



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:49 PM UTC

PDB ID : 8F4E / pdb_00008f4e
Title : RT XFEL structure of Photosystem II 250 microseconds after the third illumination at 2.09 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.09 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

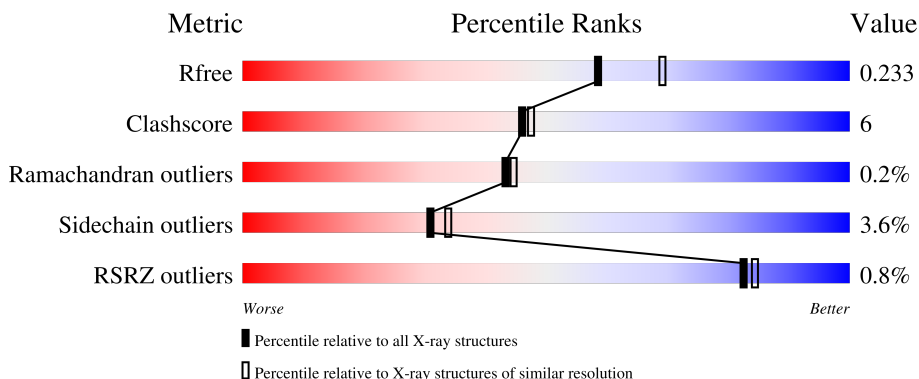
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	

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

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Mol	Chain	Length	Quality of chain
1	a	344	% 82% 14% ..
2	B	510	86% 12% ..
2	b	510	% 88% 10% .
3	C	461	87% 9% .
3	c	461	86% 11% ..
4	D	352	86% 10% ..
4	d	352	82% 14% ..
5	E	84	4% 86% 12% .
5	e	84	2% 73% 25% .
6	F	45	64% 9% . 24%
6	f	45	44% 24% 7% 24%
7	H	66	2% 91% 8% .
7	h	66	3% 80% 15% 5%
8	I	38	87% 8% 5%
8	i	38	79% 16% 5%
9	J	40	68% 22% 10%
9	j	40	2% 78% 12% 10%
10	K	46	72% 9% 20%
10	k	46	50% 30% 20%
11	L	37	86% 14%
11	l	37	86% 11% .
12	M	36	78% 14% 8%
12	m	36	75% 8% 6% 11%
13	O	272	76% 13% 10%
13	o	272	% 74% 15% 10%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	610	X	-	-	-
25	CLA	A	613	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	H	101	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	613	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	h	101	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54466 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	Total 4005	C 2631	N 666	O 695	S 13	0	4	0
2	b	505	Total 3978	C 2610	N 665	O 690	S 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	442	Total 3592	C 2355	N 601	O 621	S 15	0	11	0
3	c	451	Total 3666	C 2396	N 617	O 638	S 15	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	Total 2745	C 1818	N 448	O 467	S 12	0	2	0
4	d	341	Total 2751	C 1822	N 448	O 469	S 12	0	3	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	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	256	171	37	47	1	0	0	0
12	m	32	251	168	36	46	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	244	1870	1168	313	385	4	0	1	0
13	o	244	1874	1170	317	383	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	258	181	36	39	2	0	0	0
14	t	30	256	180	36	38	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	97	774	491	129	154	0	0	0
15	u	97	774	491	129	154	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 Ycf12.

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

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

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

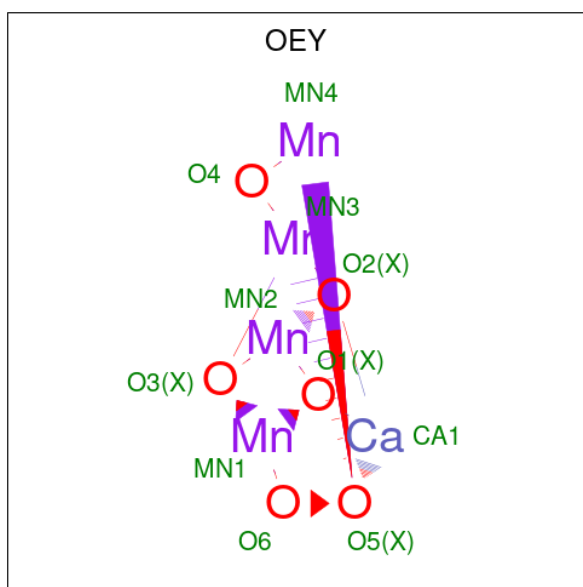
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

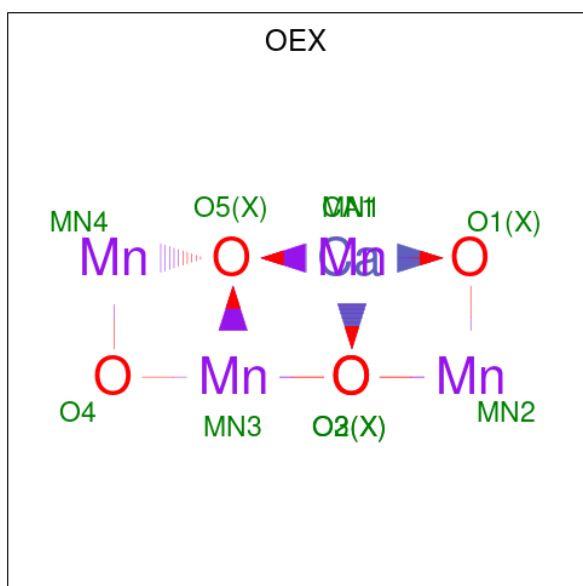
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O	S	0	0	0
			246	166	43	37				

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



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

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



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

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

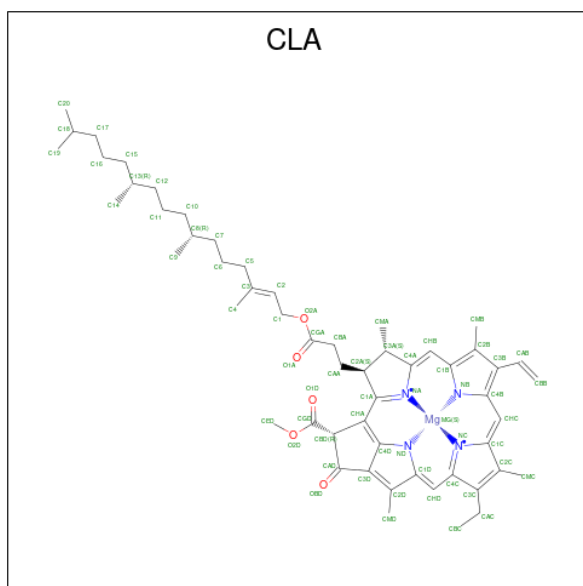
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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

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

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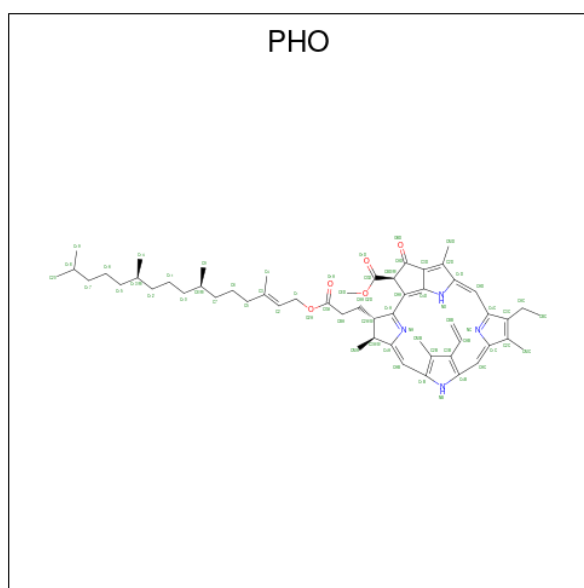
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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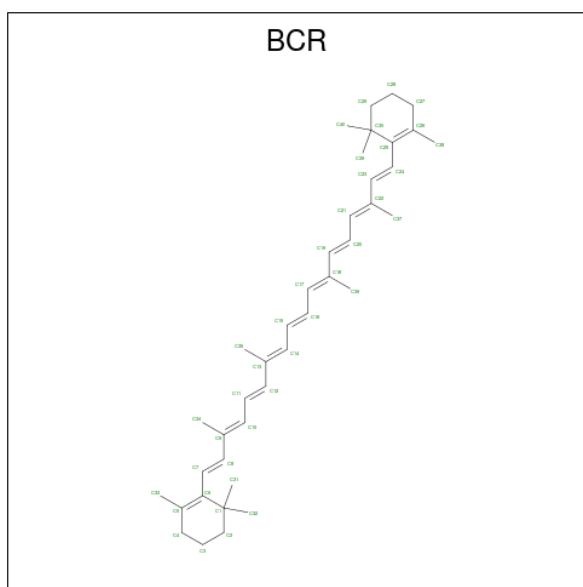
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



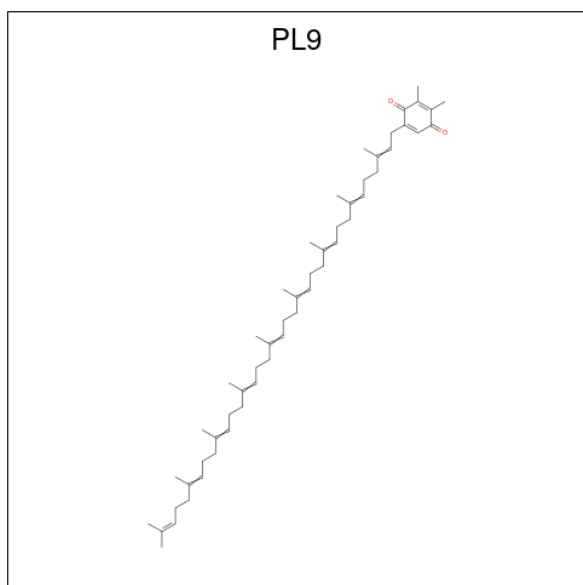
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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

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



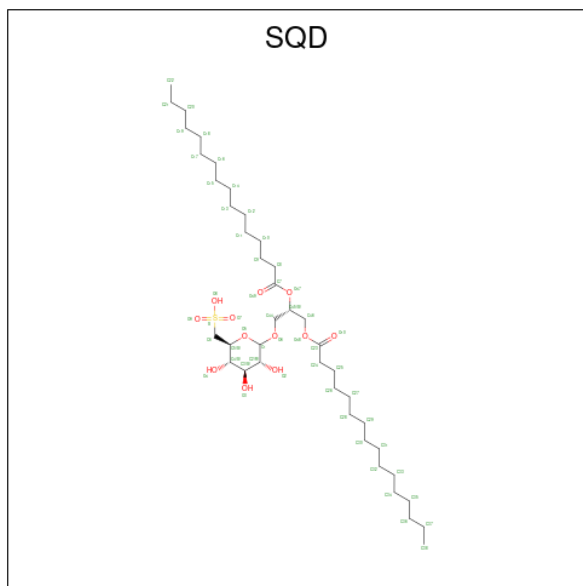
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

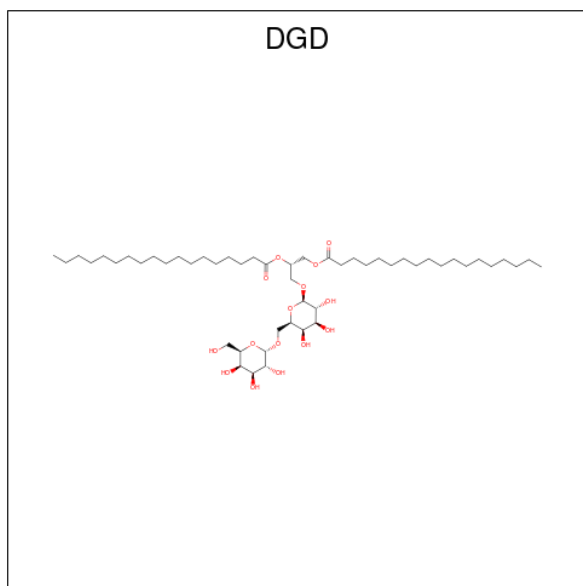
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			39	35	4			
29	F	1	Total	C	O	S	0	0
			36	25	10	1		
29	L	1	Total	C	O	S	0	0
			49	36	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O		0	0
			36	31	5			
29	f	1	Total	C	O	S	0	0
			41	28	12	1		
29	l	1	Total	C	O	S	0	0
			54	41	12	1		

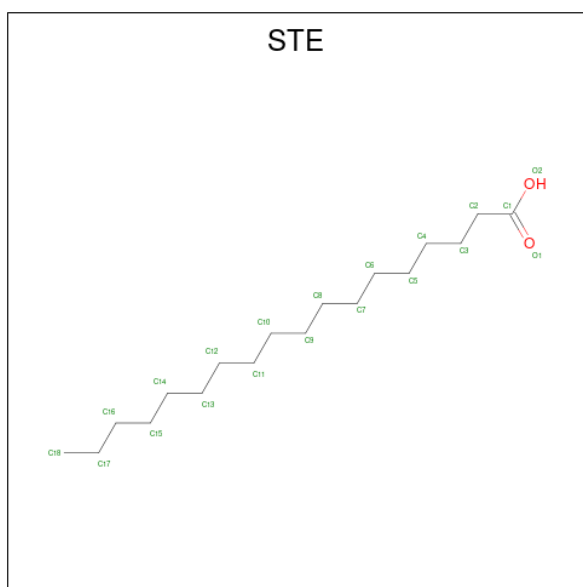
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

C₅₁H₉₆O₁₅).



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

- Molecule 31 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



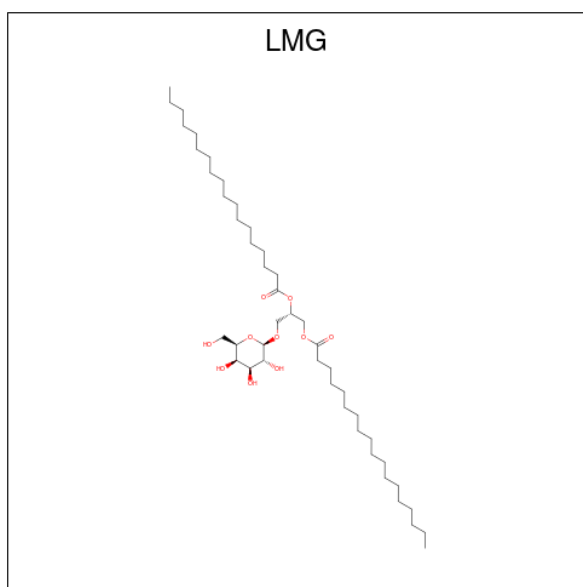
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 17 15 2	0	0
31	B	1	Total C O 12 10 2	0	0
31	B	1	Total C O 18 16 2	0	0
31	B	1	Total C O 12 10 2	0	0
31	B	1	Total C 16 16	0	0
31	C	1	Total C O 12 10 2	0	0
31	C	1	Total C O 12 10 2	0	0
31	C	1	Total C 16 16	0	0
31	D	1	Total C O 20 18 2	0	0
31	H	1	Total C 18 18	0	0
31	I	1	Total C 15 15	0	0
31	J	1	Total C O 12 10 2	0	0
31	M	1	Total C O 15 13 2	0	0
31	M	1	Total C 10 10	0	0

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

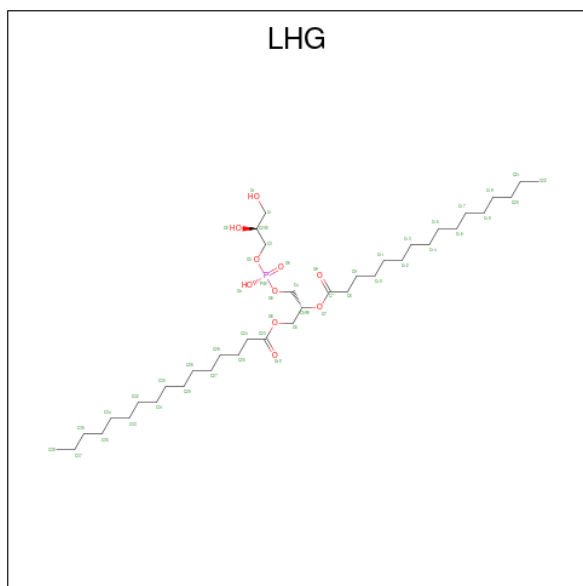
- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
32	B	1	28	24	4	0	0
32	C	1	48	38	10	0	0
32	C	1	48	38	10	0	0
32	D	1	51	41	10	0	0
32	D	1	33	27	6	0	0
32	M	1	51	41	10	0	0
32	b	1	55	45	10	0	0
32	c	1	37	27	10	0	0
32	c	1	48	38	10	0	0
32	c	1	49	39	10	0	0
32	d	1	23	21	2	0	0
32	d	1	44	34	10	0	0
32	m	1	51	41	10	0	0

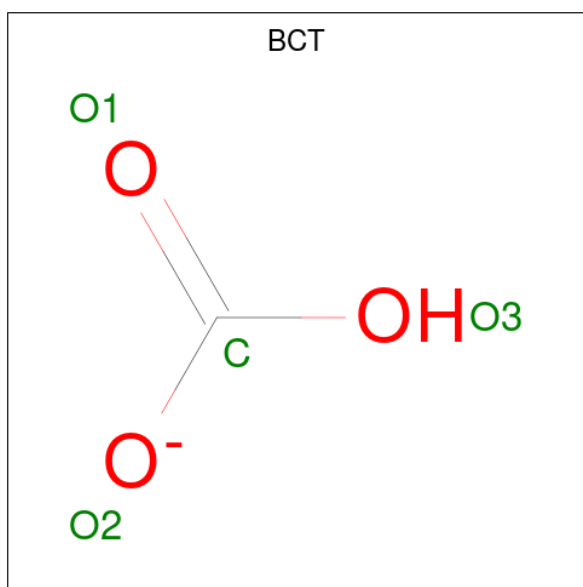
- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG)

(formula: C₃₈H₇₅O₁₀P).



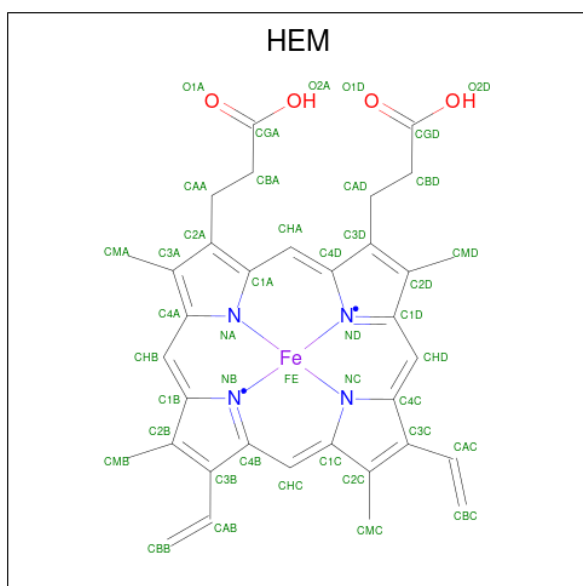
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			47	36	10	1		
33	E	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			39	28	10	1		
33	e	1	Total	C	O	P	0	0
			42	31	10	1		
33	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



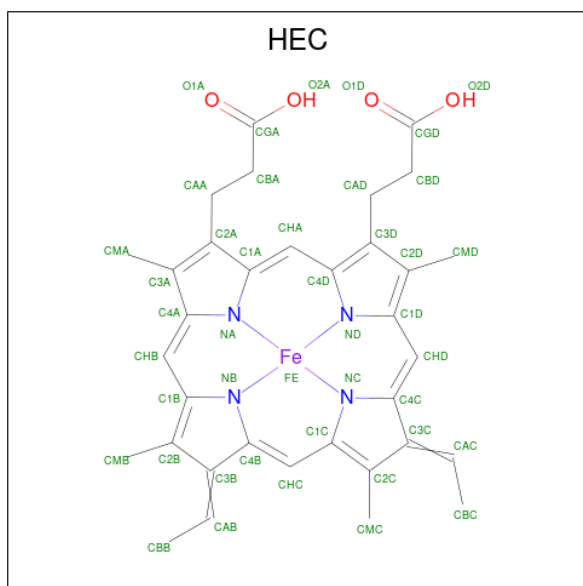
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	130	Total	O	0	4
			138	138		
37	B	191	Total	O	0	0
			191	191		
37	C	159	Total	O	0	0
			159	159		
37	D	119	Total	O	0	0
			119	119		
37	E	28	Total	O	0	0
			28	28		
37	F	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	33	Total O 33 33	0	0
37	I	21	Total O 21 21	0	0
37	J	10	Total O 10 10	0	0
37	K	5	Total O 5 5	0	0
37	L	7	Total O 7 7	0	0
37	M	4	Total O 4 4	0	0
37	O	91	Total O 91 91	0	0
37	T	13	Total O 13 13	0	0
37	U	46	Total O 46 46	0	0
37	V	58	Total O 58 58	0	0
37	Y	6	Total O 6 6	0	0
37	X	6	Total O 6 6	0	0
37	Z	8	Total O 8 8	0	0
37	R	7	Total O 7 7	0	0
37	a	117	Total O 125 125	0	4
37	b	184	Total O 184 184	0	0
37	c	166	Total O 166 166	0	0
37	d	105	Total O 105 105	0	0
37	e	26	Total O 26 26	0	0
37	f	7	Total O 7 7	0	0
37	h	23	Total O 23 23	0	0

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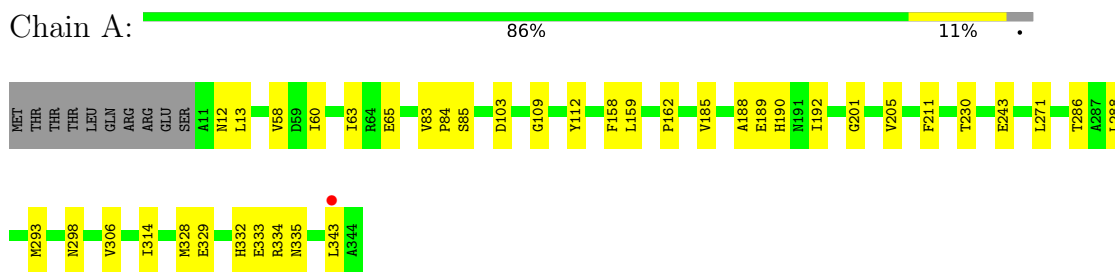
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	i	15	Total O 15 15	0	0
37	j	5	Total O 5 5	0	0
37	k	6	Total O 6 6	0	0
37	l	14	Total O 14 14	0	0
37	m	9	Total O 9 9	0	0
37	o	93	Total O 93 93	0	0
37	t	5	Total O 5 5	0	0
37	u	52	Total O 52 52	0	0
37	v	48	Total O 48 48	0	0
37	y	7	Total O 7 7	0	0
37	x	8	Total O 8 8	0	0
37	z	3	Total O 3 3	0	0
37	r	1	Total O 1 1	0	0

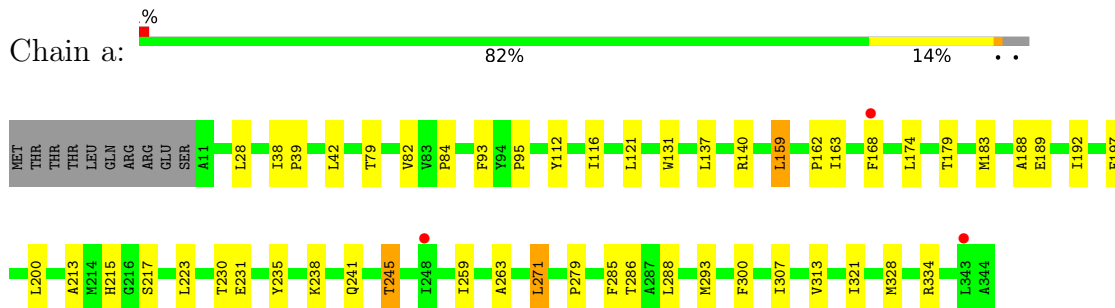
3 Residue-property plots

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.

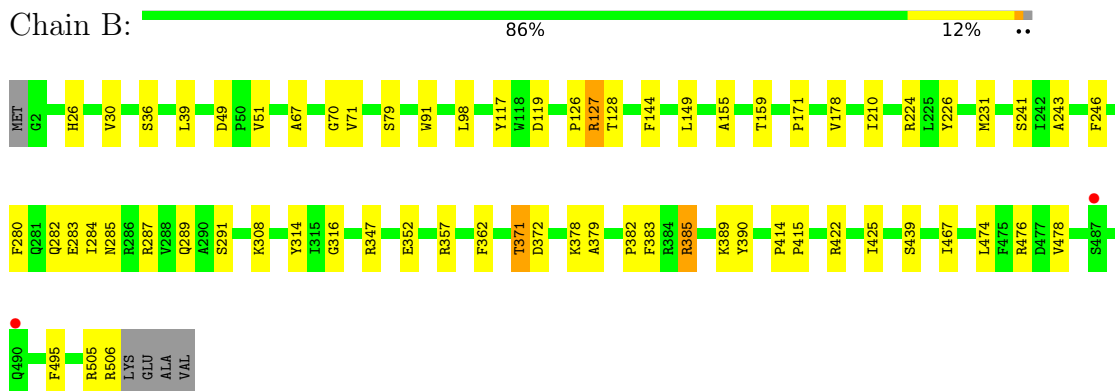
- Molecule 1: Photosystem II protein D1 1



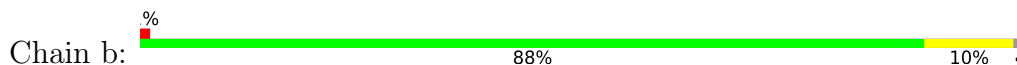
- Molecule 1: Photosystem II protein D1 1

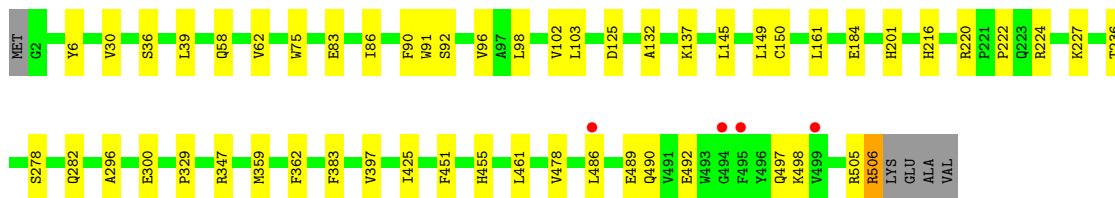


- Molecule 2: Photosystem II CP47 reaction center protein



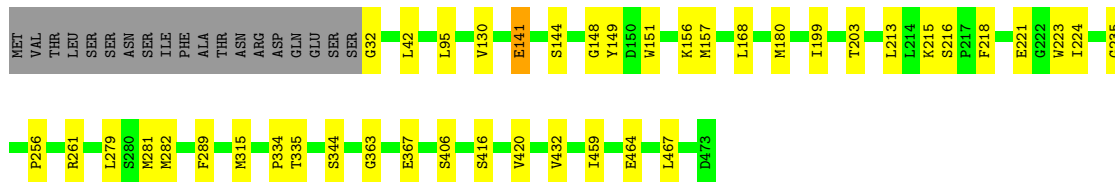
- Molecule 2: Photosystem II CP47 reaction center protein





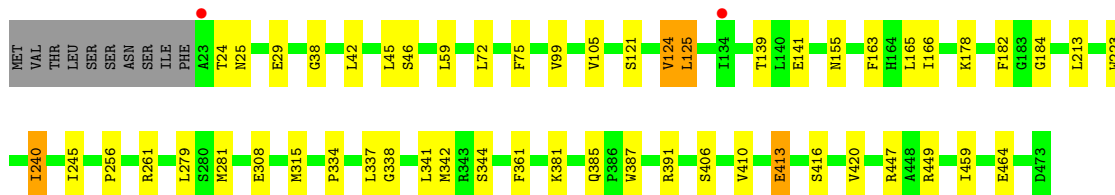
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 9% .



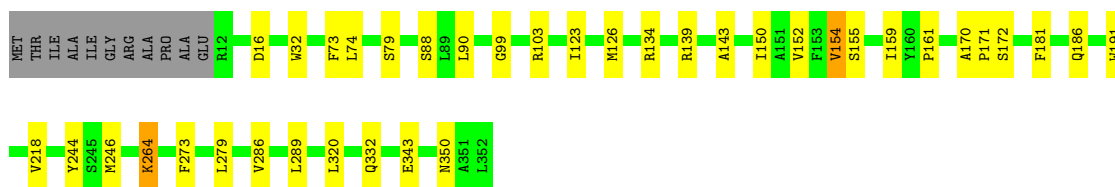
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 86% 11% ..



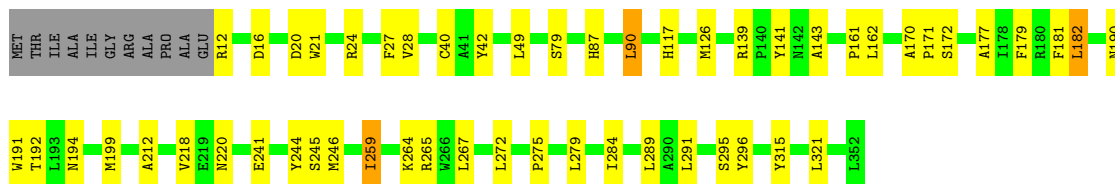
- Molecule 4: Photosystem II D2 protein

Chain D: 86% 10% ..

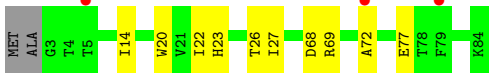
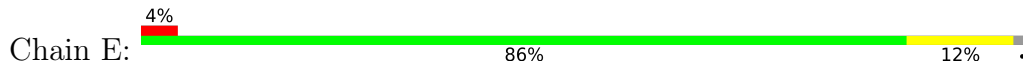


- Molecule 4: Photosystem II D2 protein

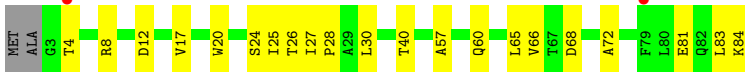
Chain d: 82% 14% ..



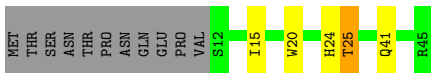
- Molecule 5: Cytochrome b559 subunit alpha



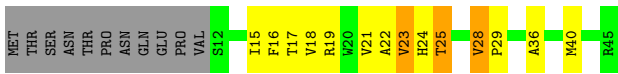
- Molecule 5: Cytochrome b559 subunit alpha



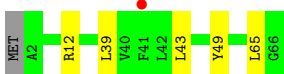
- Molecule 6: Cytochrome b559 subunit beta



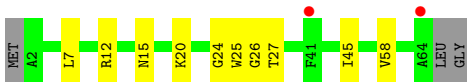
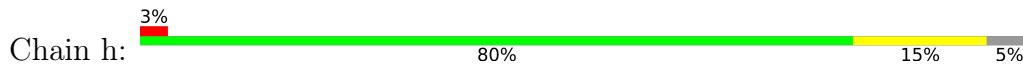
- Molecule 6: Cytochrome b559 subunit beta



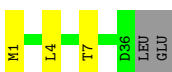
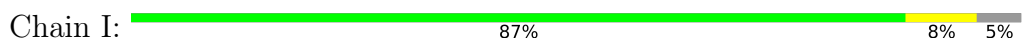
- Molecule 7: Photosystem II reaction center protein H




- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  79% 16% 5%




- Molecule 9: Photosystem II reaction center protein J

Chain J:  68% 22% 10%



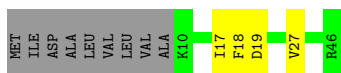
- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 78% 12% 10%



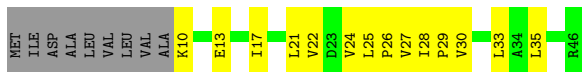
- Molecule 10: Photosystem II reaction center protein K

Chain K:  72% 9% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  50% 30% 20%




- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%




- Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 11%




- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 14% 8%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 8% 6% 11%




- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  76% 13% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  74% 15% 10%




- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 72% 22% 6%

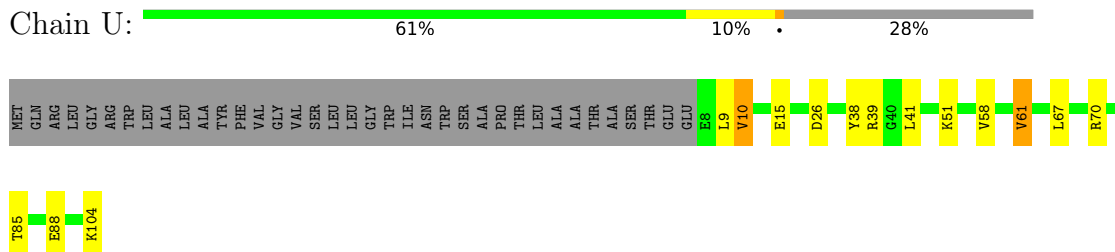


- Molecule 14: Photosystem II reaction center protein T

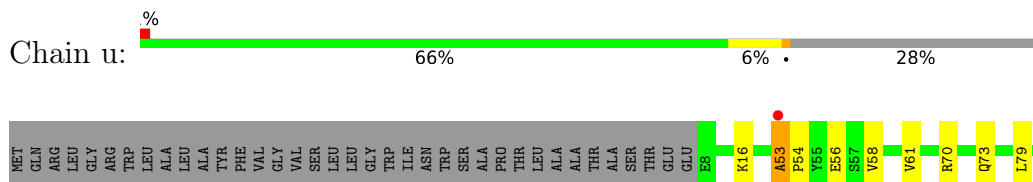
Chain t:  3% 88% 6%



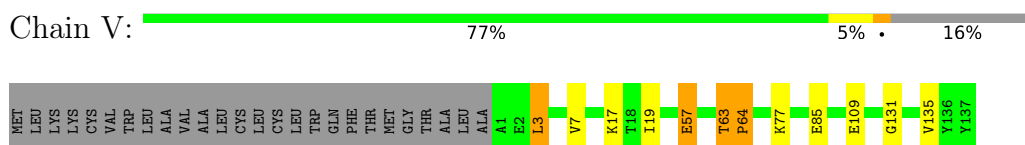
- Molecule 15: Photosystem II 12 kDa extrinsic protein



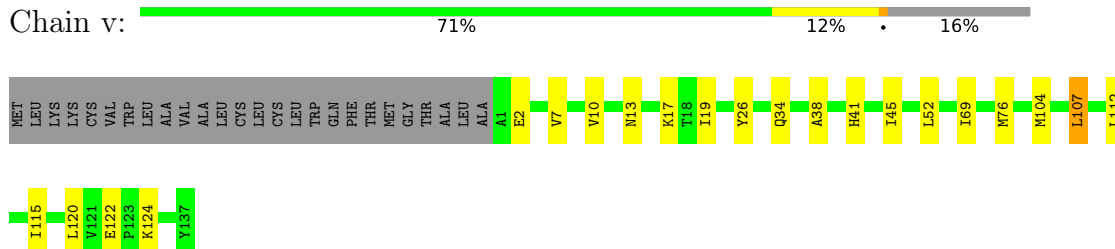
- Molecule 15: Photosystem II 12 kDa extrinsic protein



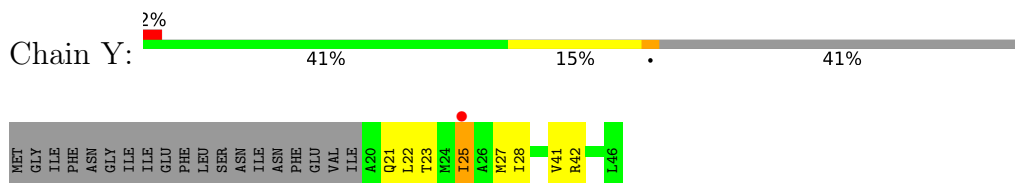
- Molecule 16: Cytochrome c-550



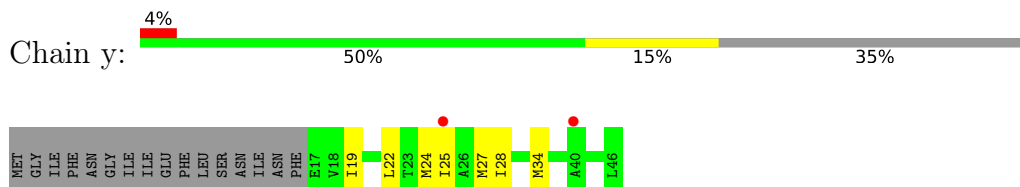
- Molecule 16: Cytochrome c-550



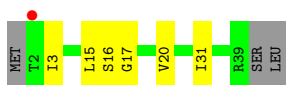
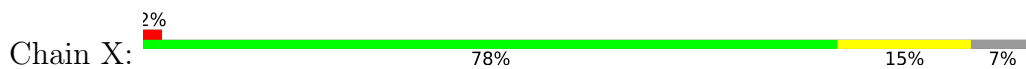
- Molecule 17: Photosystem II reaction center protein Ycf12



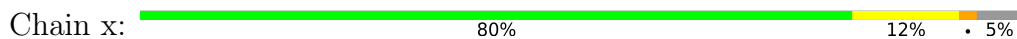
- Molecule 17: Photosystem II reaction center protein Ycf12



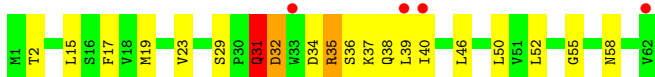
- Molecule 18: Photosystem II reaction center X protein



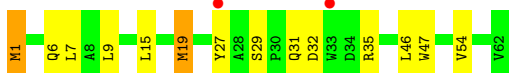
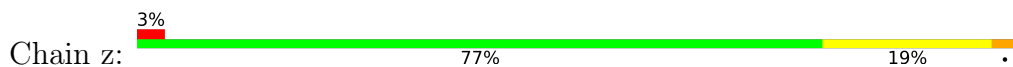
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



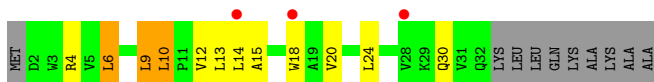
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.05Å 221.92Å 308.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.58 – 2.09 33.58 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.58-2.09) 86.0 (33.58-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.41 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.233 0.182 , 0.233	Depositor DCC
R_{free} test set	4180 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtrriage
Anisotropy	0.201	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	54466	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/3717	0.47	0/5060
1	a	0.28	0/3714	0.46	0/5056
2	B	0.34	0/4155	0.49	0/5661
2	b	0.31	0/4118	0.49	0/5611
3	C	0.32	0/3711	0.47	0/5051
3	c	0.30	0/3791	0.44	0/5158
4	D	0.35	0/2838	0.51	0/3862
4	d	0.35	0/2847	0.51	0/3874
5	E	0.26	0/688	0.42	0/940
5	e	0.24	0/683	0.43	0/932
6	F	0.31	0/284	0.41	0/387
6	f	0.25	0/284	0.49	0/387
7	H	0.33	0/523	0.49	0/713
7	h	0.32	0/511	0.50	0/697
8	I	0.31	0/293	0.46	0/396
8	i	0.33	0/293	0.45	0/396
9	J	0.27	0/263	0.40	0/356
9	j	0.26	0/263	0.44	0/356
10	K	0.27	0/303	0.44	0/416
10	k	0.25	0/303	0.41	0/416
11	L	0.36	0/311	0.46	0/422
11	l	0.32	0/303	0.48	0/412
12	M	0.31	0/249	0.53	0/341
12	m	0.34	0/244	0.48	0/334
13	O	0.32	0/1904	0.51	0/2585
13	o	0.32	0/1905	0.50	0/2583
14	T	0.36	0/257	0.54	0/349
14	t	0.32	0/255	0.48	0/346
15	U	0.30	0/785	0.48	0/1064
15	u	0.32	0/785	0.51	0/1064
16	V	0.32	0/1085	0.50	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.30	0/1085	0.46	0/1473
17	Y	0.23	0/197	0.37	0/264
17	y	0.19	0/219	0.34	0/294
18	X	0.25	0/284	0.36	0/384
18	x	0.21	0/289	0.31	0/391
19	Z	0.21	0/490	0.42	0/669
19	z	0.18	0/488	0.32	0/666
20	R	0.28	0/277	0.46	0/380
20	r	0.24	0/252	0.38	0/347
All	All	0.31	0/45246	0.48	0/61566

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3604	0	3445	26	0
1	a	3601	0	3436	41	0
2	B	4005	0	3871	42	0
2	b	3978	0	3836	41	0
3	C	3592	0	3501	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3666	0	3574	36	0
4	D	2745	0	2653	31	0
4	d	2751	0	2659	40	0
5	E	666	0	651	6	0
5	e	664	0	648	16	0
6	F	275	0	282	4	0
6	f	275	0	282	11	0
7	H	510	0	532	5	0
7	h	498	0	518	7	0
8	I	296	0	311	1	0
8	i	296	0	311	3	0
9	J	257	0	268	6	0
9	j	257	0	268	3	0
10	K	293	0	305	2	0
10	k	293	0	305	7	0
11	L	304	0	316	5	0
11	l	296	0	304	1	0
12	M	256	0	269	2	0
12	m	251	0	267	4	0
13	O	1870	0	1830	26	0
13	o	1874	0	1846	22	0
14	T	258	0	261	4	0
14	t	256	0	256	2	0
15	U	774	0	773	10	0
15	u	774	0	773	4	0
16	V	1064	0	1073	9	0
16	v	1064	0	1073	12	0
17	Y	196	0	217	5	0
17	y	218	0	241	3	0
18	X	281	0	312	4	0
18	x	286	0	314	5	0
19	Z	479	0	516	11	0
19	z	477	0	509	6	0
20	R	271	0	298	3	0
20	r	246	0	263	9	0
21	A	22	0	0	2	0
21	a	22	0	0	2	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	3	0
25	B	970	0	1067	32	0
25	C	839	0	922	16	0
25	D	130	0	144	7	0
25	H	65	0	72	2	0
25	a	260	0	288	7	0
25	b	970	0	1067	36	0
25	c	839	0	919	22	0
25	d	130	0	144	4	0
25	h	65	0	72	4	0
26	A	128	0	148	3	0
26	a	64	0	74	0	0
26	d	64	0	74	2	0
27	A	40	0	56	0	0
27	B	120	0	168	3	0
27	C	40	0	56	5	0
27	D	40	0	56	1	0
27	H	40	0	56	2	0
27	K	120	0	168	6	0
27	T	40	0	56	1	0
27	a	40	0	56	1	0
27	b	120	0	168	2	0
27	c	120	0	168	11	0
27	d	40	0	56	2	0
27	k	40	0	56	1	0
27	t	40	0	56	1	0
27	x	40	0	56	3	0
28	A	55	0	80	5	0
28	D	55	0	80	1	0
28	a	55	0	80	5	0
28	d	55	0	80	2	0
29	A	91	0	136	2	0
29	F	36	0	46	1	0
29	L	49	0	65	2	0
29	a	90	0	134	2	0
29	f	41	0	49	3	0
29	l	54	0	78	2	0
30	A	66	0	96	8	0
30	C	186	0	246	3	0
30	H	62	0	82	3	0
30	a	44	0	75	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	186	0	246	8	0
30	h	62	0	82	1	0
31	B	75	0	117	2	0
31	C	40	0	63	0	0
31	D	20	0	35	3	0
31	H	18	0	35	3	0
31	I	15	0	26	3	0
31	J	12	0	16	0	0
31	M	25	0	38	0	0
31	R	12	0	16	0	0
31	T	31	0	60	0	0
31	a	12	0	16	1	0
31	b	66	0	110	4	0
31	c	32	0	51	2	0
31	d	17	0	26	0	0
31	j	12	0	16	0	0
31	l	18	0	35	0	0
31	m	12	0	16	0	0
31	t	24	0	36	1	0
31	x	20	0	35	2	0
32	B	28	0	40	0	0
32	C	96	0	132	4	0
32	D	84	0	117	5	0
32	M	51	0	72	1	0
32	b	55	0	86	0	0
32	c	134	0	181	6	0
32	d	67	0	92	1	0
32	m	51	0	72	4	0
33	B	98	0	148	4	0
33	D	96	0	141	4	0
33	E	49	0	74	1	0
33	d	137	0	199	11	0
33	e	42	0	57	0	0
33	l	49	0	74	0	0
34	D	4	0	1	0	0
34	a	4	0	1	0	0
35	F	43	0	30	2	0
35	e	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	2	0
37	A	138	0	0	3	0
37	B	191	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	C	159	0	0	1	0
37	D	119	0	0	1	0
37	E	28	0	0	0	0
37	F	9	0	0	0	0
37	H	33	0	0	0	0
37	I	21	0	0	0	0
37	J	10	0	0	1	0
37	K	5	0	0	0	0
37	L	7	0	0	0	0
37	M	4	0	0	0	0
37	O	91	0	0	3	0
37	R	7	0	0	0	0
37	T	13	0	0	0	0
37	U	46	0	0	3	0
37	V	58	0	0	3	0
37	X	6	0	0	0	0
37	Y	6	0	0	2	0
37	Z	8	0	0	0	0
37	a	125	0	0	2	0
37	b	184	0	0	1	0
37	c	166	0	0	3	0
37	d	105	0	0	1	0
37	e	26	0	0	1	0
37	f	7	0	0	0	0
37	h	23	0	0	1	0
37	i	15	0	0	0	0
37	j	5	0	0	1	0
37	k	6	0	0	1	0
37	l	14	0	0	0	0
37	m	9	0	0	1	0
37	o	93	0	0	1	0
37	r	1	0	0	0	0
37	t	5	0	0	0	0
37	u	52	0	0	1	0
37	v	48	0	0	2	0
37	x	8	0	0	1	0
37	y	7	0	0	0	0
37	z	3	0	0	0	0
All	All	54466	0	53863	613	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 6.

All (613) 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)
37:m:209:HOH:O	14:t:1:FME:SD	2.35	0.84
25:H:101:CLA:H51	31:H:104:STE:H151	1.59	0.84
5:e:57:ALA:H	5:e:60:GLN:HE21	1.29	0.81
21:A:601[C]:OEY:O6	21:A:601[C]:OEY:O5	2.00	0.80
28:A:612:PL9:H361	6:F:25:THR:HG21	1.63	0.80
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.45	0.79
27:T:101:BCR:H311	27:T:101:BCR:HC8	1.65	0.78
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.66	0.77
25:a:610:CLA:H111	25:a:610:CLA:H52	1.67	0.76
25:b:614:CLA:H2	25:b:615:CLA:HBB2	1.69	0.74
21:a:601[C]:OEY:O6	21:a:601[C]:OEY:O5	2.06	0.73
26:A:609:PHO:HBC3	4:D:279:LEU:HD22	1.71	0.73
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.06	0.72
3:C:151:TRP:HA	3:C:157:MET:HE3	1.70	0.72
9:J:15:THR:HG22	9:J:19:MET:HE2	1.71	0.72
2:b:90:PHE:H	31:b:619:STE:H182	1.54	0.72
4:D:99:GLY:HA3	31:D:410:STE:H21	1.72	0.71
2:b:91:TRP:HE1	31:b:619:STE:H111	1.55	0.70
2:B:127:ARG:HG3	2:B:128:THR:HG23	1.74	0.70
2:B:506:ARG:NH2	37:B:702:HOH:O	2.24	0.69
3:C:148:GLY:O	3:C:156:LYS:NZ	2.25	0.69
15:u:56:GLU:O	37:u:1301:HOH:O	2.10	0.69
13:o:84:GLU:OE1	13:o:86:LYS:NZ	2.26	0.69
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.75	0.68
29:L:101:SQD:H102	25:b:613:CLA:H43	1.75	0.68
25:D:403:CLA:H141	18:X:15:LEU:HD12	1.74	0.68
30:c:517:DGD:O1A	37:c:601:HOH:O	2.12	0.68
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.74	0.68
27:t:101:BCR:HC8	27:t:101:BCR:H311	1.75	0.68
15:U:104:LYS:O	37:U:201:HOH:O	2.13	0.67
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.76	0.67
16:v:104:MET:HA	16:v:107:LEU:HD22	1.77	0.66
3:C:32:GLY:N	37:C:601:HOH:O	2.28	0.66
9:J:5:GLY:N	37:J:201:HOH:O	2.27	0.66
2:b:184:GLU:OE1	37:b:701:HOH:O	2.12	0.66
3:C:281:MET:HG3	32:C:515:LMG:H392	1.78	0.66
27:K:102:BCR:H10C	17:Y:28:ILE:HG23	1.77	0.66
28:D:405:PL9:H412	11:L:29:LEU:HD23	1.78	0.66
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.78	0.66
2:B:495:PHE:HD2	2:B:505:ARG:HH12	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:166:ILE:HG21	25:c:512:CLA:H202	1.79	0.65
1:A:103:ASP:OD1	30:A:616:DGD:O2E	2.15	0.65
15:U:88:GLU:OE2	37:U:202:HOH:O	2.14	0.65
1:a:188[C]:ALA:HB2	1:a:328[C]:MET:HB2	1.79	0.64
4:d:259:ILE:HD12	33:d:407:LHG:H291	1.77	0.64
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.32	0.64
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.79	0.64
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.79	0.64
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.12	0.63
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.80	0.63
32:C:519:LMG:H191	10:K:27:VAL:HG11	1.79	0.62
3:c:391[A]:ARG:NH1	37:c:602:HOH:O	2.32	0.62
4:d:199:MET:HG2	28:d:405:PL9:H321	1.81	0.62
25:C:502:CLA:H61	25:C:512:CLA:H42	1.82	0.62
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.82	0.62
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.81	0.62
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.31	0.62
2:b:62:VAL:HB	25:b:604:CLA:HED3	1.80	0.61
4:d:126:MET:HE3	4:d:143:ALA:O	1.99	0.61
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.82	0.61
2:b:145:LEU:HB3	25:b:603:CLA:H162	1.81	0.61
1:a:163[A]:ILE:HD11	30:c:517:DGD:HA21	1.82	0.61
1:a:334[B]:ARG:NH2	37:a:703:HOH:O	2.32	0.61
8:i:33:LYS:O	8:i:35:LYS:NZ	2.31	0.61
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.83	0.61
26:A:609:PHO:HBA2	25:D:402:CLA:H142	1.84	0.60
30:A:616:DGD:HB61	31:I:101:STE:H51	1.82	0.60
4:D:246:MET:HE3	4:D:264:LYS:HG3	1.84	0.60
2:B:474:LEU:O	4:D:134:ARG:NH1	2.33	0.60
19:Z:35:ARG:NH1	19:Z:38:GLN:OE1	2.35	0.60
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.83	0.60
15:U:58:VAL:O	15:U:61:VAL:HG22	2.02	0.60
2:B:39:LEU:HD13	31:t:103:STE:H22	1.82	0.60
2:b:102:VAL:HG11	25:b:605:CLA:H142	1.84	0.59
3:c:125:LEU:HD13	27:c:514:BCR:H361	1.82	0.59
4:d:192:THR:HG23	25:d:402:CLA:HBC2	1.83	0.59
19:z:32:ASP:HB2	19:z:35:ARG:HB2	1.84	0.59
25:b:608:CLA:H42	31:b:621:STE:H82	1.84	0.59
25:C:504:CLA:H92	30:C:517:DGD:HA92	1.83	0.59
2:B:382:PRO:HG2	2:B:385:ARG:HD2	1.85	0.59
13:O:36:GLN:O	37:O:302:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:133:VAL:O	13:O:135:SER:N	2.33	0.59
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.67	0.59
30:A:616:DGD:HBN1	8:I:7:THR:HG21	1.85	0.59
16:V:17:LYS:NZ	37:V:302:HOH:O	2.34	0.58
19:Z:23:VAL:HG22	19:Z:40:ILE:HD12	1.85	0.58
6:f:24:HIS:O	6:f:28:VAL:HG13	2.03	0.58
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.86	0.58
1:A:288:LEU:HD13	3:C:432:VAL:HG13	1.85	0.58
25:B:614:CLA:H2	25:B:615:CLA:HBB2	1.85	0.58
3:c:406:SER:HA	3:c:420:VAL:HG23	1.85	0.58
25:B:613:CLA:H102	33:B:621:LHG:H381	1.84	0.58
2:B:371:THR:HG23	2:B:372:ASP:O	2.04	0.57
1:a:189[B]:GLU:OE1	21:a:601[B]:OEY:O6	2.23	0.57
25:B:606:CLA:H191	33:B:622:LHG:H142	1.85	0.57
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.87	0.57
15:U:70:ARG:NH2	37:U:206:HOH:O	2.37	0.57
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.85	0.57
4:d:12:ARG:NH1	4:d:16:ASP:HB3	2.20	0.57
19:Z:31:GLN:CD	19:Z:32:ASP:H	2.12	0.57
1:a:286:THR:HG23	25:a:607:CLA:HED3	1.85	0.57
16:v:69:ILE:HD12	16:v:120:LEU:HD12	1.87	0.56
26:A:609:PHO:H3A	25:D:402:CLA:H142	1.88	0.56
3:c:281:MET:HG3	32:c:524:LMG:H412	1.86	0.56
5:e:26:THR:HG22	20:r:15:ALA:HB1	1.86	0.56
3:C:406:SER:HA	3:C:420:VAL:HG23	1.86	0.56
3:c:256:PRO:O	3:c:261:ARG:NH1	2.39	0.56
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.86	0.55
25:C:508:CLA:HBC3	25:C:510:CLA:H92	1.88	0.55
13:O:27:ARG:NH1	37:O:301:HOH:O	2.11	0.55
4:d:279:LEU:HD22	26:d:401:PHO:HBC3	1.88	0.55
30:A:616:DGD:HA42	2:b:98:LEU:HD11	1.89	0.55
6:f:21:VAL:O	6:f:25:THR:OG1	2.23	0.55
2:b:498:LYS:HE3	4:d:20:ASP:HA	1.89	0.55
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.89	0.55
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.88	0.55
33:B:621:LHG:H121	4:D:273:PHE:CE2	2.42	0.54
31:D:410:STE:H112	18:X:16:SER:HB3	1.90	0.54
4:d:241:GLU:CD	4:d:241:GLU:H	2.15	0.54
16:v:41:HIS:HA	16:v:45:ILE:O	2.08	0.54
20:r:6:LEU:HD12	20:r:10:LEU:HD23	1.90	0.54
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:616:DGD:HD5	2:b:75:TRP:HB3	1.88	0.54
25:c:505:CLA:H43	27:c:515:BCR:HC7	1.90	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.43	0.54
25:B:606:CLA:H142	25:B:612:CLA:H203	1.90	0.54
33:B:621:LHG:H322	12:M:18:PRO:HB3	1.89	0.53
10:k:26:PRO:O	10:k:29:PRO:HD2	2.07	0.53
1:A:271:LEU:HD11	28:A:612:PL9:HC71	1.90	0.53
35:e:101:HEM:HHC	35:e:101:HEM:HBB2	1.90	0.53
33:d:407:LHG:H281	14:t:17:PHE:CD1	2.44	0.53
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.89	0.53
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.09	0.53
2:b:222:PRO:HB3	7:h:26:GLY:HA3	1.91	0.53
18:x:15:LEU:O	18:x:19:VAL:HG23	2.09	0.52
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.90	0.52
16:v:7:VAL:O	16:v:124:LYS:NZ	2.39	0.52
2:B:117:TYR:HA	11:L:1:MET:HE1	1.92	0.52
3:C:203:THR:O	3:C:235:GLY:HA3	2.10	0.52
3:C:213:LEU:HG	25:C:506:CLA:H193	1.90	0.52
3:c:38:GLY:HA3	25:c:511:CLA:HMD2	1.90	0.52
13:O:42:ARG:O	13:O:241:ALA:HA	2.09	0.52
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.92	0.52
13:O:133:VAL:C	13:O:135:SER:H	2.17	0.52
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.91	0.52
1:A:85:SER:HA	1:A:109:GLY:HA3	1.92	0.52
25:C:505:CLA:HBC2	27:C:514:BCR:H341	1.92	0.52
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.92	0.52
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.45	0.52
16:V:77:LYS:NZ	37:V:304:HOH:O	2.42	0.52
5:e:68:ASP:O	5:e:72:ALA:HB2	2.11	0.51
1:A:201:GLY:HA3	1:A:286:THR:HB	1.91	0.51
4:D:150:ILE:O	4:D:154:VAL:HG13	2.11	0.51
10:k:21:LEU:HD13	17:y:24:MET:HE2	1.93	0.51
1:a:271:LEU:HD21	28:a:612:PL9:HC71	1.91	0.51
25:b:606:CLA:H191	33:d:406:LHG:H141	1.91	0.51
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.75	0.51
29:A:614:SQD:H251	33:D:408:LHG:H142	1.92	0.51
4:D:332:GLN:NE2	37:D:501:HOH:O	2.24	0.51
1:a:245:THR:HB	4:d:265:ARG:HE	1.76	0.50
30:c:518:DGD:HB22	32:c:520:LMG:H311	1.93	0.50
25:h:101:CLA:HBB2	27:x:101:BCR:H351	1.93	0.50
1:a:162[C]:PRO:HB3	1:a:168[C]:PHE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:45:LEU:HA	3:c:139:THR:HG22	1.94	0.50
6:f:17:THR:HG22	29:f:101:SQD:H61	1.94	0.50
25:b:602:CLA:C4D	25:b:604:CLA:H43	2.41	0.50
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.94	0.50
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.94	0.50
31:a:617:STE:O1	37:a:701:HOH:O	2.20	0.50
3:c:245:ILE:HD13	32:c:522:LMG:H371	1.93	0.50
6:f:15:ILE:H	20:r:30:GLN:NE2	2.10	0.50
13:O:72:THR:HG21	13:O:107:THR:HG23	1.94	0.50
5:e:20:TRP:O	5:e:24:SER:OG	2.25	0.50
37:A:800:HOH:O	4:D:350:ASN:HB2	2.12	0.50
25:B:603:CLA:H11	25:B:604:CLA:H42	1.93	0.50
25:C:505:CLA:H43	27:C:514:BCR:HC7	1.93	0.50
13:O:56:PRO:O	13:O:58:ASN:N	2.37	0.50
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.41	0.50
16:V:109:GLU:OE1	37:V:301:HOH:O	2.19	0.50
4:d:49:LEU:HD13	27:d:404:BCR:C15	2.42	0.50
5:e:8:ARG:NH1	5:e:12:ASP:OD2	2.43	0.50
31:D:410:STE:H152	18:X:17:GLY:HA2	1.94	0.49
25:c:510:CLA:H201	10:k:33:LEU:HD22	1.93	0.49
25:B:610:CLA:H203	25:B:612:CLA:H8	1.93	0.49
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.94	0.49
25:B:606:CLA:HMB1	25:B:606:CLA:HBB1	1.93	0.49
14:T:29:ILE:HG22	14:T:30:THR:HG23	1.94	0.49
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.48	0.49
3:C:42:LEU:HD21	25:C:511:CLA:H2A	1.94	0.49
25:C:506:CLA:H91	25:C:506:CLA:H203	1.93	0.49
25:a:610:CLA:H102	8:i:13:THR:HG23	1.94	0.49
29:f:101:SQD:H312	18:x:27:VAL:HG11	1.94	0.49
15:u:70:ARG:NH1	15:u:73:GLN:OE1	2.46	0.49
6:f:16:PHE:H	20:r:30:GLN:HE22	1.59	0.49
5:e:40:THR:HB	20:r:4:ARG:HD2	1.94	0.49
16:v:41:HIS:CD2	36:v:201:HEC:NB	2.80	0.49
1:A:211:PHE:CD1	28:A:612:PL9:H111	2.48	0.49
3:C:141:GLU:H	3:C:141:GLU:CD	2.19	0.49
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.47	0.49
28:a:612:PL9:H372	6:f:22:ALA:HA	1.93	0.49
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.48	0.49
28:A:612:PL9:H451	28:A:612:PL9:H471	1.55	0.49
1:a:321:ILE:HD11	4:d:179:PHE:HB2	1.94	0.49
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:TRP:CG	3:C:224:ILE:H	2.29	0.48
19:Z:36:SER:HA	19:Z:39:LEU:HB2	1.95	0.48
2:B:149[A]:LEU:HD21	25:B:605:CLA:HBB2	1.95	0.48
17:Y:42:ARG:NH1	37:Y:101:HOH:O	2.43	0.48
2:b:359:MET:HB2	2:b:425:ILE:HD12	1.94	0.48
12:m:4:ASN:ND2	32:m:101:LMG:O10	2.43	0.48
25:D:403:CLA:H72	25:D:403:CLA:H111	1.52	0.48
1:a:215:HIS:ND1	28:a:612:PL9:O1	2.38	0.48
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.46	0.48
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.95	0.48
18:x:8:LYS:NZ	37:x:202:HOH:O	2.45	0.48
33:D:407:LHG:HC62	11:L:15:THR:HG23	1.95	0.48
25:b:608:CLA:H111	25:b:608:CLA:H152	1.63	0.48
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.49	0.48
3:C:256:PRO:O	3:C:261:ARG:NH1	2.46	0.48
5:E:23:HIS:HB3	5:E:27:ILE:HD12	1.96	0.48
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.96	0.48
25:b:614:CLA:H2	25:b:615:CLA:CBB	2.43	0.48
4:D:186:GLN:HB2	25:D:402:CLA:HBC1	1.94	0.48
16:v:2:GLU:HB2	37:v:323:HOH:O	2.14	0.48
30:A:616:DGD:HB52	31:I:101:STE:H42	1.95	0.48
14:T:20:ALA:O	14:T:24:ARG:HB3	2.14	0.48
25:b:609:CLA:H152	25:b:611:CLA:O1A	2.14	0.48
29:l:101:SQD:H322	29:l:101:SQD:H292	1.69	0.48
3:c:178:LYS:NZ	3:c:184:GLY:O	2.47	0.47
30:c:517:DGD:HA32	30:c:517:DGD:HA61	1.46	0.47
5:E:14:ILE:O	5:E:20:TRP:NE1	2.47	0.47
19:Z:34:ASP:O	19:Z:37:LYS:HG2	2.13	0.47
1:a:279:PRO:HG2	4:d:212:ALA:HB2	1.95	0.47
3:c:46:SER:OG	3:c:141:GLU:OE2	2.28	0.47
19:z:1:MET:SD	19:z:1:MET:N	2.84	0.47
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.96	0.47
18:x:27:VAL:O	18:x:31:ILE:HG13	2.14	0.47
25:a:607:CLA:HBD	25:a:613:CLA:HAC2	1.97	0.47
3:c:381:LYS:NZ	13:o:99:ASP:OD2	2.27	0.47
5:E:26:THR:HA	20:R:15:ALA:HB1	1.96	0.47
1:a:235:TYR:OH	11:l:11:GLU:OE2	2.23	0.47
25:b:601:CLA:H43	7:h:45:ILE:HG22	1.97	0.47
25:c:505:CLA:CMD	25:c:507:CLA:HAB	2.45	0.47
4:d:21:TRP:HA	4:d:24:ARG:HG3	1.96	0.47
4:d:194:ASN:HA	4:d:295:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.14	0.47
25:b:608:CLA:H91	25:b:608:CLA:H112	1.76	0.47
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.79	0.47
13:O:27:ARG:O	13:O:27:ARG:HG2	2.15	0.47
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.97	0.47
18:x:16:SER:HB3	31:x:102:STE:H71	1.96	0.47
25:B:602:CLA:C2D	25:B:604:CLA:H2	2.44	0.47
30:A:616:DGD:HB41	31:I:101:STE:H71	1.97	0.46
2:b:36:SER:OG	27:b:617:BCR:H362	2.15	0.46
2:b:505:ARG:HG3	2:b:506:ARG:N	2.29	0.46
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.50	0.46
19:Z:29:SER:HB3	19:Z:31:GLN:HE21	1.79	0.46
1:a:82:VAL:HB	1:a:174[C]:LEU:HB2	1.97	0.46
25:b:604:CLA:HMA1	25:b:605:CLA:H3A	1.97	0.46
33:d:408:LHG:H332	33:d:408:LHG:H362	1.58	0.46
32:d:409:LMG:H121	32:d:409:LMG:H321	1.97	0.46
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.97	0.46
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.98	0.46
3:c:459:ILE:HG21	3:c:464:GLU:HG3	1.96	0.46
25:c:506:CLA:H12	25:c:506:CLA:H51	1.72	0.46
1:A:334[A]:ARG:HD3	4:D:320:LEU:HD13	1.97	0.46
32:D:406:LMG:H212	32:D:406:LMG:H182	1.55	0.46
17:Y:42:ARG:NH2	37:Y:102:HOH:O	2.45	0.46
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.50	0.46
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.98	0.46
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.97	0.46
4:D:286:VAL:HG21	25:D:402:CLA:HED2	1.97	0.46
20:R:16:ALA:O	20:R:20:VAL:HG23	2.15	0.46
32:m:101:LMG:H322	32:m:101:LMG:H291	1.62	0.46
25:B:613:CLA:H92	25:B:613:CLA:H62	1.59	0.46
14:T:1:FME:HE2	14:T:1:FME:HB2	1.87	0.46
2:b:103:LEU:HD22	25:b:605:CLA:H51	1.98	0.46
2:B:67:ALA:HA	2:B:71:VAL:O	2.15	0.46
2:B:126:PRO:HG3	7:H:12:ARG:CZ	2.46	0.46
3:C:279:LEU:CD1	25:C:509:CLA:HED2	2.45	0.46
9:J:19:MET:O	9:J:23:VAL:HG23	2.16	0.46
9:J:20:GLY:O	9:J:24:ILE:HG13	2.16	0.46
2:b:497:GLN:HE21	4:d:24:ARG:NH2	2.14	0.46
16:v:26:TYR:OH	16:v:122:GLU:OE1	2.33	0.46
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.51	0.46
30:c:519:DGD:HA82	30:c:519:DGD:HAE1	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:d:401:PHO:HBB1	26:d:401:PHO:HMB1	1.98	0.46
27:K:102:BCR:H322	19:Z:17:PHE:CE2	2.50	0.46
3:c:121:SER:CB	31:c:521:STE:H172	2.46	0.46
3:c:447:ARG:NH2	37:c:606:HOH:O	2.39	0.46
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.98	0.46
5:e:57:ALA:H	5:e:60:GLN:NE2	2.04	0.46
2:B:119:ASP:H	11:L:1:MET:CE	2.29	0.45
25:B:601:CLA:H152	25:B:601:CLA:H18	1.71	0.45
32:M:101:LMG:H371	32:M:101:LMG:H401	1.62	0.45
2:b:92:SER:O	2:b:96:VAL:HG23	2.16	0.45
25:h:101:CLA:CHA	25:h:101:CLA:HBA2	2.45	0.45
10:k:17:ILE:HD11	19:z:6:GLN:HG2	1.98	0.45
30:H:103:DGD:HBT1	30:H:103:DGD:HBH2	1.79	0.45
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	1.98	0.45
35:e:101:HEM:HMC1	35:e:101:HEM:HBC2	1.99	0.45
30:A:616:DGD:HB22	2:b:90:PHE:HD1	1.82	0.45
2:B:224:ARG:HH22	4:D:16:ASP:CG	2.23	0.45
3:C:95:LEU:HD21	25:C:501:CLA:OBD	2.16	0.45
16:V:63:THR:HG22	16:V:64:PRO:CD	2.47	0.45
29:a:614:SQD:H111	29:a:614:SQD:H142	1.40	0.45
2:b:296:ALA:HB1	2:b:300:GLU:HB2	1.98	0.45
13:o:111:ALA:O	37:o:301:HOH:O	2.20	0.45
2:B:285:ASN:O	2:B:289:GLN:HG2	2.15	0.45
2:B:357:ARG:NE	37:B:708:HOH:O	2.35	0.45
31:H:104:STE:H111	31:H:104:STE:H141	1.71	0.45
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.51	0.45
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.17	0.45
4:d:141:TYR:OH	33:d:406:LHG:O4	2.14	0.45
20:r:20:VAL:O	20:r:24:LEU:HB2	2.16	0.45
13:O:6:THR:HG22	13:O:9:ASP:CG	2.41	0.45
1:a:93:PHE:HZ	25:a:610:CLA:HAA1	1.82	0.45
13:O:110:MET:HE2	13:O:110:MET:HB3	1.83	0.45
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.99	0.45
2:B:91:TRP:HE1	31:B:619:STE:C1	2.30	0.45
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.46	0.45
25:b:613:CLA:H93	25:b:613:CLA:H61	1.65	0.45
25:b:615:CLA:H92	25:b:615:CLA:H61	1.80	0.45
2:B:495:PHE:HD2	2:B:505:ARG:NH1	2.12	0.45
25:B:611:CLA:H61	25:B:611:CLA:H102	1.73	0.45
27:C:514:BCR:H24C	27:C:514:BCR:H371	1.85	0.45
25:b:606:CLA:H61	25:b:606:CLA:H41	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:334:PRO:HA	13:o:153:THR:OG1	2.17	0.45
25:A:606:CLA:H162	25:A:606:CLA:H203	1.63	0.45
13:O:54:GLU:O	13:O:63:ALA:HB3	2.17	0.45
13:O:58:ASN:HD21	13:O:61:GLN:CD	2.22	0.45
25:c:507:CLA:H61	25:c:507:CLA:H41	1.74	0.45
25:c:512:CLA:H121	25:c:513:CLA:H151	1.99	0.45
25:h:101:CLA:H72	25:h:101:CLA:O2A	2.17	0.45
25:B:602:CLA:H161	25:B:602:CLA:H141	1.70	0.45
30:C:517:DGD:HA82	30:C:517:DGD:HAE2	1.44	0.45
4:D:126:MET:HE3	4:D:143:ALA:O	2.16	0.45
1:a:300:PHE:HZ	30:c:519:DGD:HB61	1.82	0.45
25:b:614:CLA:H161	25:b:614:CLA:H141	1.77	0.45
3:c:337:LEU:HD22	3:c:342:MET:HE3	1.98	0.45
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.52	0.44
3:c:391[B]:ARG:HG2	3:c:391[B]:ARG:HH11	1.83	0.44
16:v:13:ASN:ND2	16:v:17:LYS:HB3	2.31	0.44
2:B:280:PHE:O	2:B:284:ILE:HG13	2.17	0.44
25:B:601:CLA:H92	25:B:601:CLA:H62	1.81	0.44
25:B:611:CLA:HBB1	25:B:611:CLA:HMB1	1.99	0.44
3:C:363:GLY:O	3:C:367:GLU:HG2	2.16	0.44
4:D:152:VAL:HG21	4:D:279:LEU:HG	1.99	0.44
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.16	0.44
25:c:504:CLA:H13	25:c:508:CLA:H143	1.99	0.44
3:C:279:LEU:HD12	25:C:509:CLA:HED2	1.98	0.44
28:a:612:PL9:H321	28:a:612:PL9:H301	1.68	0.44
6:f:36:ALA:O	6:f:40:MET:HG3	2.17	0.44
10:k:28:ILE:HD11	17:y:28:ILE:HD13	1.99	0.44
1:A:230:THR:HG21	11:L:8:GLN:NE2	2.32	0.44
27:K:101:BCR:H24C	27:K:101:BCR:H371	1.80	0.44
13:O:189:ARG:HD3	15:U:9:LEU:HD22	1.99	0.44
2:b:125:ASP:HB2	2:b:132:ALA:HB3	1.98	0.44
25:c:506:CLA:H2	27:c:515:BCR:HC8	1.99	0.44
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.86	0.44
16:v:76:MET:HE1	16:v:115:ILE:HD12	2.00	0.44
20:r:9:LEU:O	20:r:13:LEU:HG	2.18	0.44
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.00	0.44
1:a:263:ALA:O	28:a:612:PL9:H152	2.16	0.44
2:b:6:TYR:OH	33:d:406:LHG:HC2	2.17	0.44
4:d:79:SER:HA	4:d:172:SER:HB3	1.99	0.44
9:j:10:LEU:O	9:j:13:VAL:HG22	2.16	0.44
25:A:606:CLA:HMB1	25:A:606:CLA:HBB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:SER:O	37:B:701:HOH:O	2.21	0.44
3:C:218:PHE:HE2	32:C:515:LMG:H131	1.81	0.44
27:a:611:BCR:H20C	27:a:611:BCR:H361	1.78	0.44
36:v:201:HEC:HMD1	37:v:322:HOH:O	2.18	0.44
25:B:613:CLA:H141	25:B:613:CLA:H161	1.70	0.44
25:B:615:CLA:H142	29:a:615:SQD:H211	2.00	0.44
25:D:403:CLA:H42	7:H:43:LEU:HD11	2.00	0.44
27:K:102:BCR:H20C	27:K:102:BCR:H361	1.83	0.44
15:U:10:VAL:HG21	15:U:15:GLU:OE2	2.18	0.44
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.73	0.44
2:B:385:ARG:HB2	13:O:165:ALA:O	2.17	0.44
2:B:422:ARG:O	2:B:425:ILE:HG12	2.18	0.44
25:B:603:CLA:HBD	25:B:604:CLA:H43	1.99	0.44
9:j:36:LEU:O	37:j:201:HOH:O	2.21	0.44
13:o:33:ASP:HB3	13:o:36:GLN:HB2	1.99	0.44
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.98	0.44
25:B:604:CLA:H41	25:B:611:CLA:H161	2.00	0.44
3:C:216:SER:HB2	32:C:515:LMG:HC8	1.99	0.44
4:D:79:SER:HA	4:D:172:SER:HB3	2.00	0.44
13:O:35:SER:OG	13:O:36:GLN:N	2.51	0.44
30:c:518:DGD:HA91	30:c:519:DGD:HB71	2.00	0.44
25:d:403:CLA:HBA2	31:x:102:STE:H21	1.98	0.44
5:e:25:ILE:HD13	20:r:18:TRP:NE1	2.33	0.44
1:A:158:PHE:O	1:A:162[A]:PRO:HG2	2.17	0.43
2:B:283:GLU:O	2:B:287:ARG:HG3	2.18	0.43
15:U:70:ARG:NH2	16:V:85:GLU:OE2	2.51	0.43
25:b:602:CLA:H141	25:b:602:CLA:H161	1.74	0.43
27:x:101:BCR:H24C	27:x:101:BCR:H371	1.81	0.43
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.53	0.43
25:C:502:CLA:HBB2	25:C:510:CLA:H152	2.01	0.43
3:c:385:GLN:HB2	3:c:387:TRP:CD1	2.53	0.43
13:o:26:ALA:O	13:o:204:VAL:N	2.48	0.43
1:A:334[B]:ARG:HD3	4:D:320:LEU:HD13	2.00	0.43
28:A:612:PL9:H422	28:A:612:PL9:H401	1.67	0.43
2:B:171:PRO:HA	7:H:65:LEU:HD12	2.00	0.43
3:C:180:MET:HG2	3:C:199:ILE:O	2.18	0.43
7:H:49:TYR:CE2	30:H:103:DGD:HB41	2.52	0.43
27:H:102:BCR:H15C	27:H:102:BCR:H351	1.89	0.43
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.01	0.43
30:a:616:DGD:HB22	30:a:616:DGD:HB51	1.80	0.43
2:b:150:CYS:HB2	25:b:602:CLA:CMC	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:601:CLA:HBB1	25:b:601:CLA:HMB3	2.00	0.43
25:b:609:CLA:H143	25:b:609:CLA:H161	1.73	0.43
27:c:516:BCR:H24C	27:c:516:BCR:H371	1.81	0.43
13:o:199:LEU:HD23	13:o:215:PHE:HB3	2.00	0.43
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.53	0.43
25:b:610:CLA:H162	25:b:610:CLA:H121	1.79	0.43
4:d:40:CYS:HB3	4:d:117:HIS:O	2.17	0.43
33:d:406:LHG:H351	33:d:406:LHG:H102	2.00	0.43
10:k:24:VAL:O	10:k:27:VAL:HG22	2.18	0.43
1:A:329[C]:GLU:HG3	37:A:770:HOH:O	2.16	0.43
2:B:414:PRO:N	2:B:415:PRO:HD2	2.33	0.43
27:K:101:BCR:H361	27:K:101:BCR:H20C	1.86	0.43
2:b:39:LEU:HD13	31:b:622:STE:H92	2.01	0.43
33:d:407:LHG:H281	33:d:407:LHG:H311	1.81	0.43
4:D:32:TRP:CD1	32:D:409:LMG:H141	2.53	0.43
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.06	0.43
2:b:145:LEU:HD22	25:b:603:CLA:H161	2.00	0.43
2:b:216:HIS:HE1	25:b:608:CLA:C1A	2.31	0.43
3:c:121:SER:O	3:c:124:VAL:HG13	2.18	0.43
3:c:464:GLU:OE2	4:d:245:SER:OG	2.35	0.43
16:V:57:GLU:CD	16:V:57:GLU:H	2.27	0.43
1:a:213:ALA:HB2	4:d:275:PRO:HG2	2.00	0.43
1:a:238:LYS:HB2	1:a:238:LYS:HE2	1.89	0.43
2:b:201:HIS:HB2	25:b:601:CLA:CHB	2.48	0.43
25:b:601:CLA:H171	30:h:102:DGD:HAW1	2.01	0.43
25:b:611:CLA:HBB1	25:b:611:CLA:HMB1	2.01	0.43
25:c:504:CLA:H62	25:c:504:CLA:H41	1.77	0.43
25:c:506:CLA:C2	27:c:515:BCR:HC8	2.49	0.43
27:c:515:BCR:H24C	27:c:515:BCR:H371	1.86	0.43
4:d:90:LEU:HA	4:d:90:LEU:HD12	1.69	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.54	0.43
1:A:185[C]:VAL:O	1:A:189[C]:GLU:HG3	2.19	0.43
29:A:614:SQD:H381	9:J:22:ILE:HD11	1.99	0.43
27:B:616:BCR:H383	29:l:101:SQD:H131	2.01	0.43
3:c:59:LEU:HD21	27:c:516:BCR:H372	2.00	0.43
5:e:26:THR:HA	20:r:15:ALA:HB1	2.00	0.43
12:m:16:LEU:HA	12:m:16:LEU:HD22	1.78	0.43
19:Z:39:LEU:HD23	19:Z:39:LEU:HA	1.82	0.43
37:d:526:HOH:O	13:o:228:HIS:HD2	2.01	0.43
4:D:90:LEU:HA	4:D:90:LEU:HD23	1.83	0.42
4:D:155:SER:HA	4:D:159:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:L:101:SQD:H172	29:L:101:SQD:H141	1.81	0.42
2:b:278:SER:O	2:b:282:GLN:HG3	2.18	0.42
2:b:497:GLN:HE21	4:d:24:ARG:HH22	1.66	0.42
25:c:501:CLA:C2D	25:c:503:CLA:H2	2.49	0.42
12:m:13:LEU:HB3	32:m:101:LMG:H401	2.00	0.42
25:B:606:CLA:H142	25:B:606:CLA:H111	1.78	0.42
27:C:514:BCR:H15C	27:C:514:BCR:H351	1.87	0.42
1:a:131:TRP:HZ2	3:c:449:ARG:HD2	1.85	0.42
1:a:217:SER:HA	4:d:272:LEU:HD12	2.02	0.42
25:b:609:CLA:H151	25:b:614:CLA:HBD	2.01	0.42
25:b:612:CLA:H172	33:d:406:LHG:H212	2.01	0.42
30:c:519:DGD:HA91	30:c:519:DGD:HA62	1.82	0.42
4:d:267:LEU:C	4:d:267:LEU:HD23	2.43	0.42
25:h:101:CLA:H143	25:h:101:CLA:H161	1.84	0.42
27:x:101:BCR:H351	27:x:101:BCR:H15C	1.94	0.42
1:A:65[C]:GLU:OE1	1:A:335[C]:ASN:ND2	2.42	0.42
2:B:241:SER:HB3	25:B:611:CLA:HED3	2.01	0.42
25:C:502:CLA:HBA2	25:C:503:CLA:H171	2.01	0.42
4:d:40:CYS:SG	25:d:403:CLA:HBB1	2.60	0.42
4:d:87:HIS:CD2	4:d:162:LEU:HD23	2.55	0.42
19:z:19:MET:HE1	19:z:47:TRP:HB2	2.02	0.42
2:B:149[A]:LEU:HD23	25:B:602:CLA:HBC1	2.02	0.42
2:b:58:GLN:C	2:b:329:PRO:HB3	2.44	0.42
2:b:478:VAL:O	4:d:139:ARG:HG2	2.19	0.42
1:A:58[A]:VAL:HB	1:A:83:VAL:HB	2.02	0.42
2:B:347:ARG:NE	37:B:703:HOH:O	2.26	0.42
25:B:613:CLA:H62	25:B:613:CLA:H41	1.78	0.42
3:C:149:TYR:CD1	3:C:157:MET:HE1	2.54	0.42
32:D:406:LMG:H211	32:D:406:LMG:H241	1.77	0.42
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.54	0.42
4:d:246:MET:HE3	4:d:264:LYS:HG2	2.02	0.42
5:e:17:VAL:HG23	9:j:7:ARG:HB2	2.01	0.42
6:f:19:ARG:O	6:f:23:VAL:HG13	2.20	0.42
7:h:12:ARG:NH2	7:h:15:ASN:O	2.51	0.42
8:i:18:LEU:HA	8:i:18:LEU:HD23	1.77	0.42
10:k:25:LEU:HB2	37:k:203:HOH:O	2.20	0.42
13:o:81:ILE:HA	13:o:100:GLY:HA3	2.02	0.42
1:A:334[C]:ARG:HD3	37:A:783:HOH:O	2.18	0.42
2:B:155:ALA:O	2:B:159:THR:OG1	2.35	0.42
25:H:101:CLA:H93	25:H:101:CLA:H62	1.84	0.42
2:b:30:VAL:HG12	25:b:604:CLA:HHD	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.00	0.42
3:C:459:ILE:HG21	3:C:464:GLU:HG3	2.01	0.42
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.55	0.42
5:E:68:ASP:O	5:E:72:ALA:HB2	2.19	0.42
13:O:37:THR:OG1	13:O:246:ALA:HB3	2.20	0.42
13:O:72:THR:CG2	13:O:107:THR:HG23	2.50	0.42
1:a:307:ILE:HG22	1:a:313:VAL:HA	2.02	0.42
25:b:601:CLA:O1D	25:b:602:CLA:HBB	2.20	0.42
27:k:101:BCR:H321	27:k:101:BCR:HC8	2.01	0.42
1:A:343[C]:LEU:HD23	1:A:343[C]:LEU:HA	1.84	0.42
2:B:49:ASP:OD2	13:o:57:LYS:HD2	2.19	0.42
33:D:408:LHG:H351	33:D:408:LHG:H383	1.74	0.42
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.02	0.42
25:B:610:CLA:H72	25:B:610:CLA:H112	1.61	0.42
27:B:616:BCR:H24C	27:B:616:BCR:H371	1.84	0.42
25:C:509:CLA:H91	25:C:509:CLA:H112	1.54	0.42
27:D:404:BCR:H381	32:D:406:LMG:H152	2.02	0.42
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.55	0.42
3:c:338:GLY:HA3	3:c:341:LEU:O	2.20	0.42
25:d:403:CLA:H111	25:d:403:CLA:H91	1.89	0.42
32:m:101:LMG:H371	32:m:101:LMG:H342	1.64	0.42
13:o:81:ILE:HG23	13:o:97:GLU:HG3	2.02	0.42
31:B:626:STE:H82	31:B:626:STE:H111	1.87	0.41
3:C:344:SER:O	13:O:75:THR:HG22	2.20	0.41
2:b:224:ARG:HG2	7:h:24:GLY:O	2.19	0.41
2:b:347:ARG:O	2:b:397:VAL:HA	2.20	0.41
33:d:406:LHG:H281	33:d:406:LHG:H311	1.60	0.41
5:e:57:ALA:N	5:e:60:GLN:HE21	2.07	0.41
1:A:306:VAL:HG12	1:A:314:ILE:HB	2.02	0.41
25:B:612:CLA:H62	25:B:612:CLA:H41	1.83	0.41
4:D:73:PHE:CE2	32:D:406:LMG:H191	2.56	0.41
25:a:607:CLA:HBB1	25:a:607:CLA:HMB3	2.02	0.41
25:b:614:CLA:H152	25:b:614:CLA:H112	1.84	0.41
25:c:509:CLA:H142	25:c:509:CLA:H111	1.67	0.41
2:B:352:GLU:OE2	2:B:378:LYS:NZ	2.53	0.41
25:B:609:CLA:H122	25:B:614:CLA:HAA1	2.02	0.41
3:C:215:LYS:HE2	3:C:221:GLU:O	2.19	0.41
25:C:507:CLA:H41	25:C:507:CLA:H61	1.88	0.41
4:d:27:PHE:HD2	4:d:28:VAL:HG23	1.85	0.41
25:B:608:CLA:HBC1	31:H:104:STE:H52	2.03	0.41
25:b:611:CLA:H172	25:b:612:CLA:HBB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:513:CLA:H202	25:c:513:CLA:H162	1.86	0.41
13:o:216:GLU:OE2	13:o:234:LYS:HD2	2.20	0.41
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.45	0.41
2:B:389:LYS:HD3	2:B:389:LYS:HA	1.75	0.41
25:B:609:CLA:HHC	25:B:609:CLA:HBB1	2.03	0.41
27:C:514:BCR:H20C	27:C:514:BCR:H361	1.91	0.41
30:C:518:DGD:HA41	4:D:74:LEU:HG	2.02	0.41
33:E:101:LHG:H302	33:E:101:LHG:H271	1.44	0.41
16:V:3:LEU:HD23	16:V:3:LEU:HA	1.84	0.41
1:a:112:TYR:O	1:a:116:ILE:HG12	2.21	0.41
32:c:524:LMG:H182	32:c:524:LMG:H152	1.84	0.41
1:A:159[C]:LEU:C	1:A:162[C]:PRO:HD2	2.45	0.41
4:D:218:VAL:HG22	4:D:244:TYR:CE1	2.56	0.41
29:F:102:SQD:H242	18:X:31:ILE:HD13	2.02	0.41
3:c:213:LEU:HD21	27:c:515:BCR:C20	2.50	0.41
28:d:405:PL9:H421	28:d:405:PL9:H401	1.88	0.41
25:C:507:CLA:H161	25:C:507:CLA:H141	1.71	0.41
1:a:159[B]:LEU:O	1:a:163[B]:ILE:HG13	2.20	0.41
32:c:522:LMG:H372	32:c:522:LMG:H402	1.69	0.41
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.55	0.41
3:c:25:ASN:HD22	3:c:45:LEU:HD11	1.86	0.41
25:c:506:CLA:HBA1	25:c:506:CLA:H3A	1.86	0.41
25:c:511:CLA:HBA1	27:c:516:BCR:H271	2.03	0.41
1:A:332[B]:HIS:O	1:A:333[B]:GLU:C	2.64	0.41
13:O:27:ARG:HG3	37:O:301:HOH:O	2.20	0.41
3:c:163:PHE:CD2	25:c:512:CLA:HAB	2.56	0.41
3:c:344:SER:O	13:o:75:THR:HG22	2.20	0.41
27:d:404:BCR:H11C	27:d:404:BCR:H341	1.89	0.41
5:e:17:VAL:N	37:e:202:HOH:O	2.49	0.41
16:v:34:GLN:HA	16:v:38:ALA:HB2	2.03	0.41
19:z:15:LEU:HG	19:z:19:MET:HE2	2.03	0.41
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	2.02	0.41
25:B:602:CLA:C3D	25:B:604:CLA:H2	2.51	0.41
25:B:608:CLA:H203	7:H:39:LEU:HD12	2.03	0.41
33:D:407:LHG:H322	14:T:21:ILE:HD11	2.01	0.41
1:a:137:LEU:HD23	1:a:137:LEU:HA	1.89	0.41
3:c:223:TRP:CD1	32:c:524:LMG:H332	2.56	0.41
5:e:30:LEU:HD11	6:f:28:VAL:HB	2.03	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.21	0.40
19:Z:31:GLN:NE2	19:Z:32:ASP:H	2.19	0.40
19:Z:55:GLY:HA2	19:Z:58:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:137:LYS:HE3	2:b:137:LYS:HB2	1.93	0.40
27:b:617:BCR:H15C	27:b:617:BCR:H351	1.82	0.40
13:o:42:ARG:O	13:o:241:ALA:HA	2.21	0.40
1:A:190[B]:HIS:ND1	1:A:298:ASN:OD1	2.55	0.40
2:B:26:HIS:O	2:B:30:VAL:HG23	2.20	0.40
27:B:617:BCR:H15C	27:B:617:BCR:H351	1.76	0.40
27:K:103:BCR:H20C	27:K:103:BCR:H361	1.81	0.40
19:Z:36:SER:O	19:Z:40:ILE:HG12	2.21	0.40
2:b:161:LEU:HD23	2:b:161:LEU:HA	1.84	0.40
3:c:121:SER:OG	31:c:521:STE:H172	2.21	0.40
25:c:507:CLA:O1D	25:c:509:CLA:H8	2.22	0.40
25:A:610:CLA:H41	25:A:610:CLA:H61	1.85	0.40
25:B:605:CLA:H91	25:B:605:CLA:H112	1.50	0.40
4:D:123:ILE:HD11	30:H:103:DGD:HAH1	2.04	0.40
10:K:17:ILE:HG23	10:K:18:PHE:CD2	2.56	0.40
1:a:197:PHE:HB3	1:a:285:PHE:O	2.21	0.40
4:d:171:PRO:HG3	4:d:181:PHE:CZ	2.56	0.40
7:h:58:VAL:HB	37:h:206:HOH:O	2.21	0.40
13:o:92:SER:HB3	13:o:131:PRO:HA	2.03	0.40
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.03	0.40
2:B:478:VAL:O	4:D:139:ARG:HG2	2.21	0.40
3:C:168:LEU:HD23	3:C:168:LEU:HA	1.91	0.40
3:C:213:LEU:HD12	3:C:213:LEU:HA	1.86	0.40
15:U:104:LYS:NZ	16:V:131:GLY:O	2.41	0.40
3:c:240:ILE:HA	3:c:240:ILE:HD13	1.72	0.40
5:e:81:GLU:O	5:e:84:LYS:HE2	2.22	0.40
29:f:101:SQD:H371	29:f:101:SQD:H342	1.87	0.40
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.56	0.40
25:B:608:CLA:H193	25:B:608:CLA:H161	1.85	0.40
3:C:223:TRP:CG	3:C:224:ILE:N	2.88	0.40
3:C:467:LEU:HD23	3:C:467:LEU:HA	1.87	0.40
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.56	0.40
27:H:102:BCR:H371	27:H:102:BCR:H24C	1.86	0.40
15:U:26:ASP:OD2	15:U:85:THR:OG1	2.36	0.40
1:a:82:VAL:HB	1:a:174[B]:LEU:HB2	2.02	0.40
1:a:159[C]:LEU:C	1:a:162[C]:PRO:HD2	2.47	0.40
1:a:183[B]:MET:HA	25:a:607:CLA:HMD1	2.02	0.40
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.10	0.40
25:b:612:CLA:H51	33:d:406:LHG:H361	2.04	0.40
27:c:515:BCR:H11C	27:c:515:BCR:H341	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/344 (133%)	451 (98%)	7 (2%)	0	100	100
1	a	458/344 (133%)	449 (98%)	8 (2%)	1 (0%)	43	44
2	B	507/510 (99%)	500 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	496 (99%)	7 (1%)	0	100	100
3	C	461/461 (100%)	451 (98%)	9 (2%)	1 (0%)	43	44
3	c	471/461 (102%)	460 (98%)	10 (2%)	1 (0%)	43	44
4	D	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
4	d	342/352 (97%)	334 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	230 (95%)	10 (4%)	3 (1%)	10	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	234 (97%)	8 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	8
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	15
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	27 (93%)	2 (7%)	0	100	100
All	All	5534/5700 (97%)	5397 (98%)	128 (2%)	9 (0%)	43	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
16	V	64	PRO
19	Z	31	GLN
13	O	62	GLU
3	c	416	SER
15	u	53	ALA
13	O	134	THR
1	a	259	ILE

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/280 (134%)	367 (98%)	7 (2%)	50	58
1	a	373/280 (133%)	360 (96%)	13 (4%)	32	35
2	B	407/407 (100%)	396 (97%)	11 (3%)	39	45
2	b	402/407 (99%)	393 (98%)	9 (2%)	45	53
3	C	361/362 (100%)	356 (99%)	5 (1%)	59	67
3	c	370/362 (102%)	357 (96%)	13 (4%)	32	35
4	D	278/283 (98%)	276 (99%)	2 (1%)	76	83
4	d	279/283 (99%)	274 (98%)	5 (2%)	51	60
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	43
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	18
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	34
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	32
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	39
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	28
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	28
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	37
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	42
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	7
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	11
13	O	206/228 (90%)	201 (98%)	5 (2%)	43	49
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	31
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	32
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	79 (94%)	5 (6%)	17	15
15	u	84/112 (75%)	82 (98%)	2 (2%)	43	49
16	V	117/138 (85%)	113 (97%)	4 (3%)	32	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	35
17	Y	19/37 (51%)	16 (84%)	3 (16%)	2	1
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	13
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	38
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	1
19	z	51/52 (98%)	44 (86%)	7 (14%)	3	2
20	R	28/33 (85%)	21 (75%)	7 (25%)	0	0
20	r	25/33 (76%)	20 (80%)	5 (20%)	1	0
All	All	4572/4654 (98%)	4410 (96%)	162 (4%)	31	35

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	60[C]	ILE
1	A	205	VAL
1	A	243	GLU
2	B	36	SER
2	B	79	SER
2	B	98	LEU
2	B	127	ARG
2	B	282	GLN
2	B	291	SER
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
2	B	467	ILE
2	B	476	ARG
3	C	130	VAL
3	C	141	GLU
3	C	144	SER
3	C	289	PHE
3	C	315	MET
4	D	154	VAL
4	D	264	LYS

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Mol	Chain	Res	Type
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
8	I	4	LEU
9	J	7	ARG
10	K	19	ASP
11	L	10	VAL
12	M	16	LEU
12	M	25	LEU
13	O	23	ASP
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	214	THR
14	T	25	GLU
15	U	10	VAL
15	U	39	ARG
15	U	51	LYS
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	19	ILE
16	V	57	GLU
17	Y	21	GLN
17	Y	25	ILE
17	Y	41	VAL
18	X	3	ILE
18	X	20	VAL
19	Z	2	THR
19	Z	15	LEU
19	Z	19	MET
19	Z	31	GLN
19	Z	32	ASP
19	Z	35	ARG
19	Z	46	LEU
19	Z	50	LEU
19	Z	52	LEU
20	R	6	LEU
20	R	10	LEU
20	R	13	LEU
20	R	21	ARG

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Mol	Chain	Res	Type
20	R	29	LYS
20	R	33	LYS
20	R	35	LEU
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	159[C]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	230	THR
1	a	231	GLU
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	83	GLU
2	b	86	ILE
2	b	149	LEU
2	b	236	THR
2	b	362	PHE
2	b	486	LEU
2	b	490	GLN
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	155	ASN
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	182	LEU
4	d	259	ILE
4	d	291	LEU

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Mol	Chain	Res	Type
4	d	321	LEU
5	e	4	THR
5	e	65	LEU
5	e	66	VAL
5	e	83	LEU
6	f	18	VAL
6	f	23	VAL
6	f	25	THR
6	f	28	VAL
7	h	7	LEU
7	h	27	THR
8	i	2	GLU
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	22	VAL
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	34	SER
13	o	49	THR
13	o	53	LYS
13	o	59	LYS
13	o	60	ARG
13	o	118	LEU
13	o	130	GLN
13	o	194	LYS
15	u	16	LYS
15	u	61	VAL
16	v	10	VAL
16	v	19	ILE
16	v	52	LEU
16	v	107	LEU
17	y	19	ILE
17	y	27	MET
17	y	34	MET
18	x	15	LEU
19	z	1	MET

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Mol	Chain	Res	Type
19	z	7	LEU
19	z	19	MET
19	z	27	TYR
19	z	29	SER
19	z	31	GLN
19	z	46	LEU
20	r	6	LEU
20	r	9	LEU
20	r	10	LEU
20	r	12	VAL
20	r	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	325	ASN
2	B	374	ASN
2	B	409	GLN
2	B	490	GLN
3	C	311	GLN
3	C	385	GLN
4	D	250	ASN
7	H	59	ASN
11	L	8	GLN
13	O	82	GLN
13	O	155	ASN
15	U	78	ASN
17	Y	45	ASN
18	X	38	GLN
19	Z	31	GLN
20	R	22	ASN
1	a	19	ASN
1	a	234	ASN
2	b	179	GLN
2	b	338	GLN
2	b	409	GLN
3	c	25	ASN
3	c	201	ASN
3	c	311	GLN
3	c	322	GLN
4	d	164	GLN

