



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:03 PM UTC

PDB ID : 3A0B / pdb_00003a0b
Title : Crystal structure of Br-substituted Photosystem II complex
Authors : Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.
Deposited on : 2009-03-16
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

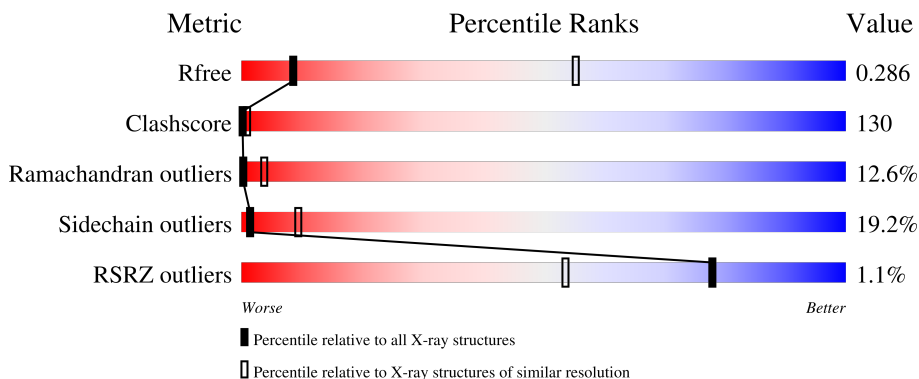
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	344	 7% 60% 27% . .
1	a	344	 7% 58% 28% 5% .
2	B	488	 14% 60% 22% . .
2	b	488	 12% 58% 26% . .
3	C	447	 14% 56% 28% .

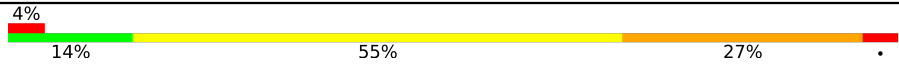


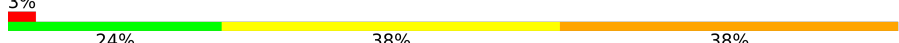

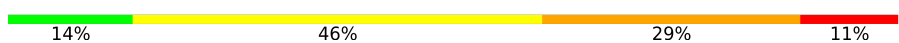

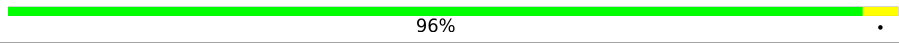
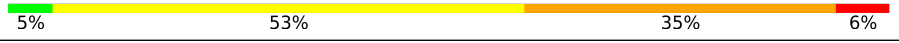
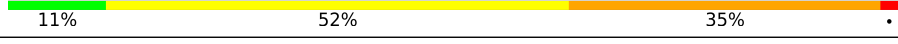
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Mol	Chain	Length	Quality of chain
3	c	447	% 14% 60% 24% .
4	D	340	% 11% 58% 26% 5%
4	d	340	% 13% 57% 26% .
5	E	83	% 13% 54% 25% 6% .
5	e	83	% 19% 54% 23% ..
6	F	44	7% 18% 39% 18% 5% 20%
6	f	44	18% 41% 16% 5% 20%
7	H	64	16% 45% 38% .
7	h	64	3% 19% 48% 31% .
8	I	35	6% 66% 26% .
8	i	35	11% 69% 14% 6%
9	J	40	10% 35% 40% 15%
9	j	40	15% 40% 30% 15%
10	K	36	3% 19% 50% 22% 8%
10	k	36	19% 47% 25% 8%
11	L	37	. 68% 24% 5%
11	l	37	3% 11% 57% 30% .
12	M	36	6% 8% 56% 28% 8%
12	m	36	3% 11% 67% 19% .
13	O	242	2% 22% 55% 18% 5%
13	o	242	% 21% 53% 23% .
14	T	30	10% 47% 37% 7%
14	t	30	17% 53% 30%
15	U	98	19% 53% 22% 5%
15	u	98	15% 58% 21% 5%

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	34	
17	x	34	
18	Y	28	
18	y	28	
19	N	24	
19	n	24	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	1003	X	-	X	-
23	CLA	A	1006	X	-	X	-
23	CLA	A	1007	X	-	-	-
23	CLA	B	1009	X	-	X	-
23	CLA	B	1010	X	-	X	-
23	CLA	B	1011	X	-	X	-
23	CLA	B	1012	X	-	X	-
23	CLA	B	1013	X	-	X	-
23	CLA	B	1014	X	-	X	-
23	CLA	B	1015	X	-	X	-
23	CLA	B	1016	X	-	X	-
23	CLA	B	1018	X	-	X	-
23	CLA	B	1019	X	-	X	-
23	CLA	B	1020	X	-	X	-
23	CLA	B	1021	X	-	X	-
23	CLA	B	1022	X	-	X	-
23	CLA	B	1023	X	-	X	-
23	CLA	B	1024	X	-	X	-
23	CLA	C	1025	X	-	X	-
23	CLA	C	1026	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	1027	X	-	X	-
23	CLA	C	1028	X	-	X	-
23	CLA	C	1029	X	-	X	-
23	CLA	C	1030	X	-	X	-
23	CLA	C	1031	X	-	X	-
23	CLA	C	1032	X	-	X	-
23	CLA	C	1033	X	-	X	-
23	CLA	C	1034	X	-	X	-
23	CLA	C	1035	X	-	-	-
23	CLA	C	1036	X	-	X	-
23	CLA	C	1037	X	-	X	-
23	CLA	D	1004	X	-	-	-
23	CLA	D	1005	X	-	X	-
23	CLA	D	1008	X	-	X	-
23	CLA	H	1017	X	-	X	-
23	CLA	a	6003	X	-	X	-
23	CLA	a	6006	X	-	X	-
23	CLA	a	6007	X	-	-	-
23	CLA	b	6009	X	-	X	-
23	CLA	b	6010	X	-	X	-
23	CLA	b	6011	X	-	X	-
23	CLA	b	6012	X	-	X	-
23	CLA	b	6013	X	-	X	-
23	CLA	b	6014	X	-	X	-
23	CLA	b	6015	X	-	X	-
23	CLA	b	6016	X	-	X	-
23	CLA	b	6017	X	-	X	-
23	CLA	b	6018	X	-	-	-
23	CLA	b	6019	X	-	X	-
23	CLA	b	6020	X	-	X	-
23	CLA	b	6021	X	-	X	-
23	CLA	b	6022	X	-	X	-
23	CLA	b	6023	X	-	X	-
23	CLA	b	6024	X	-	X	-
23	CLA	c	6025	X	-	X	-
23	CLA	c	6026	X	-	X	-
23	CLA	c	6027	X	-	X	-
23	CLA	c	6028	X	-	X	-
23	CLA	c	6029	X	-	X	-
23	CLA	c	6030	X	-	X	-
23	CLA	c	6031	X	-	X	-
23	CLA	c	6032	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	6033	X	-	X	-
23	CLA	c	6034	X	-	X	-
23	CLA	c	6035	X	-	X	-
23	CLA	c	6036	X	-	X	-
23	CLA	c	6037	X	-	X	-
23	CLA	d	6004	X	-	-	-
23	CLA	d	6005	X	-	X	-
23	CLA	d	6008	X	-	X	-
24	PHO	A	1038	X	-	X	-
24	PHO	A	1039	X	-	X	-
24	PHO	a	6039	X	-	X	-
24	PHO	d	6038	X	-	X	-
25	PQ9	D	1042	-	-	X	-
25	PQ9	d	6042	-	-	X	-
26	BCR	A	1044	-	-	X	-
26	BCR	B	1045	-	-	X	-
26	BCR	B	1047	-	-	X	-
26	BCR	B	1048	-	-	X	-
26	BCR	C	1054	-	-	X	-
26	BCR	D	1050	-	-	X	-
26	BCR	H	1049	-	-	X	-
26	BCR	K	1051	-	-	X	-
26	BCR	K	1052	-	-	X	-
26	BCR	T	6046	-	-	X	-
26	BCR	Z	1053	-	-	X	-
26	BCR	a	6044	-	-	X	-
26	BCR	b	6045	-	-	X	-
26	BCR	b	6047	-	-	X	-
26	BCR	b	6048	-	-	X	-
26	BCR	c	6054	-	-	X	-
26	BCR	d	6050	-	-	X	-
26	BCR	h	6049	-	-	X	-
26	BCR	k	6051	-	-	X	-
26	BCR	k	6052	-	-	X	-
26	BCR	t	1046	-	-	X	-
26	BCR	z	6053	-	-	X	-
27	LHG	A	1063	-	-	X	-
27	LHG	a	6063	-	-	X	-
28	BR	A	1065	-	-	X	-
29	MGE	B	1060	-	-	X	-
29	MGE	D	1062	-	-	X	-
29	MGE	J	1059	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MGE	L	1061	-	-	X	-
29	MGE	b	6060	-	-	X	-
29	MGE	d	6059	-	-	X	-
29	MGE	d	6061	-	-	X	-
29	MGE	d	6062	-	-	X	-
30	DGD	C	1055	-	-	X	-
30	DGD	C	1056	-	-	X	-
30	DGD	C	1057	-	-	X	-
30	DGD	H	1058	-	-	X	-
30	DGD	c	6055	-	-	X	-
30	DGD	c	6056	-	-	X	-
30	DGD	c	6057	-	-	X	-
30	DGD	h	6058	-	-	X	-

2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 47988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	Total 2630	C 1720	N 435	O 460	S 15	0	0	0
1	a	335	Total 2630	C 1720	N 435	O 460	S 15	0	0	0

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	485	Total 3816	C 2505	N 635	O 663	S 13	0	0	0
2	b	485	Total 3816	C 2505	N 635	O 663	S 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	447	Total 3455	C 2264	N 576	O 602	S 13	0	0	0
3	c	447	Total 3455	C 2264	N 576	O 602	S 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	340	Total 2706	C 1794	N 440	O 460	S 12	0	0	0
4	d	340	Total 2706	C 1794	N 440	O 460	S 12	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			507	339	81	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			507	339	81	85	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			287	195	45	46	1			
8	i	35	Total	C	N	O	S	0	0	0
			287	195	45	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	36	Total	C	N	O	0	0	0
			278	195	38	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	36	278	195	38	45	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	36	283	187	42	53	1	0	0	0
12	m	36	283	187	42	53	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	242	1841	1152	311	374	4	0	0	0
13	o	242	1841	1152	311	374	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	257	180	36	39	2	0	0	0
14	t	30	257	180	36	39	2	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
15	U	98	783	496	130	157	0	0	0
15	u	98	783	496	130	157	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	X	34	Total	C	N	O		0	0	0
			246	166	36	44				
17	x	34	Total	C	N	O		0	0	0
			246	166	36	44				

- Molecule 18 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	28	Total	C	N	O	S	0	0	0
			208	137	36	32	3			
18	y	28	Total	C	N	O	S	0	0	0
			208	137	36	32	3			

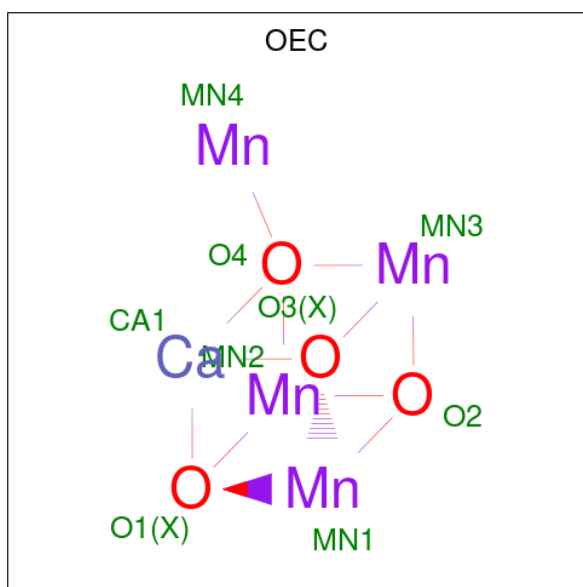
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	N	24	Total	C	N	O		0	0	0
			121	72	24	25				
19	n	24	Total	C	N	O		0	0	0
			121	72	24	25				

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

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

- Molecule 21 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn₄O₄).

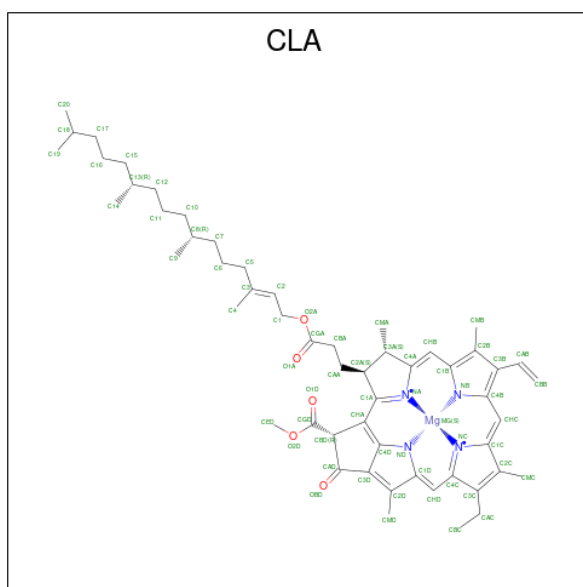


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Ca	Mn		
21	A	1	5	1	4	0	0
21	a	1	5	1	4	0	0

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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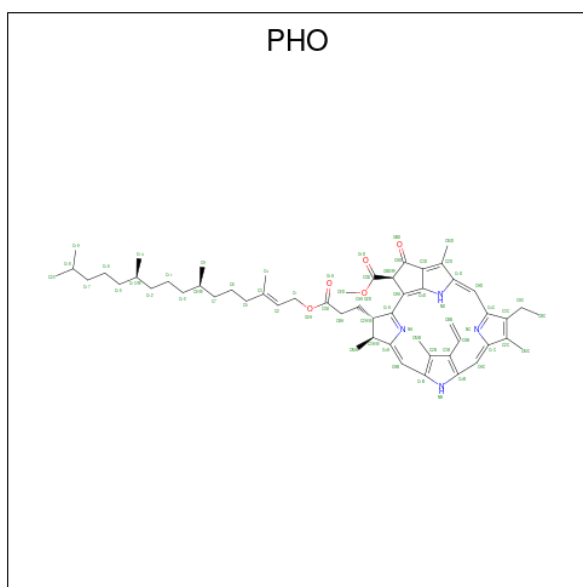
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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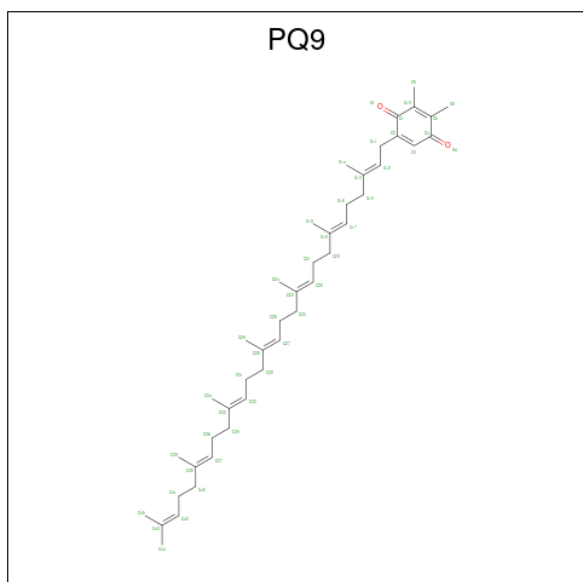
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



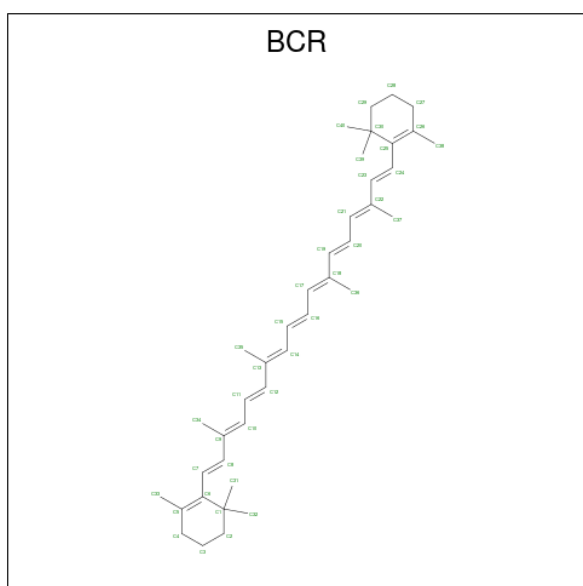
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	64	55	4	5	0	0
24	A	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0
24	d	1	64	55	4	5	0	0

- Molecule 25 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACO SA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: C₄₃H₆₄O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	1	Total	C O	0	0
			45	43 2		
25	D	1	Total	C O	0	0
			45	43 2		
25	a	1	Total	C O	0	0
			45	43 2		
25	d	1	Total	C O	0	0
			45	43 2		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



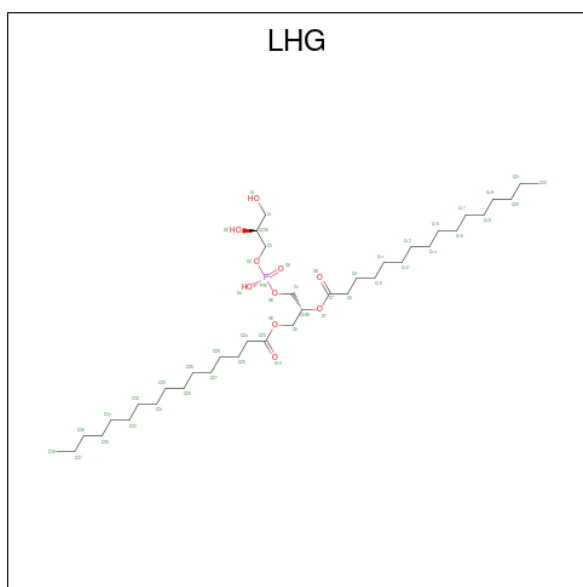
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		
26	H	1	Total	C	0	0
			40	40		
26	K	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Z	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).

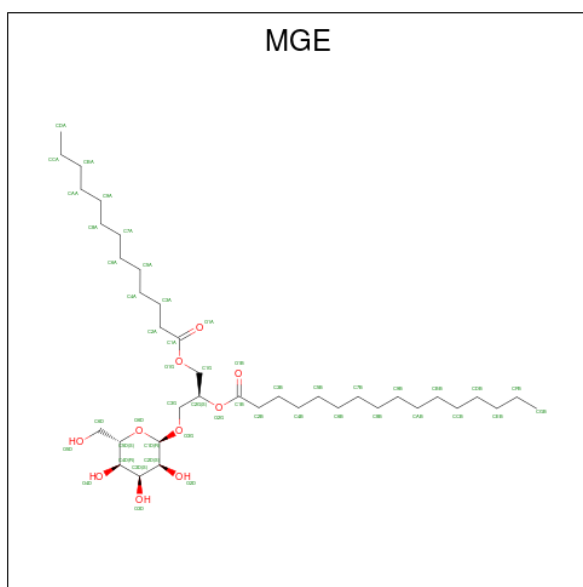


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
27	A	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 is BROMIDE ION (CCD ID: BR) (formula: Br).

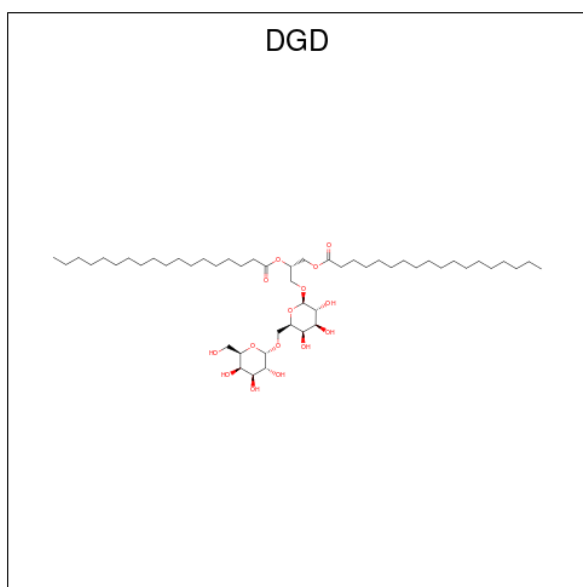
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	2	Total	Br	0	0
			2	2		
28	a	1	Total	Br	0	0
			1	1		
28	d	1	Total	Br	0	0
			1	1		

- Molecule 29 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀).



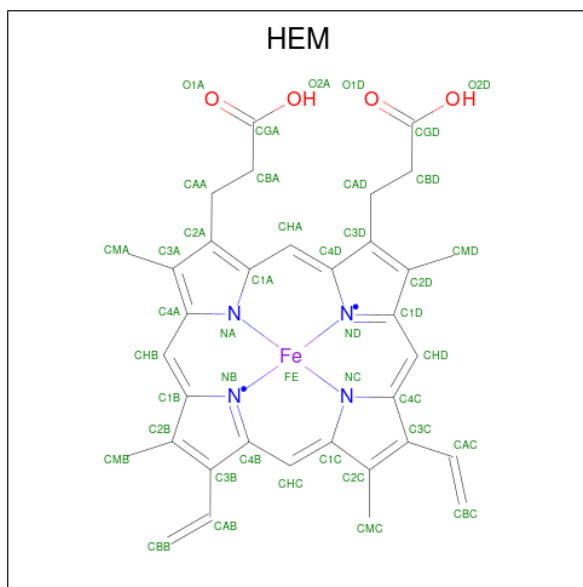
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	J	1	Total	C	O	0	0
			48	38	10		
29	L	1	Total	C	O	0	0
			48	38	10		
29	b	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			66	51	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	H	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	h	1	Total	C	O	0	0
			66	51	15		

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

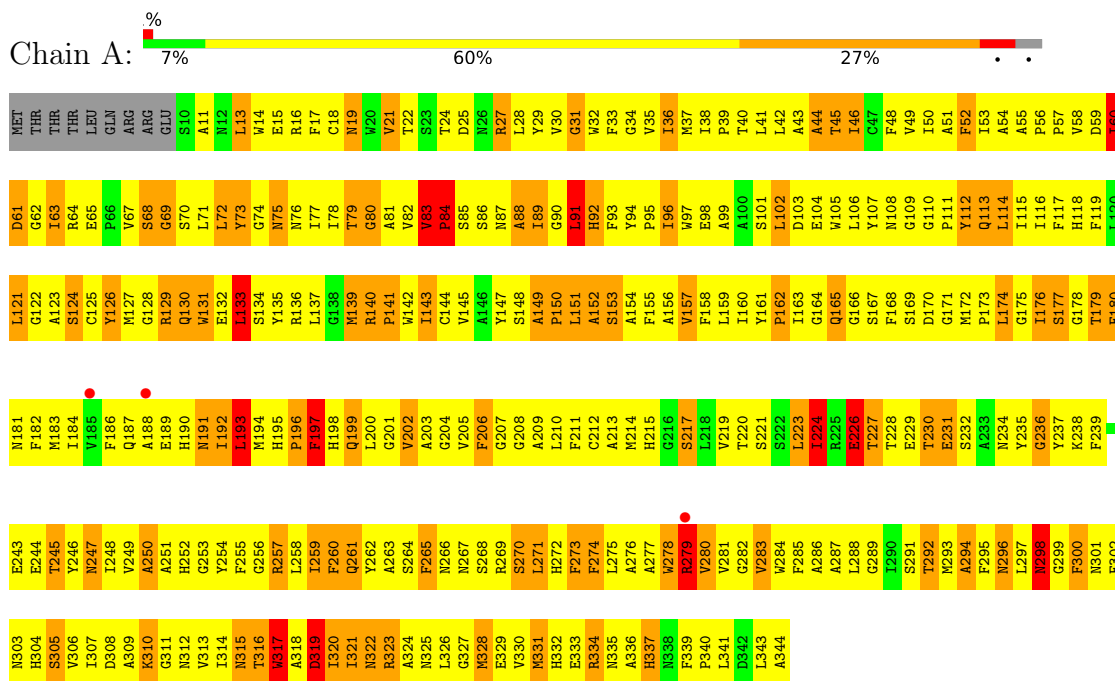


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
31	E	1	43	34	1	4	4	0	0
31	V	1	43	34	1	4	4	0	0
31	e	1	43	34	1	4	4	0	0
31	v	1	43	34	1	4	4	0	0

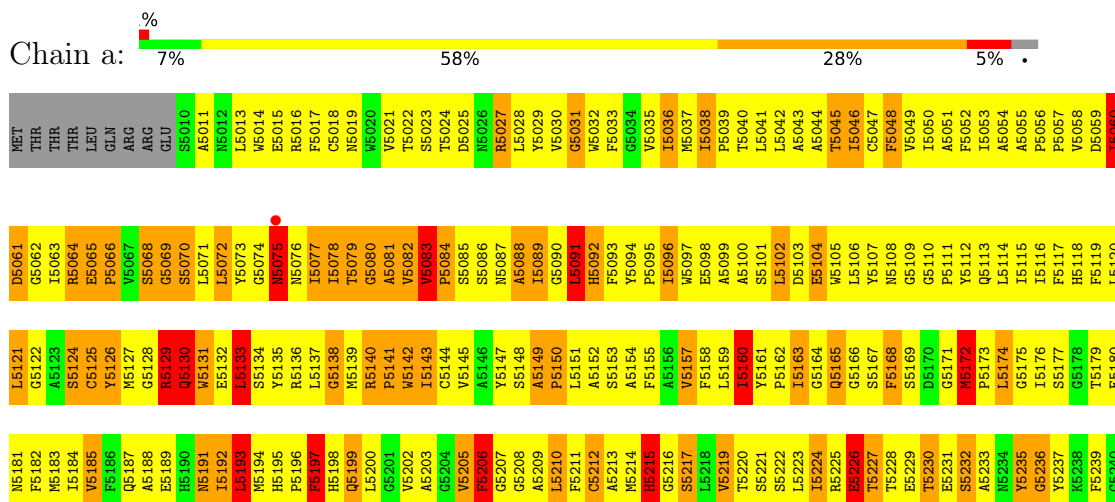
3 Residue-property plots

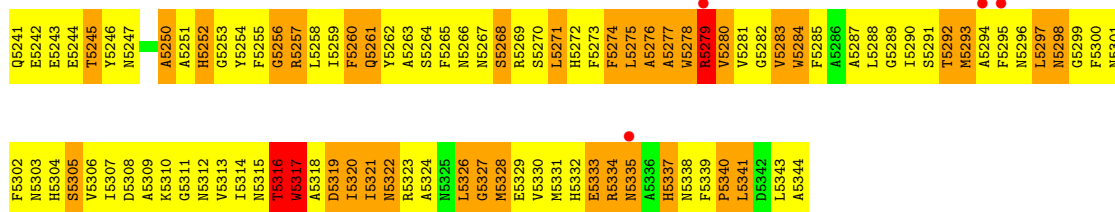
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 Q(B) protein

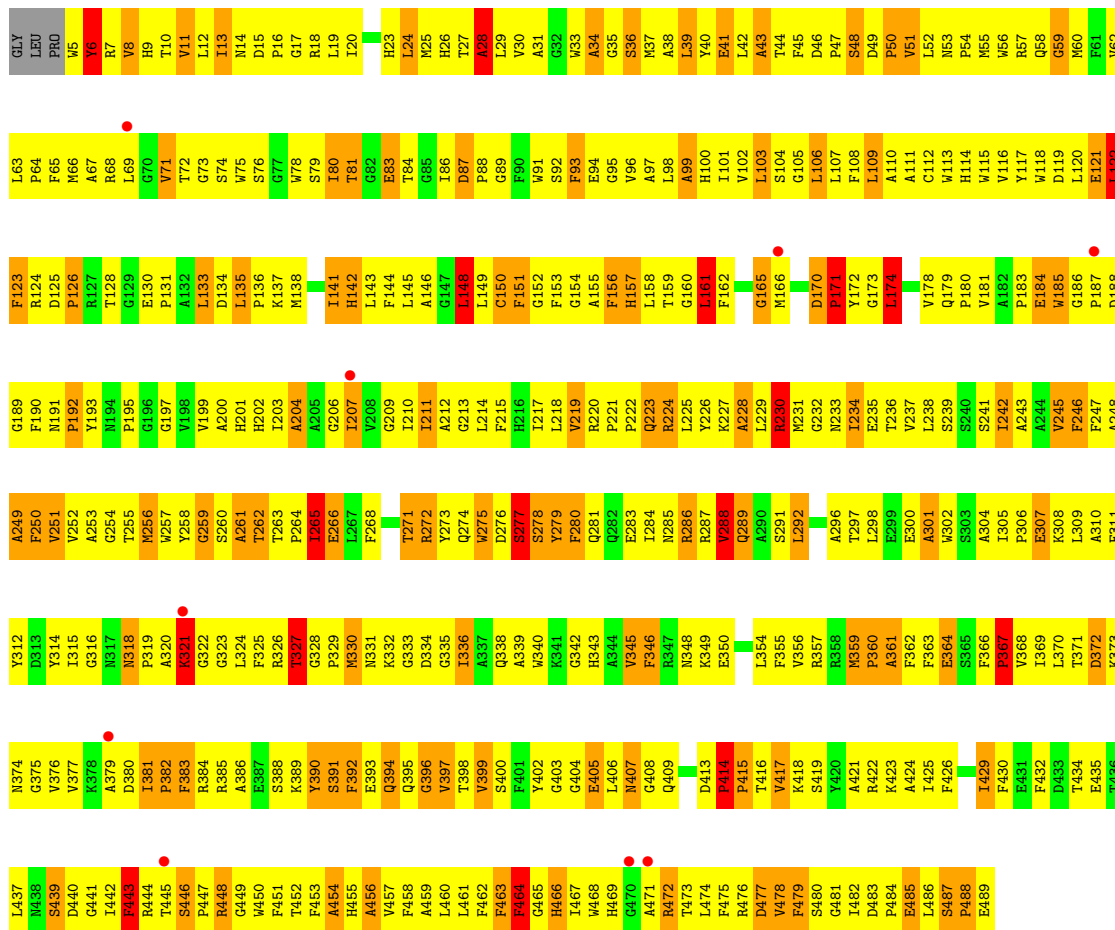
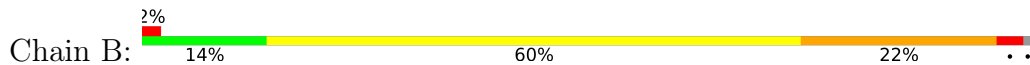


- Molecule 1: Photosystem Q(B) protein

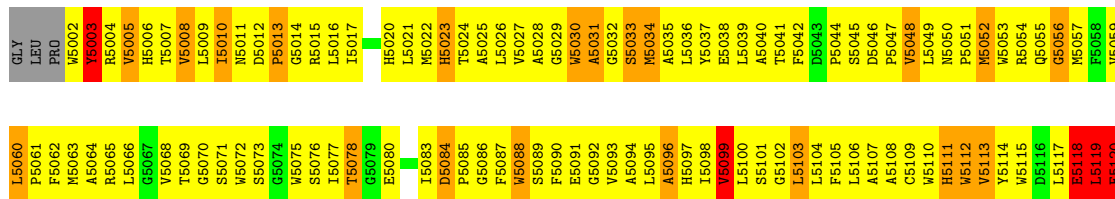
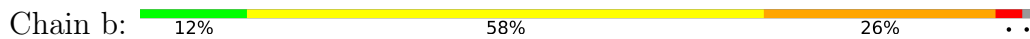




● Molecule 2: Photosystem II core light harvesting protein

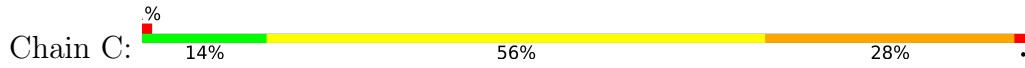


● Molecule 2: Photosystem II core light harvesting protein

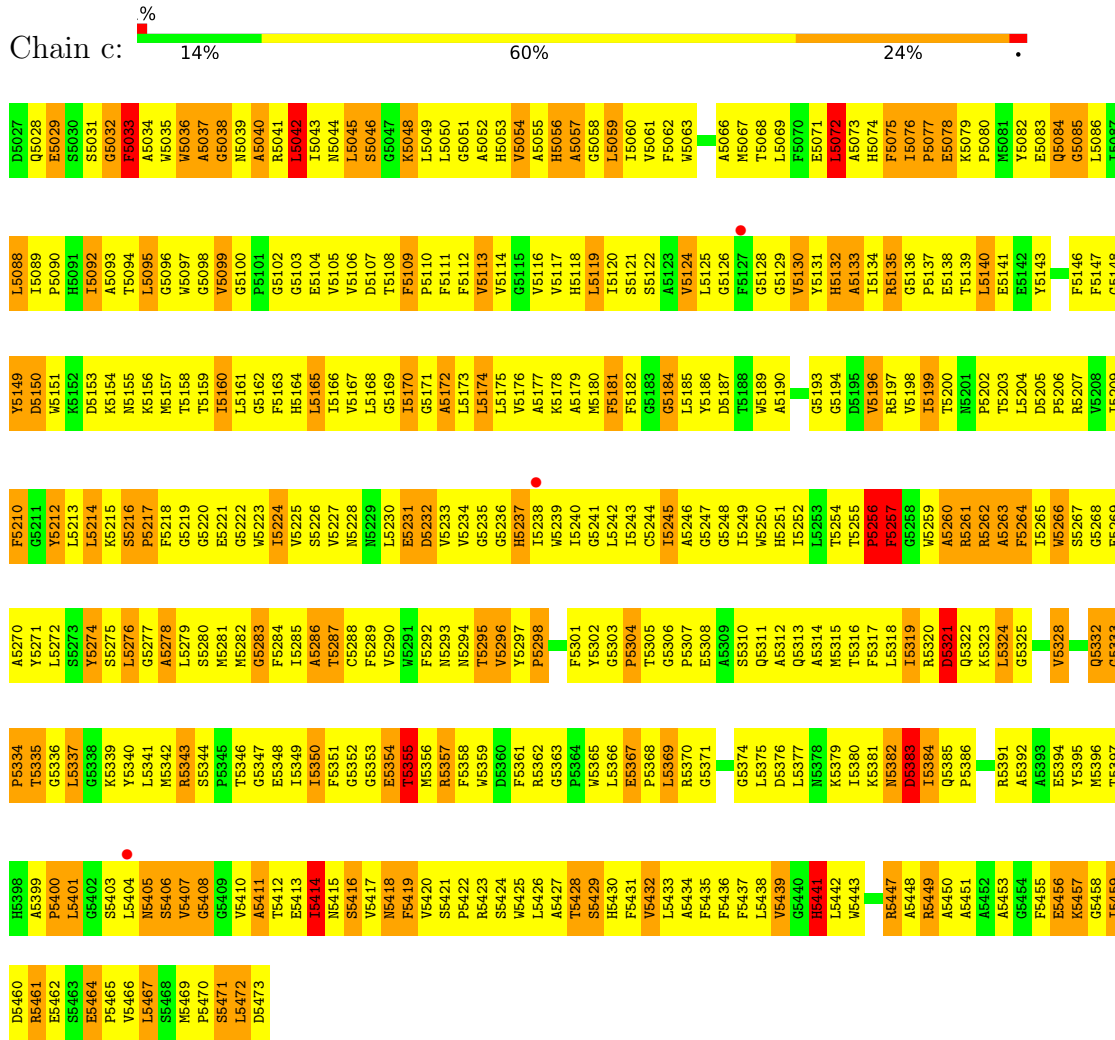


R5121	D5122	F5123	R5124	F5125	G5126	F5127	F5128	F5129	F5130	F5131	F5132	F5133	F5134	F5135	F5136	F5137	F5138	F5139	F5140	F5141	F5142	F5143	F5144	F5145	F5146	F5147	F5148	F5149	F5150	F5151	F5152	F5153	F5154	F5155	F5156	F5157	F5158	F5159	F5200	F5201	F5202	F5203	F5204	F5205	F5206	F5207	F5208	F5209	F5210	F5211	F5212	F5213	F5214	F5215	F5216	F5217	F5218	F5219	F5220	F5221	F5222	F5223	F5224	F5225	F5226	F5227	F5228	F5229	F5230	F5231	F5232	F5233	F5234	F5235	F5236	F5237	F5238	F5239	F5240																																													
A5241	V5242	F5243	F5244	F5245	A5246	F5247	F5248	F5249	A5250	G5251	F5252	F5253	F5254	F5255	F5256	F5257	F5258	F5259	F5260	F5261	F5262	F5263	F5264	F5265	F5266	F5267	F5268	F5269	F5270	F5271	F5272	F5273	F5274	F5275	F5276	F5277	F5278	F5279	F5280	F5281	F5282	F5283	F5284	F5285	F5286	F5287	F5288	F5289	F5290	F5291	F5292	F5293	F5294	F5295	F5296	F5297	F5298	F5299	F5300	F5301	F5302	F5303	F5304	F5305	F5306	F5307	F5308	F5309	F5310	F5311	F5312	F5313	F5314	F5315	F5316	F5317	F5318	F5319	F5320	F5321	F5322	F5323	F5324	F5325	F5326	F5327	F5328	F5329	F5330	F5331	F5332	F5333	F5334	F5335	F5336	F5337	F5338	F5339	F5340	F5341	F5342	F5343	F5344	F5345	F5346	F5347	F5348	F5349	F5350	F5351	F5352	F5353	F5354	F5355	F5356	F5357	F5358	F5359	F5360	F5361	F5362	F5363	F5364	F5365
K5305	L5306	F5307	F5308	F5309	F5310	F5311	F5312	F5313	F5314	F5315	F5316	F5317	F5318	F5319	F5320	F5321	F5322	F5323	F5324	F5325	F5326	F5327	F5328	F5329	F5330	F5331	F5332	F5333	F5334	F5335	F5336	F5337	F5338	F5339	F5340	F5341	F5342	F5343	F5344	F5345	F5346	F5347	F5348	F5349	F5350	F5351	F5352	F5353	F5354	F5355	F5356	F5357	F5358	F5359	F5360	F5361	F5362	F5363	F5364	F5365																																																																
L5366	L5367	K5370	N5371	F5372	F5373	F5374	F5375	F5376	F5377	F5378	F5379	F5380	F5381	F5382	F5383	F5384	F5385	F5386	F5387	F5388	F5389	F5390	F5391	F5392	F5393	F5394	F5395	F5396	F5397	F5398	F5399	F5400	F5401	F5402	F5403	F5404	F5405	F5406	F5407	F5408	F5409	F5410	F5411	F5412	F5413	F5414	F5415	F5416	F5417	F5418	F5419	F5420	F5421	F5422	F5423	F5424	F5425	F5426	F5427	F5428	F5429	F5430																																																														
F5429	D5430	E5431	E5432	F5433	F5434	F5435	F5436	F5437	F5438	F5439	F5440	F5441	F5442	F5443	F5444	F5445	F5446	F5447	F5448	F5449	F5450	F5451	F5452	F5453	F5454	F5455	F5456	F5457	F5458	F5459	F5460	F5461	F5462	F5463	F5464	F5465	F5466	F5467	F5468	F5469	F5470	F5471	F5472	F5473	F5474	F5475	F5476	F5477	F5478	F5479	F5480	F5481	F5482	F5483	F5484	F5485	F5486																																																																			
D5487	F5488	F5489	F5490	F5491	F5492	F5493	F5494	F5495	F5496	F5497	F5498	F5499	F5500	F5501	F5502	F5503	F5504	F5505	F5506	F5507	F5508	F5509	F5510	F5511	F5512	F5513	F5514	F5515	F5516	F5517	F5518	F5519	F5520	F5521	F5522	F5523	F5524	F5525	F5526	F5527	F5528	F5529	F5530	F5531	F5532	F5533	F5534	F5535	F5536	F5537	F5538	F5539	F5540	F5541	F5542	F5543	F5544	F5545	F5546	F5547	F5548	F5549	F5550	F5551	F5552	F5553	F5554	F5555	F5556	F5557	F5558	F5559	F5560	F5561	F5562	F5563	F5564	F5565																																														
D57	Q28	E29	S30	S31	G32	F33	A34	W35	W36	A37	G38	N39	A40	R41	L42	I43	M44	L45	S46	G47	K48	L49	P10	F11	G51	A52	H53	F54	A55	H56	L117	H118	L119	I120	S121	G122	F62	W63	A64	M67	T68	L69	F70	F71	L72	A73	H74	F75	I76	P77	E78	K79	P80	M81	Y82	E83	Q84	G85	L86	F147	G88	G148	I87																																																													
L88	I89	P90	H91	I92	A93	T94	L95	G96	W97	G98	V99	G100	P101	G102	G103	E104	M105	L106	L107	I108	F109	P110	F111	F112	V113	V114	G115	L116	L117	H118	L119	I120	F182	G183	S121	A122	A123	Y186	L125	G126	F127	G128	G129	Y130	Y131	H132	A133	I134	R135	V136	T200	P137	E138	N201	P202	T203	L204	E141	E142	D205	P206	R207	V208	I209	F210																																																											
Y149	D150	K151	K152	D153	K154	N155	K156	M157	L158	T159	M160	L161	G162	F163	H164	L165	I166	V167	L168	G169	I170	G171	A172	L173	L174	L175	V176	A177	K178	A179	F182	G183	S121	A122	A123	Y186	L125	G126	F127	G128	G129	Y130	Y131	H132	A133	I134	R135	V136	T200	P137	E138	N201	P202	T203	L204	E141	E142	D205	P206	R207	V208	I209	F210																																																													
G211	Y212	L213	L214	K215	S216	F217	F218	G219	G220	E221	G222	W223	I224	V225	S226	V227	F228	M229	L230	E231	N232	R233	V234	G235	G236	H237	I238	W239	W240	G241	L242	G243	C244	I245	E246	R370	G247	G248	I249	W250	H251	I252	L253	T254	T255	P256	F257	R320	D321	G258	W259	K322	A260	R261	R262	A263	F264	A392	A393	I265	G329	W266	S267	G268	E269	G333	I209	F210																																																								
Y271	L272	S273	Y274	S275	L276	G277	A278	L279	S280	M281	M282	G283	F284	I285	A286	T287	F351	G352	F353	E354	F355	M356	R357	F358	V359	B360	F361	R362	G363	P364	G365	L366	E367	P368	R370	G371	G374	L375	D376	L377	K378	K379	L380	K381	N382	D383	I384	Q385	L384	G325	R390	R391	A392	A393	F394	I395	F396	T397	G333	I209	F210																																																															
A399	P400	G401	G402	P463	P465	V466	M405	S406	V407	V410	A411	T412	E413	L414	M415	S416	V417	M418	F419	V420	S421	P422	R423	S424	V425	A426	L427	T428	S429	H430	F431	V432	L433	P434	R435	F436	F437	L438	V439	G440	H441	L442	L443	H444	R447	A448	R449	A450	A451	A452	G453	G454	F455	F456	F457	G458	T459	L460	L461	L462	L463	L464	L465	L466	L467	S468	M469	F470	L471	L472	D473																																																					

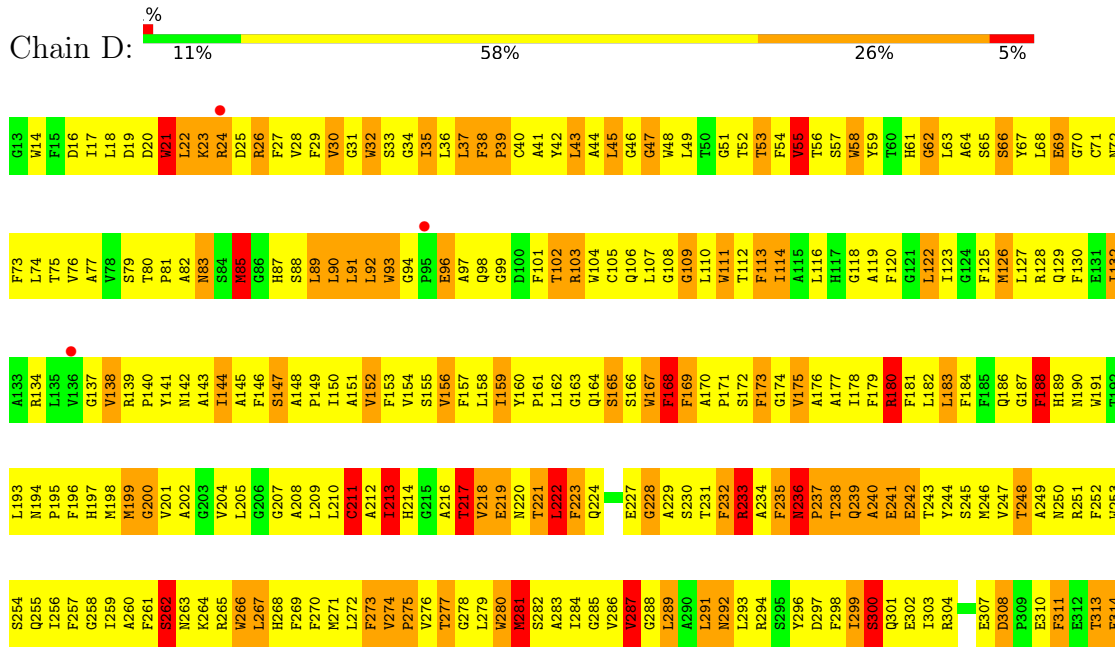
• Molecule 3: Photosystem II CP43 protein

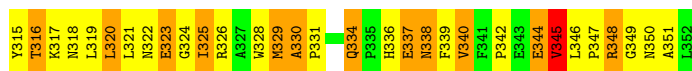


• Molecule 3: Photosystem II CP43 protein

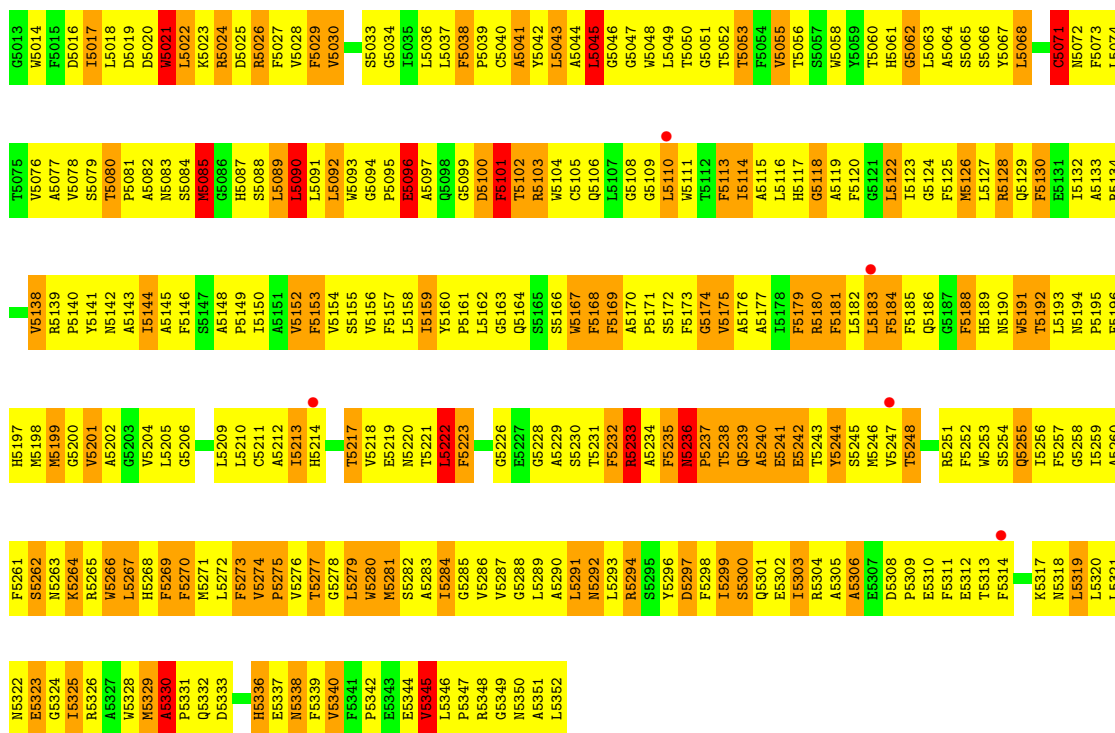
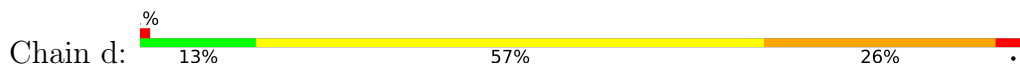


• Molecule 4: Photosystem II D2 protein

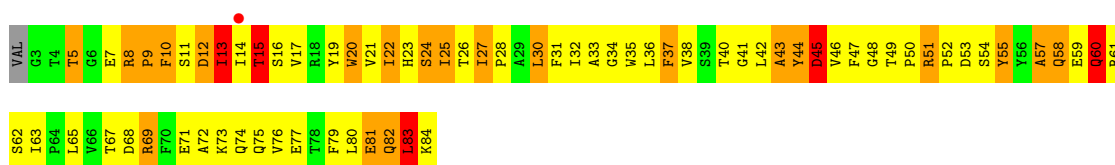
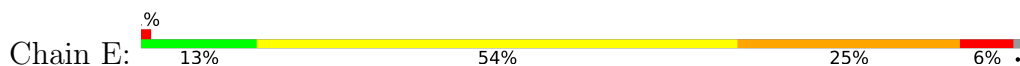




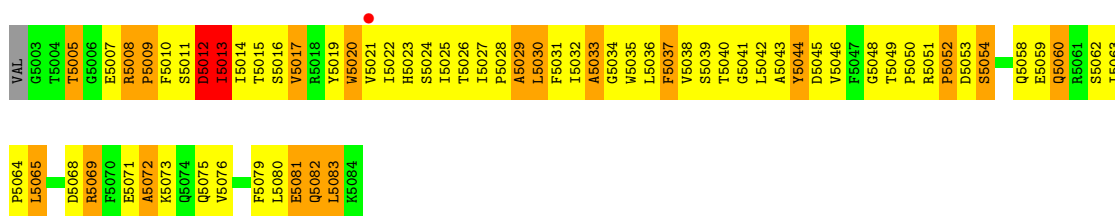
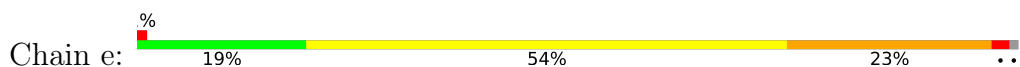
• Molecule 4: Photosystem II D2 protein



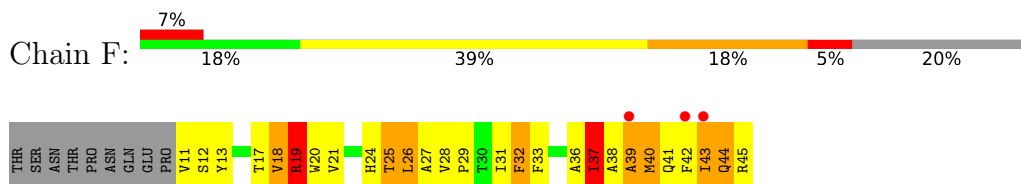
• Molecule 5: Cytochrome b559 subunit alpha



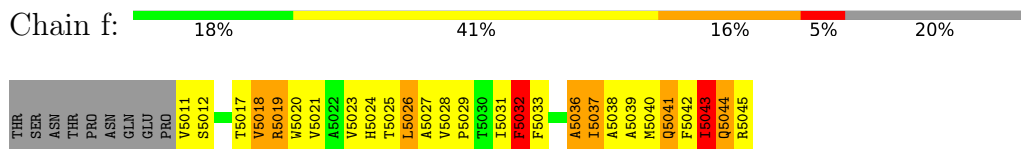
• Molecule 5: Cytochrome b559 subunit alpha



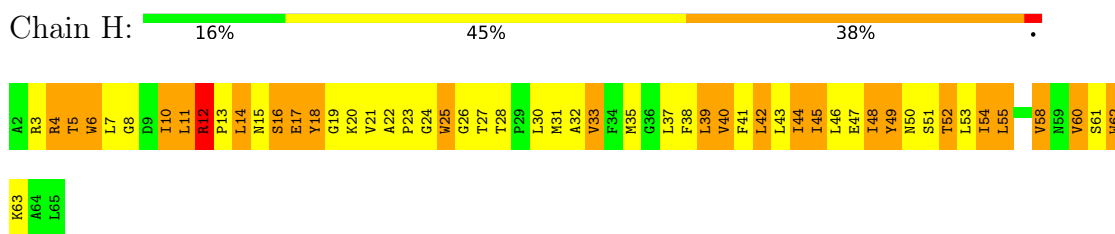
• Molecule 6: Cytochrome b559 subunit beta



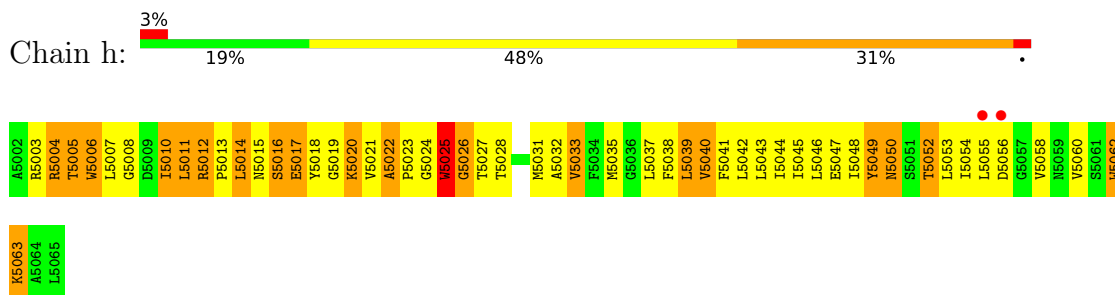
• Molecule 6: Cytochrome b559 subunit beta



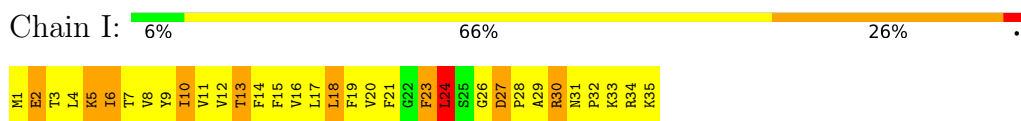
• Molecule 7: Photosystem II reaction center protein H



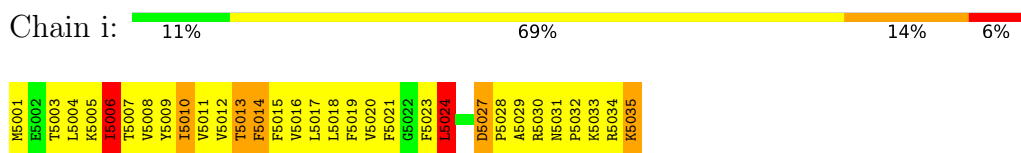
• Molecule 7: Photosystem II reaction center protein H



• Molecule 8: Photosystem II reaction center protein I



• Molecule 8: Photosystem II reaction center protein I

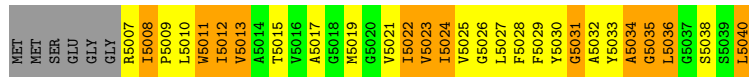


• Molecule 9: Photosystem II reaction center protein J

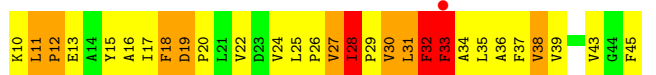
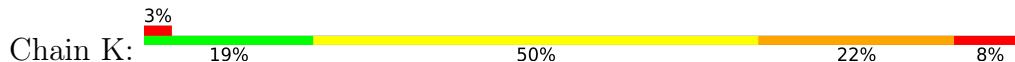




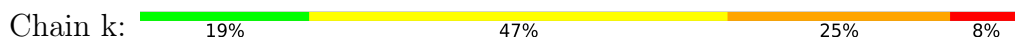
- Molecule 9: Photosystem II reaction center protein J



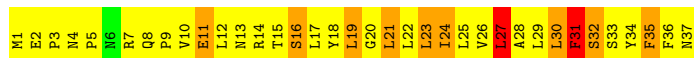
- Molecule 10: Photosystem II reaction center protein K



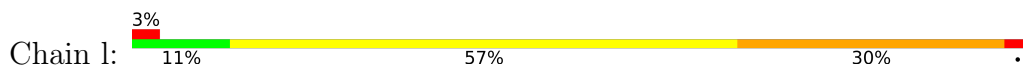
- Molecule 10: Photosystem II reaction center protein K



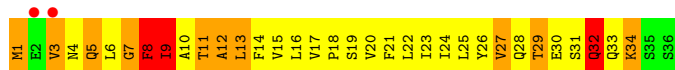
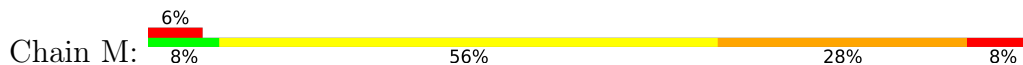
- Molecule 11: Photosystem II reaction center protein L



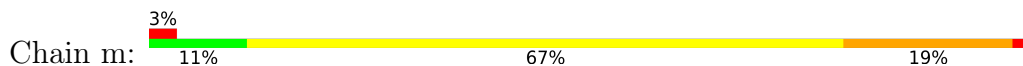
- Molecule 11: Photosystem II reaction center protein L

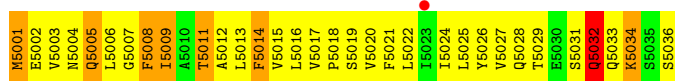


- Molecule 12: Photosystem II reaction center protein M

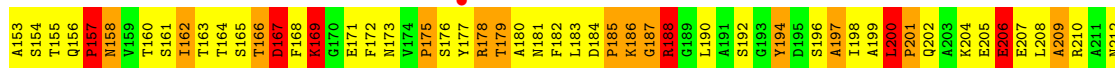
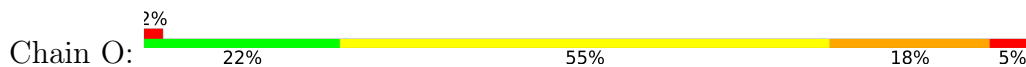


- Molecule 12: Photosystem II reaction center protein M

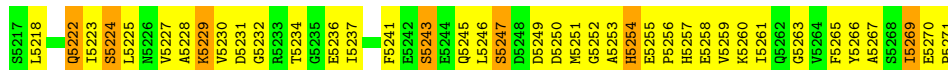
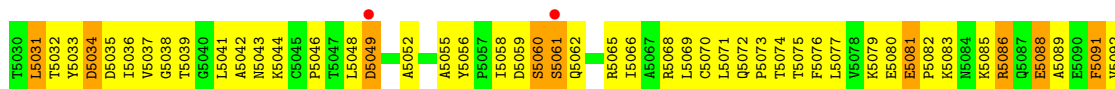




- Molecule 13: Photosystem II manganese-stabilizing polypeptide



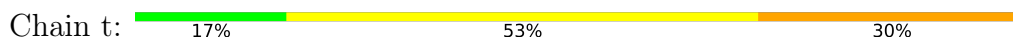
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T

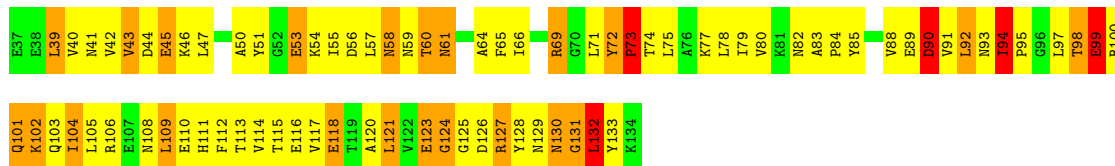


- Molecule 14: Photosystem II reaction center protein T

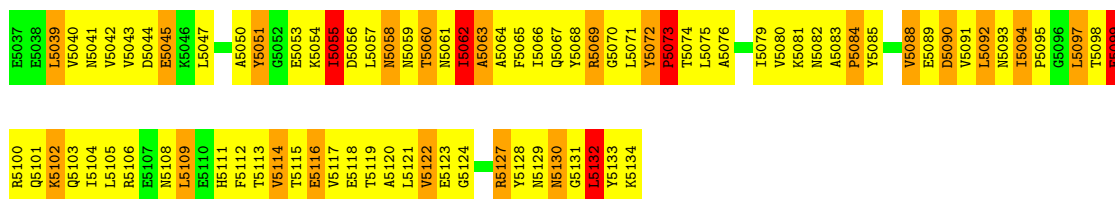
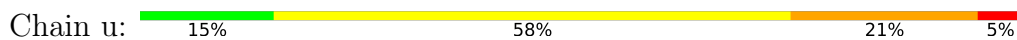




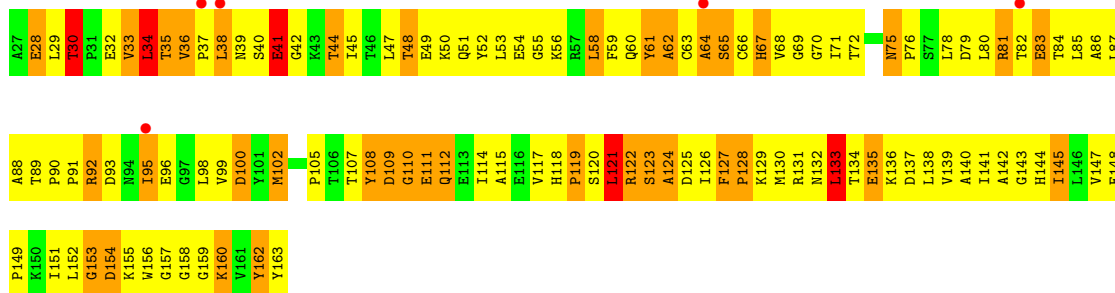
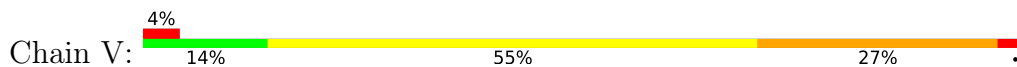
• Molecule 15: Photosystem II 12 kDa extrinsic protein



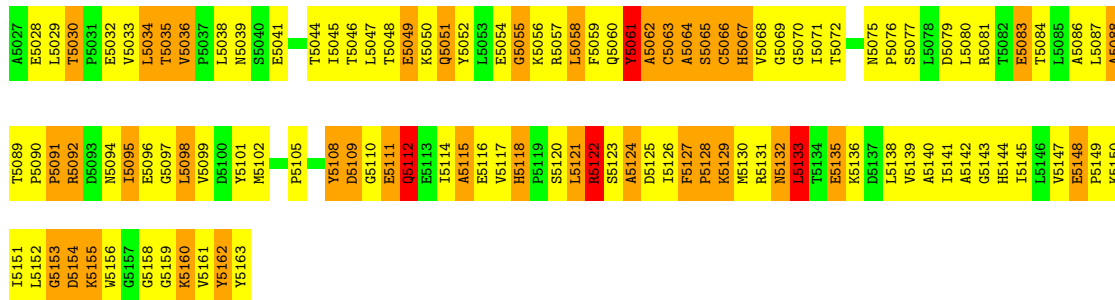
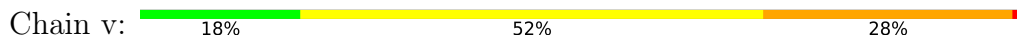
• Molecule 15: Photosystem II 12 kDa extrinsic protein




• Molecule 16: Cytochrome c-550

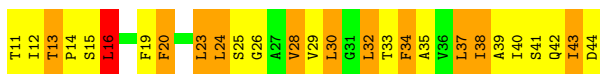


• Molecule 16: Cytochrome c-550




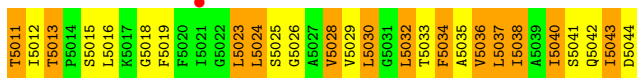
- Molecule 17: Photosystem II reaction center protein X

Chain X:  21% 44% 32% .



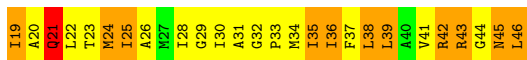
- Molecule 17: Photosystem II reaction center protein X

Chain x:  3% 24% 38% 38%

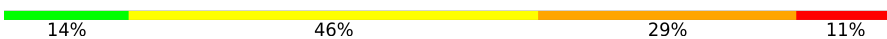


- Molecule 18: Photosystem II reaction center protein ycf12

Chain Y:  7% 50% 39% .




