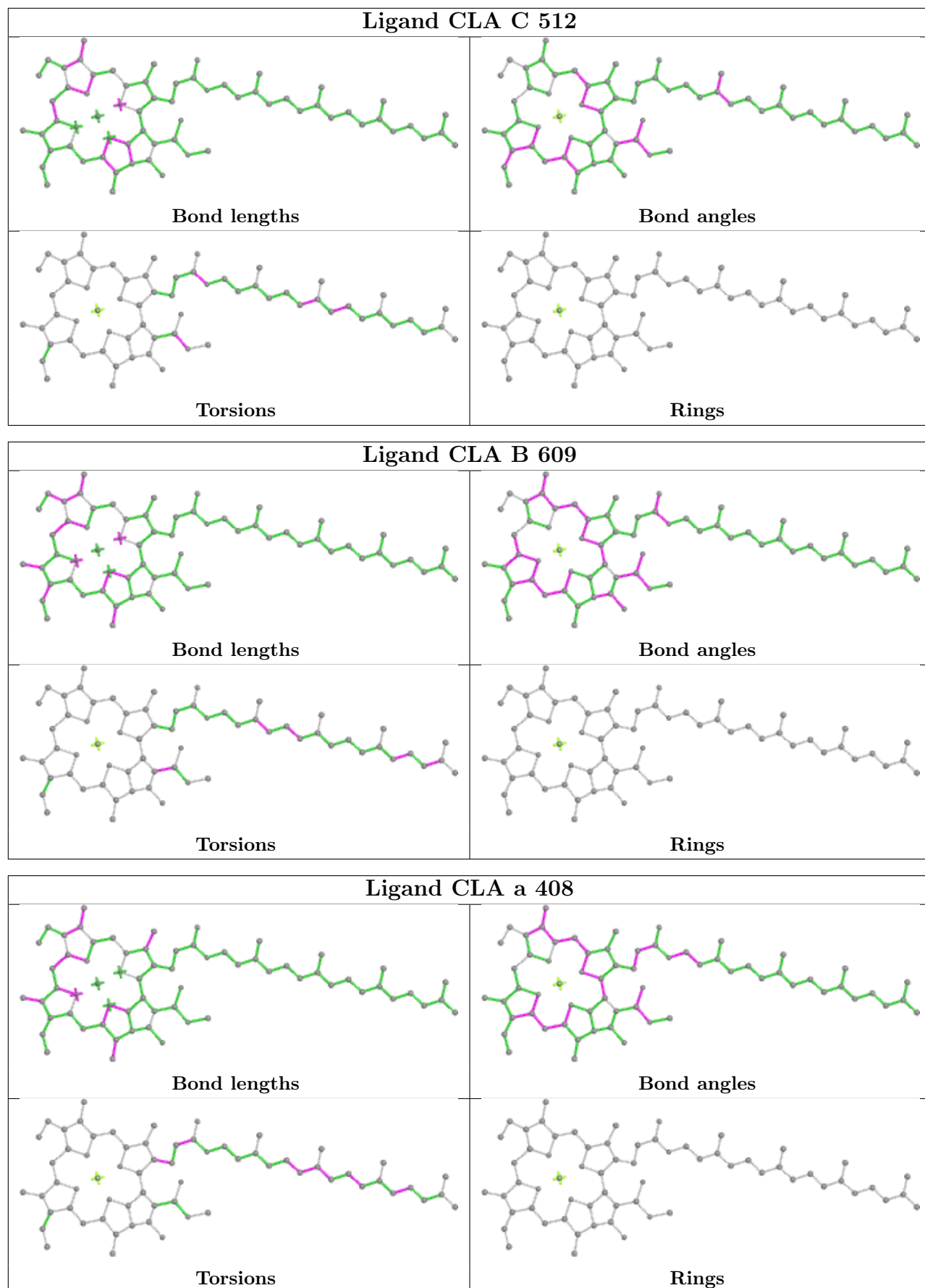


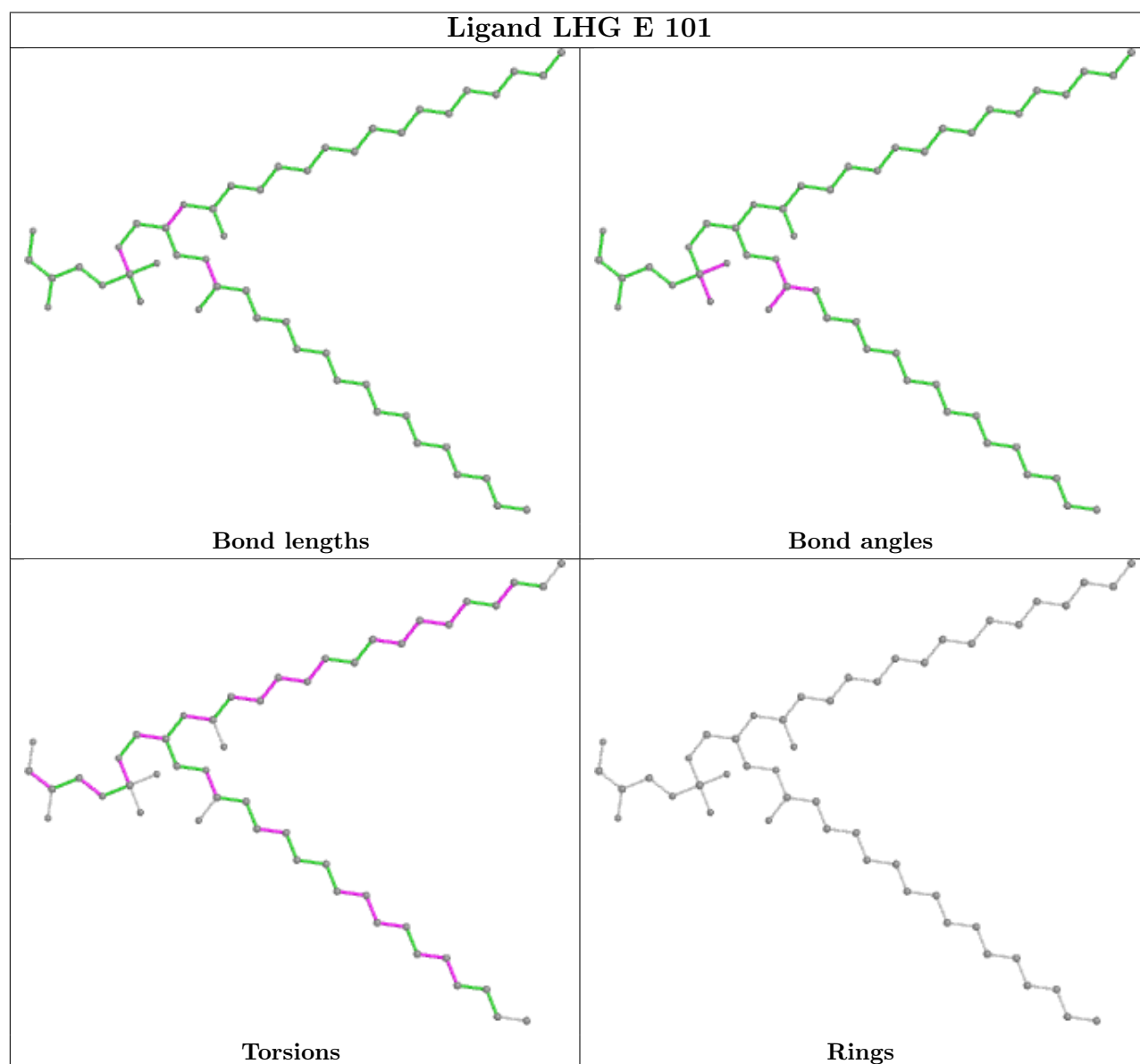
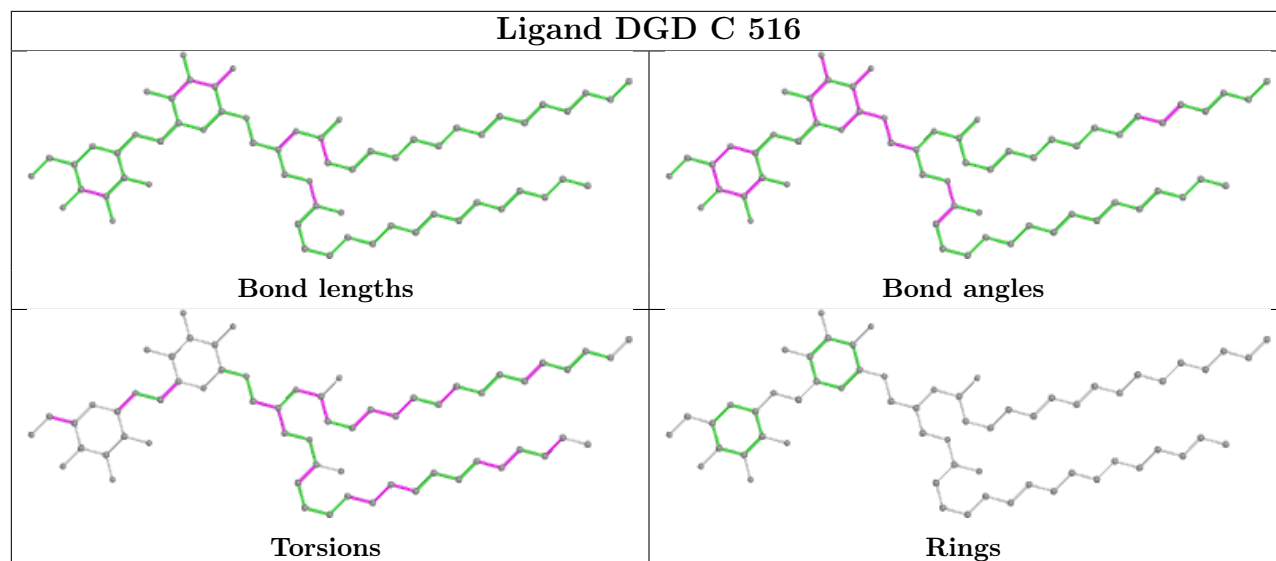


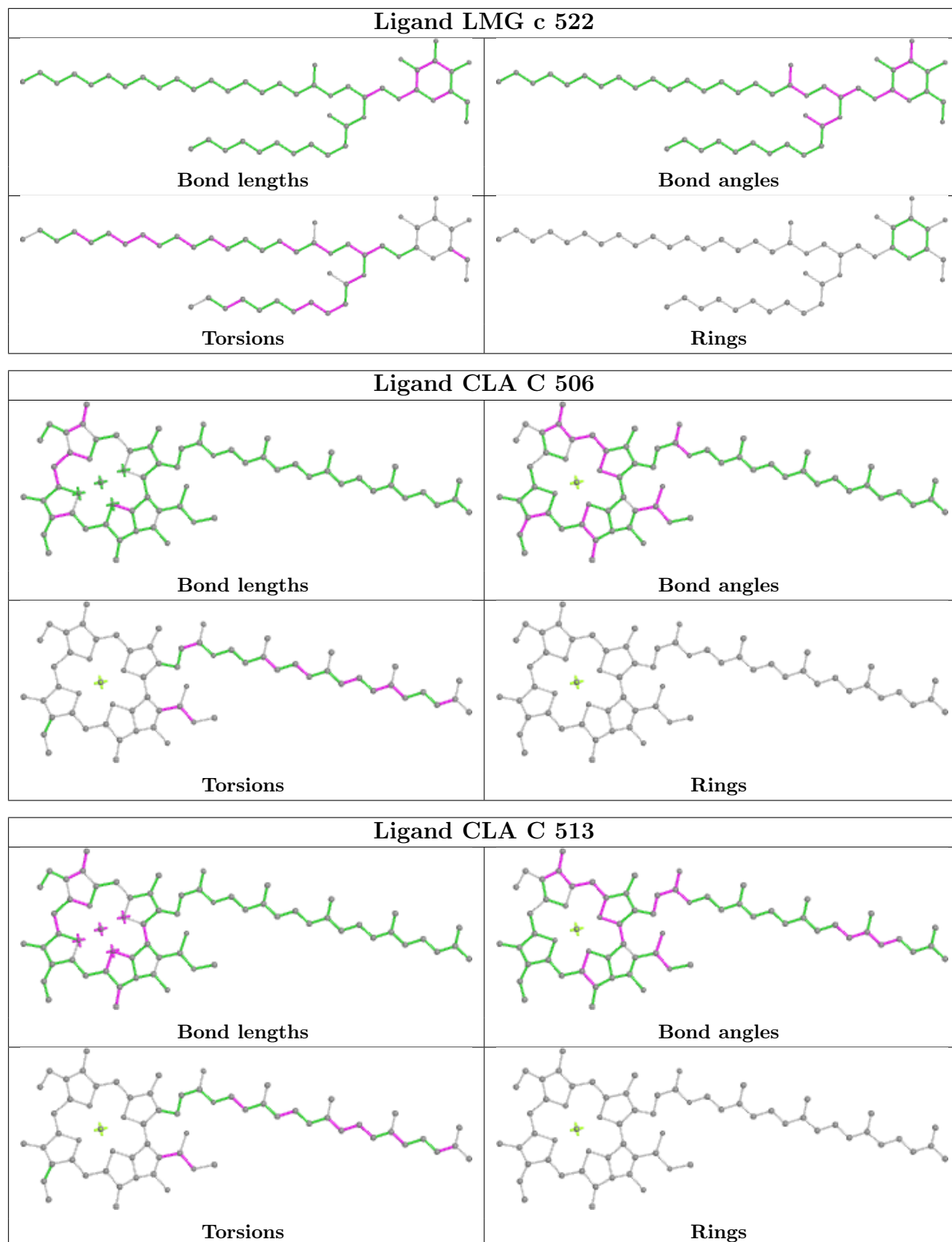


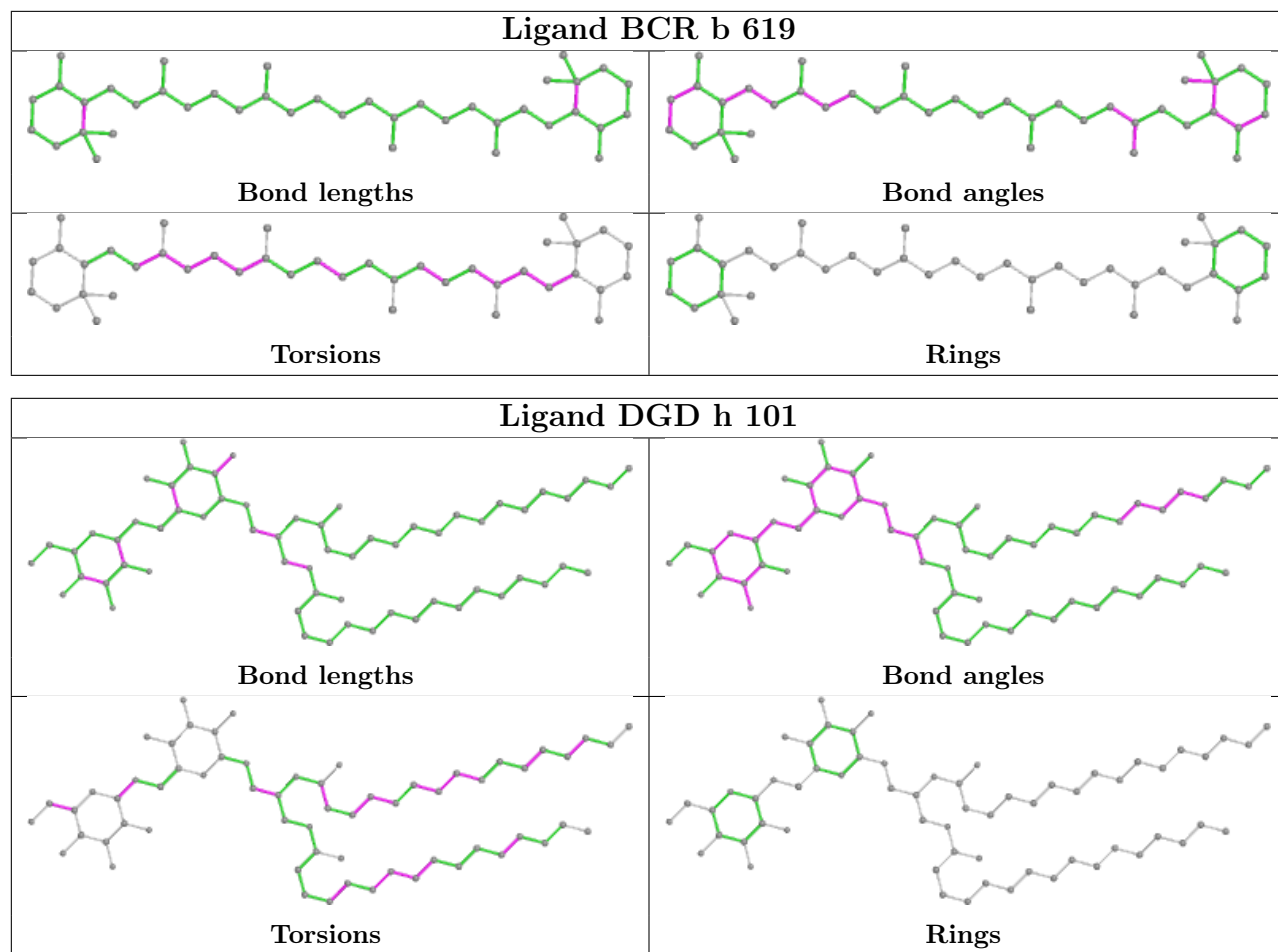


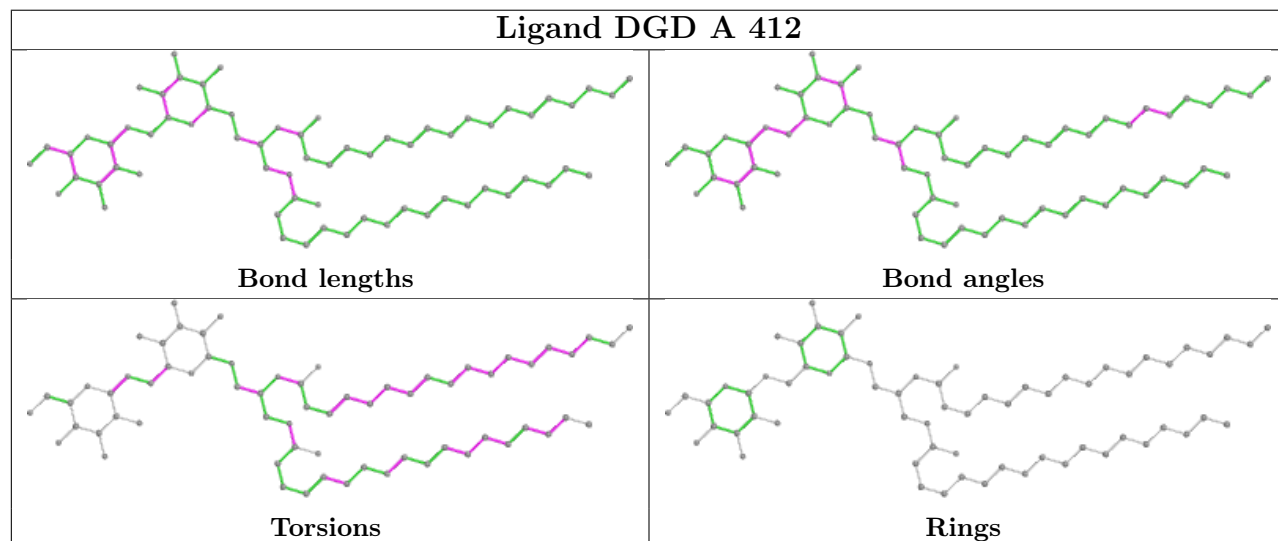
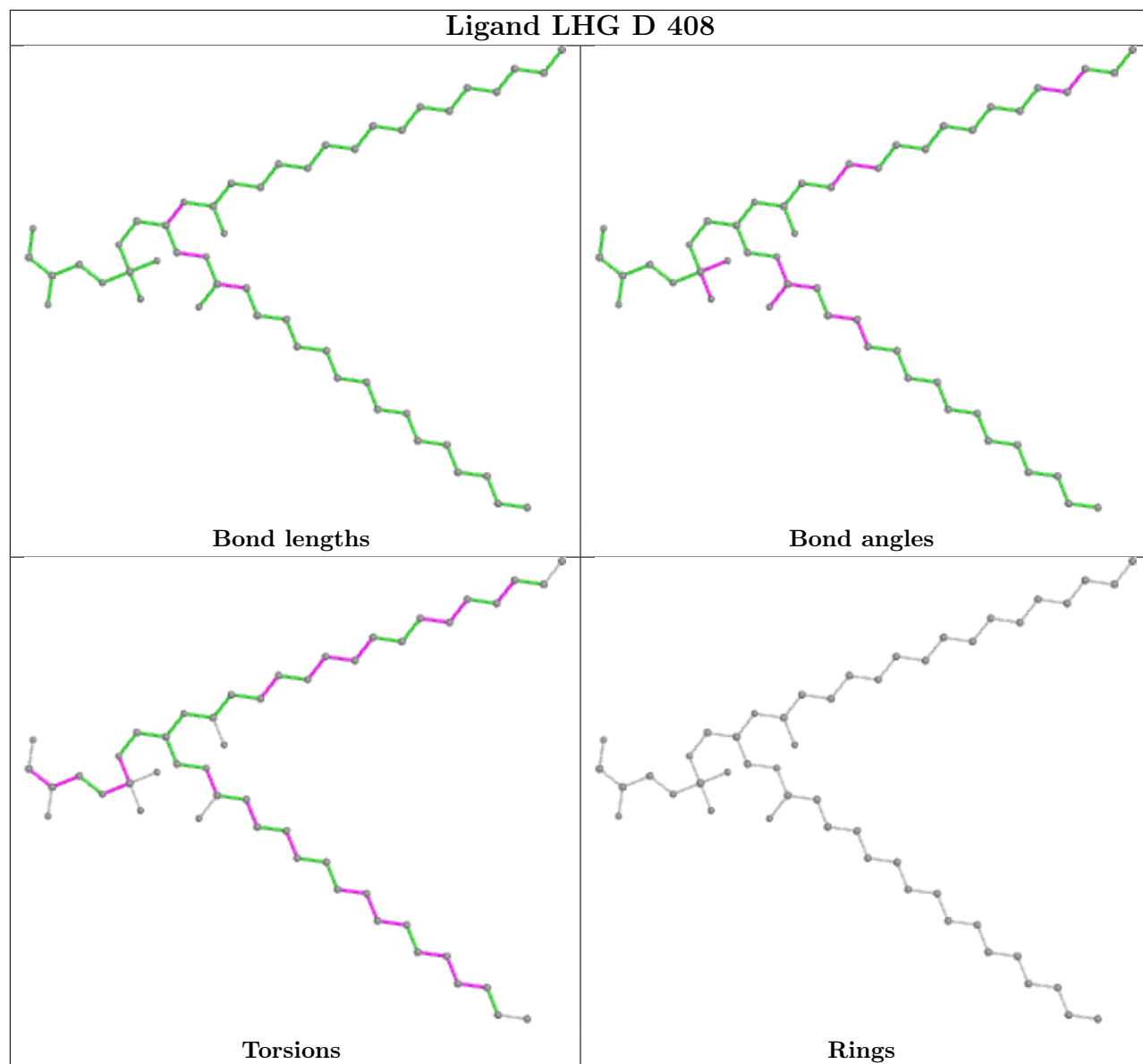


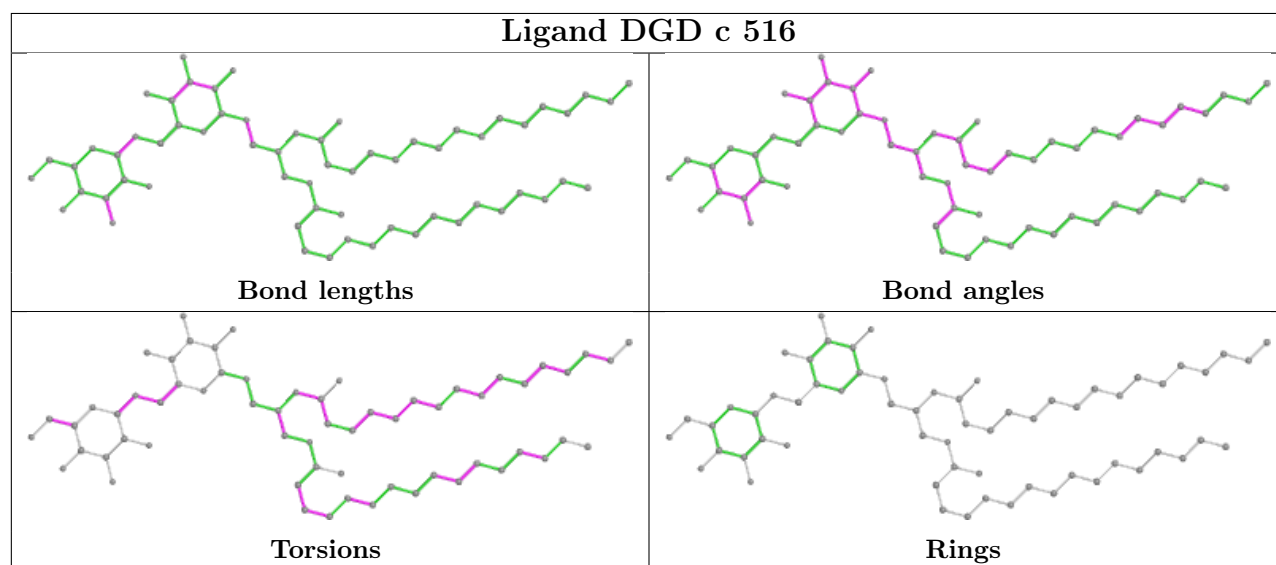
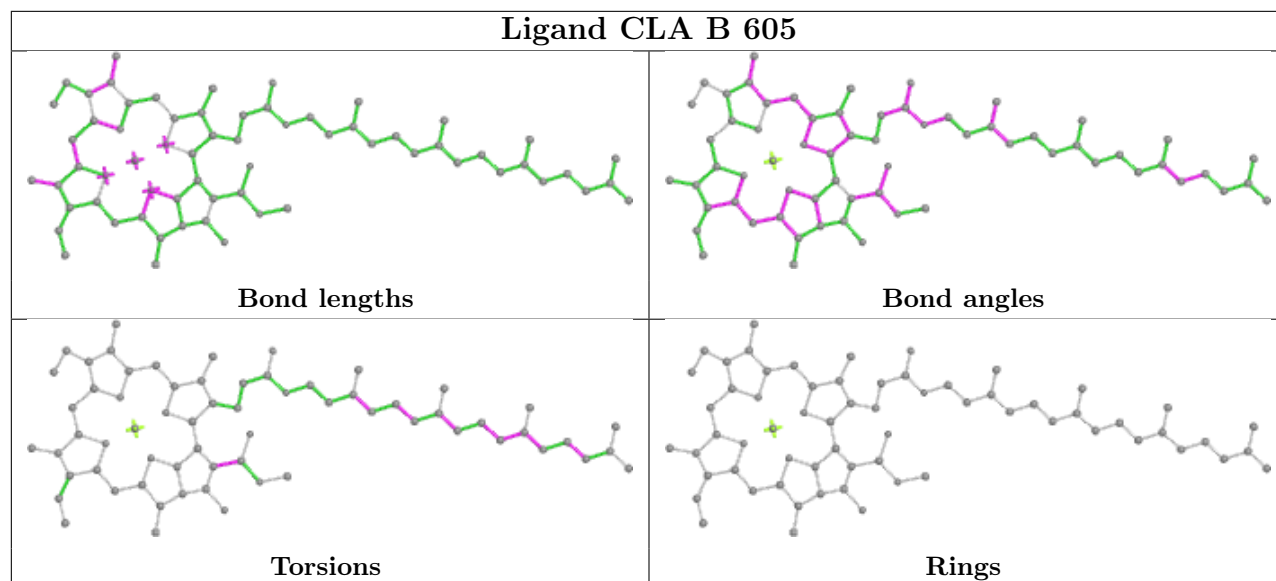
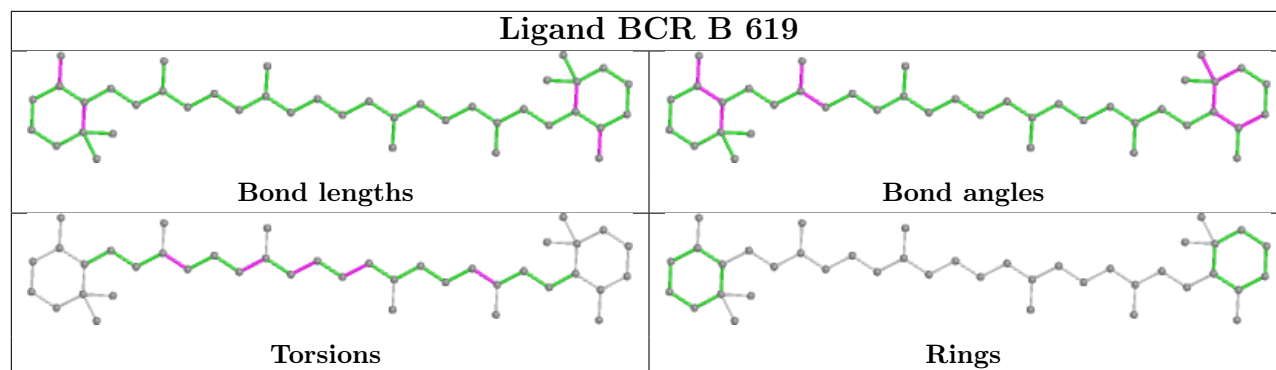


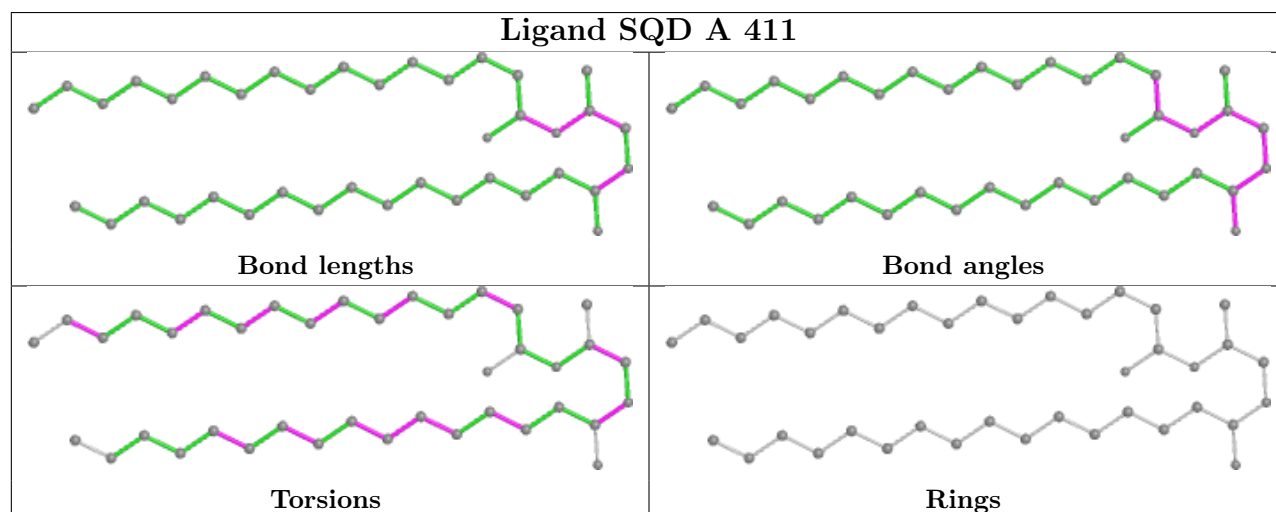
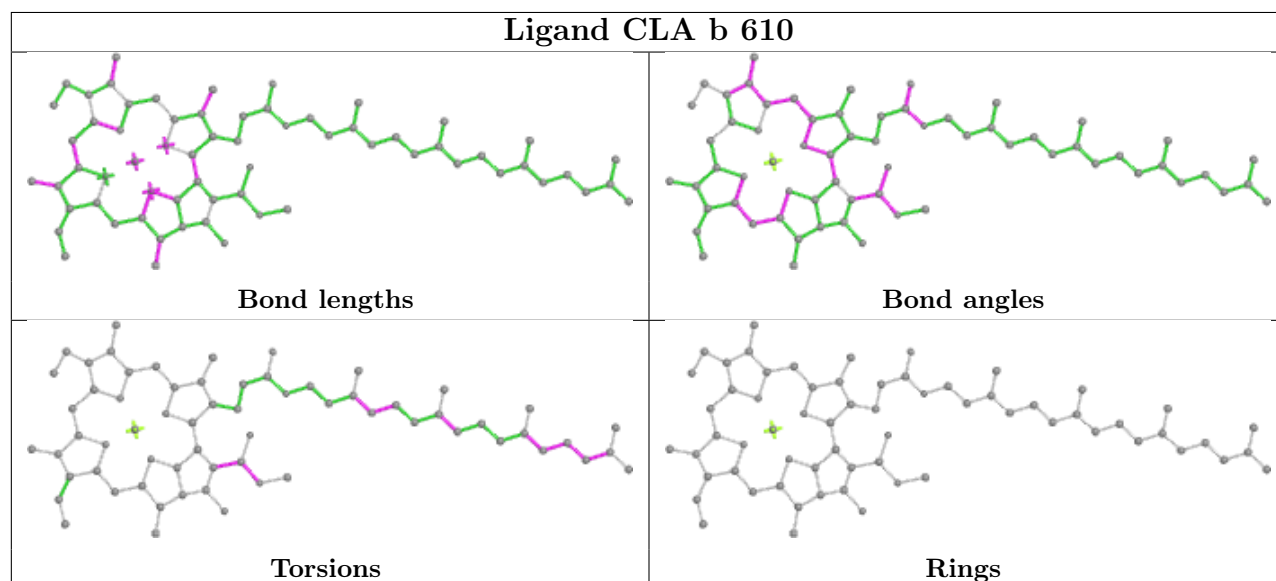
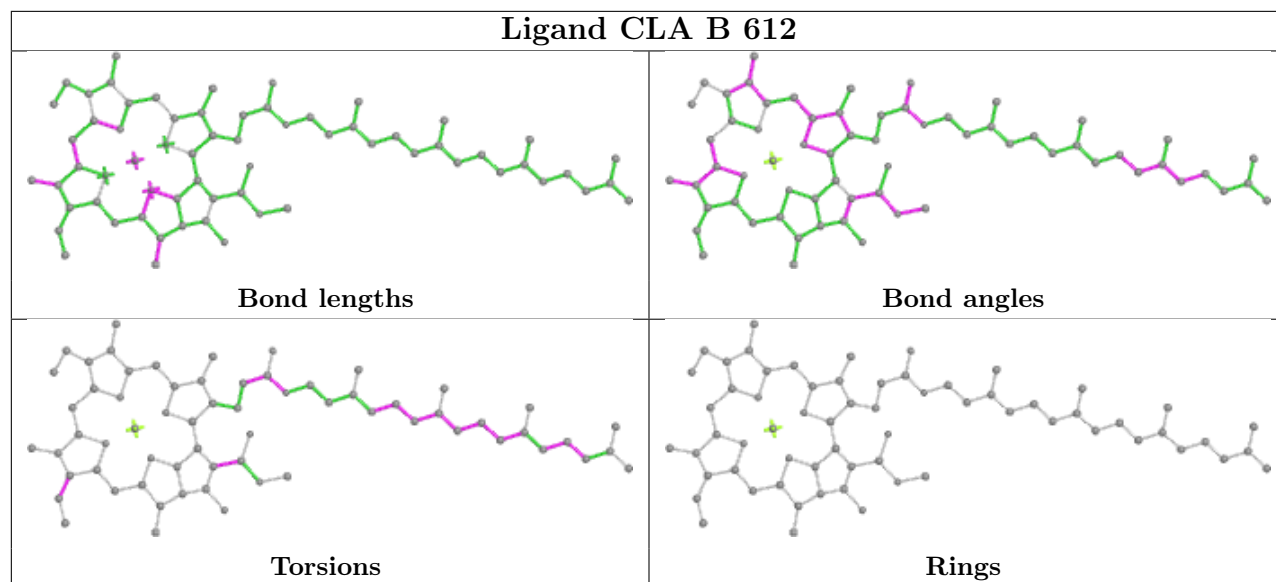


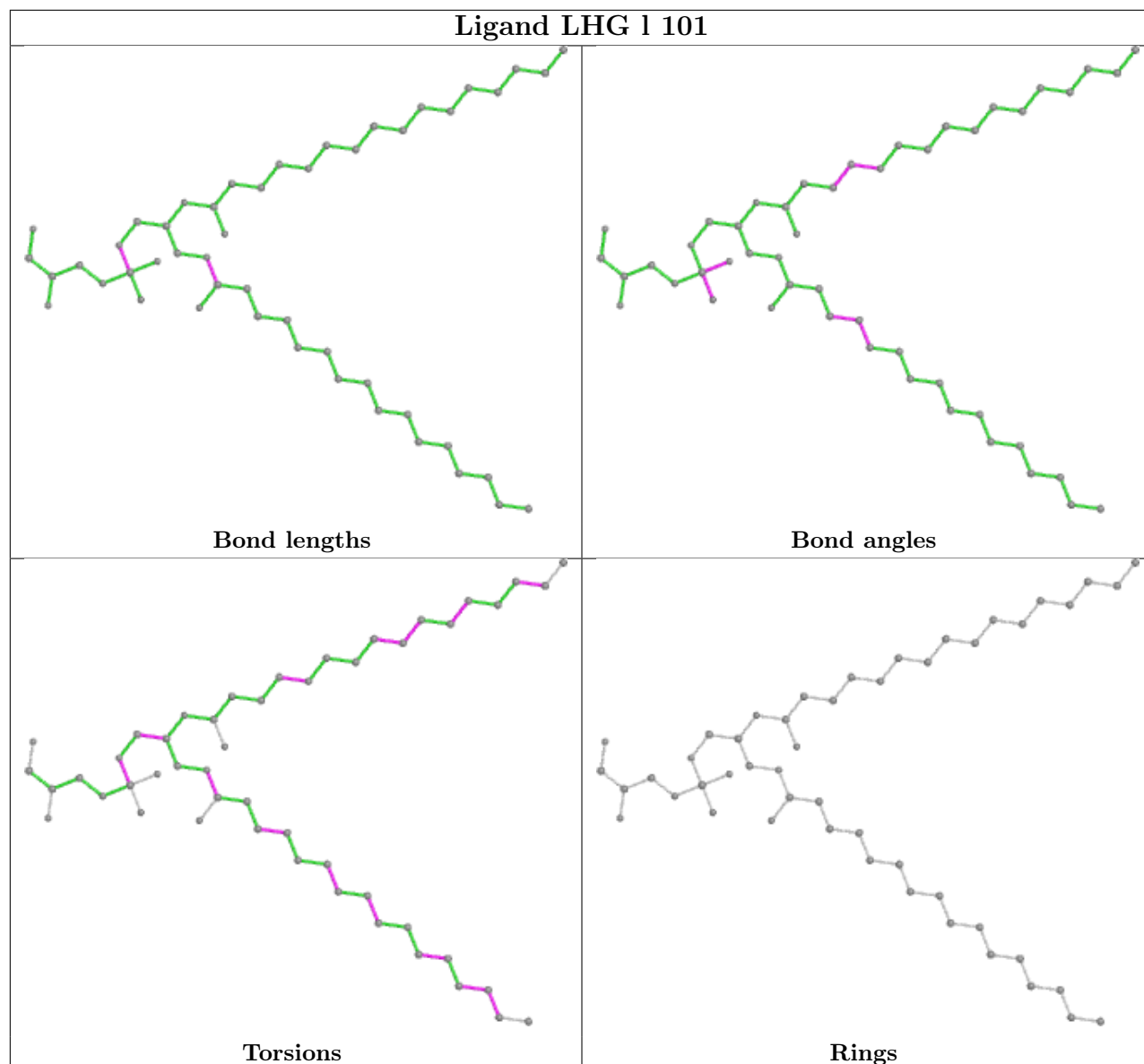
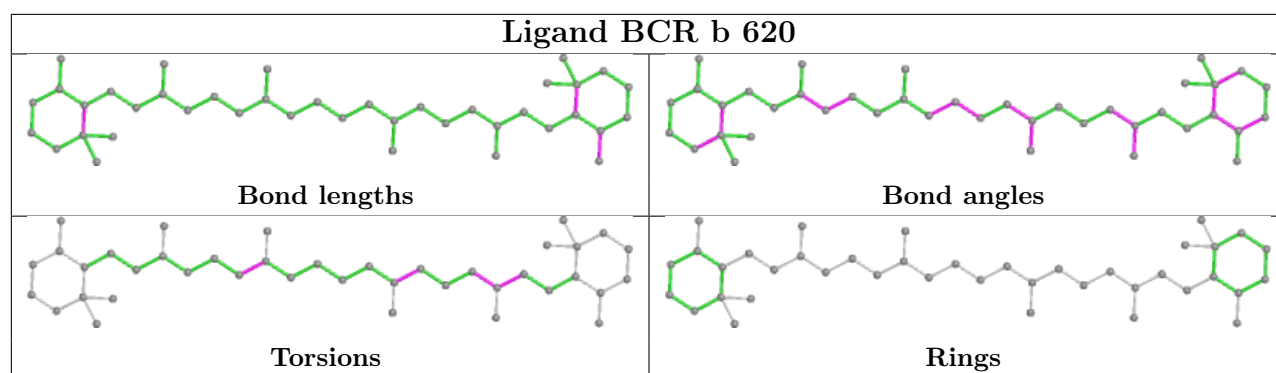


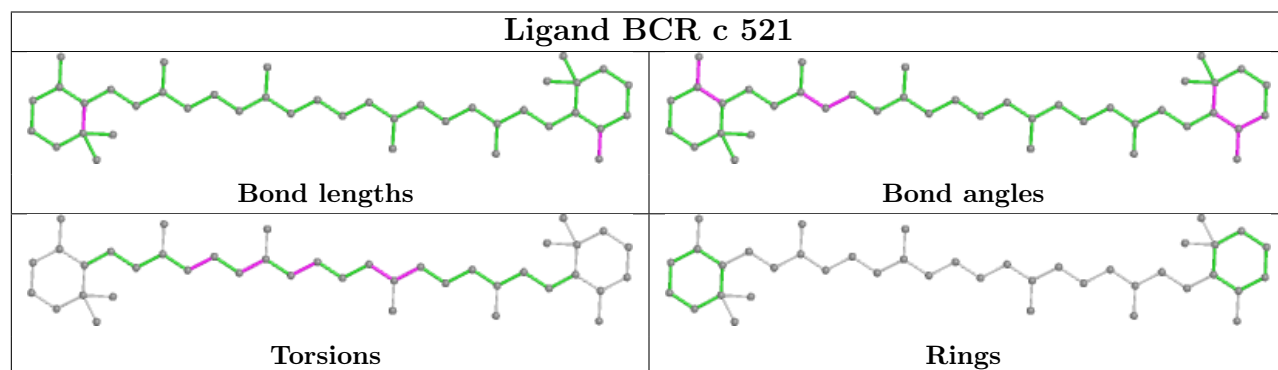
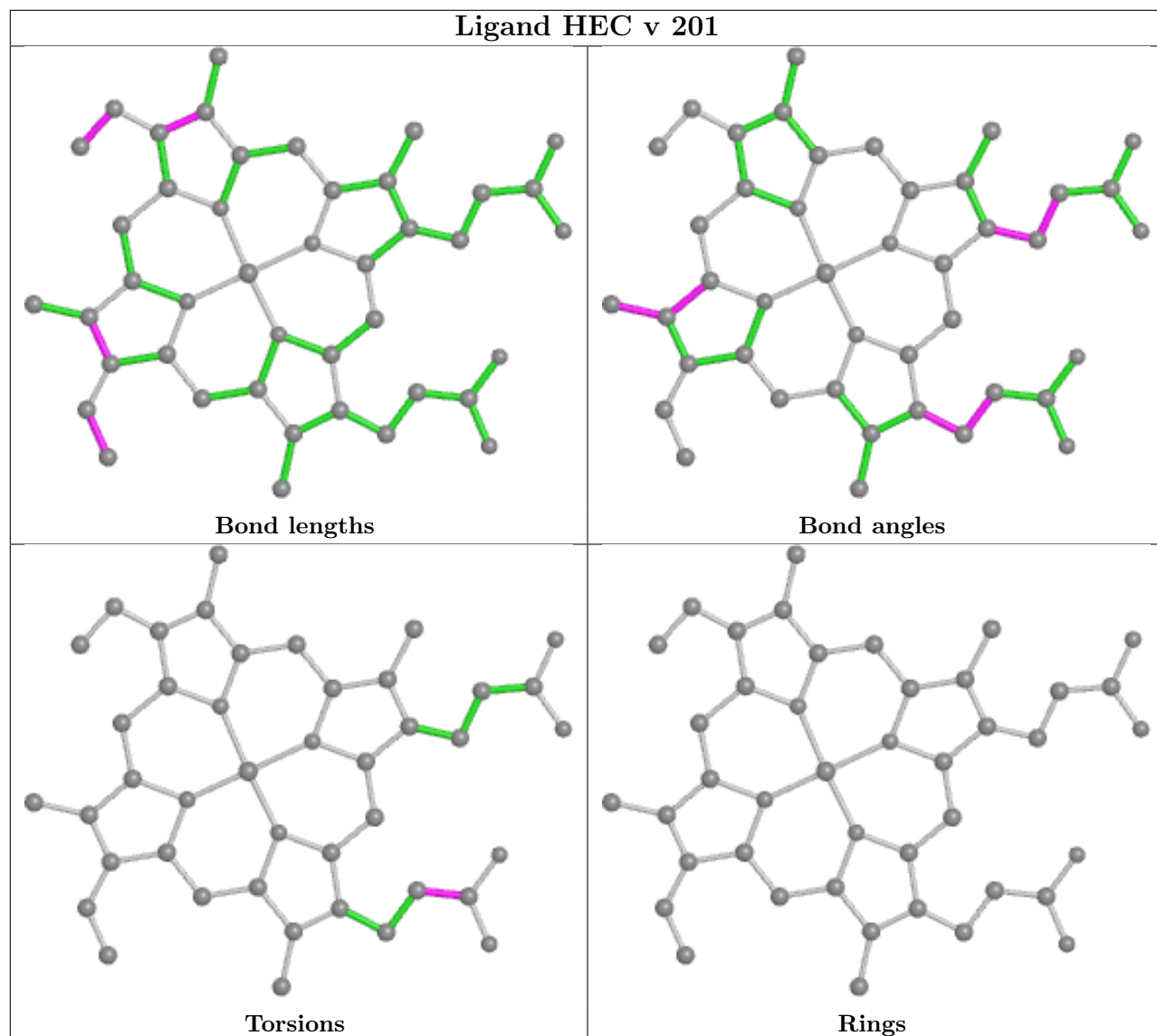


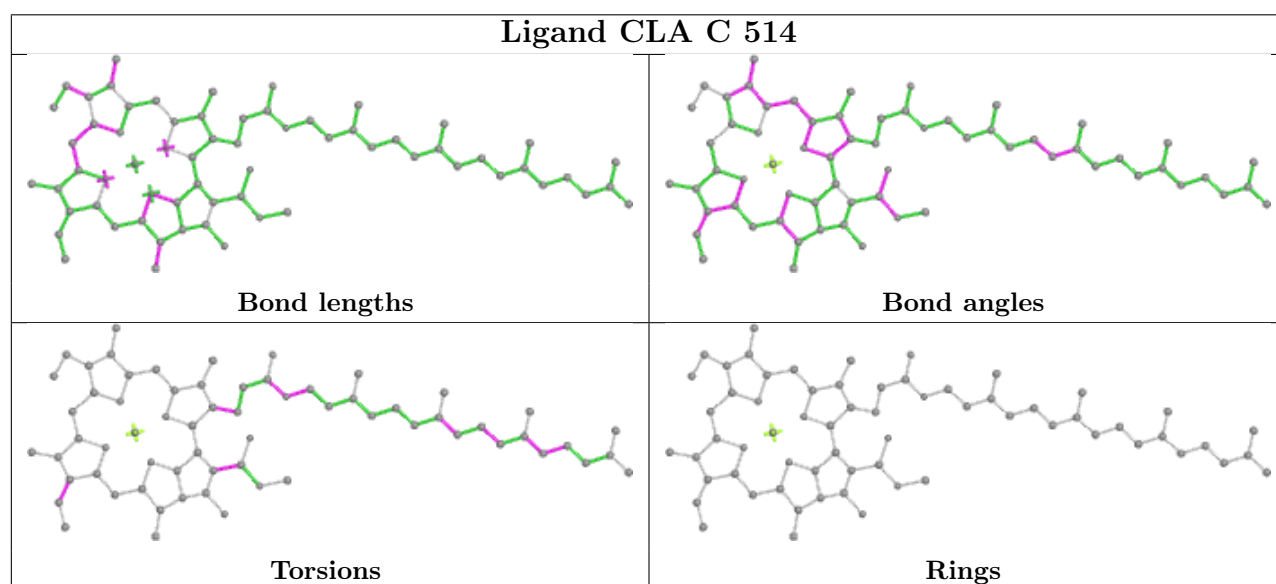
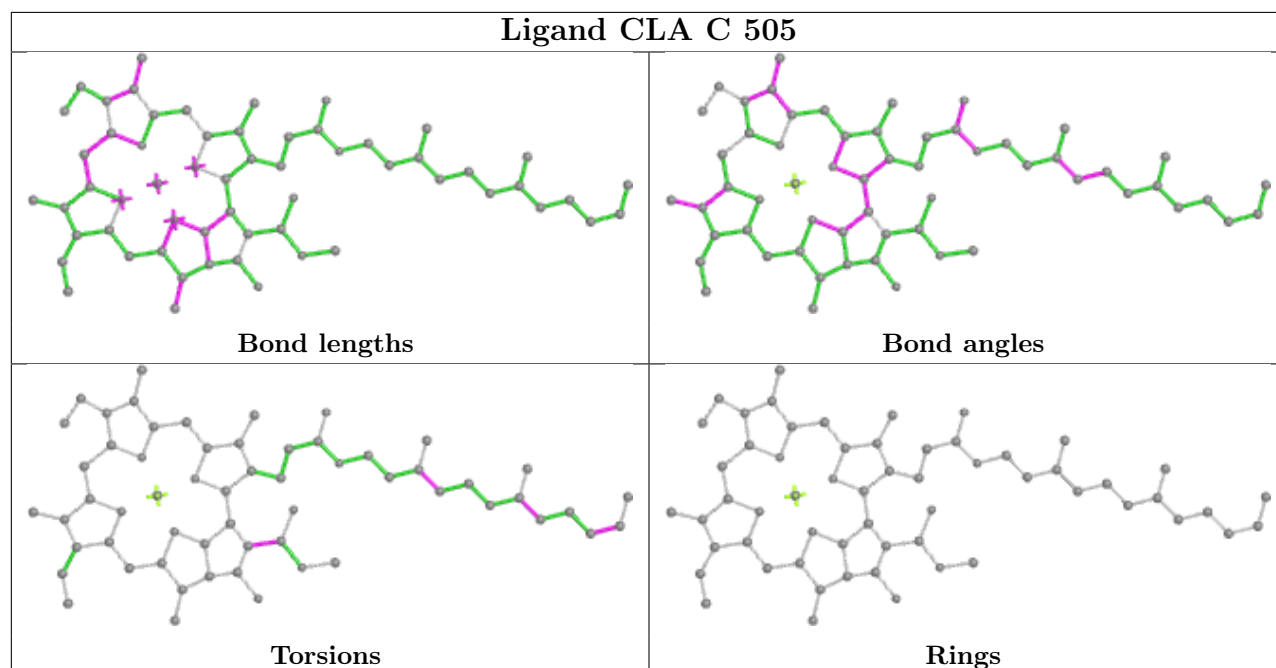
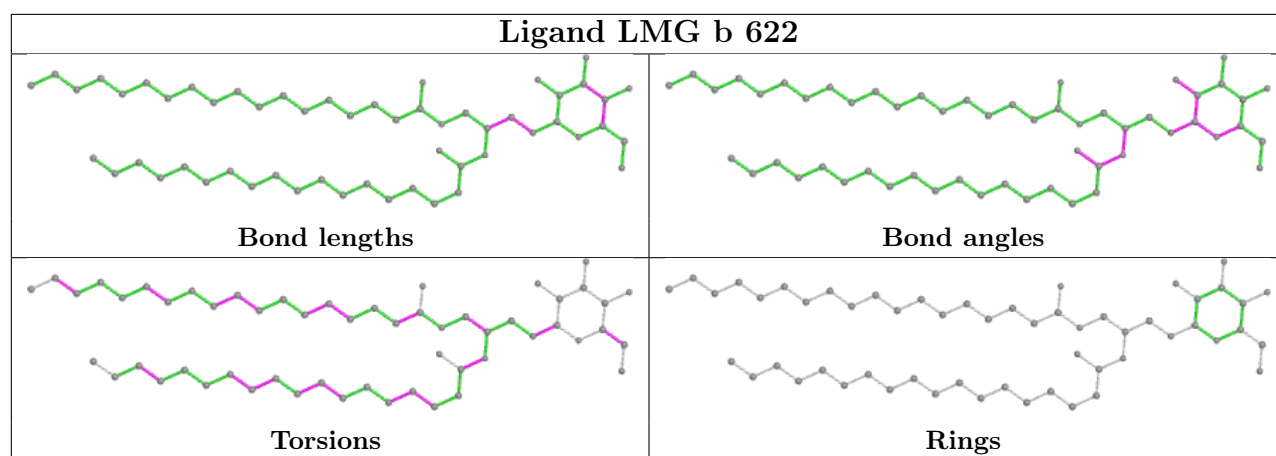