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Mol	Chain	Res	Type
5	e	60	GLN
5	e	82	GLN
7	h	59	ASN
13	o	61	GLN
13	o	109	GLN
13	o	124	ASN
17	y	45	ASN
18	x	33	GLN
19	z	31	GLN
19	z	58	ASN
20	r	30	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	1.06	1 (12%)	8,9,11	1.00	0
14	FME	t	1	14	8,9,10	1.27	1 (12%)	8,9,11	1.01	0
8	FME	I	1	8	8,9,10	1.00	0	8,9,11	1.16	1 (12%)
14	FME	T	1	14	8,9,10	1.03	0	8,9,11	0.94	0
12	FME	m	1	12	8,9,10	1.11	1 (12%)	8,9,11	0.54	0
12	FME	M	1	12	8,9,10	1.04	1 (12%)	8,9,11	1.15	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-3.03	1.42	1.46
12	m	1	FME	CA-N	-2.35	1.43	1.46
12	M	1	FME	CA-N	-2.13	1.43	1.46
8	i	1	FME	CA-N	-2.01	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.33	119.23	122.82
12	M	1	FME	CA-N-CN	-2.02	119.71	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	t	1	FME	C-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
14	t	1	FME	N-CA-CB-CG
14	T	1	FME	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	t	1	FME	1	0
14	T	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
26	PHO	d	401	-	58,69,69	2.11	11 (18%)	55,99,99	1.62	7 (12%)
31	STE	C	520	-	11,11,19	0.67	0	11,11,19	1.38	1 (9%)
25	CLA	C	501	-	69,73,73	1.29	9 (13%)	82,113,113	1.31	8 (9%)
25	CLA	a	613	37	69,73,73	1.30	9 (13%)	82,113,113	1.38	9 (10%)
25	CLA	b	604	-	69,73,73	1.09	6 (8%)	82,113,113	1.33	9 (10%)
27	BCR	c	514	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	7 (12%)
29	SQD	a	615	-	35,35,54	1.77	6 (17%)	37,37,65	1.42	5 (13%)
31	STE	B	626	-	15,15,19	0.38	0	14,14,19	0.78	0
31	STE	c	523	-	11,11,19	0.77	0	11,11,19	1.20	1 (9%)
33	LHG	B	621	-	48,48,48	0.73	1 (2%)	51,54,54	1.20	3 (5%)
31	STE	b	621	-	15,15,19	0.70	0	15,15,19	0.90	0
25	CLA	b	606	37	69,73,73	1.15	6 (8%)	82,113,113	1.31	7 (8%)
32	LMG	d	410	-	44,44,55	0.94	2 (4%)	52,52,63	1.31	6 (11%)
30	DGD	c	518	-	63,63,67	0.94	2 (3%)	77,77,81	1.29	6 (7%)
30	DGD	c	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.44	15 (19%)
25	CLA	a	610	-	69,73,73	1.27	8 (11%)	82,113,113	1.22	7 (8%)
32	LMG	C	515	-	48,48,55	0.92	4 (8%)	56,56,63	1.32	6 (10%)
25	CLA	c	506	-	69,73,73	1.27	9 (13%)	82,113,113	1.31	5 (6%)
32	LMG	M	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.40	6 (10%)
33	LHG	d	407	-	48,48,48	0.64	0	51,54,54	1.19	4 (7%)
25	CLA	C	502	-	69,73,73	1.23	7 (10%)	82,113,113	1.22	7 (8%)
25	CLA	c	502	-	69,73,73	1.18	9 (13%)	82,113,113	1.29	8 (9%)
32	LMG	B	620	-	26,26,55	0.63	0	26,26,63	1.32	1 (3%)
31	STE	B	623	-	11,11,19	0.84	0	11,11,19	1.07	0
26	PHO	a	609	-	58,69,69	2.09	8 (13%)	55,99,99	1.33	10 (18%)
27	BCR	d	404	-	41,41,41	1.11	3 (7%)	56,56,56	1.20	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	614	-	69,73,73	1.32	9 (13%)	82,113,113	1.32	7 (8%)
32	LMG	c	522	-	48,48,55	0.99	3 (6%)	56,56,63	1.31	9 (16%)
27	BCR	b	617	-	41,41,41	1.24	3 (7%)	56,56,56	1.20	6 (10%)
31	STE	C	521	-	11,11,19	0.73	0	11,11,19	1.16	0
31	STE	t	103	-	9,9,19	0.44	0	8,8,19	0.63	0
30	DGD	H	103	-	63,63,67	1.12	5 (7%)	77,77,81	1.42	11 (14%)
32	LMG	d	409	-	21,21,55	0.56	0	20,20,63	1.24	3 (15%)
25	CLA	C	505	-	69,73,73	1.33	8 (11%)	82,113,113	1.24	6 (7%)
25	CLA	A	607	37	69,73,73	1.19	6 (8%)	82,113,113	1.43	8 (9%)
25	CLA	c	505	-	69,73,73	1.11	7 (10%)	82,113,113	1.31	9 (10%)
33	LHG	D	408	-	46,46,48	0.91	1 (2%)	49,52,54	1.31	6 (12%)
21	OEY	a	601[C]	3,1,37	0,16,16	-	-	-	-	-
34	BCT	D	401	23	3,3,3	1.09	0	2,3,3	3.15	1 (50%)
27	BCR	B	618	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	4 (7%)
25	CLA	D	402	-	69,73,73	1.30	7 (10%)	82,113,113	1.32	7 (8%)
25	CLA	H	101	37	69,73,73	1.42	9 (13%)	82,113,113	1.34	5 (6%)
25	CLA	a	607	-	69,73,73	1.49	11 (15%)	82,113,113	1.30	7 (8%)
29	SQD	F	102	-	34,36,54	1.55	5 (14%)	42,45,65	1.75	11 (26%)
25	CLA	c	504	37	64,68,73	1.20	7 (10%)	76,107,113	1.33	12 (15%)
25	CLA	C	507	37	69,73,73	1.22	7 (10%)	82,113,113	1.48	8 (9%)
22	OEX	a	602[A]	3,1,37	0,15,15	-	-	-	-	-
28	PL9	A	612	-	55,55,55	0.92	2 (3%)	68,69,69	1.53	13 (19%)
30	DGD	A	616	-	67,67,67	1.08	5 (7%)	81,81,81	1.30	11 (13%)
21	OEY	A	601[C]	3,1,37	0,16,16	-	-	-	-	-
25	CLA	C	512	-	69,73,73	1.40	11 (15%)	82,113,113	1.30	9 (10%)
27	BCR	T	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.24	5 (8%)
27	BCR	A	611	-	41,41,41	0.97	2 (4%)	56,56,56	1.33	8 (14%)
25	CLA	c	503	-	69,73,73	1.30	7 (10%)	82,113,113	1.40	7 (8%)
36	HEC	v	201	16	46,50,50	1.89	4 (8%)	58,82,82	1.73	7 (12%)
25	CLA	C	508	-	69,73,73	1.27	8 (11%)	82,113,113	1.47	10 (12%)
25	CLA	B	610	-	69,73,73	1.32	10 (14%)	82,113,113	1.51	10 (12%)
25	CLA	B	603	-	69,73,73	1.45	8 (11%)	82,113,113	1.58	10 (12%)
32	LMG	b	620	-	55,55,55	0.84	2 (3%)	63,63,63	1.37	9 (14%)
22	OEX	A	602[A]	3,1,37	0,15,15	-	-	-	-	-
29	SQD	l	101	-	52,54,54	1.60	10 (19%)	62,65,65	1.69	11 (17%)
31	STE	B	619	-	16,16,19	0.71	0	16,16,19	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	B	616	-	41,41,41	1.06	3 (7%)	56,56,56	1.23	7 (12%)
25	CLA	c	501	-	69,73,73	1.13	7 (10%)	82,113,113	1.43	8 (9%)
25	CLA	b	608	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	10 (12%)
31	STE	R	101	-	11,11,19	0.74	0	11,11,19	1.14	0
25	CLA	b	605	-	69,73,73	1.43	9 (13%)	82,113,113	1.50	7 (8%)
31	STE	l	103	-	17,17,19	0.29	0	16,16,19	0.93	0
28	PL9	d	405	-	55,55,55	1.08	4 (7%)	68,69,69	1.52	11 (16%)
31	STE	B	624	-	17,17,19	0.64	0	17,17,19	1.10	0
31	STE	D	410	-	19,19,19	0.56	0	19,19,19	1.18	0
31	STE	J	101	-	11,11,19	0.68	0	11,11,19	1.28	2 (18%)
32	LMG	m	101	-	51,51,55	0.98	3 (5%)	59,59,63	1.38	8 (13%)
32	LMG	c	520	-	37,37,55	0.95	1 (2%)	45,45,63	1.33	4 (8%)
32	LMG	D	406	-	51,51,55	0.90	2 (3%)	59,59,63	1.36	5 (8%)
25	CLA	A	606	-	69,73,73	1.29	8 (11%)	82,113,113	1.16	9 (10%)
33	LHG	B	622	-	48,48,48	0.85	2 (4%)	51,54,54	1.35	7 (13%)
25	CLA	B	608	-	69,73,73	1.20	6 (8%)	82,113,113	1.29	5 (6%)
29	SQD	A	615	-	38,38,54	1.77	5 (13%)	40,40,65	1.32	3 (7%)
25	CLA	B	605	-	69,73,73	1.33	8 (11%)	82,113,113	1.38	8 (9%)
31	STE	C	522	-	15,15,19	0.39	0	14,14,19	0.74	0
25	CLA	B	615	-	64,68,73	1.47	6 (9%)	76,107,113	1.48	10 (13%)
25	CLA	C	506	-	69,73,73	1.34	8 (11%)	82,113,113	1.34	10 (12%)
33	LHG	E	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.23	6 (11%)
27	BCR	b	618	-	41,41,41	1.02	2 (4%)	56,56,56	1.28	7 (12%)
31	STE	b	622	-	19,19,19	0.63	0	19,19,19	1.05	1 (5%)
25	CLA	b	603	-	69,73,73	1.29	7 (10%)	82,113,113	1.54	11 (13%)
25	CLA	c	509	-	69,73,73	1.16	6 (8%)	82,113,113	1.46	4 (4%)
35	HEM	e	101	5,6	50,50,50	1.52	9 (18%)	67,82,82	1.27	7 (10%)
27	BCR	H	102	-	41,41,41	0.95	1 (2%)	56,56,56	1.21	6 (10%)
32	LMG	C	519	-	48,48,55	0.91	3 (6%)	56,56,63	1.34	6 (10%)
27	BCR	x	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.21	4 (7%)
25	CLA	C	510	-	69,73,73	1.25	9 (13%)	82,113,113	1.31	8 (9%)
25	CLA	c	510	-	69,73,73	1.22	8 (11%)	82,113,113	1.30	8 (9%)
30	DGD	h	102	-	63,63,67	1.03	4 (6%)	77,77,81	1.45	13 (16%)
25	CLA	D	403	-	69,73,73	1.35	9 (13%)	82,113,113	1.16	4 (4%)
25	CLA	d	403	-	69,73,73	1.26	9 (13%)	82,113,113	1.19	9 (10%)
26	PHO	A	609	-	58,69,69	2.11	10 (17%)	55,99,99	1.59	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	513	-	69,73,73	1.15	5 (7%)	82,113,113	1.26	9 (10%)
25	CLA	b	602	-	69,73,73	1.23	6 (8%)	82,113,113	1.31	9 (10%)
25	CLA	b	609	37	69,73,73	1.57	7 (10%)	82,113,113	1.42	9 (10%)
31	STE	H	104	-	17,17,19	0.44	0	16,16,19	0.57	0
27	BCR	C	514	-	41,41,41	1.10	3 (7%)	56,56,56	1.20	6 (10%)
25	CLA	c	507	37	69,73,73	1.22	8 (11%)	82,113,113	1.29	6 (7%)
25	CLA	B	606	37	69,73,73	1.37	5 (7%)	82,113,113	1.43	9 (10%)
30	DGD	a	616	-	43,43,67	0.78	2 (4%)	45,45,81	1.50	8 (17%)
33	LHG	D	407	-	48,48,48	0.77	1 (2%)	51,54,54	1.29	9 (17%)
27	BCR	K	103	-	41,41,41	1.09	2 (4%)	56,56,56	1.11	5 (8%)
33	LHG	e	102	-	41,41,48	0.78	2 (4%)	44,47,54	1.31	5 (11%)
31	STE	M	103	-	9,9,19	0.40	0	8,8,19	0.76	0
29	SQD	A	614	-	50,52,54	1.58	7 (14%)	60,63,65	1.90	15 (25%)
31	STE	t	102	-	13,13,19	0.64	0	13,13,19	1.30	2 (15%)
25	CLA	b	601	-	69,73,73	1.13	4 (5%)	82,113,113	1.38	8 (9%)
25	CLA	B	614	-	69,73,73	1.41	8 (11%)	82,113,113	1.32	5 (6%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.45	10 (17%)
28	PL9	D	405	-	55,55,55	1.02	3 (5%)	68,69,69	1.58	17 (25%)
30	DGD	C	516	-	63,63,67	1.09	4 (6%)	77,77,81	1.35	9 (11%)
30	DGD	C	518	-	63,63,67	0.98	3 (4%)	77,77,81	1.42	7 (9%)
31	STE	T	103	-	14,14,19	0.30	0	13,13,19	0.96	0
25	CLA	c	511	3	69,73,73	1.36	6 (8%)	82,113,113	1.43	6 (7%)
31	STE	x	102	-	19,19,19	0.66	0	19,19,19	0.92	1 (5%)
25	CLA	B	601	-	69,73,73	1.25	9 (13%)	82,113,113	1.35	8 (9%)
25	CLA	B	613	-	69,73,73	1.40	8 (11%)	82,113,113	1.28	9 (10%)
33	LHG	l	102	-	48,48,48	0.54	0	51,54,54	1.25	7 (13%)
31	STE	b	619	-	19,19,19	0.64	0	19,19,19	0.99	0
31	STE	b	623	-	9,9,19	0.41	0	8,8,19	0.60	0
34	BCT	a	606	23	3,3,3	1.18	0	2,3,3	2.93	1 (50%)
32	LMG	D	409	-	31,31,55	0.67	1 (3%)	33,33,63	1.22	2 (6%)
25	CLA	C	509	-	69,73,73	1.53	11 (15%)	82,113,113	1.41	11 (13%)
31	STE	j	101	-	11,11,19	0.79	0	11,11,19	1.19	1 (9%)
25	CLA	A	610	-	58,62,73	1.23	6 (10%)	68,99,113	1.34	11 (16%)
35	HEM	F	101	5,6	50,50,50	1.42	9 (18%)	67,82,82	1.10	2 (2%)
27	BCR	t	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.46	10 (17%)
31	STE	m	102	-	11,11,19	0.74	0	11,11,19	1.39	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	k	101	-	41,41,41	1.00	3 (7%)	56,56,56	1.11	3 (5%)
27	BCR	K	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	5 (8%)
31	STE	M	102	-	14,14,19	0.67	0	14,14,19	1.24	1 (7%)
32	LMG	c	524	-	49,49,55	0.90	4 (8%)	57,57,63	1.25	3 (5%)
25	CLA	d	402	-	69,73,73	1.31	9 (13%)	82,113,113	1.27	8 (9%)
25	CLA	C	503	-	69,73,73	1.28	9 (13%)	82,113,113	1.47	7 (8%)
25	CLA	b	615	-	64,68,73	1.25	7 (10%)	76,107,113	1.39	6 (7%)
25	CLA	B	604	-	69,73,73	1.24	8 (11%)	82,113,113	1.32	8 (9%)
27	BCR	b	616	-	41,41,41	0.99	3 (7%)	56,56,56	1.30	6 (10%)
25	CLA	b	610	-	69,73,73	1.27	5 (7%)	82,113,113	1.35	7 (8%)
31	STE	B	625	-	11,11,19	0.64	0	11,11,19	1.36	2 (18%)
26	PHO	A	608	-	58,69,69	1.95	10 (17%)	55,99,99	1.46	6 (10%)
25	CLA	b	613	-	69,73,73	1.26	8 (11%)	82,113,113	1.26	8 (9%)
27	BCR	D	404	-	41,41,41	1.03	2 (4%)	56,56,56	1.25	7 (12%)
29	SQD	L	101	-	47,49,54	1.66	9 (19%)	57,60,65	1.83	10 (17%)
29	SQD	a	614	-	52,54,54	1.56	6 (11%)	62,65,65	1.92	12 (19%)
25	CLA	c	508	-	68,72,73	1.36	10 (14%)	80,111,113	1.39	12 (15%)
27	BCR	c	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	5 (8%)
31	STE	a	617	-	11,11,19	0.77	0	11,11,19	0.99	0
33	LHG	d	408	-	38,38,48	0.77	1 (2%)	41,44,54	1.18	3 (7%)
25	CLA	B	612	-	69,73,73	1.21	8 (11%)	82,113,113	1.41	7 (8%)
21	OEY	A	601[B]	3,1,37	0,16,16	-	-	-	-	-
25	CLA	B	609	37	69,73,73	1.24	10 (14%)	82,113,113	1.43	11 (13%)
33	LHG	d	406	-	48,48,48	0.82	3 (6%)	51,54,54	1.35	7 (13%)
25	CLA	C	513	-	69,73,73	1.23	7 (10%)	82,113,113	1.38	8 (9%)
27	BCR	a	611	-	41,41,41	0.95	2 (4%)	56,56,56	1.17	5 (8%)
31	STE	d	411	-	16,16,19	0.65	0	16,16,19	1.13	1 (6%)
25	CLA	B	607	-	69,73,73	1.44	9 (13%)	82,113,113	1.37	10 (12%)
31	STE	I	101	-	14,14,19	0.41	0	13,13,19	0.72	0
29	SQD	f	101	-	39,41,54	1.70	9 (23%)	49,52,65	1.77	11 (22%)
30	DGD	C	517	-	63,63,67	1.05	6 (9%)	77,77,81	1.45	11 (14%)
25	CLA	C	504	37	63,67,73	1.37	10 (15%)	74,105,113	1.37	13 (17%)
28	PL9	a	612	-	55,55,55	0.72	1 (1%)	68,69,69	1.51	11 (16%)
31	STE	c	521	-	19,19,19	0.65	0	19,19,19	0.94	0
25	CLA	b	607	-	69,73,73	1.49	9 (13%)	82,113,113	1.40	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	608	37	69,73,73	1.14	6 (8%)	82,113,113	1.23	6 (7%)
25	CLA	B	602	-	69,73,73	1.27	7 (10%)	82,113,113	1.42	11 (13%)
25	CLA	C	511	3	69,73,73	1.28	8 (11%)	82,113,113	1.35	5 (6%)
27	BCR	c	516	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	3 (5%)
25	CLA	b	611	-	69,73,73	1.38	9 (13%)	82,113,113	1.34	9 (10%)
25	CLA	c	512	-	69,73,73	1.23	9 (13%)	82,113,113	1.32	7 (8%)
25	CLA	b	612	-	69,73,73	1.32	9 (13%)	82,113,113	1.42	13 (15%)
25	CLA	h	101	37	69,73,73	1.36	9 (13%)	82,113,113	1.32	9 (10%)
21	OEY	a	601[B]	3,1,37	0,16,16	-	-	-	-	-
31	STE	T	102	-	15,15,19	0.41	0	14,14,19	0.71	0
36	HEC	V	201	16	46,50,50	1.82	5 (10%)	58,82,82	1.94	6 (10%)
30	DGD	c	517	-	63,63,67	0.86	3 (4%)	77,77,81	1.35	9 (11%)
25	CLA	B	611	-	69,73,73	1.21	10 (14%)	82,113,113	1.43	11 (13%)
25	CLA	A	613	37	69,73,73	1.15	6 (8%)	82,113,113	1.25	8 (9%)
27	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.25	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	d	401	-	-	7/37/103/103	0/5/6/6
31	STE	C	520	-	-	1/9/9/17	-
25	CLA	C	501	-	1/1/15/20	7/39/115/115	-
25	CLA	a	613	37	1/1/15/20	1/39/115/115	-
25	CLA	b	604	-	1/1/15/20	12/39/115/115	-
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
29	SQD	a	615	-	-	19/37/37/69	-
31	STE	B	626	-	-	4/13/13/17	-
31	STE	c	523	-	-	4/9/9/17	-
33	LHG	B	621	-	-	21/53/53/53	-
31	STE	b	621	-	-	6/13/13/17	-
25	CLA	b	606	37	1/1/15/20	13/39/115/115	-
32	LMG	d	410	-	-	8/39/59/70	0/1/1/1
30	DGD	c	518	-	-	17/51/91/95	0/2/2/2
30	DGD	c	519	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	610	-	1/1/15/20	10/39/115/115	-
32	LMG	C	515	-	-	22/43/63/70	0/1/1/1
25	CLA	c	506	-	1/1/15/20	15/39/115/115	-
32	LMG	M	101	-	-	25/46/66/70	0/1/1/1
33	LHG	d	407	-	-	19/53/53/53	-
25	CLA	C	502	-	1/1/15/20	8/39/115/115	-
25	CLA	c	502	-	-	5/39/115/115	-
32	LMG	B	620	-	-	14/22/22/70	-
31	STE	B	623	-	-	7/9/9/17	-
26	PHO	a	609	-	-	2/37/103/103	0/5/6/6
27	BCR	d	404	-	-	10/29/63/63	0/2/2/2
25	CLA	b	614	-	1/1/15/20	9/39/115/115	-
32	LMG	c	522	-	-	29/43/63/70	0/1/1/1
27	BCR	b	617	-	-	2/29/63/63	0/2/2/2
31	STE	C	521	-	-	5/9/9/17	-
31	STE	t	103	-	-	4/7/7/17	-
30	DGD	H	103	-	-	16/51/91/95	0/2/2/2
32	LMG	d	409	-	-	8/17/17/70	-
25	CLA	C	505	-	1/1/15/20	13/39/115/115	-
25	CLA	A	607	37	-	11/39/115/115	-
25	CLA	c	505	-	1/1/15/20	12/39/115/115	-
33	LHG	D	408	-	-	23/51/51/53	-
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2
25	CLA	D	402	-	1/1/15/20	6/39/115/115	-
25	CLA	H	101	37	1/1/15/20	18/39/115/115	-
25	CLA	a	607	-	1/1/15/20	4/39/115/115	-
29	SQD	F	102	-	-	10/28/48/69	0/1/1/1
25	CLA	c	504	37	1/1/14/20	8/33/109/115	-
25	CLA	C	507	37	1/1/15/20	9/39/115/115	-
28	PL9	A	612	-	-	27/53/73/73	0/1/1/1
30	DGD	A	616	-	-	28/55/95/95	0/2/2/2
25	CLA	C	512	-	1/1/15/20	14/39/115/115	-
27	BCR	T	101	-	-	6/29/63/63	0/2/2/2
27	BCR	A	611	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	503	-	1/1/15/20	7/39/115/115	-
36	HEC	v	201	16	-	6/14/54/54	-
25	CLA	C	508	-	-	8/39/115/115	-
25	CLA	B	610	-	1/1/15/20	7/39/115/115	-
25	CLA	B	603	-	1/1/15/20	12/39/115/115	-
32	LMG	b	620	-	-	31/50/70/70	0/1/1/1
29	SQD	l	101	-	-	28/49/69/69	0/1/1/1
31	STE	B	619	-	-	7/14/14/17	-
27	BCR	B	616	-	-	8/29/63/63	0/2/2/2
25	CLA	c	501	-	1/1/15/20	4/39/115/115	-
25	CLA	b	608	-	1/1/15/20	5/39/115/115	-
31	STE	R	101	-	-	4/9/9/17	-
25	CLA	b	605	-	1/1/15/20	7/39/115/115	-
31	STE	l	103	-	-	8/15/15/17	-
28	PL9	d	405	-	-	13/53/73/73	0/1/1/1
31	STE	B	624	-	-	8/15/15/17	-
31	STE	D	410	-	-	9/17/17/17	-
31	STE	J	101	-	-	4/9/9/17	-
32	LMG	m	101	-	-	24/46/66/70	0/1/1/1
32	LMG	c	520	-	-	14/31/51/70	0/1/1/1
32	LMG	D	406	-	-	18/46/66/70	0/1/1/1
25	CLA	A	606	-	1/1/15/20	3/39/115/115	-
33	LHG	B	622	-	-	15/53/53/53	-
25	CLA	B	608	-	-	4/39/115/115	-
29	SQD	A	615	-	-	17/39/39/69	-
25	CLA	B	605	-	1/1/15/20	14/39/115/115	-
31	STE	C	522	-	-	4/13/13/17	-
25	CLA	B	615	-	1/1/14/20	6/33/109/115	-
25	CLA	C	506	-	1/1/15/20	13/39/115/115	-
33	LHG	E	101	-	-	32/53/53/53	-
27	BCR	b	618	-	-	7/29/63/63	0/2/2/2
31	STE	b	622	-	-	9/17/17/17	-
25	CLA	b	603	-	1/1/15/20	7/39/115/115	-
25	CLA	c	509	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	e	101	5,6	-	0/14/54/54	-
27	BCR	H	102	-	-	4/29/63/63	0/2/2/2
32	LMG	C	519	-	-	22/43/63/70	0/1/1/1
27	BCR	x	101	-	-	4/29/63/63	0/2/2/2
25	CLA	C	510	-	1/1/15/20	10/39/115/115	-
25	CLA	c	510	-	1/1/15/20	14/39/115/115	-
30	DGD	h	102	-	-	14/51/91/95	0/2/2/2
25	CLA	D	403	-	-	12/39/115/115	-
25	CLA	d	403	-	1/1/15/20	4/39/115/115	-
26	PHO	A	609	-	-	2/37/103/103	0/5/6/6
25	CLA	c	513	-	1/1/15/20	10/39/115/115	-
25	CLA	b	602	-	1/1/15/20	13/39/115/115	-
25	CLA	b	609	37	1/1/15/20	4/39/115/115	-
31	STE	H	104	-	-	9/15/15/17	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
25	CLA	c	507	37	1/1/15/20	12/39/115/115	-
25	CLA	B	606	37	1/1/15/20	10/39/115/115	-
30	DGD	a	616	-	-	26/45/45/95	-
33	LHG	D	407	-	-	23/53/53/53	-
27	BCR	K	103	-	-	7/29/63/63	0/2/2/2
33	LHG	e	102	-	-	25/46/46/53	-
31	STE	M	103	-	-	2/7/7/17	-
29	SQD	A	614	-	-	21/47/67/69	0/1/1/1
31	STE	t	102	-	-	3/11/11/17	-
25	CLA	b	601	-	1/1/15/20	12/39/115/115	-
25	CLA	B	614	-	1/1/15/20	12/39/115/115	-
27	BCR	K	101	-	-	11/29/63/63	0/2/2/2
28	PL9	D	405	-	-	12/53/73/73	0/1/1/1
30	DGD	C	516	-	-	18/51/91/95	0/2/2/2
30	DGD	C	518	-	-	14/51/91/95	0/2/2/2
31	STE	T	103	-	-	11/12/12/17	-
25	CLA	c	511	3	1/1/15/20	4/39/115/115	-
31	STE	x	102	-	-	6/17/17/17	-
25	CLA	B	601	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	613	-	1/1/15/20	15/39/115/115	-
33	LHG	l	102	-	-	16/53/53/53	-
31	STE	b	619	-	-	9/17/17/17	-
31	STE	b	623	-	-	2/7/7/17	-
32	LMG	D	409	-	-	18/33/33/70	-
25	CLA	C	509	-	1/1/15/20	13/39/115/115	-
31	STE	j	101	-	-	3/9/9/17	-
25	CLA	A	610	-	1/1/12/20	2/26/102/115	-
35	HEM	F	101	5,6	-	3/14/54/54	-
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
31	STE	m	102	-	-	4/9/9/17	-
27	BCR	k	101	-	-	5/29/63/63	0/2/2/2
27	BCR	K	102	-	-	6/29/63/63	0/2/2/2
31	STE	M	102	-	-	7/12/12/17	-
32	LMG	c	524	-	-	28/44/64/70	0/1/1/1
25	CLA	d	402	-	1/1/15/20	3/39/115/115	-
25	CLA	C	503	-	1/1/15/20	7/39/115/115	-
25	CLA	b	615	-	1/1/14/20	8/33/109/115	-
25	CLA	B	604	-	1/1/15/20	4/39/115/115	-
27	BCR	b	616	-	-	4/29/63/63	0/2/2/2
25	CLA	b	610	-	1/1/15/20	8/39/115/115	-
31	STE	B	625	-	-	3/9/9/17	-
26	PHO	A	608	-	-	2/37/103/103	0/5/6/6
25	CLA	b	613	-	1/1/15/20	13/39/115/115	-
27	BCR	D	404	-	-	6/29/63/63	0/2/2/2
29	SQD	L	101	-	-	19/44/64/69	0/1/1/1
29	SQD	a	614	-	-	26/49/69/69	0/1/1/1
25	CLA	c	508	-	-	3/38/114/115	-
27	BCR	c	515	-	-	6/29/63/63	0/2/2/2
31	STE	a	617	-	-	4/9/9/17	-
33	LHG	d	408	-	-	12/43/43/53	-
25	CLA	B	612	-	1/1/15/20	16/39/115/115	-
25	CLA	B	609	37	1/1/15/20	6/39/115/115	-
33	LHG	d	406	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	513	-	1/1/15/20	12/39/115/115	-
27	BCR	a	611	-	-	1/29/63/63	0/2/2/2
31	STE	d	411	-	-	11/14/14/17	-
25	CLA	B	607	-	1/1/15/20	2/39/115/115	-
31	STE	I	101	-	-	3/12/12/17	-
29	SQD	f	101	-	-	24/36/56/69	0/1/1/1
30	DGD	C	517	-	-	24/51/91/95	0/2/2/2
25	CLA	C	504	37	1/1/13/20	9/32/108/115	-
28	PL9	a	612	-	-	24/53/73/73	0/1/1/1
31	STE	c	521	-	-	11/17/17/17	-
25	CLA	b	607	-	1/1/15/20	3/39/115/115	-
25	CLA	a	608	37	1/1/15/20	12/39/115/115	-
25	CLA	B	602	-	1/1/15/20	10/39/115/115	-
25	CLA	C	511	3	1/1/15/20	8/39/115/115	-
27	BCR	c	516	-	-	4/29/63/63	0/2/2/2
25	CLA	b	611	-	1/1/15/20	8/39/115/115	-
25	CLA	c	512	-	1/1/15/20	22/39/115/115	-
25	CLA	b	612	-	1/1/15/20	4/39/115/115	-
25	CLA	h	101	37	1/1/15/20	18/39/115/115	-
31	STE	T	102	-	-	7/13/13/17	-
36	HEC	V	201	16	-	6/14/54/54	-
30	DGD	c	517	-	-	27/51/91/95	0/2/2/2
25	CLA	B	611	-	1/1/15/20	9/39/115/115	-
25	CLA	A	613	37	1/1/15/20	10/39/115/115	-
27	BCR	B	617	-	-	6/29/63/63	0/2/2/2

All (807) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	609	PHO	C1B-C2B	10.05	1.50	1.39
26	A	609	PHO	C1B-C2B	9.34	1.49	1.39
26	d	401	PHO	C1B-C2B	8.96	1.49	1.39
25	b	609	CLA	MG-NB	-8.74	1.88	2.05
26	d	401	PHO	C3B-C4B	8.68	1.50	1.41
26	A	609	PHO	C3B-C4B	8.64	1.50	1.41
26	a	609	PHO	C3B-C4B	8.07	1.49	1.41
26	A	608	PHO	C1B-C2B	8.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	605	CLA	MG-NA	7.63	2.24	2.06
25	b	607	CLA	MG-NA	7.49	2.24	2.06
25	B	615	CLA	MG-NA	7.43	2.23	2.06
26	A	608	PHO	C3B-C4B	7.36	1.49	1.41
25	B	603	CLA	MG-NA	7.01	2.22	2.06
36	v	201	HEC	CAC-C3C	6.63	1.56	1.35
36	V	201	HEC	CAC-C3C	6.54	1.56	1.35
25	C	509	CLA	MG-NA	6.48	2.21	2.06
36	v	201	HEC	CAB-C3B	6.40	1.55	1.35
25	H	101	CLA	MG-NA	6.14	2.20	2.06
36	V	201	HEC	CAB-C3B	6.13	1.54	1.35
25	B	605	CLA	MG-NA	5.77	2.20	2.06
25	b	611	CLA	MG-ND	-5.76	1.94	2.05
25	c	511	CLA	MG-NA	5.73	2.19	2.06
25	B	606	CLA	MG-NB	-5.61	1.94	2.05
25	B	607	CLA	MG-NA	5.51	2.19	2.06
25	a	607	CLA	MG-NC	5.49	2.19	2.06
25	D	402	CLA	MG-NA	5.39	2.19	2.06
25	h	101	CLA	MG-NA	5.37	2.19	2.06
36	v	201	HEC	C3D-C2D	5.33	1.52	1.38
36	V	201	HEC	C3D-C2D	5.31	1.52	1.38
35	e	101	HEM	FE-NA	5.29	2.12	1.95
25	B	613	CLA	MG-ND	-5.24	1.95	2.05
25	b	610	CLA	MG-NA	5.23	2.18	2.06
25	b	612	CLA	MG-NA	5.20	2.18	2.06
29	A	615	SQD	O47-C45	-5.19	1.38	1.47
25	B	614	CLA	MG-NA	5.14	2.18	2.06
29	L	101	SQD	O48-C23	5.07	1.48	1.33
29	a	614	SQD	O48-C23	4.90	1.47	1.33
29	a	615	SQD	O48-C23	4.88	1.47	1.33
29	F	102	SQD	O48-C23	4.85	1.47	1.33
25	B	602	CLA	MG-NA	4.84	2.17	2.06
25	B	606	CLA	MG-NA	4.78	2.17	2.06
29	A	615	SQD	O48-C23	4.76	1.47	1.33
25	C	511	CLA	MG-NA	4.73	2.17	2.06
29	f	101	SQD	O48-C23	4.72	1.47	1.33
25	C	506	CLA	MG-ND	-4.64	1.96	2.05
29	A	614	SQD	O48-C23	4.58	1.46	1.33
25	a	610	CLA	MG-ND	-4.56	1.96	2.05
29	l	101	SQD	O48-C23	4.55	1.46	1.33
25	b	603	CLA	MG-NA	4.51	2.17	2.06
25	d	402	CLA	MG-NA	4.48	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	401	PHO	C1D-C2D	4.48	1.44	1.39
27	b	617	BCR	C30-C25	-4.47	1.48	1.53
25	C	505	CLA	MG-NA	4.46	2.16	2.06
25	B	603	CLA	C1D-ND	4.43	1.43	1.37
25	C	503	CLA	MG-NA	4.40	2.16	2.06
25	b	602	CLA	MG-NA	4.38	2.16	2.06
25	C	504	CLA	MG-NA	4.38	2.16	2.06
25	C	502	CLA	MG-NB	-4.38	1.97	2.05
25	C	501	CLA	MG-NA	4.30	2.16	2.06
25	B	610	CLA	MG-NA	4.28	2.16	2.06
26	A	609	PHO	C1D-C2D	4.19	1.44	1.39
25	C	506	CLA	MG-NA	4.19	2.16	2.06
25	c	508	CLA	MG-ND	4.16	2.14	2.05
25	B	613	CLA	MG-NA	4.14	2.16	2.06
25	a	613	CLA	MG-NA	4.11	2.16	2.06
25	B	609	CLA	C1D-ND	4.11	1.43	1.37
25	C	508	CLA	MG-NA	4.10	2.16	2.06
27	c	515	BCR	C1-C6	-4.08	1.48	1.53
25	c	503	CLA	MG-NA	4.07	2.15	2.06
25	c	506	CLA	C1D-ND	4.07	1.43	1.37
25	a	607	CLA	C1D-ND	4.07	1.43	1.37
25	C	512	CLA	MG-ND	-4.03	1.97	2.05
25	C	512	CLA	MG-NB	3.97	2.13	2.05
25	b	609	CLA	C1D-ND	3.95	1.43	1.37
25	D	403	CLA	C1D-ND	3.95	1.43	1.37
25	b	613	CLA	C4B-NB	3.95	1.43	1.37
25	b	614	CLA	MG-NC	3.95	2.15	2.06
25	B	608	CLA	C1D-ND	3.93	1.43	1.37
27	C	514	BCR	C1-C6	-3.92	1.48	1.53
25	a	607	CLA	MG-NB	3.92	2.13	2.05
25	D	403	CLA	MG-ND	-3.91	1.98	2.05
28	D	405	PL9	C3-C4	-3.91	1.43	1.49
25	b	601	CLA	C1D-ND	3.91	1.43	1.37
25	b	611	CLA	C1D-ND	3.90	1.43	1.37
25	C	509	CLA	MG-ND	3.89	2.13	2.05
27	b	617	BCR	C1-C6	-3.89	1.48	1.53
25	B	607	CLA	C1D-ND	3.87	1.43	1.37
29	a	615	SQD	O47-C7	3.86	1.45	1.34
33	D	408	LHG	P-O6	3.84	1.74	1.59
25	a	608	CLA	C1D-ND	3.84	1.42	1.37
35	F	101	HEM	FE-NC	3.82	2.07	1.95
25	b	613	CLA	C1D-ND	3.80	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	C4B-NB	3.79	1.42	1.37
25	B	606	CLA	C1D-ND	3.77	1.42	1.37
35	e	101	HEM	FE-NB	3.76	2.06	1.94
25	A	606	CLA	C1B-C2B	3.75	1.51	1.43
25	B	615	CLA	C1D-ND	3.75	1.42	1.37
26	a	609	PHO	C1D-C2D	3.74	1.43	1.39
28	d	405	PL9	C6-C1	-3.73	1.42	1.48
25	d	403	CLA	C1D-ND	3.72	1.42	1.37
27	K	102	BCR	C1-C6	-3.72	1.49	1.53
29	f	101	SQD	O47-C7	3.71	1.44	1.34
25	B	604	CLA	C1B-C2B	3.71	1.51	1.43
25	d	402	CLA	C1D-ND	3.71	1.42	1.37
25	b	607	CLA	MG-NC	-3.70	1.97	2.06
25	C	506	CLA	C1D-ND	3.69	1.42	1.37
25	b	606	CLA	MG-NC	3.69	2.15	2.06
29	A	615	SQD	O47-C7	3.68	1.44	1.34
25	D	403	CLA	MG-NA	3.68	2.15	2.06
25	B	613	CLA	MG-NB	3.66	2.13	2.05
25	C	509	CLA	MG-NB	-3.65	1.98	2.05
29	l	101	SQD	O47-C7	3.65	1.44	1.34
25	d	403	CLA	MG-ND	-3.65	1.98	2.05
25	C	509	CLA	C1D-ND	3.64	1.42	1.37
25	B	614	CLA	C4B-NB	3.63	1.42	1.37
25	c	507	CLA	C1D-ND	3.62	1.42	1.37
25	c	509	CLA	C1D-ND	3.62	1.42	1.37
25	D	402	CLA	C1D-ND	3.62	1.42	1.37
29	a	614	SQD	O47-C45	-3.61	1.38	1.46
25	b	615	CLA	C1D-ND	3.61	1.42	1.37
25	A	606	CLA	C1D-ND	3.60	1.42	1.37
29	F	102	SQD	C24-C23	3.59	1.61	1.50
26	a	609	PHO	C4D-CHA	3.59	1.44	1.39
25	C	512	CLA	MG-NA	3.57	2.14	2.06
25	c	507	CLA	MG-NA	3.56	2.14	2.06
25	C	513	CLA	C1D-ND	3.55	1.42	1.37
25	C	507	CLA	MG-NA	3.54	2.14	2.06
29	L	101	SQD	O47-C7	3.54	1.44	1.34
25	b	614	CLA	C1D-ND	3.53	1.42	1.37
25	C	501	CLA	C1D-ND	3.53	1.42	1.37
25	b	610	CLA	C1D-ND	3.53	1.42	1.37
25	c	503	CLA	MG-NB	3.52	2.12	2.05
25	C	505	CLA	C1D-ND	3.51	1.42	1.37
25	B	604	CLA	MG-NB	3.51	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	615	SQD	C24-C23	3.51	1.60	1.50
25	H	101	CLA	C1D-ND	3.50	1.42	1.37
30	C	516	DGD	C4E-C3E	3.50	1.61	1.52
25	b	612	CLA	C1D-ND	3.49	1.42	1.37
27	B	617	BCR	C30-C25	-3.49	1.49	1.53
25	B	607	CLA	C4B-NB	3.47	1.42	1.37
25	c	508	CLA	C4B-NB	3.47	1.42	1.37
25	b	603	CLA	C1D-ND	3.47	1.42	1.37
25	c	503	CLA	C1D-ND	3.46	1.42	1.37
25	H	101	CLA	C4B-NB	3.45	1.42	1.37
29	a	614	SQD	O47-C7	3.45	1.44	1.34
29	l	101	SQD	O47-C45	-3.43	1.38	1.46
25	d	403	CLA	C4B-NB	3.43	1.42	1.37
25	B	604	CLA	C1D-ND	3.43	1.42	1.37
25	c	508	CLA	C1D-ND	3.42	1.42	1.37
25	c	512	CLA	C1D-ND	3.42	1.42	1.37
27	K	103	BCR	C1-C6	-3.42	1.49	1.53
25	C	511	CLA	C1D-ND	3.42	1.42	1.37
25	A	613	CLA	C1D-ND	3.41	1.42	1.37
33	B	622	LHG	O7-C5	-3.40	1.38	1.46
25	C	505	CLA	C4B-NB	3.40	1.42	1.37
25	B	612	CLA	C1D-ND	3.40	1.42	1.37
25	A	607	CLA	C1D-ND	3.39	1.42	1.37
27	t	101	BCR	C30-C25	-3.39	1.49	1.53
28	A	612	PL9	C7-C3	-3.39	1.46	1.51
29	A	614	SQD	O47-C45	-3.39	1.38	1.46
25	A	606	CLA	MG-ND	-3.38	1.99	2.05
25	c	501	CLA	C1D-ND	3.38	1.42	1.37
26	A	608	PHO	C4D-CHA	3.36	1.44	1.39
25	c	510	CLA	C1D-ND	3.36	1.42	1.37
26	A	608	PHO	CMC-C2C	-3.36	1.45	1.50
25	b	609	CLA	MG-NC	3.35	2.14	2.06
33	d	406	LHG	O7-C5	-3.35	1.38	1.46
25	a	613	CLA	C1D-ND	3.34	1.42	1.37
25	c	509	CLA	C1B-C2B	3.34	1.51	1.43
27	d	404	BCR	C1-C6	-3.33	1.49	1.53
25	B	601	CLA	C1D-ND	3.32	1.42	1.37
25	c	511	CLA	C1D-ND	3.32	1.42	1.37
27	B	616	BCR	C1-C6	-3.31	1.49	1.53
27	c	516	BCR	C30-C25	-3.31	1.49	1.53
25	C	507	CLA	C1B-C2B	3.30	1.50	1.43
25	b	614	CLA	MG-NB	3.29	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	C4B-NB	3.28	1.42	1.37
25	C	505	CLA	C1B-C2B	3.28	1.50	1.43
32	c	522	LMG	C3-C2	3.27	1.60	1.52
30	C	518	DGD	O1G-C1G	-3.27	1.37	1.45
25	c	510	CLA	MG-NA	3.27	2.14	2.06
25	B	610	CLA	C1D-ND	3.27	1.42	1.37
29	L	101	SQD	O5-C1	3.27	1.50	1.41
25	b	608	CLA	C1D-ND	3.26	1.42	1.37
25	b	605	CLA	C1D-ND	3.25	1.42	1.37
25	H	101	CLA	C1B-C2B	3.24	1.50	1.43
27	d	404	BCR	C30-C25	-3.24	1.49	1.53
25	C	507	CLA	C1D-ND	3.23	1.42	1.37
25	B	611	CLA	C1D-ND	3.23	1.42	1.37
29	A	614	SQD	C24-C23	3.22	1.60	1.50
25	B	612	CLA	C4B-NB	3.22	1.42	1.37
25	a	610	CLA	C1D-ND	3.22	1.42	1.37
32	m	101	LMG	C4-C3	3.22	1.60	1.52
25	b	610	CLA	C1B-C2B	3.21	1.50	1.43
25	a	610	CLA	C1B-C2B	3.21	1.50	1.43
25	B	614	CLA	C1D-ND	3.20	1.42	1.37
26	A	608	PHO	C1D-C2D	3.19	1.43	1.39
25	B	608	CLA	MG-NA	3.19	2.13	2.06
25	C	512	CLA	C1D-ND	3.19	1.42	1.37
25	a	607	CLA	MG-ND	-3.18	1.99	2.05
29	f	101	SQD	C24-C23	3.18	1.59	1.50
25	C	508	CLA	C1D-ND	3.18	1.42	1.37
25	C	510	CLA	C1D-ND	3.18	1.42	1.37
29	f	101	SQD	O47-C45	-3.18	1.39	1.46
25	B	608	CLA	C4B-NB	3.16	1.42	1.37
27	c	516	BCR	C1-C6	-3.15	1.49	1.53
25	A	610	CLA	C4B-NB	3.15	1.42	1.37
30	H	103	DGD	O5D-C1E	3.14	1.45	1.40
25	A	607	CLA	C4B-NB	3.14	1.42	1.37
25	B	610	CLA	C1B-C2B	3.14	1.50	1.43
25	c	513	CLA	C4B-NB	3.14	1.42	1.37
27	K	101	BCR	C1-C6	-3.13	1.49	1.53
35	F	101	HEM	CAB-C3B	3.12	1.55	1.47
25	b	615	CLA	MG-NA	3.12	2.13	2.06
29	A	614	SQD	O47-C7	3.12	1.43	1.34
25	c	511	CLA	C4B-NB	3.12	1.42	1.37
25	h	101	CLA	C4B-NB	3.12	1.42	1.37
27	K	103	BCR	C30-C25	-3.11	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	613	CLA	MG-NB	3.11	2.11	2.05
27	B	618	BCR	C1-C6	-3.10	1.49	1.53
25	c	512	CLA	C4B-NB	3.10	1.41	1.37
25	B	607	CLA	MG-NC	3.10	2.13	2.06
30	A	616	DGD	C4D-C5D	3.10	1.59	1.53
25	C	510	CLA	C4B-NB	3.09	1.41	1.37
26	A	609	PHO	C4D-CHA	3.09	1.44	1.39
25	d	402	CLA	C4B-NB	3.09	1.41	1.37
25	b	603	CLA	C1B-C2B	3.08	1.50	1.43
29	A	615	SQD	C24-C23	3.08	1.59	1.50
25	C	502	CLA	C1D-ND	3.08	1.41	1.37
25	c	508	CLA	MG-NC	3.08	2.13	2.06
27	c	514	BCR	C1-C6	-3.07	1.49	1.53
25	b	614	CLA	C4B-NB	3.07	1.41	1.37
27	C	514	BCR	C30-C25	-3.07	1.49	1.53
25	C	503	CLA	C1D-ND	3.07	1.41	1.37
25	C	511	CLA	C1B-C2B	3.06	1.50	1.43
25	B	613	CLA	C4B-NB	3.06	1.41	1.37
25	B	614	CLA	MG-NB	3.06	2.11	2.05
25	h	101	CLA	C1B-C2B	3.06	1.50	1.43
25	C	503	CLA	C1B-C2B	3.06	1.50	1.43
25	B	601	CLA	MG-NA	3.06	2.13	2.06
25	B	609	CLA	C4B-NB	3.05	1.41	1.37
25	b	604	CLA	C4B-NB	3.04	1.41	1.37
25	c	506	CLA	C4B-NB	3.04	1.41	1.37
25	A	606	CLA	C4B-NB	3.04	1.41	1.37
25	b	608	CLA	C4B-NB	3.04	1.41	1.37
25	b	613	CLA	MG-NA	3.04	2.13	2.06
25	c	505	CLA	C4B-NB	3.03	1.41	1.37
32	c	522	LMG	C4-C3	3.03	1.60	1.52
25	c	504	CLA	C4B-NB	3.03	1.41	1.37
27	K	102	BCR	C30-C25	-3.03	1.49	1.53
26	d	401	PHO	C4D-CHA	3.02	1.44	1.39
25	c	513	CLA	C1D-ND	3.02	1.41	1.37
29	L	101	SQD	O47-C45	-3.02	1.39	1.46
25	b	602	CLA	C1D-ND	3.02	1.41	1.37
27	b	618	BCR	C1-C6	-3.02	1.49	1.53
29	A	614	SQD	O5-C1	3.02	1.49	1.41
25	h	101	CLA	C1D-ND	3.02	1.41	1.37
25	B	608	CLA	C1B-C2B	3.01	1.50	1.43
25	c	511	CLA	C1B-C2B	3.01	1.50	1.43
25	c	502	CLA	C1D-ND	3.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	607	CLA	C1B-C2B	3.01	1.50	1.43
27	k	101	BCR	C1-C6	-3.00	1.49	1.53
25	B	613	CLA	C1D-ND	3.00	1.41	1.37
25	a	610	CLA	C4B-NB	2.99	1.41	1.37
27	a	611	BCR	C1-C6	-2.99	1.50	1.53
25	A	607	CLA	C1B-C2B	2.99	1.50	1.43
29	L	101	SQD	C24-C23	2.99	1.59	1.50
25	C	513	CLA	C1B-C2B	2.99	1.50	1.43
27	K	101	BCR	C30-C25	-2.98	1.50	1.53
27	A	611	BCR	C1-C6	-2.98	1.50	1.53
25	D	402	CLA	C1B-C2B	2.97	1.50	1.43
25	B	612	CLA	MG-ND	-2.97	1.99	2.05
29	f	101	SQD	O5-C1	2.97	1.49	1.41
29	l	101	SQD	O5-C1	2.97	1.49	1.41
28	d	405	PL9	C53-C6	-2.97	1.44	1.50
25	b	605	CLA	C1B-C2B	2.96	1.50	1.43
29	F	102	SQD	O5-C1	2.96	1.49	1.41
25	c	503	CLA	C1B-C2B	2.95	1.50	1.43
35	e	101	HEM	CAC-C3C	2.94	1.55	1.47
25	A	610	CLA	C1D-ND	2.94	1.41	1.37
25	c	501	CLA	C1B-C2B	2.94	1.50	1.43
25	C	512	CLA	C4B-NB	2.94	1.41	1.37
33	d	408	LHG	P-O6	2.93	1.70	1.59
25	B	607	CLA	MG-NB	-2.93	2.00	2.05
25	c	506	CLA	MG-NC	2.92	2.13	2.06
25	b	602	CLA	C1B-C2B	2.92	1.50	1.43
25	c	504	CLA	MG-NC	2.92	2.13	2.06
27	b	618	BCR	C30-C25	-2.91	1.50	1.53
25	C	504	CLA	MG-NB	2.91	2.11	2.05
25	B	602	CLA	C4B-NB	2.90	1.41	1.37
25	b	604	CLA	C1B-C2B	2.90	1.49	1.43
25	b	607	CLA	C1D-ND	2.90	1.41	1.37
28	d	405	PL9	C3-C4	-2.90	1.45	1.49
29	a	614	SQD	C24-C23	2.90	1.59	1.50
25	C	508	CLA	C1B-C2B	2.89	1.49	1.43
25	B	612	CLA	C1B-C2B	2.89	1.49	1.43
25	C	510	CLA	CHC-C1C	2.89	1.44	1.38
25	a	608	CLA	C4B-NB	2.88	1.41	1.37
25	b	615	CLA	C1B-C2B	2.88	1.49	1.43
26	A	608	PHO	C3D-C4D	2.88	1.45	1.41
27	H	102	BCR	C30-C25	-2.88	1.50	1.53
25	C	507	CLA	C4B-NB	2.87	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	614	CLA	C1B-C2B	2.87	1.49	1.43
29	a	615	SQD	O47-C45	-2.87	1.39	1.46
25	c	510	CLA	C1B-C2B	2.87	1.49	1.43
25	C	508	CLA	C3B-C4B	2.87	1.51	1.42
27	x	101	BCR	C30-C25	-2.87	1.50	1.53
25	c	512	CLA	C1B-C2B	2.86	1.49	1.43
29	A	615	SQD	C46-C45	2.86	1.57	1.50
25	B	615	CLA	C1B-C2B	2.86	1.49	1.43
25	B	607	CLA	MG-ND	-2.86	2.00	2.05
25	b	609	CLA	C1B-C2B	2.86	1.49	1.43
25	B	614	CLA	CHC-C1C	2.85	1.44	1.38
30	c	517	DGD	C3G-C2G	2.84	1.59	1.50
25	c	502	CLA	MG-NB	-2.84	2.00	2.05
25	C	504	CLA	C1D-ND	2.84	1.41	1.37
25	B	611	CLA	C4B-NB	2.83	1.41	1.37
25	b	612	CLA	C1B-C2B	2.83	1.49	1.43
25	B	612	CLA	MG-NA	2.83	2.13	2.06
25	B	602	CLA	C1B-C2B	2.83	1.49	1.43
25	D	403	CLA	MG-NB	-2.83	2.00	2.05
25	a	607	CLA	C4B-NB	2.82	1.41	1.37
25	b	604	CLA	C1D-ND	2.82	1.41	1.37
27	b	616	BCR	C1-C6	-2.82	1.50	1.53
25	C	513	CLA	C4B-NB	2.81	1.41	1.37
32	D	406	LMG	C4-C5	2.81	1.59	1.53
32	C	515	LMG	C4-C3	2.81	1.59	1.52
25	b	603	CLA	MG-NB	-2.81	2.00	2.05
25	C	503	CLA	MG-NC	2.81	2.12	2.06
35	F	101	HEM	CAC-C3C	2.80	1.54	1.47
25	D	403	CLA	C1B-C2B	2.80	1.49	1.43
25	c	506	CLA	C1B-C2B	2.80	1.49	1.43
25	c	508	CLA	CHC-C1C	2.80	1.44	1.38
25	B	609	CLA	MG-NA	2.80	2.12	2.06
25	C	504	CLA	C4B-NB	2.80	1.41	1.37
25	c	510	CLA	C4B-NB	2.80	1.41	1.37
27	B	616	BCR	C30-C25	-2.79	1.50	1.53
27	c	514	BCR	C30-C25	-2.79	1.50	1.53
25	B	605	CLA	CHC-C1C	2.79	1.44	1.38
32	c	524	LMG	C1-C2	2.79	1.60	1.52
25	C	505	CLA	CHC-C1C	2.79	1.44	1.38
25	C	510	CLA	C1B-C2B	2.78	1.49	1.43
25	B	601	CLA	CHC-C1C	2.77	1.44	1.38
25	b	611	CLA	MG-NB	2.77	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	410	LMG	C4-C5	2.77	1.58	1.53
25	C	502	CLA	C1B-C2B	2.76	1.49	1.43
25	c	501	CLA	C4B-NB	2.76	1.41	1.37
32	C	519	LMG	C4-C3	2.76	1.59	1.52
25	c	504	CLA	C1D-ND	2.76	1.41	1.37
25	c	509	CLA	MG-NA	2.76	2.12	2.06
25	A	613	CLA	C1B-C2B	2.76	1.49	1.43
27	B	618	BCR	C30-C25	-2.76	1.50	1.53
25	d	402	CLA	C1B-C2B	2.75	1.49	1.43
26	A	609	PHO	CMC-C2C	-2.74	1.46	1.50
30	A	616	DGD	O5D-C6D	-2.74	1.39	1.43
25	a	613	CLA	C4B-NB	2.74	1.41	1.37
25	B	603	CLA	C1B-C2B	2.74	1.49	1.43
25	B	611	CLA	CHC-C1C	2.74	1.44	1.38
33	E	101	LHG	P-O6	2.73	1.70	1.59
25	a	613	CLA	C1B-C2B	2.73	1.49	1.43
25	b	607	CLA	C3B-C4B	2.72	1.50	1.42
25	a	613	CLA	CHC-C1C	2.72	1.43	1.38
25	C	513	CLA	MG-NA	2.71	2.12	2.06
25	B	605	CLA	C4B-NB	2.71	1.41	1.37
25	B	605	CLA	C1D-ND	2.70	1.41	1.37
25	b	602	CLA	C4B-NB	2.70	1.41	1.37
32	c	520	LMG	C1-C2	2.70	1.60	1.52
32	b	620	LMG	C3-C2	2.70	1.59	1.52
25	b	607	CLA	CHC-C1C	2.69	1.43	1.38
25	c	511	CLA	CHC-C1C	2.69	1.43	1.38
29	l	101	SQD	C24-C23	2.69	1.58	1.50
27	T	101	BCR	C30-C25	-2.69	1.50	1.53
30	C	518	DGD	O2G-C2G	-2.69	1.40	1.46
25	B	601	CLA	C1B-C2B	2.69	1.49	1.43
25	h	101	CLA	CHC-C1C	2.69	1.43	1.38
30	A	616	DGD	C3E-C2E	2.68	1.59	1.52
30	C	516	DGD	O2G-C2G	-2.68	1.40	1.46
25	b	606	CLA	C1D-ND	2.68	1.41	1.37
27	D	404	BCR	C1-C6	-2.68	1.50	1.53
26	d	401	PHO	CMC-C2C	-2.68	1.46	1.50
25	C	509	CLA	MG-NC	-2.68	1.99	2.06
25	b	614	CLA	C1B-C2B	2.68	1.49	1.43
25	A	606	CLA	MG-NA	2.68	2.12	2.06
25	b	614	CLA	CHC-C1C	2.67	1.43	1.38
29	a	614	SQD	O5-C1	2.67	1.48	1.41
26	A	609	PHO	CMB-C2B	-2.67	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	C4B-NB	2.67	1.41	1.37
25	b	613	CLA	C1B-C2B	2.67	1.49	1.43
25	C	513	CLA	MG-NB	2.67	2.11	2.05
25	b	607	CLA	C1B-C2B	2.67	1.49	1.43
25	C	508	CLA	C4B-NB	2.67	1.41	1.37
25	b	614	CLA	CMD-C2D	-2.66	1.45	1.50
28	a	612	PL9	C53-C6	-2.66	1.45	1.50
25	B	604	CLA	MG-ND	-2.66	2.00	2.05
25	b	604	CLA	MG-NA	2.66	2.12	2.06
25	b	602	CLA	CMD-C2D	-2.65	1.45	1.50
25	a	608	CLA	C1B-C2B	2.65	1.49	1.43
30	c	519	DGD	O2G-C2G	-2.65	1.40	1.46
25	B	605	CLA	C1B-C2B	2.65	1.49	1.43
25	C	506	CLA	C4B-NB	2.64	1.41	1.37
25	b	608	CLA	MG-NC	2.64	2.12	2.06
25	c	513	CLA	C1B-C2B	2.64	1.49	1.43
25	B	601	CLA	MG-ND	-2.64	2.00	2.05
35	e	101	HEM	CAB-C3B	2.63	1.54	1.47
25	C	501	CLA	C4B-NB	2.63	1.41	1.37
25	A	610	CLA	C1B-C2B	2.63	1.49	1.43
30	C	517	DGD	C4D-C3D	2.63	1.59	1.52
25	d	403	CLA	C1B-C2B	2.62	1.49	1.43
25	b	612	CLA	MG-ND	-2.62	2.00	2.05
27	k	101	BCR	C30-C25	-2.62	1.50	1.53
25	C	501	CLA	C3B-C4B	2.61	1.50	1.42
25	b	609	CLA	C4B-NB	2.61	1.41	1.37
25	B	607	CLA	C1B-C2B	2.60	1.49	1.43
25	B	609	CLA	C1B-C2B	2.60	1.49	1.43
25	C	501	CLA	MG-ND	-2.60	2.00	2.05
35	F	101	HEM	FE-ND	2.60	2.02	1.94
25	c	502	CLA	MG-ND	2.60	2.10	2.05
33	D	407	LHG	O7-C5	-2.59	1.40	1.46
25	c	512	CLA	MG-NA	2.59	2.12	2.06
25	C	501	CLA	CHC-C1C	2.59	1.43	1.38
25	c	505	CLA	C1B-C2B	2.59	1.49	1.43
25	B	609	CLA	C3B-C4B	2.59	1.50	1.42
27	D	404	BCR	C30-C25	-2.58	1.50	1.53
25	b	615	CLA	MG-ND	-2.58	2.00	2.05
25	B	601	CLA	C3B-C4B	2.58	1.50	1.42
25	a	613	CLA	C3B-C4B	2.58	1.50	1.42
25	b	606	CLA	C4B-NB	2.58	1.41	1.37
25	C	505	CLA	MG-ND	-2.57	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	C1B-C2B	2.57	1.49	1.43
25	A	613	CLA	C3B-C4B	2.57	1.50	1.42
30	H	103	DGD	C4D-C5D	2.56	1.58	1.53
25	C	511	CLA	C3B-C4B	2.56	1.50	1.42
27	b	616	BCR	C30-C25	-2.56	1.50	1.53
26	d	401	PHO	CMD-C2D	-2.56	1.46	1.51
25	C	512	CLA	C3B-C4B	2.56	1.50	1.42
25	c	507	CLA	C1B-C2B	2.56	1.49	1.43
25	B	602	CLA	C3B-C4B	2.56	1.50	1.42
25	c	513	CLA	C3B-C4B	2.55	1.50	1.42
32	d	410	LMG	O7-C8	-2.55	1.40	1.46
32	C	519	LMG	O7-C8	-2.55	1.40	1.46
25	b	601	CLA	C1B-C2B	2.54	1.49	1.43
25	c	505	CLA	C3B-C4B	2.54	1.50	1.42
25	B	602	CLA	CHC-C1C	2.54	1.43	1.38
25	B	610	CLA	CHC-C1C	2.54	1.43	1.38
25	c	504	CLA	C1B-C2B	2.54	1.49	1.43
33	B	621	LHG	O7-C5	-2.53	1.40	1.46
25	c	511	CLA	C3B-C4B	2.53	1.50	1.42
25	H	101	CLA	C3B-C4B	2.53	1.50	1.42
25	B	602	CLA	C1D-ND	2.53	1.41	1.37
25	B	603	CLA	C4B-NB	2.52	1.41	1.37
25	C	504	CLA	C3B-C4B	2.52	1.50	1.42
25	C	509	CLA	C4B-NB	2.52	1.41	1.37
30	C	517	DGD	C1E-C2E	2.52	1.59	1.52
25	c	507	CLA	C4B-NB	2.52	1.41	1.37
25	B	611	CLA	MG-ND	-2.50	2.00	2.05
25	b	615	CLA	C4B-NB	2.50	1.41	1.37
25	A	606	CLA	C3B-C4B	2.50	1.50	1.42
26	A	608	PHO	CMD-C2D	-2.50	1.46	1.51
25	b	611	CLA	CHC-C1C	2.50	1.43	1.38
25	B	610	CLA	C4B-NB	2.50	1.41	1.37
26	A	609	PHO	CMD-C2D	-2.50	1.46	1.51
25	c	502	CLA	C1B-C2B	2.49	1.49	1.43
25	B	602	CLA	CMD-C2D	-2.49	1.45	1.50
25	c	503	CLA	CHC-C1C	2.49	1.43	1.38
25	b	611	CLA	C1B-C2B	2.49	1.49	1.43
25	D	403	CLA	CMD-C2D	-2.49	1.45	1.50
27	c	515	BCR	C30-C25	-2.49	1.50	1.53
25	D	402	CLA	CHC-C1C	2.49	1.43	1.38
30	h	102	DGD	C4D-C3D	2.48	1.58	1.52
25	c	506	CLA	MG-ND	-2.48	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	MG-ND	-2.48	2.00	2.05
25	c	509	CLA	C4B-NB	2.48	1.41	1.37
25	C	503	CLA	C4B-NB	2.48	1.41	1.37
25	b	611	CLA	C3B-C4B	2.48	1.49	1.42
26	A	609	PHO	C3D-C4D	2.48	1.44	1.41
29	l	101	SQD	O9-S	2.47	1.52	1.45
25	B	611	CLA	MG-NC	2.47	2.12	2.06
25	h	101	CLA	C3B-C4B	2.47	1.49	1.42
25	C	511	CLA	C4B-NB	2.47	1.41	1.37
25	b	607	CLA	C4B-NB	2.47	1.41	1.37
25	D	403	CLA	C4B-NB	2.46	1.41	1.37
25	B	603	CLA	C3B-C4B	2.46	1.49	1.42
26	d	401	PHO	C3D-C4D	2.46	1.44	1.41
25	b	608	CLA	CMB-C2B	-2.46	1.45	1.50
25	B	614	CLA	MG-NC	2.45	2.12	2.06
25	B	606	CLA	C4B-NB	2.45	1.41	1.37
25	B	610	CLA	MG-ND	2.45	2.10	2.05
25	b	606	CLA	C1B-C2B	2.45	1.48	1.43
33	B	622	LHG	C24-C23	2.45	1.57	1.50
25	b	614	CLA	C3B-C4B	2.45	1.49	1.42
25	A	613	CLA	CHC-C1C	2.44	1.43	1.38
25	c	505	CLA	C1D-ND	2.44	1.41	1.37
32	C	515	LMG	O1-C7	-2.44	1.39	1.43
25	b	611	CLA	CMC-C2C	-2.44	1.45	1.50
28	d	405	PL9	C31-C29	-2.44	1.46	1.51
29	A	614	SQD	O9-S	2.43	1.52	1.45
25	c	508	CLA	C3B-C4B	2.43	1.49	1.42
25	b	612	CLA	C4B-NB	2.43	1.41	1.37
25	B	611	CLA	C3B-C4B	2.43	1.49	1.42
25	a	607	CLA	MG-NA	2.43	2.12	2.06
25	C	507	CLA	C3B-C4B	2.43	1.49	1.42
25	c	508	CLA	C1B-C2B	2.43	1.48	1.43
25	c	513	CLA	CHC-C1C	2.42	1.43	1.38
29	a	614	SQD	O7-S	2.42	1.51	1.45
29	L	101	SQD	O7-S	2.42	1.51	1.45
35	F	101	HEM	FE-NA	2.42	2.03	1.95
25	b	608	CLA	C1B-C2B	2.42	1.48	1.43
25	c	505	CLA	MG-NA	2.41	2.12	2.06
30	H	103	DGD	C1E-C2E	2.41	1.59	1.52
25	c	508	CLA	CMD-C2D	-2.40	1.45	1.50
29	f	101	SQD	O7-S	2.40	1.51	1.45
25	a	610	CLA	CMC-C2C	-2.40	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	C3B-C4B	2.39	1.49	1.42
25	C	502	CLA	C3B-C4B	2.39	1.49	1.42
26	a	609	PHO	CMB-C2B	-2.39	1.46	1.51
26	d	401	PHO	CAC-C3C	-2.39	1.47	1.51
25	A	607	CLA	CHC-C1C	2.39	1.43	1.38
27	a	611	BCR	C30-C25	-2.39	1.50	1.53
25	D	403	CLA	C3B-C4B	2.38	1.49	1.42
25	B	615	CLA	CMC-C2C	-2.38	1.45	1.50
25	A	610	CLA	MG-ND	-2.38	2.01	2.05
29	L	101	SQD	O9-S	2.38	1.51	1.45
25	C	510	CLA	MG-NA	2.37	2.11	2.06
25	c	512	CLA	C3B-C4B	2.37	1.49	1.42
25	c	506	CLA	CMD-C2D	-2.37	1.45	1.50
25	H	101	CLA	CHC-C1C	2.37	1.43	1.38
25	C	513	CLA	C3B-C4B	2.37	1.49	1.42
25	C	504	CLA	CHC-C1C	2.37	1.43	1.38
26	A	609	PHO	C4D-ND	-2.37	1.35	1.38
25	d	403	CLA	CHC-C1C	2.37	1.43	1.38
25	c	510	CLA	C3B-C4B	2.36	1.49	1.42
25	C	512	CLA	CHC-C1C	2.36	1.43	1.38
25	h	101	CLA	MG-NC	-2.36	2.00	2.06
25	C	507	CLA	MG-NC	2.36	2.11	2.06
25	C	508	CLA	C1D-C2D	2.36	1.50	1.45
25	c	501	CLA	CHC-C1C	2.36	1.43	1.38
26	A	608	PHO	C4D-ND	-2.36	1.35	1.38
25	b	605	CLA	C3B-C4B	2.36	1.49	1.42
25	B	615	CLA	C3B-C4B	2.36	1.49	1.42
25	a	608	CLA	CHC-C1C	2.35	1.43	1.38
25	A	613	CLA	C4B-NB	2.35	1.40	1.37
25	C	512	CLA	MG-NC	2.34	2.11	2.06
33	e	102	LHG	P-O6	2.34	1.68	1.59
25	b	603	CLA	CHC-C1C	2.34	1.43	1.38
25	a	607	CLA	CMB-C2B	-2.34	1.46	1.50
25	c	505	CLA	CHC-C1C	2.34	1.43	1.38
25	c	510	CLA	CHC-C1C	2.34	1.43	1.38
25	C	507	CLA	CHC-C1C	2.34	1.43	1.38
25	C	503	CLA	C3B-C4B	2.34	1.49	1.42
25	c	509	CLA	CHC-C1C	2.34	1.43	1.38
32	m	101	LMG	C9-C8	2.34	1.58	1.50
25	B	603	CLA	CHC-C1C	2.33	1.43	1.38
25	C	512	CLA	CMD-C2D	-2.33	1.46	1.50
30	h	102	DGD	C4E-C3E	2.33	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	CLA	MG-NC	2.33	2.11	2.06
25	C	509	CLA	C3B-C4B	2.33	1.49	1.42
32	D	406	LMG	C7-C8	2.32	1.58	1.50
25	C	505	CLA	MG-NC	2.32	2.11	2.06
25	B	609	CLA	CHC-C1C	2.32	1.43	1.38
30	h	102	DGD	C1E-C2E	2.31	1.59	1.52
25	C	504	CLA	C1B-C2B	2.31	1.48	1.43
30	C	516	DGD	C6E-C5E	2.31	1.59	1.51
25	B	605	CLA	C3B-C4B	2.31	1.49	1.42
32	M	101	LMG	C4-C3	2.31	1.58	1.52
25	b	606	CLA	C3B-C4B	2.31	1.49	1.42
25	C	504	CLA	MG-ND	-2.31	2.01	2.05
25	C	509	CLA	CMD-C2D	-2.31	1.46	1.50
25	a	607	CLA	C3B-C4B	2.30	1.49	1.42
30	C	517	DGD	C1G-C2G	2.30	1.58	1.50
25	b	613	CLA	CHC-C1C	2.30	1.43	1.38
25	B	613	CLA	C1B-C2B	2.30	1.48	1.43
25	c	512	CLA	CHC-C1C	2.30	1.43	1.38
25	B	609	CLA	CMB-C2B	-2.30	1.46	1.50
25	C	502	CLA	C4B-NB	2.30	1.40	1.37
25	B	610	CLA	C3B-C4B	2.30	1.49	1.42
25	B	610	CLA	C1B-NB	-2.30	1.34	1.37
25	b	605	CLA	C4B-NB	2.30	1.40	1.37
25	C	506	CLA	C1B-C2B	2.30	1.48	1.43
25	C	511	CLA	CHC-C1C	2.30	1.43	1.38
25	B	609	CLA	MG-ND	-2.29	2.01	2.05
25	C	510	CLA	MG-NC	2.29	2.11	2.06
25	B	605	CLA	MG-NB	2.29	2.10	2.05
25	b	613	CLA	C3B-C4B	2.29	1.49	1.42
25	C	506	CLA	CHC-C1C	2.29	1.43	1.38
25	C	510	CLA	CMD-C2D	-2.29	1.46	1.50
25	B	615	CLA	C4B-NB	2.28	1.40	1.37
30	H	103	DGD	C6D-C5D	2.28	1.58	1.51
25	b	601	CLA	CMD-C2D	-2.28	1.46	1.50
25	B	611	CLA	C1B-C2B	2.28	1.48	1.43
27	t	101	BCR	C1-C6	-2.28	1.50	1.53
25	b	612	CLA	CMD-C2D	-2.28	1.46	1.50
25	d	403	CLA	C3B-C4B	2.28	1.49	1.42
30	a	616	DGD	C1G-C2G	2.28	1.57	1.50
26	d	401	PHO	C4D-ND	-2.27	1.35	1.38
25	C	508	CLA	CHC-C1C	2.27	1.43	1.38
25	C	501	CLA	C1B-C2B	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	409	LMG	C7-C8	2.27	1.56	1.51
29	a	615	SQD	C44-C45	2.27	1.56	1.51
25	A	610	CLA	CHC-C1C	2.26	1.43	1.38
25	b	608	CLA	C3B-C4B	2.26	1.49	1.42
25	C	511	CLA	CMB-C2B	-2.26	1.46	1.50
25	b	601	CLA	C3B-C4B	2.26	1.49	1.42
33	d	406	LHG	P-O6	2.26	1.68	1.59
25	C	510	CLA	C3B-C4B	2.26	1.49	1.42
25	a	613	CLA	CMB-C2B	-2.26	1.46	1.50
35	e	101	HEM	CMA-C3A	2.25	1.55	1.50
25	H	101	CLA	MG-NB	-2.25	2.01	2.05
25	c	506	CLA	C3B-C4B	2.25	1.49	1.42
25	a	610	CLA	CMD-C2D	-2.25	1.46	1.50
25	C	509	CLA	C1B-C2B	2.25	1.48	1.43
30	C	517	DGD	O6D-C5D	-2.25	1.38	1.44
25	B	610	CLA	MG-NB	2.25	2.10	2.05
25	c	501	CLA	CMD-C2D	-2.25	1.46	1.50
25	B	612	CLA	MG-NC	2.24	2.11	2.06
36	V	201	HEC	CMC-C2C	2.24	1.55	1.50
25	b	603	CLA	C3B-C4B	2.24	1.49	1.42
25	C	505	CLA	C3B-C4B	2.24	1.49	1.42
25	D	402	CLA	CMC-C2C	-2.24	1.46	1.50
25	A	610	CLA	C1B-NB	-2.24	1.34	1.37
28	D	405	PL9	C7-C3	-2.24	1.48	1.51
25	H	101	CLA	CMC-C2C	-2.24	1.46	1.50
25	b	608	CLA	MG-NA	2.23	2.11	2.06
25	B	604	CLA	C3B-C4B	2.23	1.49	1.42
25	b	613	CLA	CMC-C2C	-2.23	1.46	1.50
25	D	403	CLA	CMB-C2B	-2.23	1.46	1.50
29	l	101	SQD	C44-C45	2.22	1.57	1.50
25	D	402	CLA	C3B-C4B	2.22	1.49	1.42
25	B	607	CLA	CHC-C1C	2.22	1.42	1.38
32	m	101	LMG	C4-C5	2.22	1.57	1.53
25	B	604	CLA	CHC-C4B	-2.22	1.34	1.39
25	a	610	CLA	C3B-C4B	2.22	1.49	1.42
32	b	620	LMG	O1-C7	-2.21	1.39	1.43
36	v	201	HEC	C3B-C2B	-2.21	1.33	1.41
25	C	508	CLA	MG-ND	2.21	2.10	2.05
30	c	517	DGD	O2G-C2G	-2.21	1.41	1.46
25	B	611	CLA	MG-NA	2.21	2.11	2.06
25	c	504	CLA	CHC-C1C	2.21	1.42	1.38
26	A	608	PHO	CAC-C3C	-2.21	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	404	BCR	C38-C26	-2.21	1.47	1.50
25	B	605	CLA	CMD-C2D	-2.21	1.46	1.50
32	C	515	LMG	C7-C8	2.21	1.57	1.50
25	b	605	CLA	CMD-C2D	-2.20	1.46	1.50
27	A	611	BCR	C33-C5	-2.20	1.47	1.50
25	c	509	CLA	C3B-C4B	2.20	1.49	1.42
25	C	509	CLA	CMB-C2B	-2.20	1.46	1.50
26	d	401	PHO	C1D-ND	2.20	1.42	1.38
25	c	507	CLA	C3D-C4D	2.20	1.49	1.44
25	A	607	CLA	C3B-C4B	2.20	1.49	1.42
29	f	101	SQD	O9-S	2.20	1.51	1.45
25	c	502	CLA	CMD-C2D	-2.20	1.46	1.50
25	C	513	CLA	CHC-C1C	2.19	1.42	1.38
25	b	611	CLA	C4B-NB	2.19	1.40	1.37
26	d	401	PHO	CMB-C2B	-2.19	1.47	1.51
29	L	101	SQD	O5-C5	2.19	1.49	1.44
25	c	502	CLA	C3B-C4B	2.19	1.49	1.42
25	a	613	CLA	C1D-C2D	2.19	1.49	1.45
25	A	607	CLA	MG-ND	2.18	2.10	2.05
25	b	615	CLA	C3B-C4B	2.18	1.49	1.42
30	a	616	DGD	O1G-C1A	2.18	1.39	1.33
29	l	101	SQD	O7-S	2.18	1.51	1.45
25	A	606	CLA	CHC-C1C	2.18	1.42	1.38
35	e	101	HEM	CMB-C2B	2.17	1.55	1.50
29	l	101	SQD	C8-C7	2.17	1.57	1.50
27	b	617	BCR	C38-C26	-2.16	1.47	1.50
35	F	101	HEM	FE-NB	2.16	2.01	1.94
25	C	503	CLA	CHC-C1C	2.16	1.42	1.38
25	B	608	CLA	CMD-C2D	-2.16	1.46	1.50
25	h	101	CLA	O2A-CGA	2.16	1.39	1.33
25	d	402	CLA	CMB-C2B	-2.16	1.46	1.50
25	A	606	CLA	CMC-C2C	-2.16	1.46	1.50
25	C	506	CLA	C3B-C4B	2.16	1.49	1.42
25	a	608	CLA	C3B-C4B	2.16	1.49	1.42
26	A	609	PHO	CAC-C3C	-2.16	1.47	1.51
25	c	512	CLA	C1D-C2D	2.16	1.49	1.45
32	C	515	LMG	C1-C2	2.15	1.58	1.52
26	a	609	PHO	C3D-C4D	2.15	1.44	1.41
25	C	504	CLA	CMD-C2D	-2.15	1.46	1.50
26	A	608	PHO	CMB-C2B	-2.15	1.47	1.51
25	a	607	CLA	CHC-C1C	2.15	1.42	1.38
30	c	518	DGD	O6D-C5D	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	608	CLA	MG-ND	-2.14	2.01	2.05
25	c	510	CLA	CMC-C2C	-2.14	1.46	1.50
35	e	101	HEM	C3B-C2B	-2.14	1.32	1.37
25	B	612	CLA	C3B-C4B	2.14	1.49	1.42
25	c	504	CLA	C3B-C4B	2.14	1.49	1.42
30	C	517	DGD	O3G-C3G	-2.14	1.40	1.43
29	F	102	SQD	O9-S	2.14	1.51	1.45
25	B	606	CLA	CMB-C2B	-2.13	1.46	1.50
25	B	614	CLA	C3B-C4B	2.13	1.49	1.42
32	c	524	LMG	C4-C3	2.13	1.57	1.52
25	C	504	CLA	C1B-NB	-2.13	1.35	1.37
32	M	101	LMG	C4-C5	2.13	1.57	1.53
29	f	101	SQD	O5-C5	2.13	1.49	1.44
25	d	402	CLA	C3B-C4B	2.13	1.48	1.42
25	C	511	CLA	CMD-C2D	-2.13	1.46	1.50
25	h	101	CLA	CMC-C2C	-2.12	1.46	1.50
32	c	524	LMG	C4-C5	2.12	1.57	1.53
25	c	502	CLA	CMC-C2C	-2.12	1.46	1.50
25	d	403	CLA	CMB-C2B	-2.12	1.46	1.50
25	C	501	CLA	C1D-C2D	2.12	1.49	1.45
25	B	601	CLA	CMB-C2B	-2.12	1.46	1.50
25	c	507	CLA	CMB-C2B	-2.11	1.46	1.50
25	b	607	CLA	CMB-C2B	-2.11	1.46	1.50
25	b	605	CLA	CMC-C2C	-2.11	1.46	1.50
25	c	505	CLA	CMB-C2B	-2.11	1.46	1.50
30	c	517	DGD	C4D-C3D	2.11	1.57	1.52
25	c	506	CLA	CHC-C1C	2.11	1.42	1.38
25	c	501	CLA	C3B-C4B	2.10	1.48	1.42
25	c	503	CLA	C3B-C4B	2.10	1.48	1.42
32	C	519	LMG	O1-C7	-2.10	1.40	1.43
25	d	402	CLA	MG-NB	-2.10	2.01	2.05
27	C	514	BCR	C33-C5	-2.10	1.47	1.50
29	L	101	SQD	C46-C45	2.10	1.57	1.50
25	c	507	CLA	CHC-C1C	2.10	1.42	1.38
33	d	406	LHG	C24-C23	2.10	1.56	1.50
25	B	604	CLA	CMD-C2D	-2.09	1.46	1.50
25	c	512	CLA	C3D-C4D	2.09	1.48	1.44
33	e	102	LHG	O7-C5	-2.09	1.41	1.46
30	C	516	DGD	C3G-C2G	2.09	1.57	1.50
32	c	522	LMG	O1-C1	2.09	1.43	1.40
30	A	616	DGD	C3G-C2G	2.09	1.57	1.50
25	b	612	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	405	PL9	C41-C39	-2.09	1.47	1.51
25	H	101	CLA	CMB-C2B	-2.09	1.46	1.50
25	c	506	CLA	CMB-C2B	-2.08	1.46	1.50
26	a	609	PHO	CMD-C2D	-2.08	1.47	1.51
35	e	101	HEM	CMC-C2C	2.08	1.55	1.50
27	B	616	BCR	C33-C5	-2.08	1.47	1.50
29	a	615	SQD	C46-C45	2.08	1.57	1.50
29	F	102	SQD	O7-S	2.08	1.51	1.45
30	c	519	DGD	O4E-C4E	-2.08	1.37	1.43
25	C	510	CLA	CMC-C2C	-2.07	1.46	1.50
25	c	502	CLA	CHC-C1C	2.07	1.42	1.38
25	B	610	CLA	CMB-C2B	-2.07	1.46	1.50
25	d	403	CLA	MG-NA	2.07	2.11	2.06
25	C	502	CLA	CMB-C2B	-2.07	1.46	1.50
25	B	609	CLA	CMC-C2C	-2.07	1.46	1.50
25	B	608	CLA	C3B-C4B	2.07	1.48	1.42
30	H	103	DGD	O6E-C1E	2.07	1.47	1.41
25	B	612	CLA	CHC-C1C	2.07	1.42	1.38
30	A	616	DGD	C3D-C2D	2.07	1.57	1.52
25	b	612	CLA	C3C-C2C	2.06	1.41	1.36
35	F	101	HEM	CMA-C3A	2.06	1.55	1.50
25	C	506	CLA	CMC-C2C	-2.06	1.46	1.50
25	c	501	CLA	CMC-C2C	-2.06	1.46	1.50
25	A	613	CLA	C1D-C2D	2.06	1.49	1.45
25	c	507	CLA	CMC-C2C	-2.06	1.46	1.50
25	c	508	CLA	CMC-C2C	-2.06	1.46	1.50
27	k	101	BCR	C38-C26	-2.06	1.47	1.50
25	b	604	CLA	C3B-C4B	2.06	1.48	1.42
25	b	612	CLA	C3B-C4B	2.06	1.48	1.42
25	b	610	CLA	C4B-NB	2.06	1.40	1.37
27	b	616	BCR	C33-C5	-2.06	1.47	1.50
27	B	617	BCR	C1-C6	-2.05	1.51	1.53
30	h	102	DGD	C4E-C5E	2.05	1.57	1.53
25	b	614	CLA	CMB-C2B	-2.05	1.46	1.50
25	b	608	CLA	CMC-C2C	-2.05	1.46	1.50
25	b	609	CLA	CMB-C2B	-2.05	1.46	1.50
25	b	609	CLA	CMD-C2D	-2.05	1.46	1.50
25	b	611	CLA	MG-NC	2.05	2.11	2.06
25	b	610	CLA	CHC-C1C	2.05	1.42	1.38
25	B	603	CLA	MG-NC	2.04	2.11	2.06
25	C	502	CLA	CMC-C2C	-2.04	1.46	1.50
25	B	611	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	CMB-C2B	-2.04	1.46	1.50
29	A	614	SQD	C8-C7	2.04	1.56	1.50
25	B	601	CLA	CMC-C2C	-2.04	1.46	1.50
25	d	403	CLA	CMC-C2C	-2.04	1.46	1.50
25	b	607	CLA	C1D-C2D	2.04	1.49	1.45
25	B	607	CLA	C3B-C4B	2.04	1.48	1.42
30	C	518	DGD	O2E-C2E	-2.04	1.37	1.43
25	c	510	CLA	CMD-C2D	-2.03	1.46	1.50
25	C	509	CLA	CHC-C1C	2.03	1.42	1.38
25	c	502	CLA	C4B-NB	2.03	1.40	1.37
35	F	101	HEM	CMC-C2C	2.03	1.54	1.50
26	a	609	PHO	O2D-CGD	2.03	1.38	1.33
25	C	501	CLA	C1B-NB	-2.03	1.35	1.37
30	c	518	DGD	C4D-C3D	2.03	1.57	1.52
25	B	613	CLA	CHC-C1C	2.03	1.42	1.38
25	a	610	CLA	C1B-NB	-2.03	1.35	1.37
35	e	101	HEM	FE-ND	2.03	2.01	1.94
25	b	605	CLA	CMB-C2B	-2.03	1.46	1.50
36	V	201	HEC	C3B-C2B	-2.03	1.34	1.41
25	B	611	CLA	C1B-NB	-2.03	1.35	1.37
25	C	503	CLA	CMD-C2D	-2.03	1.46	1.50
30	c	519	DGD	C6D-C5D	2.02	1.57	1.51
25	b	604	CLA	CHC-C1C	2.02	1.42	1.38
28	A	612	PL9	C53-C6	-2.02	1.46	1.50
25	B	609	CLA	C3D-C4D	2.02	1.48	1.44
35	F	101	HEM	CMD-C2D	2.02	1.54	1.50
25	C	512	CLA	CMB-C2B	-2.02	1.46	1.50
25	d	402	CLA	CMD-C2D	-2.02	1.46	1.50
30	C	517	DGD	O1G-C1G	-2.02	1.40	1.45
25	C	503	CLA	MG-NB	2.02	2.09	2.05
25	B	604	CLA	C4B-NB	2.01	1.40	1.37
25	B	613	CLA	CMB-C2B	-2.01	1.46	1.50
25	c	508	CLA	CMB-C2B	-2.01	1.46	1.50
32	c	524	LMG	O8-C9	-2.01	1.40	1.45
25	D	402	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	605	CLA	CHC-C1C	2.01	1.42	1.38
25	b	606	CLA	C1B-NB	-2.01	1.35	1.37
25	a	607	CLA	CMD-C2D	-2.01	1.46	1.50
29	f	101	SQD	C46-C45	2.01	1.57	1.50
25	c	504	CLA	O2D-CGD	2.00	1.38	1.33
25	b	613	CLA	CMB-C2B	-2.00	1.46	1.50
25	b	615	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l	101	SQD	O5-C5	2.00	1.49	1.44