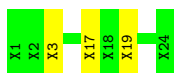
- Molecule 18: Photosystem II reaction center protein ycf12

Chain y:  14% 46% 29% 11%



- Molecule 19: Photosystem II reaction center protein Y

Chain N:  88% 12%



- Molecule 19: Photosystem II reaction center protein Y

Chain n:  96%



- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  5% 53% 35% 6%



V61
V62

- Molecule 20: Photosystem II reaction center protein Z

Chain z:  11% 52% 35%

M5001	T5002	I5003	L5004	F5005	Q5006	L5007	A5008	L5009	A5010	A5011	L5012	V5013	L5014	L5015	S5016	S5017	F5018	V5019	M5020	V5021	V5022	V5023	P5024	V5025	A5026	Y5027	A5028	S5029	P5030	Q5031	D5032	M5033	D5034	R5035	S5036	K5037	Q5038	L5039	I5040	F5041	L5042	G5043	S5044	G5045	L5046	M5047	I5048	A5049	L5050	V5051	L5052	V5053	V5054	G5055	V5056	L5057	M5058	F5059	F5060	V5061
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V5062

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.59Å 226.39Å 307.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.70 – 3.70 34.70 – 3.70	Depositor EDS
% Data completeness (in resolution range)	85.8 (34.70-3.70) 85.7 (34.70-3.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.66Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.302 , 0.358 0.286 , 0.286	Depositor DCC
R_{free} test set	4216 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	135.2	Xtrriage
Anisotropy	0.584	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47988	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: MGE, CLA, PHO, LHG, BCR, HEM, BR, PQ9, DGD, FE2, OEC

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	0.65	0/2714	1.23	45/3699 (1.2%)
1	a	0.63	0/2714	1.24	43/3699 (1.2%)
2	B	0.64	2/3951 (0.1%)	1.24	40/5383 (0.7%)
2	b	0.66	1/3951 (0.0%)	1.25	58/5383 (1.1%)
3	C	0.60	0/3568	1.21	53/4858 (1.1%)
3	c	0.59	0/3568	1.15	33/4858 (0.7%)
4	D	0.61	0/2801	1.15	26/3818 (0.7%)
4	d	0.61	0/2801	1.21	34/3818 (0.9%)
5	E	0.55	0/685	1.19	9/933 (1.0%)
5	e	0.60	0/685	1.19	7/933 (0.8%)
6	F	0.69	0/291	1.34	7/397 (1.8%)
6	f	0.74	0/291	1.14	3/397 (0.8%)
7	H	0.63	1/520 (0.2%)	1.19	5/708 (0.7%)
7	h	0.64	0/520	1.26	9/708 (1.3%)
8	I	0.67	0/294	0.97	0/395
8	i	0.63	0/294	1.02	1/395 (0.3%)
9	J	0.57	0/255	1.14	3/346 (0.9%)
9	j	0.62	0/255	1.14	2/346 (0.6%)
10	K	0.76	0/287	1.34	4/394 (1.0%)
10	k	0.64	0/287	1.34	6/394 (1.5%)
11	L	0.60	0/311	1.25	6/422 (1.4%)
11	l	0.63	0/311	1.13	4/422 (0.9%)
12	M	0.73	0/287	1.10	3/388 (0.8%)
12	m	0.63	0/287	1.13	2/388 (0.5%)
13	O	0.62	0/1872	1.15	20/2539 (0.8%)
13	o	0.60	0/1872	1.09	9/2539 (0.4%)
14	T	0.70	0/266	1.28	3/359 (0.8%)
14	t	0.70	0/266	1.24	3/359 (0.8%)
15	U	0.60	0/794	1.13	7/1076 (0.7%)
15	u	0.60	0/794	1.21	9/1076 (0.8%)
16	V	0.65	0/1085	1.34	16/1473 (1.1%)
16	v	0.61	0/1085	1.31	14/1473 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.64	0/249	1.25	3/337 (0.9%)
17	x	0.68	0/249	1.07	0/337
18	Y	0.63	0/209	1.29	3/279 (1.1%)
18	y	0.66	0/209	1.39	3/279 (1.1%)
20	Z	0.61	0/490	1.23	9/669 (1.3%)
20	z	0.66	0/490	1.25	6/669 (0.9%)
All	All	0.63	4/41858 (0.0%)	1.21	508/56946 (0.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	5453	ALA	CA-C	-10.56	1.45	1.52
2	B	456	ALA	CA-C	-6.95	1.48	1.52
2	B	454	ALA	CA-CB	-6.88	1.43	1.53
7	H	54	ILE	CA-CB	5.26	1.59	1.53

The worst 5 of 508 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	218	PHE	N-CA-C	14.16	122.34	108.75
2	B	232	GLY	N-CA-C	-13.18	99.00	114.69
2	b	5167	ASP	CA-C-N	12.99	136.07	119.84
2	b	5167	ASP	C-N-CA	12.99	136.07	119.84
2	B	466	HIS	N-CA-C	-12.56	97.06	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2630	0	2528	816	0
1	a	2630	0	2528	857	0
2	B	3816	0	3680	1011	0
2	b	3816	0	3680	1003	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3455	0	3376	834	0
3	c	3455	0	3376	863	0
4	D	2706	0	2608	803	0
4	d	2706	0	2608	803	0
5	E	666	0	651	156	0
5	e	666	0	651	127	0
6	F	282	0	291	74	0
6	f	282	0	291	67	0
7	H	507	0	529	135	0
7	h	507	0	529	129	0
8	I	287	0	308	81	0
8	i	287	0	305	59	0
9	J	249	0	262	65	0
9	j	249	0	262	36	0
10	K	278	0	289	118	0
10	k	278	0	289	124	0
11	L	304	0	316	106	0
11	l	304	0	313	132	0
12	M	283	0	297	107	0
12	m	283	0	294	118	0
13	O	1841	0	1799	298	0
13	o	1841	0	1799	322	0
14	T	257	0	262	92	0
14	t	257	0	259	82	0
15	U	783	0	779	156	0
15	u	783	0	779	146	0
16	V	1064	0	1072	198	0
16	v	1064	0	1072	183	0
17	X	246	0	269	47	0
17	x	246	0	269	51	0
18	Y	208	0	237	59	0
18	y	208	0	237	51	0
19	N	121	0	26	2	0
19	n	121	0	26	1	0
20	Z	479	0	516	130	0
20	z	479	0	513	134	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	195	0	216	169	0
23	B	975	0	1079	783	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	C	845	0	935	531	0
23	D	195	0	216	120	0
23	H	65	0	72	57	0
23	a	195	0	216	161	0
23	b	1040	0	1151	789	0
23	c	845	0	935	542	0
23	d	195	0	216	123	0
24	A	128	0	148	115	0
24	a	64	0	74	33	0
24	d	64	0	74	75	0
25	A	45	0	64	6	0
25	D	45	0	64	30	0
25	a	45	0	64	3	0
25	d	45	0	62	27	0
26	A	40	0	48	26	0
26	B	120	0	141	101	0
26	C	40	0	47	26	0
26	D	40	0	48	62	0
26	H	40	0	47	54	0
26	K	80	0	94	81	0
26	T	40	0	47	33	0
26	Z	40	0	48	41	0
26	a	40	0	48	25	0
26	b	120	0	141	102	0
26	c	40	0	47	22	0
26	d	40	0	48	58	0
26	h	40	0	47	47	0
26	k	80	0	94	81	0
26	t	40	0	47	24	0
26	z	40	0	48	40	0
27	A	49	0	74	60	0
27	a	49	0	74	53	0
28	A	2	0	0	4	0
28	a	1	0	0	1	0
28	d	1	0	0	1	0
29	B	48	0	72	46	0
29	D	48	0	72	24	0
29	J	48	0	72	32	0
29	L	48	0	72	33	0
29	b	48	0	72	52	0
29	d	144	0	216	96	0
30	C	198	0	288	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	H	66	0	96	32	0
30	c	198	0	288	136	0
30	h	66	0	96	35	0
31	E	43	0	30	10	0
31	V	43	0	30	10	0
31	e	43	0	30	11	0
31	v	43	0	30	11	0
All	All	47988	0	48413	12551	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 130.

The worst 5 of 12551 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5300:PHE:CE2	3:c:5404:LEU:HD12	1.32	1.65
26:t:1046:BCR:H371	26:t:1046:BCR:C26	1.34	1.53
26:T:6046:BCR:H371	26:T:6046:BCR:C26	1.34	1.51
23:a:6006:CLA:H171	26:d:6050:BCR:C29	1.40	1.51
23:c:6032:CLA:H2A	23:c:6032:CLA:CED	1.41	1.50

There are no symmetry-related clashes.

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	333/344 (97%)	210 (63%)	84 (25%)	39 (12%)	0 4
1	a	333/344 (97%)	214 (64%)	75 (22%)	44 (13%)	0 3
2	B	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	0 4
2	b	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	445/447 (100%)	306 (69%)	89 (20%)	50 (11%)	0	4
3	c	445/447 (100%)	316 (71%)	82 (18%)	47 (11%)	0	5
4	D	338/340 (99%)	199 (59%)	87 (26%)	52 (15%)	0	2
4	d	338/340 (99%)	214 (63%)	79 (23%)	45 (13%)	0	3
5	E	80/83 (96%)	44 (55%)	22 (28%)	14 (18%)	0	1
5	e	80/83 (96%)	51 (64%)	18 (22%)	11 (14%)	0	3
6	F	33/44 (75%)	26 (79%)	6 (18%)	1 (3%)	3	26
6	f	33/44 (75%)	26 (79%)	5 (15%)	2 (6%)	1	14
7	H	62/64 (97%)	39 (63%)	15 (24%)	8 (13%)	0	3
7	h	62/64 (97%)	38 (61%)	19 (31%)	5 (8%)	1	9
8	I	33/35 (94%)	19 (58%)	8 (24%)	6 (18%)	0	1
8	i	33/35 (94%)	24 (73%)	6 (18%)	3 (9%)	0	8
9	J	32/40 (80%)	26 (81%)	2 (6%)	4 (12%)	0	4
9	j	32/40 (80%)	26 (81%)	3 (9%)	3 (9%)	0	7
10	K	34/36 (94%)	22 (65%)	8 (24%)	4 (12%)	0	4
10	k	34/36 (94%)	23 (68%)	7 (21%)	4 (12%)	0	4
11	L	35/37 (95%)	20 (57%)	12 (34%)	3 (9%)	0	8
11	l	35/37 (95%)	22 (63%)	9 (26%)	4 (11%)	0	4
12	M	34/36 (94%)	19 (56%)	8 (24%)	7 (21%)	0	1
12	m	34/36 (94%)	24 (71%)	7 (21%)	3 (9%)	0	8
13	O	240/242 (99%)	155 (65%)	47 (20%)	38 (16%)	0	2
13	o	240/242 (99%)	163 (68%)	45 (19%)	32 (13%)	0	3
14	T	28/30 (93%)	18 (64%)	5 (18%)	5 (18%)	0	1
14	t	28/30 (93%)	20 (71%)	7 (25%)	1 (4%)	2	23
15	U	96/98 (98%)	56 (58%)	24 (25%)	16 (17%)	0	2
15	u	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	2
16	V	135/137 (98%)	91 (67%)	25 (18%)	19 (14%)	0	3
16	v	135/137 (98%)	90 (67%)	28 (21%)	17 (13%)	0	4
17	X	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	3	26
17	x	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	3	26
18	Y	26/28 (93%)	19 (73%)	5 (19%)	2 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	26/28 (93%)	19 (73%)	3 (12%)	4 (15%)	0	2
20	Z	60/62 (97%)	39 (65%)	10 (17%)	11 (18%)	0	1
20	z	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	6
All	All	5118/5250 (98%)	3365 (66%)	1106 (22%)	647 (13%)	0	4

5 of 647 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	75	ASN
1	A	79	THR
1	A	80	GLY
1	A	84	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	219 (81%)	51 (19%)	1	10
1	a	270/279 (97%)	214 (79%)	56 (21%)	1	8
2	B	386/388 (100%)	323 (84%)	63 (16%)	2	14
2	b	386/388 (100%)	325 (84%)	61 (16%)	2	15
3	C	349/349 (100%)	287 (82%)	62 (18%)	2	12
3	c	349/349 (100%)	283 (81%)	66 (19%)	1	10
4	D	275/275 (100%)	220 (80%)	55 (20%)	1	9
4	d	275/275 (100%)	229 (83%)	46 (17%)	2	14
5	E	72/73 (99%)	58 (81%)	14 (19%)	1	9
5	e	72/73 (99%)	61 (85%)	11 (15%)	3	16
6	F	29/38 (76%)	21 (72%)	8 (28%)	0	3
6	f	29/38 (76%)	21 (72%)	8 (28%)	0	3
7	H	54/54 (100%)	38 (70%)	16 (30%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	54/54 (100%)	42 (78%)	12 (22%)	1	7
8	I	32/32 (100%)	27 (84%)	5 (16%)	2	15
8	i	32/32 (100%)	27 (84%)	5 (16%)	2	15
9	J	24/28 (86%)	12 (50%)	12 (50%)	0	0
9	j	24/28 (86%)	14 (58%)	10 (42%)	0	0
10	K	29/29 (100%)	21 (72%)	8 (28%)	0	3
10	k	29/29 (100%)	23 (79%)	6 (21%)	1	8
11	L	35/35 (100%)	28 (80%)	7 (20%)	1	9
11	l	35/35 (100%)	29 (83%)	6 (17%)	2	13
12	M	33/33 (100%)	27 (82%)	6 (18%)	2	11
12	m	33/33 (100%)	28 (85%)	5 (15%)	3	16
13	O	200/206 (97%)	170 (85%)	30 (15%)	3	16
13	o	200/206 (97%)	163 (82%)	37 (18%)	1	10
14	T	27/27 (100%)	18 (67%)	9 (33%)	0	1
14	t	27/27 (100%)	20 (74%)	7 (26%)	0	4
15	U	85/85 (100%)	72 (85%)	13 (15%)	3	16
15	u	85/85 (100%)	72 (85%)	13 (15%)	3	16
16	V	117/117 (100%)	98 (84%)	19 (16%)	2	14
16	v	117/117 (100%)	97 (83%)	20 (17%)	2	13
17	X	27/27 (100%)	17 (63%)	10 (37%)	0	0
17	x	27/27 (100%)	15 (56%)	12 (44%)	0	0
18	Y	21/21 (100%)	13 (62%)	8 (38%)	0	0
18	y	21/21 (100%)	12 (57%)	9 (43%)	0	0
20	Z	52/52 (100%)	40 (77%)	12 (23%)	1	6
20	z	52/52 (100%)	37 (71%)	15 (29%)	0	2
All	All	4234/4296 (99%)	3421 (81%)	813 (19%)	1	9

5 of 813 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	5341	LEU
3	c	5382	ASN
20	z	5009	LEU

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Mol	Chain	Res	Type
2	b	5120	PHE
1	a	5337	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	5332	GLN
18	y	5003	GLN
5	e	5075	GLN
13	o	5150	ASN
10	K	40	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 6 are monoatomic - leaving 124 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
23	CLA	d	6005	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MGE	J	1059	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	b	6024	-	69,73,73	1.89	19 (27%)	82,113,113	2.67	34 (41%)
23	CLA	d	6004	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
23	CLA	b	6021	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
25	PQ9	D	1042	-	45,45,45	4.10	17 (37%)	56,57,57	5.08	25 (44%)
23	CLA	b	6013	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	C	1032	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6029	-	69,73,73	1.91	18 (26%)	82,113,113	2.58	27 (32%)
23	CLA	c	6025	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
30	DGD	C	1056	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	b	6019	-	69,73,73	1.89	18 (26%)	82,113,113	2.65	36 (43%)
23	CLA	B	1013	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	C	1035	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
24	PHO	a	6039	-	58,69,69	2.94	13 (22%)	55,99,99	3.53	19 (34%)
24	PHO	d	6038	-	58,69,69	2.98	14 (24%)	55,99,99	3.44	20 (36%)
26	BCR	k	6051	-	41,41,41	3.99	16 (39%)	56,56,56	6.51	29 (51%)
23	CLA	C	1028	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	B	1018	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	B	1023	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
29	MGE	d	6061	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
25	PQ9	a	6043	-	45,45,45	4.39	21 (46%)	56,57,57	4.90	20 (35%)
23	CLA	a	6006	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	C	1029	-	69,73,73	1.91	18 (26%)	82,113,113	2.58	27 (32%)
26	BCR	t	1046	-	41,41,41	4.03	17 (41%)	56,56,56	6.58	24 (42%)
23	CLA	C	1026	-	69,73,73	1.85	18 (26%)	82,113,113	2.55	29 (35%)
23	CLA	A	1003	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
25	PQ9	A	1043	-	45,45,45	4.25	17 (37%)	56,57,57	4.94	22 (39%)
23	CLA	A	1007	-	69,73,73	1.89	18 (26%)	82,113,113	2.53	30 (36%)
23	CLA	B	1012	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6036	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	c	6054	-	41,41,41	4.00	17 (41%)	56,56,56	6.93	24 (42%)
30	DGD	C	1055	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	c	6031	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	B	1022	-	69,73,73	1.87	17 (24%)	82,113,113	2.60	31 (37%)
26	BCR	Z	1053	-	41,41,41	4.01	16 (39%)	56,56,56	6.65	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	A	1044	-	41,41,41	3.84	16 (39%)	56,56,56	6.30	30 (53%)
30	DGD	C	1057	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	D	1005	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
23	CLA	B	1020	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
31	HEM	e	6040	6	50,50,50	1.88	8 (16%)	67,82,82	1.34	5 (7%)
23	CLA	b	6022	-	69,73,73	1.87	17 (24%)	82,113,113	2.60	31 (37%)
29	MGE	L	1061	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	D	1008	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
25	PQ9	d	6042	-	45,45,45	4.12	15 (33%)	56,57,57	5.08	26 (46%)
23	CLA	c	6030	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	z	6053	-	41,41,41	4.01	16 (39%)	56,56,56	6.64	26 (46%)
23	CLA	B	1015	-	69,73,73	1.95	20 (28%)	82,113,113	2.80	37 (45%)
23	CLA	C	1030	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6028	-	69,73,73	1.94	16 (23%)	82,113,113	2.47	28 (34%)
30	DGD	c	6055	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
26	BCR	b	6045	-	41,41,41	4.01	17 (41%)	56,56,56	6.58	26 (46%)
23	CLA	b	6009	-	69,73,73	1.91	18 (26%)	82,113,113	2.44	28 (34%)
23	CLA	C	1034	-	69,73,73	1.97	17 (24%)	82,113,113	2.70	29 (35%)
23	CLA	B	1014	-	69,73,73	1.89	19 (27%)	82,113,113	2.59	29 (35%)
23	CLA	C	1036	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	H	1049	-	41,41,41	4.02	17 (41%)	56,56,56	6.31	21 (37%)
26	BCR	h	6049	-	41,41,41	4.02	17 (41%)	56,56,56	6.31	20 (35%)
26	BCR	B	1047	-	41,41,41	3.99	16 (39%)	56,56,56	7.22	26 (46%)
23	CLA	b	6017	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
23	CLA	c	6035	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	b	6015	-	69,73,73	1.95	19 (27%)	82,113,113	2.80	37 (45%)
26	BCR	B	1045	-	41,41,41	4.01	17 (41%)	56,56,56	6.58	27 (48%)
23	CLA	c	6034	-	69,73,73	1.90	16 (23%)	82,113,113	2.54	26 (31%)
23	CLA	C	1025	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	b	6048	-	41,41,41	4.03	17 (41%)	56,56,56	6.42	22 (39%)
23	CLA	C	1037	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	a	6003	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	C	1054	-	41,41,41	4.00	17 (41%)	56,56,56	6.93	24 (42%)
23	CLA	a	6007	-	69,73,73	1.89	18 (26%)	82,113,113	2.53	30 (36%)
29	MGE	b	6060	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	A	1038	-	58,69,69	2.98	14 (24%)	55,99,99	3.43	20 (36%)
23	CLA	D	1004	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
23	CLA	B	1011	2	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	H	1017	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
24	PHO	A	1039	-	58,69,69	2.94	13 (22%)	55,99,99	3.52	19 (34%)
23	CLA	c	6026	-	69,73,73	1.85	18 (26%)	82,113,113	2.55	29 (35%)
23	CLA	C	1031	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	C	1033	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	a	6044	-	41,41,41	3.84	16 (39%)	56,56,56	6.30	29 (51%)
23	CLA	c	6032	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	b	6018	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	b	6014	-	69,73,73	1.89	19 (27%)	82,113,113	2.59	30 (36%)
23	CLA	c	6027	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
27	LHG	A	1063	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	B	1009	-	69,73,73	1.90	17 (24%)	82,113,113	2.44	28 (34%)
26	BCR	K	1052	-	41,41,41	4.02	17 (41%)	56,56,56	5.60	21 (37%)
26	BCR	b	6047	-	41,41,41	3.99	16 (39%)	56,56,56	7.22	26 (46%)
30	DGD	c	6056	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	B	1024	-	69,73,73	1.88	19 (27%)	82,113,113	2.67	34 (41%)
23	CLA	c	6033	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6037	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
31	HEM	V	1041	16	50,50,50	1.88	8 (16%)	67,82,82	1.35	5 (7%)
23	CLA	b	6011	2	69,73,73	1.93	17 (24%)	82,113,113	2.48	28 (34%)
26	BCR	K	1051	-	41,41,41	3.99	16 (39%)	56,56,56	6.52	29 (51%)
23	CLA	b	6012	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	T	6046	-	41,41,41	4.04	17 (41%)	56,56,56	7.68	28 (50%)
30	DGD	h	6058	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	B	1021	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	B	1048	-	41,41,41	4.03	17 (41%)	56,56,56	6.42	22 (39%)
23	CLA	B	1016	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
29	MGE	d	6059	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	b	6016	-	69,73,73	1.94	16 (23%)	82,113,113	2.47	27 (32%)
29	MGE	D	1062	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	C	1027	-	69,73,73	1.94	16 (23%)	82,113,113	2.47	28 (34%)
23	CLA	b	6023	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	HEM	E	1040	6	50,50,50	1.87	7 (14%)	67,82,82	1.34	5 (7%)
26	BCR	D	1050	-	41,41,41	3.94	16 (39%)	56,56,56	6.35	28 (50%)
29	MGE	B	1060	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	A	1006	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
27	LHG	a	6063	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	d	6008	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
26	BCR	d	6050	-	41,41,41	3.94	16 (39%)	56,56,56	6.35	28 (50%)
30	DGD	H	1058	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
31	HEM	v	6041	-	50,50,50	1.87	8 (16%)	67,82,82	1.34	5 (7%)
23	CLA	b	6010	-	69,73,73	1.92	19 (27%)	82,113,113	2.74	31 (37%)
30	DGD	c	6057	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	B	1010	-	69,73,73	1.91	19 (27%)	82,113,113	2.73	31 (37%)
29	MGE	d	6062	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	B	1019	-	69,73,73	1.89	18 (26%)	82,113,113	2.65	36 (43%)
26	BCR	k	6052	-	41,41,41	4.03	17 (41%)	56,56,56	5.22	21 (37%)
23	CLA	b	6020	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	6005	-	2/2/15/20	17/39/115/115	-
29	MGE	J	1059	-	-	23/43/63/63	0/1/1/1
23	CLA	b	6024	-	2/2/15/20	14/39/115/115	-
23	CLA	d	6004	-	1/1/15/20	16/39/115/115	-
23	CLA	b	6021	-	3/3/15/20	20/39/115/115	-
25	PQ9	D	1042	-	-	7/41/61/61	0/1/1/1
23	CLA	b	6013	-	1/1/15/20	17/39/115/115	-
23	CLA	C	1032	-	1/1/15/20	16/39/115/115	-
23	CLA	c	6029	-	3/3/15/20	17/39/115/115	-
23	CLA	c	6025	-	2/2/15/20	21/39/115/115	-
30	DGD	C	1056	-	-	31/55/95/95	0/2/2/2
23	CLA	b	6019	-	3/3/15/20	23/39/115/115	-
23	CLA	B	1013	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	1035	-	1/1/15/20	21/39/115/115	-
24	PHO	a	6039	-	1/1/17/22	19/37/103/103	0/5/6/6
24	PHO	d	6038	-	2/2/17/22	19/37/103/103	0/5/6/6
26	BCR	k	6051	-	-	15/29/63/63	0/2/2/2
23	CLA	C	1028	-	4/4/15/20	18/39/115/115	-
23	CLA	B	1018	-	1/1/15/20	11/39/115/115	-
23	CLA	B	1023	-	3/3/15/20	19/39/115/115	-
29	MGE	d	6061	-	-	24/43/63/63	0/1/1/1
25	PQ9	a	6043	-	-	10/41/61/61	0/1/1/1
23	CLA	a	6006	-	1/1/15/20	22/39/115/115	-
23	CLA	C	1029	-	3/3/15/20	17/39/115/115	-
26	BCR	t	1046	-	-	14/29/63/63	0/2/2/2
23	CLA	C	1026	-	2/2/15/20	16/39/115/115	-
23	CLA	A	1003	-	1/1/15/20	18/39/115/115	-
25	PQ9	A	1043	-	-	11/41/61/61	0/1/1/1
23	CLA	A	1007	-	2/2/15/20	22/39/115/115	-
23	CLA	B	1012	-	1/1/15/20	22/39/115/115	-
23	CLA	c	6036	-	3/3/15/20	25/39/115/115	-
26	BCR	c	6054	-	-	14/29/63/63	0/2/2/2
30	DGD	C	1055	-	-	27/55/95/95	0/2/2/2
23	CLA	c	6031	-	4/4/15/20	14/39/115/115	-
23	CLA	B	1022	-	3/3/15/20	16/39/115/115	-
26	BCR	Z	1053	-	-	13/29/63/63	0/2/2/2
26	BCR	A	1044	-	-	10/29/63/63	0/2/2/2
30	DGD	C	1057	-	-	19/55/95/95	0/2/2/2
23	CLA	D	1005	-	2/2/15/20	17/39/115/115	-
23	CLA	B	1020	-	2/2/15/20	19/39/115/115	-
31	HEM	e	6040	6	-	3/14/54/54	-
23	CLA	b	6022	-	3/3/15/20	16/39/115/115	-
29	MGE	L	1061	-	-	24/43/63/63	0/1/1/1
23	CLA	D	1008	-	1/1/15/20	22/39/115/115	-
25	PQ9	d	6042	-	-	8/41/61/61	0/1/1/1
23	CLA	c	6030	-	1/1/15/20	16/39/115/115	-
26	BCR	z	6053	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	1015	-	1/1/15/20	19/39/115/115	-
23	CLA	C	1030	-	1/1/15/20	16/39/115/115	-
23	CLA	c	6028	-	4/4/15/20	18/39/115/115	-
30	DGD	c	6055	-	-	27/55/95/95	0/2/2/2
26	BCR	b	6045	-	-	8/29/63/63	0/2/2/2
23	CLA	b	6009	-	4/4/15/20	18/39/115/115	-
23	CLA	C	1034	-	5/5/15/20	25/39/115/115	-
23	CLA	B	1014	-	2/2/15/20	19/39/115/115	-
23	CLA	C	1036	-	3/3/15/20	25/39/115/115	-
26	BCR	H	1049	-	-	15/29/63/63	0/2/2/2
26	BCR	h	6049	-	-	15/29/63/63	0/2/2/2
26	BCR	B	1047	-	-	15/29/63/63	0/2/2/2
23	CLA	b	6017	-	2/2/15/20	21/39/115/115	-
23	CLA	c	6035	-	1/1/15/20	21/39/115/115	-
23	CLA	b	6015	-	1/1/15/20	19/39/115/115	-
26	BCR	B	1045	-	-	8/29/63/63	0/2/2/2
23	CLA	c	6034	-	5/5/15/20	27/39/115/115	-
23	CLA	C	1025	-	2/2/15/20	21/39/115/115	-
26	BCR	b	6048	-	-	17/29/63/63	0/2/2/2
23	CLA	C	1037	-	3/3/15/20	16/39/115/115	-
23	CLA	a	6003	-	1/1/15/20	18/39/115/115	-
26	BCR	C	1054	-	-	14/29/63/63	0/2/2/2
23	CLA	a	6007	-	2/2/15/20	22/39/115/115	-
29	MGE	b	6060	-	-	22/43/63/63	0/1/1/1
24	PHO	A	1038	-	2/2/17/22	19/37/103/103	0/5/6/6
23	CLA	D	1004	-	1/1/15/20	16/39/115/115	-
23	CLA	B	1011	2	1/1/15/20	16/39/115/115	-
23	CLA	H	1017	-	2/2/15/20	21/39/115/115	-
24	PHO	A	1039	-	1/1/17/22	19/37/103/103	0/5/6/6
23	CLA	c	6026	-	2/2/15/20	16/39/115/115	-
23	CLA	C	1031	-	4/4/15/20	14/39/115/115	-
23	CLA	C	1033	-	3/3/15/20	24/39/115/115	-
26	BCR	a	6044	-	-	10/29/63/63	0/2/2/2
23	CLA	c	6032	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	6018	-	1/1/15/20	11/39/115/115	-
23	CLA	b	6014	-	2/2/15/20	19/39/115/115	-
23	CLA	c	6027	-	4/4/15/20	19/39/115/115	-
27	LHG	A	1063	-	-	26/53/53/53	-
23	CLA	B	1009	-	4/4/15/20	18/39/115/115	-
26	BCR	K	1052	-	-	20/29/63/63	0/2/2/2
26	BCR	b	6047	-	-	15/29/63/63	0/2/2/2
30	DGD	c	6056	-	-	31/55/95/95	0/2/2/2
23	CLA	B	1024	-	2/2/15/20	14/39/115/115	-
23	CLA	c	6033	-	3/3/15/20	24/39/115/115	-
23	CLA	c	6037	-	3/3/15/20	16/39/115/115	-
31	HEM	V	1041	16	-	7/14/54/54	-
23	CLA	b	6011	2	1/1/15/20	16/39/115/115	-
26	BCR	K	1051	-	-	15/29/63/63	0/2/2/2
23	CLA	b	6012	-	1/1/15/20	23/39/115/115	-
26	BCR	T	6046	-	-	9/20/63/63	-
30	DGD	h	6058	-	-	36/55/95/95	0/2/2/2
23	CLA	B	1021	-	3/3/15/20	20/39/115/115	-
26	BCR	B	1048	-	-	17/29/63/63	0/2/2/2
23	CLA	B	1016	-	1/1/15/20	20/39/115/115	-
29	MGE	d	6059	-	-	23/43/63/63	0/1/1/1
23	CLA	b	6016	-	1/1/15/20	20/39/115/115	-
29	MGE	D	1062	-	-	24/43/63/63	0/1/1/1
23	CLA	C	1027	-	4/4/15/20	18/39/115/115	-
23	CLA	b	6023	-	3/3/15/20	19/39/115/115	-
31	HEM	E	1040	6	-	3/14/54/54	-
26	BCR	D	1050	-	-	12/29/63/63	0/2/2/2
29	MGE	B	1060	-	-	24/43/63/63	0/1/1/1
23	CLA	A	1006	-	1/1/15/20	23/39/115/115	-
27	LHG	a	6063	-	-	26/53/53/53	-
23	CLA	d	6008	-	1/1/15/20	22/39/115/115	-
26	BCR	d	6050	-	-	12/29/63/63	0/2/2/2
30	DGD	H	1058	-	-	36/55/95/95	0/2/2/2
31	HEM	v	6041	-	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	6010	-	1/1/15/20	15/39/115/115	-
30	DGD	c	6057	-	-	19/55/95/95	0/2/2/2
23	CLA	B	1010	-	1/1/15/20	15/39/115/115	-
29	MGE	d	6062	-	-	24/43/63/63	0/1/1/1
23	CLA	B	1019	-	3/3/15/20	23/39/115/115	-
26	BCR	k	6052	-	-	20/29/63/63	0/2/2/2
23	CLA	b	6020	2	2/2/15/20	19/39/115/115	-

The worst 5 of 1717 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	6043	PQ9	C27-C28	15.14	1.67	1.33
24	A	1039	PHO	OBD-CAD	14.54	1.41	1.22
24	A	1038	PHO	OBD-CAD	14.53	1.41	1.22
24	a	6039	PHO	OBD-CAD	14.51	1.41	1.22
24	d	6038	PHO	OBD-CAD	14.50	1.41	1.22

The worst 5 of 2826 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	1047	BCR	C7-C8-C9	34.70	177.56	126.23
26	b	6047	BCR	C7-C8-C9	34.65	177.50	126.23
26	C	1054	BCR	C7-C8-C9	28.08	167.78	126.23
26	c	6054	BCR	C7-C8-C9	28.06	167.74	126.23
26	T	6046	BCR	C7-C8-C9	27.21	166.48	126.23

5 of 156 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	1003	CLA	ND
23	A	1006	CLA	ND
23	A	1007	CLA	ND
23	A	1007	CLA	C13
23	B	1009	CLA	C8

5 of 2210 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	1003	CLA	C14-C13-C15-C16
23	A	1006	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	A	1006	CLA	C3A-C2A-CAA-CBA
23	A	1006	CLA	C4C-C3C-CAC-CBC
23	A	1006	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

122 monomers are involved in 4438 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	6005	CLA	69	0
29	J	1059	MGE	32	0
23	b	6024	CLA	38	0
23	d	6004	CLA	20	0
23	b	6021	CLA	71	0
25	D	1042	PQ9	30	0
23	b	6013	CLA	85	0
23	C	1032	CLA	61	0
23	c	6029	CLA	46	0
23	c	6025	CLA	53	0
30	C	1056	DGD	57	0
23	b	6019	CLA	81	0
23	B	1013	CLA	84	0
23	C	1035	CLA	20	0
24	a	6039	PHO	33	0
24	d	6038	PHO	75	0
26	k	6051	BCR	48	0
23	C	1028	CLA	34	0
23	B	1018	CLA	23	0
23	B	1023	CLA	80	0
29	d	6061	MGE	29	0
25	a	6043	PQ9	3	0
23	a	6006	CLA	78	0
23	C	1029	CLA	46	0
26	t	1046	BCR	24	0
23	C	1026	CLA	33	0
23	A	1003	CLA	63	0
25	A	1043	PQ9	6	0
23	A	1007	CLA	20	0
23	B	1012	CLA	65	0
23	c	6036	CLA	51	0
26	c	6054	BCR	22	0
30	C	1055	DGD	34	0
23	c	6031	CLA	69	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1022	CLA	70	0
26	Z	1053	BCR	41	0
26	A	1044	BCR	26	0
30	C	1057	DGD	61	0
23	D	1005	CLA	69	0
23	B	1020	CLA	69	0
31	e	6040	HEM	11	0
23	b	6022	CLA	71	0
29	L	1061	MGE	33	0
23	D	1008	CLA	33	0
25	d	6042	PQ9	27	0
23	c	6030	CLA	29	0
26	z	6053	BCR	40	0
23	B	1015	CLA	31	0
23	C	1030	CLA	29	0
23	c	6028	CLA	35	0
30	c	6055	DGD	34	0
26	b	6045	BCR	29	0
23	b	6009	CLA	50	0
23	C	1034	CLA	87	0
23	B	1014	CLA	84	0
23	C	1036	CLA	49	0
26	H	1049	BCR	54	0
26	h	6049	BCR	47	0
26	B	1047	BCR	39	0
23	b	6017	CLA	56	0
23	c	6035	CLA	32	0
23	b	6015	CLA	29	0
26	B	1045	BCR	29	0
23	c	6034	CLA	82	0
23	C	1025	CLA	54	0
26	b	6048	BCR	40	0
23	C	1037	CLA	25	0
23	a	6003	CLA	72	0
26	C	1054	BCR	26	0
23	a	6007	CLA	19	0
29	b	6060	MGE	52	0
24	A	1038	PHO	81	0
23	D	1004	CLA	19	0
23	B	1011	CLA	107	0
23	H	1017	CLA	57	0
24	A	1039	PHO	34	0

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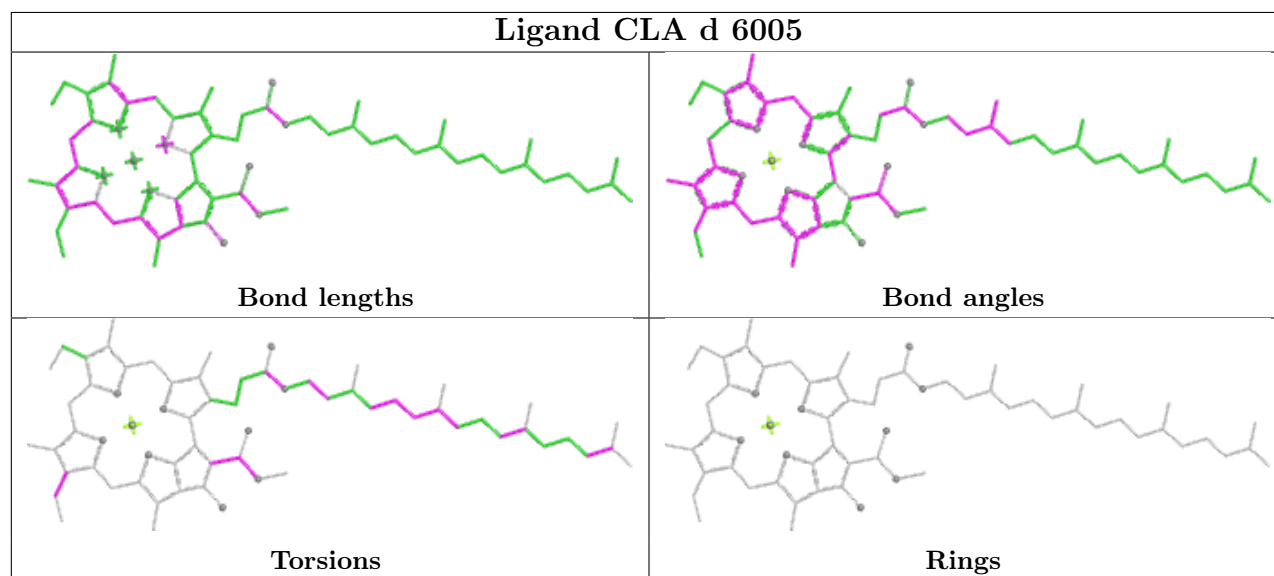
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	6026	CLA	31	0
23	C	1031	CLA	63	0
23	C	1033	CLA	64	0
26	a	6044	BCR	25	0
23	c	6032	CLA	59	0
23	b	6018	CLA	19	0
23	b	6014	CLA	80	0
23	c	6027	CLA	46	0
27	A	1063	LHG	60	0
23	B	1009	CLA	49	0
26	K	1052	BCR	47	0
26	b	6047	BCR	38	0
30	c	6056	DGD	53	0
23	B	1024	CLA	38	0
23	c	6033	CLA	65	0
23	c	6037	CLA	26	0
31	V	1041	HEM	10	0
23	b	6011	CLA	109	0
26	K	1051	BCR	43	0
23	b	6012	CLA	58	0
26	T	6046	BCR	33	0
30	h	6058	DGD	35	0
23	B	1021	CLA	75	0
26	B	1048	BCR	38	0
23	B	1016	CLA	62	0
29	d	6059	MGE	33	0
23	b	6016	CLA	58	0
29	D	1062	MGE	24	0
23	C	1027	CLA	48	0
23	b	6023	CLA	77	0
31	E	1040	HEM	10	0
26	D	1050	BCR	62	0
29	B	1060	MGE	46	0
23	A	1006	CLA	93	0
27	a	6063	LHG	53	0
23	d	6008	CLA	35	0
26	d	6050	BCR	58	0
30	H	1058	DGD	32	0
31	v	6041	HEM	11	0
23	b	6010	CLA	52	0
30	c	6057	DGD	52	0
23	B	1010	CLA	49	0

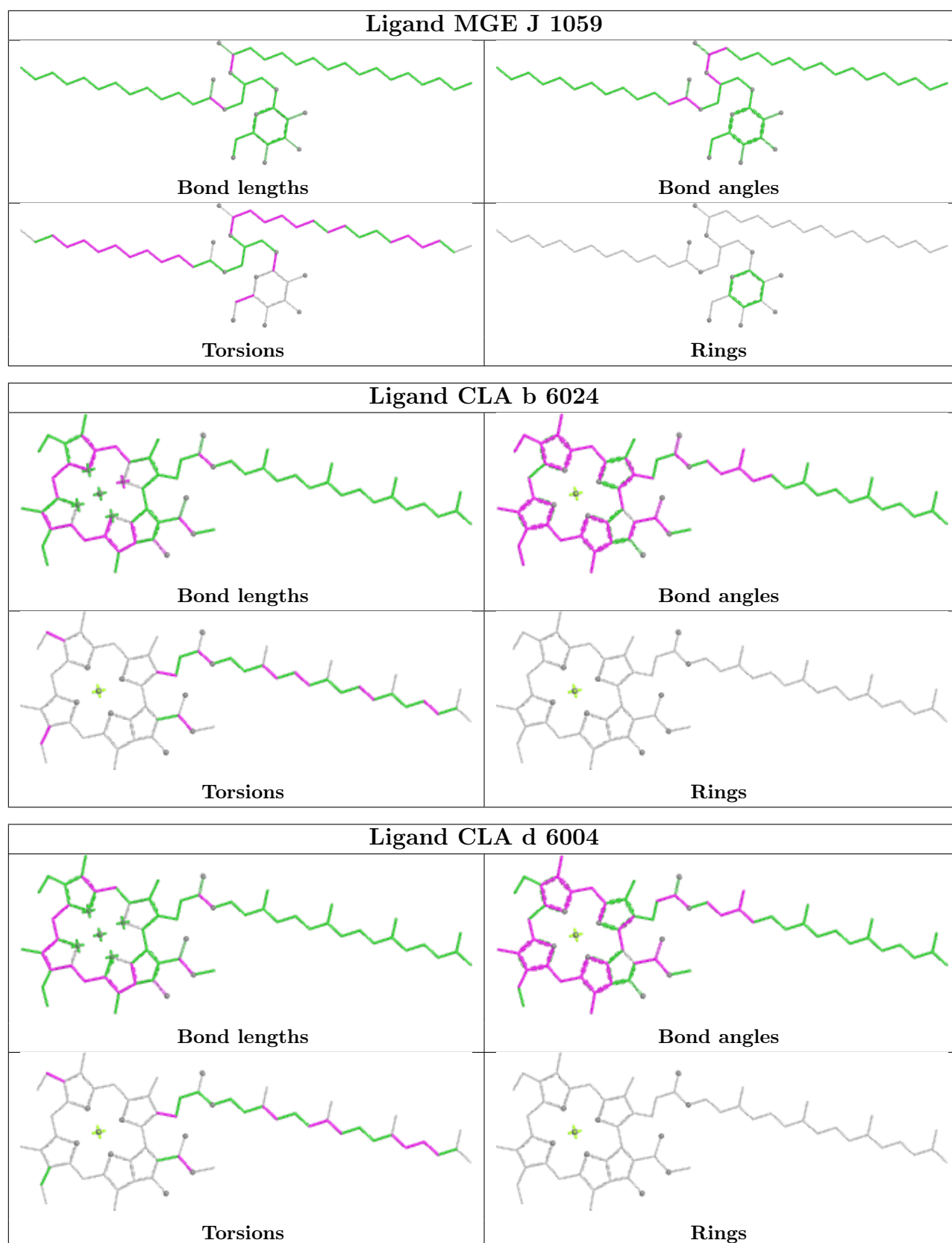
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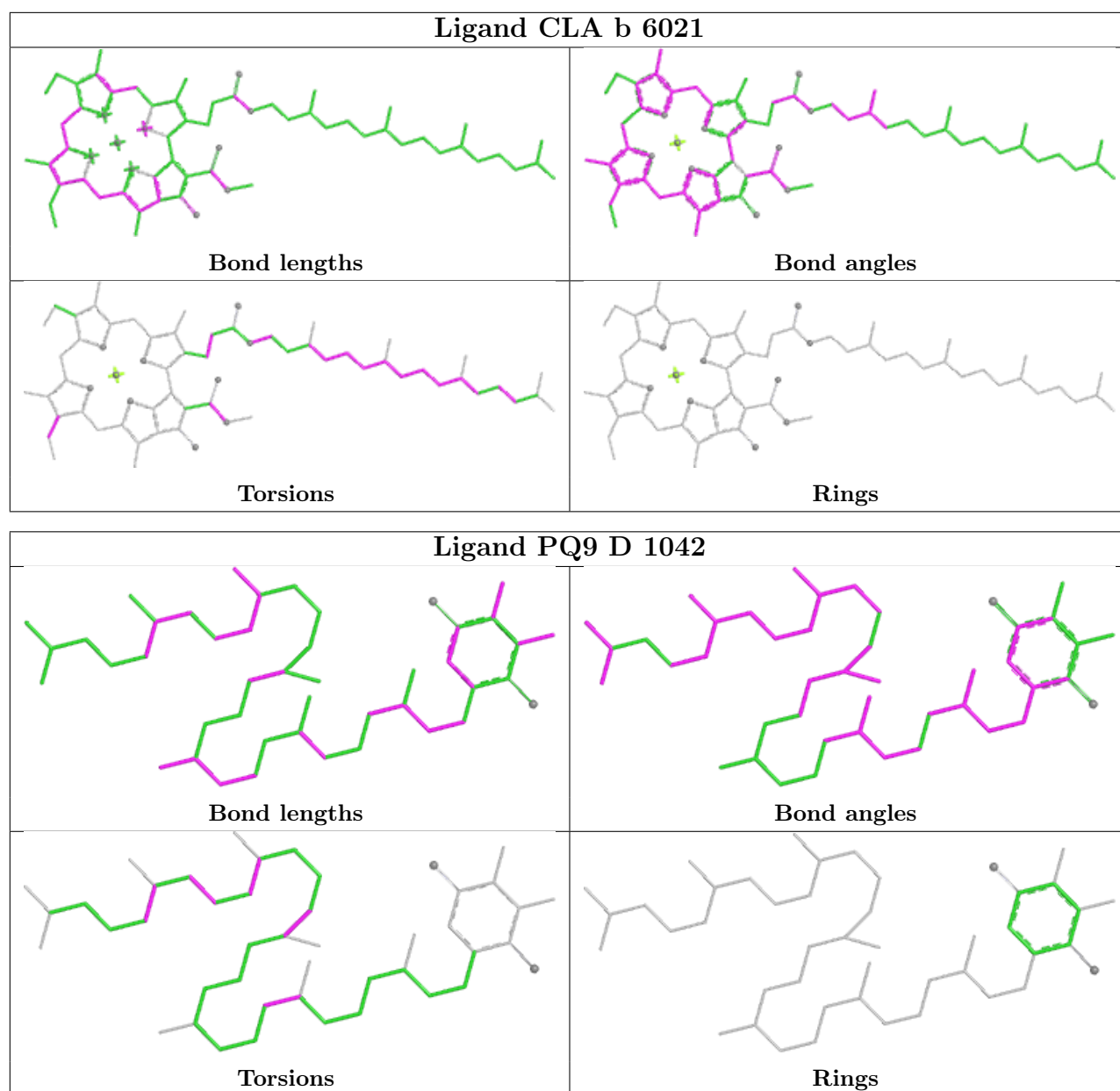
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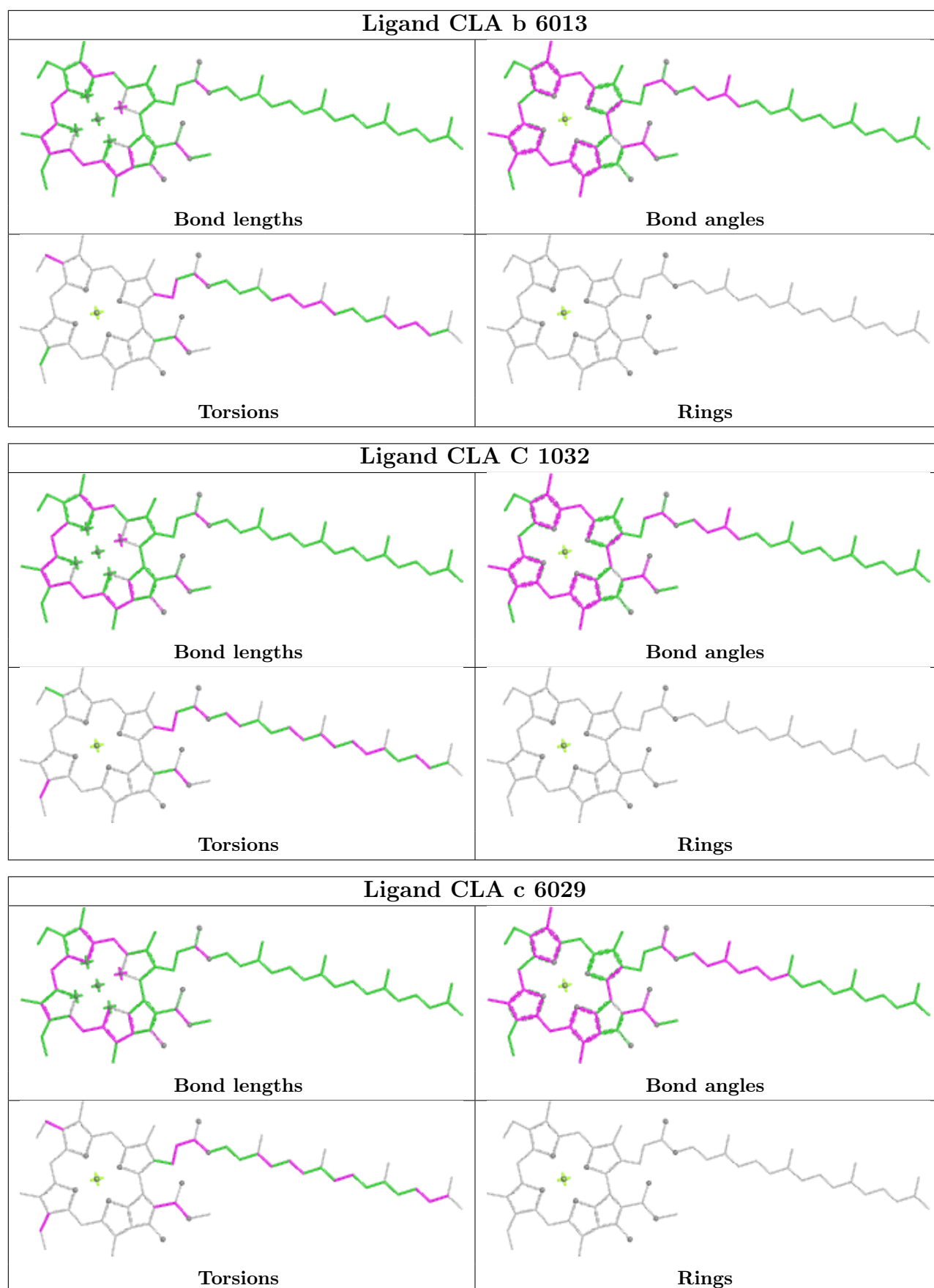
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	6062	MGE	35	0
23	B	1019	CLA	85	0
26	k	6052	BCR	43	0
23	b	6020	CLA	71	0

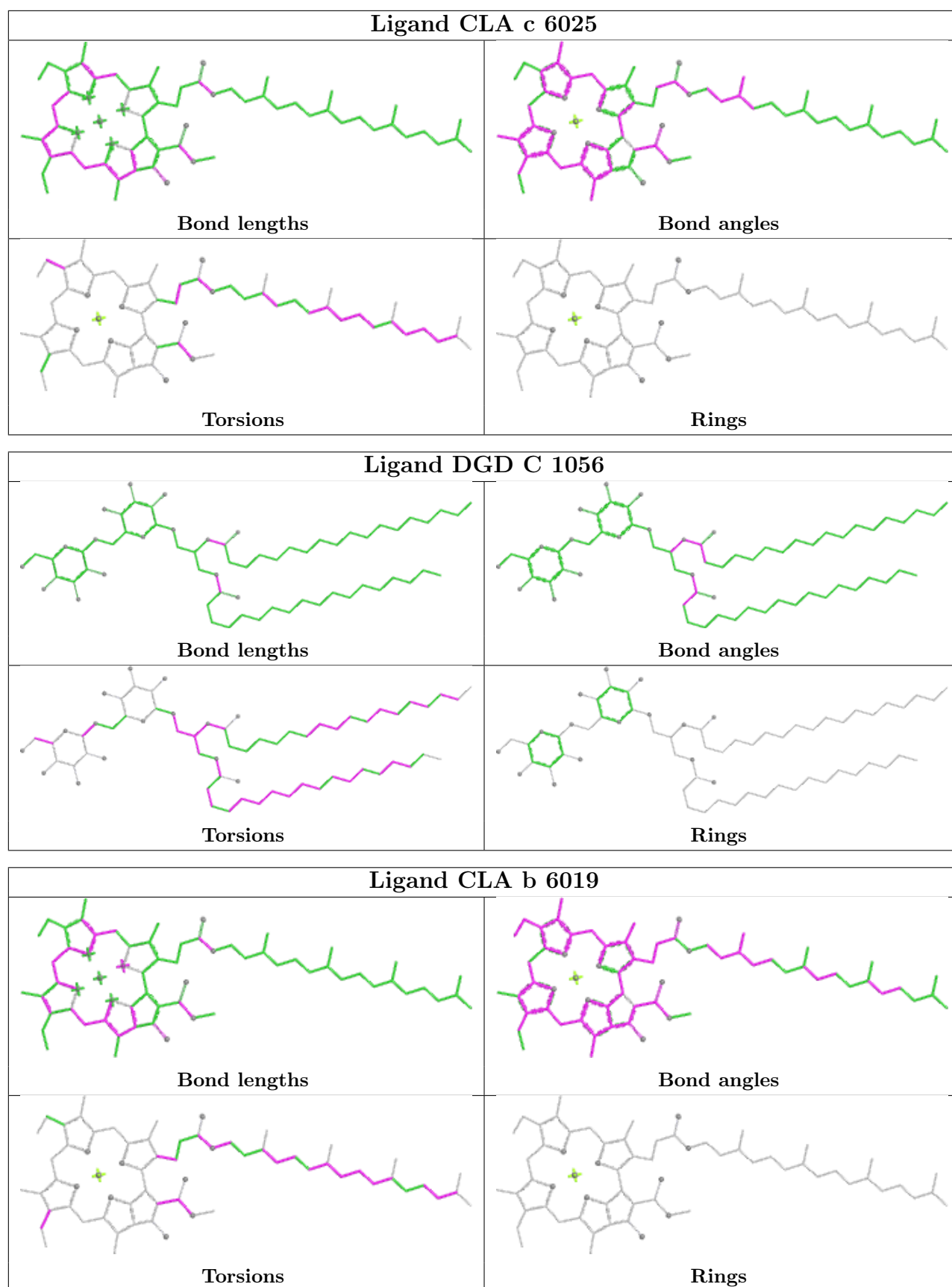
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

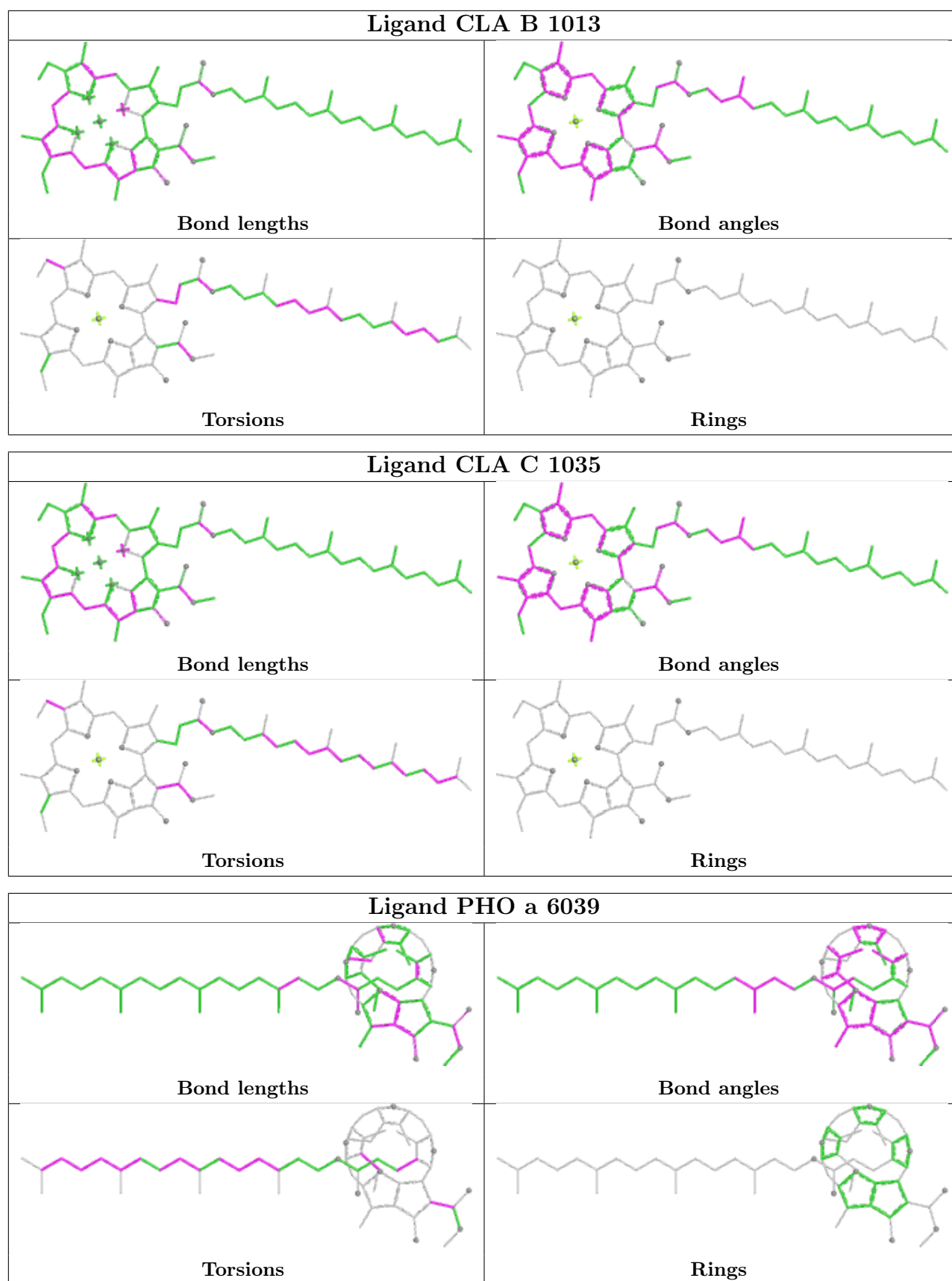


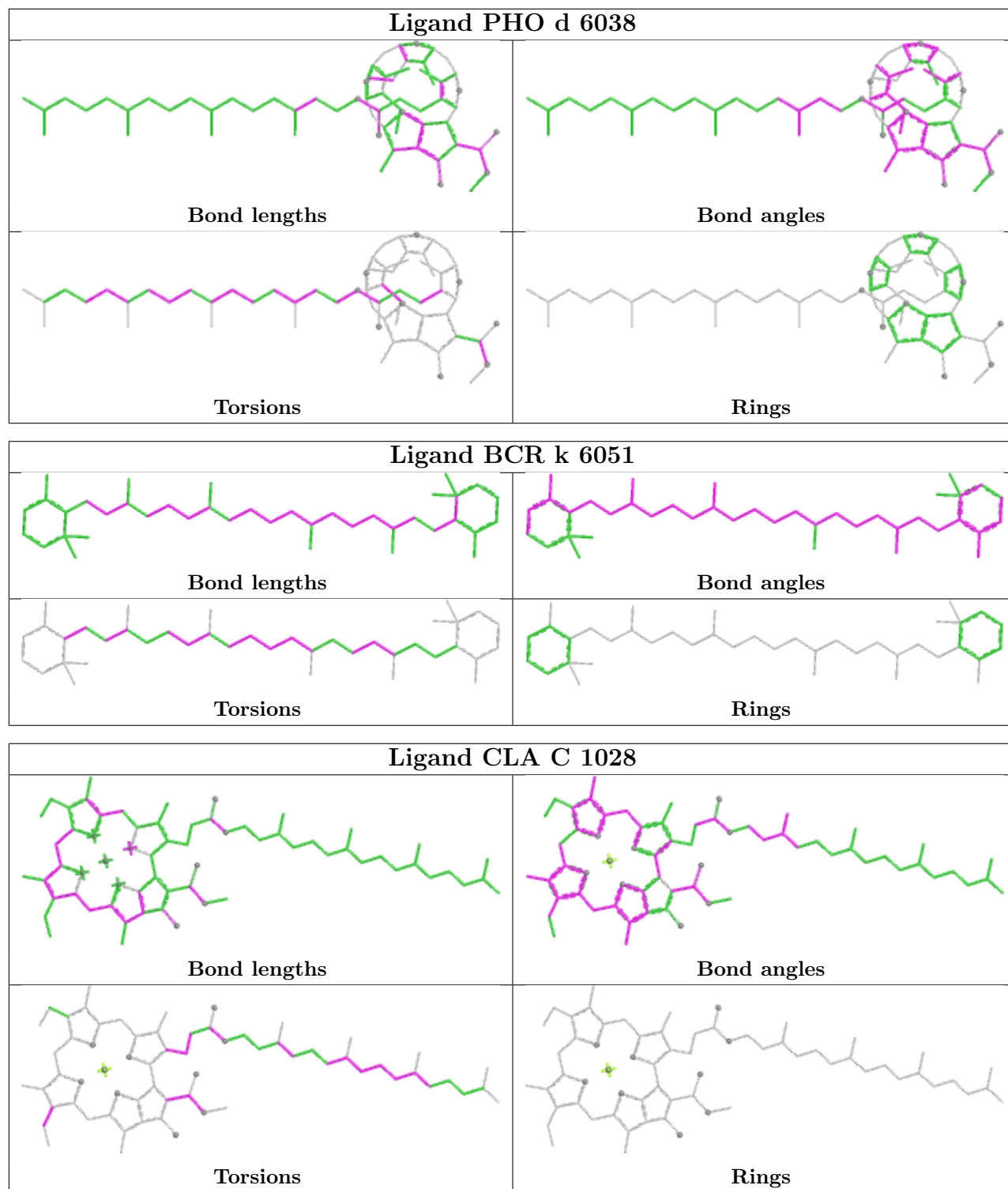


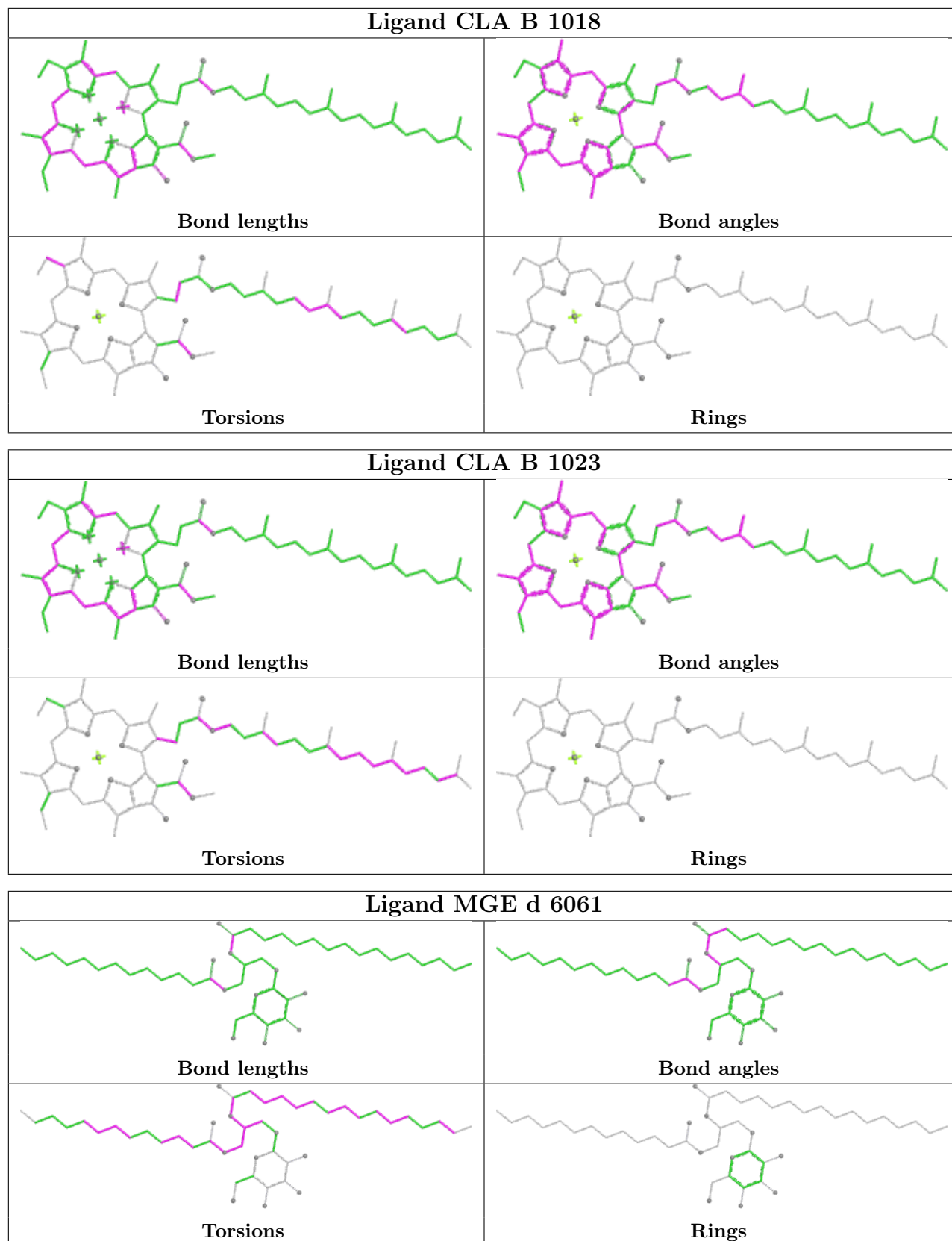


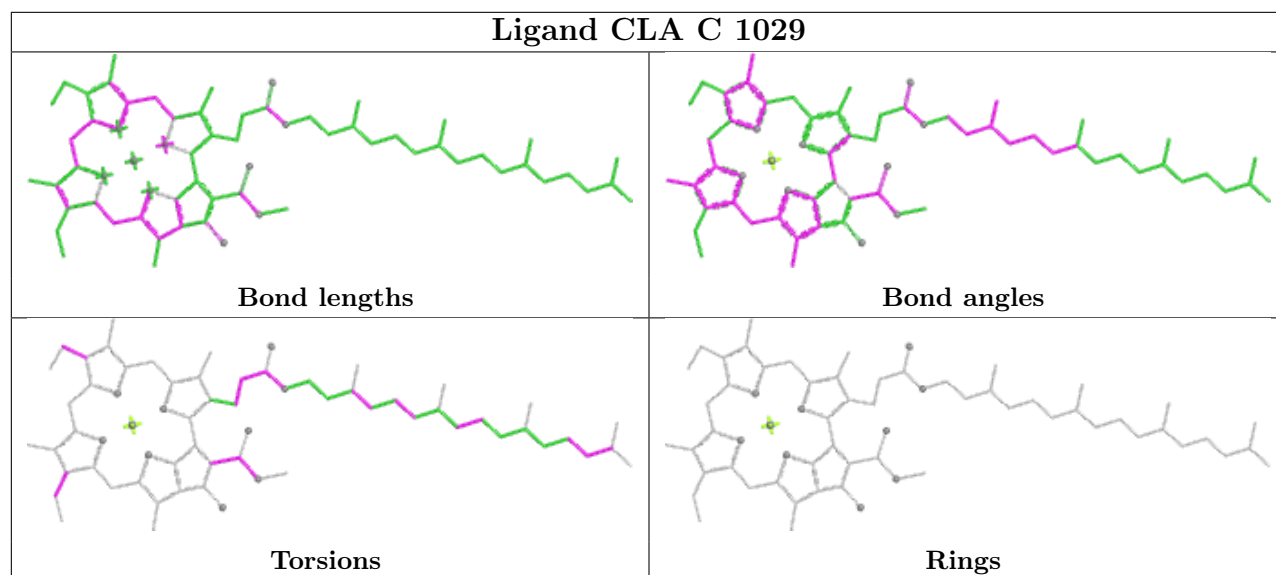
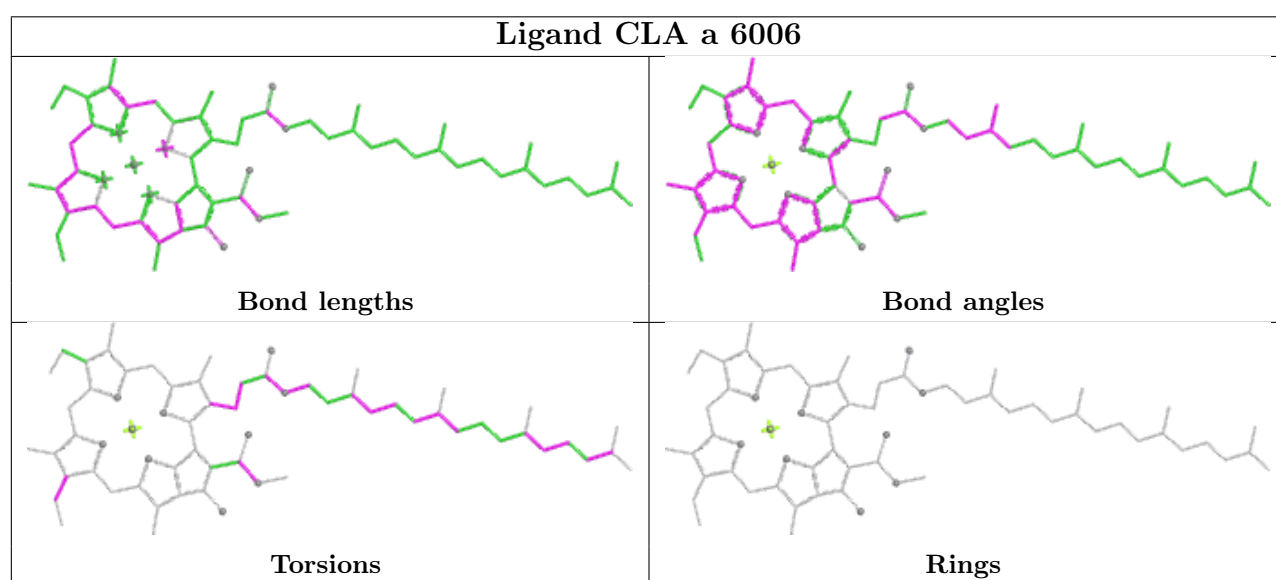
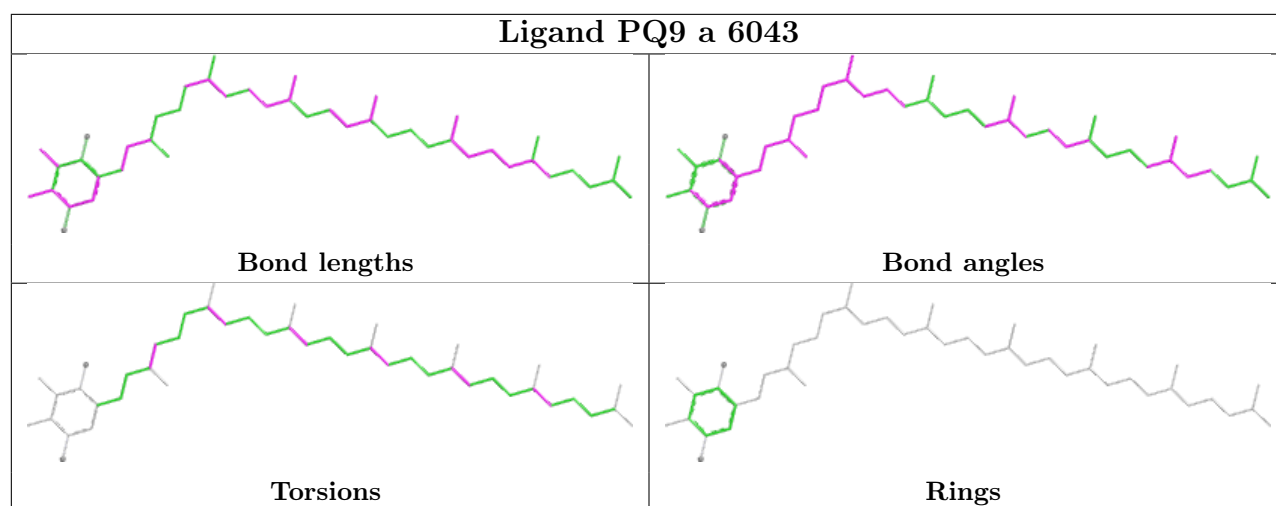