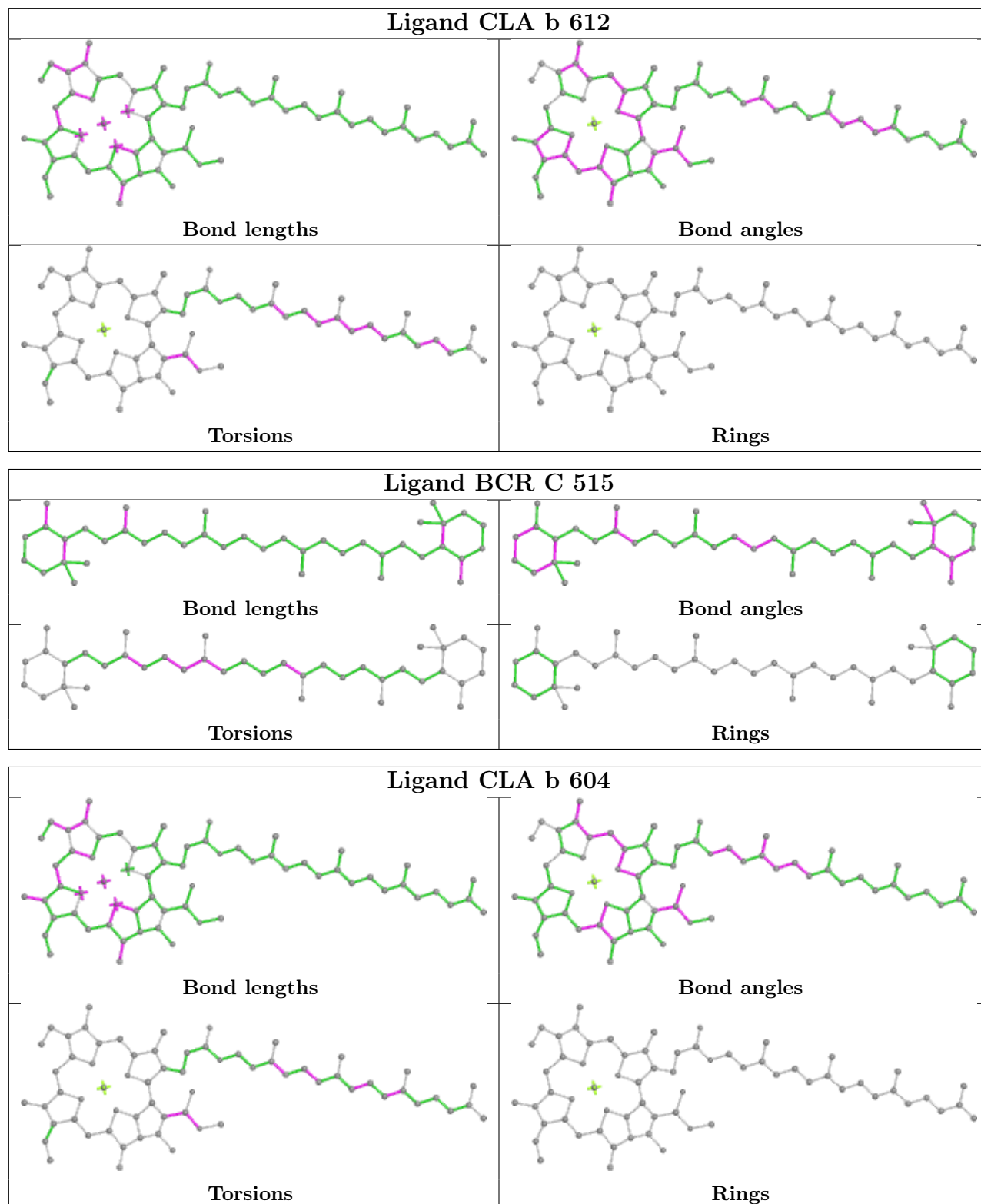


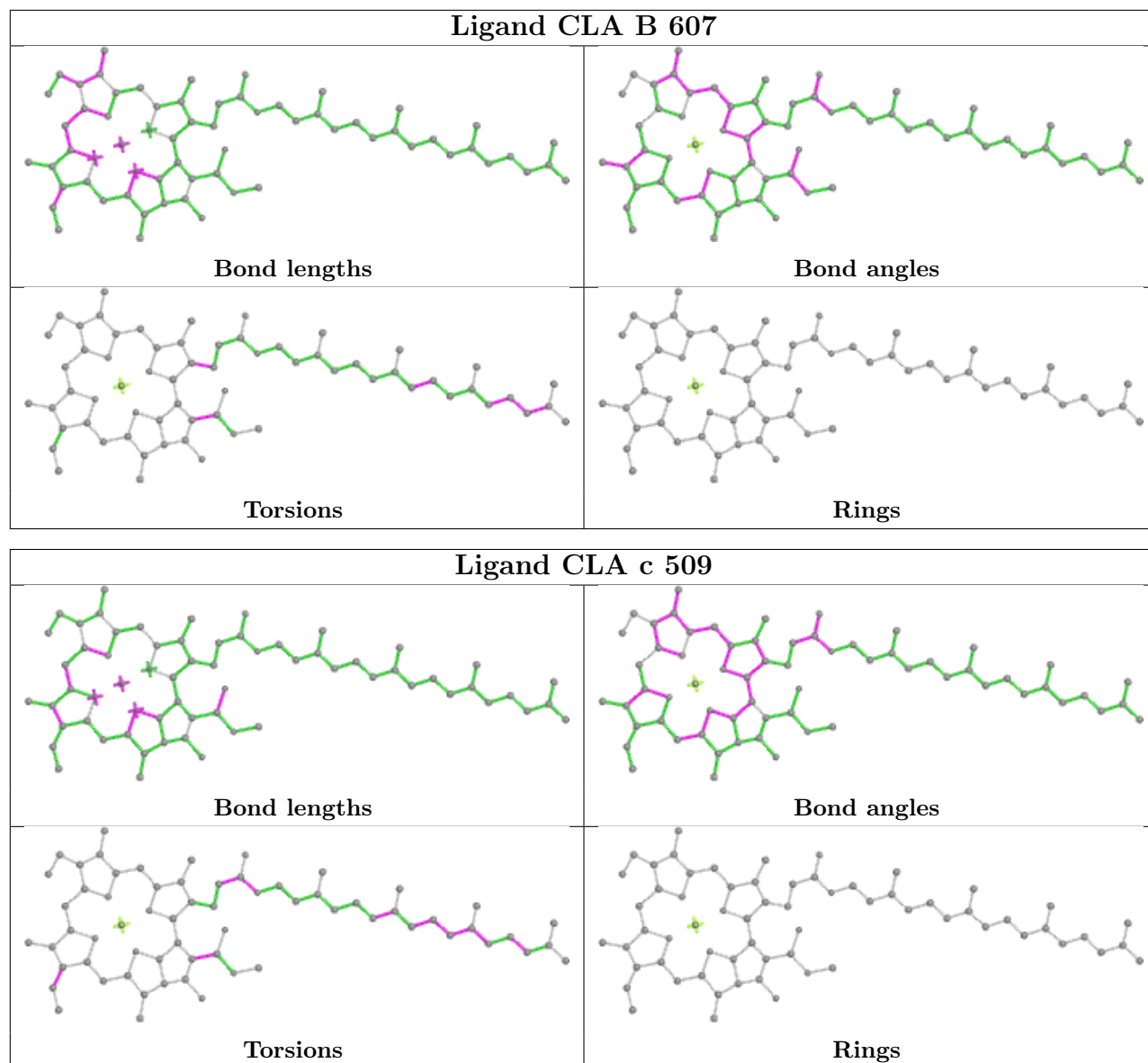


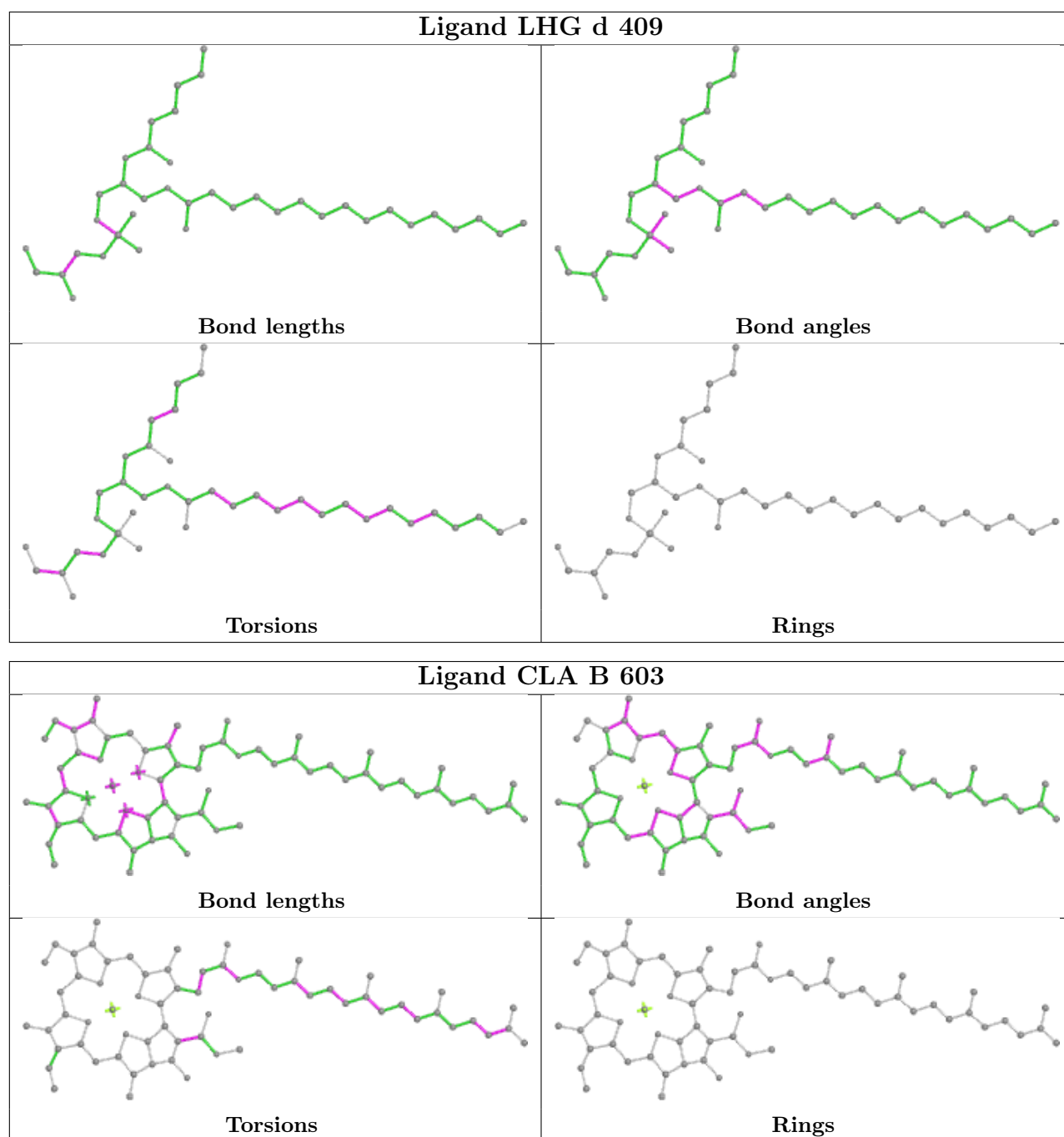


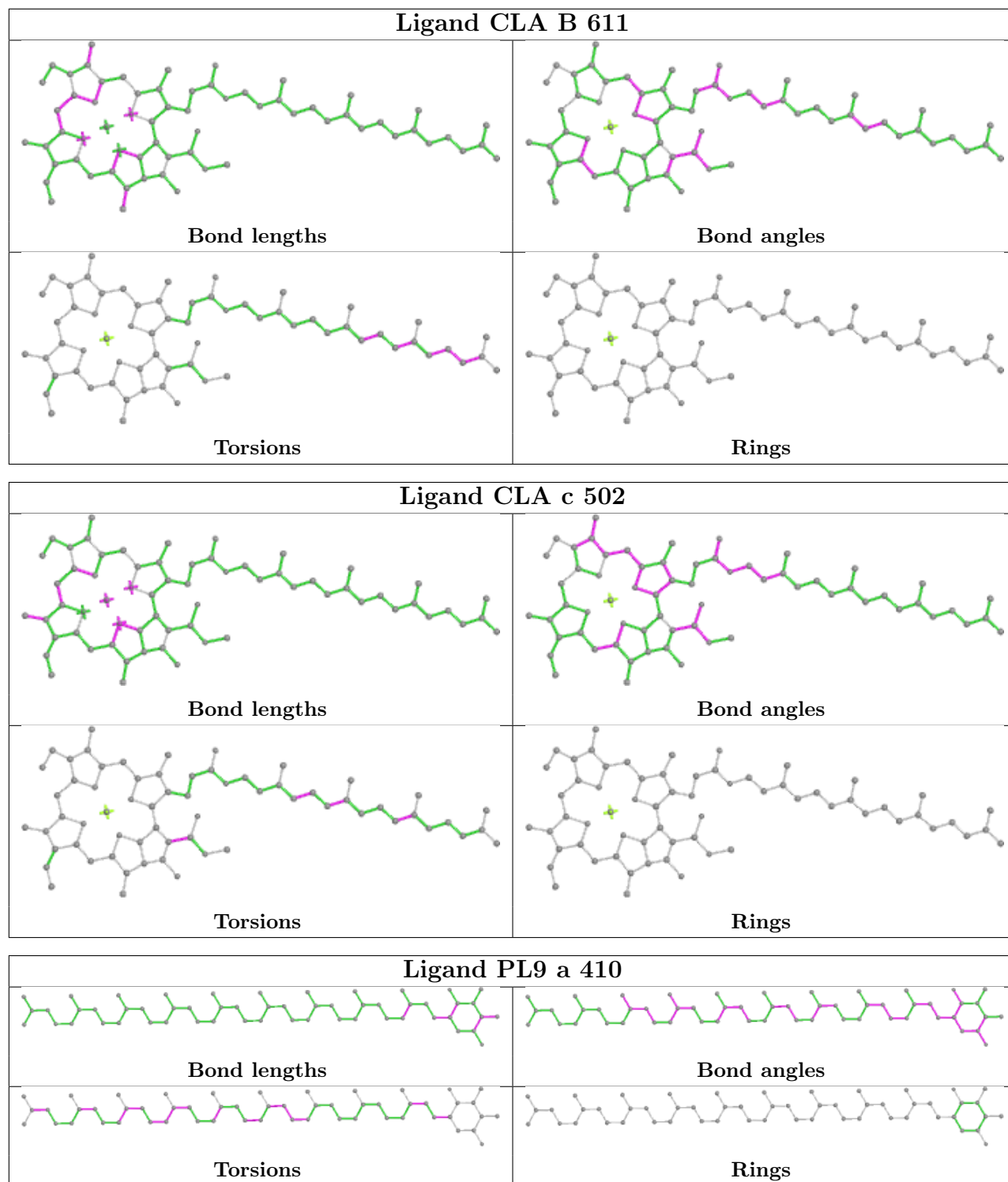


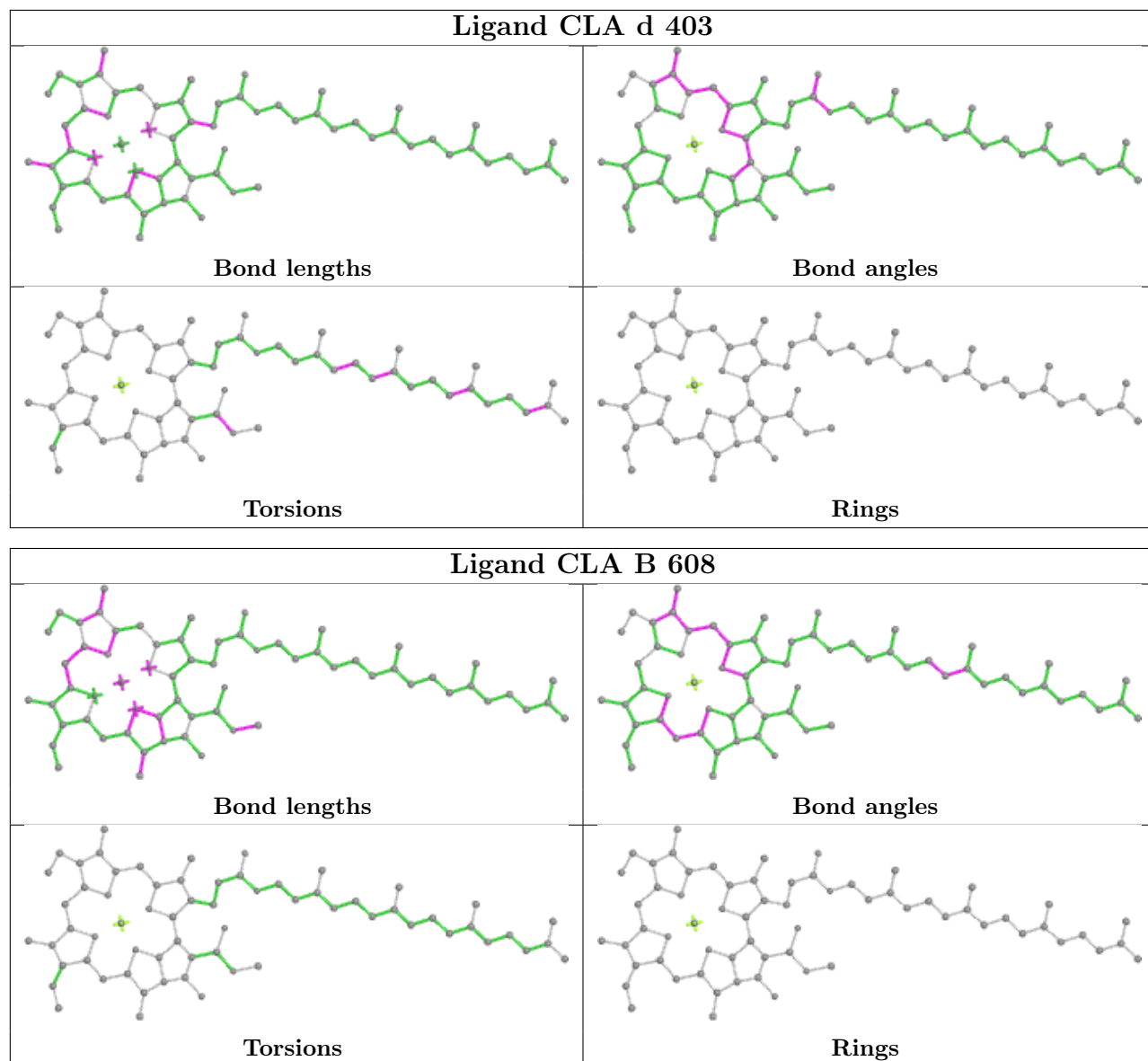


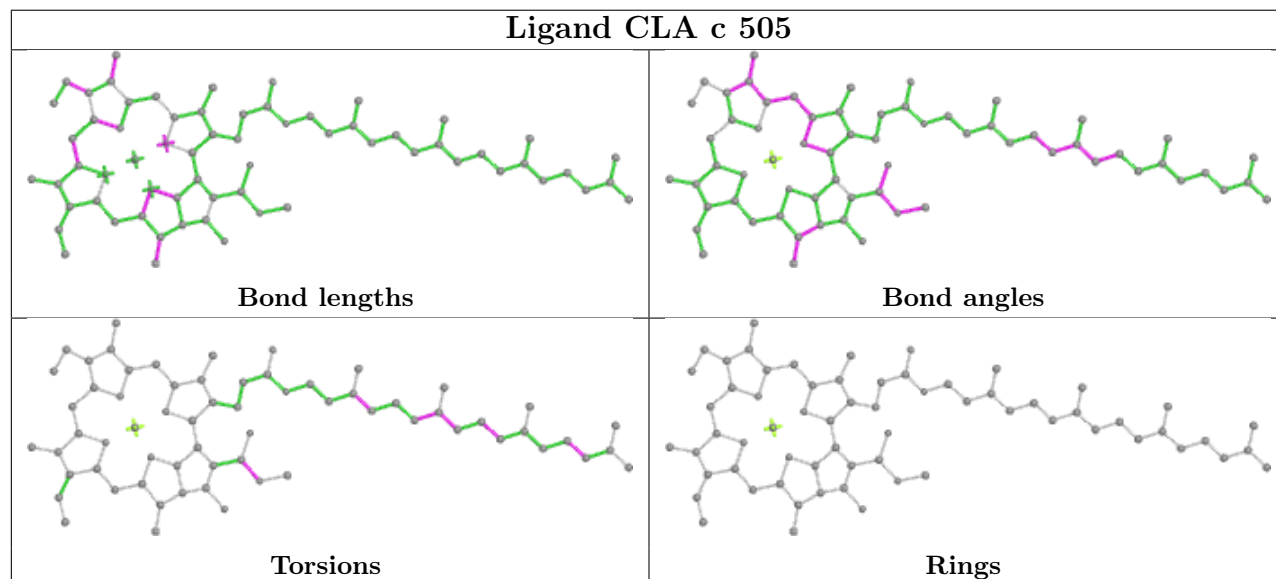
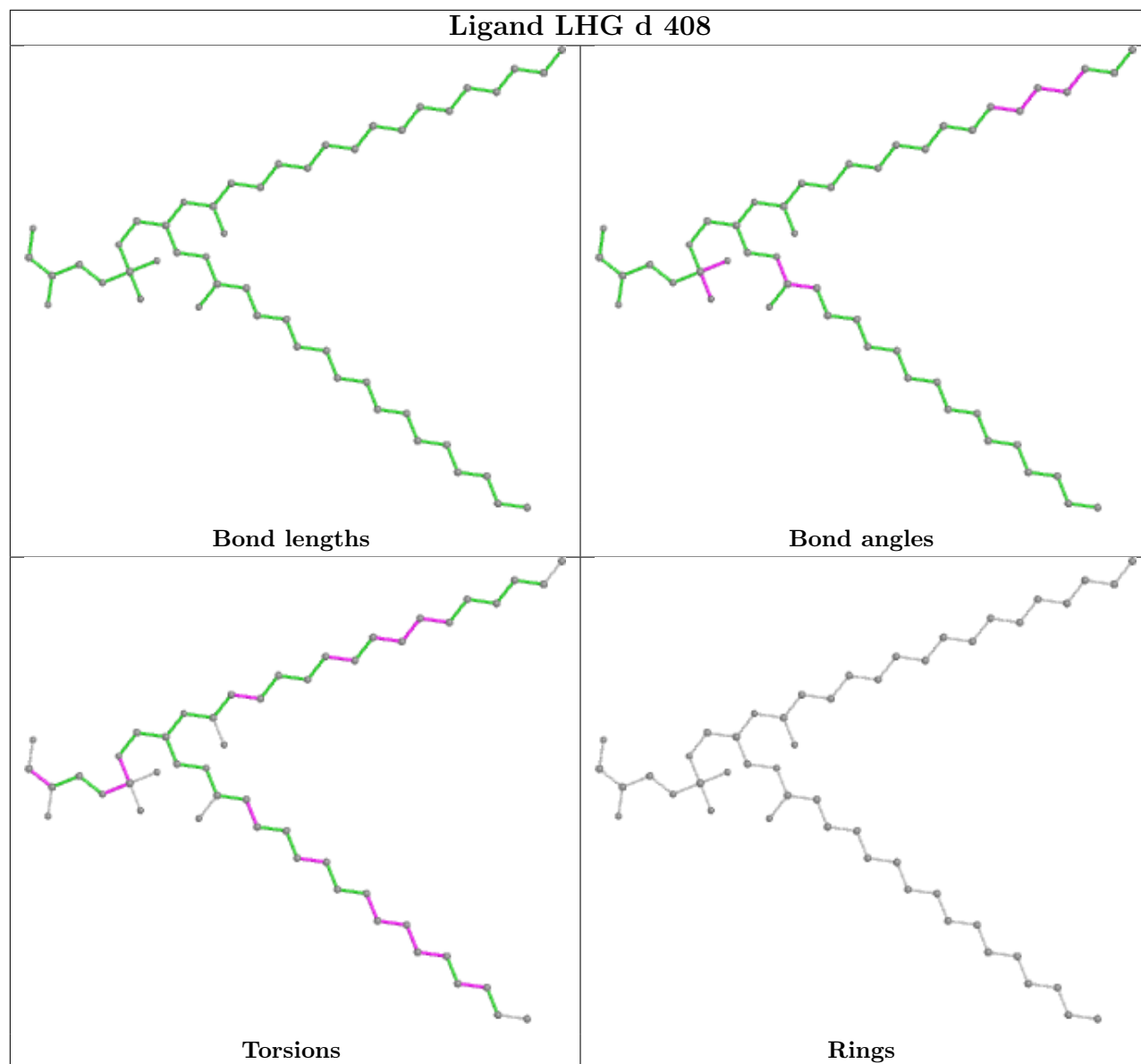


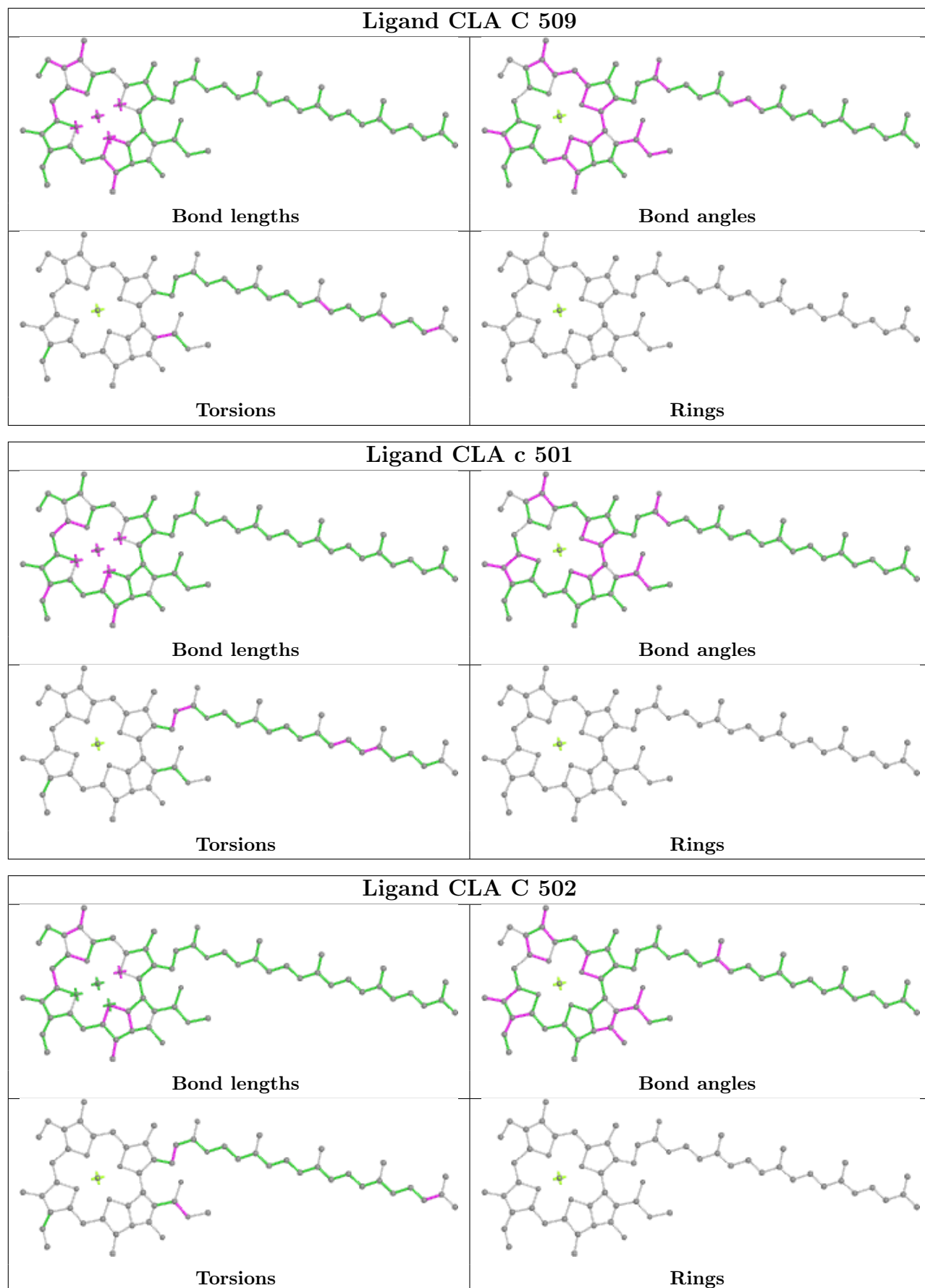


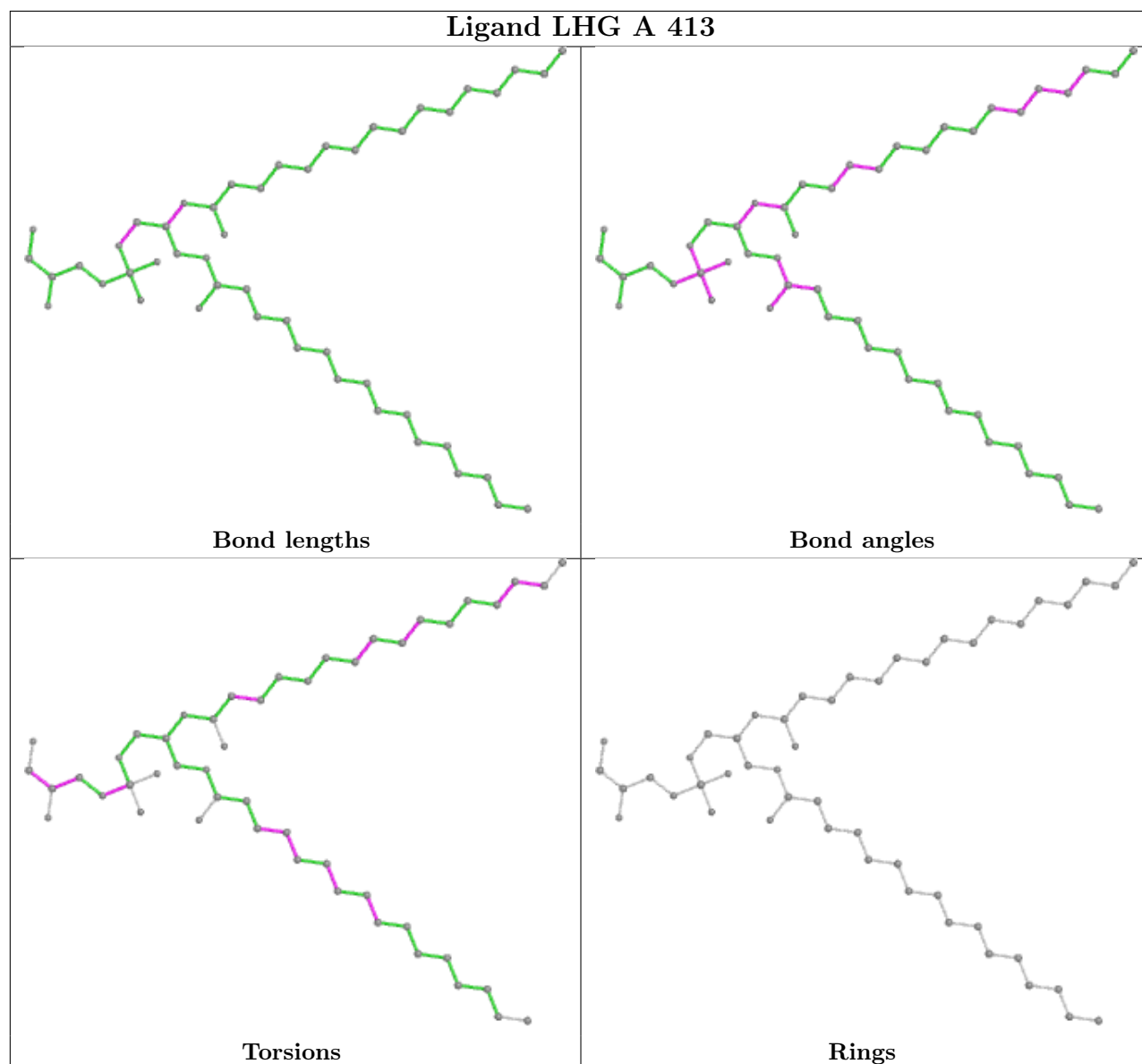
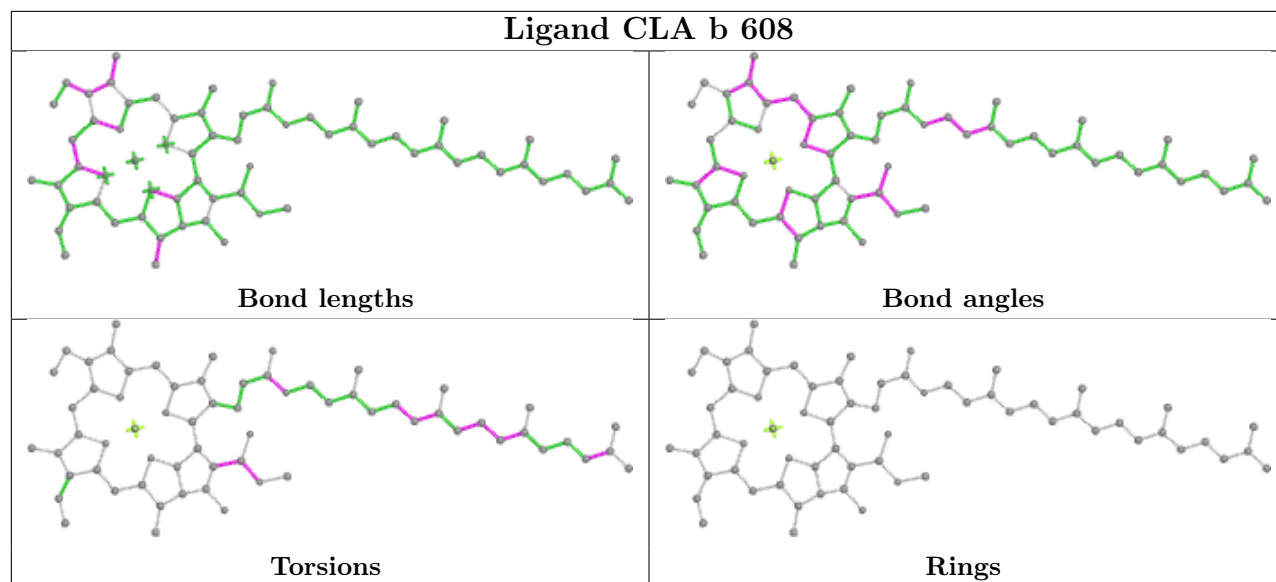


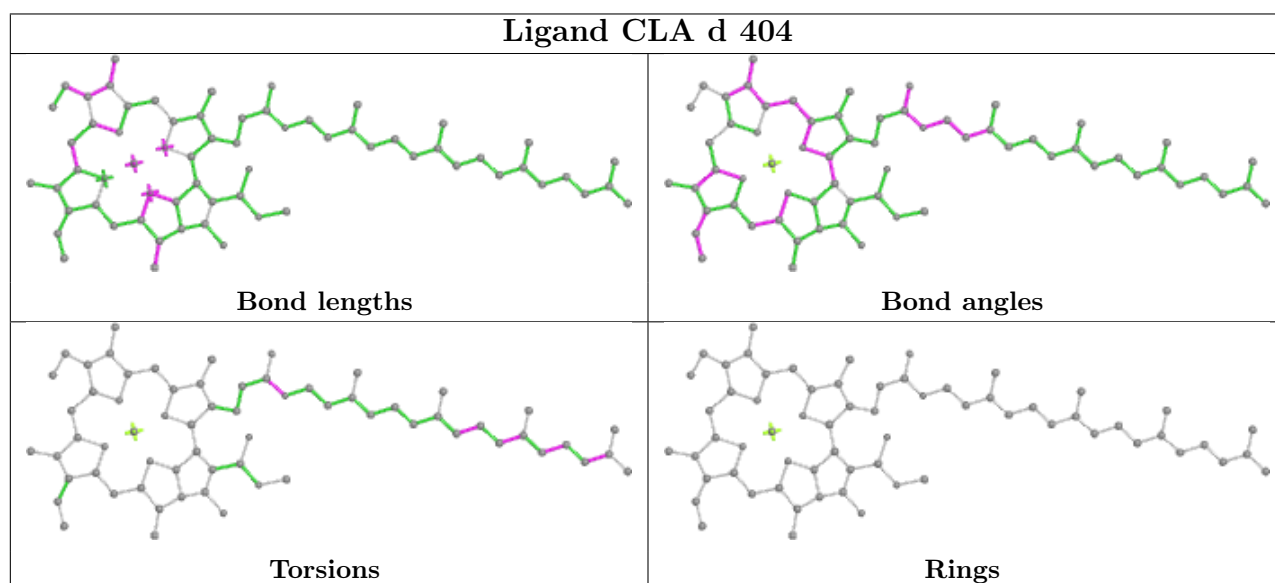
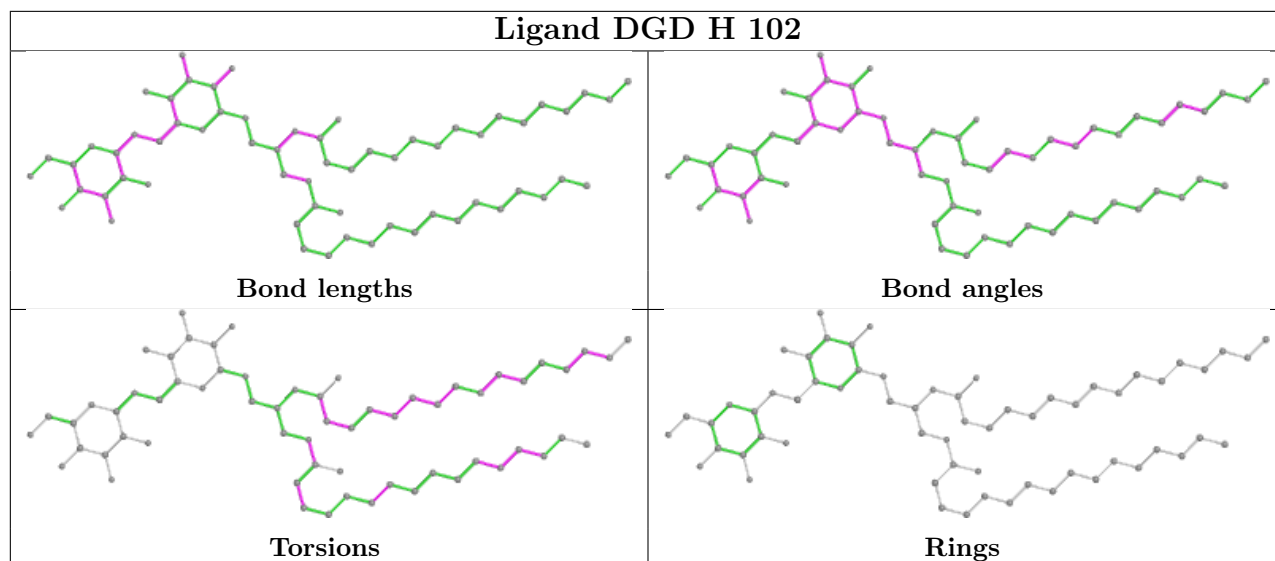


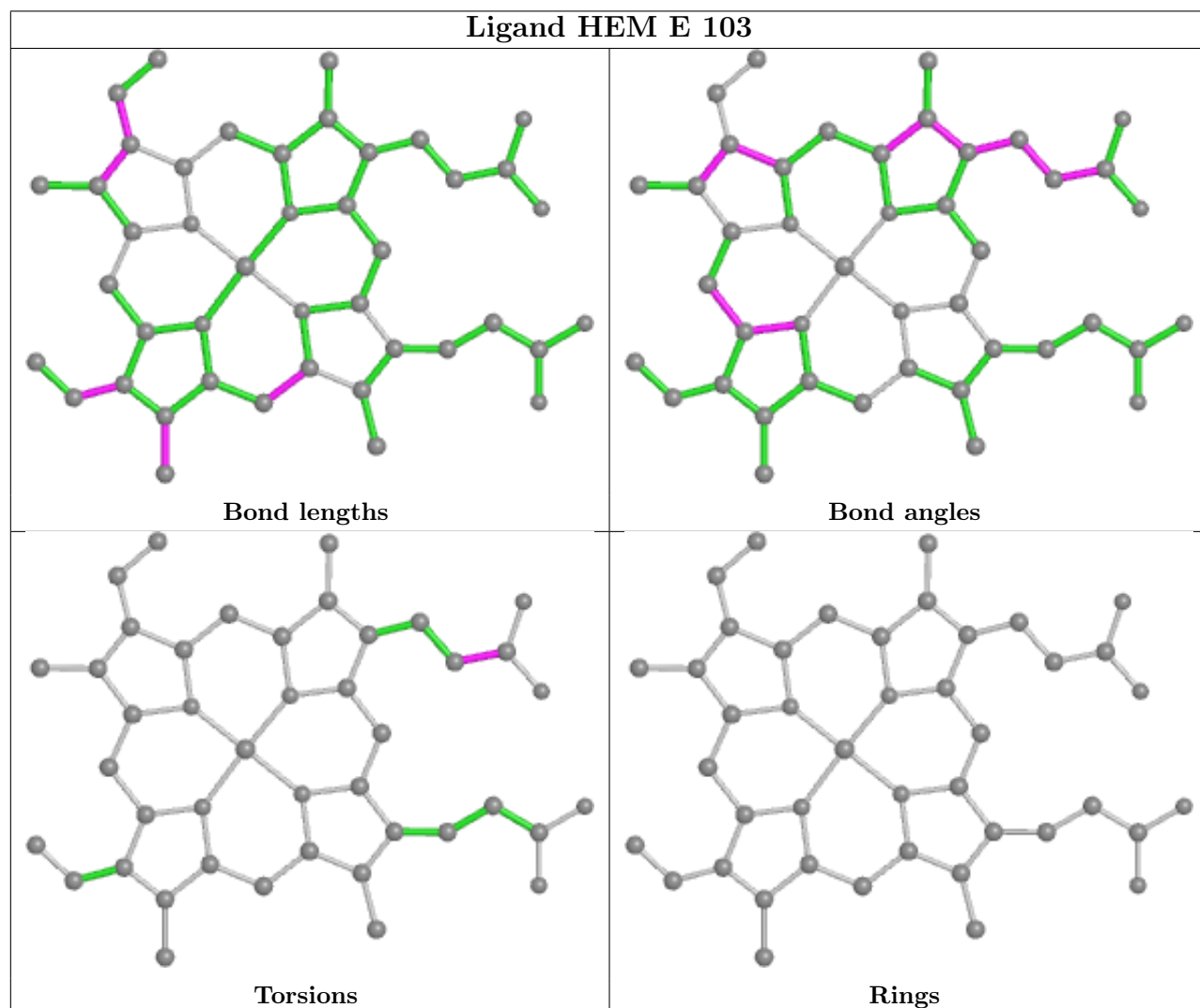
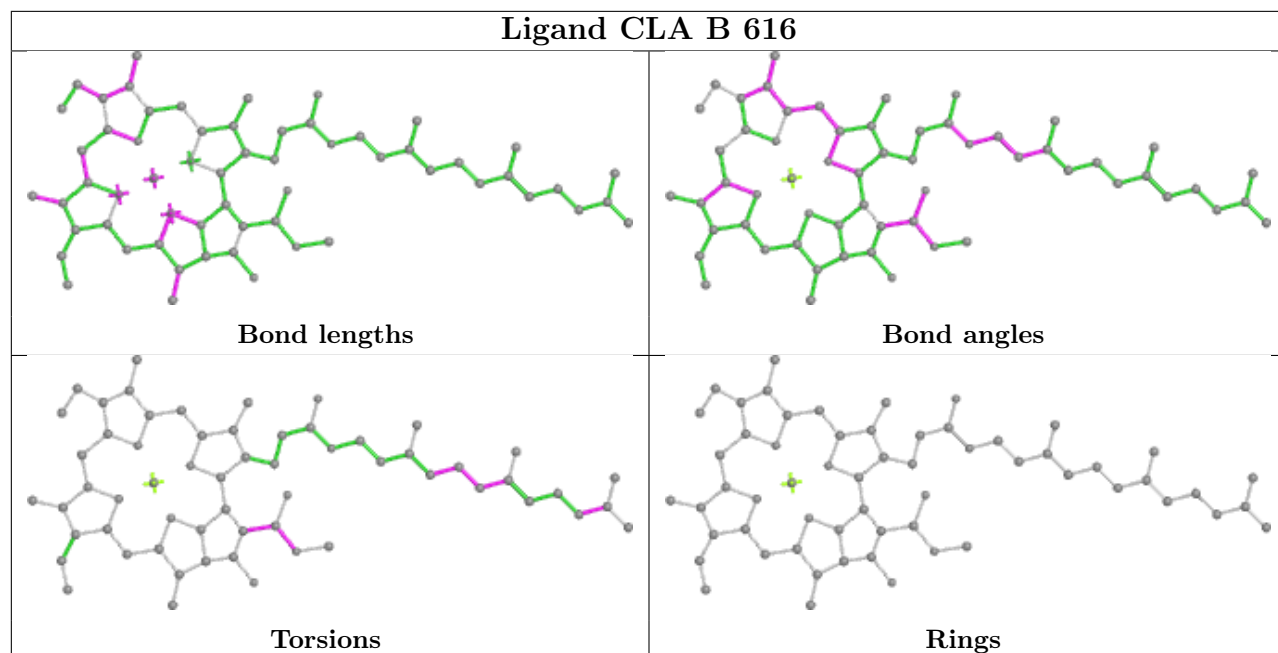