All (1138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	C4A-NA-C1A	8.87	110.73	106.68
36	V	201	HEC	CBB-CAB-C3B	-8.82	109.80	127.43
25	c	511	CLA	C4A-NA-C1A	8.60	110.60	106.68
25	C	507	CLA	C4A-NA-C1A	8.54	110.58	106.68
25	B	603	CLA	C4A-NA-C1A	8.40	110.51	106.68
25	b	603	CLA	C4A-NA-C1A	7.82	110.25	106.68
25	b	605	CLA	C4A-NA-C1A	7.81	110.24	106.68
25	C	511	CLA	C4A-NA-C1A	7.79	110.23	106.68
25	C	508	CLA	C4A-NA-C1A	7.69	110.19	106.68
25	c	503	CLA	C4A-NA-C1A	7.62	110.16	106.68
25	H	101	CLA	C4A-NA-C1A	7.45	110.08	106.68
25	C	503	CLA	C4A-NA-C1A	7.37	110.04	106.68
25	B	614	CLA	C4A-NA-C1A	7.34	110.03	106.68
25	C	513	CLA	C4A-NA-C1A	7.32	110.02	106.68
25	B	615	CLA	C4A-NA-C1A	7.22	109.97	106.68
25	C	506	CLA	C4A-NA-C1A	7.11	109.92	106.68
25	c	506	CLA	C4A-NA-C1A	6.98	109.86	106.68
36	v	201	HEC	CBC-CAC-C3C	-6.94	113.56	127.43
36	v	201	HEC	CBB-CAB-C3B	-6.91	113.62	127.43
25	b	606	CLA	C4A-NA-C1A	6.88	109.82	106.68
25	B	608	CLA	C4A-NA-C1A	6.82	109.79	106.68
36	V	201	HEC	CBC-CAC-C3C	-6.76	113.93	127.43
25	B	610	CLA	C4A-NA-C1A	6.75	109.76	106.68
25	A	607	CLA	C4A-NA-C1A	6.74	109.76	106.68
25	b	615	CLA	C4A-NA-C1A	6.73	109.75	106.68
25	b	610	CLA	C4A-NA-C1A	6.67	109.72	106.68
25	C	510	CLA	C4A-NA-C1A	6.63	109.71	106.68
25	B	606	CLA	C4A-NA-C1A	6.61	109.69	106.68
25	B	607	CLA	C4A-NA-C1A	6.59	109.68	106.68
29	a	614	SQD	O6-C1-C2	6.56	118.24	108.27
29	a	614	SQD	C1-O5-C5	-6.52	100.98	113.72
25	c	501	CLA	C4A-NA-C1A	6.50	109.64	106.68
25	c	507	CLA	C4A-NA-C1A	6.48	109.63	106.68
25	b	614	CLA	C4A-NA-C1A	6.45	109.62	106.68
25	a	607	CLA	C4A-NA-C1A	6.30	109.56	106.68
25	B	611	CLA	C4A-NA-C1A	6.30	109.55	106.68
25	b	609	CLA	C4A-NA-C1A	6.28	109.54	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	612	CLA	C4A-NA-C1A	6.16	109.49	106.68
29	A	614	SQD	O6-C1-C2	6.15	117.61	108.27
25	B	605	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	h	101	CLA	C4A-NA-C1A	6.08	109.45	106.68
25	C	505	CLA	C4A-NA-C1A	6.02	109.42	106.68
25	c	510	CLA	C4A-NA-C1A	6.01	109.42	106.68
25	C	509	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	D	402	CLA	C4A-NA-C1A	5.92	109.38	106.68
29	L	101	SQD	O6-C1-C2	5.92	117.26	108.27
25	b	612	CLA	C4A-NA-C1A	5.84	109.34	106.68
28	a	612	PL9	C7-C3-C4	5.78	121.67	116.91
25	C	501	CLA	C4A-NA-C1A	5.75	109.30	106.68
25	c	502	CLA	C4A-NA-C1A	5.70	109.28	106.68
25	b	602	CLA	C4A-NA-C1A	5.59	109.23	106.68
26	A	608	PHO	C4D-CHA-CBD	-5.58	105.78	108.45
25	d	402	CLA	C4A-NA-C1A	5.57	109.22	106.68
25	c	504	CLA	C4A-NA-C1A	5.46	109.17	106.68
29	l	101	SQD	O6-C1-C2	5.43	116.52	108.27
25	b	604	CLA	C4A-NA-C1A	5.33	109.11	106.68
25	a	608	CLA	C4A-NA-C1A	5.32	109.11	106.68
28	A	612	PL9	C7-C3-C4	5.27	121.25	116.91
25	A	613	CLA	C4A-NA-C1A	5.25	109.07	106.68
25	c	505	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	b	608	CLA	C4A-NA-C1A	5.15	109.03	106.68
25	b	611	CLA	C4A-NA-C1A	5.12	109.01	106.68
29	a	615	SQD	O47-C7-C8	5.10	122.52	111.48
25	c	512	CLA	C4A-NA-C1A	5.10	109.01	106.68
25	c	513	CLA	C4A-NA-C1A	5.08	109.00	106.68
25	D	403	CLA	C4A-NA-C1A	5.06	108.99	106.68
25	B	604	CLA	C4A-NA-C1A	5.05	108.98	106.68
29	l	101	SQD	O47-C7-C8	5.04	122.39	111.48
25	b	605	CLA	O2D-CGD-O1D	-4.92	114.27	123.85
26	A	609	PHO	C1-C2-C3	-4.89	118.19	126.20
29	A	614	SQD	O47-C7-C8	4.89	122.05	111.48
28	d	405	PL9	C7-C3-C4	4.83	120.89	116.91
25	B	601	CLA	C4A-NA-C1A	4.82	108.88	106.68
29	A	614	SQD	C1-C2-C3	-4.79	99.93	110.01
25	C	504	CLA	C4A-NA-C1A	4.78	108.86	106.68
25	b	601	CLA	C4A-NA-C1A	4.74	108.84	106.68
25	a	613	CLA	C4A-NA-C1A	4.74	108.84	106.68
25	B	613	CLA	C4A-NA-C1A	4.73	108.84	106.68
25	c	501	CLA	O2D-CGD-O1D	-4.68	114.73	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	508	CLA	C4A-NA-C1A	4.68	108.82	106.68
29	L	101	SQD	O7-S-C6	4.68	113.75	106.76
25	A	606	CLA	C4A-NA-C1A	4.66	108.81	106.68
25	b	607	CLA	C4A-NA-C1A	4.66	108.81	106.68
29	F	102	SQD	C1-O5-C5	-4.66	104.62	113.72
25	B	609	CLA	C4A-NA-C1A	4.64	108.80	106.68
25	C	512	CLA	C4A-NA-C1A	4.59	108.77	106.68
33	d	407	LHG	O4-P-O5	4.57	133.71	112.44
30	C	518	DGD	O3G-C3G-C2G	-4.54	99.77	110.82
26	d	401	PHO	C4D-CHA-CBD	-4.49	106.30	108.45
25	B	612	CLA	C1-C2-C3	-4.46	118.89	126.20
33	e	102	LHG	O4-P-O5	4.45	133.13	112.44
26	d	401	PHO	C1-C2-C3	-4.41	118.97	126.20
29	f	101	SQD	O7-S-C6	4.37	113.27	106.76
28	A	612	PL9	C7-C3-C2	-4.35	118.26	123.39
33	B	621	LHG	O4-P-O5	4.31	132.51	112.44
33	E	101	LHG	O4-P-O5	4.29	132.39	112.44
33	B	622	LHG	O4-P-O5	4.28	132.38	112.44
25	b	609	CLA	C1-C2-C3	-4.28	119.19	126.20
29	f	101	SQD	O6-C1-C2	4.25	114.73	108.27
33	D	408	LHG	O4-P-O5	4.25	132.21	112.44
33	d	406	LHG	O4-P-O5	4.25	132.20	112.44
25	C	502	CLA	C4A-NA-C1A	4.24	108.61	106.68
25	b	613	CLA	C4A-NA-C1A	4.23	108.61	106.68
29	f	101	SQD	O9-S-O7	-4.23	100.08	113.82
33	D	407	LHG	O4-P-O5	4.21	132.04	112.44
34	D	401	BCT	O2-C-O1	4.20	130.41	119.68
30	C	517	DGD	O3G-C3G-C2G	-4.19	100.61	110.82
25	a	610	CLA	C4A-NA-C1A	4.19	108.59	106.68
33	l	102	LHG	O4-P-O5	4.19	131.92	112.44
25	B	609	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
25	B	605	CLA	C3B-C4B-NB	-4.17	106.81	110.53
25	c	512	CLA	C1-C2-C3	-4.16	119.38	126.20
33	d	408	LHG	O4-P-O5	4.13	131.68	112.44
27	B	616	BCR	C2-C1-C6	4.10	116.39	110.44
28	a	612	PL9	C7-C3-C2	-4.08	118.58	123.39
28	D	405	PL9	C7-C3-C4	4.07	120.27	116.91
25	d	403	CLA	C4A-NA-C1A	4.07	108.54	106.68
25	a	613	CLA	C1-C2-C3	-4.06	119.55	126.20
29	A	614	SQD	O7-S-C6	4.02	112.76	106.76
25	B	615	CLA	O2D-CGD-O1D	-4.01	116.04	123.85
25	B	610	CLA	O2D-CGD-CBD	4.01	118.23	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	610	CLA	O2D-CGD-O1D	-4.00	116.07	123.85
25	a	613	CLA	C3B-C4B-NB	-3.97	106.99	110.53
29	f	101	SQD	O5-C5-C4	3.96	116.84	109.70
29	A	614	SQD	C1-O5-C5	-3.96	105.98	113.72
26	d	401	PHO	O1D-CGD-CBD	3.94	130.70	124.72
34	a	606	BCT	O2-C-O1	3.93	129.73	119.68
30	a	616	DGD	O3G-C3G-C2G	-3.93	101.68	111.77
30	H	103	DGD	O3G-C3G-C2G	-3.93	101.27	110.82
30	c	519	DGD	O3G-C3G-C2G	-3.92	101.29	110.82
25	c	509	CLA	O2A-CGA-O1A	-3.91	113.84	123.63
25	b	614	CLA	C3B-C4B-NB	-3.88	107.06	110.53
26	A	608	PHO	CMB-C2B-C3B	3.88	132.43	124.68
29	a	614	SQD	O47-C7-C8	3.86	119.83	111.48
25	b	605	CLA	O2D-CGD-CBD	3.85	117.97	111.23
26	A	609	PHO	O2D-CGD-O1D	-3.84	116.36	123.85
25	b	615	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
29	F	102	SQD	O9-S-C6	3.82	112.46	106.76
27	b	616	BCR	C2-C1-C6	3.82	115.98	110.44
25	B	602	CLA	C3B-C4B-NB	-3.81	107.13	110.53
29	L	101	SQD	C1-C2-C3	-3.80	102.01	110.01
29	a	614	SQD	O9-S-O7	-3.79	101.48	113.82
25	c	508	CLA	C3B-C4B-NB	-3.79	107.15	110.53
25	B	603	CLA	C3B-C4B-NB	-3.78	107.16	110.53
25	A	607	CLA	O2D-CGD-O1D	-3.78	116.50	123.85
27	K	101	BCR	C15-C16-C17	-3.77	115.81	123.52
25	B	601	CLA	O2D-CGD-CBD	3.76	117.81	111.23
29	A	614	SQD	O9-S-O7	-3.75	101.61	113.82
25	A	610	CLA	O2D-CGD-O1D	-3.75	116.54	123.85
25	B	603	CLA	C1-C2-C3	-3.75	120.06	126.20
27	K	101	BCR	C11-C10-C9	-3.74	122.03	127.28
25	C	509	CLA	C3B-C4B-NB	-3.73	107.20	110.53
30	h	102	DGD	O3G-C3G-C2G	-3.72	101.77	110.82
26	A	609	PHO	O1D-CGD-CBD	3.71	130.35	124.72
27	B	617	BCR	C15-C14-C13	-3.71	122.08	127.28
25	c	513	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
29	A	615	SQD	O48-C23-C24	3.67	123.03	111.83
29	L	101	SQD	O48-C23-C24	3.67	123.03	111.83
25	d	402	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
26	d	401	PHO	CMB-C2B-C3B	3.65	131.99	124.68
25	c	505	CLA	C3B-C4B-NB	-3.65	107.27	110.53
26	d	401	PHO	C2B-C1B-NB	-3.65	106.80	109.43
25	B	614	CLA	C3B-C4B-NB	-3.64	107.28	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	508	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
35	e	101	HEM	CBD-CAD-C3D	-3.61	102.54	112.53
29	L	101	SQD	O5-C5-C4	3.61	116.21	109.70
25	B	607	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
25	C	513	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
25	c	501	CLA	O2D-CGD-CBD	3.59	117.50	111.23
25	b	612	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
25	a	610	CLA	C1-C2-C3	-3.58	120.33	126.20
25	C	507	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
29	L	101	SQD	O47-C7-C8	3.58	119.23	111.48
29	L	101	SQD	O9-S-O7	-3.57	102.20	113.82
25	A	610	CLA	C4A-NA-C1A	3.56	108.30	106.68
25	b	601	CLA	C1-C2-C3	-3.55	120.38	126.20
25	h	101	CLA	C3B-C4B-NB	-3.55	107.36	110.53
25	b	611	CLA	C1-C2-C3	-3.54	120.39	126.20
29	A	615	SQD	O47-C7-C8	3.54	119.15	111.48
25	c	510	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
25	c	507	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	B	611	CLA	C3B-C4B-NB	-3.53	107.38	110.53
27	K	101	BCR	C15-C14-C13	-3.53	122.33	127.28
25	b	607	CLA	C3B-C4B-NB	-3.53	107.38	110.53
30	C	516	DGD	O3G-C3G-C2G	-3.52	102.25	110.82
33	d	406	LHG	O8-C23-C24	3.52	122.57	111.83
26	A	609	PHO	C2B-C1B-NB	-3.52	106.89	109.43
25	c	511	CLA	C3B-C4B-NB	-3.52	107.39	110.53
25	b	609	CLA	CAA-CBA-CGA	-3.51	103.25	113.21
25	b	610	CLA	O2D-CGD-CBD	3.49	117.34	111.23
25	C	510	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
25	b	602	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
29	a	615	SQD	O48-C23-C24	3.48	122.45	111.83
28	D	405	PL9	C22-C23-C24	-3.47	119.67	127.62
25	c	503	CLA	C1-C2-C3	-3.47	120.52	126.20
29	a	614	SQD	O48-C23-C24	3.46	122.40	111.83
25	b	604	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
25	b	601	CLA	CHB-C4A-NA	3.43	129.36	124.40
27	t	101	BCR	C3-C4-C5	-3.43	107.95	114.06
25	B	603	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
25	B	602	CLA	C4A-NA-C1A	3.42	108.24	106.68
27	c	515	BCR	C11-C10-C9	-3.41	122.49	127.28
25	B	609	CLA	CHB-C4A-NA	3.41	129.32	124.40
32	c	524	LMG	O6-C1-O1	-3.41	101.98	110.04
25	C	512	CLA	O2D-CGD-O1D	-3.41	117.22	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
30	c	517	DGD	O3G-C3G-C2G	-3.40	102.56	110.82
36	V	201	HEC	C4D-ND-C1D	3.40	111.36	105.82
25	H	101	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
32	m	101	LMG	O1-C7-C8	-3.39	102.57	110.82
25	B	609	CLA	O2A-CGA-O1A	-3.39	115.15	123.63
25	b	611	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
26	A	609	PHO	C4D-CHA-CBD	-3.38	106.83	108.45
30	C	517	DGD	O6D-C1D-O3G	-3.37	102.08	110.04
25	C	511	CLA	C1-C2-C3	-3.36	120.69	126.20
25	B	607	CLA	C3B-C4B-NB	-3.35	107.54	110.53
27	b	617	BCR	C15-C14-C13	-3.34	122.59	127.28
25	C	510	CLA	C3B-C4B-NB	-3.34	107.55	110.53
25	C	501	CLA	C3B-C4B-NB	-3.34	107.55	110.53
25	a	608	CLA	CHB-C4A-NA	3.33	129.21	124.40
35	F	101	HEM	CBD-CAD-C3D	-3.33	103.33	112.53
25	B	610	CLA	CHD-C4C-NC	3.32	129.37	124.23
25	b	613	CLA	C1-C2-C3	-3.32	120.76	126.20
29	l	101	SQD	O48-C23-C24	3.31	121.92	111.83
25	C	502	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
25	B	604	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
36	v	201	HEC	C4D-ND-C1D	3.28	111.16	105.82
27	x	101	BCR	C27-C26-C25	3.27	127.13	122.70
29	l	101	SQD	O7-S-C6	3.26	111.63	106.76
25	b	609	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
25	c	508	CLA	C1-C2-C3	-3.26	120.86	126.20
30	a	616	DGD	C1G-C2G-C3G	-3.26	104.28	111.80
26	d	401	PHO	O2D-CGD-O1D	-3.25	117.51	123.85
25	C	506	CLA	C3B-C4B-NB	-3.25	107.63	110.53
25	B	606	CLA	C3B-C4B-NB	-3.25	107.63	110.53
26	A	608	PHO	C2B-C1B-NB	-3.24	107.09	109.43
26	A	609	PHO	CMB-C2B-C3B	3.24	131.16	124.68
27	A	611	BCR	C27-C26-C25	3.24	127.08	122.70
25	H	101	CLA	C3B-C4B-NB	-3.23	107.64	110.53
25	c	502	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
25	b	603	CLA	C1-C2-C3	-3.23	120.90	126.20
25	b	608	CLA	C3B-C4B-NB	-3.23	107.65	110.53
32	d	410	LMG	O6-C1-O1	-3.22	102.43	110.04
25	C	512	CLA	CHB-C4A-NA	3.22	129.05	124.40
28	d	405	PL9	C7-C3-C2	-3.22	119.59	123.39
30	c	518	DGD	O6D-C1D-O3G	-3.22	102.43	110.04
25	c	512	CLA	C3B-C4B-NB	-3.22	107.66	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	606	CLA	CMB-C2B-C1B	-3.22	120.52	125.42
25	C	504	CLA	C3B-C4B-NB	-3.21	107.67	110.53
25	B	601	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
25	D	402	CLA	C3B-C4B-NB	-3.20	107.67	110.53
30	h	102	DGD	C1D-C2D-C3D	-3.20	103.28	110.01
25	B	601	CLA	C3B-C4B-NB	-3.20	107.67	110.53
25	C	503	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
27	B	618	BCR	C29-C30-C25	3.20	115.08	110.44
27	T	101	BCR	C27-C26-C25	3.19	127.02	122.70
28	d	405	PL9	C37-C38-C39	-3.19	120.31	127.62
30	c	518	DGD	O3G-C3G-C2G	-3.19	103.06	110.82
27	T	101	BCR	C2-C1-C6	3.19	115.07	110.44
25	c	508	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
25	B	604	CLA	C7-C6-C5	-3.18	104.79	113.26
25	B	602	CLA	O2A-CGA-O1A	-3.18	115.68	123.63
25	C	505	CLA	C3B-C4B-NB	-3.17	107.70	110.53
25	A	610	CLA	O2D-CGD-CBD	3.17	116.77	111.23
25	B	610	CLA	CHB-C4A-NA	3.17	128.97	124.40
28	D	405	PL9	C7-C3-C2	-3.16	119.66	123.39
27	d	404	BCR	C27-C26-C25	3.16	126.97	122.70
25	B	613	CLA	C3B-C4B-NB	-3.16	107.71	110.53
29	F	102	SQD	O9-S-O7	-3.16	103.55	113.82
29	l	101	SQD	O9-S-O7	-3.15	103.57	113.82
25	A	613	CLA	C3B-C4B-NB	-3.15	107.72	110.53
25	c	504	CLA	O2A-CGA-O1A	-3.15	115.75	123.63
29	a	614	SQD	C44-O6-C1	-3.14	107.05	113.80
25	B	602	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
25	B	611	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
25	d	403	CLA	C3B-C4B-NB	-3.12	107.74	110.53
25	b	606	CLA	C3B-C4B-NB	-3.12	107.74	110.53
25	B	610	CLA	CHD-C1D-ND	-3.12	120.41	124.80
25	b	612	CLA	O2D-CGD-CBD	3.11	116.66	111.23
30	H	103	DGD	C1D-C2D-C3D	-3.11	103.47	110.01
25	B	611	CLA	C1-C2-C3	-3.10	121.11	126.20
25	c	513	CLA	C3B-C4B-NB	-3.10	107.76	110.53
31	x	102	STE	C3-C2-C1	-3.09	106.44	114.51
25	A	607	CLA	CHB-C4A-NA	3.09	128.86	124.40
30	C	517	DGD	O2D-C2D-C1D	-3.09	102.72	110.08
30	C	518	DGD	O6D-C1D-O3G	-3.08	102.76	110.04
25	C	501	CLA	O2A-CGA-O1A	-3.08	115.93	123.63
25	B	601	CLA	CHB-C4A-NA	3.08	128.84	124.40
25	C	512	CLA	C3B-C4B-NB	-3.07	107.79	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
25	B	606	CLA	CHB-C1B-NB	3.06	128.64	124.05
29	a	614	SQD	O8-S-C6	3.06	111.88	105.97
31	M	102	STE	C3-C2-C1	-3.06	106.53	114.51
33	d	408	LHG	O8-C23-C24	3.06	121.15	111.83
29	A	614	SQD	O5-C1-C2	-3.04	104.12	110.37
29	l	101	SQD	C1-C2-C3	-3.04	103.62	110.01
32	D	406	LMG	O1-C1-C2	-3.03	103.66	108.27
27	x	101	BCR	C2-C1-C6	3.03	114.84	110.44
25	C	509	CLA	CHD-C1D-ND	-3.03	120.54	124.80
25	C	505	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
30	h	102	DGD	C3D-C4D-C5D	-3.02	104.76	110.23
32	b	620	LMG	O2-C2-C1	-3.02	102.89	110.08
27	b	617	BCR	C27-C26-C25	3.01	126.78	122.70
25	B	613	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
27	T	101	BCR	C3-C4-C5	-3.01	108.68	114.06
29	a	614	SQD	C1-C2-C3	-3.01	103.67	110.01
27	C	514	BCR	C15-C16-C17	-3.01	117.36	123.52
25	A	613	CLA	CHB-C4A-NA	3.01	128.74	124.40
36	V	201	HEC	CBD-CAD-C3D	-3.00	104.22	112.53
25	b	613	CLA	O2A-CGA-O1A	-3.00	116.12	123.63
33	D	407	LHG	O8-C23-C24	3.00	120.99	111.83
29	f	101	SQD	O48-C23-C24	3.00	120.98	111.83
29	F	102	SQD	O6-C1-C2	3.00	112.83	108.27
32	C	515	LMG	C1-O6-C5	-2.99	107.88	113.72
25	h	101	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
25	h	101	CLA	CHB-C4A-NA	2.98	128.70	124.40
25	a	613	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	B	605	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
33	e	102	LHG	O8-C23-C24	2.97	120.90	111.83
25	C	503	CLA	C7-C6-C5	-2.97	105.35	113.26
32	m	101	LMG	O7-C10-O9	-2.97	116.76	123.70
28	d	405	PL9	C12-C13-C14	-2.97	120.83	127.62
25	b	604	CLA	C1-C2-C3	-2.97	121.34	126.20
28	d	405	PL9	C22-C23-C24	-2.95	120.87	127.62
32	b	620	LMG	O1-C1-C2	-2.95	103.80	108.27
27	C	514	BCR	C2-C1-C6	2.94	114.71	110.44
27	K	102	BCR	C27-C26-C25	2.94	126.68	122.70
25	c	513	CLA	O2D-CGD-CBD	2.94	116.37	111.23
25	b	608	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
26	A	608	PHO	CMA-C3A-C4A	-2.94	108.28	114.61
25	b	601	CLA	O2D-CGD-O1D	-2.93	118.14	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	c	503	CLA	C3B-C4B-NB	-2.93	107.91	110.53
28	d	405	PL9	C7-C8-C9	-2.93	121.78	126.83
26	a	609	PHO	C2B-C1B-NB	-2.93	107.31	109.43
29	F	102	SQD	C1-C2-C3	-2.92	103.86	110.01
27	c	514	BCR	C2-C1-C6	2.92	114.68	110.44
30	C	516	DGD	O6D-C1D-O3G	-2.92	103.15	110.04
25	C	507	CLA	CHB-C4A-NA	2.92	128.61	124.40
25	B	612	CLA	C3B-C4B-NB	-2.92	107.93	110.53
25	C	508	CLA	O2D-CGD-CBD	2.91	116.32	111.23
25	B	605	CLA	O2D-CGD-CBD	2.91	116.32	111.23
27	d	404	BCR	C11-C10-C9	-2.91	123.20	127.28
32	c	520	LMG	O6-C1-O1	-2.91	103.17	110.04
27	K	101	BCR	C2-C1-C6	2.91	114.66	110.44
27	c	514	BCR	C27-C26-C25	2.90	126.63	122.70
25	B	609	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	c	505	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
27	H	102	BCR	C2-C1-C6	2.90	114.66	110.44
25	A	606	CLA	CHB-C4A-NA	2.90	128.59	124.40
29	F	102	SQD	O48-C23-C24	2.90	120.68	111.83
25	A	613	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
25	a	608	CLA	O2A-CGA-O1A	-2.90	116.38	123.63
25	a	610	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
32	b	620	LMG	C1-O6-C5	-2.89	108.08	113.72
31	b	622	STE	C3-C2-C1	-2.88	106.98	114.51
25	a	608	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
33	B	622	LHG	O8-C23-C24	2.87	120.59	111.83
30	H	103	DGD	O2D-C2D-C1D	-2.87	103.23	110.08
25	B	603	CLA	O2D-CGD-CBD	2.87	116.24	111.23
31	m	102	STE	O2-C1-C2	2.85	123.01	114.00
29	a	614	SQD	O7-S-C6	2.85	111.01	106.76
32	M	101	LMG	C38-C37-C36	-2.85	99.97	114.37
27	c	515	BCR	C15-C16-C17	-2.85	117.69	123.52
27	H	102	BCR	C16-C15-C14	-2.84	117.71	123.52
25	B	614	CLA	C7-C6-C5	-2.84	105.70	113.26
25	C	504	CLA	CMB-C2B-C1B	-2.84	121.10	125.42
25	A	607	CLA	O2A-CGA-O1A	-2.83	116.54	123.63
28	A	612	PL9	C20-C19-C21	2.83	120.15	115.23
25	C	507	CLA	C3B-C4B-NB	-2.83	108.00	110.53
28	D	405	PL9	C35-C34-C36	2.83	120.14	115.23
30	A	616	DGD	O6D-C1D-O3G	-2.83	103.35	110.04
25	b	613	CLA	C3B-C4B-NB	-2.83	108.01	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	612	CLA	CHB-C4A-NA	2.83	128.48	124.40
28	D	405	PL9	C36-C34-C33	-2.82	114.83	121.17
27	c	514	BCR	C33-C5-C6	-2.82	121.40	124.48
25	C	508	CLA	C3B-C4B-NB	-2.82	108.01	110.53
25	C	512	CLA	O2D-CGD-CBD	2.82	116.16	111.23
33	B	622	LHG	C11-C10-C9	-2.81	100.15	114.37
29	L	101	SQD	C3-C4-C5	2.81	115.32	110.23
27	H	102	BCR	C27-C26-C25	2.81	126.50	122.70
27	K	102	BCR	C33-C5-C6	-2.80	121.42	124.48
25	b	611	CLA	CHB-C4A-NA	2.80	128.45	124.40
25	C	513	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	c	512	CLA	CHB-C4A-NA	2.80	128.44	124.40
25	d	402	CLA	O2A-CGA-O1A	-2.80	116.64	123.63
25	b	607	CLA	O2D-CGD-CBD	2.79	116.11	111.23
25	A	607	CLA	C1-C2-C3	-2.79	121.63	126.20
29	A	614	SQD	C45-O47-C7	-2.79	111.12	117.80
27	c	516	BCR	C27-C26-C25	2.78	126.47	122.70
25	b	607	CLA	CHB-C4A-NA	2.78	128.42	124.40
27	t	101	BCR	C2-C1-C6	2.78	114.48	110.44
25	b	604	CLA	C3B-C4B-NB	-2.78	108.05	110.53
28	d	405	PL9	C40-C39-C41	2.78	120.06	115.23
25	C	504	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
35	e	101	HEM	C3B-C2B-C1B	2.78	108.50	106.41
27	A	611	BCR	C11-C10-C9	-2.77	123.39	127.28
33	B	622	LHG	O8-C23-O10	-2.77	116.69	123.63
25	B	611	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
32	d	410	LMG	O2-C2-C1	-2.77	103.48	110.08
25	c	513	CLA	CHB-C4A-NA	2.76	128.38	124.40
25	A	606	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	C	512	CLA	C1-C2-C3	-2.76	121.68	126.20
36	V	201	HEC	CAD-CBD-CGD	-2.75	106.37	113.67
27	K	101	BCR	C27-C26-C25	2.75	126.42	122.70
25	c	505	CLA	C1-C2-C3	-2.75	121.70	126.20
25	B	607	CLA	O2D-CGD-CBD	2.74	116.03	111.23
27	b	616	BCR	C27-C26-C25	2.74	126.41	122.70
25	A	607	CLA	C3B-C4B-NB	-2.74	108.08	110.53
25	b	607	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
25	b	602	CLA	C3B-C4B-NB	-2.74	108.09	110.53
27	B	618	BCR	C2-C1-C6	2.73	114.41	110.44
32	C	519	LMG	O6-C1-O1	-2.73	103.60	110.04
32	m	101	LMG	C1-O6-C5	-2.72	108.41	113.72
36	v	201	HEC	CAD-CBD-CGD	-2.72	106.46	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	101	HEM	C3B-C4B-NB	-2.72	107.52	109.47
25	c	506	CLA	C1-C2-C3	-2.72	121.75	126.20
25	c	505	CLA	O2D-CGD-CBD	2.72	115.98	111.23
25	c	510	CLA	C3B-C4B-NB	-2.72	108.11	110.53
25	a	610	CLA	O2D-CGD-CBD	2.71	115.97	111.23
25	b	615	CLA	CHB-C4A-NA	2.71	128.31	124.40
25	b	604	CLA	O2A-CGA-O1A	-2.70	116.86	123.63
25	c	509	CLA	CHB-C4A-NA	2.70	128.30	124.40
27	D	404	BCR	C3-C4-C5	-2.70	109.24	114.06
25	b	606	CLA	CHB-C4A-NA	2.70	128.30	124.40
30	c	517	DGD	O6D-C1D-O3G	-2.70	103.66	110.04
28	A	612	PL9	C27-C28-C29	-2.70	121.44	127.62
25	a	607	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
27	a	611	BCR	C27-C26-C25	2.70	126.35	122.70
27	B	617	BCR	C2-C1-C6	2.70	114.36	110.44
27	b	618	BCR	C15-C16-C17	-2.69	118.01	123.52
25	C	506	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
26	a	609	PHO	OBD-CAD-CBD	-2.69	121.88	125.82
25	B	602	CLA	O2D-CGD-CBD	2.69	115.93	111.23
26	a	609	PHO	O2A-CGA-O1A	-2.68	116.91	123.63
25	B	608	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
33	E	101	LHG	O8-C23-C24	2.68	120.00	111.83
25	c	505	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
27	c	515	BCR	C33-C5-C6	-2.68	121.56	124.48
27	b	617	BCR	C8-C7-C6	-2.68	119.84	127.00
28	D	405	PL9	C7-C8-C9	-2.68	122.22	126.83
25	b	608	CLA	C1-C2-C3	-2.67	121.82	126.20
33	d	406	LHG	O8-C23-O10	-2.67	116.96	123.63
27	c	515	BCR	C27-C26-C25	2.67	126.31	122.70
27	k	101	BCR	C27-C26-C25	2.67	126.31	122.70
27	K	101	BCR	C24-C23-C22	-2.67	122.29	126.23
25	b	612	CLA	C1D-ND-C4D	2.67	108.18	106.31
25	C	503	CLA	C3B-C4B-NB	-2.66	108.15	110.53
25	B	606	CLA	CMB-C2B-C3B	2.66	132.81	126.55
28	D	405	PL9	C20-C19-C21	2.66	119.85	115.23
26	a	609	PHO	CMB-C2B-C3B	2.66	130.00	124.68
25	B	604	CLA	CAA-CBA-CGA	-2.66	105.65	113.21
25	b	602	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	D	403	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
30	c	519	DGD	O5D-C1E-C2E	2.66	112.31	108.27
32	D	406	LMG	O3-C3-C2	-2.66	104.11	110.38
25	c	509	CLA	C3B-C4B-NB	-2.66	108.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	402	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
28	D	405	PL9	C27-C28-C29	-2.65	121.55	127.62
31	t	102	STE	C3-C2-C1	-2.65	107.58	114.51
25	c	512	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
25	c	508	CLA	CHD-C1D-ND	-2.65	121.07	124.80
25	c	508	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
25	B	605	CLA	CGD-CBD-CAD	-2.65	102.27	110.85
25	C	504	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
31	B	625	STE	O2-C1-C2	2.65	122.37	114.00
25	B	611	CLA	CHB-C4A-NA	2.65	128.22	124.40
25	b	607	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
29	l	101	SQD	O5-C5-C4	2.64	114.47	109.70
25	A	613	CLA	O2D-CGD-CBD	2.64	115.85	111.23
25	C	513	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	D	402	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
27	b	616	BCR	C15-C14-C13	-2.64	123.58	127.28
25	c	506	CLA	C3B-C4B-NB	-2.63	108.18	110.53
33	D	407	LHG	C27-C26-C25	-2.62	101.11	114.37
30	c	517	DGD	O3E-C3E-C2E	-2.62	104.19	110.38
27	k	101	BCR	C33-C5-C6	-2.62	121.63	124.48
30	h	102	DGD	CDB-CCB-CBB	-2.62	101.14	114.37
29	f	101	SQD	C1-C2-C3	-2.61	104.51	110.01
29	A	614	SQD	O47-C7-O49	-2.61	117.59	123.70
30	C	516	DGD	CDB-CCB-CBB	-2.61	101.16	114.37
25	C	509	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
25	C	511	CLA	CHB-C4A-NA	2.61	128.17	124.40
30	c	519	DGD	C3G-C2G-C1G	-2.61	105.69	111.78
25	C	502	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
25	h	101	CLA	CHD-C1D-ND	-2.61	121.13	124.80
25	b	612	CLA	C1-C2-C3	-2.61	121.92	126.20
33	D	408	LHG	O8-C23-C24	2.61	119.80	111.83
25	b	602	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
27	c	514	BCR	C15-C14-C13	-2.61	123.62	127.28
25	a	613	CLA	O2D-CGD-CBD	2.61	115.79	111.23
30	a	616	DGD	CDB-CCB-CBB	-2.60	101.20	114.37
33	D	407	LHG	C18-C17-C16	-2.60	101.21	114.37
25	B	601	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
25	C	508	CLA	CHD-C1D-ND	-2.60	121.14	124.80
25	c	503	CLA	CHB-C4A-NA	2.60	128.15	124.40
32	C	519	LMG	O1-C7-C8	-2.60	104.49	110.82
25	b	614	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	B	612	CLA	O2A-CGA-O1A	-2.60	117.12	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
32	b	620	LMG	O7-C10-O9	-2.59	117.64	123.70
25	c	502	CLA	C1-C2-C3	-2.59	121.95	126.20
28	D	405	PL9	C40-C39-C41	2.59	119.73	115.23
25	B	604	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
30	C	517	DGD	CDB-CCB-CBB	-2.59	101.28	114.37
30	h	102	DGD	O6D-C1D-O3G	-2.59	103.92	110.04
27	C	514	BCR	C27-C26-C25	2.59	126.20	122.70
30	H	103	DGD	C3E-C4E-C5E	-2.59	105.54	110.23
25	B	611	CLA	CMB-C2B-C3B	2.59	132.64	126.55
27	b	616	BCR	C3-C4-C5	-2.59	109.44	114.06
28	D	405	PL9	C42-C43-C44	-2.58	121.71	127.62
30	A	616	DGD	C3G-C2G-C1G	-2.58	105.78	111.78
27	D	404	BCR	C28-C27-C26	-2.57	109.47	114.06
27	b	618	BCR	C11-C10-C9	-2.57	123.68	127.28
30	C	518	DGD	CDB-CCB-CBB	-2.57	101.40	114.37
29	a	614	SQD	C3-C4-C5	2.56	114.88	110.23
29	l	101	SQD	C1-O5-C5	-2.56	108.71	113.72
25	D	402	CLA	C1-C2-C3	-2.56	122.00	126.20
25	B	609	CLA	CHC-C1C-NC	2.56	128.17	124.31
28	a	612	PL9	C37-C38-C39	-2.55	121.78	127.62
25	b	603	CLA	C3B-C4B-NB	-2.55	108.25	110.53
28	a	612	PL9	C22-C23-C24	-2.55	121.78	127.62
25	C	509	CLA	C1-C2-C3	-2.55	122.02	126.20
28	A	612	PL9	C12-C13-C14	-2.55	121.79	127.62
30	h	102	DGD	O6E-C1E-O5D	-2.55	104.02	110.04
25	c	504	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
29	F	102	SQD	O8-S-C6	2.55	110.89	105.97
32	D	406	LMG	O6-C1-O1	-2.55	104.02	110.04
30	C	517	DGD	C1D-C2D-C3D	-2.55	104.65	110.01
25	c	510	CLA	CHB-C4A-NA	2.55	128.08	124.40
25	C	509	CLA	CHD-C1D-C2D	2.55	130.78	125.49
29	a	614	SQD	O9-S-C6	2.55	110.56	106.76
25	b	615	CLA	C3B-C4B-NB	-2.55	108.26	110.53
25	d	403	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
29	A	614	SQD	O48-C23-C24	2.54	119.58	111.83
25	B	615	CLA	CAA-CBA-CGA	-2.54	106.00	113.21
33	l	102	LHG	O8-C23-C24	2.54	119.57	111.83
33	E	101	LHG	C11-C10-C9	-2.54	101.54	114.37
25	c	502	CLA	C3B-C4B-NB	-2.54	108.27	110.53
35	e	101	HEM	CHB-C1B-NB	2.53	127.50	124.37
25	B	611	CLA	C11-C12-C13	-2.53	107.55	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	517	DGD	C3D-C4D-C5D	-2.53	105.65	110.23
25	A	610	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
32	b	620	LMG	C3-C4-C5	-2.53	105.65	110.23
30	A	616	DGD	C4E-C3E-C2E	-2.53	106.39	110.83
25	a	607	CLA	C3B-C4B-NB	-2.53	108.27	110.53
30	c	517	DGD	CDB-CCB-CBB	-2.53	101.59	114.37
25	a	613	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	c	522	LMG	O6-C1-O1	-2.53	104.08	110.04
25	a	608	CLA	O2D-CGD-CBD	2.52	115.64	111.23
26	a	609	PHO	C4D-CHA-CBD	-2.52	107.24	108.45
33	l	102	LHG	C20-C19-C18	-2.52	101.61	114.37
30	A	616	DGD	CDB-CCB-CBB	-2.52	101.62	114.37
25	C	507	CLA	C1-C2-C3	-2.52	122.06	126.20
30	C	518	DGD	C3G-C2G-C1G	-2.52	105.91	111.78
25	b	611	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	c	504	CLA	C3B-C4B-NB	-2.52	108.28	110.53
30	C	517	DGD	C6D-O5D-C1E	2.52	119.20	113.80
25	C	508	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
25	c	501	CLA	C1-C2-C3	-2.51	122.08	126.20
25	D	402	CLA	C4-C3-C5	2.51	119.59	115.23
33	d	406	LHG	C11-C10-C9	-2.51	101.67	114.37
25	B	606	CLA	CED-O2D-CGD	2.51	121.61	115.92
25	C	503	CLA	O1D-CGD-CBD	2.51	129.47	124.52
25	b	607	CLA	CHB-C1B-NB	2.51	127.81	124.05
30	c	519	DGD	CAB-C9B-C8B	-2.51	101.68	114.37
25	d	403	CLA	C1-C2-C3	-2.51	122.08	126.20
30	H	103	DGD	O6D-C1D-O3G	-2.51	104.12	110.04
25	b	611	CLA	C11-C12-C13	-2.51	107.63	115.97
30	C	517	DGD	O2G-C1B-O1B	-2.50	117.85	123.70
27	t	101	BCR	C33-C5-C6	-2.50	121.75	124.48
25	a	610	CLA	O2A-CGA-O1A	-2.50	117.36	123.63
32	c	522	LMG	C4-C3-C2	2.50	115.22	110.83
25	b	603	CLA	C11-C12-C13	-2.50	107.65	115.97
25	c	506	CLA	CHB-C4A-NA	2.50	128.01	124.40
28	A	612	PL9	C22-C23-C24	-2.50	121.91	127.62
29	f	101	SQD	C1-O5-C5	-2.49	108.85	113.72
25	A	610	CLA	CHD-C1D-ND	-2.49	121.29	124.80
25	b	603	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
26	a	609	PHO	O1D-CGD-CBD	2.49	128.50	124.72
27	c	516	BCR	C33-C5-C6	-2.49	121.77	124.48
25	c	501	CLA	C3B-C4B-NB	-2.48	108.31	110.53
25	B	607	CLA	CHC-C4B-NB	2.48	127.78	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	403	CLA	CHB-C4A-NA	2.48	127.98	124.40
25	B	602	CLA	CHB-C1B-NB	2.48	127.77	124.05
28	D	405	PL9	O2-C1-C6	2.48	124.42	120.48
25	B	607	CLA	CHB-C1B-NB	2.48	127.77	124.05
25	B	607	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
28	A	612	PL9	O2-C1-C6	2.48	124.42	120.48
25	B	601	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
25	d	402	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
25	b	609	CLA	CHC-C4B-NB	2.47	127.75	124.05
30	H	103	DGD	CDB-CCB-CBB	-2.47	101.89	114.37
27	c	514	BCR	C15-C16-C17	-2.47	118.47	123.52
25	C	512	CLA	O2A-CGA-O1A	-2.46	117.46	123.63
25	C	503	CLA	CHB-C4A-NA	2.46	127.96	124.40
30	a	616	DGD	CBB-CAB-C9B	-2.46	101.92	114.37
27	D	404	BCR	C2-C1-C6	2.46	114.01	110.44
25	C	501	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
25	A	613	CLA	C16-C15-C13	-2.45	107.81	115.97
25	B	604	CLA	O1D-CGD-CBD	2.45	129.36	124.52
25	c	504	CLA	CMB-C2B-C3B	2.45	132.32	126.55
25	a	610	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	C	508	CLA	CHB-C4A-NA	2.45	127.94	124.40
27	C	514	BCR	C33-C5-C6	-2.45	121.81	124.48
25	B	612	CLA	CED-O2D-CGD	2.45	121.47	115.92
25	A	610	CLA	CHB-C4A-NA	2.45	127.93	124.40
25	b	601	CLA	O2D-CGD-CBD	2.45	115.50	111.23
27	t	101	BCR	C27-C26-C25	2.45	126.01	122.70
29	f	101	SQD	C3-C4-C5	2.44	114.66	110.23
25	C	501	CLA	CHB-C1B-NB	2.44	127.71	124.05
32	M	101	LMG	C40-C39-C38	-2.44	102.04	114.37
32	d	410	LMG	O1-C1-C2	-2.44	104.57	108.27
27	c	515	BCR	C7-C8-C9	-2.44	122.63	126.23
25	C	506	CLA	O2A-CGA-O1A	-2.44	117.54	123.63
29	f	101	SQD	O5-C1-C2	-2.43	105.37	110.37
25	B	610	CLA	CHD-C1D-C2D	2.43	130.54	125.49
27	K	102	BCR	C8-C7-C6	-2.43	120.51	127.00
25	b	602	CLA	O2D-CGD-CBD	2.43	115.47	111.23
25	a	608	CLA	C3B-C4B-NB	-2.43	108.36	110.53
25	a	613	CLA	CHD-C1D-ND	-2.43	121.39	124.80
25	b	613	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
25	c	504	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
30	C	517	DGD	C5B-C4B-C3B	-2.42	102.11	114.37
33	D	408	LHG	C27-C26-C25	-2.42	102.11	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	BCR	C27-C26-C25	2.42	125.98	122.70
25	B	610	CLA	C3B-C4B-NB	-2.42	108.37	110.53
25	B	602	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
25	H	101	CLA	O2D-CGD-CBD	2.42	115.46	111.23
28	a	612	PL9	C7-C8-C9	-2.42	122.66	126.83
33	l	102	LHG	C18-C17-C16	-2.42	102.14	114.37
25	c	507	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
25	B	609	CLA	O2D-CGD-CBD	2.42	115.46	111.23
28	A	612	PL9	O2-C1-C2	-2.42	116.33	121.83
25	A	613	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	a	607	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	B	603	CLA	O2A-CGA-O1A	-2.42	117.59	123.63
25	C	507	CLA	C2A-C1A-CHA	2.41	128.05	123.87
25	c	502	CLA	CHD-C1D-ND	-2.40	121.42	124.80
32	m	101	LMG	O3-C3-C2	-2.40	104.71	110.38
28	D	405	PL9	C37-C38-C39	-2.40	122.12	127.62
25	C	506	CLA	C1-C2-C3	-2.40	122.26	126.20
25	C	510	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
27	d	404	BCR	C30-C25-C26	-2.40	119.36	122.64
27	B	617	BCR	C3-C4-C5	-2.40	109.78	114.06
36	v	201	HEC	CHA-C4D-ND	2.40	128.21	123.86
26	d	401	PHO	C3B-C4B-NB	-2.40	105.90	107.46
28	d	405	PL9	C32-C33-C34	-2.40	122.14	127.62
25	B	613	CLA	C1-C2-C3	-2.40	122.27	126.20
25	b	602	CLA	CHD-C1D-ND	-2.40	121.43	124.80
30	c	519	DGD	CDB-CCB-CBB	-2.39	102.26	114.37
27	b	618	BCR	C27-C26-C25	2.39	125.94	122.70
25	B	604	CLA	CHD-C1D-ND	-2.39	121.43	124.80
29	a	615	SQD	C9-C8-C7	-2.39	104.92	113.69
25	c	508	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
27	t	101	BCR	C11-C10-C9	-2.39	123.92	127.28
30	c	517	DGD	O1G-C1A-O1A	-2.39	117.65	123.63
30	A	616	DGD	O5D-C6D-C5D	-2.39	104.03	109.42
29	f	101	SQD	O47-C7-C8	2.39	119.71	110.93
26	A	608	PHO	O1D-CGD-CBD	2.39	128.35	124.72
27	B	617	BCR	C35-C13-C14	-2.39	118.95	122.82
29	f	101	SQD	O9-S-C6	2.39	110.32	106.76
32	m	101	LMG	C40-C39-C38	-2.39	102.31	114.37
28	a	612	PL9	C27-C28-C29	-2.39	122.16	127.62
25	B	615	CLA	C1-C2-C3	2.39	130.10	126.20
33	D	408	LHG	C11-C10-C9	-2.39	102.31	114.37
25	B	615	CLA	C3B-C4B-NB	-2.38	108.40	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	606	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
31	C	520	STE	C3-C2-C1	-2.38	108.30	114.51
25	B	614	CLA	CHB-C4A-NA	2.38	127.83	124.40
30	c	519	DGD	O6E-C5E-C4E	2.38	113.99	109.70
25	c	508	CLA	O2D-CGD-CBD	2.38	115.39	111.23
25	A	610	CLA	C1-C2-C3	-2.38	122.30	126.20
27	B	616	BCR	C29-C30-C25	2.38	113.89	110.44
30	c	518	DGD	O2E-C2E-C1E	-2.38	104.41	110.08
25	d	403	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	a	609	PHO	C1-C2-C3	-2.37	122.31	126.20
36	v	201	HEC	CBD-CAD-C3D	-2.37	105.98	112.53
25	C	511	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
28	A	612	PL9	C36-C34-C33	-2.37	115.85	121.17
25	b	603	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
30	c	518	DGD	CDB-CCB-CBB	-2.37	102.40	114.37
27	T	101	BCR	C7-C8-C9	-2.37	122.73	126.23
25	B	610	CLA	C1-C2-C3	-2.37	122.32	126.20
25	c	507	CLA	CHB-C4A-NA	2.37	127.81	124.40
25	C	502	CLA	C1-C2-C3	-2.36	122.32	126.20
25	C	501	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	C	509	CLA	CHB-C1B-NB	2.36	127.59	124.05
25	C	510	CLA	O2D-CGD-CBD	2.36	115.36	111.23
25	h	101	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
32	C	515	LMG	C38-C37-C36	-2.36	102.46	114.37
25	B	613	CLA	CHB-C4A-NA	2.36	127.80	124.40
25	b	601	CLA	C2D-C1D-ND	-2.35	107.80	110.13
27	b	618	BCR	C7-C8-C9	-2.35	122.75	126.23
33	l	102	LHG	C11-C10-C9	-2.35	102.48	114.37
33	d	407	LHG	O8-C23-C24	2.35	119.00	111.83
25	C	510	CLA	CHB-C4A-NA	2.35	127.79	124.40
30	C	517	DGD	C7B-C6B-C5B	-2.35	102.49	114.37
25	b	604	CLA	CHD-C1D-ND	-2.35	121.50	124.80
27	c	516	BCR	C11-C10-C9	-2.35	123.99	127.28
25	A	610	CLA	CMB-C2B-C3B	2.35	132.07	126.55
26	A	608	PHO	O2A-CGA-O1A	-2.35	117.76	123.63
25	c	513	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
25	c	508	CLA	CHD-C1D-C2D	2.34	130.36	125.49
27	d	404	BCR	C38-C26-C25	-2.34	121.93	124.48
35	e	101	HEM	CAB-C3B-C2B	-2.34	120.81	128.43
25	b	613	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	B	601	CLA	CMB-C2B-C3B	2.34	132.05	126.55
25	A	610	CLA	CHD-C4C-NC	2.34	127.86	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	517	DGD	O5D-C6D-C5D	-2.34	104.15	109.42
25	C	508	CLA	CHD-C1D-C2D	2.34	130.35	125.49
28	D	405	PL9	C12-C13-C14	-2.34	122.27	127.62
25	C	509	CLA	CMB-C2B-C3B	2.34	132.05	126.55
25	c	505	CLA	C11-C10-C8	-2.34	108.20	115.97
27	t	101	BCR	C15-C14-C13	-2.34	124.00	127.28
25	c	503	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
27	D	404	BCR	C38-C26-C25	-2.34	121.93	124.48
25	b	610	CLA	CHD-C1D-C2D	2.33	130.34	125.49
28	A	612	PL9	C7-C8-C9	-2.33	122.81	126.83
27	K	102	BCR	C30-C25-C26	-2.33	119.45	122.64
26	a	609	PHO	CMD-C2D-C3D	2.33	129.34	124.68
29	L	101	SQD	O9-S-C6	2.33	110.24	106.76
25	c	506	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
27	A	611	BCR	C16-C15-C14	-2.33	118.75	123.52
25	c	513	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
25	a	613	CLA	CHD-C1D-C2D	2.33	130.33	125.49
27	D	404	BCR	C7-C8-C9	-2.33	122.80	126.23
27	a	611	BCR	C11-C10-C9	-2.32	124.02	127.28
33	E	101	LHG	C20-C19-C18	-2.32	102.65	114.37
32	c	520	LMG	C38-C37-C36	-2.32	102.65	114.37
30	c	519	DGD	O6D-C1D-O3G	-2.32	104.57	110.04
25	b	612	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
25	C	513	CLA	O2D-CGD-CBD	2.31	115.28	111.23
25	a	607	CLA	O1D-CGD-CBD	2.31	129.08	124.52
25	C	506	CLA	CHB-C4A-NA	2.31	127.74	124.40
25	C	512	CLA	CAA-CBA-CGA	-2.31	106.64	113.21
33	D	407	LHG	C20-C19-C18	-2.31	102.67	114.37
30	C	516	DGD	CAB-C9B-C8B	-2.31	102.68	114.37
25	b	607	CLA	CMB-C2B-C3B	2.31	131.99	126.55
32	d	410	LMG	C40-C39-C38	-2.31	102.69	114.37
25	b	610	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	b	614	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
25	a	607	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
25	C	502	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	x	101	BCR	C3-C4-C5	-2.31	109.94	114.06
30	C	516	DGD	O5D-C6D-C5D	-2.30	104.23	109.42
27	K	102	BCR	C16-C15-C14	-2.30	118.81	123.52
32	B	620	LMG	C38-C37-C36	-2.30	102.73	114.37
32	D	406	LMG	C38-C37-C36	-2.30	102.75	114.37
33	e	102	LHG	C11-C10-C9	-2.30	102.75	114.37
25	c	508	CLA	CHD-C4C-NC	2.30	127.79	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	516	DGD	C3D-C4D-C5D	-2.29	106.07	110.23
27	K	103	BCR	C24-C23-C22	-2.29	122.84	126.23
35	e	101	HEM	CBA-CAA-C2A	-2.29	106.20	112.53
25	b	609	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
32	b	620	LMG	O8-C28-O10	-2.29	117.91	123.63
30	c	519	DGD	C8B-C7B-C6B	-2.29	102.81	114.37
25	b	606	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
32	M	101	LMG	C1-O6-C5	-2.29	109.25	113.72
27	B	618	BCR	C15-C16-C17	-2.28	118.85	123.52
31	j	101	STE	O2-C1-C2	2.28	121.21	114.00
25	B	602	CLA	C7-C6-C5	-2.28	107.18	113.26
29	l	101	SQD	O6-C44-C45	2.28	116.37	110.82
33	D	407	LHG	O8-C23-O10	-2.28	117.92	123.63
27	D	404	BCR	C27-C26-C25	2.28	125.78	122.70
27	t	101	BCR	C15-C16-C17	-2.28	118.86	123.52
25	B	605	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
25	c	508	CLA	CHB-C1B-NB	2.28	127.46	124.05
25	c	505	CLA	CMD-C2D-C3D	2.28	132.91	127.69
25	b	612	CLA	C7-C6-C5	-2.28	107.20	113.26
33	l	102	LHG	C5-O7-C7	-2.28	112.35	117.80
27	a	611	BCR	C7-C8-C9	-2.28	122.87	126.23
25	A	606	CLA	C7-C6-C5	-2.27	107.20	113.26
27	B	616	BCR	C3-C4-C5	-2.27	110.00	114.06
25	C	513	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
27	b	616	BCR	C33-C5-C6	-2.27	122.01	124.48
31	d	411	STE	O2-C1-C2	2.27	121.16	114.00
32	c	520	LMG	C40-C39-C38	-2.27	102.92	114.37
33	B	622	LHG	C18-C17-C16	-2.26	102.92	114.37
33	D	408	LHG	C18-C17-C16	-2.26	102.93	114.37
30	c	517	DGD	O5D-C6D-C5D	-2.26	104.32	109.42
25	b	605	CLA	CHB-C4A-NA	2.26	127.66	124.40
30	c	519	DGD	O3G-C1D-C2D	-2.26	104.84	108.27
28	a	612	PL9	O2-C1-C2	-2.26	116.69	121.83
25	b	601	CLA	C11-C10-C8	-2.26	108.46	115.97
32	c	522	LMG	O3-C3-C2	-2.26	105.05	110.38
25	C	504	CLA	O2D-CGD-CBD	2.26	115.17	111.23
31	J	101	STE	O2-C1-C2	2.26	121.13	114.00
27	b	616	BCR	C35-C13-C14	-2.26	119.16	122.82
25	A	613	CLA	CMB-C2B-C3B	2.26	131.85	126.55
25	h	101	CLA	CHD-C4C-NC	2.26	127.73	124.23
25	B	612	CLA	CHB-C4A-NA	2.25	127.65	124.40
25	b	608	CLA	CMB-C2B-C3B	2.25	131.85	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	612	CLA	C16-C15-C13	-2.25	108.47	115.97
28	a	612	PL9	C40-C39-C41	2.25	119.14	115.23
36	v	201	HEC	CHB-C1B-NB	2.25	127.93	123.86
25	B	615	CLA	O1D-CGD-CBD	2.25	128.95	124.52
25	C	513	CLA	CHD-C1D-ND	-2.24	121.64	124.80
25	b	604	CLA	O1D-CGD-CBD	2.24	128.94	124.52
32	D	409	LMG	O1-C7-C8	-2.24	106.01	111.77
32	b	620	LMG	C40-C39-C38	-2.24	103.05	114.37
33	d	408	LHG	C27-C26-C25	-2.24	103.05	114.37
25	b	609	CLA	C3B-C4B-NB	-2.24	108.53	110.53
27	c	514	BCR	C11-C10-C9	-2.24	124.14	127.28
28	D	405	PL9	C50-C49-C48	-2.24	115.94	122.66
27	A	611	BCR	C8-C7-C6	-2.24	121.02	127.00
25	B	602	CLA	CMB-C2B-C3B	2.24	131.81	126.55
29	A	615	SQD	O48-C23-O10	-2.24	118.03	123.63
25	B	609	CLA	C1-C2-C3	-2.24	122.53	126.20
27	K	103	BCR	C2-C1-C6	2.23	113.68	110.44
27	B	616	BCR	C33-C5-C6	-2.23	122.05	124.48
25	C	504	CLA	CHD-C4C-NC	2.23	127.69	124.23
30	c	519	DGD	O3D-C3D-C4D	-2.23	105.11	110.38
25	B	605	CLA	CHB-C4A-NA	2.23	127.62	124.40
25	b	610	CLA	CHD-C1D-ND	-2.23	121.66	124.80
25	b	607	CLA	CHD-C1D-ND	-2.23	121.67	124.80
27	B	617	BCR	C15-C16-C17	-2.23	118.96	123.52
36	V	201	HEC	C1D-C2D-C3D	-2.23	104.27	106.82
27	T	101	BCR	C30-C25-C26	-2.23	119.59	122.64
25	c	505	CLA	CHB-C4A-NA	2.23	127.61	124.40
25	b	608	CLA	CHC-C4B-NB	2.22	127.39	124.05
25	C	504	CLA	CHD-C1D-ND	-2.22	121.67	124.80
30	h	102	DGD	O3E-C3E-C2E	-2.22	105.14	110.38
29	F	102	SQD	O5-C1-C2	-2.22	105.81	110.37
31	t	102	STE	O2-C1-C2	2.22	121.02	114.00
27	K	101	BCR	C33-C5-C6	-2.22	122.06	124.48
33	B	621	LHG	C20-C19-C18	-2.22	103.15	114.37
25	d	402	CLA	CMB-C2B-C3B	2.22	131.77	126.55
25	C	511	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
25	c	504	CLA	CHB-C4A-NA	2.22	127.60	124.40
32	C	519	LMG	C40-C39-C38	-2.22	103.16	114.37
30	C	517	DGD	CBB-CAB-C9B	-2.22	103.16	114.37
35	e	101	HEM	C1B-NB-C4B	2.22	107.83	105.21
25	B	609	CLA	CHA-C1A-NA	-2.21	121.38	126.39
25	B	602	CLA	C4-C3-C5	2.21	119.07	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	101	LMG	C1-C2-C3	-2.21	105.36	110.01
25	b	605	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
25	B	613	CLA	CHC-C4B-NB	2.21	127.36	124.05
32	C	519	LMG	C38-C37-C36	-2.21	103.21	114.37
27	K	101	BCR	C7-C8-C9	-2.21	122.97	126.23
25	B	604	CLA	CHB-C4A-NA	2.21	127.58	124.40
25	b	611	CLA	O1D-CGD-CBD	2.21	128.87	124.52
25	c	510	CLA	C16-C15-C13	-2.21	108.63	115.97
33	E	101	LHG	C18-C17-C16	-2.20	103.23	114.37
30	A	616	DGD	CBB-CAB-C9B	-2.20	103.23	114.37
30	c	519	DGD	C6B-C5B-C4B	-2.20	103.23	114.37
30	H	103	DGD	CAB-C9B-C8B	-2.20	103.24	114.37
27	C	514	BCR	C7-C8-C9	-2.20	122.98	126.23
27	A	611	BCR	C2-C1-C6	2.20	113.64	110.44
32	D	406	LMG	O2-C2-C1	-2.20	104.83	110.08
25	A	607	CLA	O2D-CGD-CBD	2.20	115.07	111.23
25	b	612	CLA	C2D-C1D-ND	-2.20	107.95	110.13
27	B	616	BCR	C27-C26-C25	2.19	125.66	122.70
31	J	101	STE	C3-C2-C1	-2.19	108.81	114.51
25	c	511	CLA	CHB-C4A-NA	2.18	127.55	124.40
25	B	609	CLA	C2A-C1A-CHA	2.18	127.65	123.87
32	d	409	LMG	O7-C10-O9	-2.18	117.72	123.33
26	a	609	PHO	O2D-CGD-O1D	-2.18	119.60	123.85
32	M	101	LMG	O3-C3-C2	-2.18	105.23	110.38
25	B	615	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
25	C	502	CLA	O2D-CGD-CBD	2.18	115.04	111.23
30	a	616	DGD	C5B-C4B-C3B	-2.18	103.36	114.37
27	t	101	BCR	C7-C8-C9	-2.18	123.01	126.23
27	B	616	BCR	C30-C25-C26	-2.18	119.66	122.64
27	K	103	BCR	C15-C14-C13	-2.18	124.22	127.28
33	e	102	LHG	C20-C19-C18	-2.18	103.37	114.37
28	d	405	PL9	C20-C19-C21	2.17	119.00	115.23
33	B	622	LHG	C20-C19-C18	-2.17	103.38	114.37
25	b	611	CLA	C11-C10-C8	-2.17	108.74	115.97
30	C	516	DGD	C6B-C5B-C4B	-2.17	103.38	114.37
25	c	501	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
25	C	503	CLA	C6-C5-C3	2.17	118.76	113.47
25	B	609	CLA	O1D-CGD-CBD	2.17	128.80	124.52
25	B	611	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	b	608	CLA	CED-O2D-CGD	2.17	120.83	115.92
29	l	101	SQD	C25-C24-C23	-2.17	105.75	113.69
25	C	507	CLA	O2A-CGA-O1A	-2.17	118.21	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	h	102	DGD	CBB-CAB-C9B	-2.17	103.42	114.37
25	b	606	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
25	b	614	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
30	c	518	DGD	CBB-CAB-C9B	-2.17	103.42	114.37
30	a	616	DGD	CFB-CEB-CDB	-2.17	103.42	114.37
27	a	611	BCR	C29-C30-C25	2.17	113.58	110.44
29	A	614	SQD	O9-S-C6	2.16	109.99	106.76
25	A	606	CLA	C3B-C4B-NB	-2.16	108.60	110.53
25	c	508	CLA	CMB-C2B-C3B	2.16	131.64	126.55
26	a	609	PHO	C1-O2A-CGA	-2.16	111.42	116.65
25	D	402	CLA	O2D-CGD-CBD	2.16	115.01	111.23
25	B	615	CLA	O2D-CGD-CBD	2.16	115.01	111.23
25	b	609	CLA	O1D-CGD-CBD	2.16	128.78	124.52
25	d	402	CLA	C3B-C4B-NB	-2.16	108.60	110.53
25	C	509	CLA	CHD-C4C-NC	2.16	127.58	124.23
33	l	102	LHG	O8-C23-O10	-2.16	118.23	123.63
25	b	603	CLA	C4-C3-C5	2.16	118.97	115.23
25	b	610	CLA	C2D-C1D-ND	-2.16	107.99	110.13
27	b	618	BCR	C31-C1-C6	2.16	113.62	110.24
27	A	611	BCR	C37-C22-C21	-2.16	119.32	122.82
32	M	101	LMG	O2-C2-C1	-2.15	104.94	110.08
25	c	503	CLA	C7-C6-C5	-2.15	107.52	113.26
25	b	604	CLA	CHB-C4A-NA	2.15	127.51	124.40
27	b	617	BCR	C33-C5-C6	-2.15	122.13	124.48
25	c	501	CLA	CHB-C4A-NA	2.15	127.51	124.40
30	h	102	DGD	O6E-C5E-C6E	-2.15	101.11	106.44
32	C	515	LMG	O8-C28-O10	-2.15	118.25	123.63
33	d	406	LHG	C20-C19-C18	-2.15	103.51	114.37
25	b	615	CLA	O2D-CGD-CBD	2.15	114.99	111.23
25	B	612	CLA	CAC-C3C-C4C	2.15	127.58	124.79
35	F	101	HEM	CBA-CAA-C2A	-2.15	106.60	112.53
25	B	610	CLA	C11-C12-C13	-2.15	108.83	115.97
29	F	102	SQD	C46-C45-C44	-2.14	106.75	113.67
27	C	514	BCR	C15-C14-C13	-2.14	124.27	127.28
27	B	617	BCR	C27-C26-C25	2.14	125.60	122.70
30	A	616	DGD	C5B-C4B-C3B	-2.14	103.54	114.37
25	B	607	CLA	C6-C7-C8	-2.14	108.85	115.97
25	c	513	CLA	C1-C2-C3	-2.14	122.69	126.20
28	A	612	PL9	O1-C4-C3	-2.14	118.47	120.73
25	C	509	CLA	CHB-C4A-NA	2.14	127.49	124.40
27	b	617	BCR	C11-C10-C9	-2.14	124.28	127.28
32	C	519	LMG	O3-C3-C2	-2.14	105.34	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	615	SQD	O49-C7-C8	-2.14	115.43	123.78
25	B	614	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
27	A	611	BCR	C33-C5-C6	-2.13	122.16	124.48
27	B	618	BCR	C37-C22-C21	-2.13	119.36	122.82
30	A	616	DGD	CFB-CEB-CDB	-2.13	103.59	114.37
25	B	615	CLA	CHB-C1B-NB	2.13	127.25	124.05
30	c	519	DGD	O2D-C2D-C1D	-2.13	105.00	110.08
25	C	510	CLA	CMB-C2B-C3B	2.13	131.56	126.55
25	b	603	CLA	CHB-C4A-NA	2.13	127.47	124.40
25	b	607	CLA	CHD-C4C-NC	2.13	127.53	124.23
25	b	608	CLA	C7-C6-C5	-2.13	107.59	113.26
27	A	611	BCR	C15-C14-C13	-2.13	124.29	127.28
28	a	612	PL9	C32-C33-C34	-2.13	122.75	127.62
25	B	613	CLA	CHB-C1B-NB	2.13	127.24	124.05
33	D	407	LHG	C11-C10-C9	-2.13	103.61	114.37
32	d	410	LMG	O1-C7-C8	-2.13	105.64	110.82
26	A	609	PHO	O2D-CGD-CBD	2.13	113.28	110.95
30	h	102	DGD	C1D-O6D-C5D	-2.13	109.57	113.72
25	b	605	CLA	C1-C2-C3	-2.13	122.71	126.20
25	A	607	CLA	CHD-C1D-ND	-2.13	121.81	124.80
33	d	407	LHG	O8-C23-O10	-2.13	118.31	123.63
25	B	606	CLA	CHC-C4B-NB	2.12	127.23	124.05
25	b	614	CLA	CHB-C1B-NB	2.12	127.23	124.05
25	a	610	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	C	508	CLA	CMB-C2B-C3B	2.12	131.53	126.55
25	B	605	CLA	C1-C2-C3	-2.12	122.73	126.20
25	c	512	CLA	CHD-C1D-ND	-2.12	121.82	124.80
30	H	103	DGD	C3G-C2G-C1G	-2.12	106.85	111.78
25	c	510	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
32	d	409	LMG	C38-C37-C36	-2.11	103.68	114.37
30	h	102	DGD	C7B-C6B-C5B	-2.11	103.69	114.37
25	b	606	CLA	C1-O2A-CGA	2.11	121.76	116.65
28	d	405	PL9	C8-C7-C3	2.11	117.49	112.03
25	C	505	CLA	CHB-C4A-NA	2.11	127.45	124.40
32	c	522	LMG	C40-C39-C38	-2.11	103.70	114.37
27	t	101	BCR	C31-C1-C6	2.11	113.55	110.24
33	B	621	LHG	C11-C10-C9	-2.11	103.70	114.37
32	D	409	LMG	C38-C37-C36	-2.11	103.70	114.37
25	b	607	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
33	E	101	LHG	C27-C26-C25	-2.11	103.71	114.37
27	b	618	BCR	C29-C30-C25	2.11	113.50	110.44
29	a	615	SQD	O48-C23-O10	-2.11	118.36	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	605	CLA	CHB-C1B-NB	2.10	127.21	124.05
32	C	515	LMG	C40-C39-C38	-2.10	103.73	114.37
25	c	513	CLA	CMB-C2B-C3B	2.10	131.50	126.55
27	H	102	BCR	C29-C30-C25	2.10	113.49	110.44
32	b	620	LMG	C8-O7-C10	2.10	122.83	117.80
27	K	103	BCR	C28-C27-C26	-2.10	110.31	114.06
30	c	519	DGD	C3D-C4D-C5D	-2.10	106.42	110.23
30	a	616	DGD	CAB-C9B-C8B	-2.10	103.75	114.37
29	F	102	SQD	O5-C5-C4	2.10	113.48	109.70
25	B	607	CLA	CMB-C2B-C3B	2.10	131.49	126.55
32	d	410	LMG	O7-C10-O9	-2.10	118.80	123.70
25	c	504	CLA	CHD-C1D-ND	-2.10	121.85	124.80
25	c	507	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
32	c	520	LMG	O8-C28-O10	-2.10	118.38	123.63
25	C	504	CLA	CHC-C1C-NC	2.10	127.47	124.31
25	d	403	CLA	CHD-C1D-ND	-2.10	121.85	124.80
32	c	522	LMG	C38-C37-C36	-2.10	103.77	114.37
25	c	511	CLA	C1-C2-C3	-2.10	122.76	126.20
29	F	102	SQD	C3-C4-C5	2.10	114.03	110.23
27	d	404	BCR	C3-C4-C5	-2.09	110.32	114.06
30	H	103	DGD	C4E-C3E-C2E	-2.09	107.15	110.83
25	A	610	CLA	C3B-C4B-NB	-2.09	108.66	110.53
25	d	402	CLA	C4-C3-C5	2.09	118.86	115.23
25	a	607	CLA	CHC-C4B-NB	2.09	127.19	124.05
32	b	620	LMG	O6-C5-C6	2.09	111.63	106.44
25	b	613	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
25	H	101	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	B	615	CLA	CMB-C2B-C3B	2.09	131.47	126.55
25	C	506	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	b	608	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
25	C	506	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
25	C	504	CLA	C4-C3-C5	2.09	118.85	115.23
25	c	504	CLA	C1-C2-C3	-2.09	122.78	126.20
25	b	608	CLA	CHB-C4A-NA	2.09	127.41	124.40
30	C	516	DGD	O2D-C2D-C1D	-2.09	105.10	110.08
25	C	510	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
31	B	625	STE	C3-C2-C1	-2.09	109.07	114.51
25	C	504	CLA	C1-C2-C3	-2.08	122.78	126.20
30	a	616	DGD	C7B-C6B-C5B	-2.08	103.83	114.37
25	C	504	CLA	CMB-C2B-C3B	2.08	131.45	126.55
25	d	403	CLA	CHA-C1A-NA	-2.08	121.68	126.39
31	c	523	STE	O2-C1-C2	2.08	120.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	514	BCR	C7-C8-C9	-2.08	123.16	126.23
29	A	614	SQD	O8-S-C6	2.08	109.99	105.97
25	c	504	CLA	C6-C7-C8	-2.08	109.05	115.97
25	b	612	CLA	CHA-C1A-NA	-2.08	121.68	126.39
25	B	608	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	B	613	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
27	H	102	BCR	C35-C13-C14	-2.08	119.45	122.82
25	d	402	CLA	O2D-CGD-CBD	2.08	114.86	111.23
25	B	602	CLA	CHA-C1A-NA	-2.07	121.69	126.39
30	H	103	DGD	C8B-C7B-C6B	-2.07	103.88	114.37
32	c	524	LMG	C40-C39-C38	-2.07	103.88	114.37
25	b	604	CLA	C4-C3-C5	2.07	118.83	115.23
29	l	101	SQD	O5-C1-C2	-2.07	106.11	110.37
30	h	102	DGD	CAB-C9B-C8B	-2.07	103.90	114.37
30	c	517	DGD	O6E-C5E-C4E	2.07	113.43	109.70
30	c	519	DGD	C7A-C6A-C5A	-2.07	103.90	114.37
25	C	506	CLA	CHA-C4D-ND	2.07	136.82	132.55
27	b	617	BCR	C30-C25-C26	-2.07	119.81	122.64
28	a	612	PL9	C20-C19-C21	2.07	118.82	115.23
27	K	101	BCR	C35-C13-C14	-2.07	119.47	122.82
32	c	524	LMG	C38-C37-C36	-2.07	103.92	114.37
25	b	602	CLA	C1-C2-C3	-2.07	122.81	126.20
25	A	606	CLA	C11-C12-C13	-2.07	109.10	115.97
25	B	603	CLA	CGD-CBD-CAD	-2.07	104.16	110.85
25	A	606	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	h	101	CLA	O2D-CGD-CBD	2.06	114.84	111.23
26	A	609	PHO	C3D-C4D-ND	2.06	110.35	107.71
32	C	515	LMG	O5-C6-C5	-2.06	104.31	111.33
26	A	609	PHO	C3B-C4B-NB	-2.06	106.12	107.46
30	c	517	DGD	C5B-C4B-C3B	-2.06	103.94	114.37
25	B	611	CLA	O1D-CGD-CBD	2.06	128.58	124.52
32	d	409	LMG	C40-C39-C38	-2.06	103.95	114.37
25	c	504	CLA	CHD-C4C-NC	2.06	127.43	124.23
25	b	615	CLA	O1D-CGD-CBD	2.06	128.58	124.52
25	B	603	CLA	C11-C10-C8	-2.06	109.12	115.97
28	D	405	PL9	O1-C4-C3	-2.06	118.56	120.73
25	b	606	CLA	C4-C3-C5	2.06	118.80	115.23
25	C	513	CLA	CHD-C1D-C2D	2.06	129.76	125.49
25	c	507	CLA	CHA-C1A-NA	-2.06	121.74	126.39
25	B	607	CLA	CHA-C1A-NA	-2.06	121.74	126.39
25	B	603	CLA	CHA-C4D-ND	2.06	136.79	132.55
32	c	522	LMG	C6-C5-C4	-2.05	107.98	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	CHB-C4A-NA	2.05	127.36	124.40
25	d	403	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
25	B	611	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	B	608	CLA	CHC-C4B-NB	2.05	127.12	124.05
33	B	622	LHG	O3-P-O5	-2.05	100.82	108.94
30	c	519	DGD	O3E-C3E-C2E	-2.05	105.55	110.38
30	c	518	DGD	O5D-C6D-C5D	-2.05	104.81	109.42
25	b	613	CLA	CED-O2D-CGD	2.05	120.56	115.92
25	D	403	CLA	O2D-CGD-CBD	2.05	114.81	111.23
25	B	608	CLA	C3B-C4B-NB	-2.05	108.70	110.53
32	c	522	LMG	C42-C41-C40	-2.05	104.02	114.37
33	D	407	LHG	C29-C28-C27	-2.05	104.02	114.37
27	a	611	BCR	C2-C1-C6	2.04	113.41	110.44
25	b	601	CLA	C11-C12-C13	-2.04	109.17	115.97
30	A	616	DGD	O3G-C3G-C2G	-2.04	105.85	110.82
25	b	611	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
29	a	614	SQD	O4-C4-C3	-2.04	105.56	110.38
32	c	522	LMG	O2-C2-C1	-2.04	105.21	110.08
25	c	504	CLA	O1A-CGA-CBA	2.04	131.76	123.78
27	b	618	BCR	C37-C22-C21	-2.04	119.51	122.82
25	B	606	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
32	c	522	LMG	O7-C10-O9	-2.04	118.94	123.70
25	b	602	CLA	CHD-C1D-C2D	2.04	129.73	125.49
33	D	408	LHG	C29-C28-C27	-2.04	104.07	114.37
28	D	405	PL9	C8-C7-C3	2.04	117.30	112.03
30	C	518	DGD	O6E-C5E-C4E	2.04	113.37	109.70
29	A	614	SQD	O6-C44-C45	-2.04	105.86	110.82
27	B	616	BCR	C24-C23-C22	-2.04	123.22	126.23
30	H	103	DGD	C7B-C6B-C5B	-2.04	104.07	114.37
32	m	101	LMG	C1-C2-C3	-2.04	105.73	110.01
30	A	616	DGD	CAB-C9B-C8B	-2.04	104.08	114.37
28	d	405	PL9	C36-C34-C33	-2.04	116.60	121.17
27	k	101	BCR	C38-C26-C25	-2.04	122.26	124.48
25	B	606	CLA	CHB-C4A-NA	2.04	127.34	124.40
32	m	101	LMG	C38-C37-C36	-2.04	104.08	114.37
33	D	407	LHG	O8-C6-C5	-2.03	102.53	108.40
25	C	508	CLA	C3C-C4C-NC	-2.03	107.83	110.43
25	C	507	CLA	O1D-CGD-CBD	2.03	128.53	124.52
25	c	502	CLA	O1D-CGD-CBD	2.03	128.53	124.52
27	K	101	BCR	C3-C4-C5	-2.03	110.43	114.06
25	c	501	CLA	C2D-C1D-ND	-2.03	108.11	110.13
32	C	519	LMG	O2-C2-C1	-2.03	105.23	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	502	CLA	CHB-C4A-NA	2.03	127.33	124.40
33	d	407	LHG	C27-C26-C25	-2.03	104.10	114.37
25	c	510	CLA	O1D-CGD-CBD	2.03	128.52	124.52
33	d	406	LHG	C27-C26-C25	-2.03	104.11	114.37
25	c	502	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	b	603	CLA	CAA-CBA-CGA	-2.03	107.44	113.21
27	t	101	BCR	C35-C13-C12	2.03	121.19	118.09
25	A	606	CLA	CAA-CBA-CGA	-2.03	107.45	113.21
25	C	506	CLA	CMB-C2B-C3B	2.03	131.32	126.55
25	C	502	CLA	C4D-CHA-C1A	2.03	123.66	121.24
25	b	609	CLA	CHB-C4A-NA	2.03	127.32	124.40
25	h	101	CLA	CHD-C1D-C2D	2.03	129.70	125.49
28	A	612	PL9	C35-C34-C36	2.03	118.74	115.23
25	a	613	CLA	CHB-C1B-NB	2.02	127.09	124.05
25	d	403	CLA	CHB-C1B-NB	2.02	127.09	124.05
25	b	603	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
30	C	516	DGD	O3D-C3D-C4D	-2.02	105.61	110.38
25	C	504	CLA	CHA-C1A-NA	-2.02	121.82	126.39
27	x	101	BCR	C11-C10-C9	-2.02	124.45	127.28
31	m	102	STE	O2-C1-O1	-2.02	118.14	123.33
25	c	503	CLA	CHD-C1D-ND	-2.02	121.96	124.80
25	c	511	CLA	C2A-C1A-CHA	2.02	127.37	123.87
25	C	509	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
29	A	614	SQD	O2-C2-C1	2.02	114.88	110.08
32	C	515	LMG	O6-C1-O1	-2.01	105.28	110.04
25	b	612	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
25	C	501	CLA	CHD-C1D-C2D	2.01	129.68	125.49
28	a	612	PL9	C35-C34-C36	2.01	118.72	115.23
28	D	405	PL9	O2-C1-C2	-2.01	117.25	121.83
25	C	505	CLA	O2D-CGD-CBD	2.01	114.75	111.23
29	L	101	SQD	O5-C1-C2	-2.01	106.24	110.37
25	B	603	CLA	CHA-C1A-NA	-2.01	121.84	126.39
32	m	101	LMG	C6-C5-C4	-2.01	108.09	113.02
25	B	613	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
28	A	612	PL9	C42-C43-C44	-2.01	123.03	127.62
30	h	102	DGD	O5D-C6D-C5D	-2.01	104.89	109.42
25	b	614	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
27	D	404	BCR	C2-C3-C4	-2.01	106.86	111.28
25	C	505	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
30	C	518	DGD	O6E-C1E-O5D	-2.01	105.30	110.04
27	H	102	BCR	C1-C6-C5	-2.01	119.89	122.64
30	C	518	DGD	C5B-C4B-C3B	-2.01	104.23	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	612	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
25	C	512	CLA	CHA-C1A-NA	-2.00	121.85	126.39
33	d	406	LHG	C18-C17-C16	-2.00	104.24	114.37
25	A	610	CLA	C3D-C4D-ND	2.00	113.24	109.99
27	d	404	BCR	C2-C1-C6	2.00	113.35	110.44
33	e	102	LHG	C18-C17-C16	-2.00	104.24	114.37
30	A	616	DGD	O5D-C1E-C2E	2.00	111.31	108.27
25	b	603	CLA	O2D-CGD-CBD	2.00	114.73	111.23
29	A	614	SQD	C9-C8-C7	-2.00	106.36	113.69

All (64) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
25	D	402	CLA	ND
25	H	101	CLA	ND
25	a	607	CLA	ND
25	a	608	CLA	ND
25	a	610	CLA	ND
25	a	613	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	c	501	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	402	CLA	ND
25	d	403	CLA	ND
25	h	101	CLA	ND

All (1874) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C4B-C3B-CAB-CBB
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C14-C13-C15-C16
25	B	614	CLA	C2B-C3B-CAB-CBB
25	B	614	CLA	C4B-C3B-CAB-CBB
25	C	504	CLA	C4-C3-C5-C6
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C4B-C3B-CAB-CBB
25	H	101	CLA	C1A-C2A-CAA-CBA
25	H	101	CLA	C6-C7-C8-C9
25	a	608	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	C4-C3-C5-C6
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
25	c	506	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C3A-C2A-CAA-CBA
25	c	507	CLA	C2B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
25	c	513	CLA	CAD-CBD-CGD-O1D
25	c	513	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CBD-CGD-O2D-CED
25	h	101	CLA	C1A-C2A-CAA-CBA
25	h	101	CLA	C3A-C2A-CAA-CBA
25	h	101	CLA	C2B-C3B-CAB-CBB
25	h	101	CLA	C4B-C3B-CAB-CBB
27	B	618	BCR	C35-C13-C14-C15
27	B	618	BCR	C20-C21-C22-C37
27	C	514	BCR	C11-C12-C13-C14
27	D	404	BCR	C37-C22-C23-C24
27	D	404	BCR	C22-C23-C24-C25
27	K	101	BCR	C7-C8-C9-C34
27	K	101	BCR	C11-C10-C9-C8
27	K	101	BCR	C16-C17-C18-C36
27	T	101	BCR	C7-C8-C9-C10
27	T	101	BCR	C7-C8-C9-C34
27	b	618	BCR	C11-C12-C13-C14
27	b	618	BCR	C11-C12-C13-C35
27	b	618	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	c	515	BCR	C7-C8-C9-C10
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C17-C18-C19-C20
28	A	612	PL9	C12-C13-C14-C15
28	A	612	PL9	C12-C13-C14-C16
28	A	612	PL9	C17-C18-C19-C21
28	A	612	PL9	C22-C23-C24-C26
28	A	612	PL9	C32-C33-C34-C35
28	A	612	PL9	C32-C33-C34-C36
28	A	612	PL9	C35-C34-C36-C37
28	A	612	PL9	C37-C38-C39-C40
28	A	612	PL9	C45-C44-C46-C47
28	D	405	PL9	C32-C33-C34-C36
28	a	612	PL9	C22-C23-C24-C26
28	a	612	PL9	C27-C28-C29-C31
28	a	612	PL9	C32-C33-C34-C36
28	a	612	PL9	C42-C43-C44-C45
28	d	405	PL9	C27-C28-C29-C31
28	d	405	PL9	C40-C39-C41-C42
29	A	615	SQD	O47-C45-C46-O48
29	F	102	SQD	C45-C44-O6-C1
29	F	102	SQD	O10-C23-O48-C46
29	F	102	SQD	C24-C23-O48-C46
29	L	101	SQD	C8-C7-O47-C45
29	L	101	SQD	O10-C23-O48-C46
29	L	101	SQD	C24-C23-O48-C46
29	a	614	SQD	O6-C44-C45-O47
29	a	615	SQD	O47-C45-C46-O48
29	a	615	SQD	O49-C7-O47-C45
29	a	615	SQD	C8-C7-O47-C45
29	f	101	SQD	O5-C1-O6-C44
29	f	101	SQD	C8-C7-O47-C45
29	f	101	SQD	C5-C6-S-O7
29	l	101	SQD	C2-C1-O6-C44
29	l	101	SQD	O5-C1-O6-C44
29	l	101	SQD	O6-C44-C45-O47
29	l	101	SQD	O49-C7-O47-C45
29	l	101	SQD	C8-C7-O47-C45
30	A	616	DGD	O1B-C1B-O2G-C2G
30	a	616	DGD	C1G-C2G-C3G-O3G
30	a	616	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
32	C	515	LMG	O6-C1-O1-C7
32	C	515	LMG	O9-C10-O7-C8
32	D	409	LMG	O1-C7-C8-C9
32	D	409	LMG	O1-C7-C8-O7
32	c	522	LMG	C11-C10-O7-C8
32	c	524	LMG	C2-C1-O1-C7
32	c	524	LMG	O6-C1-O1-C7
32	c	524	LMG	C29-C28-O8-C9
32	m	101	LMG	O6-C1-O1-C7
33	B	621	LHG	C4-O6-P-O3
33	B	621	LHG	C4-O6-P-O4
33	B	622	LHG	O1-C1-C2-C3
33	B	622	LHG	C3-O3-P-O4
33	D	407	LHG	O1-C1-C2-C3
33	D	407	LHG	C3-O3-P-O4
33	D	407	LHG	C3-O3-P-O6
33	D	407	LHG	C4-O6-P-O3
33	D	407	LHG	C4-O6-P-O4
33	D	408	LHG	C1-C2-C3-O3
33	D	408	LHG	O2-C2-C3-O3
33	D	408	LHG	C3-O3-P-O5
33	D	408	LHG	C3-O3-P-O6
33	E	101	LHG	O1-C1-C2-C3
33	E	101	LHG	C4-O6-P-O3
33	E	101	LHG	C4-O6-P-O4
33	E	101	LHG	C4-O6-P-O5
33	d	406	LHG	C3-O3-P-O4
33	d	406	LHG	C3-O3-P-O6
33	d	407	LHG	O1-C1-C2-C3
33	d	407	LHG	C4-O6-P-O3
33	d	407	LHG	C4-O6-P-O4
33	d	407	LHG	C4-O6-P-O5
33	d	408	LHG	C4-O6-P-O4
33	e	102	LHG	O1-C1-C2-C3
33	e	102	LHG	C1-C2-C3-O3
33	e	102	LHG	C3-O3-P-O4
33	e	102	LHG	C3-O3-P-O5
33	e	102	LHG	C3-O3-P-O6
33	e	102	LHG	O10-C23-O8-C6
33	e	102	LHG	C24-C23-O8-C6
33	l	102	LHG	C4-O6-P-O3
36	V	201	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	V	201	HEC	C4B-C3B-CAB-CBB
36	V	201	HEC	C2C-C3C-CAC-CBC
36	V	201	HEC	C4C-C3C-CAC-CBC
36	v	201	HEC	C2B-C3B-CAB-CBB
36	v	201	HEC	C4B-C3B-CAB-CBB
36	v	201	HEC	C2C-C3C-CAC-CBC
36	v	201	HEC	C4C-C3C-CAC-CBC
25	h	101	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	h	101	CLA	CBD-CGD-O2D-CED
32	c	524	LMG	O10-C28-O8-C9
28	a	612	PL9	C47-C48-C49-C51
32	c	522	LMG	C29-C28-O8-C9
25	H	101	CLA	O1A-CGA-O2A-C1
29	f	101	SQD	O10-C23-O48-C46
32	M	101	LMG	O10-C28-O8-C9
32	c	522	LMG	O10-C28-O8-C9
25	c	513	CLA	O1D-CGD-O2D-CED
29	L	101	SQD	O49-C7-O47-C45
29	f	101	SQD	O49-C7-O47-C45
25	B	615	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	H	101	CLA	CBA-CGA-O2A-C1
29	a	615	SQD	C24-C23-O48-C46
29	f	101	SQD	C24-C23-O48-C46
32	c	520	LMG	C11-C10-O7-C8
25	C	501	CLA	CBD-CGD-O2D-CED
25	C	513	CLA	CBD-CGD-O2D-CED
25	a	608	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
30	A	616	DGD	C2B-C1B-O2G-C2G
32	C	515	LMG	C11-C10-O7-C8
32	D	409	LMG	C11-C10-O7-C8
25	b	613	CLA	C4-C3-C5-C6
28	A	612	PL9	C25-C24-C26-C27
28	A	612	PL9	C40-C39-C41-C42
25	C	504	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	613	CLA	C2-C3-C5-C6
28	A	612	PL9	C18-C19-C21-C22
28	A	612	PL9	C43-C44-C46-C47
28	D	405	PL9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
28	a	612	PL9	C28-C29-C31-C32
28	d	405	PL9	C38-C39-C41-C42
25	c	512	CLA	C2A-CAA-CBA-CGA
28	D	405	PL9	C47-C48-C49-C51
25	h	101	CLA	C3-C5-C6-C7
32	M	101	LMG	C29-C28-O8-C9
32	d	410	LMG	C10-C11-C12-C13
28	a	612	PL9	C22-C23-C24-C25
28	A	612	PL9	C37-C38-C39-C41
28	a	612	PL9	C42-C43-C44-C46
29	a	615	SQD	O10-C23-O48-C46
32	D	409	LMG	O9-C10-O7-C8
32	b	620	LMG	O9-C10-O7-C8
32	c	522	LMG	O9-C10-O7-C8
28	D	405	PL9	C47-C48-C49-C50
25	b	606	CLA	CBD-CGD-O2D-CED
33	D	407	LHG	O2-C2-C3-O3
25	c	511	CLA	O1D-CGD-O2D-CED
30	A	616	DGD	O6E-C5E-C6E-O5E
32	C	519	LMG	C11-C10-O7-C8
32	b	620	LMG	C11-C10-O7-C8
28	d	405	PL9	C47-C48-C49-C51
32	c	524	LMG	C4-C5-C6-O5
25	b	606	CLA	C4-C3-C5-C6
28	a	612	PL9	C40-C39-C41-C42
25	b	606	CLA	C2-C3-C5-C6
28	A	612	PL9	C38-C39-C41-C42
28	A	612	PL9	C39-C41-C42-C43
28	A	612	PL9	C44-C46-C47-C48
30	A	616	DGD	C4E-C5E-C6E-O5E
25	b	603	CLA	C13-C15-C16-C17
32	b	620	LMG	O10-C28-O8-C9
32	m	101	LMG	C29-C28-O8-C9
25	C	511	CLA	CBD-CGD-O2D-CED
25	D	403	CLA	CBD-CGD-O2D-CED
25	H	101	CLA	CBD-CGD-O2D-CED
33	d	407	LHG	C28-C29-C30-C31
28	a	612	PL9	C32-C33-C34-C35
33	E	101	LHG	O10-C23-O8-C6
32	C	515	LMG	O6-C5-C6-O5
28	a	612	PL9	C37-C38-C39-C41
33	d	406	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	a	612	PL9	C47-C48-C49-C50
25	H	101	CLA	C3-C5-C6-C7
33	E	101	LHG	C24-C23-O8-C6
32	c	520	LMG	O6-C5-C6-O5
32	c	524	LMG	O6-C5-C6-O5
25	B	611	CLA	CBD-CGD-O2D-CED
31	b	622	STE	C4-C5-C6-C7
25	c	507	CLA	C4-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
28	a	612	PL9	C38-C39-C41-C42
25	A	607	CLA	C14-C13-C15-C16
25	B	609	CLA	C14-C13-C15-C16
25	B	612	CLA	C11-C12-C13-C14
25	B	613	CLA	C11-C12-C13-C14
25	B	614	CLA	C11-C10-C8-C9
25	C	503	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	615	CLA	C6-C7-C8-C9
25	c	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	512	CLA	C6-C7-C8-C9
25	d	403	CLA	C11-C12-C13-C14
25	h	101	CLA	C11-C10-C8-C9
25	h	101	CLA	C14-C13-C15-C16
29	a	614	SQD	C11-C12-C13-C14
31	H	104	STE	C11-C12-C13-C14
29	f	101	SQD	C2-C1-O6-C44
32	m	101	LMG	C2-C1-O1-C7
33	e	102	LHG	O2-C2-C3-O3
25	b	615	CLA	O1D-CGD-O2D-CED
27	B	616	BCR	C7-C8-C9-C34
27	B	617	BCR	C7-C8-C9-C34
27	B	618	BCR	C37-C22-C23-C24
27	C	514	BCR	C11-C12-C13-C35
27	K	102	BCR	C11-C12-C13-C35
27	K	102	BCR	C37-C22-C23-C24
27	K	103	BCR	C37-C22-C23-C24
27	b	617	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	c	515	BCR	C7-C8-C9-C34
27	c	515	BCR	C11-C12-C13-C35
27	t	101	BCR	C7-C8-C9-C34
27	x	101	BCR	C7-C8-C9-C34
25	b	605	CLA	C2A-CAA-CBA-CGA
33	E	101	LHG	C27-C28-C29-C30
30	a	616	DGD	O1A-C1A-O1G-C1G
25	C	509	CLA	C3-C5-C6-C7
32	C	515	LMG	C4-C5-C6-O5
30	A	616	DGD	O2G-C2G-C3G-O3G
25	b	604	CLA	C5-C6-C7-C8
29	A	614	SQD	C23-C24-C25-C26
31	B	623	STE	C4-C5-C6-C7
25	a	608	CLA	O1D-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	C8-C10-C11-C12
25	C	507	CLA	C13-C15-C16-C17
25	C	512	CLA	C5-C6-C7-C8
25	c	509	CLA	C13-C15-C16-C17
29	a	614	SQD	C23-C24-C25-C26
32	d	410	LMG	C28-C29-C30-C31
33	E	101	LHG	C23-C24-C25-C26
28	d	405	PL9	C42-C43-C44-C46
25	B	610	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	D	403	CLA	C11-C10-C8-C7
25	b	608	CLA	C11-C12-C13-C15
25	b	614	CLA	C11-C12-C13-C15
25	c	512	CLA	CBA-CGA-O2A-C1
32	c	524	LMG	C15-C16-C17-C18
31	B	624	STE	C1-C2-C3-C4
28	A	612	PL9	C34-C36-C37-C38
25	C	506	CLA	C13-C15-C16-C17
25	a	610	CLA	C10-C11-C12-C13
32	c	522	LMG	O6-C5-C6-O5
30	a	616	DGD	C1A-C2A-C3A-C4A
32	D	409	LMG	C28-C29-C30-C31
25	B	601	CLA	C13-C15-C16-C17
25	C	513	CLA	C15-C16-C17-C18
25	H	101	CLA	C13-C15-C16-C17
25	b	604	CLA	C10-C11-C12-C13
25	b	606	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C2A-CAA-CBA-CGA
25	h	101	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C5-C6-C7-C8
25	C	506	CLA	C8-C10-C11-C12
25	b	602	CLA	C5-C6-C7-C8
25	b	611	CLA	C15-C16-C17-C18
25	b	614	CLA	C15-C16-C17-C18
25	c	512	CLA	C15-C16-C17-C18
29	A	614	SQD	C7-C8-C9-C10
29	A	615	SQD	C7-C8-C9-C10
29	L	101	SQD	C23-C24-C25-C26
32	D	409	LMG	C10-C11-C12-C13
32	c	520	LMG	C28-C29-C30-C31
32	c	522	LMG	C10-C11-C12-C13
33	d	406	LHG	C23-C24-C25-C26
33	l	102	LHG	C23-C24-C25-C26
25	C	513	CLA	O1D-CGD-O2D-CED
30	C	518	DGD	O1A-C1A-O1G-C1G
29	l	101	SQD	C11-C10-C9-C8
25	B	612	CLA	C5-C6-C7-C8
25	C	503	CLA	C5-C6-C7-C8
25	C	507	CLA	C10-C11-C12-C13
25	C	509	CLA	C5-C6-C7-C8
25	C	509	CLA	C8-C10-C11-C12
25	c	509	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
33	d	406	LHG	O2-C2-C3-O3
32	b	620	LMG	C29-C28-O8-C9
29	A	615	SQD	C23-C24-C25-C26
33	d	406	LHG	C7-C8-C9-C10
25	B	612	CLA	C8-C10-C11-C12
25	C	505	CLA	C5-C6-C7-C8
25	C	501	CLA	O1D-CGD-O2D-CED
25	A	613	CLA	C15-C16-C17-C18
25	B	606	CLA	C10-C11-C12-C13
25	h	101	CLA	C13-C15-C16-C17
32	b	620	LMG	C28-C29-C30-C31
25	b	606	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	C15-C16-C17-C18
25	b	601	CLA	CBD-CGD-O2D-CED
31	T	102	STE	C5-C6-C7-C8
32	m	101	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7
25	b	602	CLA	C13-C15-C16-C17
33	e	102	LHG	C23-C24-C25-C26
32	C	519	LMG	O9-C10-O7-C8
33	d	406	LHG	C1-C2-C3-O3
32	C	519	LMG	C29-C28-O8-C9
25	B	610	CLA	C8-C10-C11-C12
25	B	610	CLA	C13-C15-C16-C17
25	B	613	CLA	C5-C6-C7-C8
25	C	506	CLA	C15-C16-C17-C18
25	a	607	CLA	C15-C16-C17-C18
25	a	608	CLA	C8-C10-C11-C12
25	b	613	CLA	C13-C15-C16-C17
25	B	609	CLA	C15-C16-C17-C18
25	C	508	CLA	C10-C11-C12-C13
25	c	503	CLA	C5-C6-C7-C8
25	b	610	CLA	C8-C10-C11-C12
25	c	505	CLA	C15-C16-C17-C18
25	c	512	CLA	C8-C10-C11-C12
32	c	520	LMG	O9-C10-O7-C8
25	B	605	CLA	C13-C15-C16-C17
25	b	606	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17
25	C	510	CLA	CBD-CGD-O2D-CED
30	a	616	DGD	O1B-C1B-O2G-C2G
30	c	518	DGD	C2E-C1E-O5D-C6D
32	C	519	LMG	C2-C1-O1-C7
25	b	613	CLA	C8-C10-C11-C12
29	l	101	SQD	C29-C30-C31-C32
30	a	616	DGD	C2A-C1A-O1G-C1G
25	c	510	CLA	C15-C16-C17-C18
25	c	512	CLA	O1A-CGA-O2A-C1
33	d	408	LHG	C33-C34-C35-C36
27	B	616	BCR	C16-C17-C18-C36
27	B	616	BCR	C20-C21-C22-C37
27	B	617	BCR	C20-C21-C22-C37
27	D	404	BCR	C20-C21-C22-C37
27	K	101	BCR	C35-C13-C14-C15
27	K	102	BCR	C20-C21-C22-C37
27	T	101	BCR	C20-C21-C22-C37
27	c	514	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
27	c	515	BCR	C35-C13-C14-C15
27	c	516	BCR	C20-C21-C22-C37
27	d	404	BCR	C16-C17-C18-C36
27	t	101	BCR	C35-C13-C14-C15
25	B	605	CLA	C15-C16-C17-C18
27	H	102	BCR	C11-C12-C13-C35
27	K	102	BCR	C7-C8-C9-C34
27	d	404	BCR	C37-C22-C23-C24
27	x	101	BCR	C11-C12-C13-C35
31	b	622	STE	C2-C3-C4-C5
33	d	406	LHG	O1-C1-C2-C3
33	d	408	LHG	O1-C1-C2-C3
31	B	623	STE	C1-C2-C3-C4
29	L	101	SQD	C46-C45-O47-C7
32	D	409	LMG	C9-C8-O7-C10
25	A	613	CLA	C16-C17-C18-C20
25	B	604	CLA	C16-C17-C18-C19
25	B	613	CLA	C16-C17-C18-C20
25	b	613	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C20
25	c	512	CLA	C13-C15-C16-C17
27	B	618	BCR	C12-C13-C14-C15
27	K	101	BCR	C16-C17-C18-C19
27	b	618	BCR	C12-C13-C14-C15
27	c	514	BCR	C12-C13-C14-C15
27	d	404	BCR	C16-C17-C18-C19
27	x	101	BCR	C11-C10-C9-C8
29	L	101	SQD	O5-C1-O6-C44
30	c	518	DGD	O6E-C1E-O5D-C6D
32	C	519	LMG	O6-C1-O1-C7
30	c	519	DGD	C2A-C1A-O1G-C1G
25	c	503	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
31	J	101	STE	C1-C2-C3-C4
25	B	603	CLA	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C19
25	b	603	CLA	C15-C16-C17-C18
25	b	614	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	f	101	SQD	C32-C33-C34-C35
31	H	104	STE	C5-C6-C7-C8
32	C	519	LMG	C12-C13-C14-C15
30	C	517	DGD	C5A-C6A-C7A-C8A
30	C	517	DGD	C8A-C9A-CAA-CBA
31	H	104	STE	C7-C8-C9-C10
31	c	523	STE	C5-C6-C7-C8
32	C	519	LMG	C17-C18-C19-C20
32	M	101	LMG	C29-C30-C31-C32
32	c	522	LMG	C39-C40-C41-C42
33	B	621	LHG	C27-C28-C29-C30
33	D	408	LHG	C33-C34-C35-C36
33	d	406	LHG	C17-C18-C19-C20
30	C	516	DGD	O6E-C5E-C6E-O5E
31	d	411	STE	C10-C11-C12-C13
32	b	620	LMG	C17-C18-C19-C20
33	B	621	LHG	C31-C32-C33-C34
33	D	408	LHG	C11-C12-C13-C14
29	A	614	SQD	C16-C17-C18-C19
29	L	101	SQD	C26-C27-C28-C29
29	a	614	SQD	C17-C18-C19-C20
30	A	616	DGD	CEA-CFA-CGA-CHA
30	c	517	DGD	C2A-C3A-C4A-C5A
30	c	519	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	C2B-C3B-C4B-C5B
30	h	102	DGD	C6B-C7B-C8B-C9B
31	H	104	STE	C2-C3-C4-C5
31	T	103	STE	C11-C12-C13-C14
31	c	523	STE	C3-C4-C5-C6
31	x	102	STE	C4-C5-C6-C7
32	C	519	LMG	C30-C31-C32-C33
32	D	406	LMG	C30-C31-C32-C33
32	M	101	LMG	C13-C14-C15-C16
33	D	408	LHG	C9-C10-C11-C12
33	D	408	LHG	C27-C28-C29-C30
33	E	101	LHG	C18-C19-C20-C21
33	d	407	LHG	C33-C34-C35-C36
33	e	102	LHG	O1-C1-C2-O2
29	F	102	SQD	C30-C31-C32-C33
29	l	101	SQD	C11-C12-C13-C14
30	c	517	DGD	C7B-C8B-C9B-CAB
31	B	624	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
32	M	101	LMG	C35-C36-C37-C38
32	b	620	LMG	C34-C35-C36-C37
32	d	409	LMG	C37-C38-C39-C40
33	D	408	LHG	C32-C33-C34-C35
33	E	101	LHG	C26-C27-C28-C29
33	E	101	LHG	C30-C31-C32-C33
25	A	607	CLA	C4B-C3B-CAB-CBB
25	b	609	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
31	c	521	STE	C1-C2-C3-C4
32	m	101	LMG	C10-C11-C12-C13
33	D	408	LHG	C29-C30-C31-C32
32	b	620	LMG	O6-C5-C6-O5
25	B	603	CLA	C16-C17-C18-C19
25	B	604	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C20
29	A	614	SQD	C27-C28-C29-C30
30	c	517	DGD	C9B-CAB-CBB-CCB
31	x	102	STE	C11-C12-C13-C14
33	e	102	LHG	C11-C10-C9-C8
25	b	601	CLA	C15-C16-C17-C18
31	d	411	STE	C3-C4-C5-C6
31	d	411	STE	C5-C6-C7-C8
33	e	102	LHG	C27-C28-C29-C30
25	A	607	CLA	C6-C7-C8-C10
25	B	605	CLA	C6-C7-C8-C10
25	B	605	CLA	C12-C13-C15-C16
25	c	510	CLA	C11-C10-C8-C7
29	f	101	SQD	C28-C29-C30-C31
29	f	101	SQD	C30-C31-C32-C33
30	C	517	DGD	C3B-C4B-C5B-C6B
30	c	517	DGD	C5B-C6B-C7B-C8B
31	t	102	STE	C11-C10-C9-C8
31	x	102	STE	C2-C3-C4-C5
32	M	101	LMG	C32-C33-C34-C35
33	d	406	LHG	C11-C10-C9-C8
28	d	405	PL9	C47-C48-C49-C50
33	D	408	LHG	C7-C8-C9-C10
25	B	613	CLA	C8-C10-C11-C12
25	b	609	CLA	C13-C15-C16-C17
25	c	504	CLA	C8-C10-C11-C12
29	A	615	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	a	614	SQD	C10-C11-C12-C13
29	l	101	SQD	C33-C34-C35-C36
30	A	616	DGD	CBA-CCA-CDA-CEA
30	C	518	DGD	CBB-CCB-CDB-CEB
30	c	519	DGD	C3A-C4A-C5A-C6A
31	T	103	STE	C9-C10-C11-C12
32	c	524	LMG	C19-C20-C21-C22
32	c	524	LMG	C29-C30-C31-C32
32	d	409	LMG	C34-C35-C36-C37
25	c	512	CLA	C3A-C2A-CAA-CBA
26	d	401	PHO	C3A-C2A-CAA-CBA
31	x	102	STE	C3-C4-C5-C6
32	c	522	LMG	C36-C37-C38-C39
33	B	622	LHG	C28-C29-C30-C31
29	A	615	SQD	C26-C27-C28-C29
33	D	408	LHG	C30-C31-C32-C33
25	b	613	CLA	C5-C6-C7-C8
25	C	511	CLA	O1D-CGD-O2D-CED
29	l	101	SQD	C7-C8-C9-C10
32	C	515	LMG	C16-C17-C18-C19
27	k	101	BCR	C19-C20-C21-C22
25	B	613	CLA	C16-C17-C18-C19
25	b	606	CLA	C16-C17-C18-C20
30	A	616	DGD	O6D-C5D-C6D-O5D
30	c	517	DGD	C3A-C4A-C5A-C6A
32	b	620	LMG	C40-C41-C42-C43
33	l	102	LHG	C14-C15-C16-C17
33	l	102	LHG	C25-C26-C27-C28
25	b	610	CLA	C13-C15-C16-C17
30	c	517	DGD	CAB-CBB-CCB-CDB
32	B	620	LMG	C33-C34-C35-C36
25	D	403	CLA	O1D-CGD-O2D-CED
30	C	518	DGD	C2A-C1A-O1G-C1G
29	a	614	SQD	C29-C30-C31-C32
32	b	620	LMG	C11-C12-C13-C14
33	D	407	LHG	C13-C14-C15-C16
33	E	101	LHG	C32-C33-C34-C35
30	c	518	DGD	C1B-C2B-C3B-C4B
32	C	519	LMG	C28-C29-C30-C31
33	B	621	LHG	C23-C24-C25-C26
29	f	101	SQD	C31-C32-C33-C34
30	C	517	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	H	103	DGD	CCA-CDA-CEA-CFA
30	a	616	DGD	C7B-C8B-C9B-CAB
31	T	102	STE	C6-C7-C8-C9
31	b	619	STE	C6-C7-C8-C9
31	c	521	STE	C9-C10-C11-C12
33	E	101	LHG	C24-C25-C26-C27
33	d	406	LHG	C16-C17-C18-C19
30	A	616	DGD	C2B-C3B-C4B-C5B
30	C	518	DGD	C5A-C6A-C7A-C8A
30	C	518	DGD	C6A-C7A-C8A-C9A
32	b	620	LMG	C16-C17-C18-C19
32	m	101	LMG	C15-C16-C17-C18
33	d	408	LHG	C30-C31-C32-C33
29	A	614	SQD	C14-C15-C16-C17
31	T	103	STE	C13-C14-C15-C16
32	D	406	LMG	C17-C18-C19-C20
32	M	101	LMG	C33-C34-C35-C36
33	D	407	LHG	C32-C33-C34-C35
33	E	101	LHG	C12-C13-C14-C15
30	A	616	DGD	CBB-CCB-CDB-CEB
30	c	518	DGD	CCA-CDA-CEA-CFA
31	H	104	STE	C4-C5-C6-C7
33	B	621	LHG	C12-C13-C14-C15
33	B	622	LHG	C11-C12-C13-C14
33	E	101	LHG	C11-C10-C9-C8
25	b	602	CLA	C16-C17-C18-C20
31	x	102	STE	C1-C2-C3-C4
25	A	607	CLA	C2B-C3B-CAB-CBB
25	B	605	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C2B-C3B-CAB-CBB
25	a	608	CLA	C2B-C3B-CAB-CBB
25	b	604	CLA	C2B-C3B-CAB-CBB
27	D	404	BCR	C23-C24-C25-C30
27	K	102	BCR	C1-C6-C7-C8
27	K	102	BCR	C5-C6-C7-C8
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
30	C	518	DGD	CAB-CBB-CCB-CDB
30	a	616	DGD	C4B-C5B-C6B-C7B
30	h	102	DGD	C3B-C4B-C5B-C6B
30	h	102	DGD	C5B-C6B-C7B-C8B
30	C	516	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
32	B	620	LMG	C36-C37-C38-C39
32	c	520	LMG	C33-C34-C35-C36
33	D	408	LHG	C15-C16-C17-C18
33	d	408	LHG	C25-C26-C27-C28
30	A	616	DGD	CCA-CDA-CEA-CFA
31	T	102	STE	C7-C8-C9-C10
31	c	521	STE	C5-C6-C7-C8
32	B	620	LMG	C31-C32-C33-C34
32	d	410	LMG	C34-C35-C36-C37
33	D	408	LHG	C14-C15-C16-C17
33	l	102	LHG	C32-C33-C34-C35
31	c	523	STE	C2-C3-C4-C5
32	c	524	LMG	O9-C10-O7-C8
28	A	612	PL9	C20-C19-C21-C22
28	D	405	PL9	C35-C34-C36-C37
29	l	101	SQD	C25-C26-C27-C28
31	c	521	STE	C3-C4-C5-C6
27	B	617	BCR	C18-C19-C20-C21
25	B	606	CLA	C5-C6-C7-C8
25	b	601	CLA	C13-C15-C16-C17
28	a	612	PL9	C33-C34-C36-C37
29	a	615	SQD	C14-C15-C16-C17
30	H	103	DGD	CCB-CDB-CEB-CFB
30	a	616	DGD	CEA-CFA-CGA-CHA
30	a	616	DGD	C5B-C6B-C7B-C8B
31	J	101	STE	C5-C6-C7-C8
31	b	622	STE	C13-C14-C15-C16
31	j	101	STE	C2-C3-C4-C5
33	l	102	LHG	C11-C12-C13-C14
25	B	611	CLA	O1D-CGD-O2D-CED
25	B	606	CLA	C11-C12-C13-C14
25	b	605	CLA	C14-C13-C15-C16
31	T	103	STE	C10-C11-C12-C13
32	M	101	LMG	C12-C13-C14-C15
32	c	522	LMG	C14-C15-C16-C17
29	a	614	SQD	C24-C25-C26-C27
29	a	615	SQD	C11-C10-C9-C8
30	C	518	DGD	C2A-C3A-C4A-C5A
32	D	406	LMG	C14-C15-C16-C17
32	d	409	LMG	C36-C37-C38-C39
33	d	406	LHG	C29-C30-C31-C32
30	C	517	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
31	B	624	STE	C7-C8-C9-C10
31	C	521	STE	C3-C4-C5-C6
31	T	103	STE	C7-C8-C9-C10
31	d	411	STE	C9-C10-C11-C12
25	C	509	CLA	C10-C11-C12-C13
31	b	621	STE	C4-C5-C6-C7
31	b	621	STE	C5-C6-C7-C8
29	L	101	SQD	C7-C8-C9-C10
31	B	625	STE	C5-C6-C7-C8
31	d	411	STE	C11-C12-C13-C14
32	C	519	LMG	C32-C33-C34-C35
32	b	620	LMG	C14-C15-C16-C17
32	c	522	LMG	C34-C35-C36-C37
30	A	616	DGD	C2A-C3A-C4A-C5A
30	a	616	DGD	C8B-C9B-CAB-CBB
30	a	616	DGD	CAB-CBB-CCB-CDB
30	c	518	DGD	CBB-CCB-CDB-CEB
31	D	410	STE	C2-C3-C4-C5
32	m	101	LMG	C30-C31-C32-C33
29	l	101	SQD	C24-C23-O48-C46
32	B	620	LMG	C28-C29-C30-C31
31	T	103	STE	C14-C15-C16-C17
32	C	515	LMG	C34-C35-C36-C37
29	A	615	SQD	C14-C15-C16-C17
29	A	615	SQD	C18-C19-C20-C21
29	a	614	SQD	C18-C19-C20-C21
31	l	103	STE	C14-C15-C16-C17
27	C	514	BCR	C7-C8-C9-C34
27	d	404	BCR	C7-C8-C9-C34
33	D	407	LHG	C23-C24-C25-C26
29	a	615	SQD	C10-C11-C12-C13
30	a	616	DGD	CEB-CFB-CGB-CHB
31	c	521	STE	C10-C11-C12-C13
33	d	408	LHG	C27-C28-C29-C30
27	b	616	BCR	C21-C22-C23-C24
33	d	406	LHG	C25-C26-C27-C28
25	B	602	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C19
25	c	506	CLA	C16-C17-C18-C20
33	D	407	LHG	C11-C10-C9-C8
28	A	612	PL9	C23-C24-C26-C27
29	a	614	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
30	a	616	DGD	C3B-C4B-C5B-C6B
33	D	408	LHG	C11-C10-C9-C8
33	E	101	LHG	C15-C16-C17-C18
25	b	607	CLA	C2C-C3C-CAC-CBC
25	C	509	CLA	C13-C15-C16-C17
31	c	521	STE	C11-C12-C13-C14
32	c	522	LMG	C30-C31-C32-C33
32	c	524	LMG	C30-C31-C32-C33
30	C	518	DGD	C3A-C4A-C5A-C6A
31	H	104	STE	C3-C4-C5-C6
32	c	524	LMG	C33-C34-C35-C36
25	B	603	CLA	C3-C5-C6-C7
30	c	517	DGD	O6E-C5E-C6E-O5E
25	b	602	CLA	C8-C10-C11-C12
25	b	615	CLA	C5-C6-C7-C8
29	A	615	SQD	C10-C11-C12-C13
31	C	521	STE	C5-C6-C7-C8
32	B	620	LMG	C32-C33-C34-C35
25	B	605	CLA	C8-C10-C11-C12
25	b	610	CLA	C15-C16-C17-C18
25	b	606	CLA	C16-C17-C18-C19
29	A	615	SQD	C12-C13-C14-C15
33	e	102	LHG	C11-C12-C13-C14
29	a	614	SQD	C27-C28-C29-C30
30	c	519	DGD	CBB-CCB-CDB-CEB
31	a	617	STE	C5-C6-C7-C8
32	c	520	LMG	C38-C39-C40-C41
33	D	407	LHG	C28-C29-C30-C31
33	D	407	LHG	C29-C30-C31-C32
33	d	406	LHG	C32-C33-C34-C35
30	H	103	DGD	C1A-C2A-C3A-C4A
25	h	101	CLA	C8-C10-C11-C12
32	c	520	LMG	C31-C32-C33-C34
33	d	407	LHG	C29-C30-C31-C32
32	C	515	LMG	O1-C7-C8-O7
29	l	101	SQD	C28-C29-C30-C31
30	A	616	DGD	C4B-C5B-C6B-C7B
30	C	516	DGD	CCB-CDB-CEB-CFB
31	C	522	STE	C7-C8-C9-C10
32	D	406	LMG	C35-C36-C37-C38
25	B	611	CLA	C10-C11-C12-C13
25	c	507	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	d	410	LMG	O6-C5-C6-O5
29	L	101	SQD	C13-C14-C15-C16
29	l	101	SQD	C18-C19-C20-C21
31	T	103	STE	C12-C13-C14-C15
33	e	102	LHG	C18-C19-C20-C21
29	a	614	SQD	C15-C16-C17-C18
30	C	517	DGD	C6A-C7A-C8A-C9A
31	B	619	STE	C2-C3-C4-C5
33	d	408	LHG	C32-C33-C34-C35
25	A	613	CLA	C16-C17-C18-C19
25	B	602	CLA	C16-C17-C18-C20
30	C	516	DGD	C6B-C7B-C8B-C9B
31	a	617	STE	C3-C4-C5-C6
31	m	102	STE	C5-C6-C7-C8
32	b	620	LMG	C23-C24-C25-C26
32	c	524	LMG	C12-C13-C14-C15
30	c	517	DGD	C4B-C5B-C6B-C7B
28	d	405	PL9	C43-C44-C46-C47
29	A	615	SQD	C24-C25-C26-C27
29	F	102	SQD	C25-C26-C27-C28
33	B	621	LHG	C15-C16-C17-C18
33	B	621	LHG	C17-C18-C19-C20
33	D	407	LHG	C16-C17-C18-C19
33	E	101	LHG	C11-C12-C13-C14
33	e	102	LHG	C14-C15-C16-C17
25	b	609	CLA	C2A-CAA-CBA-CGA
25	H	101	CLA	O1D-CGD-O2D-CED
29	L	101	SQD	C24-C25-C26-C27
30	c	519	DGD	CAA-CBA-CCA-CDA
33	d	406	LHG	C31-C32-C33-C34
30	c	518	DGD	C7B-C8B-C9B-CAB
25	B	607	CLA	C15-C16-C17-C18
25	B	612	CLA	C10-C11-C12-C13
25	C	508	CLA	C13-C15-C16-C17
25	C	512	CLA	C13-C15-C16-C17
29	a	615	SQD	C30-C31-C32-C33
33	d	407	LHG	C32-C33-C34-C35
32	c	520	LMG	C36-C37-C38-C39
33	B	622	LHG	C25-C26-C27-C28
33	B	622	LHG	O1-C1-C2-O2
33	D	407	LHG	O1-C1-C2-O2
29	F	102	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	l	101	SQD	C16-C17-C18-C19
31	T	102	STE	C14-C15-C16-C17
33	E	101	LHG	C31-C32-C33-C34
25	C	508	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	B	604	CLA	C13-C15-C16-C17
25	C	512	CLA	C15-C16-C17-C18
31	t	103	STE	C2-C3-C4-C5
32	C	519	LMG	C31-C32-C33-C34
33	l	102	LHG	C29-C30-C31-C32
33	E	101	LHG	O6-C4-C5-C6
33	l	102	LHG	O6-C4-C5-C6
25	B	602	CLA	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	B	603	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C15
25	B	610	CLA	C11-C10-C8-C7
25	B	612	CLA	C12-C13-C15-C16
25	B	614	CLA	C11-C10-C8-C7
25	C	503	CLA	C11-C10-C8-C7
25	C	505	CLA	C11-C10-C8-C7
25	C	505	CLA	C12-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C7
25	C	511	CLA	C11-C12-C13-C15
25	C	512	CLA	C6-C7-C8-C10
25	b	601	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C15
25	c	509	CLA	C6-C7-C8-C10
25	c	510	CLA	C6-C7-C8-C10
25	c	510	CLA	C12-C13-C15-C16
25	c	512	CLA	C12-C13-C15-C16
25	h	101	CLA	C11-C12-C13-C15
30	c	519	DGD	C9B-CAB-CBB-CCB
32	C	515	LMG	C14-C15-C16-C17
32	C	515	LMG	C38-C39-C40-C41
25	c	504	CLA	C11-C12-C13-C14
25	B	604	CLA	C8-C10-C11-C12
25	B	613	CLA	C15-C16-C17-C18
30	A	616	DGD	C7B-C8B-C9B-CAB
33	B	622	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	c	518	DGD	C4E-C5E-C6E-O5E
31	B	624	STE	C4-C5-C6-C7
25	A	607	CLA	C10-C11-C12-C13
25	b	601	CLA	C10-C11-C12-C13
33	D	407	LHG	C25-C26-C27-C28
31	a	617	STE	C4-C5-C6-C7
31	b	619	STE	C11-C12-C13-C14
31	b	621	STE	C2-C3-C4-C5
30	a	616	DGD	C2B-C1B-O2G-C2G
25	B	603	CLA	C14-C13-C15-C16
25	C	506	CLA	C14-C13-C15-C16
25	a	608	CLA	C14-C13-C15-C16
25	b	601	CLA	C6-C7-C8-C9
25	b	603	CLA	C14-C13-C15-C16
25	b	608	CLA	C14-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C9
25	c	502	CLA	C6-C7-C8-C9
25	c	510	CLA	C6-C7-C8-C9
25	c	510	CLA	C14-C13-C15-C16
25	h	101	CLA	C11-C12-C13-C14
29	a	614	SQD	C25-C26-C27-C28
30	A	616	DGD	C8B-C9B-CAB-CBB
30	H	103	DGD	C7B-C8B-C9B-CAB
33	D	407	LHG	C14-C15-C16-C17
33	l	102	LHG	C16-C17-C18-C19
29	L	101	SQD	C27-C28-C29-C30
30	c	519	DGD	CCA-CDA-CEA-CFA
32	D	406	LMG	C18-C19-C20-C21
33	E	101	LHG	C33-C34-C35-C36
25	B	603	CLA	CBA-CGA-O2A-C1
33	d	407	LHG	C11-C12-C13-C14
32	C	515	LMG	C36-C37-C38-C39
33	e	102	LHG	O9-C7-O7-C5
31	x	102	STE	C5-C6-C7-C8
29	a	614	SQD	O6-C44-C45-C46
29	a	615	SQD	C44-C45-C46-O48
29	l	101	SQD	O6-C44-C45-C46
30	A	616	DGD	C1G-C2G-C3G-O3G
32	C	519	LMG	O1-C7-C8-C9
32	c	522	LMG	C7-C8-C9-O8
32	m	101	LMG	C7-C8-C9-O8
31	D	410	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	m	101	LMG	C11-C12-C13-C14
33	E	101	LHG	C17-C18-C19-C20
30	c	518	DGD	C8A-C9A-CAA-CBA
32	c	524	LMG	C14-C15-C16-C17
25	C	511	CLA	CBA-CGA-O2A-C1
30	h	102	DGD	O6E-C5E-C6E-O5E
29	A	615	SQD	C17-C18-C19-C20
30	c	517	DGD	CCA-CDA-CEA-CFA
31	d	411	STE	C2-C3-C4-C5
31	l	103	STE	C7-C8-C9-C10
33	B	621	LHG	C29-C30-C31-C32
31	B	625	STE	C4-C5-C6-C7
33	B	621	LHG	C11-C12-C13-C14
27	A	611	BCR	C35-C13-C14-C15
27	c	514	BCR	C35-C13-C14-C15
27	d	404	BCR	C20-C21-C22-C37
27	t	101	BCR	C20-C21-C22-C37
25	C	502	CLA	C13-C15-C16-C17
30	c	517	DGD	C8A-C9A-CAA-CBA
33	B	621	LHG	C13-C14-C15-C16
25	C	509	CLA	CBD-CGD-O2D-CED
32	d	409	LMG	C31-C32-C33-C34
25	a	610	CLA	C5-C6-C7-C8
30	c	517	DGD	CCB-CDB-CEB-CFB
32	c	522	LMG	C33-C34-C35-C36
32	C	515	LMG	C33-C34-C35-C36
32	D	409	LMG	C33-C34-C35-C36
33	d	407	LHG	C10-C11-C12-C13
27	K	101	BCR	C7-C8-C9-C10
29	l	101	SQD	O10-C23-O48-C46
30	A	616	DGD	CEB-CFB-CGB-CHB
32	D	406	LMG	O6-C5-C6-O5
25	C	504	CLA	C11-C12-C13-C14
29	l	101	SQD	C13-C14-C15-C16
29	l	101	SQD	C26-C27-C28-C29
30	A	616	DGD	C4D-C5D-C6D-O5D
32	C	515	LMG	C30-C31-C32-C33
29	l	101	SQD	C23-C24-C25-C26
30	C	516	DGD	C2B-C3B-C4B-C5B
30	C	517	DGD	C3A-C4A-C5A-C6A
31	T	103	STE	C5-C6-C7-C8
31	b	623	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	D	407	LHG	C17-C18-C19-C20
29	A	615	SQD	C28-C29-C30-C31
31	D	410	STE	C11-C10-C9-C8
30	c	517	DGD	O6D-C5D-C6D-O5D
29	a	615	SQD	C17-C18-C19-C20
30	A	616	DGD	C5B-C6B-C7B-C8B
30	a	616	DGD	C9A-CAA-CBA-CCA
30	c	518	DGD	C6A-C7A-C8A-C9A
32	M	101	LMG	C38-C39-C40-C41
33	d	407	LHG	C13-C14-C15-C16
25	c	506	CLA	C16-C17-C18-C19
30	C	517	DGD	C1B-C2B-C3B-C4B
27	A	611	BCR	C16-C17-C18-C19
27	B	617	BCR	C11-C10-C9-C8
27	c	516	BCR	C11-C10-C9-C8
32	m	101	LMG	C19-C20-C21-C22
33	D	407	LHG	C15-C16-C17-C18
27	b	618	BCR	C22-C23-C24-C25
29	A	614	SQD	C8-C7-O47-C45
31	B	619	STE	C9-C10-C11-C12
25	C	505	CLA	C2-C3-C5-C6
30	c	519	DGD	CDA-CEA-CFA-CGA
29	l	101	SQD	C9-C10-C11-C12
30	a	616	DGD	C8A-C9A-CAA-CBA
32	D	409	LMG	C12-C13-C14-C15
32	b	620	LMG	C22-C23-C24-C25
25	C	513	CLA	C16-C17-C18-C19
30	h	102	DGD	C7A-C8A-C9A-CAA
32	c	524	LMG	C31-C32-C33-C34
29	l	101	SQD	C19-C20-C21-C22
30	C	516	DGD	C4A-C5A-C6A-C7A
30	c	518	DGD	C4A-C5A-C6A-C7A
30	h	102	DGD	CCA-CDA-CEA-CFA
32	c	522	LMG	C40-C41-C42-C43
33	B	621	LHG	C18-C19-C20-C21
33	E	101	LHG	C10-C11-C12-C13
29	A	614	SQD	C17-C18-C19-C20
30	c	518	DGD	CDA-CEA-CFA-CGA
31	l	103	STE	C1-C2-C3-C4
31	b	622	STE	C10-C11-C12-C13
32	D	406	LMG	C39-C40-C41-C42
31	b	619	STE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	b	620	LMG	C24-C25-C26-C27
30	c	518	DGD	CBA-CCA-CDA-CEA
30	c	519	DGD	CBA-CCA-CDA-CEA
31	B	623	STE	C6-C7-C8-C9
32	b	620	LMG	C38-C39-C40-C41
33	B	622	LHG	C27-C28-C29-C30
32	c	524	LMG	C20-C21-C22-C23
29	A	615	SQD	C11-C12-C13-C14
29	a	614	SQD	C12-C13-C14-C15
29	l	101	SQD	C35-C36-C37-C38
25	C	505	CLA	C10-C11-C12-C13
33	d	406	LHG	C12-C13-C14-C15
31	b	623	STE	C7-C8-C9-C10
32	M	101	LMG	C17-C18-C19-C20
32	c	522	LMG	C42-C43-C44-C45
32	d	409	LMG	C33-C34-C35-C36
32	c	520	LMG	C4-C5-C6-O5
32	B	620	LMG	C37-C38-C39-C40
28	d	405	PL9	C42-C43-C44-C45
25	A	610	CLA	C5-C6-C7-C8
30	a	616	DGD	CDA-CEA-CFA-CGA
25	A	607	CLA	C15-C16-C17-C18
33	B	622	LHG	C23-C24-C25-C26
25	C	510	CLA	C4-C3-C5-C6
28	d	405	PL9	C30-C29-C31-C32
30	c	517	DGD	CDB-CEB-CFB-CGB
28	a	612	PL9	C43-C44-C46-C47
31	R	101	STE	C3-C4-C5-C6
25	C	513	CLA	CBA-CGA-O2A-C1
30	a	616	DGD	C1B-C2B-C3B-C4B
31	T	102	STE	C3-C4-C5-C6
29	A	614	SQD	C26-C27-C28-C29
31	B	623	STE	C2-C3-C4-C5
31	b	621	STE	C10-C11-C12-C13
31	l	103	STE	C4-C5-C6-C7
32	c	522	LMG	C38-C39-C40-C41
33	d	407	LHG	O1-C1-C2-O2
25	A	607	CLA	C6-C7-C8-C9
25	B	601	CLA	C11-C12-C13-C14
25	B	602	CLA	C6-C7-C8-C9
25	B	605	CLA	C11-C12-C13-C14
25	B	610	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	B	612	CLA	C14-C13-C15-C16
25	C	505	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C9
25	C	510	CLA	C11-C10-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	b	601	CLA	C14-C13-C15-C16
25	b	604	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	507	CLA	C6-C7-C8-C9
25	c	512	CLA	C11-C12-C13-C14
25	c	512	CLA	C14-C13-C15-C16
31	H	104	STE	C12-C13-C14-C15
33	d	406	LHG	C27-C28-C29-C30
25	C	502	CLA	C4B-C3B-CAB-CBB
30	C	518	DGD	CAA-CBA-CCA-CDA
30	c	517	DGD	C5A-C6A-C7A-C8A
25	b	601	CLA	O1D-CGD-O2D-CED
25	c	509	CLA	CAA-CBA-CGA-O2A
31	t	103	STE	C5-C6-C7-C8
33	B	621	LHG	C30-C31-C32-C33
32	D	406	LMG	C36-C37-C38-C39
30	A	616	DGD	C2E-C1E-O5D-C6D
25	b	605	CLA	C15-C16-C17-C18
31	m	102	STE	C3-C4-C5-C6
32	c	522	LMG	C29-C30-C31-C32
33	E	101	LHG	C9-C10-C11-C12
31	t	103	STE	C7-C8-C9-C10
32	d	410	LMG	C11-C10-O7-C8
31	B	626	STE	C5-C6-C7-C8
30	c	518	DGD	CDB-CEB-CFB-CGB
33	E	101	LHG	C35-C36-C37-C38
25	D	402	CLA	C2C-C3C-CAC-CBC
30	c	517	DGD	CBB-CCB-CDB-CEB
25	A	607	CLA	C11-C12-C13-C15
25	B	601	CLA	C11-C12-C13-C15
25	B	603	CLA	C11-C12-C13-C15
25	B	606	CLA	C6-C7-C8-C10
25	B	613	CLA	C12-C13-C15-C16
25	C	505	CLA	C6-C7-C8-C10
25	C	506	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	509	CLA	C12-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C10
25	D	403	CLA	C6-C7-C8-C10
25	H	101	CLA	C6-C7-C8-C10
25	a	608	CLA	C11-C10-C8-C7
25	a	608	CLA	C12-C13-C15-C16
25	a	610	CLA	C12-C13-C15-C16
25	b	601	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C10-C8-C7
25	b	603	CLA	C12-C13-C15-C16
25	b	604	CLA	C12-C13-C15-C16
25	b	608	CLA	C12-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C7
25	c	505	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C12-C13-C15
33	d	407	LHG	C35-C36-C37-C38
32	c	524	LMG	C35-C36-C37-C38
25	c	501	CLA	O1D-CGD-O2D-CED
25	C	505	CLA	C4-C3-C5-C6
28	A	612	PL9	C15-C14-C16-C17
28	d	405	PL9	C45-C44-C46-C47
25	C	508	CLA	C15-C16-C17-C18
29	A	614	SQD	C10-C11-C12-C13
30	C	516	DGD	O1G-C1A-C2A-C3A
28	a	612	PL9	C18-C19-C21-C22
30	C	517	DGD	CDA-CEA-CFA-CGA
29	A	615	SQD	C44-C45-C46-O48
29	F	102	SQD	O5-C1-O6-C44
29	A	614	SQD	C9-C10-C11-C12
33	E	101	LHG	C28-C29-C30-C31
25	B	603	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
29	a	614	SQD	C24-C23-O48-C46
32	M	101	LMG	C31-C32-C33-C34
25	b	601	CLA	C3-C5-C6-C7
25	a	608	CLA	C16-C17-C18-C20
30	C	517	DGD	CBB-CCB-CDB-CEB
30	C	518	DGD	C2B-C3B-C4B-C5B
31	J	101	STE	C6-C7-C8-C9
32	c	524	LMG	C17-C18-C19-C20
31	M	103	STE	C1-C2-C3-C4
32	D	409	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
32	C	519	LMG	C40-C41-C42-C43
33	B	622	LHG	C1-C2-C3-O3
29	a	614	SQD	C26-C27-C28-C29
31	b	622	STE	C11-C12-C13-C14
32	C	519	LMG	C18-C19-C20-C21
33	B	622	LHG	C16-C17-C18-C19
28	A	612	PL9	C19-C21-C22-C23
32	D	409	LMG	C7-C8-C9-O8
32	C	519	LMG	C37-C38-C39-C40
29	l	101	SQD	C17-C18-C19-C20
30	A	616	DGD	CFA-CGA-CHA-CIA
30	a	616	DGD	CBB-CCB-CDB-CEB
32	d	409	LMG	C35-C36-C37-C38
26	d	401	PHO	C1A-C2A-CAA-CBA
25	c	503	CLA	C15-C16-C17-C18
30	C	517	DGD	C5B-C6B-C7B-C8B
32	C	515	LMG	C32-C33-C34-C35
33	d	407	LHG	C9-C10-C11-C12
25	B	610	CLA	C4-C3-C5-C6
29	a	615	SQD	C11-C12-C13-C14
31	b	621	STE	C9-C10-C11-C12
25	B	610	CLA	C2-C3-C5-C6
31	d	411	STE	C12-C13-C14-C15
33	l	102	LHG	C34-C35-C36-C37
25	C	506	CLA	C16-C17-C18-C20
30	C	518	DGD	C4B-C5B-C6B-C7B
27	B	616	BCR	C1-C6-C7-C8
27	K	103	BCR	C23-C24-C25-C30
30	h	102	DGD	O2G-C1B-C2B-C3B
29	A	614	SQD	C24-C25-C26-C27
25	A	606	CLA	C15-C16-C17-C18
30	A	616	DGD	CDB-CEB-CFB-CGB
32	c	522	LMG	C32-C33-C34-C35
29	f	101	SQD	C26-C27-C28-C29
25	c	504	CLA	C11-C12-C13-C15
29	a	614	SQD	O47-C45-C46-O48
32	C	519	LMG	O1-C7-C8-O7
32	D	409	LMG	O7-C8-C9-O8
32	M	101	LMG	O7-C8-C9-O8
32	c	522	LMG	O7-C8-C9-O8
32	m	101	LMG	O7-C8-C9-O8
31	B	619	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	A	612	PL9	C4-C3-C7-C8
28	D	405	PL9	C4-C3-C7-C8
28	a	612	PL9	C4-C3-C7-C8
29	l	101	SQD	C34-C35-C36-C37
31	b	619	STE	C4-C5-C6-C7
31	m	102	STE	C4-C5-C6-C7
32	c	522	LMG	C15-C16-C17-C18
27	d	404	BCR	C18-C19-C20-C21
25	C	510	CLA	C2-C3-C5-C6
29	a	614	SQD	C11-C10-C9-C8
33	l	102	LHG	C24-C25-C26-C27
25	C	513	CLA	C16-C17-C18-C20
25	a	608	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C20
29	a	615	SQD	C15-C16-C17-C18
30	c	517	DGD	C7A-C8A-C9A-CAA
31	M	103	STE	C4-C5-C6-C7
31	T	102	STE	C10-C11-C12-C13
31	c	521	STE	C11-C10-C9-C8
32	c	524	LMG	C11-C12-C13-C14
25	A	607	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C12-C13-C14
25	B	614	CLA	C6-C7-C8-C9
25	a	608	CLA	C11-C10-C8-C9
25	c	504	CLA	C11-C10-C8-C9
32	D	406	LMG	C34-C35-C36-C37
30	C	517	DGD	O6E-C1E-O5D-C6D
30	H	103	DGD	C4E-C5E-C6E-O5E
27	d	404	BCR	C14-C15-C16-C17
25	B	609	CLA	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C19
31	D	410	STE	C7-C8-C9-C10
32	c	522	LMG	C31-C32-C33-C34
32	C	519	LMG	C14-C15-C16-C17
33	d	406	LHG	C33-C34-C35-C36
30	C	518	DGD	O6D-C5D-C6D-O5D
33	E	101	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
25	c	505	CLA	C5-C6-C7-C8
25	c	507	CLA	C15-C16-C17-C18
29	L	101	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
31	a	617	STE	C2-C3-C4-C5
32	b	620	LMG	C15-C16-C17-C18
33	D	407	LHG	C1-C2-C3-O3
29	F	102	SQD	C28-C29-C30-C31
30	C	517	DGD	C7B-C8B-C9B-CAB
27	K	103	BCR	C16-C17-C18-C36
27	a	611	BCR	C16-C17-C18-C36
27	b	616	BCR	C20-C21-C22-C37
27	b	617	BCR	C16-C17-C18-C36
27	b	618	BCR	C20-C21-C22-C37
27	k	101	BCR	C35-C13-C14-C15
30	H	103	DGD	C3A-C4A-C5A-C6A
30	c	517	DGD	C4A-C5A-C6A-C7A
31	B	624	STE	C9-C10-C11-C12
25	c	502	CLA	C16-C17-C18-C20
32	d	409	LMG	C40-C41-C42-C43
29	A	614	SQD	C11-C10-C9-C8
25	B	614	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C12-C13-C15
25	C	507	CLA	C11-C10-C8-C7
25	b	606	CLA	C11-C12-C13-C15
25	b	611	CLA	C12-C13-C15-C16
25	c	505	CLA	C6-C7-C8-C10
25	c	506	CLA	C11-C10-C8-C7
25	c	512	CLA	C6-C7-C8-C10
32	c	524	LMG	C10-C11-C12-C13
29	A	615	SQD	C19-C20-C21-C22
31	c	521	STE	C15-C16-C17-C18
30	A	616	DGD	C2A-C1A-O1G-C1G
25	C	513	CLA	O1A-CGA-O2A-C1
32	C	519	LMG	O10-C28-O8-C9
29	f	101	SQD	C5-C6-S-O8
29	l	101	SQD	C45-C44-O6-C1
30	C	517	DGD	C5D-C6D-O5D-C1E
30	c	518	DGD	C5D-C6D-O5D-C1E
25	C	510	CLA	O1D-CGD-O2D-CED
32	m	101	LMG	C29-C30-C31-C32
25	B	612	CLA	C4-C3-C5-C6
25	C	506	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
30	c	518	DGD	O6E-C5E-C6E-O5E
30	C	517	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
32	D	409	LMG	C37-C38-C39-C40
33	d	407	LHG	C12-C13-C14-C15
29	a	614	SQD	O10-C23-O48-C46
30	a	616	DGD	C2B-C3B-C4B-C5B
30	C	516	DGD	C6A-C7A-C8A-C9A
31	T	103	STE	C11-C10-C9-C8
33	D	408	LHG	C16-C17-C18-C19
32	D	406	LMG	C20-C21-C22-C23
31	B	623	STE	C7-C8-C9-C10
25	C	512	CLA	C3-C5-C6-C7
30	c	517	DGD	C1A-C2A-C3A-C4A
33	E	101	LHG	C34-C35-C36-C37
33	e	102	LHG	C26-C27-C28-C29
25	c	510	CLA	C5-C6-C7-C8
33	l	102	LHG	O6-C4-C5-O7
29	a	614	SQD	C19-C20-C21-C22
30	A	616	DGD	O6E-C1E-O5D-C6D
32	M	101	LMG	C7-C8-C9-O8
32	m	101	LMG	O1-C7-C8-C9
32	M	101	LMG	C28-C29-C30-C31
35	F	101	HEM	C4C-C3C-CAC-CBC
25	B	608	CLA	C16-C17-C18-C19
25	c	512	CLA	C4-C3-C5-C6
25	B	605	CLA	CBD-CGD-O2D-CED
25	c	510	CLA	C2-C3-C5-C6
31	D	410	STE	C9-C10-C11-C12
31	m	102	STE	C6-C7-C8-C9
33	B	621	LHG	C16-C17-C18-C19
25	D	403	CLA	C8-C10-C11-C12
26	d	401	PHO	C5-C6-C7-C8
30	h	102	DGD	C5A-C6A-C7A-C8A
32	D	406	LMG	C37-C38-C39-C40
29	A	614	SQD	O6-C44-C45-O47
30	C	516	DGD	O1G-C1G-C2G-O2G
32	m	101	LMG	O1-C7-C8-O7
30	c	517	DGD	C4D-C5D-C6D-O5D
25	B	602	CLA	C11-C12-C13-C14
25	C	510	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C19
25	c	502	CLA	C16-C17-C18-C19
25	b	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	a	616	DGD	C3A-C4A-C5A-C6A
31	I	101	STE	C4-C5-C6-C7
31	M	102	STE	C11-C10-C9-C8
32	m	101	LMG	C16-C17-C18-C19
29	a	615	SQD	C18-C19-C20-C21
33	D	408	LHG	C25-C26-C27-C28
30	H	103	DGD	C1B-C2B-C3B-C4B
31	M	102	STE	C5-C6-C7-C8
31	b	622	STE	C6-C7-C8-C9
30	H	103	DGD	O2G-C1B-C2B-C3B
25	B	615	CLA	C2-C1-O2A-CGA
30	C	517	DGD	C2E-C1E-O5D-C6D
33	D	408	LHG	C13-C14-C15-C16
30	a	616	DGD	C5A-C6A-C7A-C8A
29	L	101	SQD	C19-C20-C21-C22
30	c	519	DGD	CDB-CEB-CFB-CGB
29	a	614	SQD	C13-C14-C15-C16
32	D	409	LMG	C30-C31-C32-C33
32	m	101	LMG	C17-C18-C19-C20
25	a	610	CLA	C4-C3-C5-C6
25	A	607	CLA	C3-C5-C6-C7
25	C	506	CLA	C2-C3-C5-C6
32	D	406	LMG	C11-C12-C13-C14
32	D	409	LMG	C36-C37-C38-C39
25	b	602	CLA	O1A-CGA-O2A-C1
25	c	506	CLA	O1A-CGA-O2A-C1
25	C	509	CLA	O1D-CGD-O2D-CED
32	d	410	LMG	C40-C41-C42-C43
33	d	406	LHG	O1-C1-C2-O2
32	b	620	LMG	C30-C31-C32-C33
25	b	614	CLA	C8-C10-C11-C12
25	b	607	CLA	C4C-C3C-CAC-CBC
31	I	101	STE	C9-C10-C11-C12
25	C	503	CLA	C1A-C2A-CAA-CBA
25	C	504	CLA	C4B-C3B-CAB-CBB
25	H	101	CLA	C4B-C3B-CAB-CBB
25	a	613	CLA	C1A-C2A-CAA-CBA
25	b	614	CLA	C4B-C3B-CAB-CBB
25	c	511	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	CBA-CGA-O2A-C1
32	c	524	LMG	C37-C38-C39-C40
32	C	515	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
28	d	405	PL9	C28-C29-C31-C32
27	D	404	BCR	C7-C8-C9-C10
25	B	601	CLA	C16-C17-C18-C20
25	B	602	CLA	C2A-CAA-CBA-CGA
28	A	612	PL9	C47-C48-C49-C50
33	d	407	LHG	O6-C4-C5-C6
28	d	405	PL9	C27-C28-C29-C30
29	a	615	SQD	C29-C30-C31-C32
30	c	519	DGD	C5B-C6B-C7B-C8B
33	d	407	LHG	C31-C32-C33-C34
25	A	613	CLA	C12-C13-C15-C16
25	B	603	CLA	C11-C10-C8-C7
25	B	612	CLA	C6-C7-C8-C10
25	B	612	CLA	C11-C12-C13-C15
25	B	614	CLA	C12-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C10
25	C	504	CLA	C6-C7-C8-C10
25	C	509	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C12-C13-C15
25	H	101	CLA	C11-C10-C8-C7
25	b	605	CLA	C11-C10-C8-C7
25	b	615	CLA	C6-C7-C8-C10
25	c	513	CLA	C11-C12-C13-C15
31	B	619	STE	C11-C12-C13-C14
30	H	103	DGD	C7A-C8A-C9A-CAA
31	B	619	STE	C7-C8-C9-C10
32	b	620	LMG	C39-C40-C41-C42
33	D	407	LHG	C35-C36-C37-C38
32	b	620	LMG	C37-C38-C39-C40
30	c	518	DGD	C8B-C9B-CAB-CBB
32	C	519	LMG	C11-C12-C13-C14
25	C	506	CLA	C16-C17-C18-C19
30	c	517	DGD	C8B-C9B-CAB-CBB
29	A	614	SQD	O49-C7-O47-C45
33	E	101	LHG	O6-C4-C5-O7
33	d	407	LHG	O6-C4-C5-O7
33	D	408	LHG	C34-C35-C36-C37
25	B	612	CLA	C6-C7-C8-C9
25	B	614	CLA	C11-C12-C13-C14
25	C	508	CLA	C14-C13-C15-C16
25	D	403	CLA	C11-C10-C8-C9
25	b	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C11-C12-C13-C14
25	c	505	CLA	C6-C7-C8-C9
25	D	403	CLA	C13-C15-C16-C17
32	C	519	LMG	C16-C17-C18-C19
32	c	522	LMG	C16-C17-C18-C19
27	K	101	BCR	C13-C14-C15-C16
25	c	508	CLA	C10-C11-C12-C13
31	c	523	STE	C7-C8-C9-C10
30	c	517	DGD	C2B-C3B-C4B-C5B
32	B	620	LMG	C34-C35-C36-C37
32	b	620	LMG	O1-C7-C8-O7
30	c	519	DGD	C8B-C9B-CAB-CBB
30	C	517	DGD	C4A-C5A-C6A-C7A
30	C	516	DGD	O1G-C1G-C2G-C3G
32	C	515	LMG	O1-C7-C8-C9
32	b	620	LMG	O1-C7-C8-C9
33	e	102	LHG	C4-C5-C6-O8
25	b	610	CLA	C4-C3-C5-C6
29	A	614	SQD	C29-C30-C31-C32
25	c	512	CLA	C2-C3-C5-C6
30	c	519	DGD	C7B-C8B-C9B-CAB
32	d	409	LMG	C39-C40-C41-C42
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	H	101	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O2D
32	b	620	LMG	O6-C1-O1-C7
33	B	622	LHG	C7-C8-C9-C10
25	B	608	CLA	C16-C17-C18-C20
29	a	615	SQD	C31-C32-C33-C34
30	H	103	DGD	C6B-C7B-C8B-C9B
32	D	409	LMG	C13-C14-C15-C16
30	h	102	DGD	C9A-CAA-CBA-CCA
31	j	101	STE	C3-C4-C5-C6
32	M	101	LMG	C14-C15-C16-C17
25	B	606	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	H	101	CLA	CAD-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
27	K	101	BCR	C9-C10-C11-C12
27	d	404	BCR	C13-C14-C15-C16
33	B	621	LHG	C4-O6-P-O5
33	D	407	LHG	C4-O6-P-O5
33	d	406	LHG	C3-O3-P-O5
33	d	407	LHG	C3-O3-P-O5
33	e	102	LHG	C4-O6-P-O3
33	e	102	LHG	C4-O6-P-O5
33	l	102	LHG	C4-O6-P-O5
30	a	616	DGD	CFA-CGA-CHA-CIA
25	D	403	CLA	C16-C17-C18-C20
25	C	502	CLA	C2B-C3B-CAB-CBB
25	H	101	CLA	C2B-C3B-CAB-CBB
25	b	609	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
29	f	101	SQD	C29-C30-C31-C32
33	d	408	LHG	C2-C3-O3-P
31	B	619	STE	C12-C13-C14-C15
25	b	615	CLA	C11-C12-C13-C15
31	B	625	STE	C1-C2-C3-C4
31	M	102	STE	C1-C2-C3-C4
31	C	520	STE	C7-C8-C9-C10
33	d	406	LHG	C30-C31-C32-C33
31	l	103	STE	C10-C11-C12-C13
32	C	519	LMG	C13-C14-C15-C16
32	M	101	LMG	C30-C31-C32-C33
32	C	515	LMG	C39-C40-C41-C42
31	t	102	STE	C5-C6-C7-C8
25	a	607	CLA	C16-C17-C18-C19
32	M	101	LMG	C10-C11-C12-C13
29	L	101	SQD	C30-C31-C32-C33
29	f	101	SQD	C44-C45-O47-C7
32	b	620	LMG	C9-C8-O7-C10
32	c	524	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
31	b	619	STE	C2-C3-C4-C5
32	b	620	LMG	C32-C33-C34-C35
31	l	103	STE	C15-C16-C17-C18
27	B	616	BCR	C9-C10-C11-C12
32	D	406	LMG	C33-C34-C35-C36
33	e	102	LHG	O6-C4-C5-C6
30	c	517	DGD	C6B-C7B-C8B-C9B
32	c	520	LMG	C40-C41-C42-C43
25	C	512	CLA	C10-C11-C12-C13
25	b	607	CLA	C13-C15-C16-C17
25	A	613	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C10-C8-C9
25	B	606	CLA	C6-C7-C8-C9
25	C	505	CLA	C6-C7-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C14
25	D	403	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	611	CLA	C14-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C9
25	c	505	CLA	C11-C10-C8-C9
25	c	505	CLA	C14-C13-C15-C16
25	b	613	CLA	C11-C12-C13-C15
32	D	406	LMG	C16-C17-C18-C19
27	C	514	BCR	C11-C10-C9-C8
27	H	102	BCR	C11-C10-C9-C8
33	e	102	LHG	O6-C4-C5-O7
29	f	101	SQD	C24-C25-C26-C27
32	m	101	LMG	C14-C15-C16-C17
33	B	621	LHG	O10-C23-O8-C6
32	c	524	LMG	C40-C41-C42-C43
29	A	615	SQD	C27-C28-C29-C30
32	b	620	LMG	C13-C14-C15-C16
32	b	620	LMG	C2-C1-O1-C7
25	c	513	CLA	C3-C5-C6-C7
25	B	612	CLA	C16-C17-C18-C20
30	C	516	DGD	C9B-CAB-CBB-CCB
32	b	620	LMG	O7-C8-C9-O8
33	e	102	LHG	O7-C5-C6-O8
32	D	406	LMG	C19-C20-C21-C22
30	A	616	DGD	CFB-CGB-CHB-CIB