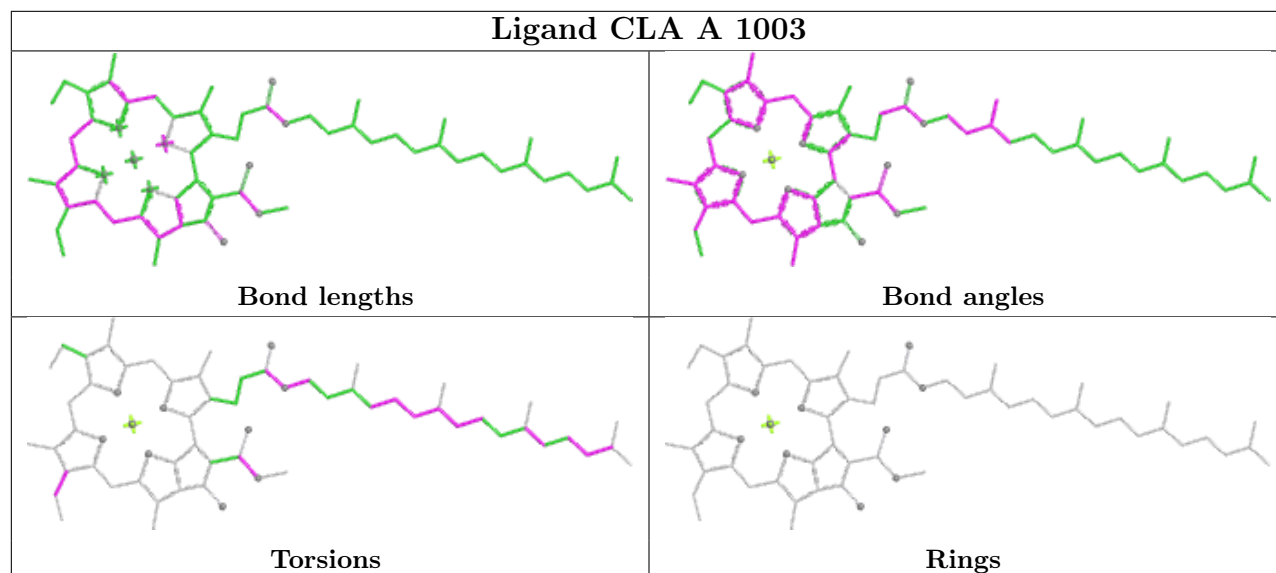
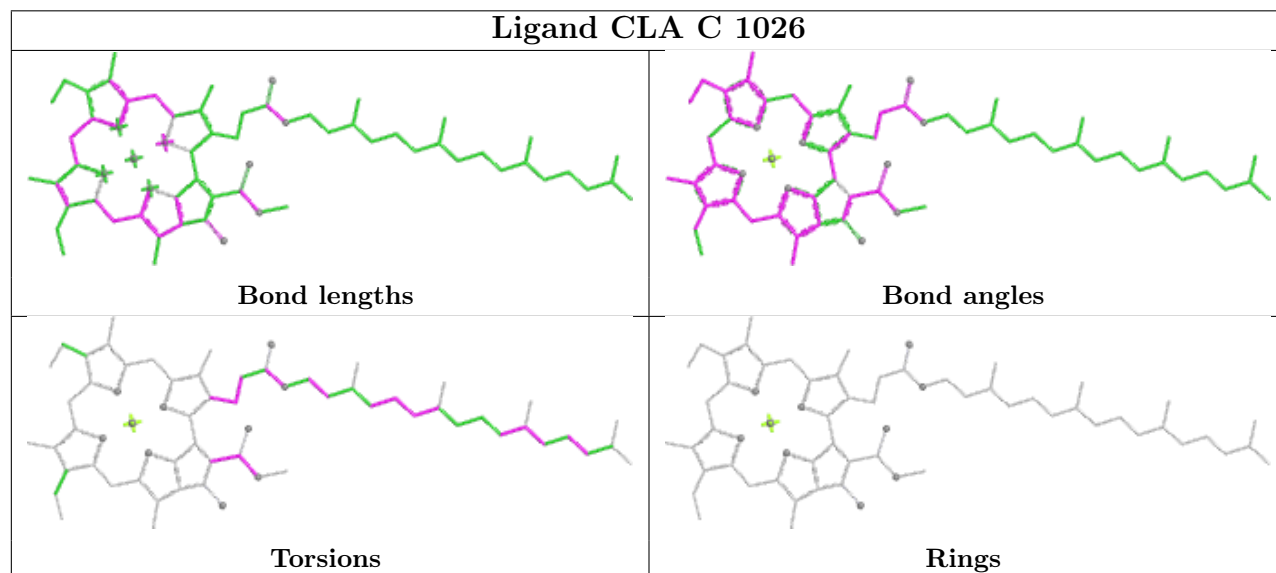
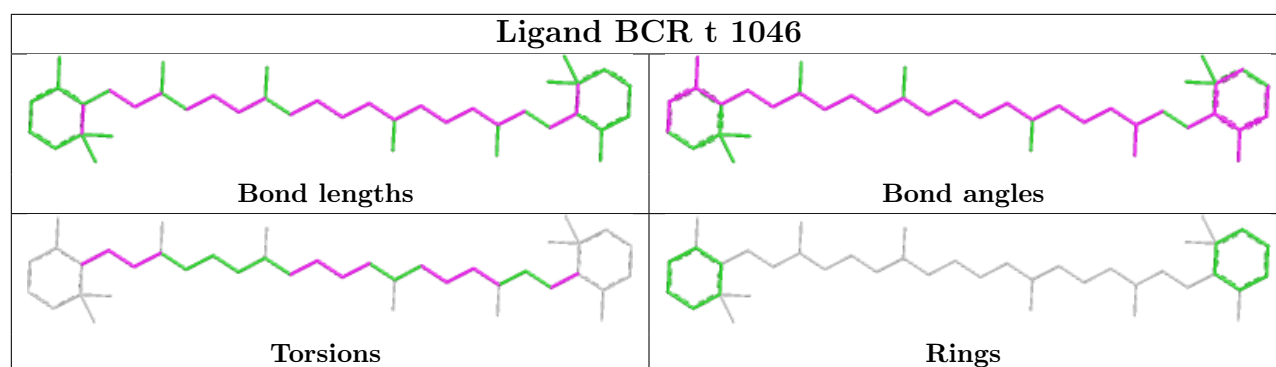


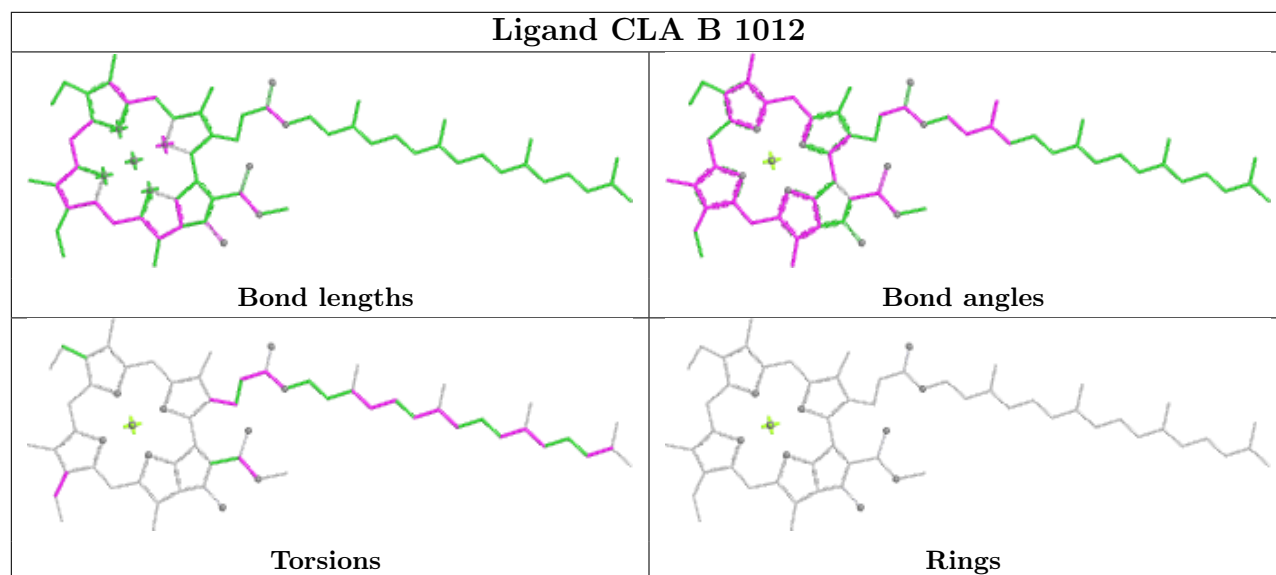
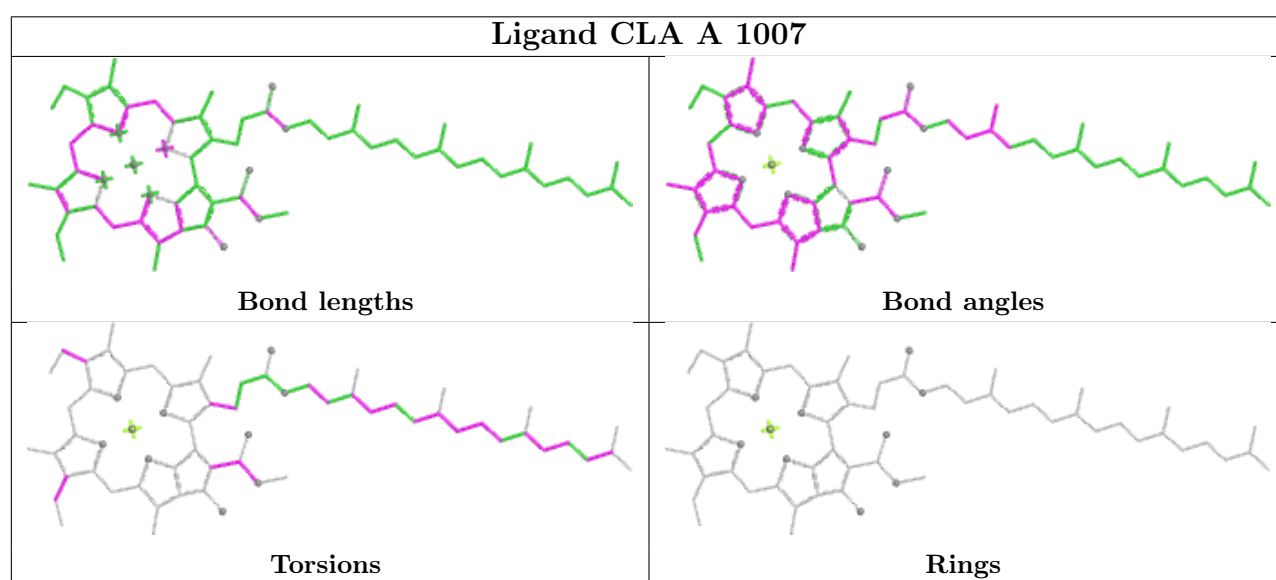
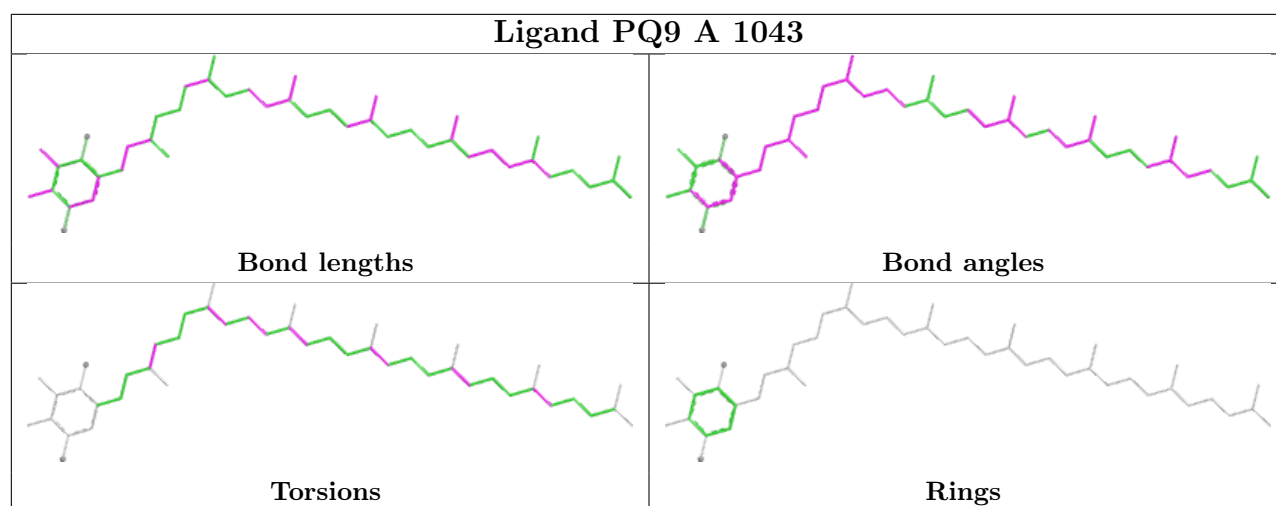


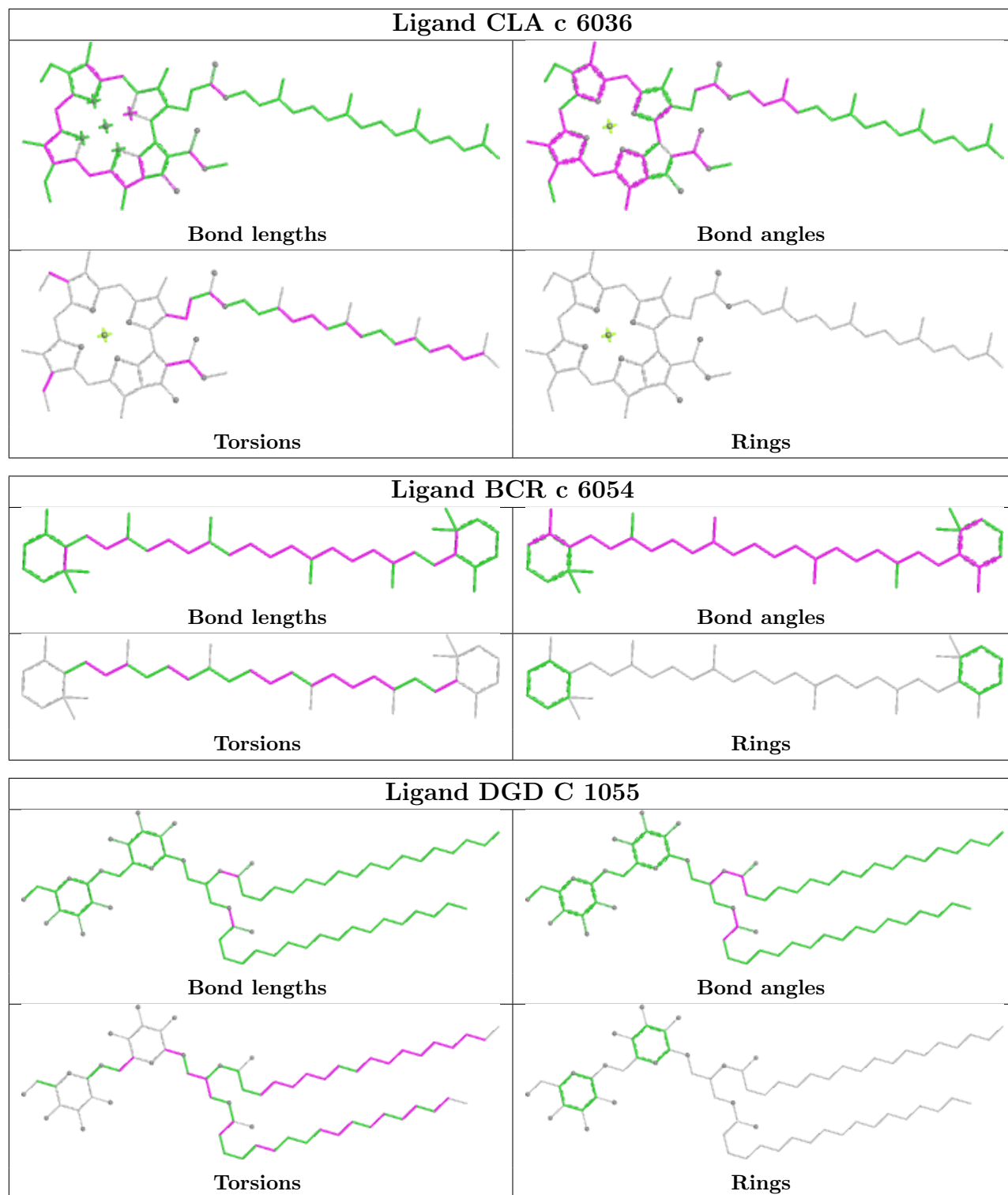


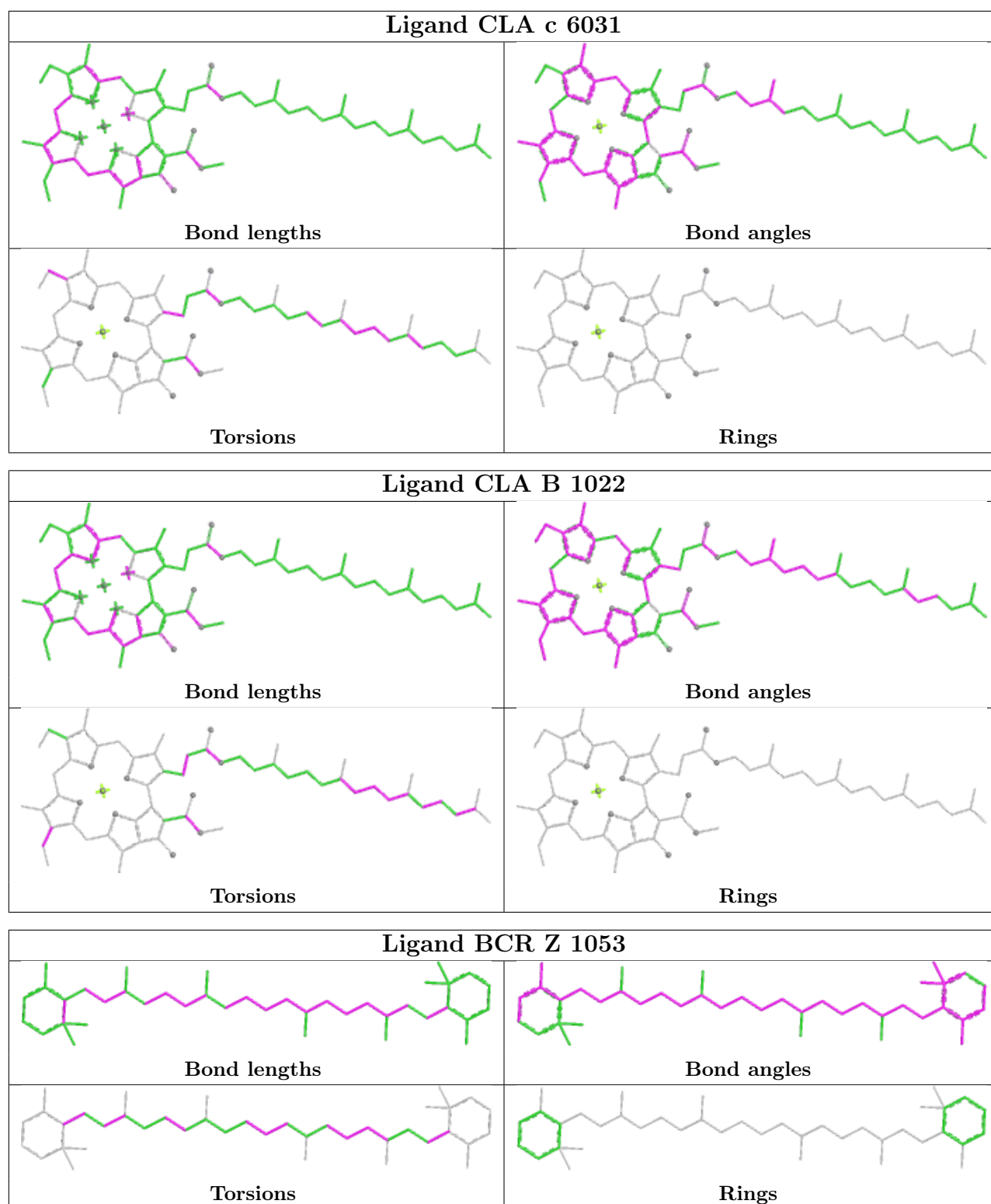


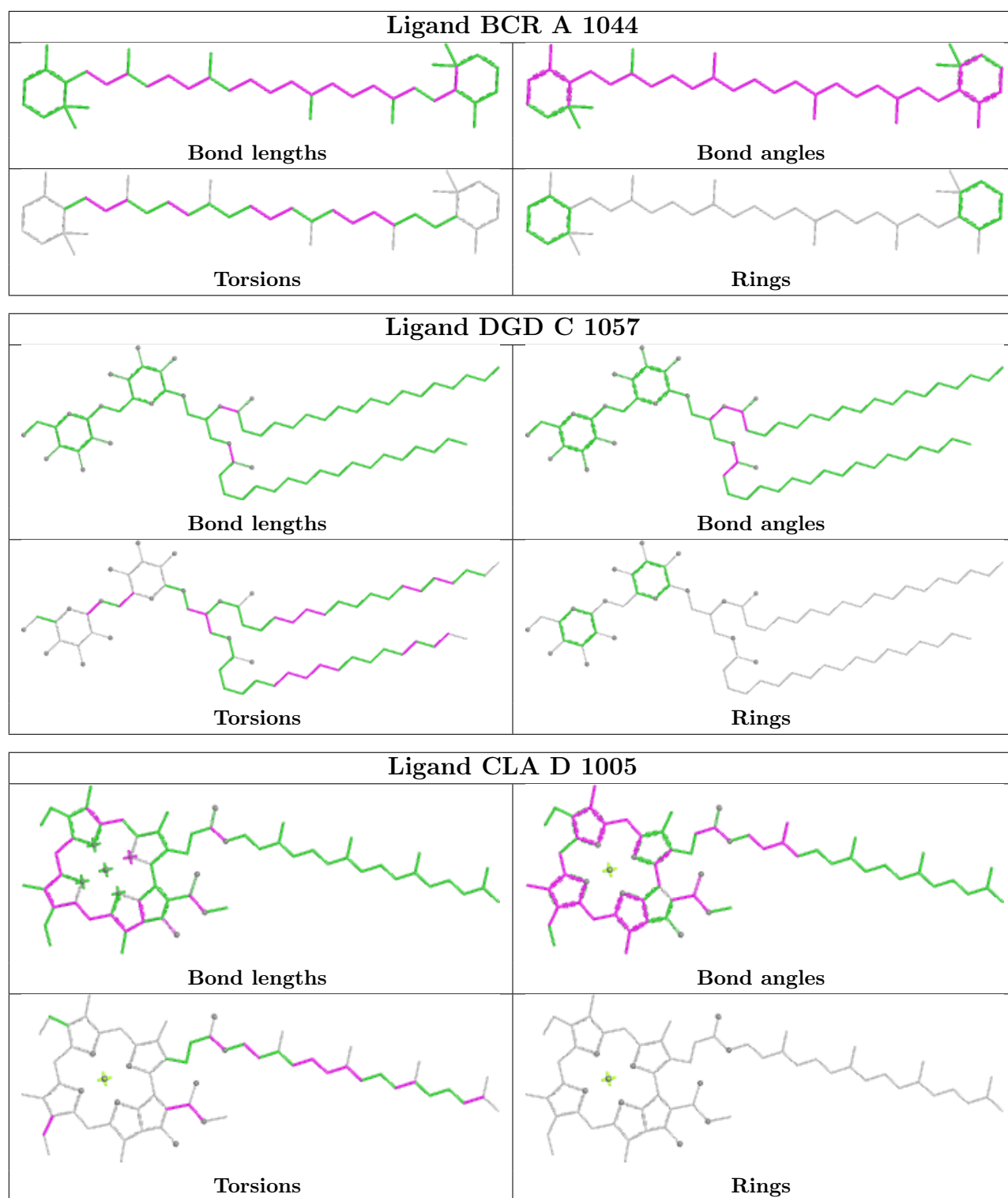


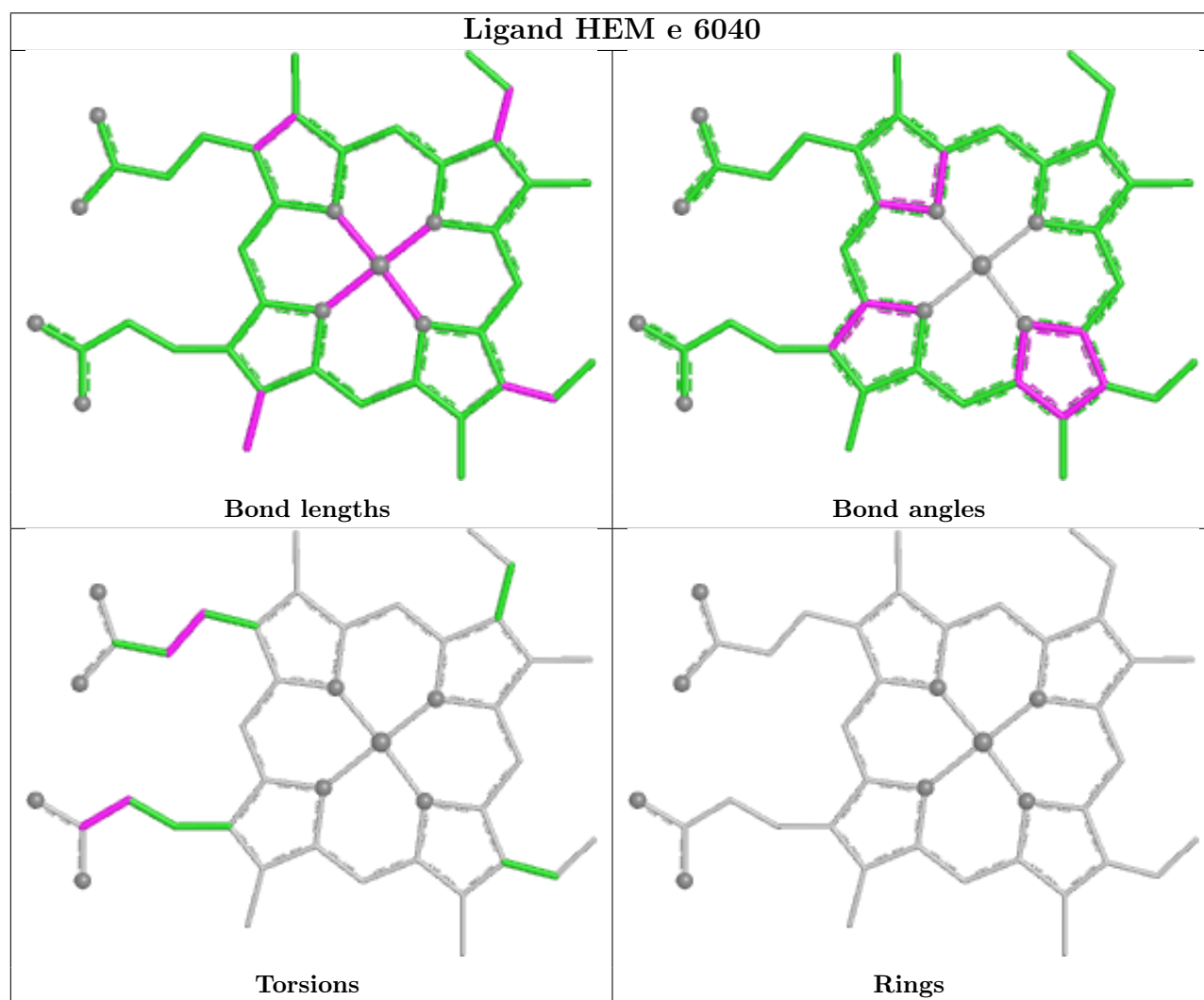
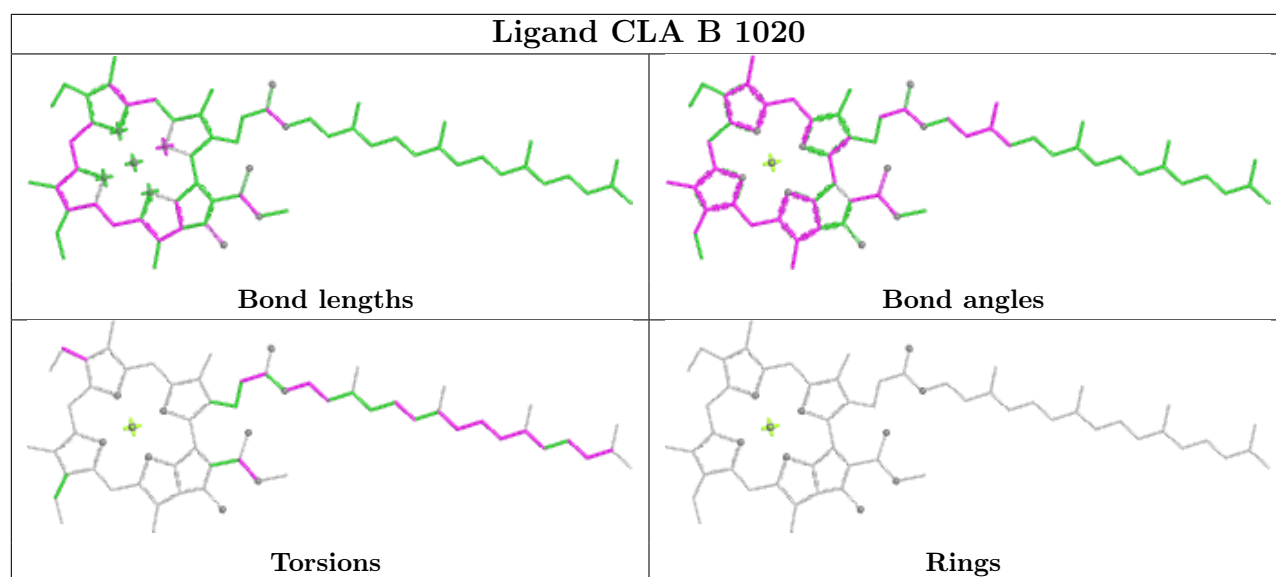


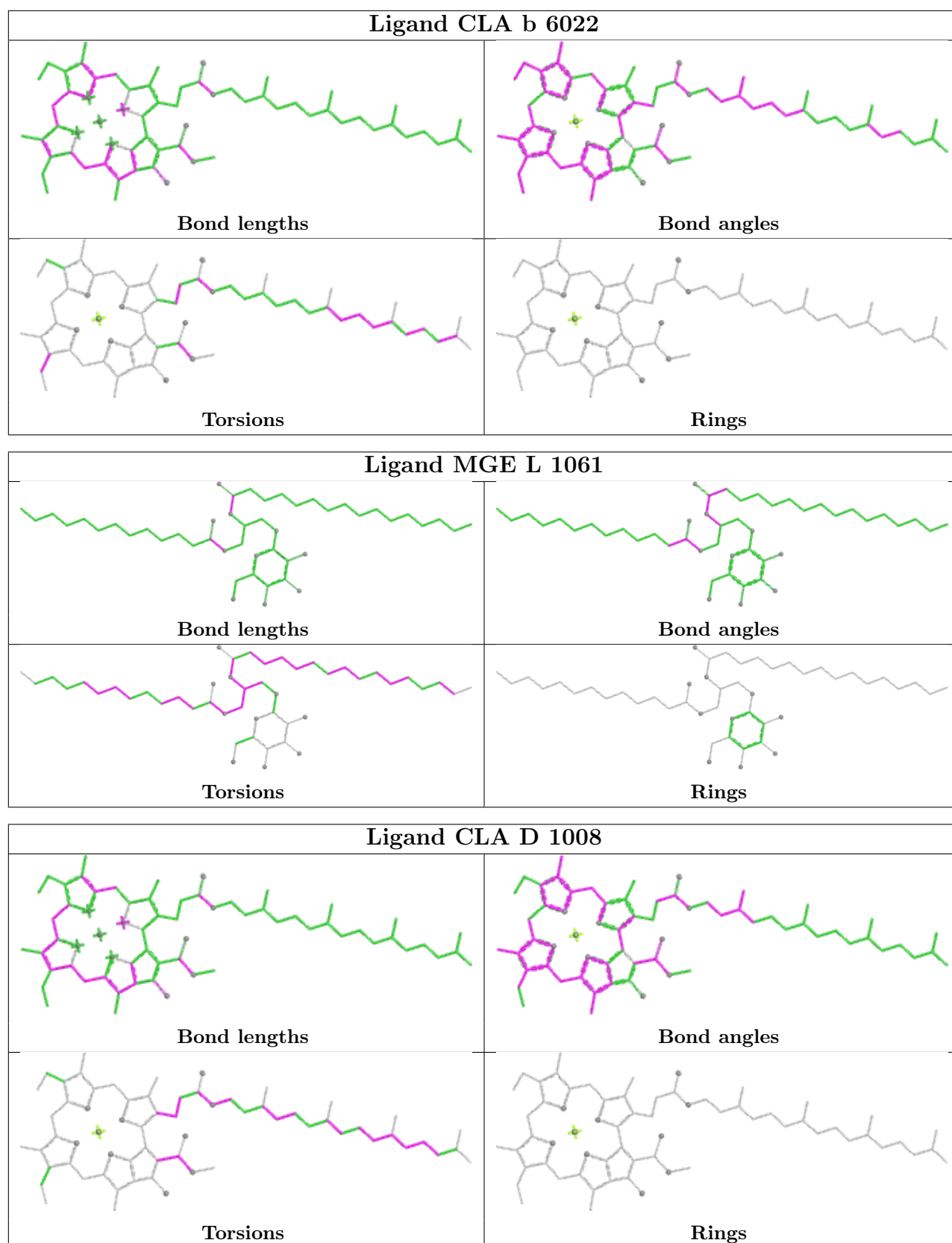


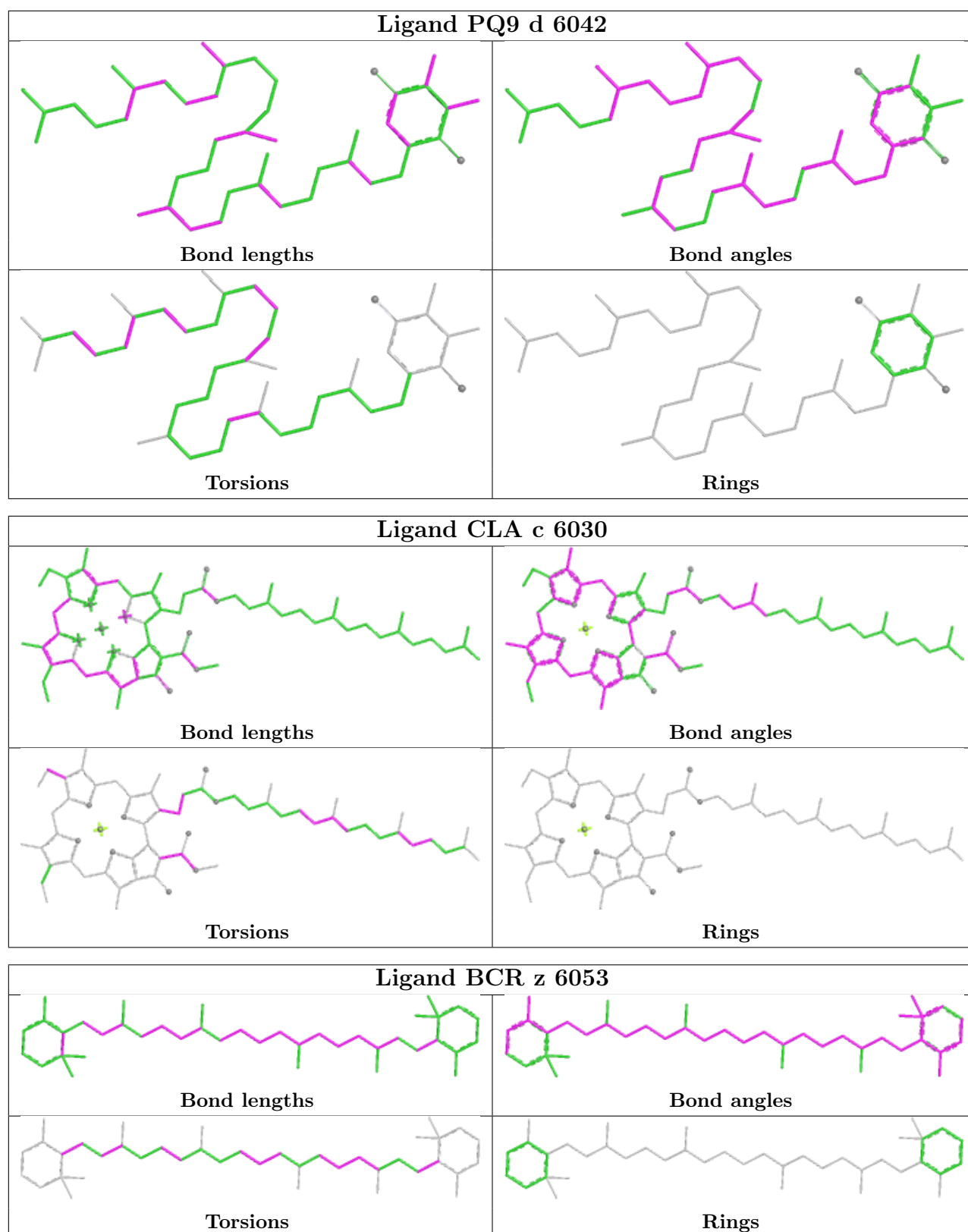


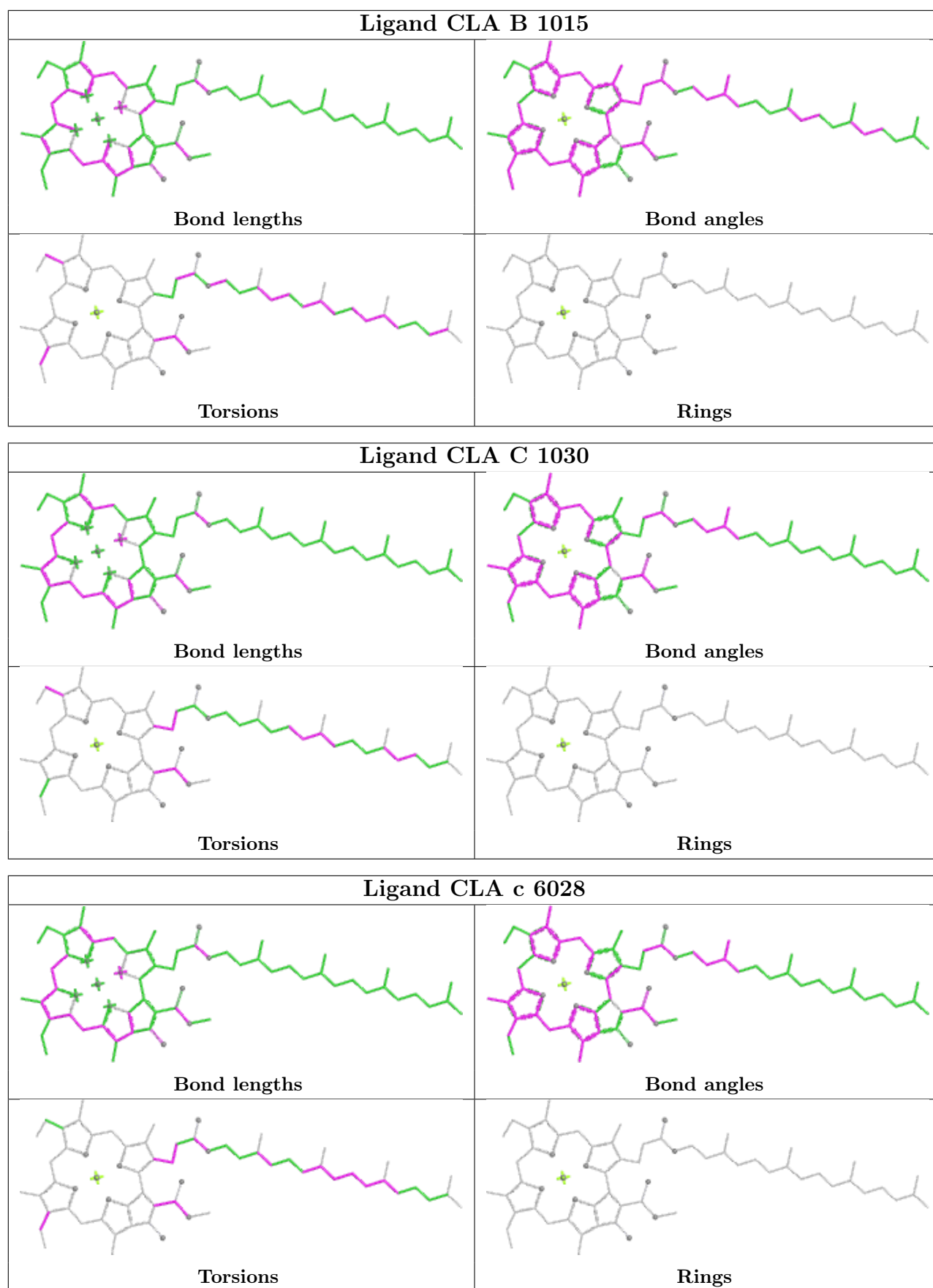


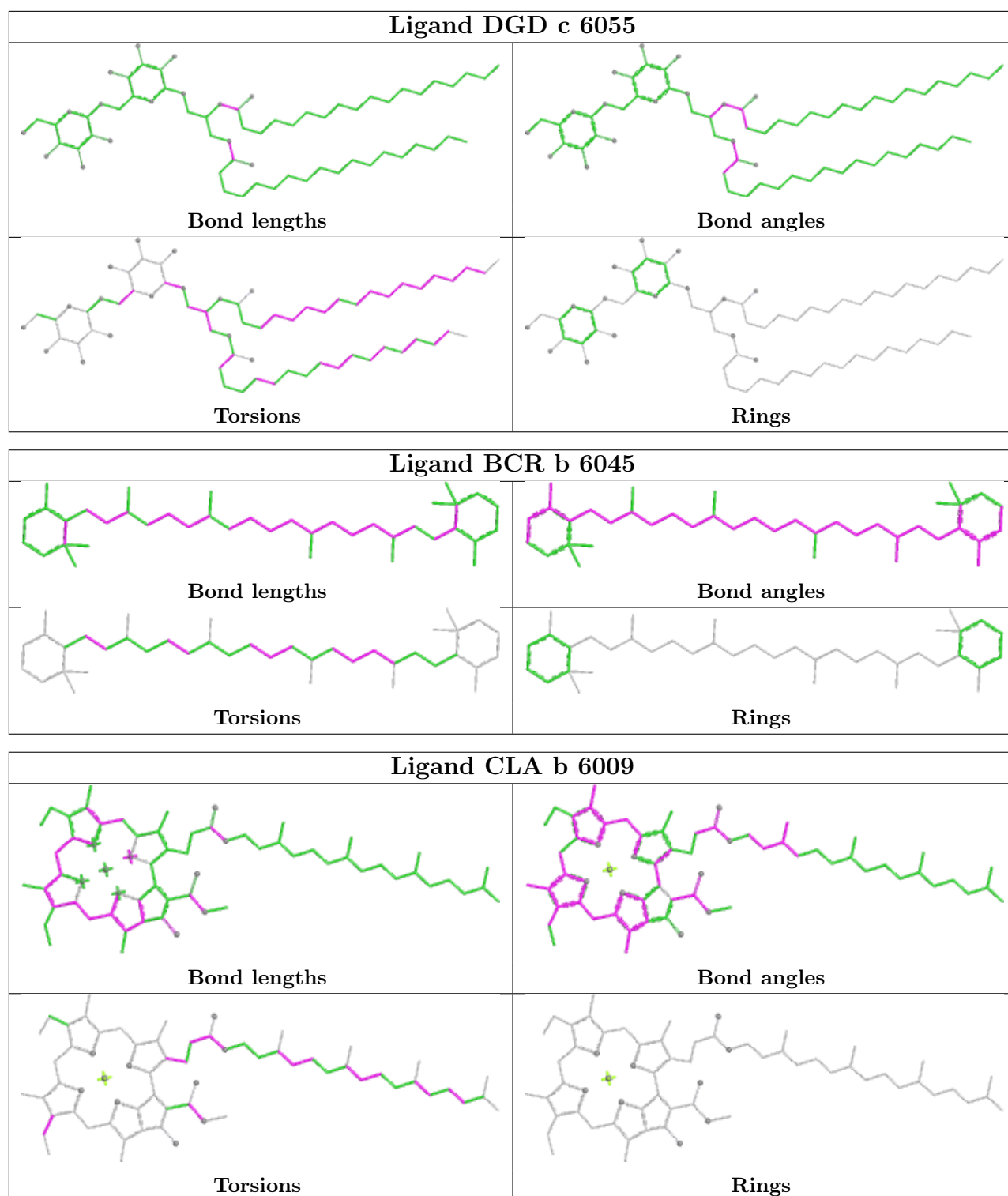


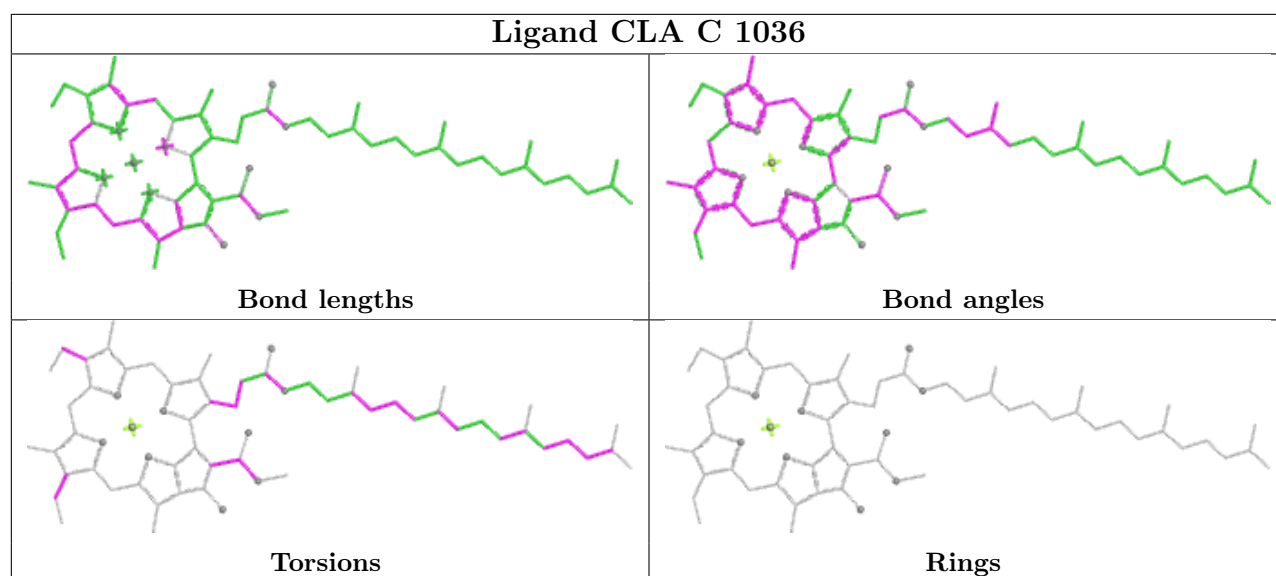
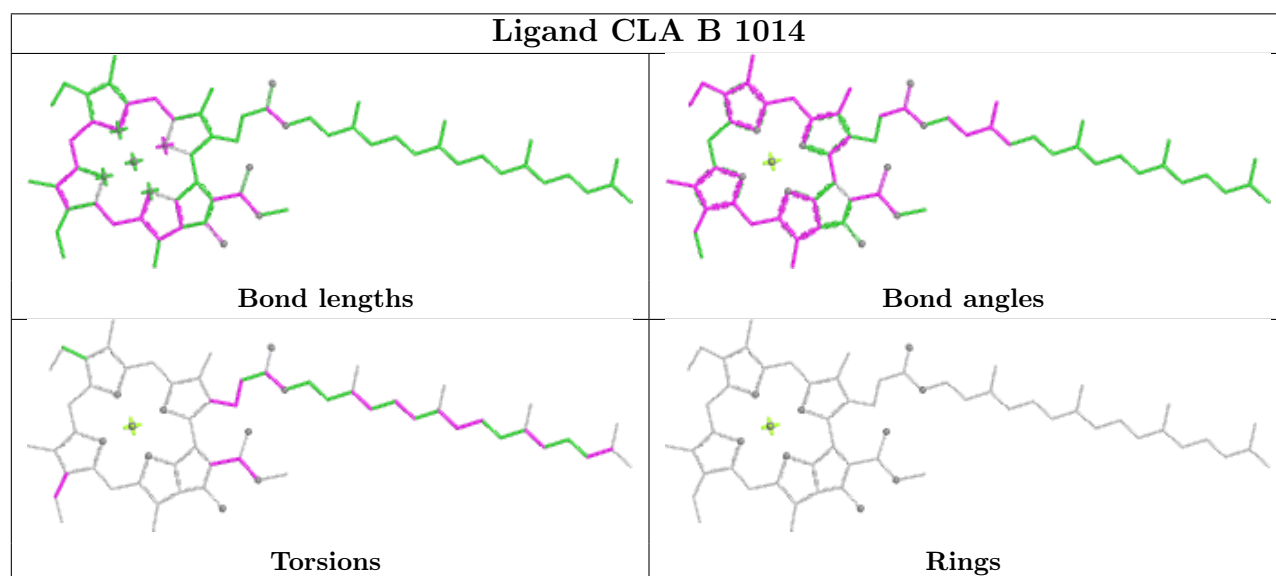
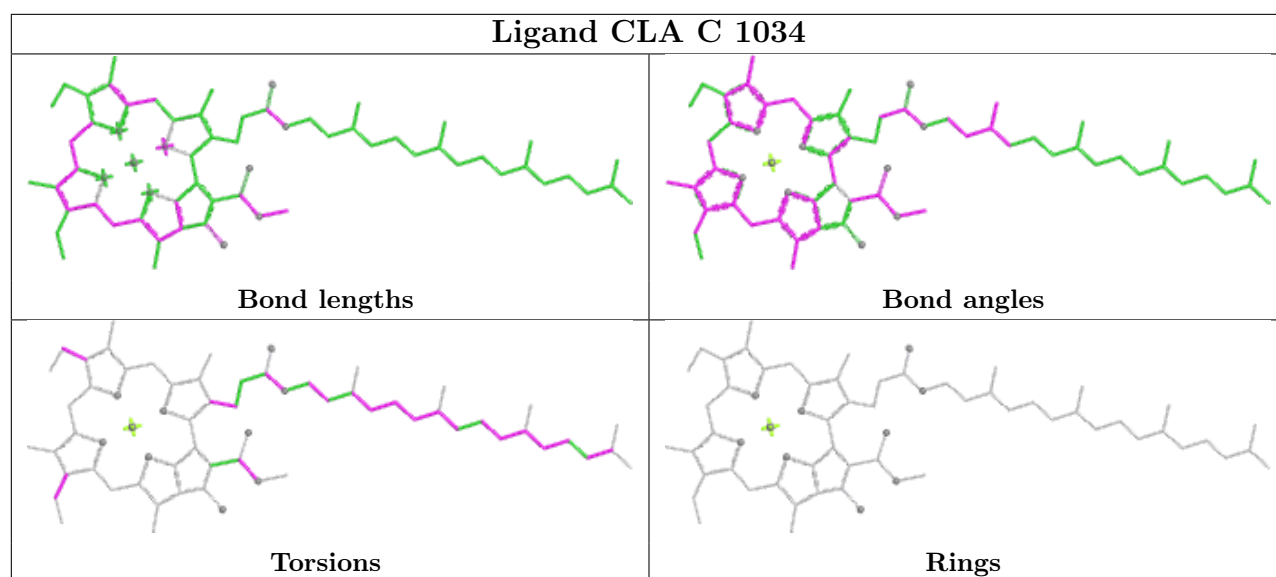


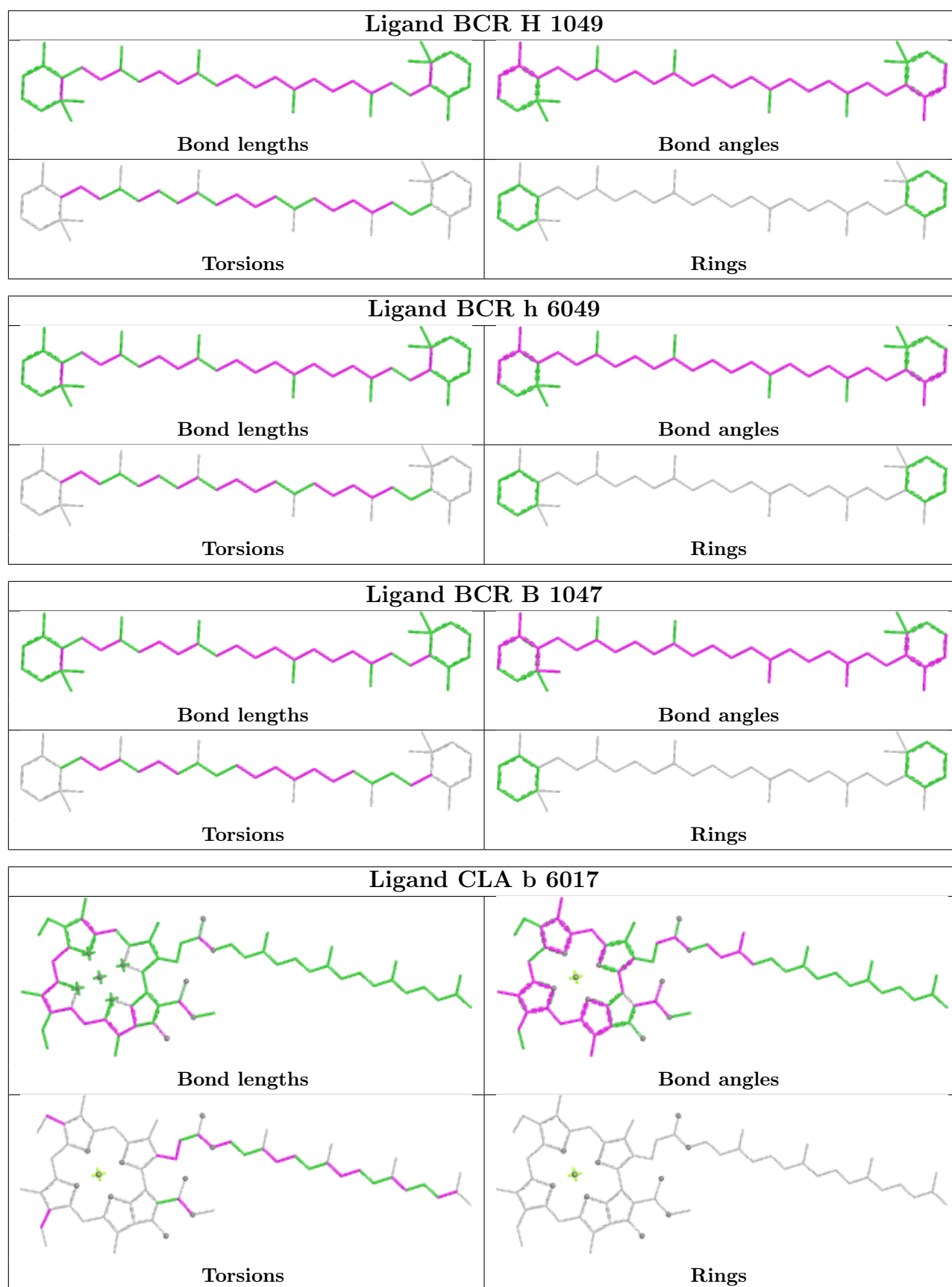


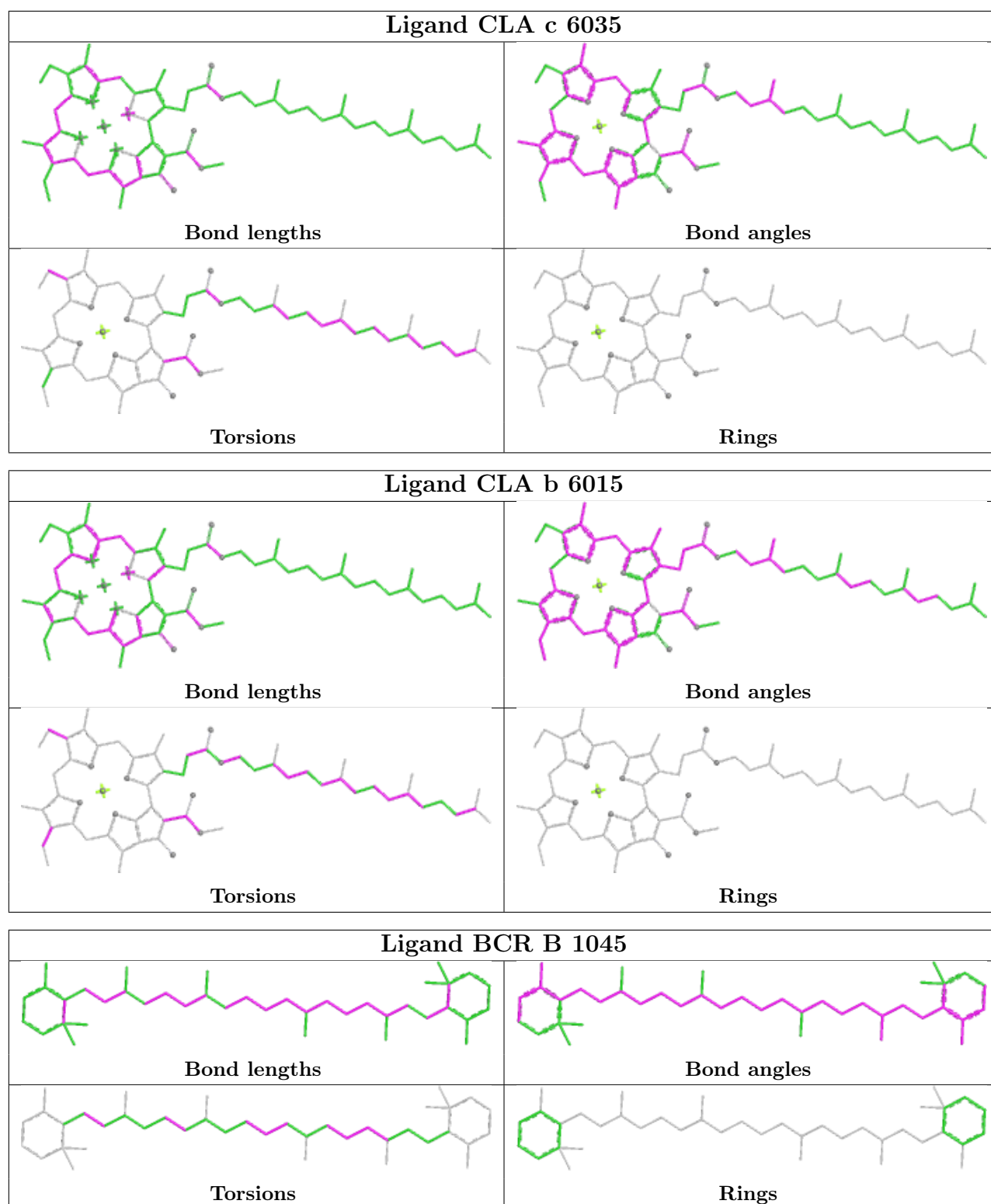


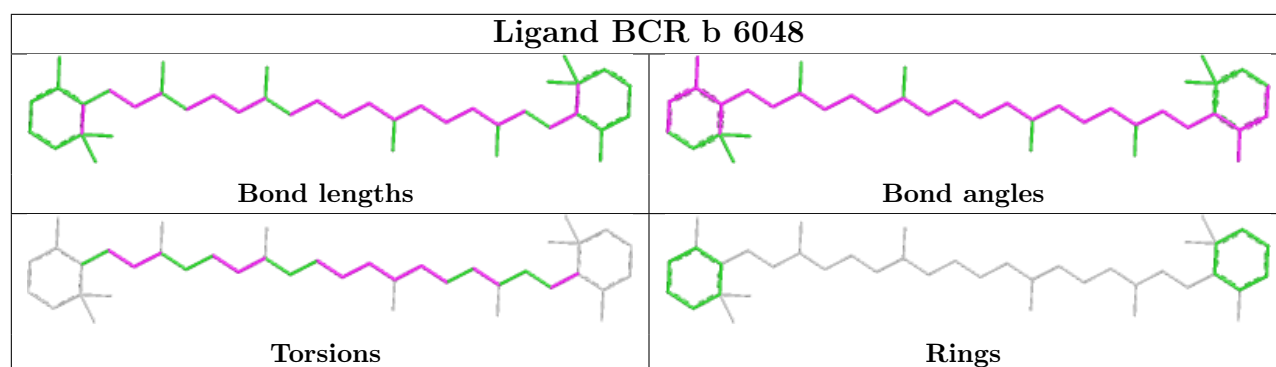
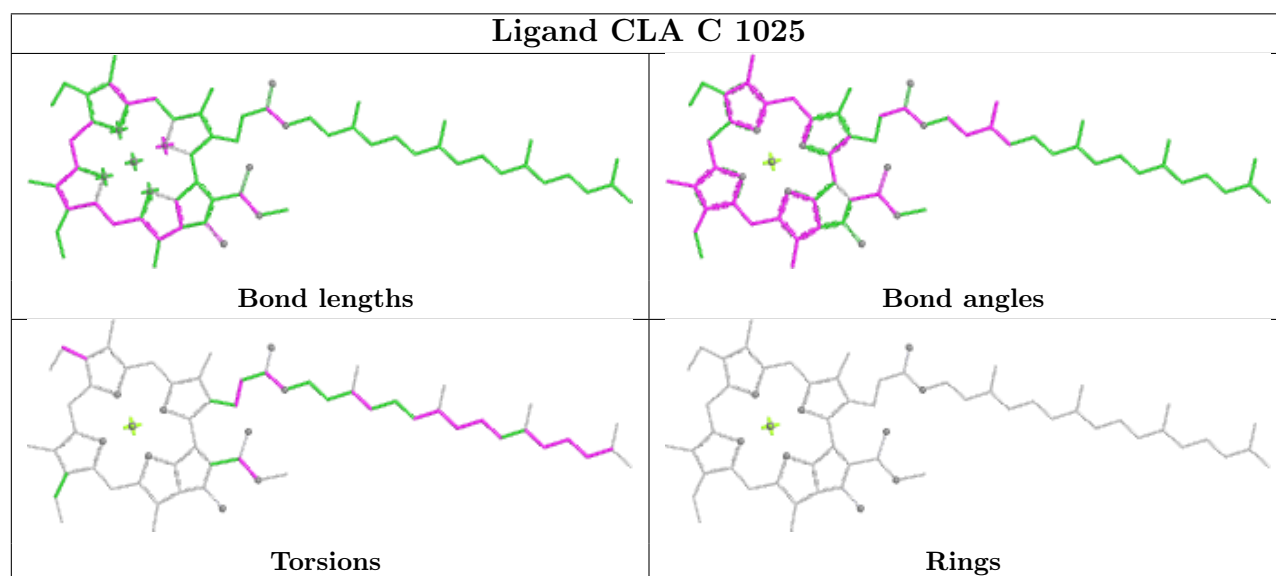
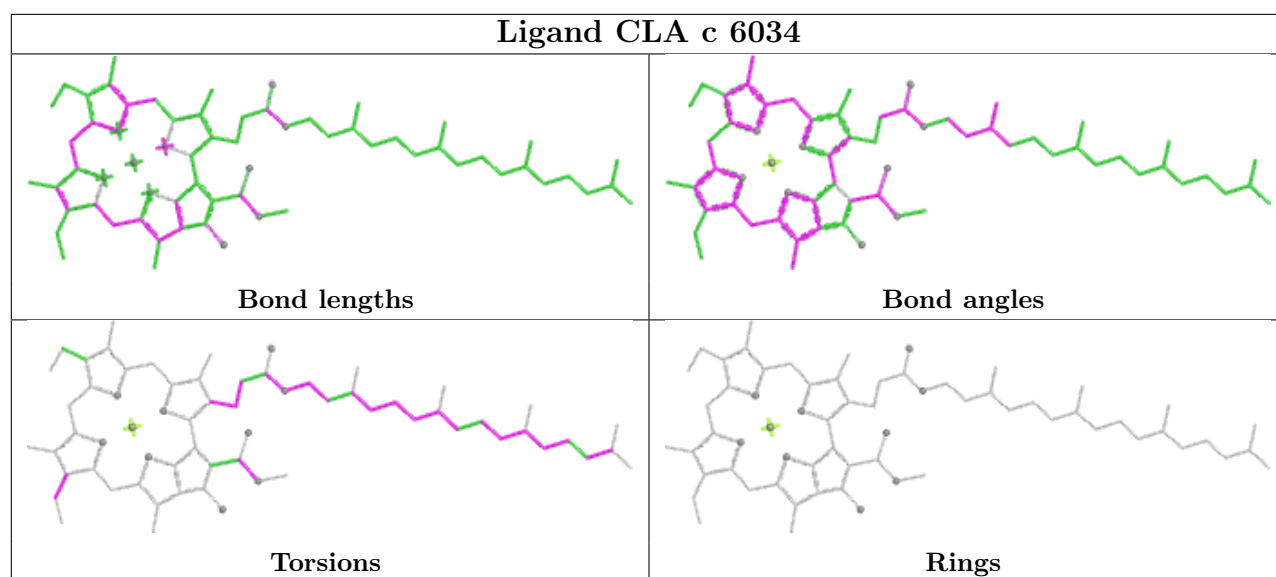