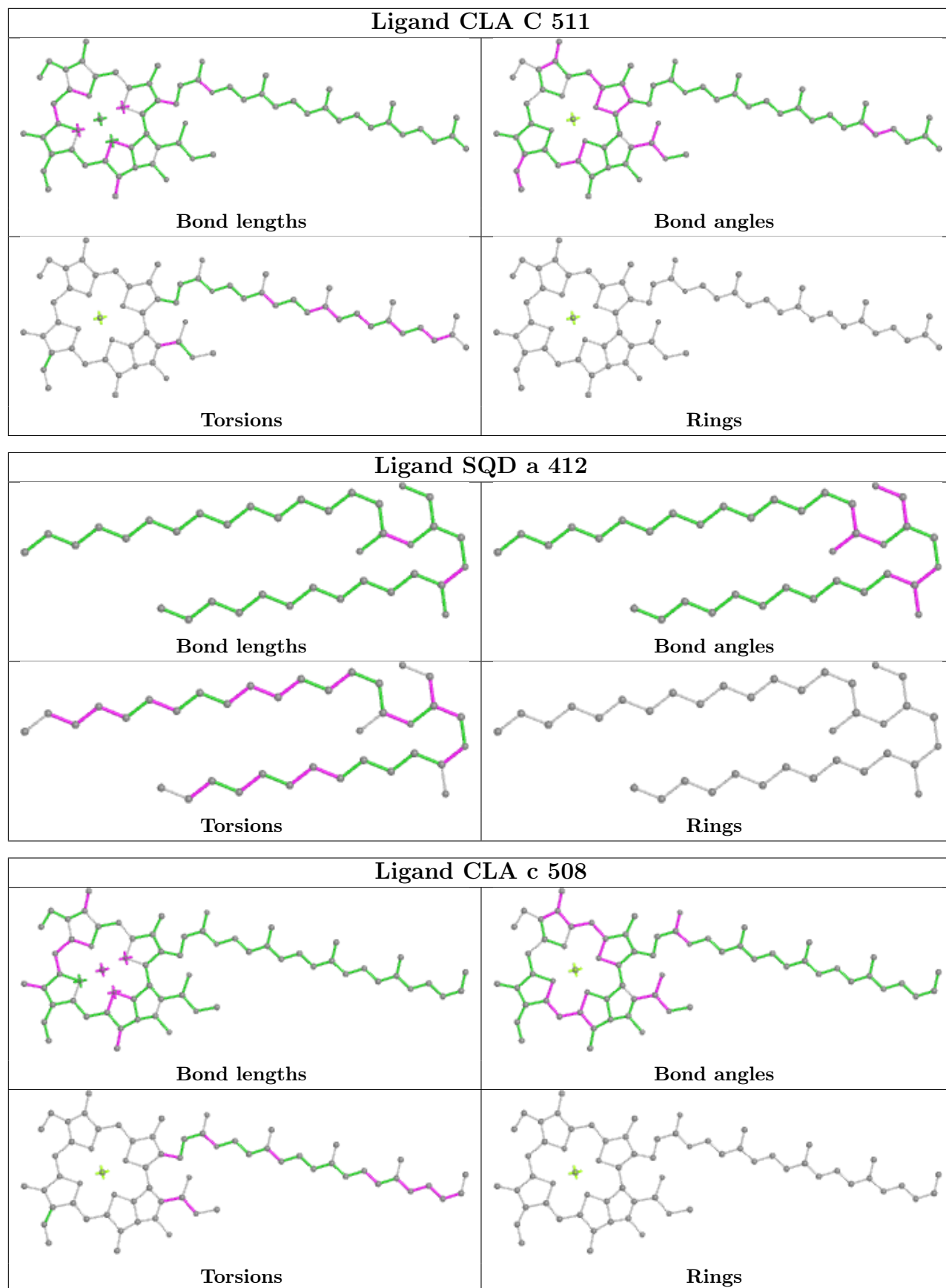


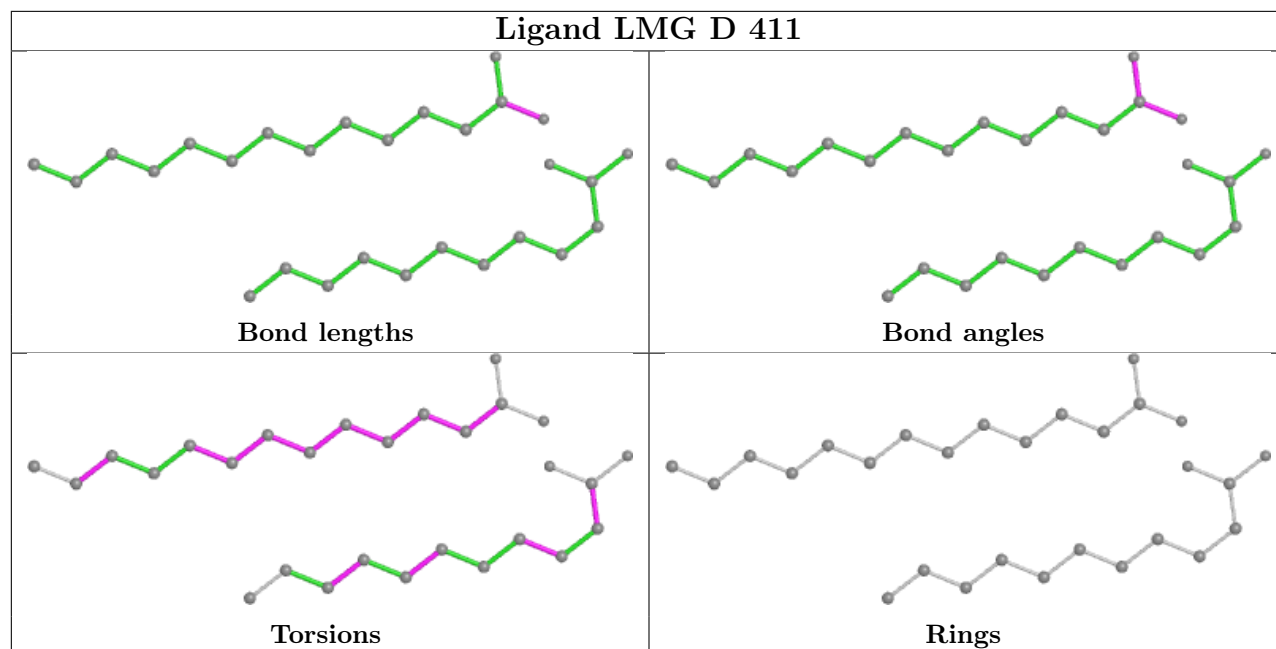












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.63	3 (0%) 84 86	27, 35, 53, 81	0
1	a	334/334 (100%)	-0.59	1 (0%) 94 94	26, 36, 63, 84	0
2	B	505/505 (100%)	-0.51	7 (1%) 75 77	27, 39, 67, 107	0
2	b	505/505 (100%)	-0.41	12 (2%) 59 62	27, 42, 78, 104	0
3	C	442/451 (98%)	-0.47	1 (0%) 95 95	29, 42, 59, 81	0
3	c	451/451 (100%)	-0.42	4 (0%) 84 86	31, 46, 68, 109	0
4	D	341/341 (100%)	-0.50	0 100 100	27, 36, 53, 90	0
4	d	341/341 (100%)	-0.46	3 (0%) 84 86	28, 40, 62, 92	0
5	E	81/82 (98%)	-0.11	3 (3%) 41 45	39, 56, 74, 91	0
5	e	82/82 (100%)	0.23	5 (6%) 21 22	44, 63, 85, 94	0
6	F	34/34 (100%)	-0.58	2 (5%) 22 23	42, 48, 69, 86	0
6	f	34/34 (100%)	-0.46	0 100 100	49, 54, 83, 98	0
7	H	65/65 (100%)	-0.17	0 100 100	37, 45, 66, 87	0
7	h	63/65 (96%)	-0.12	2 (3%) 47 51	43, 54, 69, 78	0
8	I	35/36 (97%)	-0.49	0 100 100	32, 43, 73, 80	0
8	i	35/36 (97%)	-0.21	3 (8%) 10 10	33, 46, 83, 90	0
9	J	36/36 (100%)	0.19	4 (11%) 5 5	43, 54, 80, 104	0
9	j	36/36 (100%)	0.06	4 (11%) 5 5	42, 58, 93, 101	0
10	K	37/37 (100%)	-0.26	0 100 100	46, 60, 75, 77	0
10	k	37/37 (100%)	-0.05	1 (2%) 54 58	59, 67, 76, 82	0
11	L	37/37 (100%)	-0.46	0 100 100	29, 36, 75, 75	0
11	l	36/37 (97%)	-0.43	0 100 100	29, 37, 72, 83	0
12	M	32/33 (96%)	-0.36	1 (3%) 49 52	32, 38, 69, 75	0
12	m	31/33 (93%)	-0.42	0 100 100	32, 38, 57, 71	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.13	12 (4%) 29 31	28, 48, 85, 150	0
13	o	244/244 (100%)	-0.26	12 (4%) 29 31	29, 46, 88, 133	0
14	T	29/30 (96%)	-0.77	1 (3%) 45 48	29, 37, 67, 74	0
14	t	29/30 (96%)	-0.60	2 (6%) 16 17	31, 37, 89, 92	0
15	U	97/97 (100%)	-0.34	2 (2%) 63 66	36, 49, 77, 103	0
15	u	97/97 (100%)	-0.50	1 (1%) 82 84	36, 46, 64, 91	0
16	V	137/137 (100%)	-0.63	0 100 100	34, 46, 62, 92	0
16	v	137/137 (100%)	-0.36	3 (2%) 62 65	36, 53, 76, 99	0
17	Y	27/30 (90%)	1.63	11 (40%) 0 0	57, 79, 114, 120	0
17	y	30/30 (100%)	0.39	1 (3%) 46 50	64, 78, 94, 111	0
18	X	38/38 (100%)	-0.13	3 (7%) 12 12	42, 53, 78, 83	0
18	x	38/38 (100%)	0.14	1 (2%) 56 59	52, 63, 87, 96	0
19	Z	62/62 (100%)	0.40	8 (12%) 3 3	55, 69, 115, 123	0
19	z	62/62 (100%)	0.77	12 (19%) 1 1	62, 79, 121, 127	0
20	R	34/34 (100%)	1.39	7 (20%) 1 0	66, 75, 95, 103	0
20	r	31/34 (91%)	2.19	17 (54%) 0 0	79, 93, 106, 110	0
All	All	5300/5326 (99%)	-0.35	149 (2%) 53 56	26, 44, 80, 150	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	20	ALA	8.4
13	O	60	ARG	7.9
19	z	33	TRP	7.2
13	o	3	GLN	7.0
13	O	3	GLN	6.3
9	J	5	GLY	6.0
13	o	58	ASN	5.7
13	O	61	GLN	5.5
13	O	59	LYS	5.2
1	A	13	LEU	5.2
9	j	7	ARG	5.1
13	O	62	GLU	5.0
20	r	26	TYR	4.8
5	e	79	PHE	4.7
2	B	502	VAL	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	o	56	PRO	4.5
9	J	7	ARG	4.5
9	j	8	ILE	4.3
17	Y	45	ASN	4.3
18	x	2	THR	4.3
3	c	23	ALA	4.3
17	Y	41	VAL	4.2
6	F	12	SER	4.2
17	Y	21	GLN	4.1
9	J	6	GLY	4.1
13	o	5	LEU	4.1
18	X	2	THR	4.1
17	Y	43	ARG	4.0
19	z	31	GLN	4.0
17	Y	42	ARG	3.9
20	r	3	TRP	3.8
13	O	5	LEU	3.8
13	O	56	PRO	3.8
19	z	62	VAL	3.7
20	r	2	ASP	3.6
17	Y	23	THR	3.5
20	r	6	LEU	3.5
8	i	36	ASP	3.5
19	Z	33	TRP	3.5
2	b	127	ARG	3.5
19	z	35	ARG	3.4
20	R	3	TRP	3.4
20	R	6	LEU	3.4
13	O	4	THR	3.3
9	j	5	GLY	3.3
2	B	506	ARG	3.3
18	X	3	ILE	3.3
20	r	25	PRO	3.3
20	r	4	ARG	3.3
20	r	28	VAL	3.3
13	o	4	THR	3.2
18	X	39	ARG	3.2
14	t	28	ARG	3.2
20	R	21	ARG	3.2
19	Z	1	MET	3.2
20	r	14	LEU	3.2
20	r	27	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	3.1
2	b	486	LEU	3.1
20	r	24	LEU	3.1
13	o	61	GLN	3.1
19	z	30	PRO	3.0
1	a	11	ALA	3.0
3	c	143	TYR	3.0
20	R	29	LYS	3.0
9	J	8	ILE	3.0
20	R	32	GLN	3.0
5	E	79	PHE	2.9
20	r	9	LEU	2.9
20	r	10	LEU	2.9
13	O	63	ALA	2.9
20	R	31	VAL	2.9
17	y	19	ILE	2.8
20	r	13	LEU	2.8
19	z	41	PHE	2.8
9	j	6	GLY	2.8
2	B	505	ARG	2.8
2	b	506	ARG	2.8
20	r	5	VAL	2.7
19	Z	62	VAL	2.6
17	Y	37	PHE	2.6
19	z	60	PHE	2.6
6	F	13	TYR	2.6
13	O	23	ASP	2.6
19	z	61	VAL	2.6
19	Z	30	PRO	2.6
19	Z	3	ILE	2.6
15	U	8	GLU	2.6
15	U	67	LEU	2.6
14	t	29	ILE	2.6
16	v	15	GLU	2.6
8	i	34	ARG	2.6
1	A	12	ASN	2.5
19	z	32	ASP	2.5
13	O	57	LYS	2.5
2	b	502	VAL	2.5
2	b	128	THR	2.5
5	E	84	LYS	2.5
4	d	227[A]	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Z	35	ARG	2.5
1	A	11	ALA	2.5
16	v	16	GLY	2.5
2	b	487	SER	2.4
17	Y	25	ILE	2.4
2	B	296	ALA	2.4
2	b	489	GLU	2.4
2	B	294	SER	2.4
3	c	193	GLY	2.4
13	o	246	ALA	2.4
5	e	71	GLU	2.4
7	h	10	ILE	2.3
7	h	6	TRP	2.3
5	e	61	ARG	2.3
8	i	35	LYS	2.3
20	r	29	LYS	2.3
3	C	143	TYR	2.3
5	e	72	ALA	2.3
15	u	53	ALA	2.3
12	M	33	GLN	2.2
19	z	34	ASP	2.2
13	O	64	GLU	2.2
2	b	161	LEU	2.2
19	z	37	LYS	2.2
19	Z	38	GLN	2.2
13	o	62	GLU	2.2
2	b	126	PRO	2.2
13	o	54	GLU	2.2
20	r	7	VAL	2.2
20	R	2	ASP	2.2
5	E	15	THR	2.2
13	o	57	LYS	2.1
20	r	16	ALA	2.1
4	d	226	GLY	2.1
13	o	207	ARG	2.1
19	Z	4	LEU	2.1
4	d	236	ASN	2.1
17	Y	24	MET	2.1
2	B	504	THR	2.1
14	T	29	ILE	2.1
2	b	490	GLN	2.1
2	b	289	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	z	59	PHE	2.1
5	e	15	THR	2.0
10	k	17	ILE	2.0
3	c	146	PHE	2.0
16	v	22	THR	2.0
2	B	486	LEU	2.0
17	Y	39	LEU	2.0
13	o	55	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.96	0.16	41,55,69,80	0
14	FME	T	1	10/11	0.96	0.14	33,58,80,90	0
8	FME	i	1	10/11	0.96	0.18	39,54,68,78	0
12	FME	m	1	10/11	0.96	0.16	37,54,75,81	0
8	FME	I	1	10/11	0.97	0.14	48,61,72,83	0
14	FME	t	1	10/11	0.97	0.10	36,55,82,88	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	UNL	H	103	53/-	0.74	0.32	44,89,115,116	0
32	UNL	c	523	28/-	0.75	0.22	55,80,93,95	0
32	UNL	a	414	28/-	0.78	0.29	44,66,82,84	0
32	UNL	x	101	55/-	0.78	0.31	43,71,92,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	LMG	c	522	48/55	0.80	0.26	42,89,123,138	0
28	DGD	A	412	66/66	0.82	0.23	41,75,100,124	0
32	UNL	E	102	28/-	0.82	0.32	66,88,97,103	0
32	UNL	c	520	55/-	0.82	0.23	48,72,94,101	0
33	LMG	d	410	23/55	0.82	0.27	43,73,104,105	0
32	UNL	B	624	46/-	0.83	0.20	55,68,83,87	0
33	LMG	b	622	55/55	0.84	0.27	48,80,99,104	0
32	UNL	b	621	55/-	0.84	0.23	42,68,96,118	0
32	UNL	B	625	28/-	0.84	0.41	47,67,91,99	0
28	DGD	a	413	44/66	0.85	0.18	36,62,86,88	0
29	LHG	E	101	49/49	0.85	0.23	54,88,118,126	0
33	LMG	D	410	33/55	0.85	0.20	34,61,107,111	0
29	LHG	e	101	42/49	0.85	0.30	68,92,115,158	0
27	SQD	a	412	36/54	0.85	0.19	40,72,101,113	0
23	CLA	c	512	65/65	0.85	0.19	45,68,99,114	0
32	UNL	b	623	40/-	0.86	0.21	52,68,91,100	0
32	UNL	b	625	55/-	0.86	0.19	50,73,87,98	0
32	UNL	b	626	26/-	0.86	0.28	52,65,76,78	0
23	CLA	b	602	65/65	0.86	0.21	55,76,104,110	0
32	UNL	B	626	47/-	0.86	0.34	54,73,88,96	0
25	BCR	x	102	40/40	0.87	0.16	40,62,84,87	0
26	PL9	A	409	55/55	0.87	0.26	35,70,101,113	0
32	UNL	C	522	28/-	0.87	0.18	41,61,81,83	0
26	PL9	a	410	55/55	0.87	0.23	42,77,101,112	0
32	UNL	t	102	26/-	0.87	0.25	56,75,87,88	0
32	UNL	j	101	28/-	0.88	0.16	53,67,81,85	0
23	CLA	C	514	65/65	0.88	0.22	48,77,110,115	0
25	BCR	H	101	40/40	0.88	0.15	35,51,65,69	0
25	BCR	K	101	40/40	0.88	0.16	38,60,75,91	0
25	BCR	k	101	40/40	0.88	0.17	45,71,86,89	0
32	UNL	B	620	43/-	0.88	0.15	41,59,81,83	0
27	SQD	b	601	49/54	0.88	0.17	47,68,101,117	0
27	SQD	f	101	41/54	0.89	0.22	58,91,129,142	0
32	UNL	m	102	28/-	0.89	0.18	38,58,78,78	0
23	CLA	c	513	65/65	0.89	0.23	47,74,109,113	0
32	UNL	D	412	55/-	0.89	0.26	35,65,88,94	0
23	CLA	B	616	60/65	0.90	0.17	24,45,91,96	0
32	UNL	b	624	44/-	0.90	0.20	48,68,88,89	0
33	LMG	C	501	48/55	0.90	0.17	40,67,86,111	0
33	LMG	C	519	48/55	0.90	0.20	53,85,105,121	0
32	UNL	d	412	43/-	0.90	0.20	50,62,78,83	0
33	LMG	D	411	28/55	0.90	0.18	34,58,76,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	D	404	65/65	0.90	0.17	26,47,133,138	0
32	UNL	l	102	53/-	0.90	0.19	36,55,96,102	0
32	UNL	C	521	28/-	0.90	0.14	35,50,62,67	0
32	UNL	T	102	47/-	0.91	0.21	34,52,79,81	0
27	SQD	A	411	39/54	0.91	0.23	43,73,96,111	0
27	SQD	B	621	54/54	0.91	0.16	43,67,104,121	0
27	SQD	F	101	36/54	0.91	0.16	48,76,102,107	0
23	CLA	B	601	65/65	0.91	0.16	36,65,116,139	0
23	CLA	C	513	65/65	0.91	0.17	35,62,112,146	0
32	UNL	B	622	34/-	0.91	0.16	38,55,71,72	0
23	CLA	a	408	65/65	0.91	0.16	22,41,107,114	0
32	UNL	I	101	41/-	0.91	0.14	42,62,95,99	0
33	LMG	c	519	37/55	0.91	0.18	45,74,99,105	0
32	UNL	J	101	28/-	0.91	0.23	48,62,74,75	0
33	LMG	c	524	49/55	0.91	0.15	31,60,96,125	0
32	UNL	M	103	26/-	0.91	0.20	36,54,72,72	0
23	CLA	c	508	64/65	0.92	0.15	32,54,97,122	0
25	BCR	d	405	40/40	0.92	0.16	39,59,110,121	0
33	LMG	D	407	51/55	0.92	0.18	34,64,86,98	0
28	DGD	c	517	62/66	0.92	0.15	37,62,94,112	0
23	CLA	d	404	65/65	0.92	0.16	31,56,111,137	0
25	BCR	C	515	40/40	0.92	0.15	24,46,60,75	0
32	UNL	C	523	47/-	0.92	0.15	47,60,78,78	0
25	BCR	D	405	40/40	0.92	0.15	34,50,95,115	0
23	CLA	b	617	60/65	0.92	0.14	33,50,94,105	0
32	UNL	B	623	28/-	0.92	0.12	36,52,70,76	0
23	CLA	c	511	65/65	0.93	0.17	45,66,85,88	0
27	SQD	a	411	54/54	0.93	0.16	45,75,97,102	0
28	DGD	c	518	62/66	0.93	0.15	30,63,82,92	0
23	CLA	c	502	65/65	0.93	0.15	36,52,71,82	0
33	LMG	M	101	51/55	0.93	0.13	33,54,75,89	0
23	CLA	c	503	65/65	0.93	0.19	33,54,68,71	0
23	CLA	c	507	65/65	0.93	0.15	35,51,66,69	0
23	CLA	C	503	65/65	0.93	0.14	37,51,67,80	0
28	DGD	C	516	62/66	0.93	0.15	27,44,87,103	0
28	DGD	C	517	62/66	0.93	0.14	40,62,111,122	0
33	LMG	d	411	44/55	0.93	0.14	41,63,94,112	0
33	LMG	m	101	51/55	0.93	0.14	37,60,85,98	0
25	BCR	T	101	40/40	0.94	0.13	30,50,64,70	0
25	BCR	Z	101	40/40	0.94	0.17	41,63,81,84	0
25	BCR	b	618	40/40	0.94	0.13	31,50,67,67	0
28	DGD	h	101	62/66	0.94	0.13	35,55,69,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	BCR	b	620	40/40	0.94	0.14	34,58,75,80	0
29	LHG	d	407	49/49	0.94	0.16	38,59,98,112	0
29	LHG	d	409	39/49	0.94	0.14	35,56,75,81	0
25	BCR	c	514	40/40	0.94	0.21	44,65,80,80	0
25	BCR	c	521	40/40	0.94	0.18	39,61,68,74	0
23	CLA	b	605	65/65	0.94	0.16	25,42,84,98	0
23	CLA	b	607	65/65	0.94	0.12	30,48,78,87	0
23	CLA	c	509	65/65	0.94	0.22	37,56,73,83	0
23	CLA	c	510	65/65	0.94	0.16	39,57,78,89	0
23	CLA	b	615	65/65	0.94	0.17	24,46,85,89	0
23	CLA	b	616	65/65	0.94	0.14	33,48,69,80	0
23	CLA	C	506	65/65	0.94	0.19	27,46,69,79	0
23	CLA	B	606	65/65	0.94	0.13	26,43,85,94	0
25	BCR	B	618	40/40	0.94	0.12	29,45,68,69	0
25	BCR	B	619	40/40	0.94	0.12	33,49,66,84	0
23	CLA	B	615	65/65	0.94	0.15	27,46,70,81	0
25	BCR	C	520	40/40	0.94	0.18	42,60,75,79	0
23	CLA	c	504	60/65	0.94	0.14	36,54,83,87	0
32	UNL	M	102	37/-	0.94	0.13	37,51,63,73	0
23	CLA	c	505	65/65	0.94	0.17	31,48,70,79	0
23	CLA	c	506	65/65	0.94	0.16	35,60,114,126	0
28	DGD	H	102	62/66	0.94	0.13	32,52,68,76	0
26	PL9	D	406	55/55	0.95	0.13	22,38,49,55	0
23	CLA	C	512	65/65	0.95	0.14	37,58,76,83	0
29	LHG	D	409	47/49	0.95	0.14	36,56,90,108	0
27	SQD	A	410	52/54	0.95	0.15	37,68,94,102	0
23	CLA	A	405	65/65	0.95	0.13	23,41,104,122	0
23	CLA	B	604	65/65	0.95	0.14	25,41,92,98	0
23	CLA	c	501	65/65	0.95	0.15	30,46,58,67	0
23	CLA	A	407	54/65	0.95	0.14	25,38,83,85	0
25	BCR	b	619	40/40	0.95	0.11	33,46,58,62	0
23	CLA	a	406	65/65	0.95	0.14	31,48,99,114	0
25	BCR	B	617	40/40	0.95	0.13	32,48,61,67	0
25	BCR	c	515	40/40	0.95	0.15	32,52,66,80	0
23	CLA	B	613	65/65	0.95	0.14	24,36,71,82	0
23	CLA	C	507	65/65	0.95	0.14	27,49,103,114	0
23	CLA	C	508	65/65	0.95	0.15	29,44,66,71	0
23	CLA	C	511	65/65	0.95	0.13	35,55,81,86	0
23	CLA	b	614	65/65	0.95	0.15	23,41,92,97	0
28	DGD	C	518	62/66	0.96	0.12	32,58,86,104	0
23	CLA	C	509	65/65	0.96	0.12	28,51,114,130	0
23	CLA	b	606	65/65	0.96	0.14	27,43,57,61	0

Continued on next page...

Continued from previous page...

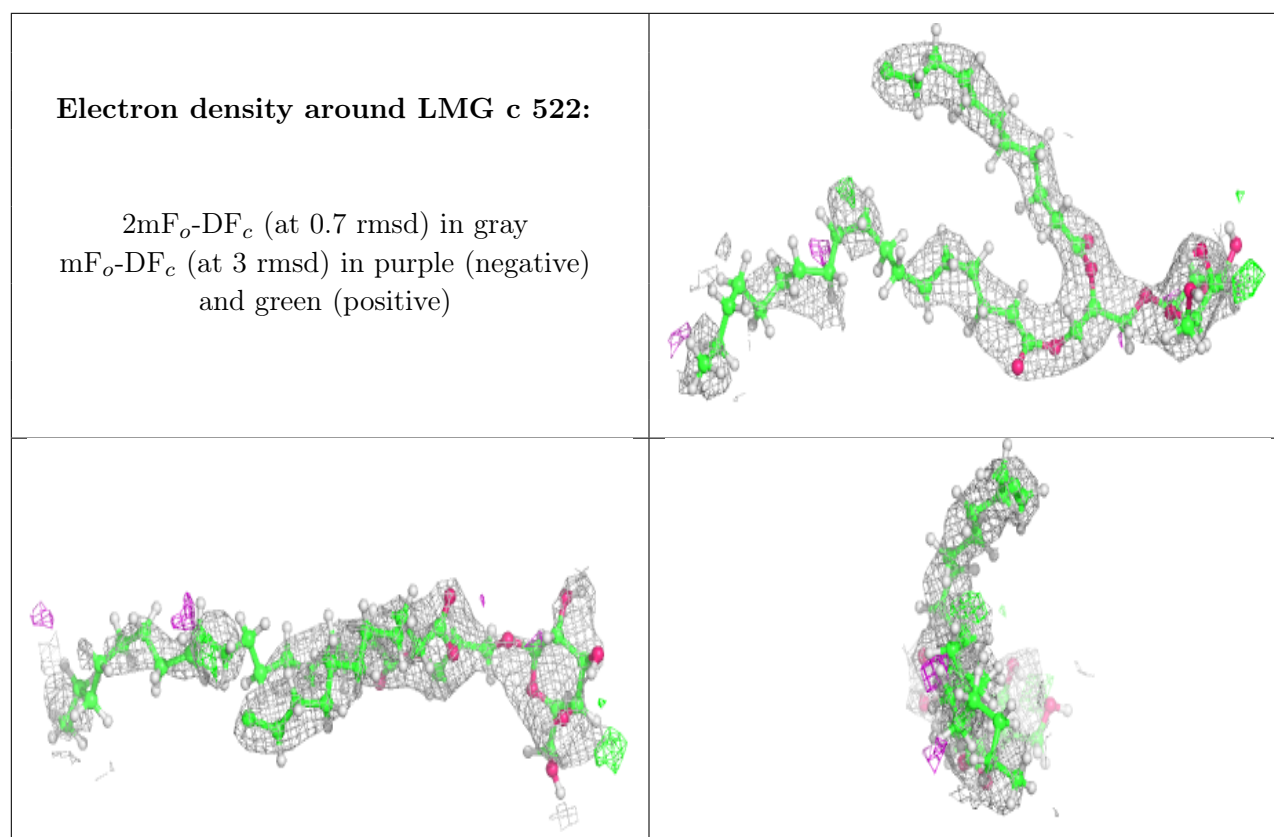
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	DGD	c	516	62/66	0.96	0.12	25,46,78,94	0
23	CLA	C	510	65/65	0.96	0.14	35,51,71,72	0
23	CLA	b	608	65/65	0.96	0.12	23,42,73,81	0
23	CLA	b	610	65/65	0.96	0.12	27,48,67,93	0
29	LHG	A	413	49/49	0.96	0.13	31,53,82,87	0
23	CLA	b	613	65/65	0.96	0.16	24,40,56,65	0
23	CLA	d	402	65/65	0.96	0.12	26,39,50,54	0
23	CLA	d	403	65/65	0.96	0.12	24,41,75,83	0
25	BCR	t	101	40/40	0.96	0.10	31,45,57,65	0
23	CLA	B	605	65/65	0.96	0.17	23,39,55,60	0
29	LHG	l	101	49/49	0.96	0.12	38,51,63,81	0
24	PHO	A	406	64/64	0.96	0.12	20,35,49,55	0
24	PHO	a	407	64/64	0.96	0.14	24,36,48,50	0
25	BCR	A	408	40/40	0.96	0.10	25,37,50,51	0
26	PL9	d	406	55/55	0.96	0.13	27,41,49,54	0
23	CLA	B	603	65/65	0.96	0.15	26,42,69,76	0
23	CLA	B	609	65/65	0.96	0.12	23,42,59,66	0
23	CLA	C	504	65/65	0.96	0.12	30,50,63,68	0
23	CLA	D	403	65/65	0.96	0.11	22,37,58,68	0
23	CLA	C	505	59/65	0.96	0.14	30,52,92,107	0
23	CLA	B	610	65/65	0.96	0.16	25,39,55,62	0
23	CLA	B	602	65/65	0.96	0.15	28,44,72,77	0
23	CLA	B	614	65/65	0.96	0.14	25,46,93,105	0
23	CLA	b	603	65/65	0.96	0.16	28,50,75,82	0
23	CLA	b	604	65/65	0.96	0.15	28,44,70,74	0
25	BCR	a	409	40/40	0.96	0.11	25,42,57,63	0
34	HEM	E	103	43/43	0.96	0.14	39,53,69,76	0
23	CLA	b	609	65/65	0.97	0.12	27,48,72,79	0
23	CLA	B	607	65/65	0.97	0.12	18,41,77,85	0
23	CLA	b	611	65/65	0.97	0.13	26,41,59,70	0
23	CLA	b	612	65/65	0.97	0.11	26,38,58,62	0
23	CLA	D	402	65/65	0.97	0.12	22,35,54,60	0
23	CLA	B	611	65/65	0.97	0.12	20,34,47,48	0
29	LHG	D	408	49/49	0.97	0.11	30,46,62,65	0
24	PHO	D	401	64/64	0.97	0.10	26,37,47,51	0
23	CLA	B	612	65/65	0.97	0.16	23,38,55,59	0
29	LHG	L	101	49/49	0.97	0.13	31,46,63,69	0
24	PHO	d	401	64/64	0.97	0.11	32,45,59,68	0
29	LHG	d	408	49/49	0.97	0.12	27,48,66,67	0
23	CLA	a	405	65/65	0.97	0.12	25,37,55,65	0
23	CLA	C	502	65/65	0.97	0.12	25,43,59,68	0
23	CLA	A	404	65/65	0.97	0.12	19,33,54,68	0

Continued on next page...

Continued from previous page...

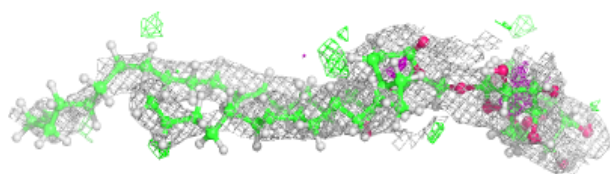
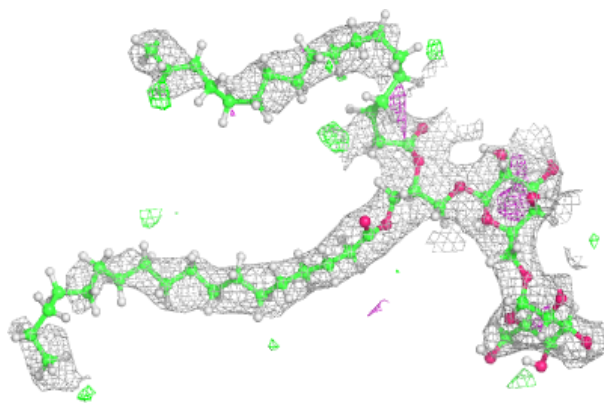
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	HEM	e	102	43/43	0.97	0.12	46,63,79,83	0
23	CLA	B	608	65/65	0.98	0.11	24,40,58,65	0
31	BCT	a	404	4/4	0.98	0.23	27,36,48,58	0
35	HEC	V	201	43/43	0.98	0.11	28,38,50,51	0
35	HEC	v	201	43/43	0.98	0.15	37,45,57,61	0
21	FE2	A	401	1/1	0.99	0.09	32,32,32,32	0
21	FE2	a	401	1/1	0.99	0.07	39,39,39,39	0
22	CL	A	402	1/1	0.99	0.06	36,36,36,36	0
22	CL	A	403	1/1	0.99	0.09	36,36,36,36	0
30	OEX	A	414	10/10	0.99	0.11	31,36,39,42	0
30	OEX	a	415	10/10	0.99	0.11	29,33,38,39	0
31	BCT	A	415	4/4	0.99	0.24	32,35,39,42	0
22	CL	a	402	1/1	1.00	0.08	34,34,34,34	0
22	CL	a	403	1/1	1.00	0.03	32,32,32,32	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.

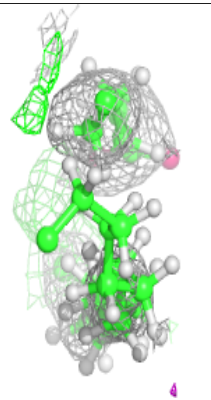
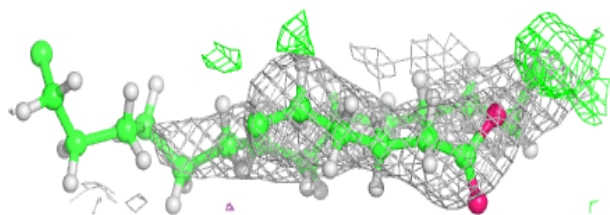
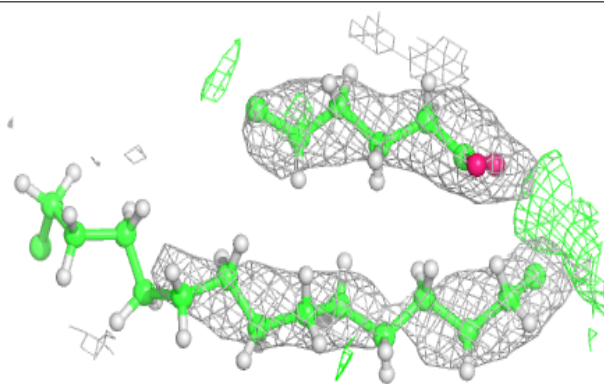


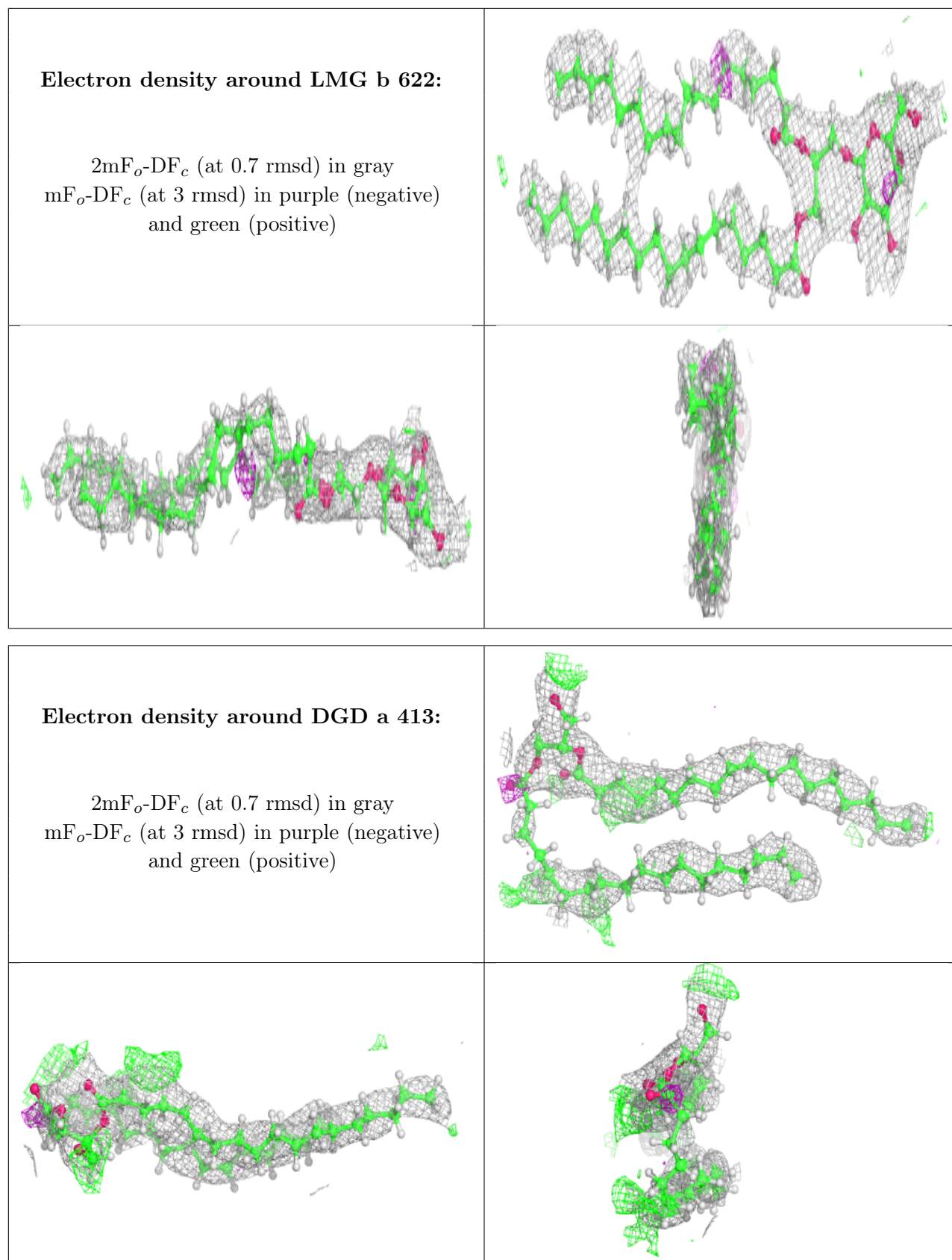
Electron density around DGD A 412:

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

**Electron density around LMG d 410:**

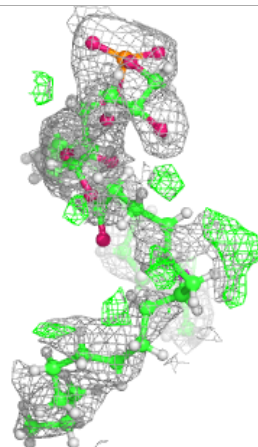
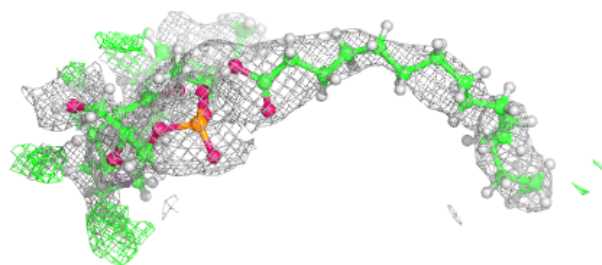
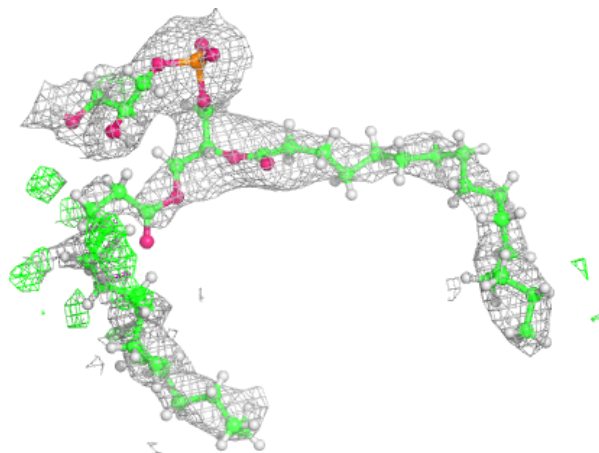
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



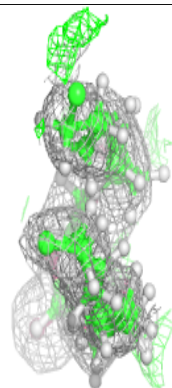
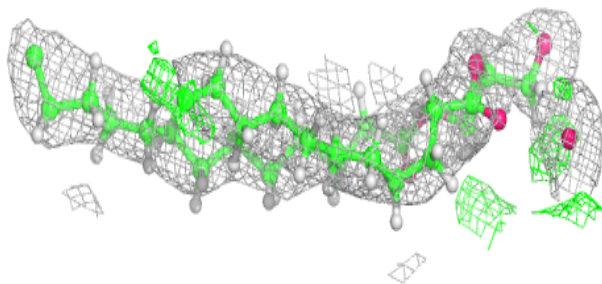
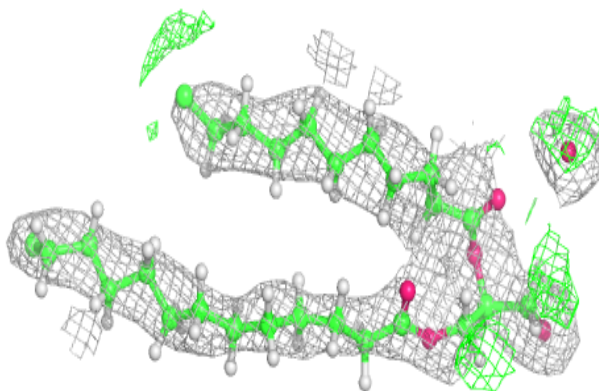


Electron density around LHG E 101:

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

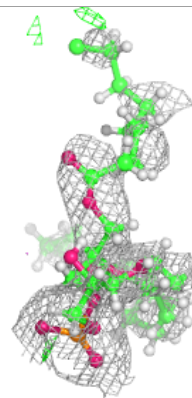
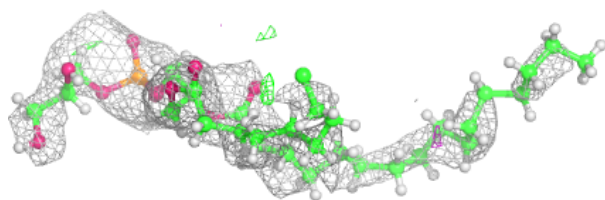
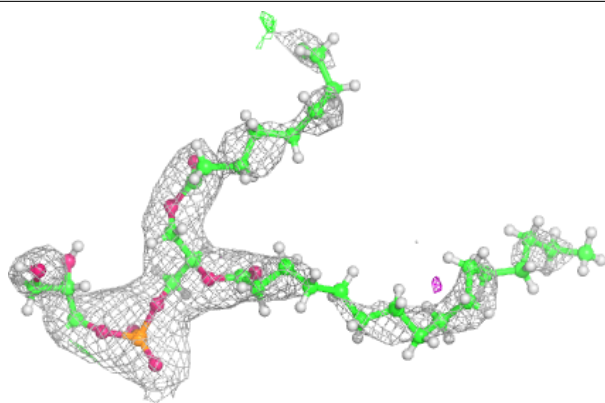
**Electron density around LMG D 410:**

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



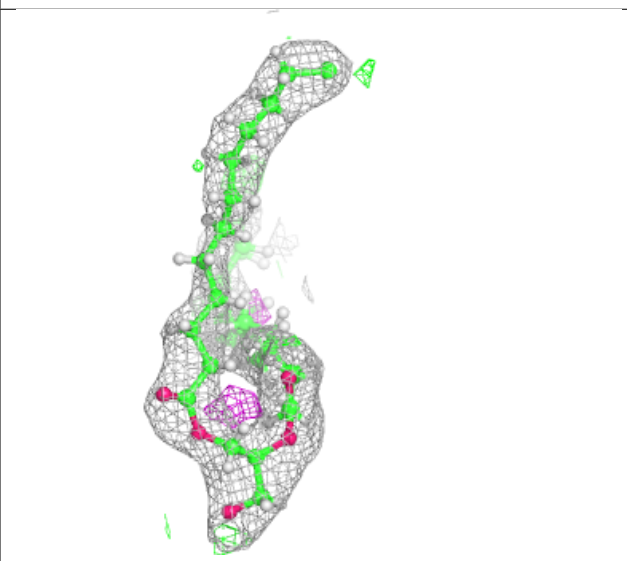
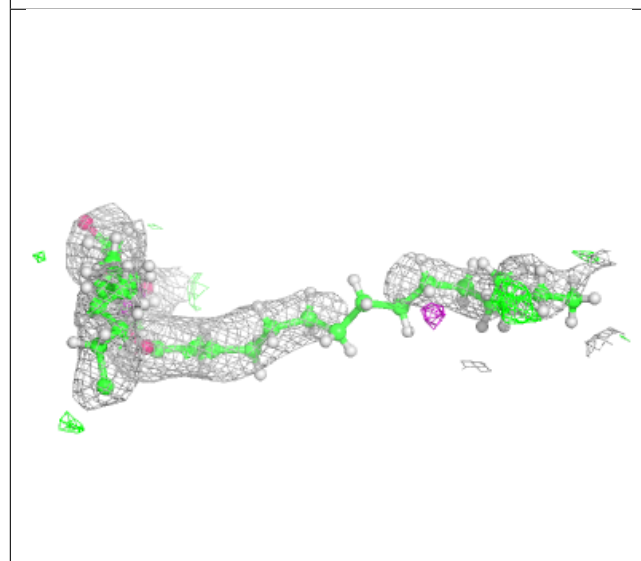
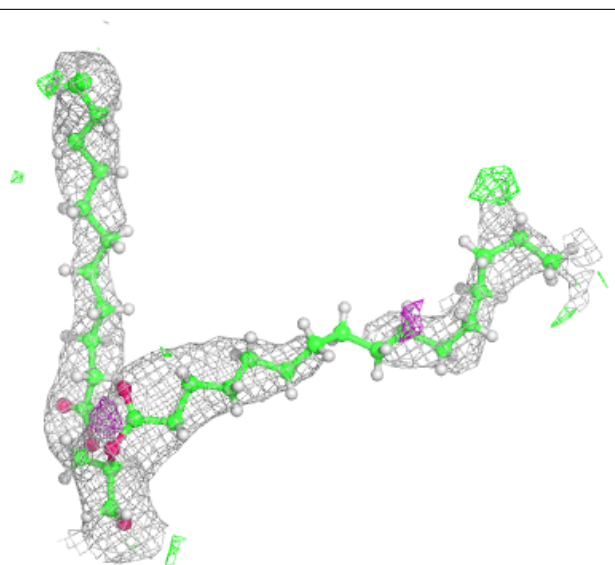
Electron density around LHG e 101:

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



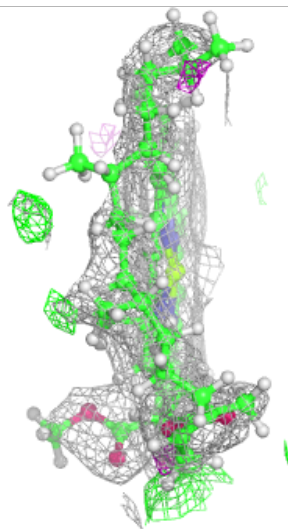
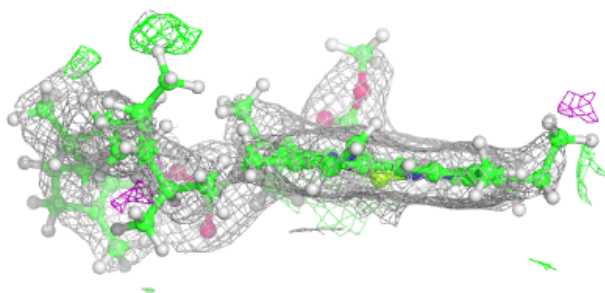
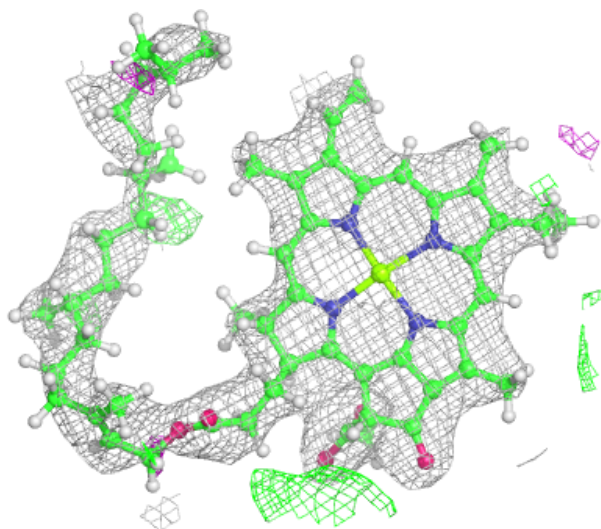
Electron density around SQD a 412:

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



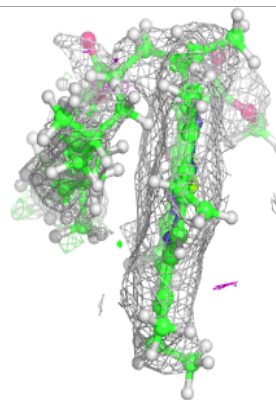
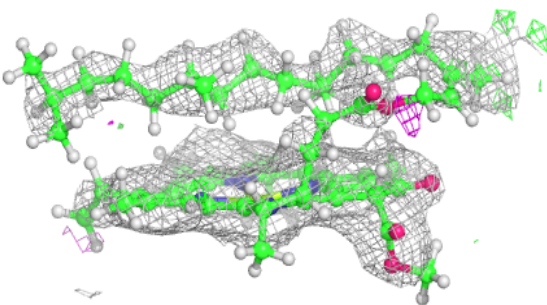
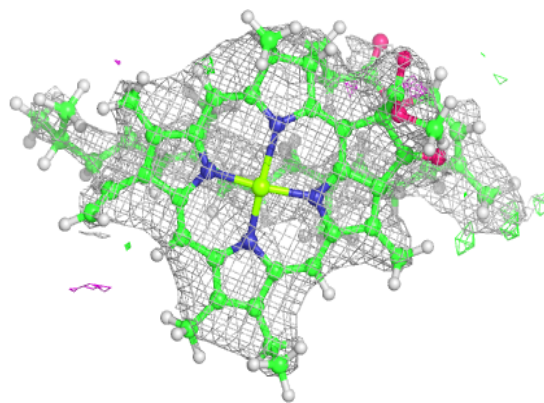
Electron density around CLA c 512:

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

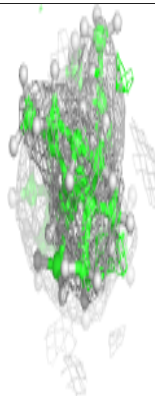
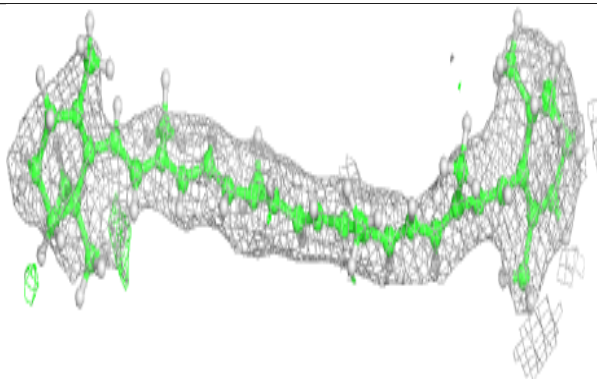
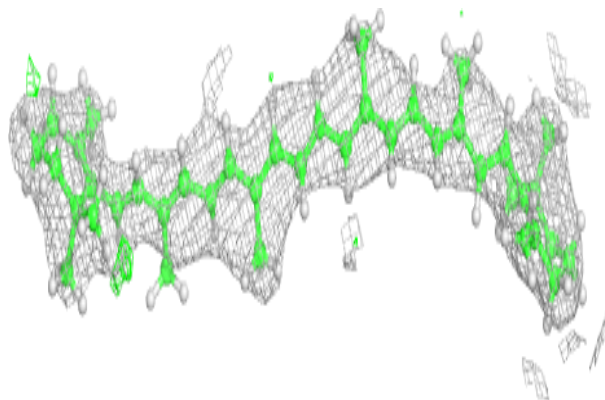


Electron density around CLA b 602:

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

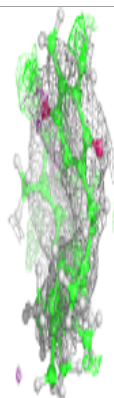
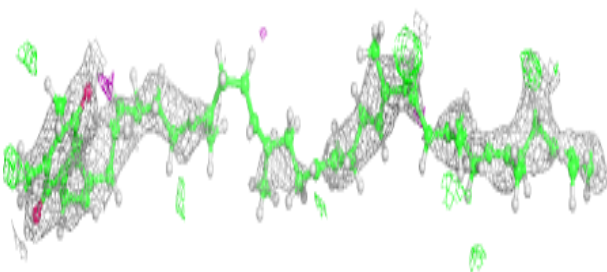
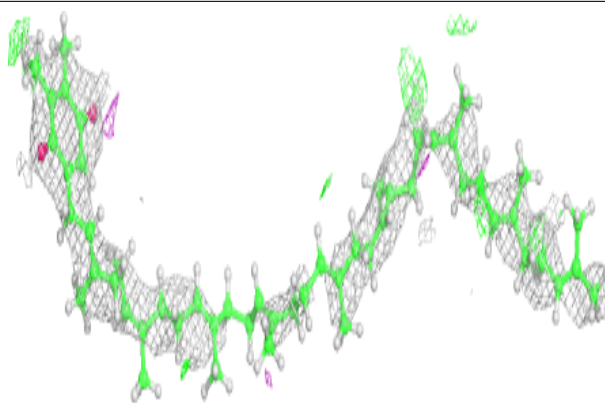
**Electron density around BCR x 102:**

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

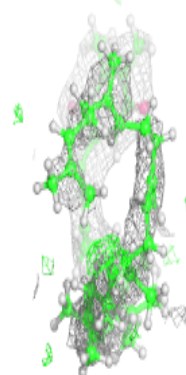
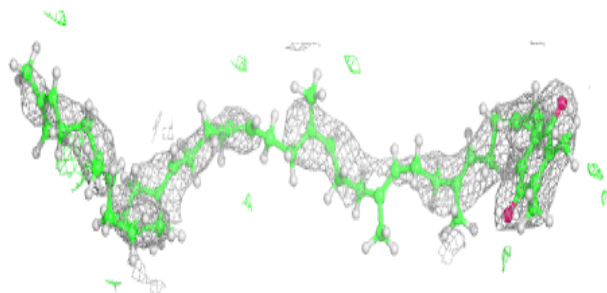
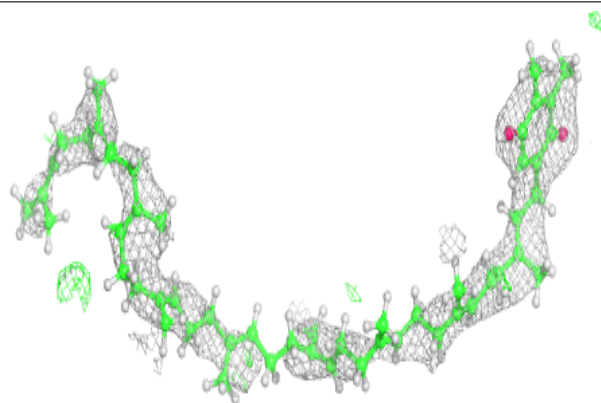


Electron density around PL9 A 409:

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

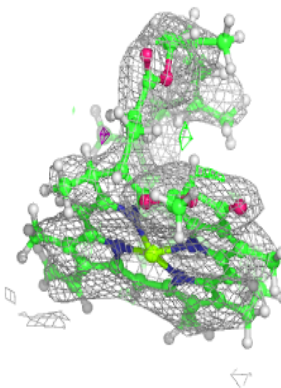
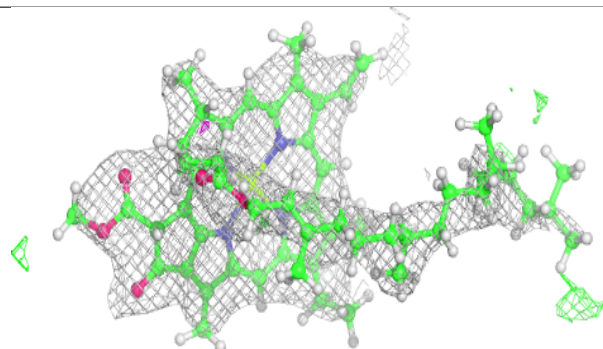
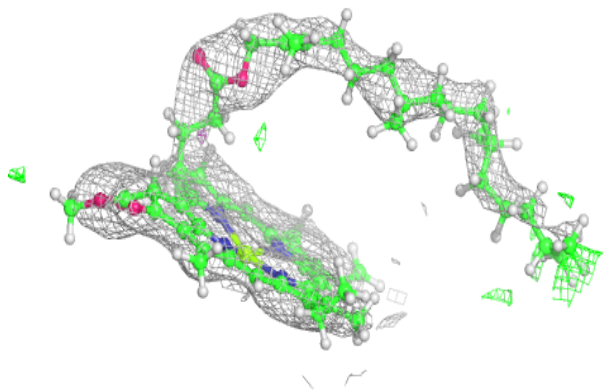
**Electron density around PL9 a 410:**

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

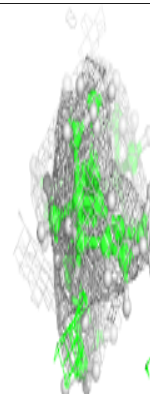
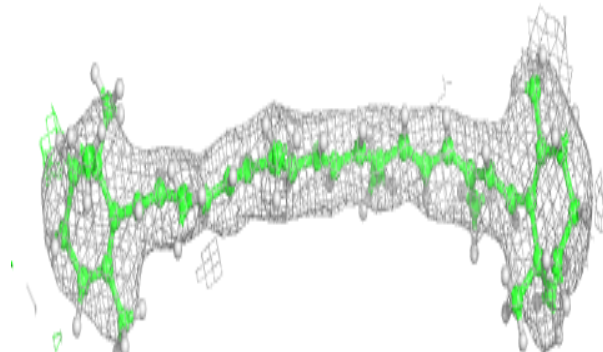
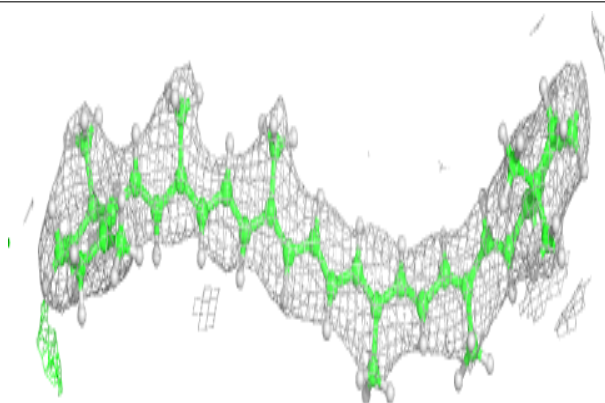


Electron density around CLA C 514:

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

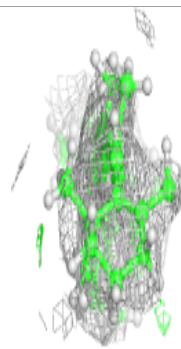
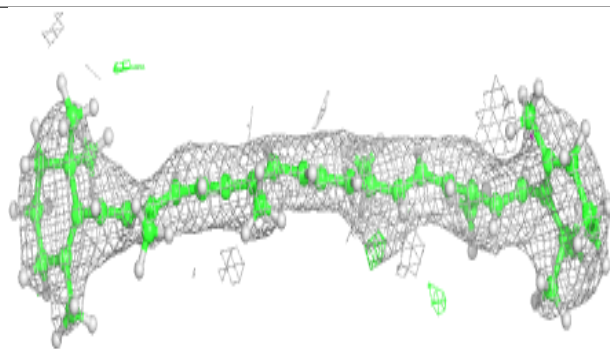
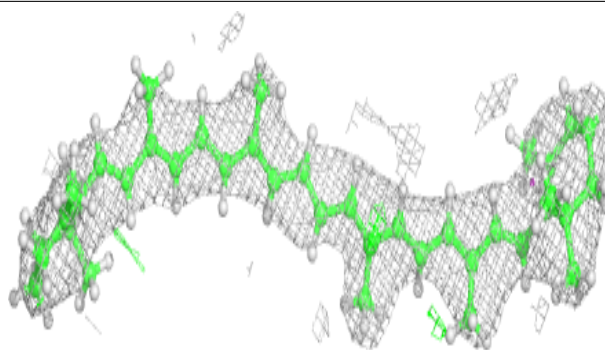
**Electron density around BCR H 101:**

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

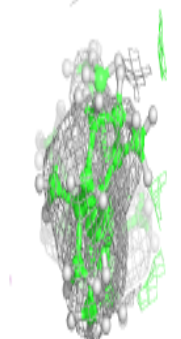
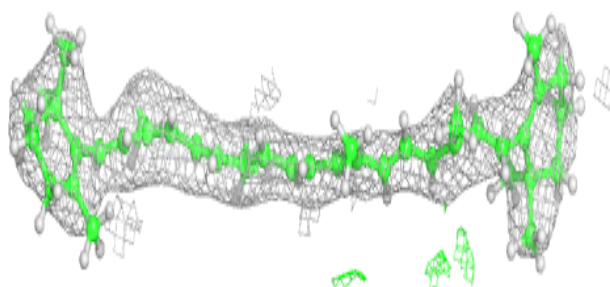
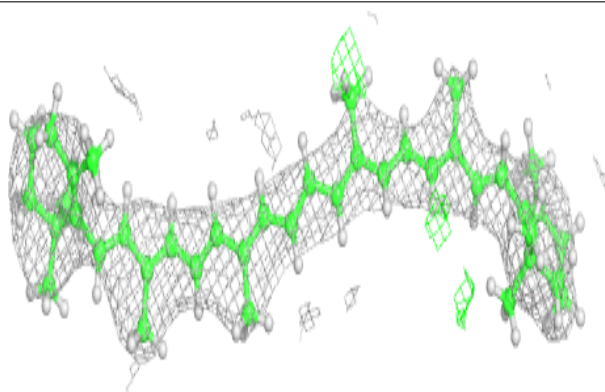


Electron density around BCR K 101:

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

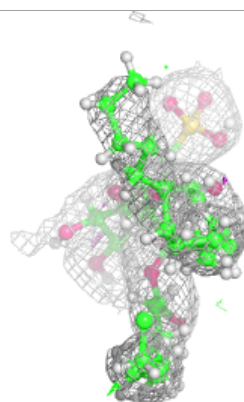
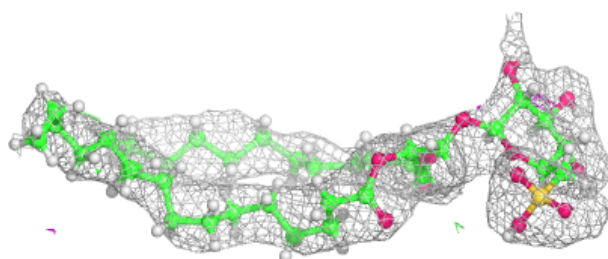
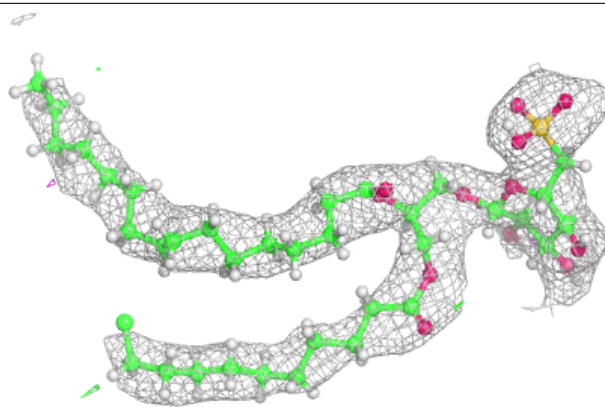
**Electron density around BCR k 101:**

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

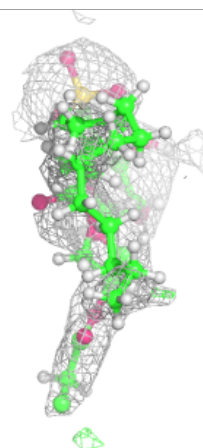
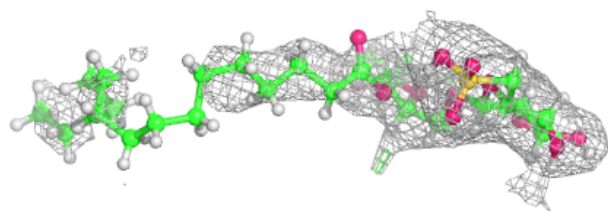
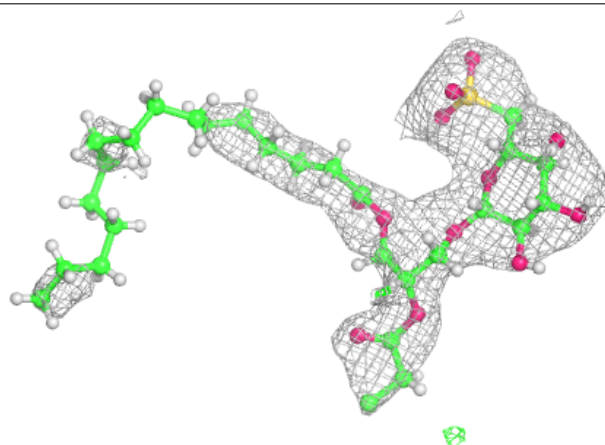


Electron density around SQD b 601:

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

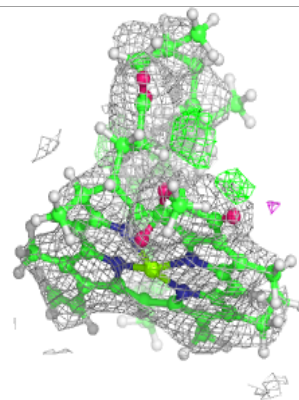
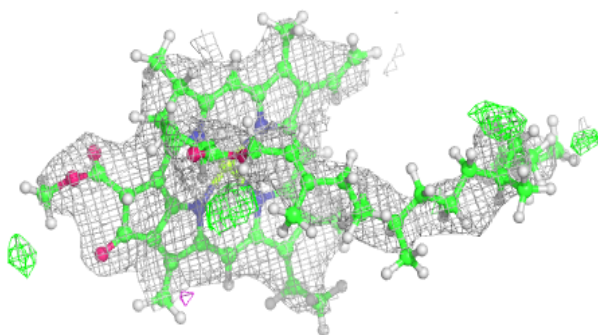
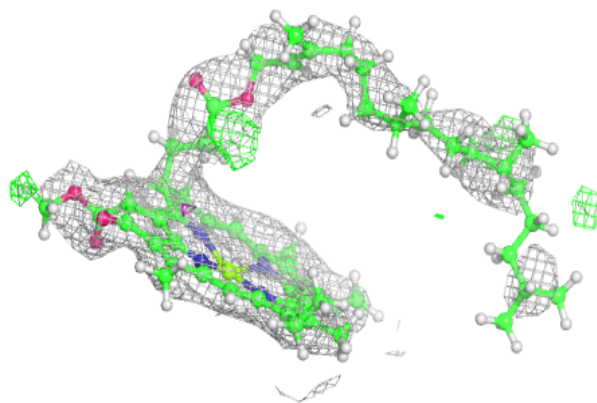
**Electron density around SQD f 101:**

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



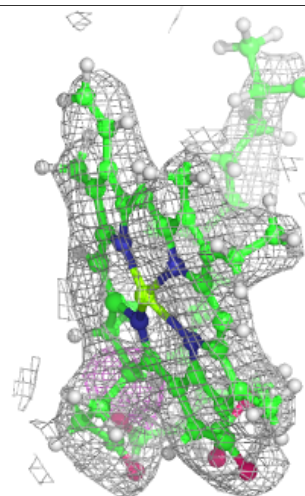
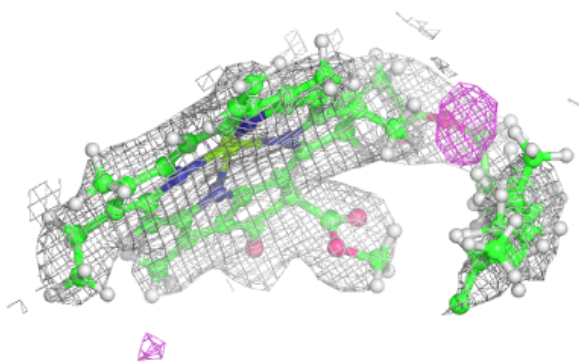
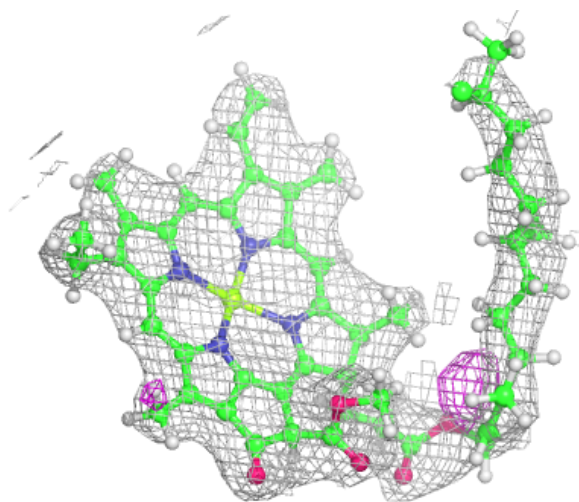
Electron density around CLA c 513:

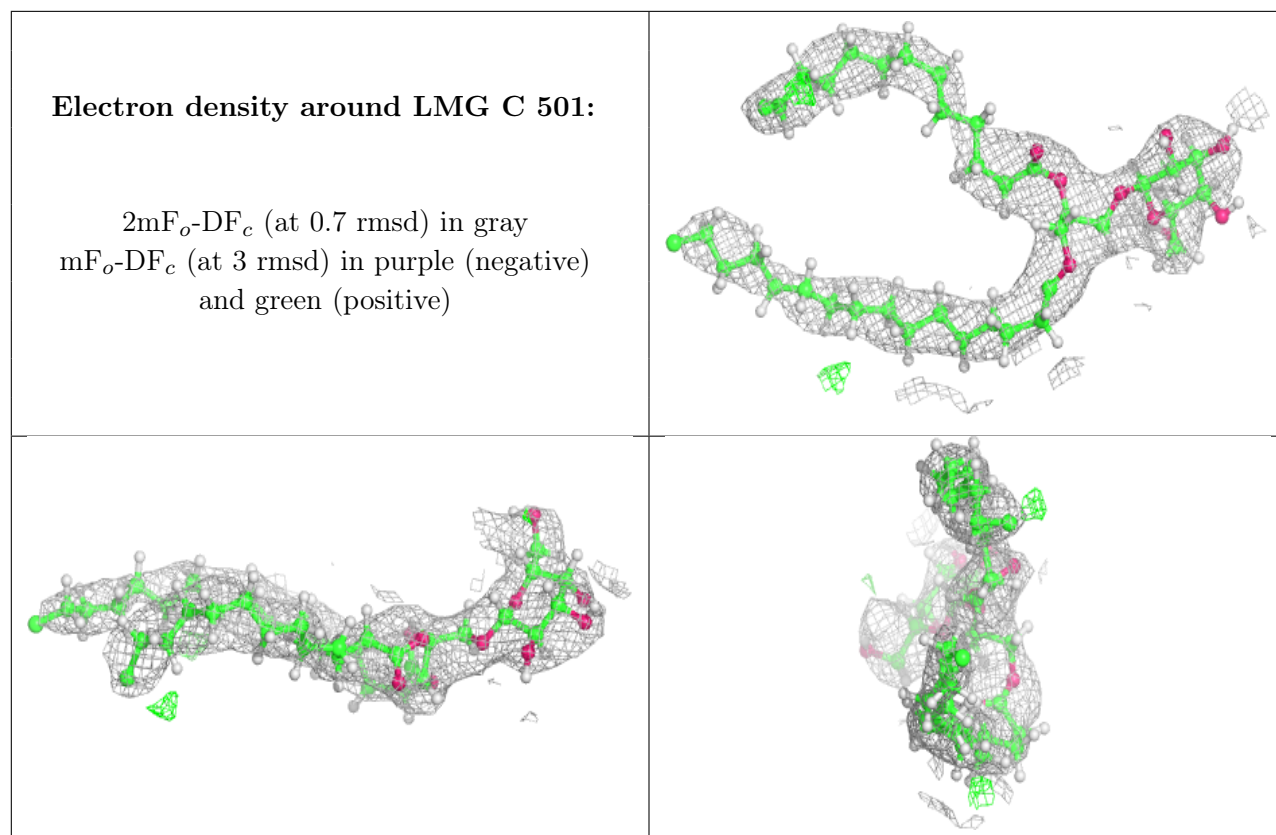
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 616:

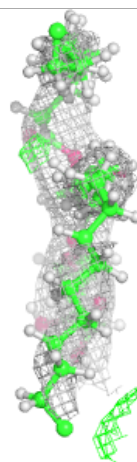
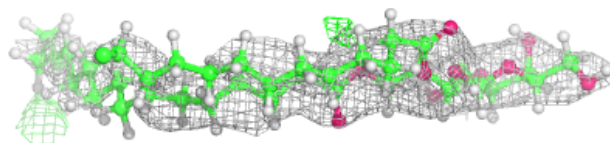
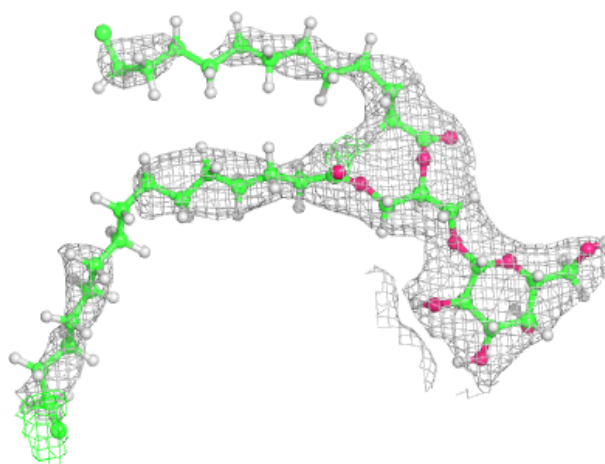
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





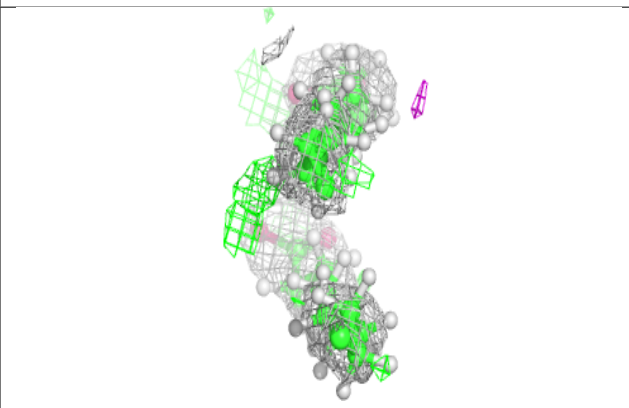
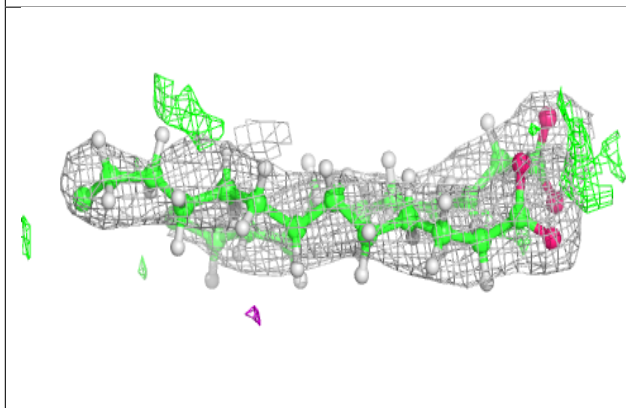
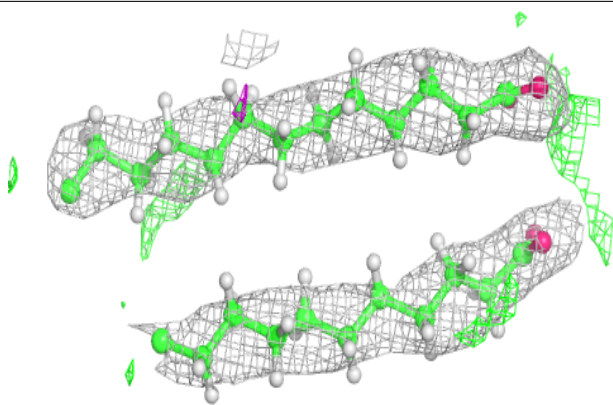
Electron density around LMG C 519:

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

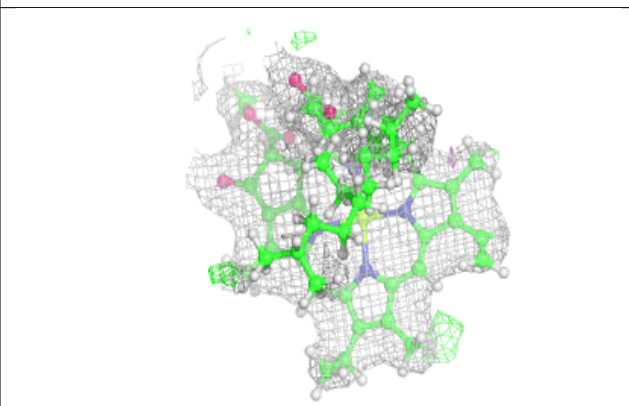
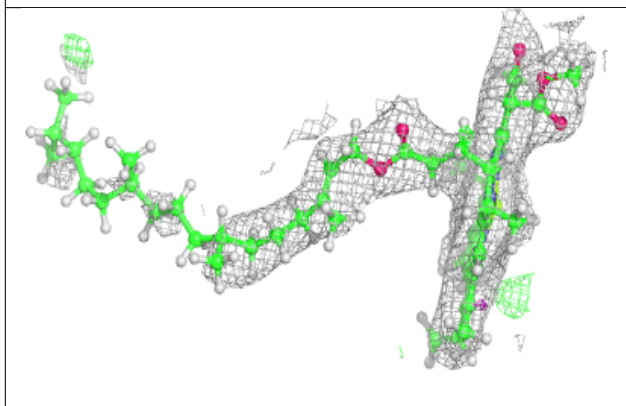
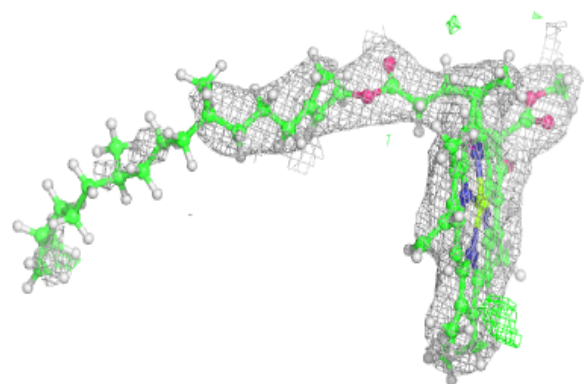


Electron density around LMG D 411:

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

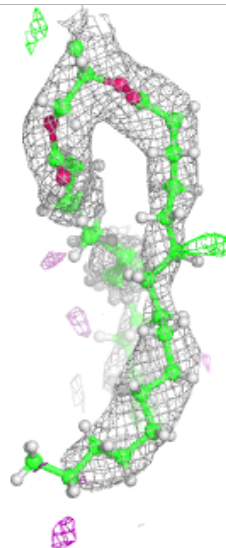
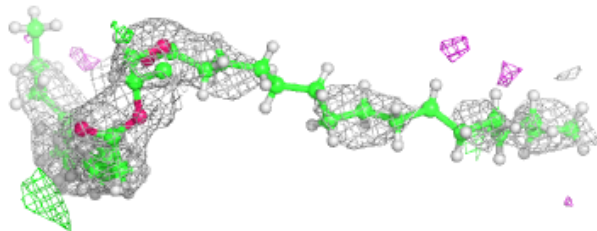
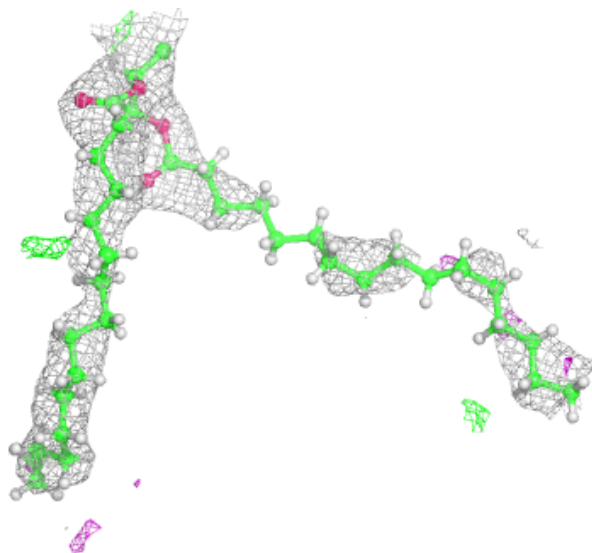
**Electron density around CLA D 404:**

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



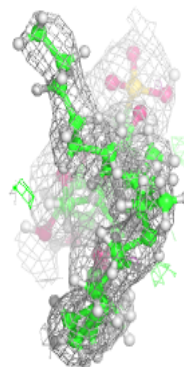
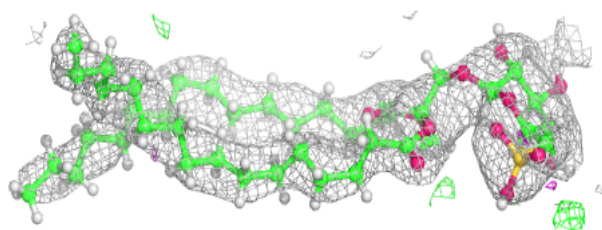
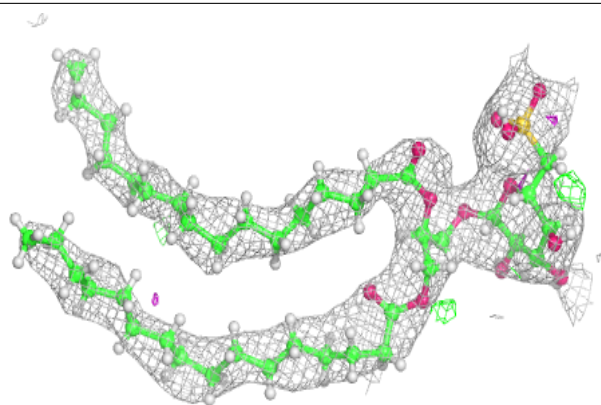
Electron density around SQD A 411:

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

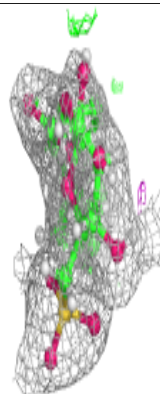
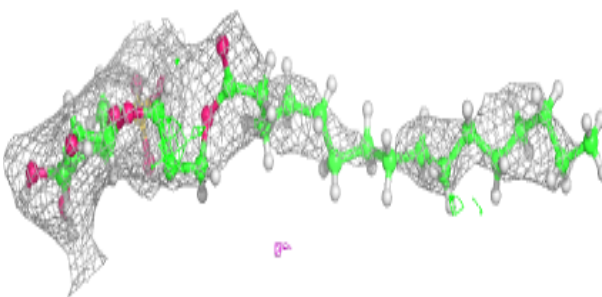
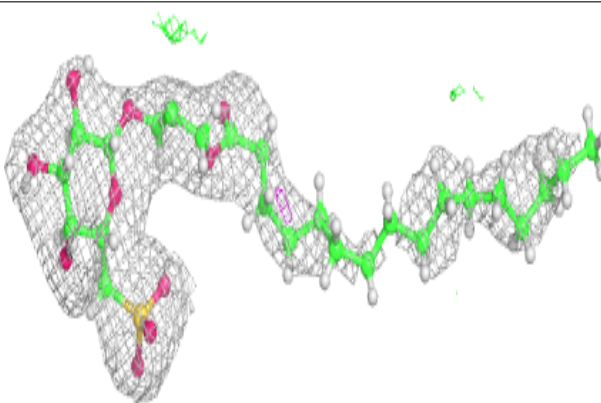


Electron density around SQD B 621:

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

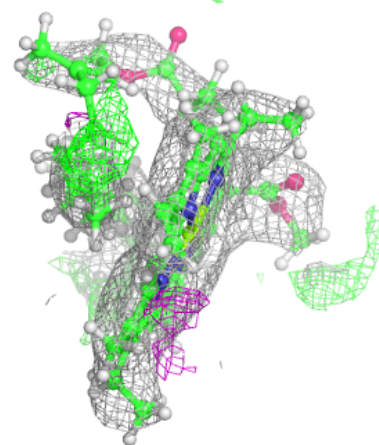
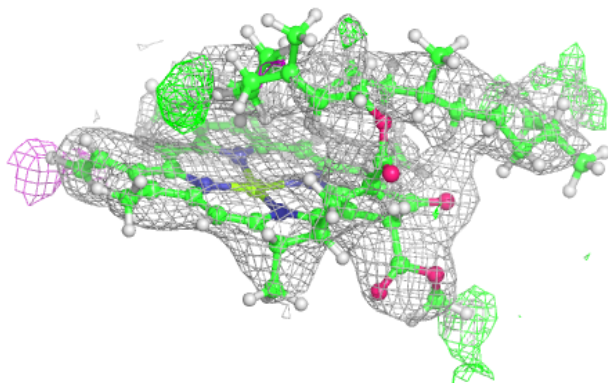
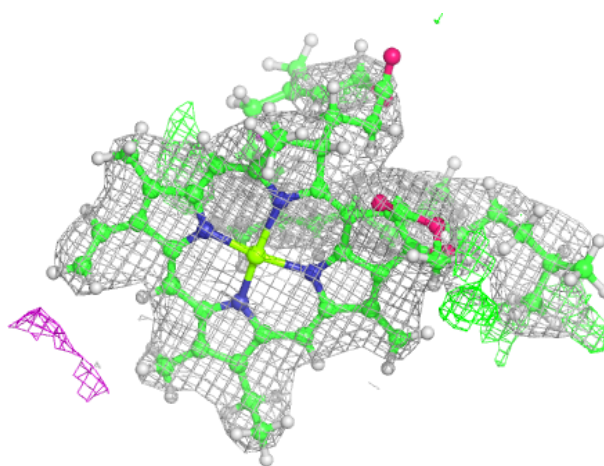
**Electron density around SQD F 101:**

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



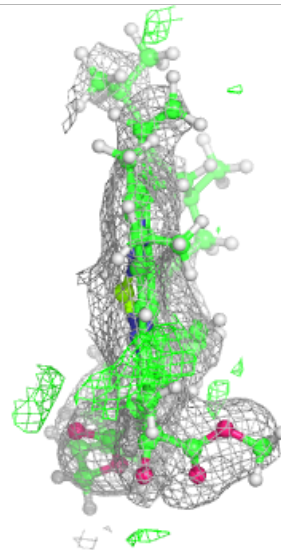
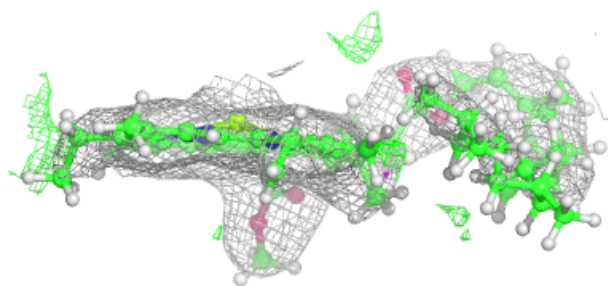
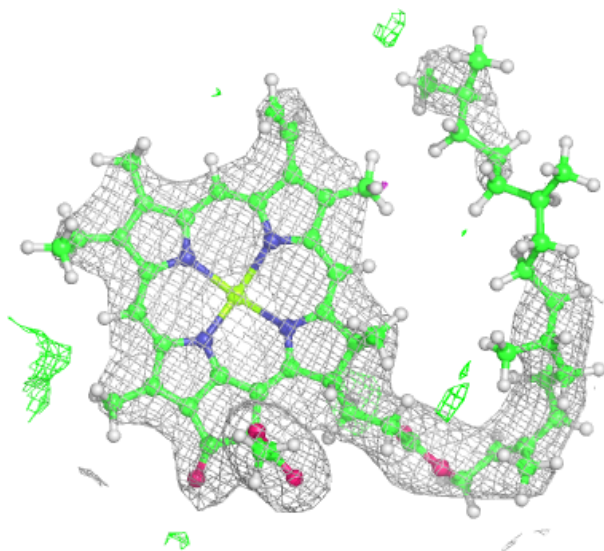
Electron density around CLA B 601:

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



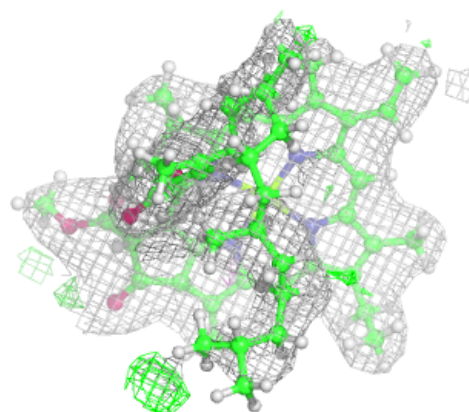
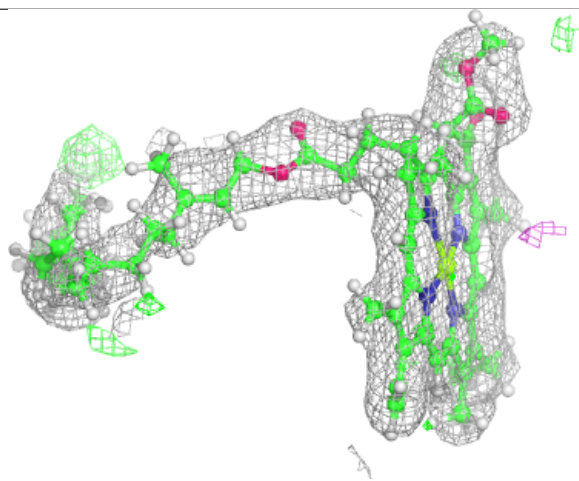
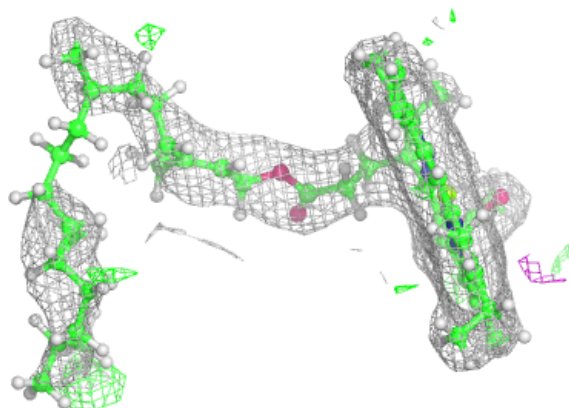
Electron density around CLA C 513:

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



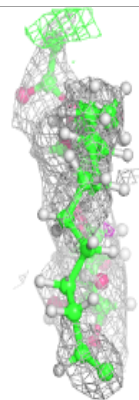
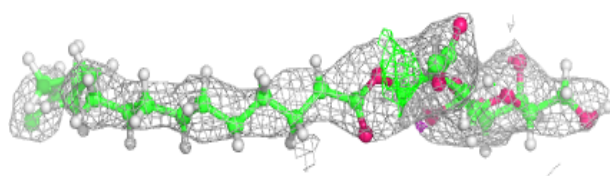
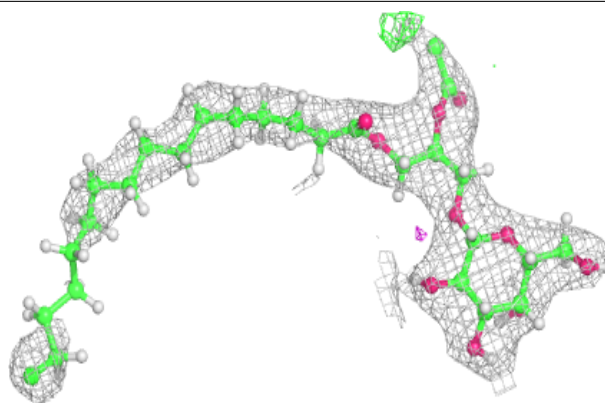
Electron density around CLA a 408:

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

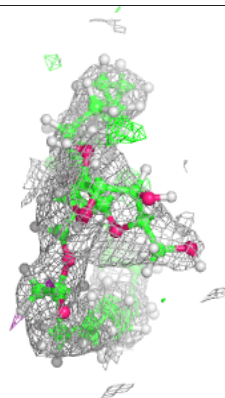
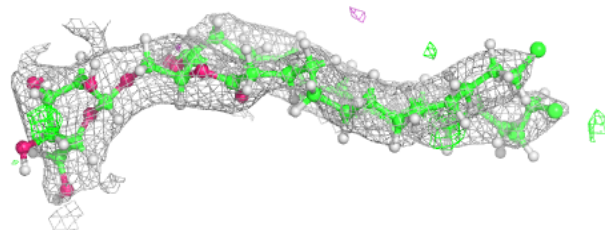
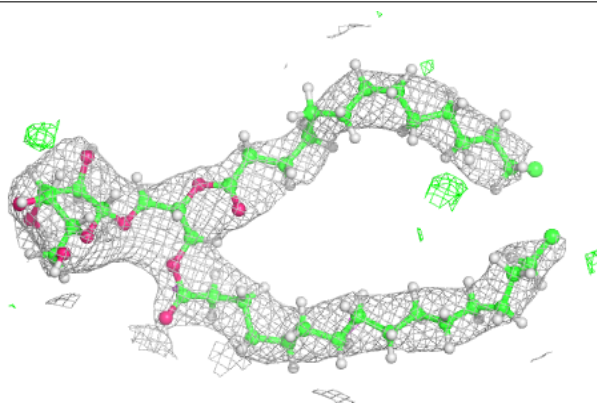


Electron density around LMG c 519:

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

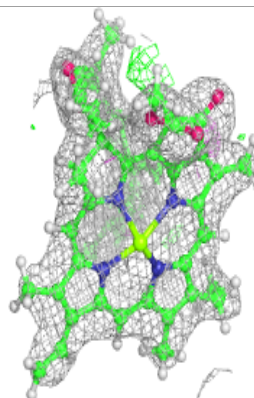
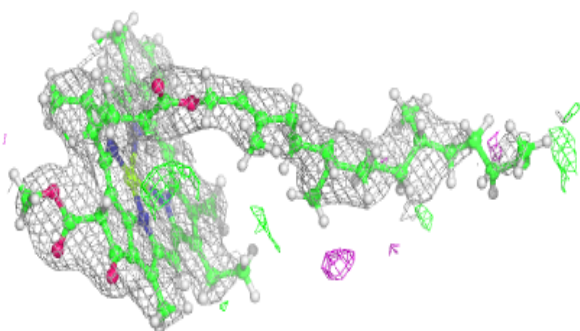
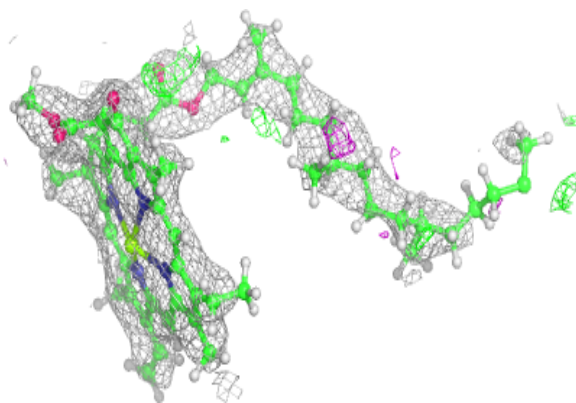
**Electron density around LMG c 524:**

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

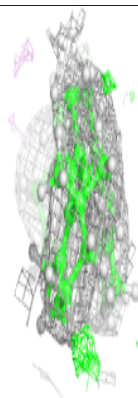
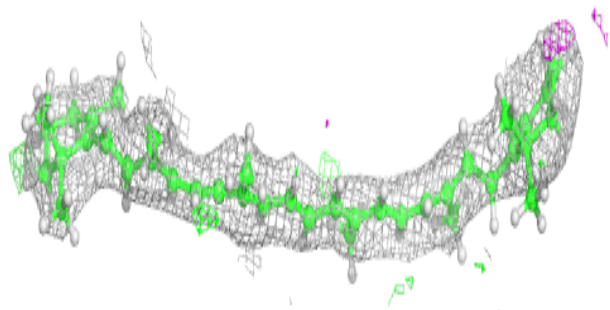
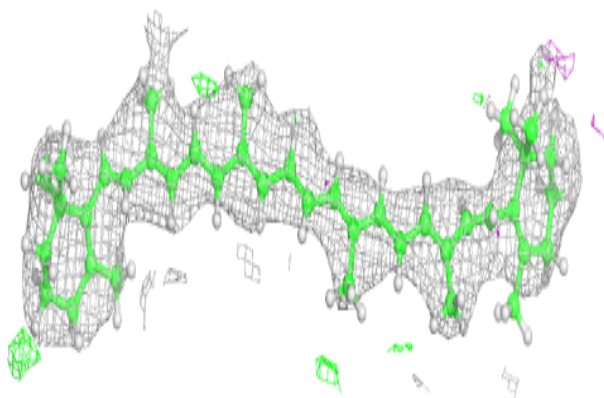


Electron density around CLA c 508:

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

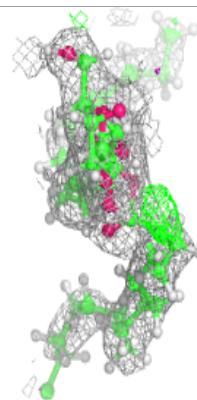
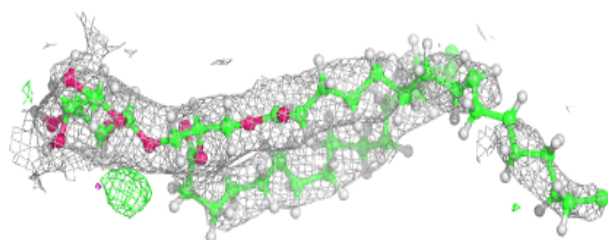
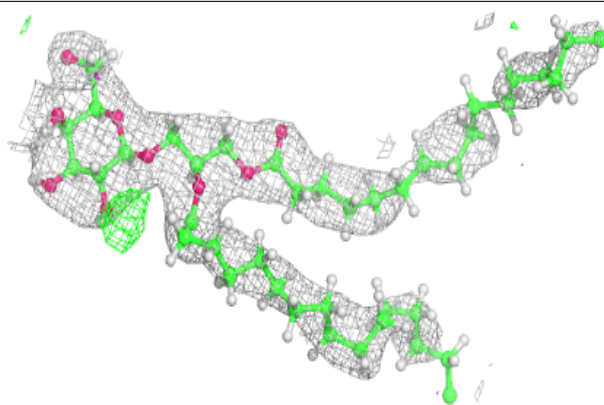
**Electron density around BCR d 405:**

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

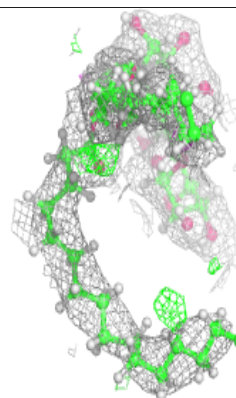
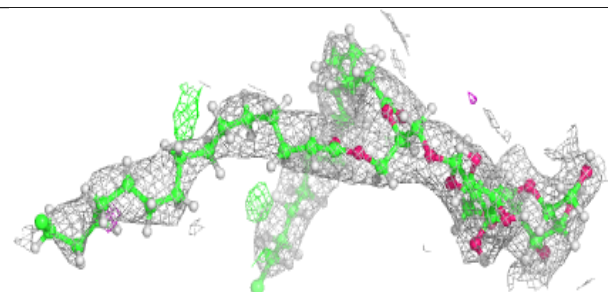
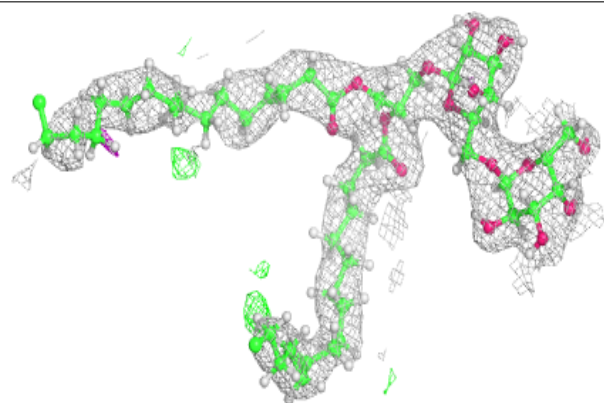


Electron density around LMG D 407:

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

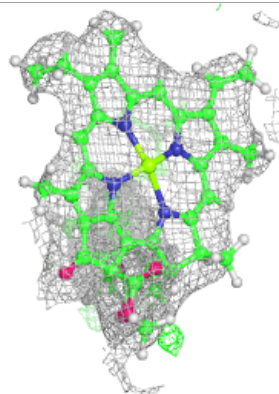
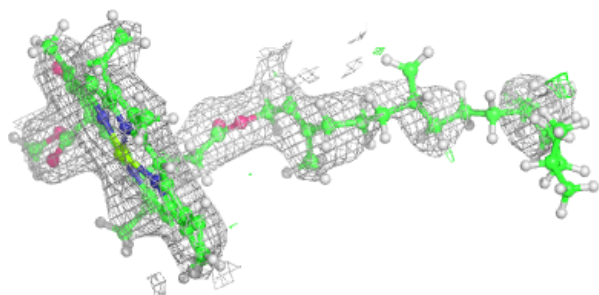
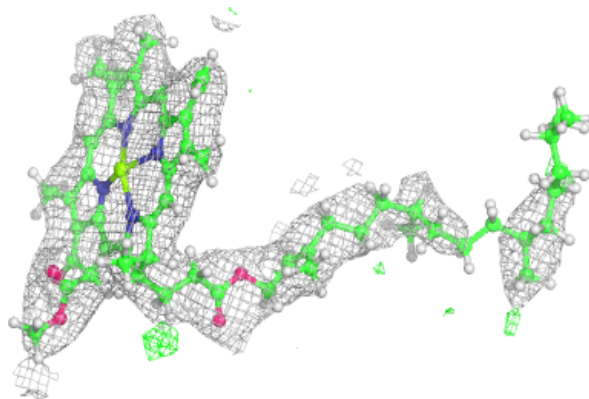
**Electron density around DGD c 517:**

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

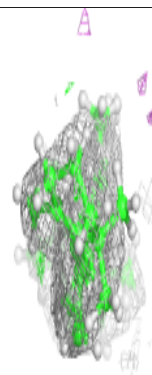
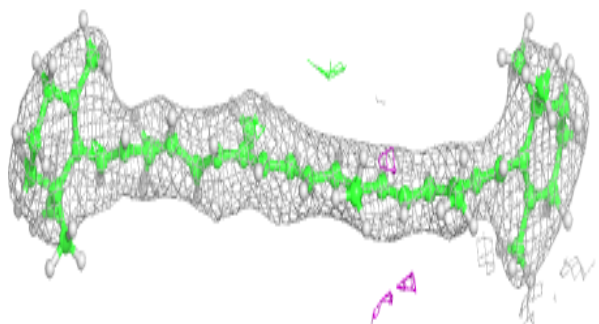
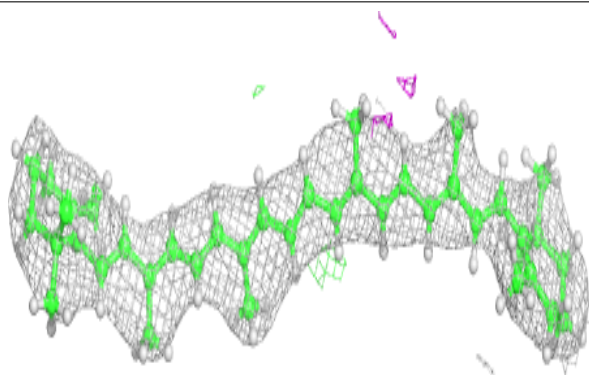


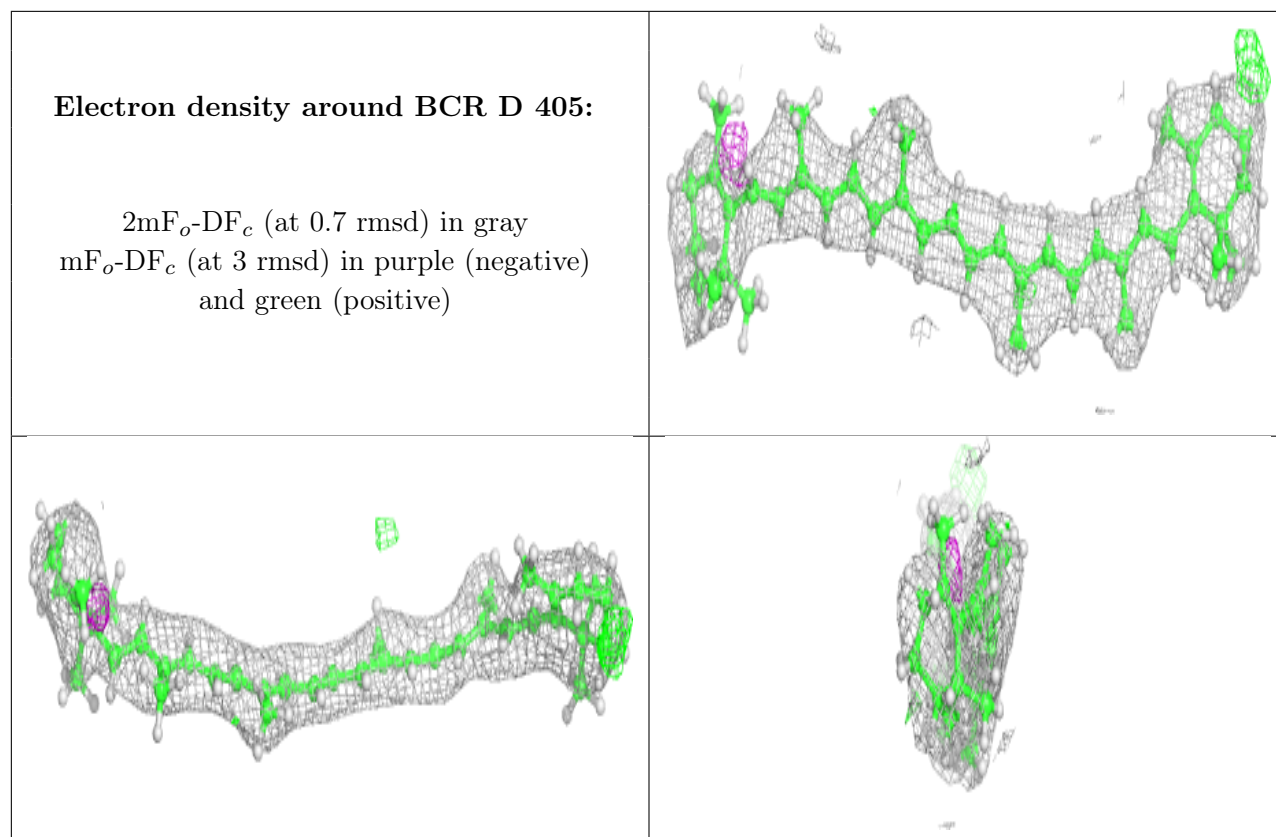
Electron density around CLA d 404:

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

**Electron density around BCR C 515:**

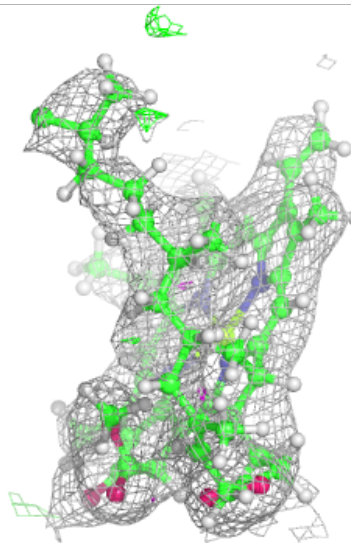
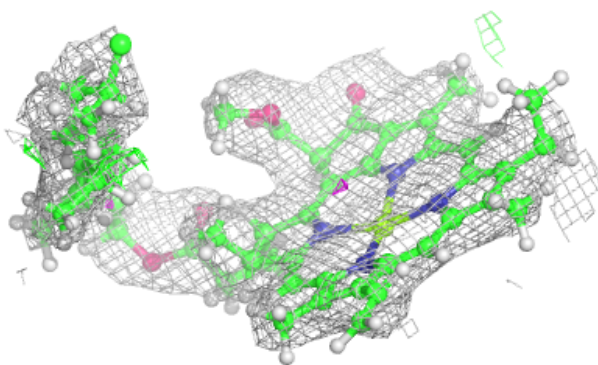
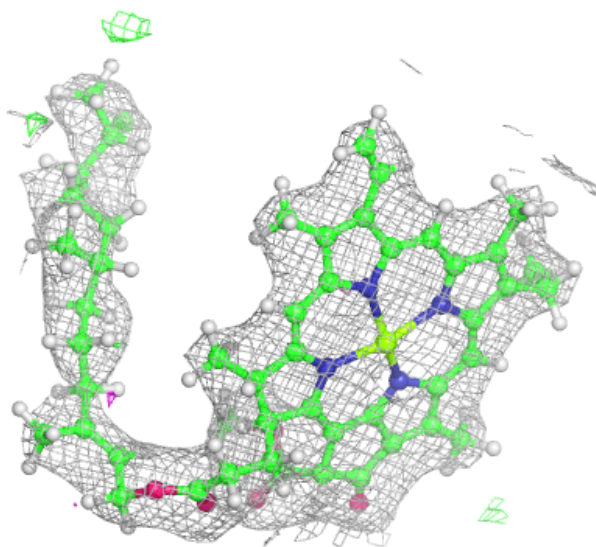
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





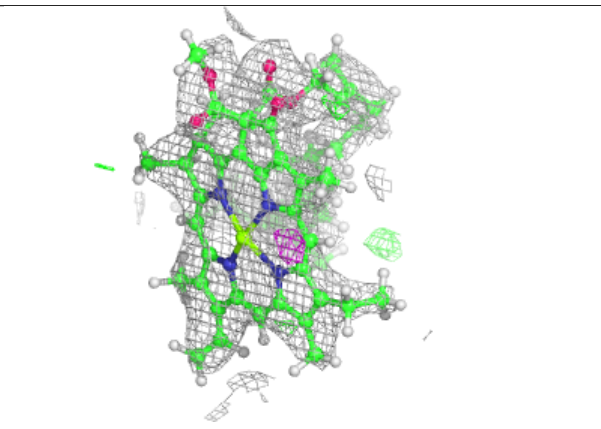
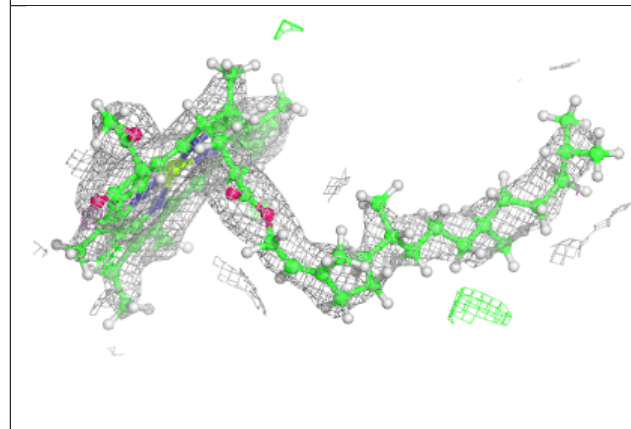
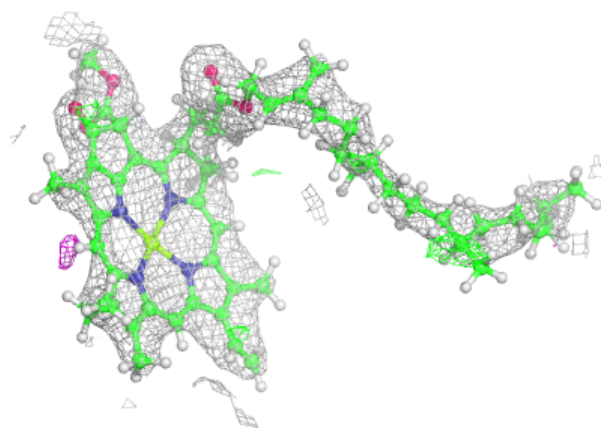
Electron density around CLA b 617:

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



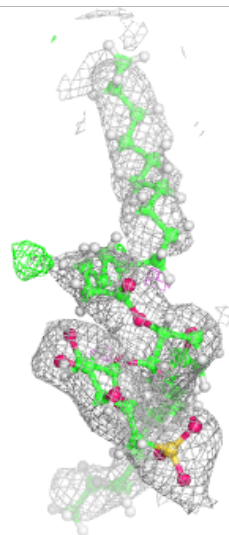
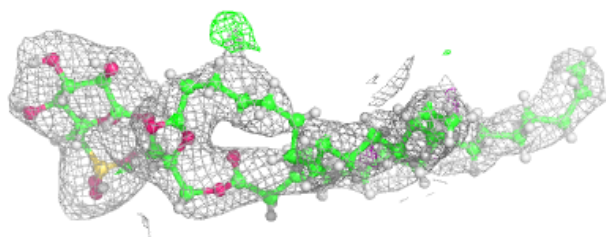
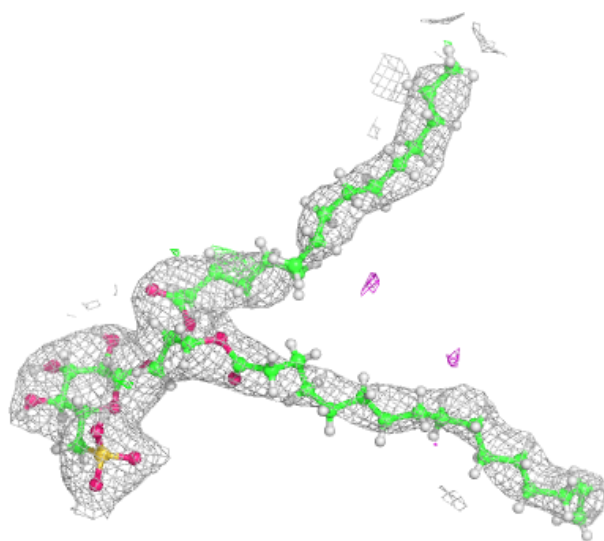
Electron density around CLA c 511:

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



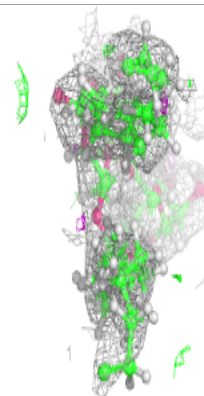
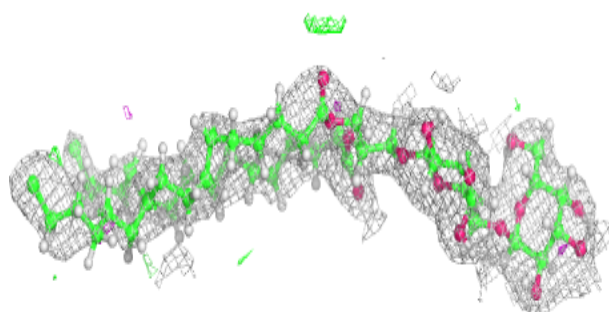
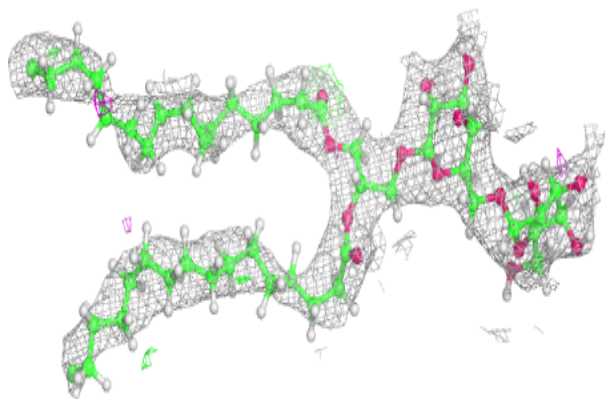
Electron density around SQD a 411:

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

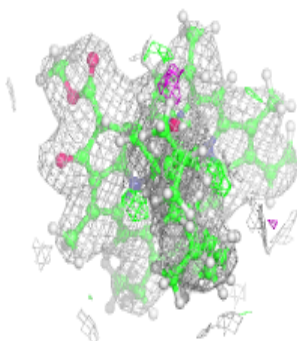
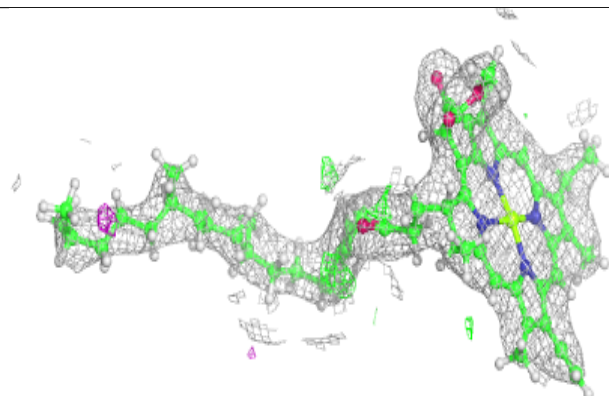
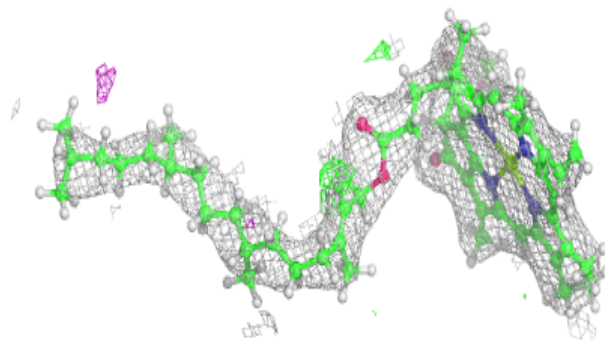


Electron density around DGD c 518:

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

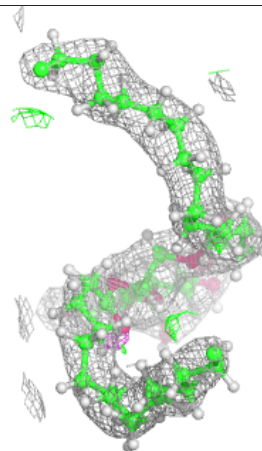
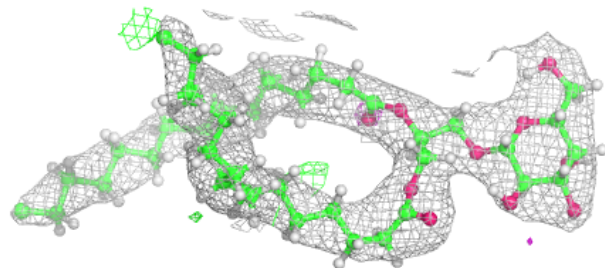
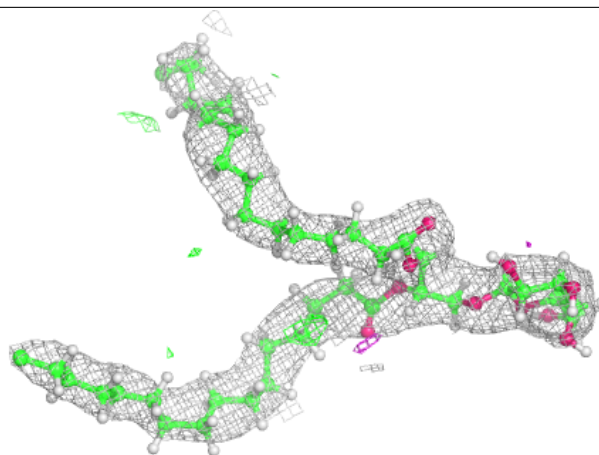
**Electron density around CLA c 502:**

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



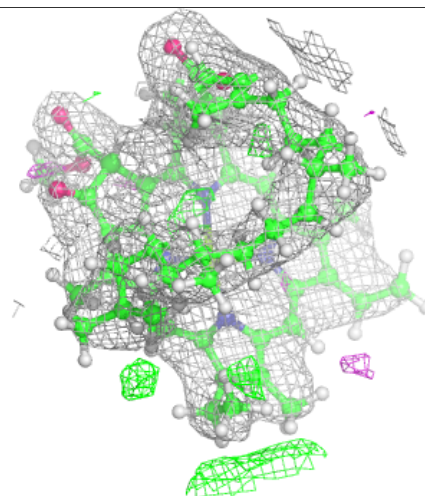
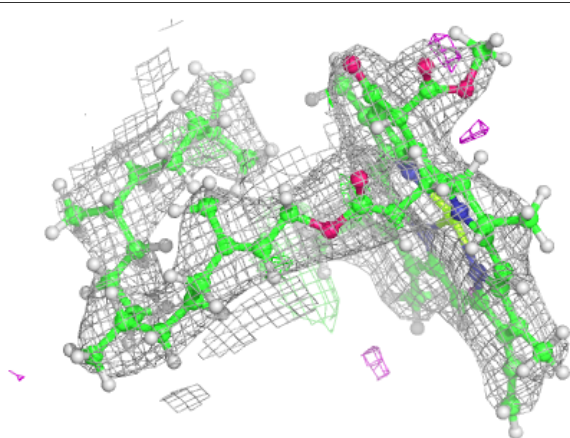
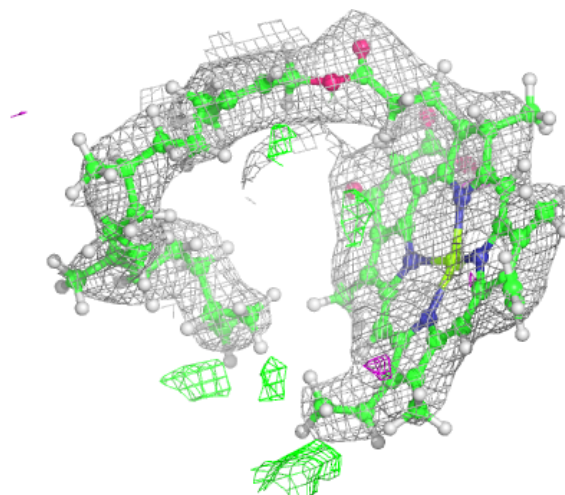
Electron density around LMG M 101:

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



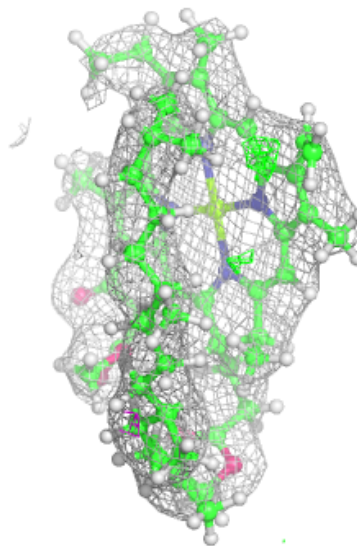
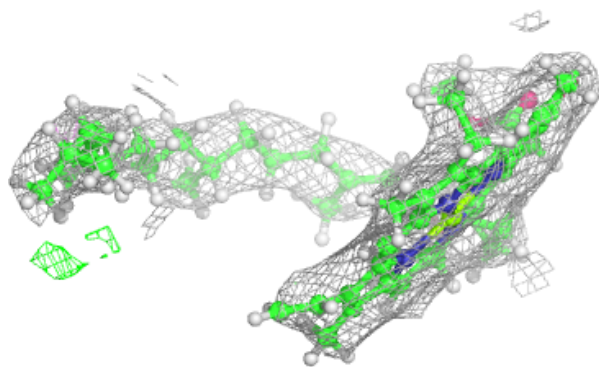
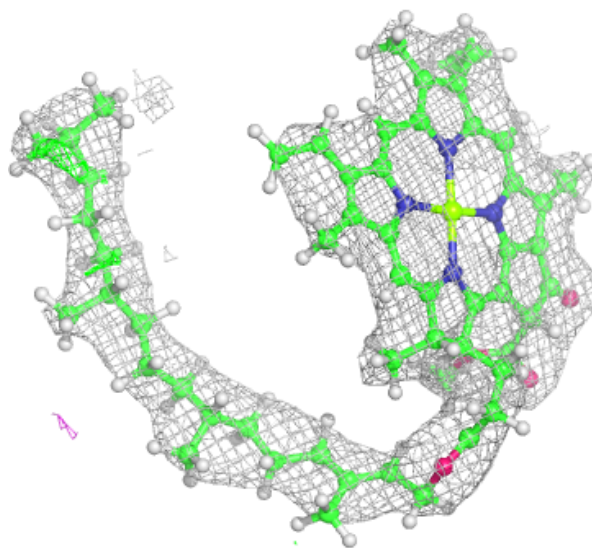
Electron density around CLA c 503:

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



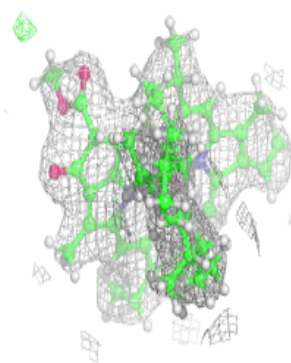
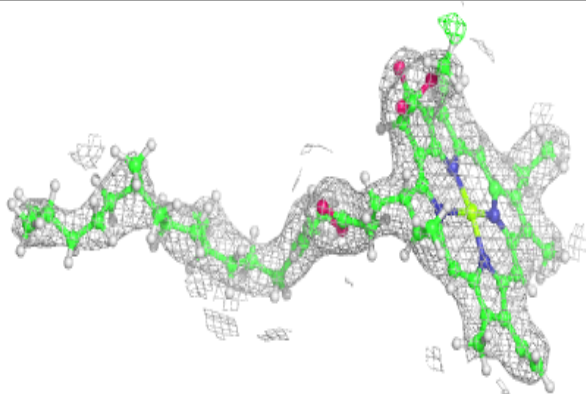
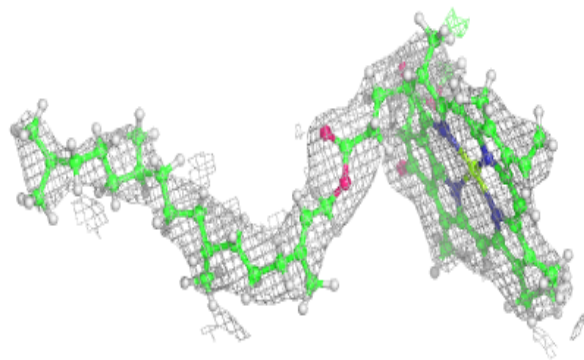
Electron density around CLA c 507:

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

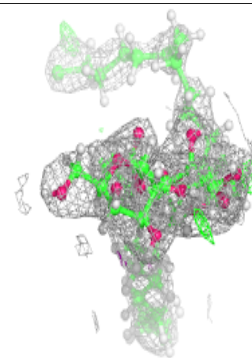
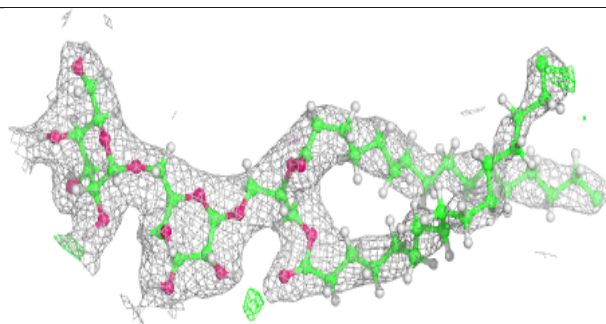
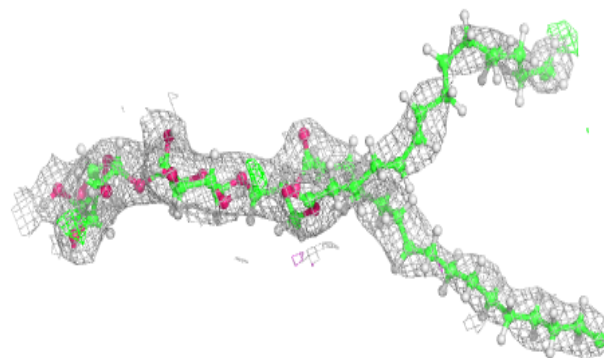


Electron density around CLA C 503:

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

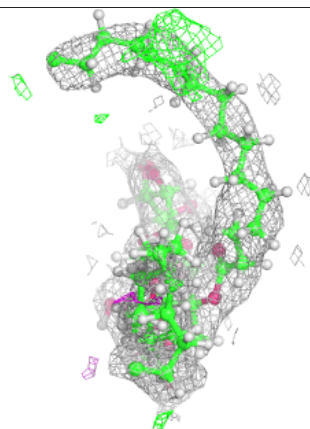
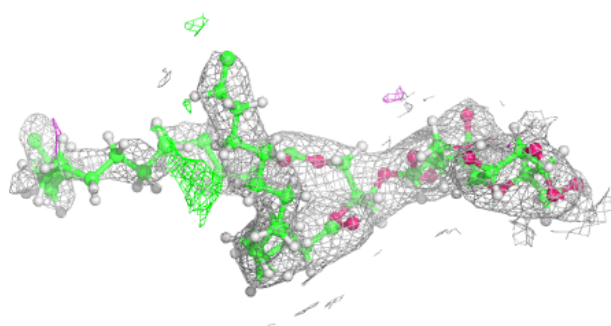
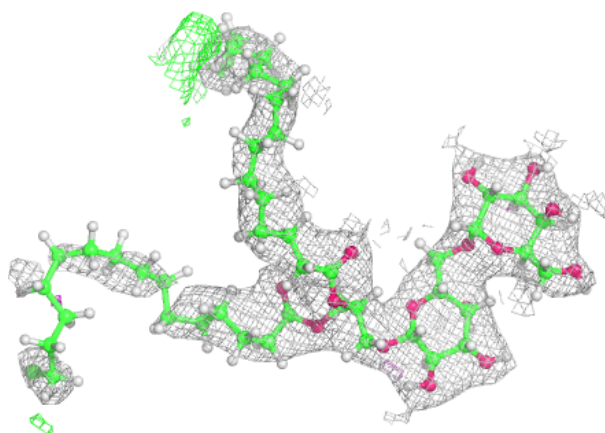
**Electron density around DGD C 516:**

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

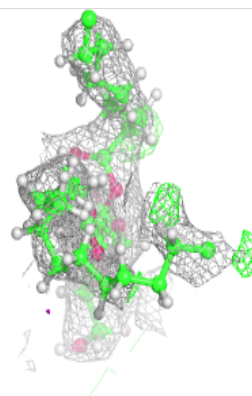
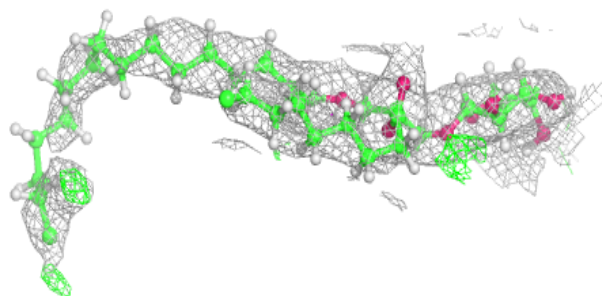
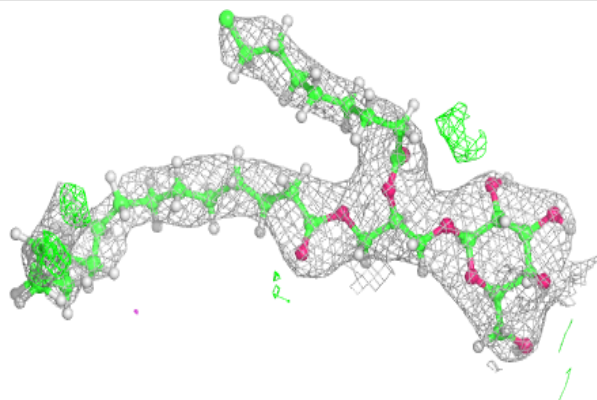


Electron density around DGD C 517:

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

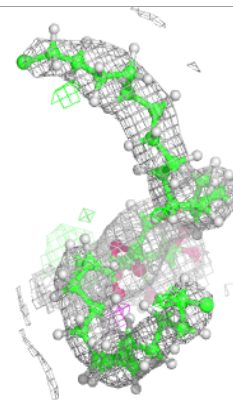
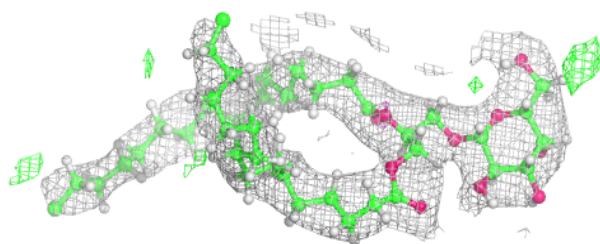
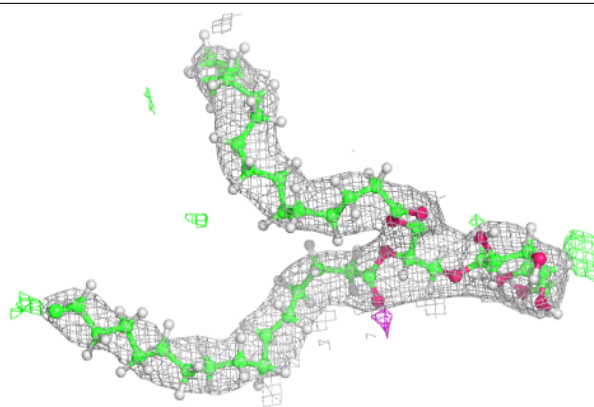
**Electron density around LMG d 411:**

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

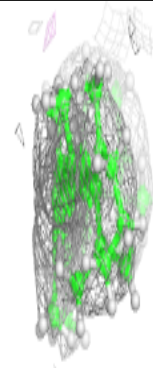
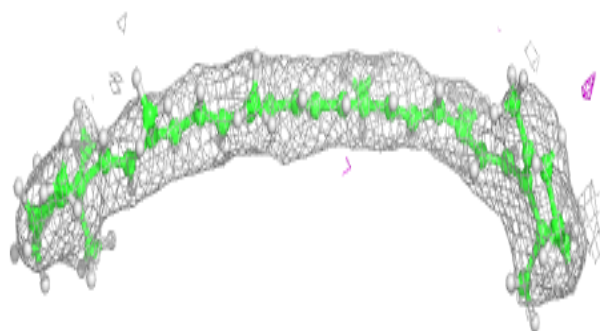
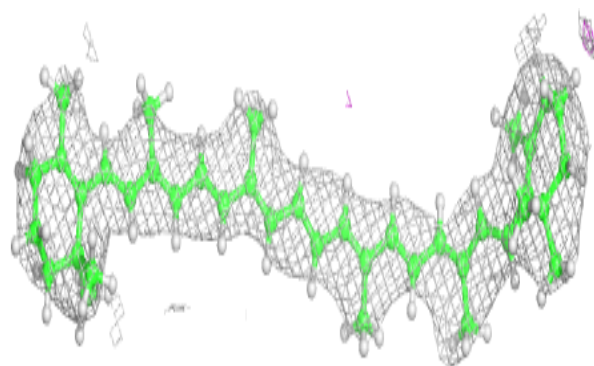


Electron density around LMG m 101:

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

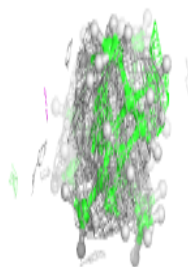
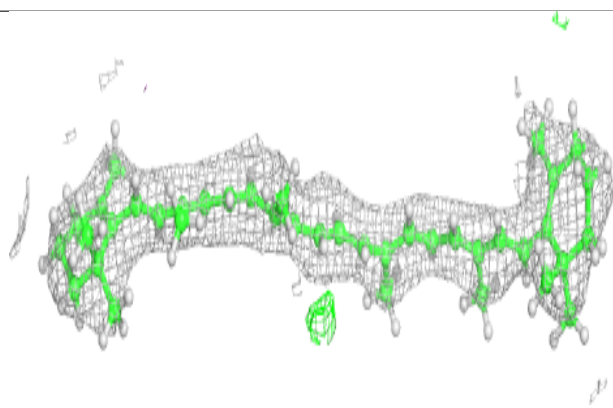
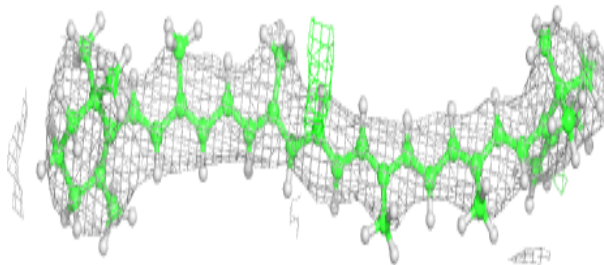
**Electron density around BCR T 101:**

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

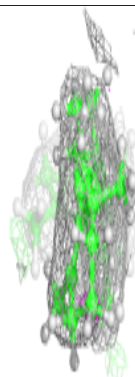
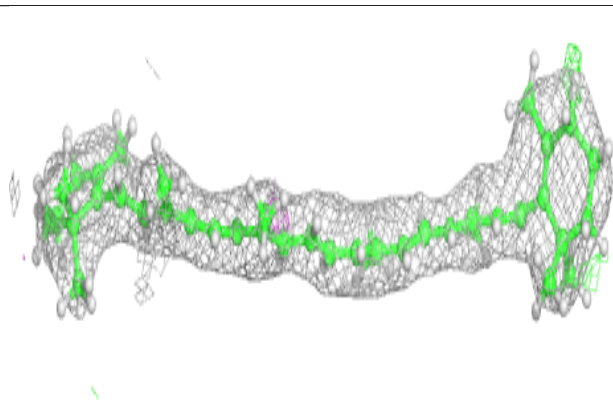
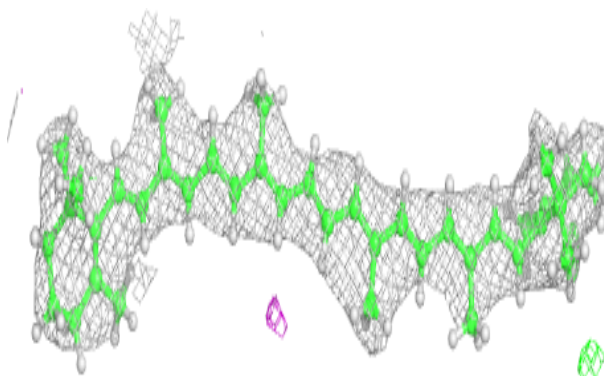


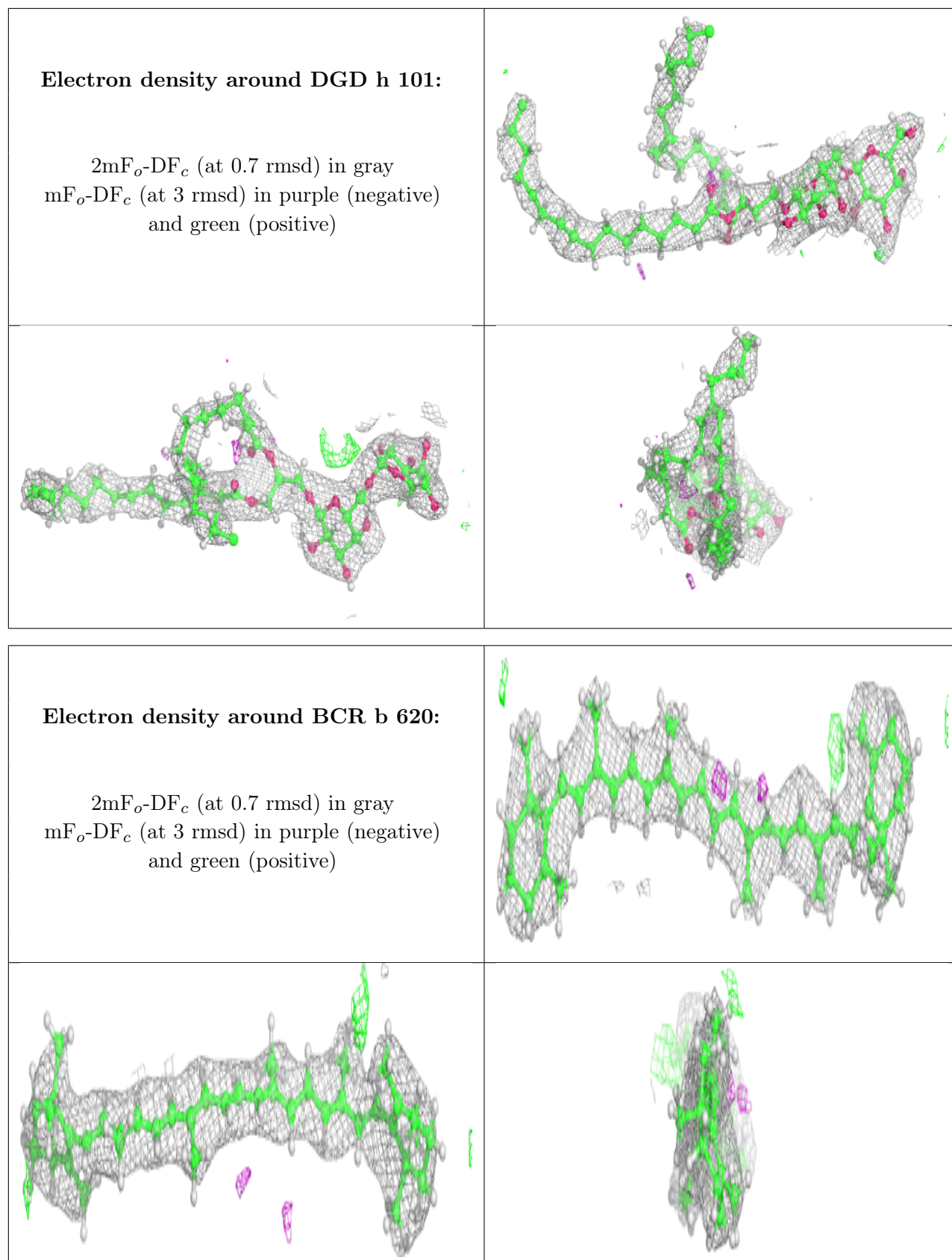
Electron density around BCR Z 101:

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

**Electron density around BCR b 618:**

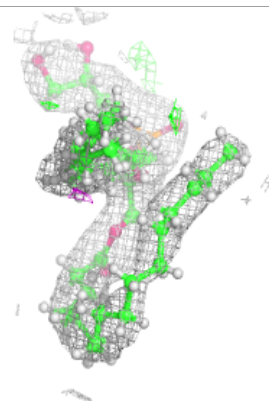
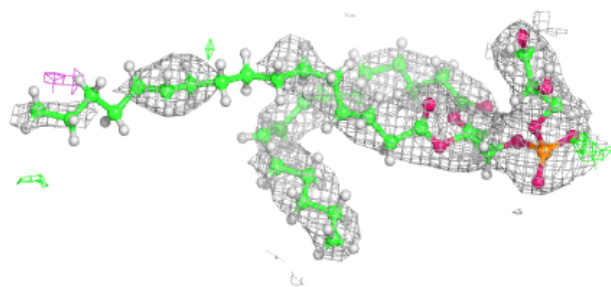
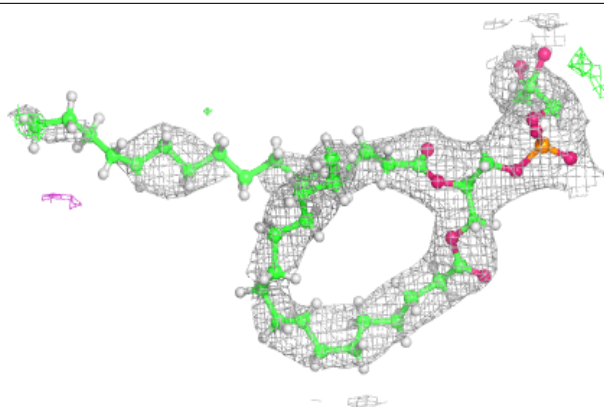
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



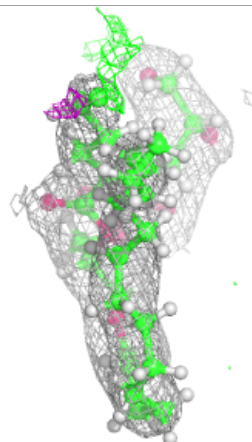
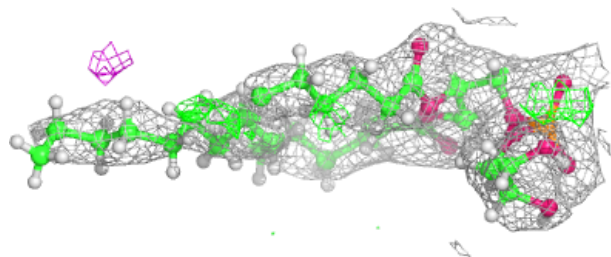
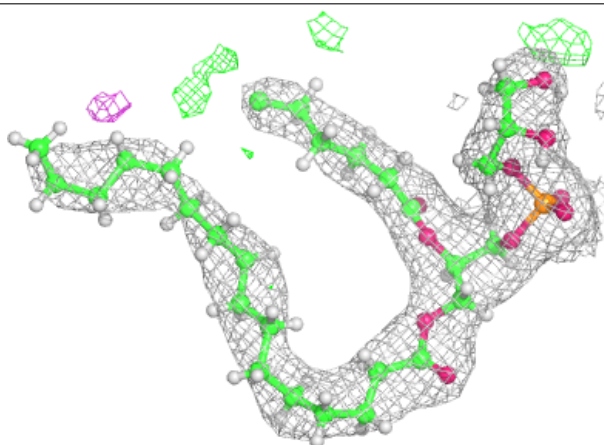


Electron density around LHG d 407:

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

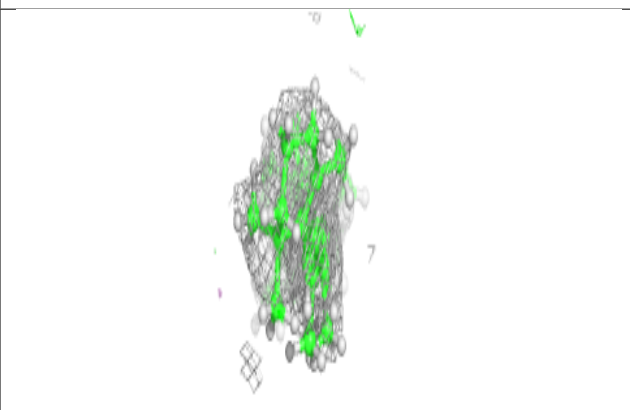
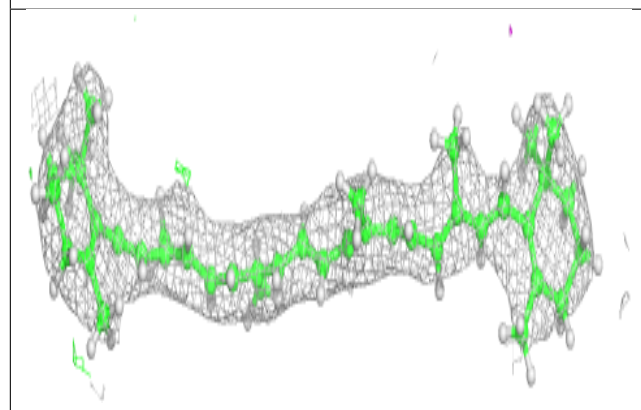
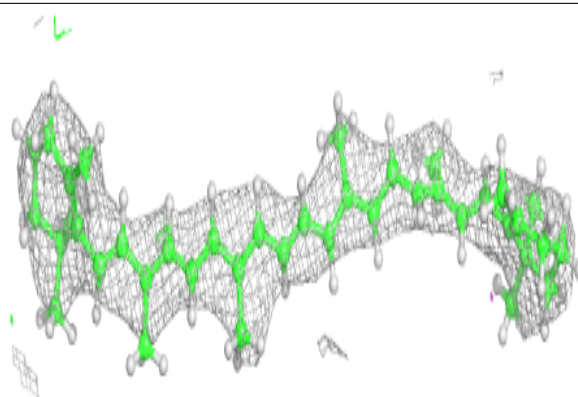
**Electron density around LHG d 409:**

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

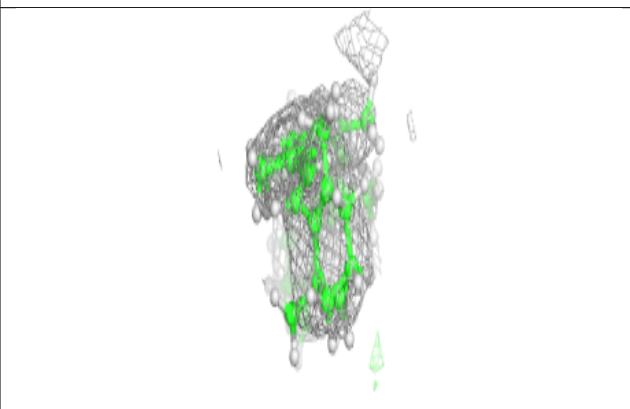
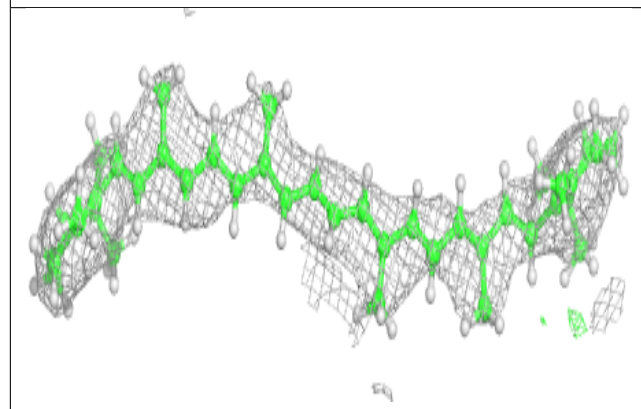
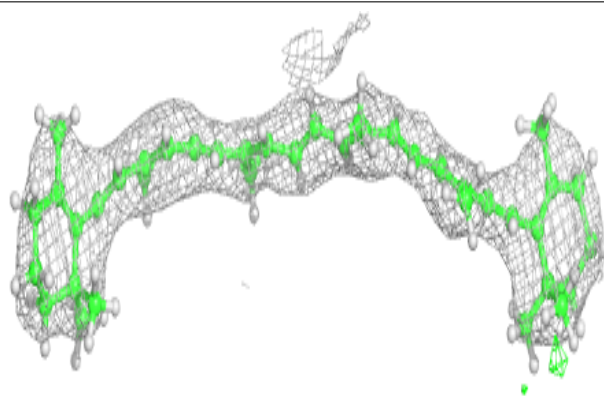


Electron density around BCR c 514:

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

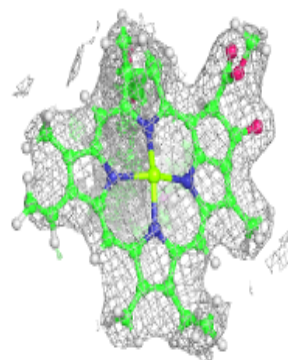
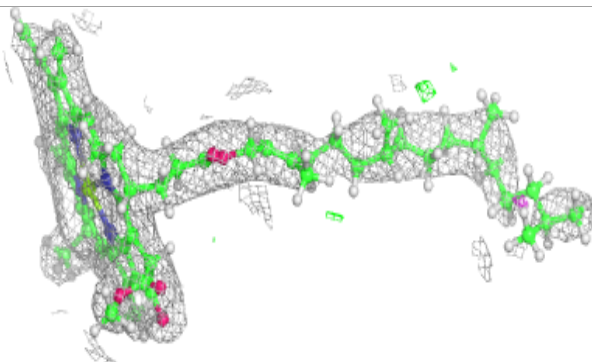
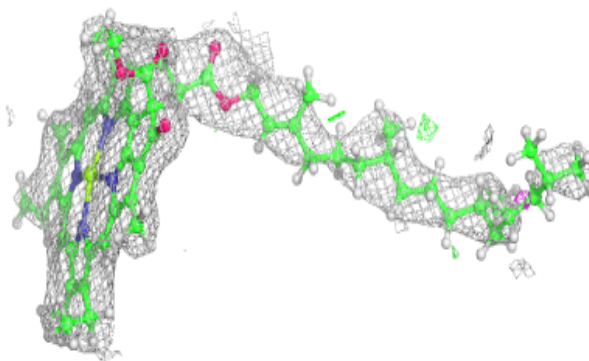
**Electron density around BCR c 521:**

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

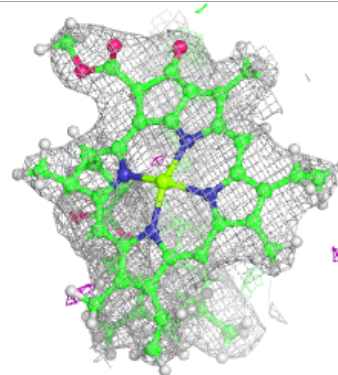
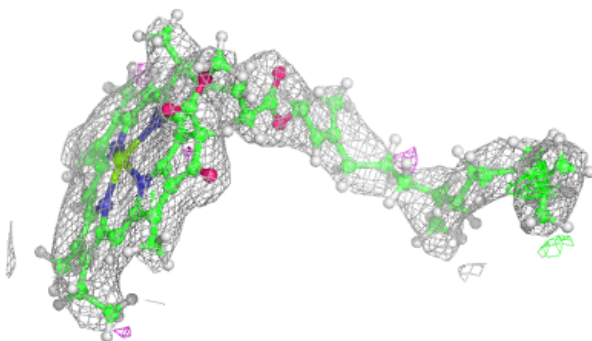
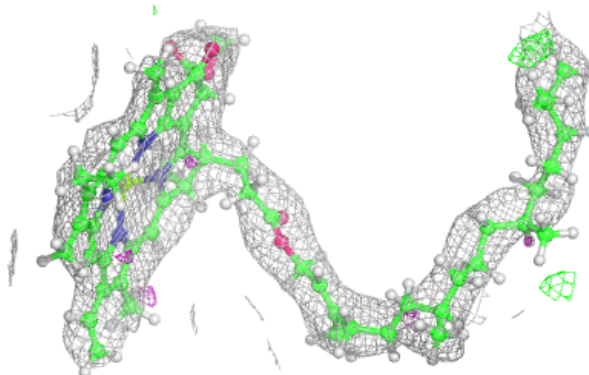


Electron density around CLA b 605:

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

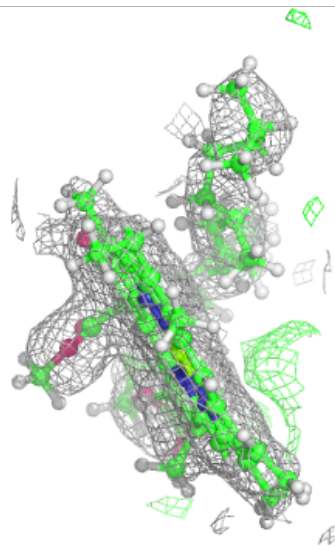
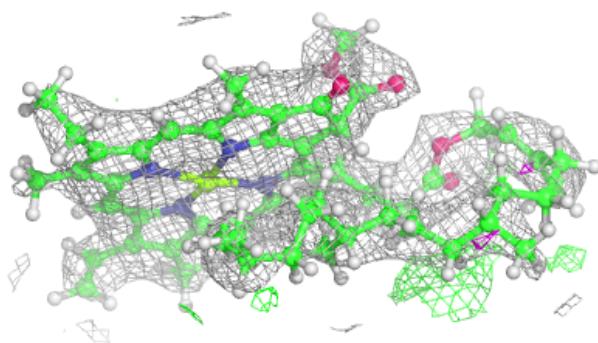
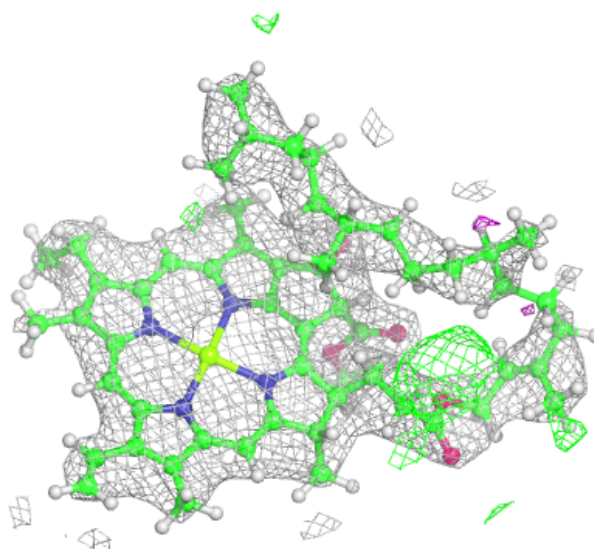
**Electron density around CLA b 607:**

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



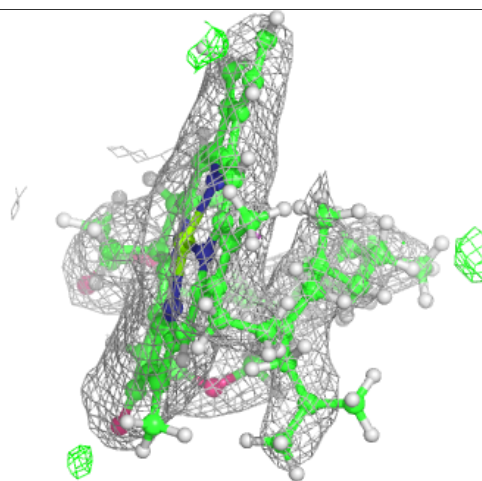
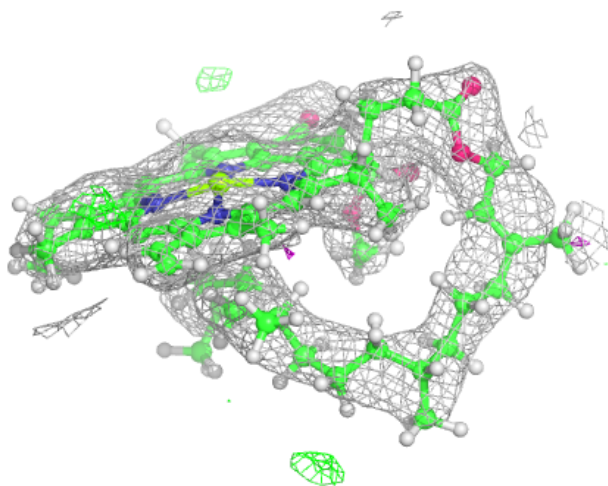
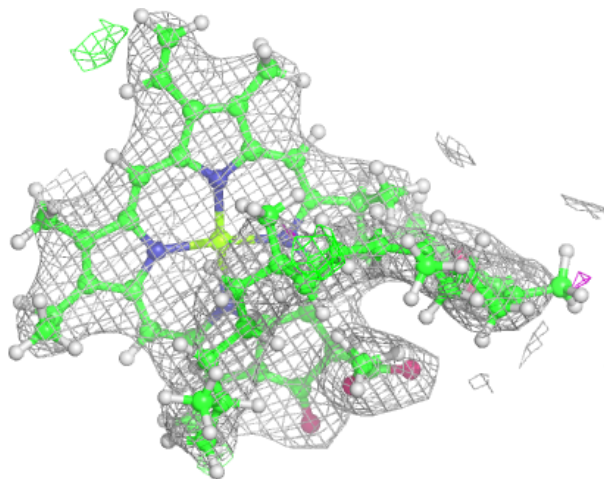
Electron density around CLA c 509:

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



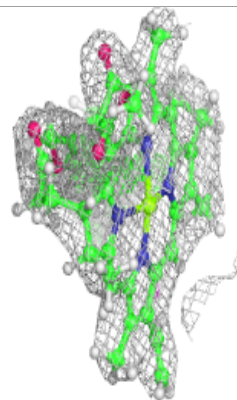
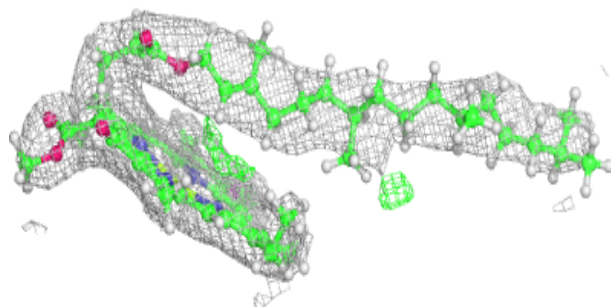
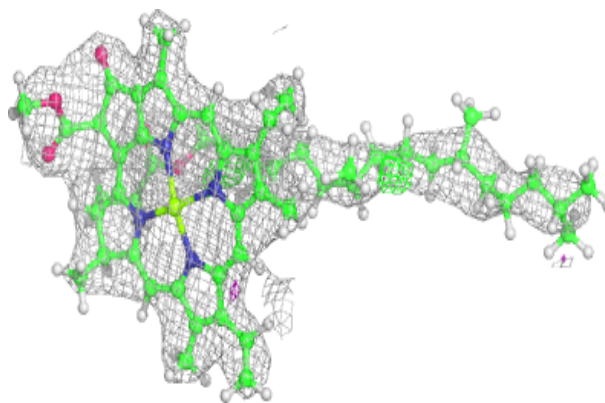
Electron density around CLA c 510:

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



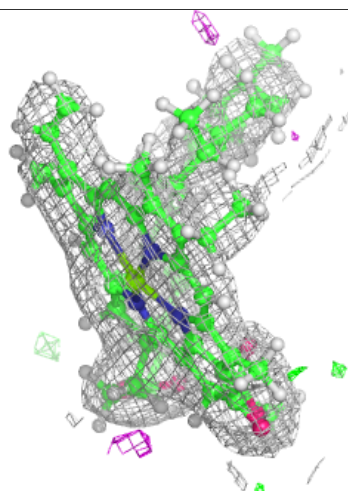
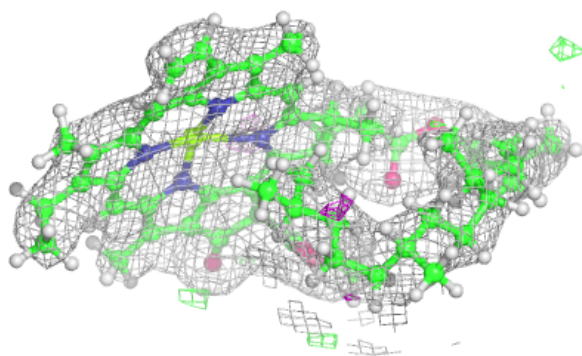
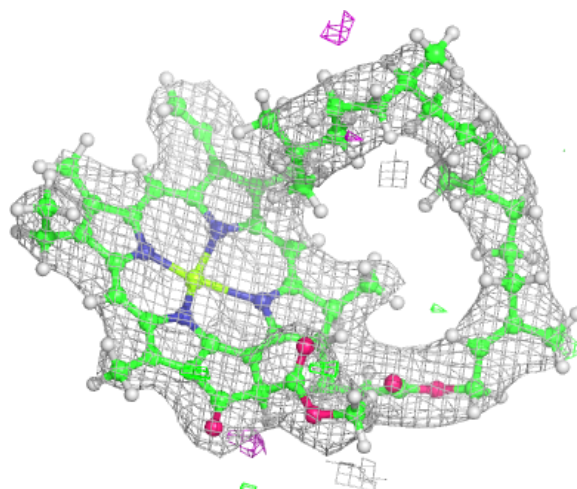
Electron density around CLA b 615:

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



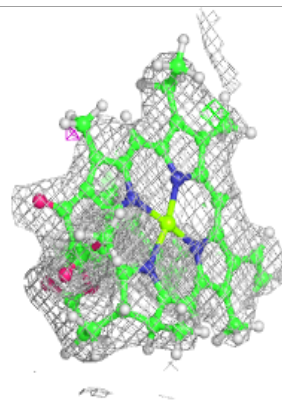
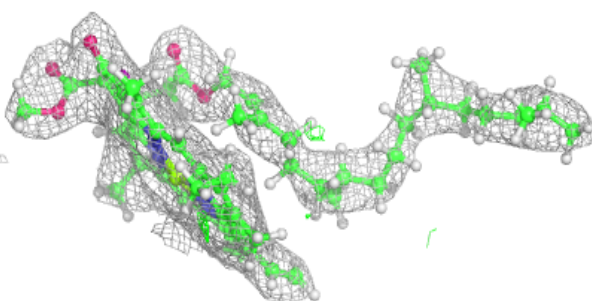
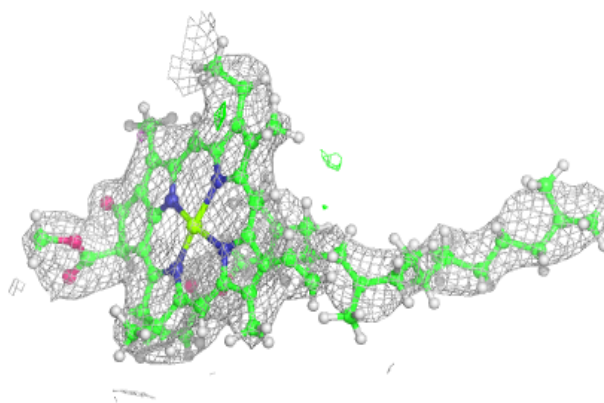
Electron density around CLA b 616:

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

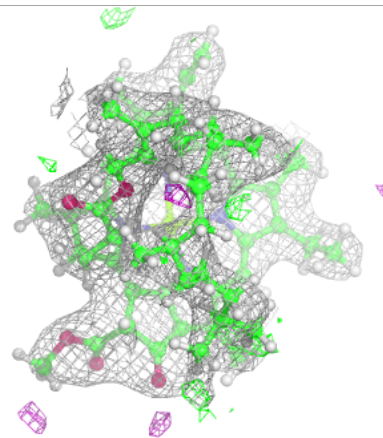
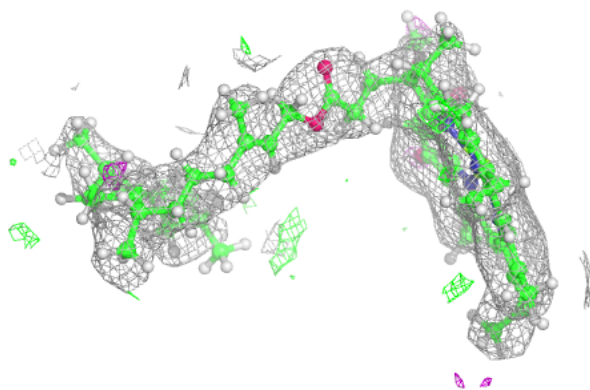
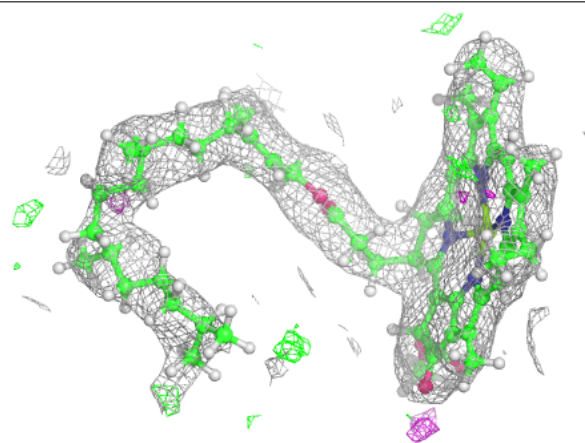


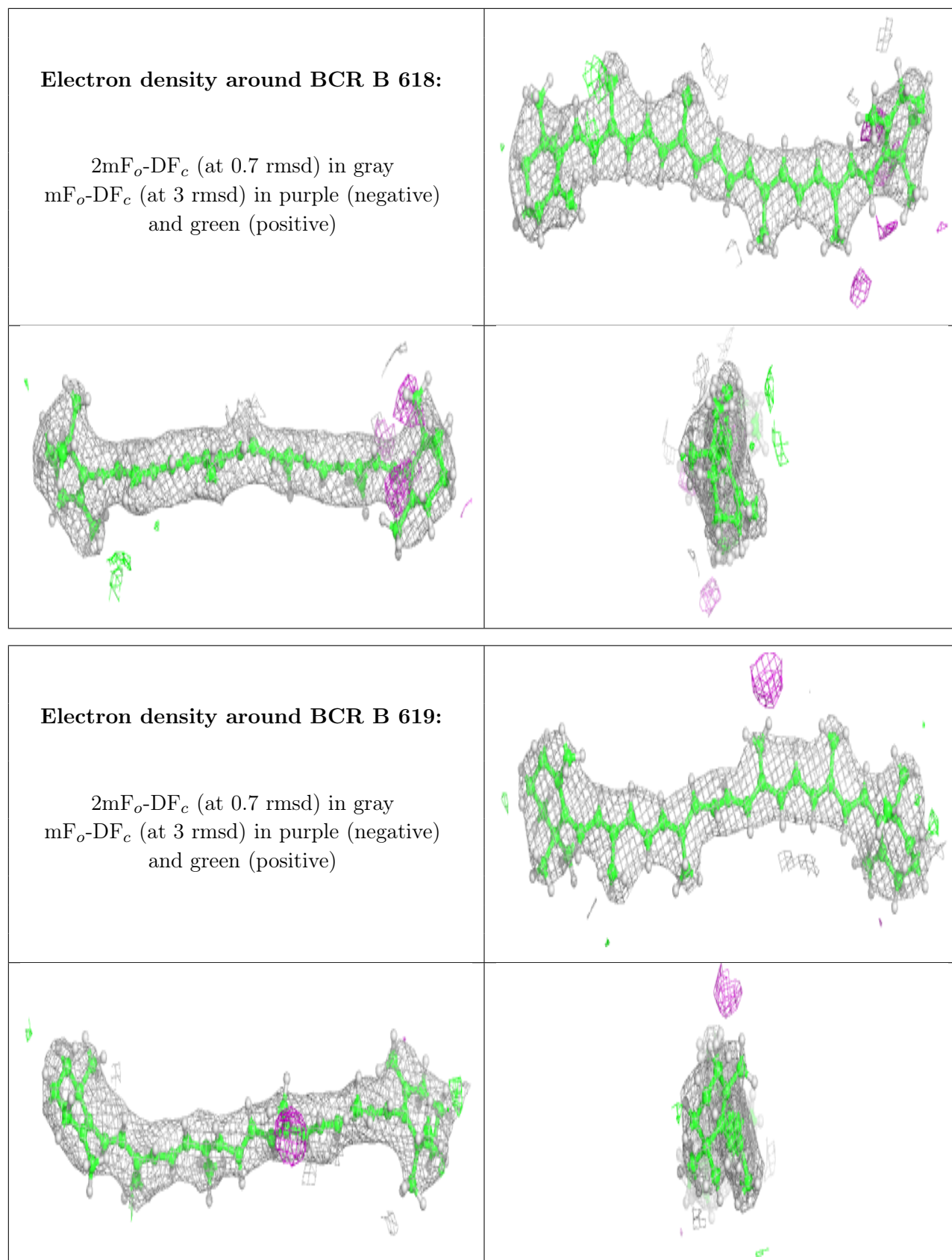
Electron density around CLA C 506:

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

**Electron density around CLA B 606:**

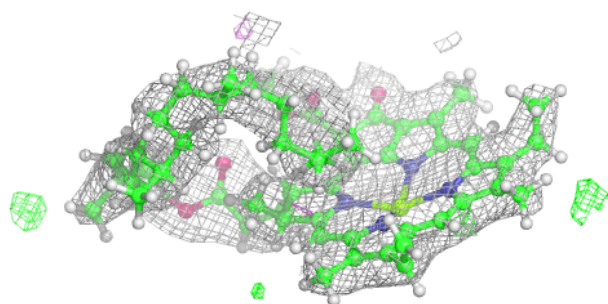
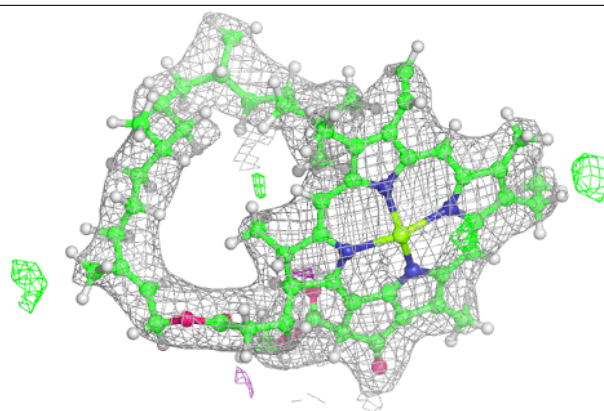
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



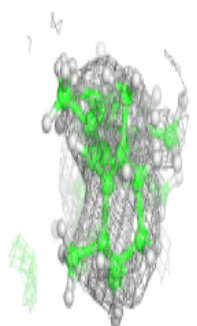
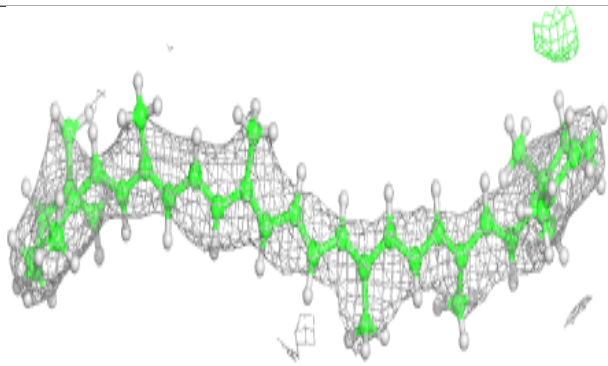
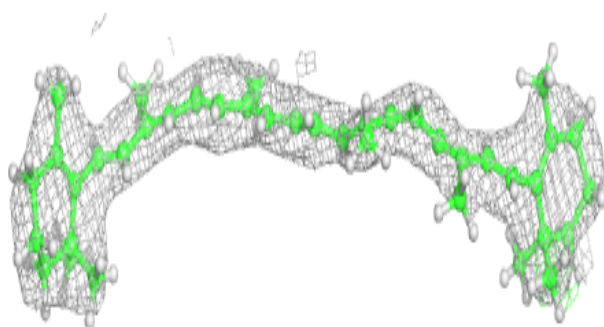


Electron density around CLA B 615:

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

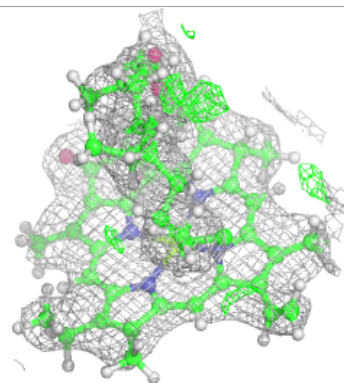
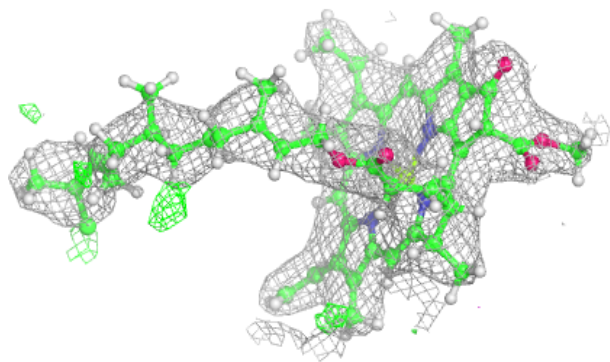
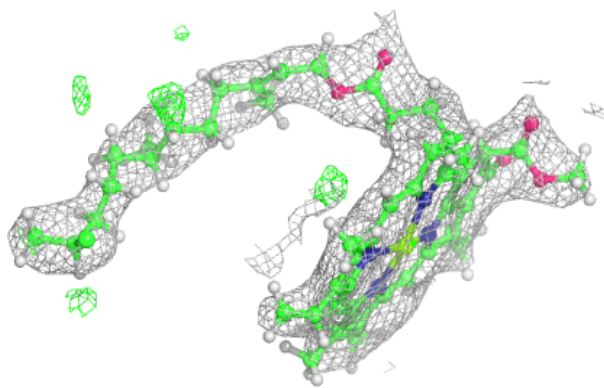
**Electron density around BCR C 520:**

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

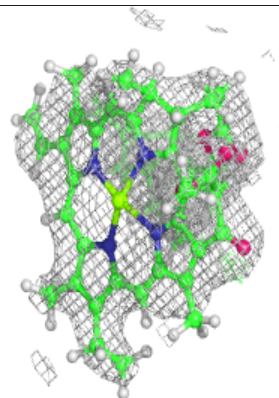
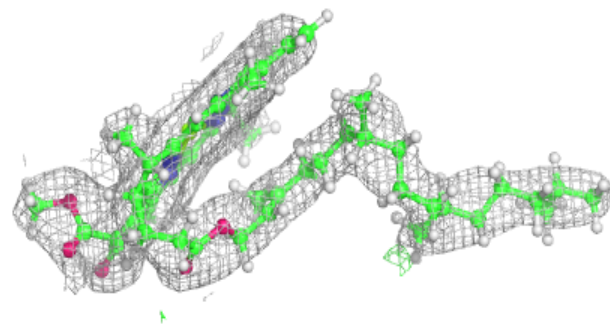
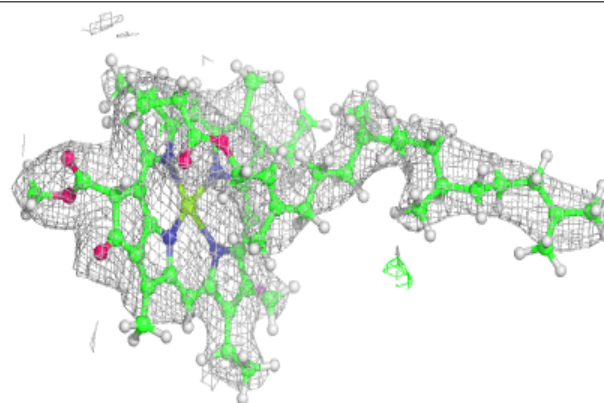


Electron density around CLA c 504:

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

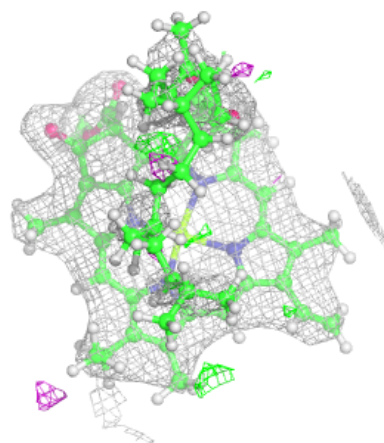
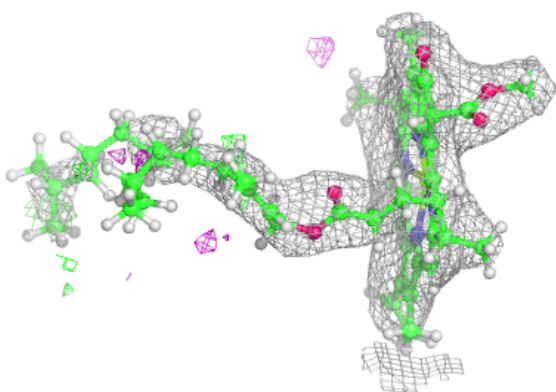
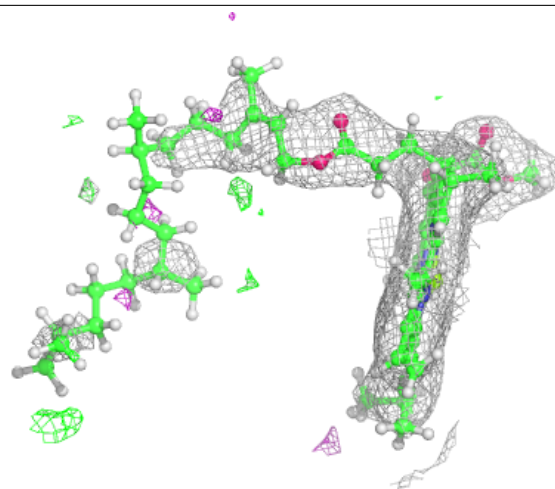
**Electron density around CLA c 505:**

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



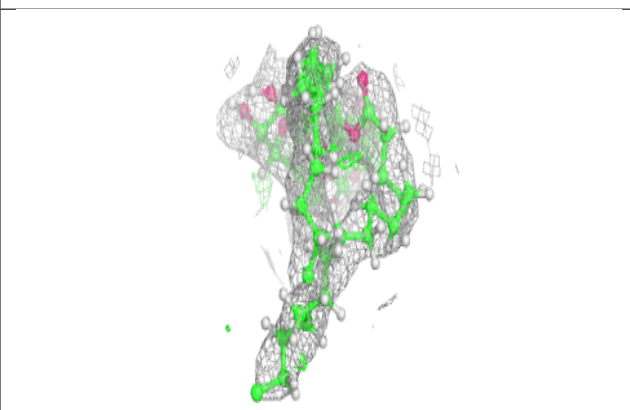
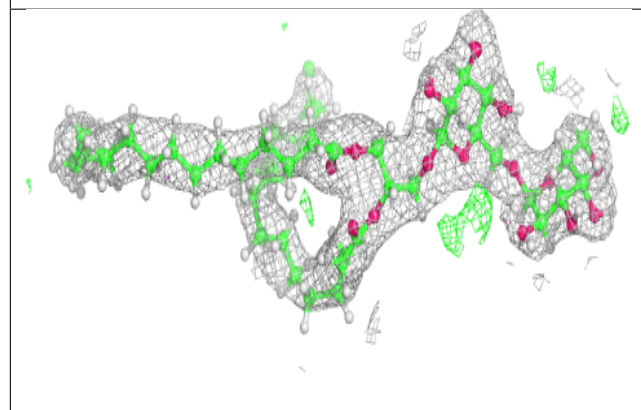
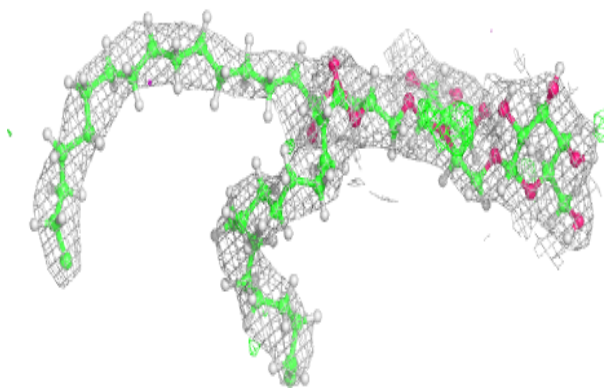
Electron density around CLA c 506:

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

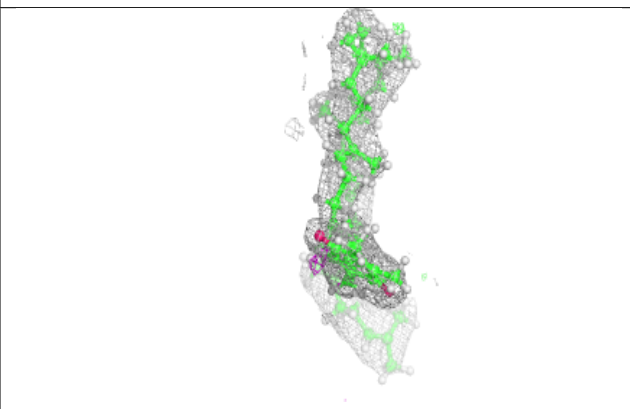
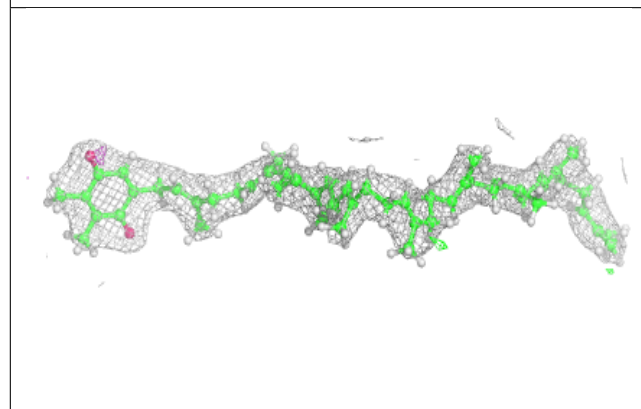
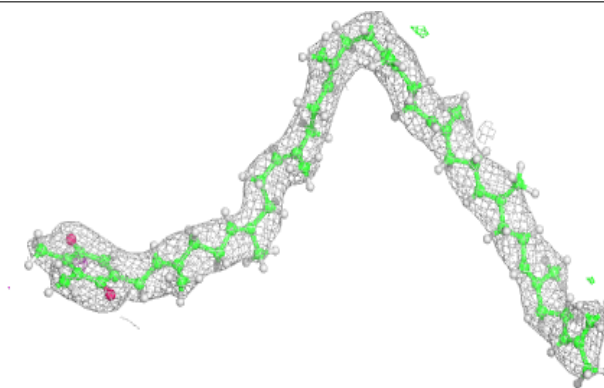


Electron density around DGD H 102:

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

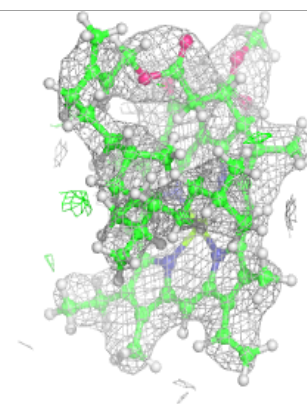
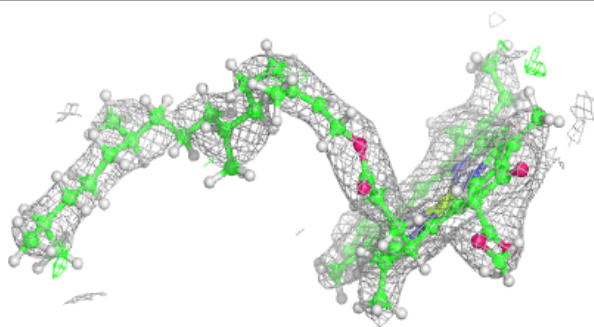
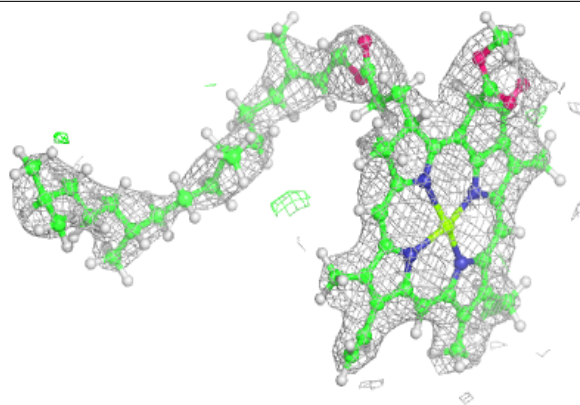
**Electron density around PL9 D 406:**

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

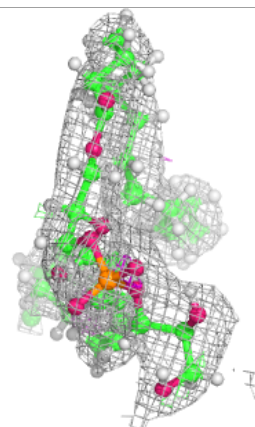
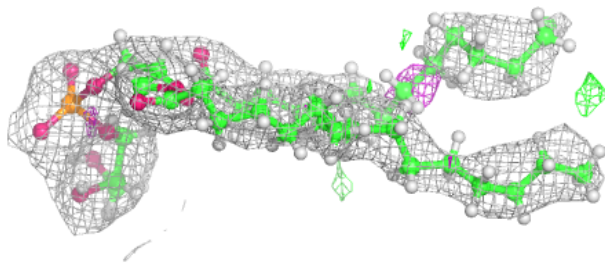
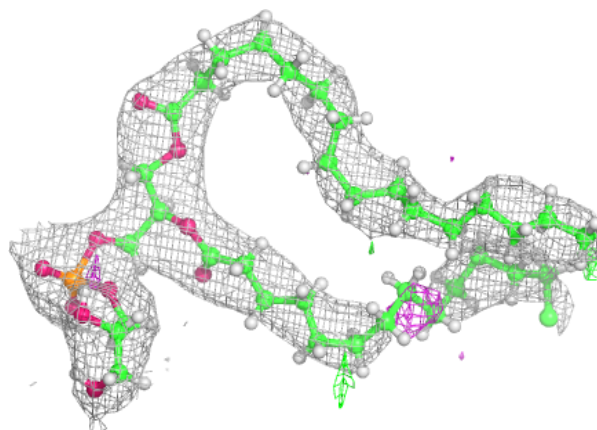


Electron density around CLA C 512:

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

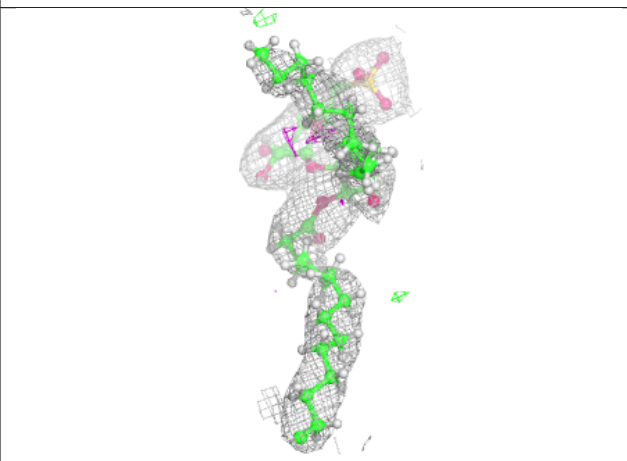
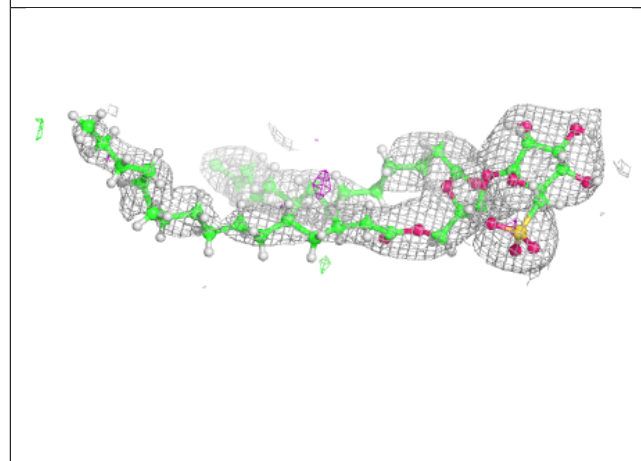
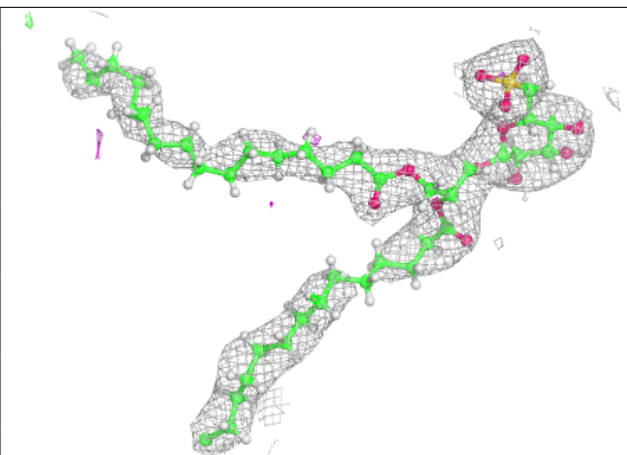
**Electron density around LHG D 409:**

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

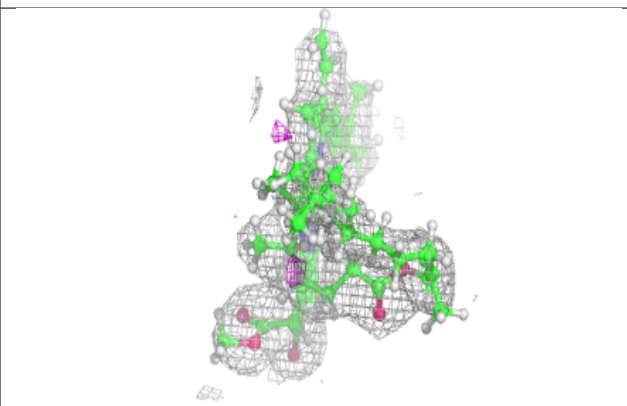
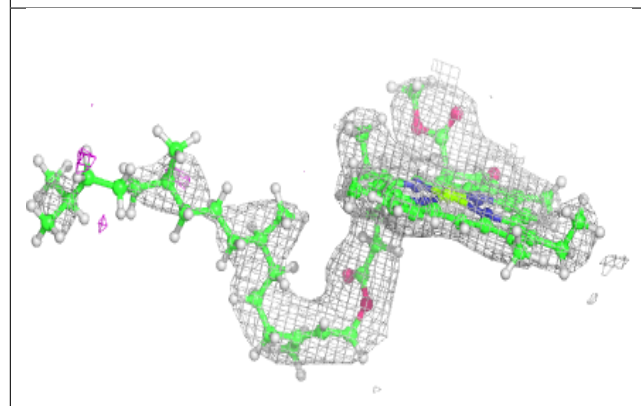
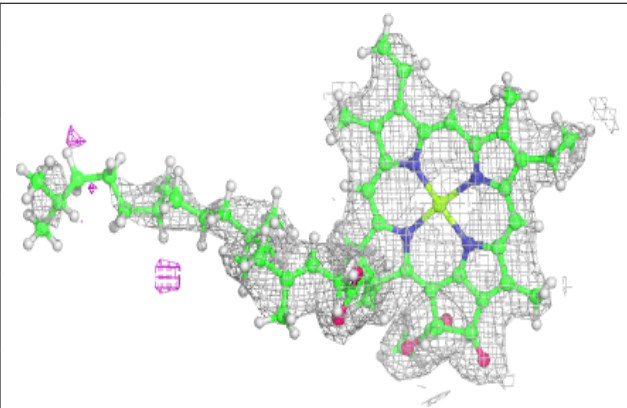


Electron density around SQD A 410:

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

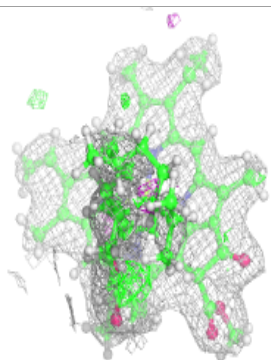
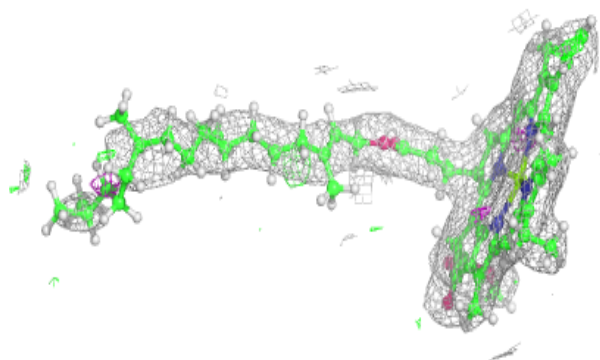
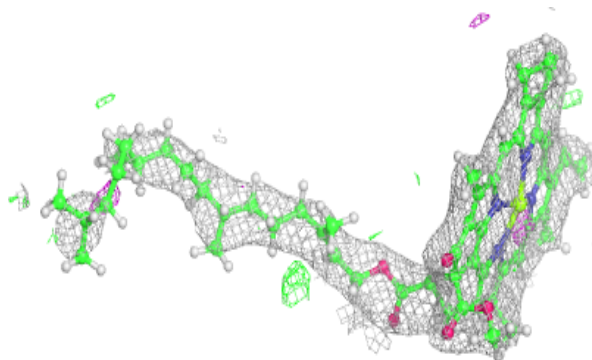
**Electron density around CLA A 405:**

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

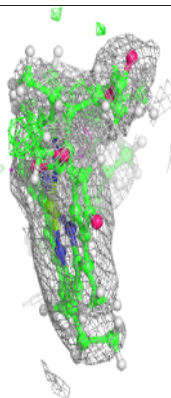
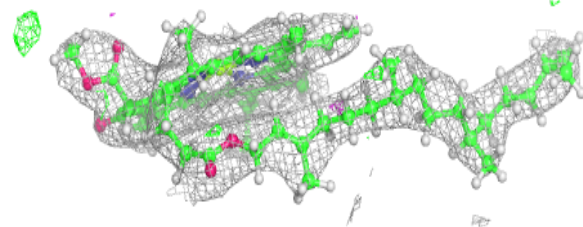
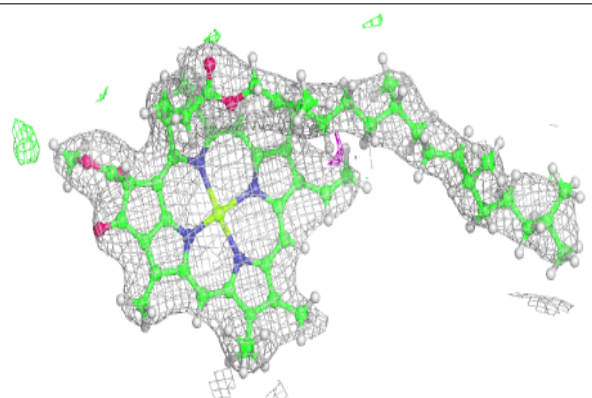


Electron density around CLA B 604:

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

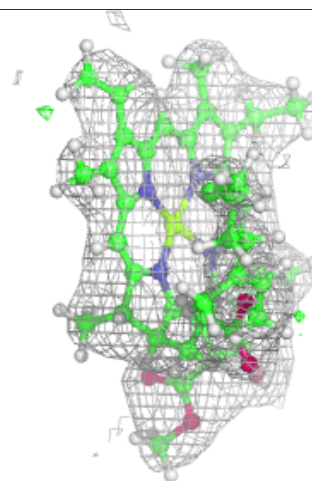
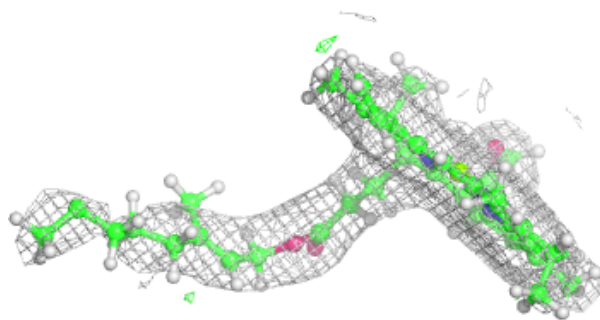
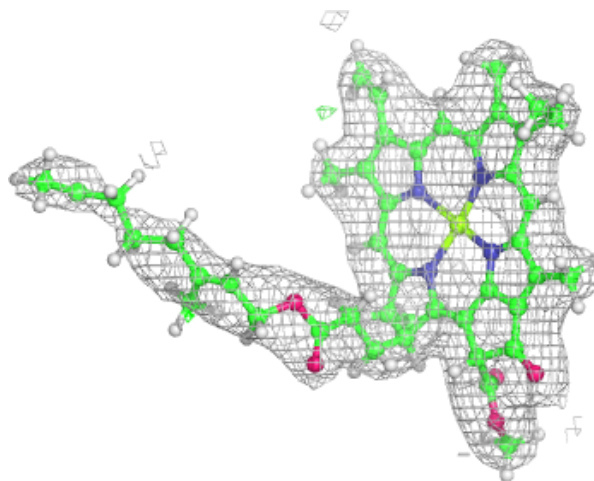
**Electron density around CLA c 501:**

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



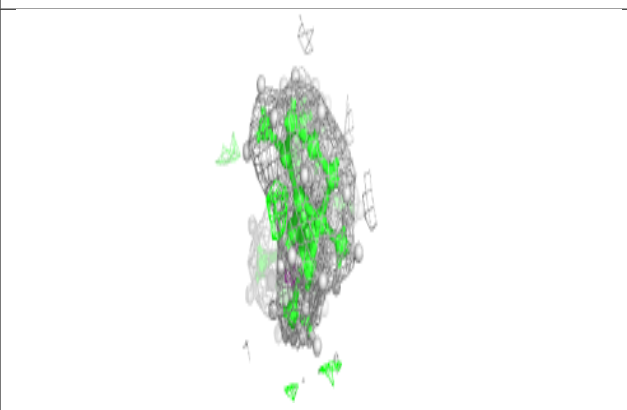
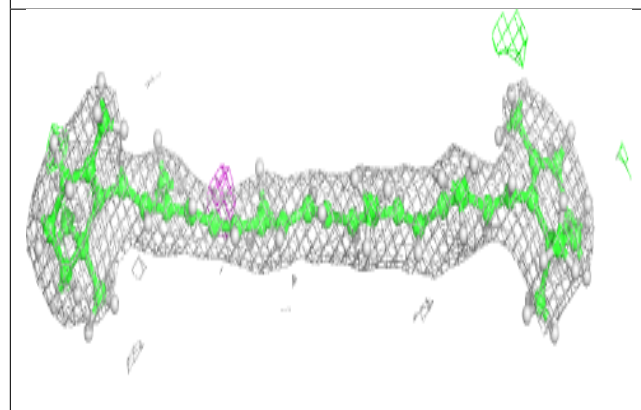
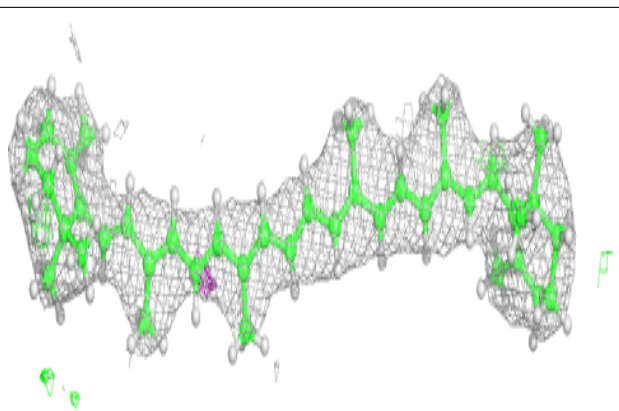
Electron density around CLA A 407:

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

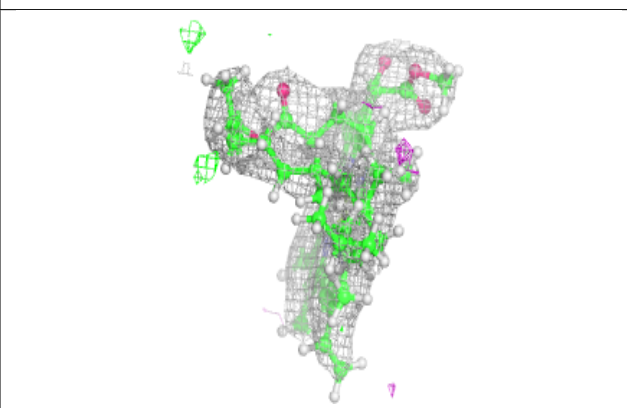
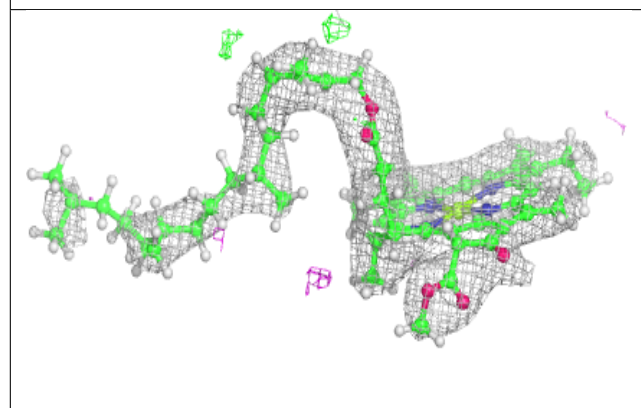
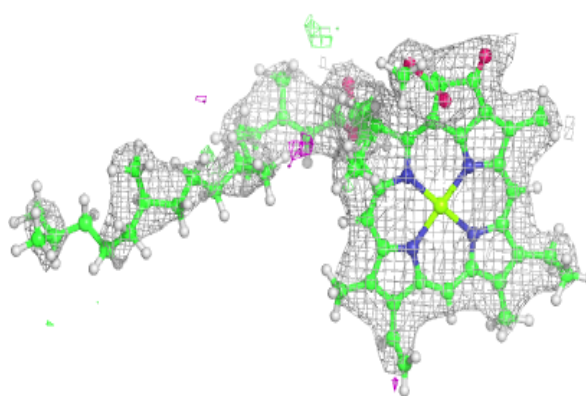


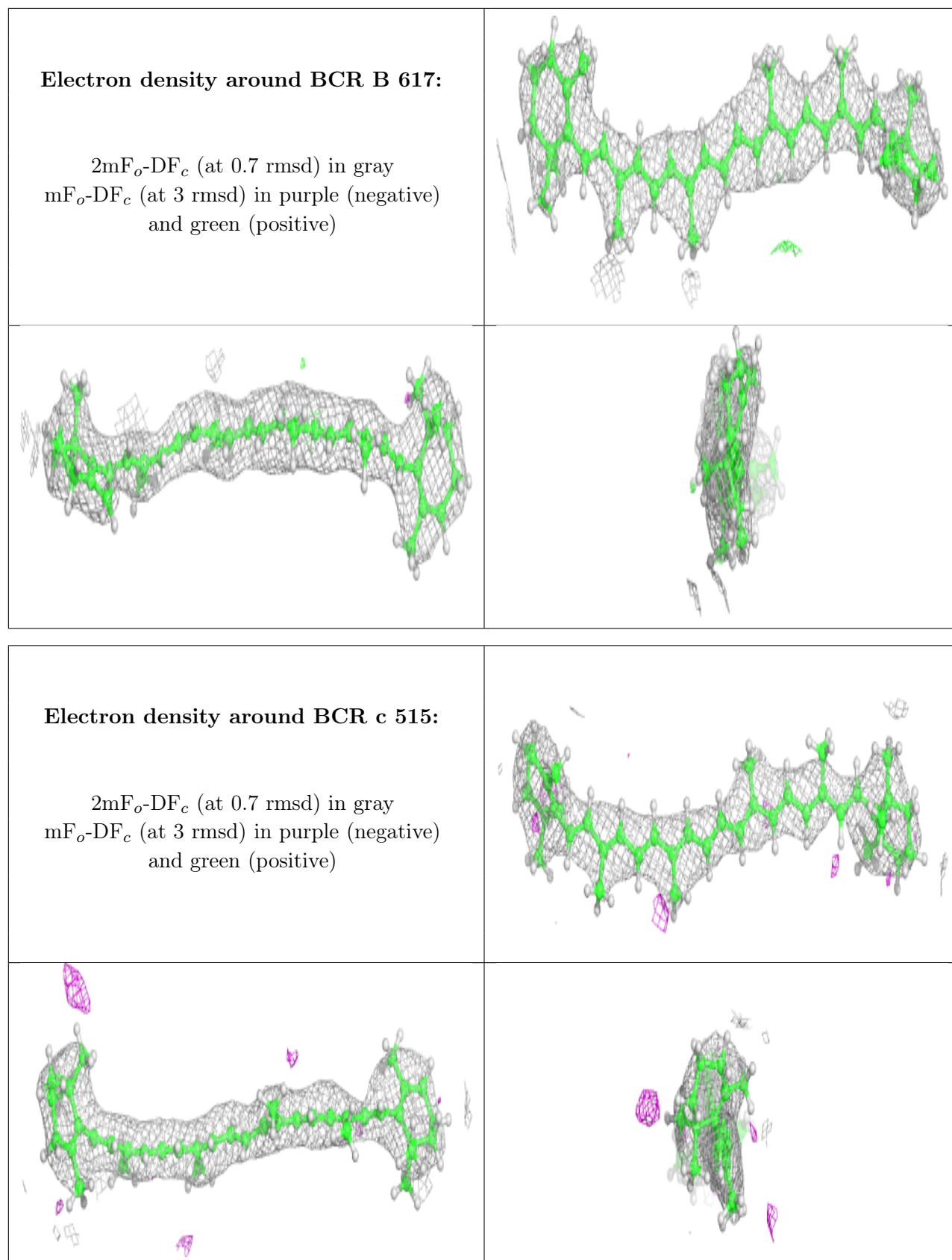
Electron density around BCR b 619:

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

**Electron density around CLA a 406:**

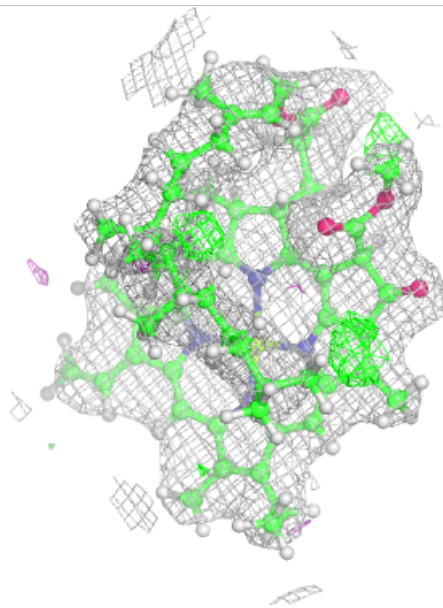
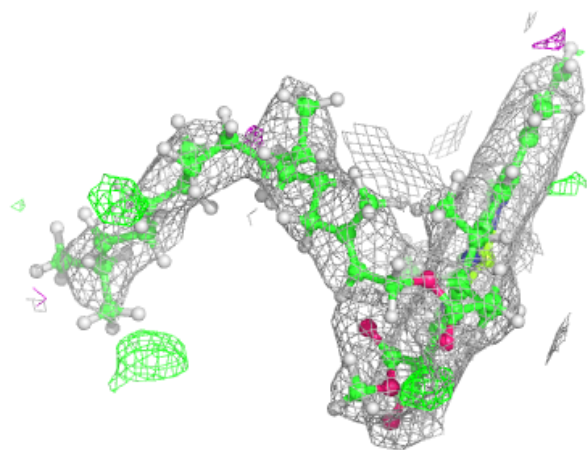
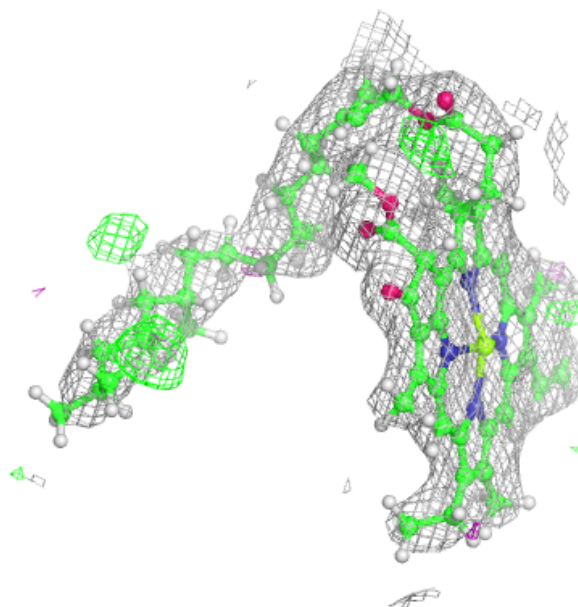
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





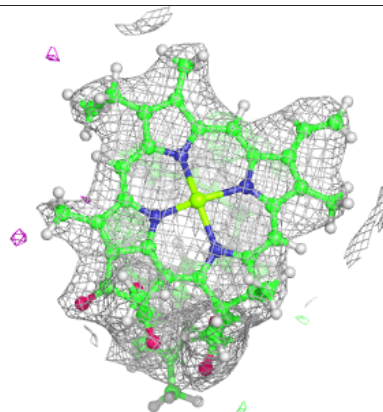
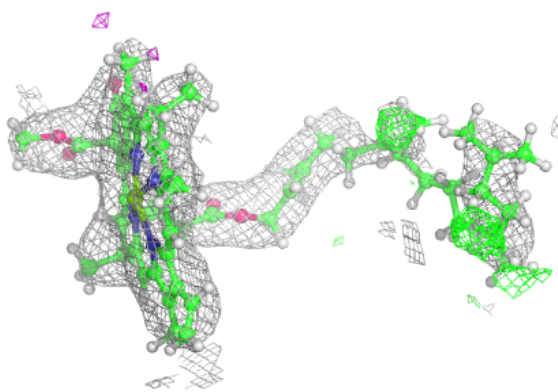
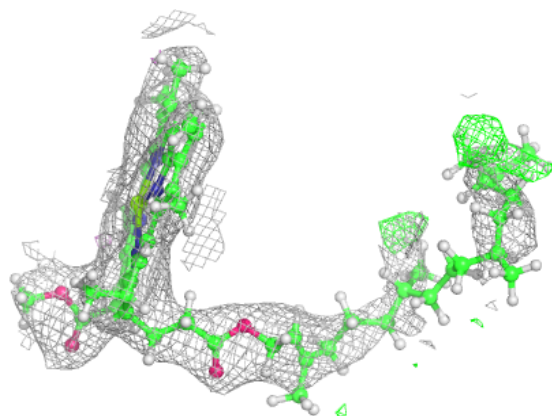
Electron density around CLA B 613:

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



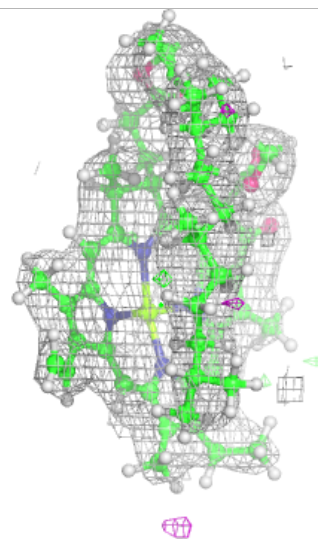
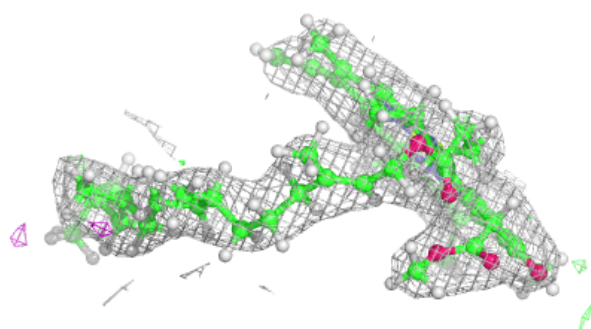
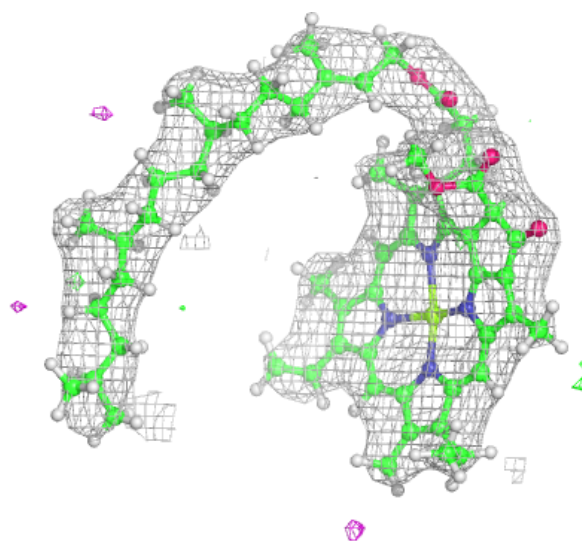
Electron density around CLA C 507:

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



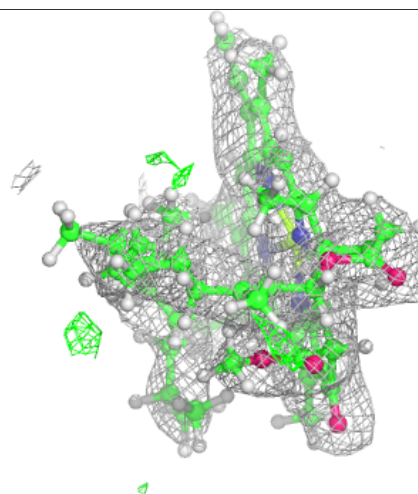
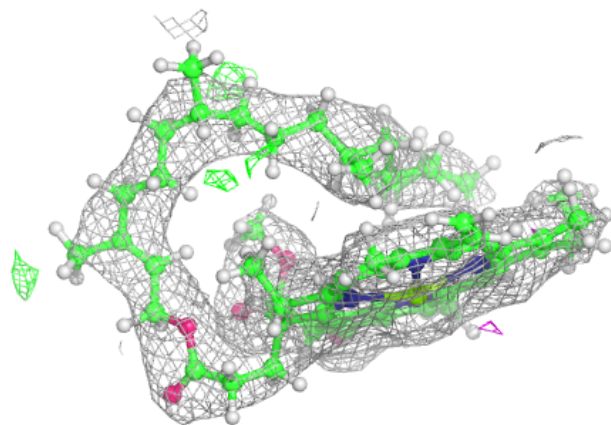
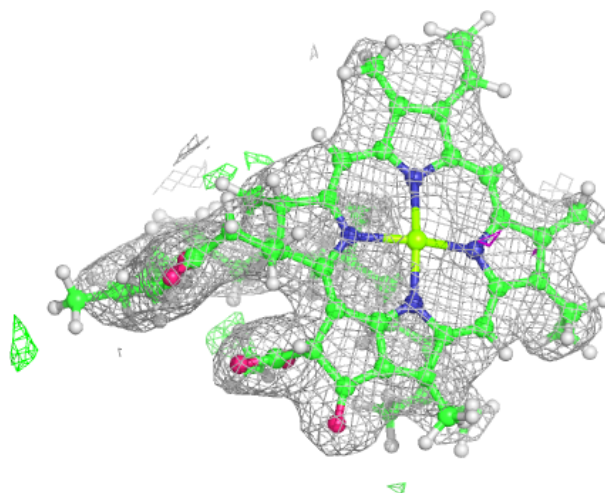
Electron density around CLA C 508:

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



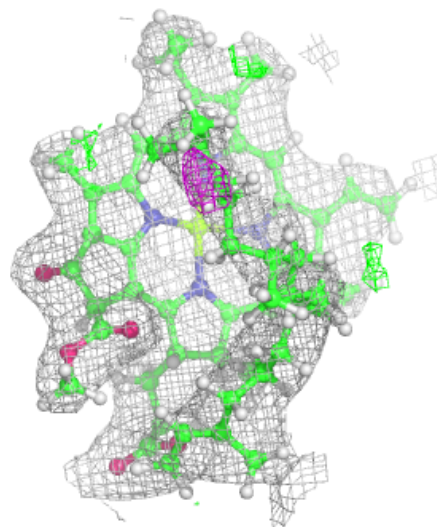
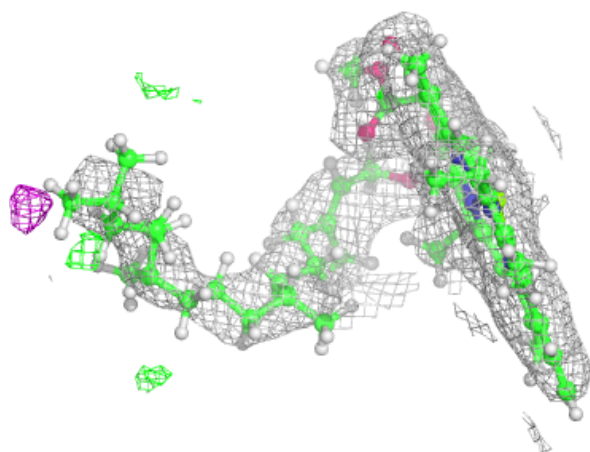
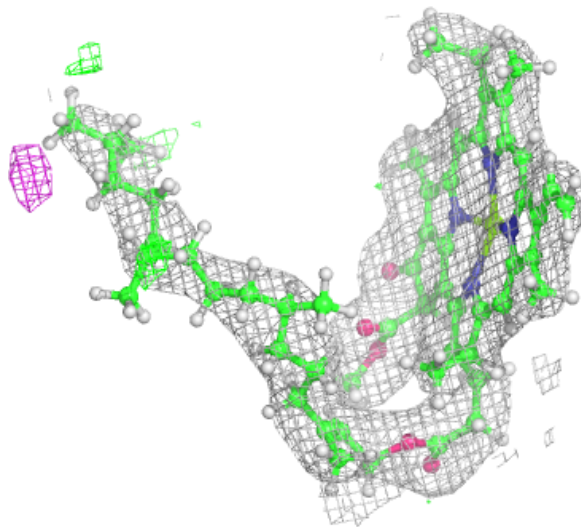
Electron density around CLA C 511:

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



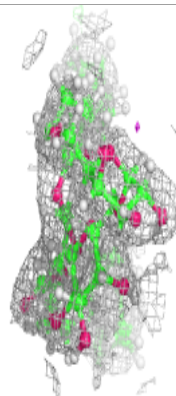
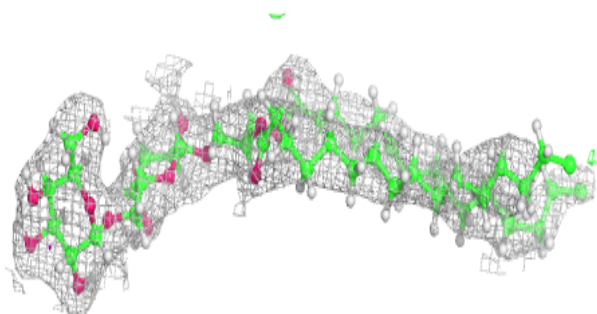
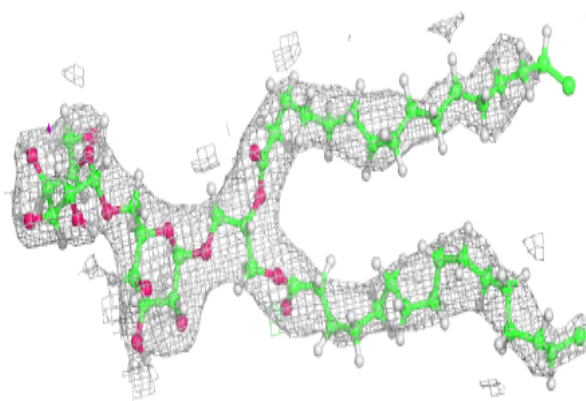
Electron density around CLA b 614:

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

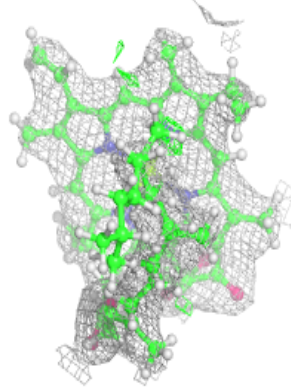
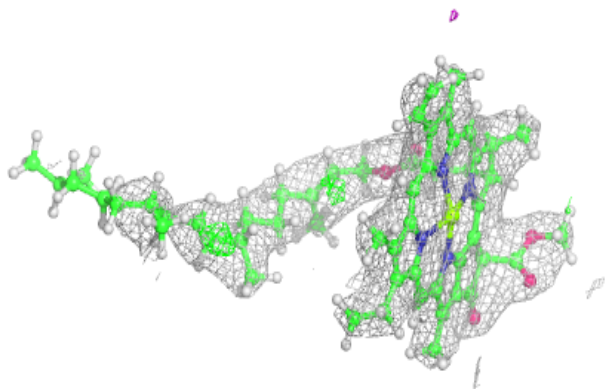
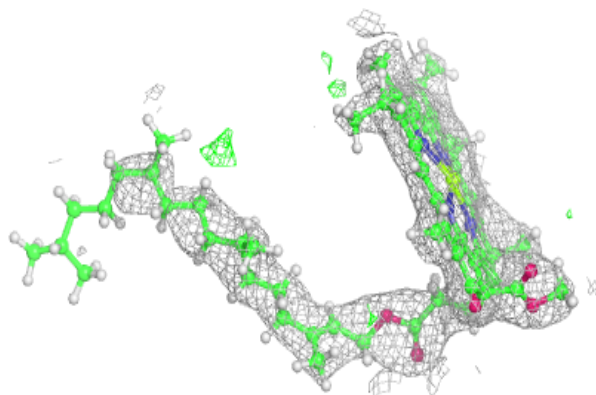


Electron density around DGD C 518:

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

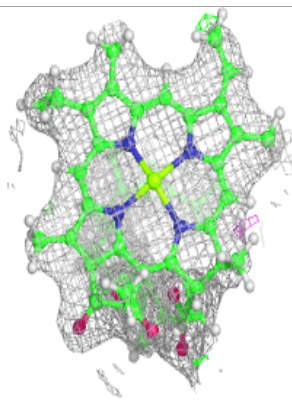
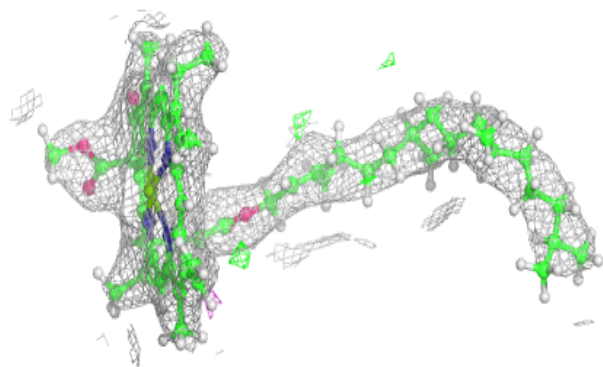
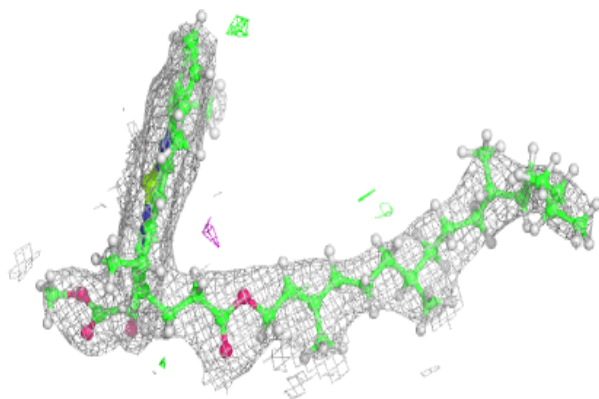
**Electron density around CLA C 509:**

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

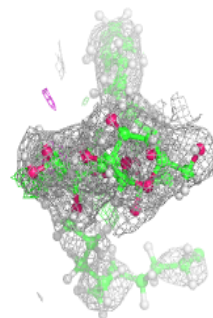
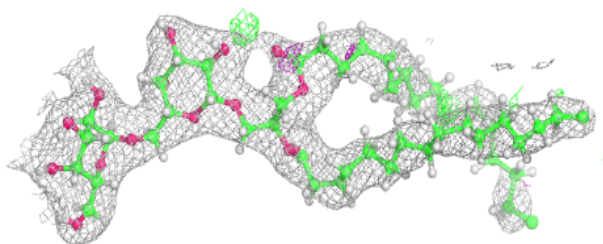
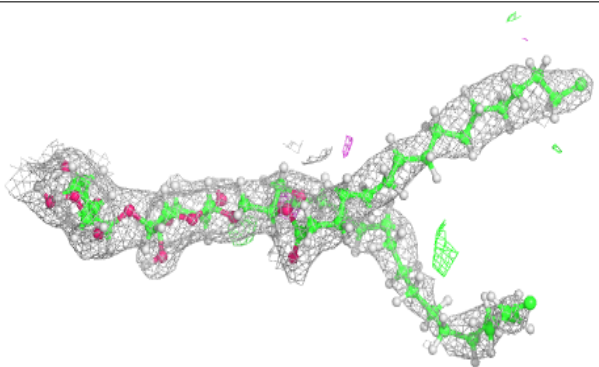


Electron density around CLA b 606:

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

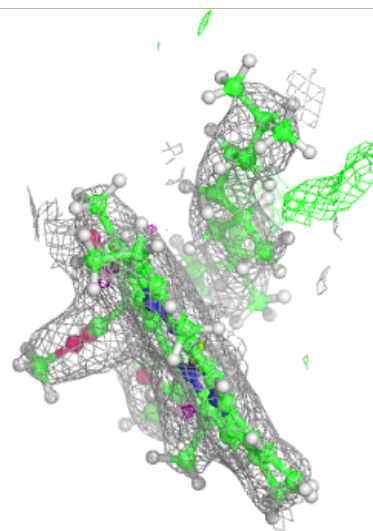
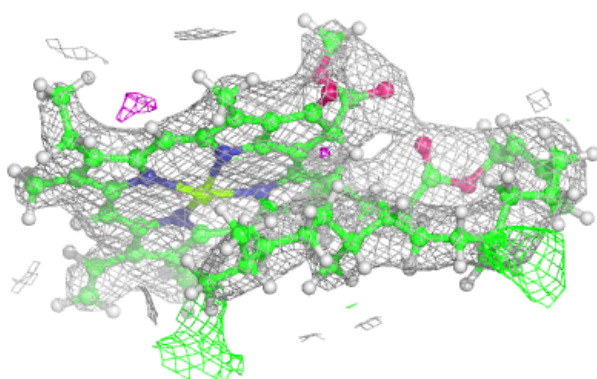
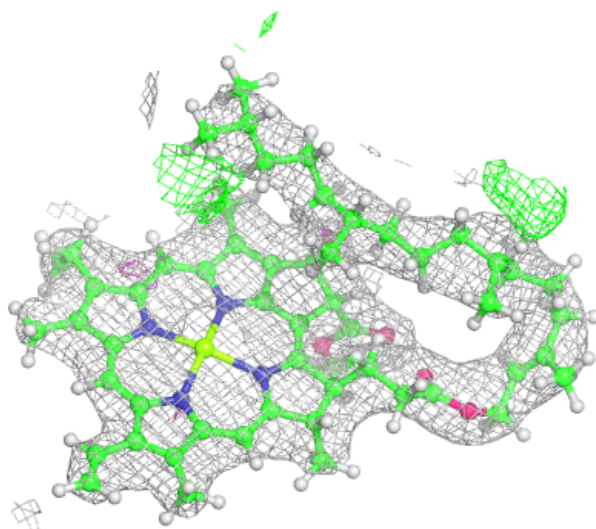
**Electron density around DGD c 516:**

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



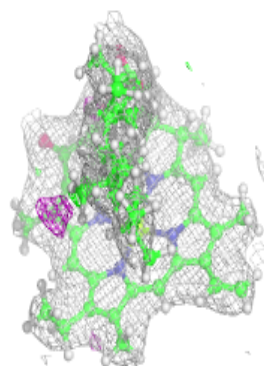
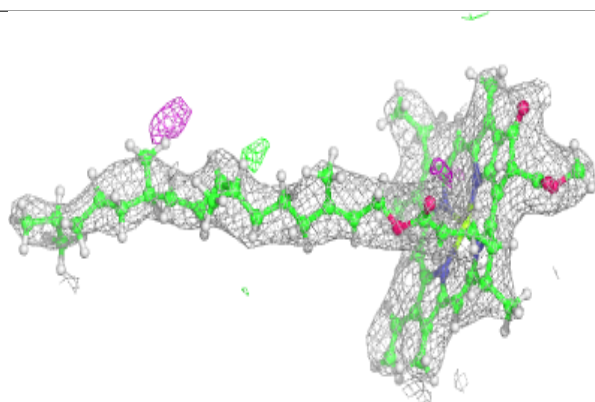
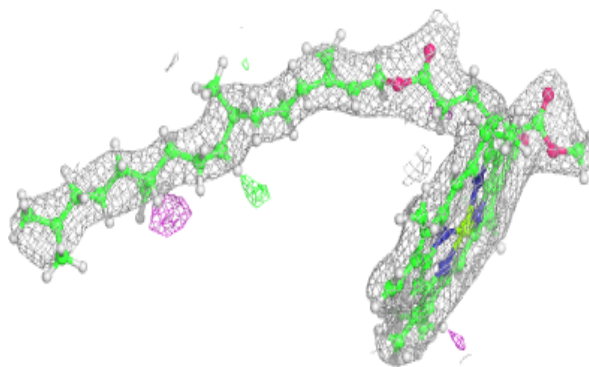
Electron density around CLA C 510:

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

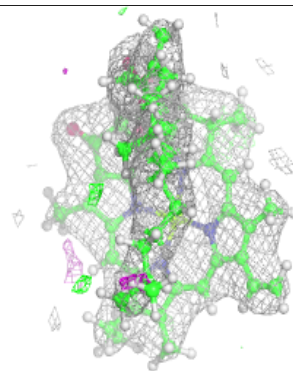
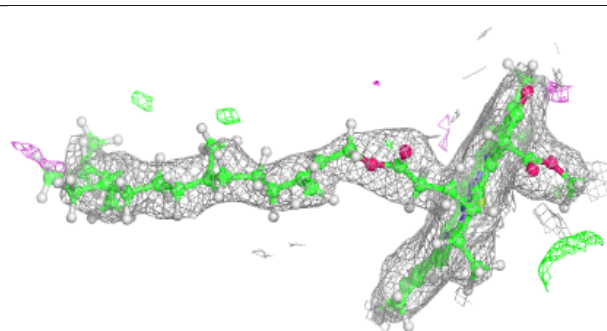
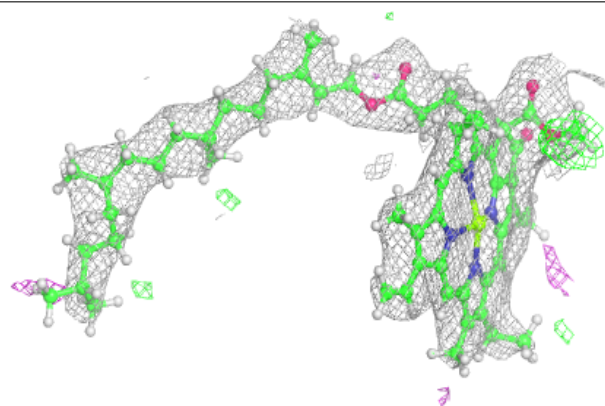


Electron density around CLA b 608:

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

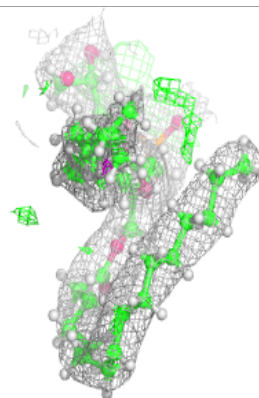
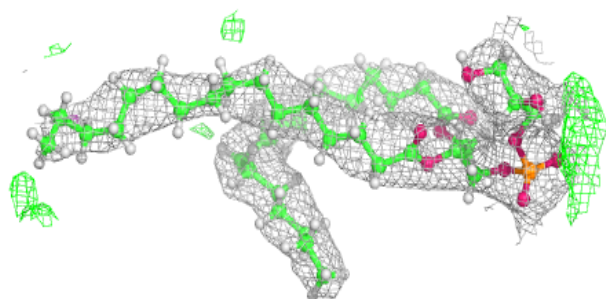
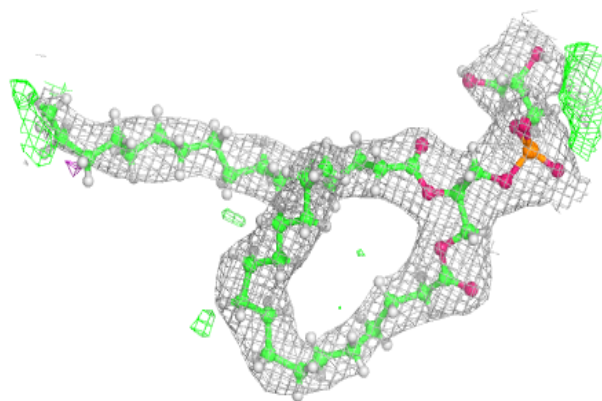
**Electron density around CLA b 610:**

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

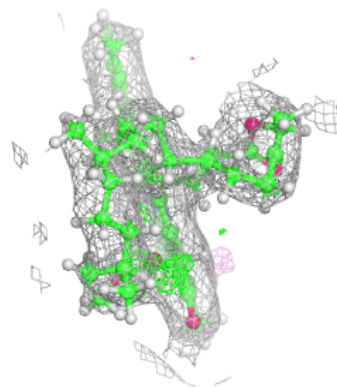
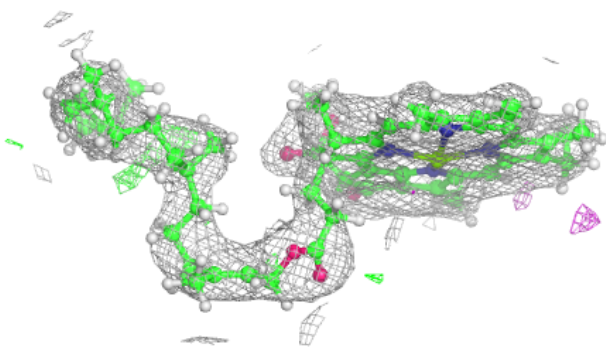
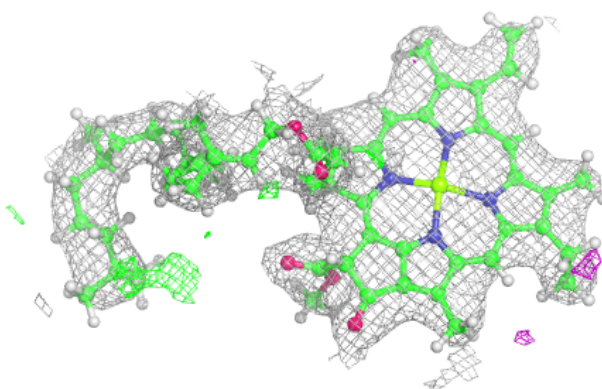


Electron density around LHG A 413:

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

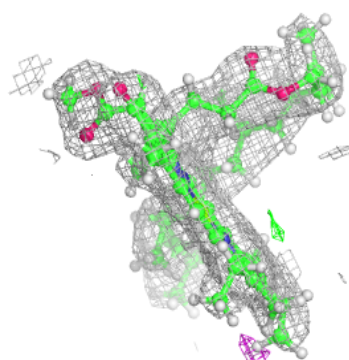
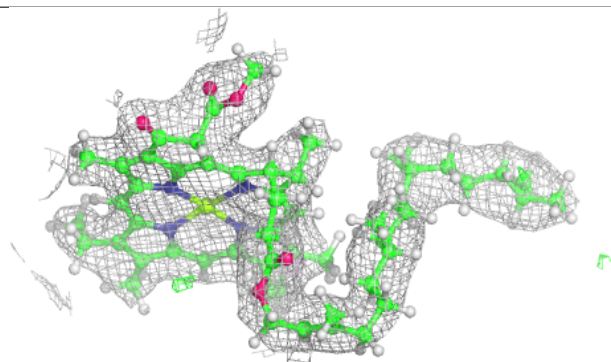
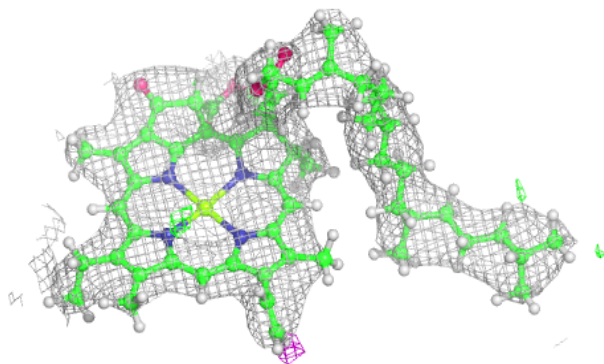
**Electron density around CLA b 613:**

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

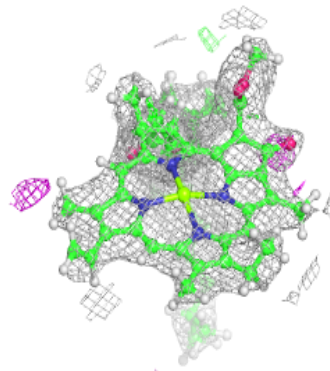
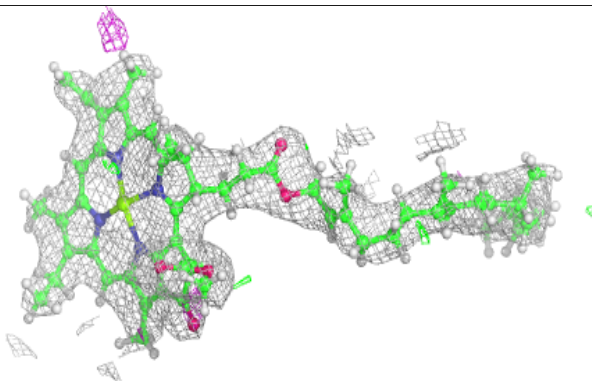
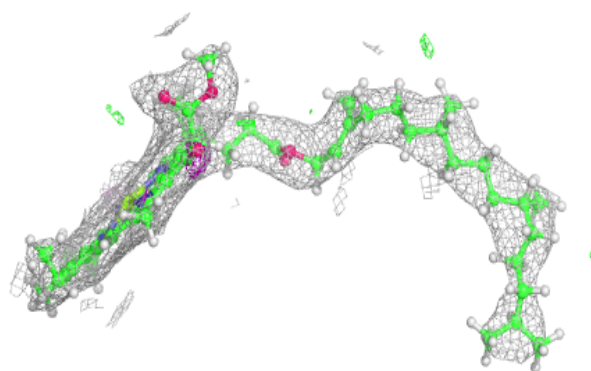


Electron density around CLA d 402:

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

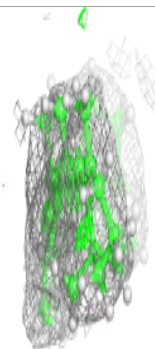
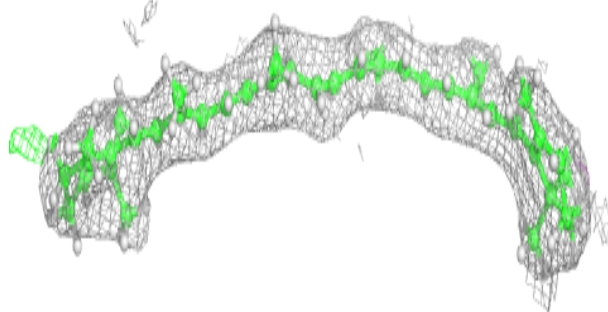
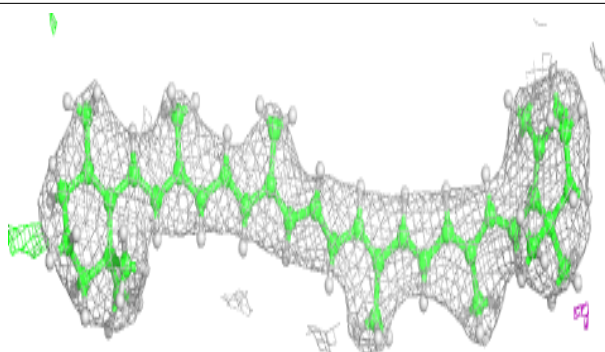
**Electron density around CLA d 403:**

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

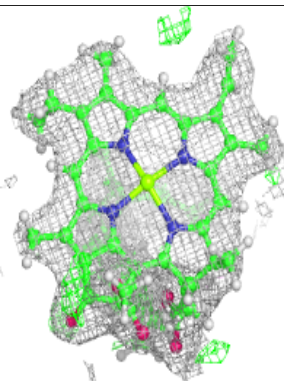
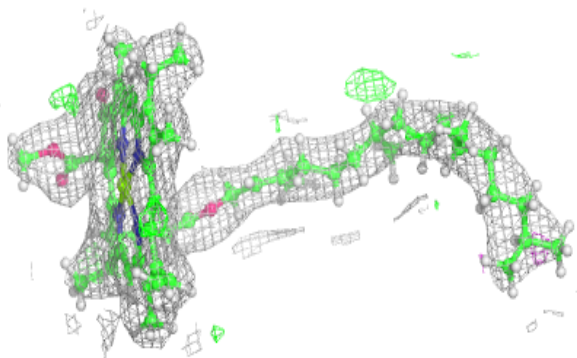
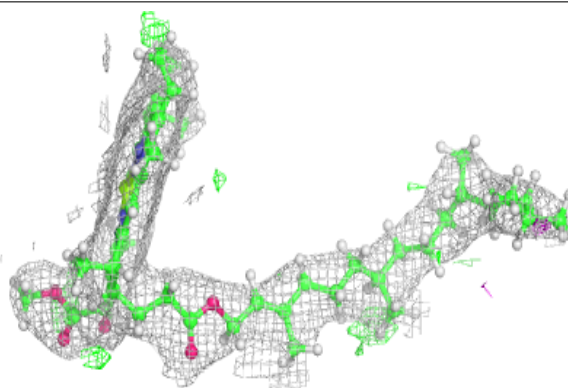


Electron density around BCR t 101:

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

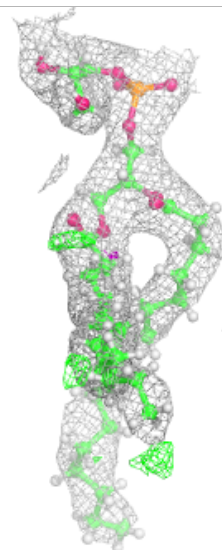
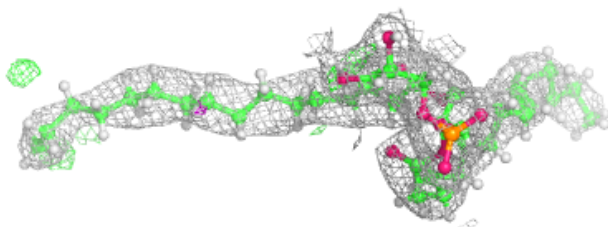
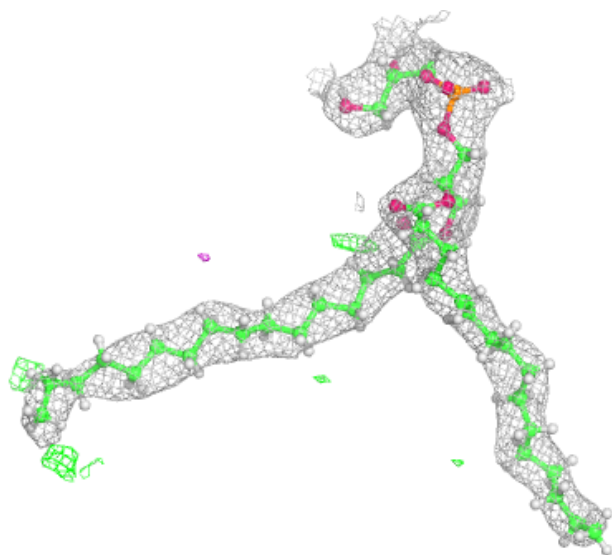
**Electron density around CLA B 605:**

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



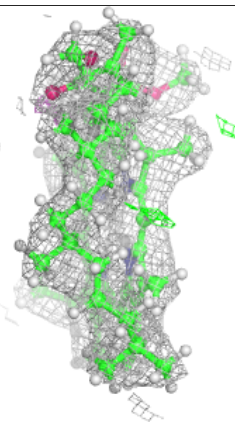
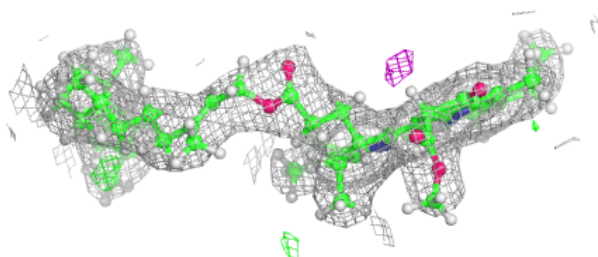
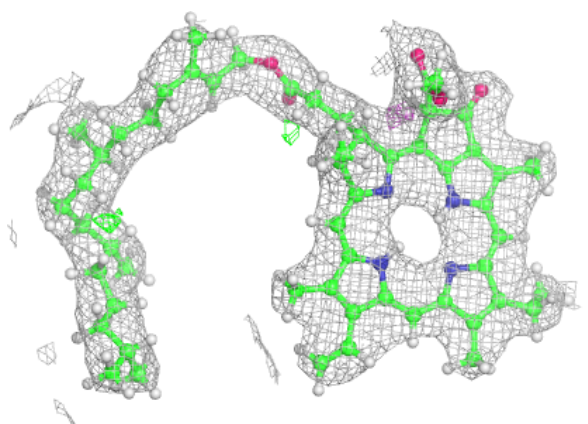
Electron density around LHG 1 101:

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

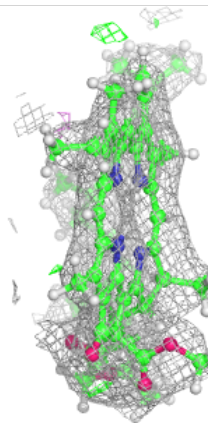
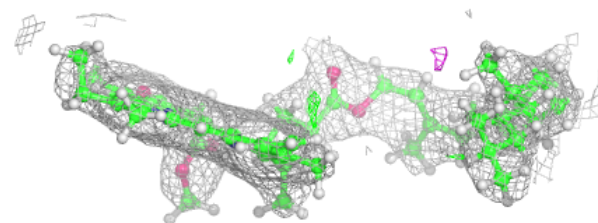
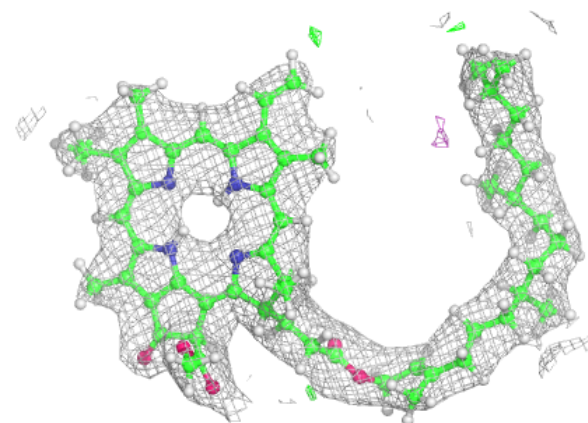


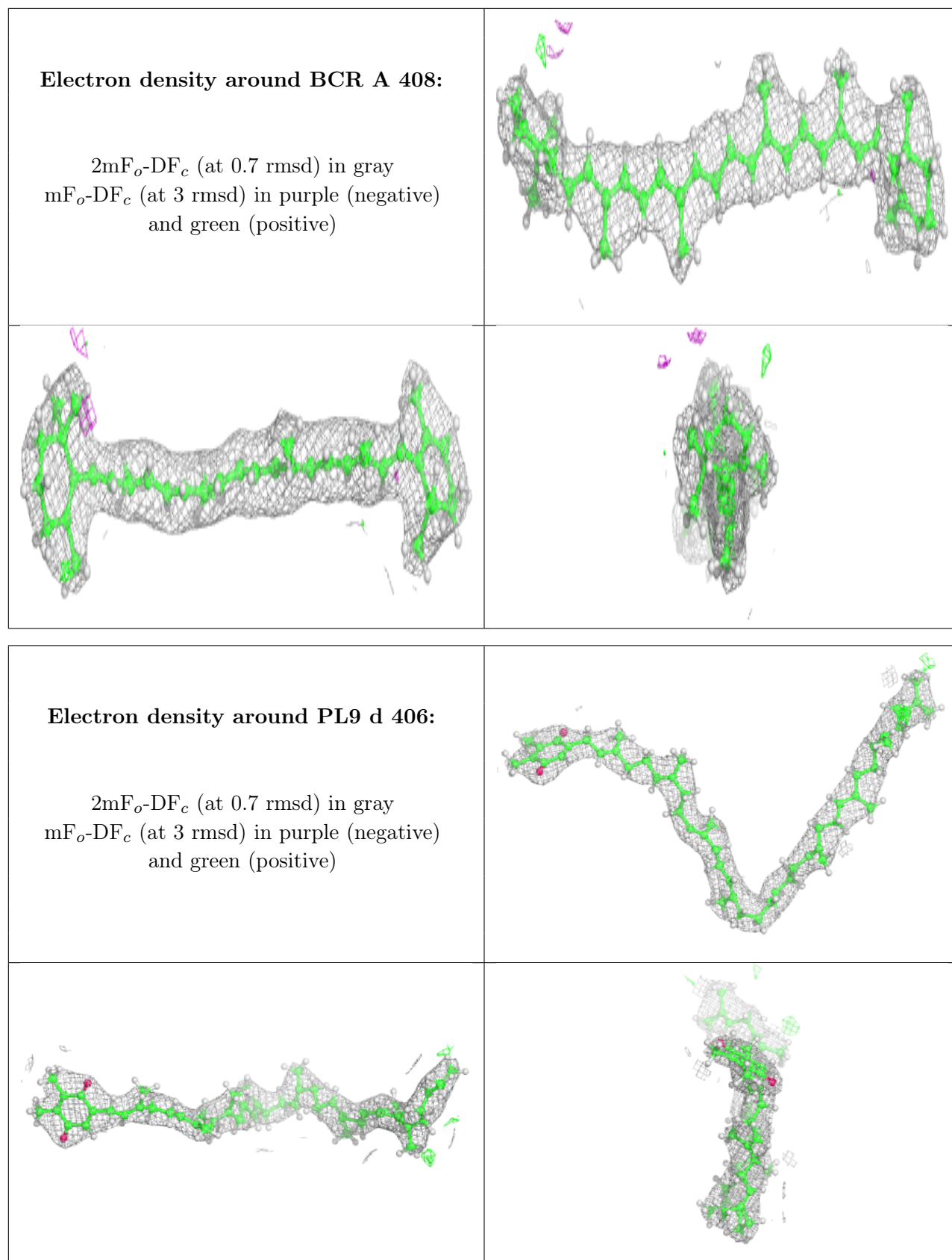
Electron density around PHO A 406:

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

**Electron density around PHO a 407:**

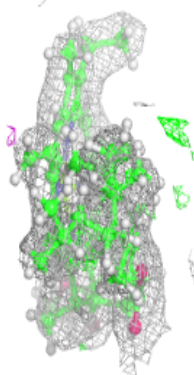
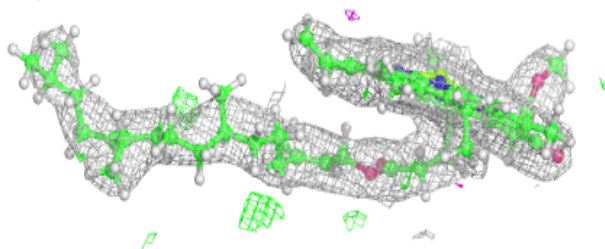
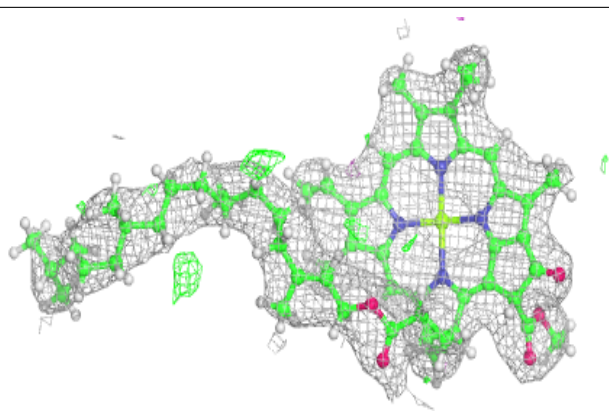
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



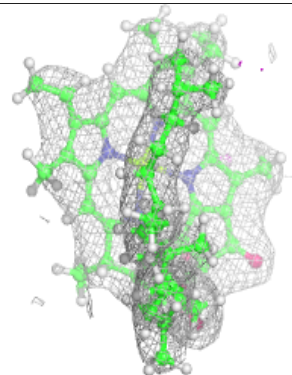
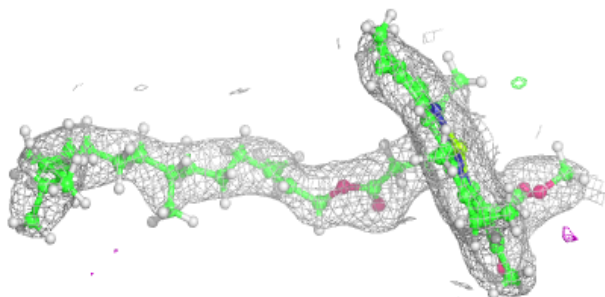
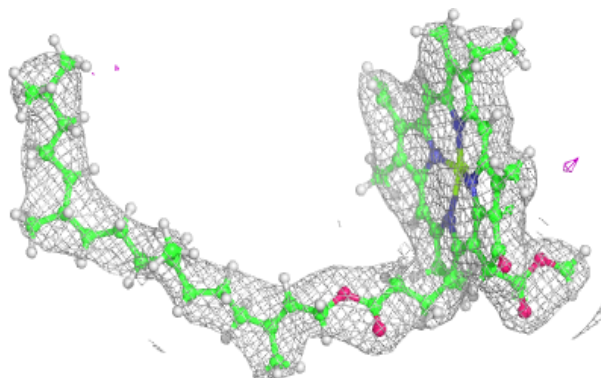


Electron density around CLA B 603:

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

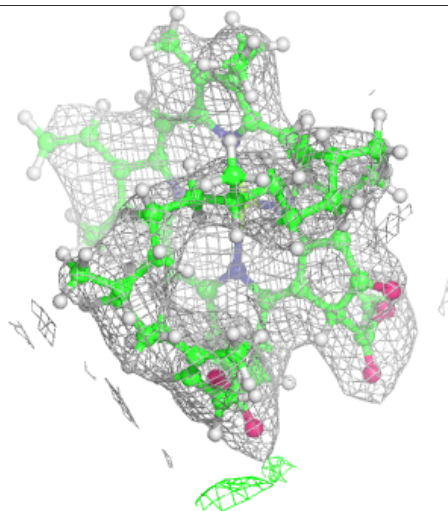
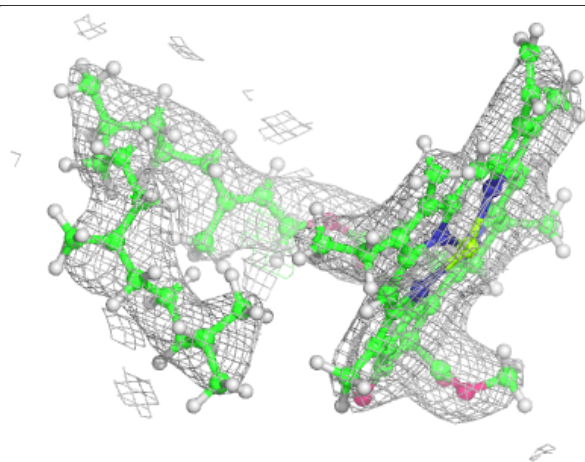
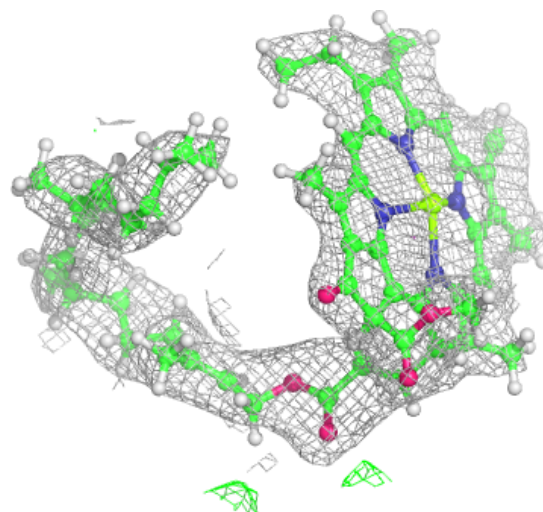
**Electron density around CLA B 609:**

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



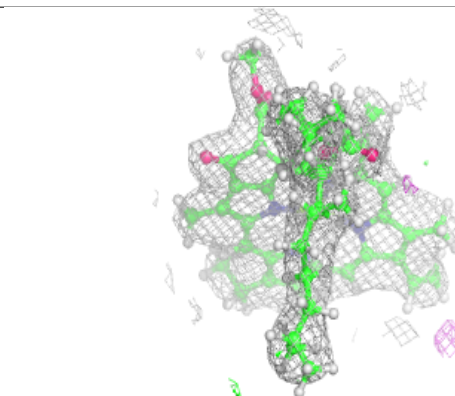
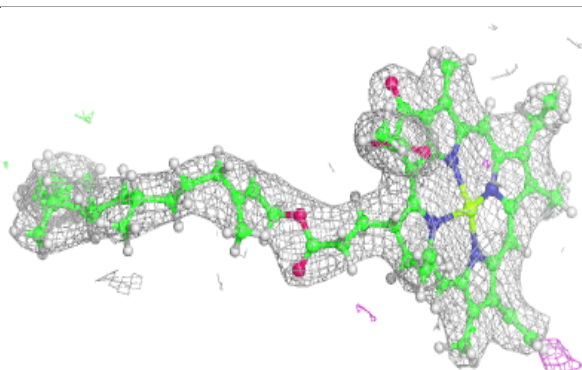
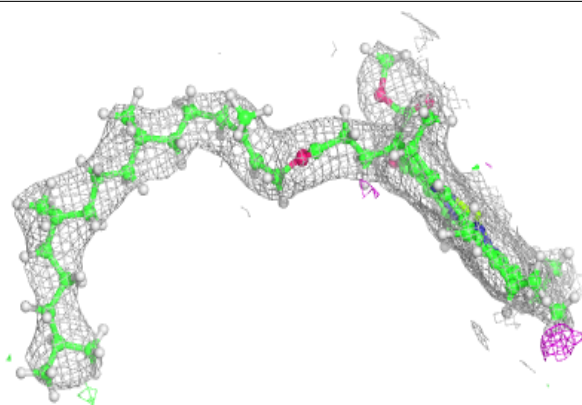
Electron density around CLA C 504:

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

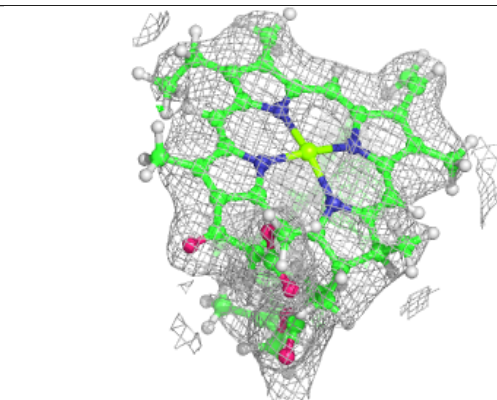
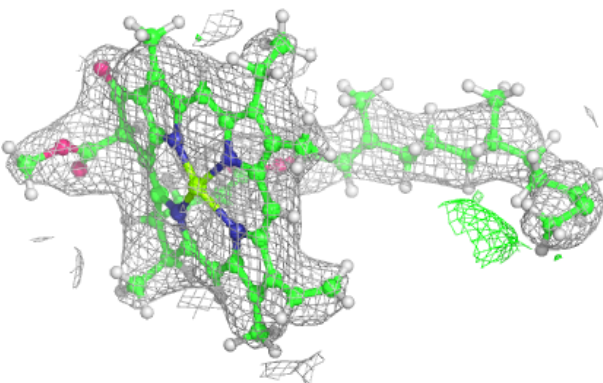
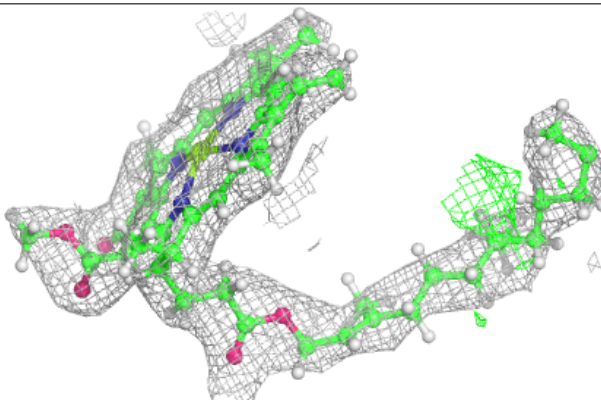


Electron density around CLA D 403:

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

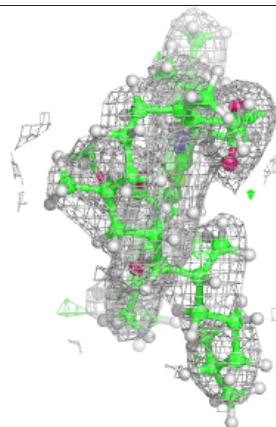
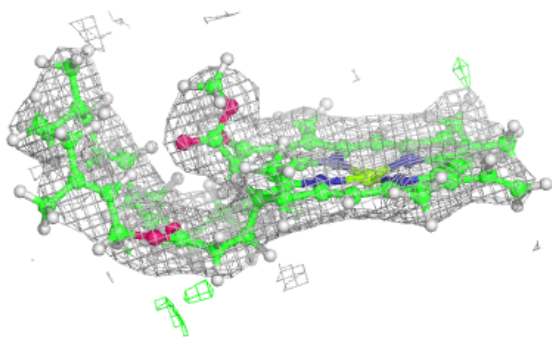
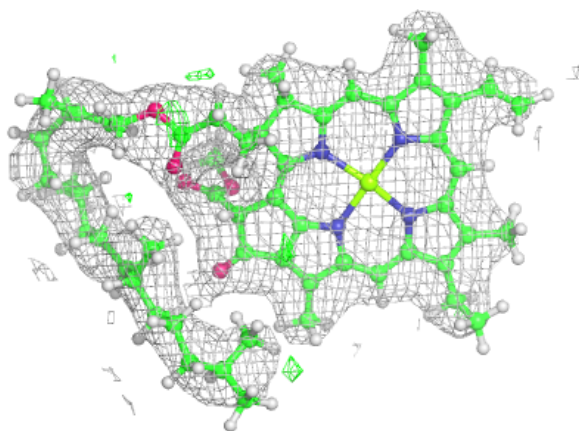
**Electron density around CLA C 505:**

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

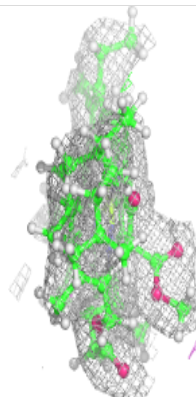
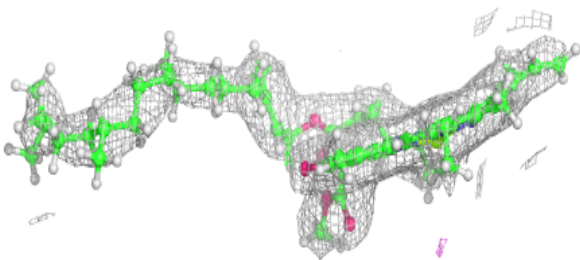
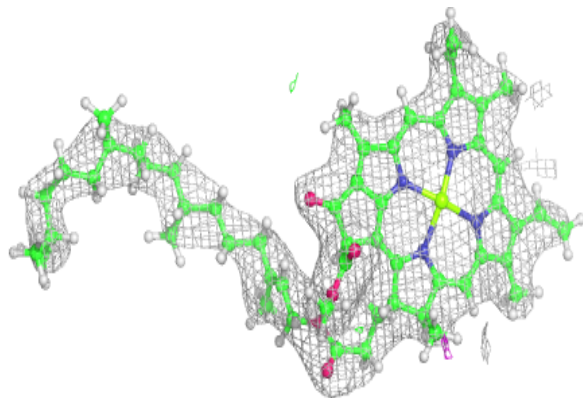


Electron density around CLA B 610:

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

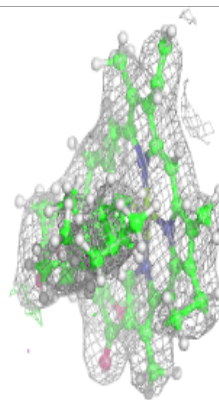
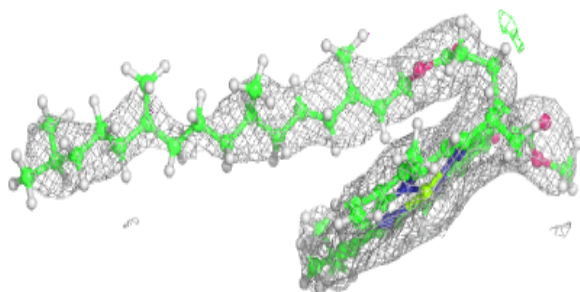
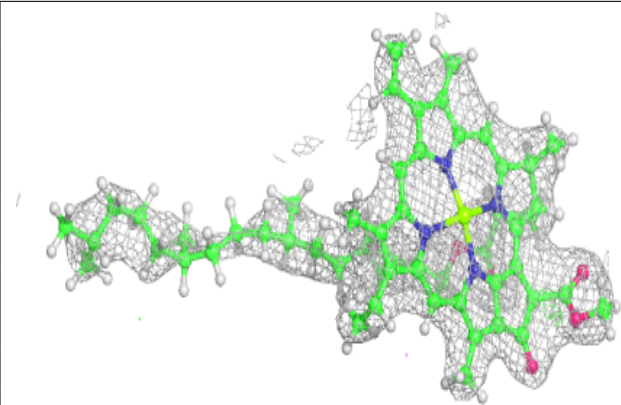
**Electron density around CLA B 602:**

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

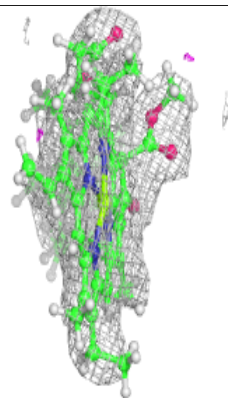
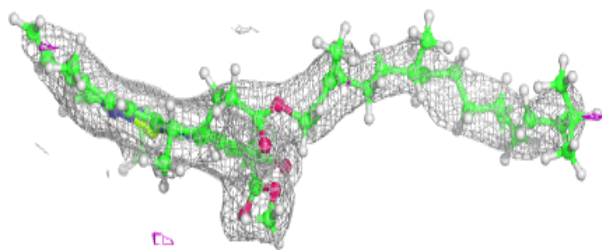
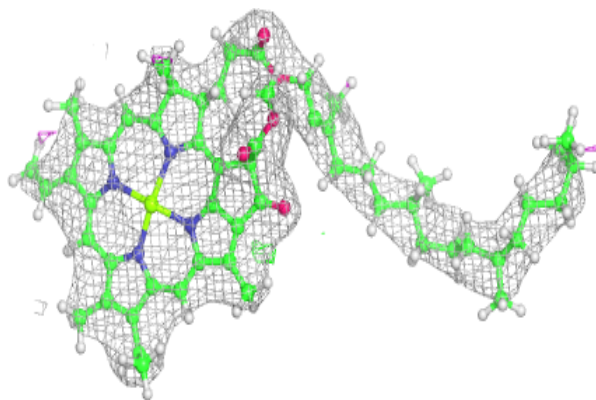


Electron density around CLA B 614:

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

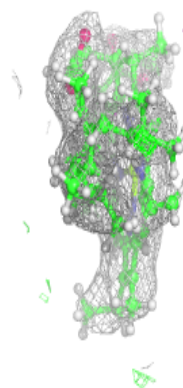
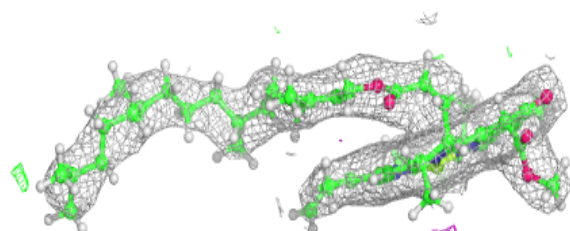
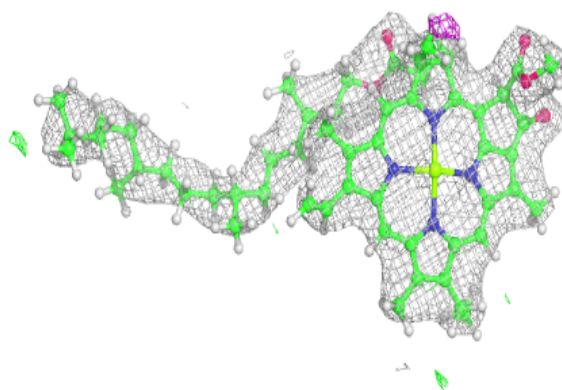
**Electron density around CLA b 603:**

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

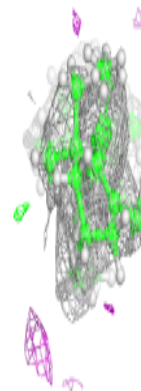
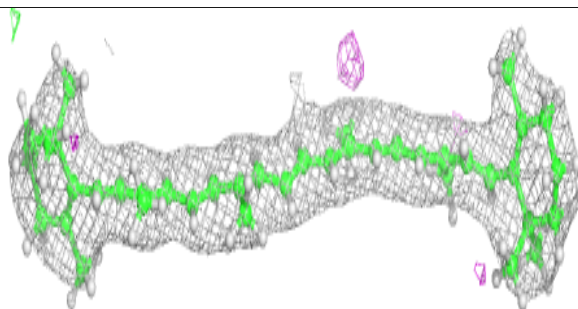
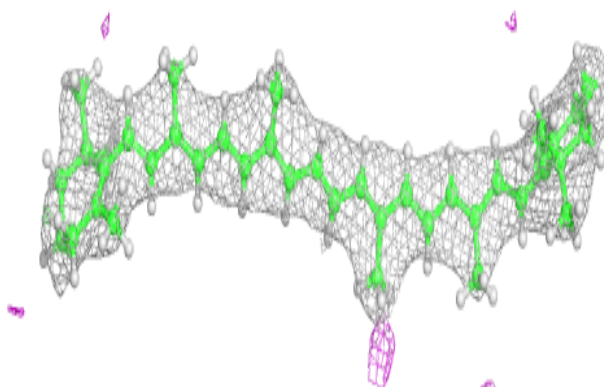


Electron density around CLA b 604:

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

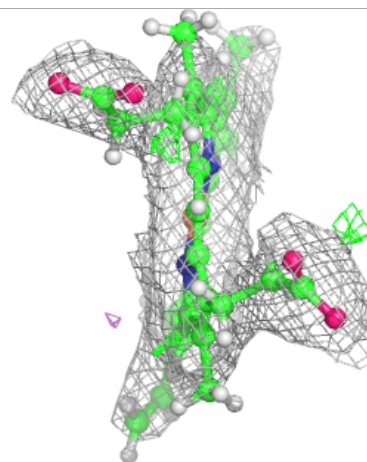
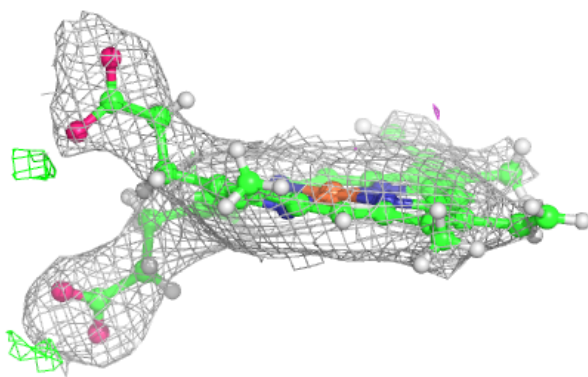
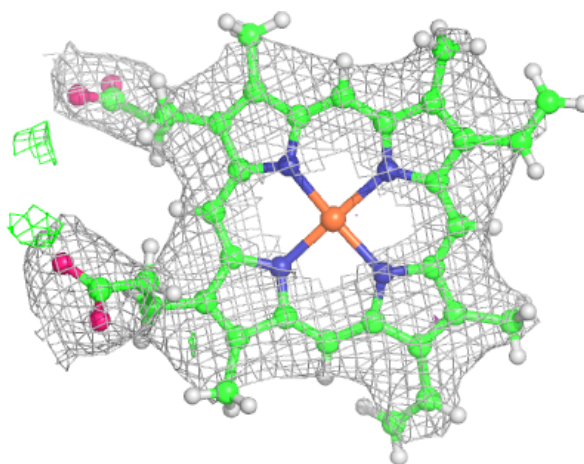
**Electron density around BCR a 409:**

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



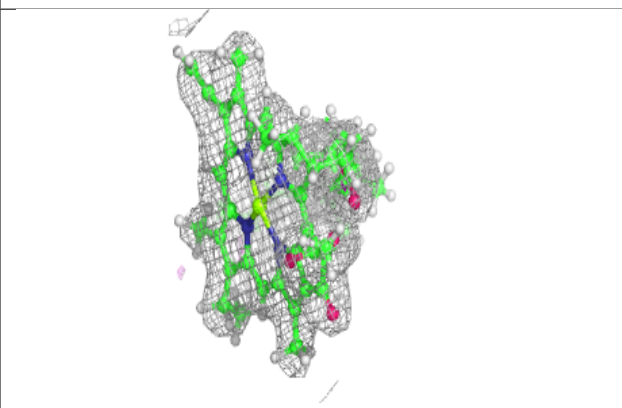
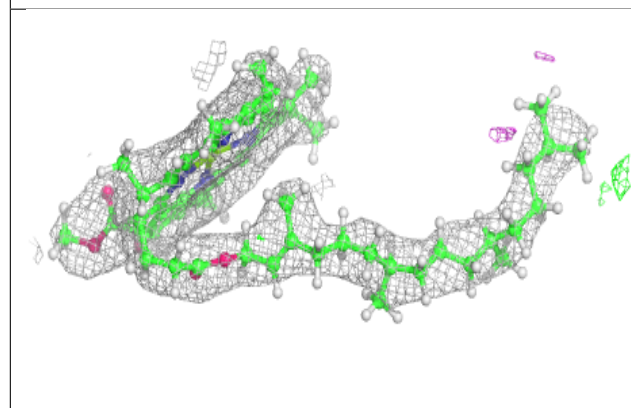
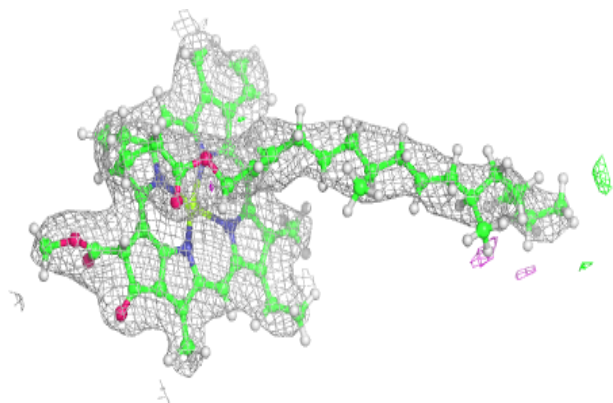
Electron density around HEM E 103:

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

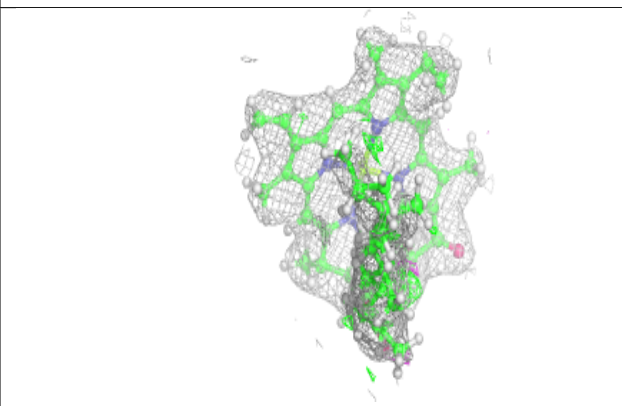
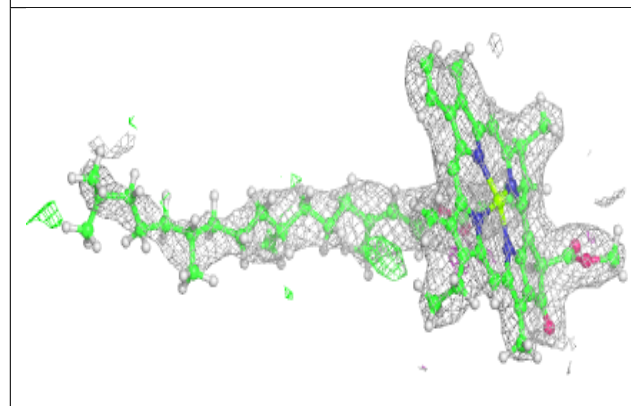
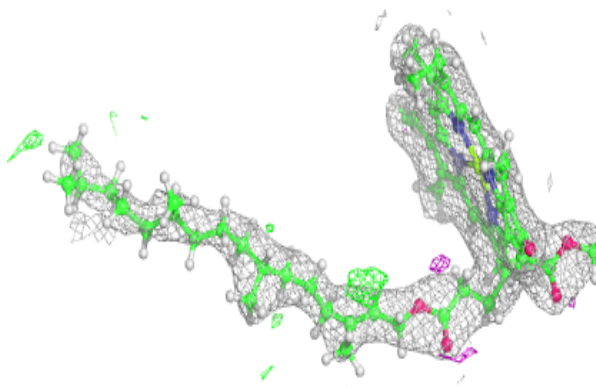


Electron density around CLA b 609:

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

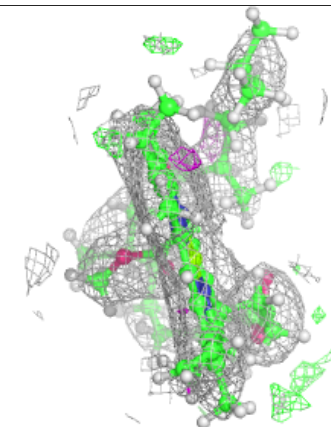
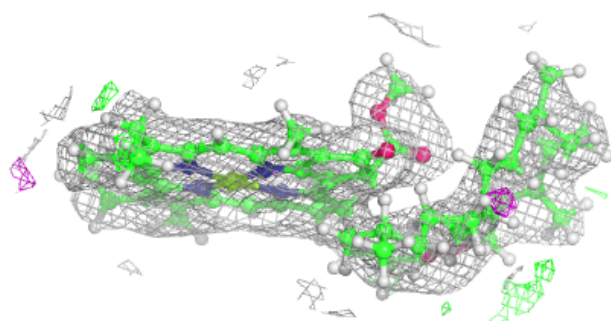
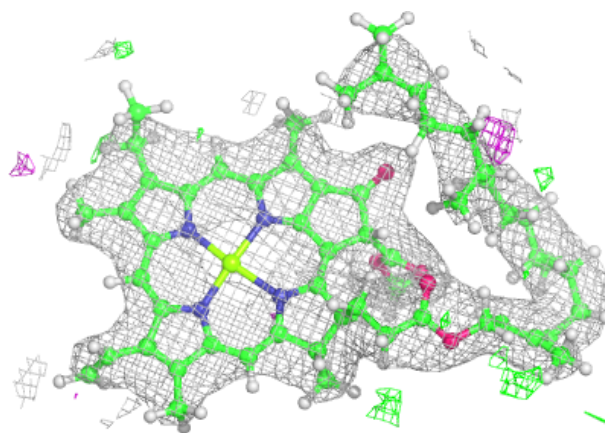
**Electron density around CLA B 607:**

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



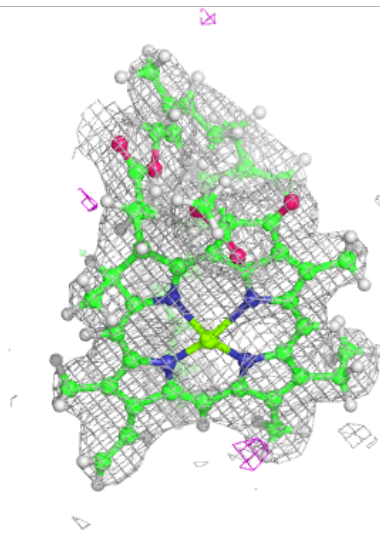
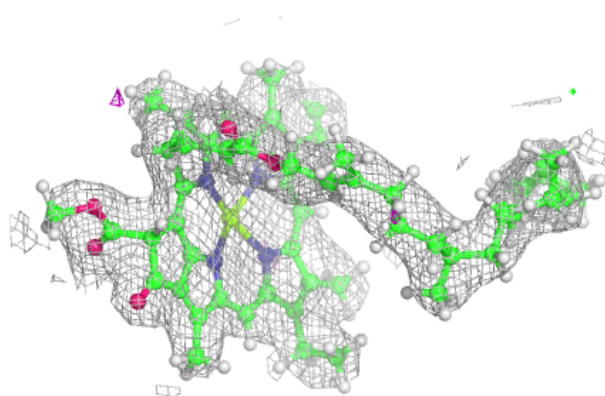
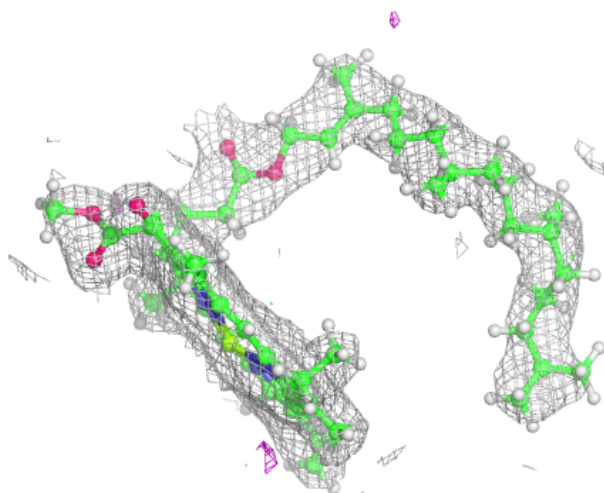
Electron density around CLA b 611:

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



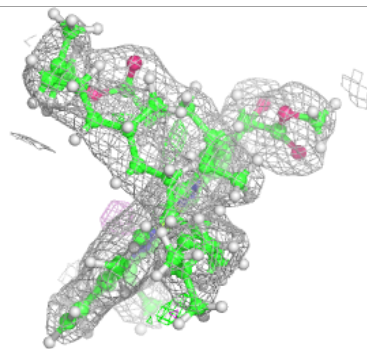
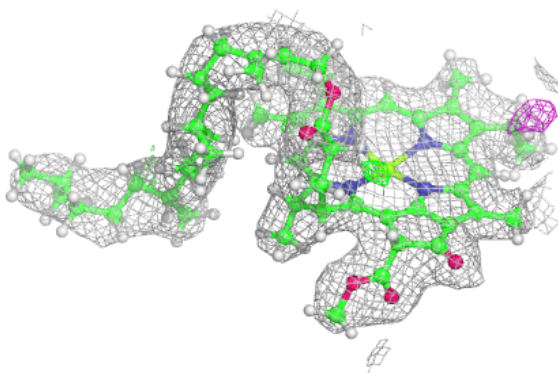
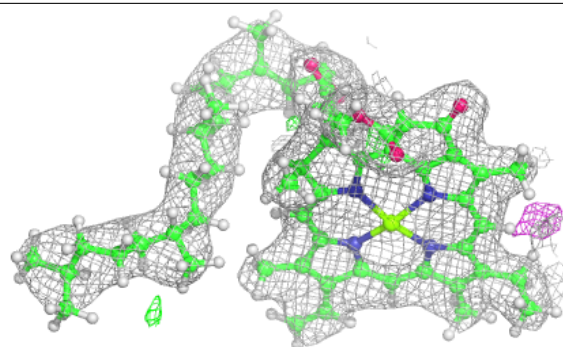
Electron density around CLA b 612:

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

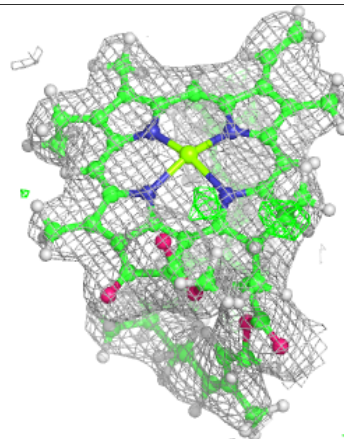
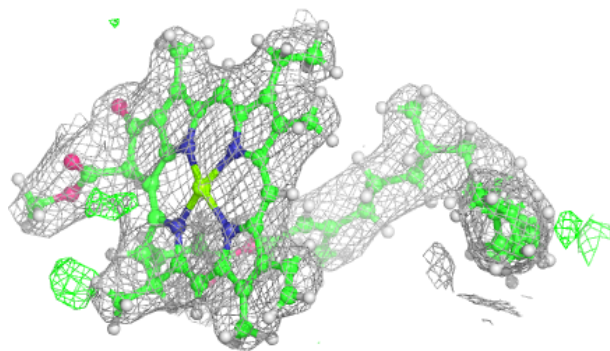
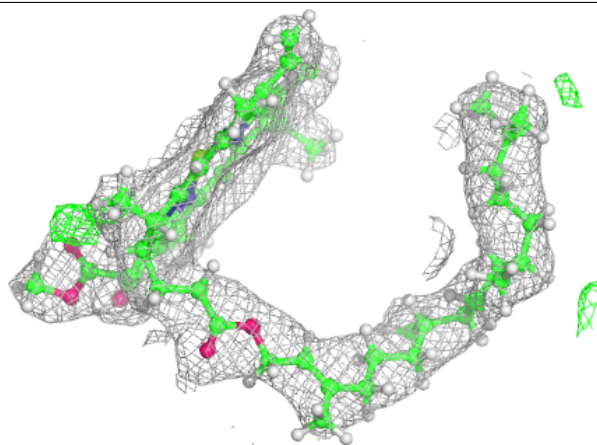


Electron density around CLA D 402:

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

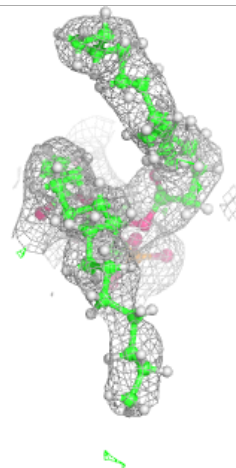
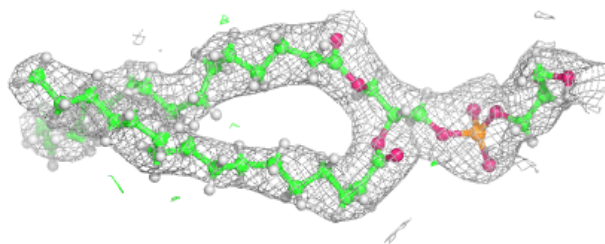
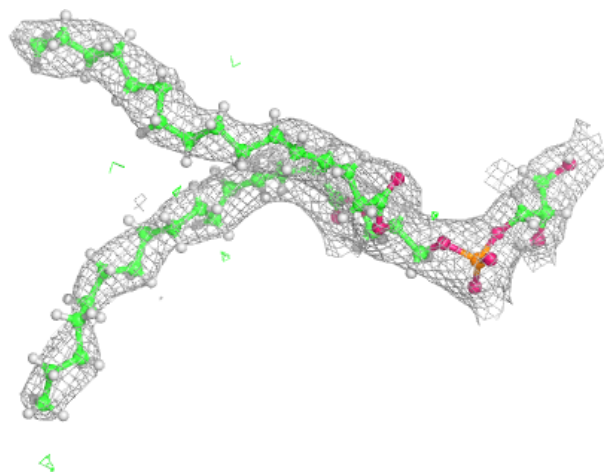
**Electron density around CLA B 611:**

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



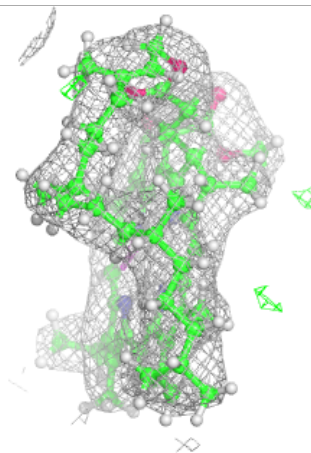
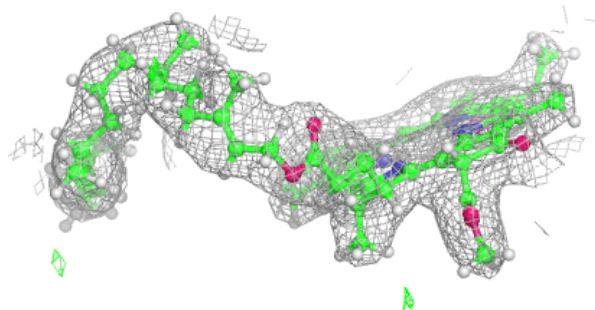
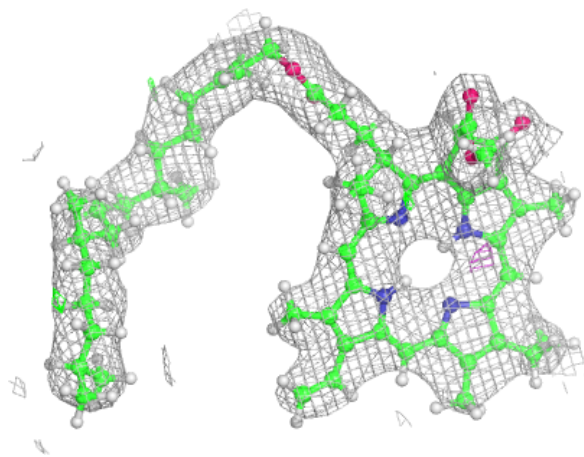
Electron density around LHG D 408:

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



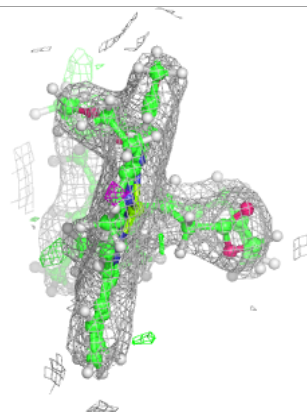
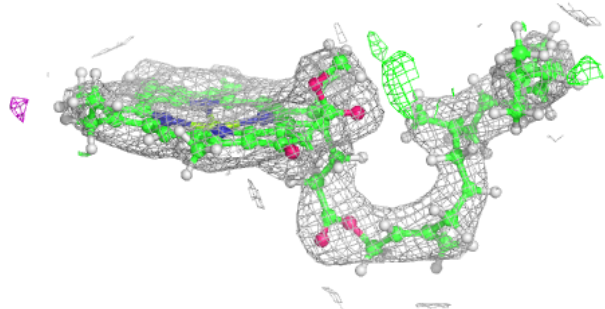
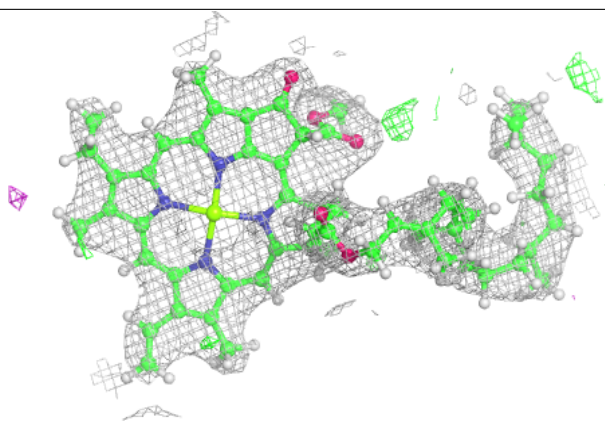
Electron density around PHO D 401:

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



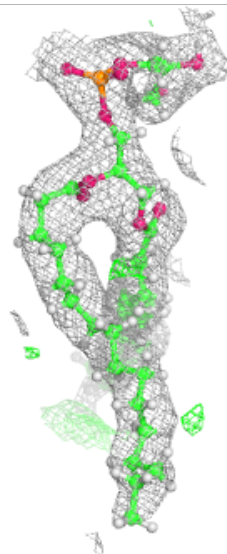
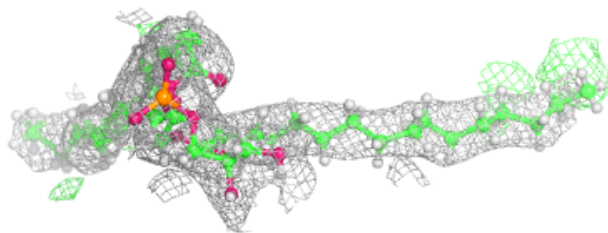
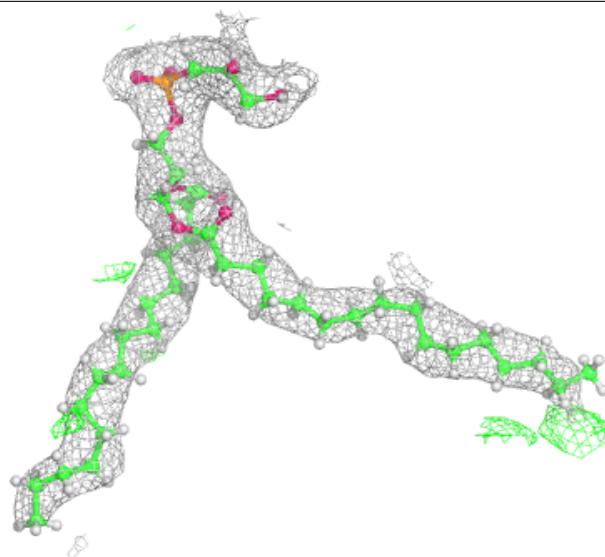
Electron density around CLA B 612:

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



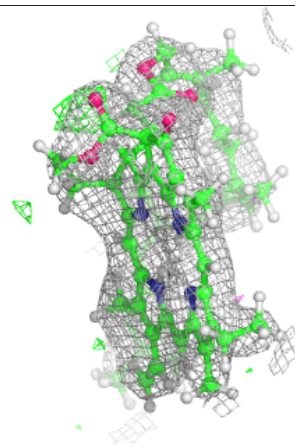
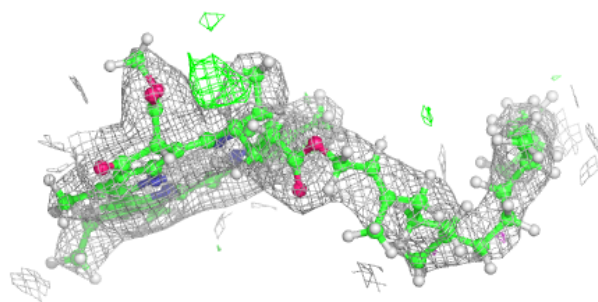
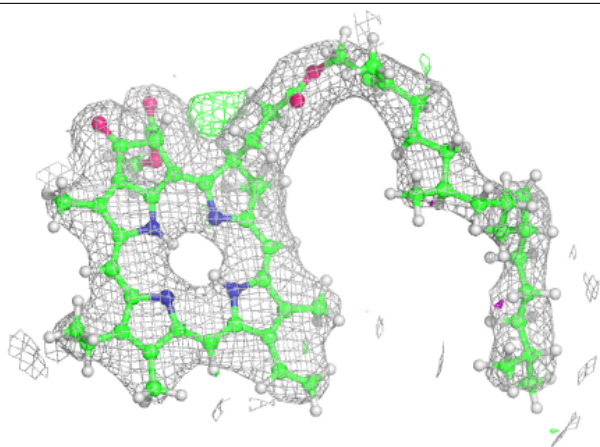
Electron density around LHG L 101:

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



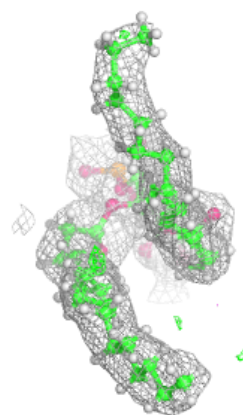
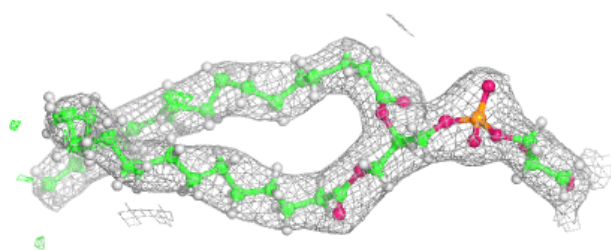
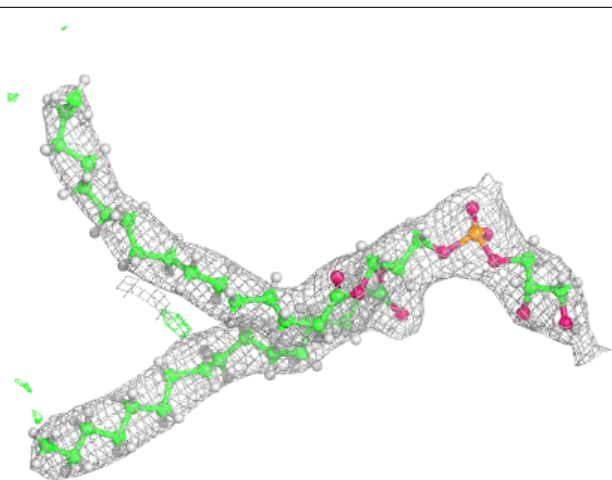
Electron density around PHO d 401:

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



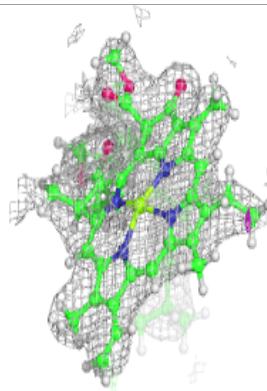
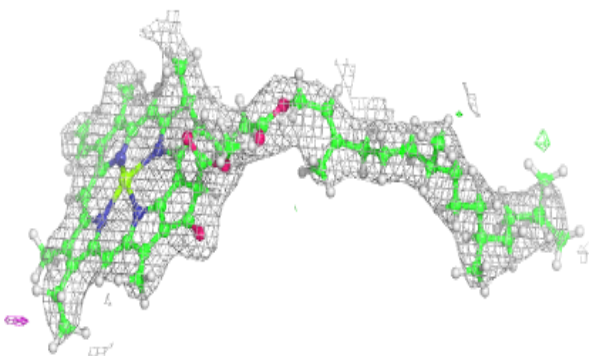
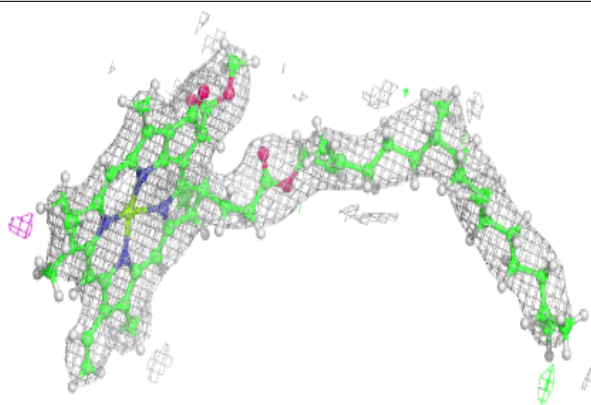
Electron density around LHG d 408:

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

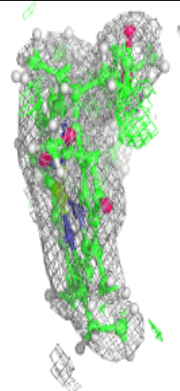
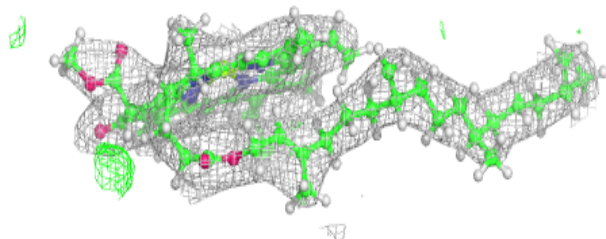
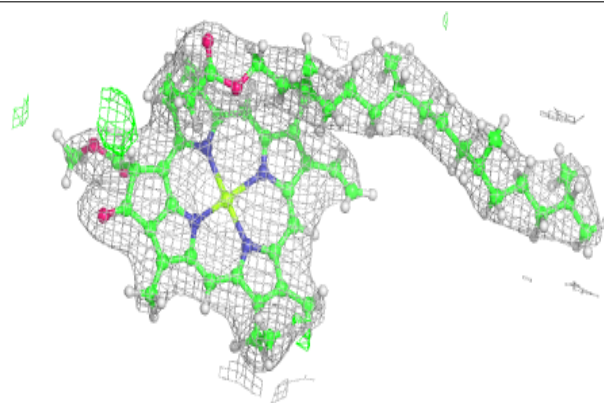


Electron density around CLA a 405:

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

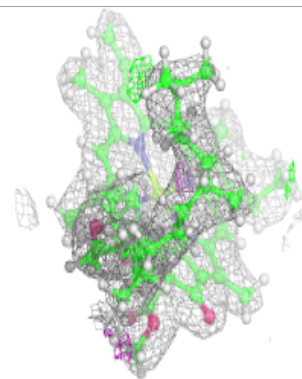
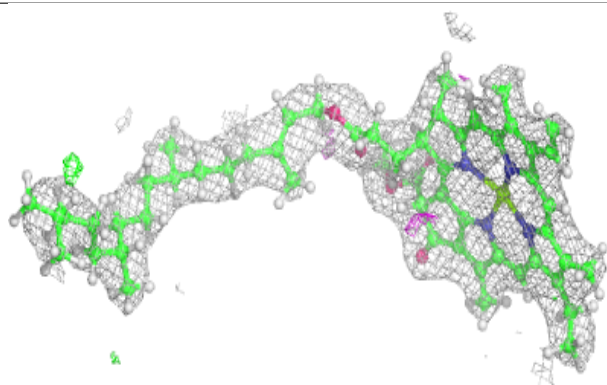
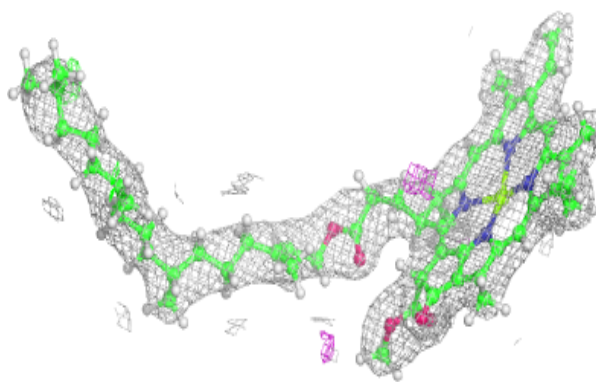
**Electron density around CLA C 502:**

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

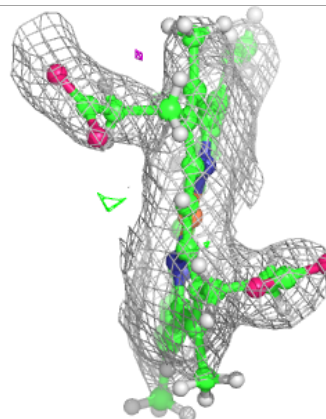
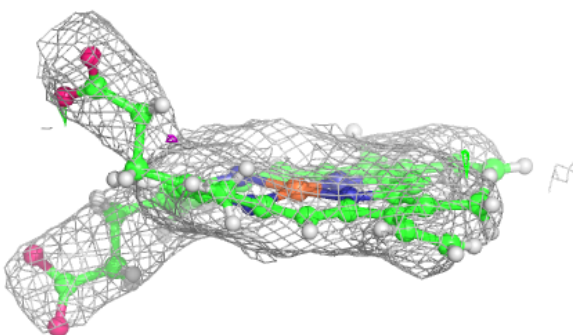
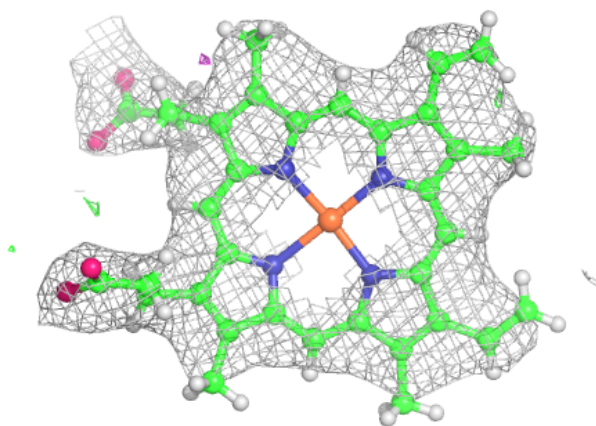


Electron density around CLA A 404:

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

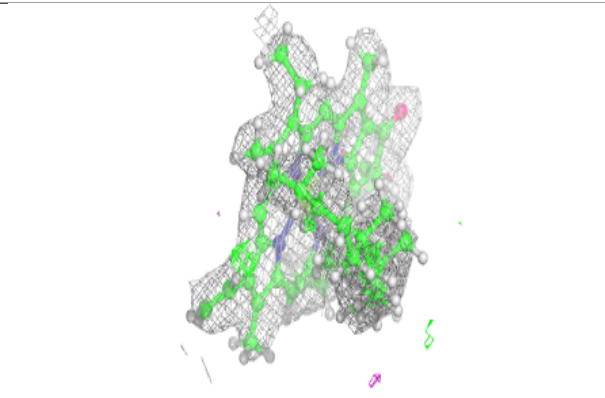
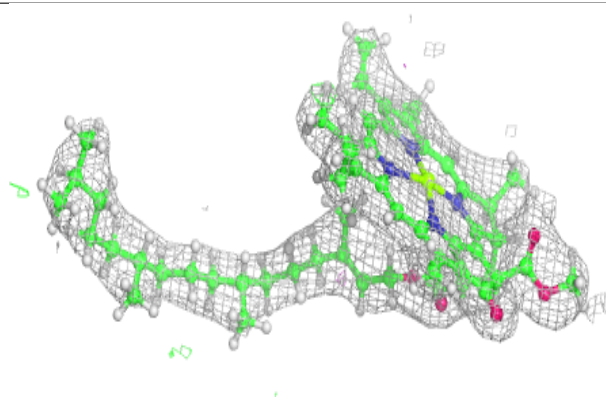
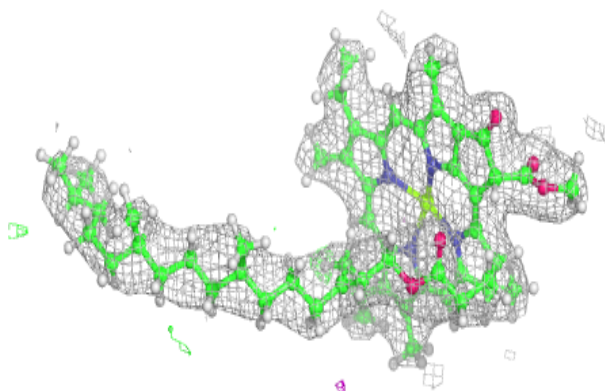
**Electron density around HEM e 102:**

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

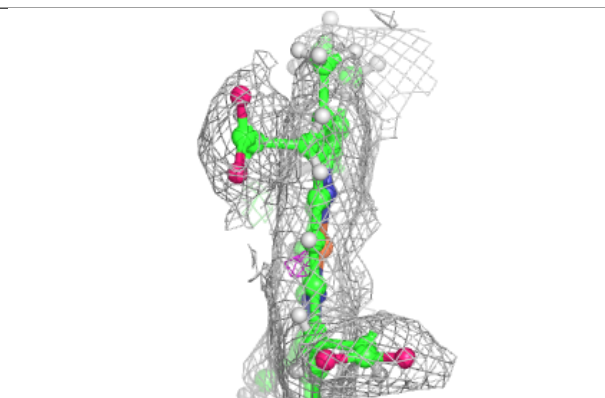
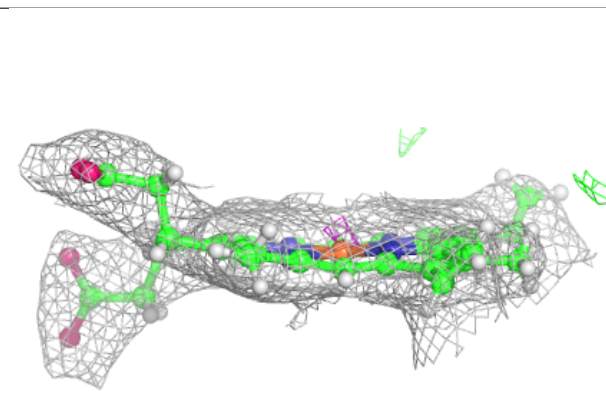
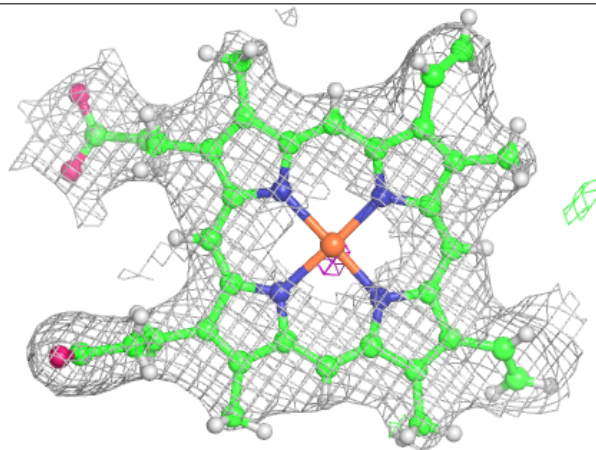


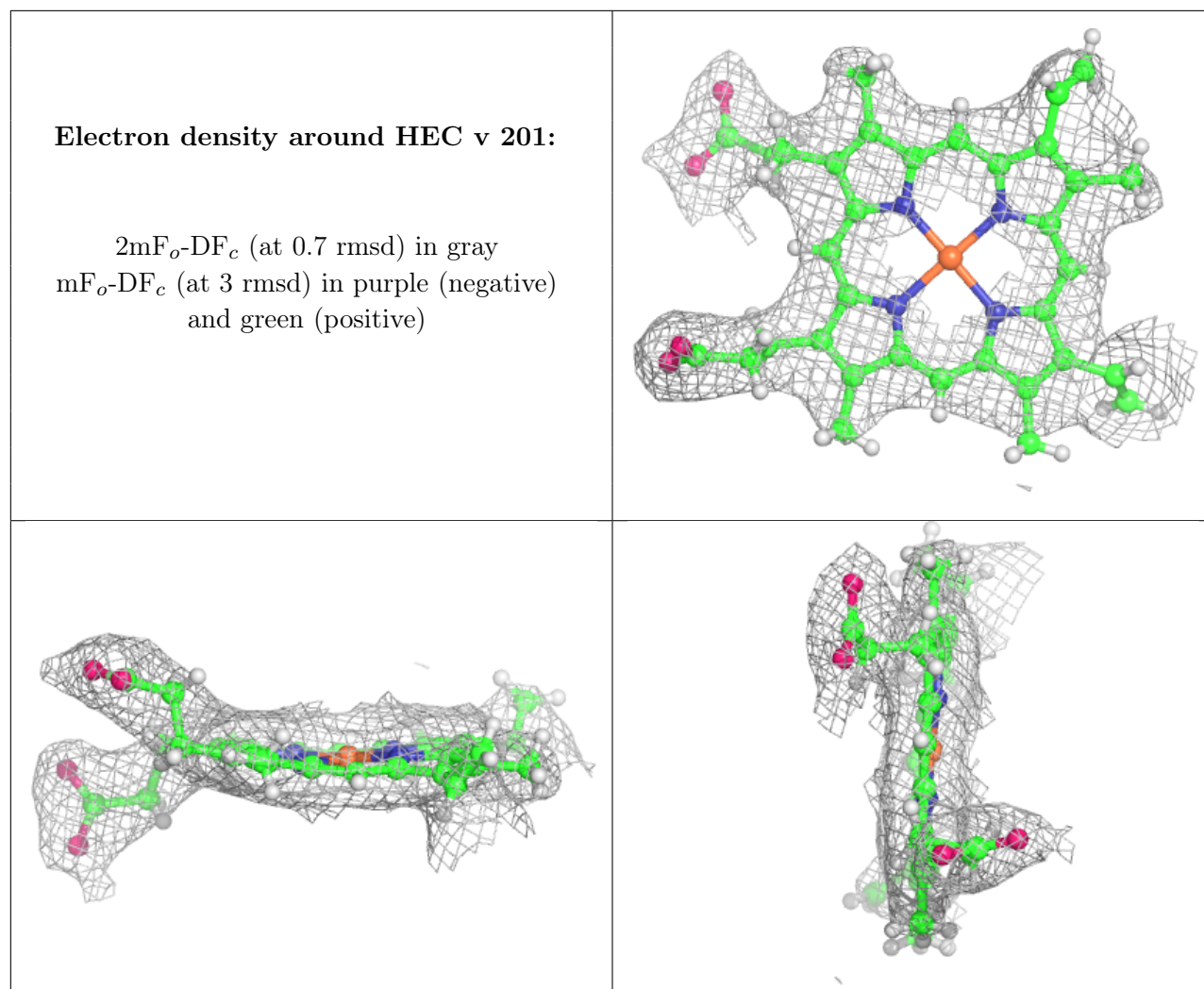
Electron density around CLA B 608:

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

**Electron density around HEC V 201:**

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





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

There are no such residues in this entry.