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Mol	Chain	Res	Type	Atoms
32	C	515	LMG	C19-C20-C21-C22
27	c	516	BCR	C15-C16-C17-C18
30	A	616	DGD	C3B-C4B-C5B-C6B
25	C	513	CLA	C8-C10-C11-C12
30	C	516	DGD	O6D-C5D-C6D-O5D
29	l	101	SQD	C27-C28-C29-C30
25	B	613	CLA	C4-C3-C5-C6
28	a	612	PL9	C30-C29-C31-C32
25	C	513	CLA	C13-C15-C16-C17
32	c	524	LMG	C18-C19-C20-C21
25	B	612	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
30	C	516	DGD	C4D-C5D-C6D-O5D
27	T	101	BCR	C21-C22-C23-C24
25	b	612	CLA	C13-C15-C16-C17
31	b	619	STE	C3-C4-C5-C6
30	h	102	DGD	CDB-CEB-CFB-CGB
32	C	515	LMG	C17-C18-C19-C20
25	C	501	CLA	C2A-CAA-CBA-CGA
31	B	624	STE	C11-C12-C13-C14
30	c	519	DGD	C1B-C2B-C3B-C4B
28	d	405	PL9	C15-C14-C16-C17
29	A	615	SQD	O48-C23-C24-C25
31	T	103	STE	C15-C16-C17-C18
31	l	103	STE	C13-C14-C15-C16
25	A	613	CLA	C14-C13-C15-C16
25	B	614	CLA	C14-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C9
25	a	610	CLA	C6-C7-C8-C9
25	a	610	CLA	C14-C13-C15-C16
31	b	621	STE	C3-C4-C5-C6
25	A	613	CLA	C13-C15-C16-C17
32	M	101	LMG	C18-C19-C20-C21
25	D	402	CLA	C4B-C3B-CAB-CBB
25	B	611	CLA	C8-C10-C11-C12
25	A	606	CLA	C13-C15-C16-C17
30	c	519	DGD	O6D-C5D-C6D-O5D
30	h	102	DGD	CBB-CCB-CDB-CEB
30	C	517	DGD	C7A-C8A-C9A-CAA
25	a	610	CLA	CBA-CGA-O2A-C1
32	c	520	LMG	C29-C28-O8-C9
32	B	620	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
33	D	407	LHG	C30-C31-C32-C33
32	M	101	LMG	C34-C35-C36-C37
25	A	607	CLA	C12-C13-C15-C16
25	B	613	CLA	C11-C12-C13-C15
25	C	503	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C10-C8-C7
25	b	612	CLA	C11-C10-C8-C7
25	h	101	CLA	C12-C13-C15-C16
25	b	603	CLA	C8-C10-C11-C12
32	d	410	LMG	C11-C12-C13-C14
25	B	607	CLA	C10-C11-C12-C13
25	B	601	CLA	C16-C17-C18-C19
28	a	612	PL9	C7-C8-C9-C10
31	I	101	STE	C11-C10-C9-C8
25	H	101	CLA	C3A-C2A-CAA-CBA
28	A	612	PL9	C13-C14-C16-C17
31	d	411	STE	C1-C2-C3-C4
30	a	616	DGD	C6B-C7B-C8B-C9B
32	M	101	LMG	C15-C16-C17-C18
27	K	101	BCR	C20-C21-C22-C37
27	x	101	BCR	C20-C21-C22-C37
30	C	516	DGD	CBA-CCA-CDA-CEA
29	F	102	SQD	C44-C45-C46-O48
25	d	402	CLA	C2-C1-O2A-CGA
30	H	103	DGD	CAA-CBA-CCA-CDA
32	D	406	LMG	C32-C33-C34-C35
32	B	620	LMG	C30-C31-C32-C33
31	B	624	STE	O1-C1-C2-C3
31	D	410	STE	O2-C1-C2-C3
25	b	610	CLA	C2-C3-C5-C6
32	c	522	LMG	O1-C7-C8-C9
31	D	410	STE	C5-C6-C7-C8
33	B	622	LHG	C13-C14-C15-C16
25	B	605	CLA	C11-C10-C8-C9
25	B	613	CLA	C6-C7-C8-C9
25	C	503	CLA	C14-C13-C15-C16
25	C	507	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
25	c	503	CLA	C11-C12-C13-C14
25	c	513	CLA	C11-C12-C13-C14
25	c	509	CLA	C16-C17-C18-C19
32	m	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
29	f	101	SQD	C46-C45-O47-C7
32	C	515	LMG	C9-C8-O7-C10
31	B	626	STE	C4-C5-C6-C7
25	c	508	CLA	C4-C3-C5-C6
25	c	505	CLA	C13-C15-C16-C17
25	C	505	CLA	CBD-CGD-O2D-CED
29	A	614	SQD	O10-C23-O48-C46
33	D	408	LHG	C35-C36-C37-C38
25	b	611	CLA	C10-C11-C12-C13
32	c	520	LMG	C34-C35-C36-C37
31	B	624	STE	O2-C1-C2-C3
32	c	524	LMG	C38-C39-C40-C41
25	C	504	CLA	C2B-C3B-CAB-CBB
25	b	602	CLA	C2B-C3B-CAB-CBB
25	b	606	CLA	C2B-C3B-CAB-CBB
25	b	614	CLA	C2B-C3B-CAB-CBB
27	B	616	BCR	C5-C6-C7-C8
27	C	514	BCR	C23-C24-C25-C30
27	D	404	BCR	C23-C24-C25-C26
27	H	102	BCR	C23-C24-C25-C30
27	K	103	BCR	C1-C6-C7-C8
27	b	616	BCR	C1-C6-C7-C8
27	c	514	BCR	C1-C6-C7-C8
27	c	515	BCR	C1-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
31	J	101	STE	C3-C4-C5-C6
29	A	614	SQD	C24-C23-O48-C46
25	c	506	CLA	C8-C10-C11-C12
30	h	102	DGD	CBA-CCA-CDA-CEA
30	h	102	DGD	CAB-CBB-CCB-CDB
35	F	101	HEM	CAD-CBD-CGD-O1D
25	H	101	CLA	C4-C3-C5-C6
28	a	612	PL9	C45-C44-C46-C47
32	D	406	LMG	C38-C39-C40-C41
25	A	613	CLA	C11-C12-C13-C15
25	B	602	CLA	C11-C10-C8-C7
25	B	609	CLA	C12-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C10
25	a	610	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C12-C13-C15
25	c	505	CLA	C11-C10-C8-C7
25	c	507	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C2A-CAA-CBA-CGA
33	D	408	LHG	C12-C13-C14-C15
29	A	614	SQD	C11-C12-C13-C14
31	b	622	STE	C14-C15-C16-C17
30	H	103	DGD	C9A-CAA-CBA-CCA
30	C	517	DGD	C2B-C3B-C4B-C5B
25	c	504	CLA	C4-C3-C5-C6
31	j	101	STE	C7-C8-C9-C10
25	c	509	CLA	CAA-CBA-CGA-O1A
33	B	622	LHG	C24-C25-C26-C27
32	C	515	LMG	C12-C13-C14-C15
31	D	410	STE	O1-C1-C2-C3
25	C	513	CLA	C11-C10-C8-C9
33	B	621	LHG	C35-C36-C37-C38
30	C	518	DGD	CBA-CCA-CDA-CEA
32	C	519	LMG	C38-C39-C40-C41
32	M	101	LMG	C16-C17-C18-C19
32	B	620	LMG	C11-C12-C13-C14
32	c	520	LMG	C39-C40-C41-C42
31	D	410	STE	C10-C11-C12-C13
25	H	101	CLA	C15-C16-C17-C18
28	A	612	PL9	C12-C11-C9-C10
31	b	619	STE	O1-C1-C2-C3
26	A	609	PHO	C2C-C3C-CAC-CBC
25	B	612	CLA	C2-C3-C5-C6
25	C	508	CLA	O1A-CGA-O2A-C1
25	a	610	CLA	O1A-CGA-O2A-C1
32	B	620	LMG	O7-C10-C11-C12
31	b	622	STE	C12-C13-C14-C15
30	C	516	DGD	C5B-C6B-C7B-C8B
30	H	103	DGD	CBB-CCB-CDB-CEB
31	B	619	STE	C1-C2-C3-C4
29	a	614	SQD	C44-C45-C46-O48
31	l	103	STE	C11-C10-C9-C8
32	m	101	LMG	C28-C29-C30-C31
29	A	614	SQD	C15-C16-C17-C18
31	d	411	STE	O2-C1-C2-C3
25	A	610	CLA	C4-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
28	a	612	PL9	C35-C34-C36-C37
25	a	607	CLA	C16-C17-C18-C20
25	c	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
35	F	101	HEM	CAD-CBD-CGD-O2D
33	D	408	LHG	C31-C32-C33-C34
25	B	608	CLA	C15-C16-C17-C18
31	d	411	STE	O1-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O2D
36	v	201	HEC	CAD-CBD-CGD-O2D
25	C	511	CLA	C16-C17-C18-C19
25	b	601	CLA	C16-C17-C18-C19
25	b	614	CLA	C13-C15-C16-C17
32	c	522	LMG	C11-C12-C13-C14
26	A	608	PHO	CHA-CBD-CGD-O1D
26	A	609	PHO	CHA-CBD-CGD-O1D
27	B	616	BCR	C11-C10-C9-C34
27	K	103	BCR	C11-C10-C9-C34
27	b	618	BCR	C35-C13-C14-C15
25	h	101	CLA	C10-C11-C12-C13
31	M	102	STE	C7-C8-C9-C10
29	L	101	SQD	C12-C13-C14-C15
25	C	505	CLA	C16-C17-C18-C19
25	C	512	CLA	C4-C3-C5-C6
29	f	101	SQD	O6-C44-C45-O47
32	c	522	LMG	O1-C7-C8-O7
31	H	104	STE	C11-C10-C9-C8
32	B	620	LMG	C12-C13-C14-C15
33	l	102	LHG	C17-C18-C19-C20
25	C	513	CLA	C11-C10-C8-C7
31	B	623	STE	O2-C1-C2-C3
33	B	622	LHG	O2-C2-C3-O3
25	C	504	CLA	C6-C7-C8-C9
25	H	101	CLA	C11-C10-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	610	CLA	C11-C12-C13-C14
30	c	517	DGD	C5D-C6D-O5D-C1E
32	c	524	LMG	C8-C7-O1-C1
36	V	201	HEC	CAD-CBD-CGD-O1D
25	D	402	CLA	C2-C1-O2A-CGA
31	B	626	STE	C11-C10-C9-C8
25	b	608	CLA	C15-C16-C17-C18
30	H	103	DGD	CBA-CCA-CDA-CEA
25	a	610	CLA	C2-C3-C5-C6
25	c	511	CLA	C3-C5-C6-C7
31	M	102	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	d	411	STE	C6-C7-C8-C9
30	C	517	DGD	C2D-C1D-O3G-C3G
33	D	408	LHG	C23-C24-C25-C26
26	A	608	PHO	O2A-C1-C2-C3
26	a	609	PHO	O2A-C1-C2-C3
28	D	405	PL9	C32-C33-C34-C35
30	a	616	DGD	CCB-CDB-CEB-CFB
32	c	524	LMG	C16-C17-C18-C19
27	B	616	BCR	C14-C15-C16-C17
27	K	101	BCR	C14-C15-C16-C17
25	b	612	CLA	C16-C17-C18-C19
31	b	619	STE	O2-C1-C2-C3
29	F	102	SQD	C31-C32-C33-C34
25	c	513	CLA	C5-C6-C7-C8
31	B	626	STE	C6-C7-C8-C9
33	d	406	LHG	C26-C27-C28-C29
36	v	201	HEC	CAD-CBD-CGD-O1D
31	c	521	STE	C4-C5-C6-C7
25	C	508	CLA	CBA-CGA-O2A-C1
28	D	405	PL9	C44-C46-C47-C48
32	b	620	LMG	C7-C8-C9-O8
33	E	101	LHG	C4-C5-C6-O8
29	l	101	SQD	C24-C25-C26-C27
32	b	620	LMG	C18-C19-C20-C21
25	c	507	CLA	C3-C5-C6-C7
31	c	521	STE	O2-C1-C2-C3
31	H	104	STE	C15-C16-C17-C18
30	C	517	DGD	C9B-CAB-CBB-CCB
25	c	501	CLA	C2A-CAA-CBA-CGA
30	c	517	DGD	O1G-C1A-C2A-C3A
29	a	615	SQD	C9-C10-C11-C12
31	C	522	STE	C12-C13-C14-C15
25	B	614	CLA	C16-C17-C18-C19
32	m	101	LMG	C38-C39-C40-C41
31	T	103	STE	C6-C7-C8-C9
31	R	101	STE	C2-C3-C4-C5
31	C	522	STE	C4-C5-C6-C7
33	B	621	LHG	C19-C20-C21-C22
29	L	101	SQD	C28-C29-C30-C31
32	m	101	LMG	C11-C10-O7-C8
33	E	101	LHG	O7-C5-C6-O8
25	B	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C14-C13-C15-C16
25	B	608	CLA	C14-C13-C15-C16
25	C	501	CLA	C14-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C14
25	b	614	CLA	C11-C12-C13-C14
25	c	510	CLA	C11-C10-C8-C9
29	a	615	SQD	O48-C23-C24-C25
31	B	623	STE	O1-C1-C2-C3
31	c	521	STE	O1-C1-C2-C3
32	C	515	LMG	C28-C29-C30-C31
27	t	101	BCR	C7-C8-C9-C10
30	A	616	DGD	C6A-C7A-C8A-C9A
33	B	621	LHG	C11-C10-C9-C8
33	D	407	LHG	C33-C34-C35-C36
28	a	612	PL9	C12-C13-C14-C15
30	c	519	DGD	C8A-C9A-CAA-CBA
25	C	502	CLA	C11-C12-C13-C15
25	C	507	CLA	C6-C7-C8-C10
25	C	511	CLA	C6-C7-C8-C10
25	D	402	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C12-C13-C15
25	b	605	CLA	C6-C7-C8-C10
25	b	606	CLA	C11-C10-C8-C7
25	c	509	CLA	C11-C12-C13-C15
26	d	401	PHO	C11-C10-C8-C7
29	L	101	SQD	C11-C10-C9-C8
31	C	522	STE	C3-C4-C5-C6
25	C	501	CLA	C2B-C3B-CAB-CBB
25	D	402	CLA	C2B-C3B-CAB-CBB
25	d	402	CLA	C2B-C3B-CAB-CBB
27	A	611	BCR	C1-C6-C7-C8
27	A	611	BCR	C23-C24-C25-C26
27	B	617	BCR	C23-C24-C25-C26
27	B	617	BCR	C23-C24-C25-C30
27	C	514	BCR	C23-C24-C25-C26
27	H	102	BCR	C23-C24-C25-C26
27	K	103	BCR	C5-C6-C7-C8
27	K	103	BCR	C23-C24-C25-C26
27	b	616	BCR	C5-C6-C7-C8
27	c	514	BCR	C5-C6-C7-C8
27	c	515	BCR	C5-C6-C7-C8
27	d	404	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	d	404	BCR	C23-C24-C25-C30
27	t	101	BCR	C5-C6-C7-C8
33	E	101	LHG	O9-C7-O7-C5
25	C	506	CLA	C2-C1-O2A-CGA
25	c	505	CLA	C10-C11-C12-C13
32	c	520	LMG	C30-C31-C32-C33
28	D	405	PL9	C24-C26-C27-C28
28	a	612	PL9	C24-C26-C27-C28
32	M	101	LMG	C36-C37-C38-C39
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	611	CLA	CAA-CBA-CGA-O2A
30	c	519	DGD	O1G-C1A-C2A-C3A
25	B	601	CLA	C15-C16-C17-C18
30	H	103	DGD	C5A-C6A-C7A-C8A
32	D	409	LMG	C11-C12-C13-C14
33	d	408	LHG	C31-C32-C33-C34
25	B	611	CLA	CBA-CGA-O2A-C1
26	d	401	PHO	O1D-CGD-O2D-CED
32	D	406	LMG	C12-C13-C14-C15
28	A	612	PL9	C33-C34-C36-C37
25	h	101	CLA	C15-C16-C17-C18
32	D	409	LMG	C31-C32-C33-C34
31	t	103	STE	C4-C5-C6-C7
29	a	614	SQD	O47-C7-C8-C9
29	f	101	SQD	O48-C23-C24-C25
30	c	517	DGD	O2G-C1B-C2B-C3B
29	f	101	SQD	C4-C5-C6-S
31	M	102	STE	O2-C1-C2-C3
25	B	605	CLA	C4-C3-C5-C6
31	t	102	STE	C2-C3-C4-C5
32	d	410	LMG	O7-C10-C11-C12
25	B	609	CLA	CBD-CGD-O2D-CED
27	c	514	BCR	C11-C10-C9-C34
29	a	614	SQD	C34-C35-C36-C37
31	b	622	STE	C9-C10-C11-C12
33	B	621	LHG	C10-C11-C12-C13
31	M	102	STE	O1-C1-C2-C3
32	B	620	LMG	O10-C28-C29-C30
33	d	408	LHG	C35-C36-C37-C38
29	L	101	SQD	C16-C17-C18-C19
31	C	521	STE	C1-C2-C3-C4
31	C	521	STE	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	R	101	STE	O1-C1-C2-C3
25	c	512	CLA	O1D-CGD-O2D-CED
32	M	101	LMG	C39-C40-C41-C42
25	B	601	CLA	C1A-C2A-CAA-CBA
25	C	501	CLA	C4B-C3B-CAB-CBB
25	C	503	CLA	C4B-C3B-CAB-CBB
25	C	507	CLA	C4B-C3B-CAB-CBB
25	b	602	CLA	C4B-C3B-CAB-CBB
25	b	603	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C1A-C2A-CAA-CBA
25	d	402	CLA	C4B-C3B-CAB-CBB
30	c	517	DGD	O6E-C1E-O5D-C6D
25	B	611	CLA	CAA-CBA-CGA-O2A
32	b	620	LMG	O7-C10-C11-C12
32	m	101	LMG	O8-C28-C29-C30
25	B	613	CLA	C2-C3-C5-C6
28	D	405	PL9	C46-C47-C48-C49
27	c	516	BCR	C13-C14-C15-C16
26	d	401	PHO	CBD-CGD-O2D-CED
30	H	103	DGD	O1A-C1A-O1G-C1G
25	b	601	CLA	C16-C17-C18-C20
25	h	101	CLA	C16-C17-C18-C19
31	R	101	STE	O2-C1-C2-C3
32	B	620	LMG	O9-C10-C11-C12
29	A	614	SQD	O47-C7-C8-C9
30	C	517	DGD	O2G-C1B-C2B-C3B
31	T	102	STE	C4-C5-C6-C7
33	B	621	LHG	C28-C29-C30-C31
33	E	101	LHG	C25-C26-C27-C28
25	A	613	CLA	C4C-C3C-CAC-CBC
26	d	401	PHO	C16-C17-C18-C20
25	B	611	CLA	C13-C15-C16-C17
29	f	101	SQD	C5-C6-S-O9
25	C	505	CLA	C15-C16-C17-C18
28	D	405	PL9	C30-C29-C31-C32
25	B	612	CLA	C2-C1-O2A-CGA
25	a	607	CLA	C2-C1-O2A-CGA
30	C	518	DGD	C8B-C9B-CAB-CBB
25	B	606	CLA	C12-C13-C15-C16
25	a	608	CLA	C11-C12-C13-C15
25	b	605	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	C12-C13-C15-C16
33	l	102	LHG	C24-C23-O8-C6
29	a	614	SQD	C9-C10-C11-C12
31	b	619	STE	C14-C15-C16-C17
25	C	512	CLA	O2A-C1-C2-C3
25	D	403	CLA	O2A-C1-C2-C3
32	M	101	LMG	C20-C21-C22-C23
33	l	102	LHG	C28-C29-C30-C31
32	c	524	LMG	C36-C37-C38-C39
25	b	602	CLA	C2A-CAA-CBA-CGA
25	A	606	CLA	C16-C17-C18-C20
25	B	602	CLA	C13-C15-C16-C17
25	B	606	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C19
30	C	517	DGD	C2A-C3A-C4A-C5A
25	B	611	CLA	O1A-CGA-O2A-C1
25	A	613	CLA	C8-C10-C11-C12
25	B	613	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C11-C10-C8-C9
27	K	101	BCR	C15-C16-C17-C18
28	a	612	PL9	C20-C19-C21-C22
29	a	614	SQD	O49-C7-C8-C9
32	m	101	LMG	O10-C28-C29-C30
32	c	522	LMG	C35-C36-C37-C38
29	f	101	SQD	O5-C5-C6-S
30	C	516	DGD	CDB-CEB-CFB-CGB
32	c	522	LMG	C17-C18-C19-C20
25	b	611	CLA	CAA-CBA-CGA-O1A
25	B	614	CLA	C10-C11-C12-C13
30	c	518	DGD	C9A-CAA-CBA-CCA
32	c	522	LMG	C12-C13-C14-C15
27	B	618	BCR	C11-C12-C13-C14
25	B	611	CLA	CAA-CBA-CGA-O1A
25	B	612	CLA	CAA-CBA-CGA-O1A
29	A	614	SQD	O49-C7-C8-C9
29	a	615	SQD	O10-C23-C24-C25
30	C	516	DGD	O1B-C1B-C2B-C3B
30	c	517	DGD	O1B-C1B-C2B-C3B
33	e	102	LHG	O10-C23-C24-C25
25	D	402	CLA	C15-C16-C17-C18
30	C	517	DGD	C2G-C3G-O3G-C1D
30	c	519	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
31	C	521	STE	O1-C1-C2-C3
33	e	102	LHG	O8-C23-C24-C25
29	f	101	SQD	O6-C44-C45-C46
32	M	101	LMG	O1-C7-C8-C9
30	C	516	DGD	C1B-C2B-C3B-C4B
25	C	512	CLA	C2-C3-C5-C6
29	f	101	SQD	O10-C23-C24-C25
25	B	606	CLA	CAD-CBD-CGD-O2D
25	B	615	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
26	a	609	PHO	CAD-CBD-CGD-O2D
25	b	612	CLA	CAA-CBA-CGA-O2A
33	d	408	LHG	O8-C23-C24-C25
32	c	522	LMG	C37-C38-C39-C40
25	b	602	CLA	C10-C11-C12-C13
25	c	510	CLA	CAA-CBA-CGA-O2A
32	m	101	LMG	C36-C37-C38-C39
28	D	405	PL9	C2-C3-C7-C8
25	b	613	CLA	O1A-CGA-O2A-C1
30	A	616	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

140 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	d	401	PHO	2	0
25	C	501	CLA	1	0
25	a	613	CLA	1	0
25	b	604	CLA	4	0
27	c	514	BCR	2	0
29	a	615	SQD	1	0
31	B	626	STE	1	0
33	B	621	LHG	3	0
31	b	621	STE	1	0
25	b	606	CLA	2	0
30	c	518	DGD	2	0
30	c	519	DGD	4	0
25	a	610	CLA	3	0
32	C	515	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	506	CLA	4	0
32	M	101	LMG	1	0
33	d	407	LHG	3	0
25	C	502	CLA	3	0
27	d	404	BCR	2	0
25	b	614	CLA	5	0
32	c	522	LMG	2	0
27	b	617	BCR	2	0
31	t	103	STE	1	0
30	H	103	DGD	3	0
32	d	409	LMG	1	0
25	C	505	CLA	2	0
25	c	505	CLA	3	0
33	D	408	LHG	2	0
21	a	601[C]	OEY	1	0
25	D	402	CLA	4	0
25	H	101	CLA	2	0
25	a	607	CLA	4	0
29	F	102	SQD	1	0
25	c	504	CLA	2	0
25	C	507	CLA	2	0
28	A	612	PL9	5	0
30	A	616	DGD	8	0
21	A	601[C]	OEY	1	0
25	C	512	CLA	1	0
27	T	101	BCR	1	0
25	c	503	CLA	2	0
36	v	201	HEC	2	0
25	C	508	CLA	1	0
25	B	610	CLA	2	0
25	B	603	CLA	2	0
29	l	101	SQD	2	0
31	B	619	STE	1	0
27	B	616	BCR	2	0
25	c	501	CLA	2	0
25	b	608	CLA	4	0
25	b	605	CLA	3	0
28	d	405	PL9	2	0
31	D	410	STE	3	0
32	m	101	LMG	4	0
32	c	520	LMG	1	0
32	D	406	LMG	4	0

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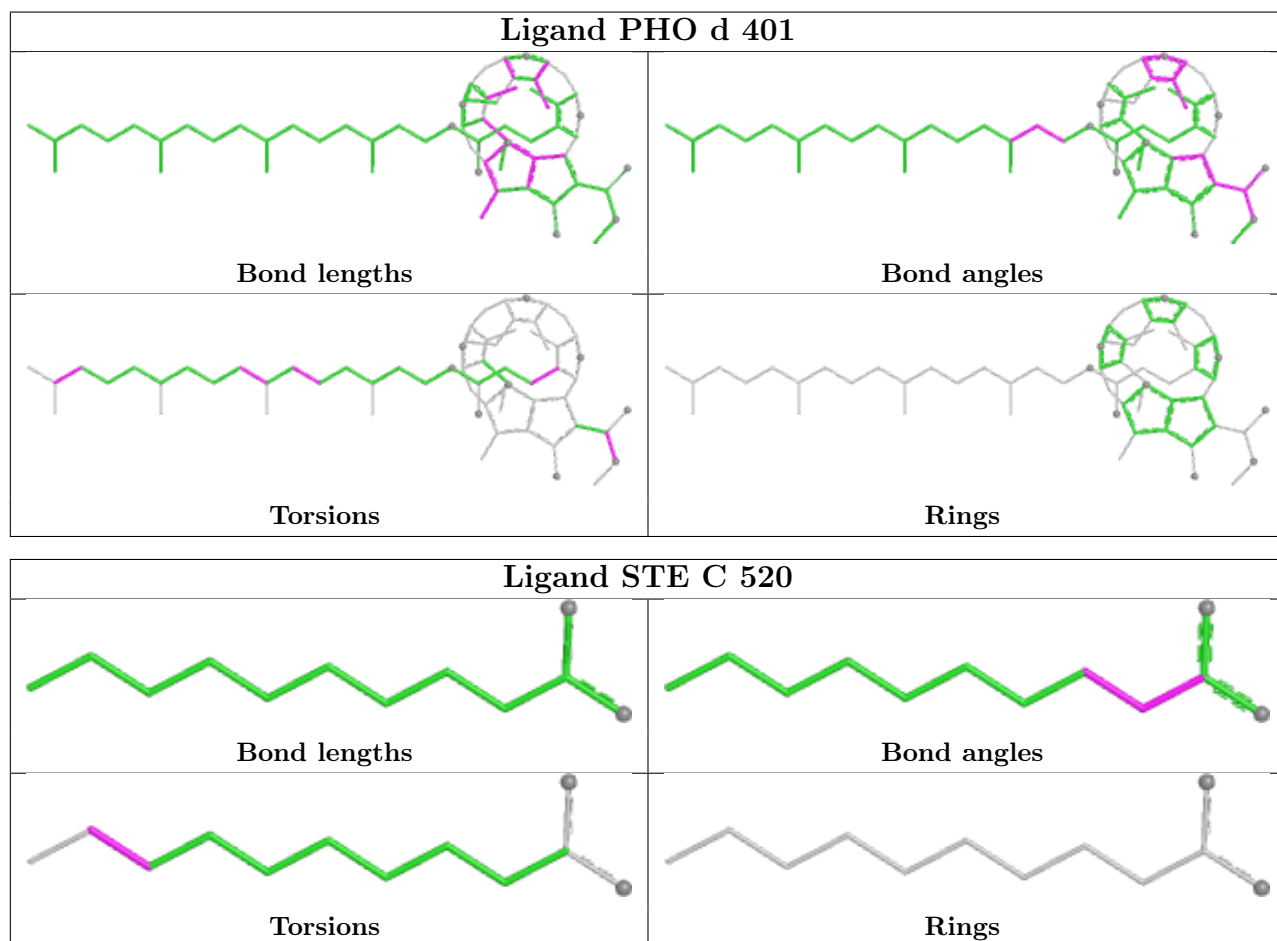
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	606	CLA	2	0
33	B	622	LHG	1	0
25	B	608	CLA	3	0
25	B	605	CLA	2	0
25	B	615	CLA	2	0
25	C	506	CLA	2	0
33	E	101	LHG	1	0
31	b	622	STE	1	0
25	b	603	CLA	2	0
25	c	509	CLA	2	0
35	e	101	HEM	2	0
27	H	102	BCR	2	0
32	C	519	LMG	1	0
27	x	101	BCR	3	0
25	C	510	CLA	2	0
25	c	510	CLA	1	0
30	h	102	DGD	1	0
25	D	403	CLA	3	0
25	d	403	CLA	3	0
26	A	609	PHO	3	0
25	c	513	CLA	2	0
25	b	602	CLA	4	0
25	b	609	CLA	3	0
31	H	104	STE	3	0
27	C	514	BCR	5	0
25	c	507	CLA	3	0
25	B	606	CLA	4	0
30	a	616	DGD	1	0
33	D	407	LHG	2	0
27	K	103	BCR	1	0
29	A	614	SQD	2	0
25	b	601	CLA	5	0
25	B	614	CLA	2	0
27	K	101	BCR	2	0
28	D	405	PL9	1	0
30	C	518	DGD	1	0
25	c	511	CLA	3	0
31	x	102	STE	2	0
25	B	601	CLA	2	0
25	B	613	CLA	4	0
31	b	619	STE	2	0
32	D	409	LMG	1	0

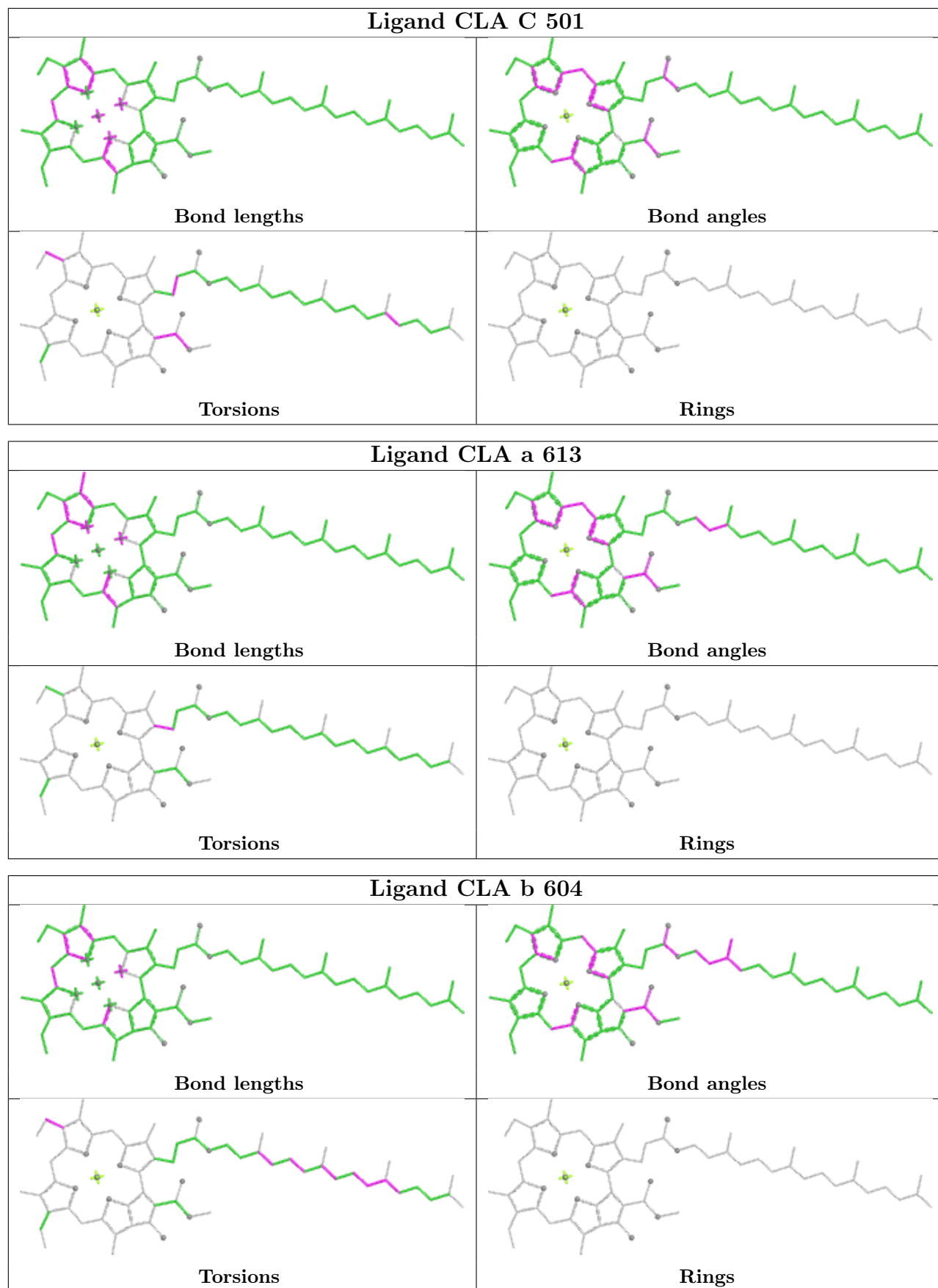
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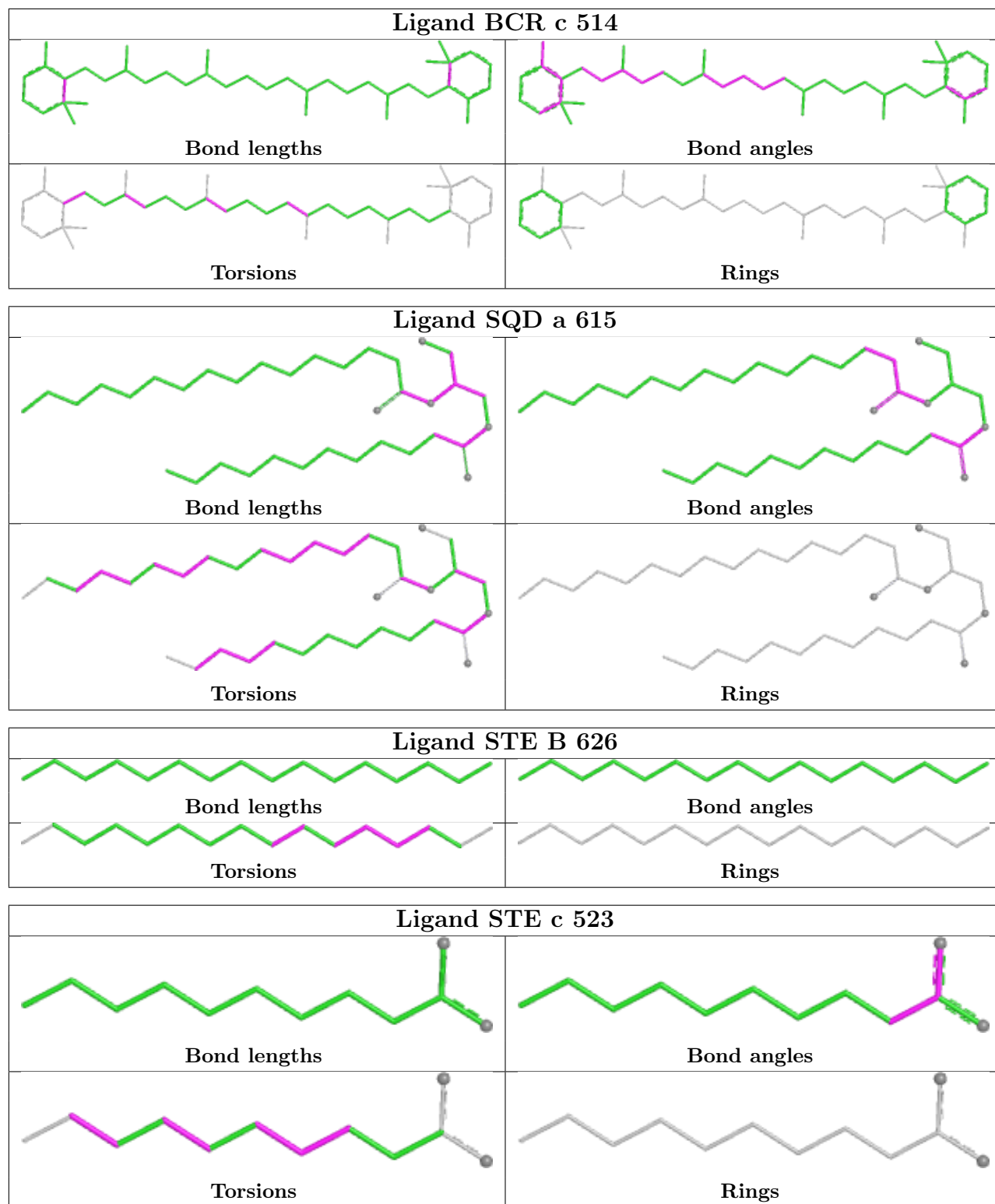
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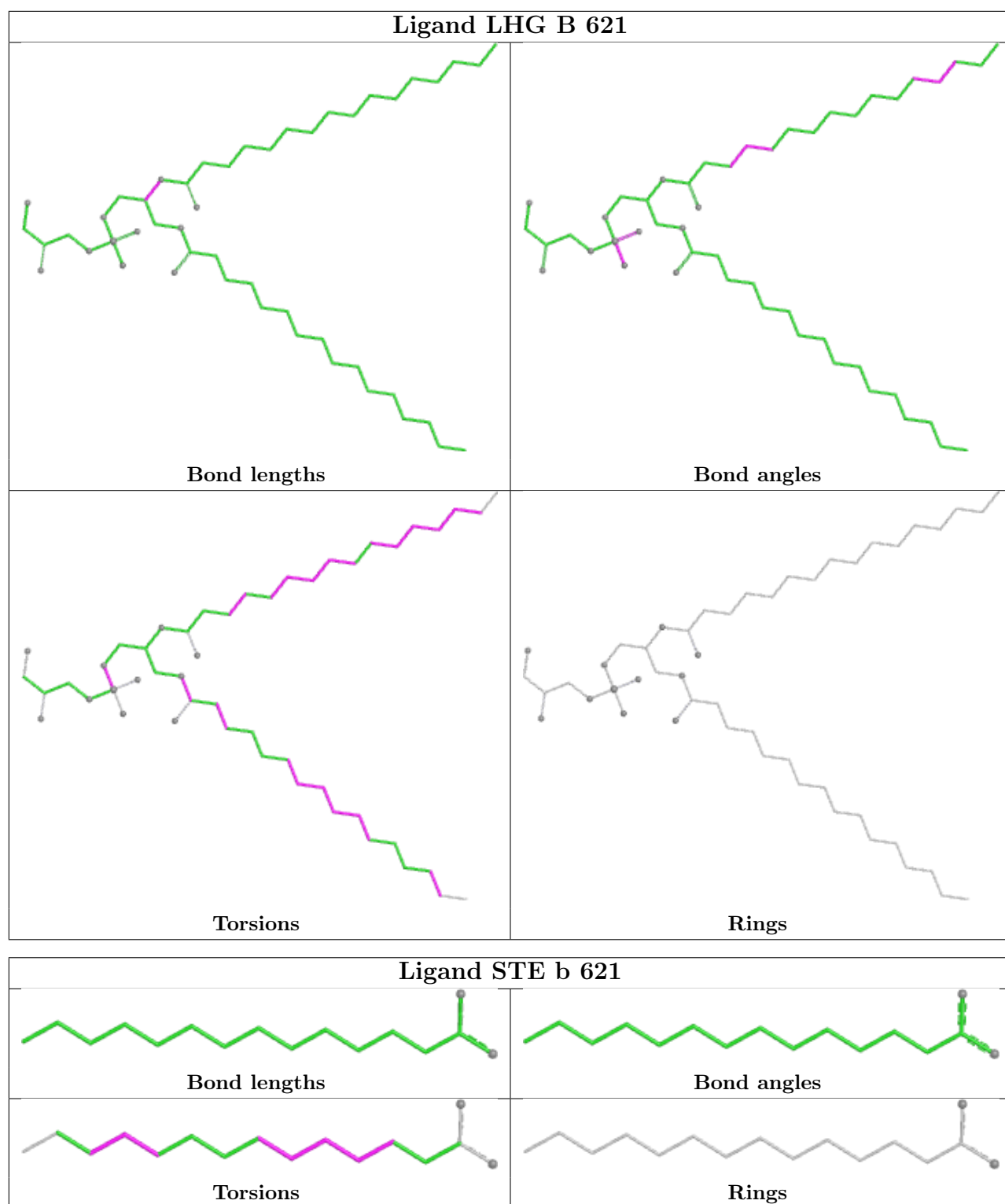
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	509	CLA	3	0
25	A	610	CLA	1	0
35	F	101	HEM	2	0
27	t	101	BCR	1	0
27	k	101	BCR	1	0
27	K	102	BCR	3	0
32	c	524	LMG	3	0
25	d	402	CLA	1	0
25	C	503	CLA	1	0
25	b	615	CLA	3	0
25	B	604	CLA	5	0
25	b	610	CLA	1	0
25	b	613	CLA	2	0
27	D	404	BCR	1	0
29	L	101	SQD	2	0
29	a	614	SQD	1	0
25	c	508	CLA	1	0
27	c	515	BCR	6	0
31	a	617	STE	1	0
33	d	408	LHG	1	0
25	B	612	CLA	3	0
21	A	601[B]	OEY	1	0
25	B	609	CLA	2	0
33	d	406	LHG	7	0
27	a	611	BCR	1	0
31	I	101	STE	3	0
29	f	101	SQD	3	0
30	C	517	DGD	2	0
25	C	504	CLA	1	0
28	a	612	PL9	5	0
31	c	521	STE	2	0
25	B	602	CLA	4	0
25	C	511	CLA	1	0
27	c	516	BCR	3	0
25	b	611	CLA	3	0
25	c	512	CLA	3	0
25	b	612	CLA	3	0
25	h	101	CLA	4	0
21	a	601[B]	OEY	1	0
30	c	517	DGD	3	0
25	B	611	CLA	4	0
27	B	617	BCR	1	0

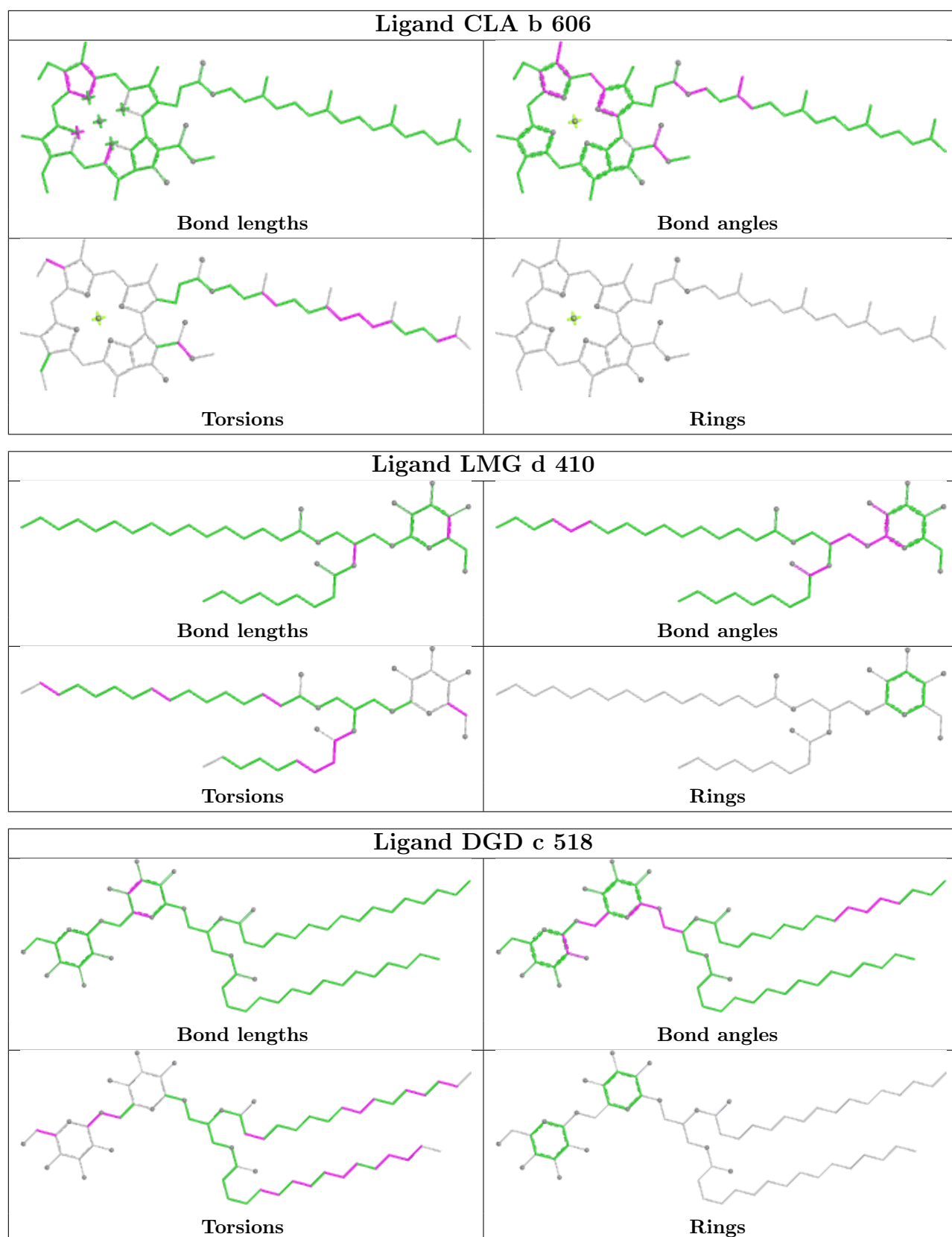
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

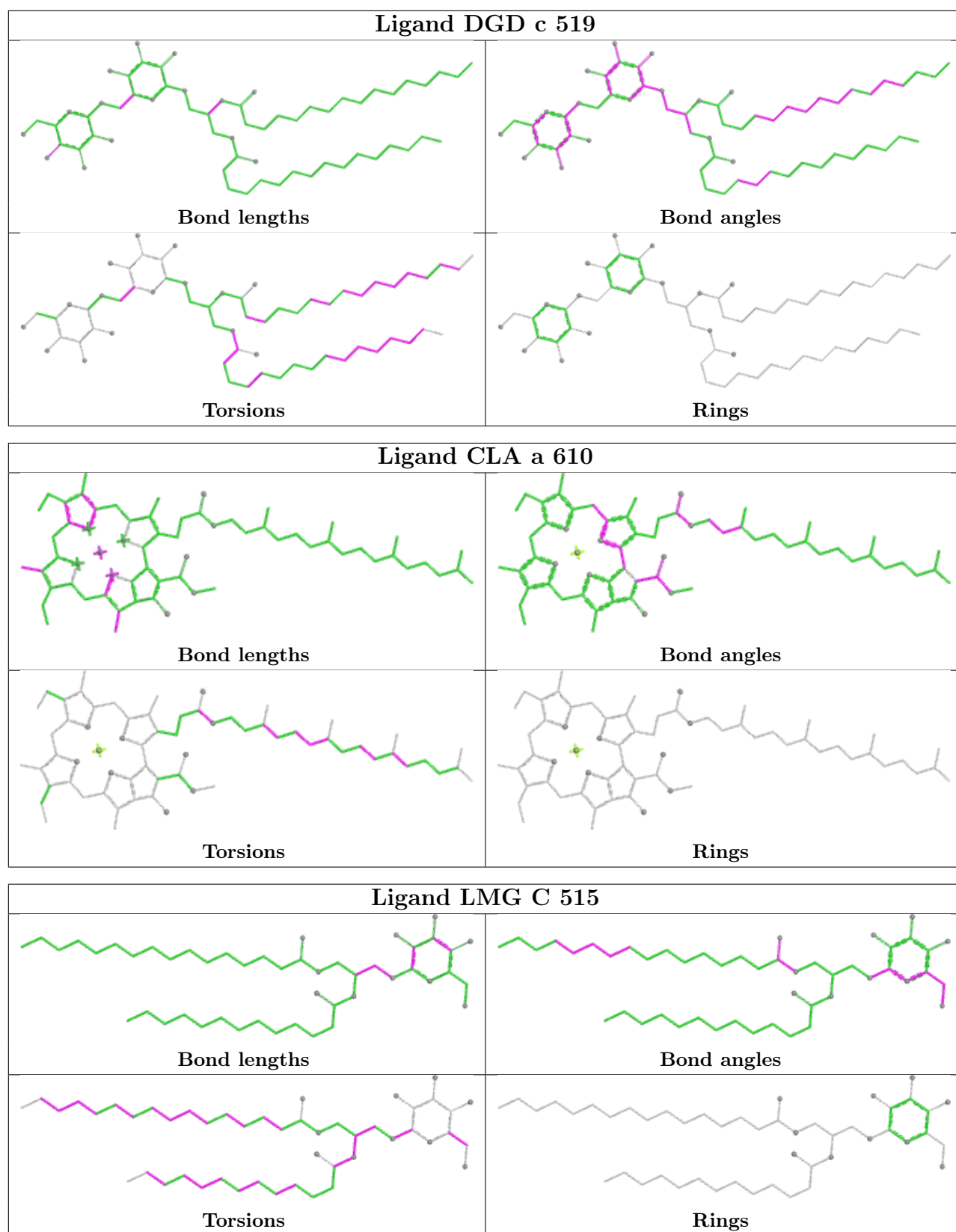


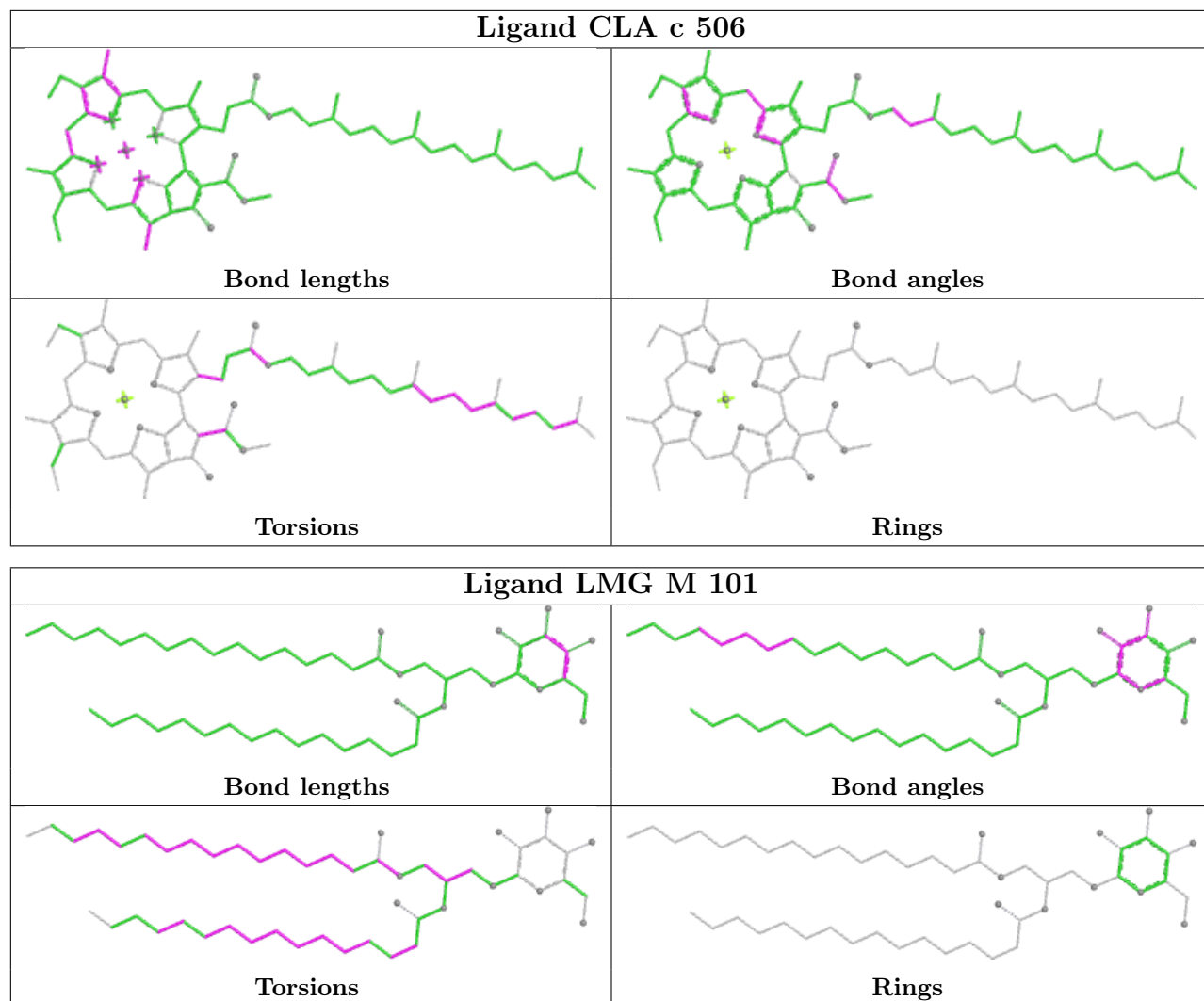


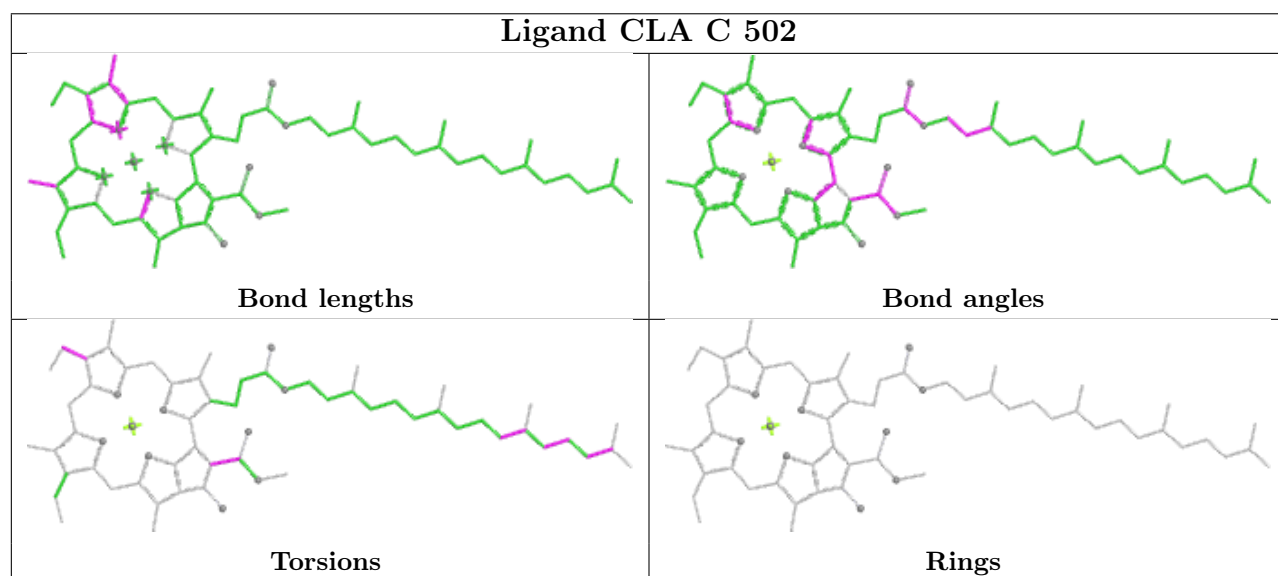
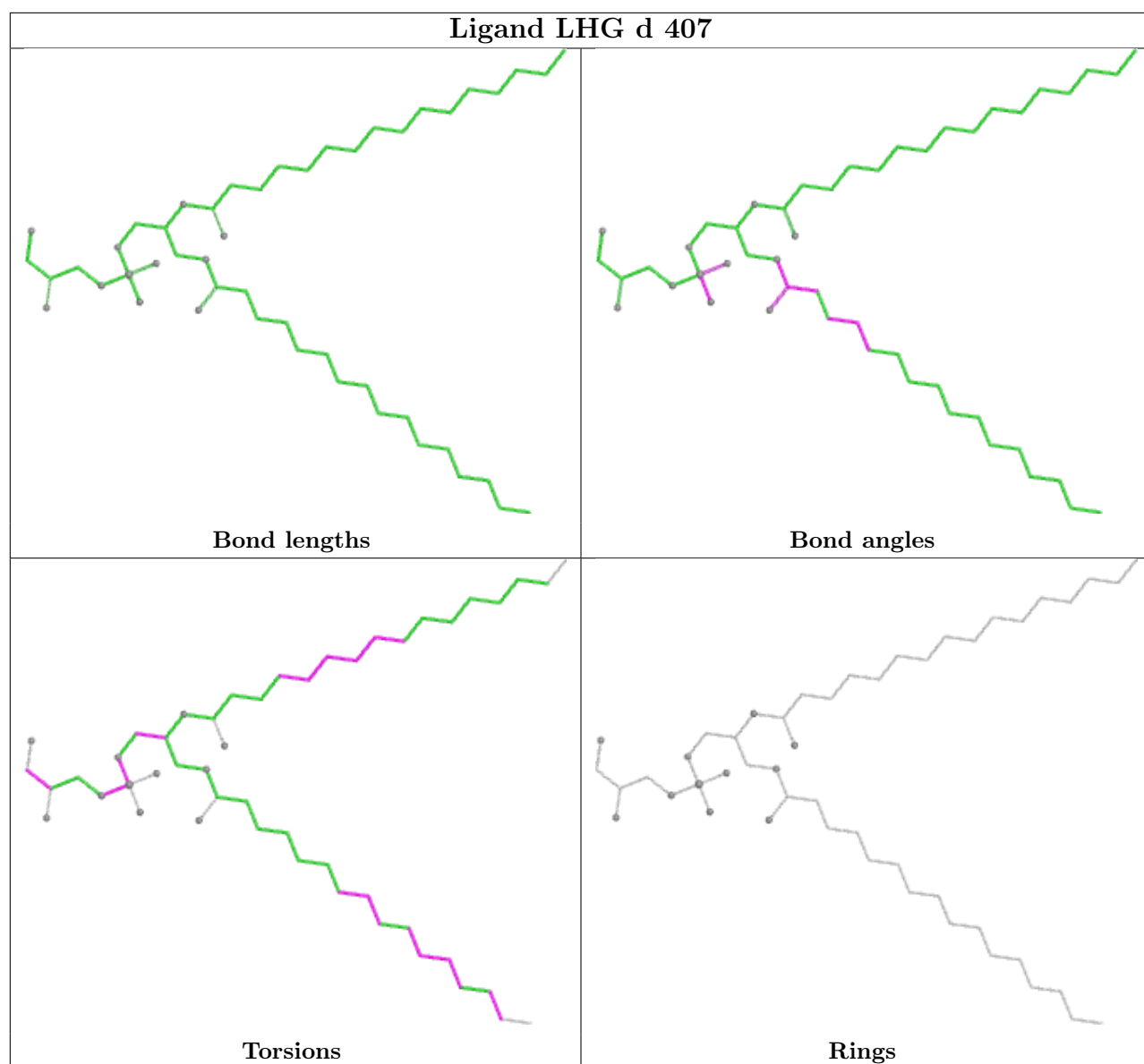


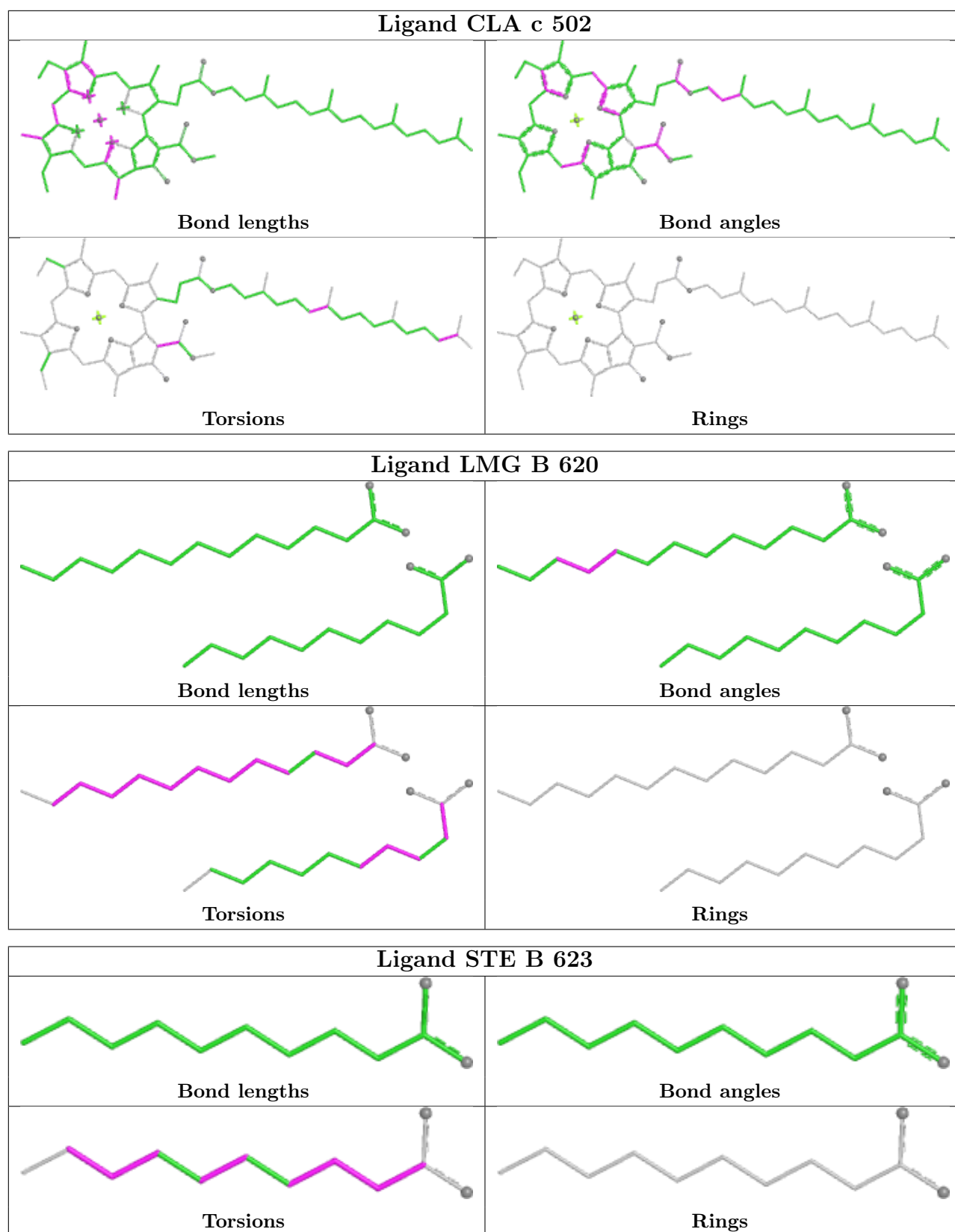


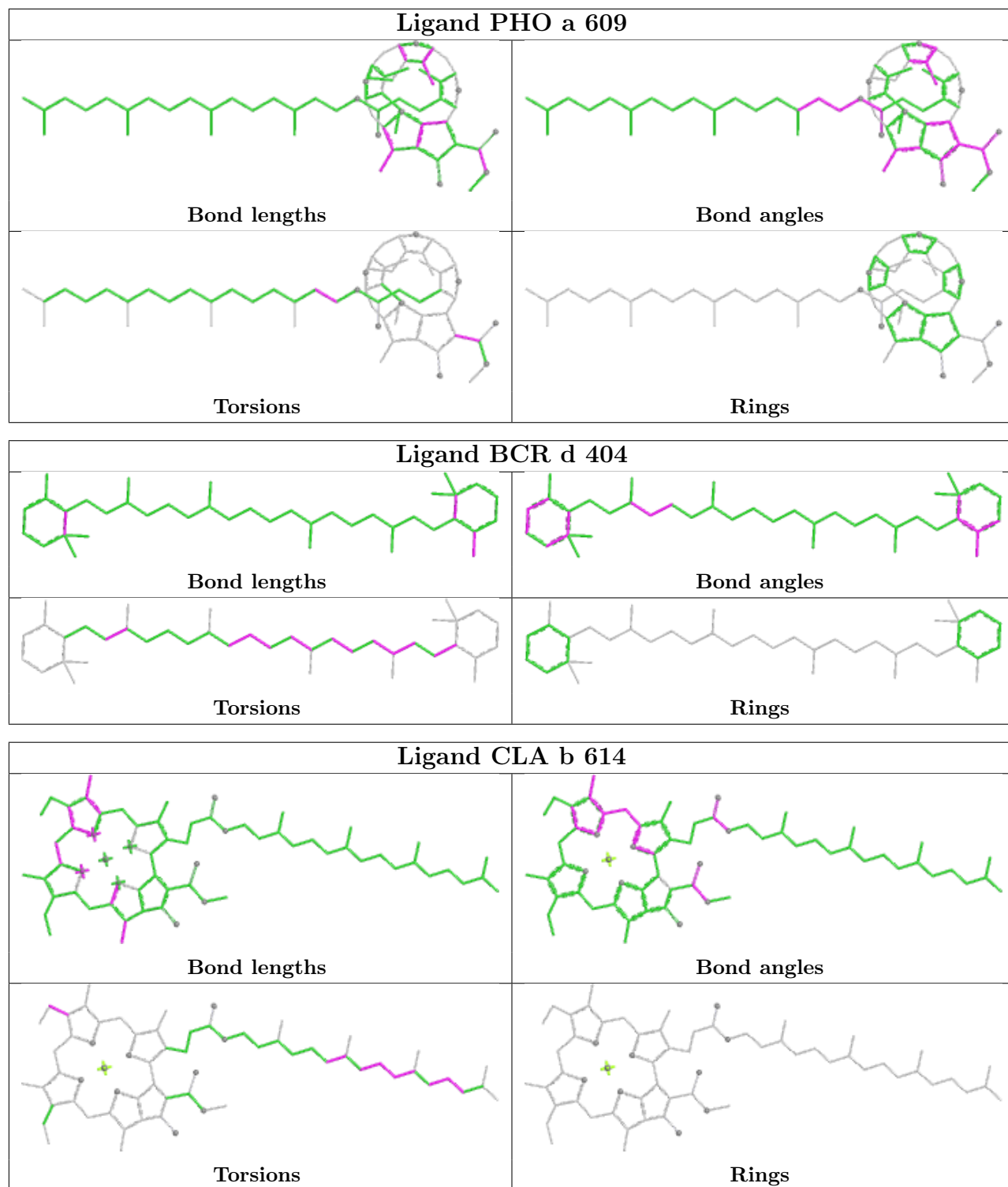


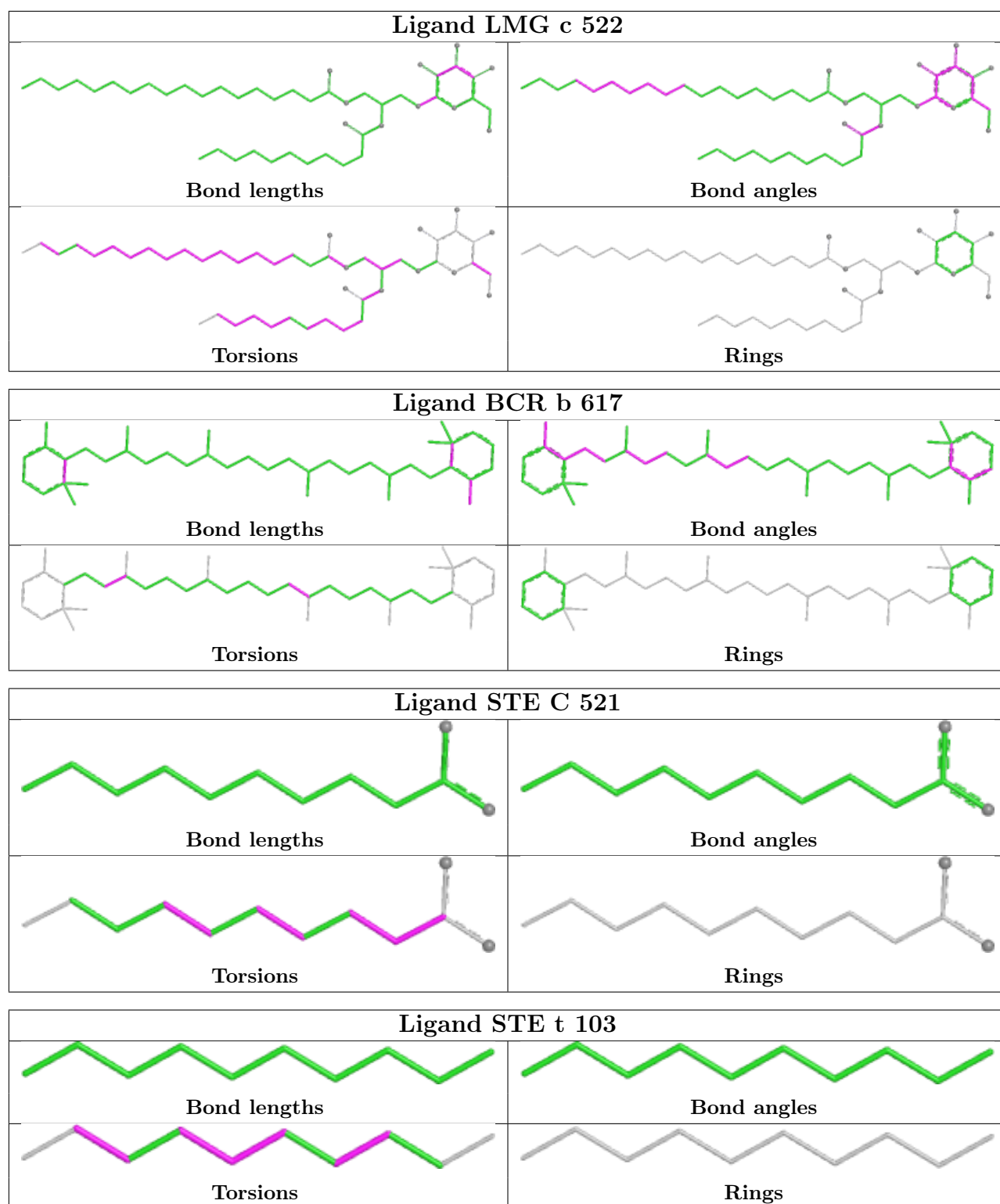


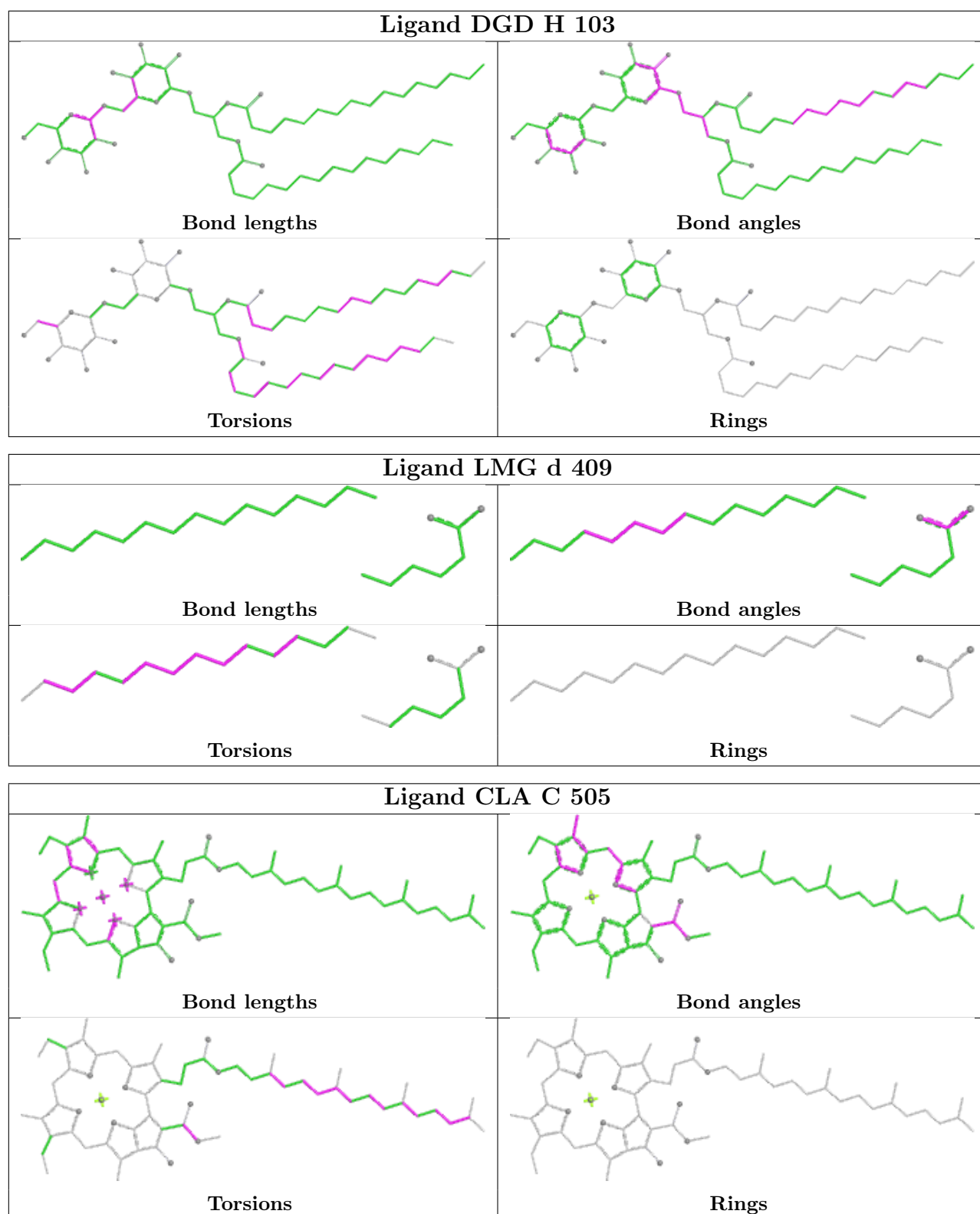


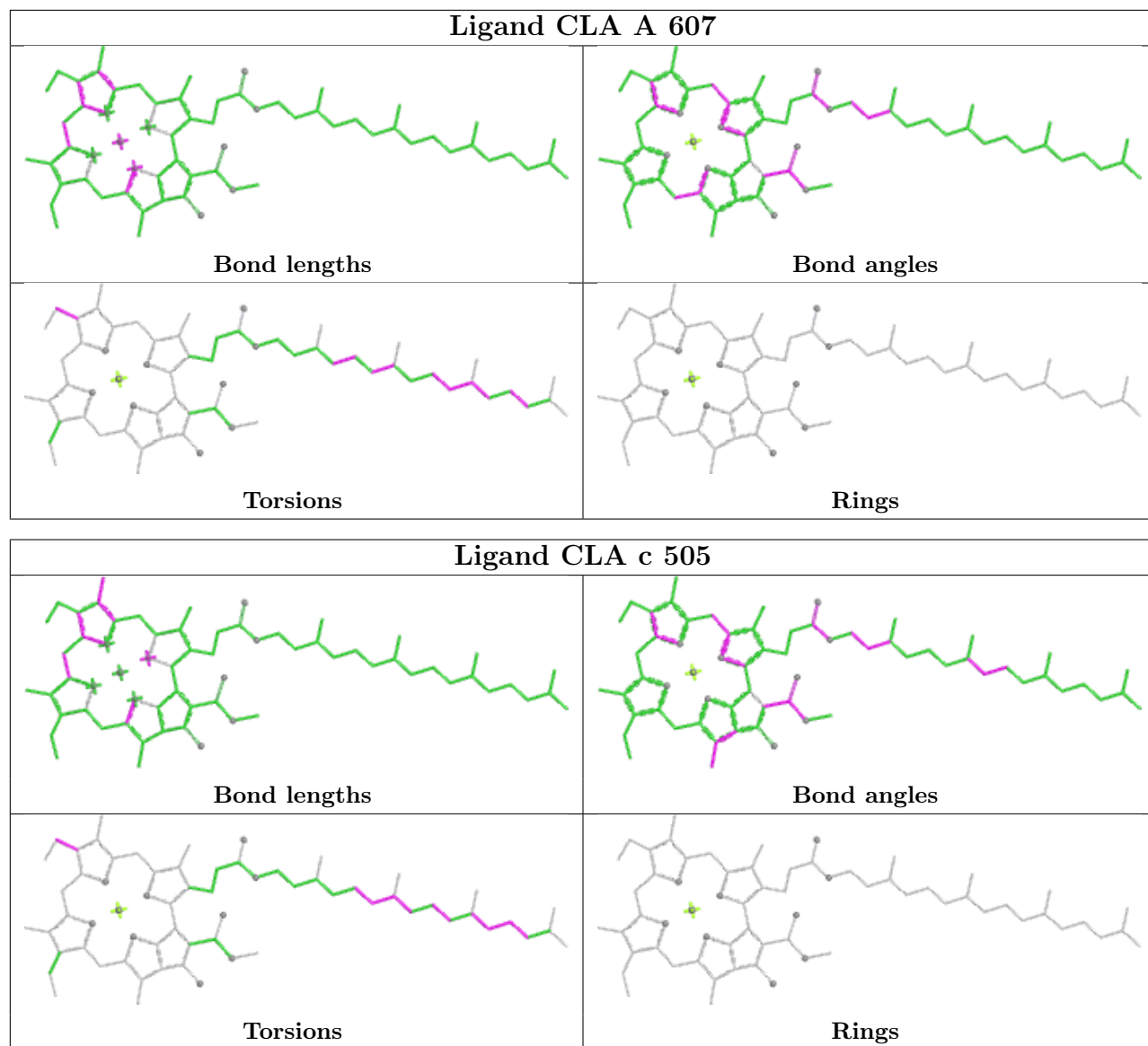


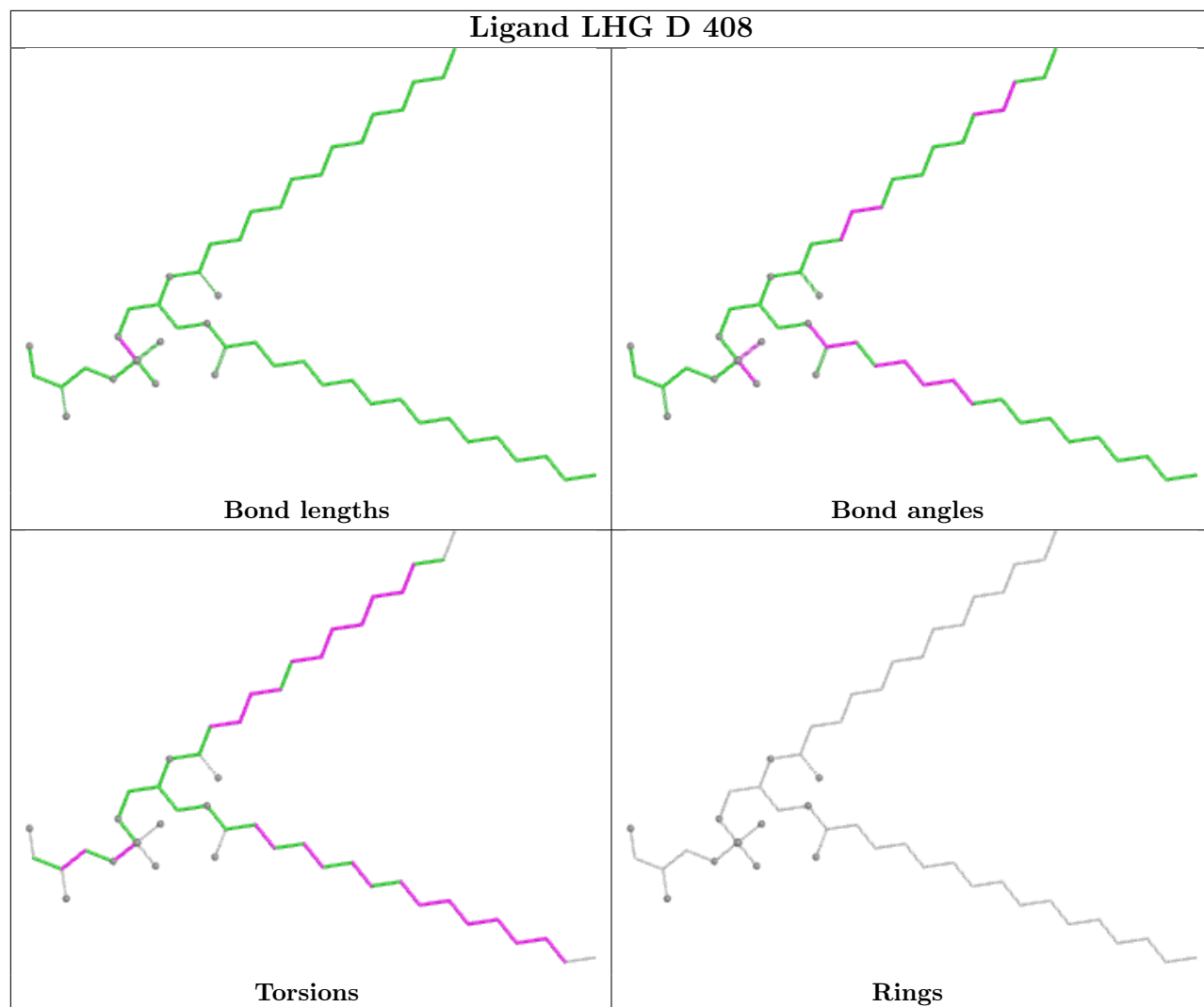


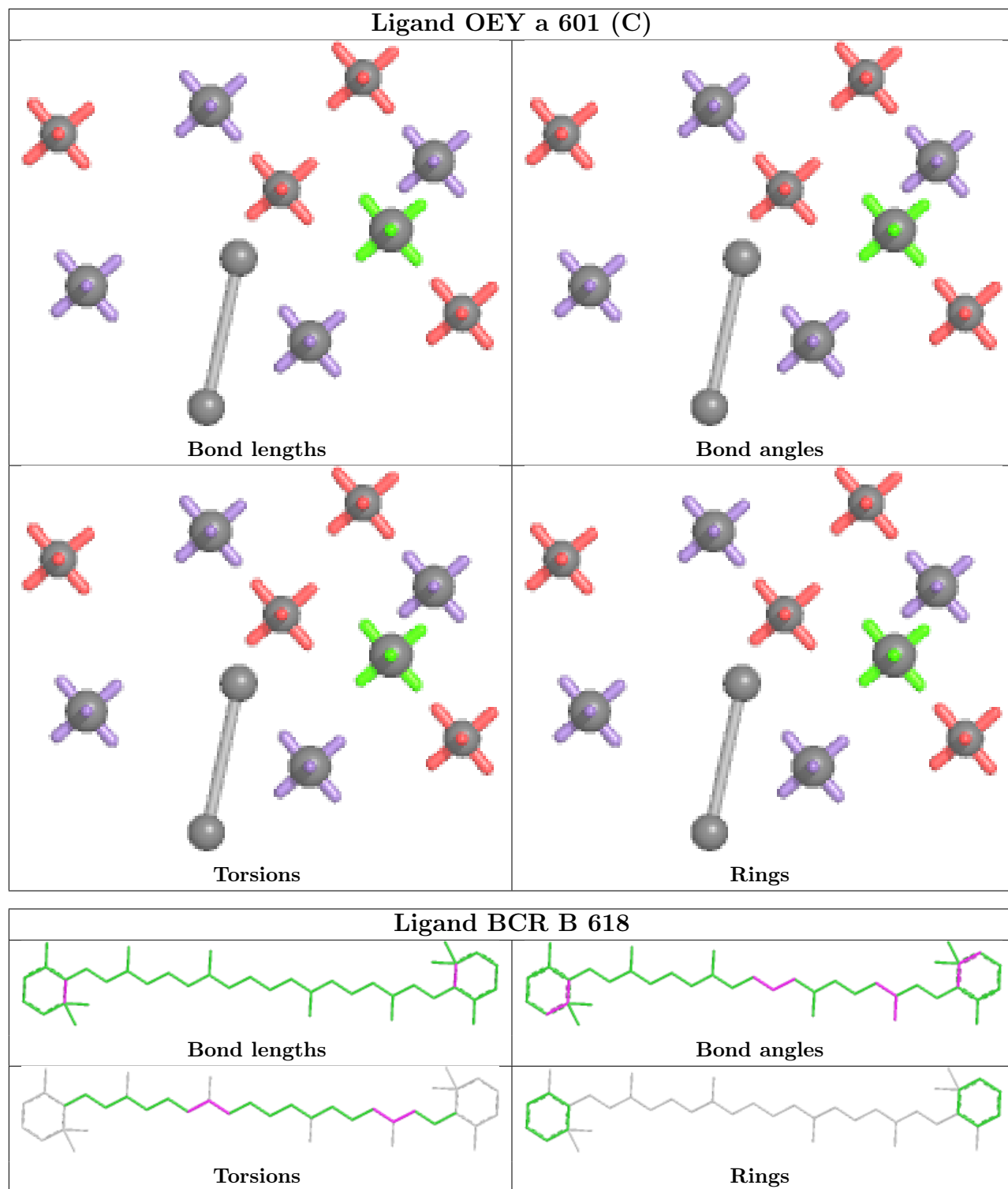


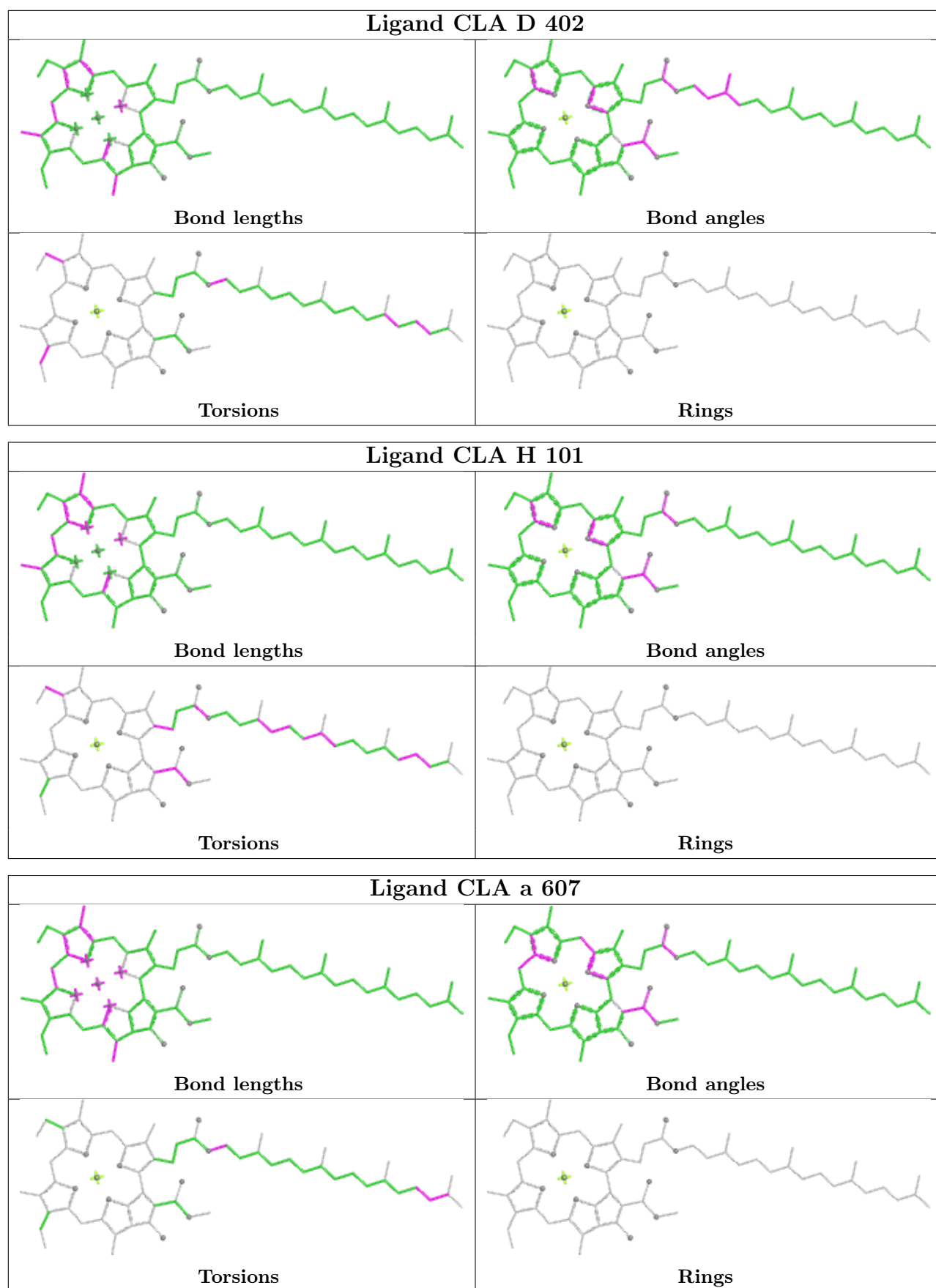


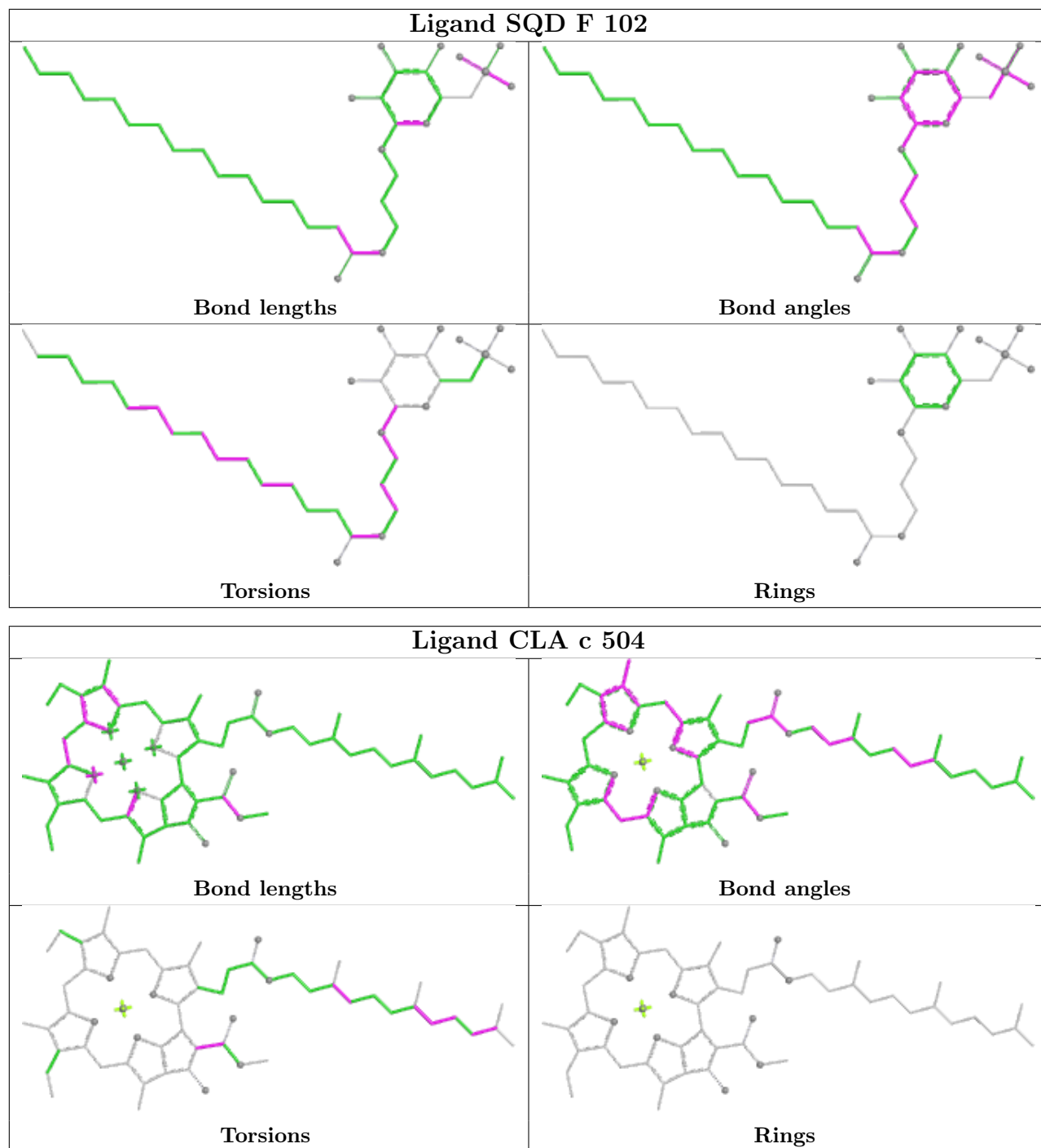


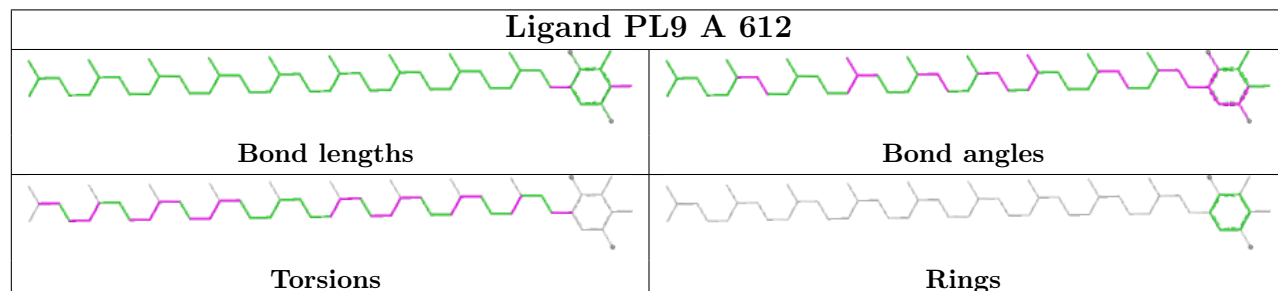
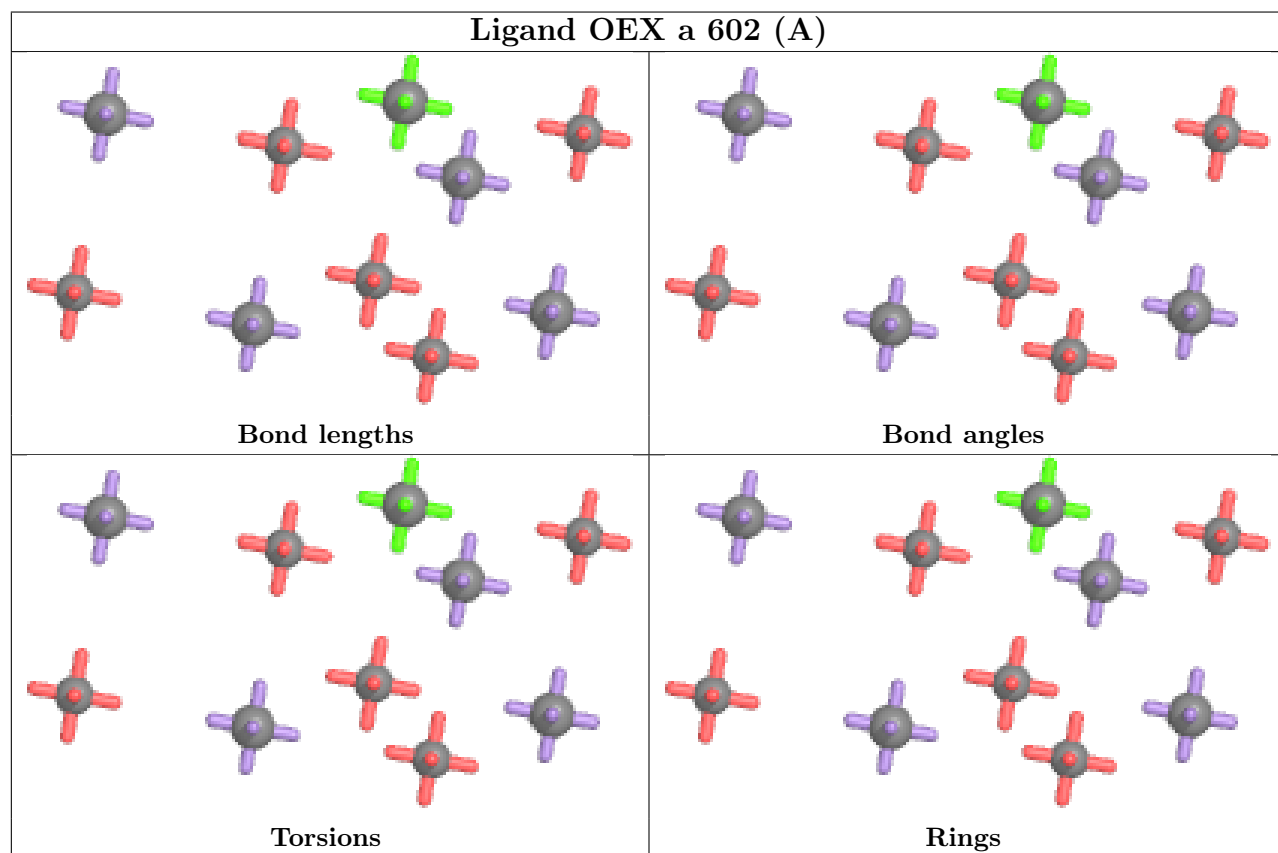
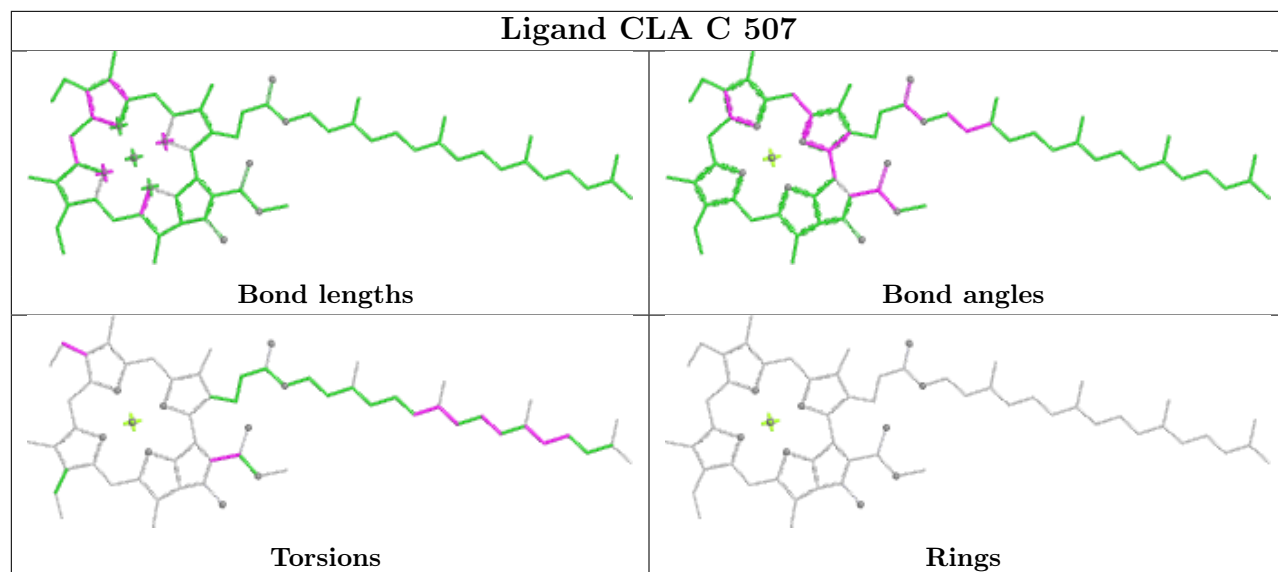