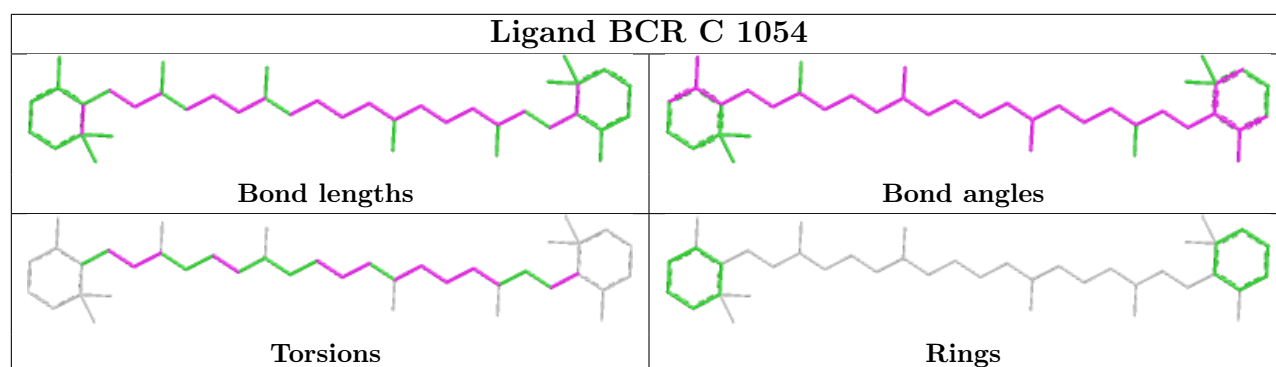
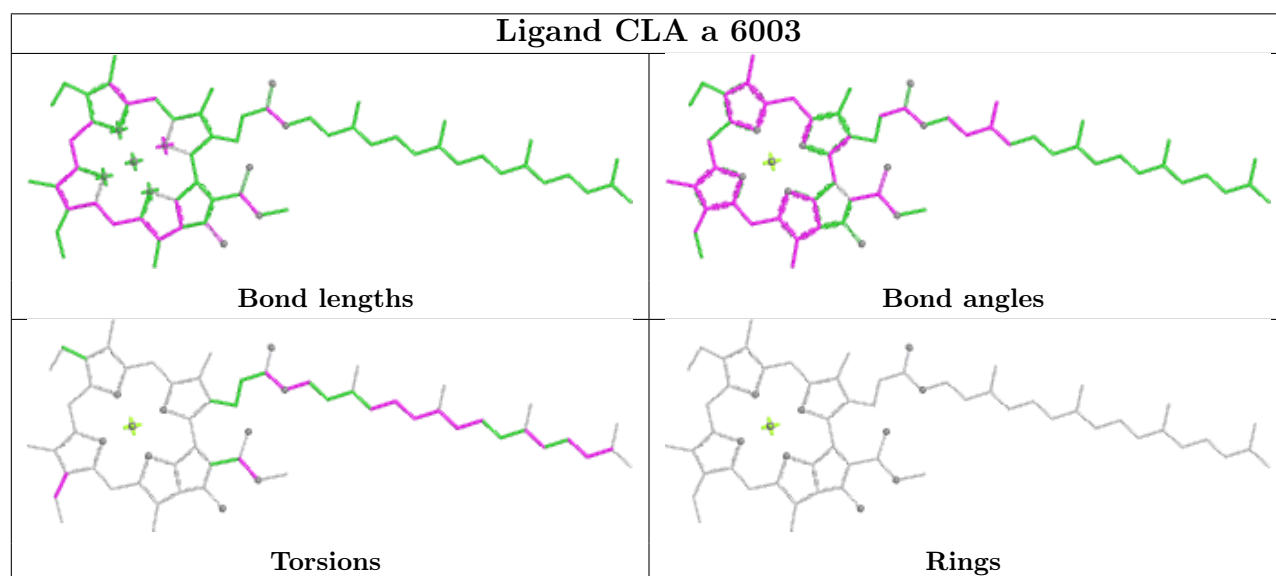
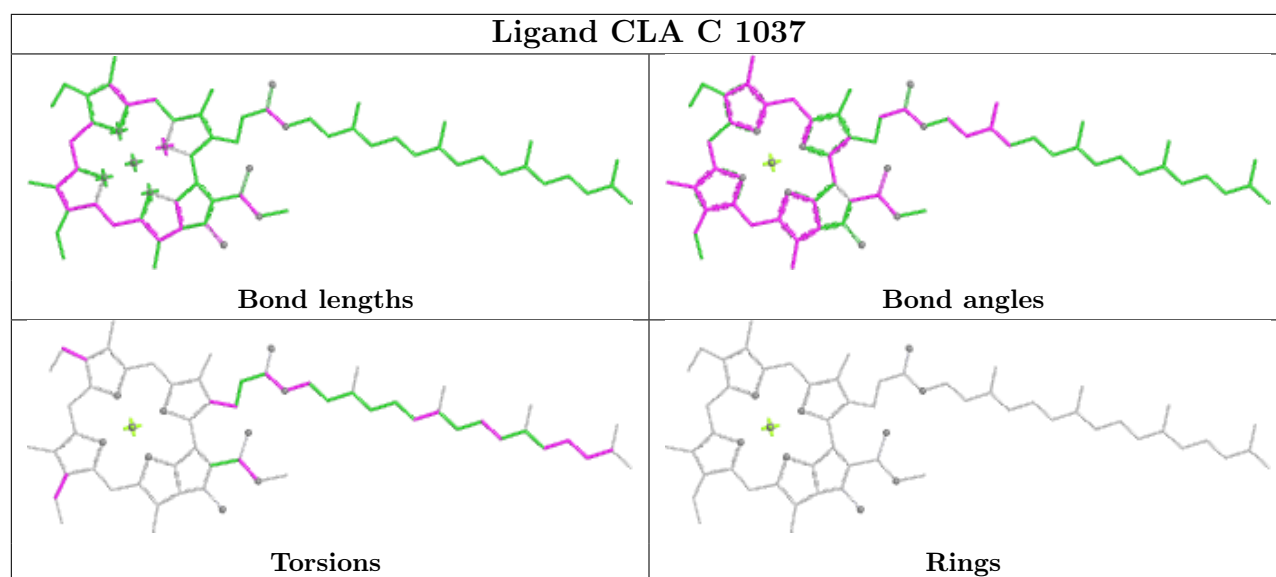


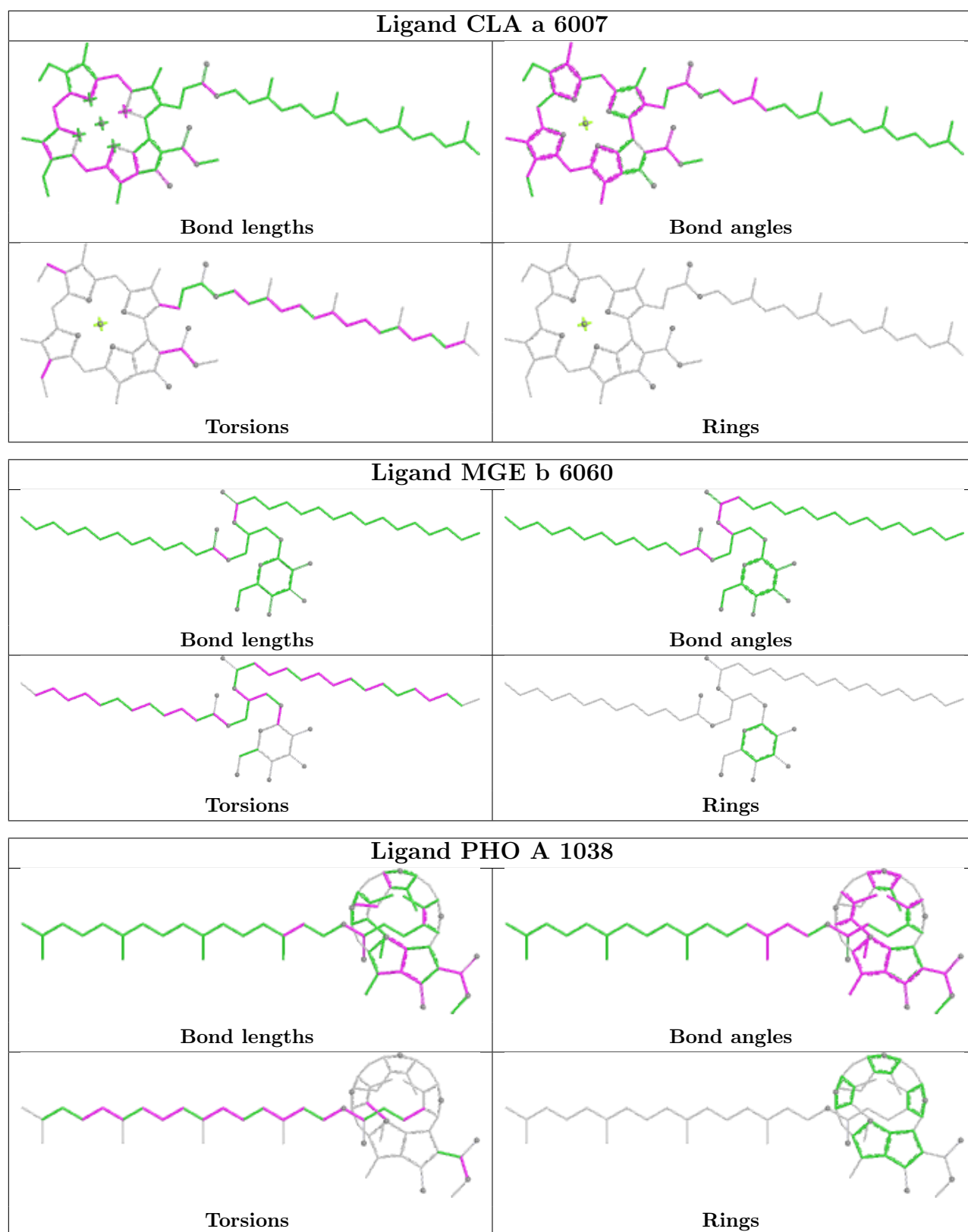


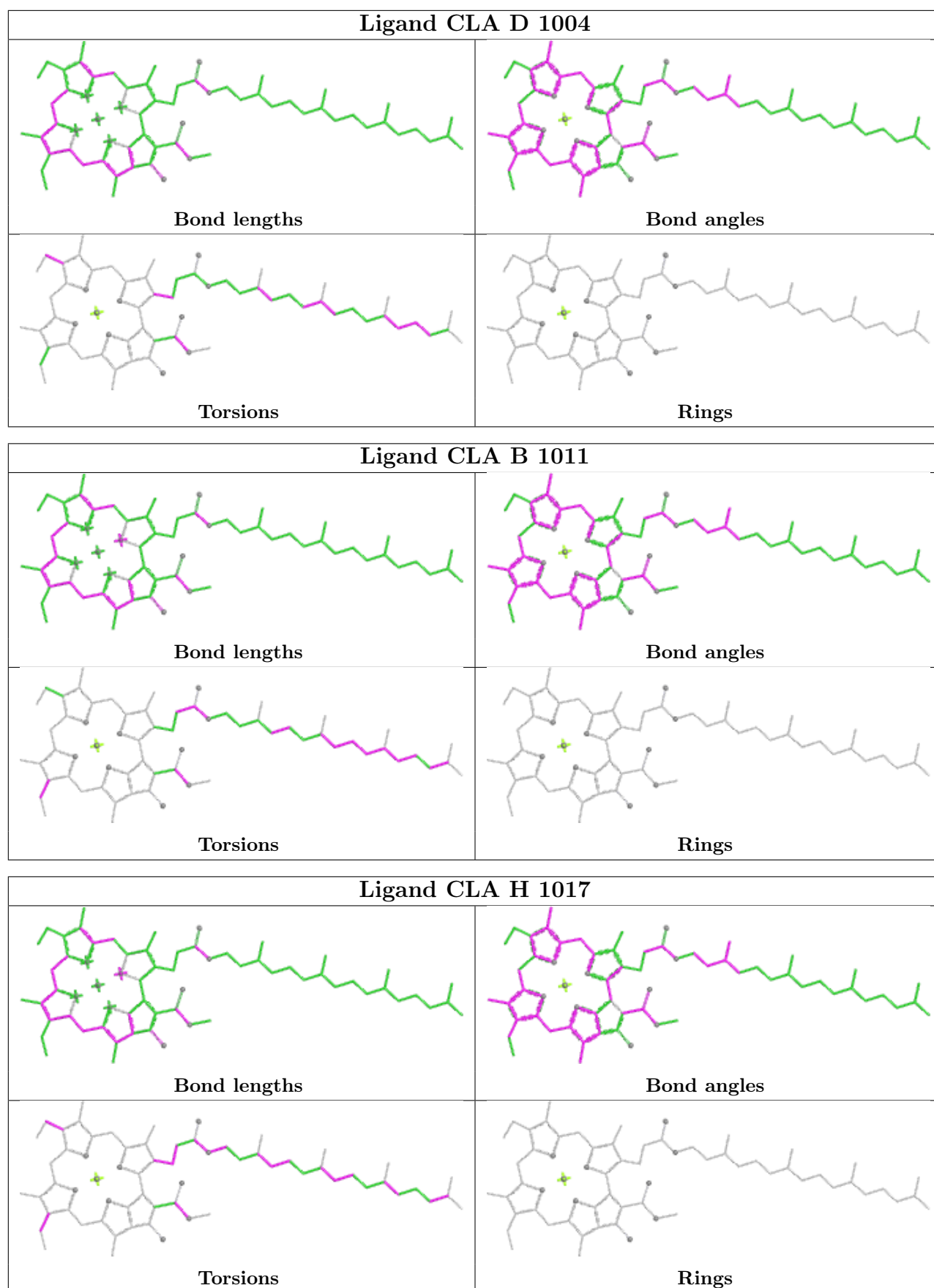


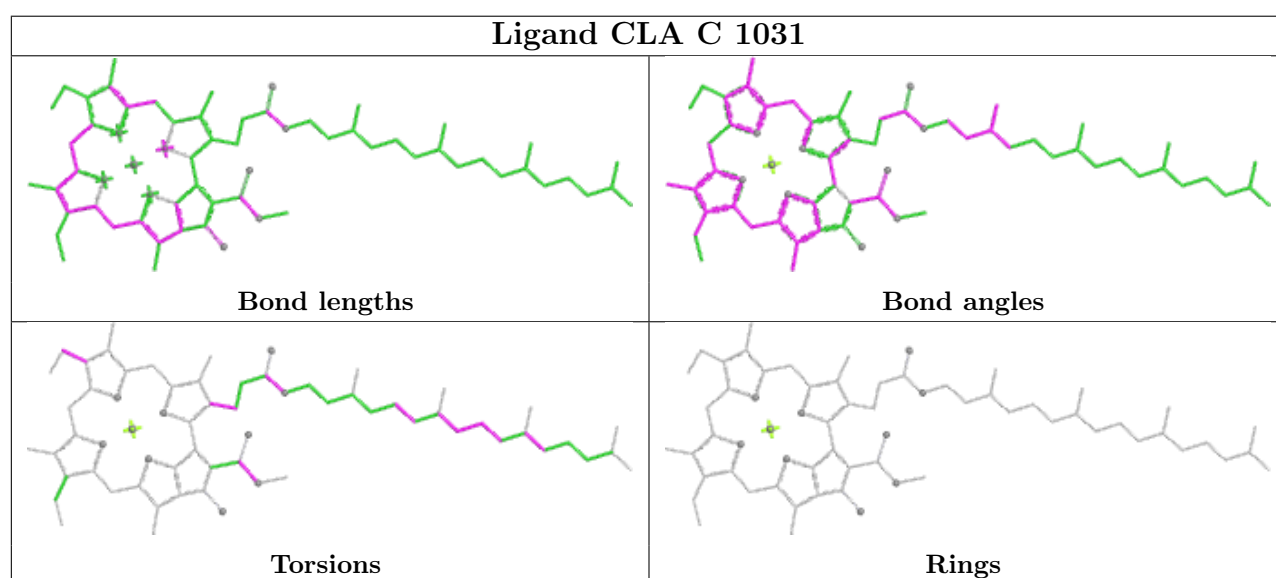
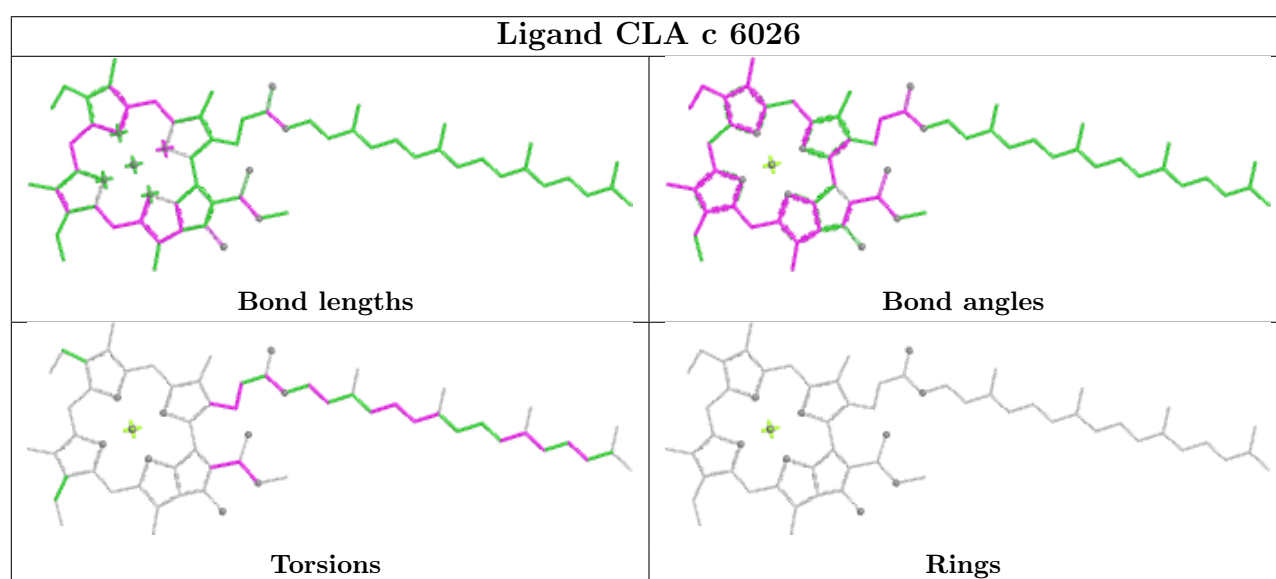
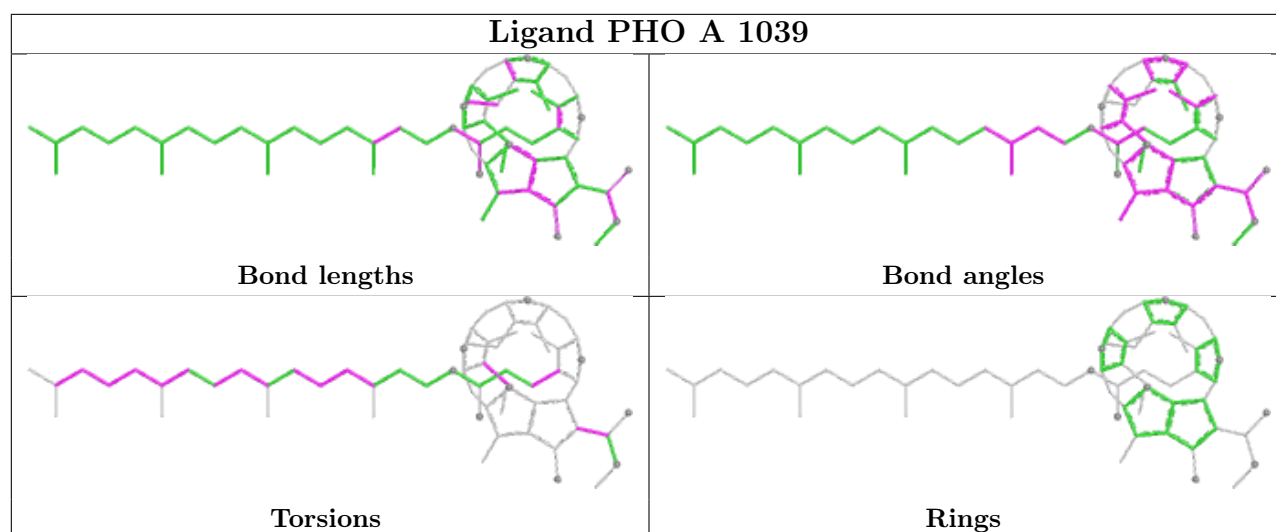


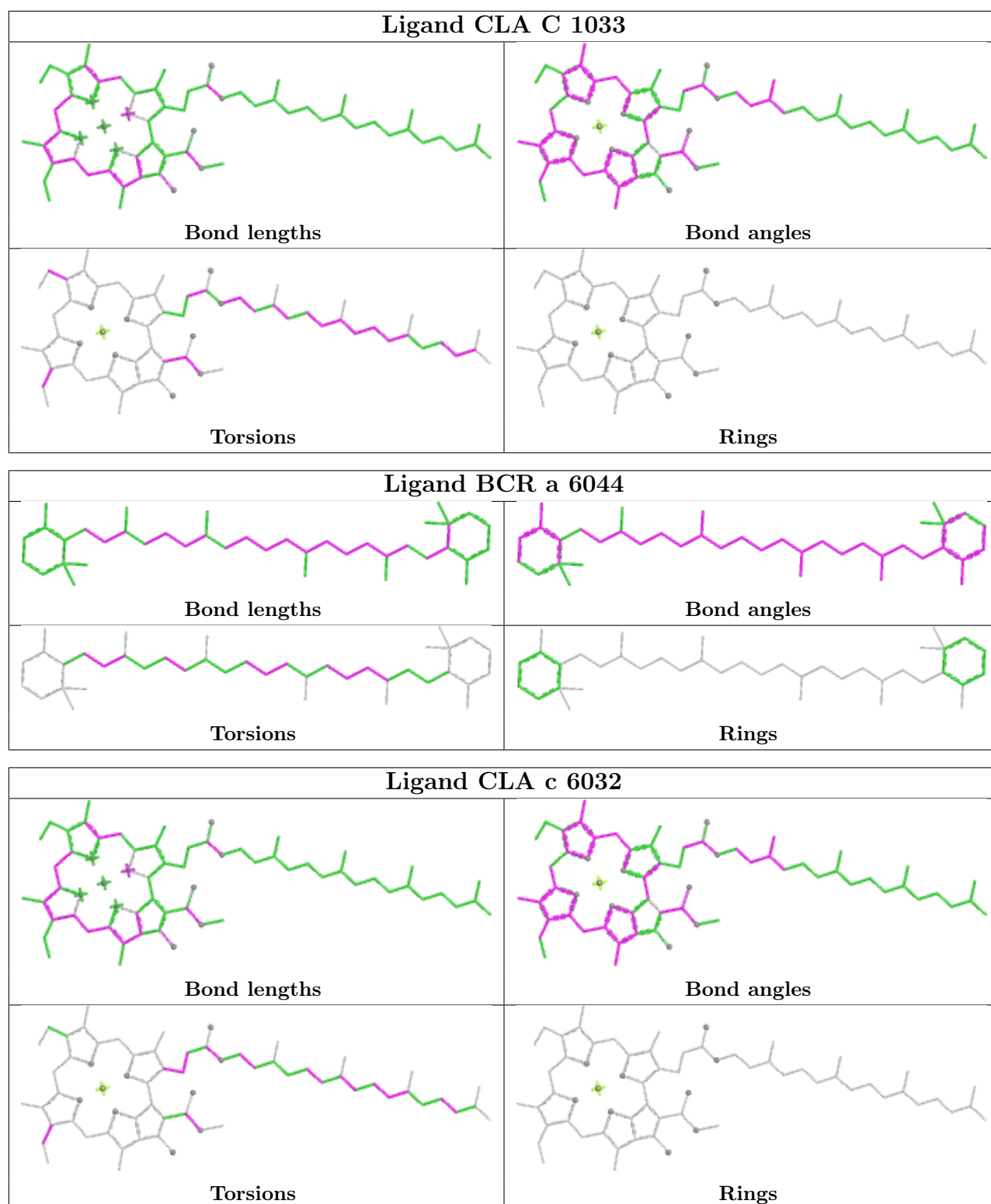


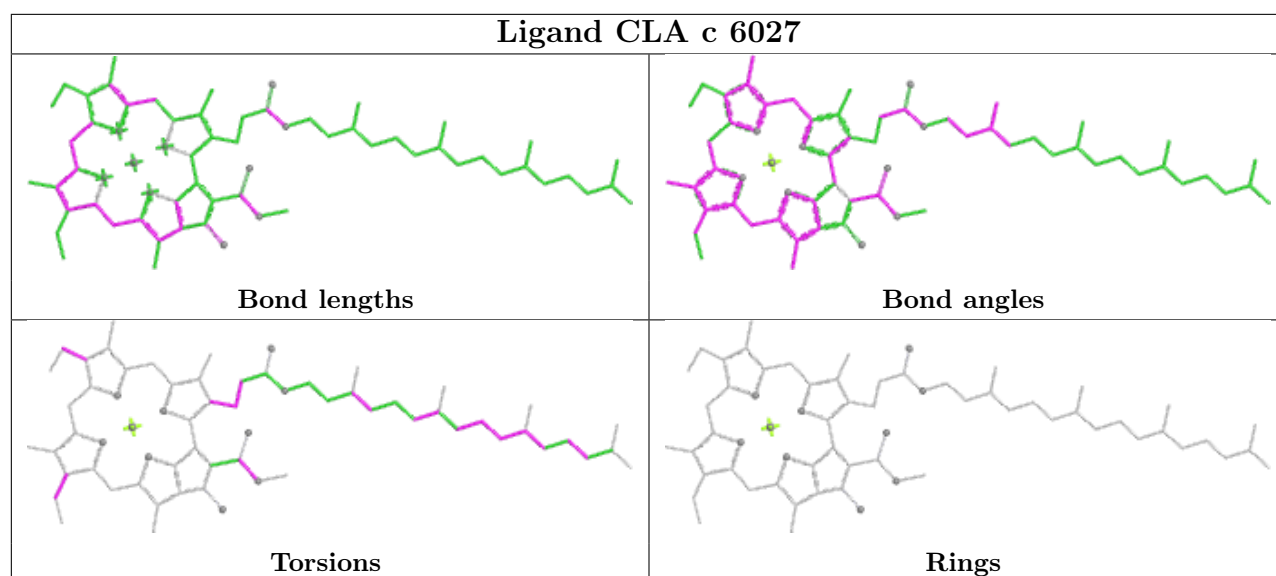
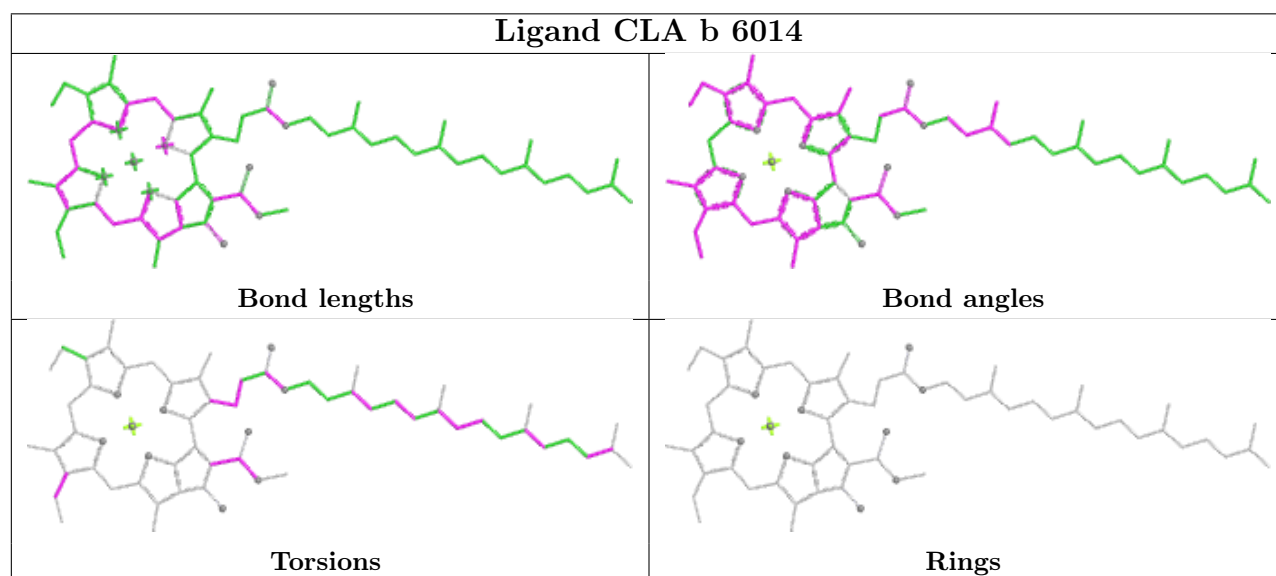
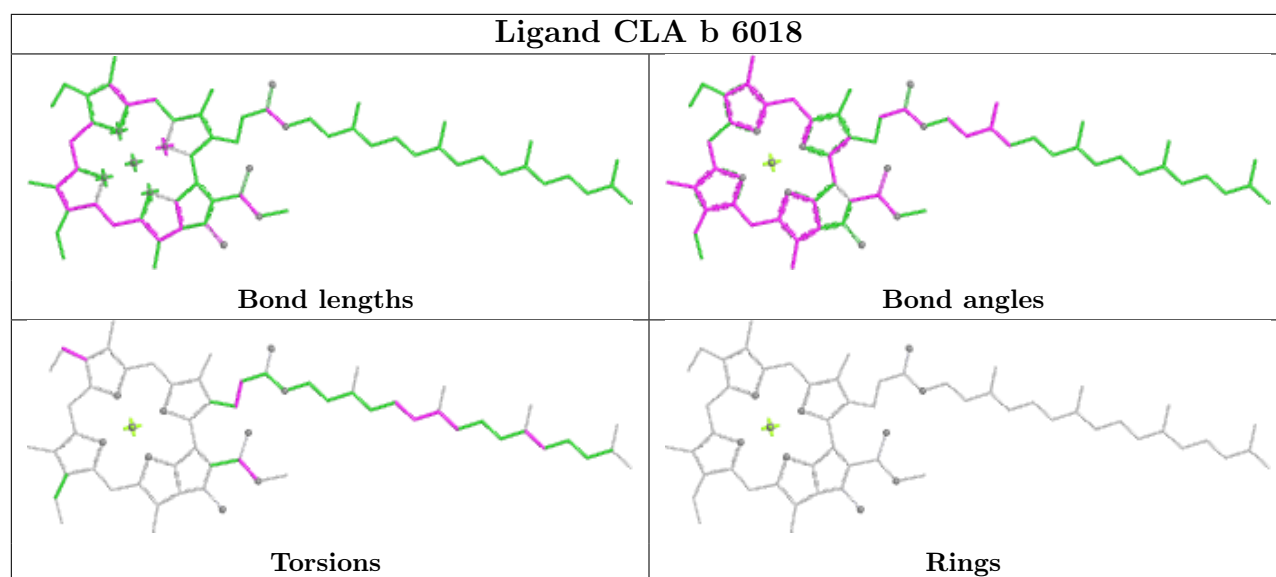


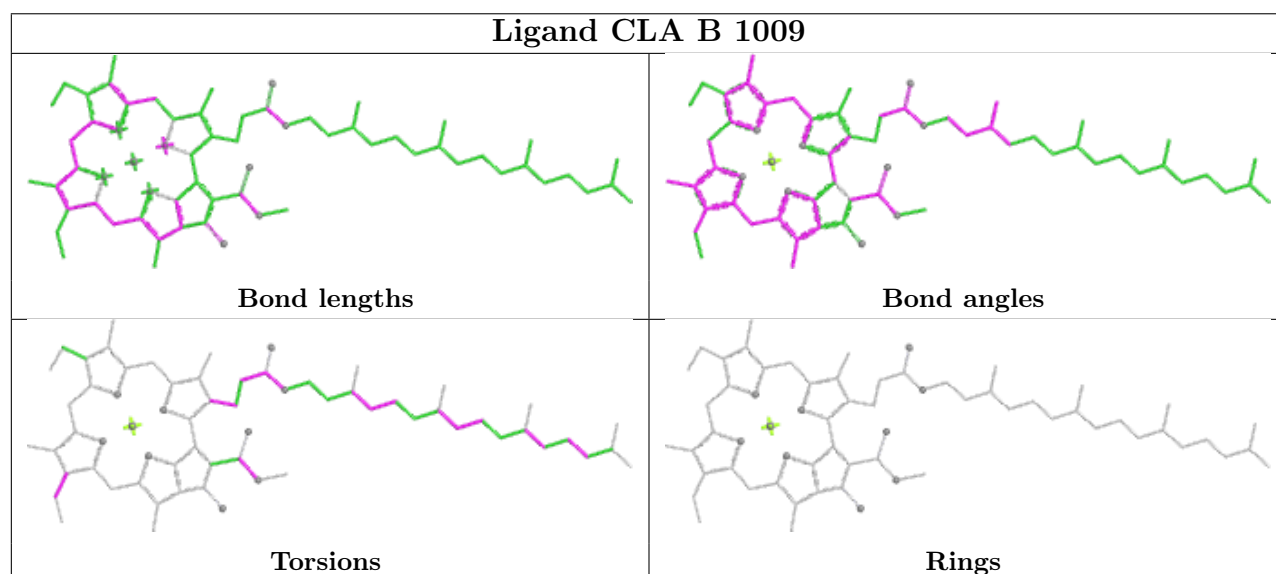
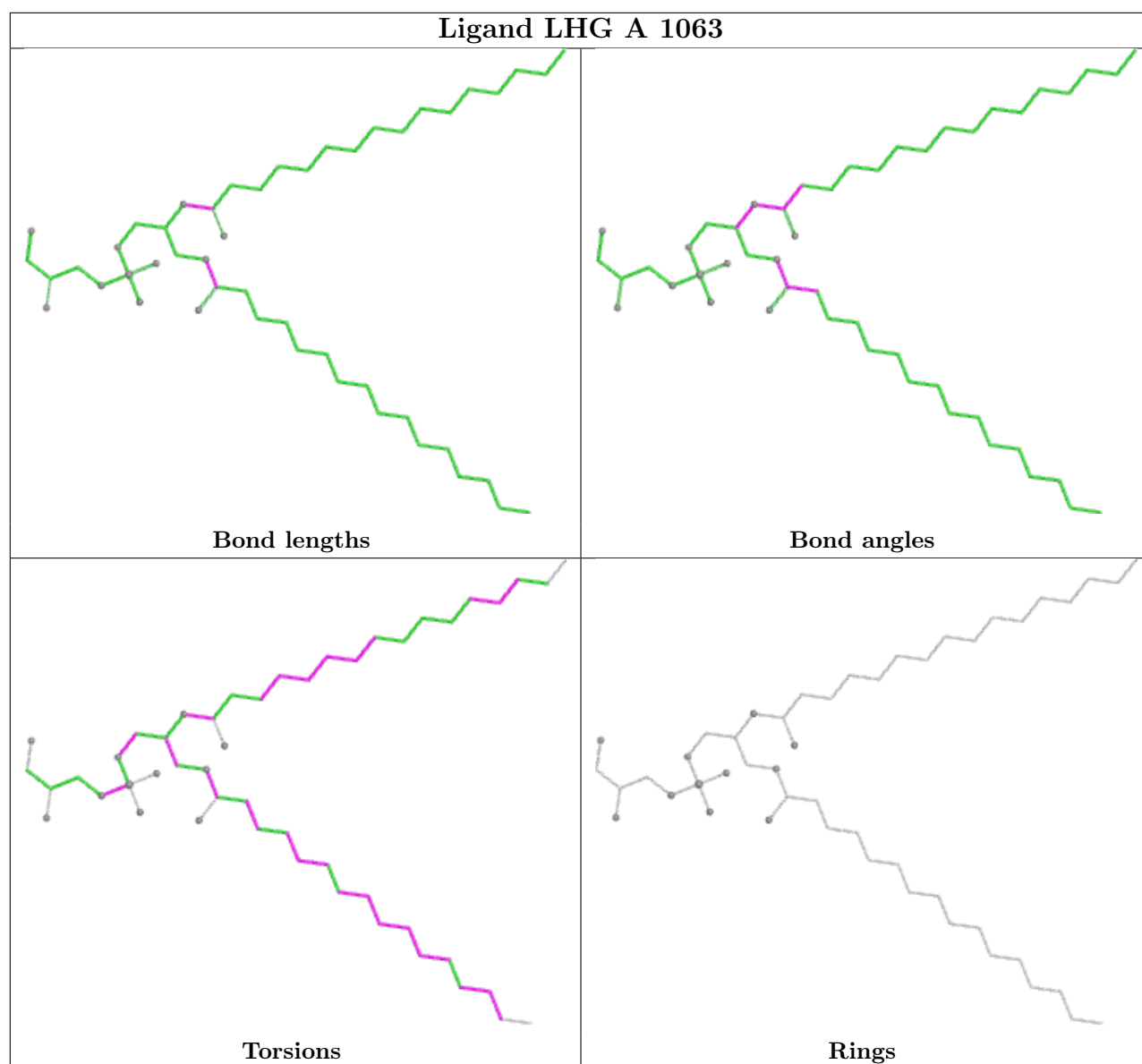