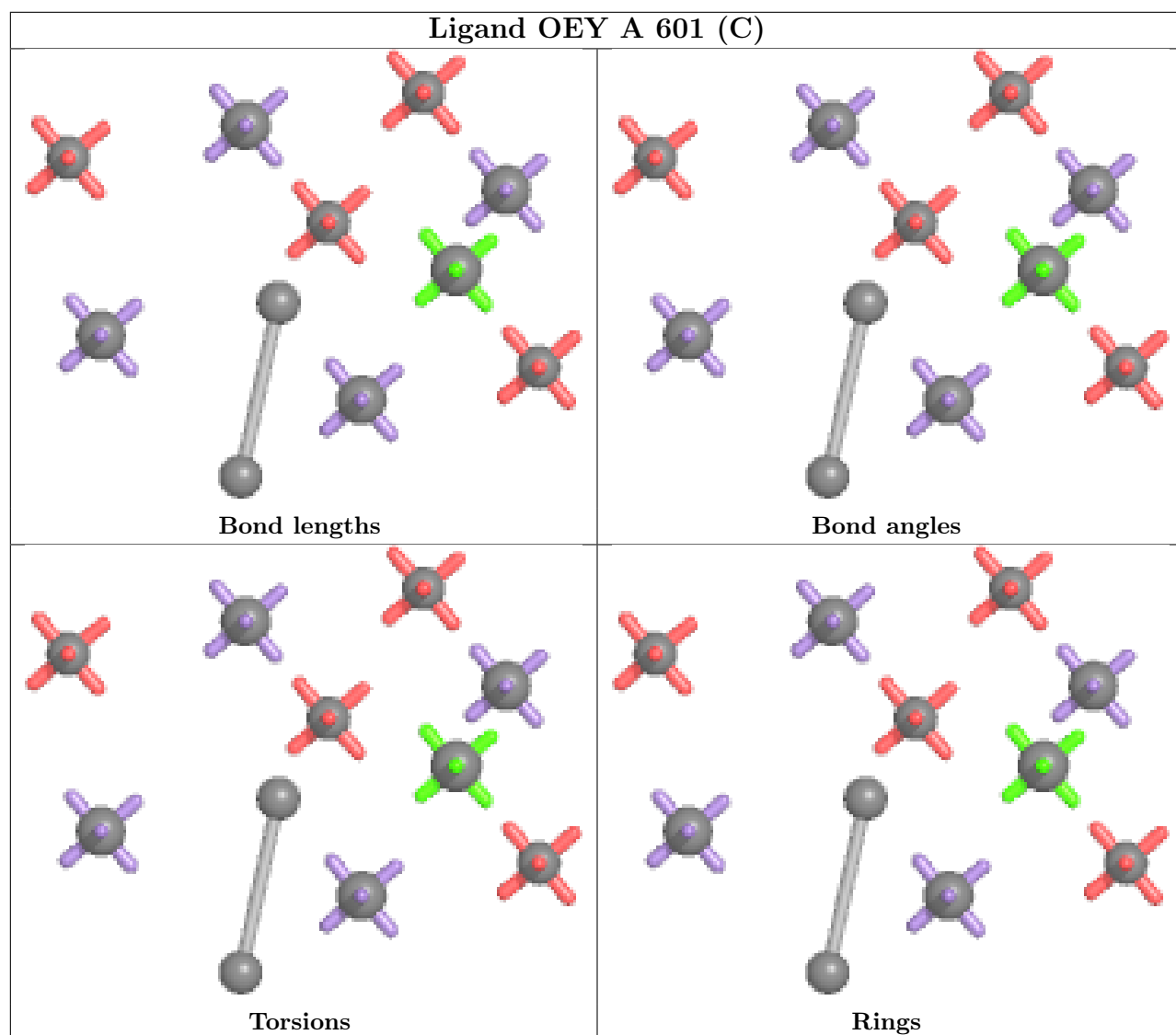
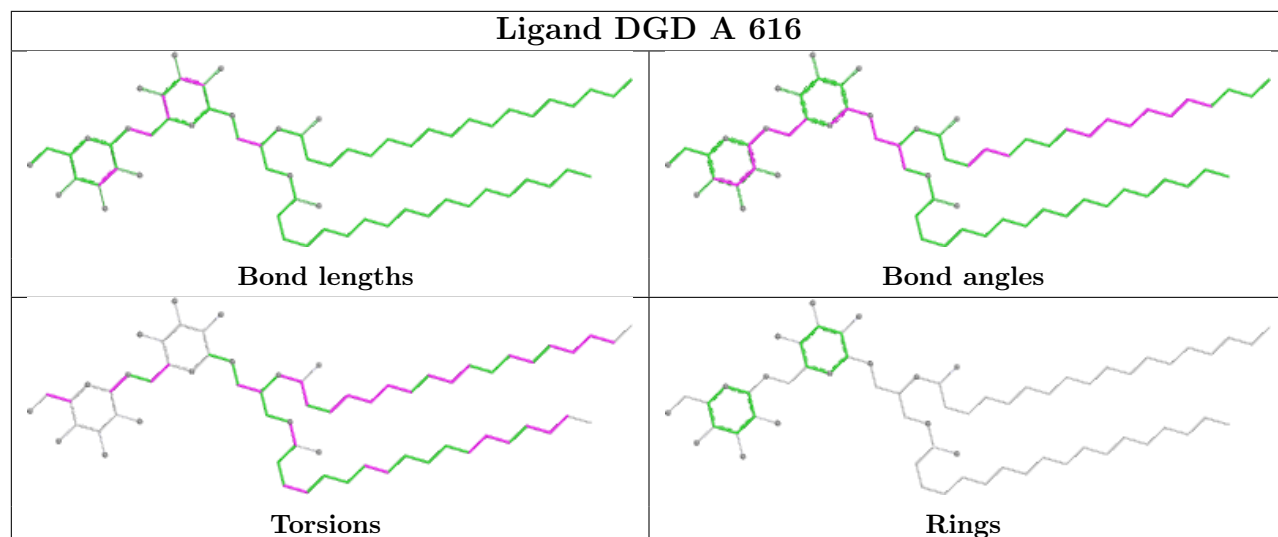


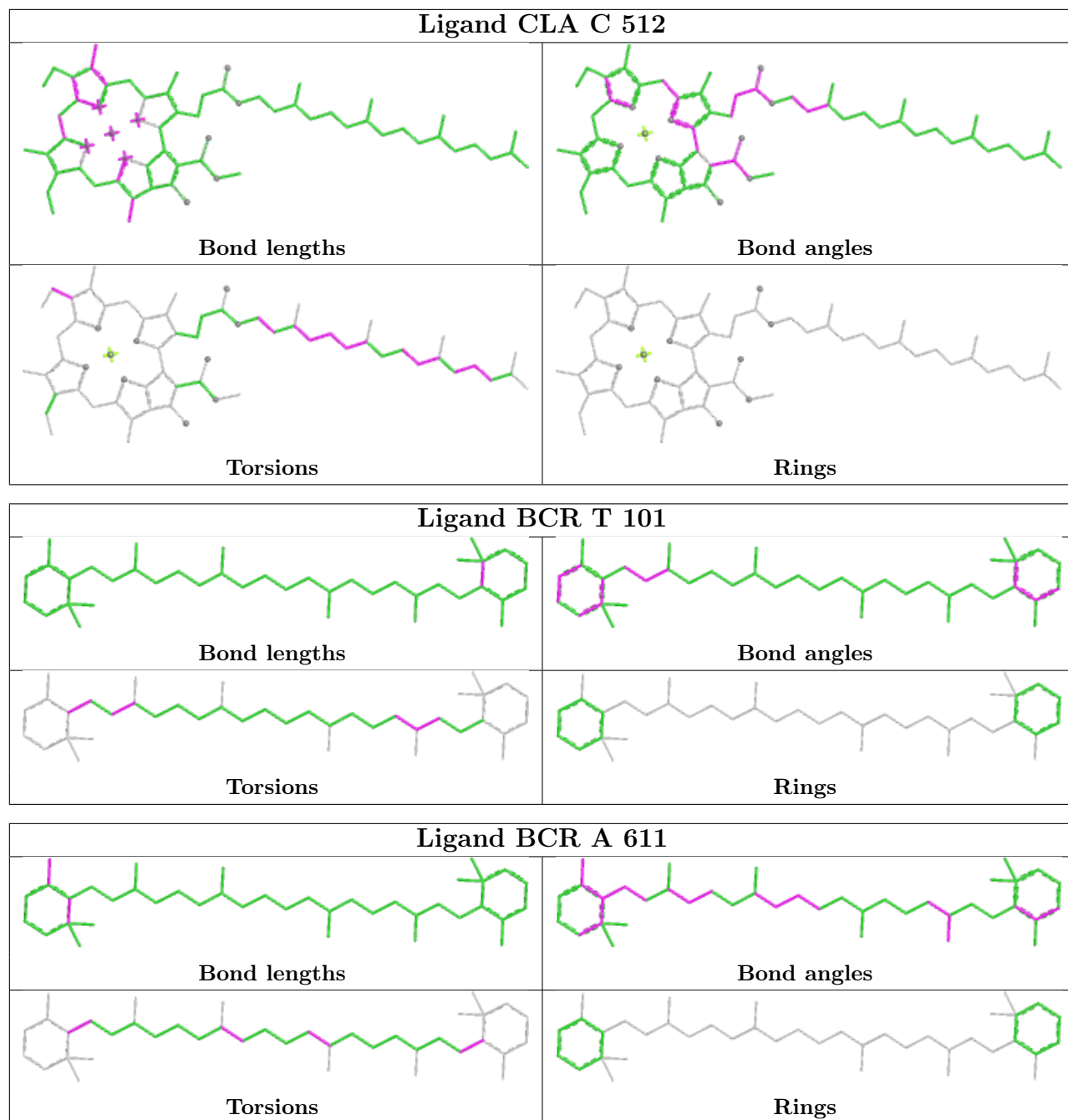


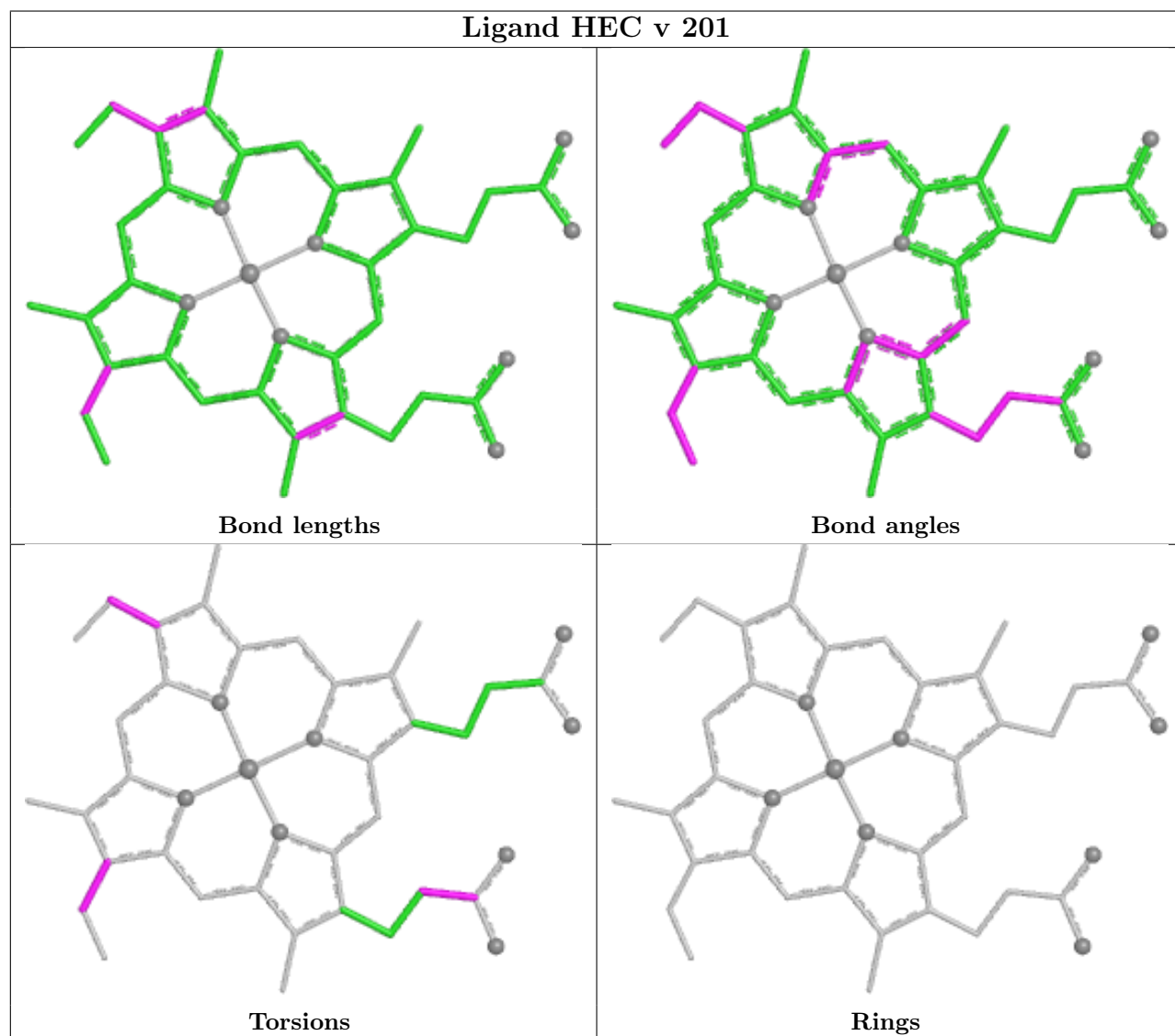
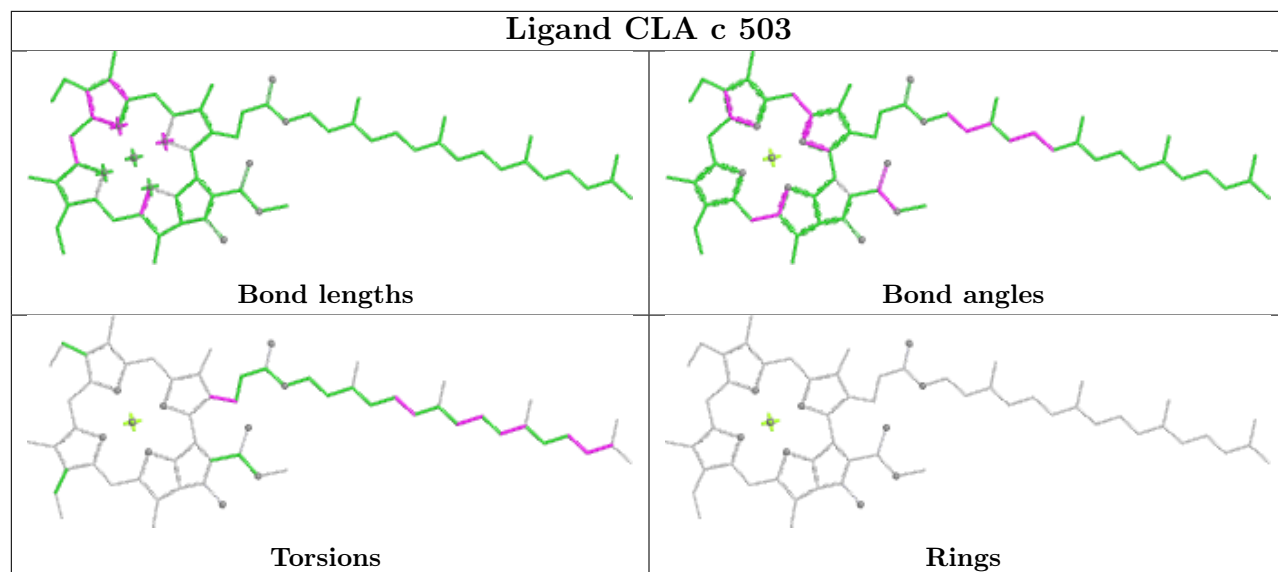


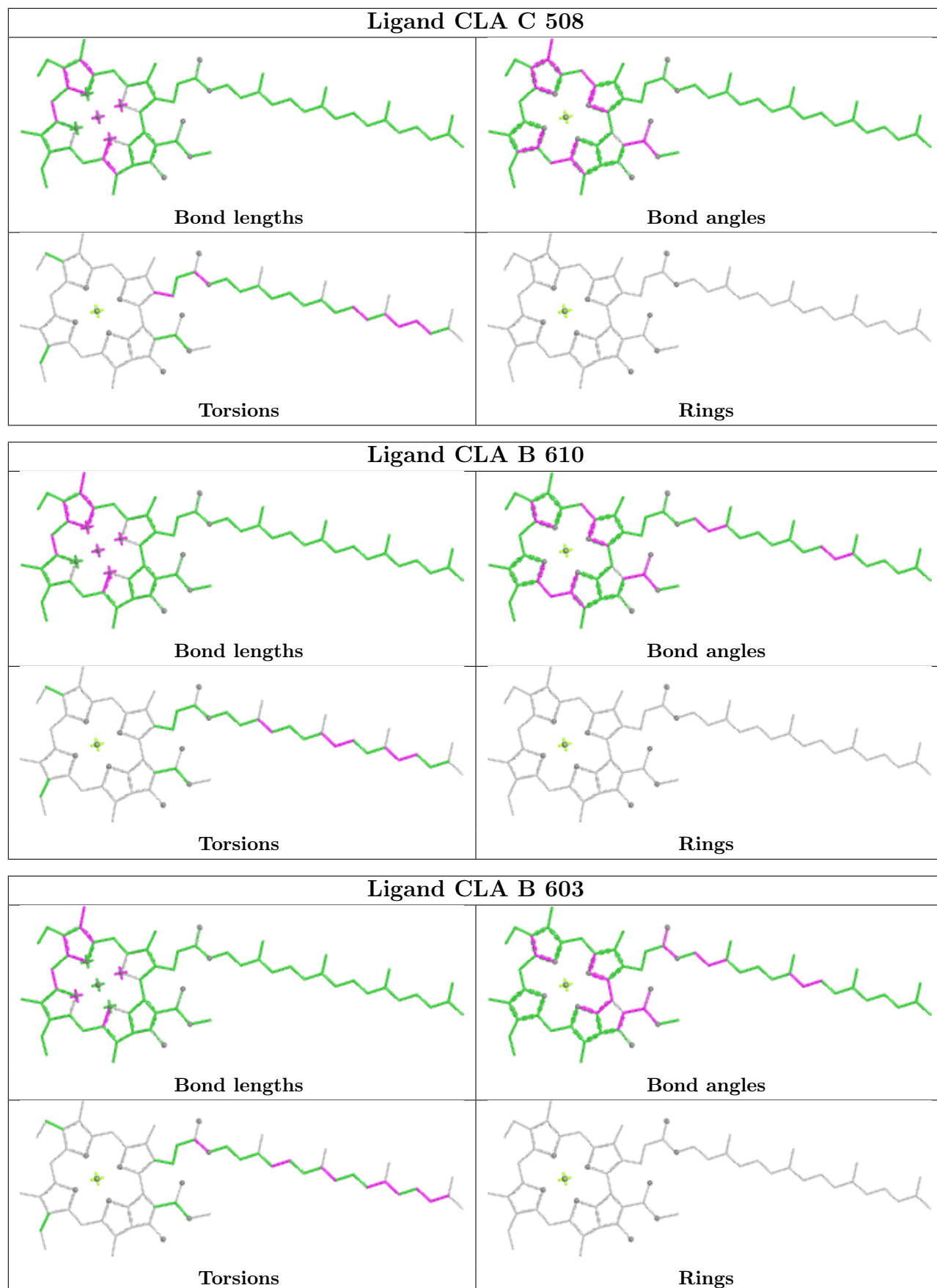


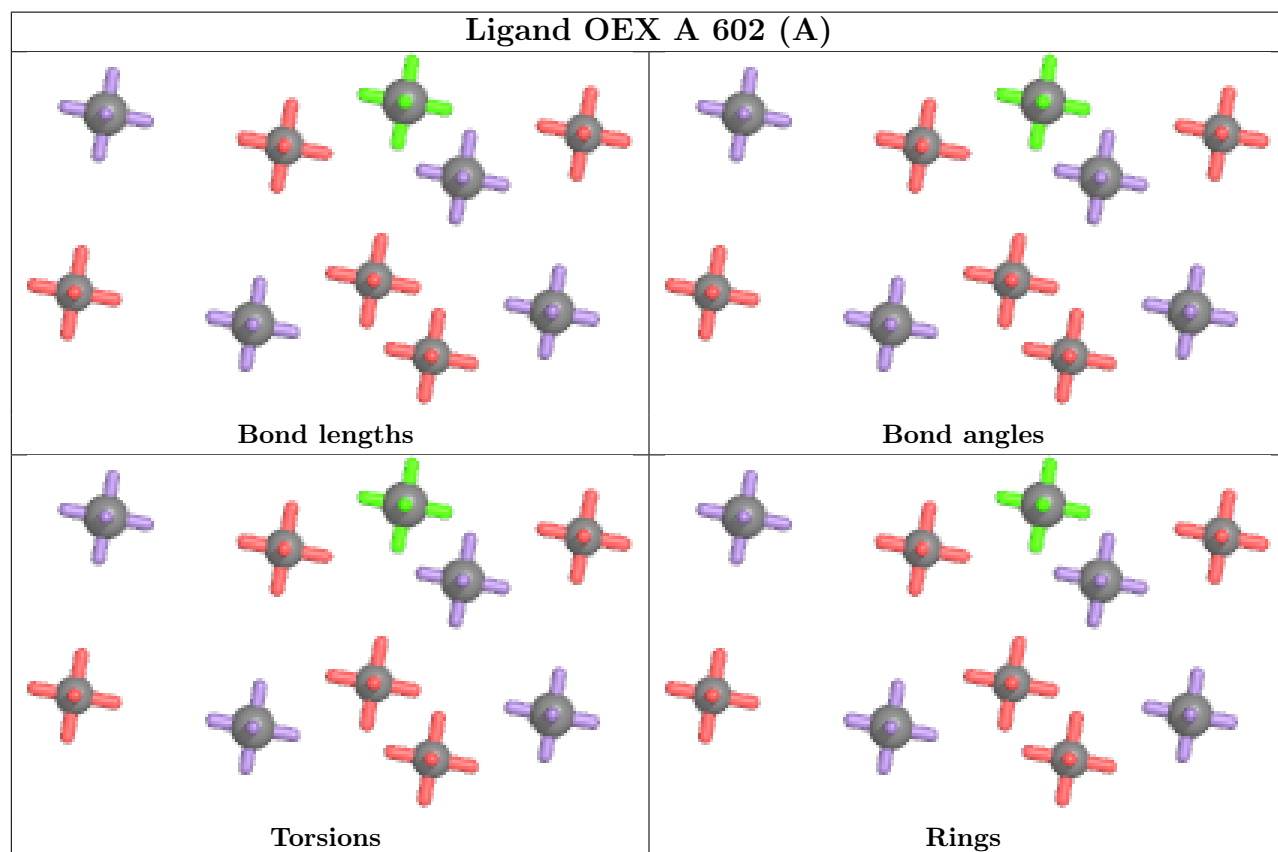
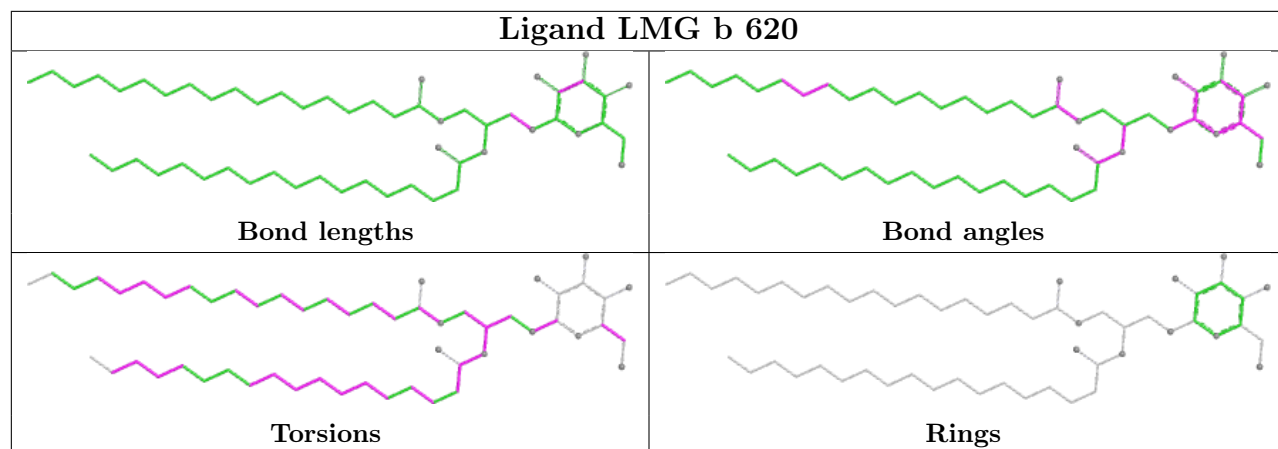


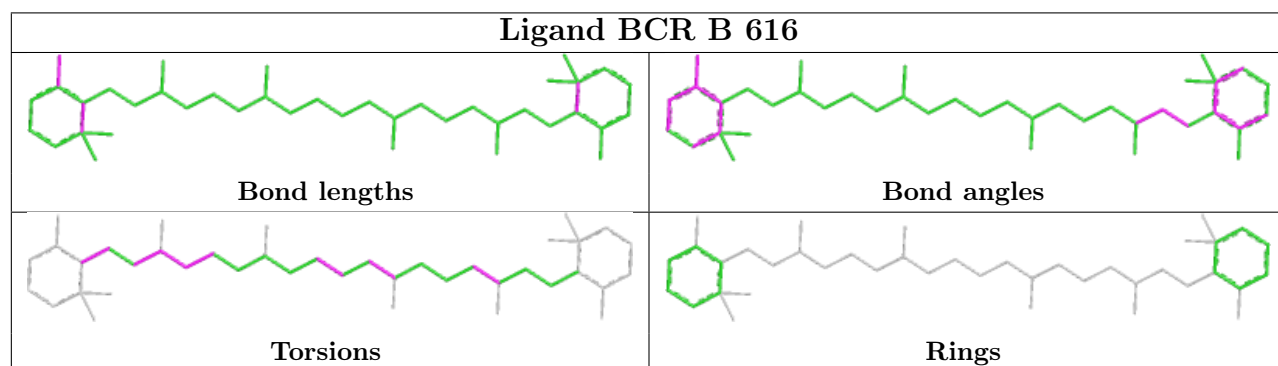
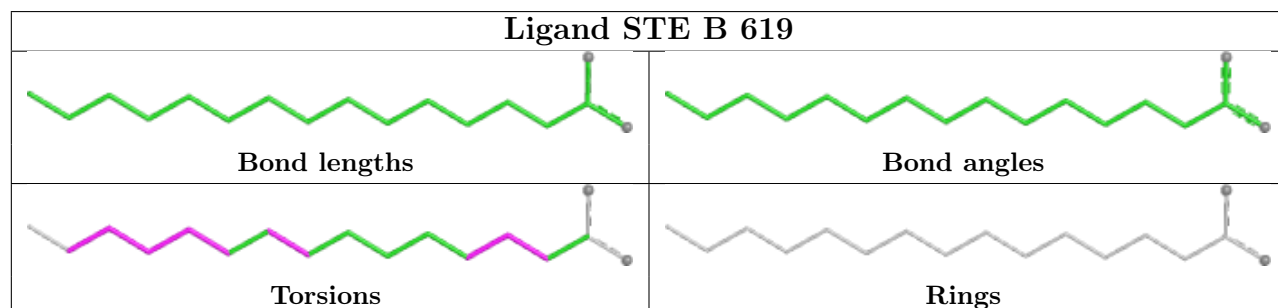
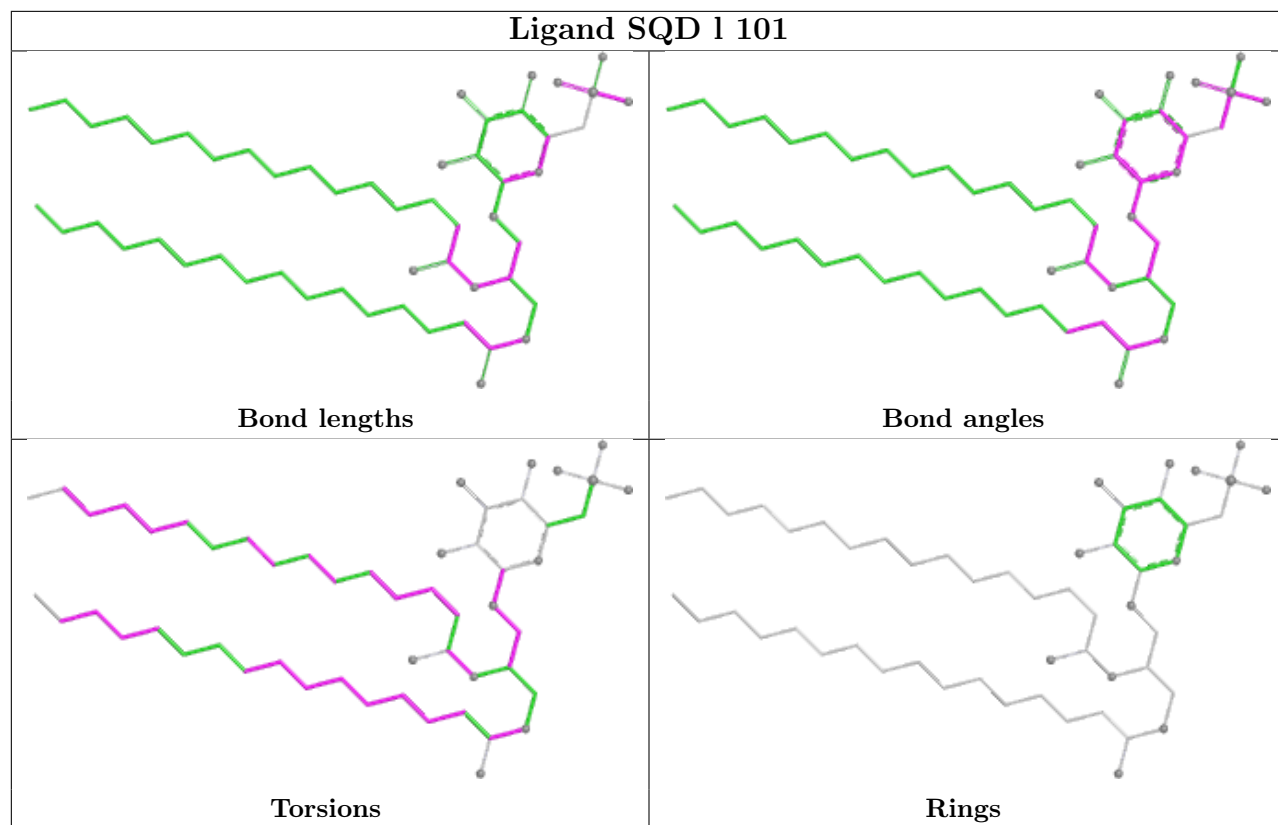


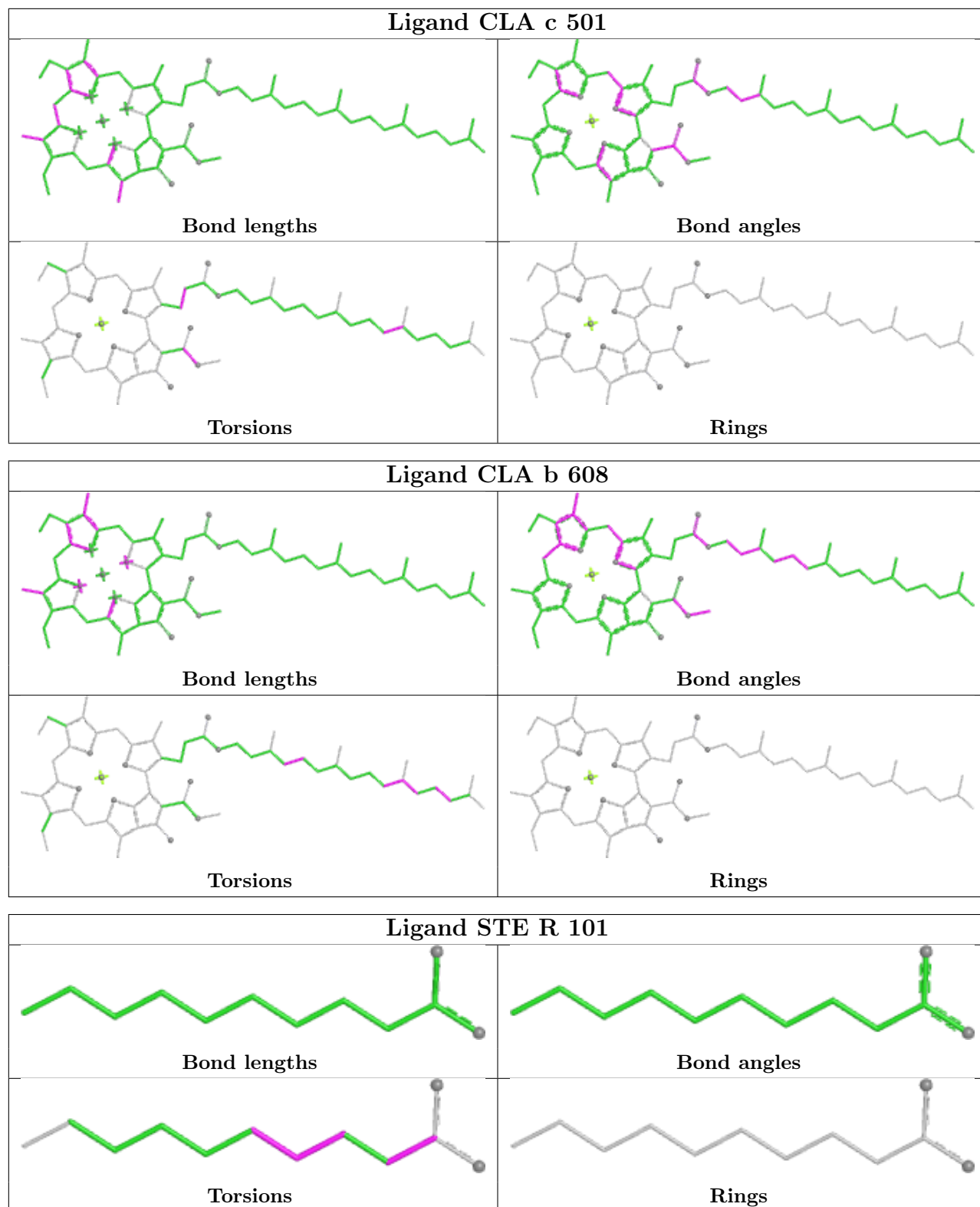


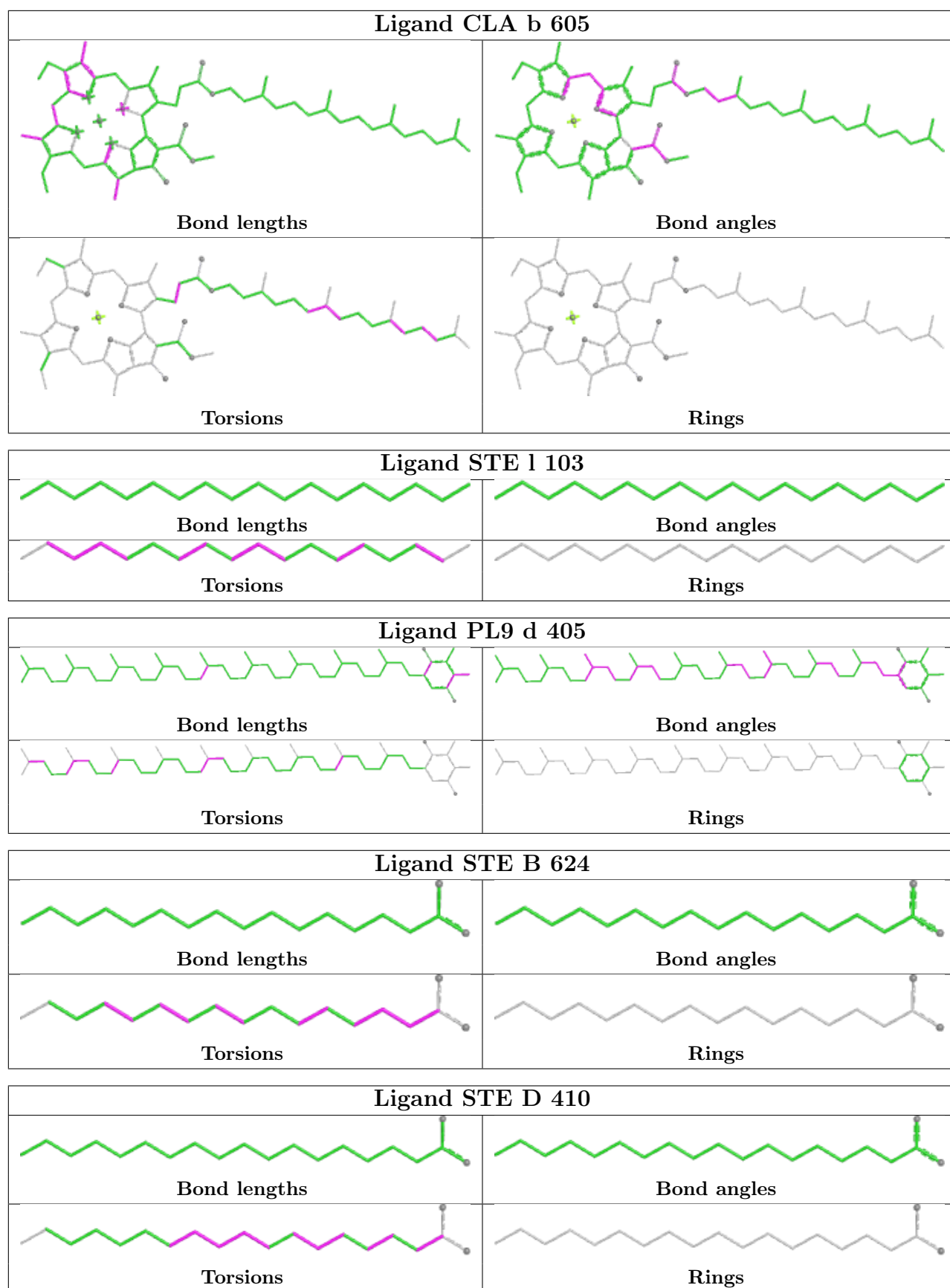


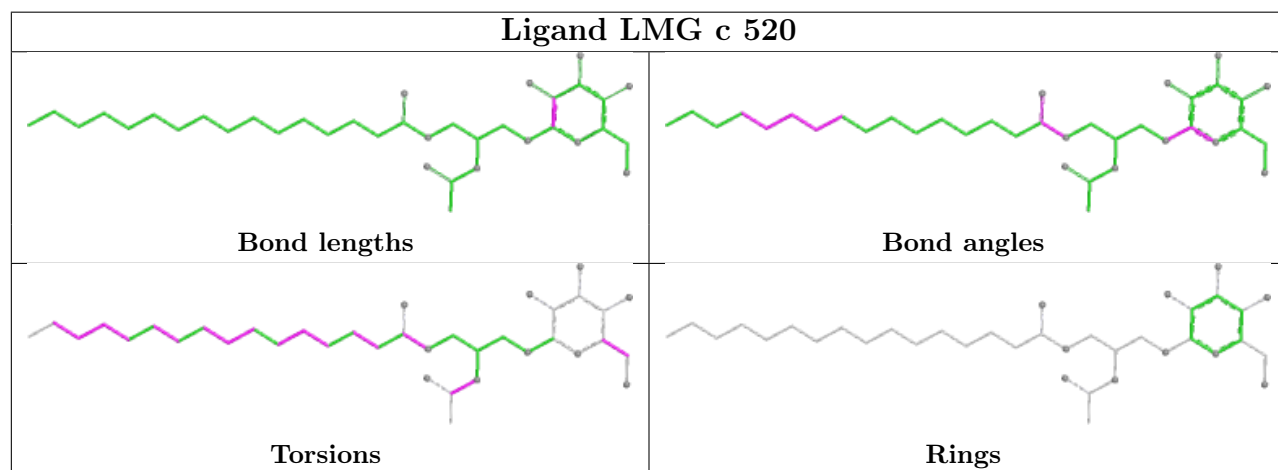
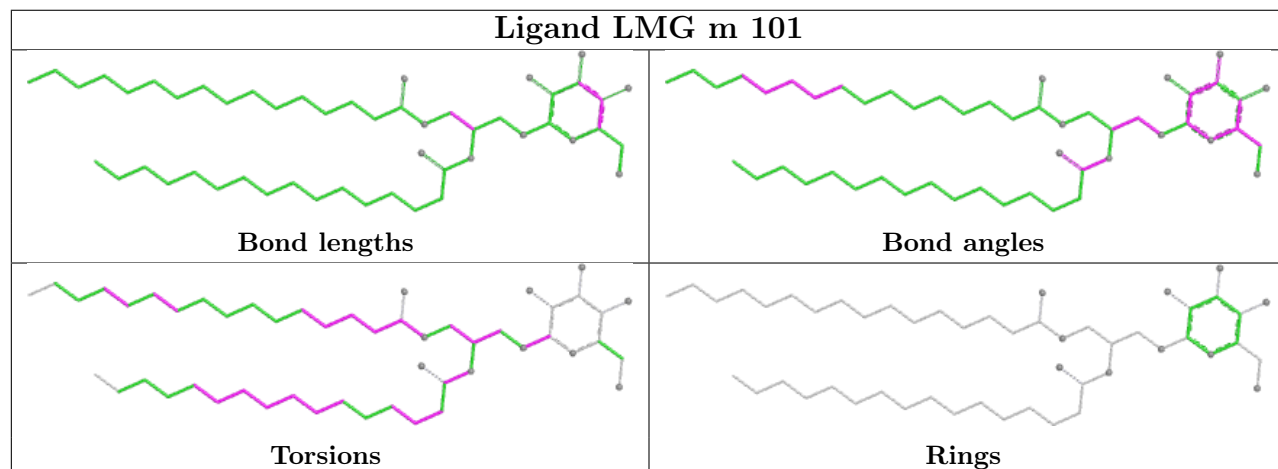
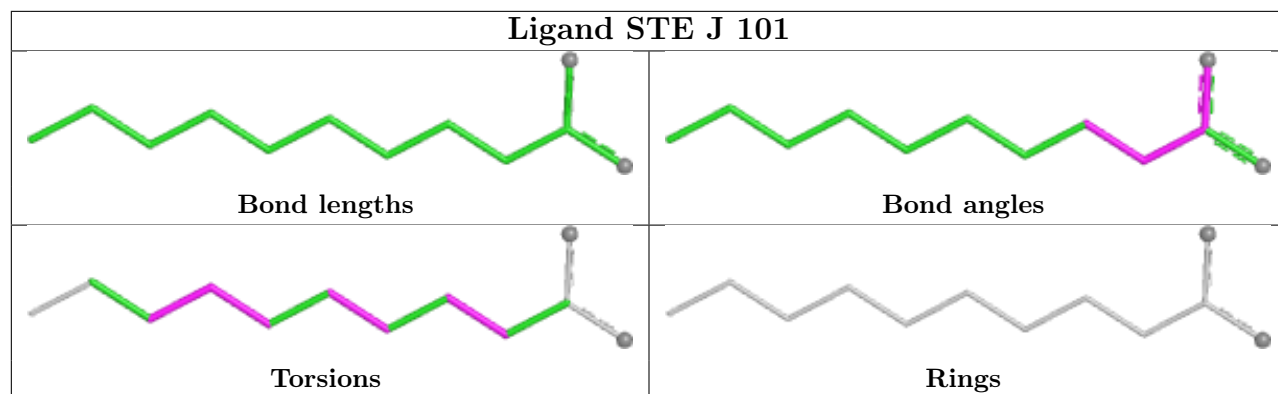


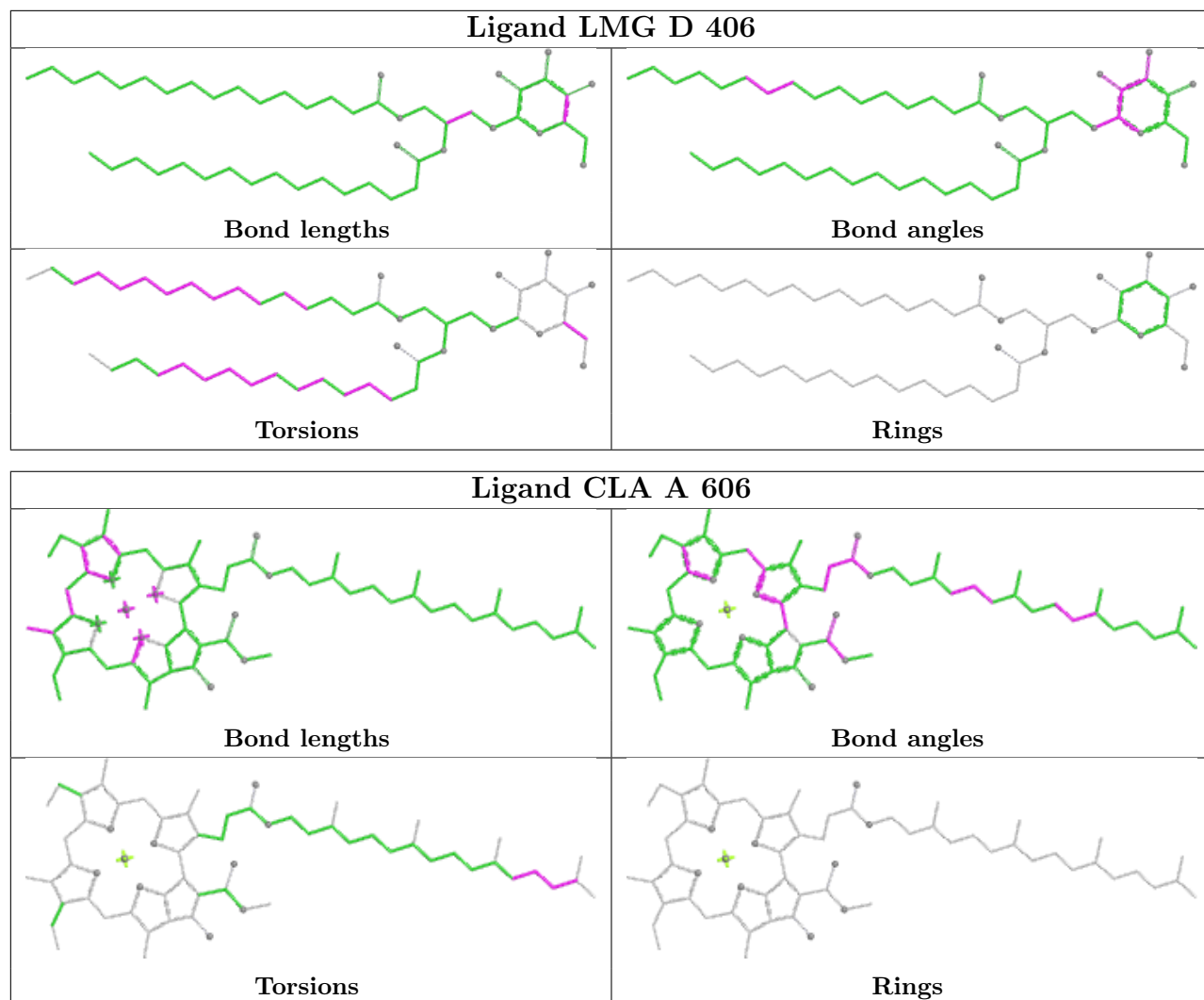


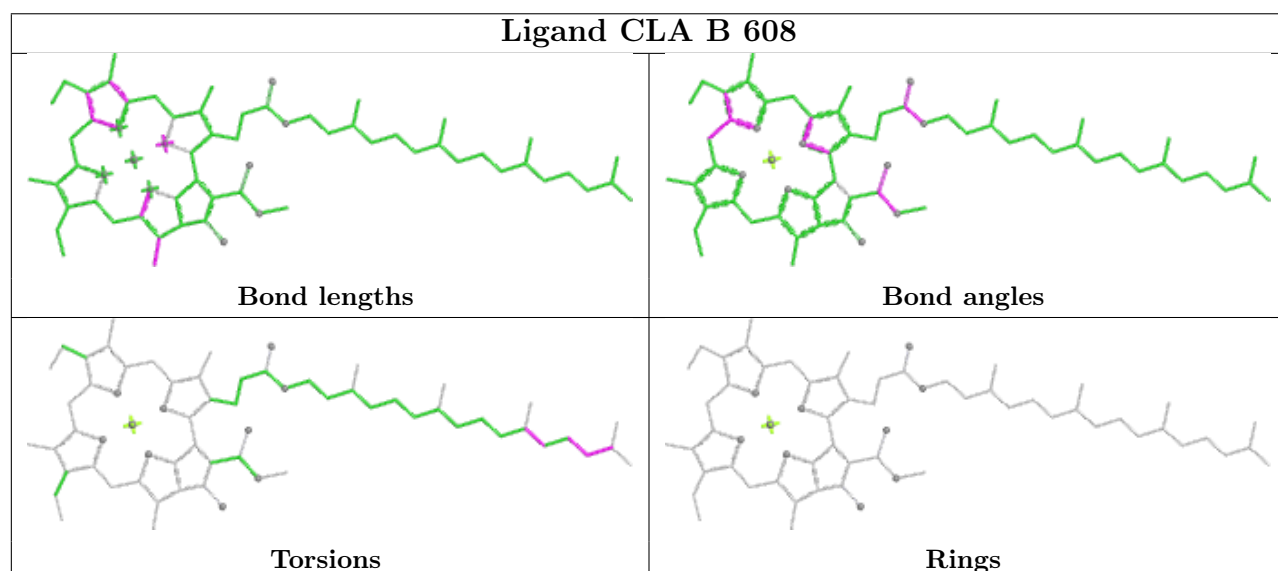
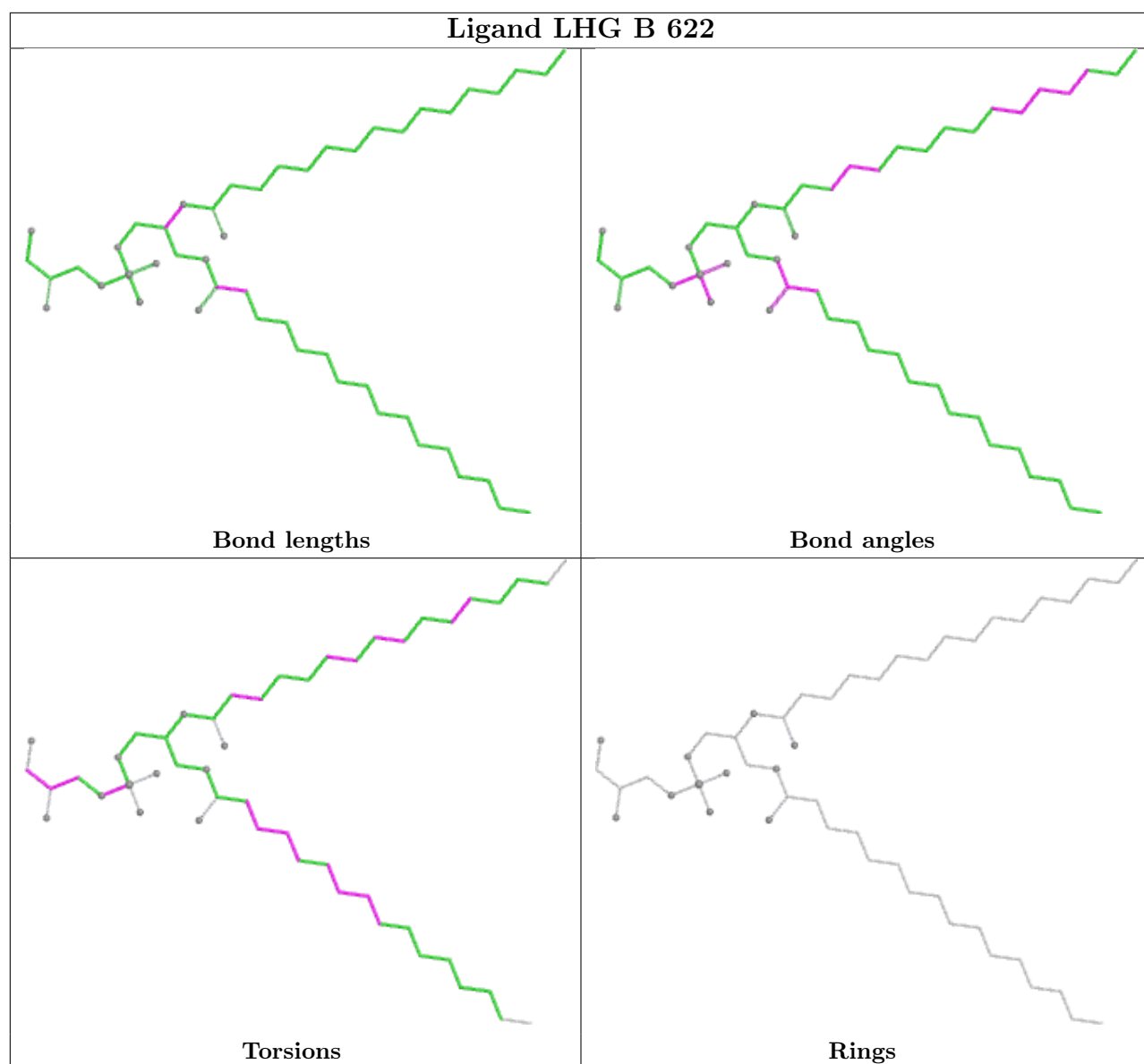


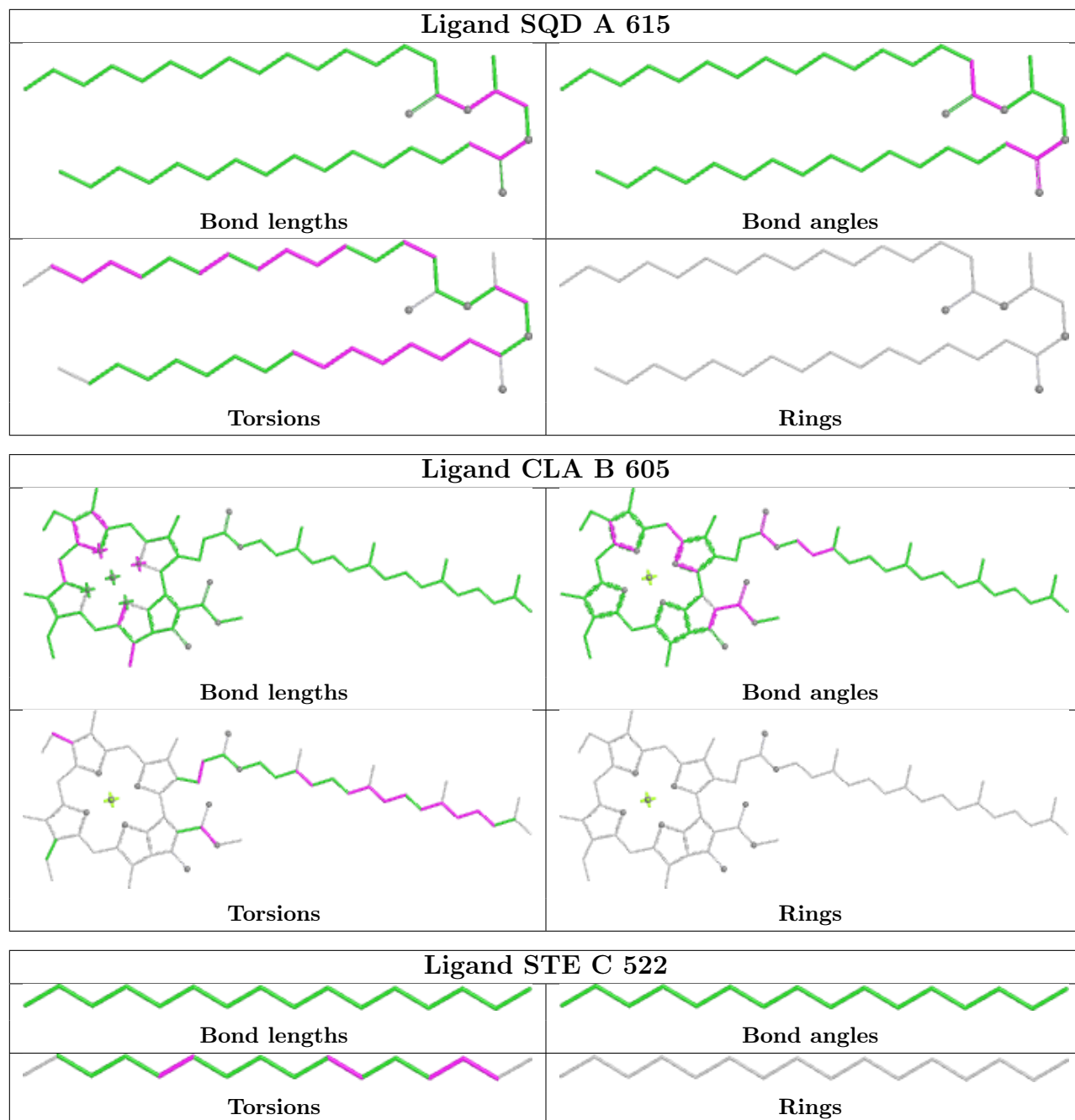


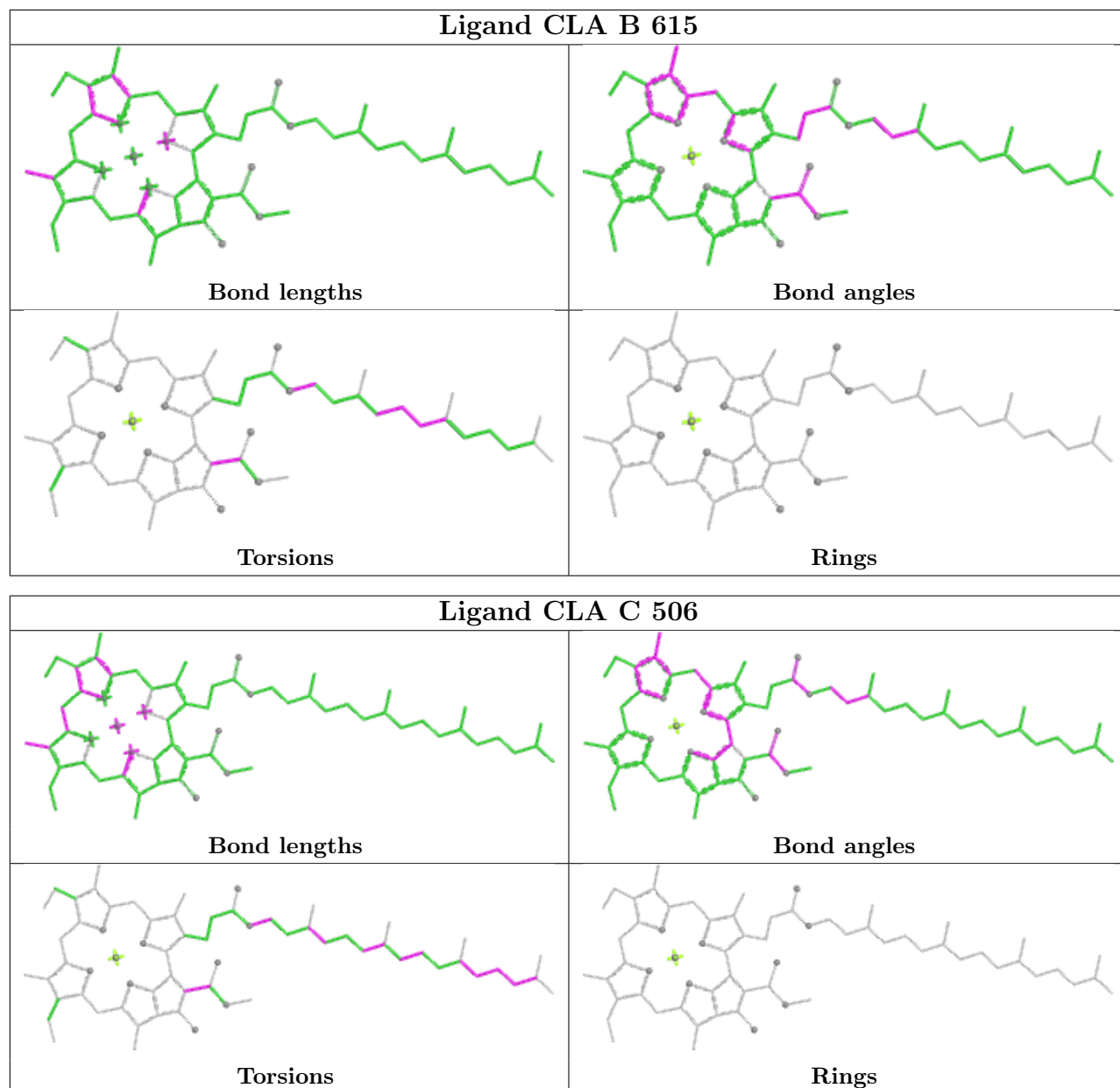


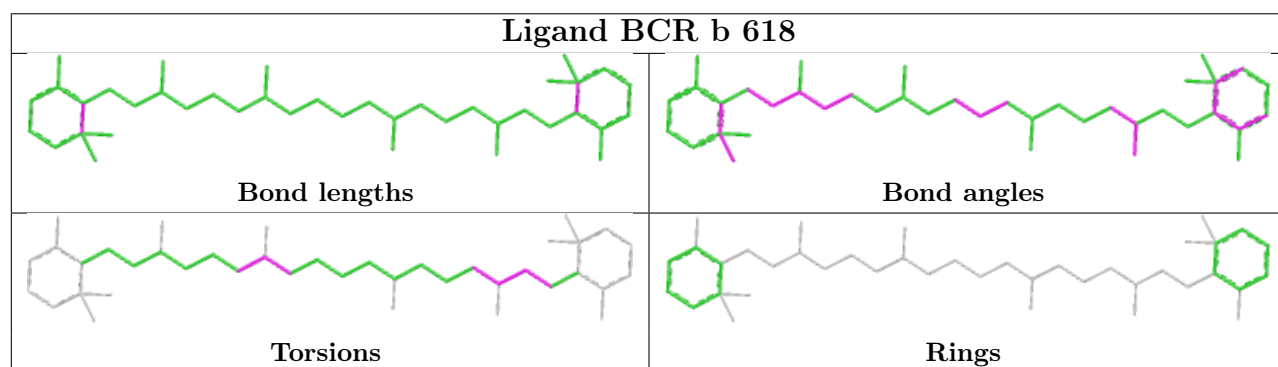
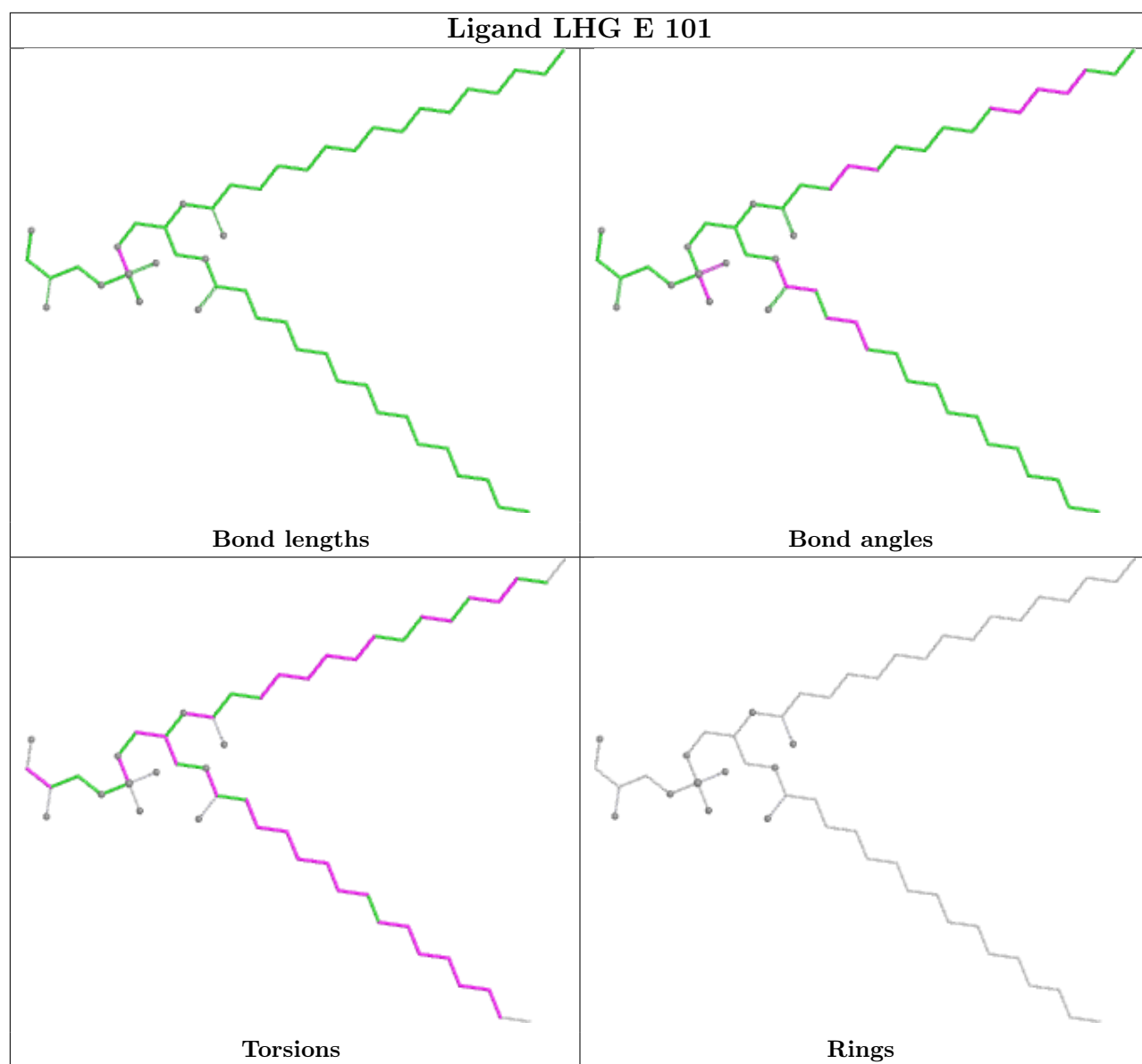


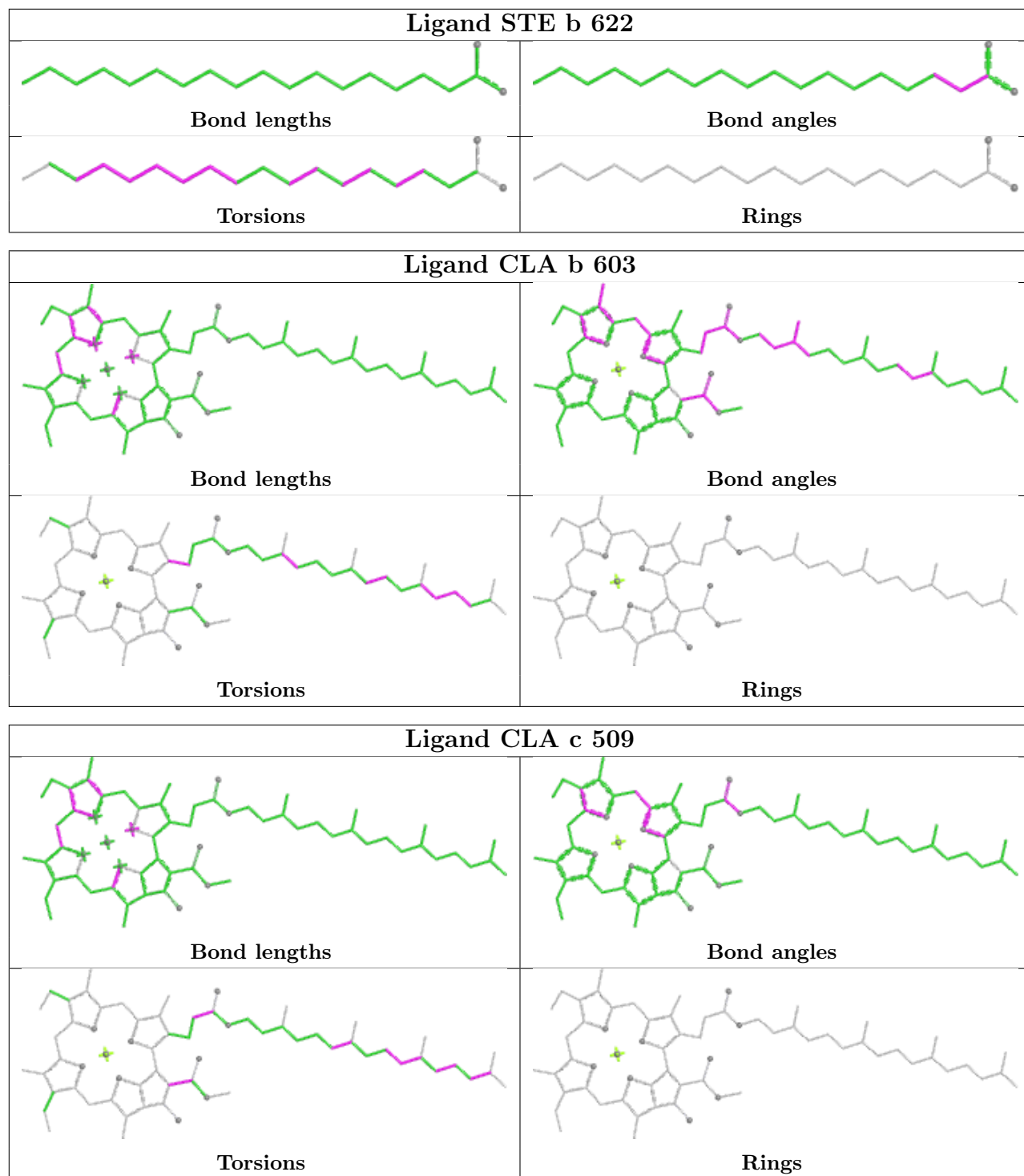


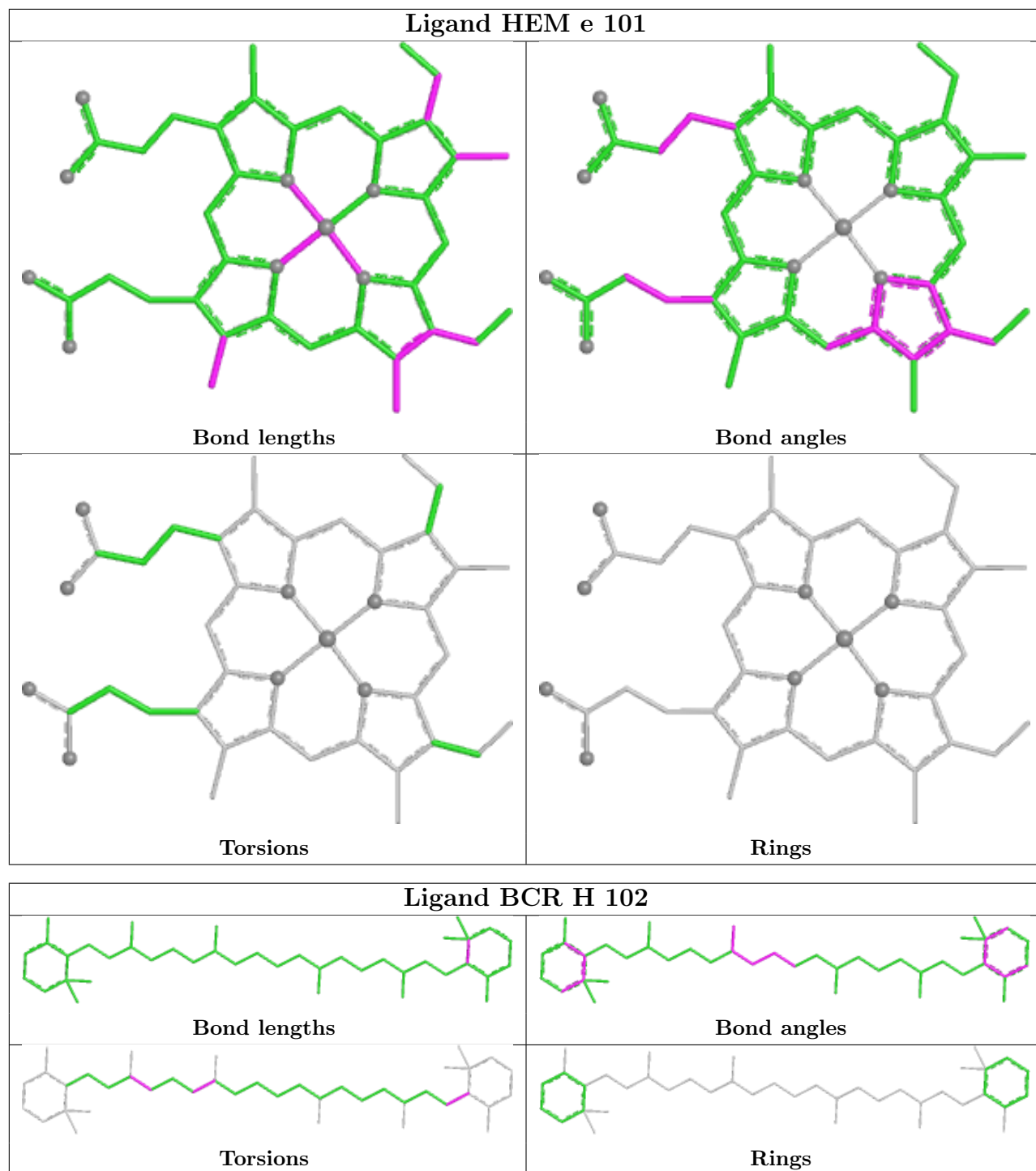


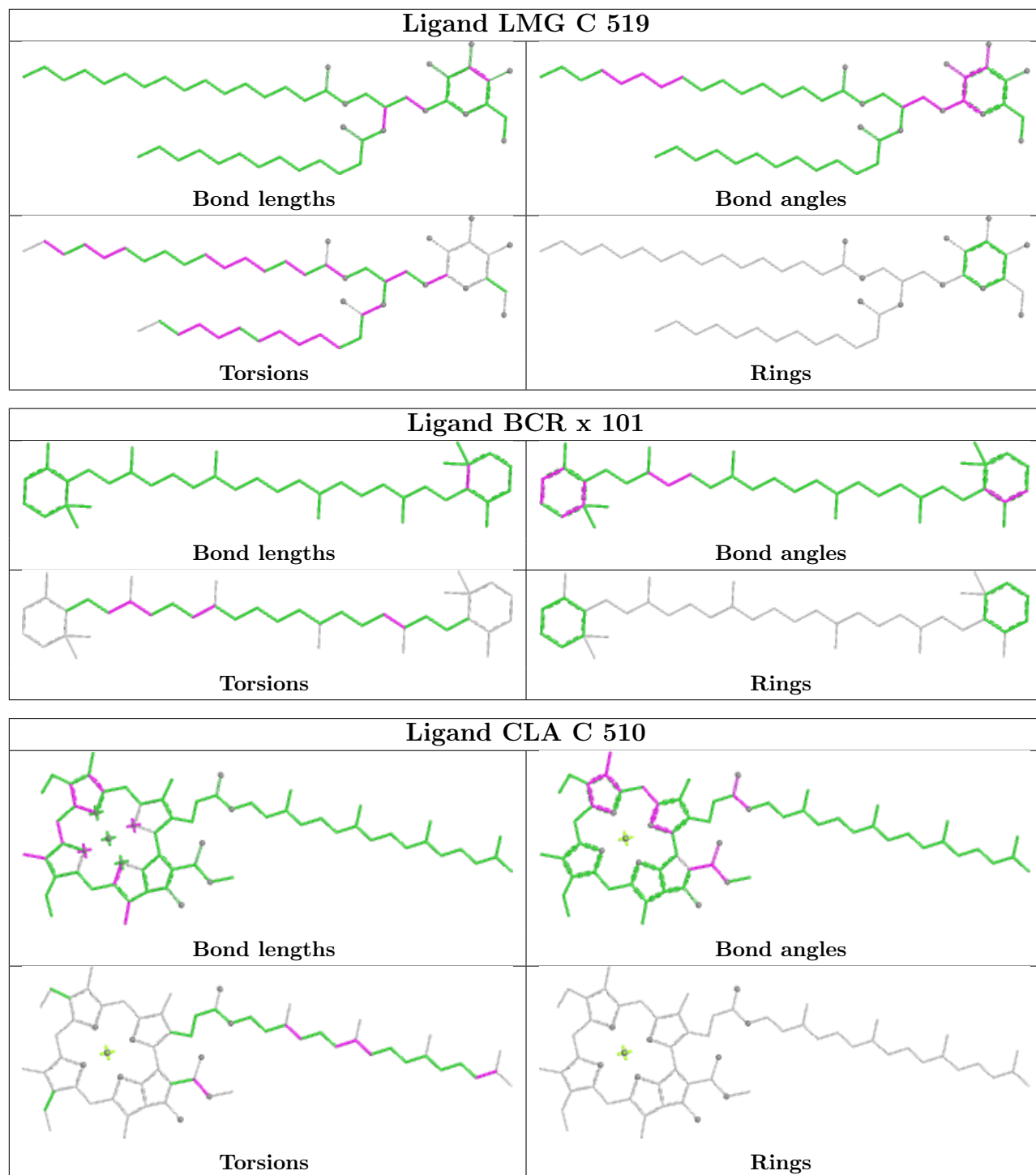


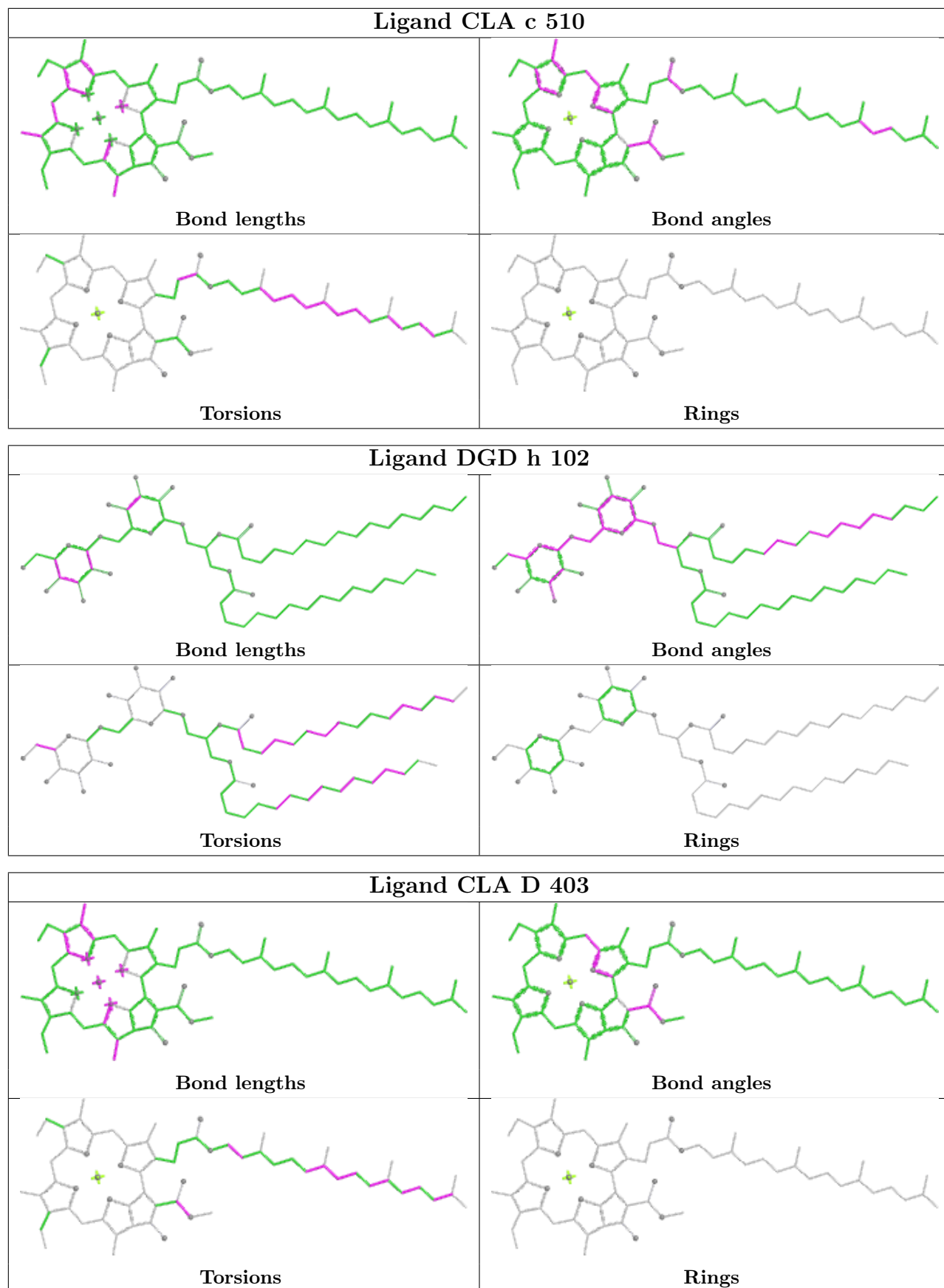


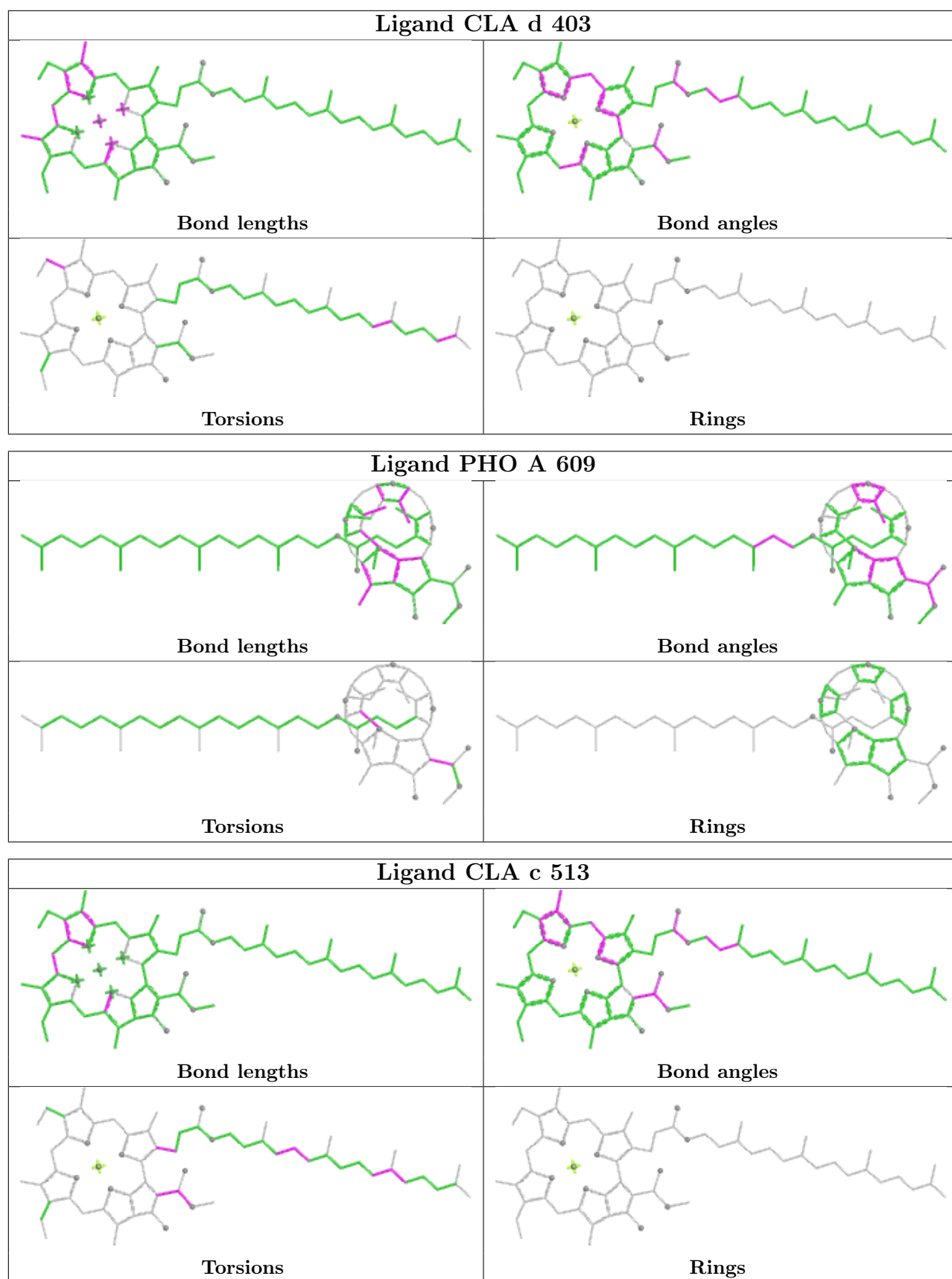


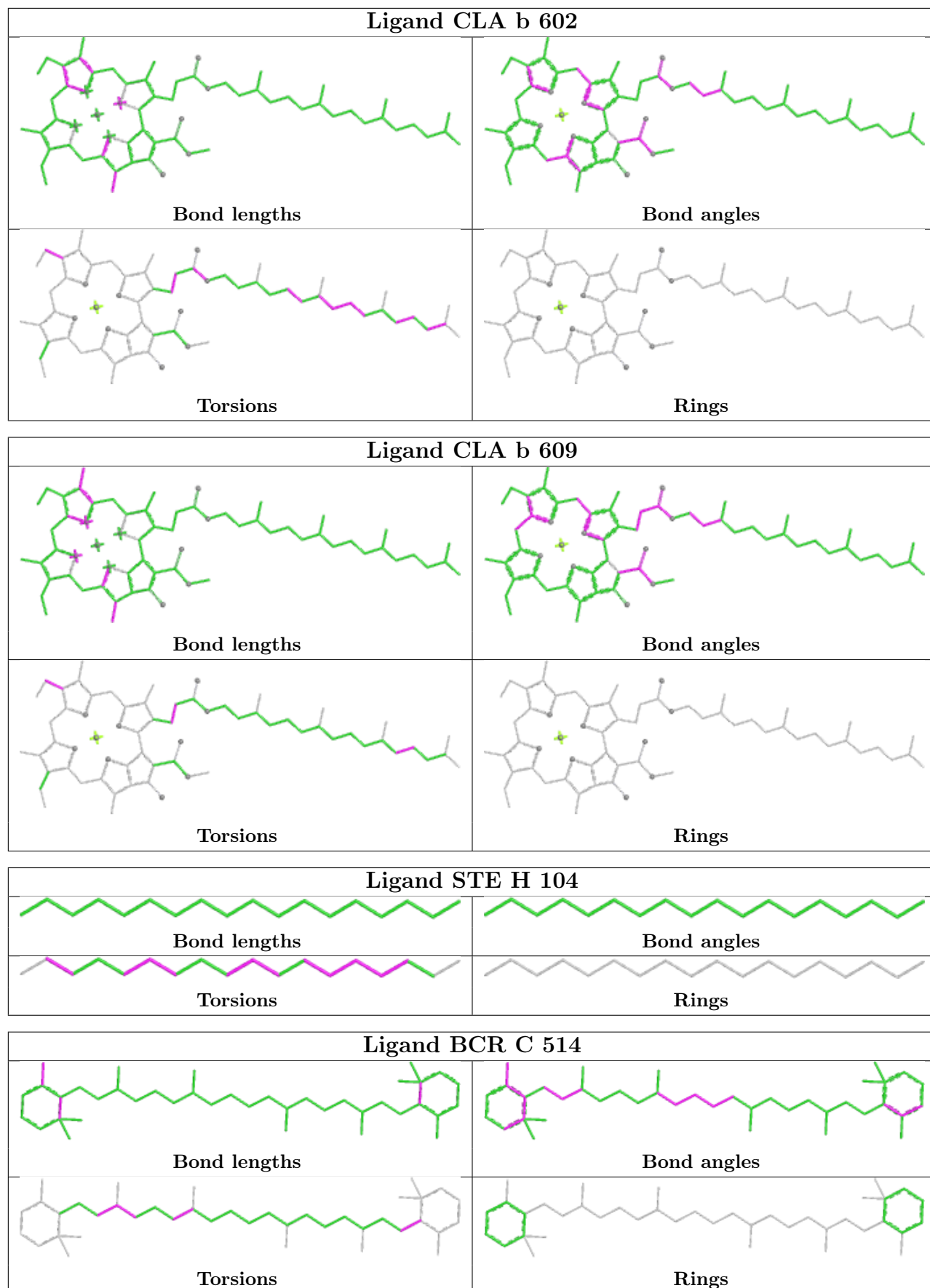


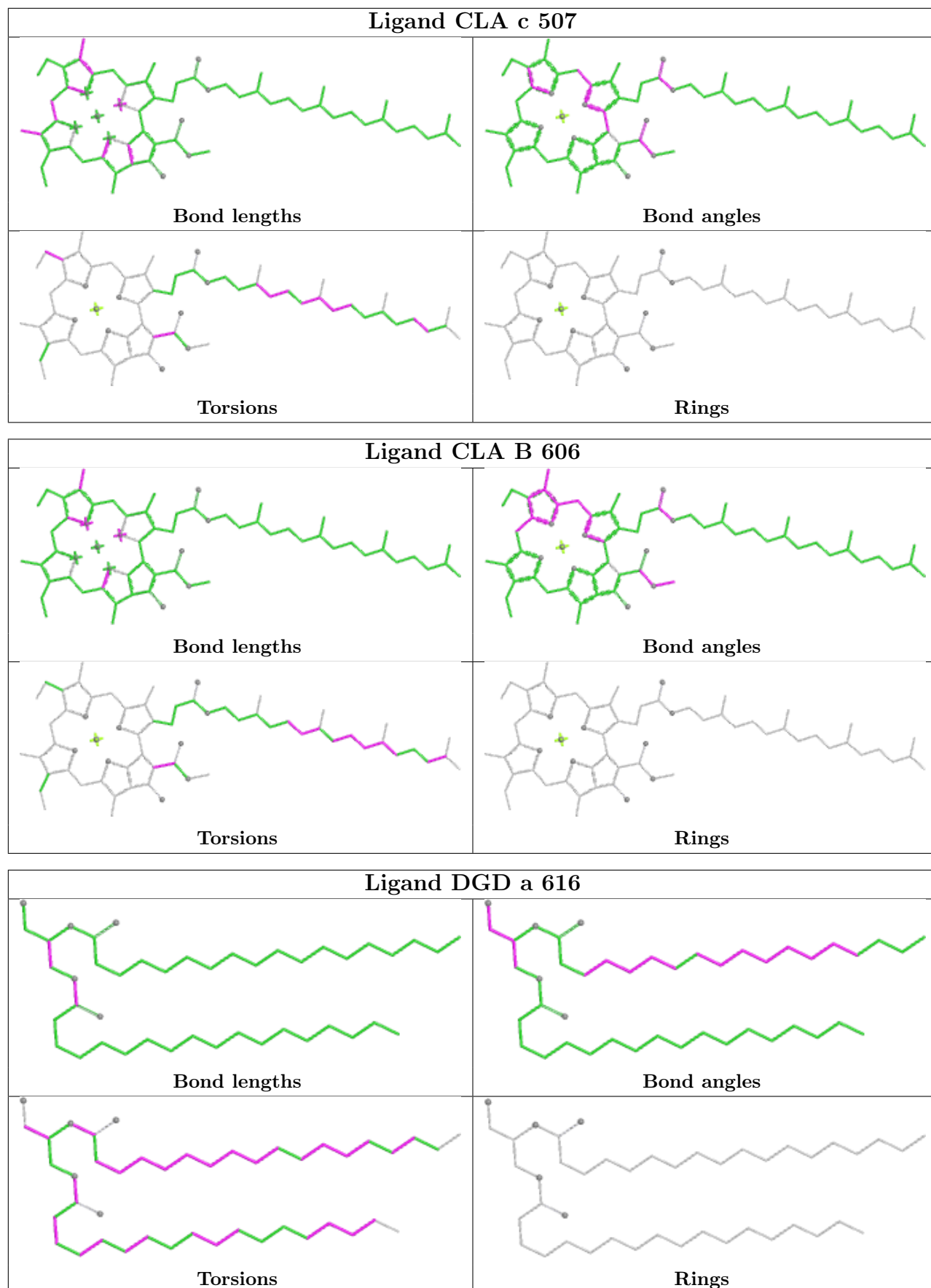


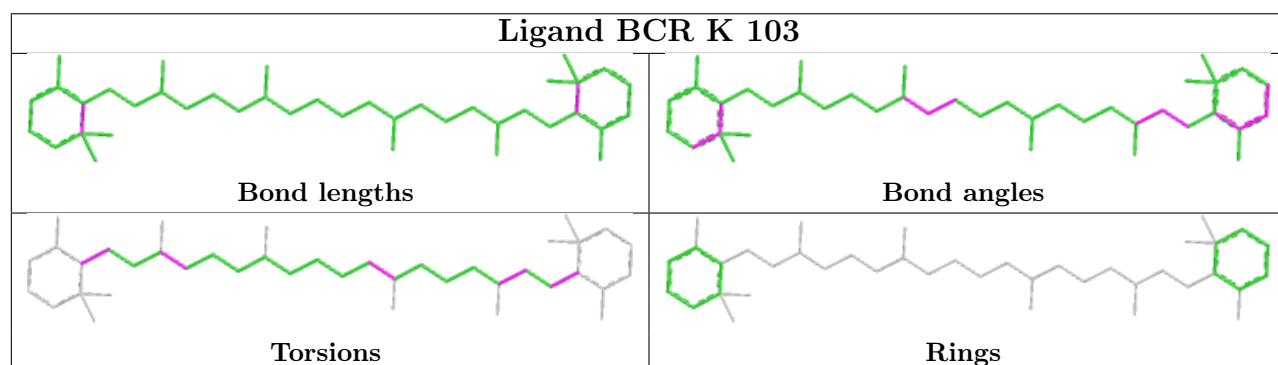
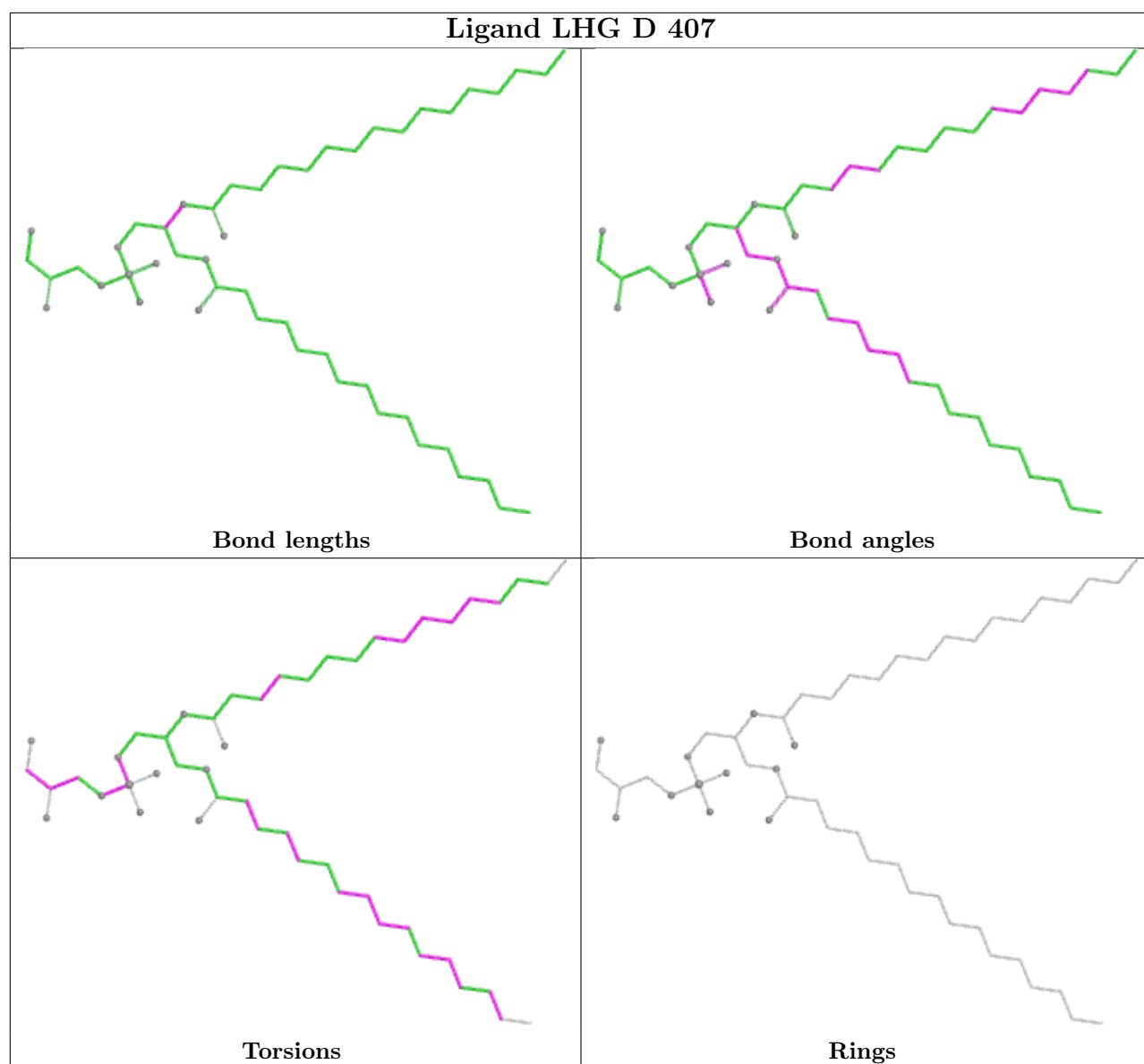


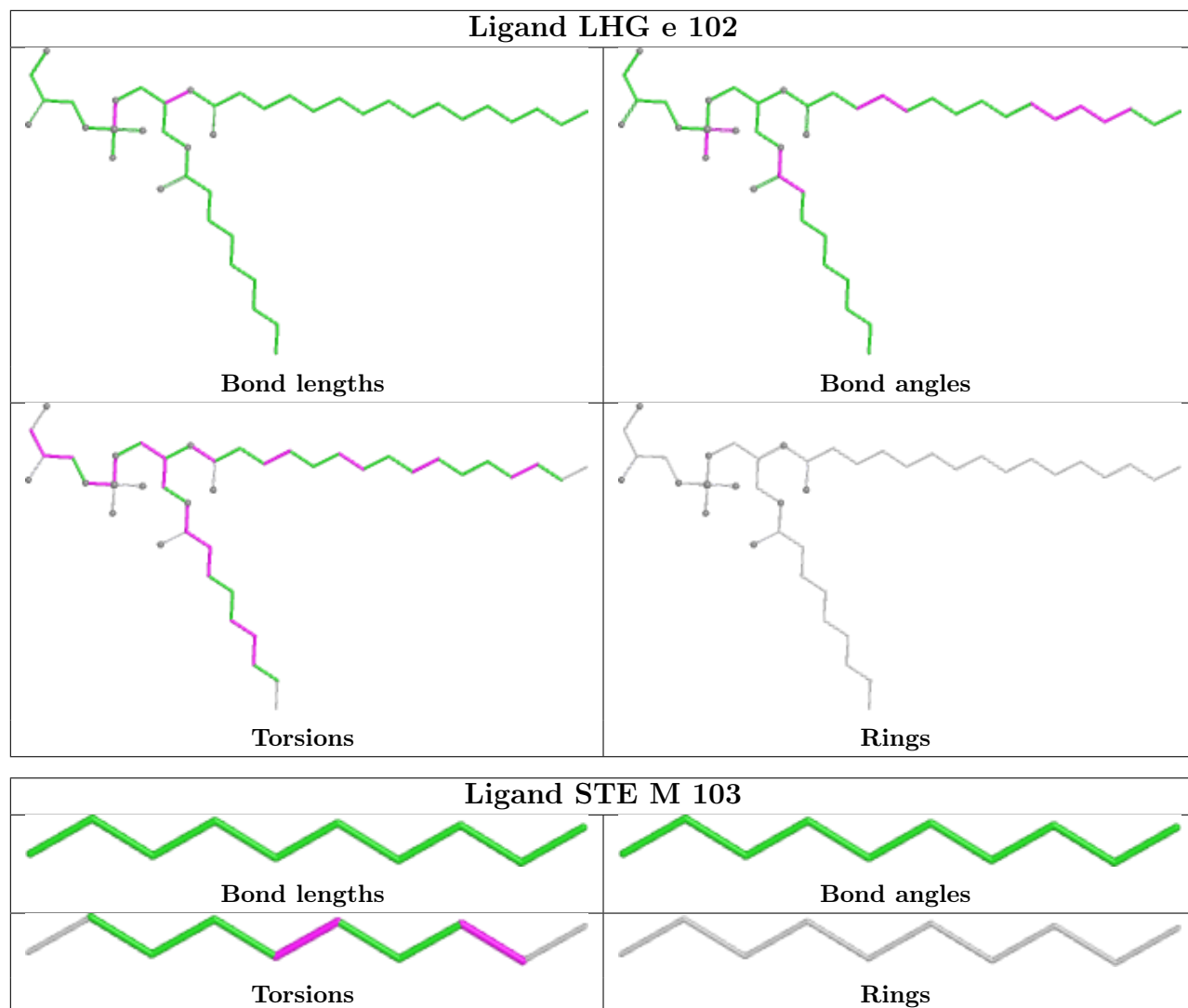


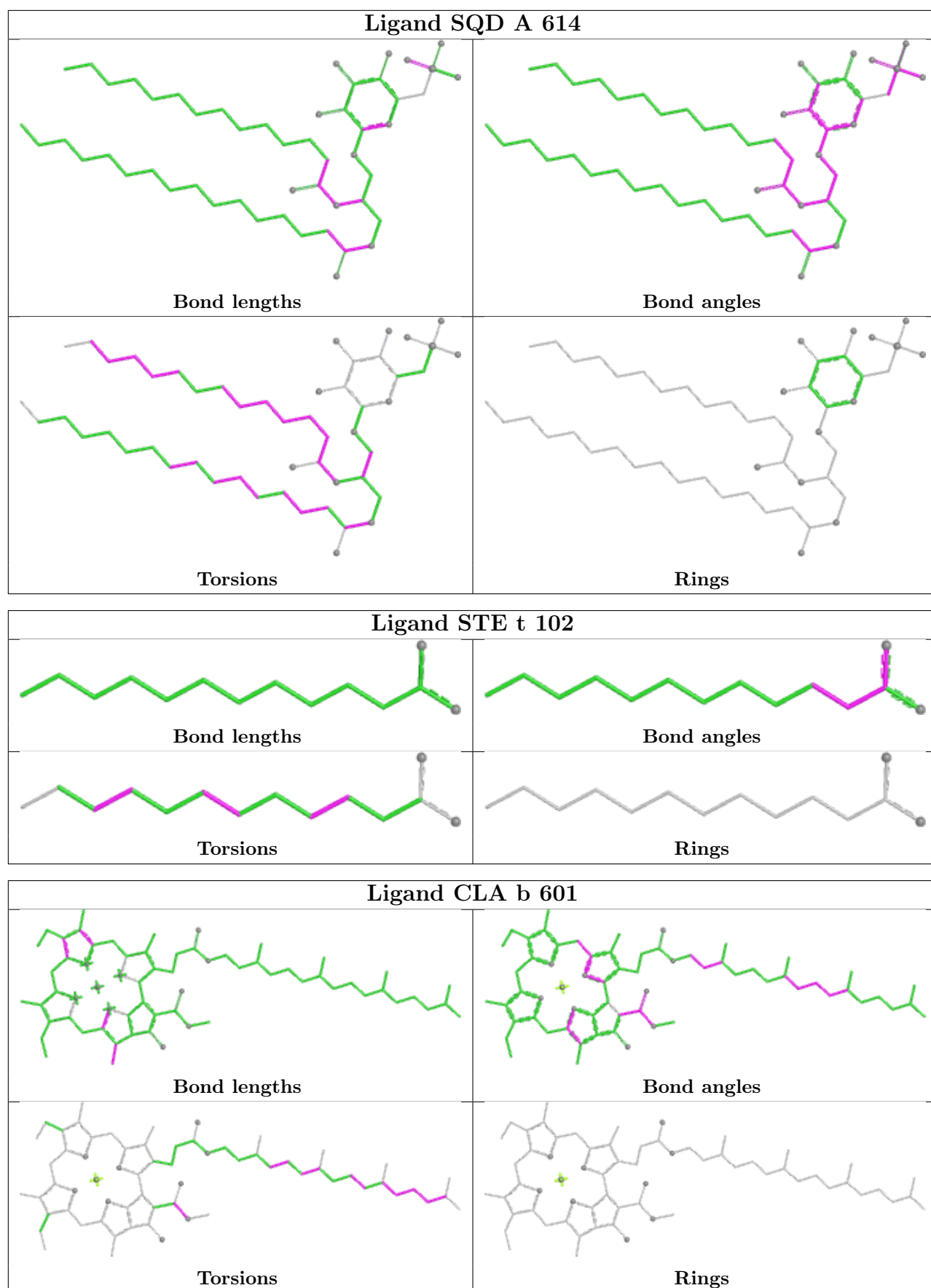


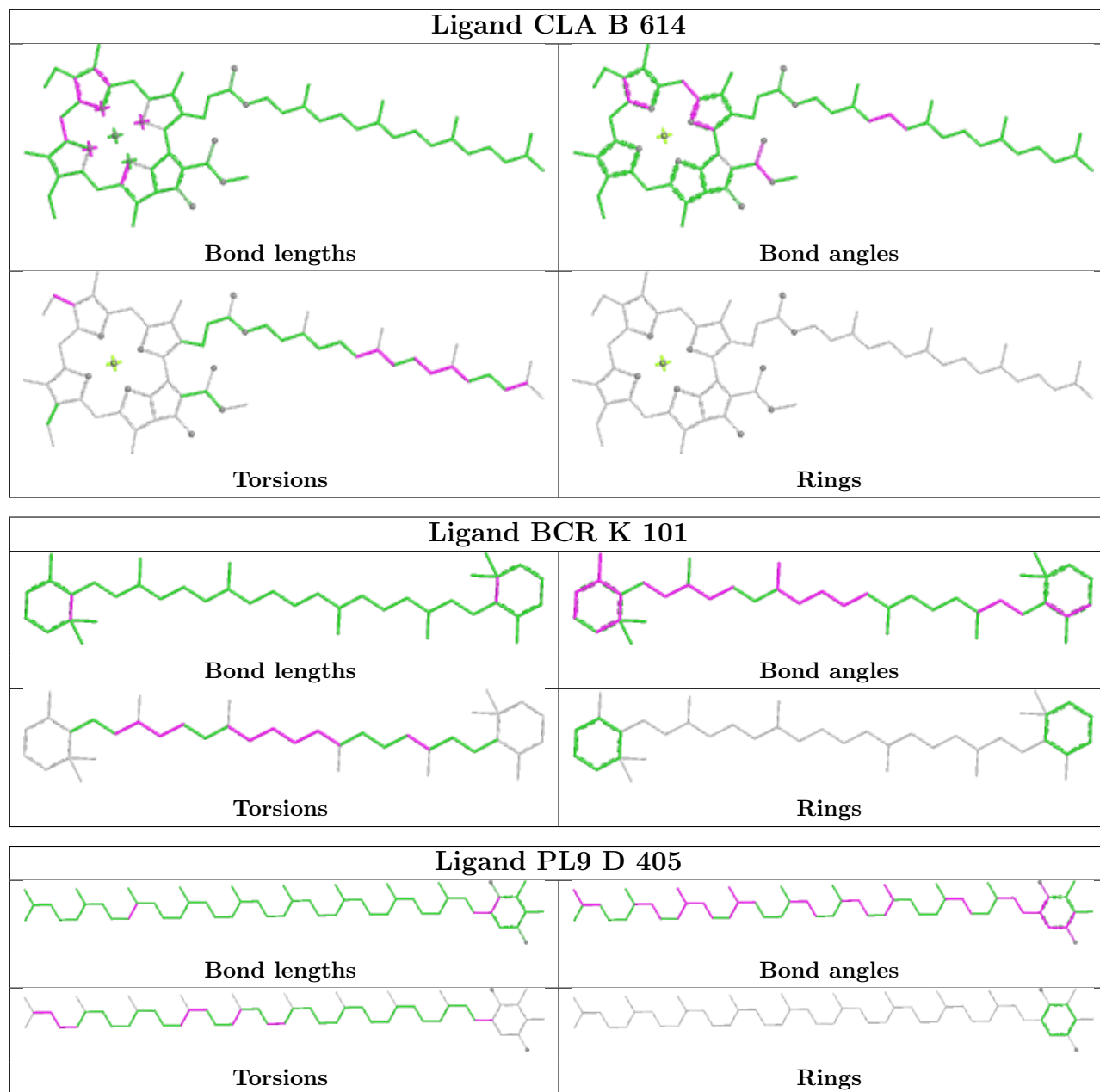


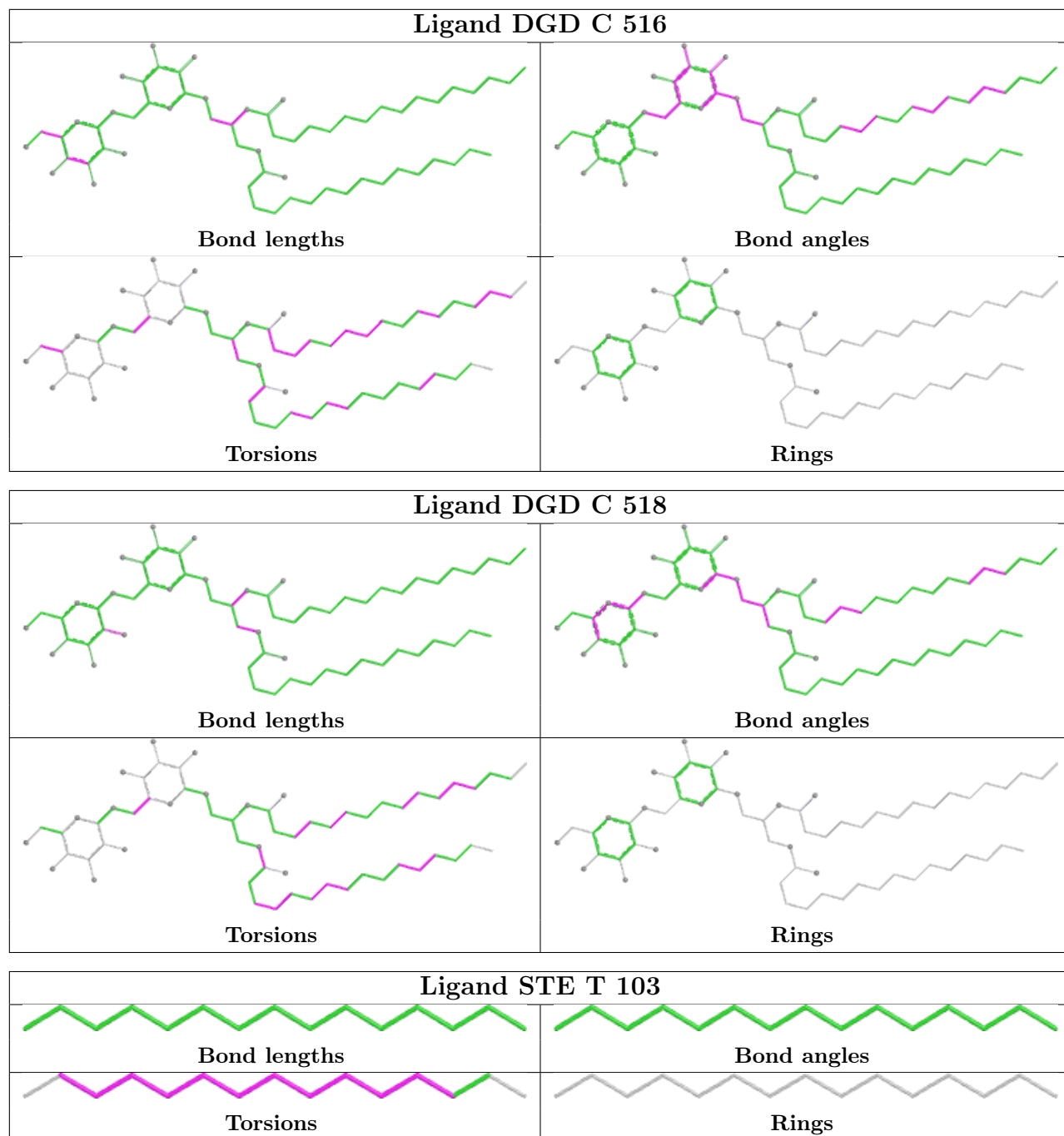


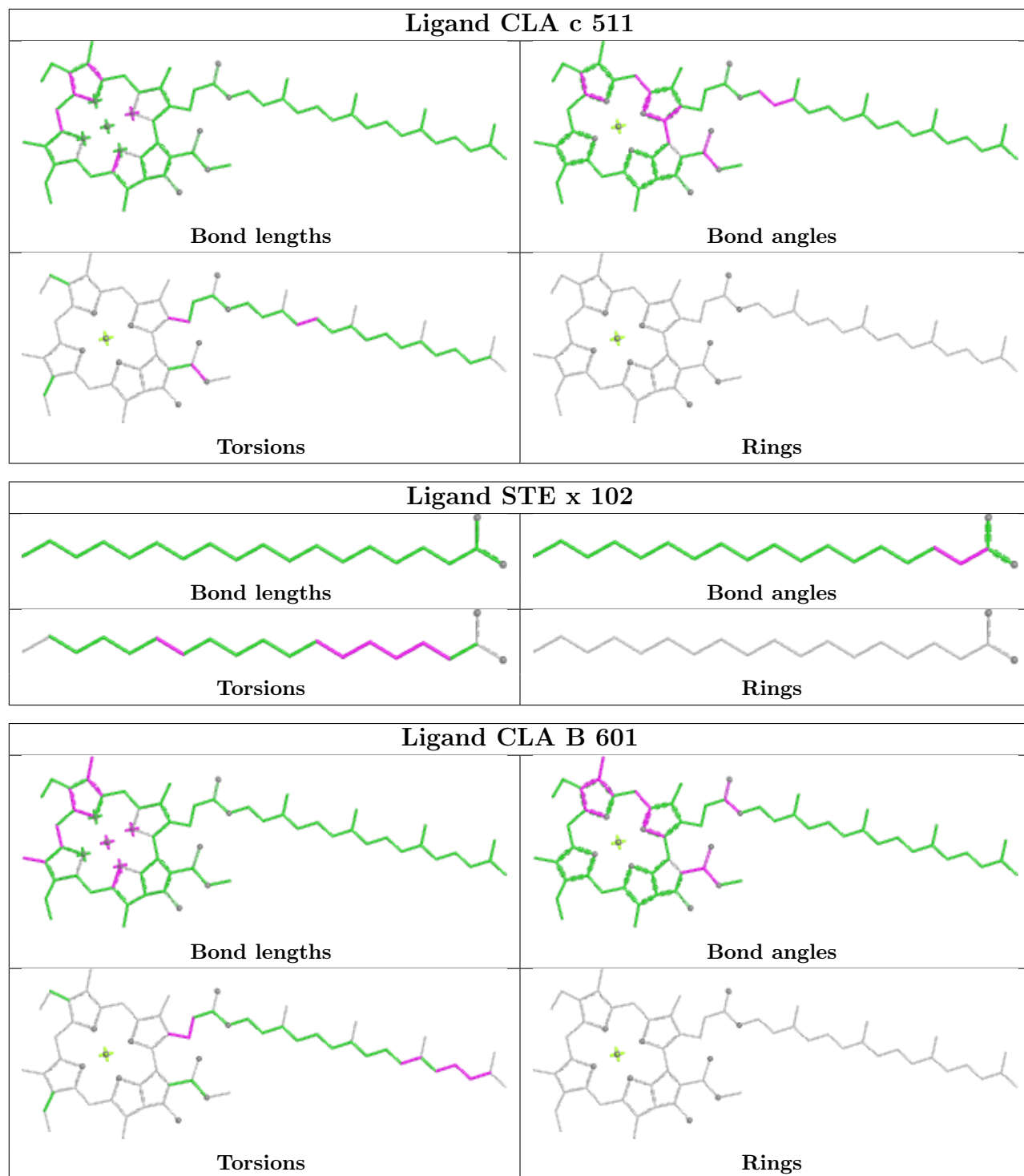


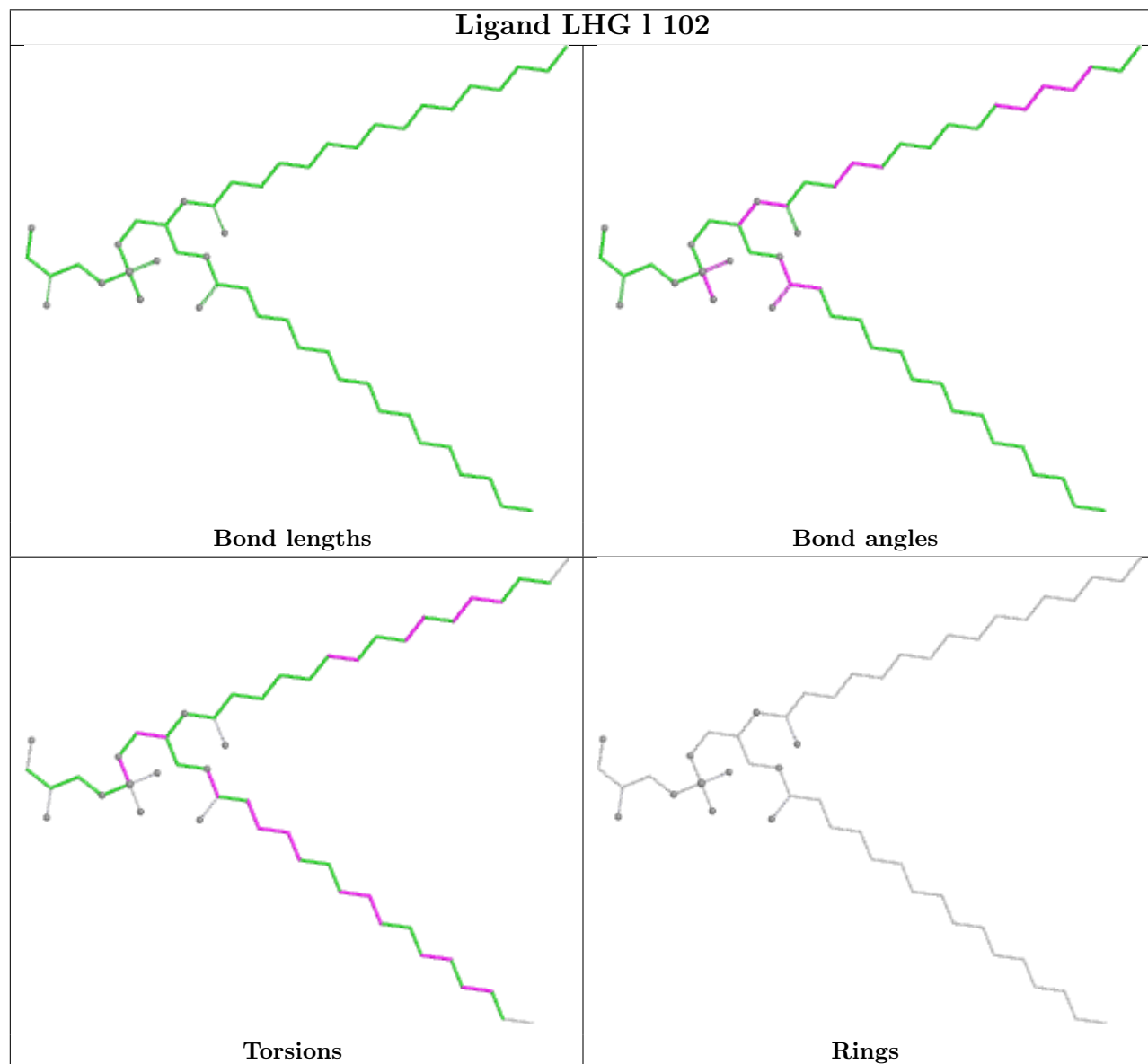
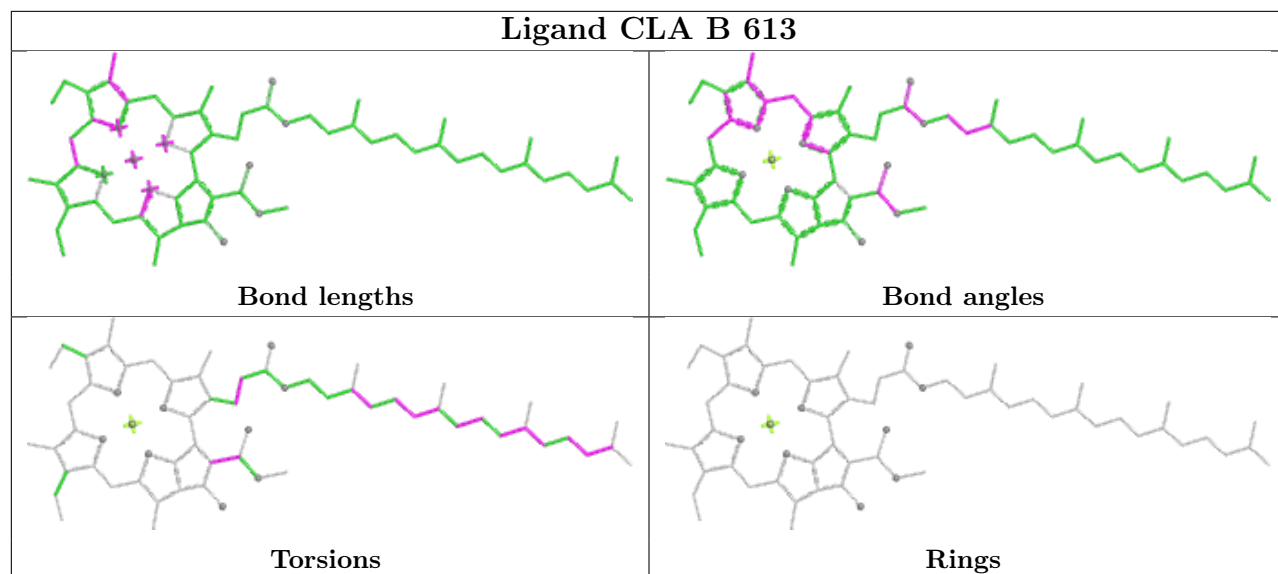


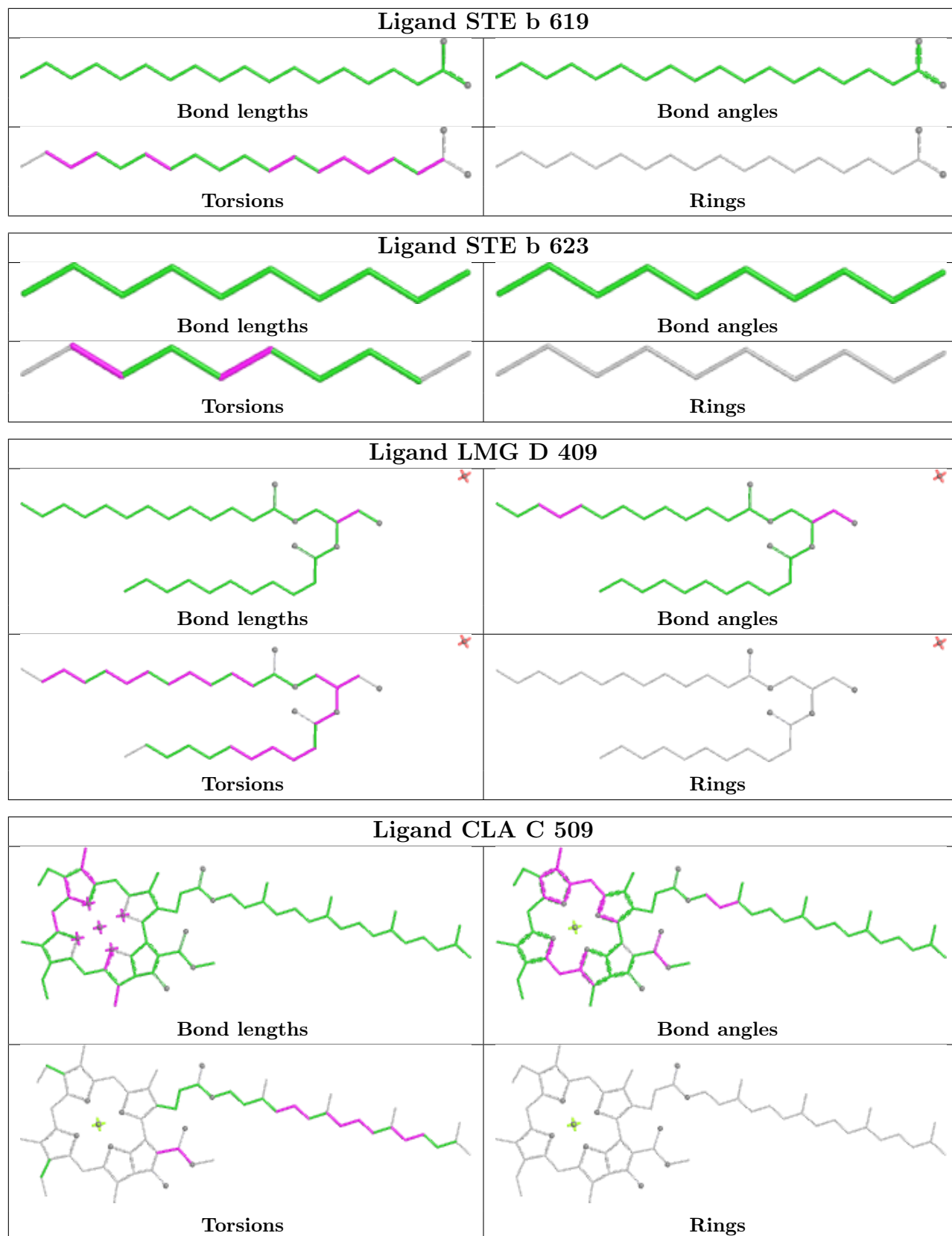


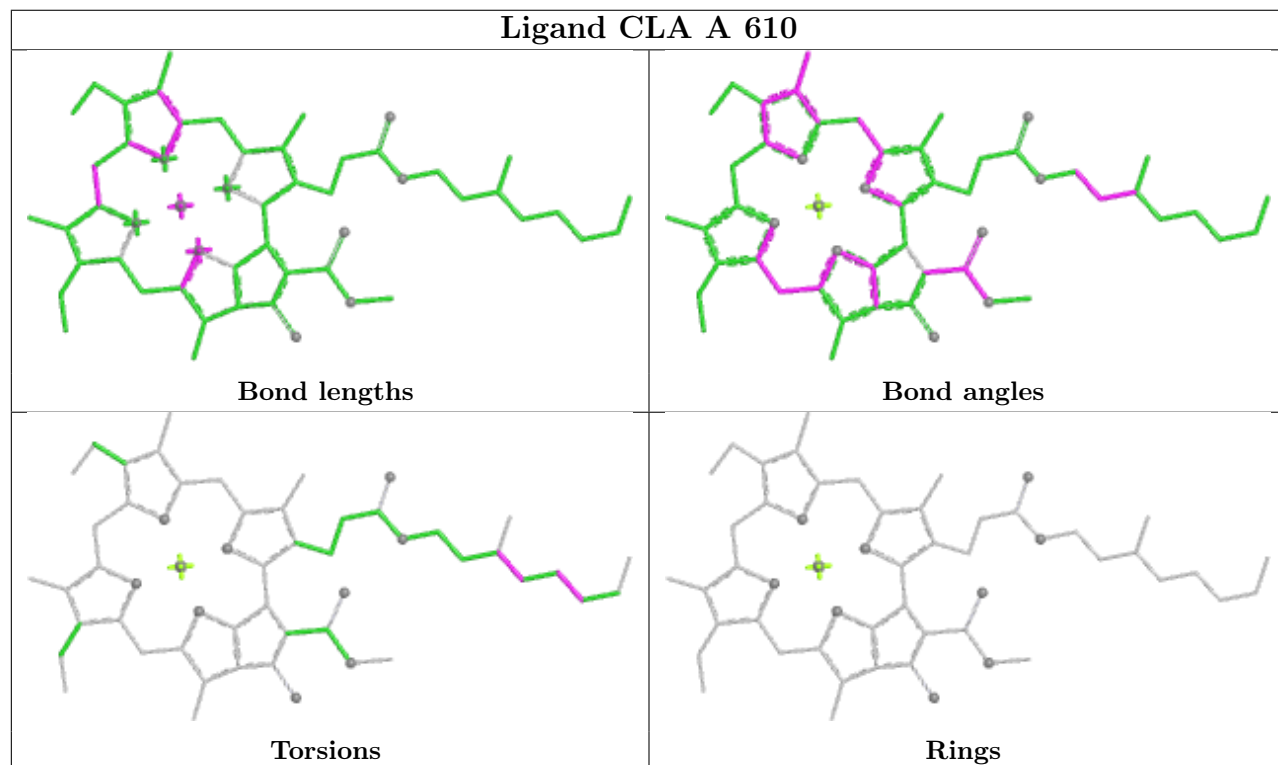
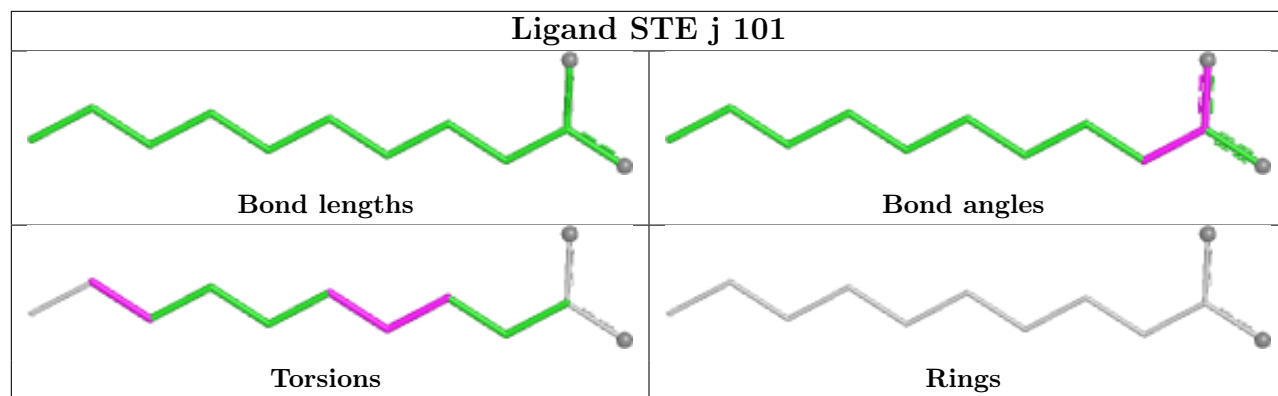


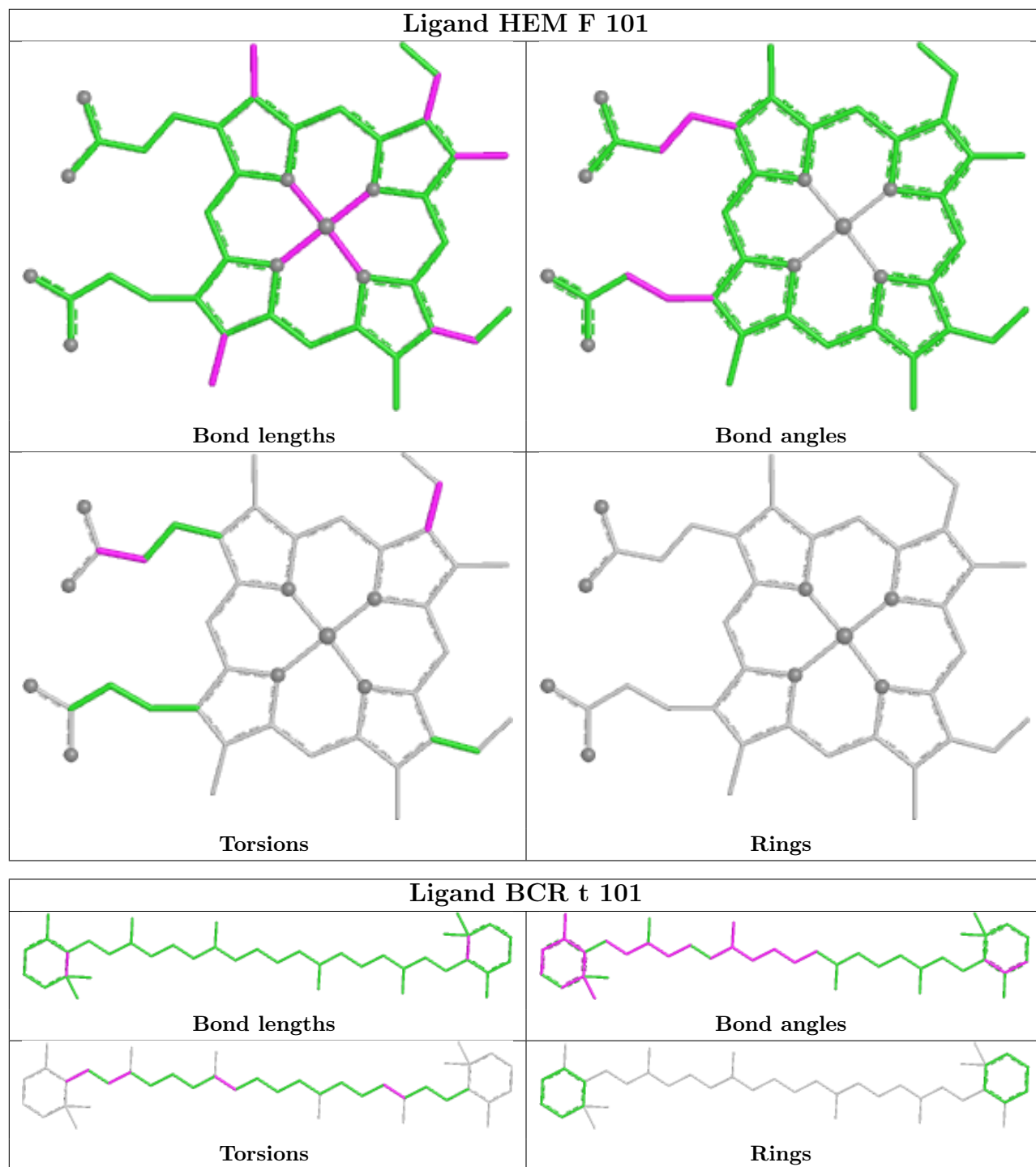


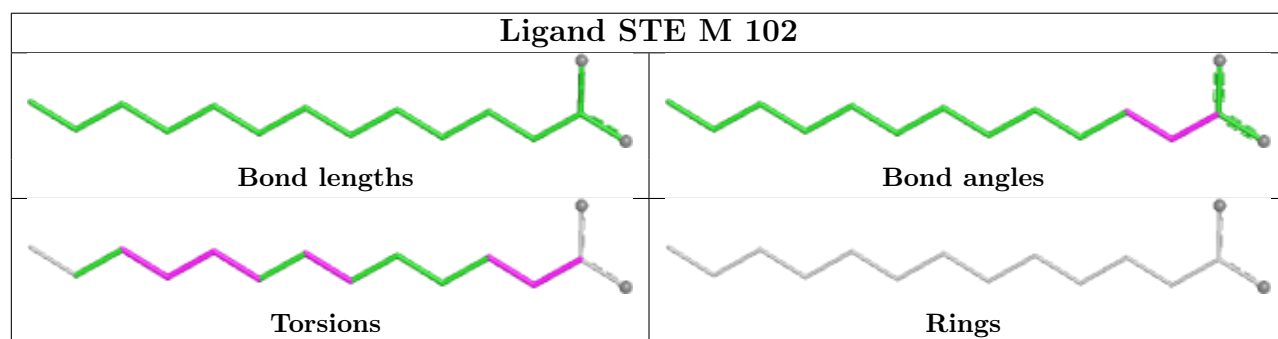
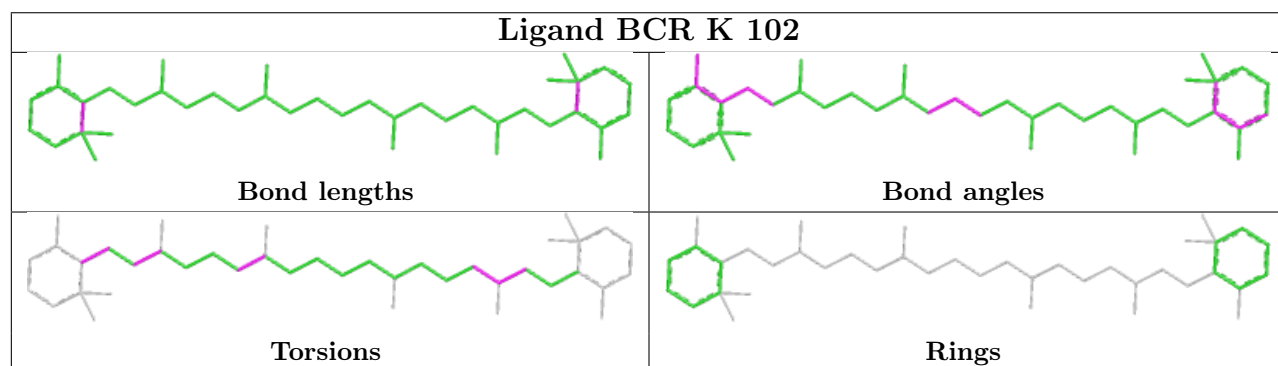
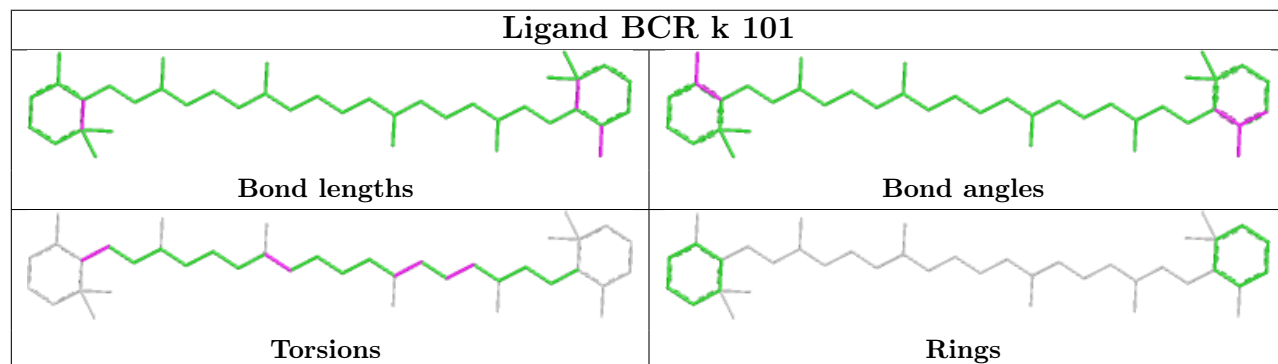
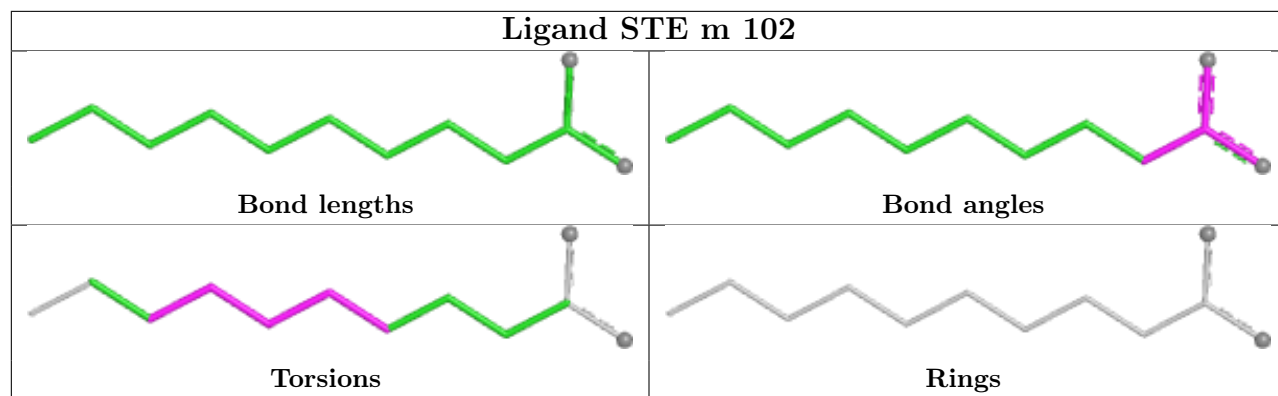


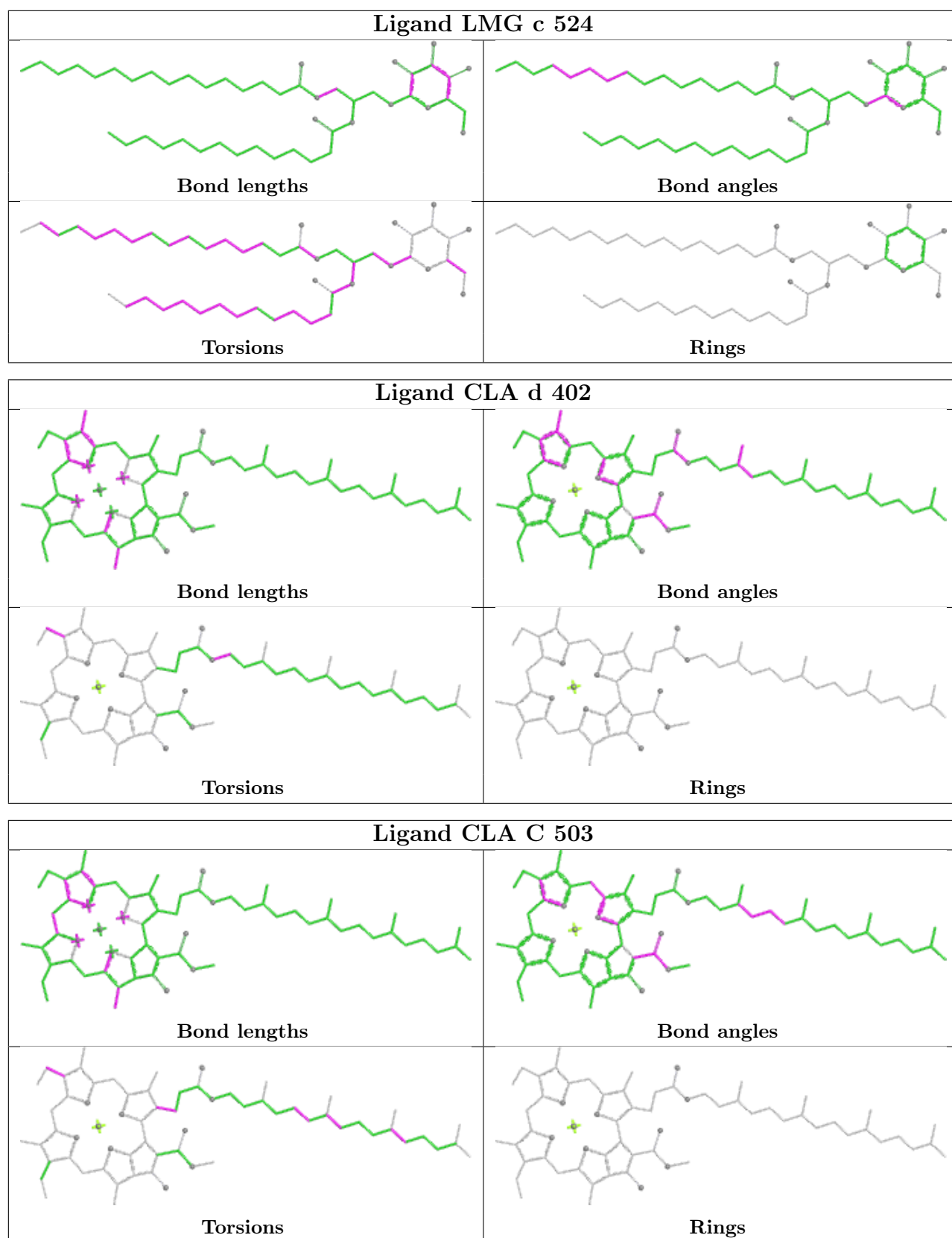


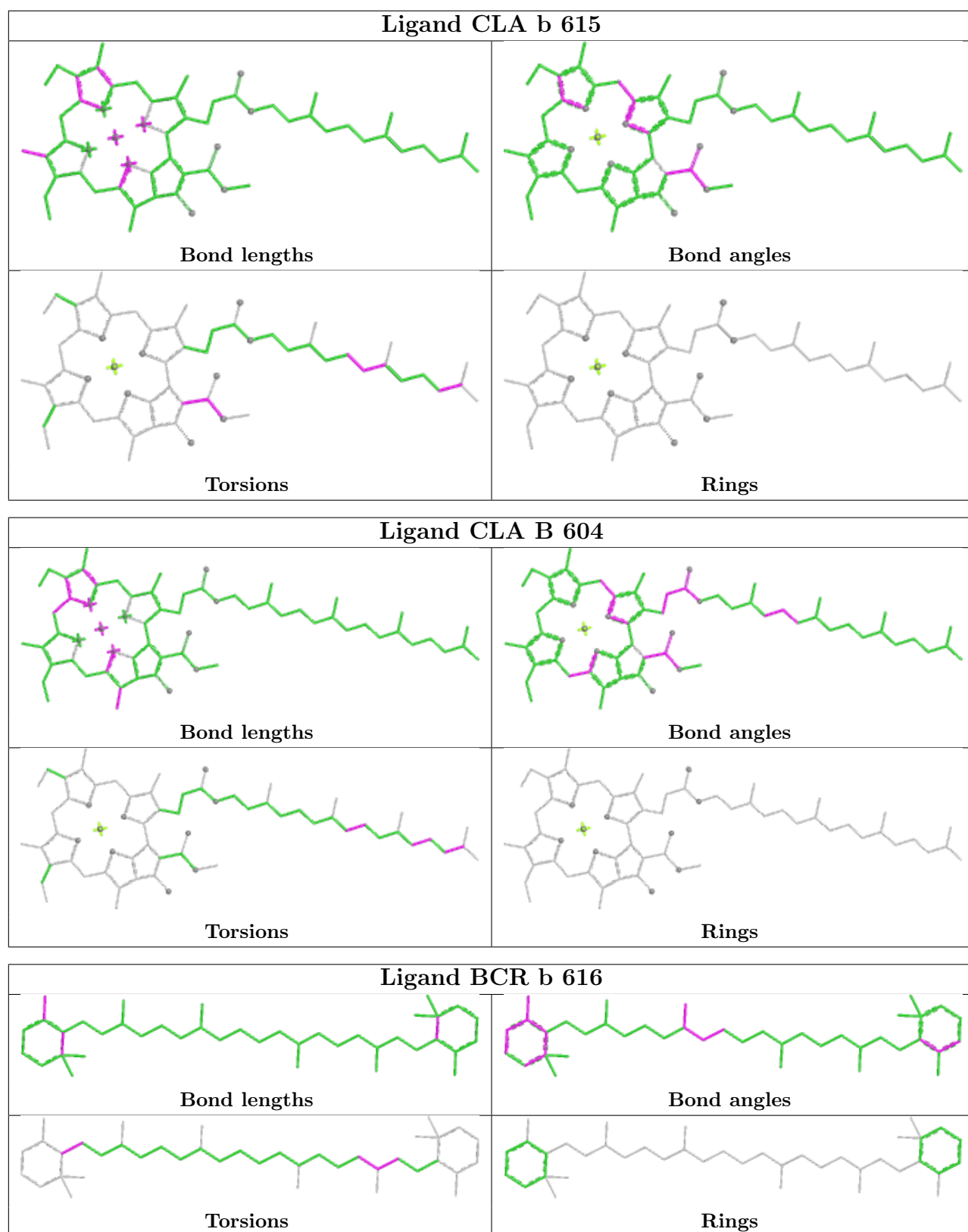


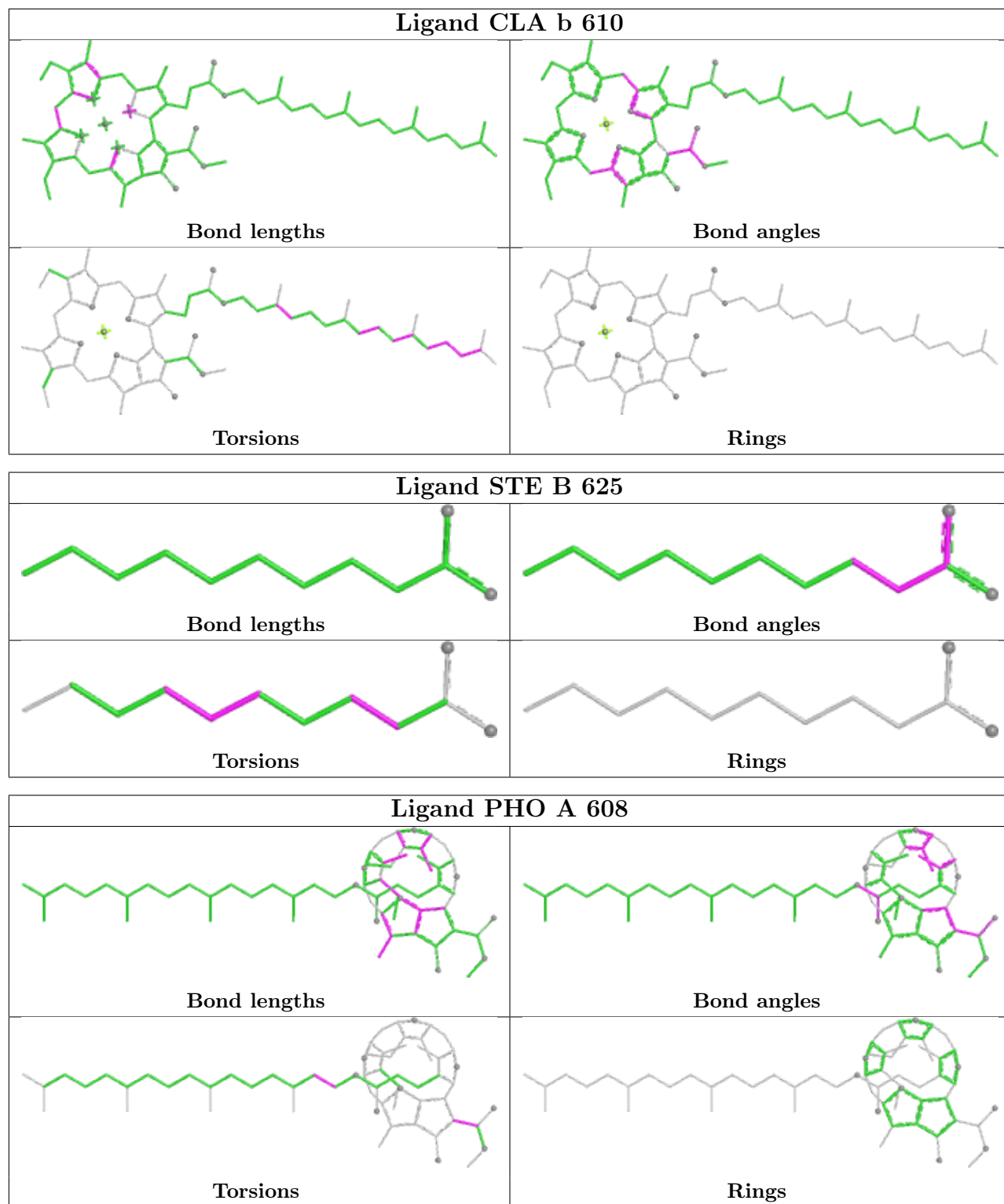


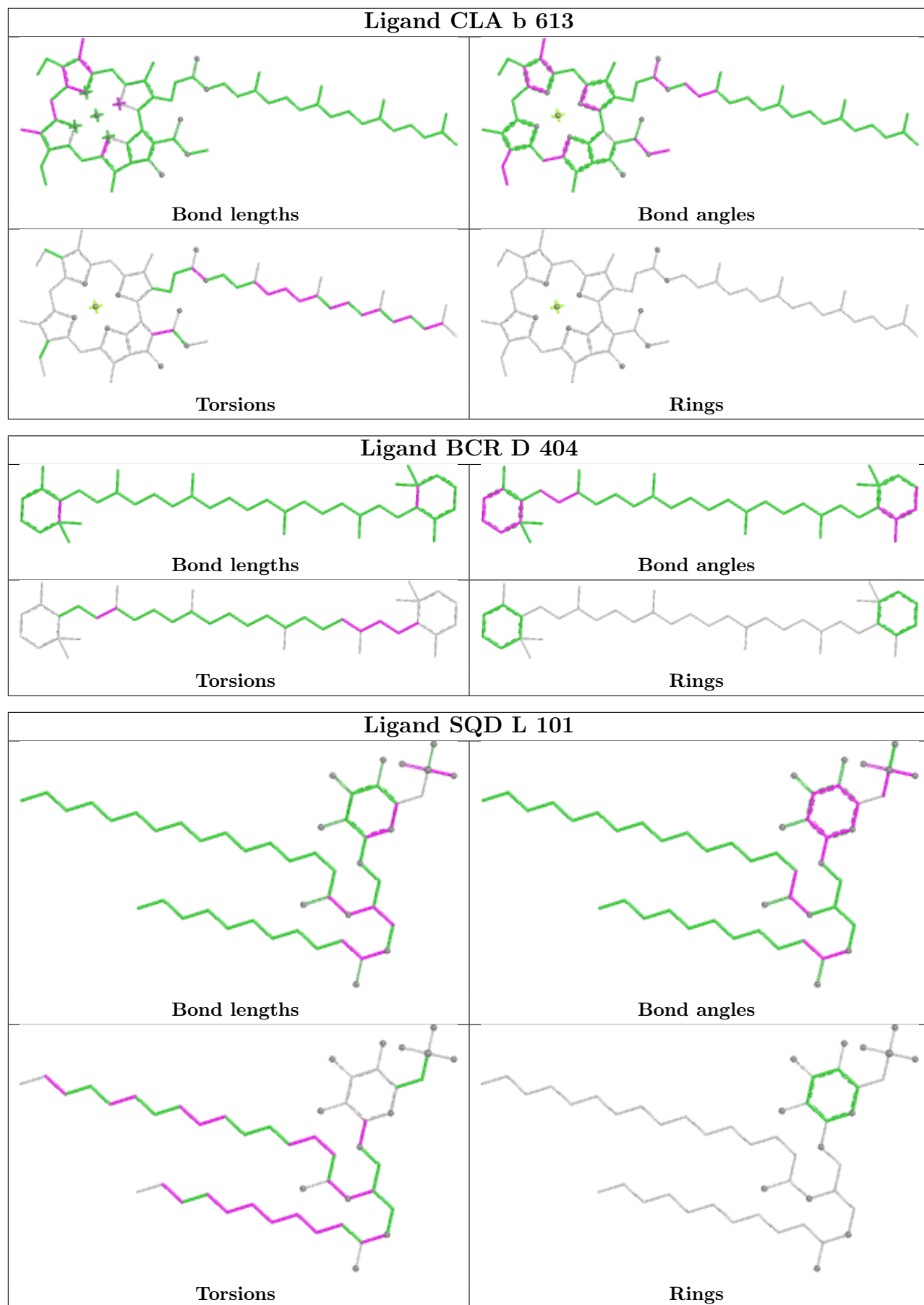


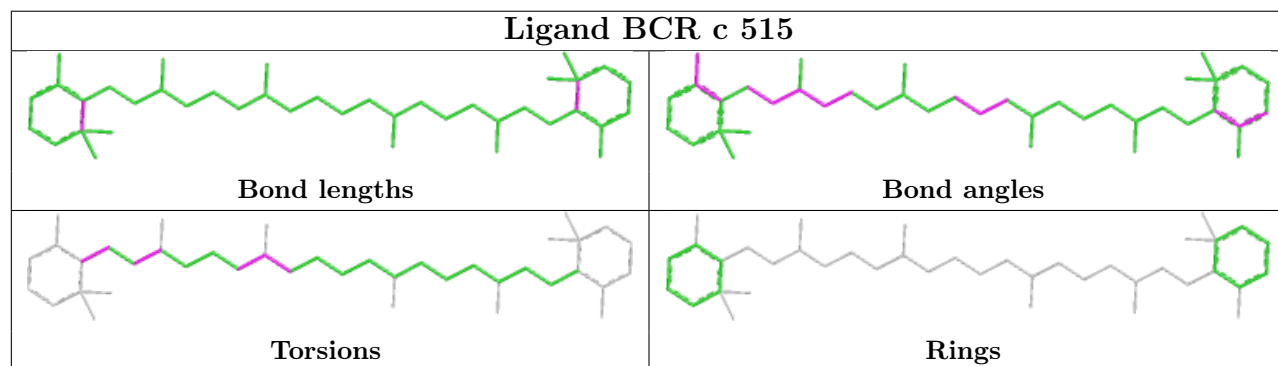
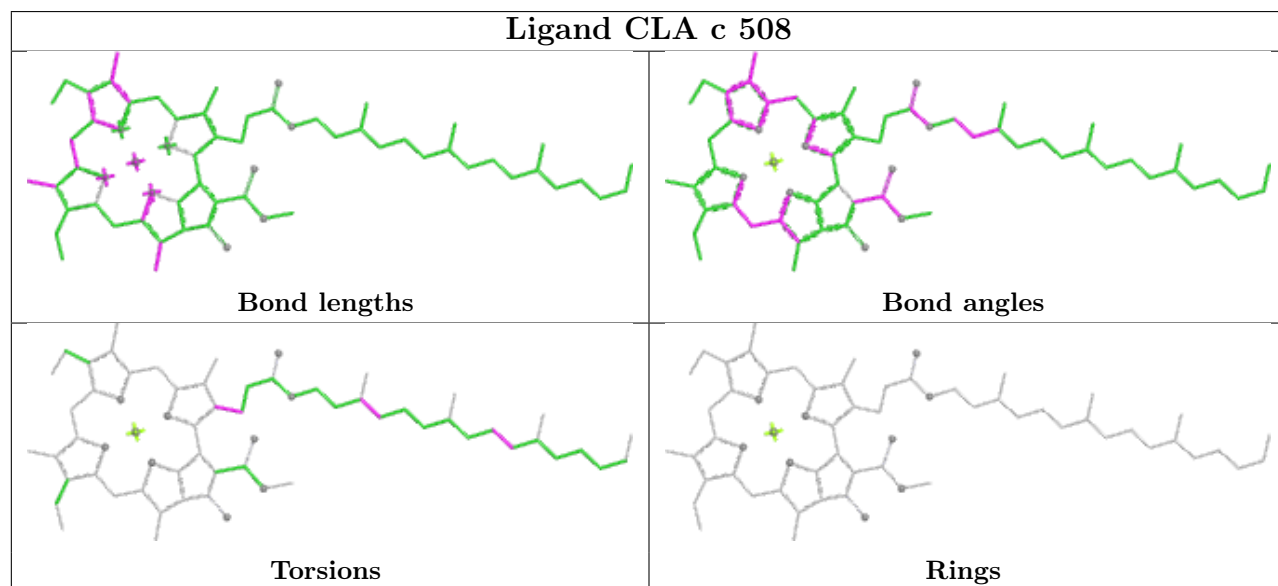
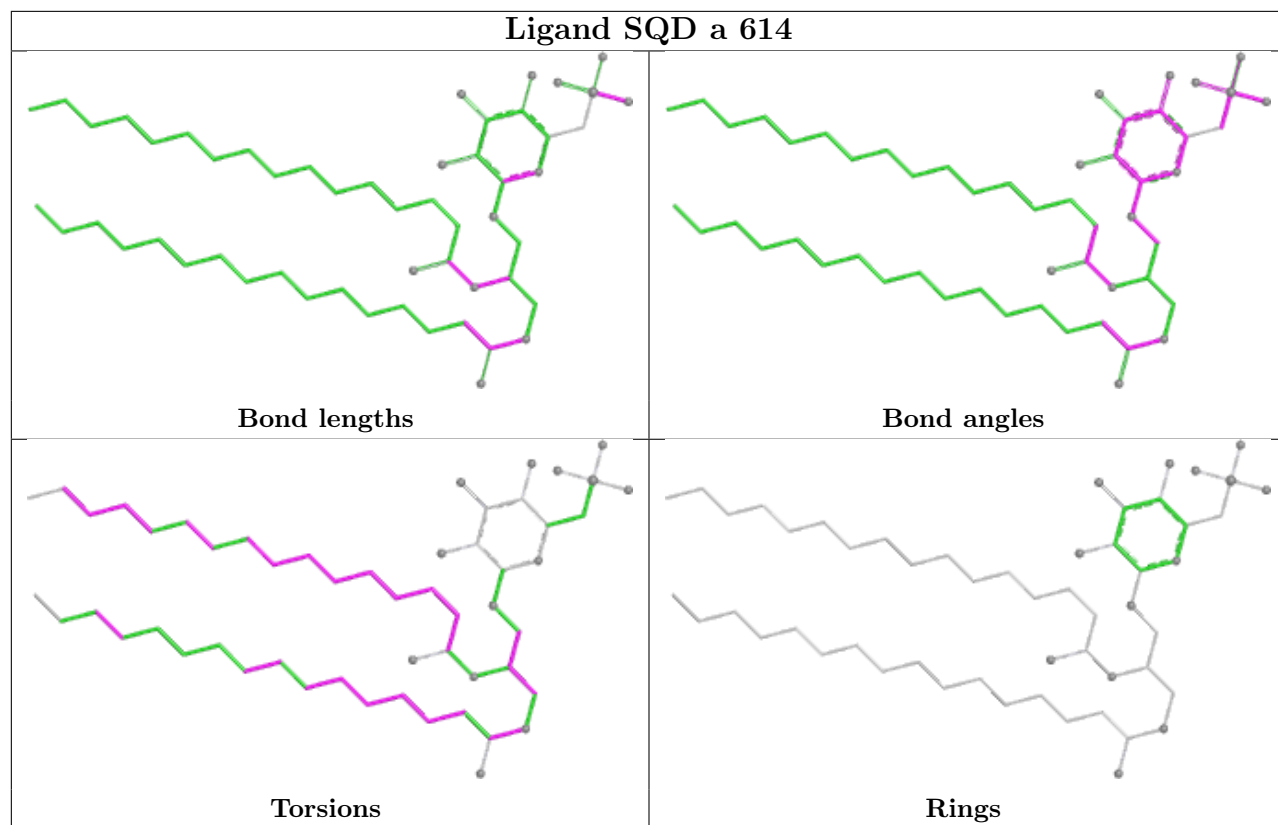


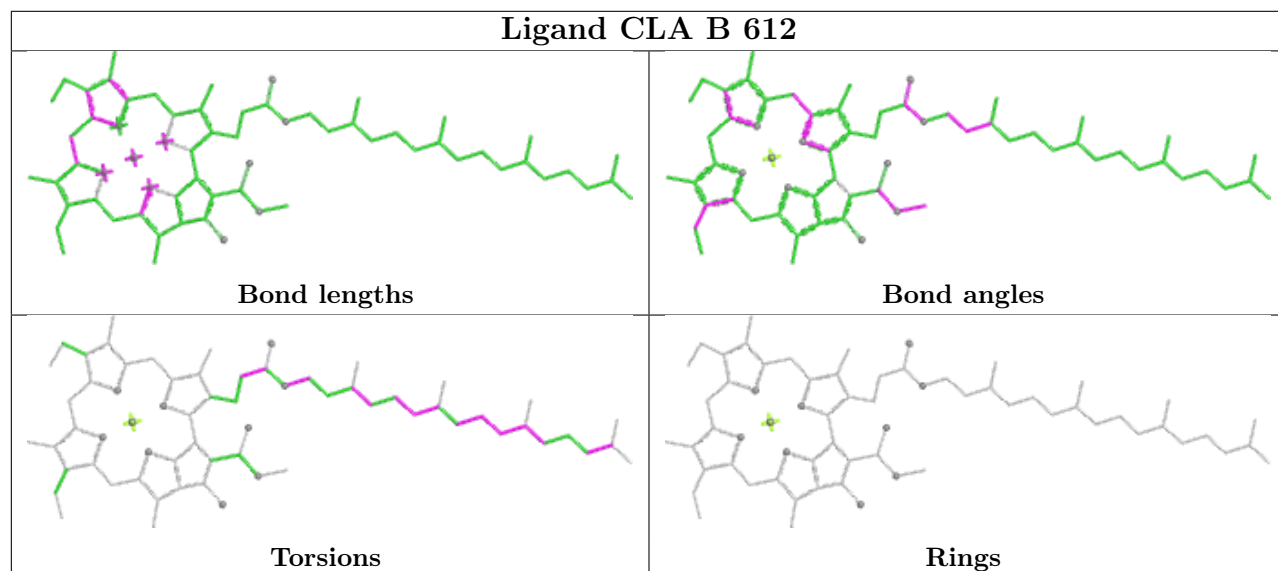
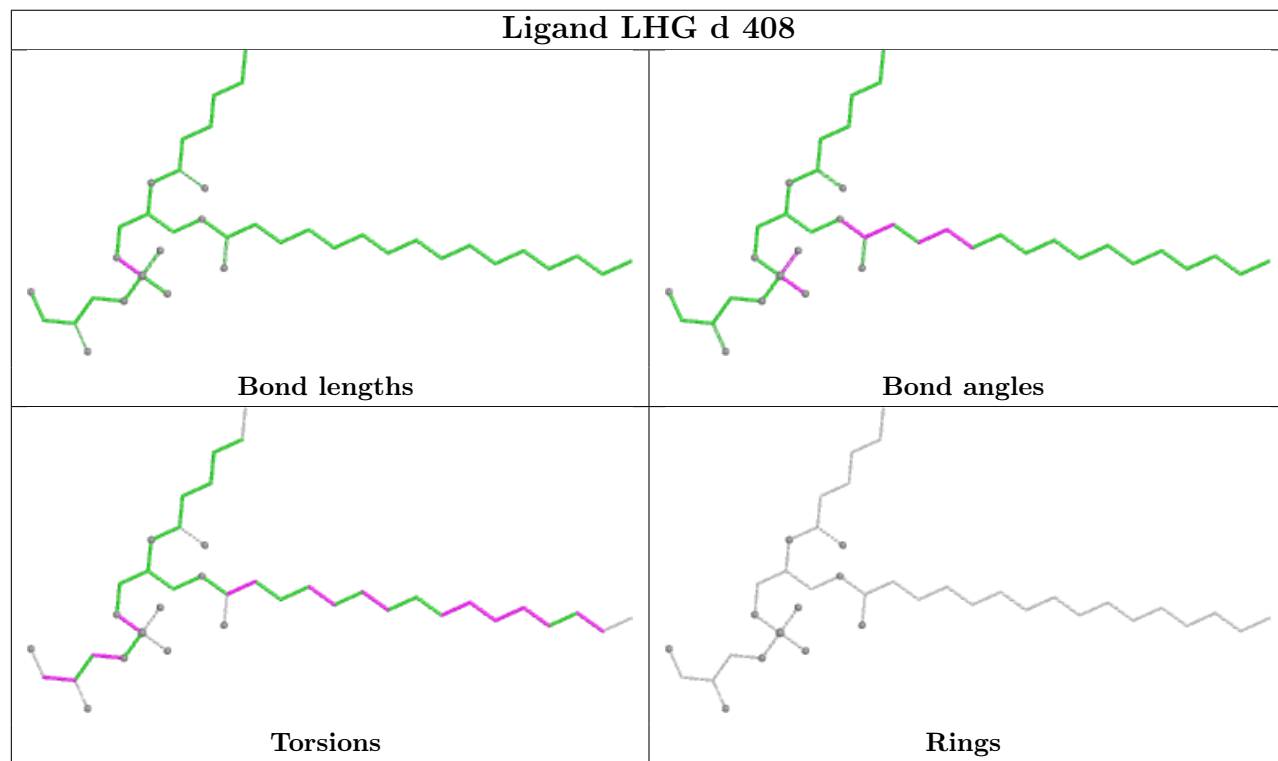
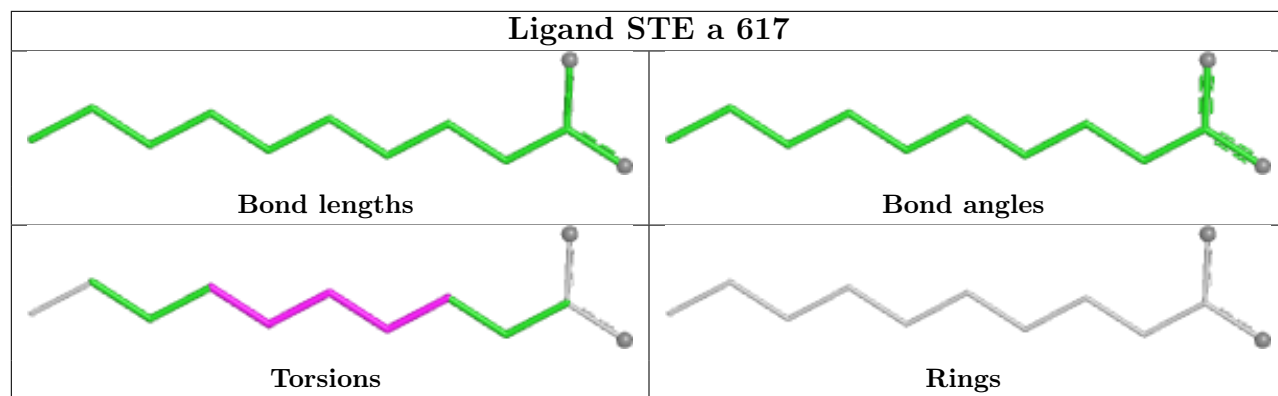


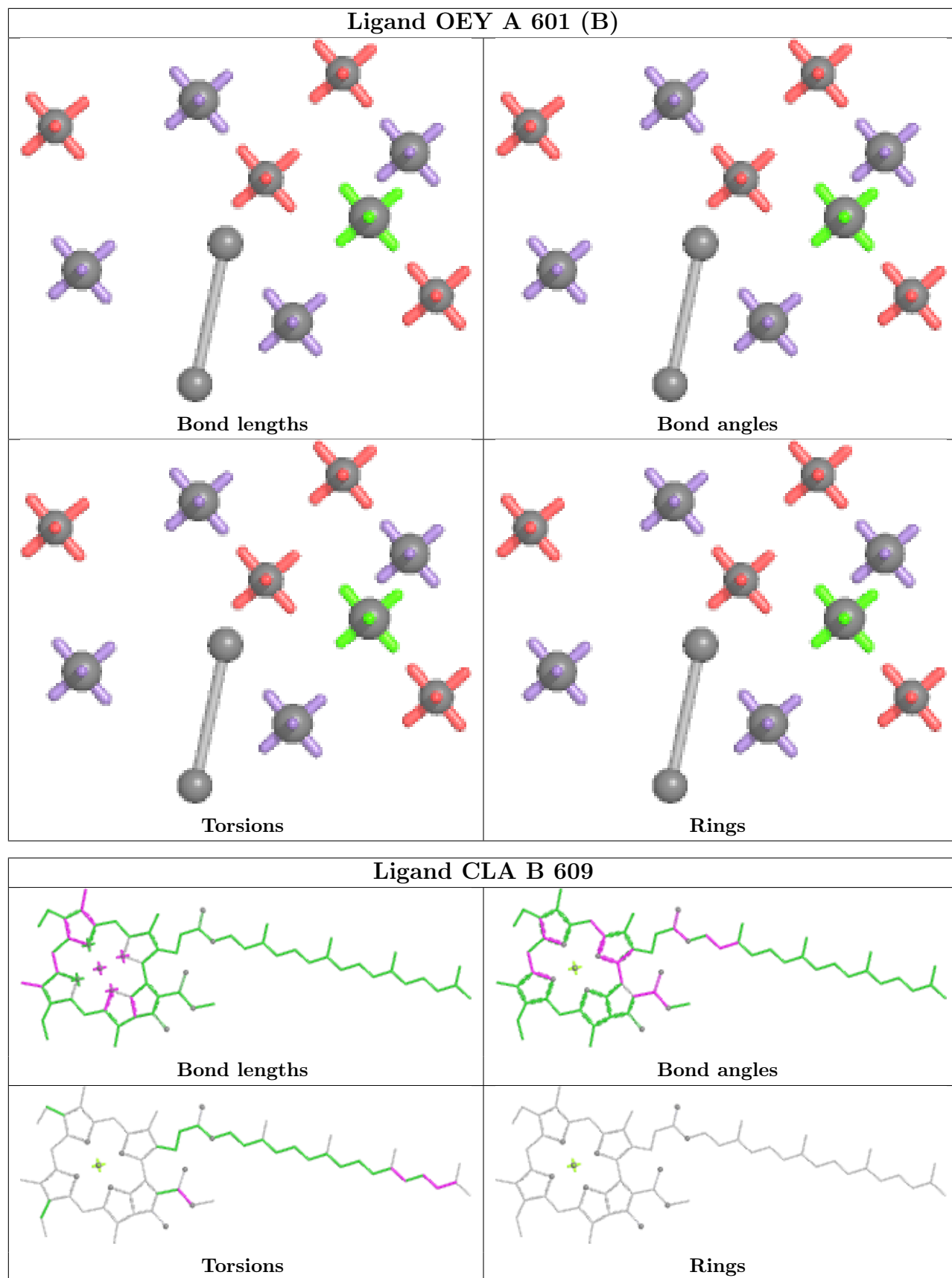


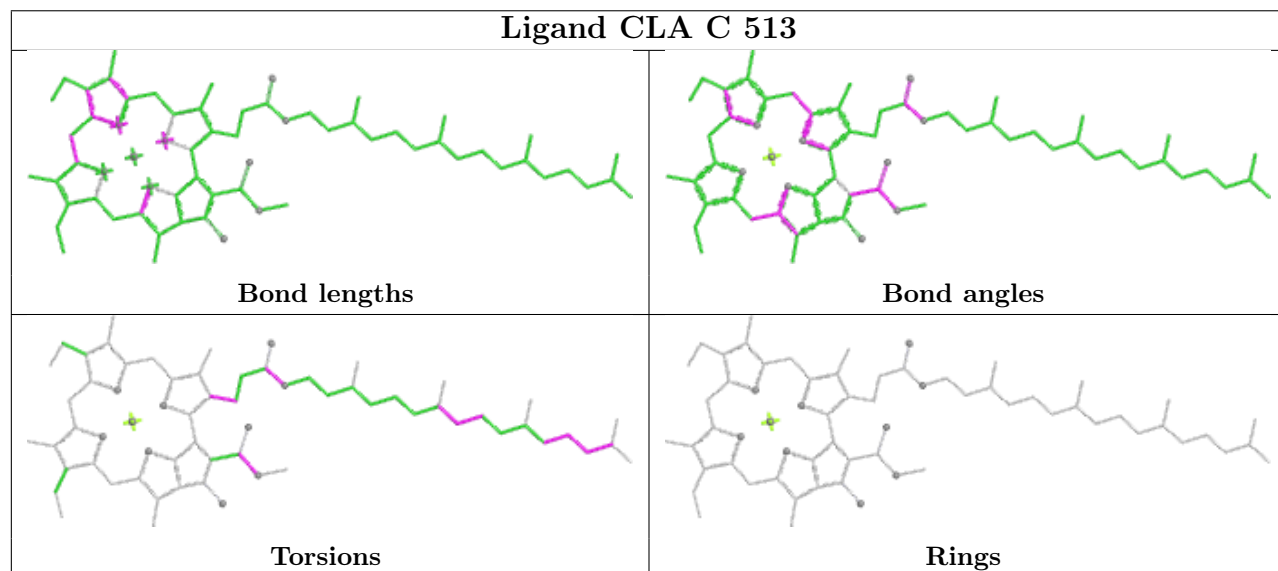
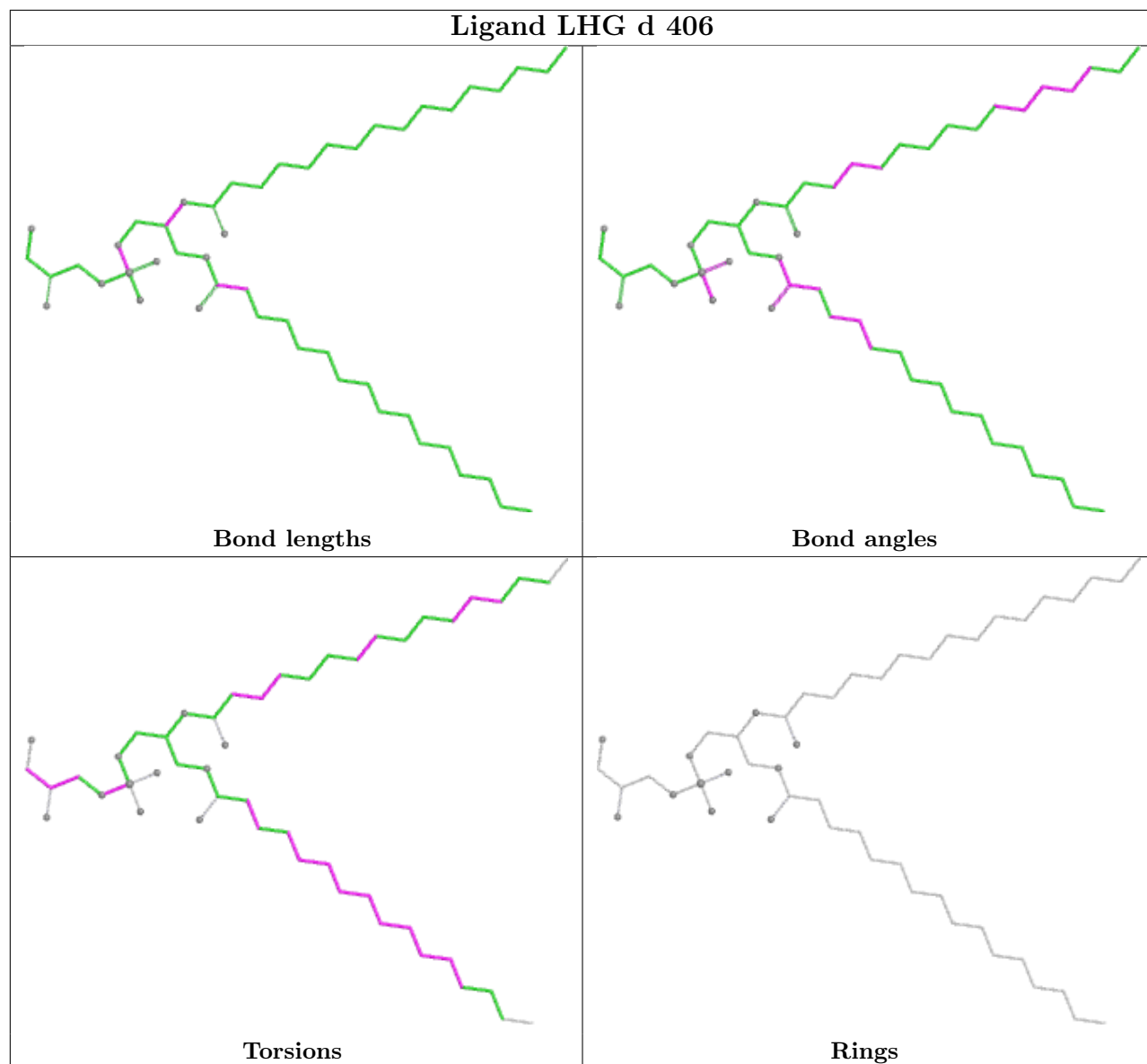


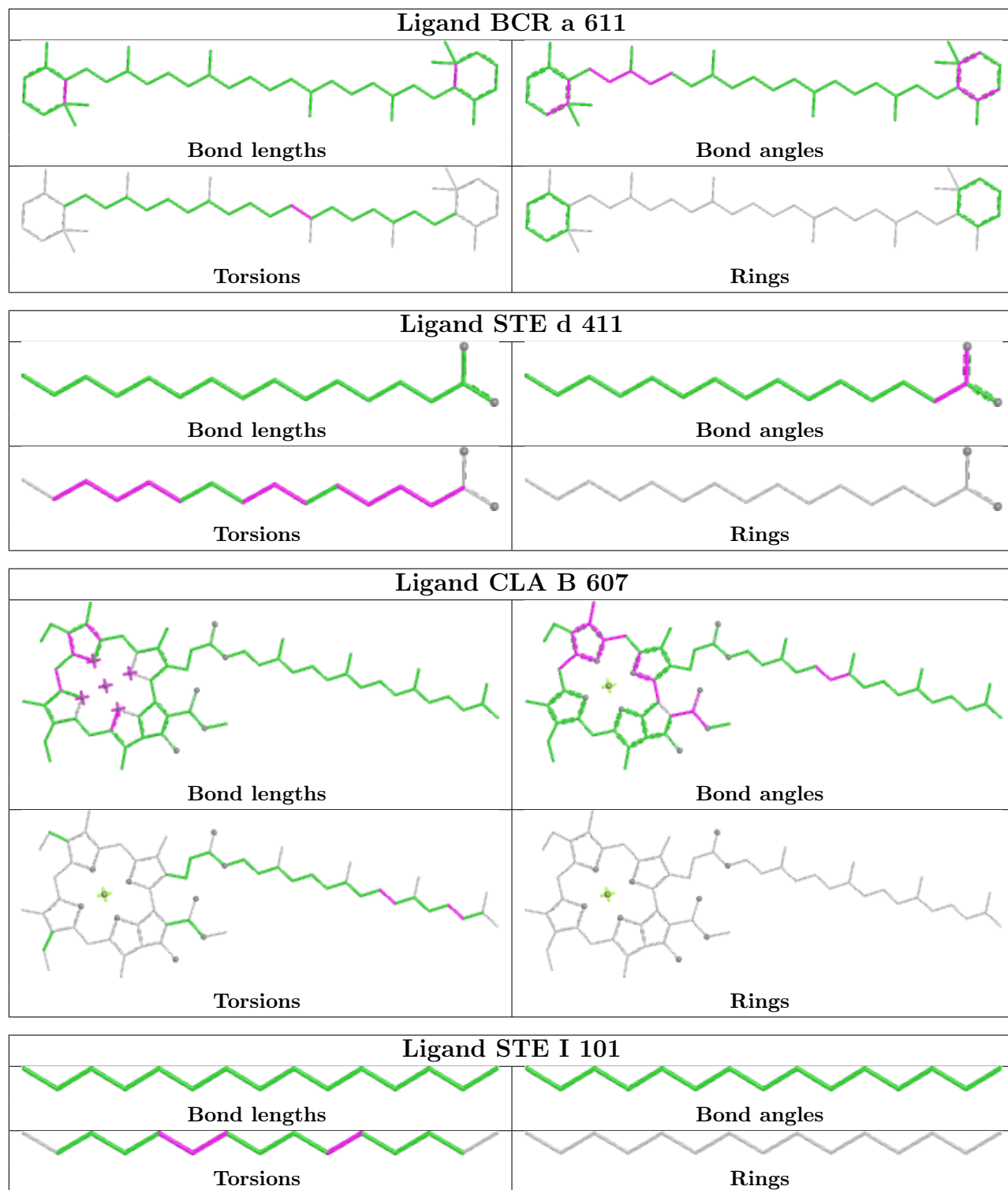


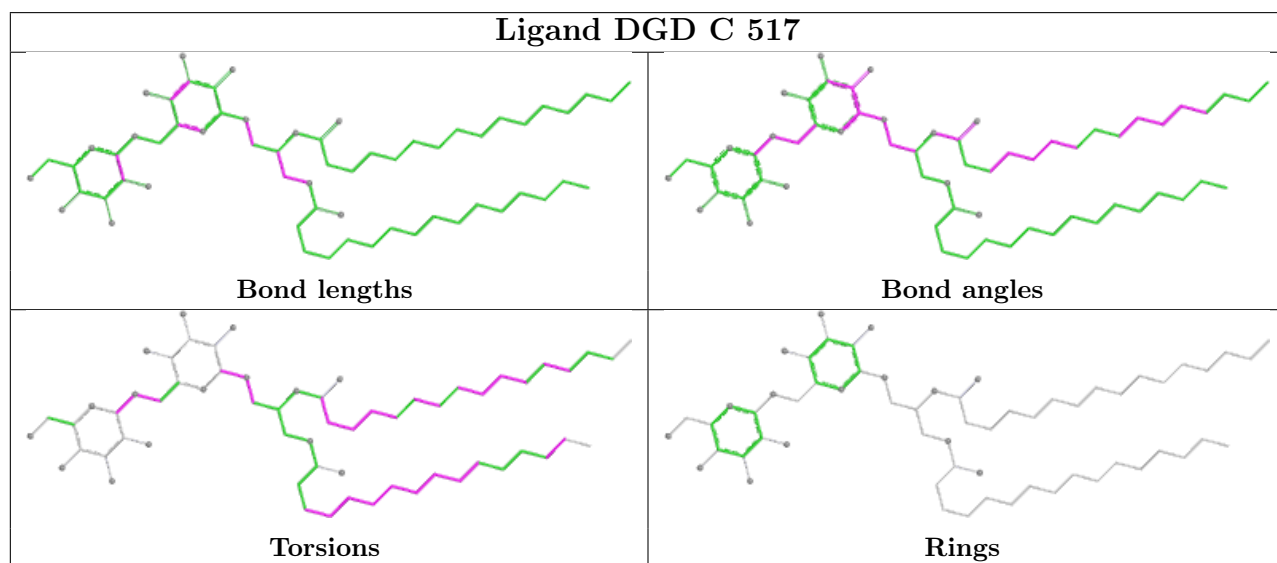
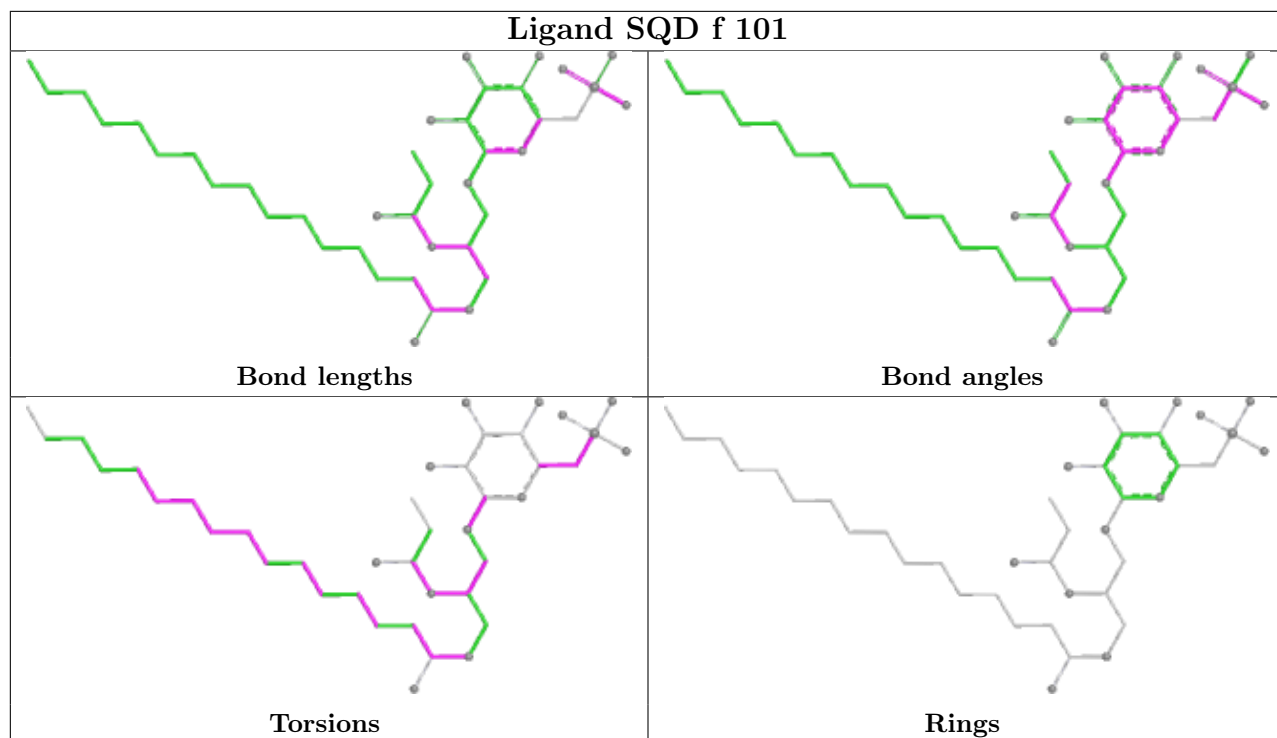