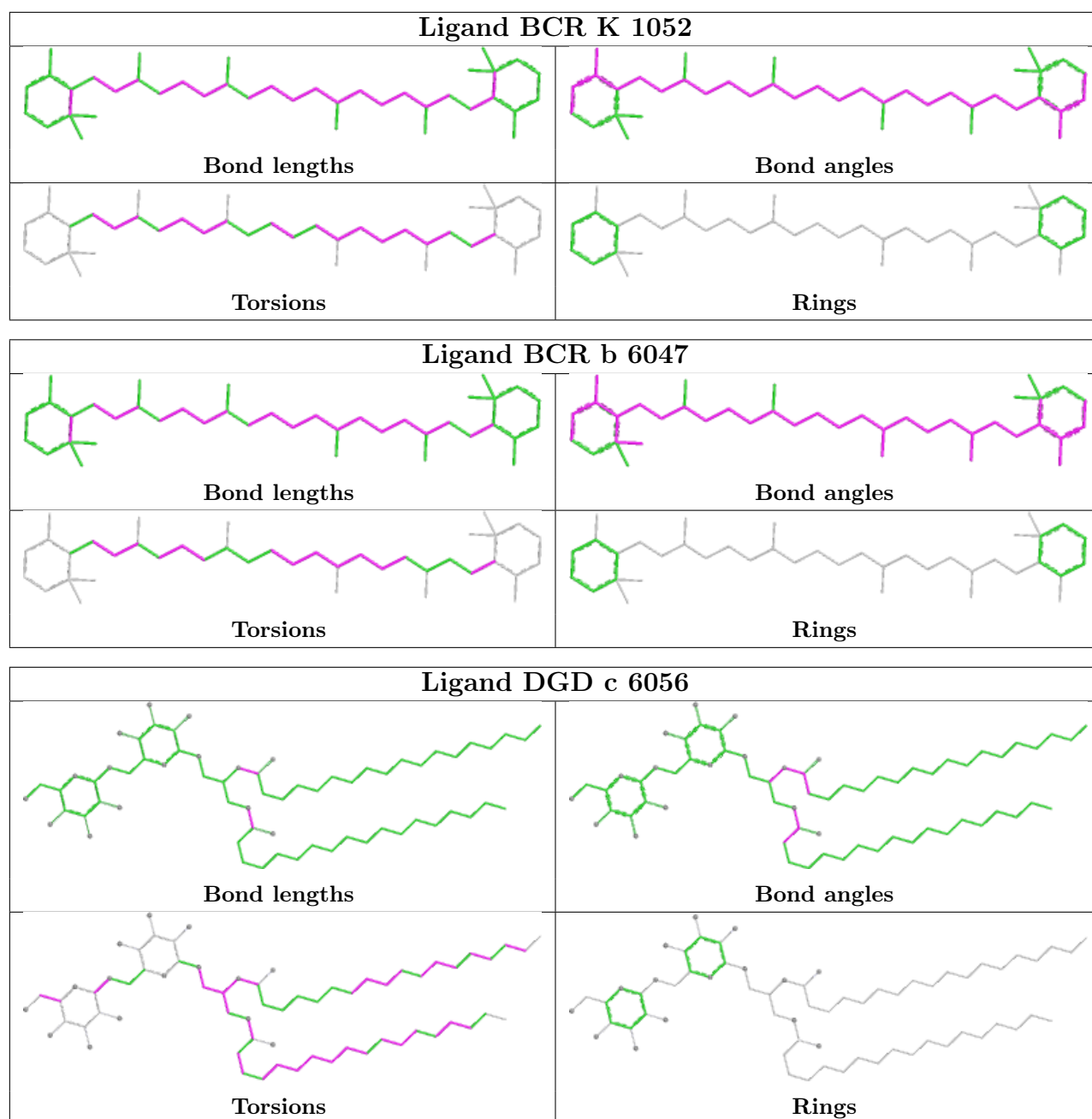


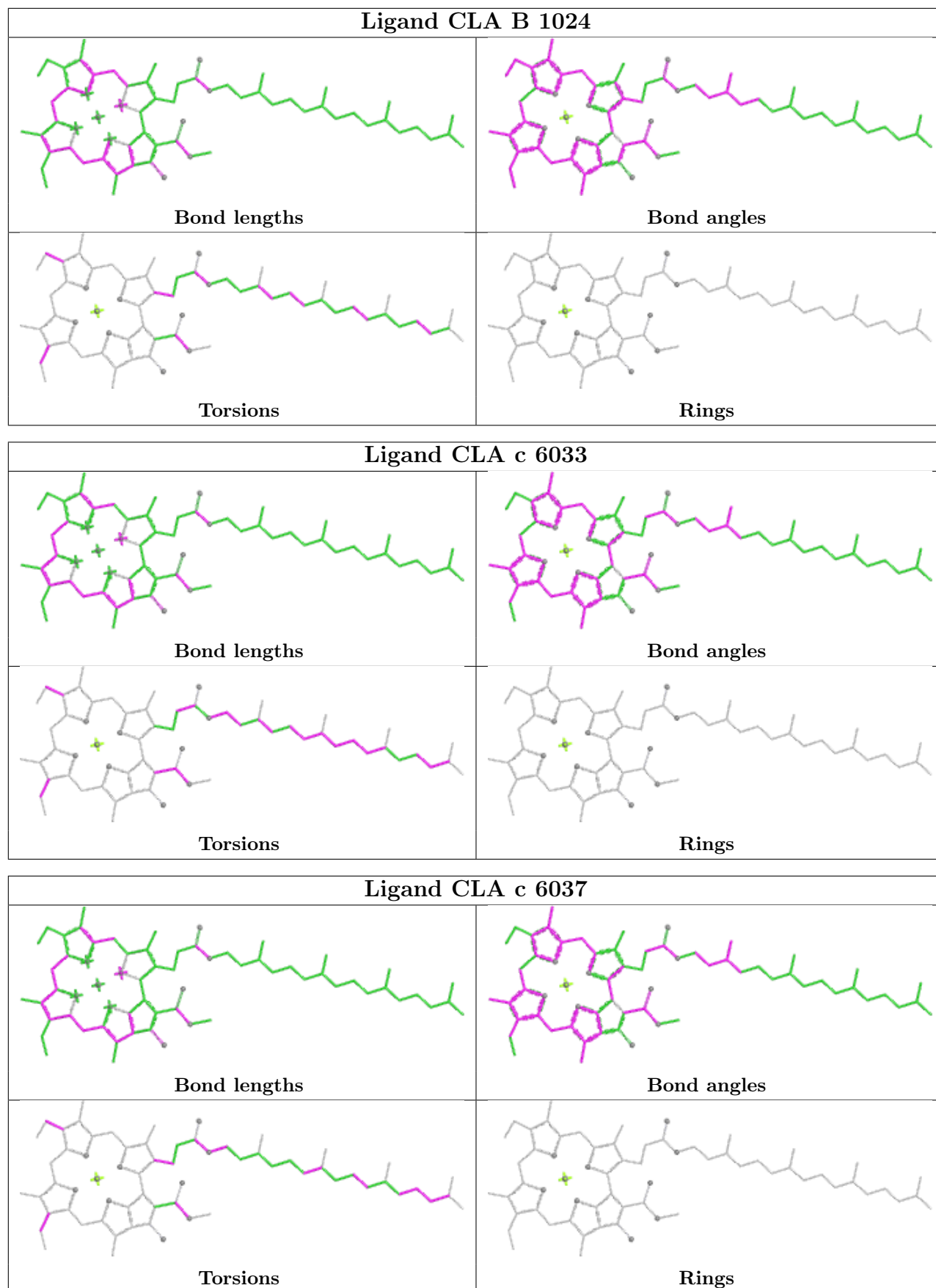


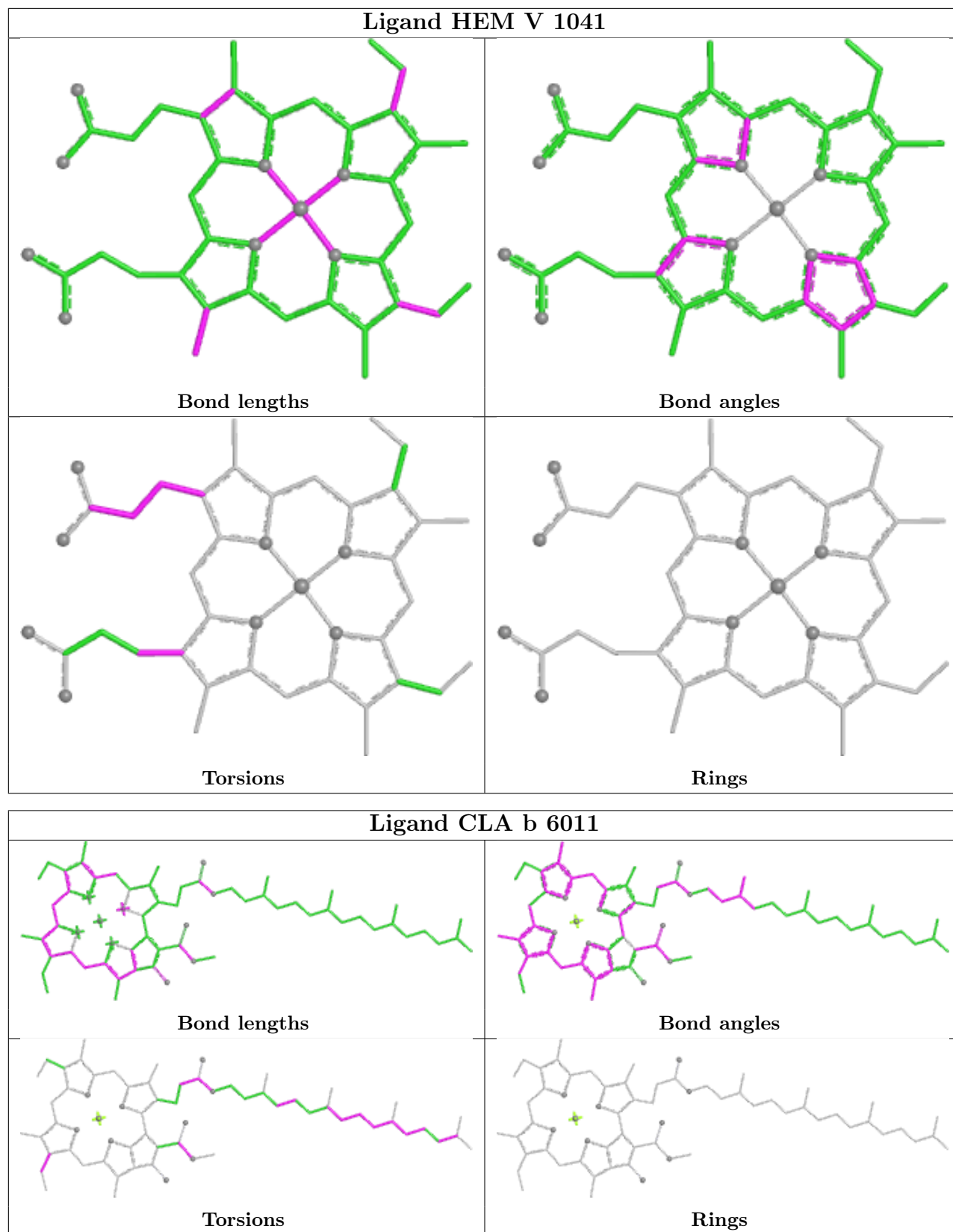


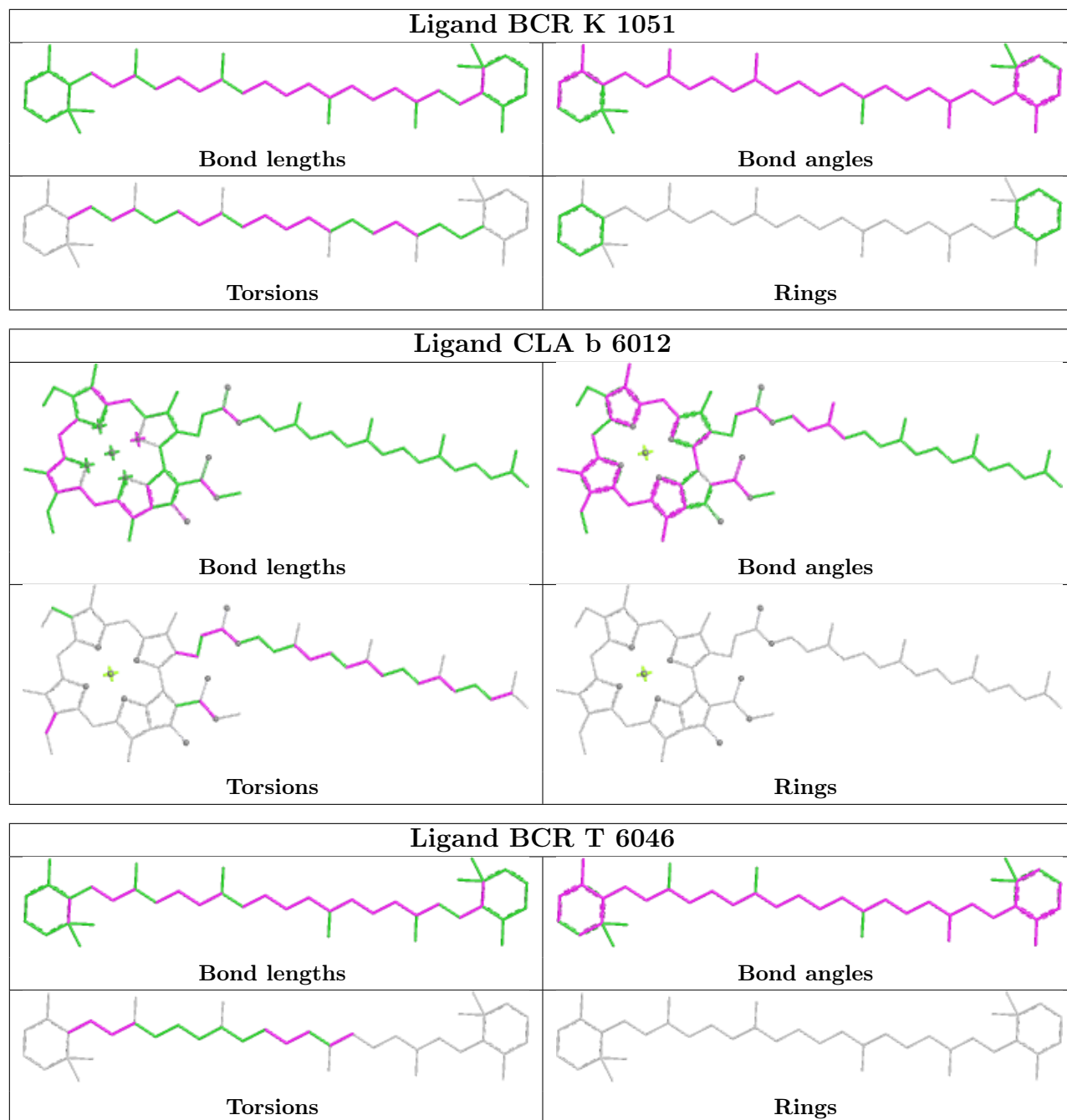


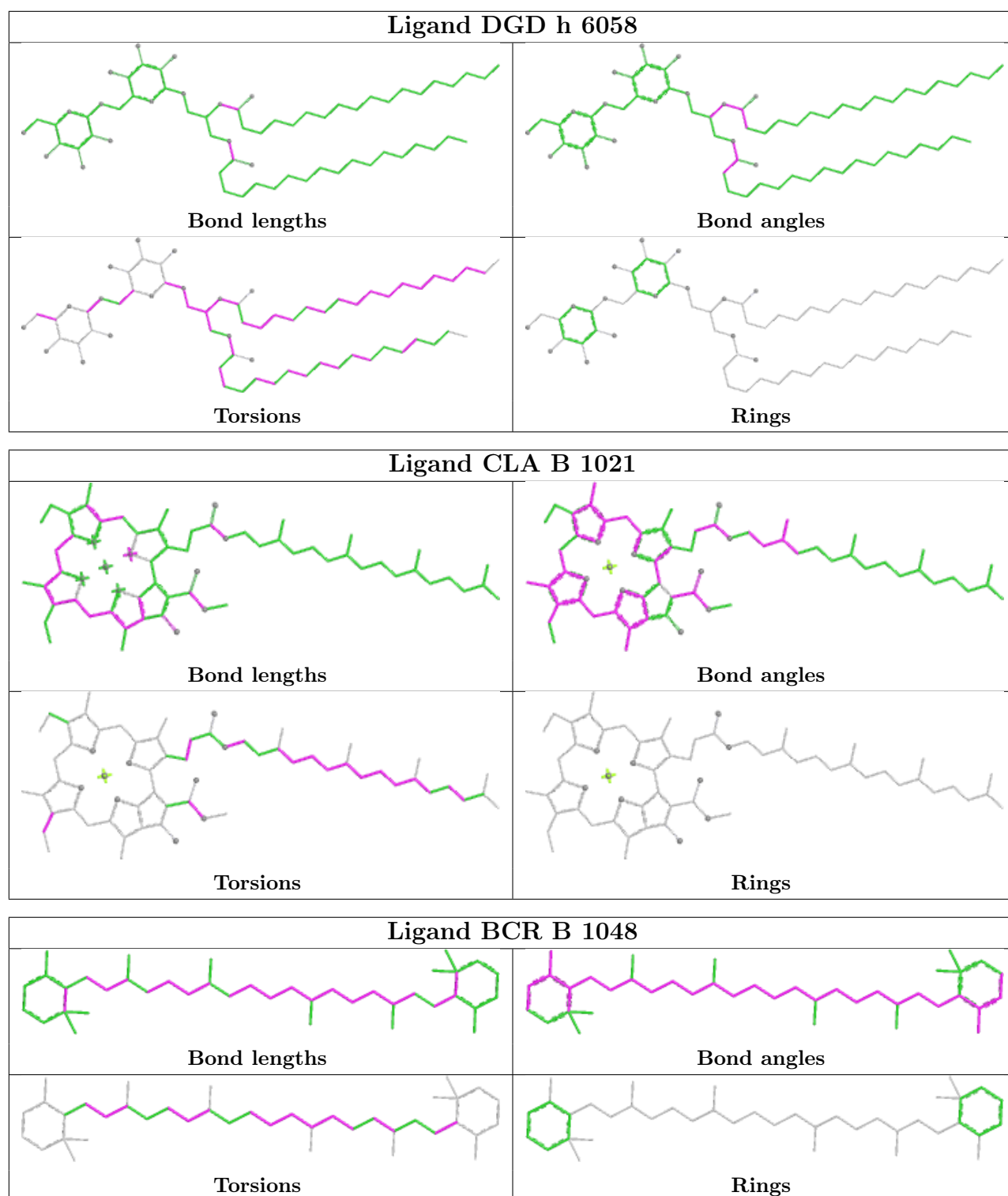


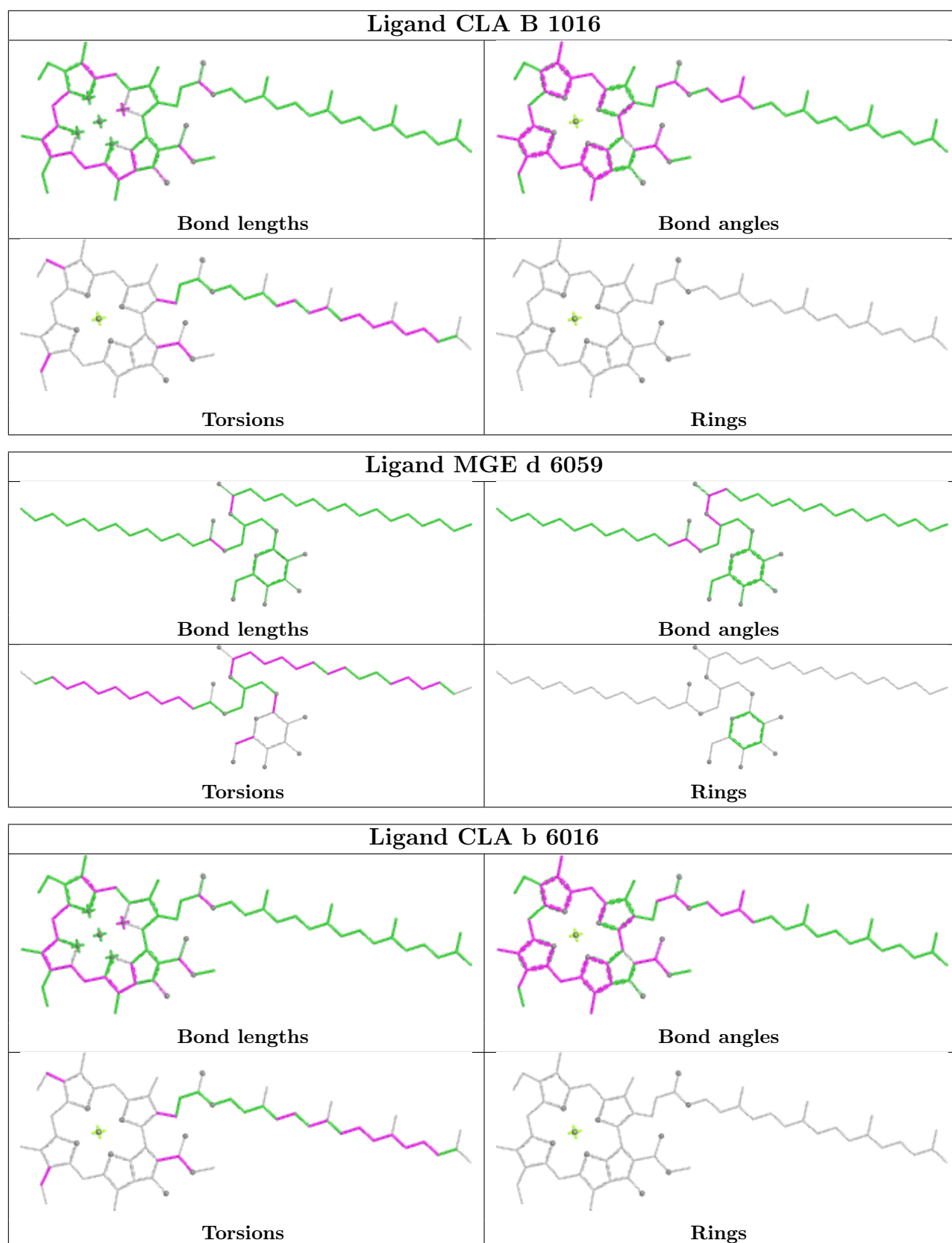


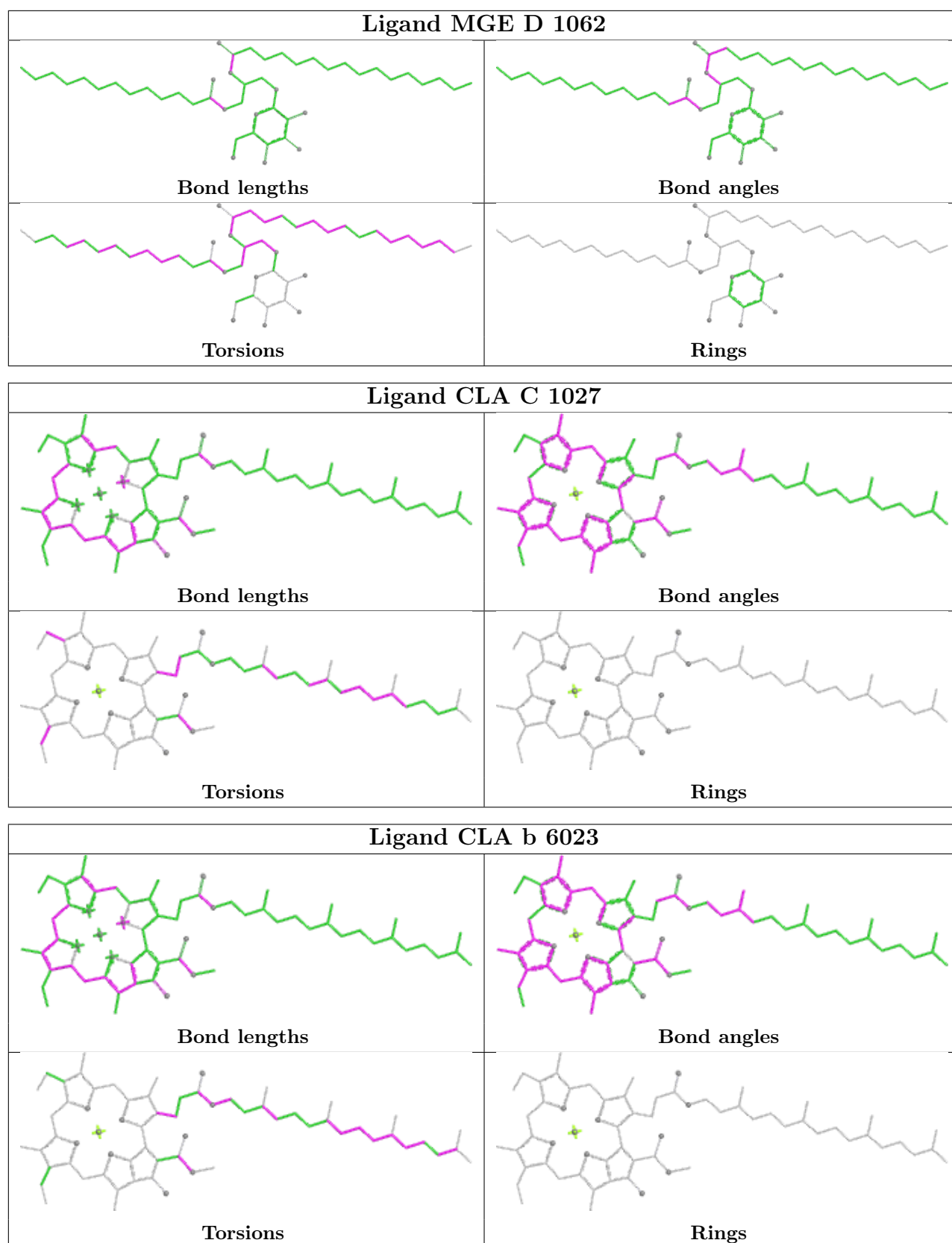


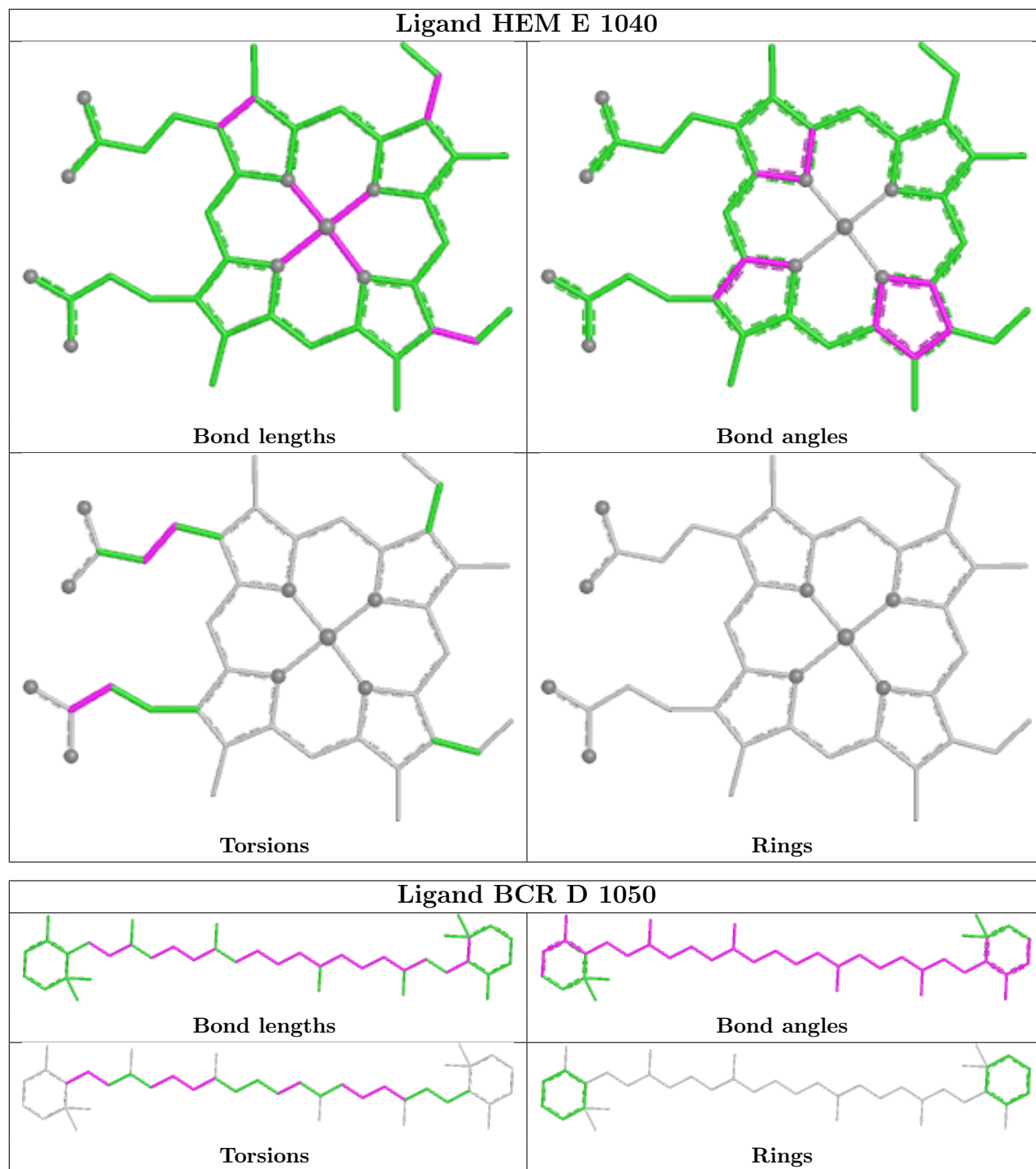


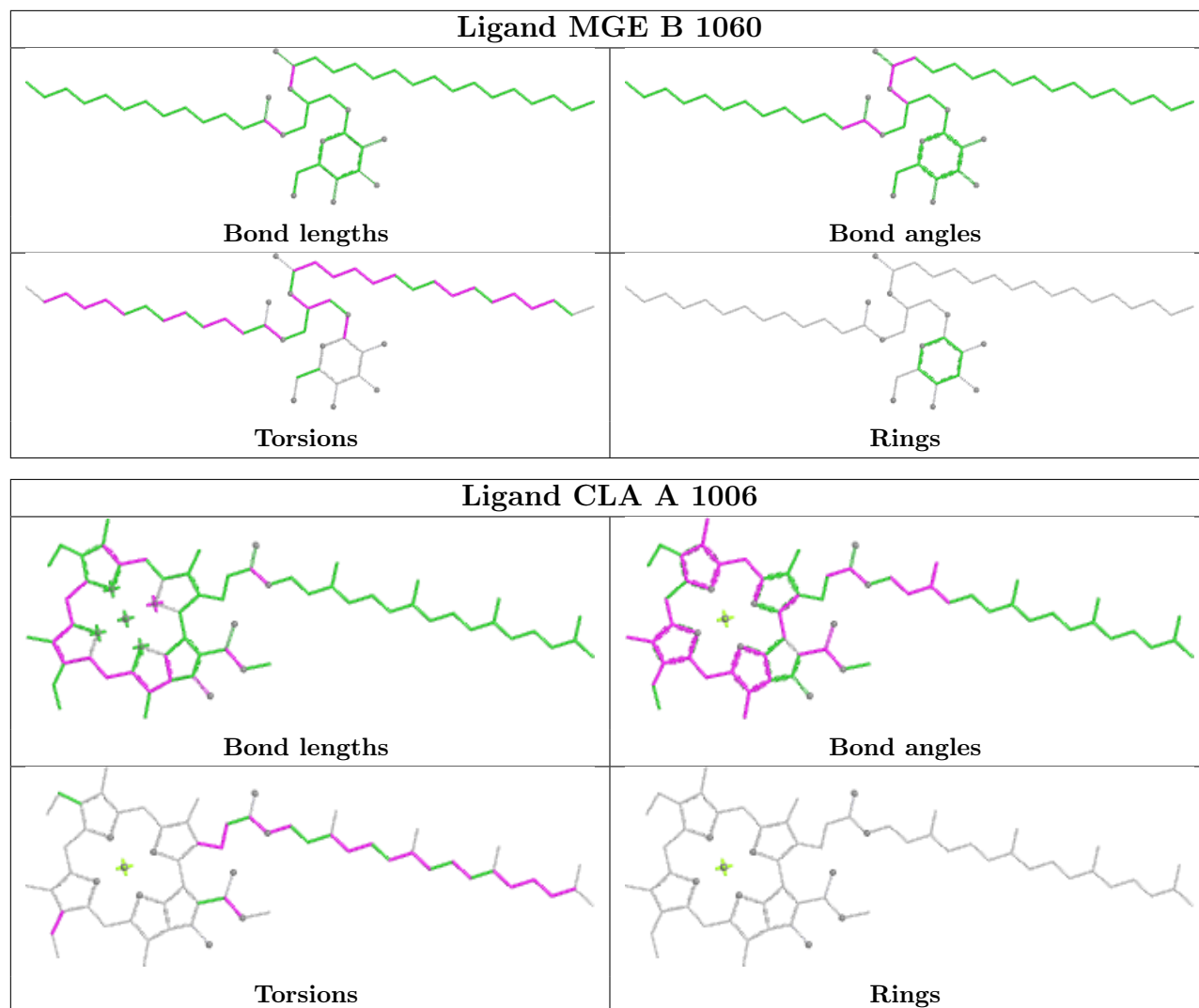


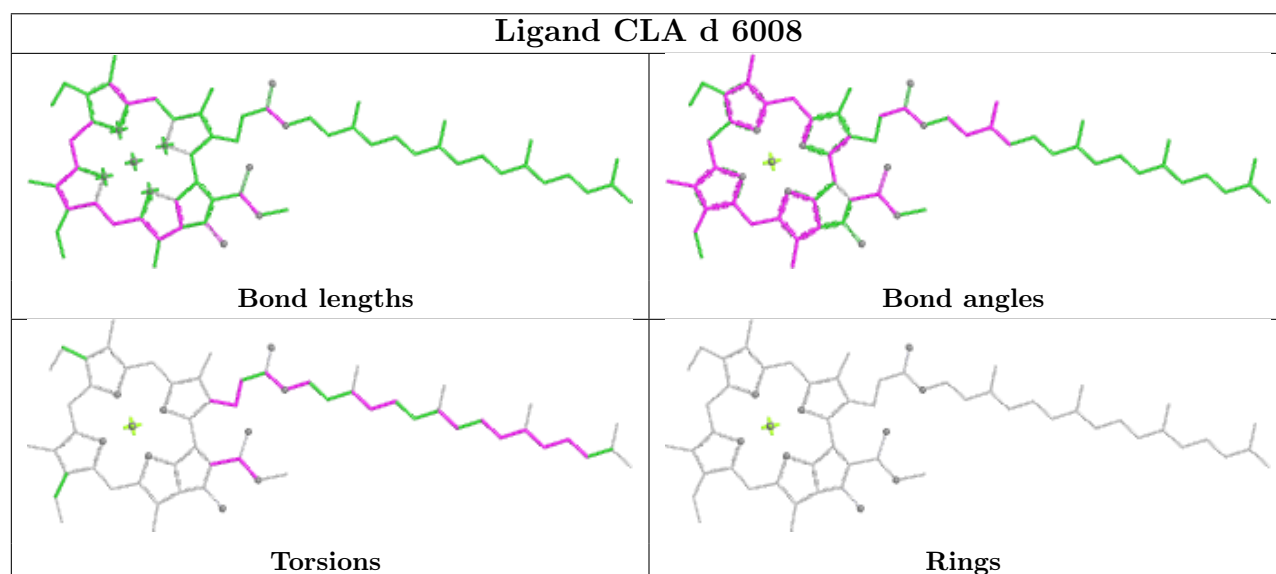
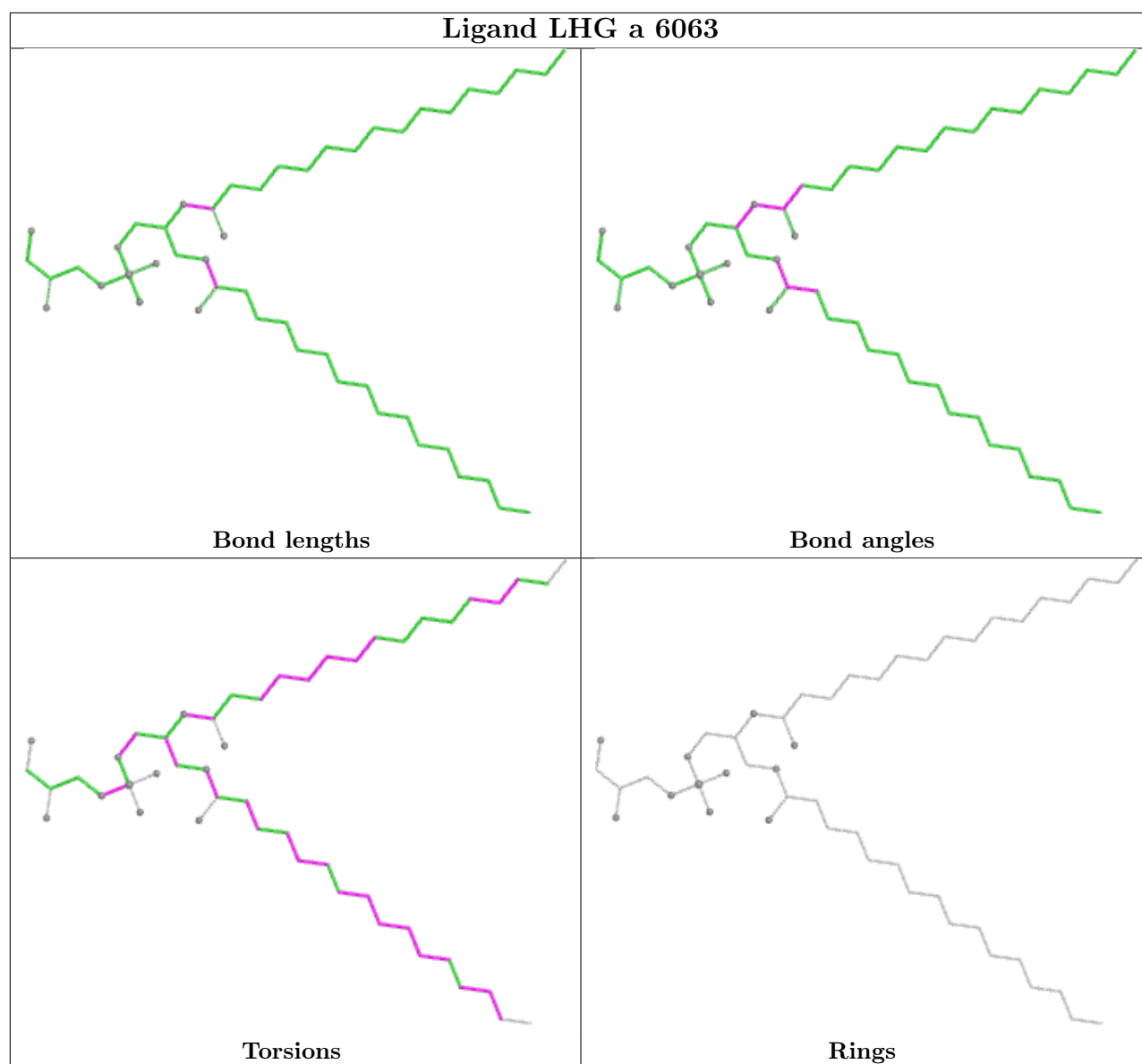


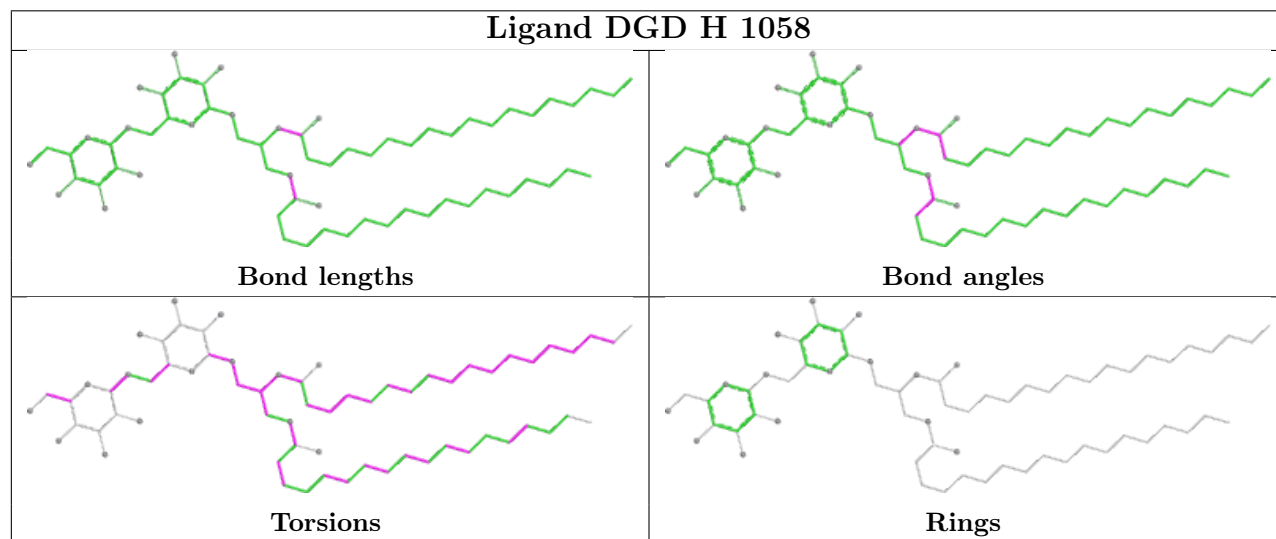
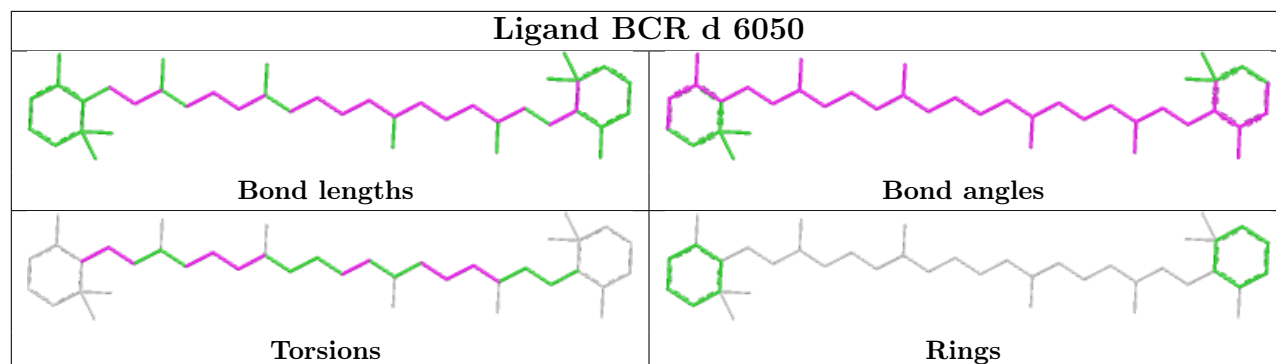


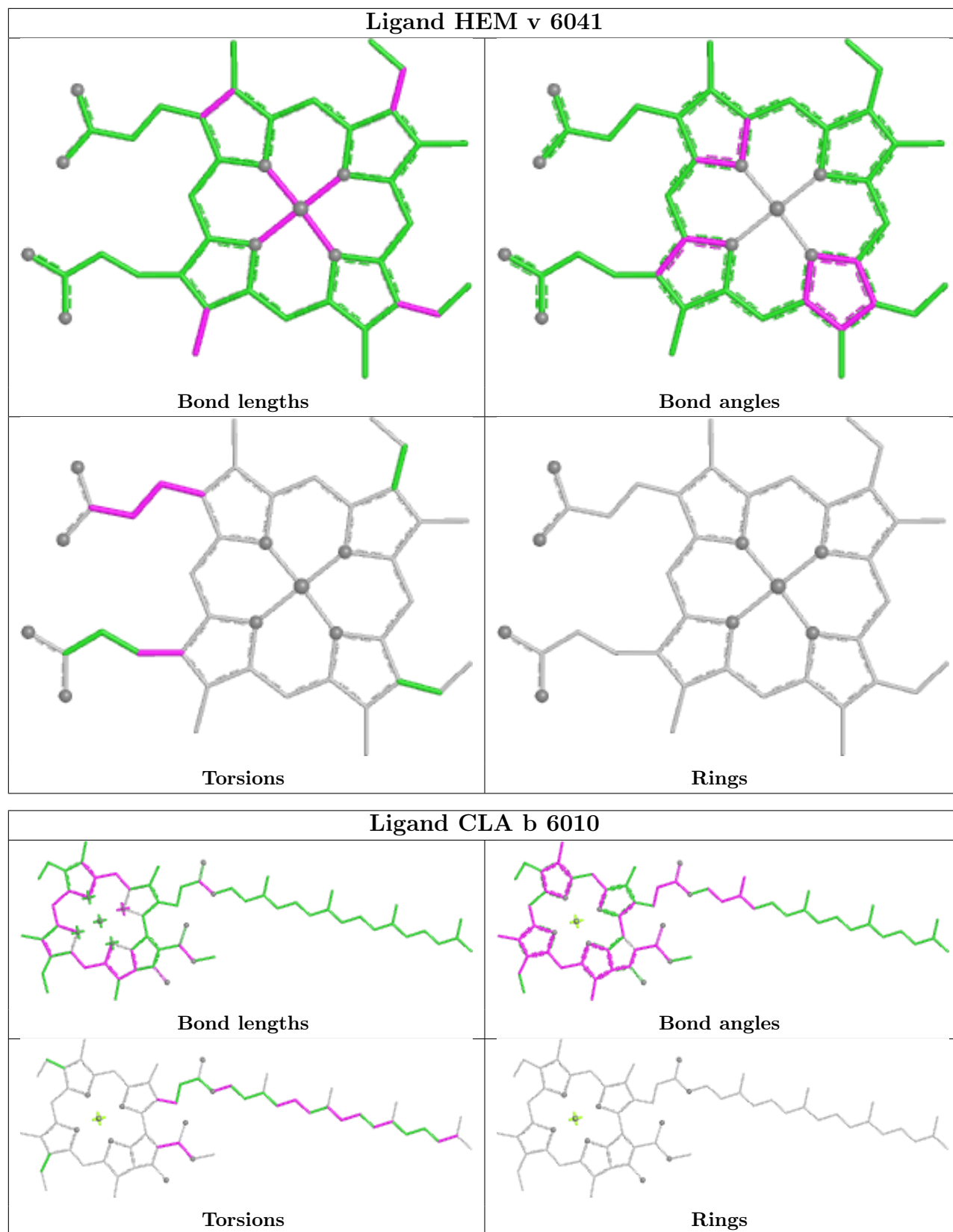


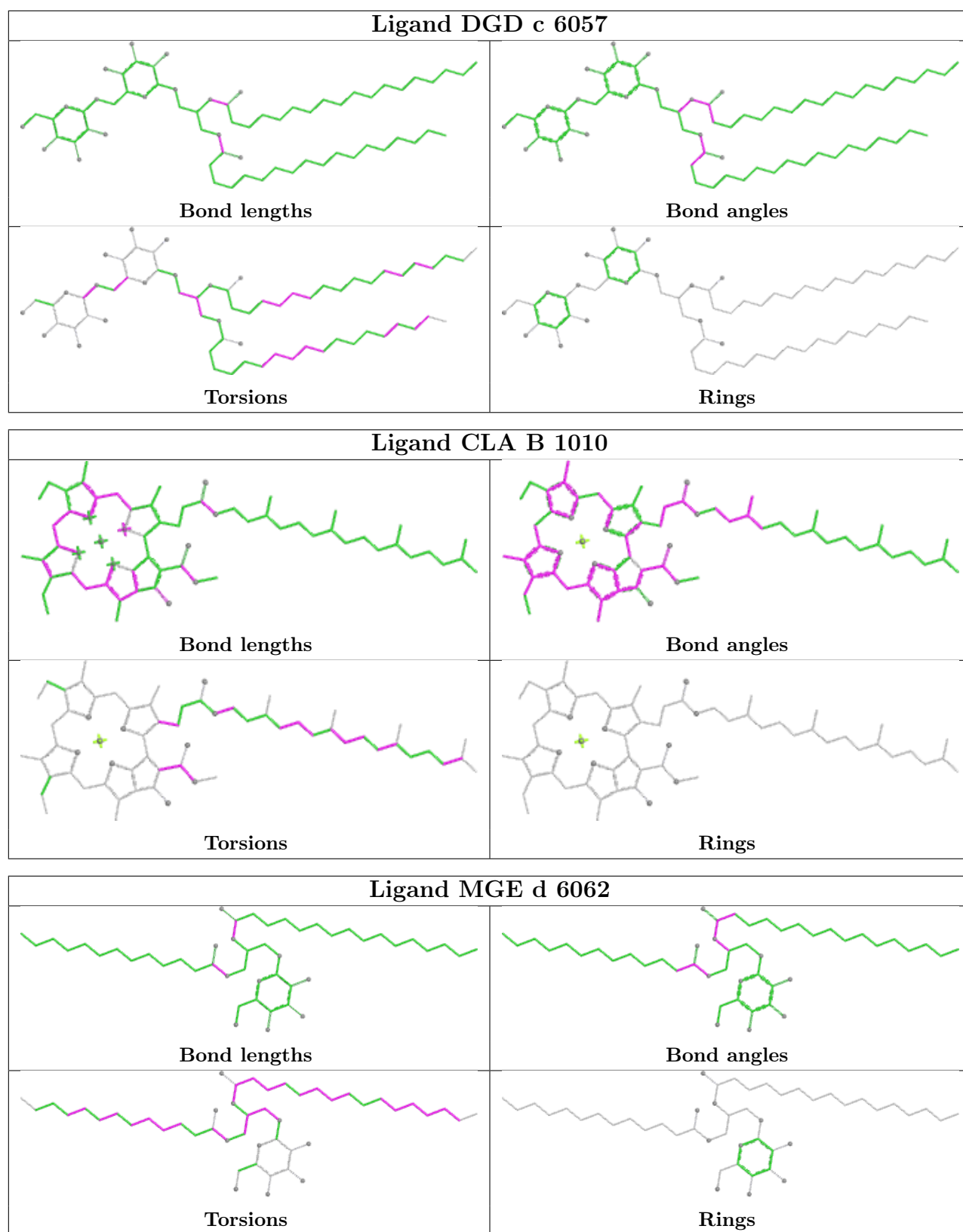


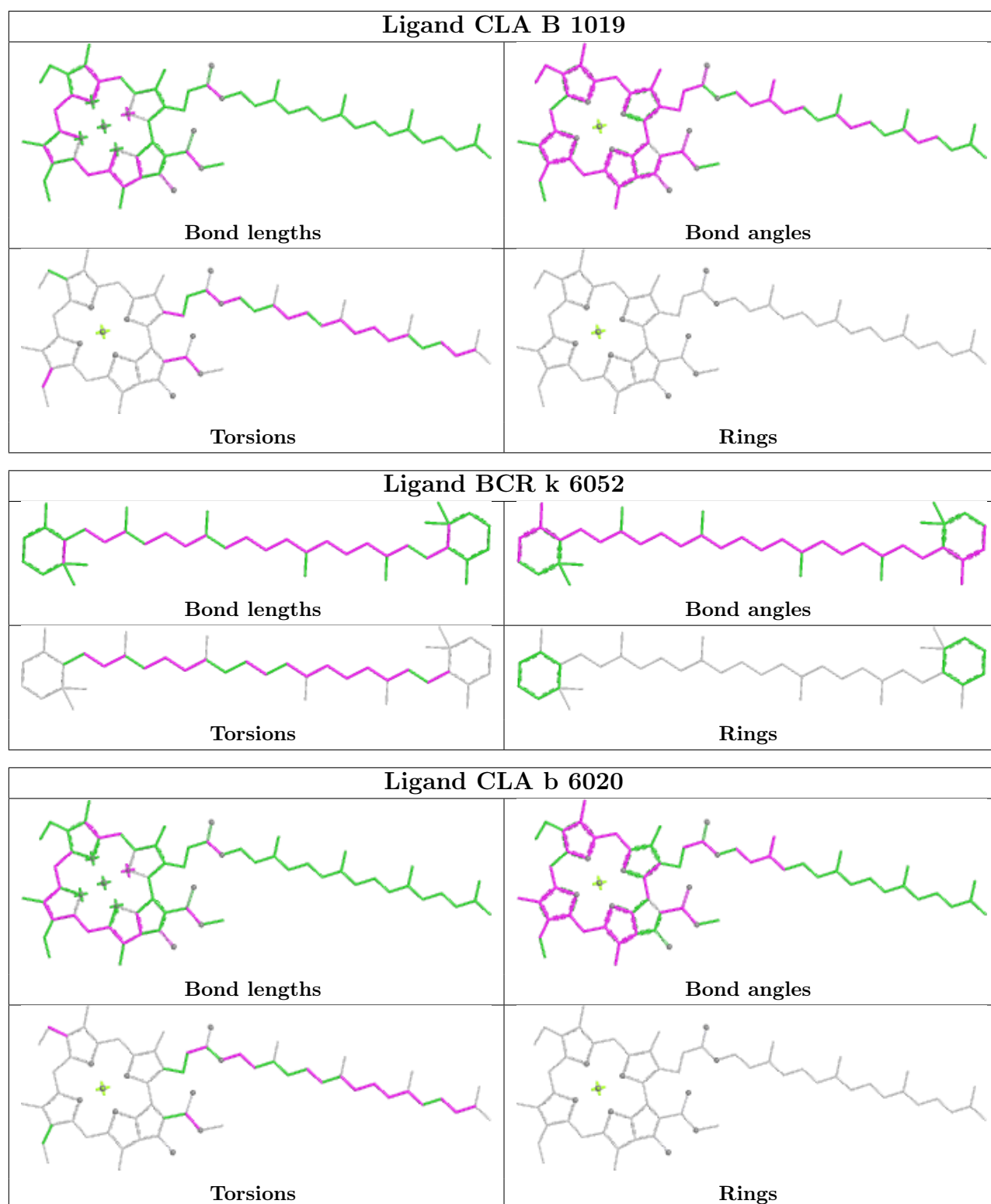












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	335/344 (97%)	-0.23	3 (0%) 81 58	97, 127, 162, 173	0
1	a	335/344 (97%)	-0.13	5 (1%) 72 46	101, 131, 166, 178	0
2	B	485/488 (99%)	-0.25	9 (1%) 66 42	94, 130, 157, 181	0
2	b	485/488 (99%)	-0.29	1 (0%) 91 80	102, 129, 161, 183	0
3	C	447/447 (100%)	-0.17	6 (1%) 75 50	100, 143, 170, 185	0
3	c	447/447 (100%)	-0.16	3 (0%) 84 63	102, 150, 173, 187	0
4	D	340/340 (100%)	-0.24	3 (0%) 81 58	94, 127, 165, 187	0
4	d	340/340 (100%)	-0.16	5 (1%) 72 46	92, 133, 172, 191	0
5	E	82/83 (98%)	-0.29	1 (1%) 76 51	117, 156, 184, 186	0
5	e	82/83 (98%)	-0.10	1 (1%) 76 51	126, 160, 181, 186	0
6	F	35/44 (79%)	-0.04	3 (8%) 16 14	139, 147, 160, 163	0
6	f	35/44 (79%)	-0.28	0 100 100	143, 152, 160, 163	0
7	H	64/64 (100%)	-0.35	0 100 100	119, 143, 165, 170	0
7	h	64/64 (100%)	-0.26	2 (3%) 51 32	120, 143, 164, 169	0
8	I	35/35 (100%)	-0.49	0 100 100	127, 137, 166, 173	0
8	i	35/35 (100%)	-0.53	0 100 100	124, 141, 175, 176	0
9	J	34/40 (85%)	-0.16	0 100 100	127, 142, 165, 175	0
9	j	34/40 (85%)	-0.24	0 100 100	131, 146, 172, 174	0
10	K	36/36 (100%)	-0.29	1 (2%) 55 34	132, 145, 153, 155	0
10	k	36/36 (100%)	-0.09	0 100 100	140, 151, 162, 164	0
11	L	37/37 (100%)	-0.26	0 100 100	102, 123, 178, 184	0
11	l	37/37 (100%)	-0.32	1 (2%) 56 35	110, 130, 181, 188	0
12	M	36/36 (100%)	-0.13	2 (5%) 30 20	101, 119, 171, 174	0
12	m	36/36 (100%)	-0.26	1 (2%) 55 34	100, 121, 171, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/242 (100%)	-0.15	4 (1%) 69 43	108, 133, 165, 186	0
13	o	242/242 (100%)	-0.16	2 (0%) 82 60	114, 139, 164, 186	0
14	T	30/30 (100%)	-0.40	0 100 100	105, 124, 173, 178	0
14	t	30/30 (100%)	-0.38	0 100 100	101, 115, 173, 181	0
15	U	98/98 (100%)	-0.38	0 100 100	108, 123, 143, 158	0
15	u	98/98 (100%)	-0.34	0 100 100	112, 128, 143, 167	0
16	V	137/137 (100%)	-0.13	5 (3%) 46 29	104, 131, 160, 170	0
16	v	137/137 (100%)	-0.20	0 100 100	114, 145, 165, 176	0
17	X	34/34 (100%)	-0.11	0 100 100	148, 155, 164, 170	0
17	x	34/34 (100%)	-0.28	1 (2%) 53 33	151, 159, 169, 175	0
18	Y	28/28 (100%)	-0.18	0 100 100	164, 178, 189, 192	0
18	y	28/28 (100%)	0.06	0 100 100	170, 181, 191, 196	0
19	N	0/24	-	-	-	-
19	n	0/24	-	-	-	-
20	Z	62/62 (100%)	-0.16	0 100 100	138, 161, 180, 186	0
20	z	62/62 (100%)	-0.24	0 100 100	144, 164, 184, 187	0
All	All	5194/5298 (98%)	-0.21	59 (1%) 78 53	92, 136, 172, 196	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	39	ALA	5.8
1	a	5279	ARG	5.8
4	D	95	PRO	5.5
11	l	5017	LEU	4.5
1	A	279	ARG	4.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	LHG	a	6063	49/49	0.61	0.18	186,196,200,200	0
27	LHG	A	1063	49/49	0.62	0.19	181,187,194,195	0
23	CLA	C	1034	65/65	0.68	0.20	134,147,172,174	0
30	DGD	C	1057	66/66	0.69	0.18	125,140,187,193	0
26	BCR	z	6053	40/40	0.70	0.14	159,176,186,187	0
23	CLA	c	6034	65/65	0.70	0.18	87,162,181,181	0
23	CLA	c	6027	65/65	0.72	0.19	178,195,198,200	0
26	BCR	b	6047	40/40	0.72	0.17	114,127,145,147	0
23	CLA	c	6037	65/65	0.73	0.13	184,188,191,200	0
23	CLA	B	1009	65/65	0.73	0.15	119,178,184,185	0
26	BCR	B	1047	40/40	0.74	0.15	101,136,157,157	0
26	BCR	d	6050	40/40	0.74	0.15	149,160,166,167	0
23	CLA	b	6009	65/65	0.76	0.13	160,177,200,200	0
26	BCR	h	6049	40/40	0.76	0.17	156,175,191,192	0
23	CLA	C	1037	65/65	0.77	0.15	180,185,188,200	0
26	BCR	b	6045	40/40	0.78	0.17	145,156,167,168	0
29	MGE	d	6059	48/48	0.78	0.15	164,168,198,200	0
26	BCR	a	6044	40/40	0.78	0.21	154,160,163,166	0
26	BCR	A	1044	40/40	0.79	0.17	147,156,158,159	0
30	DGD	C	1056	66/66	0.79	0.16	155,171,183,188	0
26	BCR	D	1050	40/40	0.79	0.15	149,153,161,162	0
23	CLA	C	1032	65/65	0.80	0.19	153,166,174,176	0
26	BCR	b	6048	40/40	0.80	0.16	141,147,158,159	0
30	DGD	c	6057	66/66	0.80	0.13	128,149,183,184	0
23	CLA	B	1024	65/65	0.81	0.13	105,177,179,180	0
26	BCR	t	1046	40/40	0.82	0.14	144,156,163,163	0
23	CLA	c	6032	65/65	0.82	0.15	144,175,181,182	0
23	CLA	C	1025	65/65	0.82	0.20	131,170,180,200	0
30	DGD	c	6056	66/66	0.82	0.14	170,175,181,183	0
26	BCR	Z	1053	40/40	0.82	0.16	141,166,178,178	0
23	CLA	b	6024	65/65	0.83	0.14	172,183,186,187	0
29	MGE	d	6062	48/48	0.83	0.17	130,155,167,168	0
29	MGE	J	1059	48/48	0.83	0.12	152,158,185,186	0
23	CLA	b	6014	65/65	0.84	0.14	163,171,179,200	0
26	BCR	B	1045	40/40	0.84	0.16	146,156,169,170	0
23	CLA	C	1027	65/65	0.84	0.15	167,183,190,200	0
26	BCR	B	1048	40/40	0.84	0.14	148,155,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	PHO	d	6038	64/64	0.84	0.17	136,147,150,150	0
26	BCR	T	6046	40/40	0.84	0.15	140,149,154,157	0
29	MGE	d	6061	48/48	0.85	0.19	141,152,165,169	0
23	CLA	c	6025	65/65	0.85	0.16	145,170,178,200	0
26	BCR	c	6054	40/40	0.85	0.18	174,177,183,183	0
23	CLA	d	6008	65/65	0.85	0.17	172,175,185,200	0
26	BCR	K	1051	40/40	0.85	0.23	175,179,182,183	0
23	CLA	c	6031	65/65	0.85	0.15	173,182,185,186	0
23	CLA	c	6033	65/65	0.86	0.16	84,142,180,180	0
25	PQ9	d	6042	45/45	0.86	0.25	137,146,167,168	0
23	CLA	B	1014	65/65	0.86	0.12	123,169,174,176	0
29	MGE	B	1060	48/48	0.86	0.18	151,170,182,184	0
23	CLA	c	6036	65/65	0.87	0.13	177,180,184,200	0
29	MGE	L	1061	48/48	0.87	0.20	141,144,154,155	0
29	MGE	b	6060	48/48	0.87	0.21	158,178,191,192	0
23	CLA	B	1022	65/65	0.87	0.12	135,155,159,161	0
26	BCR	k	6052	40/40	0.87	0.24	158,179,200,200	0
23	CLA	C	1033	65/65	0.87	0.14	117,131,162,164	0
23	CLA	b	6021	65/65	0.87	0.14	125,132,157,160	0
25	PQ9	A	1043	45/45	0.87	0.34	138,151,171,171	30
26	BCR	H	1049	40/40	0.87	0.16	155,162,188,188	0
23	CLA	c	6030	65/65	0.87	0.12	100,154,174,175	0
23	CLA	C	1028	65/65	0.88	0.14	141,154,159,168	0
23	CLA	c	6029	65/65	0.88	0.15	151,170,173,200	0
23	CLA	b	6022	65/65	0.88	0.10	133,148,156,157	0
23	CLA	b	6013	65/65	0.88	0.15	139,154,161,172	0
23	CLA	a	6003	65/65	0.88	0.18	121,130,145,193	0
23	CLA	b	6023	65/65	0.89	0.14	149,183,189,190	0
23	CLA	c	6035	65/65	0.89	0.18	170,173,177,200	0
23	CLA	C	1036	65/65	0.89	0.12	162,166,179,200	0
23	CLA	b	6011	65/65	0.89	0.14	156,159,165,170	0
26	BCR	K	1052	40/40	0.89	0.25	153,171,178,179	0
23	CLA	b	6012	65/65	0.89	0.17	146,153,159,198	0
24	PHO	A	1038	64/64	0.89	0.14	122,144,147,148	0
24	PHO	a	6039	64/64	0.89	0.15	151,165,169,170	0
23	CLA	c	6028	65/65	0.89	0.14	147,157,160,162	0
23	CLA	C	1029	65/65	0.89	0.13	146,156,159,200	0
25	PQ9	a	6043	45/45	0.89	0.31	135,149,185,185	30
23	CLA	C	1026	65/65	0.89	0.13	128,133,146,149	0
23	CLA	b	6015	65/65	0.89	0.15	137,149,155,164	0
30	DGD	c	6055	66/66	0.89	0.15	147,153,165,166	0
23	CLA	a	6006	65/65	0.89	0.11	140,145,197,200	0

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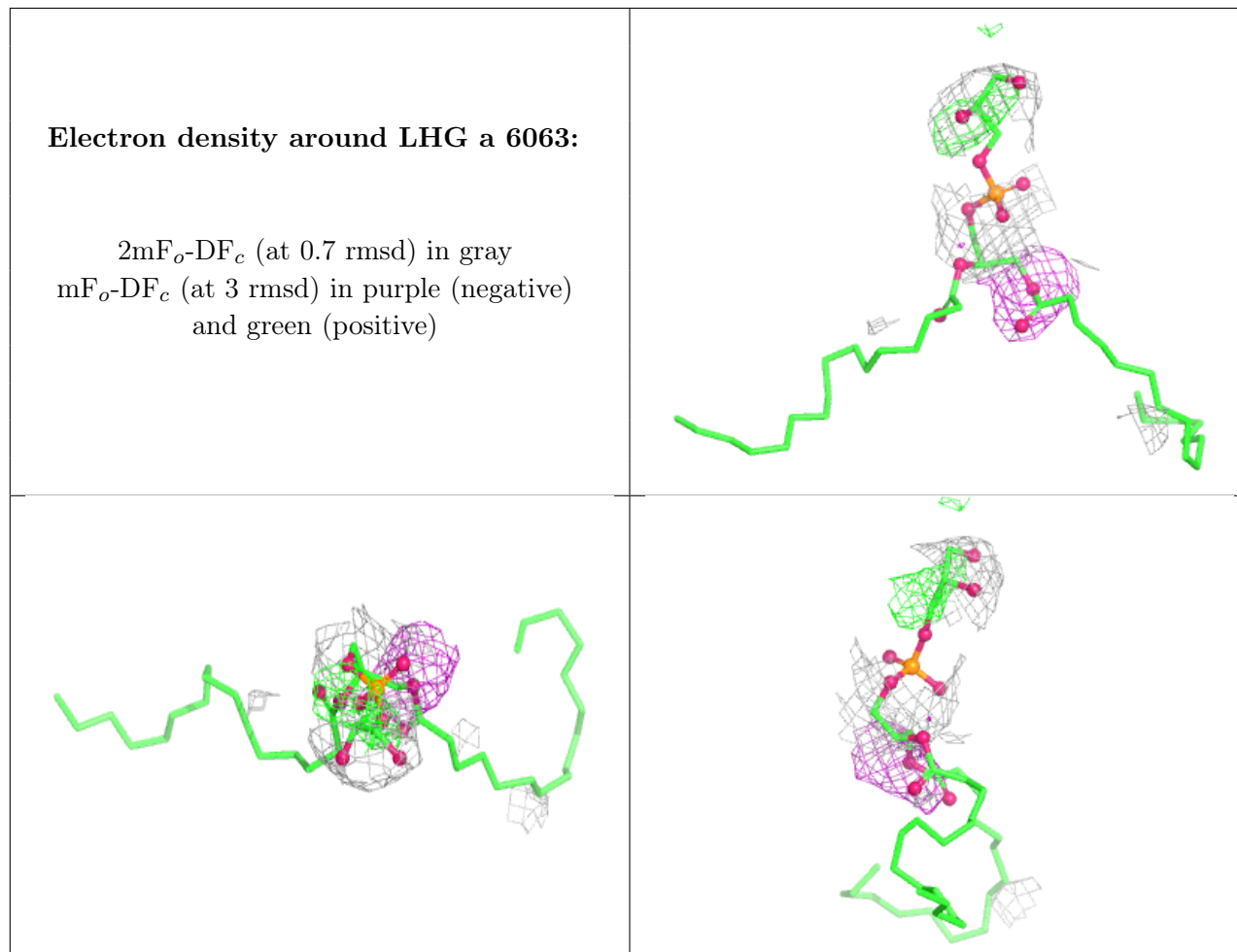
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	a	6007	65/65	0.89	0.17	143,149,179,183	0
30	DGD	h	6058	66/66	0.89	0.19	140,153,163,170	0
31	HEM	e	6040	43/43	0.89	0.16	171,184,185,185	0
23	CLA	A	1007	65/65	0.90	0.13	137,141,171,183	0
23	CLA	B	1015	65/65	0.90	0.12	133,146,153,175	0
23	CLA	B	1016	65/65	0.90	0.12	87,143,150,150	0
23	CLA	A	1003	65/65	0.90	0.18	122,129,147,149	0
30	DGD	C	1055	66/66	0.90	0.19	131,140,147,152	0
23	CLA	D	1008	65/65	0.90	0.15	159,167,182,200	0
23	CLA	B	1023	65/65	0.90	0.15	155,179,185,200	0
30	DGD	H	1058	66/66	0.90	0.18	131,150,165,166	0
23	CLA	B	1013	65/65	0.90	0.14	131,157,165,168	0
23	CLA	d	6005	65/65	0.90	0.12	90,100,117,118	0
29	MGE	D	1062	48/48	0.90	0.17	129,148,165,165	0
23	CLA	b	6016	65/65	0.90	0.14	76,148,153,155	0
23	CLA	b	6020	65/65	0.90	0.17	75,148,170,173	0
23	CLA	B	1020	65/65	0.91	0.15	113,151,177,179	0
23	CLA	C	1030	65/65	0.91	0.11	92,145,175,176	0
23	CLA	C	1031	65/65	0.91	0.17	164,170,179,200	0
23	CLA	A	1006	65/65	0.91	0.14	119,124,190,192	0
31	HEM	E	1040	43/43	0.91	0.21	141,181,194,198	0
26	BCR	C	1054	40/40	0.91	0.15	158,165,169,170	0
23	CLA	b	6018	65/65	0.92	0.15	142,154,162,165	0
23	CLA	b	6019	65/65	0.92	0.10	124,150,155,193	0
23	CLA	B	1021	65/65	0.92	0.10	104,129,142,146	0
23	CLA	H	1017	65/65	0.92	0.12	116,169,174,200	0
23	CLA	B	1012	65/65	0.92	0.14	148,152,159,176	0
24	PHO	A	1039	64/64	0.92	0.13	149,151,160,161	0
23	CLA	C	1035	65/65	0.92	0.18	155,167,173,200	0
23	CLA	B	1019	65/65	0.92	0.09	121,156,158,200	0
23	CLA	B	1010	65/65	0.92	0.15	115,164,166,169	0
26	BCR	k	6051	40/40	0.92	0.15	187,193,197,197	0
23	CLA	c	6026	65/65	0.92	0.11	140,144,157,170	0
23	CLA	D	1004	65/65	0.93	0.16	101,131,139,142	0
23	CLA	D	1005	65/65	0.93	0.10	101,108,116,157	0
23	CLA	b	6017	65/65	0.93	0.12	118,165,168,200	0
23	CLA	B	1011	65/65	0.93	0.13	144,159,161,166	0
28	BR	a	6065	1/1	0.93	0.09	164,164,164,164	0
28	BR	d	6064	1/1	0.93	0.07	130,130,130,130	0
25	PQ9	D	1042	45/45	0.94	0.18	131,145,154,155	0
23	CLA	d	6004	65/65	0.94	0.14	111,128,134,134	0
23	CLA	B	1018	65/65	0.94	0.13	111,158,165,168	0

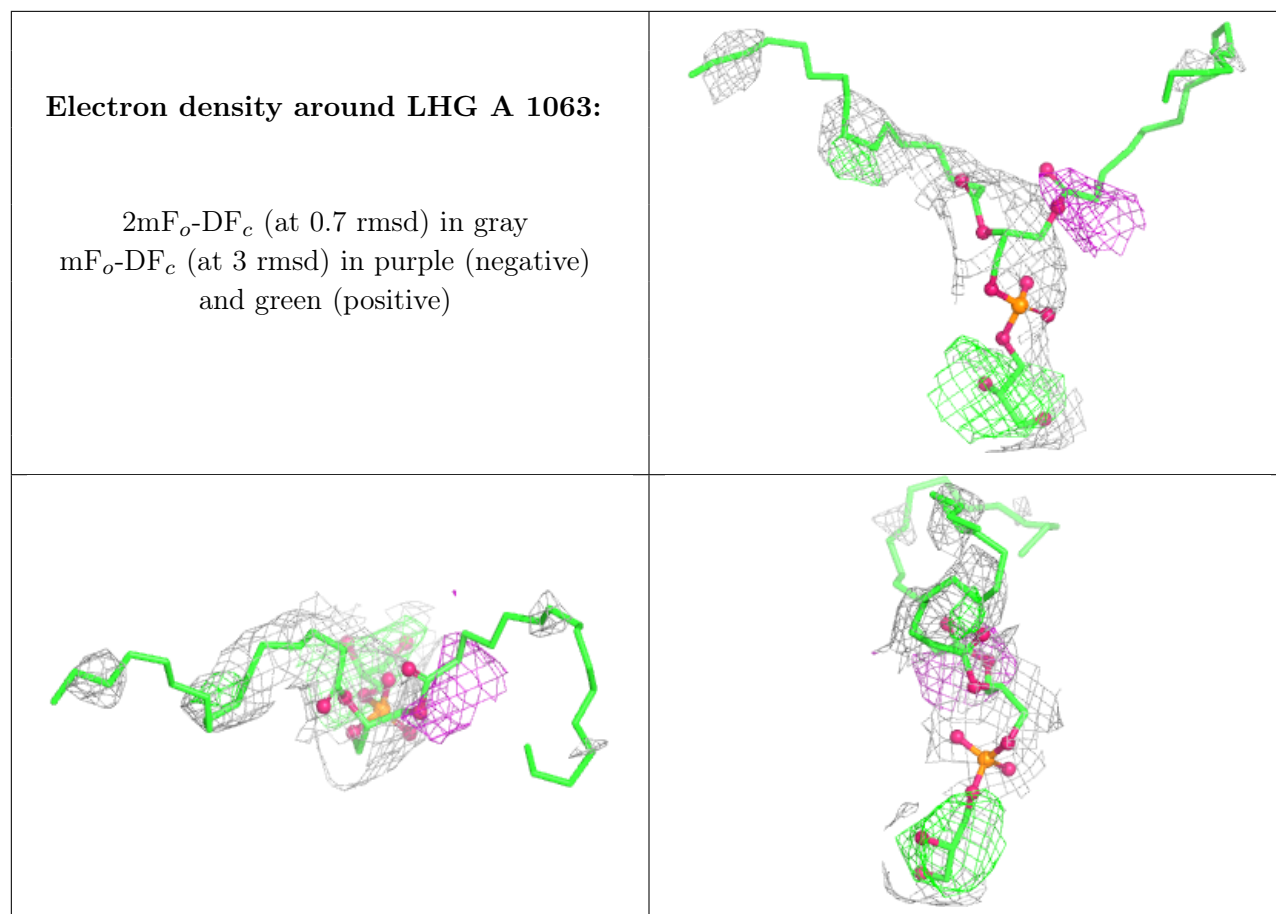
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	BR	A	1064	1/1	0.94	0.10	113,113,113,113	0
23	CLA	b	6010	65/65	0.95	0.12	93,165,169,170	0
22	FE2	a	6002	1/1	0.95	0.04	149,149,149,149	0
28	BR	A	1065	1/1	0.96	0.06	158,158,158,158	0
31	HEM	v	6041	43/43	0.96	0.14	99,135,139,140	0
22	FE2	A	1002	1/1	0.97	0.09	125,125,125,125	0
31	HEM	V	1041	43/43	0.97	0.16	81,131,132,133	0
21	OEC	a	6001	5/9	0.98	0.11	87,94,106,107	0
21	OEC	A	1001	5/9	0.99	0.09	79,94,115,119	0

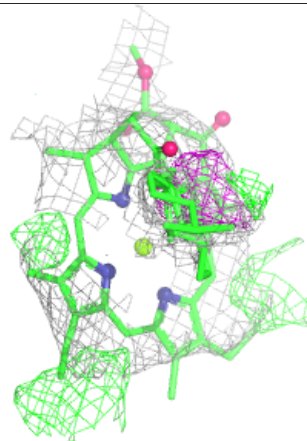
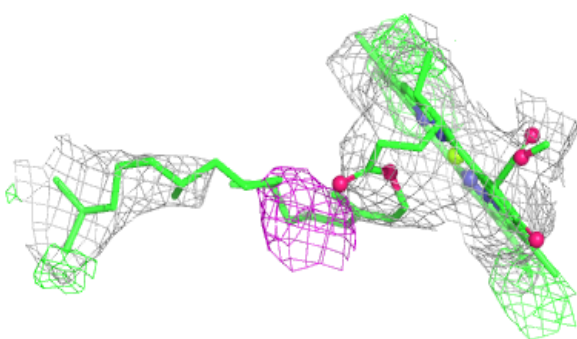
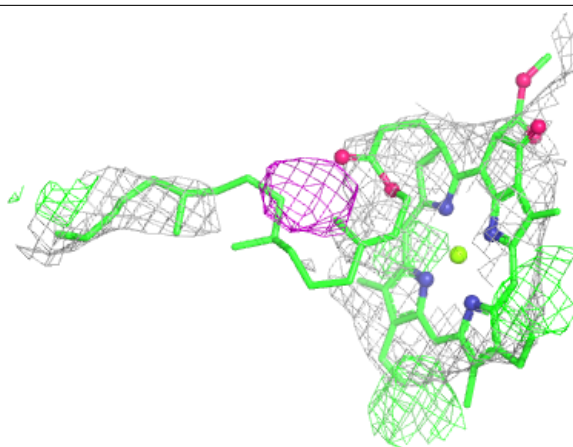
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



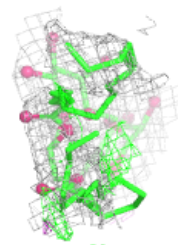
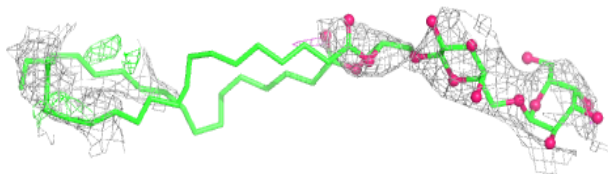
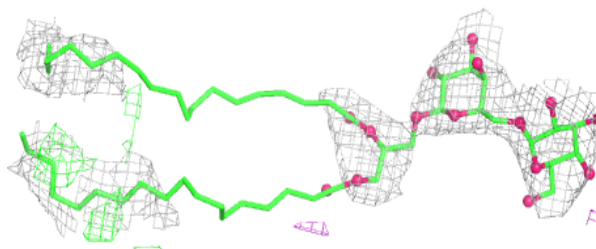


Electron density around CLA C 1034:

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

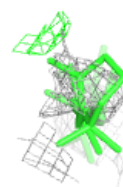
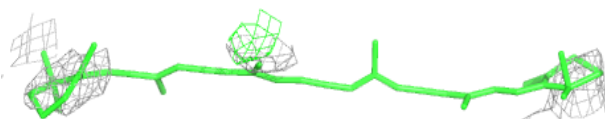
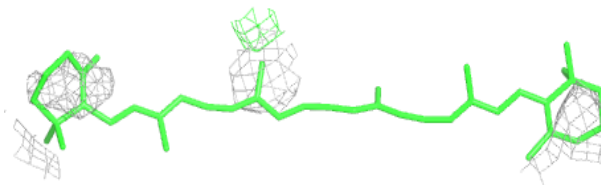
**Electron density around DGD C 1057:**

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

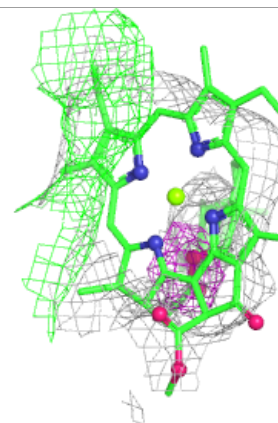
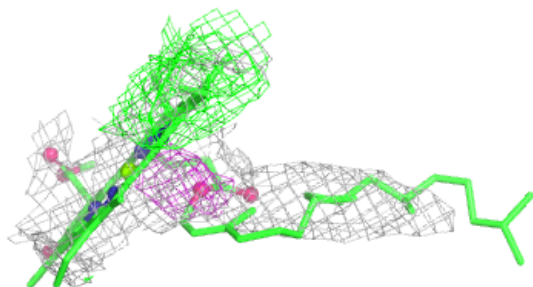
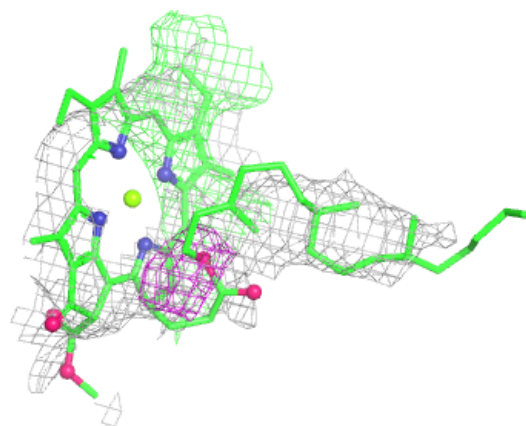


Electron density around BCR z 6053:

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

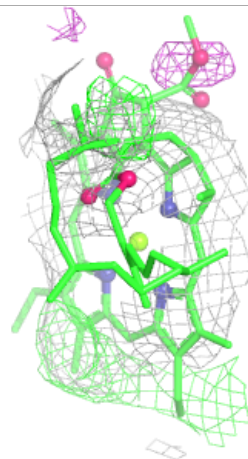
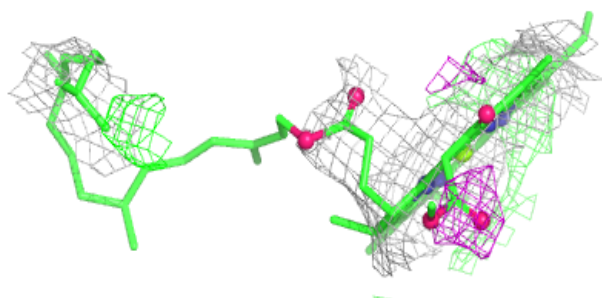
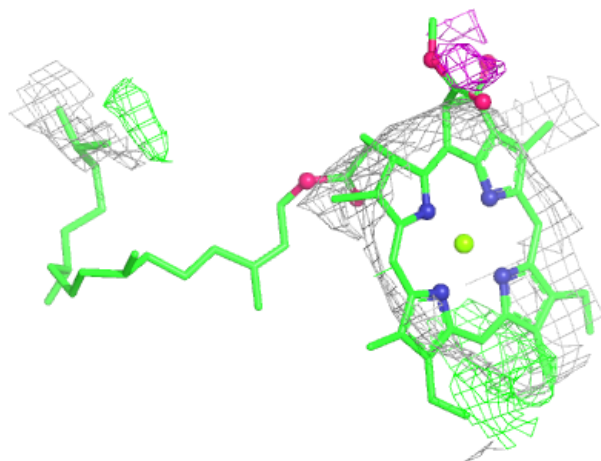
**Electron density around CLA c 6034:**

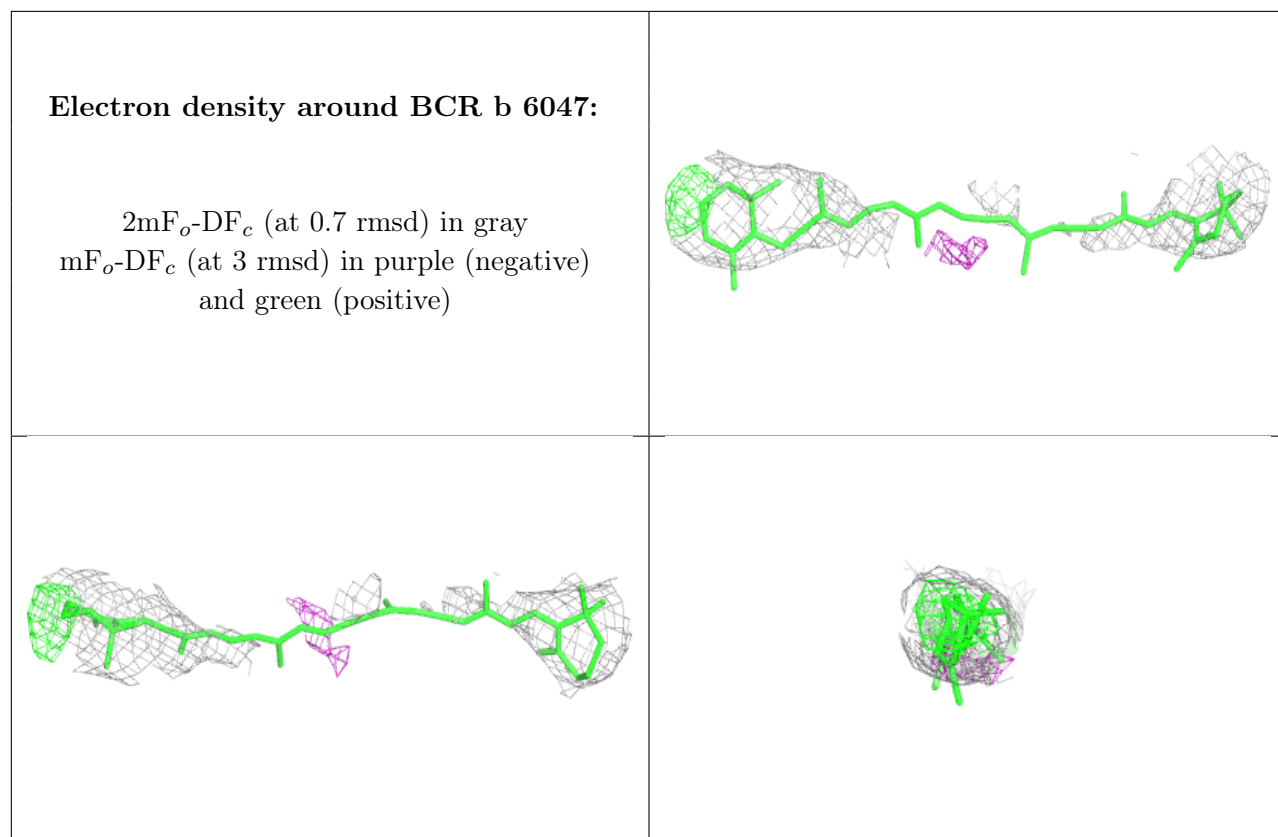
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 6027:

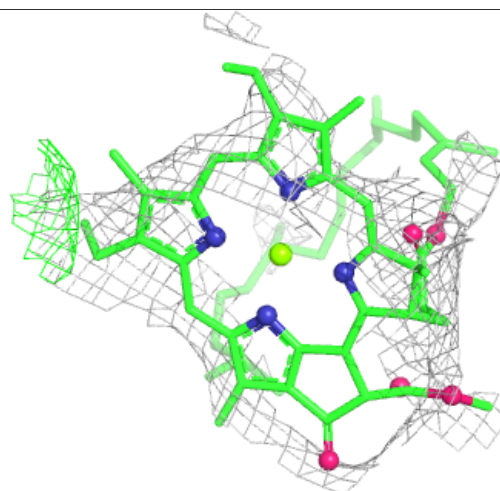
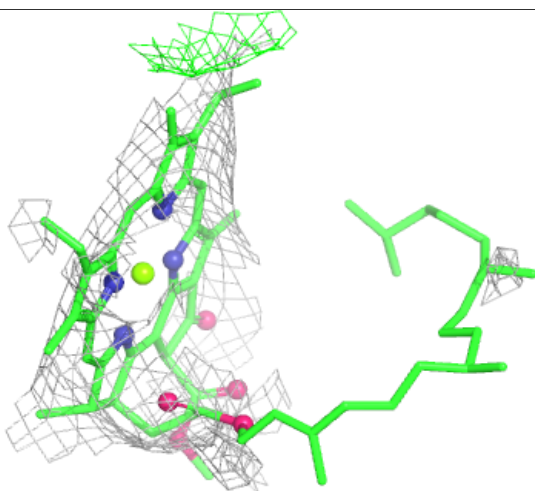
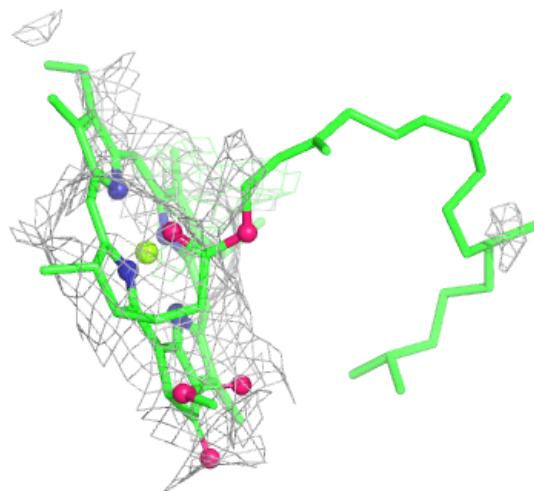
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





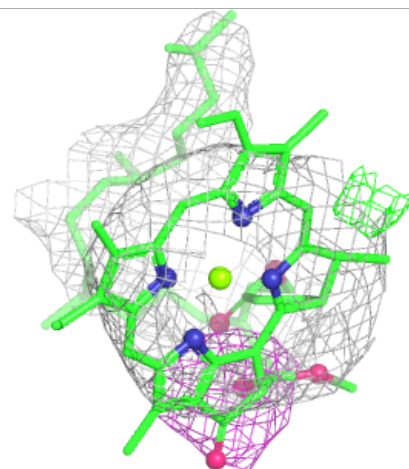
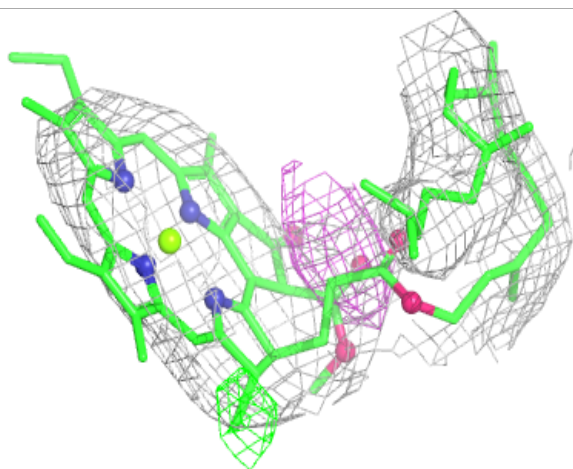
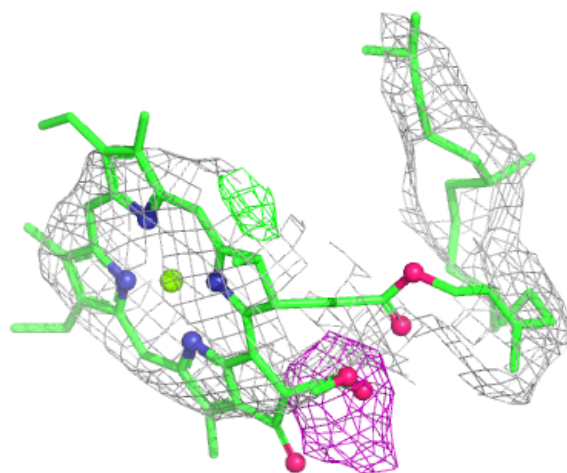
Electron density around CLA c 6037:

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



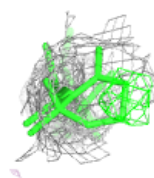
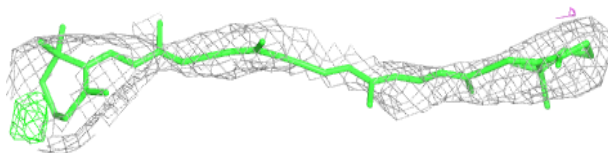
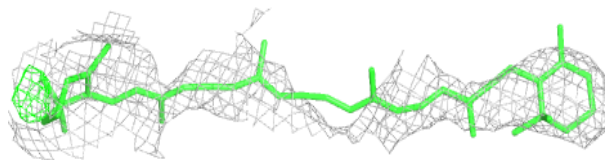
Electron density around CLA B 1009:

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

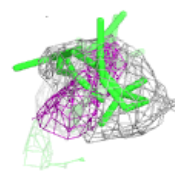
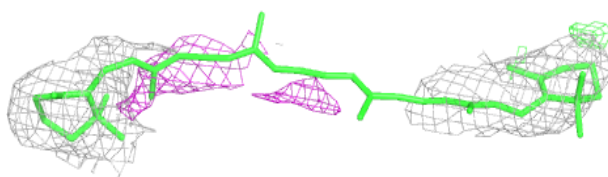
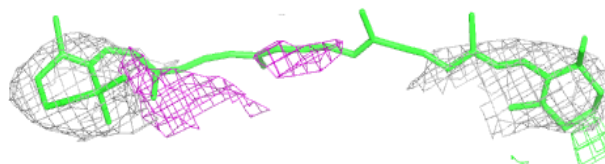


Electron density around BCR B 1047:

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

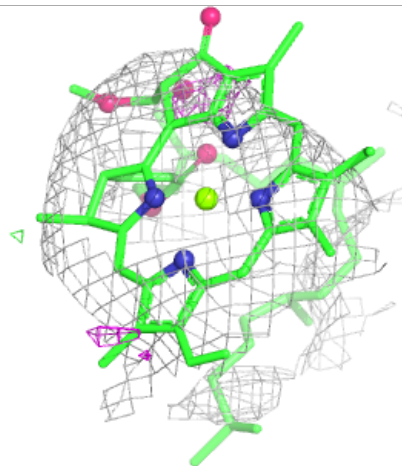
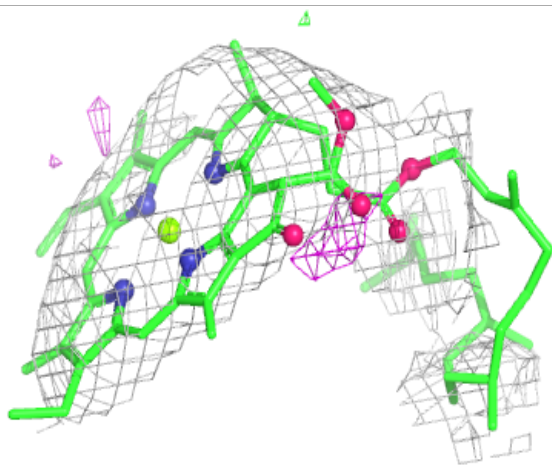
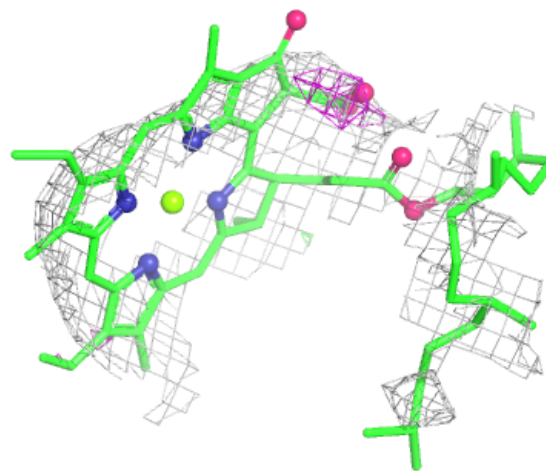
**Electron density around BCR d 6050:**

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



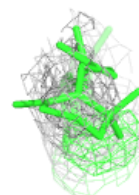
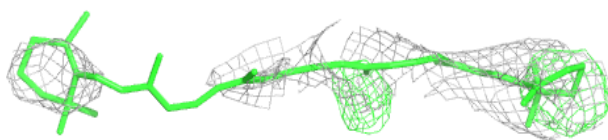
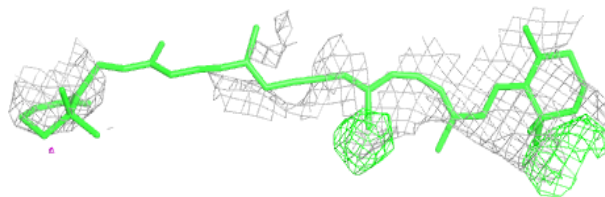
Electron density around CLA b 6009:

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

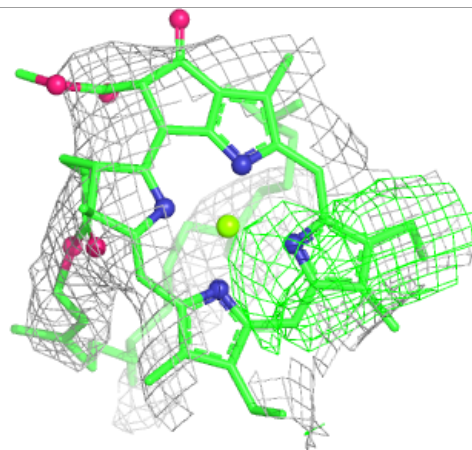
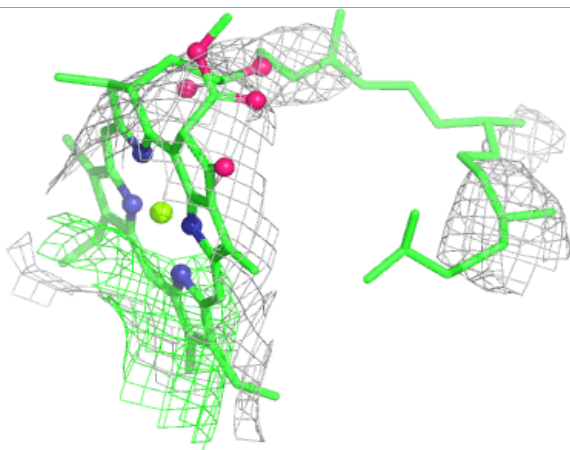
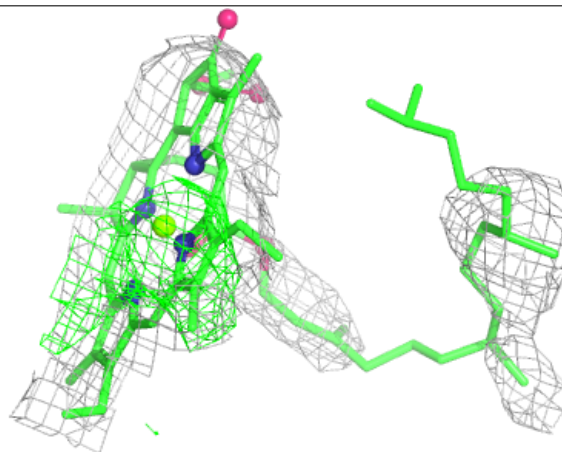


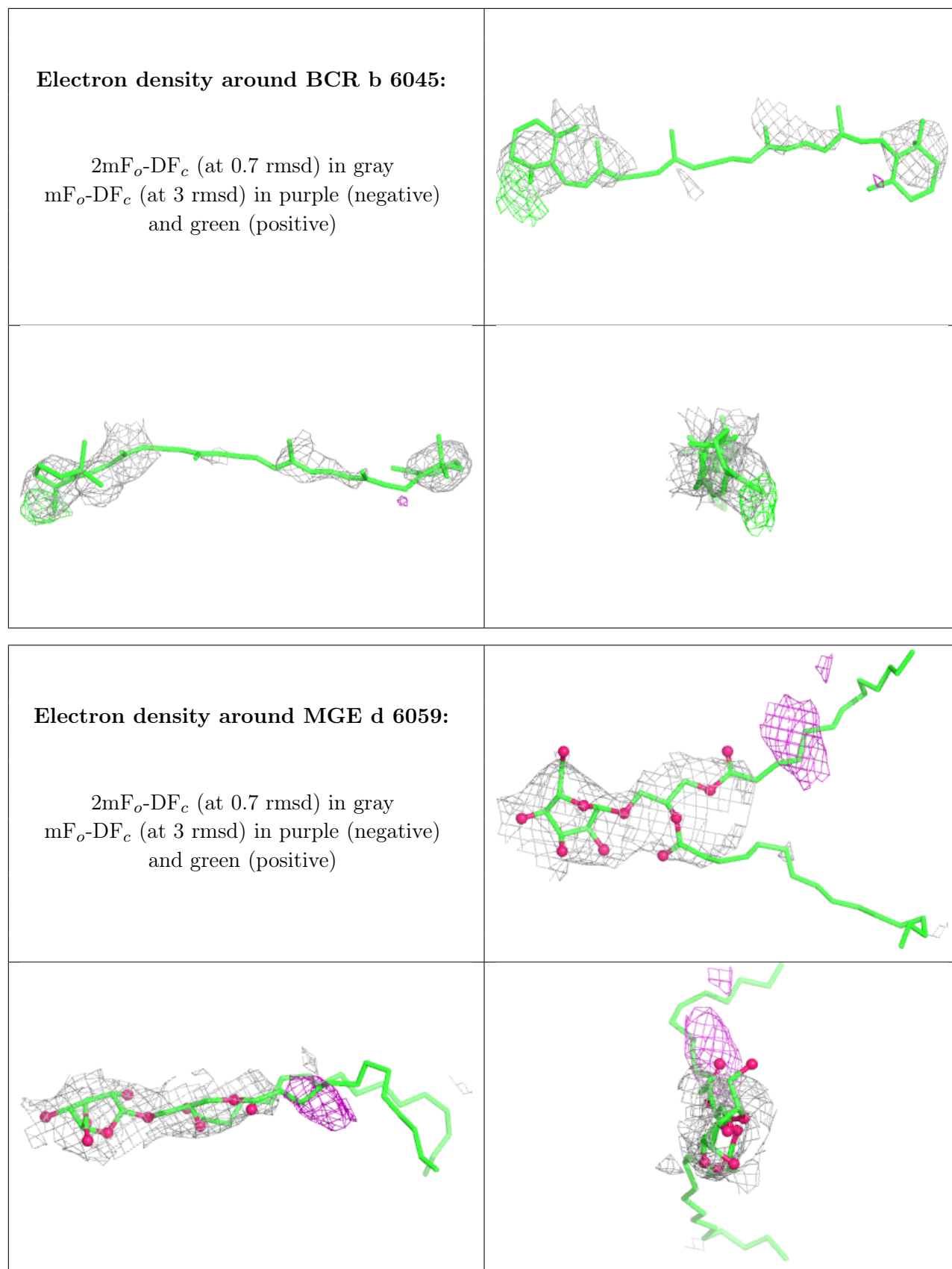
Electron density around BCR h 6049:

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

**Electron density around CLA C 1037:**

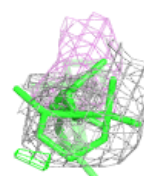
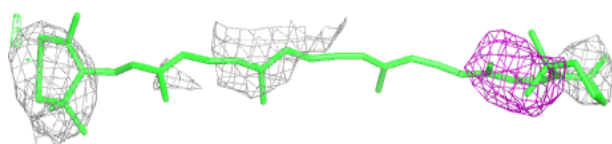
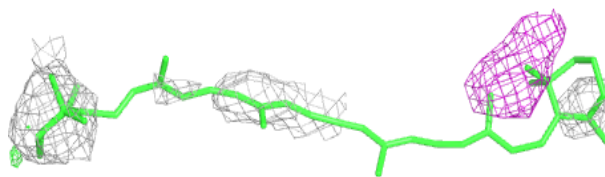
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



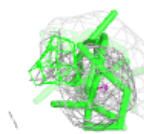
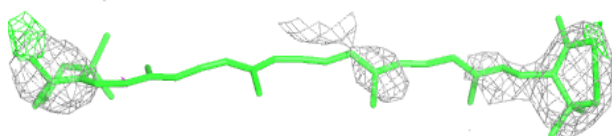
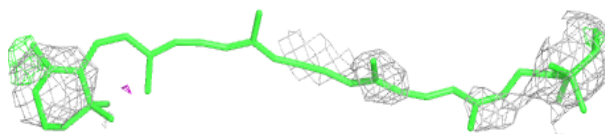


Electron density around BCR a 6044:

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

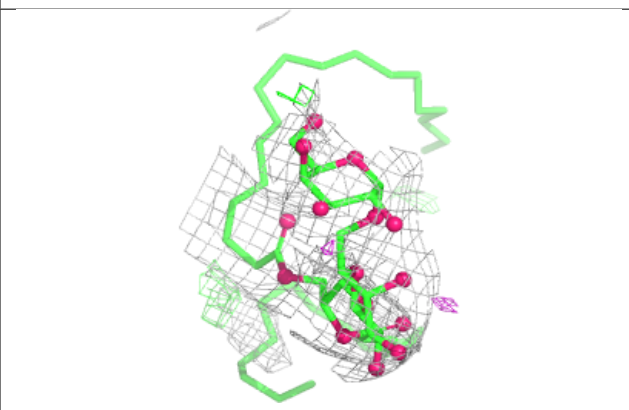
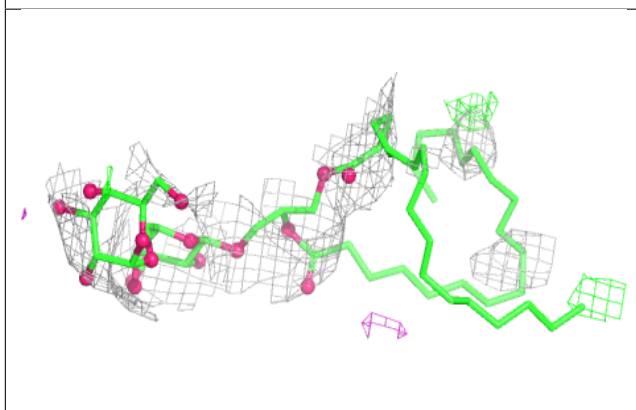
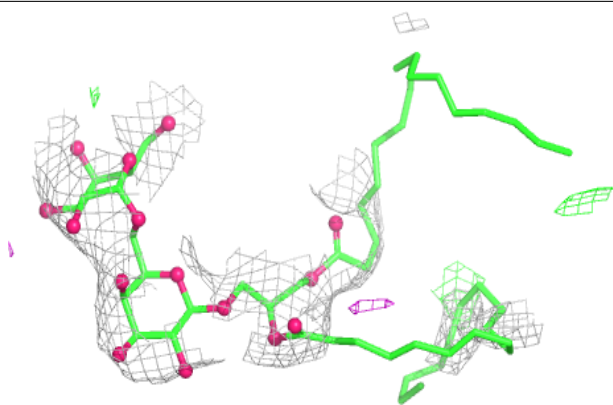
**Electron density around BCR A 1044:**

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

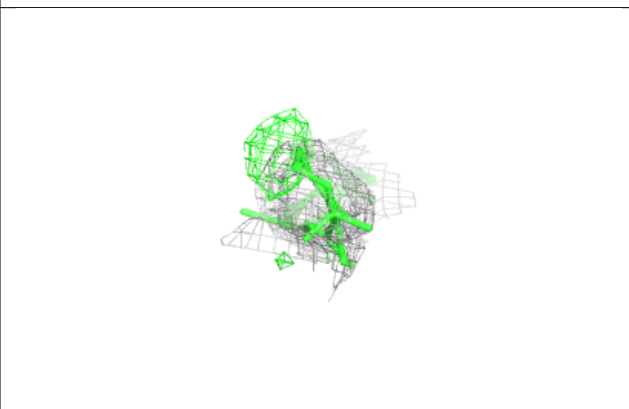
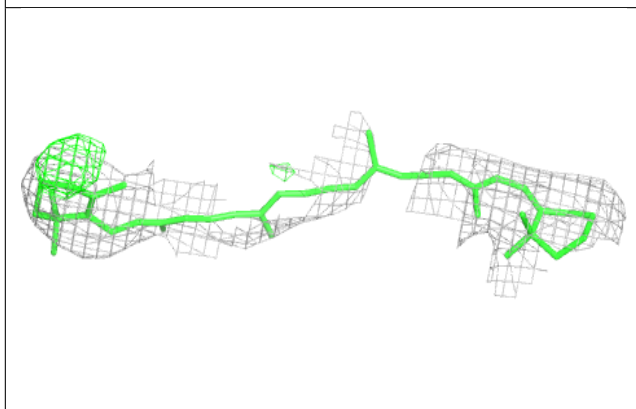


Electron density around DGD C 1056:

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

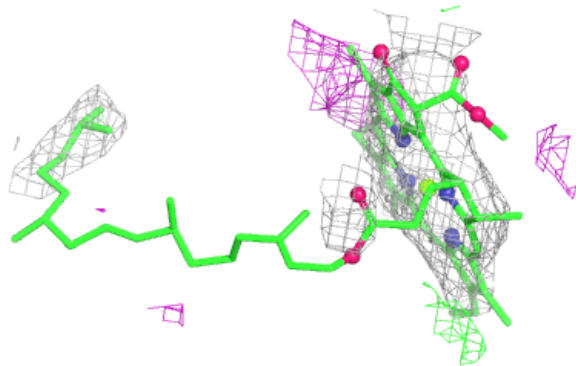
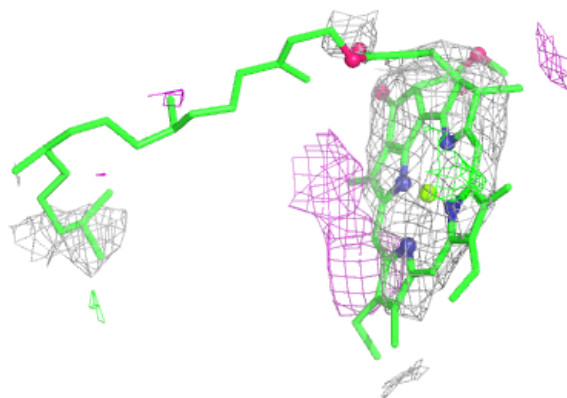
**Electron density around BCR D 1050:**

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

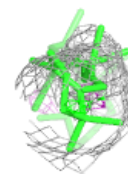
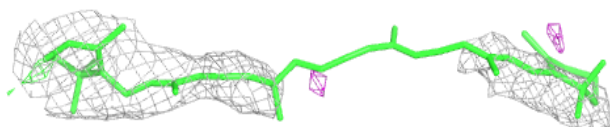
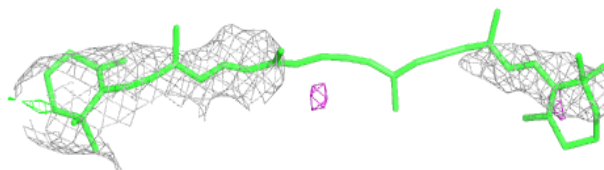


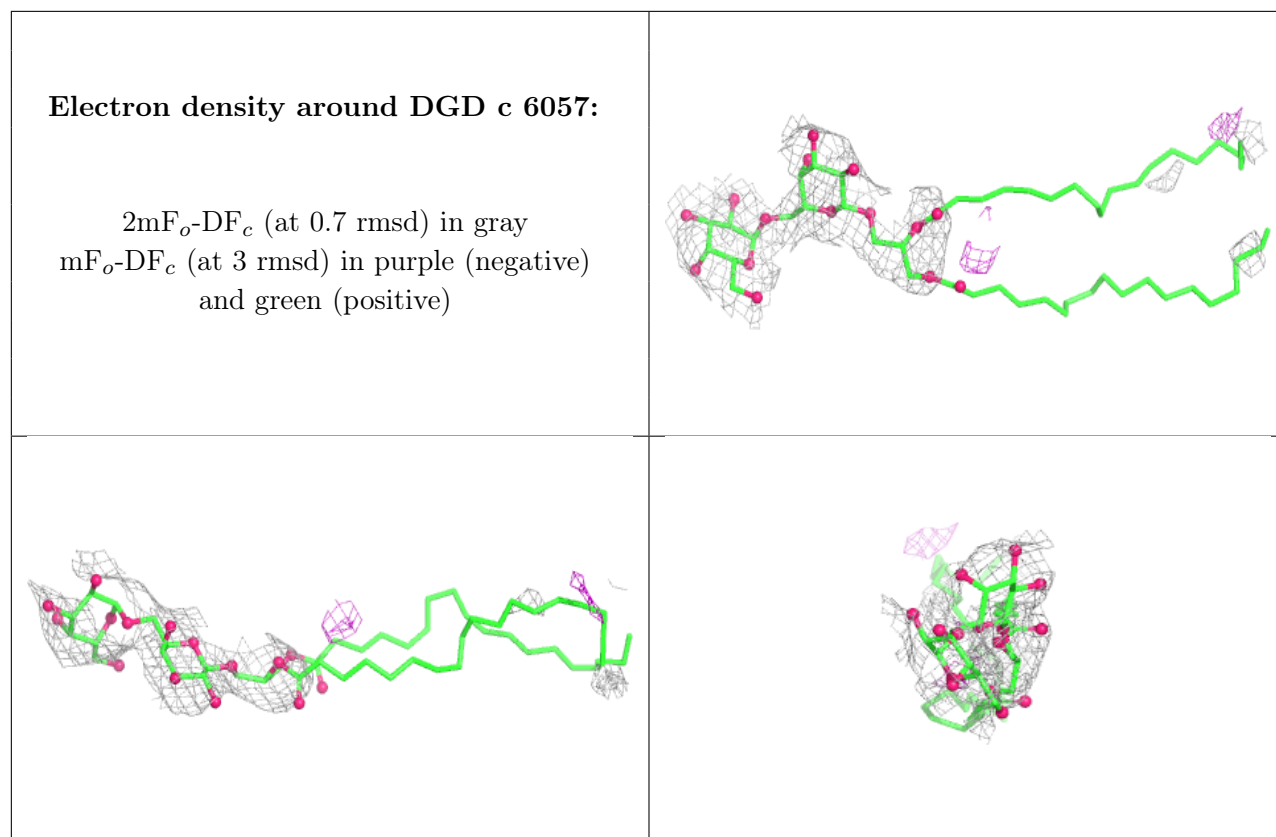
Electron density around CLA C 1032:

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

**Electron density around BCR b 6048:**

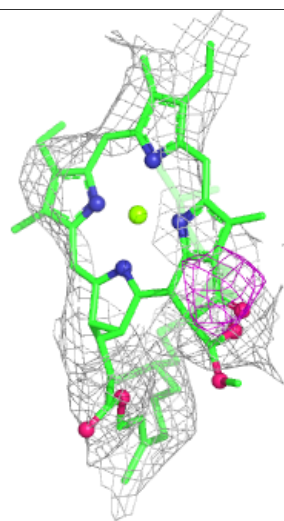
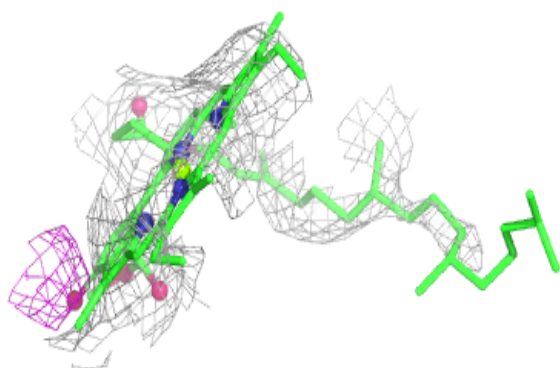
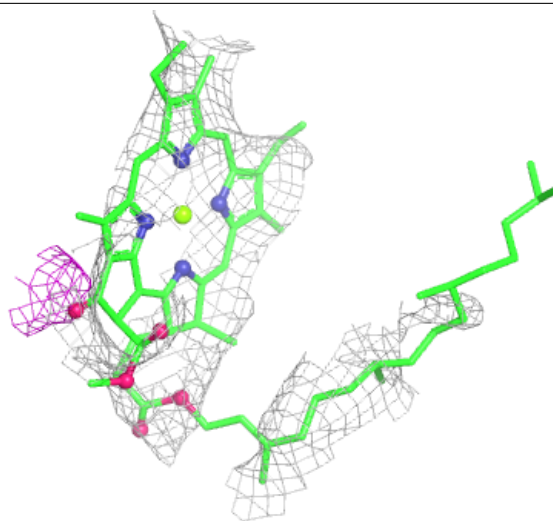
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)





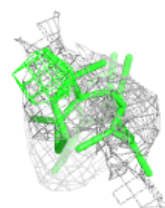
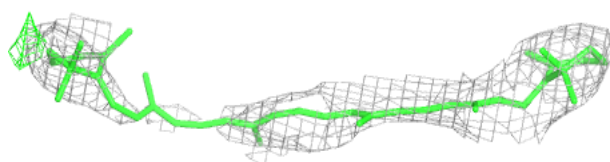
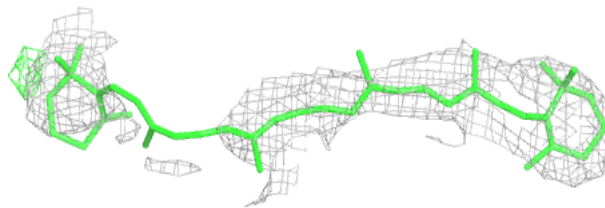
Electron density around CLA B 1024:

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

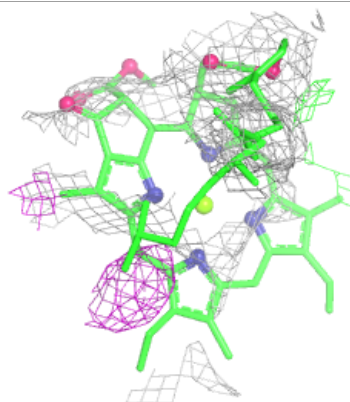
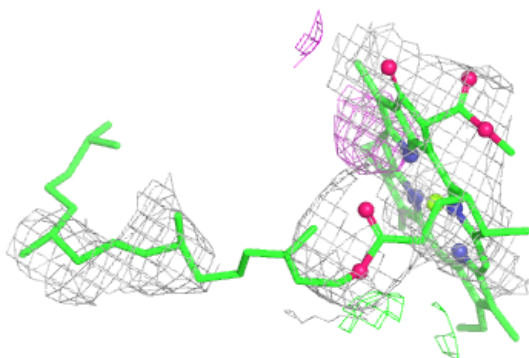
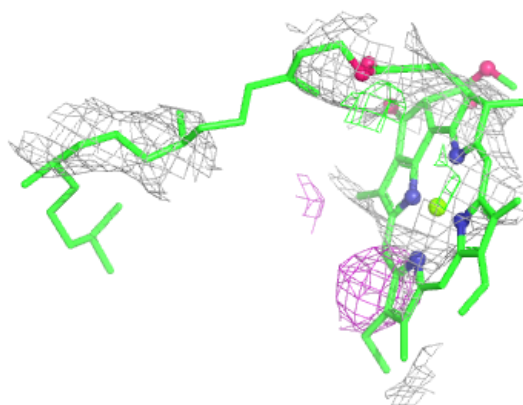


Electron density around BCR t 1046:

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

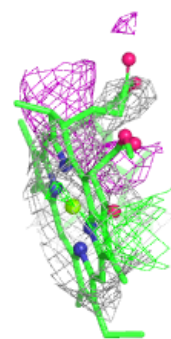
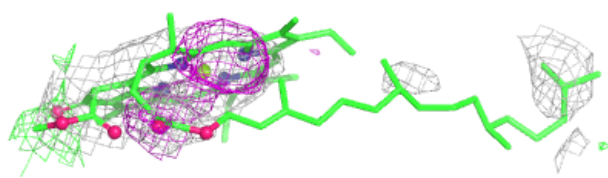
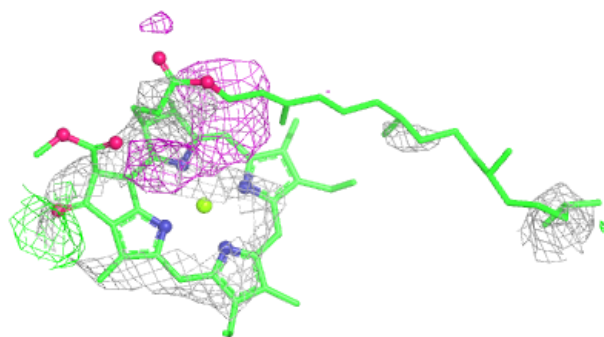
**Electron density around CLA c 6032:**

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

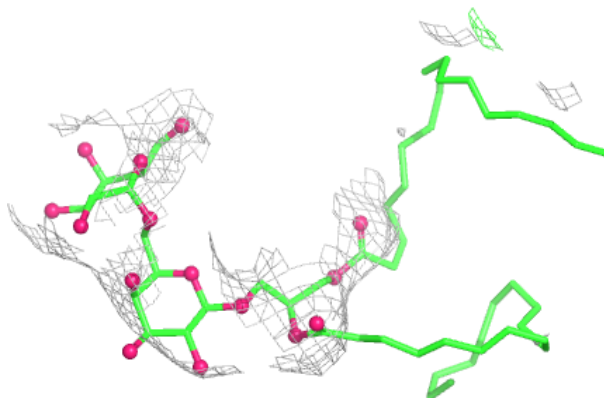


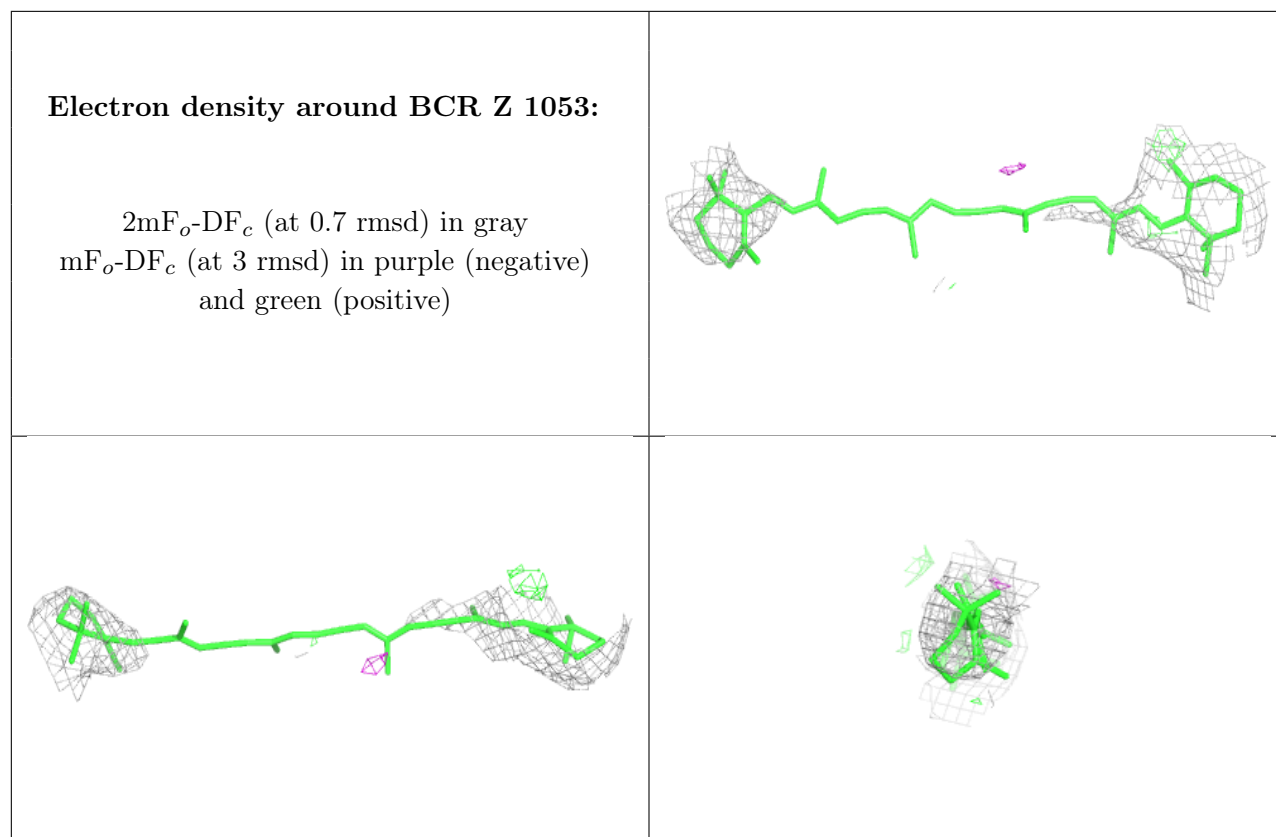
Electron density around CLA C 1025:

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

**Electron density around DGD c 6056:**

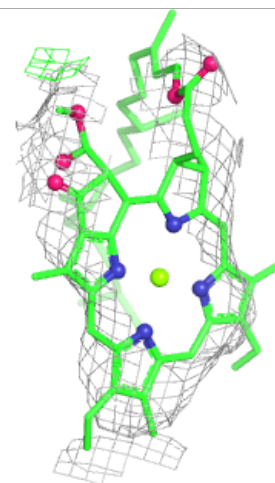
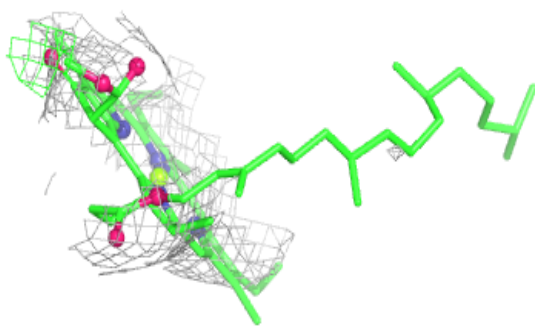
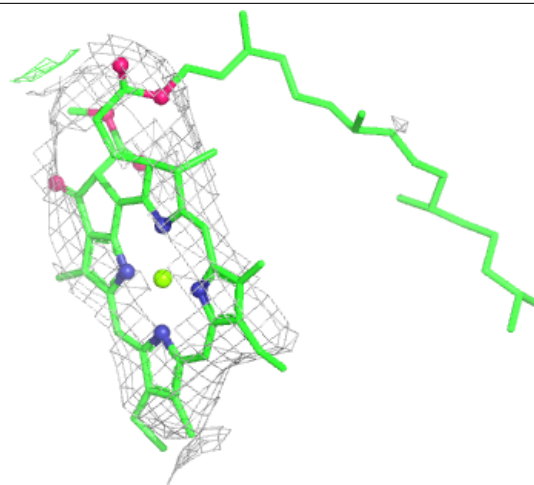
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





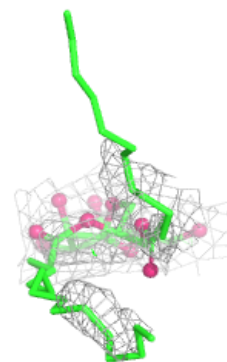
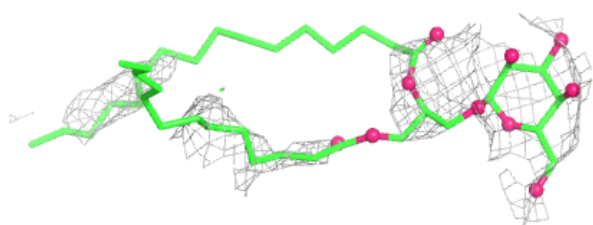
Electron density around CLA b 6024:

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

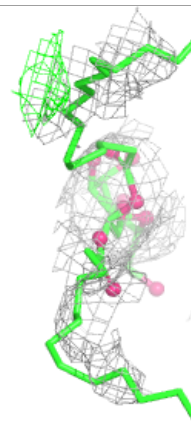
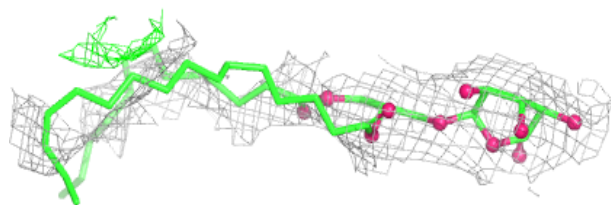
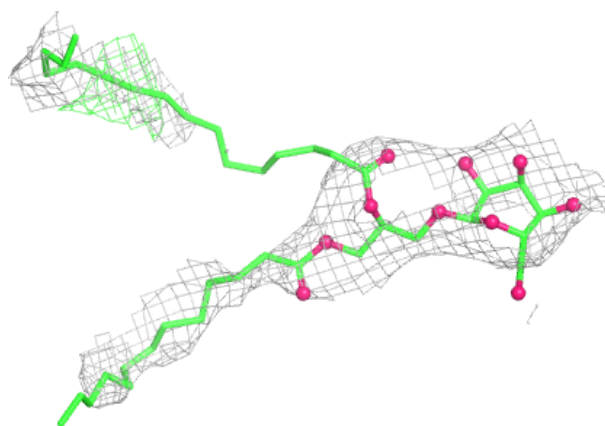


Electron density around MGE d 6062:

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

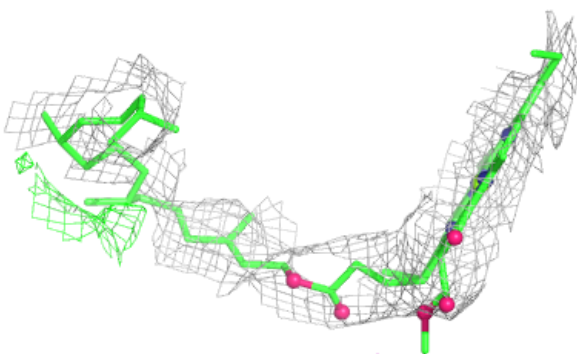
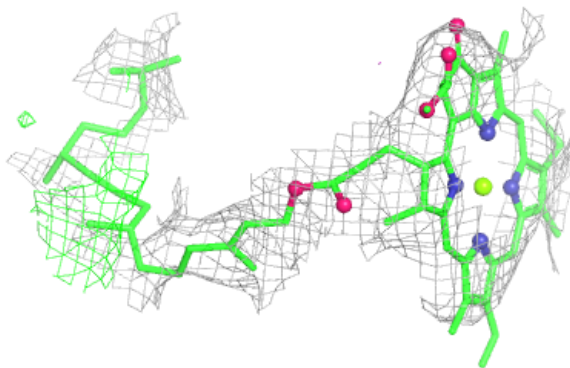
**Electron density around MGE J 1059:**

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

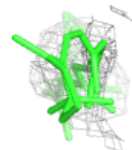
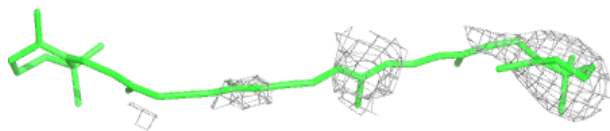
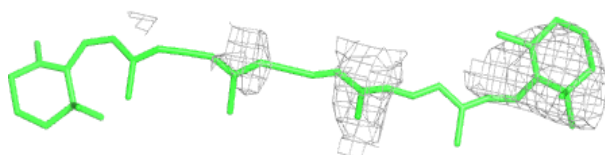


Electron density around CLA b 6014:

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

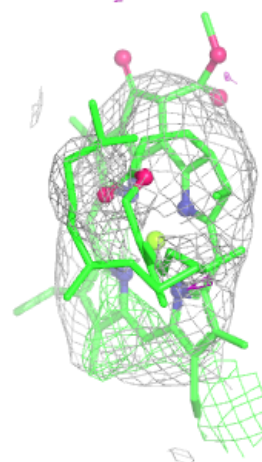
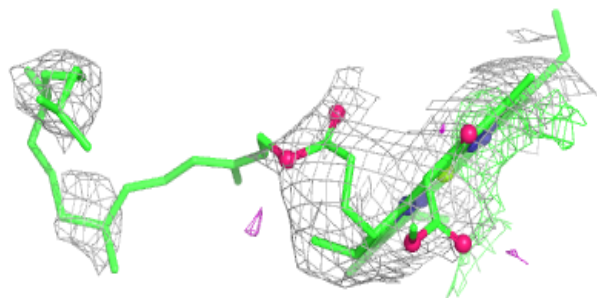
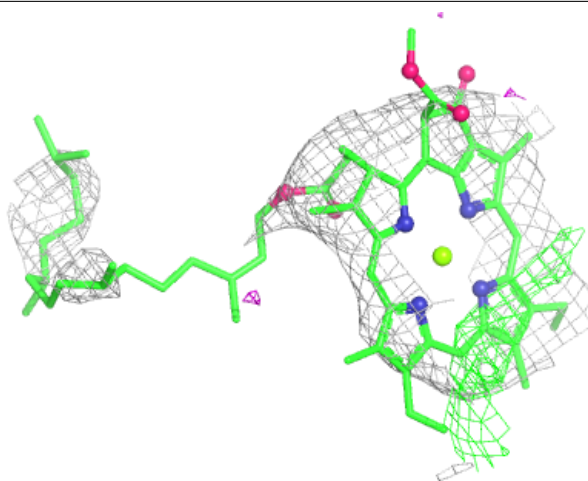
**Electron density around BCR B 1045:**

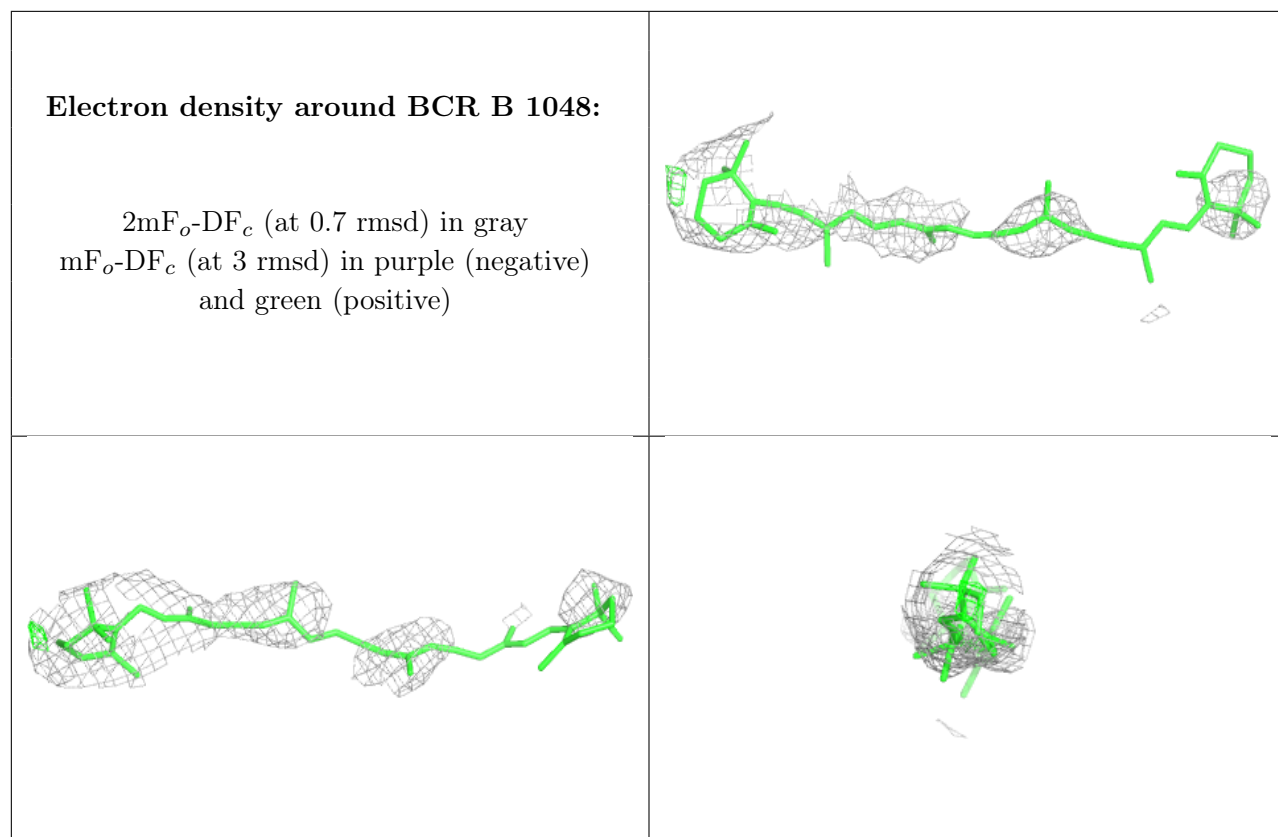
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



Electron density around CLA C 1027:

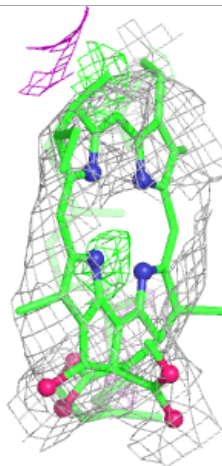
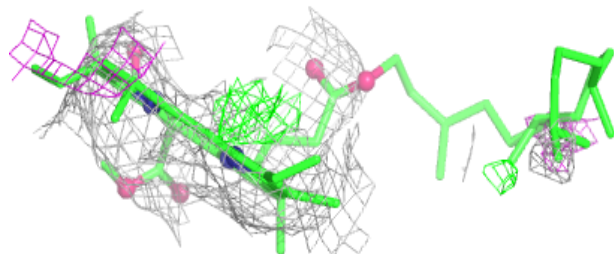
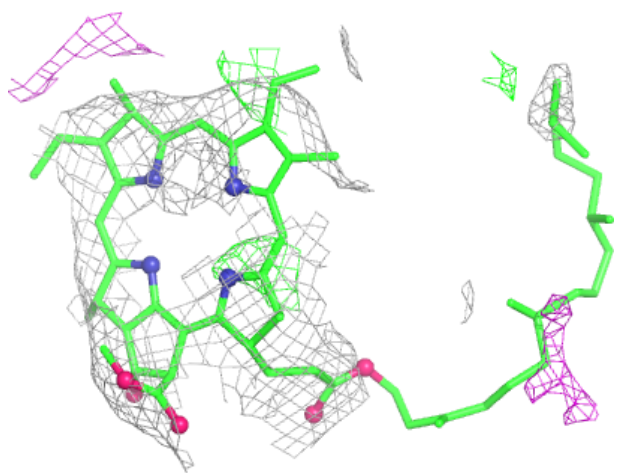
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

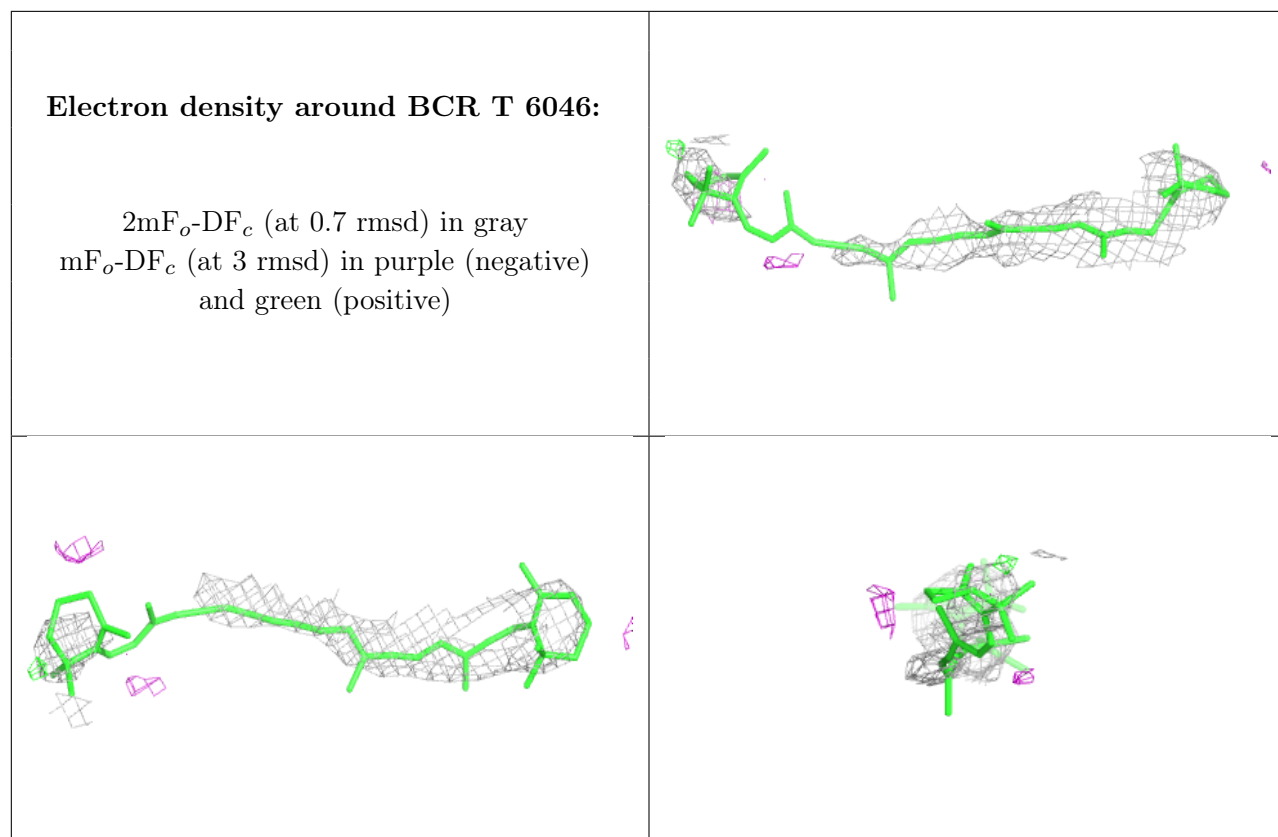




Electron density around PHO d 6038:

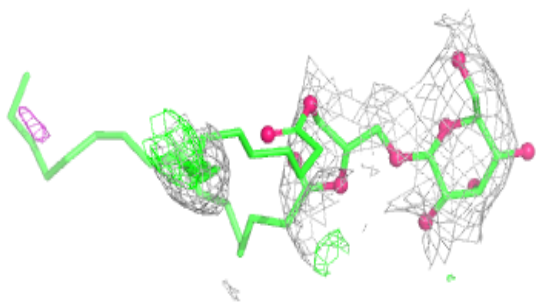
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





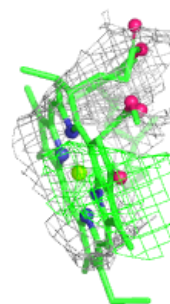
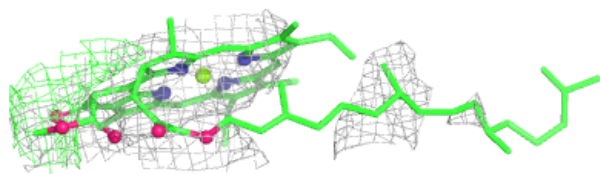
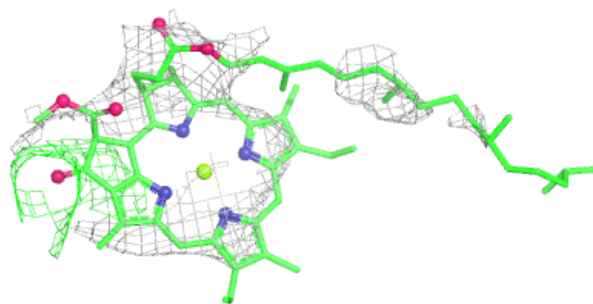
Electron density around MGE d 6061:

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

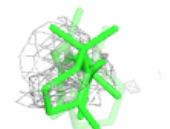
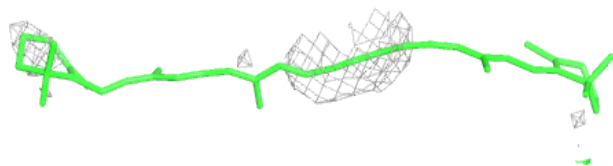
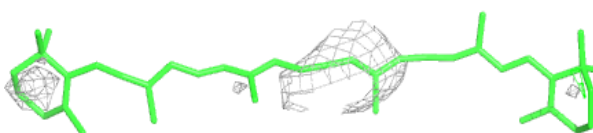


Electron density around CLA c 6025:

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

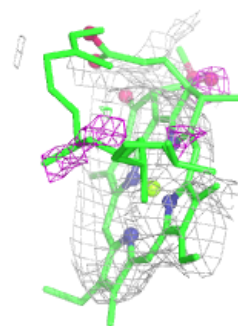
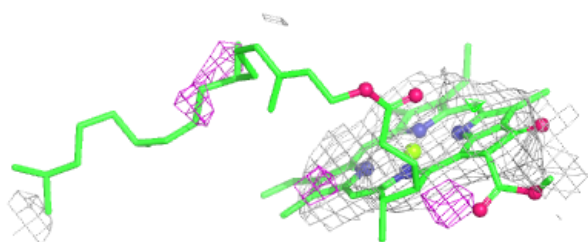
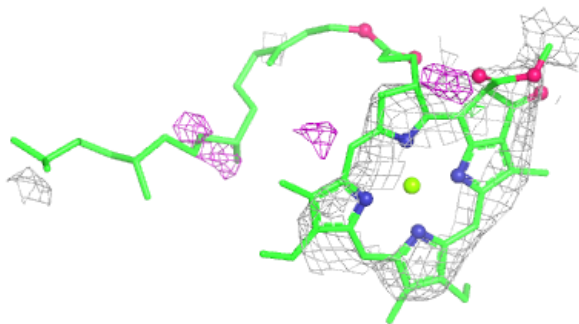
**Electron density around BCR c 6054:**

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

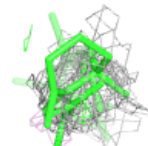
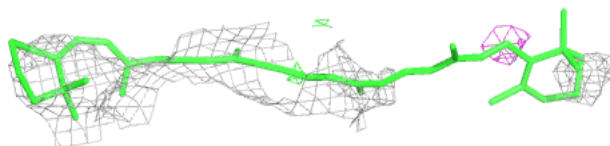
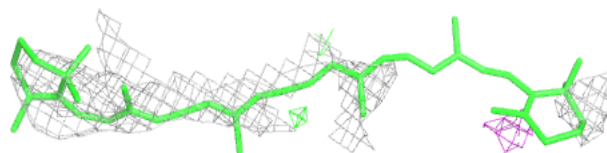


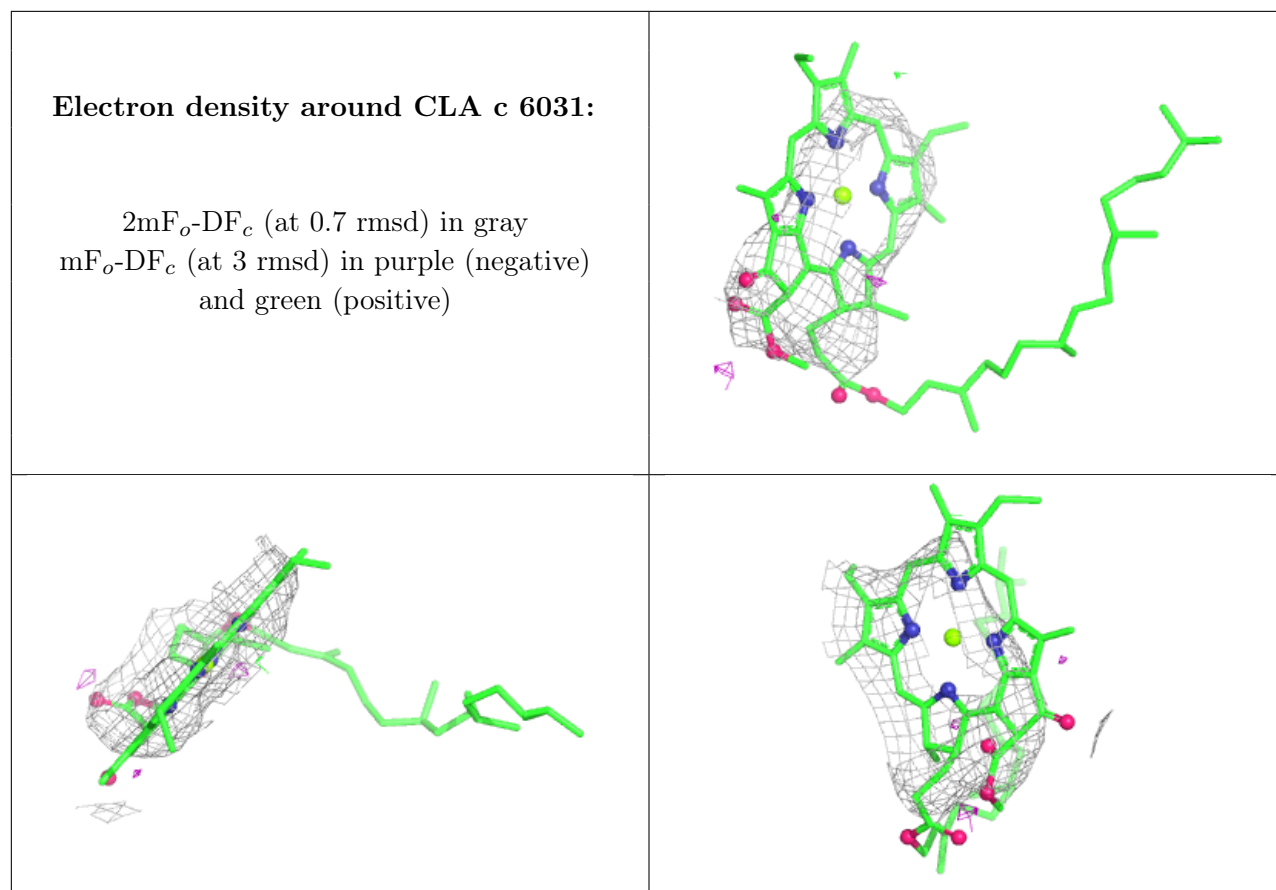
Electron density around CLA d 6008:

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

**Electron density around BCR K 1051:**

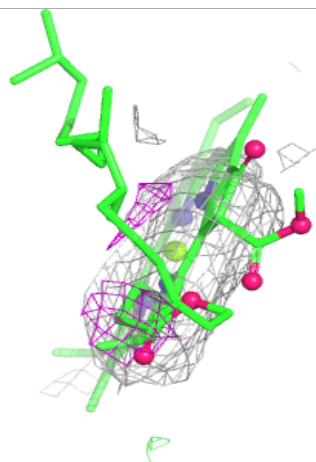
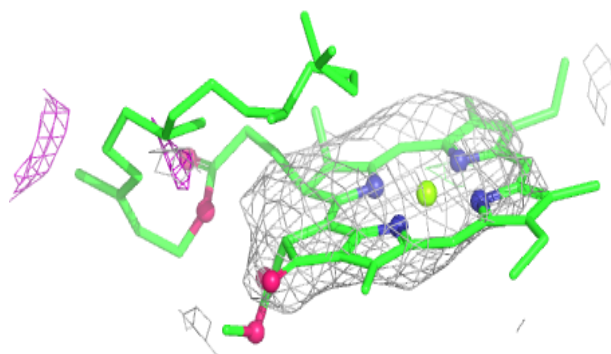
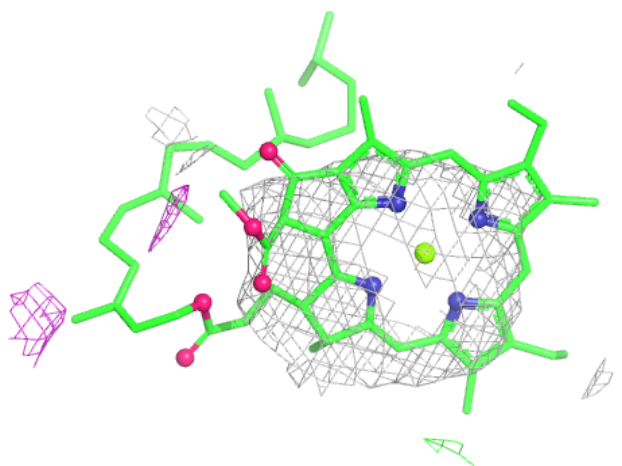
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





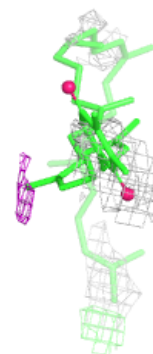
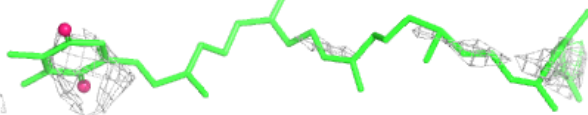
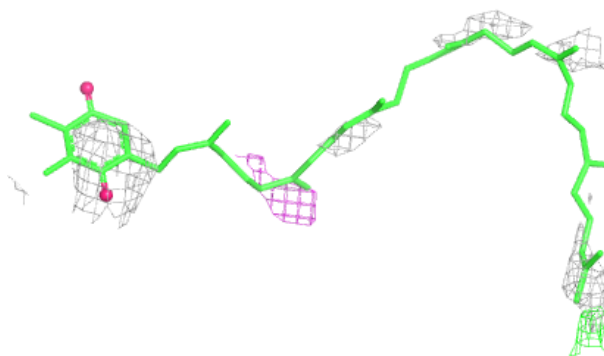
Electron density around CLA c 6033:

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

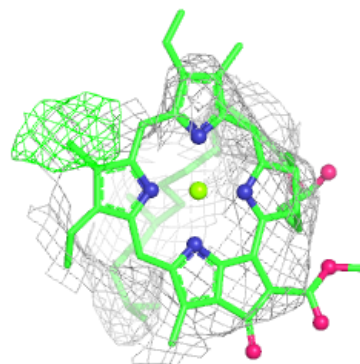
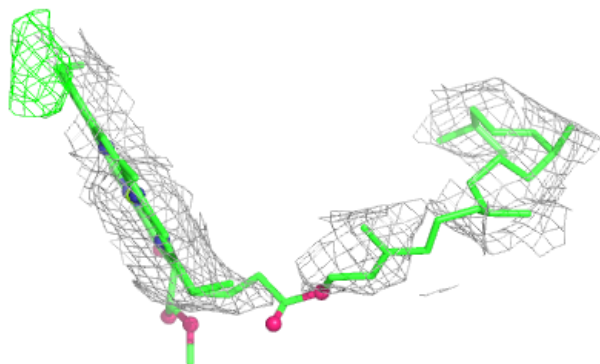
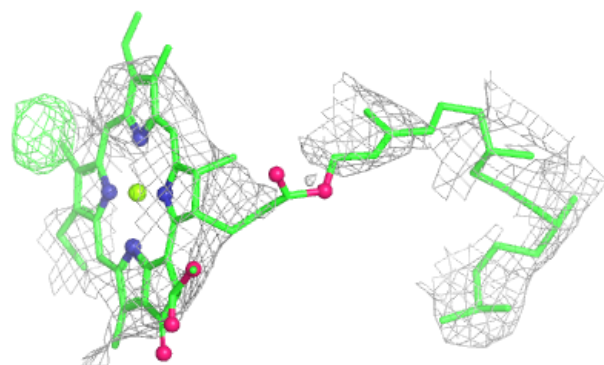


Electron density around PQ9 d 6042:

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

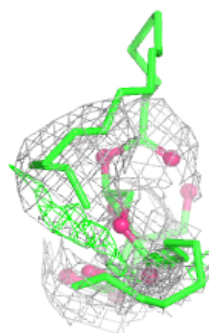
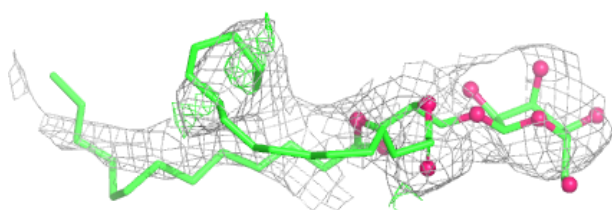
**Electron density around CLA B 1014:**

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

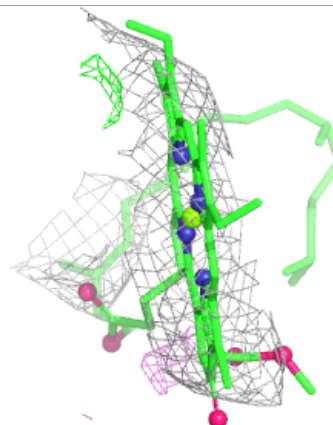
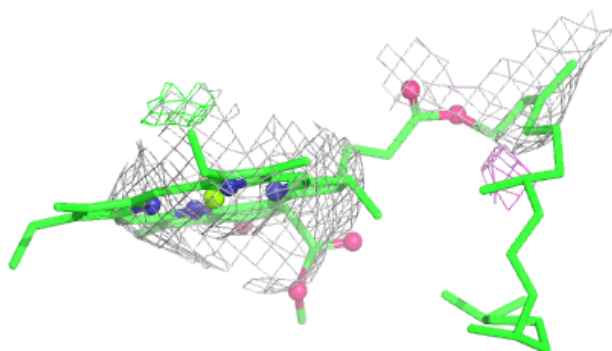
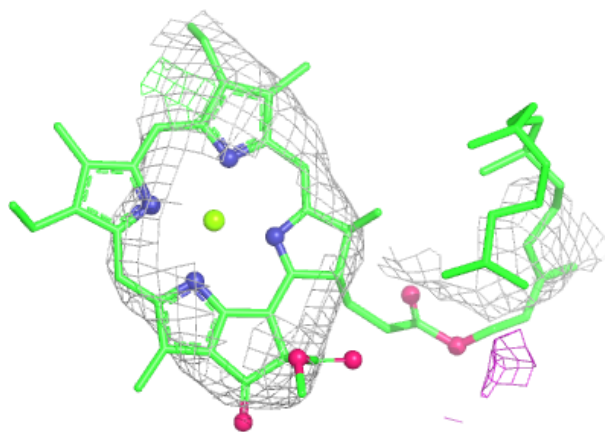


Electron density around MGE B 1060:

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

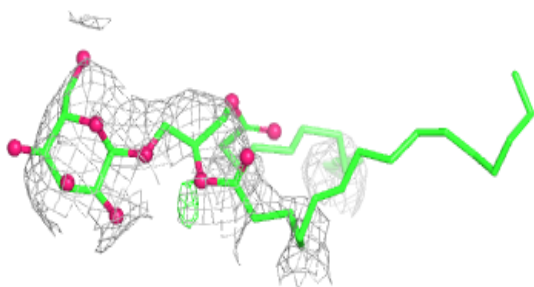
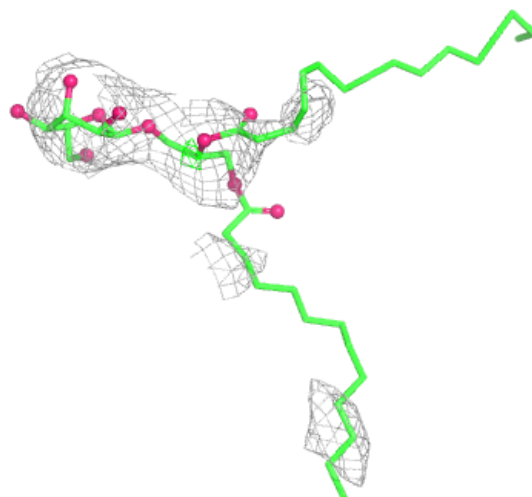
**Electron density around CLA c 6036:**

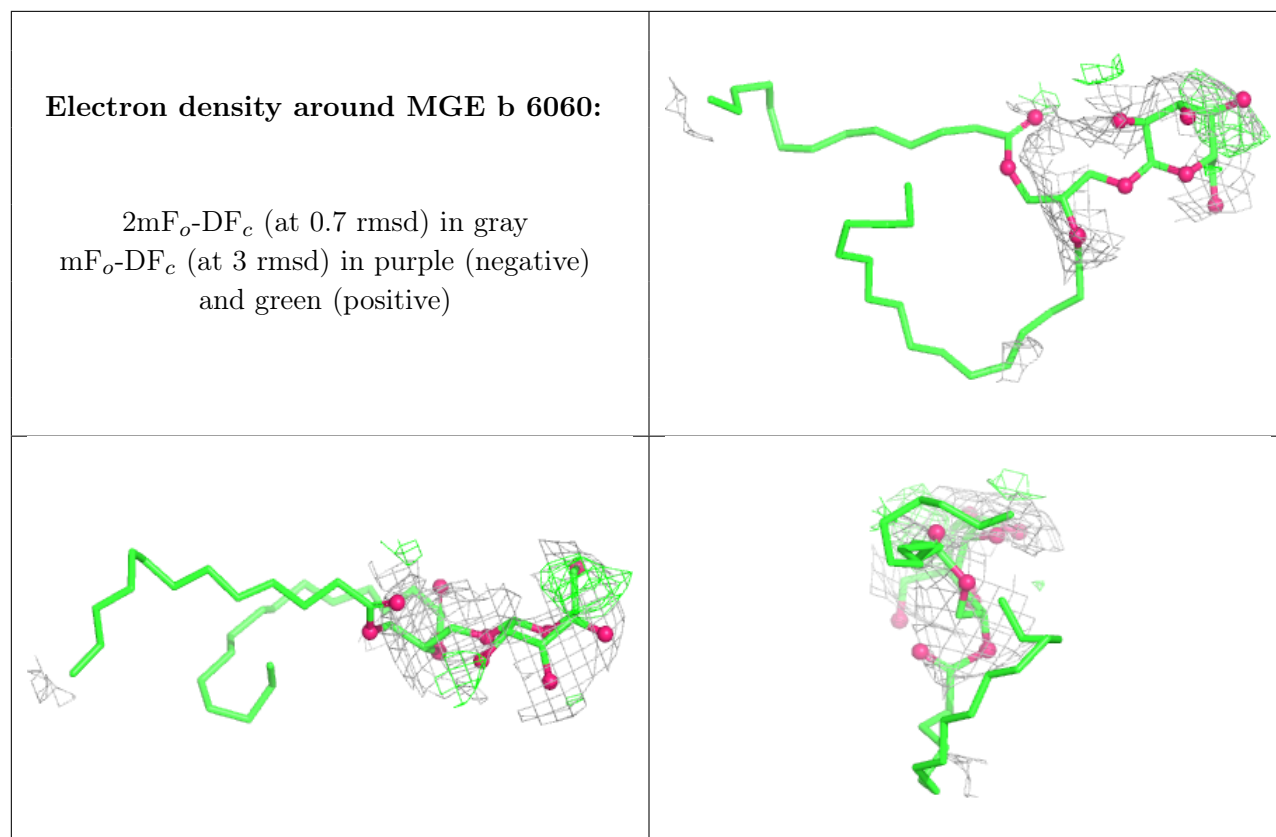
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MGE L 1061:

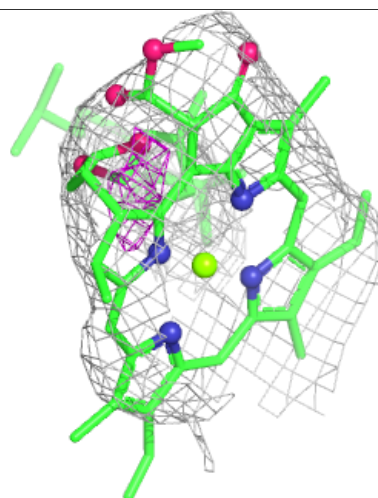
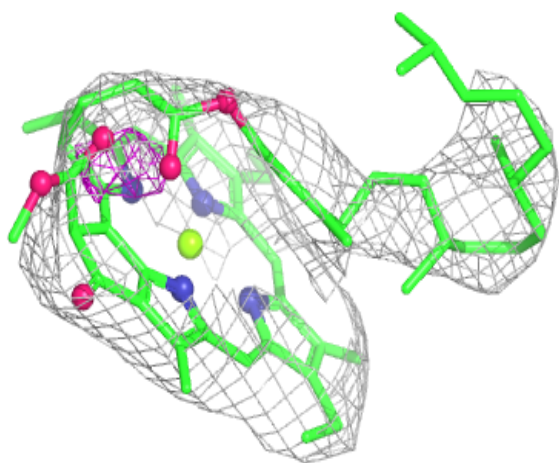
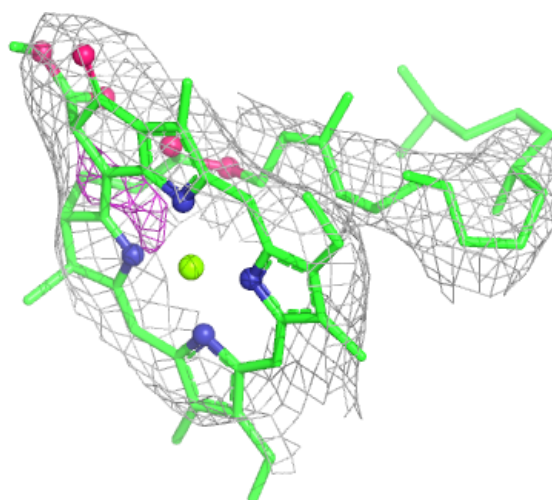
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

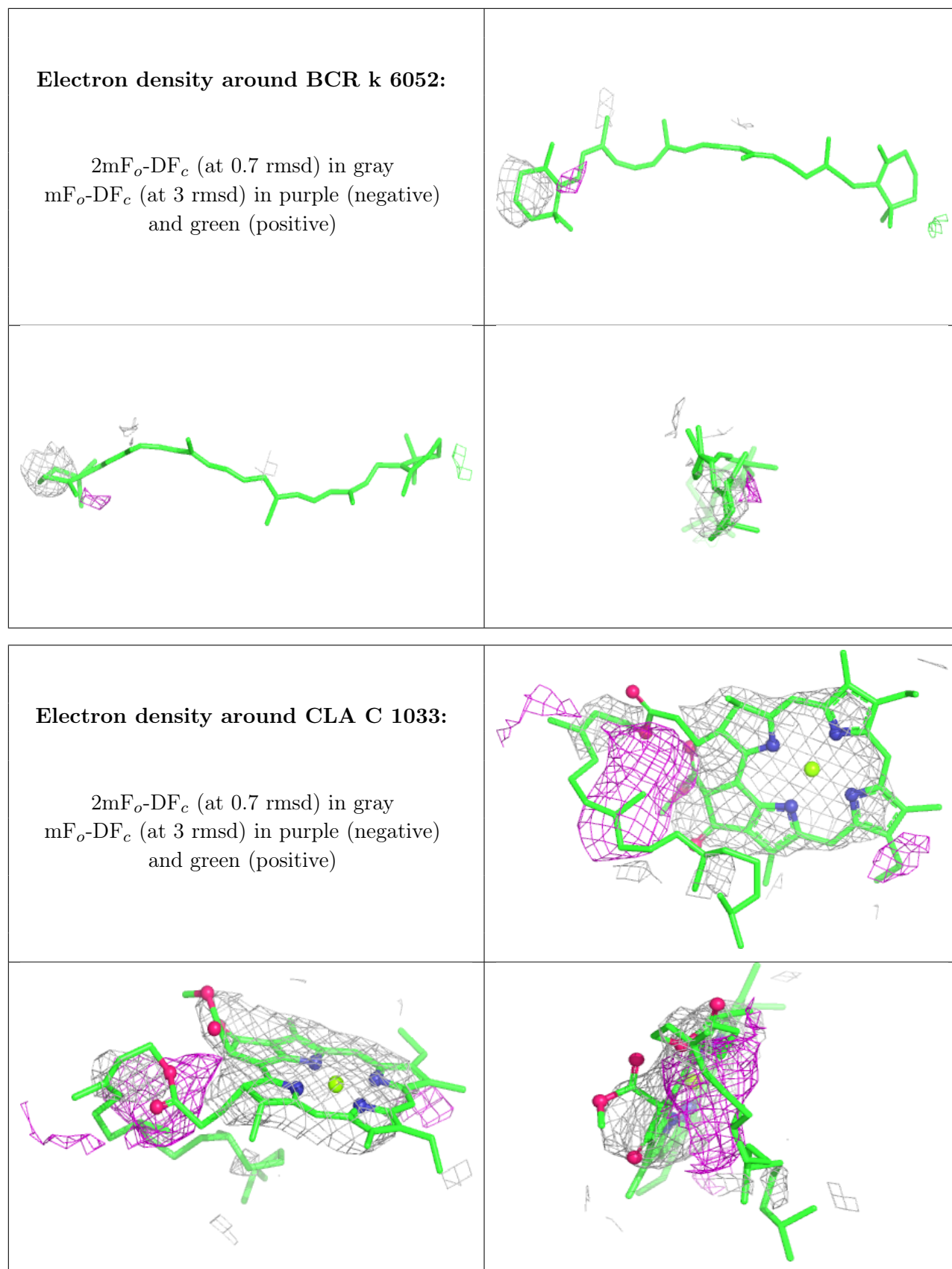




Electron density around CLA B 1022:

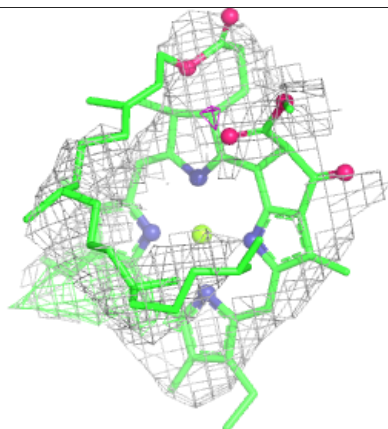
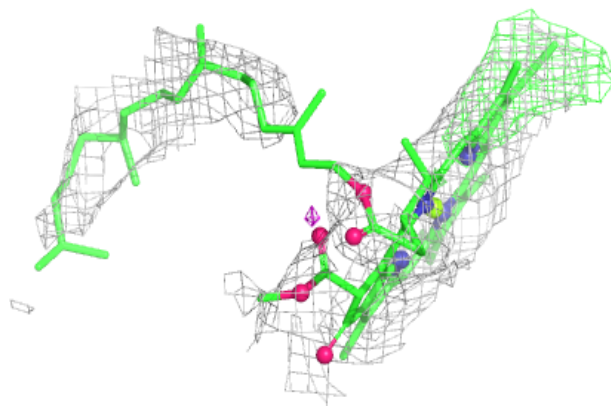
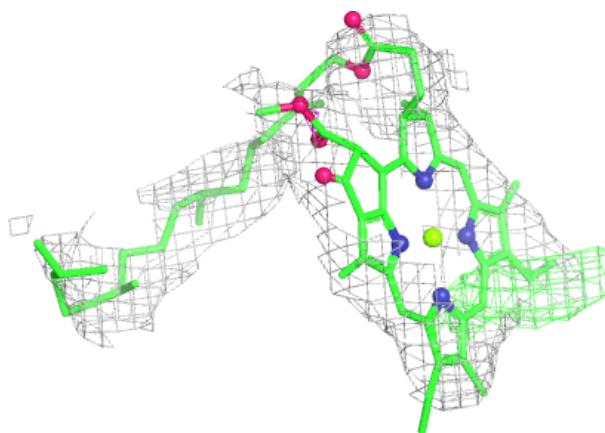
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



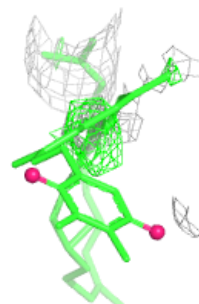
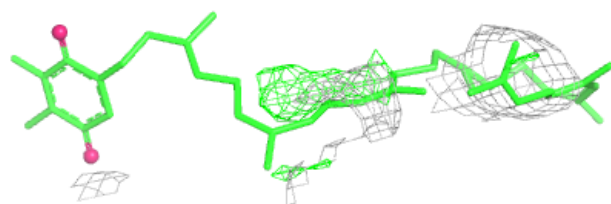
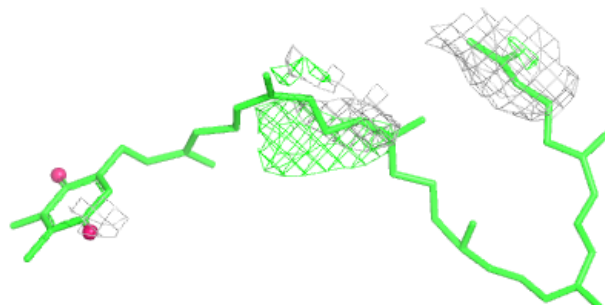


Electron density around CLA b 6021:

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

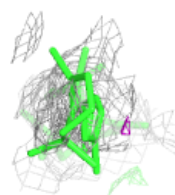
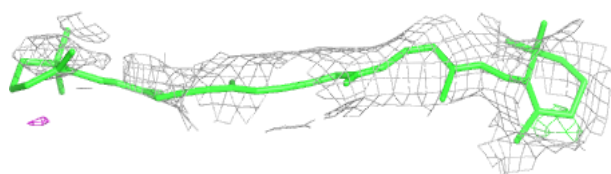
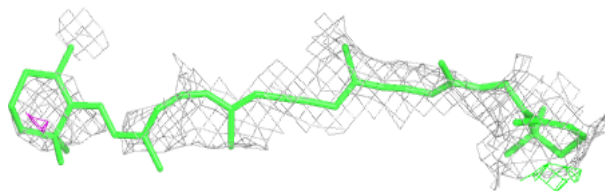
**Electron density around PQ9 A 1043:**

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

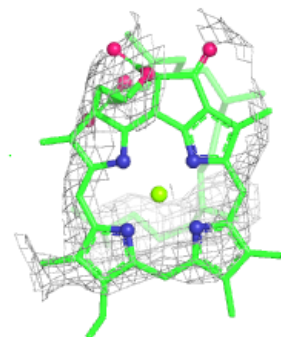
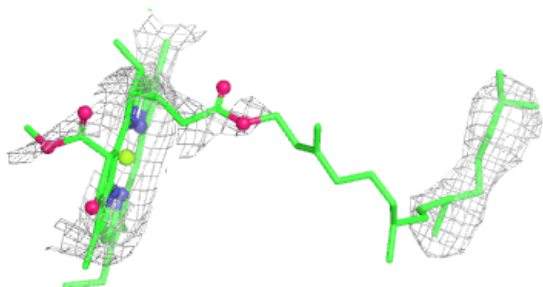


Electron density around BCR H 1049:

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

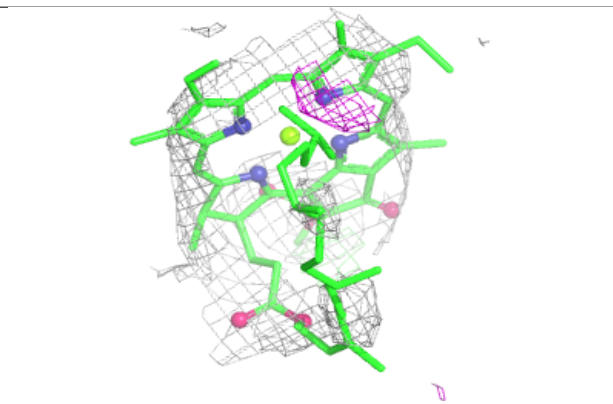
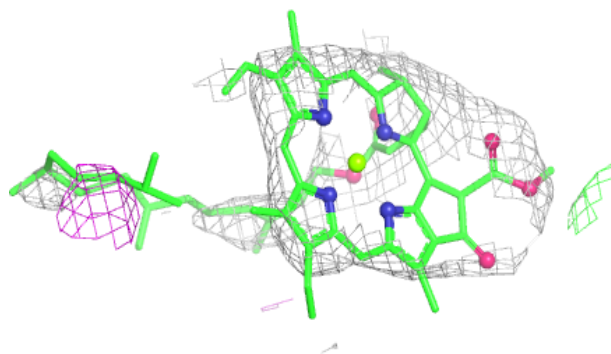
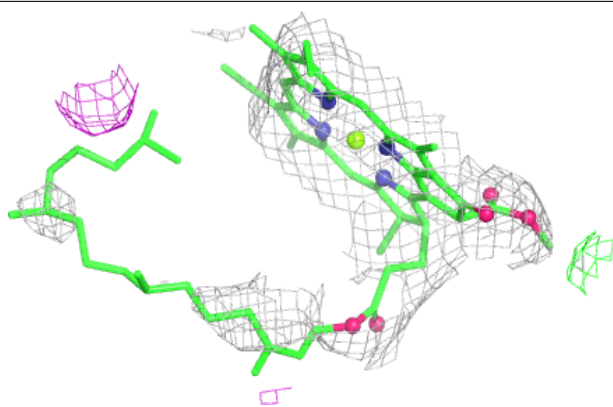
**Electron density around CLA c 6030:**

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

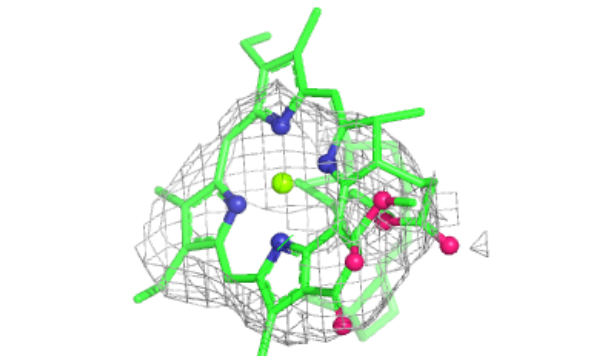
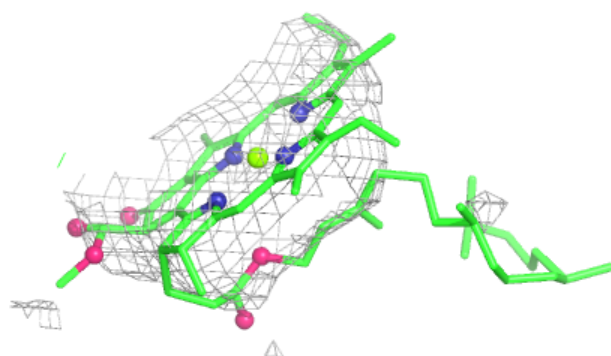
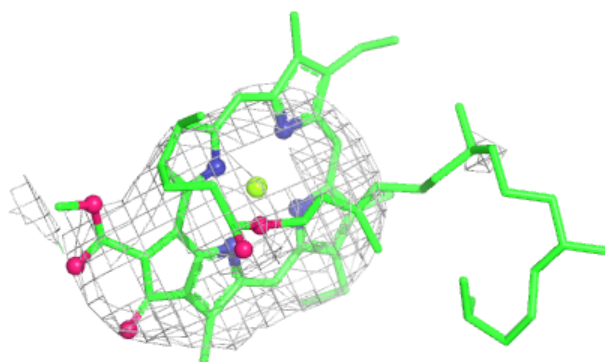


Electron density around CLA C 1028:

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

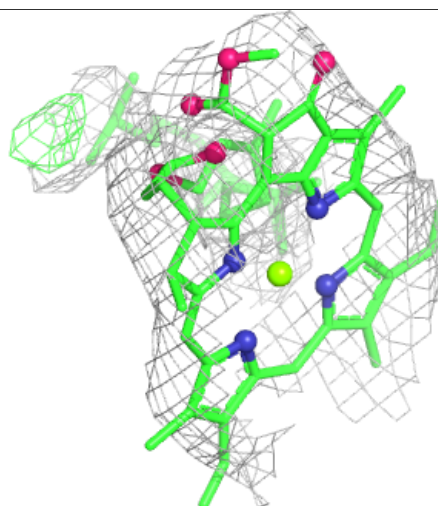
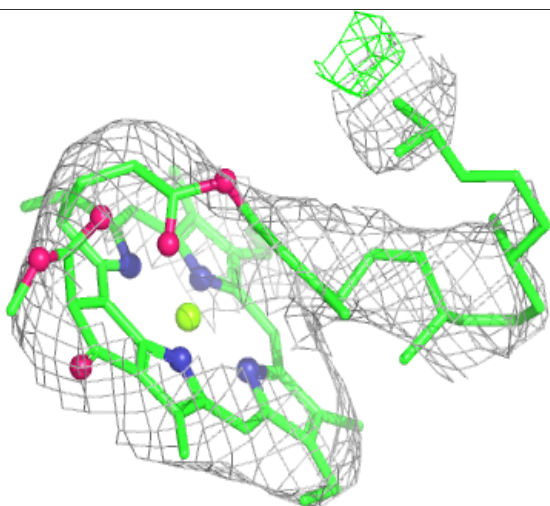
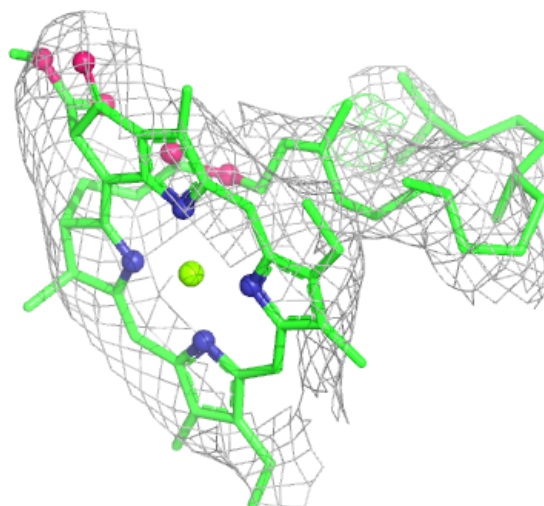
**Electron density around CLA c 6029:**

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



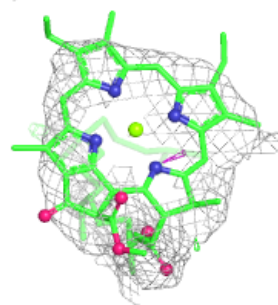
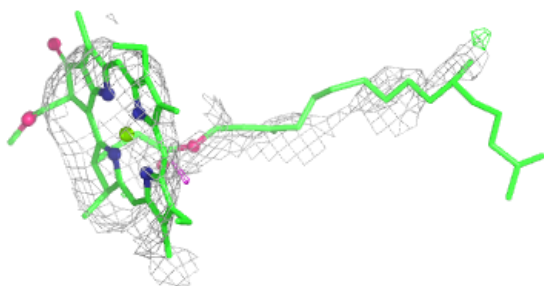
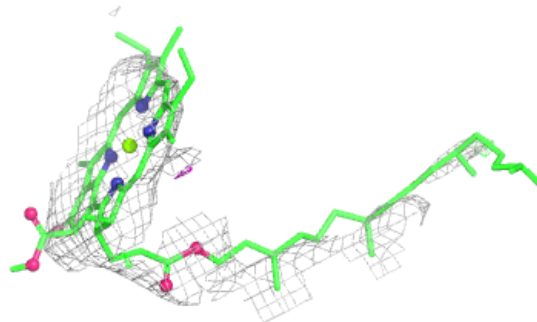
Electron density around CLA b 6022:

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

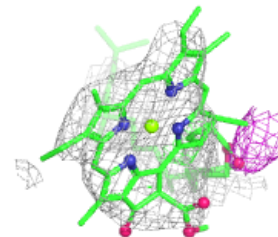
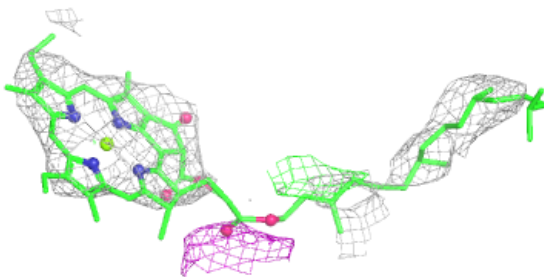
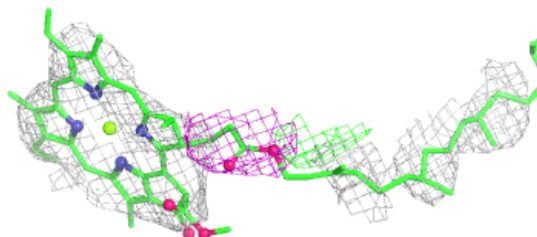


Electron density around CLA b 6013:

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

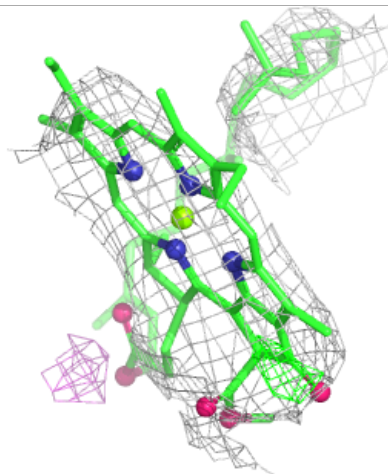
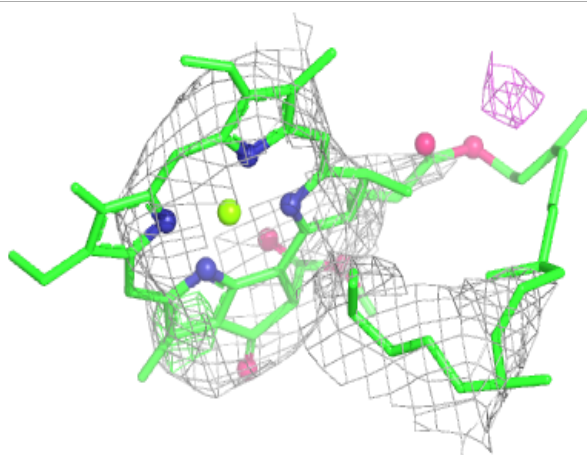
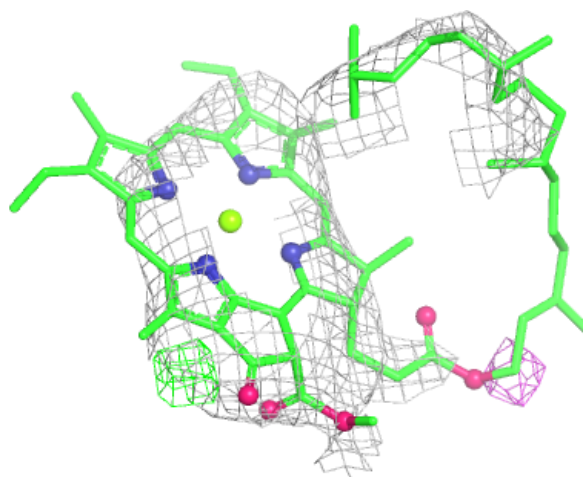
**Electron density around CLA a 6003:**

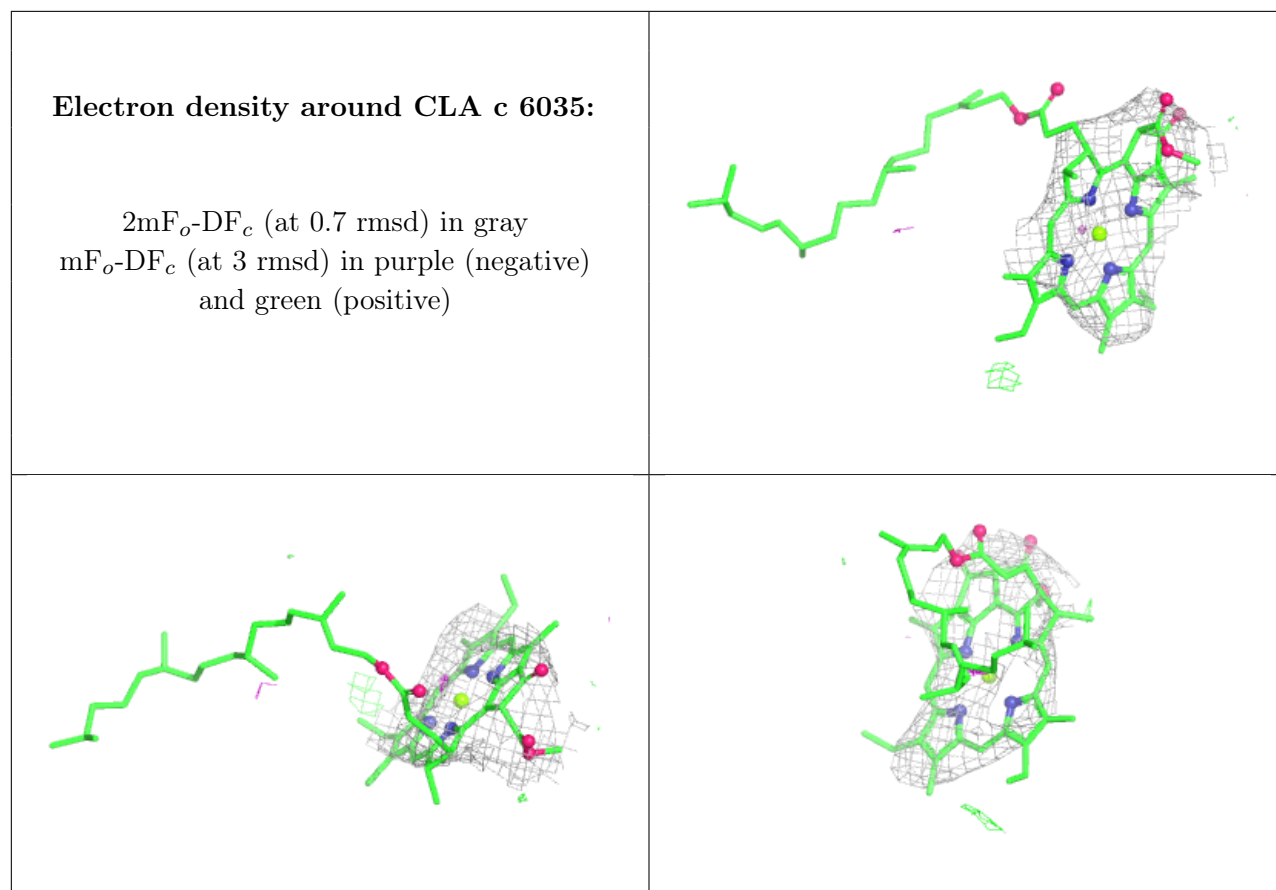
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 6023:

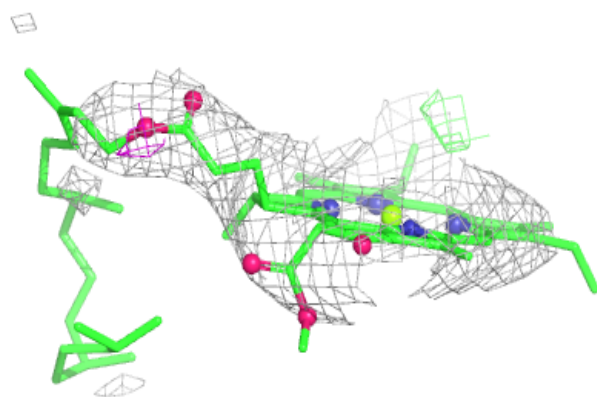
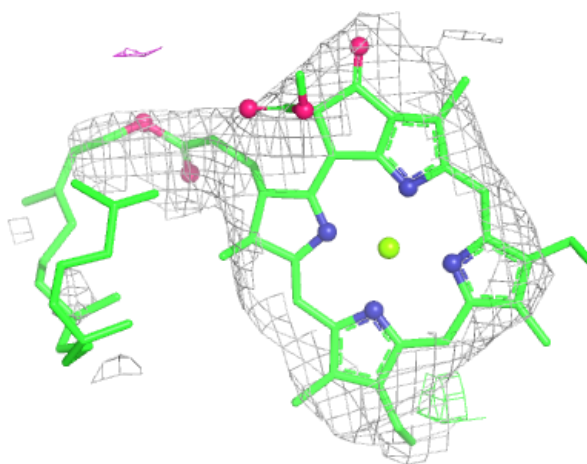
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





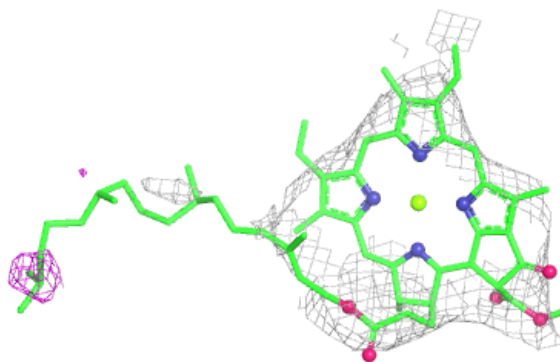
Electron density around CLA C 1036:

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

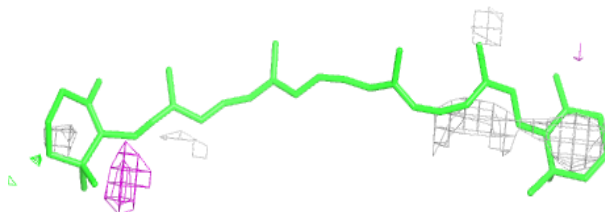


Electron density around CLA b 6011:

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

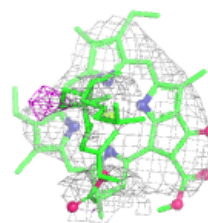
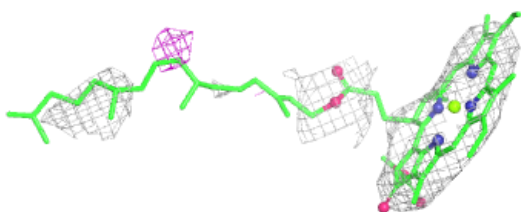
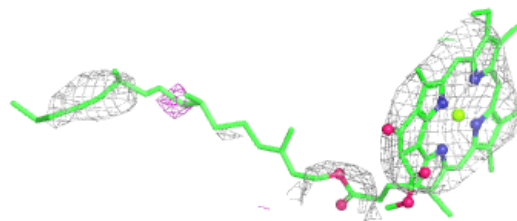
**Electron density around BCR K 1052:**

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

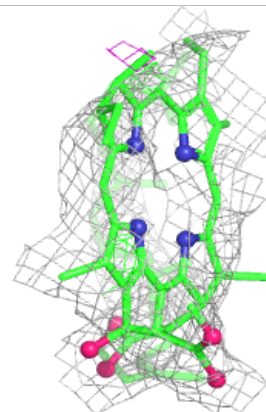
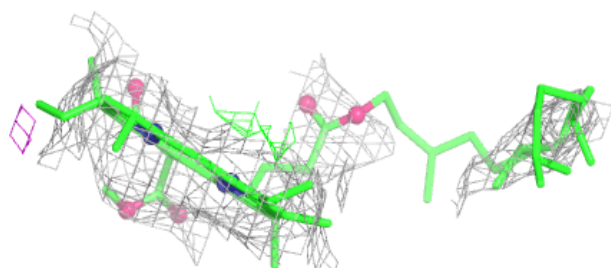
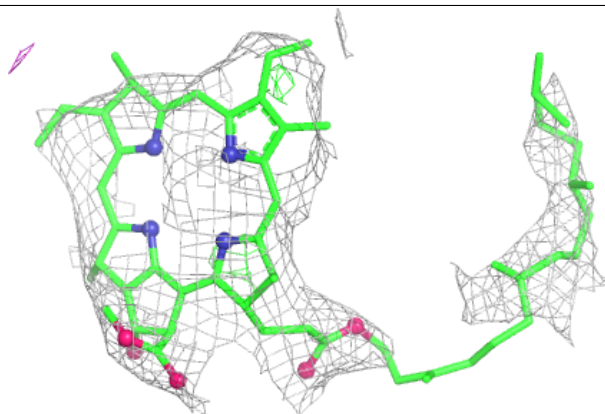


Electron density around CLA b 6012:

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

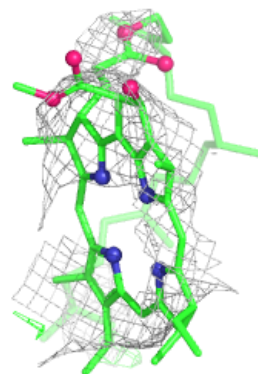
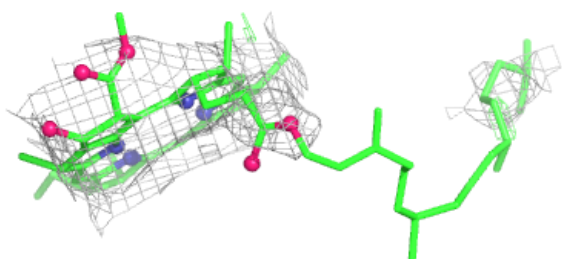
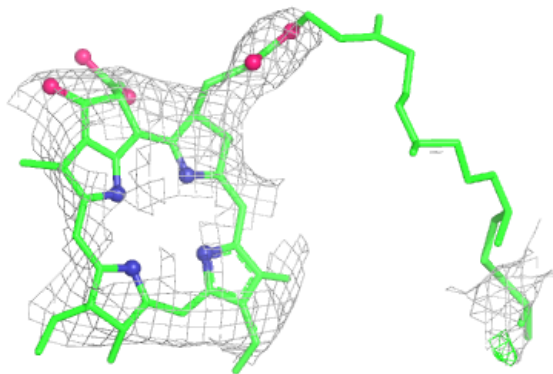
**Electron density around PHO A 1038:**

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

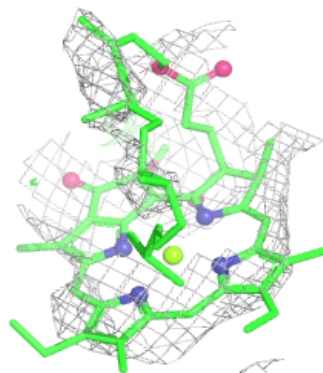
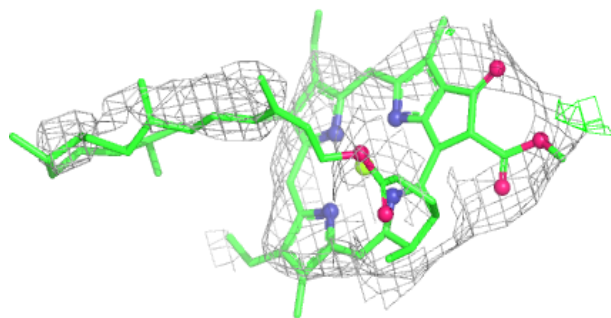
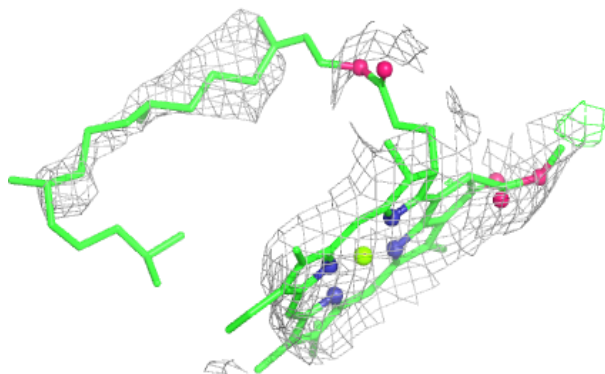


Electron density around PHO a 6039:

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

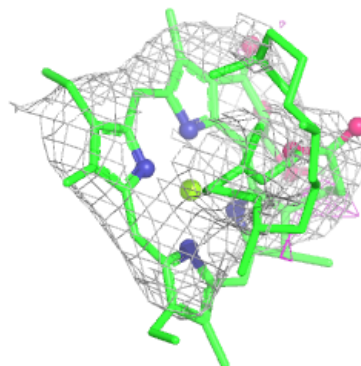
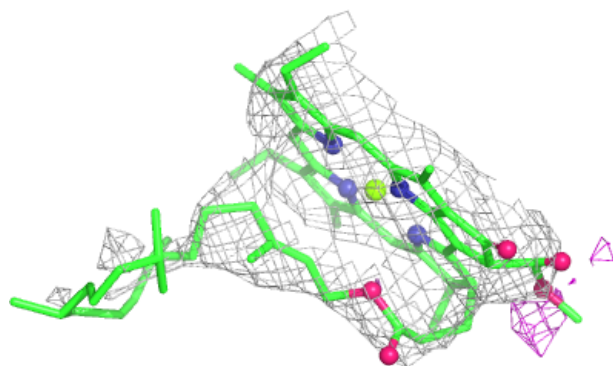
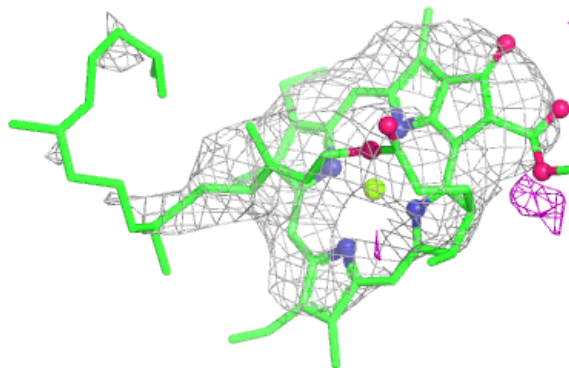
**Electron density around CLA c 6028:**

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

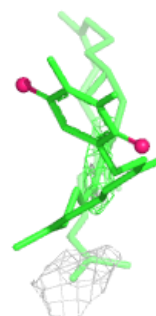
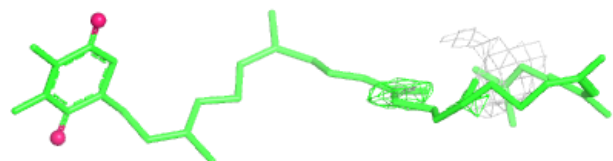
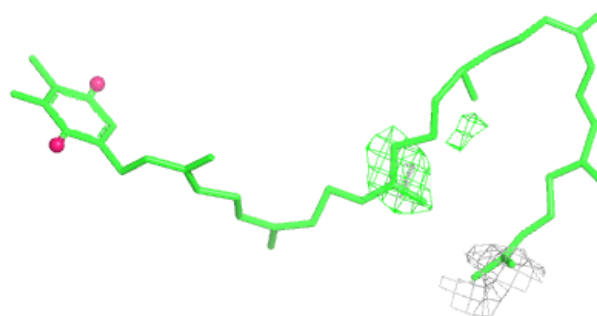


Electron density around CLA C 1029:

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

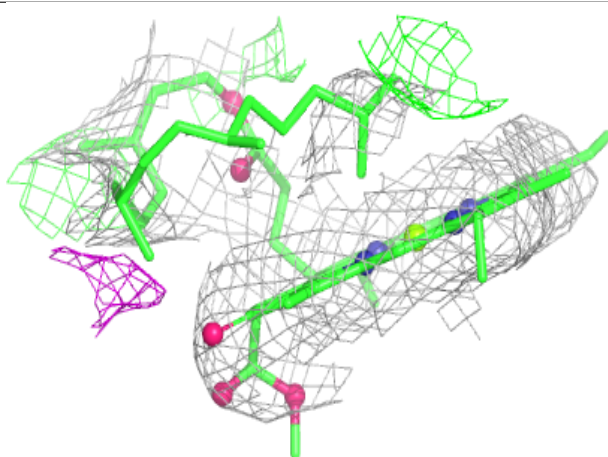
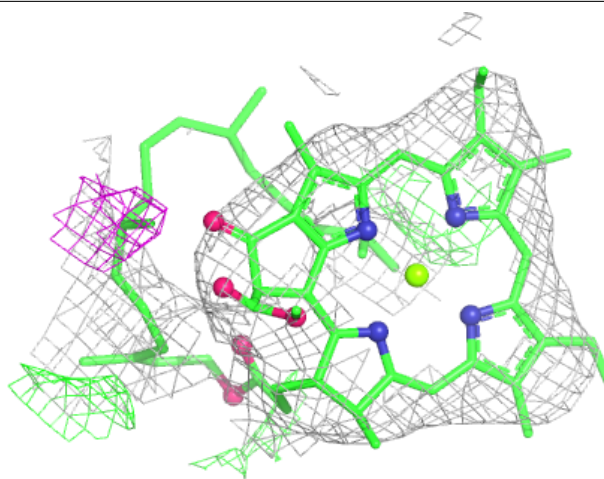
**Electron density around PQ9 a 6043:**

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



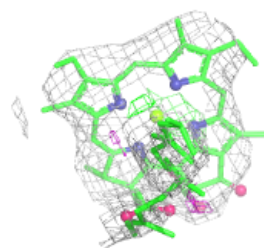
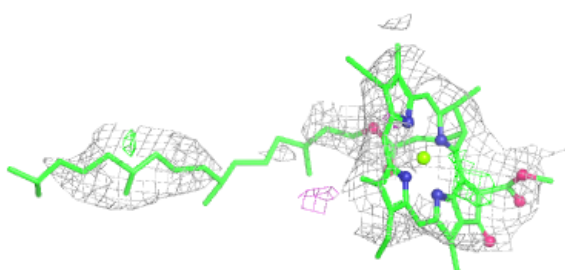
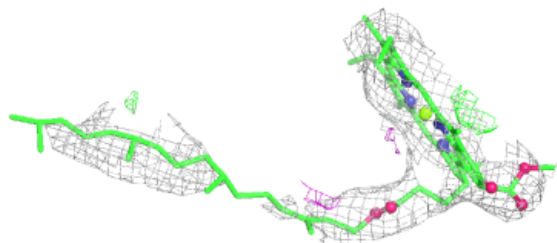
Electron density around CLA C 1026:

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

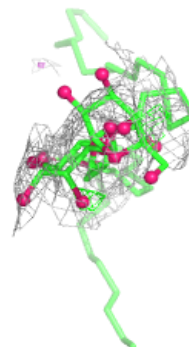
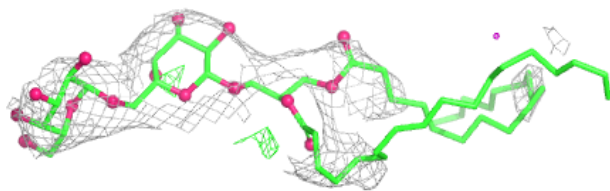


Electron density around CLA b 6015:

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

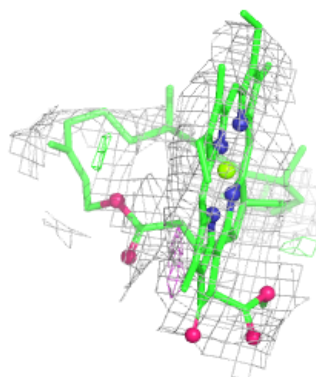
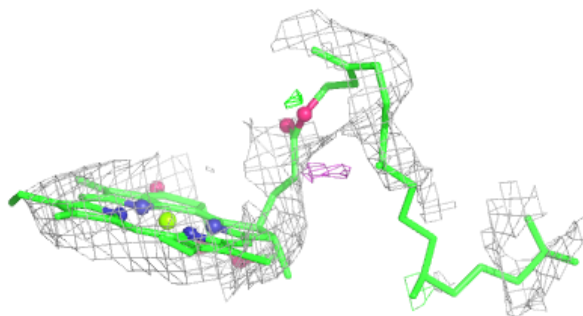
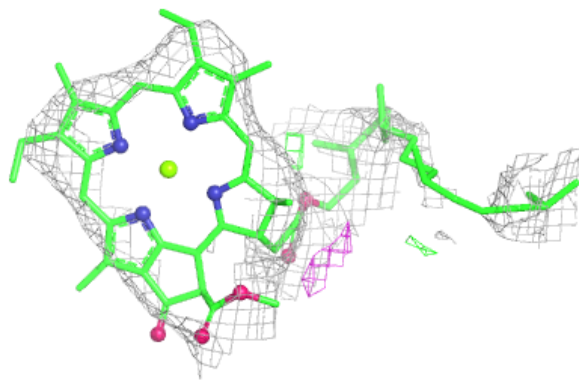
**Electron density around DGD c 6055:**

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

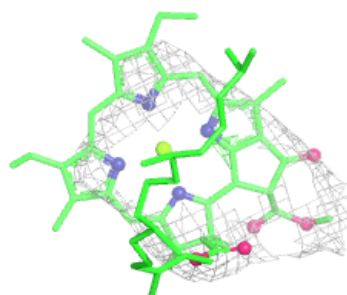
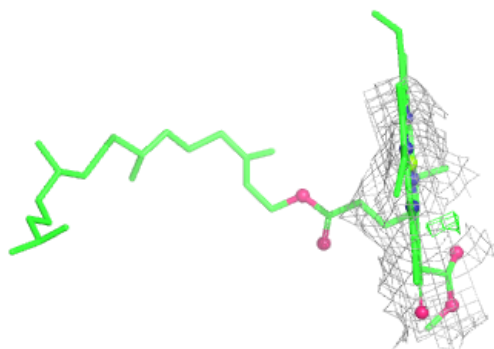
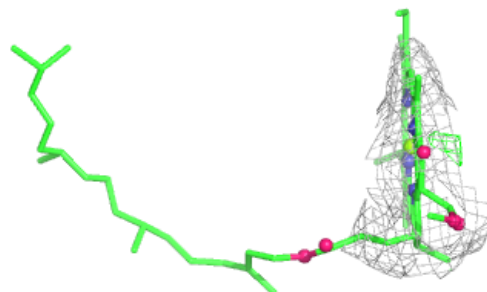


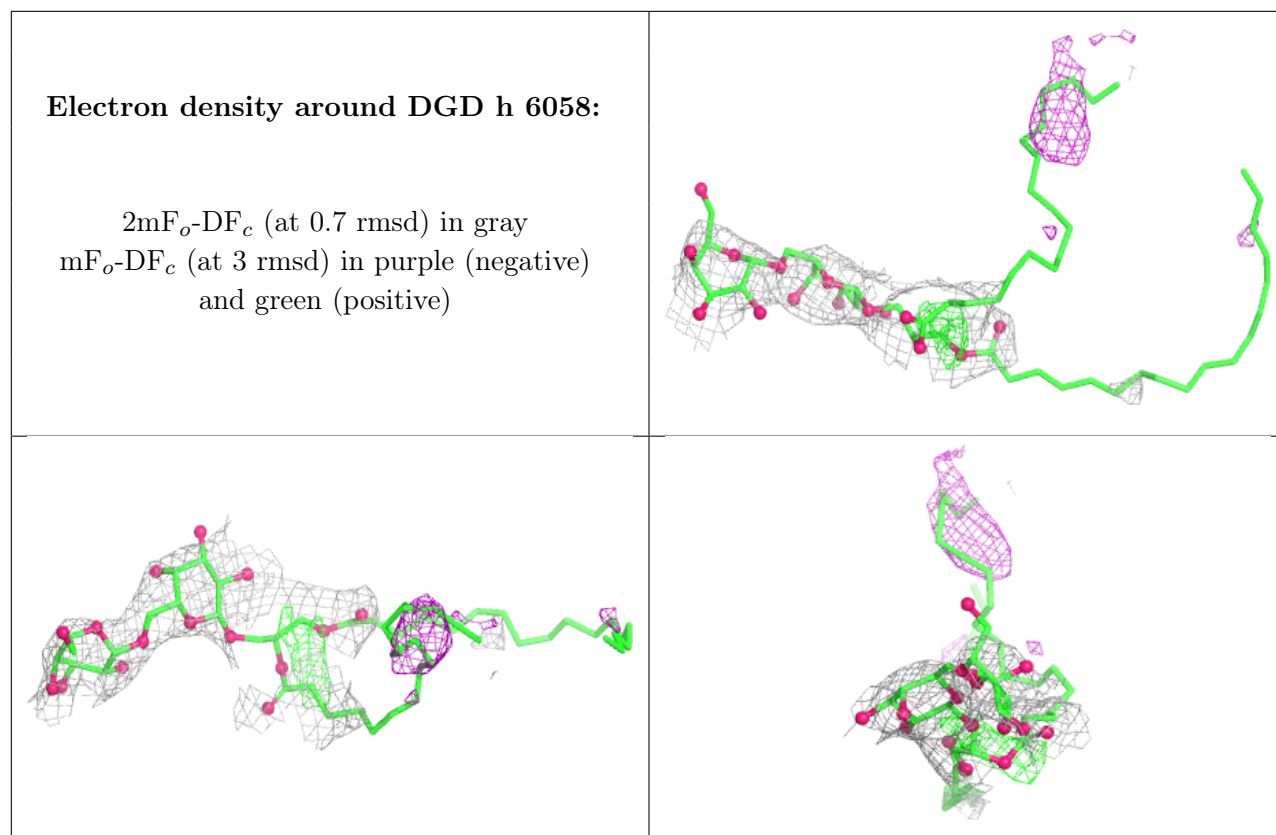
Electron density around CLA a 6006:

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

**Electron density around CLA a 6007:**

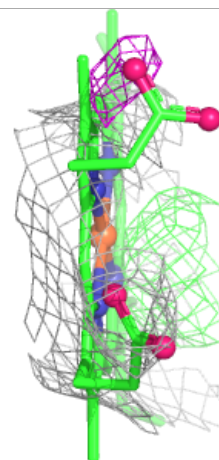
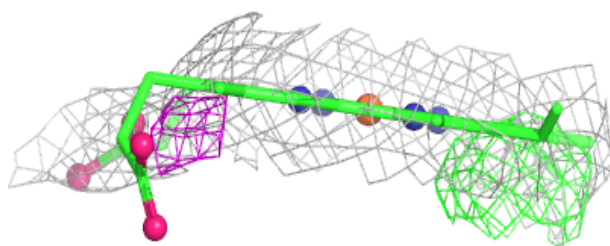
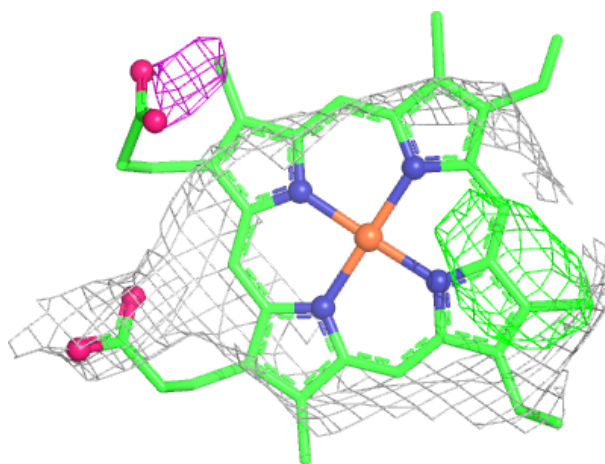
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





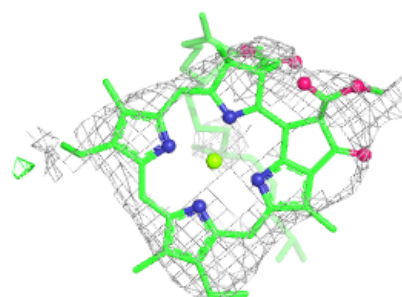
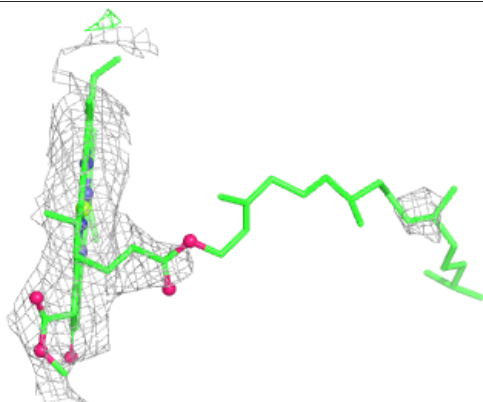
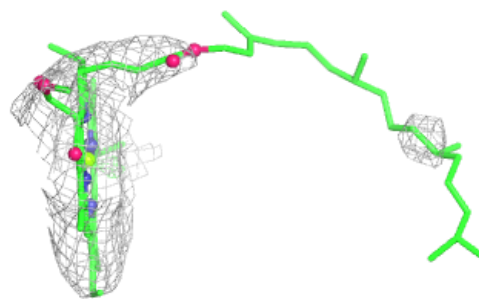
Electron density around HEM e 6040:

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

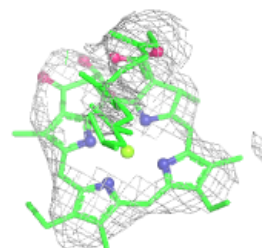
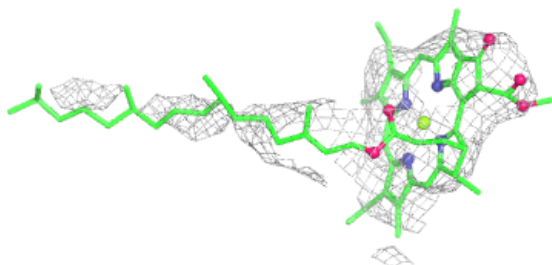
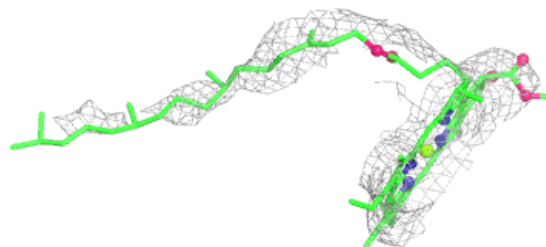


Electron density around CLA A 1007:

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

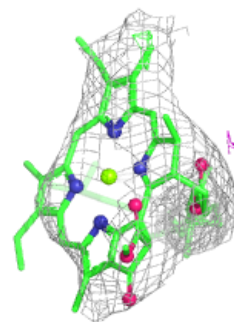
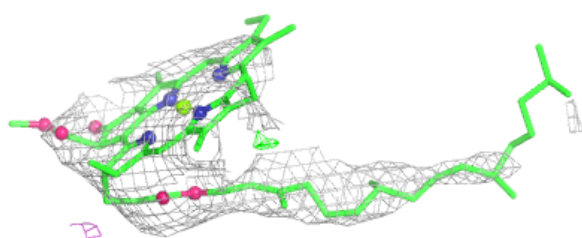
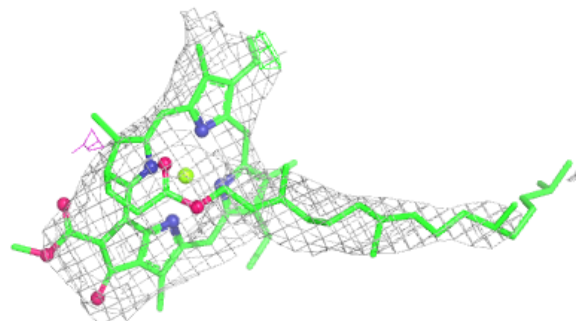
**Electron density around CLA B 1015:**

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

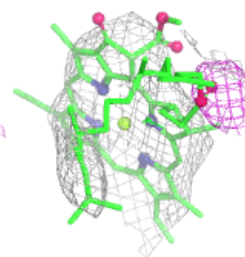
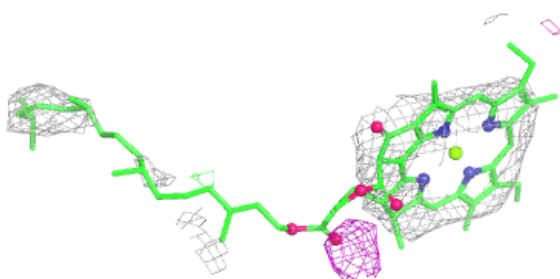
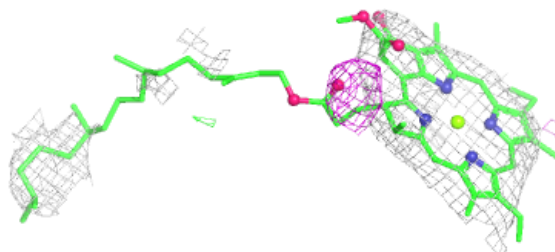


Electron density around CLA B 1016:

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

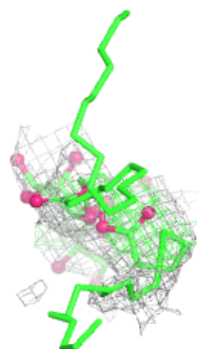
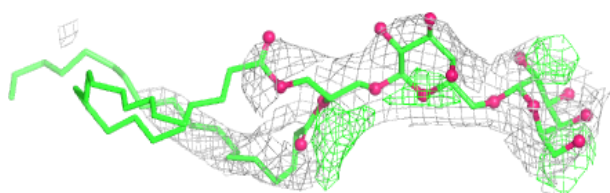
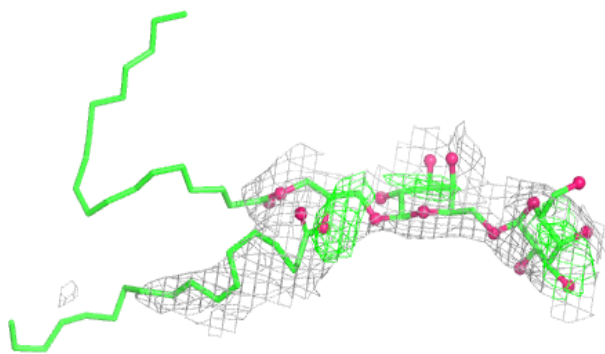
**Electron density around CLA A 1003:**

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

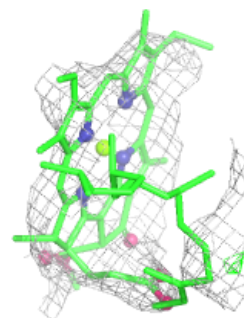
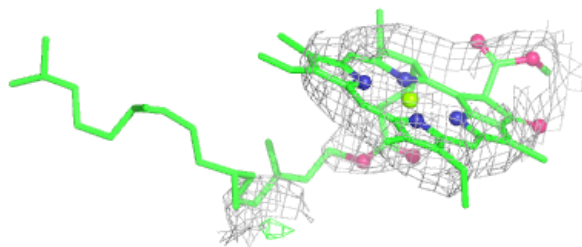
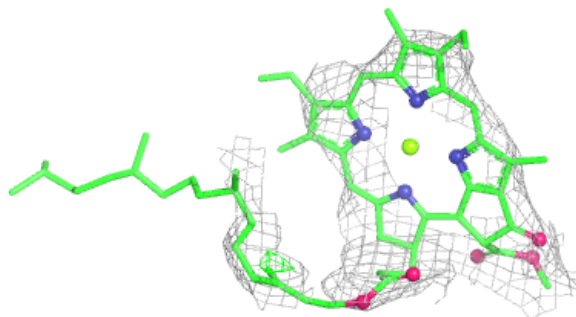


Electron density around DGD C 1055:

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

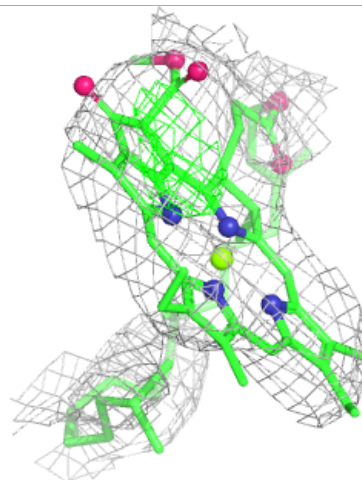
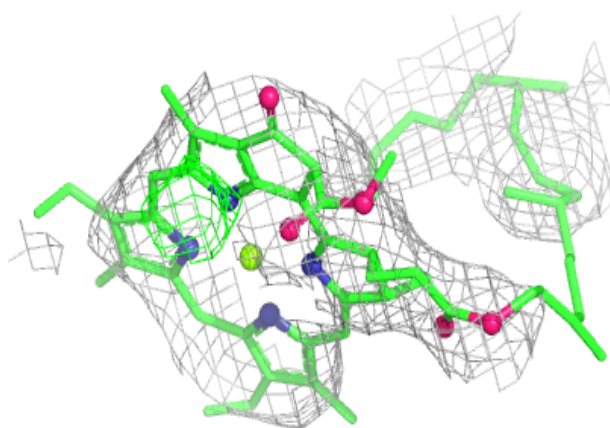
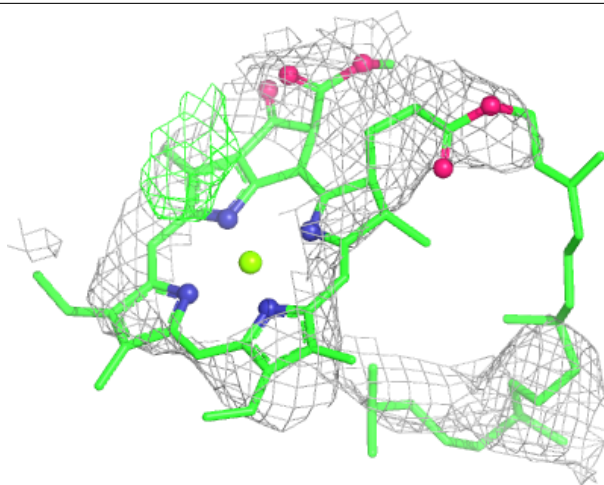
**Electron density around CLA D 1008:**

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



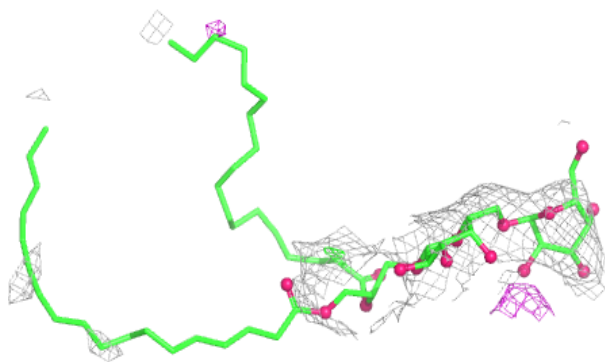
Electron density around CLA B 1023:

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

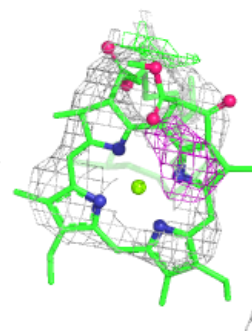
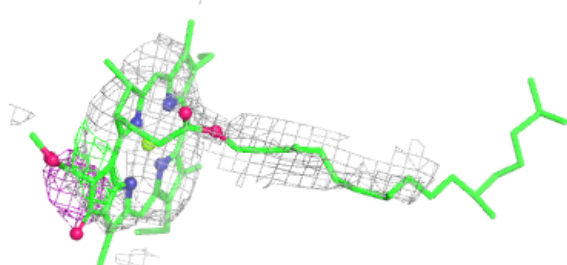
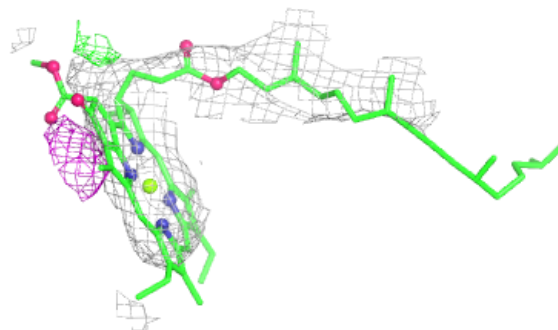


Electron density around DGD H 1058:

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

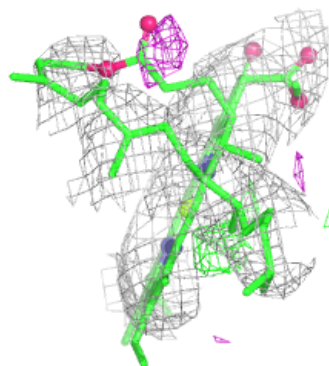
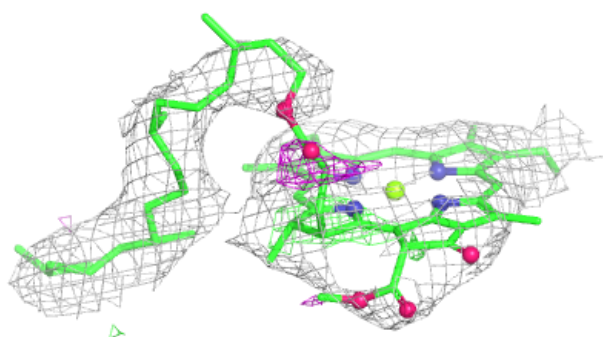
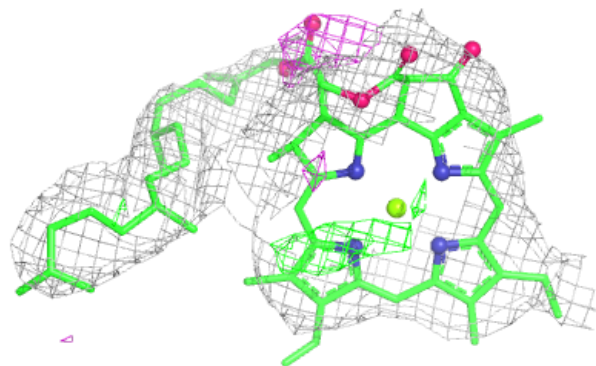
**Electron density around CLA B 1013:**

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

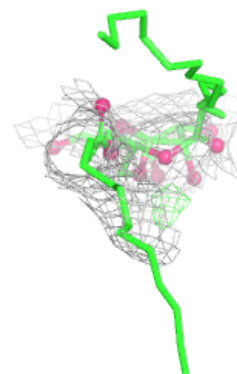
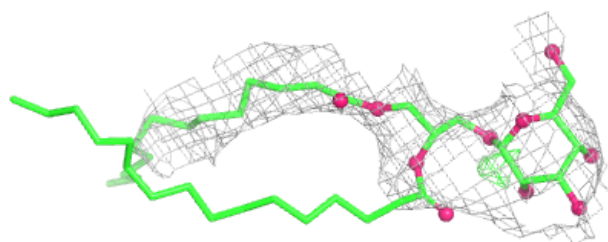
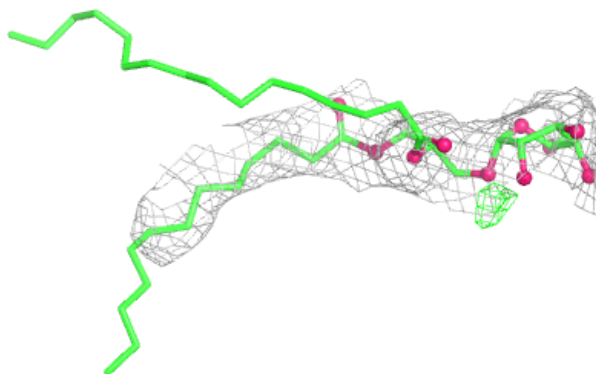


Electron density around CLA d 6005:

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

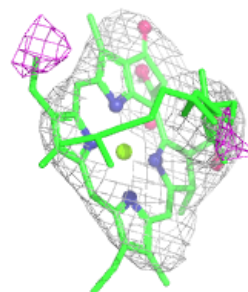
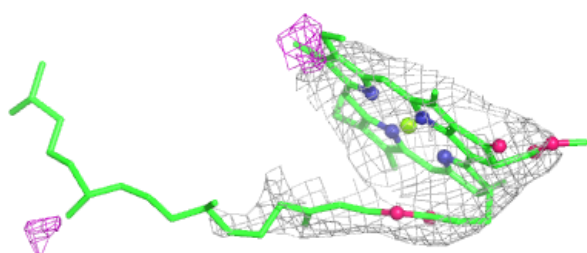
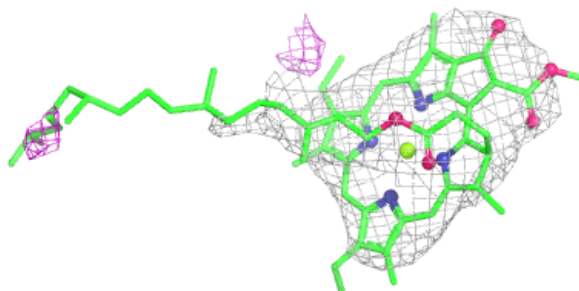
**Electron density around MGE D 1062:**

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

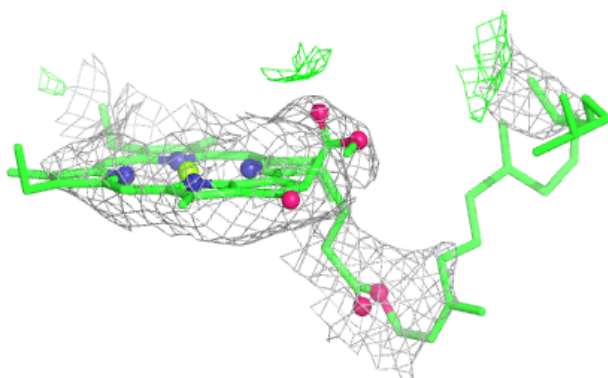
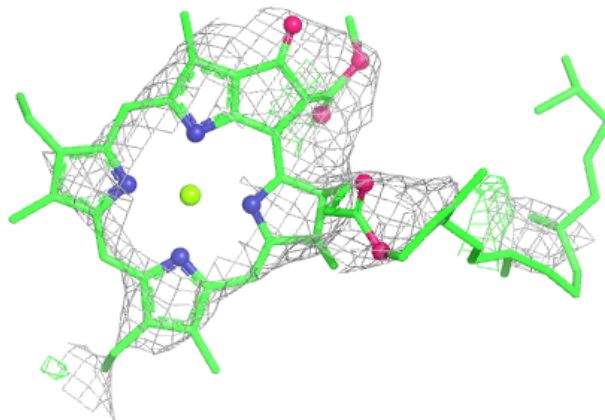


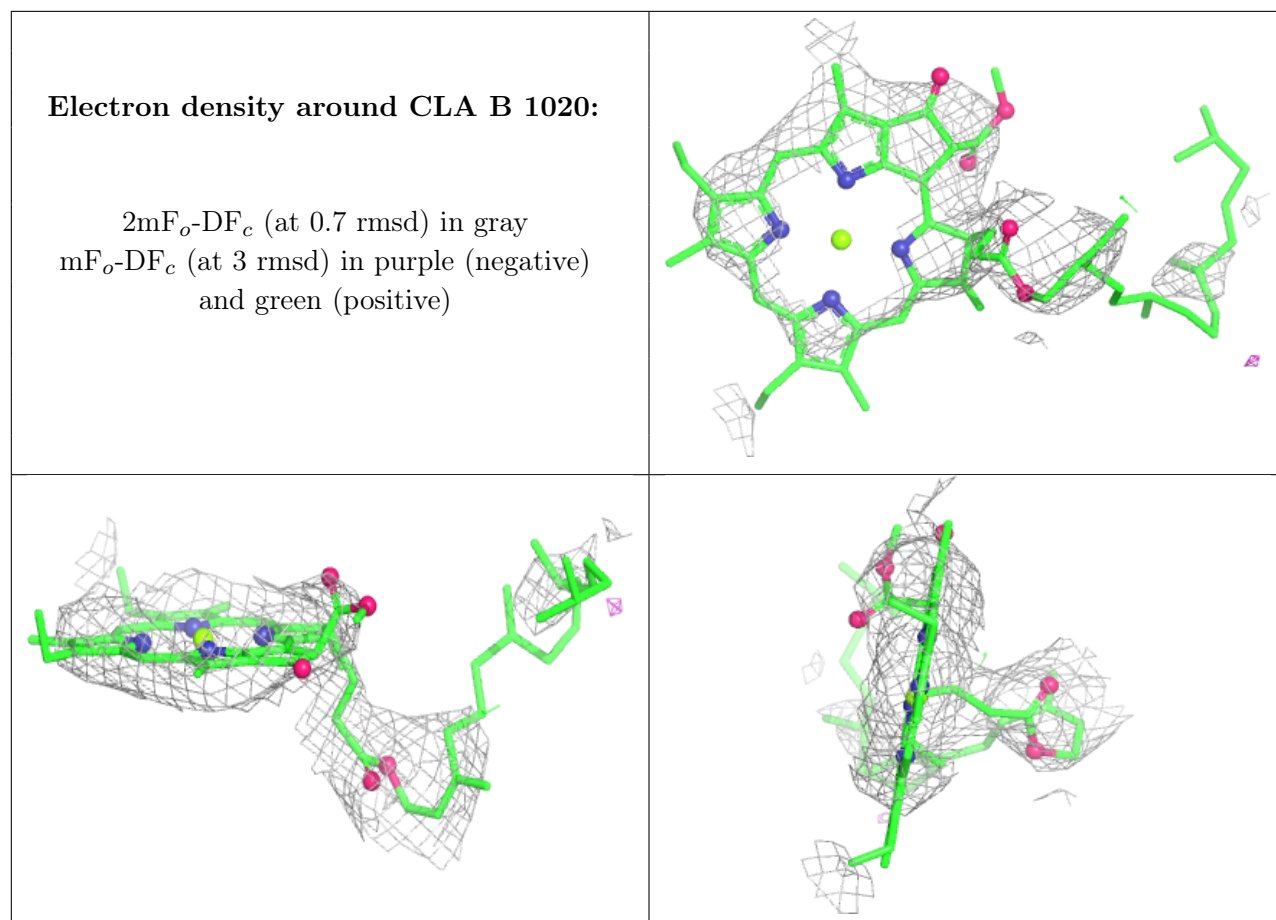
Electron density around CLA b 6016:

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

**Electron density around CLA b 6020:**

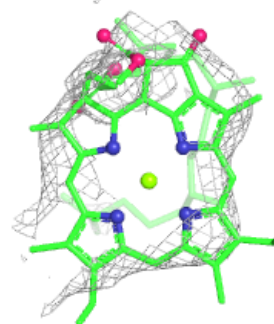
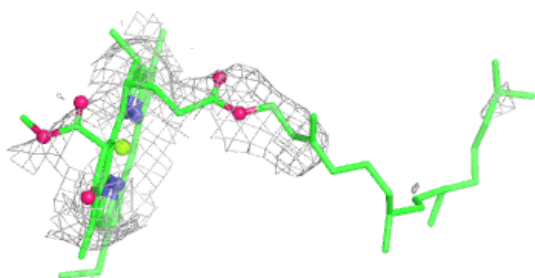
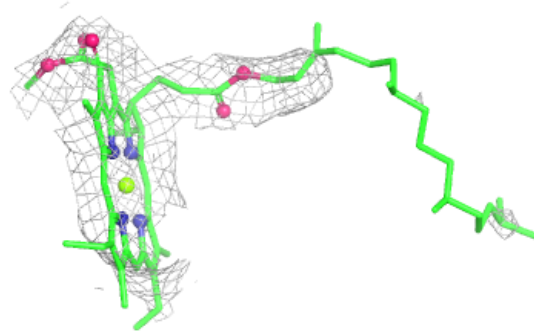
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



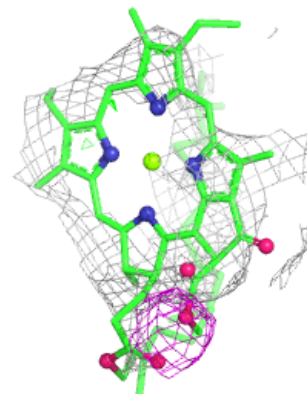
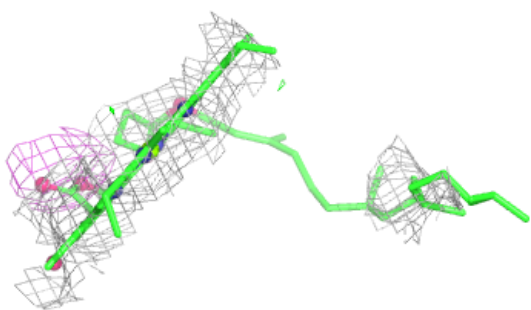
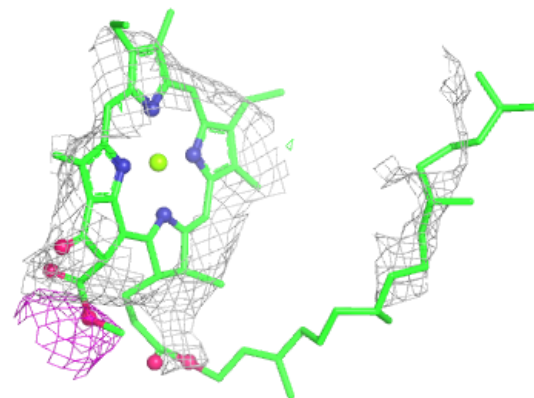


Electron density around CLA C 1030:

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

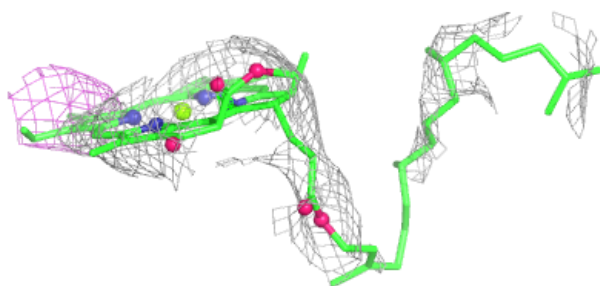
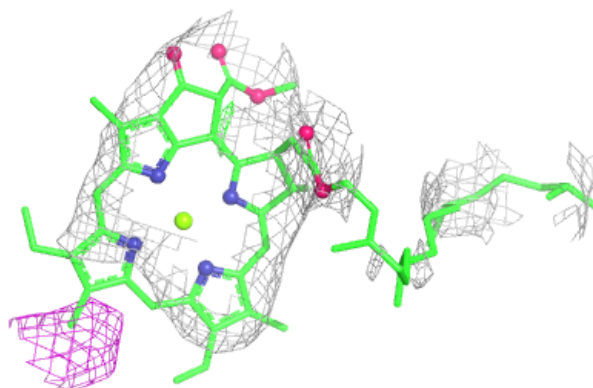
**Electron density around CLA C 1031:**

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



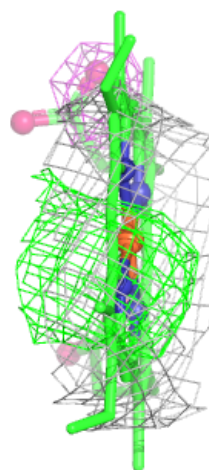
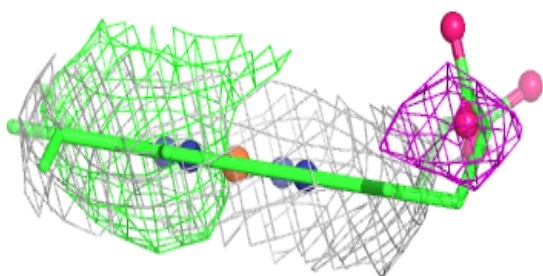
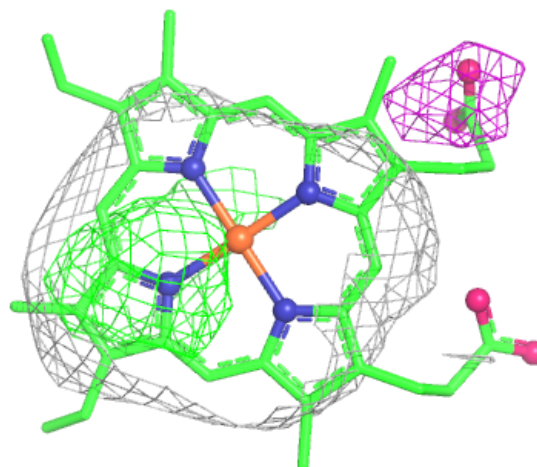
Electron density around CLA A 1006:

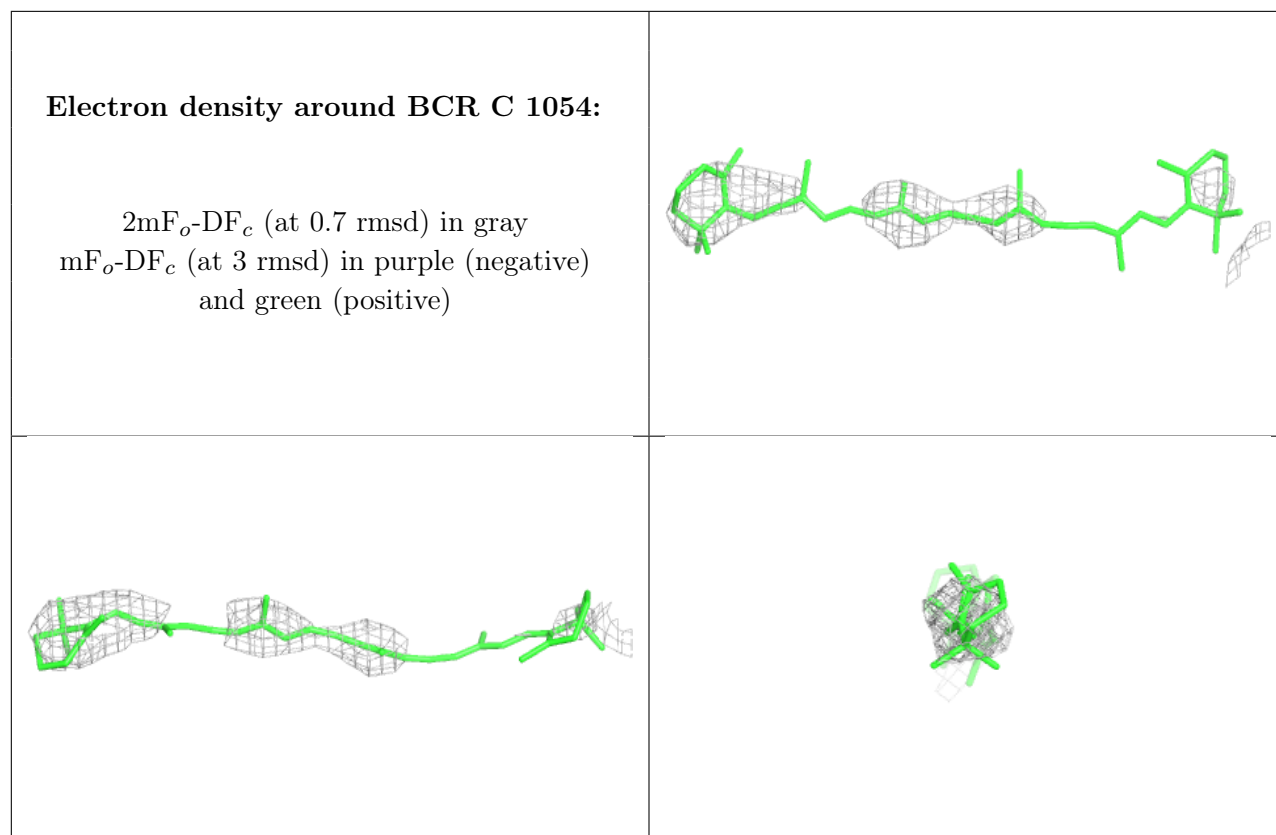
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

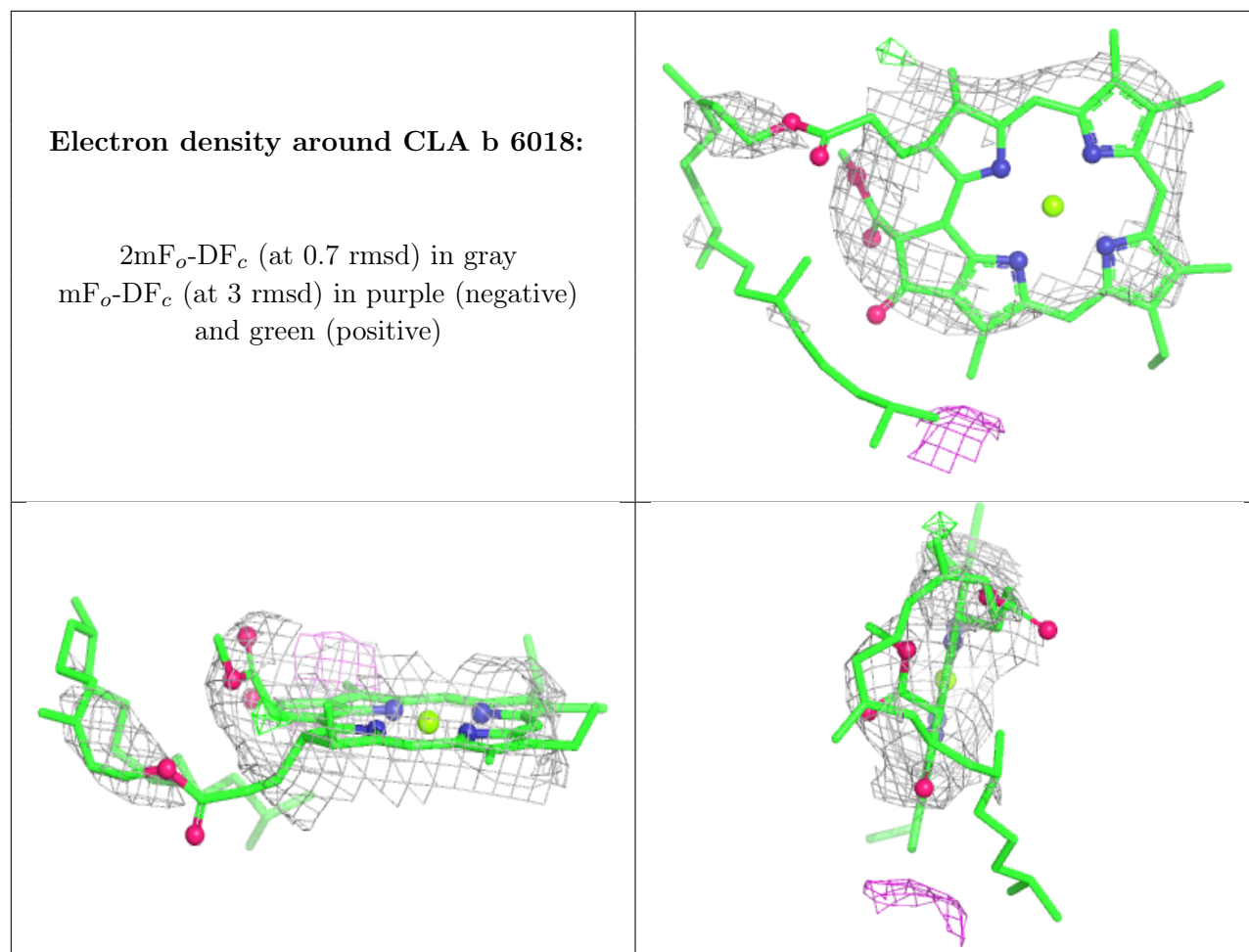


Electron density around HEM E 1040:

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

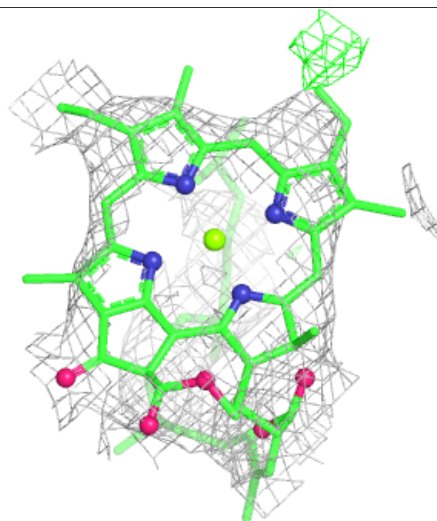
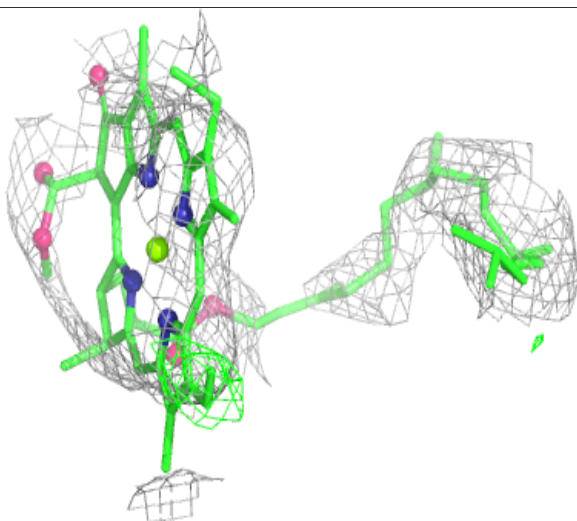
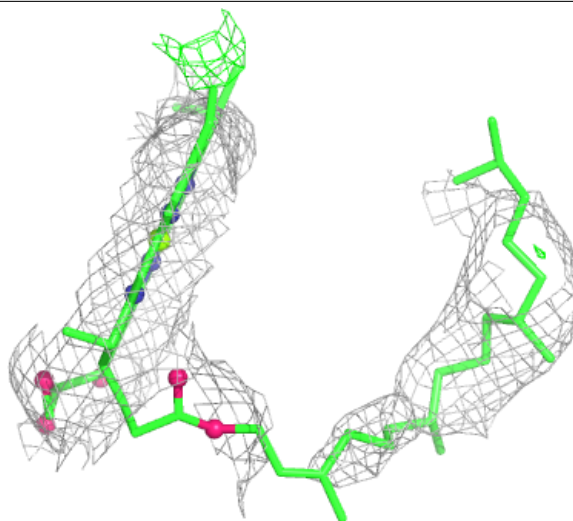






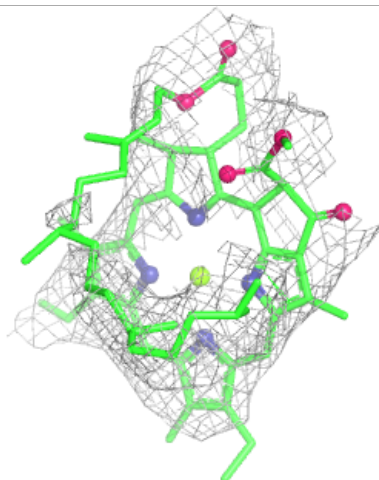
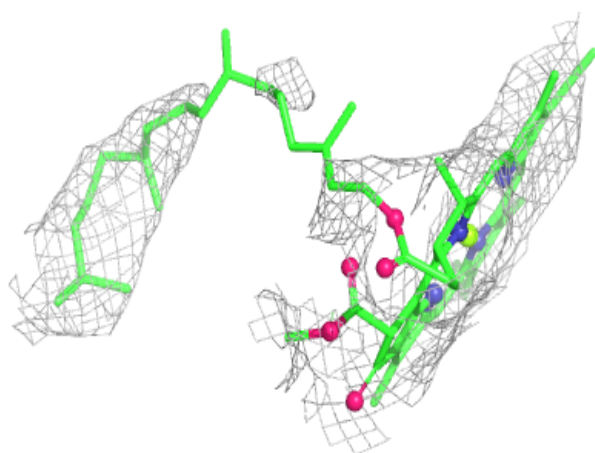
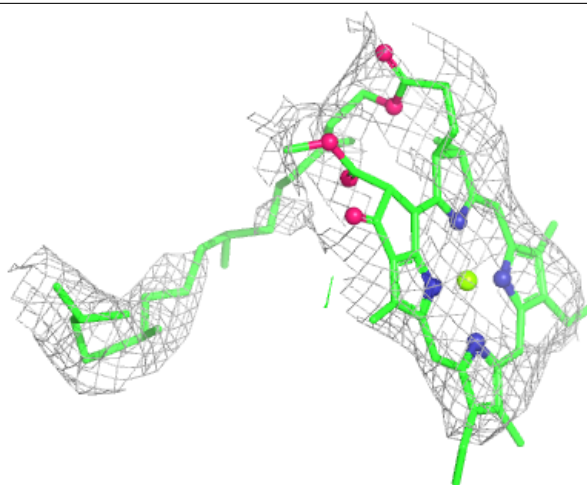
Electron density around CLA b 6019:

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



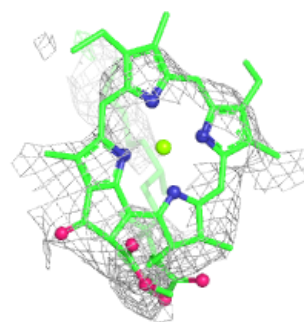
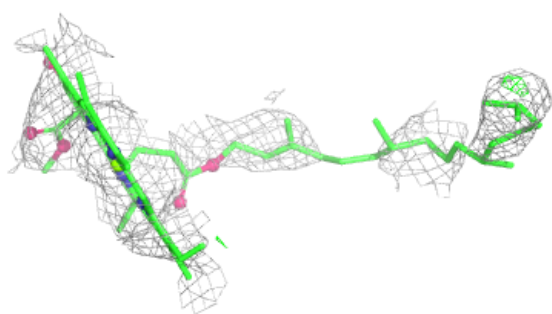
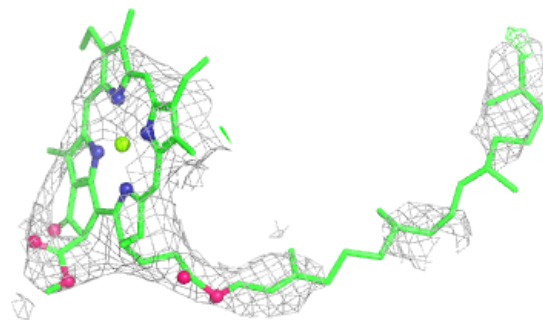
Electron density around CLA B 1021:

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

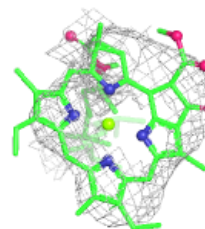
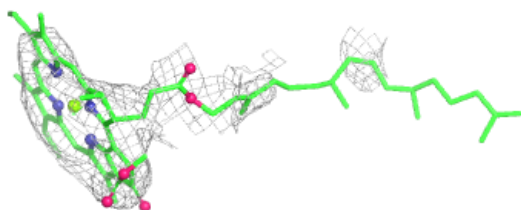
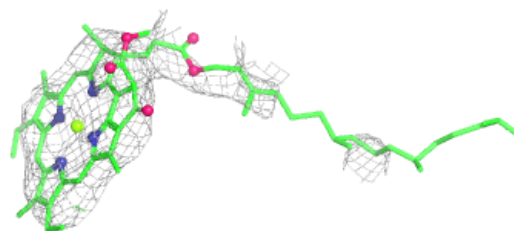


Electron density around CLA H 1017:

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

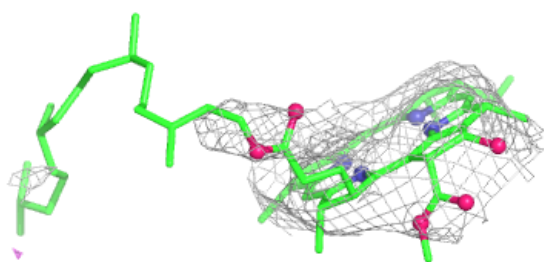
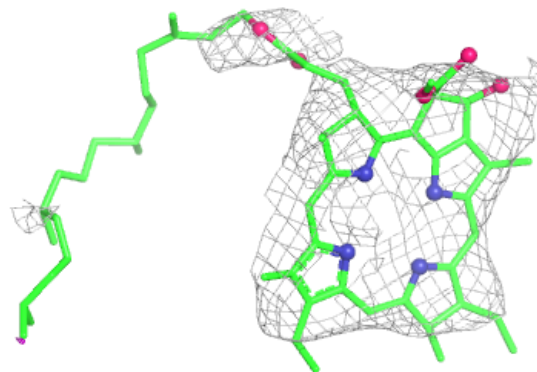
**Electron density around CLA B 1012:**

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

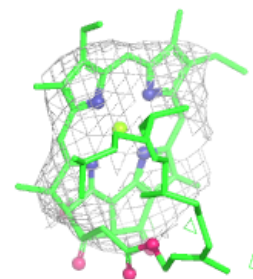
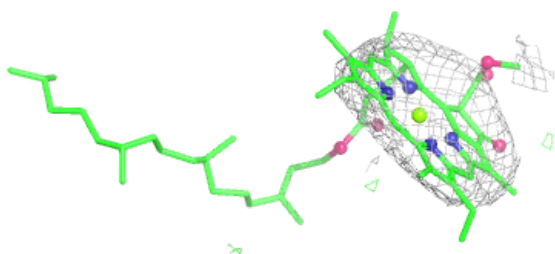
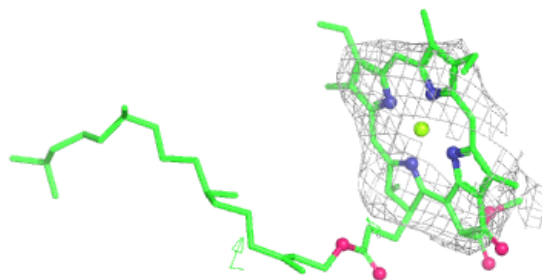


Electron density around PHO A 1039:

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

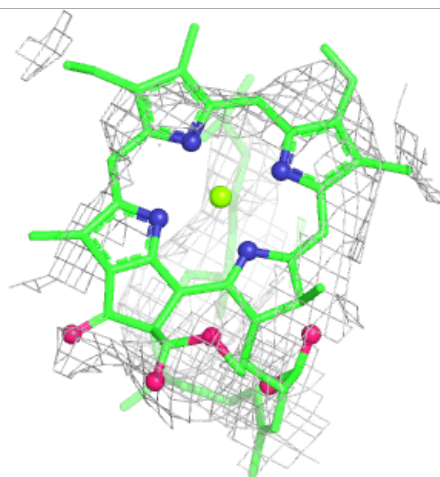
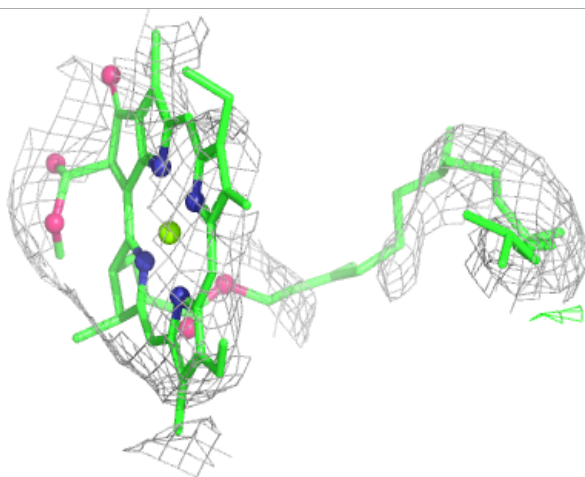
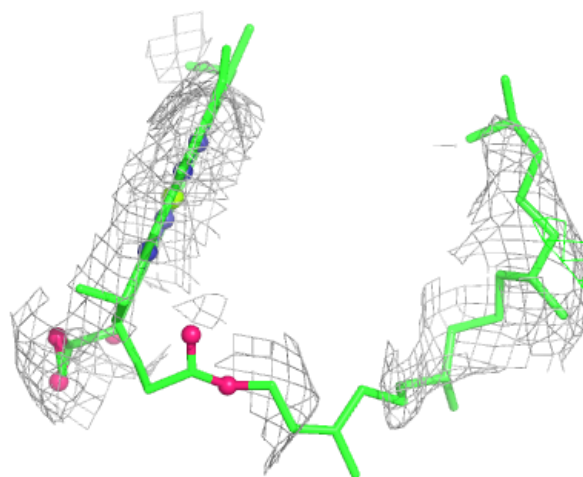
**Electron density around CLA C 1035:**

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



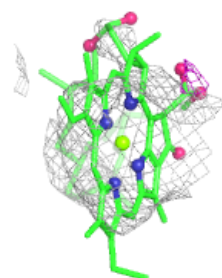
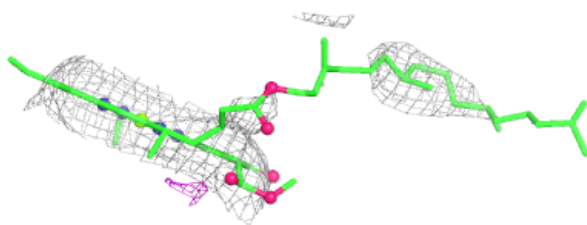
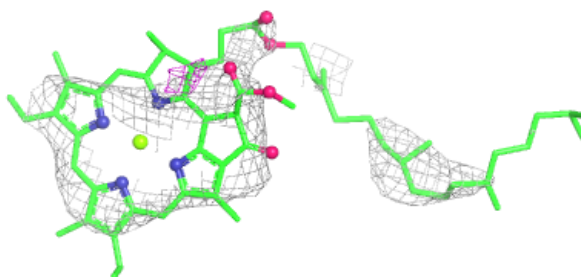
Electron density around CLA B 1019:

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

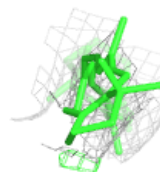
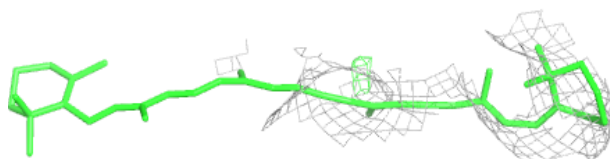
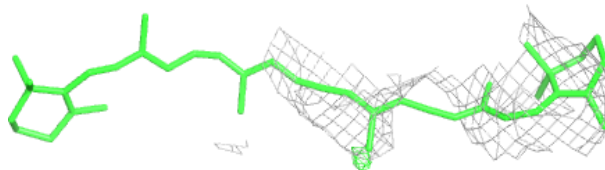


Electron density around CLA B 1010:

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

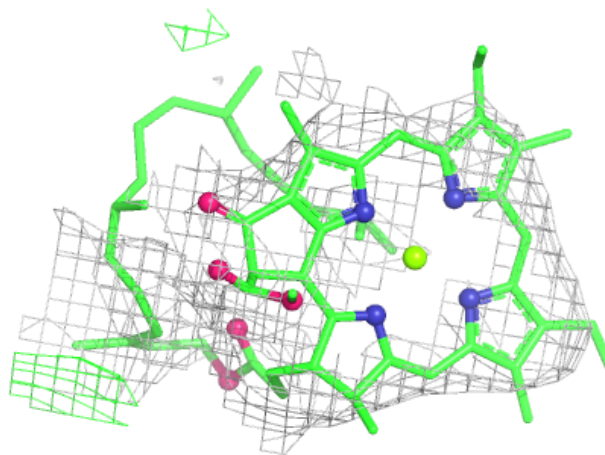
**Electron density around BCR k 6051:**

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



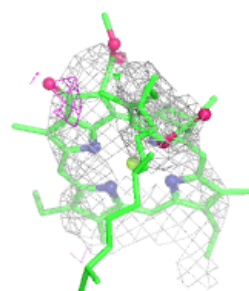
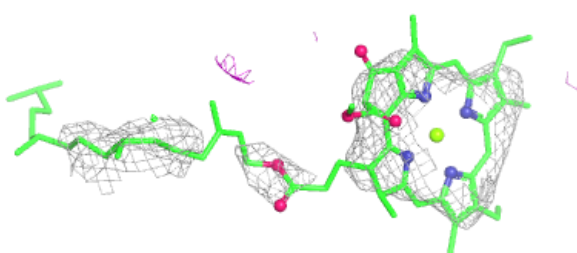
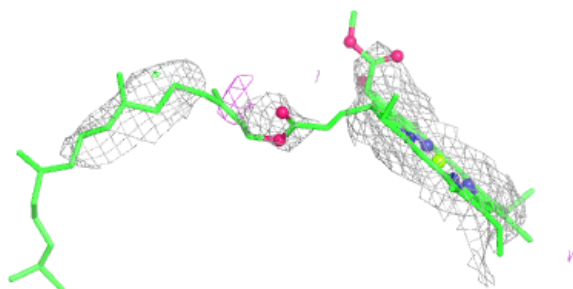
Electron density around CLA c 6026:

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

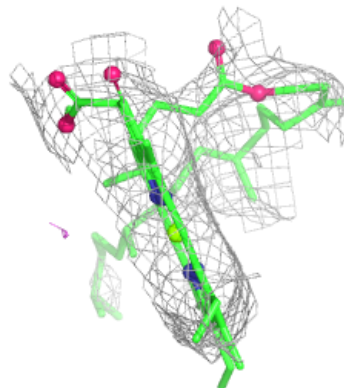
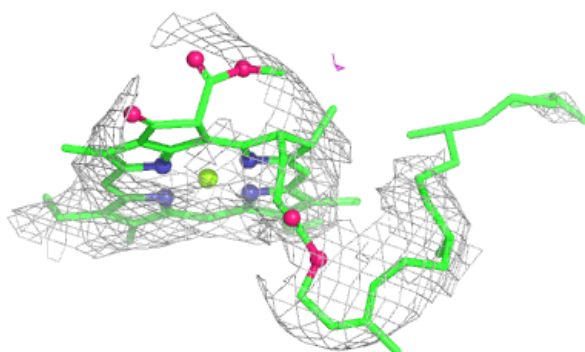
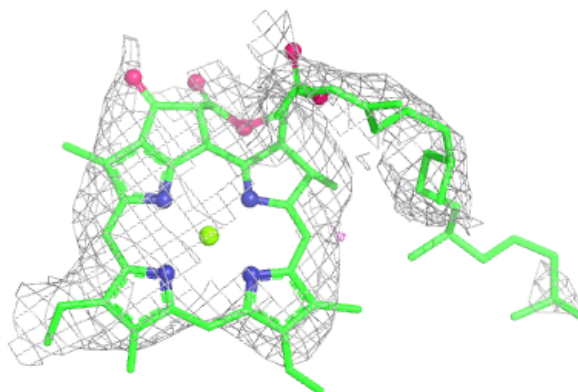


Electron density around CLA D 1004:

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

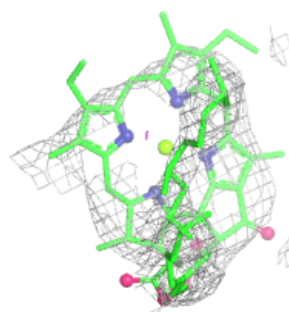
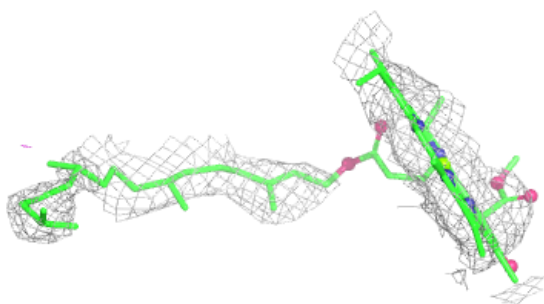
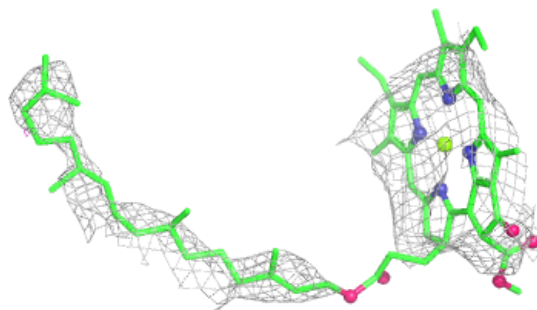
**Electron density around CLA D 1005:**

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

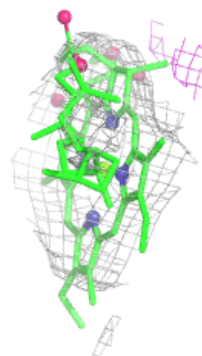
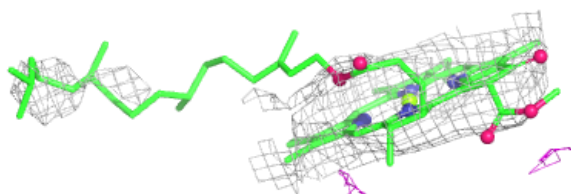
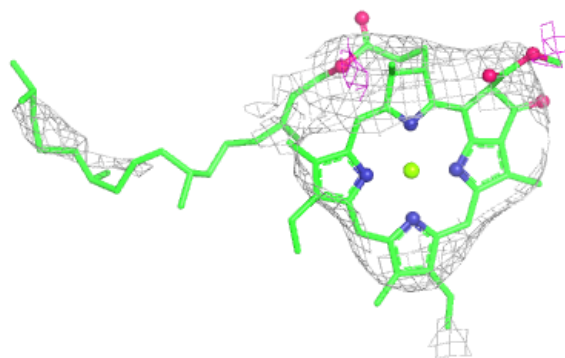


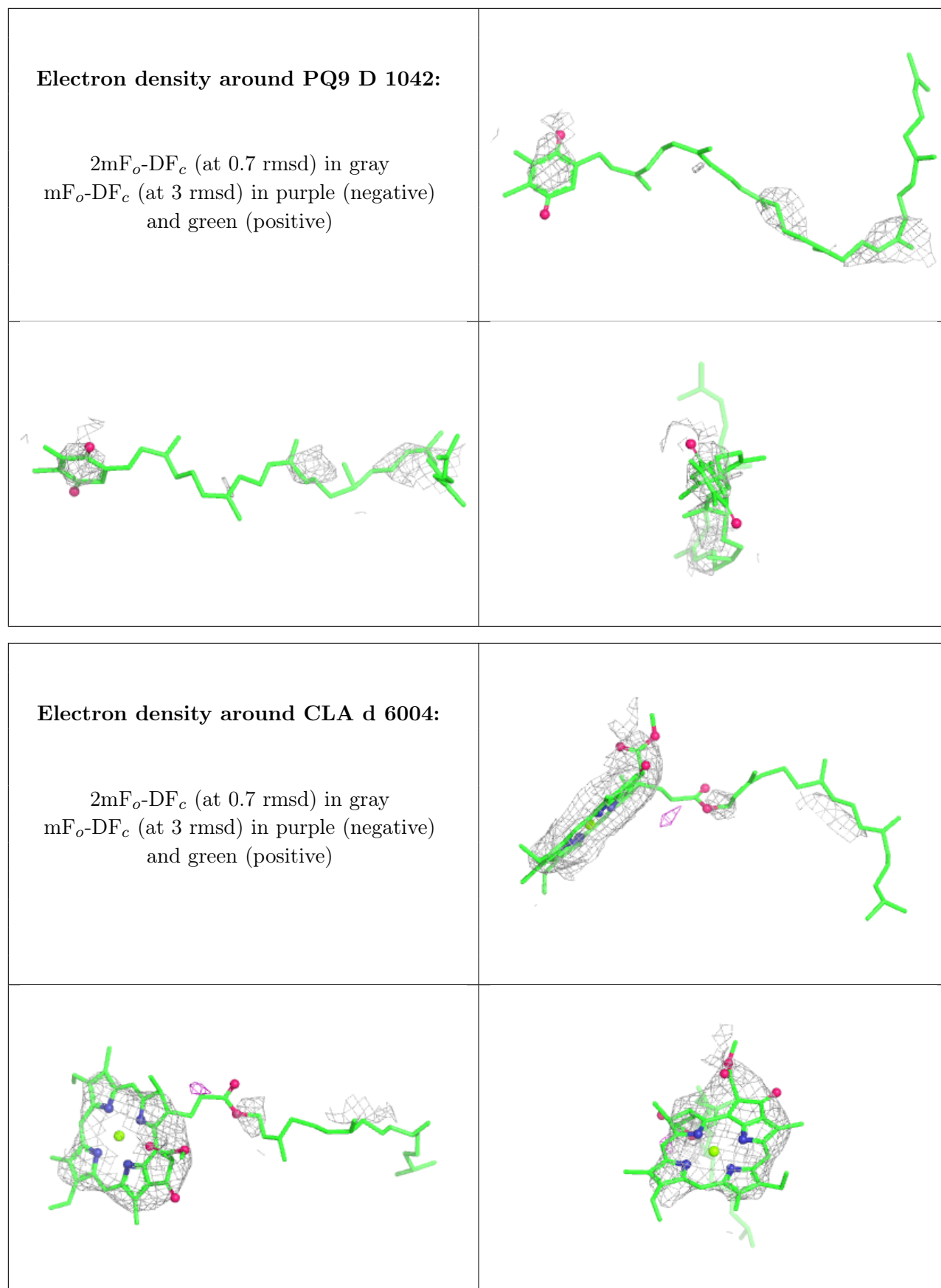
Electron density around CLA b 6017:

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

**Electron density around CLA B 1011:**

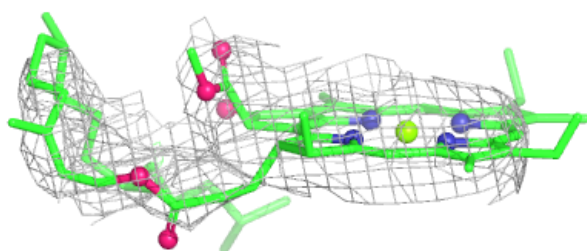
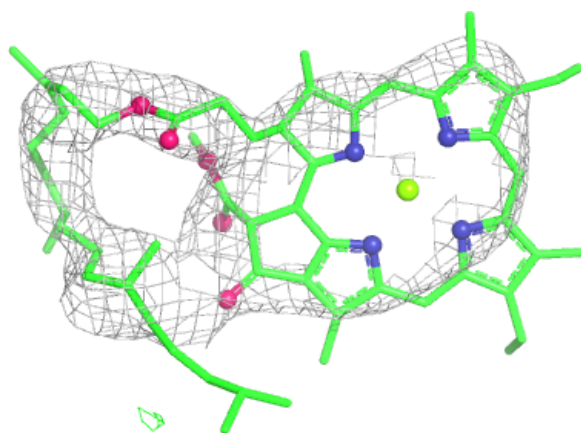
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



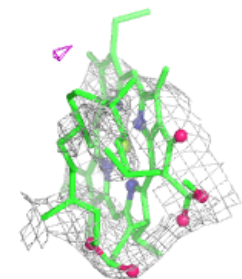
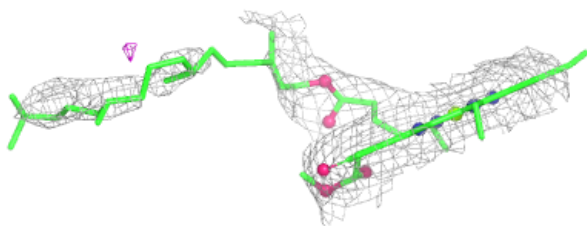
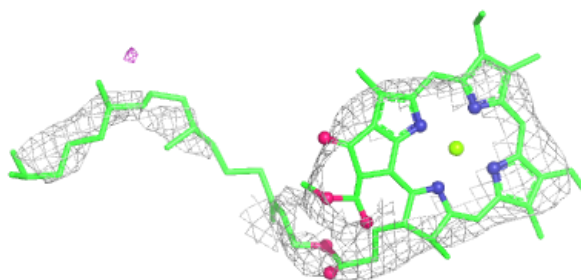


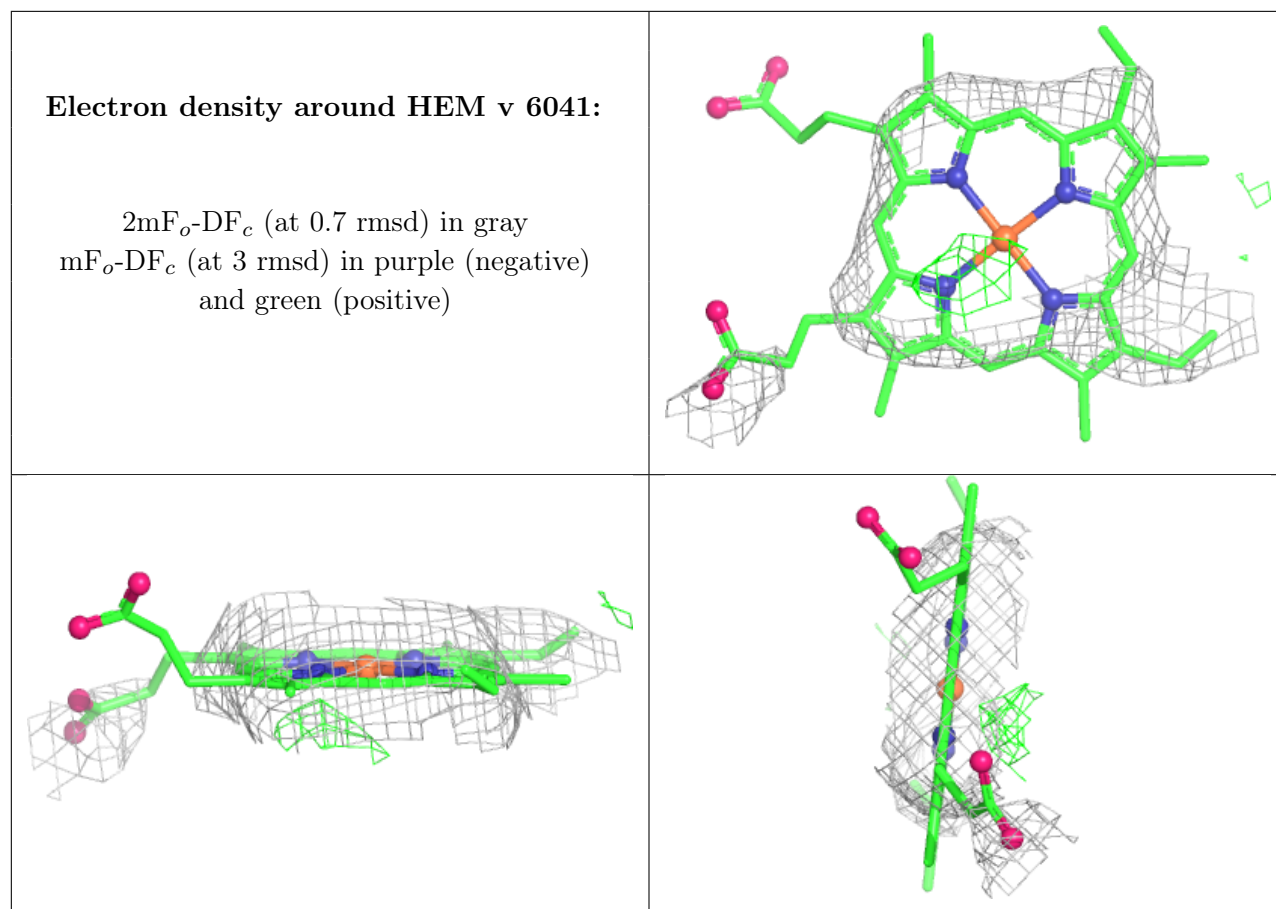
Electron density around CLA B 1018:

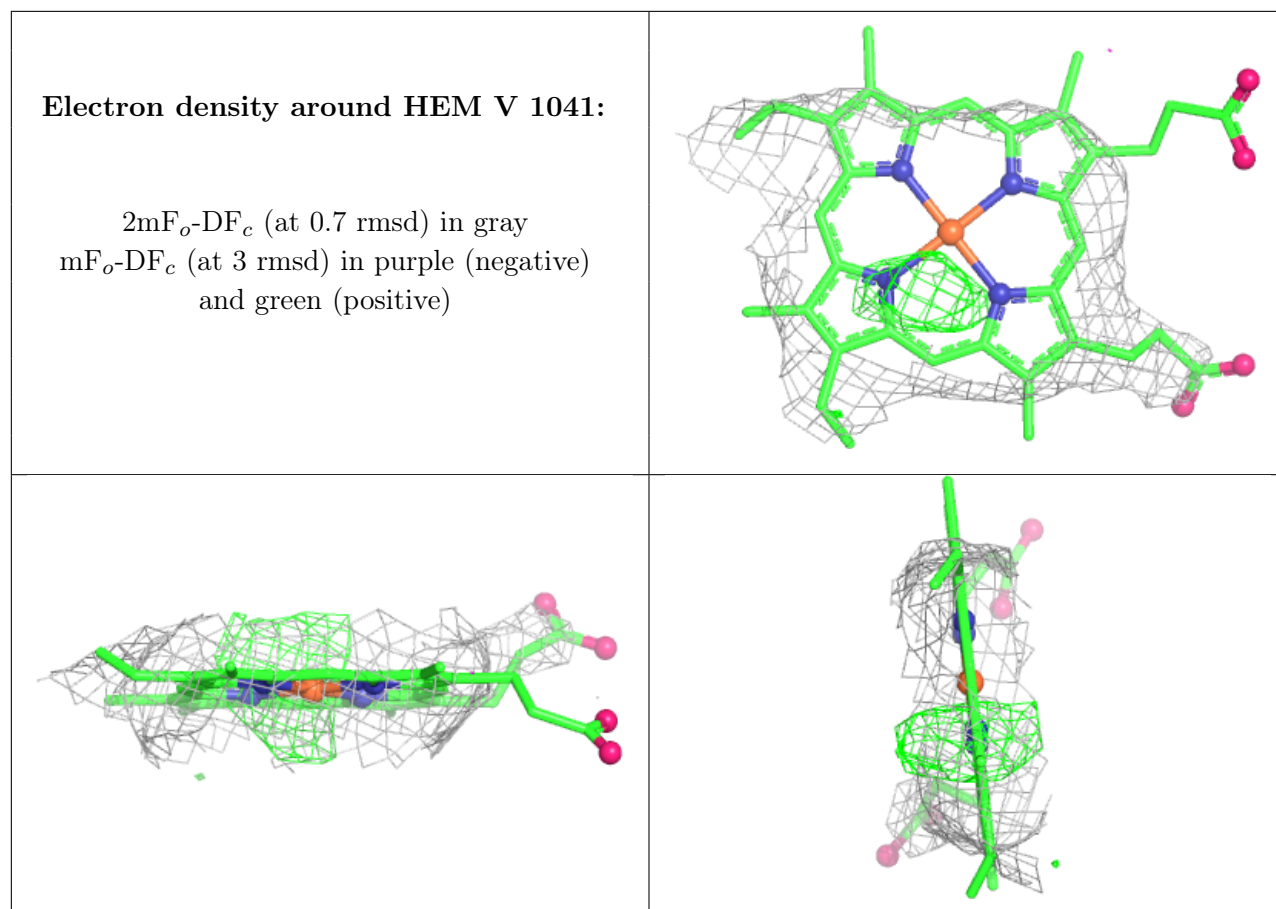
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA b 6010:**

$2mF_o-DF_c$ (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.