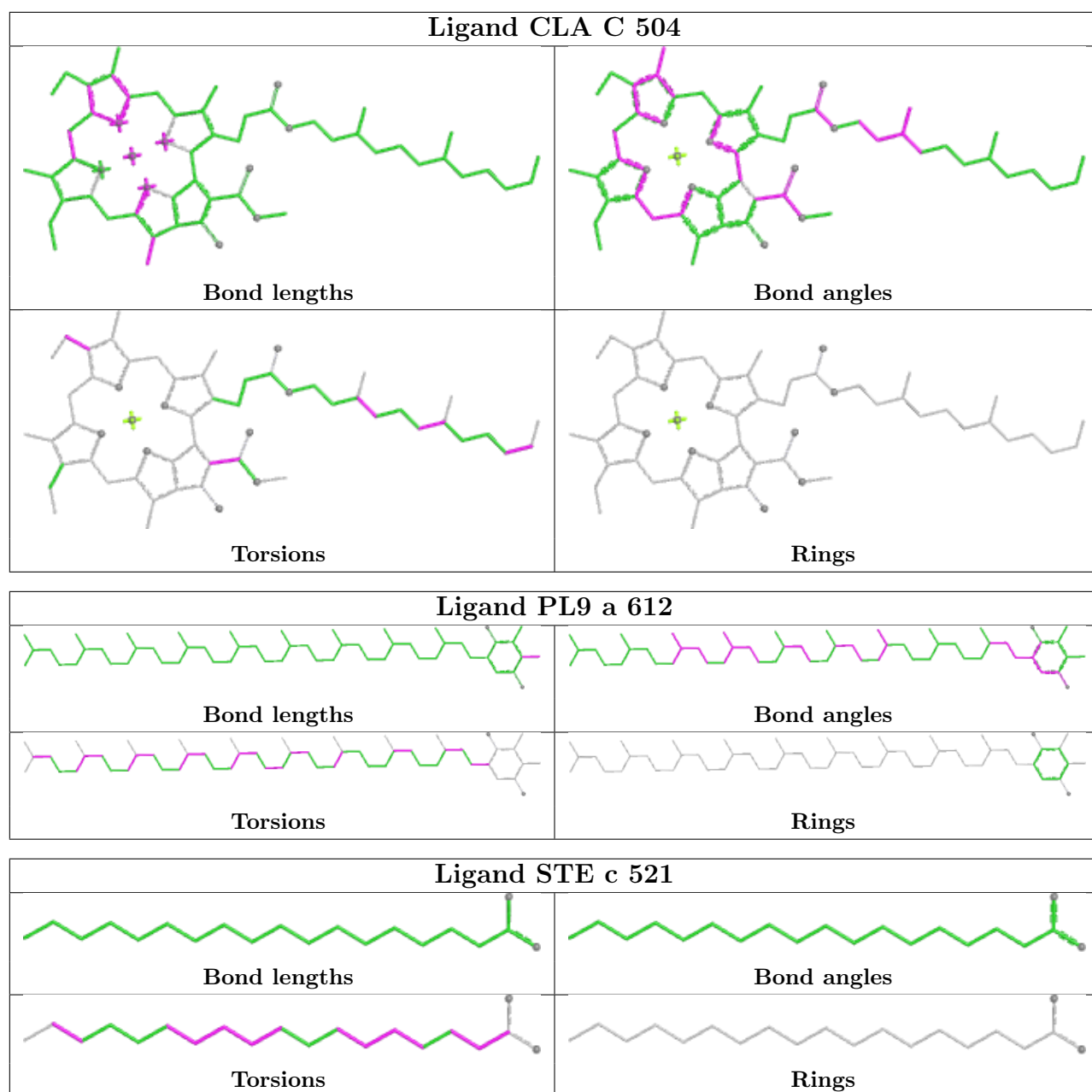


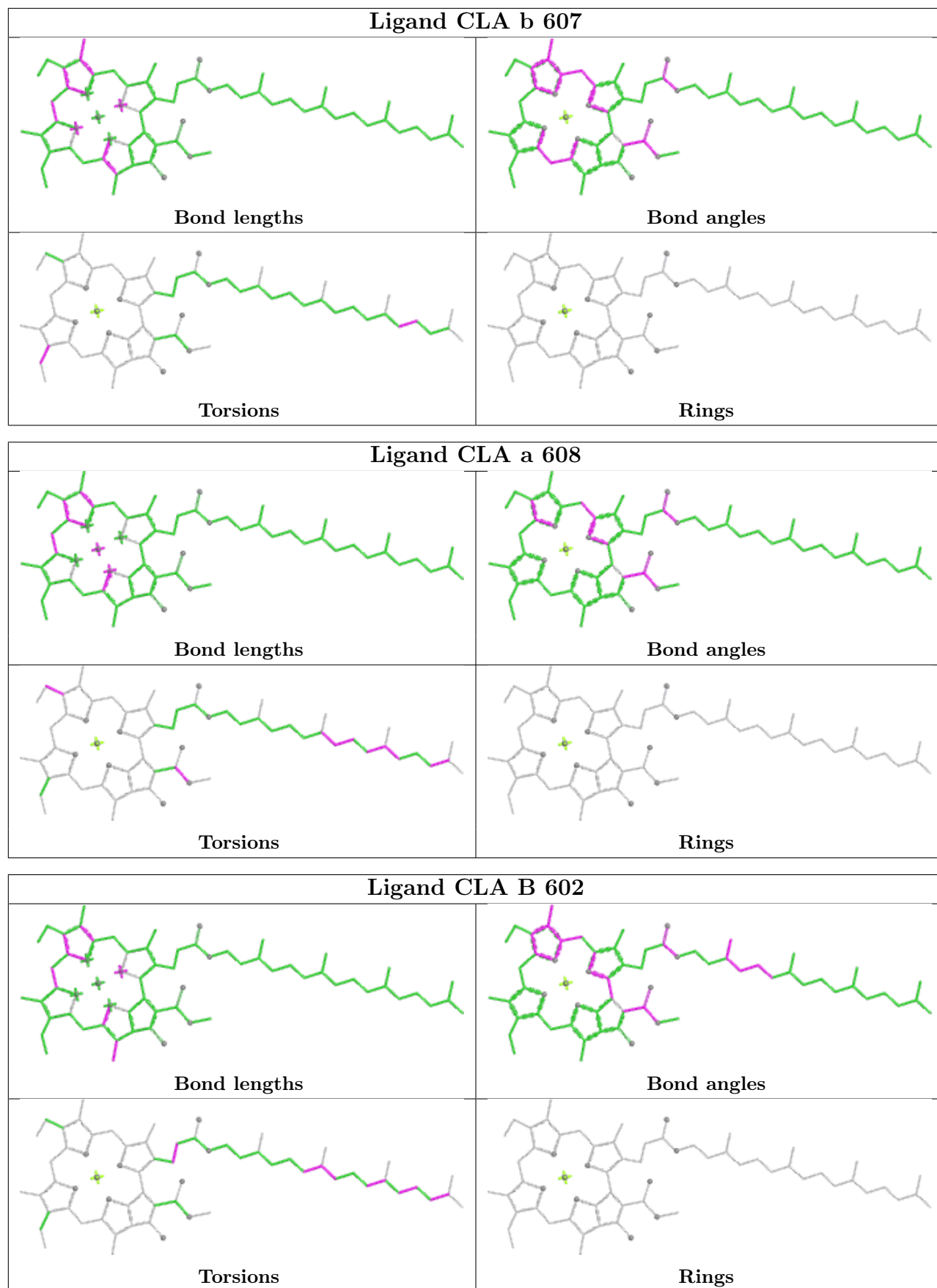


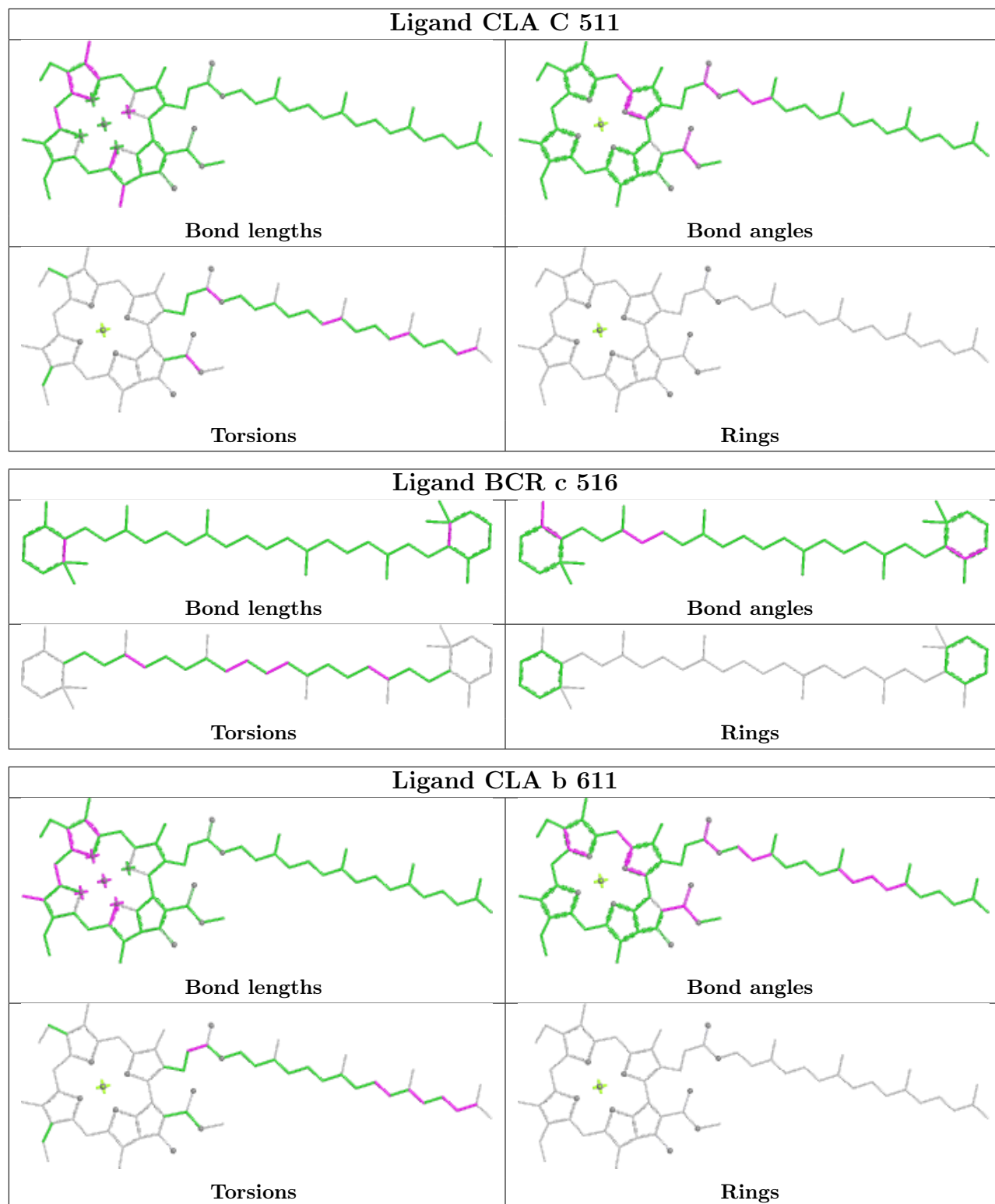


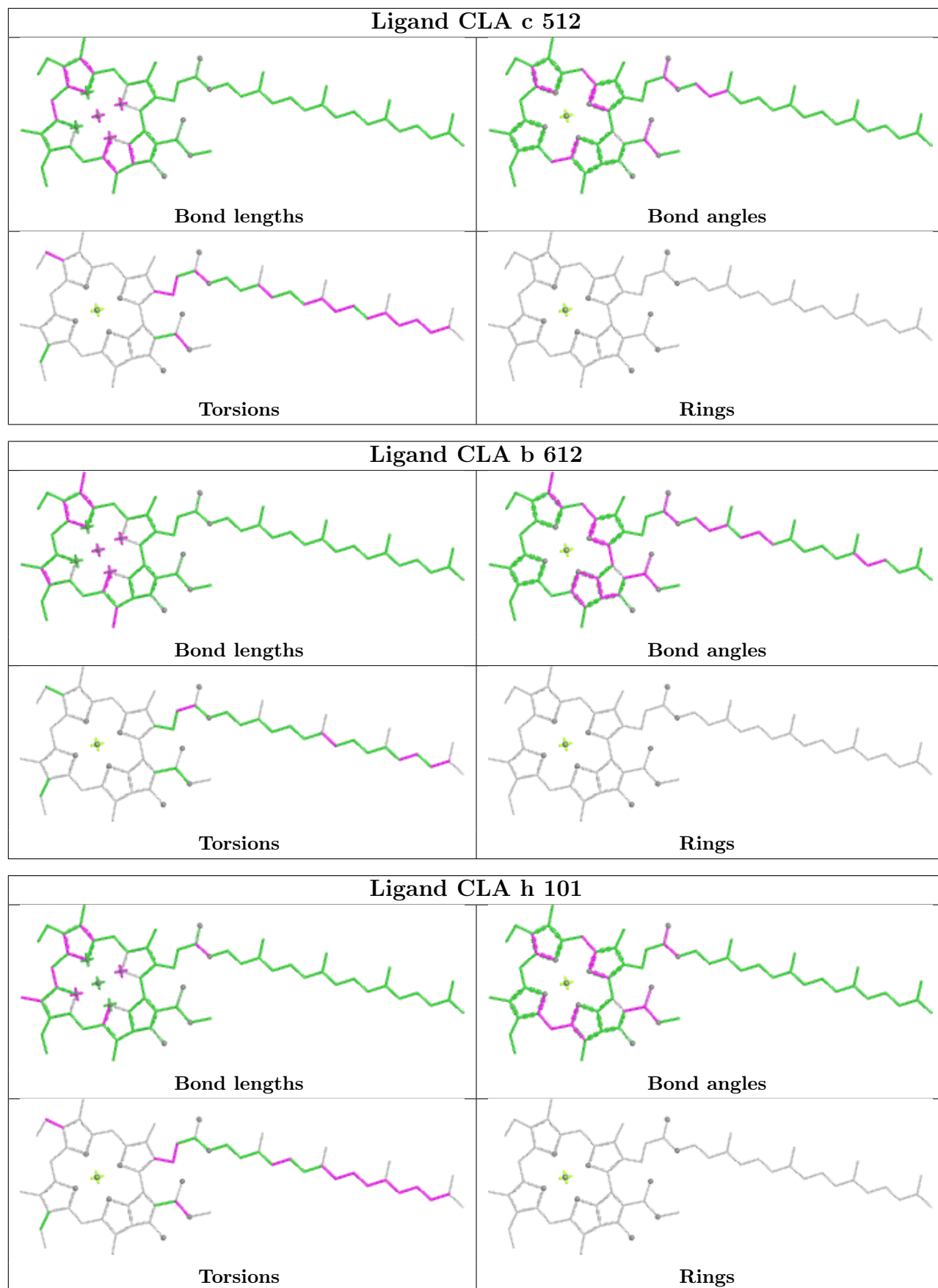


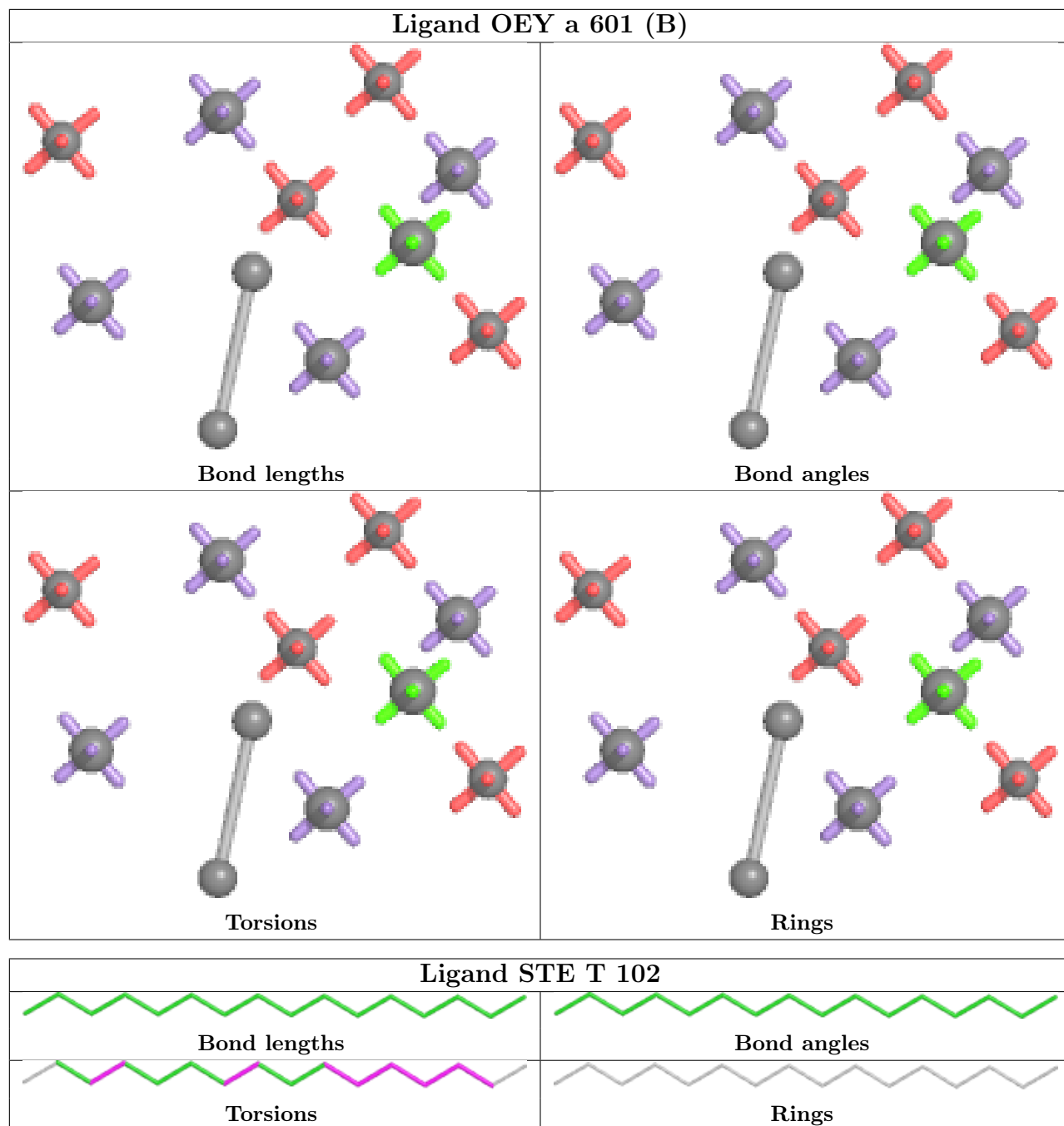


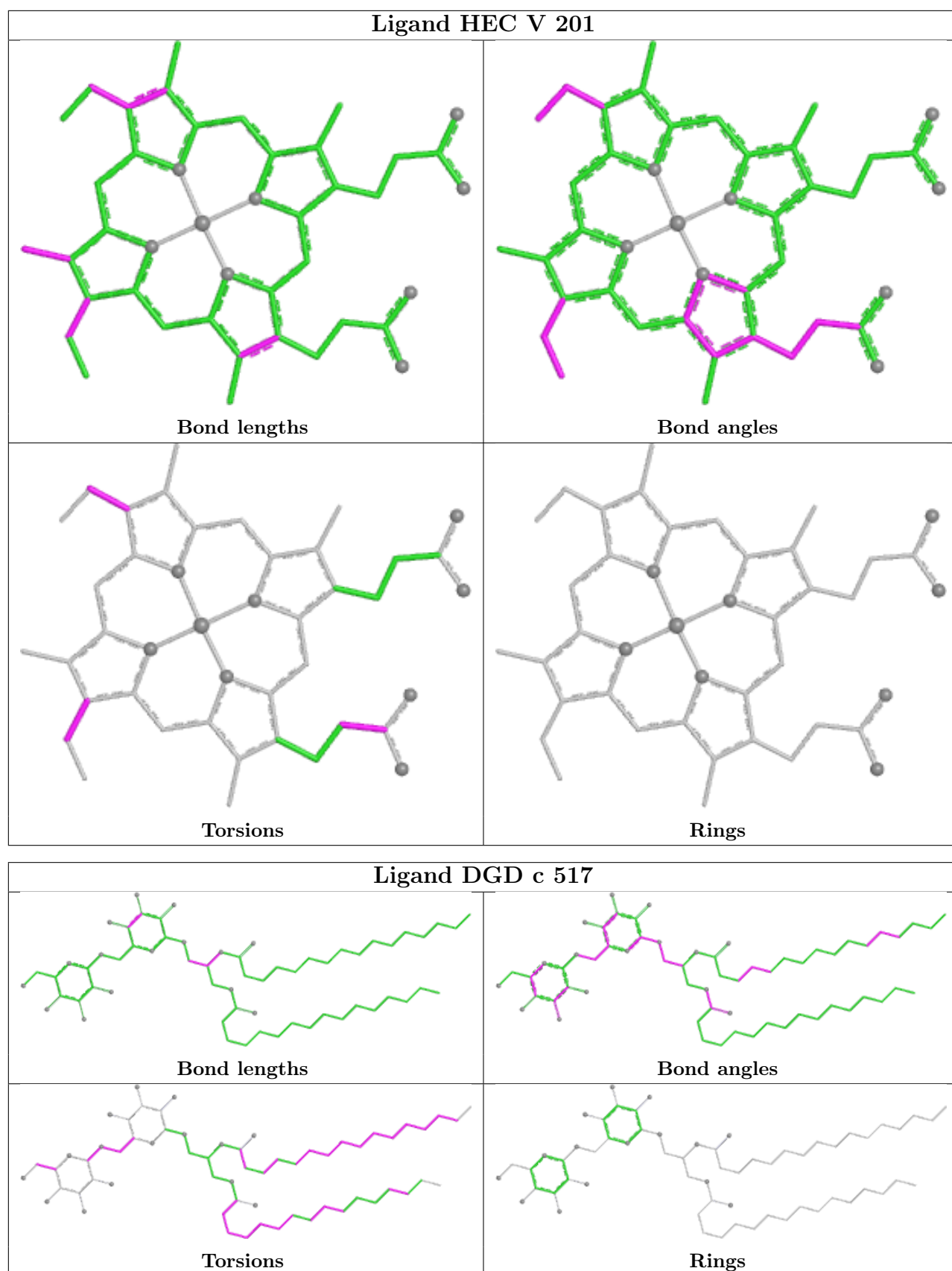


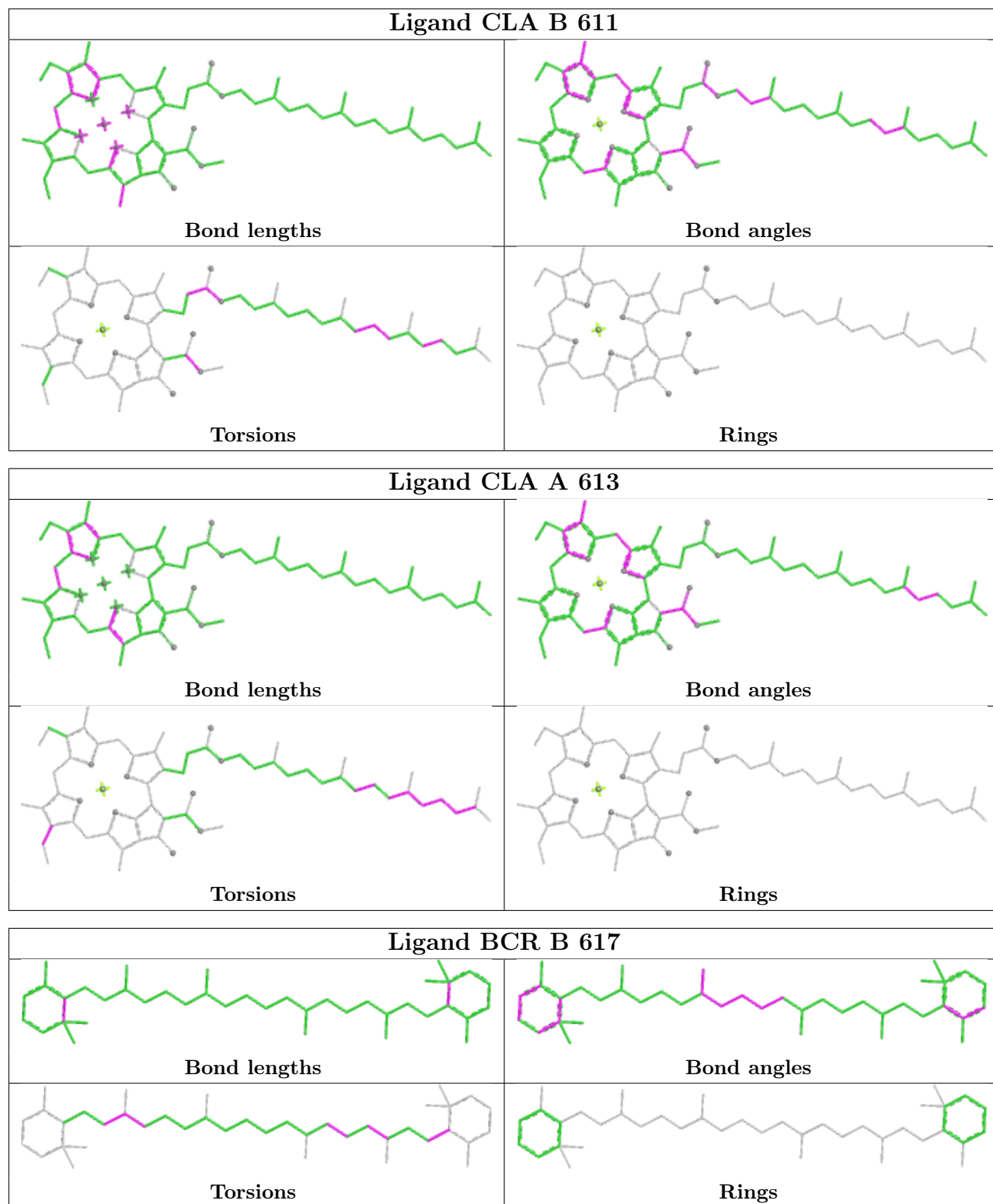












5.7 Other polymers [\(i\)](#)

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	334/344 (97%)	-0.25	1 (0%) 90 91	9, 30, 50, 82	64 (19%)
1	a	334/344 (97%)	-0.16	3 (0%) 81 83	9, 32, 58, 81	64 (19%)
2	B	505/510 (99%)	-0.34	2 (0%) 88 90	19, 35, 62, 88	4 (0%)
2	b	505/510 (99%)	-0.19	4 (0%) 82 84	27, 39, 71, 112	0
3	C	442/461 (95%)	-0.24	0 100 100	9, 38, 54, 75	11 (2%)
3	c	451/461 (97%)	-0.14	2 (0%) 88 90	10, 42, 62, 99	12 (2%)
4	D	341/352 (96%)	-0.44	0 100 100	10, 32, 49, 73	2 (0%)
4	d	341/352 (96%)	-0.30	0 100 100	11, 36, 60, 80	3 (0%)
5	E	82/84 (97%)	0.37	3 (3%) 45 47	34, 53, 70, 85	1 (1%)
5	e	82/84 (97%)	0.45	2 (2%) 59 62	42, 60, 78, 86	0
6	F	34/45 (75%)	0.06	0 100 100	40, 45, 59, 87	0
6	f	34/45 (75%)	0.26	0 100 100	44, 52, 79, 92	0
7	H	65/66 (98%)	-0.04	1 (1%) 72 74	35, 42, 58, 72	0
7	h	63/66 (95%)	0.21	2 (3%) 50 53	42, 51, 62, 66	0
8	I	35/38 (92%)	-0.25	0 100 100	35, 41, 68, 77	0
8	i	35/38 (92%)	-0.06	0 100 100	34, 43, 77, 88	0
9	J	36/40 (90%)	0.09	0 100 100	38, 51, 78, 86	0
9	j	36/40 (90%)	0.41	1 (2%) 55 57	41, 54, 87, 92	0
10	K	37/46 (80%)	0.13	0 100 100	46, 52, 69, 77	0
10	k	37/46 (80%)	0.19	0 100 100	51, 57, 72, 78	0
11	L	37/37 (100%)	-0.41	0 100 100	27, 31, 61, 68	0
11	l	36/37 (97%)	-0.46	0 100 100	30, 33, 68, 88	0
12	M	32/36 (88%)	-0.37	0 100 100	30, 35, 58, 71	0
12	m	31/36 (86%)	-0.33	0 100 100	31, 36, 54, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.09	1 (0%) 88 90	27, 44, 80, 133	1 (0%)
13	o	244/272 (89%)	-0.08	2 (0%) 82 84	29, 42, 79, 123	0
14	T	29/32 (90%)	-0.44	1 (3%) 48 50	28, 33, 57, 71	0
14	t	29/32 (90%)	-0.37	1 (3%) 48 50	30, 34, 71, 87	0
15	U	97/134 (72%)	-0.08	0 100 100	34, 45, 71, 88	0
15	u	97/134 (72%)	-0.15	1 (1%) 79 81	33, 42, 58, 84	0
16	V	137/163 (84%)	-0.20	0 100 100	33, 42, 58, 77	0
16	v	137/163 (84%)	-0.02	0 100 100	36, 48, 66, 86	0
17	Y	27/46 (58%)	0.96	1 (3%) 45 47	55, 75, 93, 95	0
17	y	30/46 (65%)	0.84	2 (6%) 24 25	64, 76, 89, 104	0
18	X	38/41 (92%)	0.12	1 (2%) 57 60	41, 53, 67, 74	0
18	x	39/41 (95%)	0.24	0 100 100	50, 60, 87, 102	0
19	Z	62/62 (100%)	0.85	4 (6%) 25 26	57, 69, 111, 126	0
19	z	62/62 (100%)	0.74	2 (3%) 50 53	61, 72, 115, 119	0
20	R	34/41 (82%)	0.83	1 (2%) 53 56	61, 69, 81, 84	0
20	r	31/41 (75%)	1.23	3 (9%) 13 14	73, 88, 108, 116	0
All	All	5302/5700 (93%)	-0.12	41 (0%) 82 84	9, 40, 73, 133	162 (3%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	3.8
20	R	35	LEU	3.7
1	a	248	ILE	3.4
9	j	6	GLY	3.0
5	e	79	PHE	3.0
19	Z	62	VAL	2.9
17	Y	25	ILE	2.8
2	b	486	LEU	2.7
19	Z	33	TRP	2.7
7	H	41	PHE	2.6
19	z	33	TRP	2.6
2	b	499	VAL	2.6
1	a	343[A]	LEU	2.6
3	c	23	ALA	2.6
13	o	57	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
15	u	53	ALA	2.5
7	h	41	PHE	2.5
3	c	134	ILE	2.5
2	b	495	PHE	2.4
13	O	60	ARG	2.4
14	t	30	THR	2.4
5	E	72	ALA	2.4
20	r	28	VAL	2.4
1	A	343[A]	LEU	2.3
2	B	487	SER	2.3
2	B	490	GLN	2.3
14	T	30	THR	2.2
1	a	168[A]	PHE	2.2
5	E	5	THR	2.2
17	y	40	ALA	2.2
19	z	27	TYR	2.2
5	E	79	PHE	2.2
19	Z	40	ILE	2.2
5	e	4	THR	2.2
2	b	494	GLY	2.1
17	y	25	ILE	2.1
7	h	64	ALA	2.1
20	r	18	TRP	2.1
18	X	2	THR	2.0
19	Z	39	LEU	2.0
20	r	14	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.92	0.11	44,51,67,72	0
14	FME	t	1	10/11	0.93	0.09	33,38,54,78	0
12	FME	m	1	10/11	0.95	0.09	33,45,62,66	0
14	FME	T	1	10/11	0.95	0.07	33,41,57,63	0
8	FME	I	1	10/11	0.96	0.07	39,49,57,57	0
8	FME	i	1	10/11	0.96	0.09	37,50,52,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	STE	H	104	18/20	0.73	0.20	52,68,74,75	0
31	STE	b	622	20/20	0.75	0.15	47,57,75,76	0
32	LMG	b	620	55/55	0.78	0.17	50,66,81,84	0
33	LHG	E	101	49/49	0.78	0.15	52,74,93,101	0
32	LMG	d	409	23/55	0.79	0.18	49,63,69,72	0
31	STE	x	102	20/20	0.80	0.16	43,54,63,69	0
32	LMG	c	522	48/55	0.80	0.15	51,71,81,87	0
31	STE	b	623	10/20	0.81	0.14	44,50,52,55	0
31	STE	a	617	12/20	0.81	0.12	50,56,71,72	0
25	CLA	h	101	65/65	0.82	0.13	52,66,86,94	0
28	PL9	A	612	55/55	0.82	0.16	39,62,73,75	0
28	PL9	a	612	55/55	0.82	0.17	46,67,79,83	0
31	STE	B	626	16/20	0.82	0.15	48,58,64,69	0
31	STE	t	103	10/20	0.82	0.14	43,53,58,60	0
33	LHG	e	102	42/49	0.82	0.14	58,80,99,107	0
31	STE	m	102	12/20	0.83	0.15	48,52,66,67	0
31	STE	B	624	18/20	0.83	0.13	41,50,72,75	0
30	DGD	a	616	44/66	0.83	0.14	36,52,82,85	0
31	STE	c	523	12/20	0.83	0.12	57,67,75,76	0
29	SQD	a	615	36/54	0.84	0.13	30,52,69,74	0
31	STE	B	625	12/20	0.84	0.13	49,56,65,65	0
32	LMG	D	409	33/55	0.84	0.14	37,52,69,72	0
31	STE	B	619	17/20	0.84	0.13	37,49,69,70	0
31	STE	b	621	16/20	0.85	0.14	53,59,78,79	0
31	STE	J	101	12/20	0.85	0.13	49,54,61,65	0
30	DGD	A	616	66/66	0.85	0.12	47,57,66,70	0
32	LMG	C	515	48/55	0.85	0.12	40,54,65,71	0
31	STE	b	619	20/20	0.85	0.13	40,52,66,68	0
31	STE	c	521	20/20	0.86	0.12	44,55,77,78	0
29	SQD	A	615	39/54	0.86	0.13	40,51,77,78	0
31	STE	I	101	15/20	0.86	0.15	43,51,64,65	0
31	STE	C	521	12/20	0.86	0.12	43,50,56,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	STE	T	102	16/20	0.86	0.15	36,45,56,61	0
31	STE	R	101	12/20	0.86	0.14	63,68,83,84	0
32	LMG	c	520	37/55	0.87	0.11	49,59,71,73	0
32	LMG	B	620	28/55	0.87	0.13	37,48,61,67	0
29	SQD	f	101	41/54	0.87	0.14	65,78,88,91	0
31	STE	C	522	16/20	0.87	0.14	37,52,58,59	0
31	STE	d	411	17/20	0.87	0.13	49,52,64,66	0
31	STE	C	520	12/20	0.88	0.11	34,44,52,56	0
31	STE	j	101	12/20	0.88	0.11	51,57,60,61	0
29	SQD	l	101	54/54	0.88	0.11	38,60,76,82	0
25	CLA	H	101	65/65	0.88	0.11	39,53,77,84	0
32	LMG	c	524	49/55	0.88	0.10	39,54,70,76	0
31	STE	T	103	15/20	0.88	0.14	45,53,69,73	0
32	LMG	m	101	51/55	0.88	0.10	34,49,63,71	0
31	STE	D	410	20/20	0.88	0.12	35,45,64,73	0
31	STE	B	623	12/20	0.88	0.11	39,47,59,59	0
31	STE	l	103	18/20	0.89	0.12	37,44,63,64	0
29	SQD	L	101	49/54	0.89	0.10	42,58,80,82	0
32	LMG	C	519	48/55	0.89	0.12	43,65,81,85	0
27	BCR	K	102	40/40	0.90	0.10	43,51,61,62	0
29	SQD	a	614	54/54	0.90	0.10	38,59,75,81	0
27	BCR	d	404	40/40	0.90	0.11	38,47,79,85	0
31	STE	t	102	14/20	0.90	0.09	38,43,50,54	0
27	BCR	k	101	40/40	0.90	0.11	50,57,65,70	0
29	SQD	F	102	36/54	0.90	0.12	48,64,72,75	0
27	BCR	c	514	40/40	0.91	0.10	46,56,63,65	0
31	STE	M	102	15/20	0.91	0.10	36,43,60,62	0
27	BCR	x	101	40/40	0.91	0.10	38,53,61,64	0
32	LMG	M	101	51/55	0.91	0.09	33,46,61,62	0
27	BCR	H	102	40/40	0.91	0.09	34,45,55,57	0
30	DGD	C	517	62/66	0.91	0.10	36,45,83,98	0
27	BCR	B	617	40/40	0.92	0.07	27,36,46,48	0
27	BCR	D	404	40/40	0.92	0.10	33,43,70,79	0
30	DGD	H	103	62/66	0.92	0.09	34,42,50,52	0
25	CLA	c	512	65/65	0.92	0.10	47,55,78,83	0
30	DGD	h	102	62/66	0.92	0.09	34,45,52,54	0
25	CLA	C	513	65/65	0.92	0.09	45,55,79,83	0
27	BCR	K	103	40/40	0.92	0.11	42,48,58,59	0
27	BCR	b	618	40/40	0.92	0.09	33,43,53,55	0
29	SQD	A	614	52/54	0.92	0.10	33,52,68,74	0
31	STE	M	103	10/20	0.92	0.10	35,46,53,54	0
27	BCR	c	516	40/40	0.93	0.11	47,52,61,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	LMG	D	406	51/55	0.93	0.10	32,47,64,68	0
25	CLA	C	512	65/65	0.93	0.10	39,48,69,79	0
25	CLA	c	513	65/65	0.93	0.10	48,60,86,92	0
27	BCR	t	101	40/40	0.93	0.07	27,39,48,48	0
27	BCR	K	101	40/40	0.93	0.10	41,53,58,60	0
25	CLA	B	605	65/65	0.93	0.09	26,34,63,72	0
25	CLA	C	510	65/65	0.93	0.08	31,43,51,53	0
27	BCR	b	616	40/40	0.93	0.08	28,42,48,51	0
27	BCR	B	618	40/40	0.93	0.08	31,42,50,52	0
30	DGD	c	518	62/66	0.93	0.09	39,47,75,81	0
27	BCR	C	514	40/40	0.93	0.09	31,41,49,50	0
25	CLA	C	511	65/65	0.94	0.09	36,48,57,62	0
27	BCR	A	611	40/40	0.94	0.07	26,34,38,39	0
27	BCR	T	101	40/40	0.94	0.07	29,38,47,48	0
30	DGD	C	516	62/66	0.94	0.10	30,35,70,79	0
28	PL9	D	405	55/55	0.94	0.07	24,31,40,42	0
30	DGD	C	518	62/66	0.94	0.08	31,43,61,66	0
25	CLA	c	503	65/65	0.94	0.08	36,44,50,55	0
27	BCR	b	617	40/40	0.94	0.07	29,39,45,49	0
25	CLA	c	508	64/65	0.94	0.09	36,42,77,93	0
30	DGD	c	519	62/66	0.94	0.08	33,46,66,68	0
25	CLA	c	509	65/65	0.94	0.10	38,46,56,58	0
32	LMG	d	410	44/55	0.94	0.09	38,48,71,76	0
25	CLA	c	511	65/65	0.94	0.10	44,53,59,63	0
33	LHG	B	622	49/49	0.94	0.09	32,41,53,61	0
33	LHG	D	408	47/49	0.94	0.10	31,40,69,74	0
25	CLA	C	502	65/65	0.94	0.08	33,39,49,58	0
33	LHG	d	406	49/49	0.94	0.10	32,45,59,65	0
25	CLA	C	501	65/65	0.94	0.07	26,35,45,45	0
34	BCT	a	606	4/4	0.94	0.08	33,36,41,45	0
28	PL9	d	405	55/55	0.95	0.07	25,34,39,41	0
25	CLA	B	614	65/65	0.95	0.07	25,35,51,62	0
25	CLA	B	615	60/65	0.95	0.09	28,35,74,82	0
25	CLA	d	402	65/65	0.95	0.07	21,32,51,55	0
25	CLA	d	403	65/65	0.95	0.08	34,42,70,74	0
25	CLA	A	607	65/65	0.95	0.09	23,32,80,84	0
26	PHO	A	609	64/64	0.95	0.06	27,32,38,42	0
26	PHO	a	609	64/64	0.95	0.06	26,31,36,39	0
26	PHO	d	401	64/64	0.95	0.07	28,38,44,46	0
25	CLA	B	609	65/65	0.95	0.07	25,32,37,42	0
27	BCR	B	616	40/40	0.95	0.07	31,36,46,55	0
25	CLA	C	503	65/65	0.95	0.07	35,41,45,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	a	607	65/65	0.95	0.07	24,29,37,47	0
25	CLA	a	608	65/65	0.95	0.08	28,37,85,93	0
25	CLA	b	601	65/65	0.95	0.08	31,39,52,55	0
25	CLA	b	603	65/65	0.95	0.08	25,33,62,71	0
25	CLA	b	605	65/65	0.95	0.07	30,37,62,65	0
25	CLA	b	607	65/65	0.95	0.07	32,40,53,56	0
25	CLA	b	608	65/65	0.95	0.07	32,43,54,64	0
25	CLA	b	609	65/65	0.95	0.08	30,37,43,49	0
27	BCR	a	611	40/40	0.95	0.07	23,32,42,45	0
25	CLA	b	614	65/65	0.95	0.07	29,39,51,56	0
25	CLA	b	615	60/65	0.95	0.08	33,40,77,79	0
25	CLA	c	502	65/65	0.95	0.07	33,41,53,59	0
25	CLA	C	506	65/65	0.95	0.09	30,41,74,79	0
27	BCR	c	515	40/40	0.95	0.08	32,44,50,53	0
25	CLA	c	504	60/65	0.95	0.08	30,42,68,72	0
25	CLA	c	505	65/65	0.95	0.08	31,39,58,60	0
25	CLA	c	506	65/65	0.95	0.08	37,43,71,77	0
25	CLA	c	507	65/65	0.95	0.07	32,40,49,55	0
25	CLA	C	507	65/65	0.95	0.07	29,38,49,51	0
25	CLA	C	508	65/65	0.95	0.08	33,39,83,94	0
33	LHG	d	408	39/49	0.95	0.09	34,44,55,60	0
25	CLA	c	510	65/65	0.95	0.07	33,45,52,54	0
33	LHG	l	102	49/49	0.95	0.07	32,41,46,49	0
25	CLA	C	509	65/65	0.95	0.08	32,40,53,55	0
25	CLA	a	613	65/65	0.96	0.06	25,30,40,42	0
25	CLA	B	604	65/65	0.96	0.07	26,31,39,42	0
25	CLA	b	602	65/65	0.96	0.07	27,33,56,68	0
25	CLA	A	606	65/65	0.96	0.06	21,27,37,41	0
25	CLA	b	604	65/65	0.96	0.07	25,34,42,45	0
25	CLA	C	504	59/65	0.96	0.07	35,41,66,72	0
25	CLA	b	606	65/65	0.96	0.07	25,33,54,60	0
26	PHO	A	608	64/64	0.96	0.05	21,27,33,37	0
25	CLA	C	505	65/65	0.96	0.08	28,36,58,65	0
25	CLA	B	606	65/65	0.96	0.07	21,30,54,57	0
25	CLA	B	607	65/65	0.96	0.06	25,33,47,50	0
25	CLA	b	610	65/65	0.96	0.06	25,33,45,50	0
25	CLA	b	611	65/65	0.96	0.07	25,33,39,45	0
25	CLA	b	612	65/65	0.96	0.07	26,31,64,67	0
25	CLA	b	613	65/65	0.96	0.07	27,37,63,73	0
25	CLA	B	608	65/65	0.96	0.07	28,37,49,52	0
25	CLA	A	610	54/65	0.96	0.07	22,30,58,60	0
25	CLA	c	501	65/65	0.96	0.07	29,38,46,48	0

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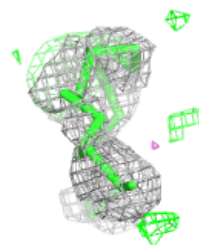
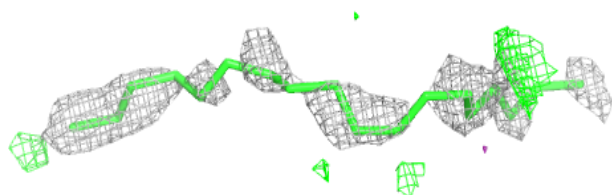
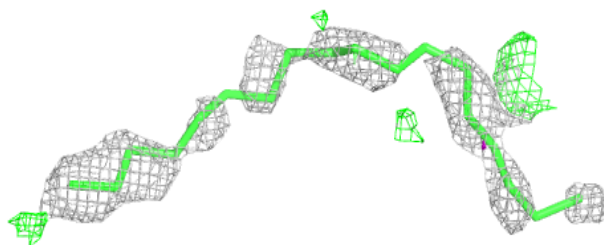
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	B	610	65/65	0.96	0.06	23,30,40,43	0
33	LHG	B	621	49/49	0.96	0.07	30,36,45,53	0
25	CLA	B	611	65/65	0.96	0.07	24,31,40,47	0
33	LHG	D	407	49/49	0.96	0.07	25,35,45,46	0
25	CLA	B	612	65/65	0.96	0.06	22,30,56,65	0
25	CLA	B	613	65/65	0.96	0.08	26,36,57,67	0
25	CLA	B	601	65/65	0.96	0.07	28,36,49,54	0
33	LHG	d	407	49/49	0.96	0.07	30,40,47,52	0
25	CLA	B	602	65/65	0.96	0.07	25,31,52,54	0
25	CLA	B	603	65/65	0.96	0.07	25,30,63,65	0
30	DGD	c	517	62/66	0.96	0.08	27,38,58,67	0
25	CLA	a	610	65/65	0.96	0.08	24,31,66,74	0
35	HEM	e	101	43/43	0.96	0.09	54,58,72,85	0
25	CLA	D	403	65/65	0.97	0.07	28,34,77,92	0
25	CLA	A	613	65/65	0.97	0.06	21,28,41,45	0
35	HEM	F	101	43/43	0.97	0.08	42,48,58,63	0
25	CLA	D	402	65/65	0.97	0.06	22,28,47,52	0
34	BCT	D	401	4/4	0.98	0.07	35,37,38,38	0
22	OEX	a	602[A]	10/10	0.98	0.03	35,37,42,42	10
24	CL	A	604	1/1	0.98	0.04	34,34,34,34	0
22	OEX	A	602[A]	10/10	0.98	0.03	36,38,41,43	10
36	HEC	V	201	43/43	0.98	0.07	29,36,44,52	0
36	HEC	v	201	43/43	0.98	0.06	29,38,41,44	0
21	OEY	A	601[C]	11/11	0.99	0.03	29,31,35,37	11
23	FE2	a	603	1/1	0.99	0.02	36,36,36,36	0
21	OEY	a	601[B]	11/11	0.99	0.03	20,25,29,30	11
24	CL	A	605	1/1	0.99	0.08	31,31,31,31	0
24	CL	a	604	1/1	0.99	0.04	32,32,32,32	0
24	CL	a	605	1/1	0.99	0.09	34,34,34,34	0
21	OEY	a	601[C]	11/11	0.99	0.03	30,32,34,36	11
21	OEY	A	601[B]	11/11	0.99	0.03	20,24,27,30	11
23	FE2	A	603	1/1	1.00	0.01	28,28,28,28	0

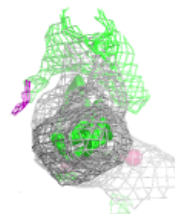
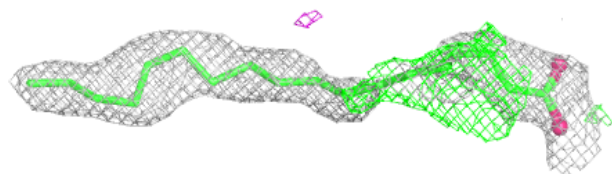
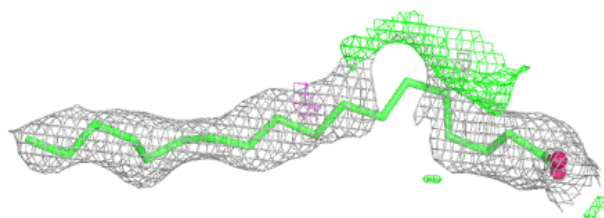
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

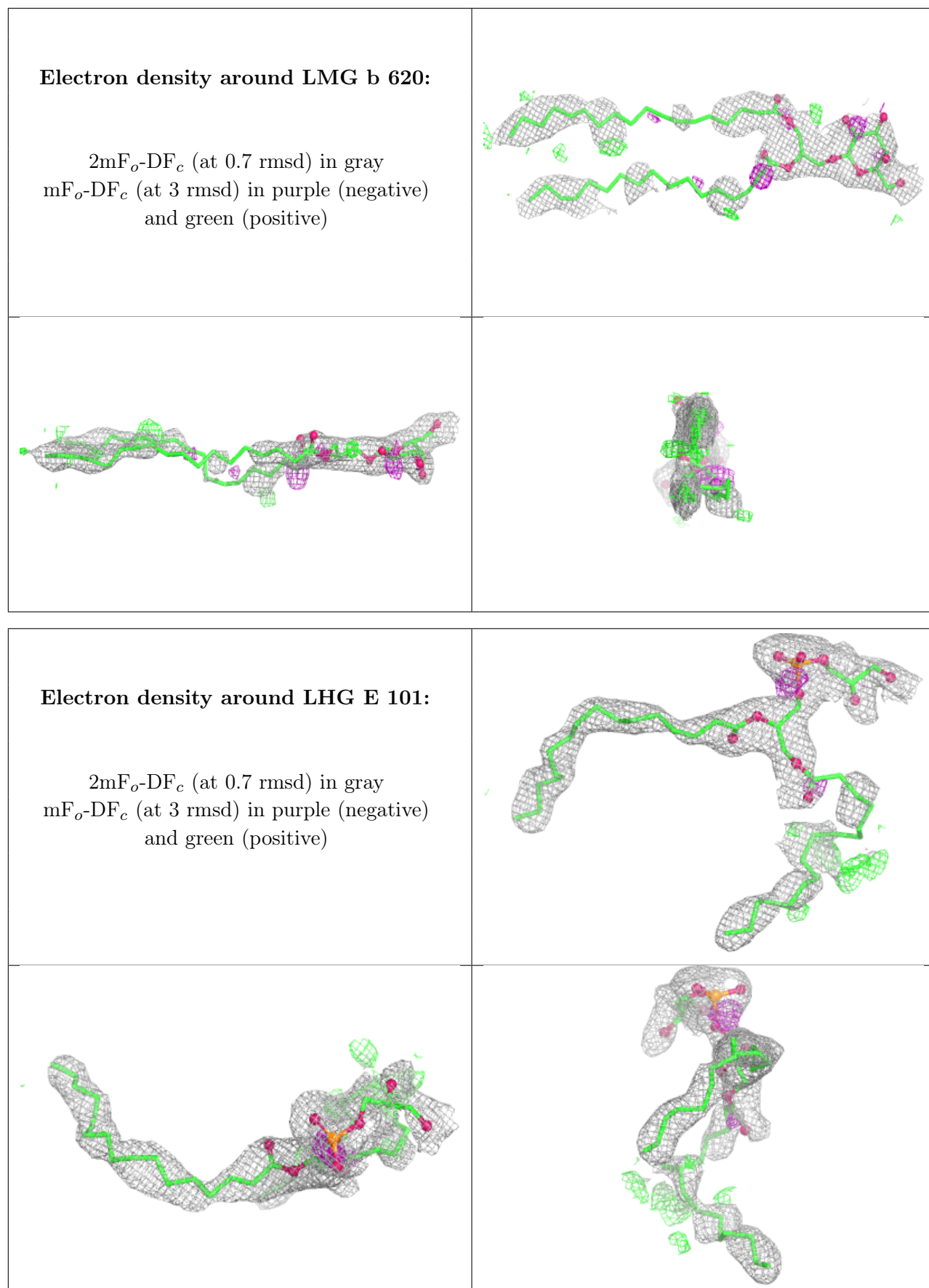
Electron density around STE H 104:

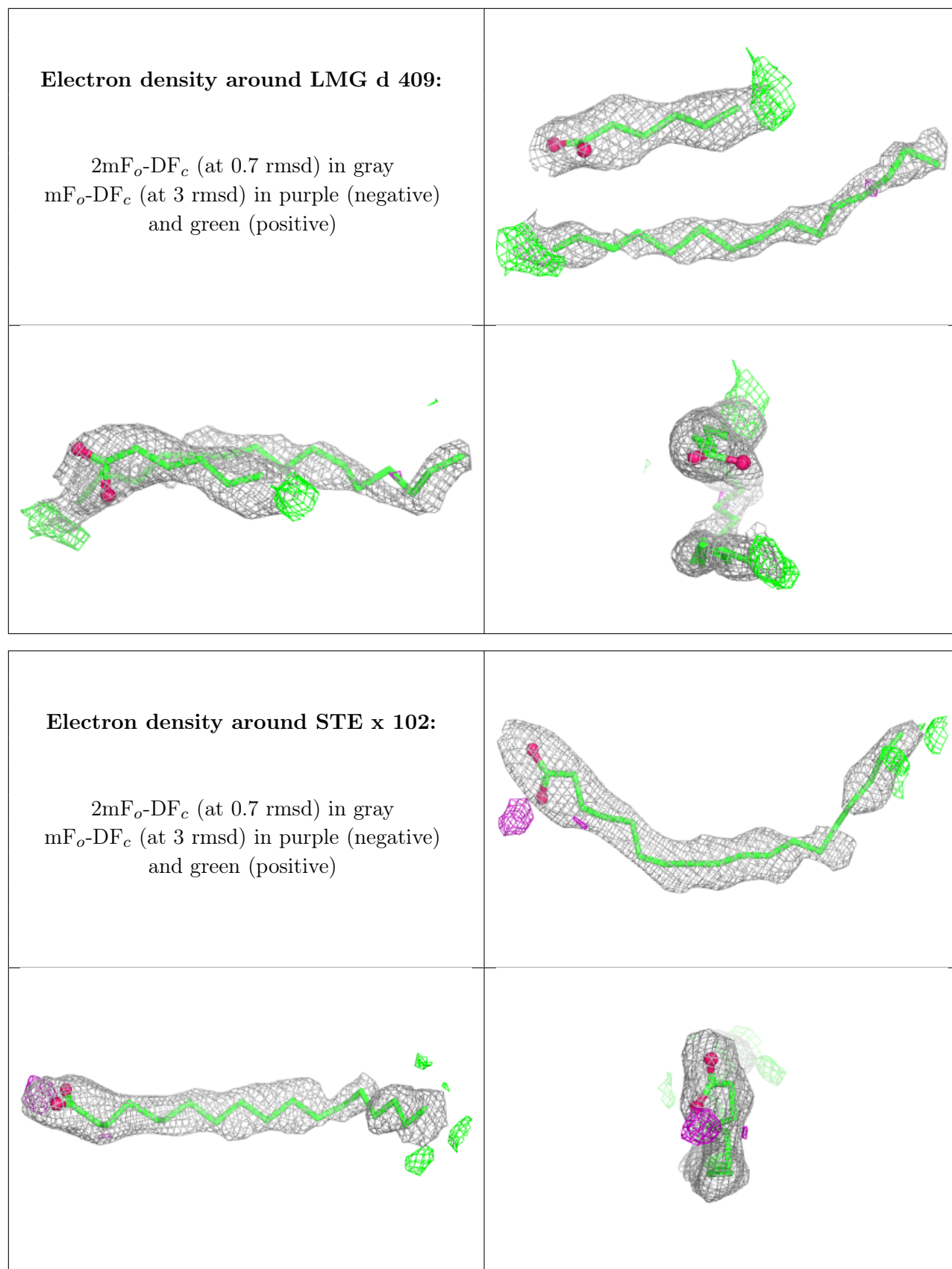
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around STE b 622:**

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

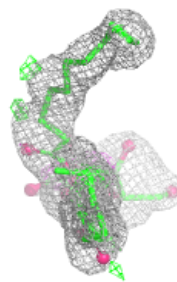
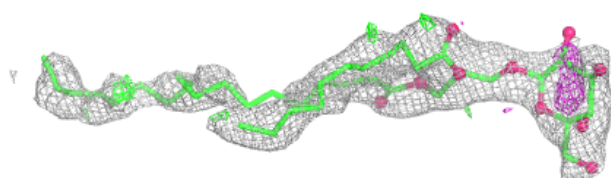
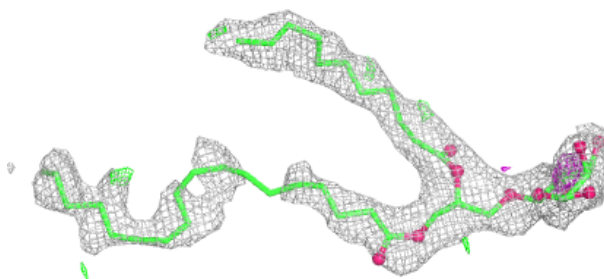




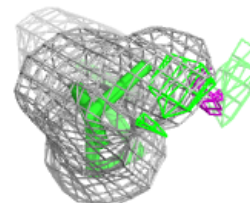
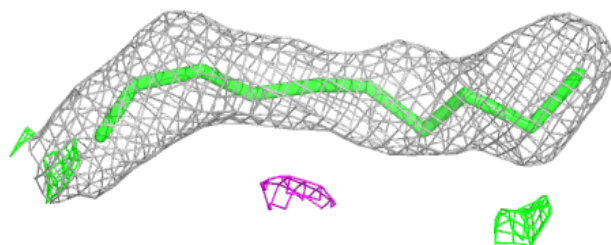
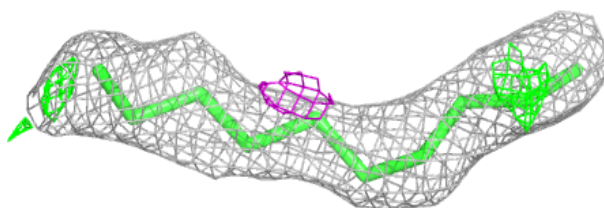


Electron density around LMG c 522:

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

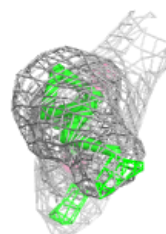
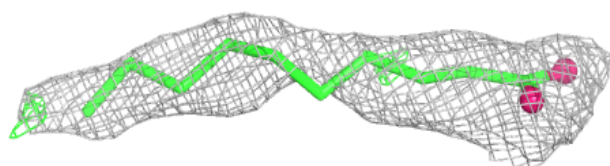
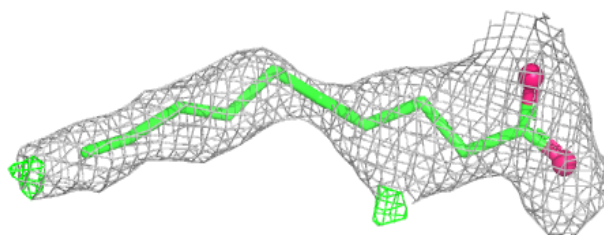
**Electron density around STE b 623:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

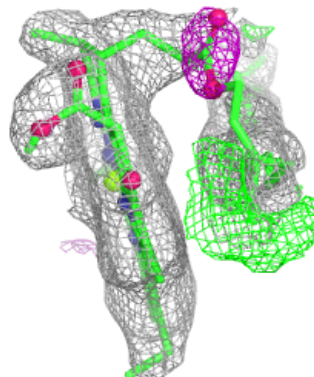
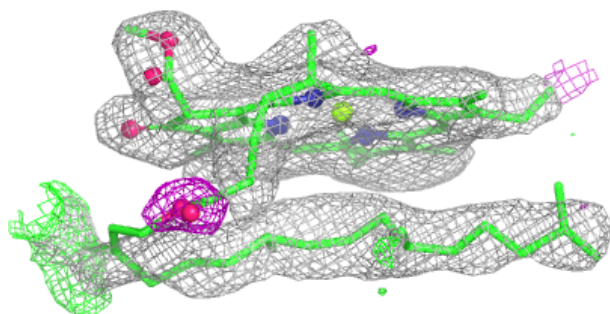
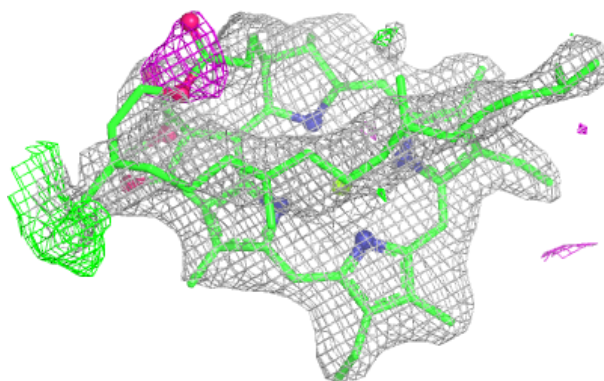


Electron density around STE a 617:

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

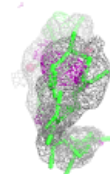
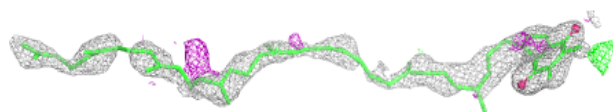
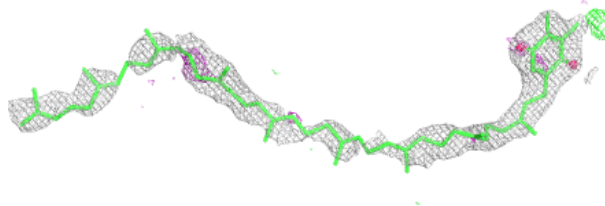
**Electron density around CLA h 101:**

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

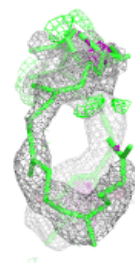
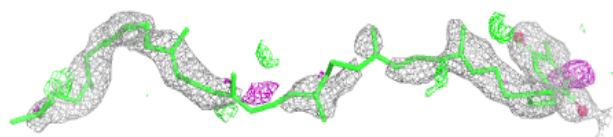
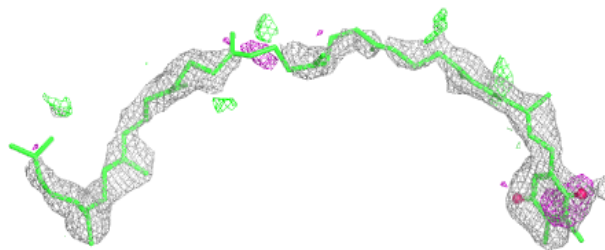


Electron density around PL9 A 612:

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

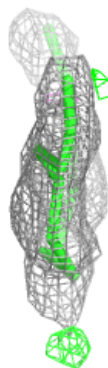
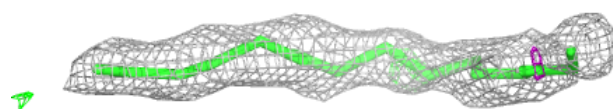
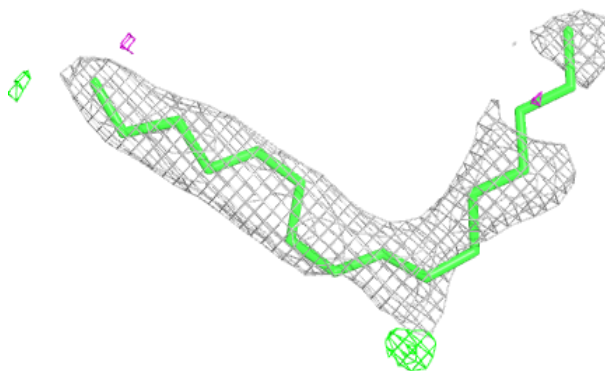
**Electron density around PL9 a 612:**

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

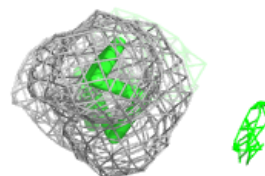
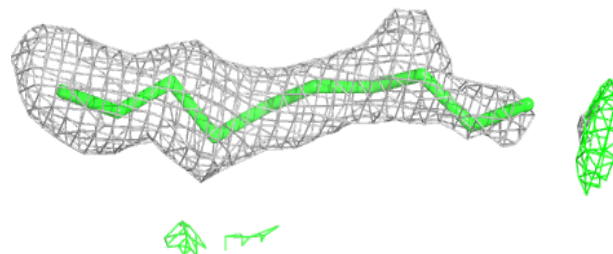
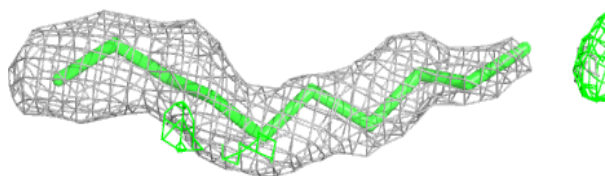


Electron density around STE B 626:

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

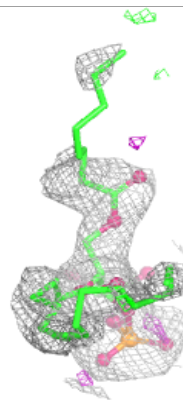
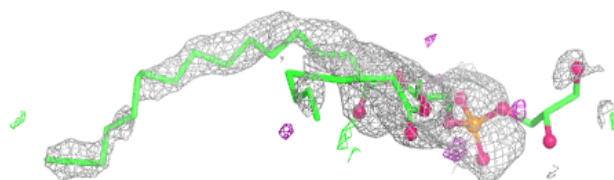
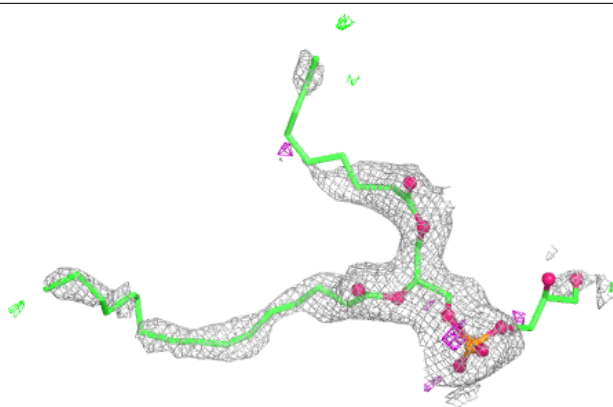
**Electron density around STE t 103:**

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

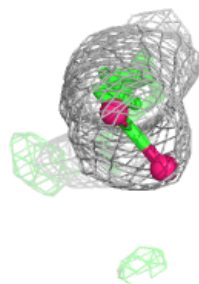
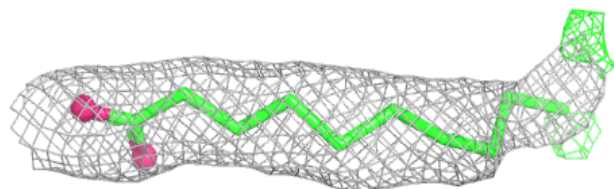
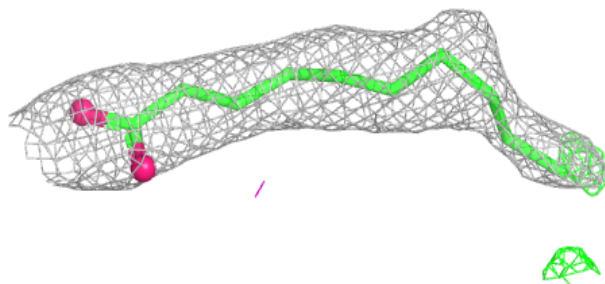


Electron density around LHG e 102:

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

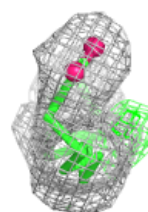
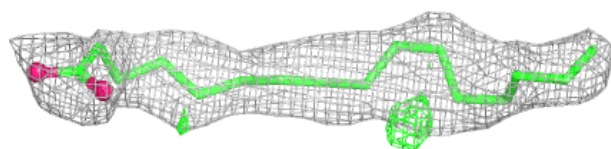
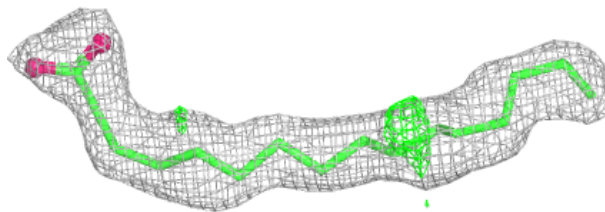
**Electron density around STE m 102:**

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

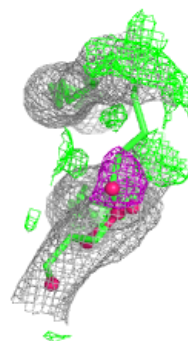
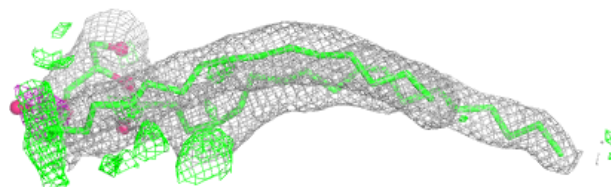
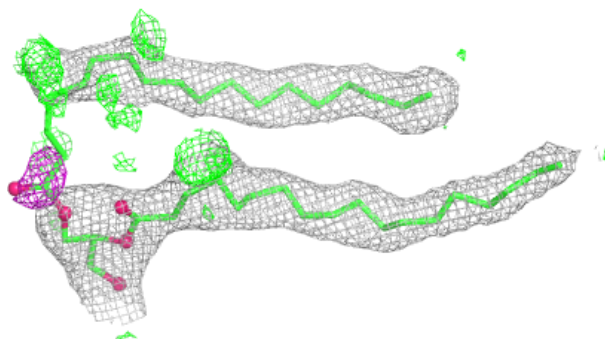


Electron density around STE B 624:

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

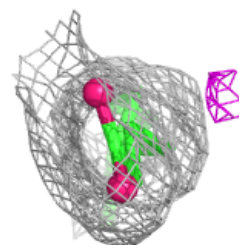
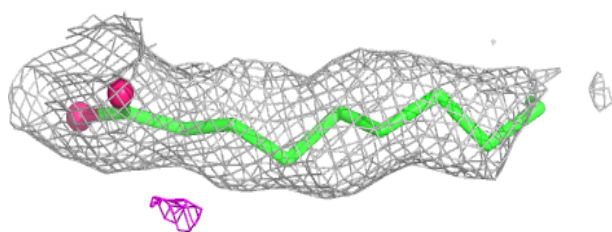
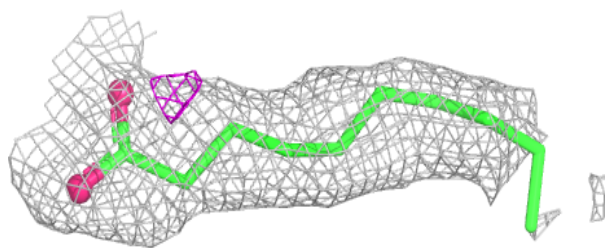
**Electron density around DGD a 616:**

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



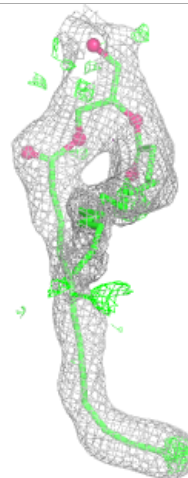
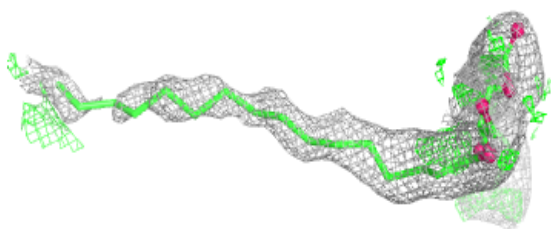
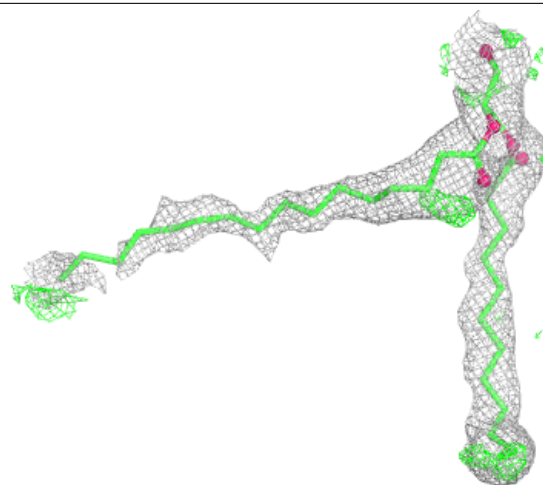
Electron density around STE c 523:

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



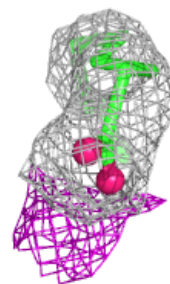
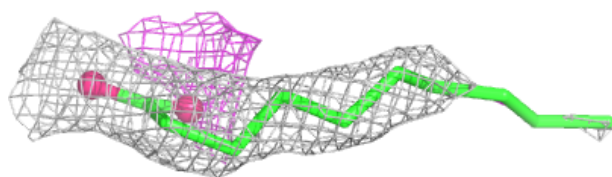
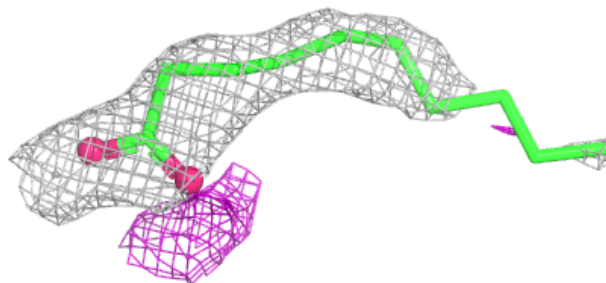
Electron density around SQD a 615:

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

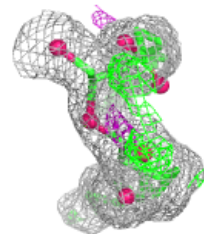
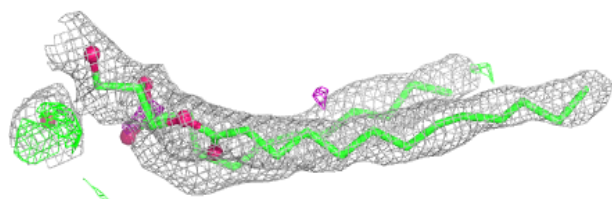
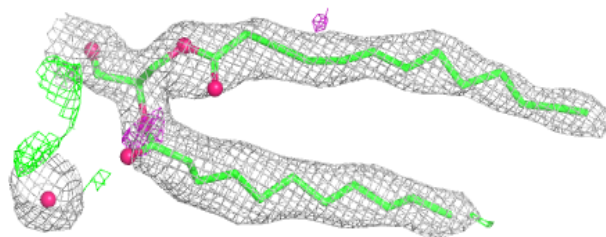


Electron density around STE B 625:

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

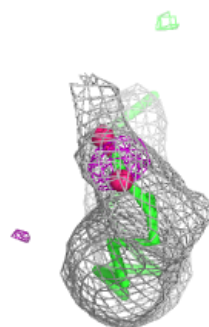
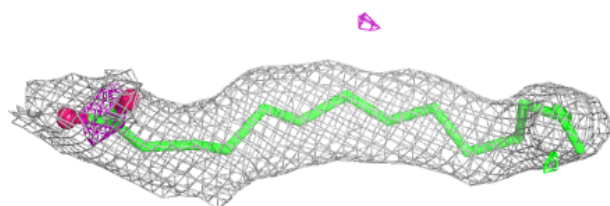
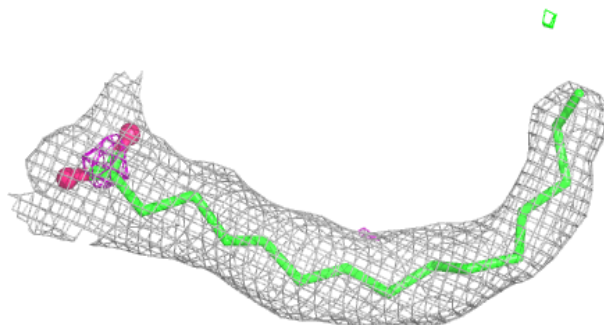
**Electron density around LMG D 409:**

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

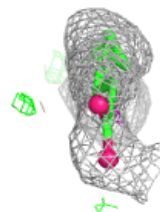
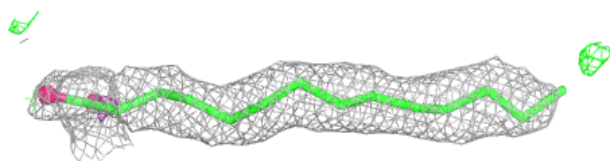
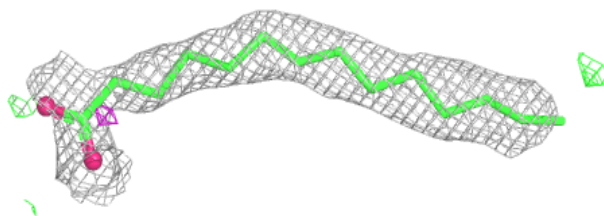


Electron density around STE B 619:

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

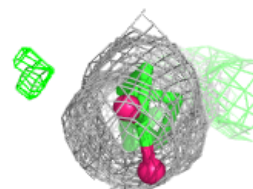
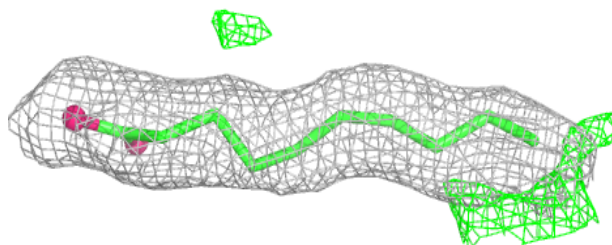
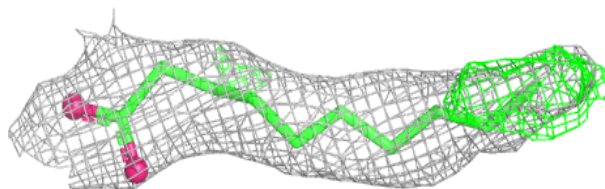
**Electron density around STE b 621:**

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

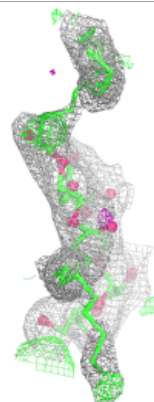
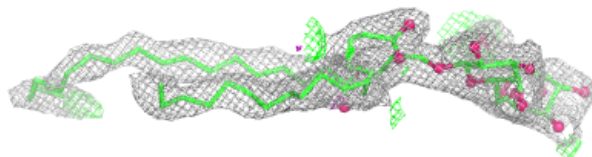
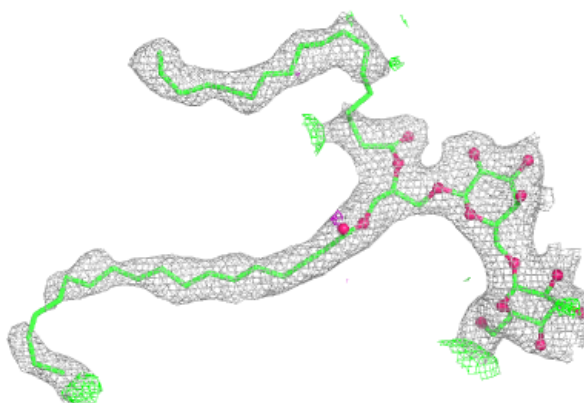


Electron density around STE J 101:

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

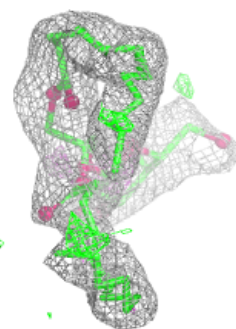
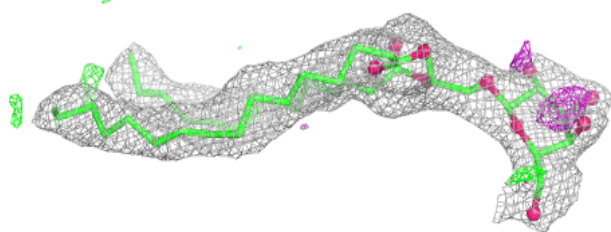
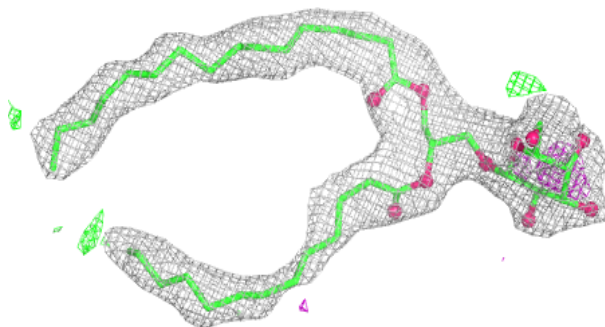
**Electron density around DGD A 616:**

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

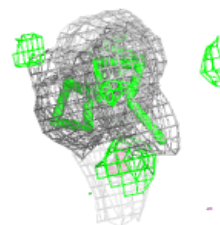
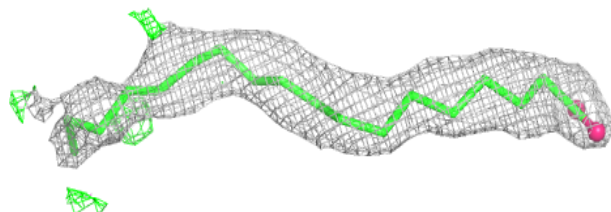
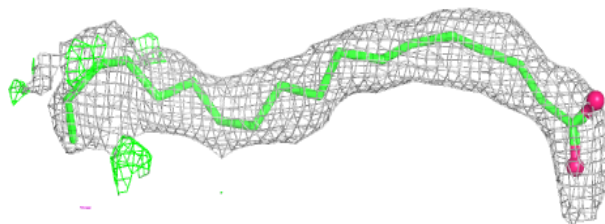


Electron density around LMG C 515:

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

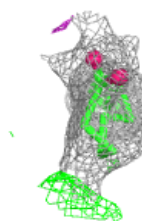
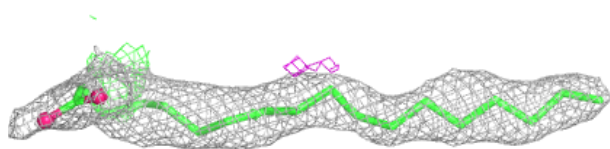
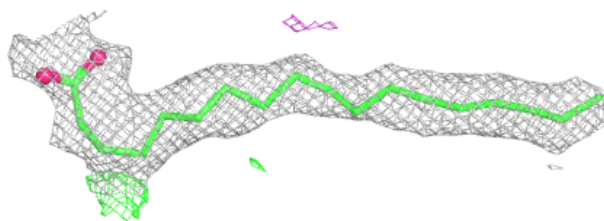
**Electron density around STE b 619:**

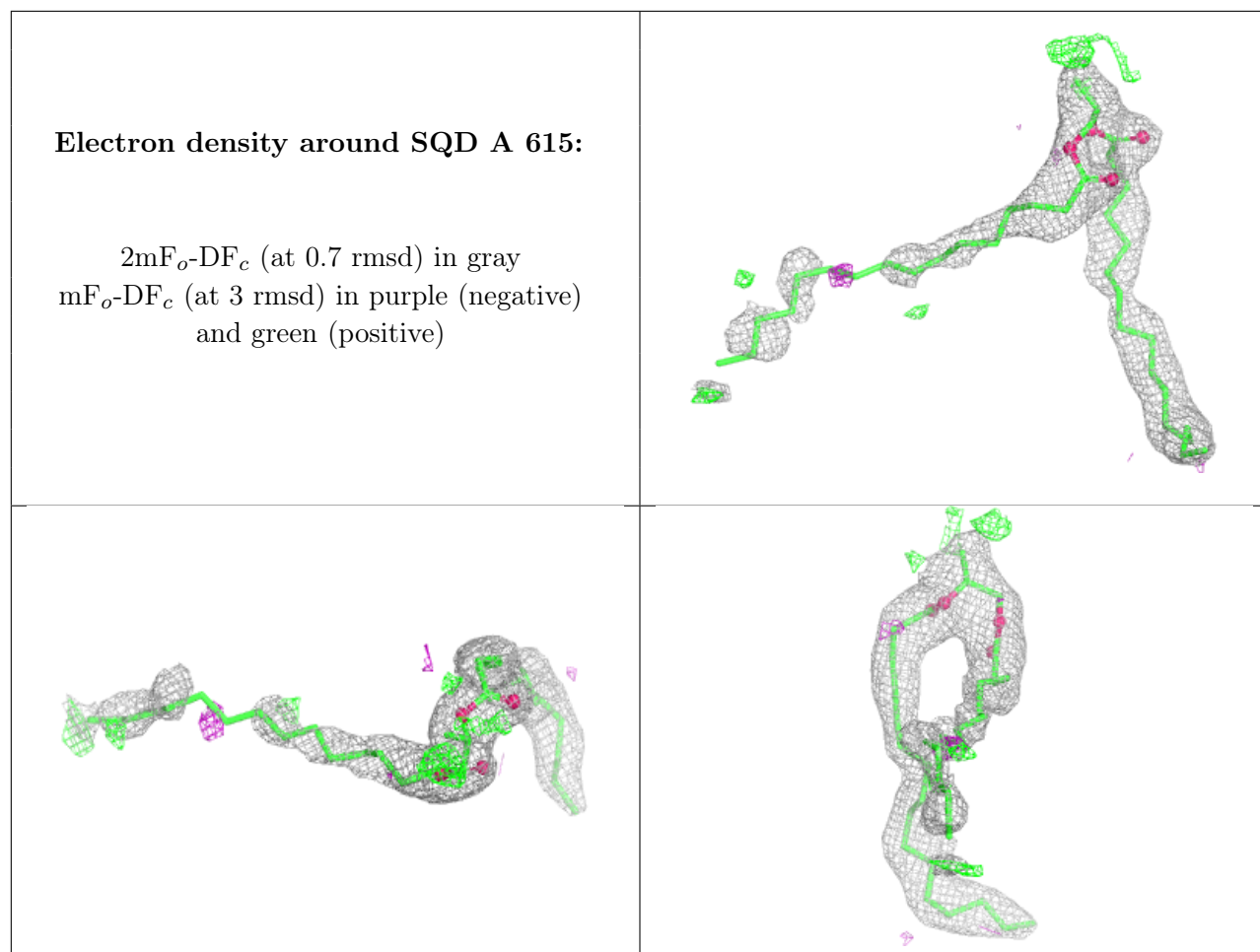
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around STE c 521:

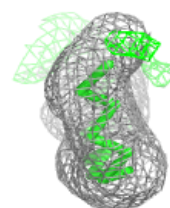
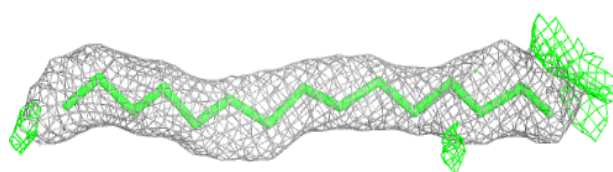
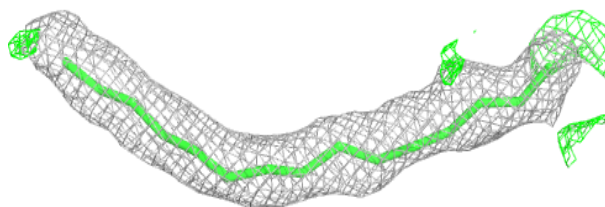
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



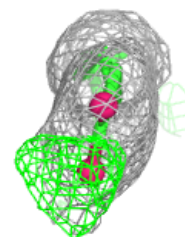
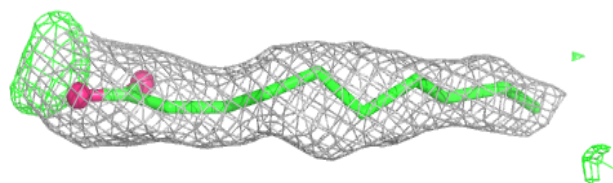
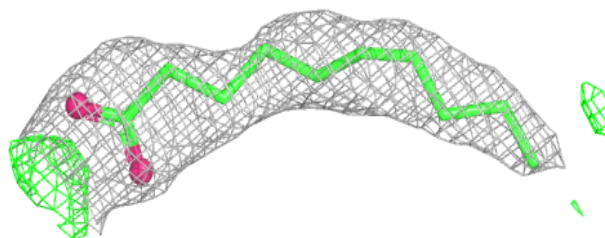


Electron density around STE I 101:

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

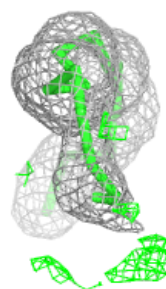
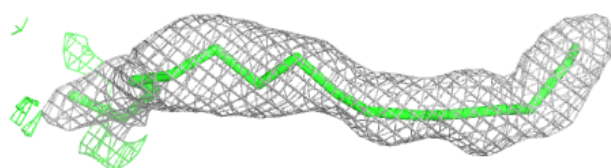
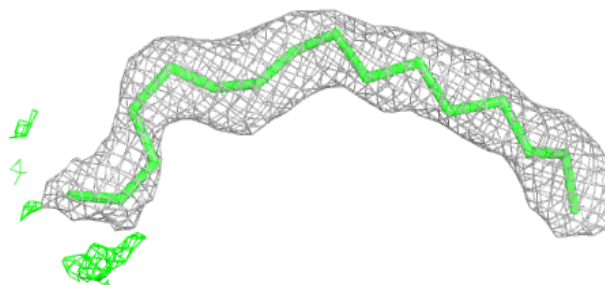
**Electron density around STE C 521:**

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

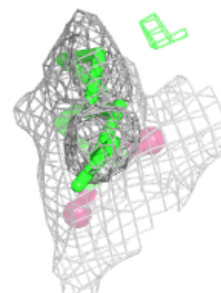
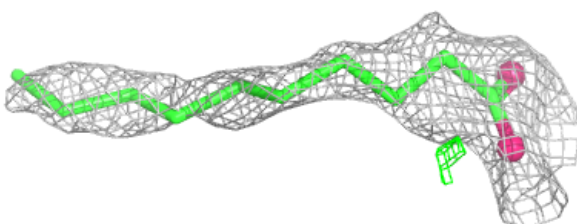
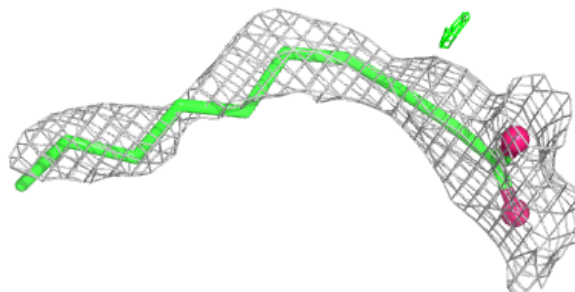


Electron density around STE T 102:

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

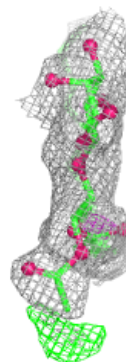
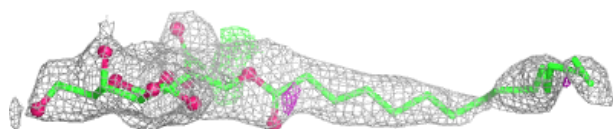
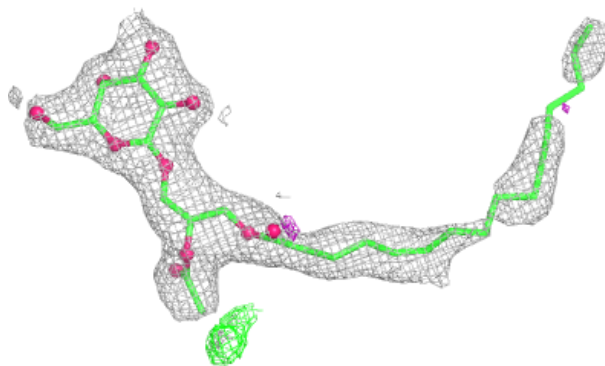
**Electron density around STE R 101:**

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

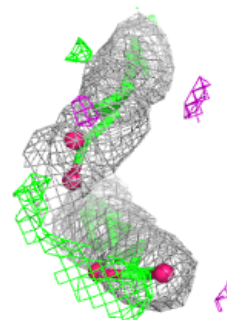
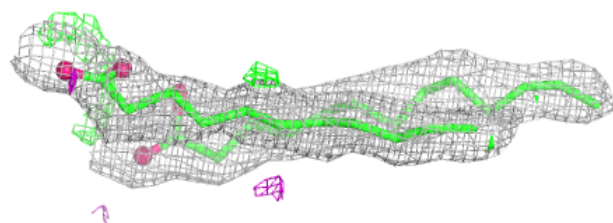
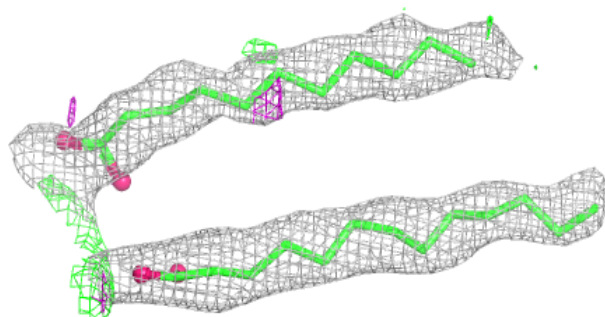


Electron density around LMG c 520:

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

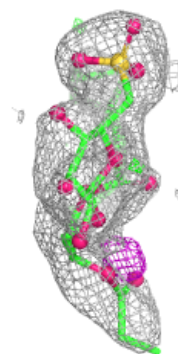
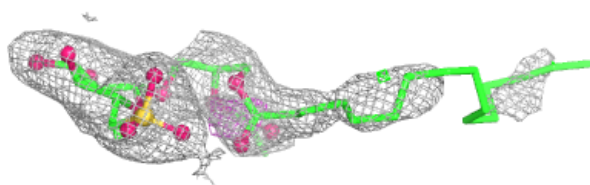
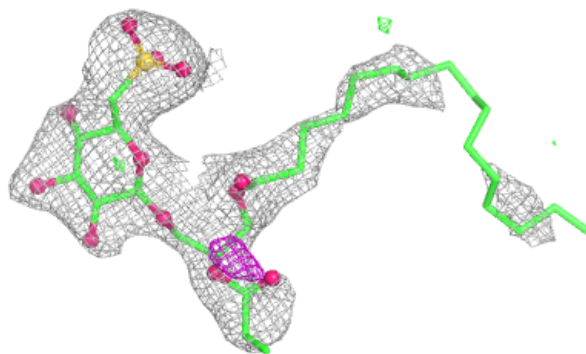
**Electron density around LMG B 620:**

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

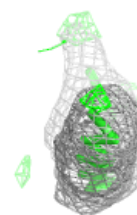
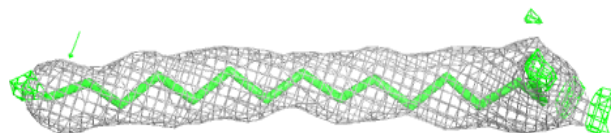
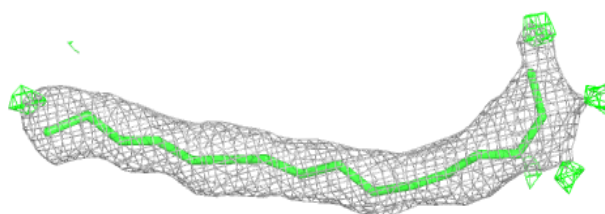


Electron density around SQD f 101:

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

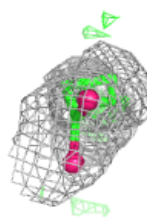
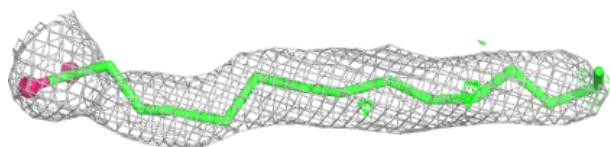
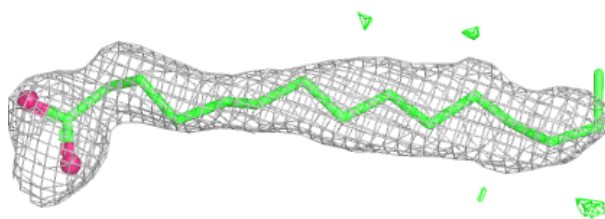
**Electron density around STE C 522:**

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

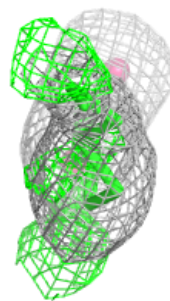
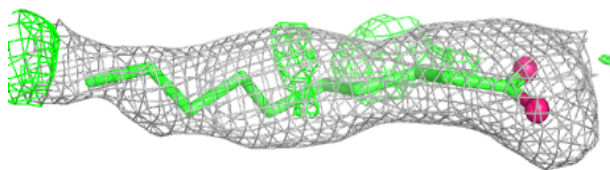
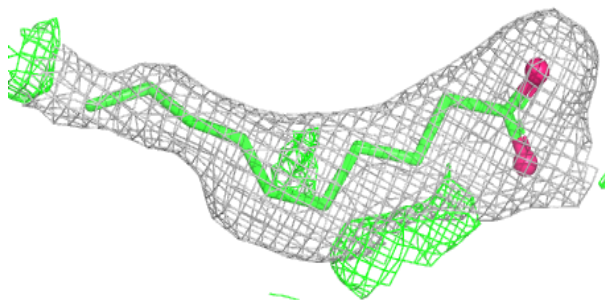


Electron density around STE d 411:

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

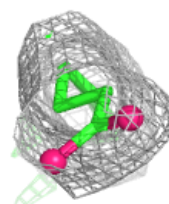
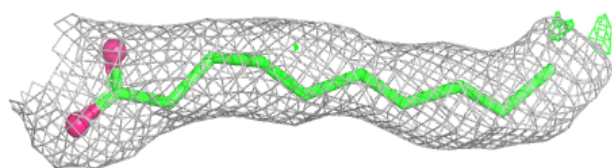
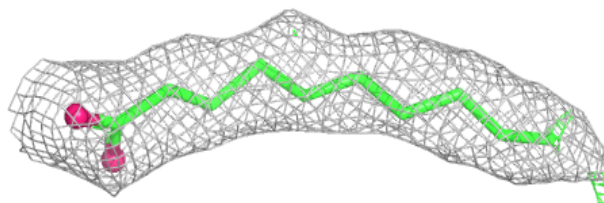
**Electron density around STE C 520:**

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

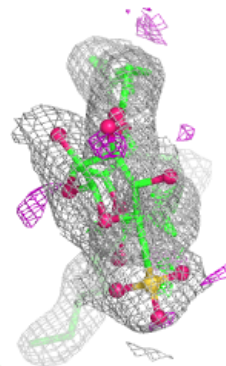
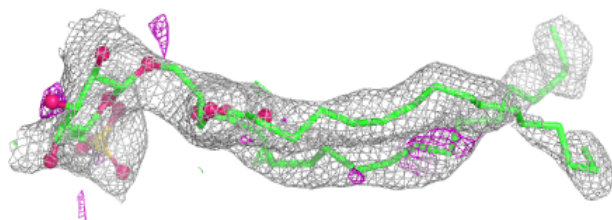
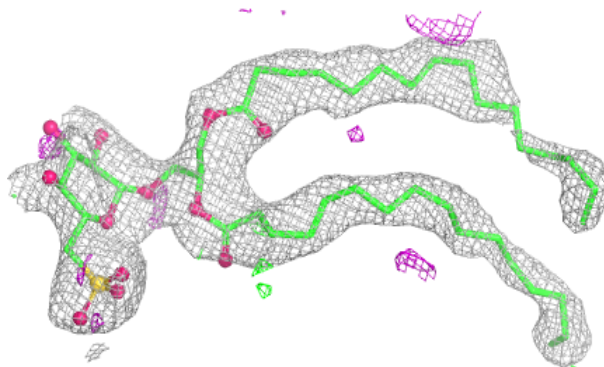


Electron density around STE j 101:

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

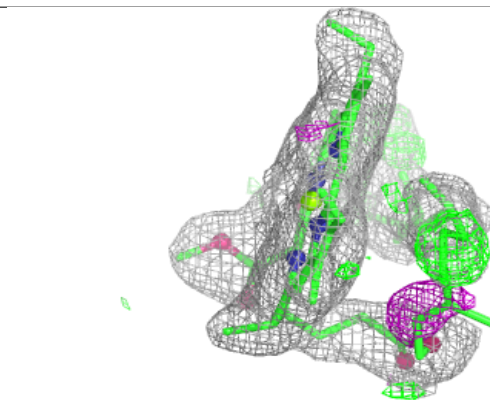
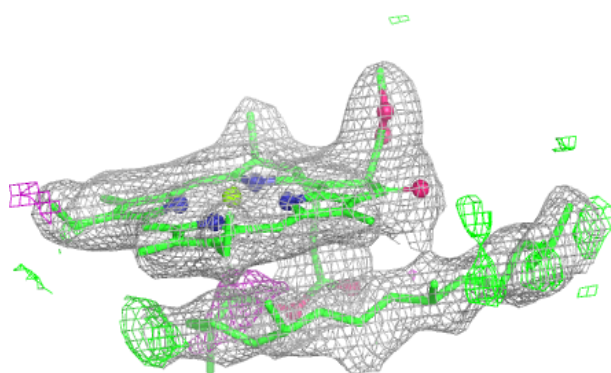
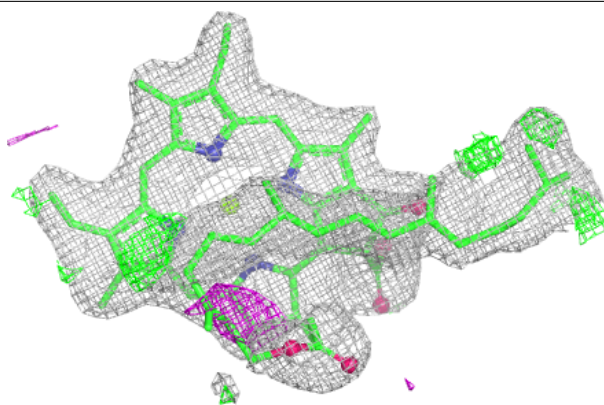
**Electron density around SQD 1 101:**

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

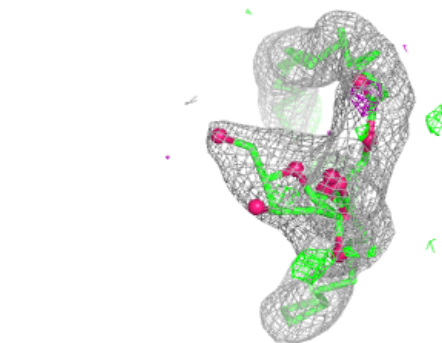
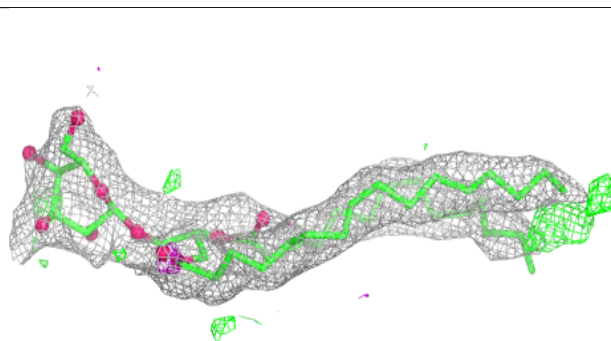
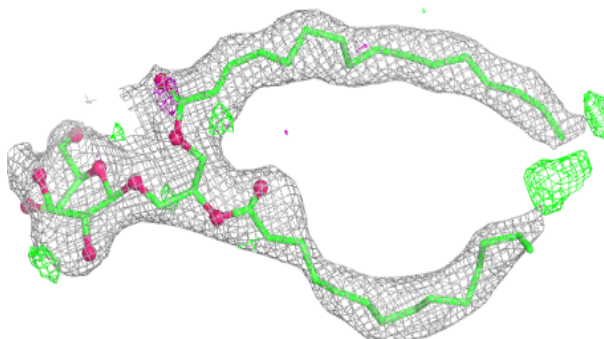


Electron density around CLA H 101:

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

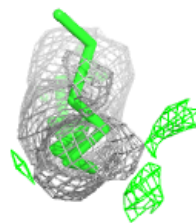
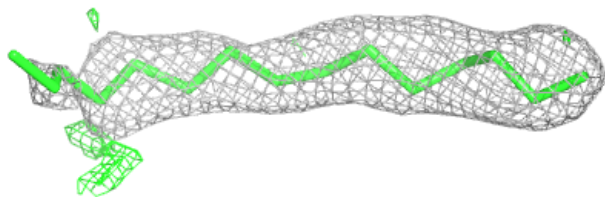
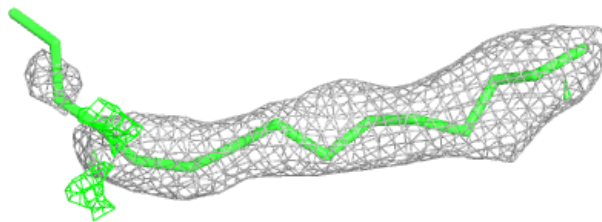
**Electron density around LMG c 524:**

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

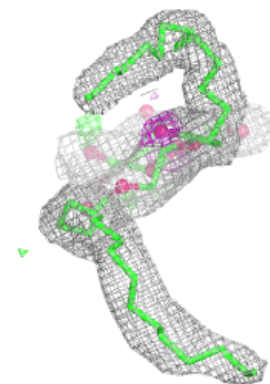
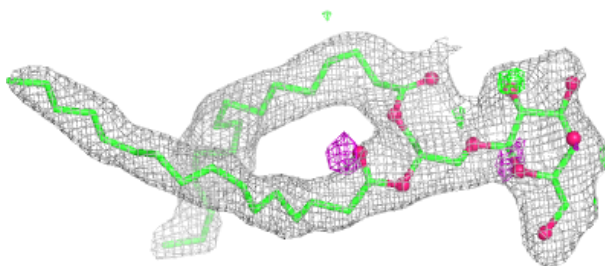
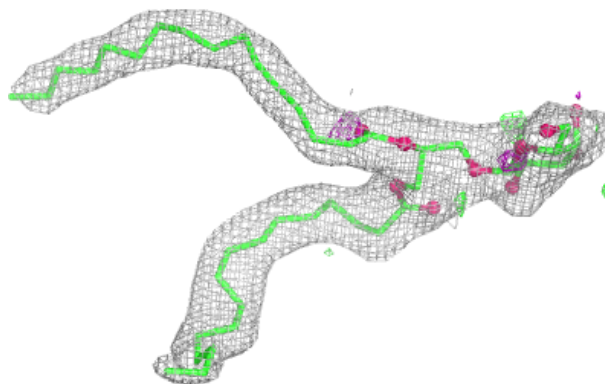


Electron density around STE T 103:

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

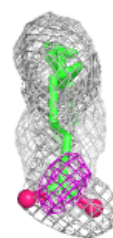
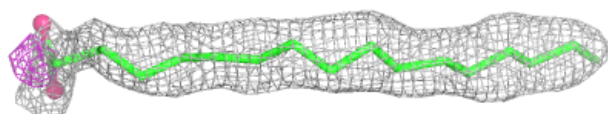
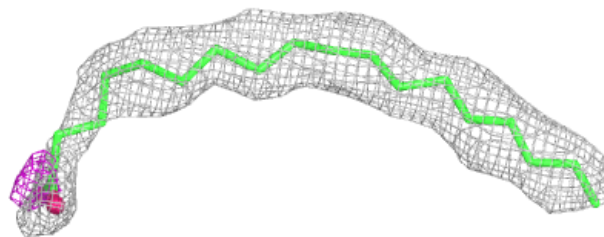
**Electron density around LMG m 101:**

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

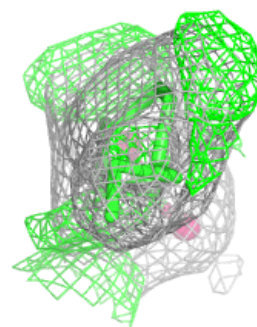
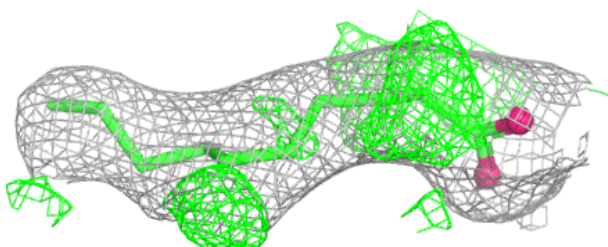
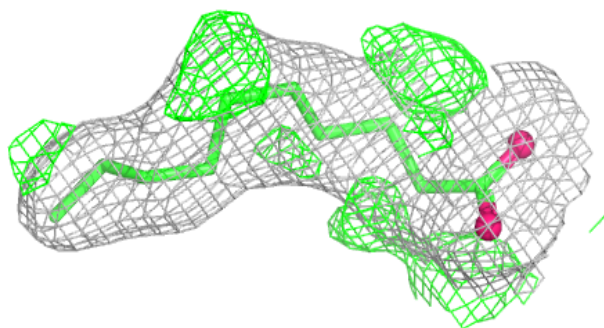


Electron density around STE D 410:

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

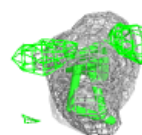
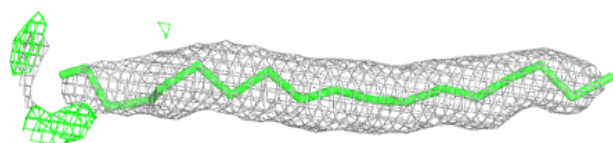
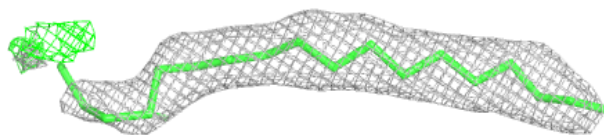
**Electron density around STE B 623:**

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

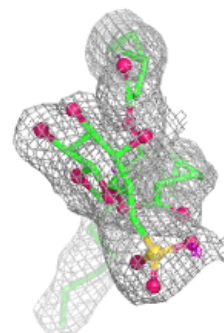
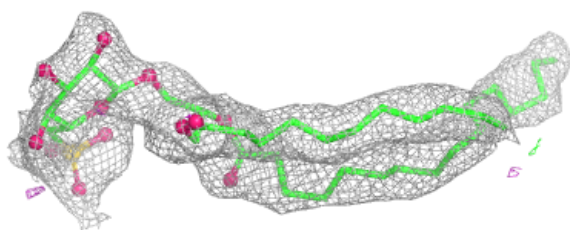
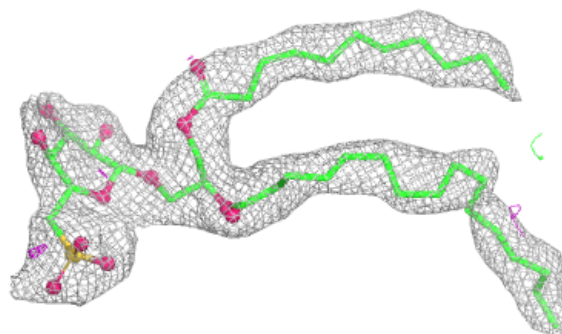


Electron density around STE I 103:

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

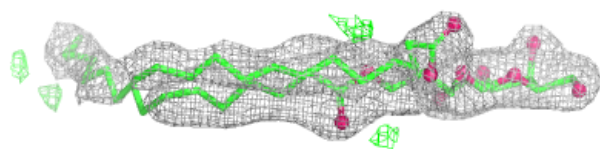
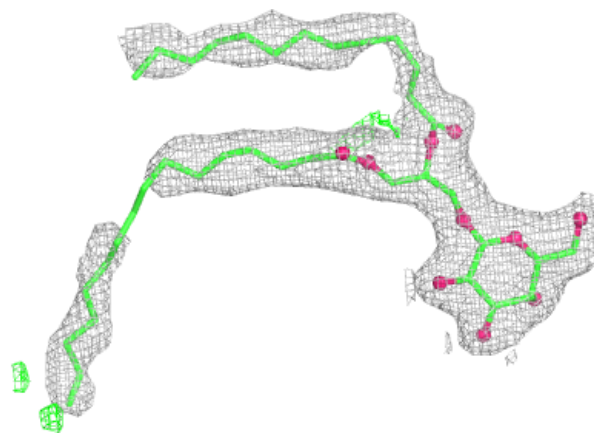
**Electron density around SQD L 101:**

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

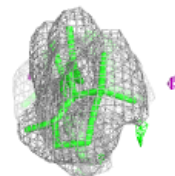
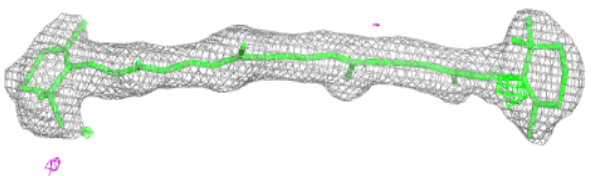
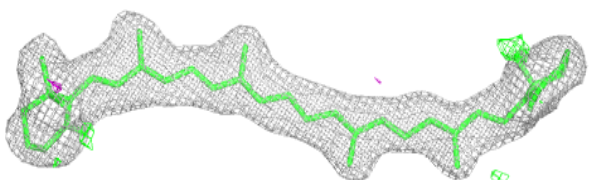


Electron density around LMG C 519:

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

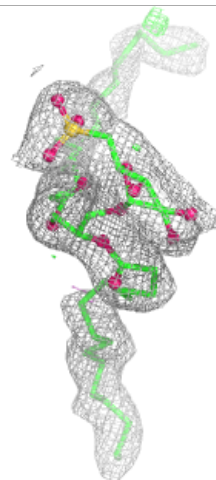
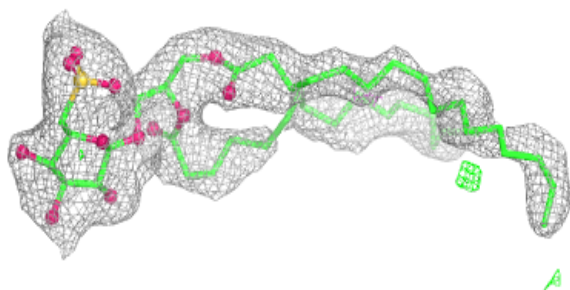
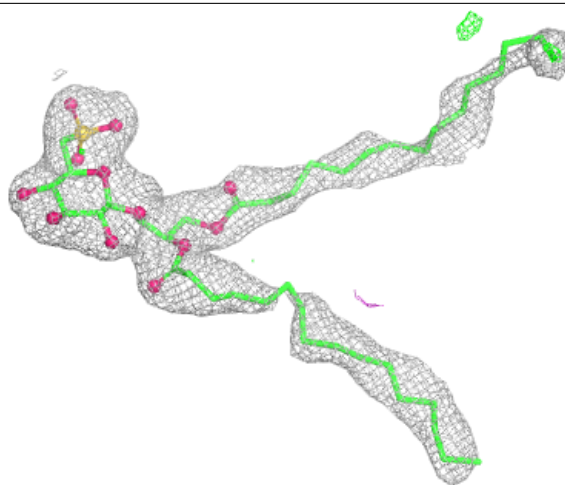
**Electron density around BCR K 102:**

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



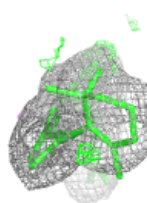
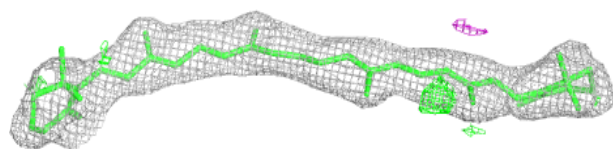
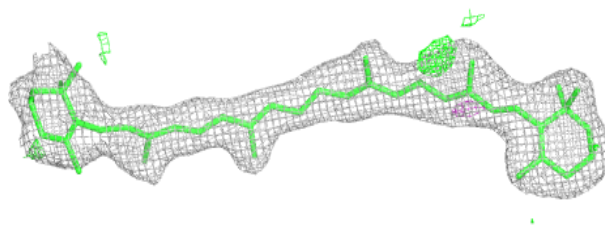
Electron density around SQD a 614:

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

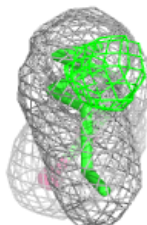
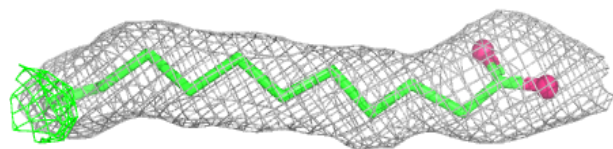
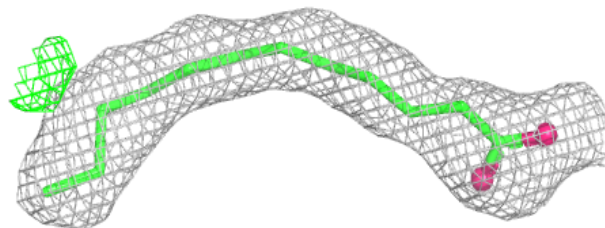


Electron density around BCR d 404:

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

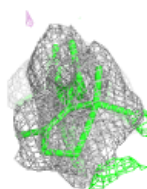
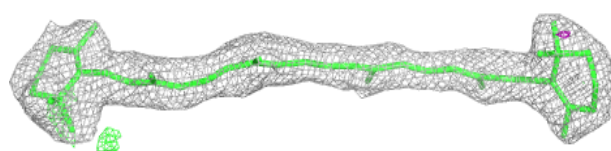
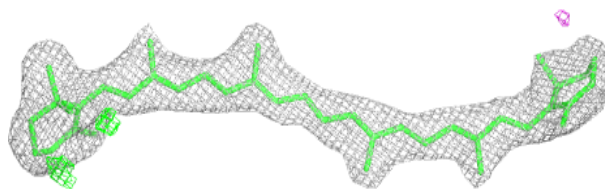
**Electron density around STE t 102:**

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

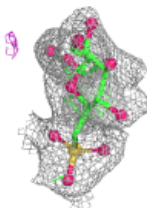
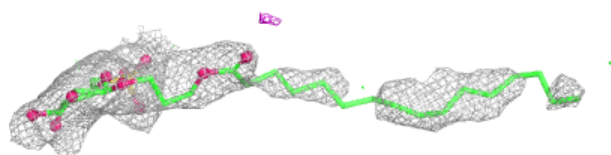
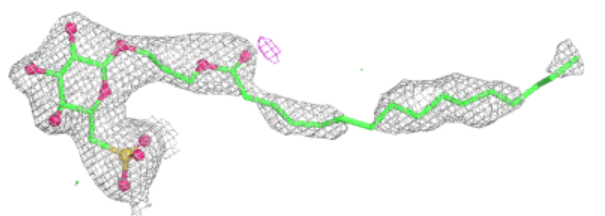


Electron density around BCR k 101:

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

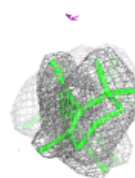
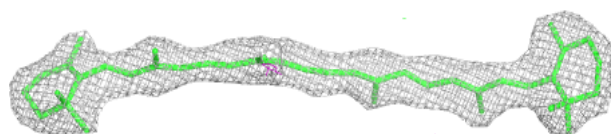
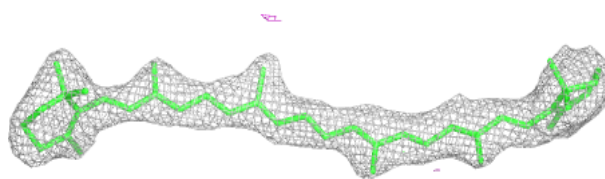
**Electron density around SQD F 102:**

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

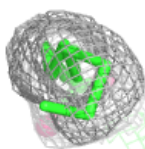
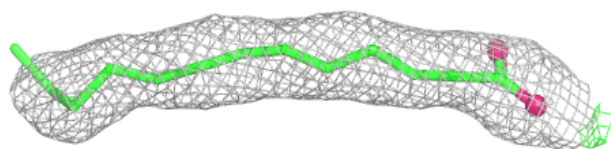
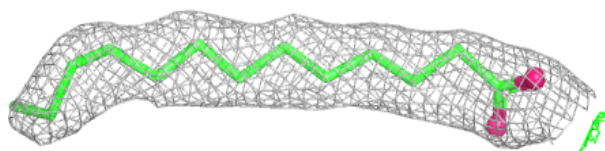


Electron density around BCR c 514:

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

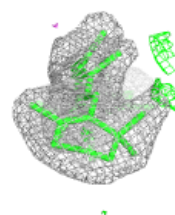
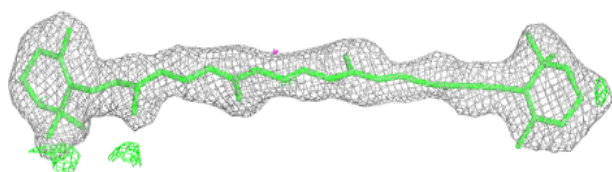
**Electron density around STE M 102:**

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

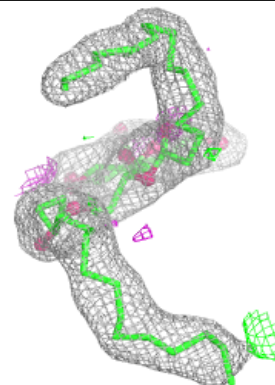
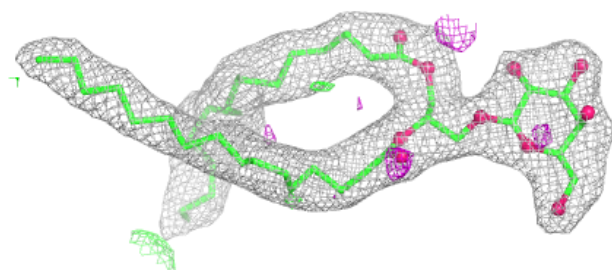
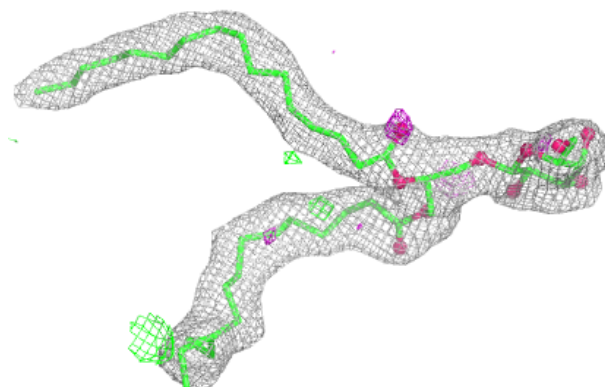


Electron density around BCR x 101:

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

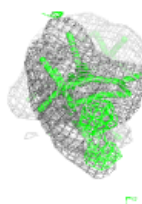
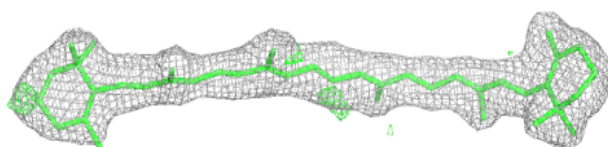
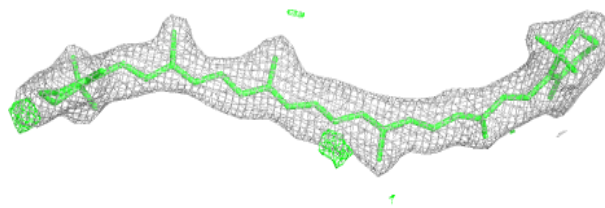
**Electron density around LMG M 101:**

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

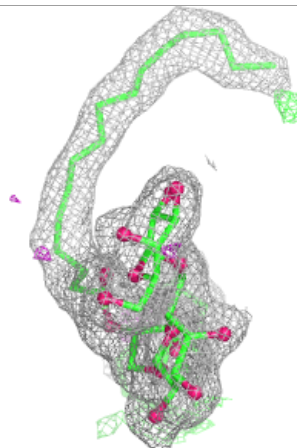
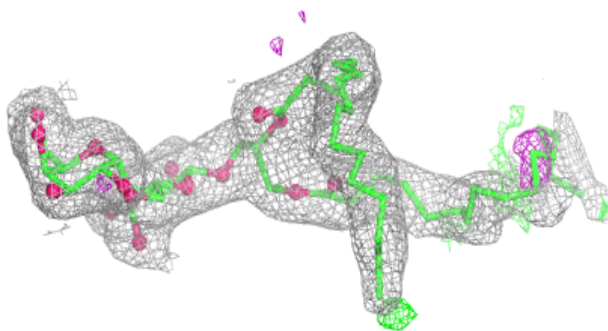
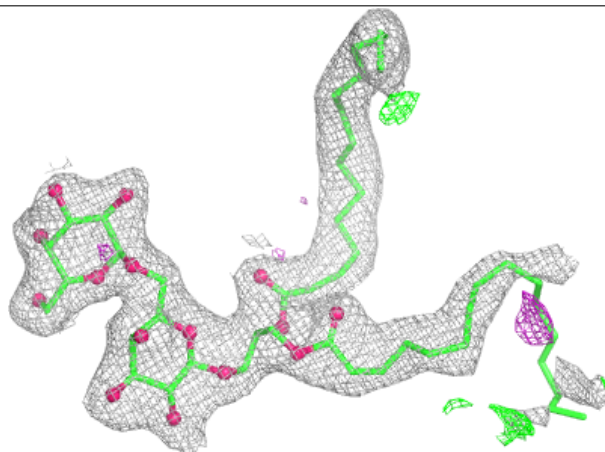


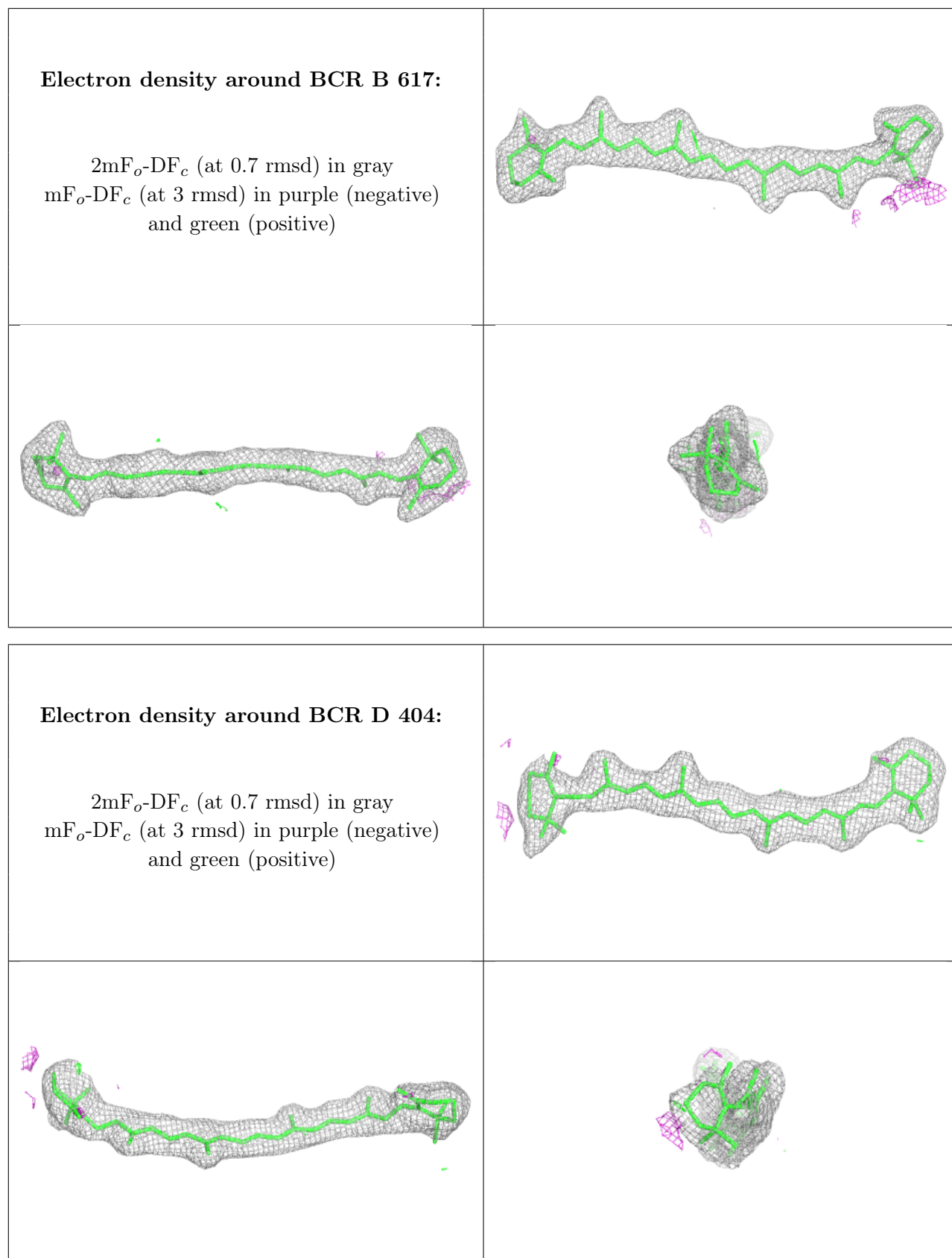
Electron density around BCR H 102:

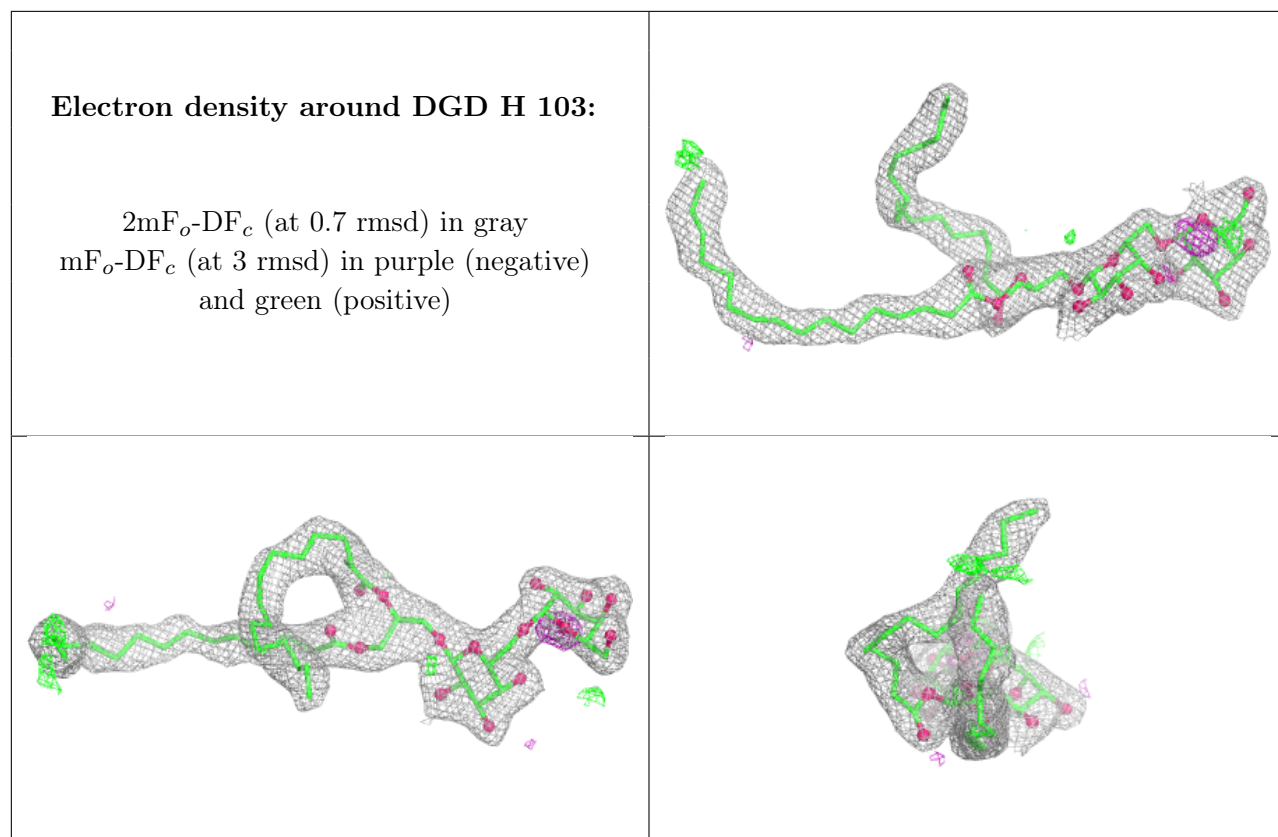
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DGD C 517:**

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

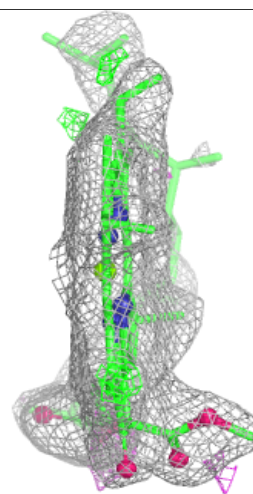
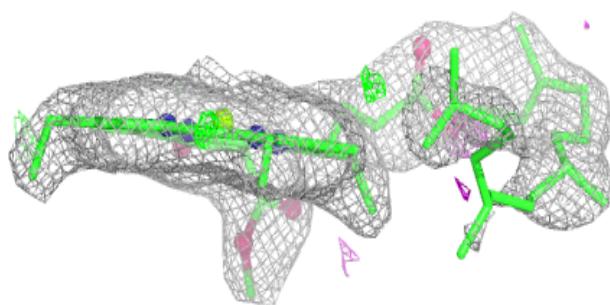
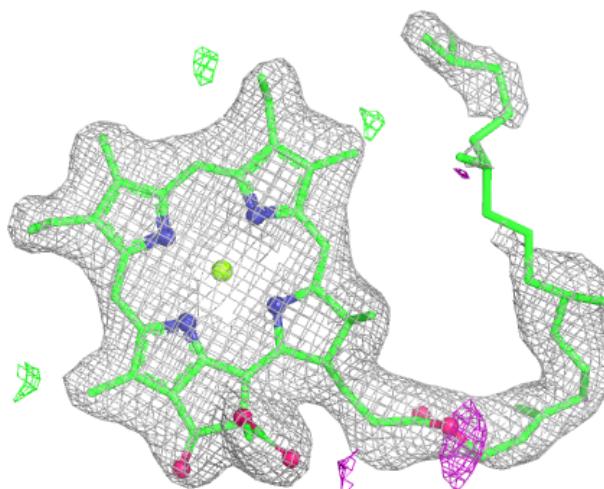


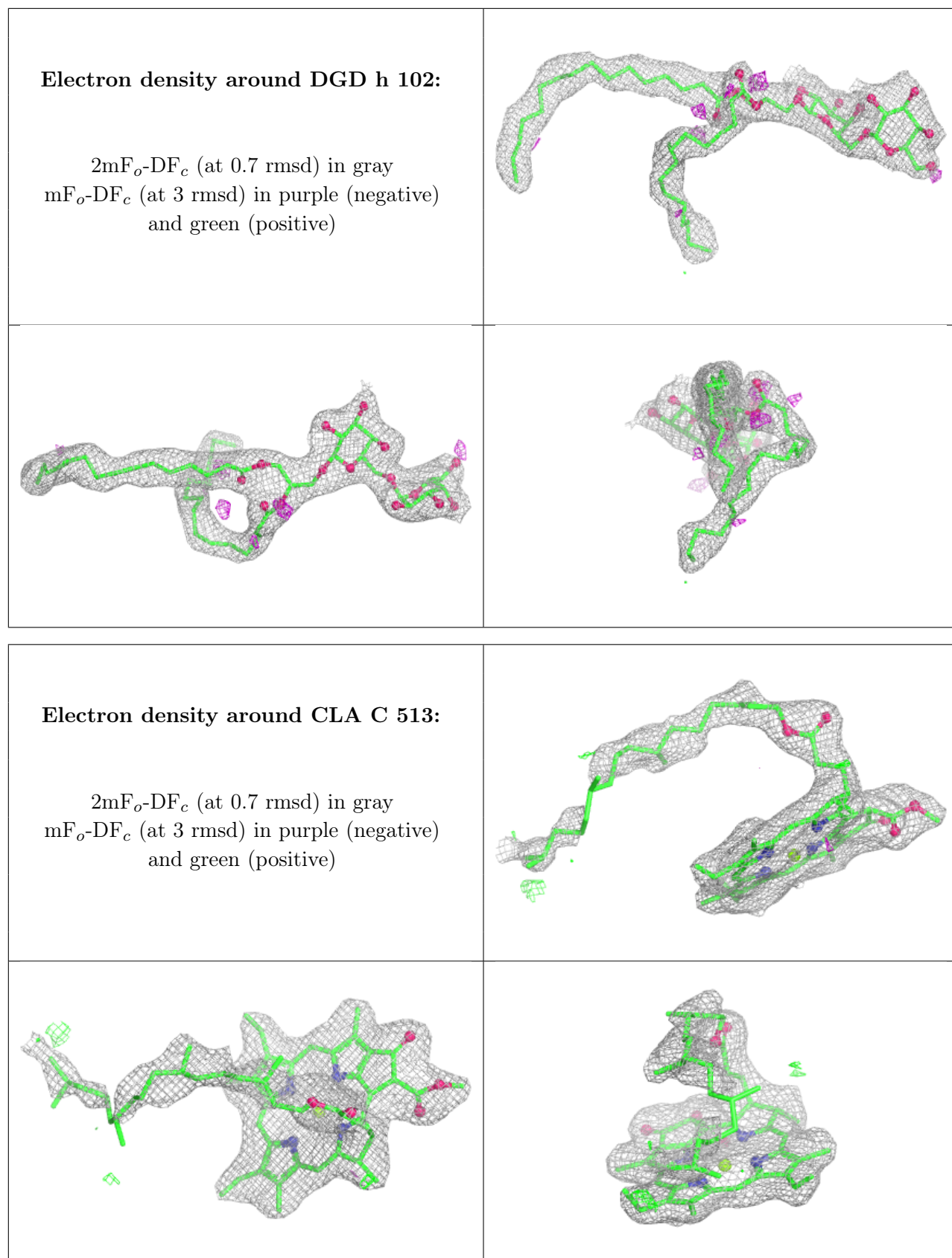


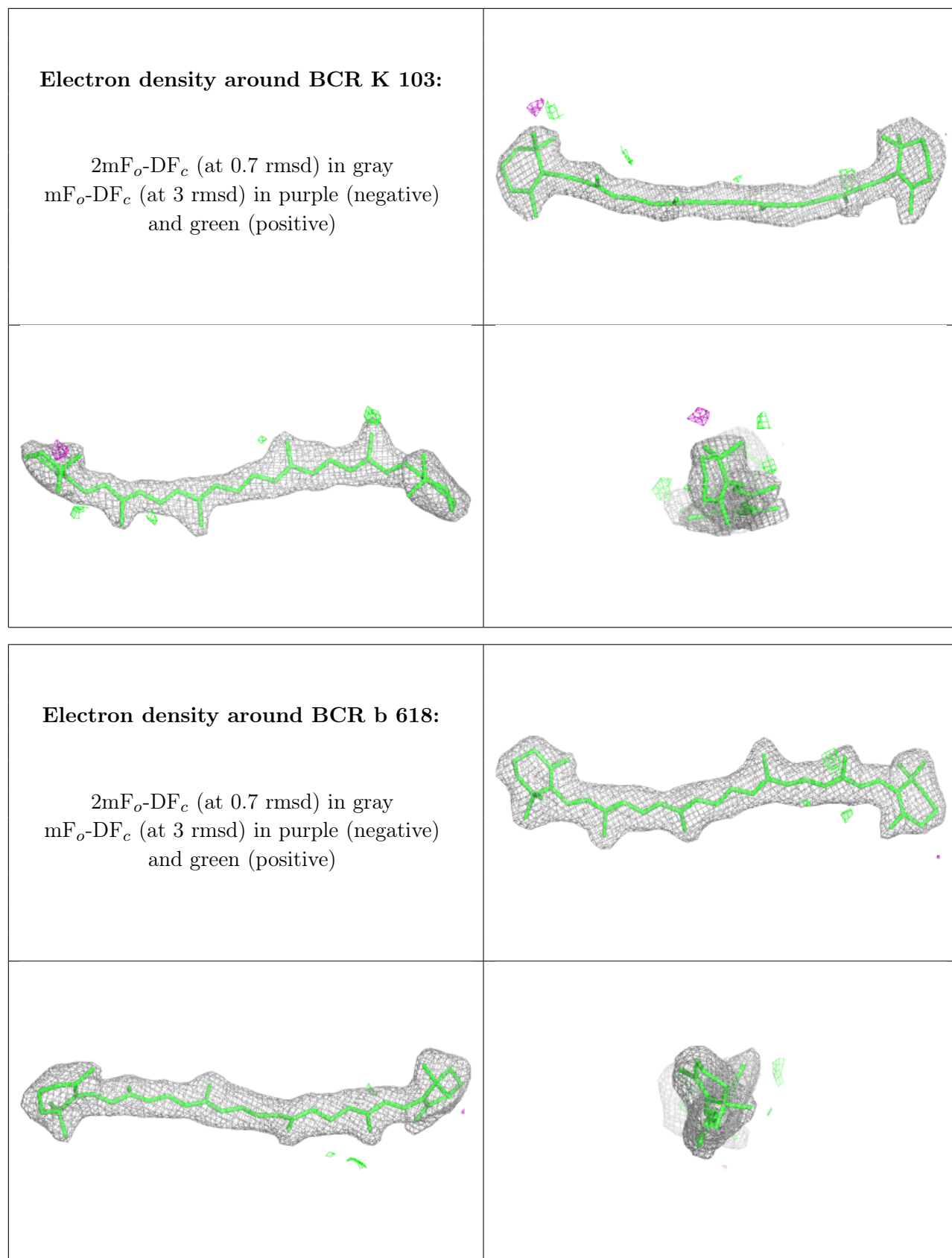


Electron density around CLA c 512:

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

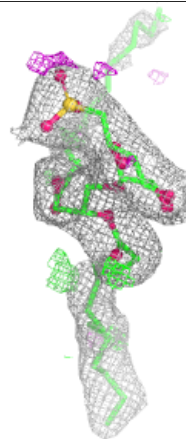
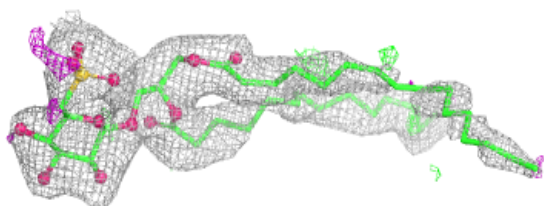
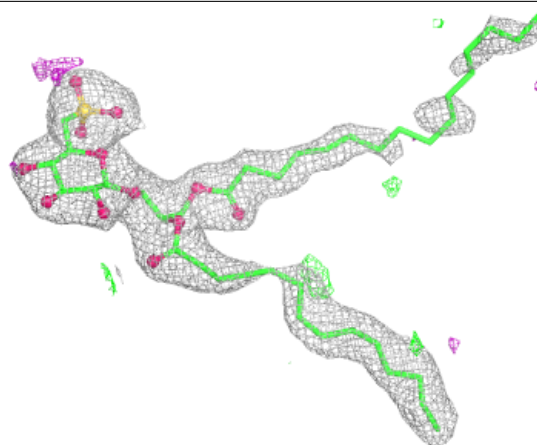




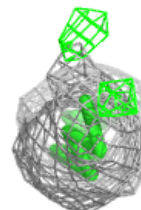
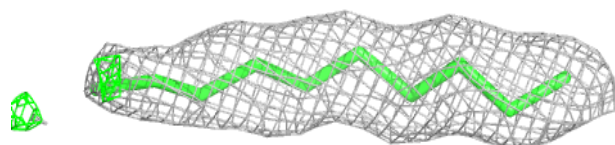
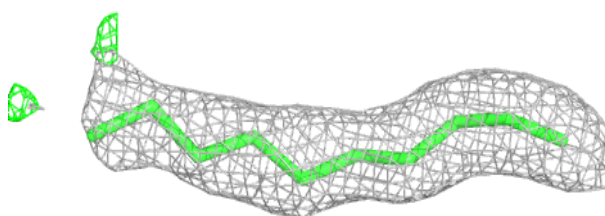


Electron density around SQD A 614:

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

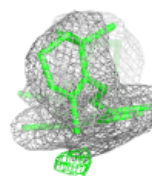
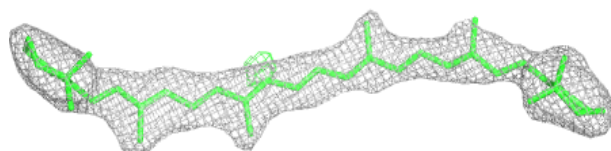
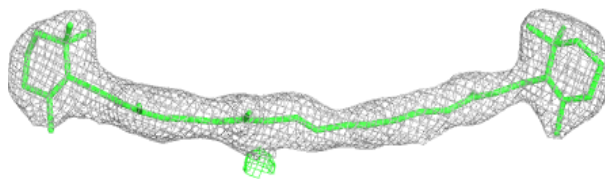
**Electron density around STE M 103:**

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

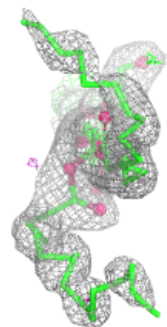
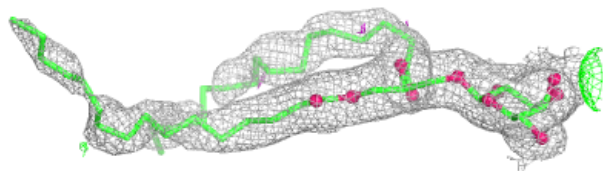
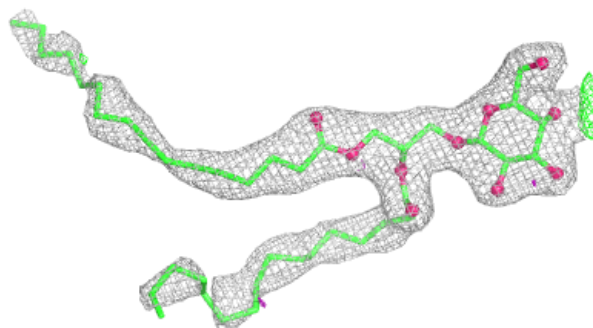


Electron density around BCR c 516:

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

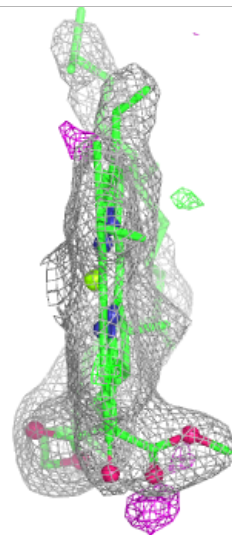
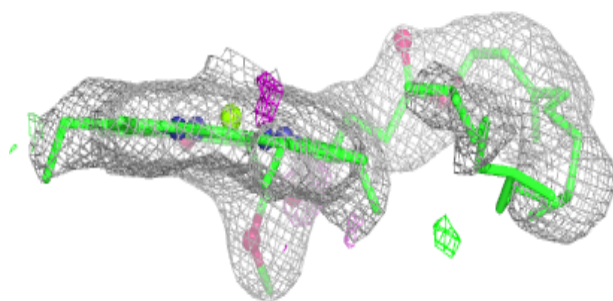
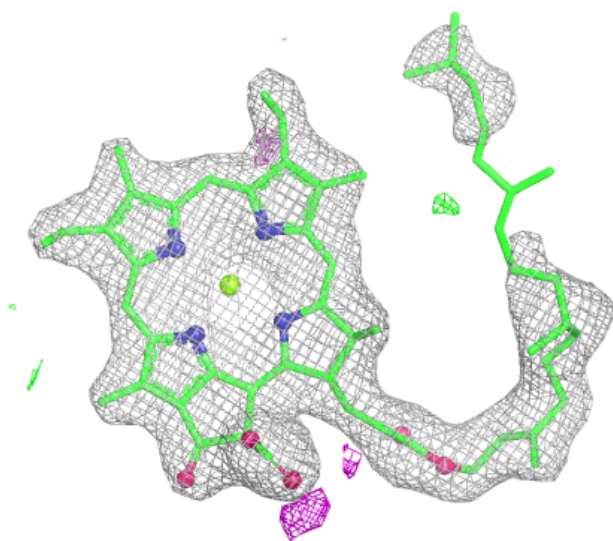
**Electron density around LMG D 406:**

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



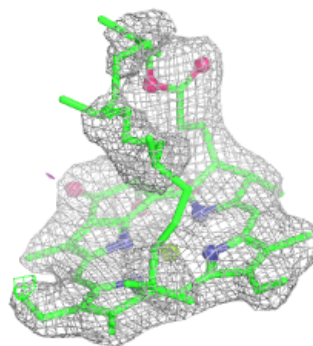
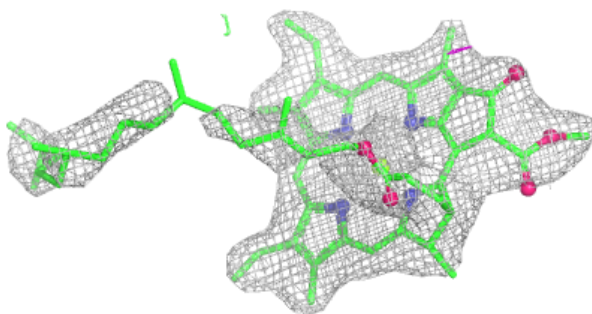
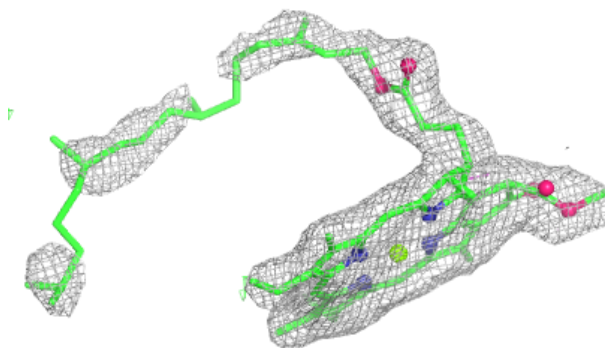
Electron density around CLA C 512:

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

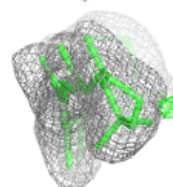
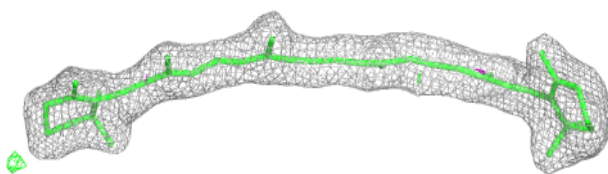
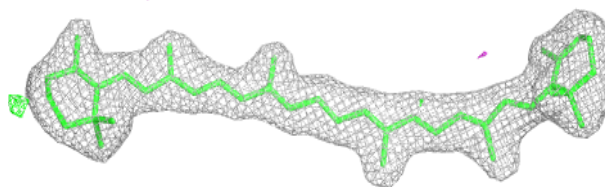


Electron density around CLA c 513:

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

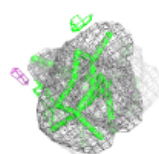
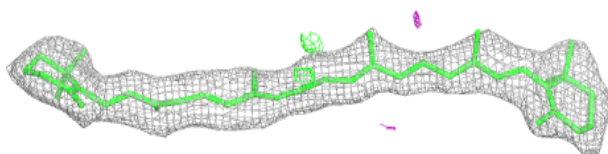
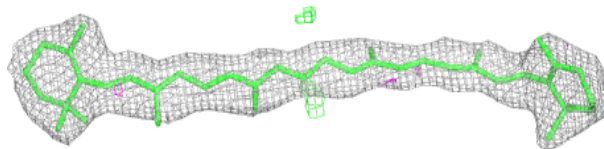
**Electron density around BCR t 101:**

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

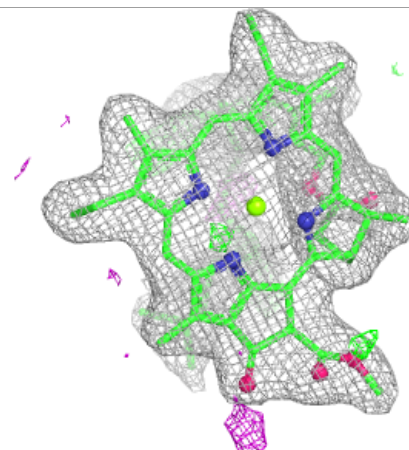
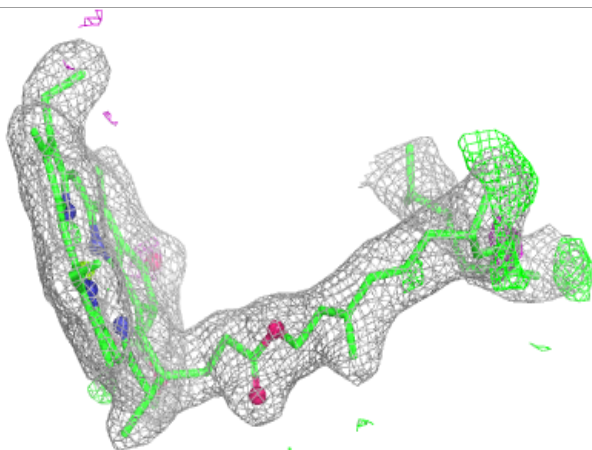
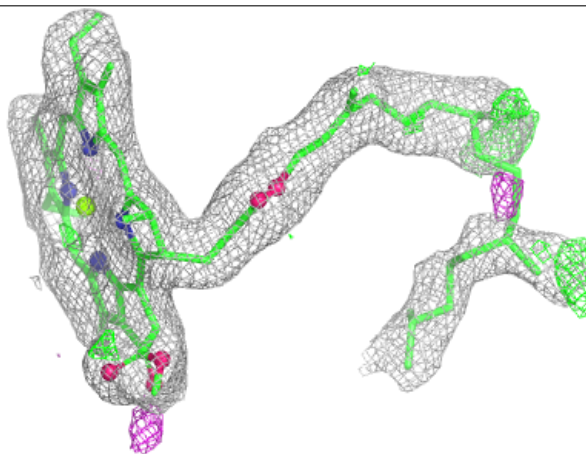


Electron density around BCR K 101:

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

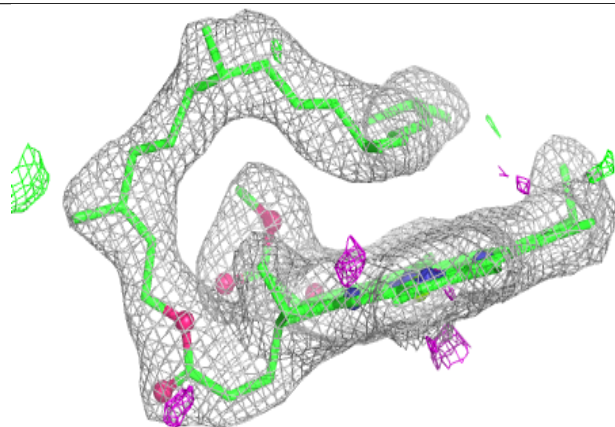
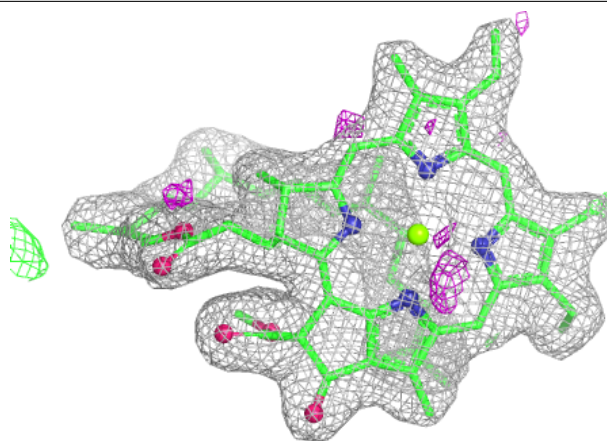
**Electron density around CLA B 605:**

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

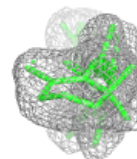
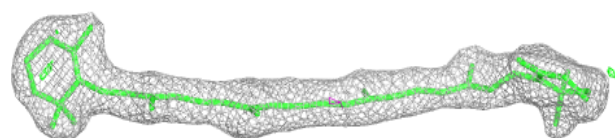
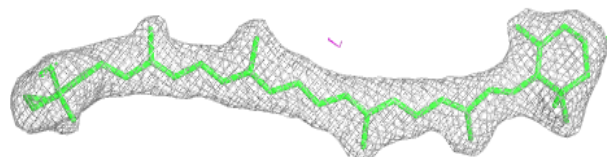


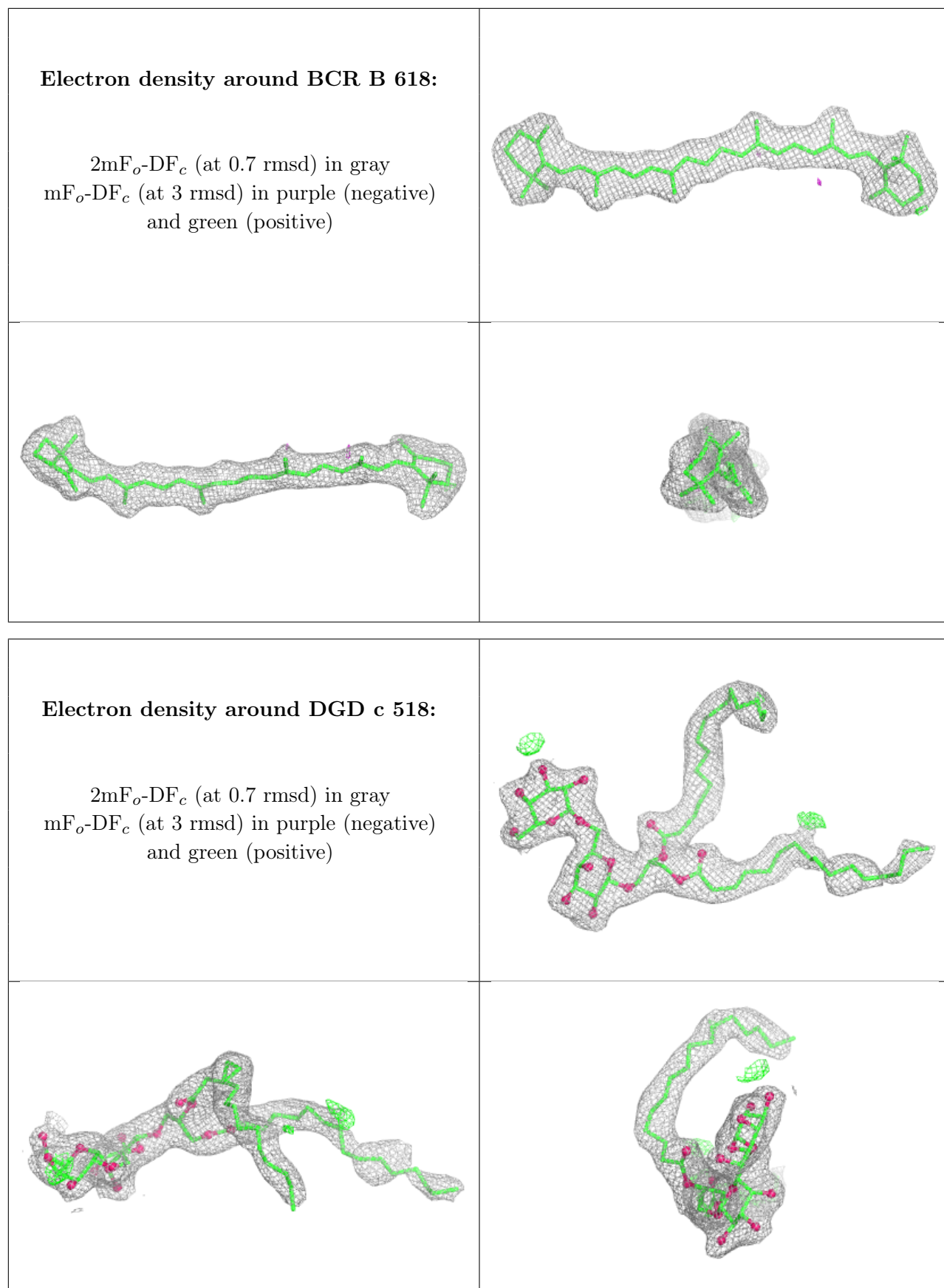
Electron density around CLA C 510:

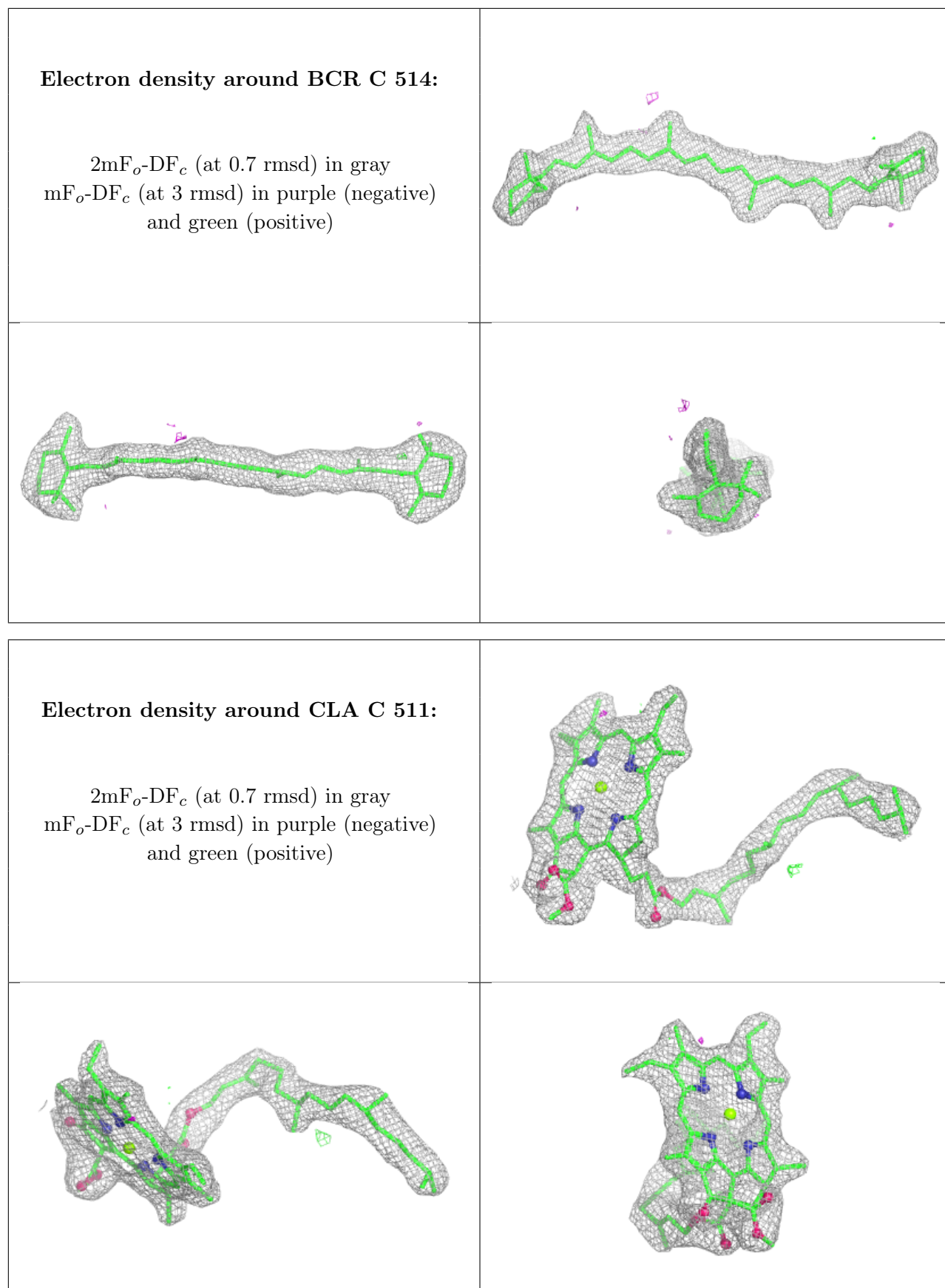
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

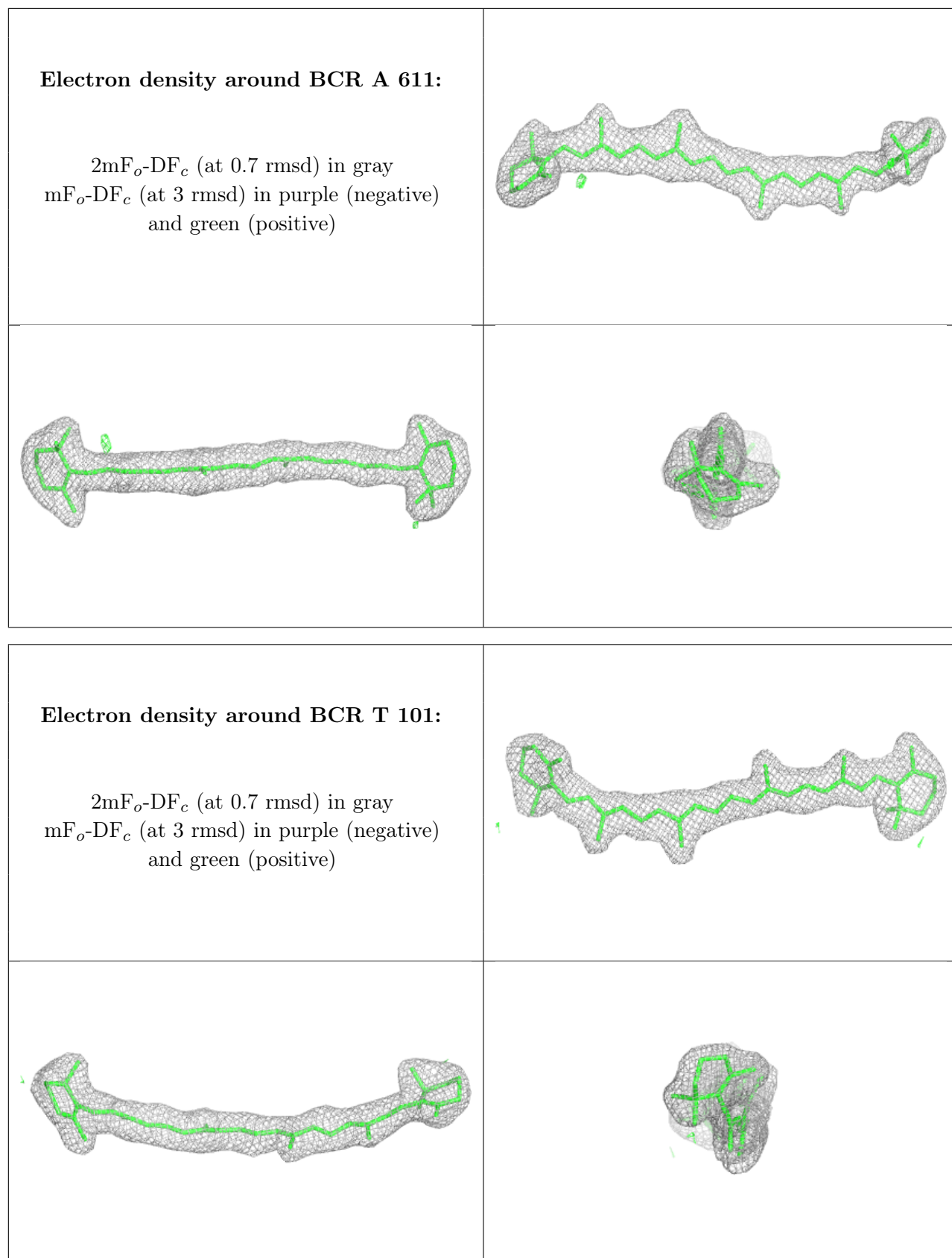
**Electron density around BCR b 616:**

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



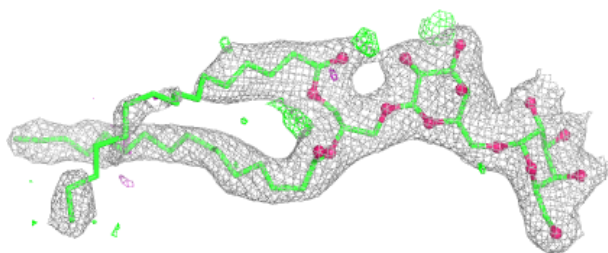
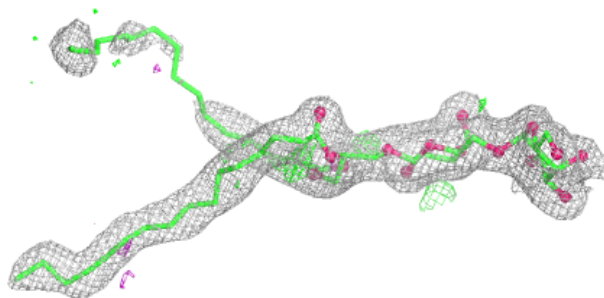




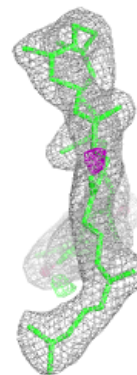
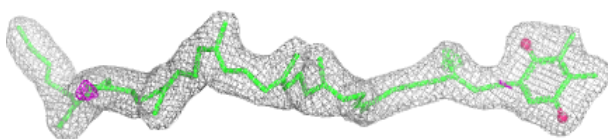
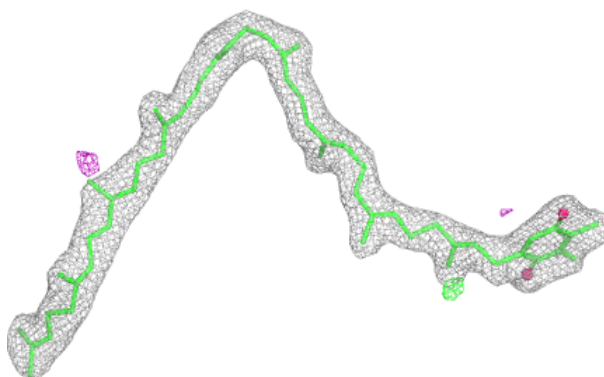


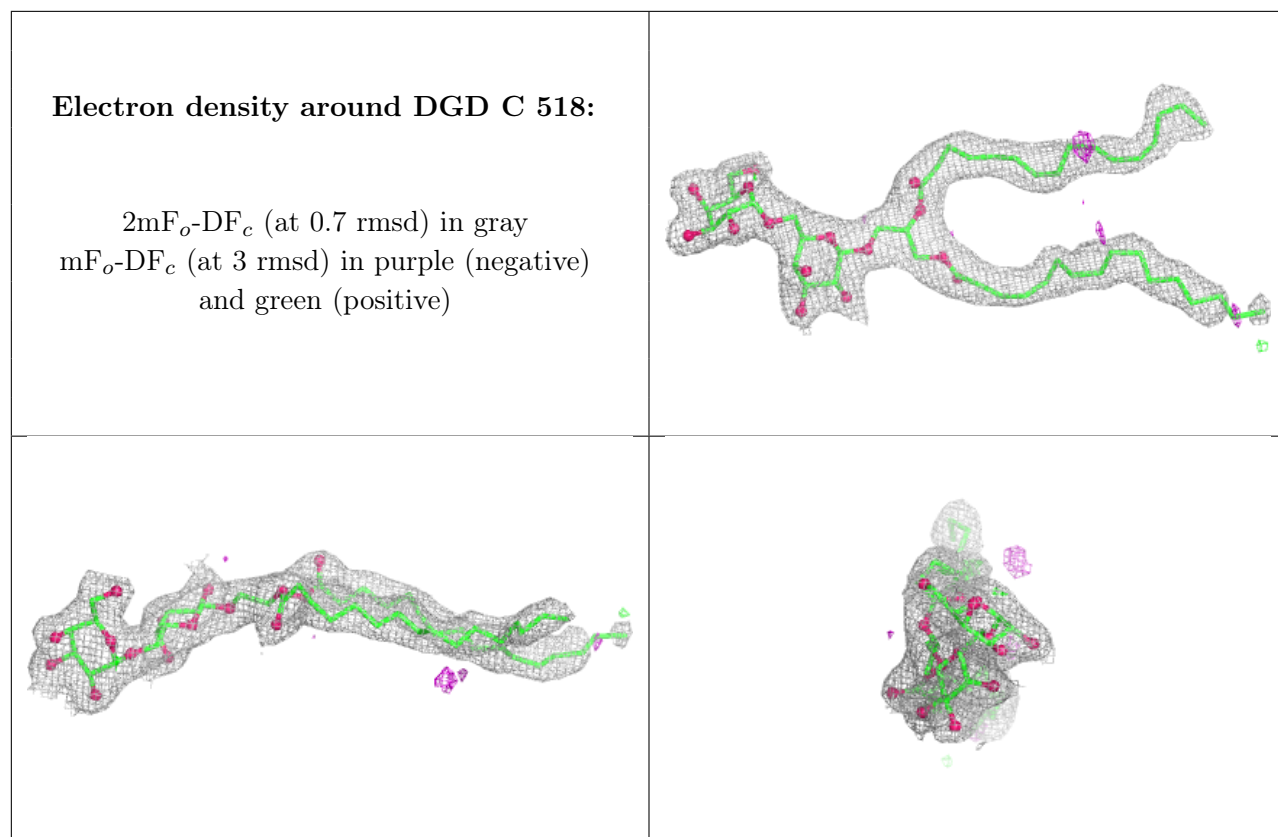
Electron density around DGD C 516:

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

**Electron density around PL9 D 405:**

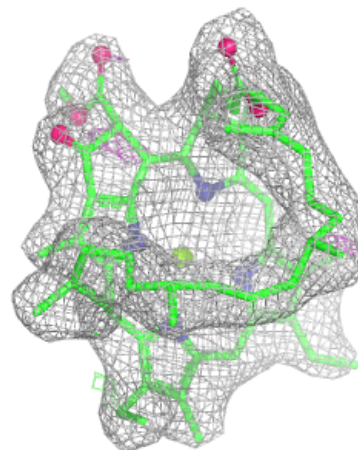
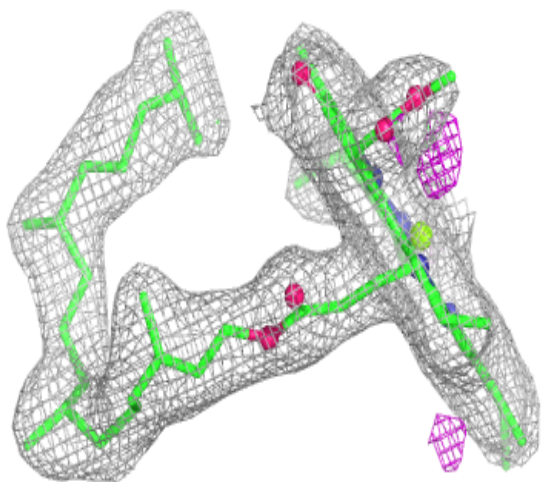
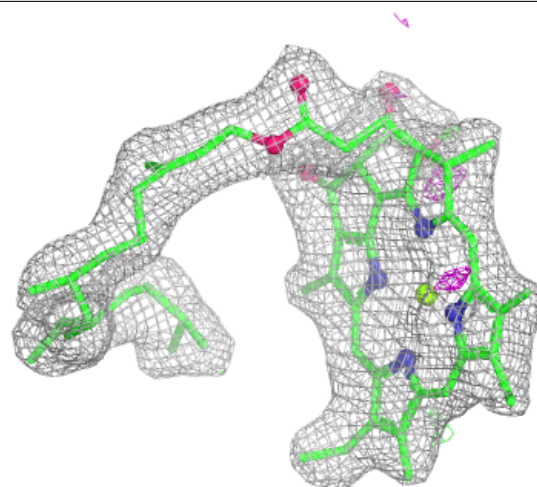
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





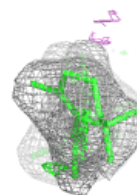
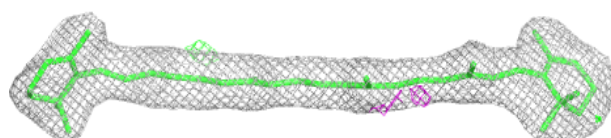
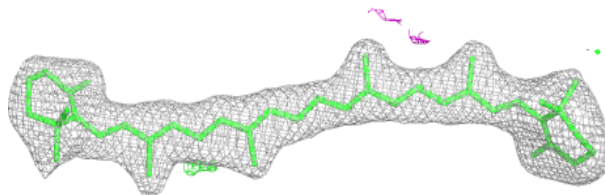
Electron density around CLA c 503:

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

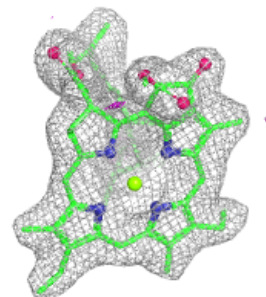
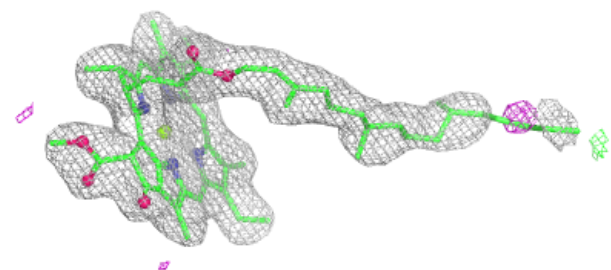
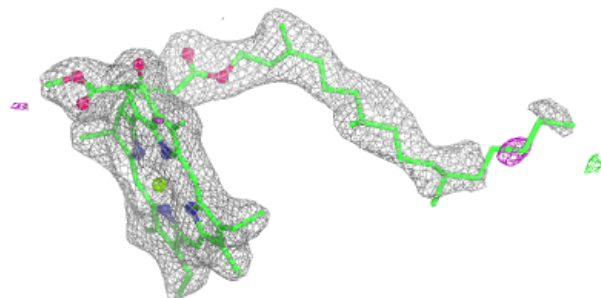


Electron density around BCR b 617:

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

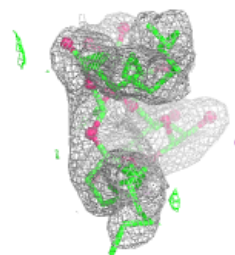
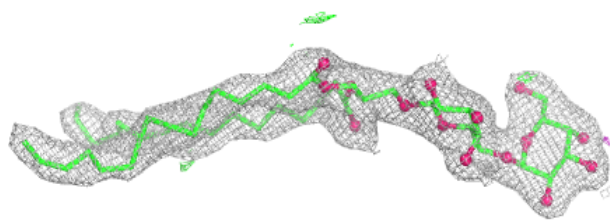
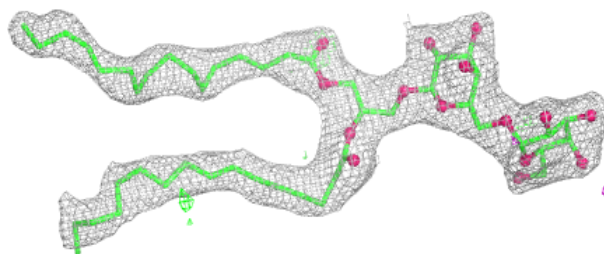
**Electron density around CLA c 508:**

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



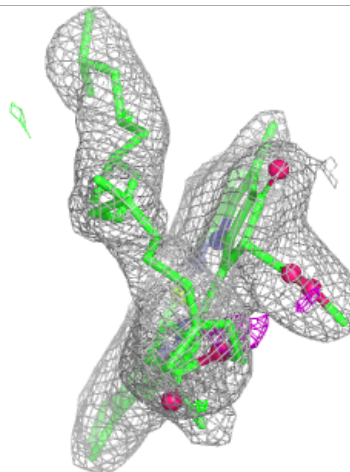
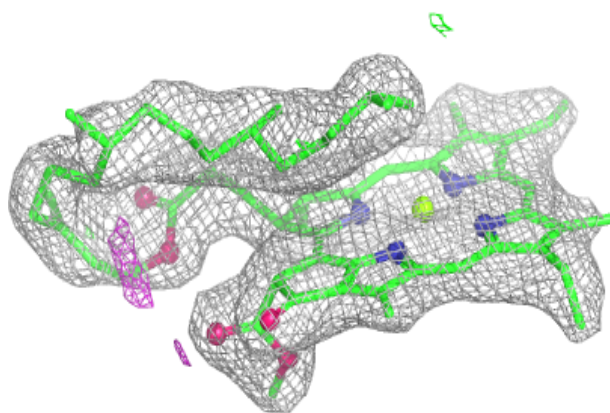
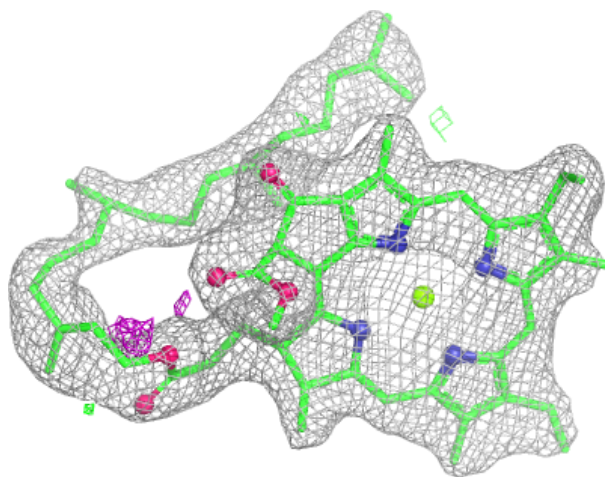
Electron density around DGD c 519:

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



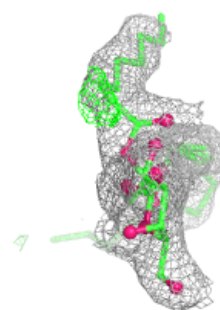
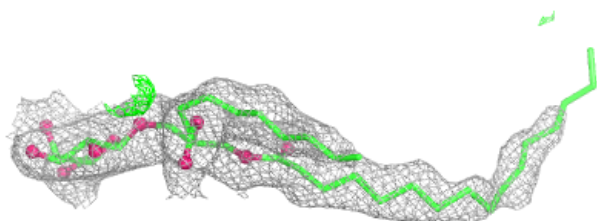
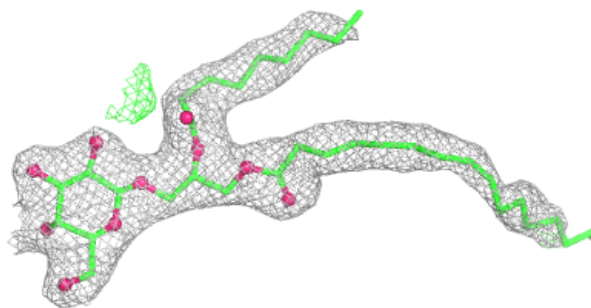
Electron density around CLA c 509:

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

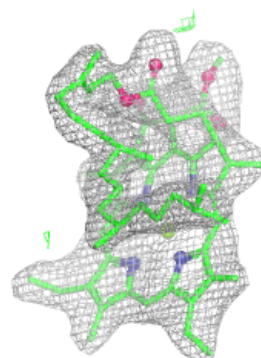
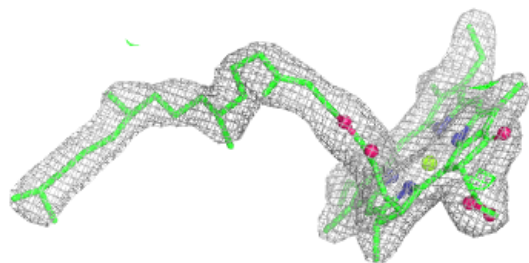
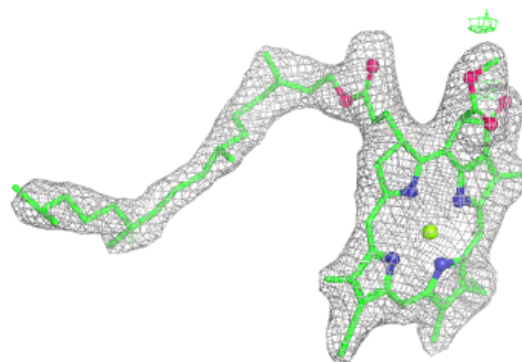


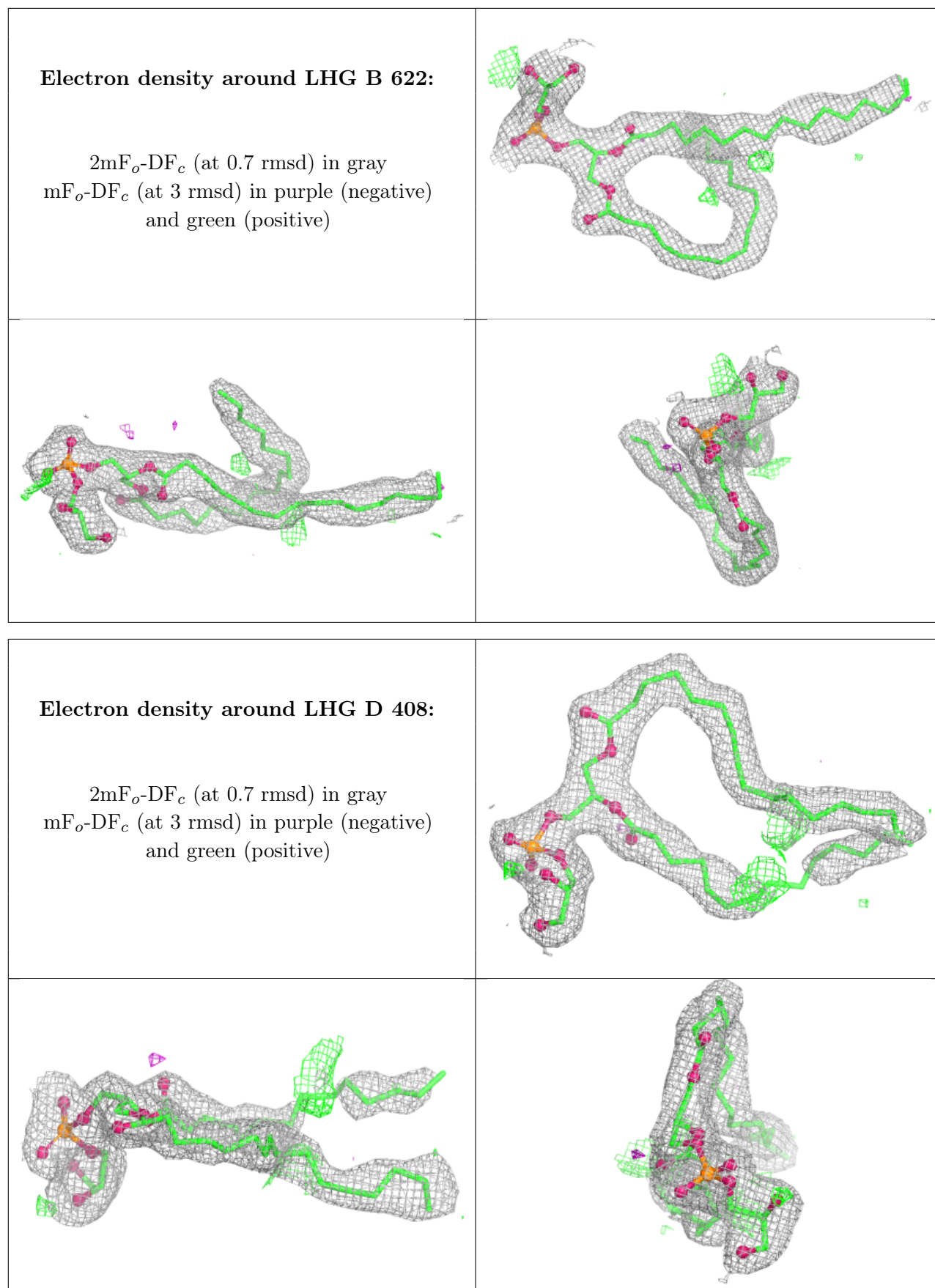
Electron density around LMG d 410:

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

**Electron density around CLA c 511:**

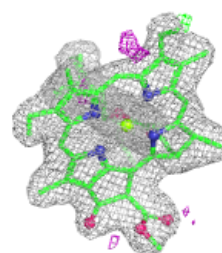
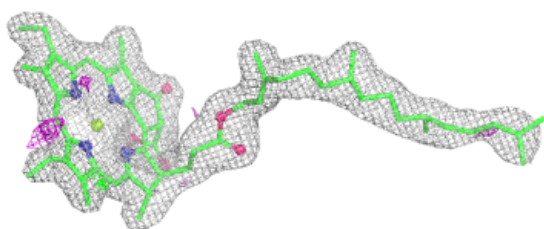
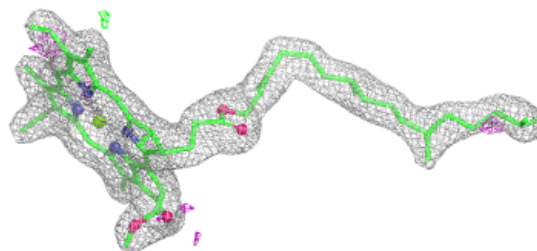
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



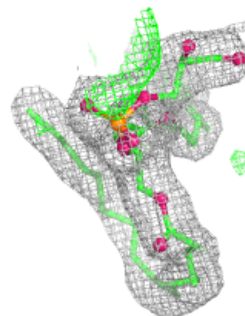
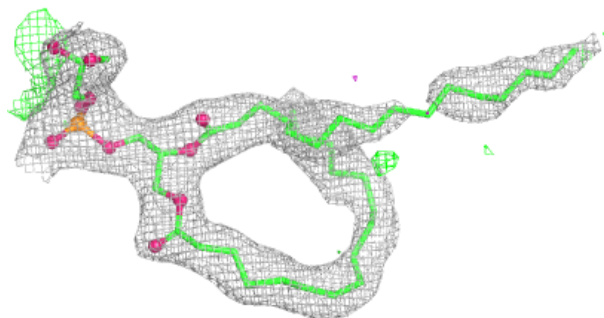


Electron density around CLA C 502:

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

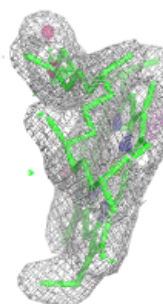
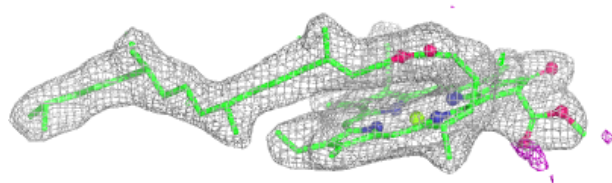
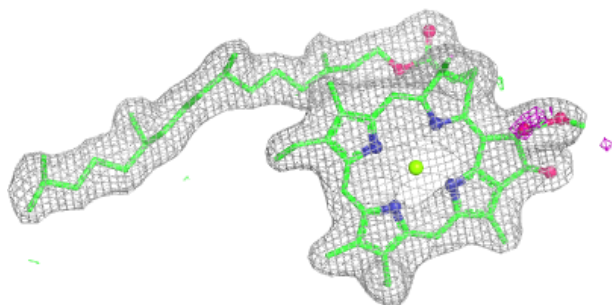
**Electron density around LHG d 406:**

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

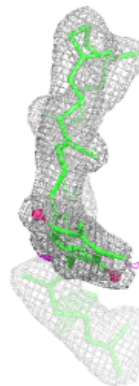
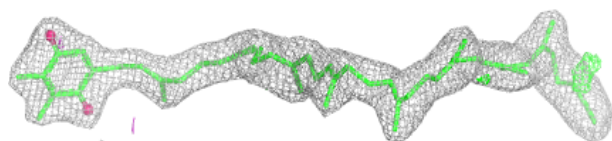
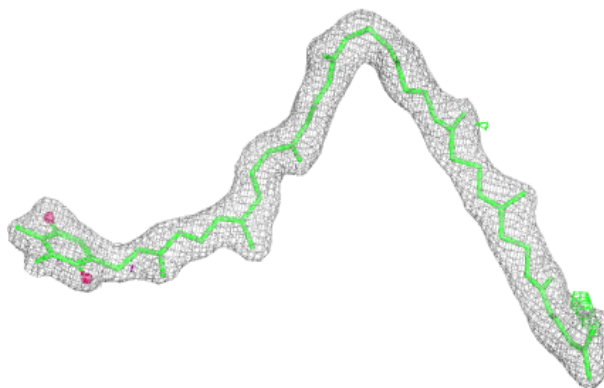


Electron density around CLA C 501:

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

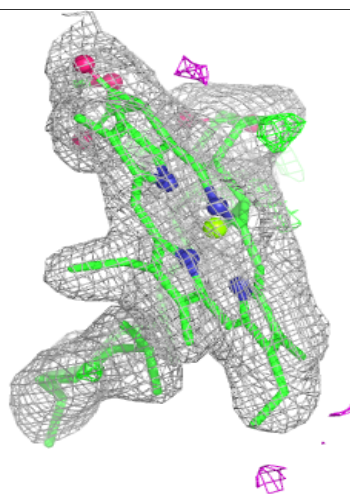
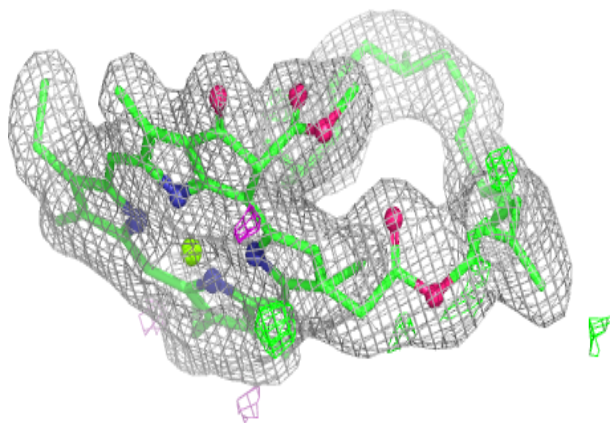
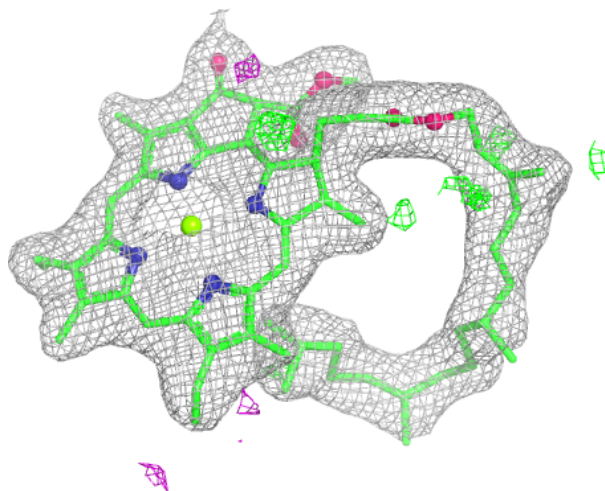
**Electron density around PL9 d 405:**

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



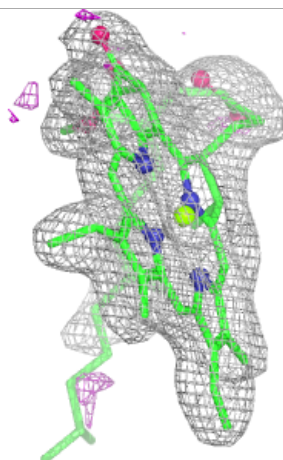
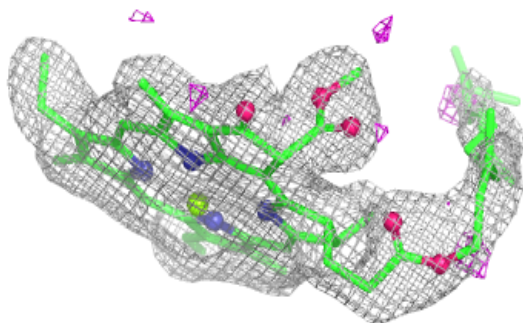
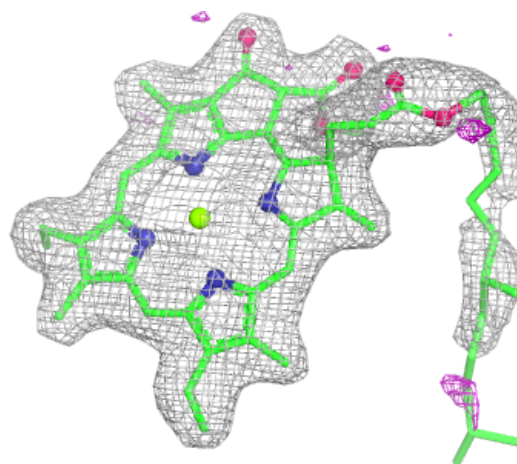
Electron density around CLA B 614:

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



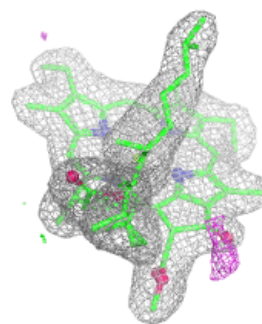
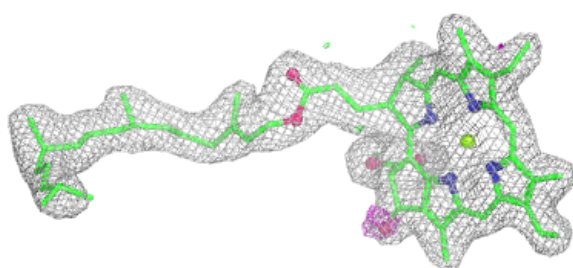
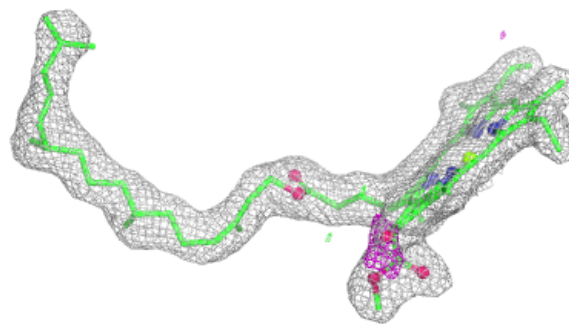
Electron density around CLA B 615:

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

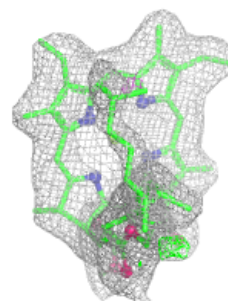
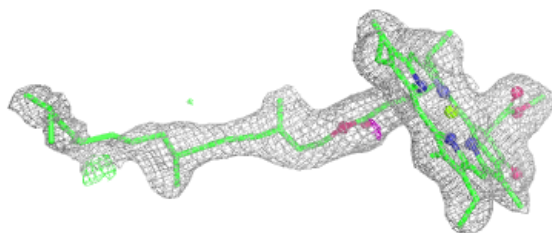
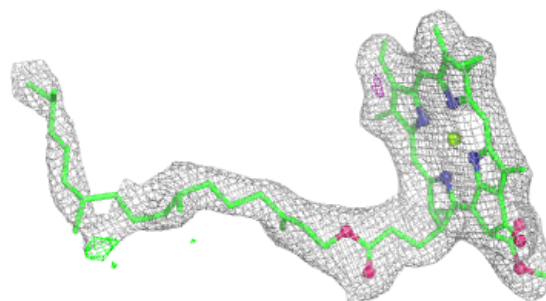


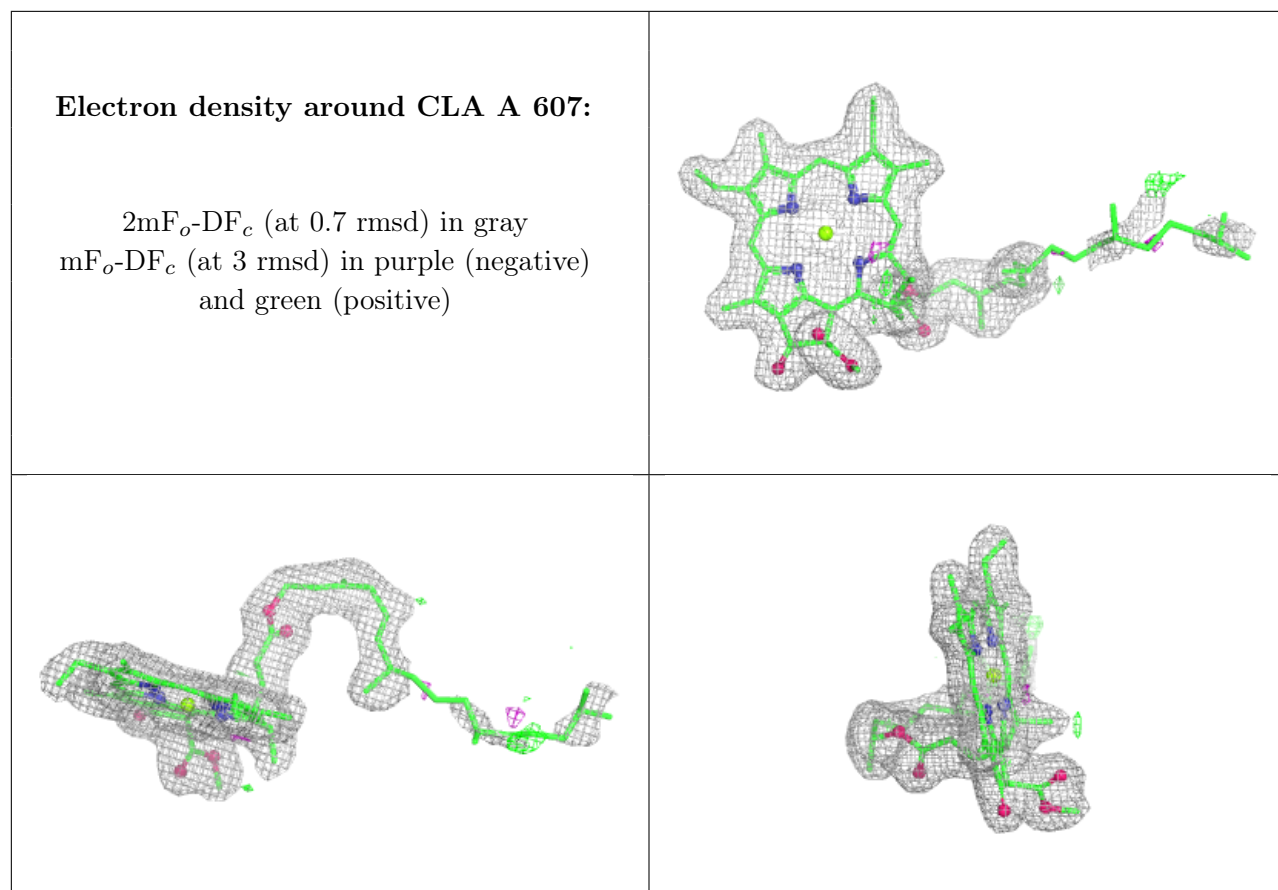
Electron density around CLA d 402:

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

**Electron density around CLA d 403:**

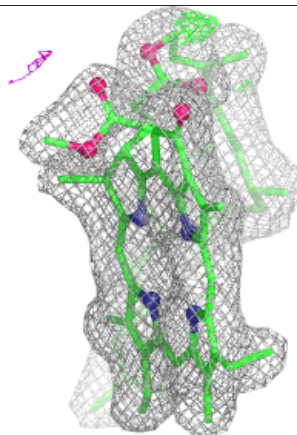
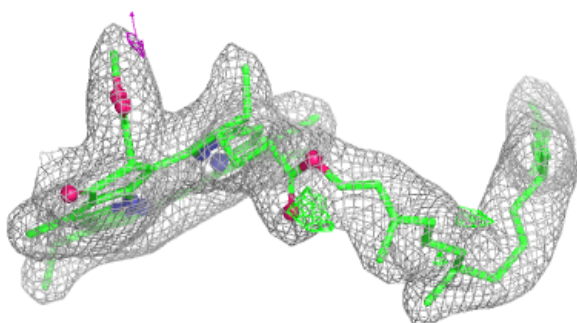
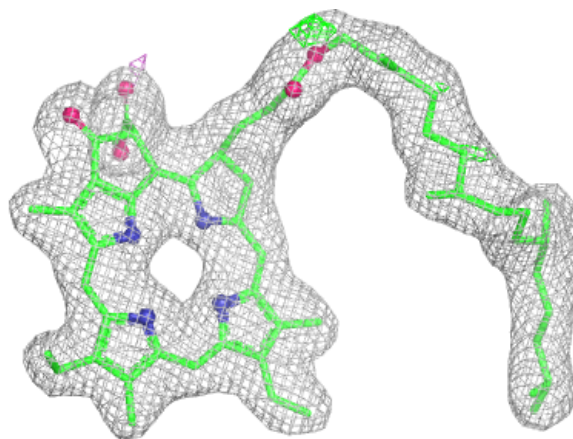
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





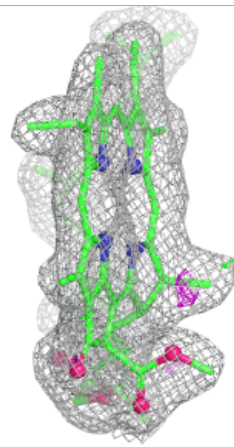
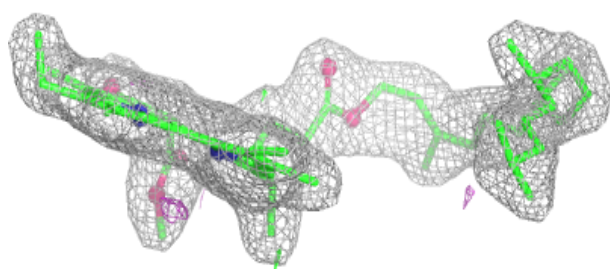
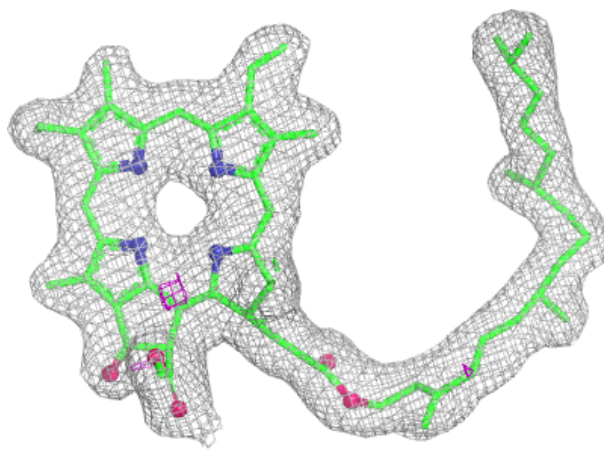
Electron density around PHO A 609:

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



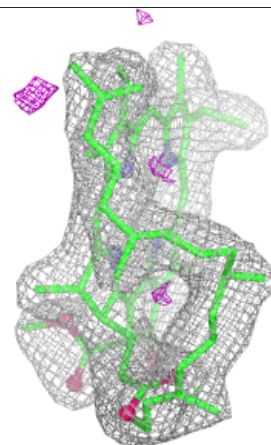
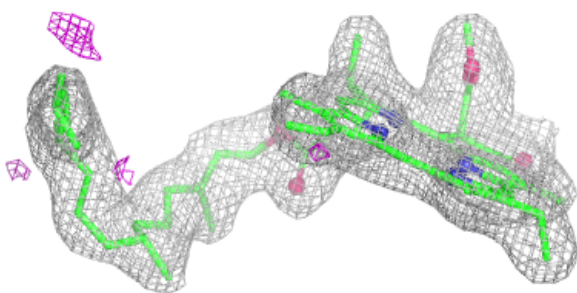
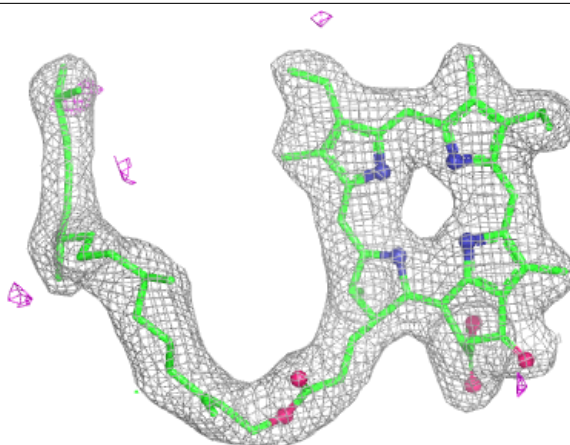
Electron density around PHO a 609:

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



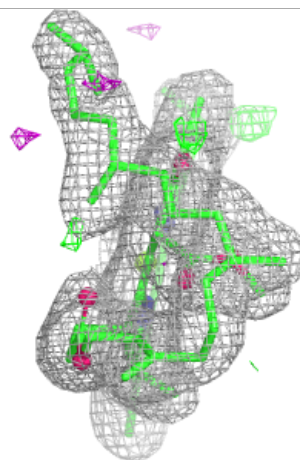
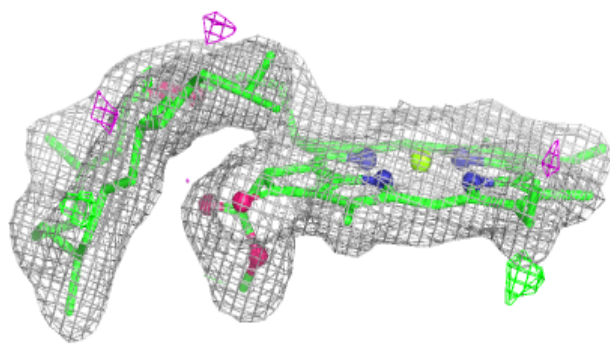
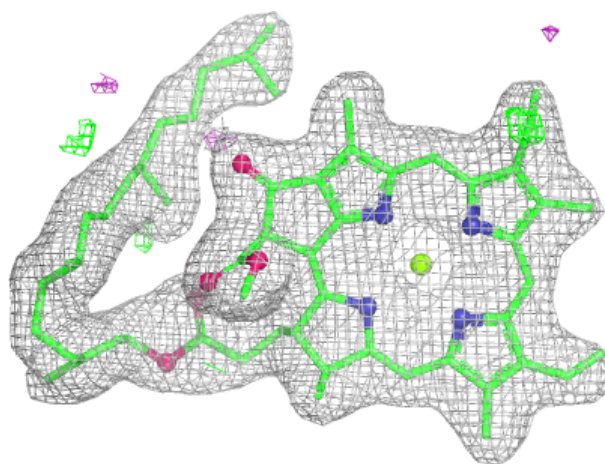
Electron density around PHO d 401:

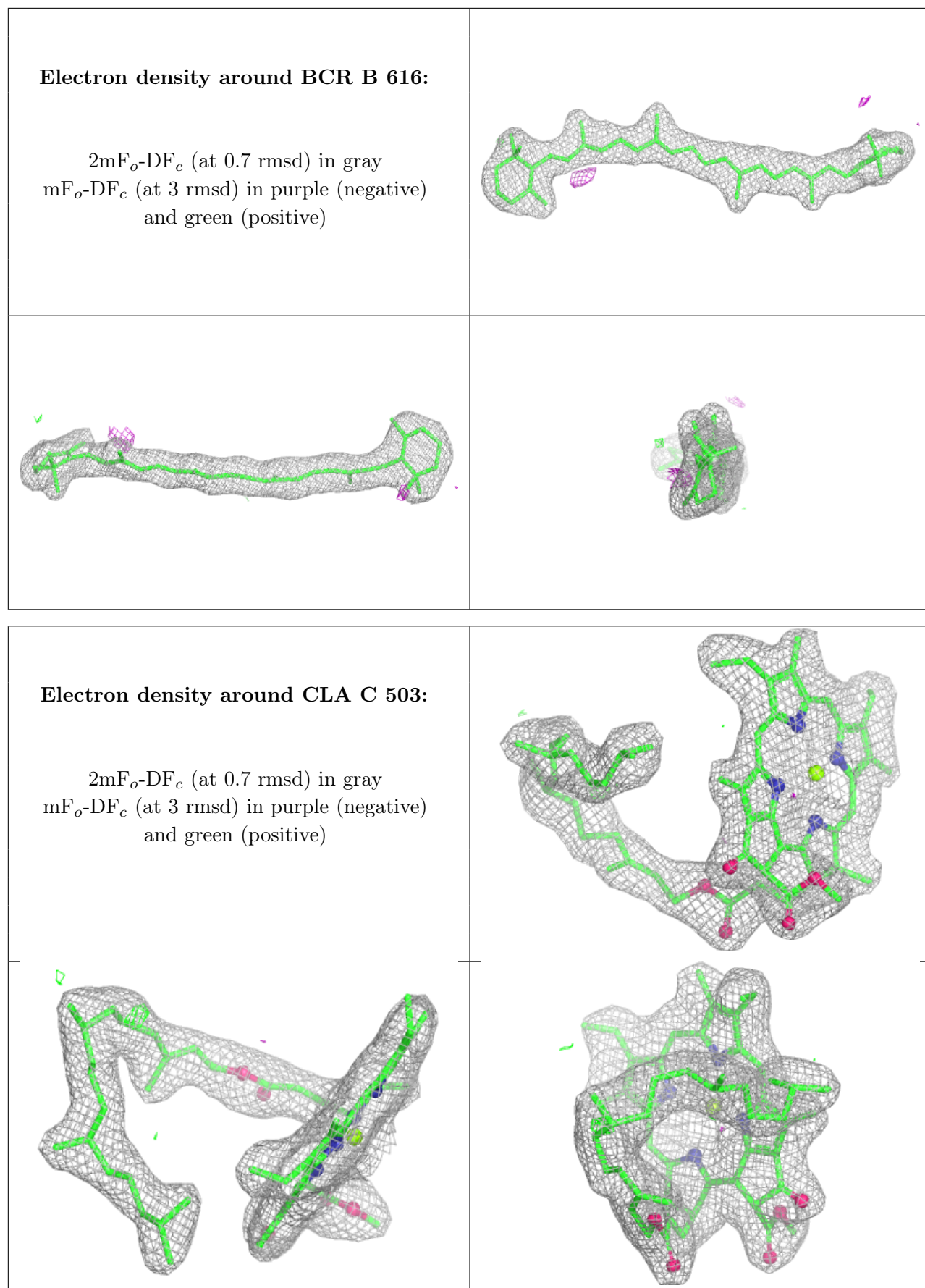
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 609:

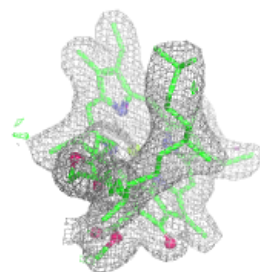
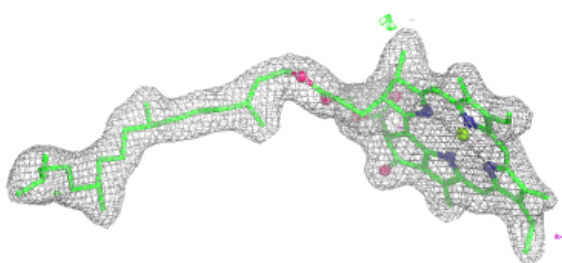
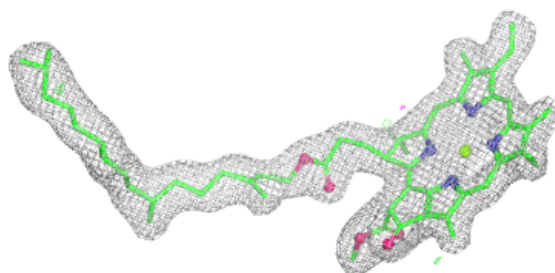
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



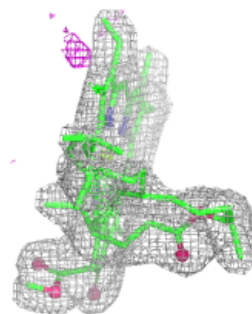
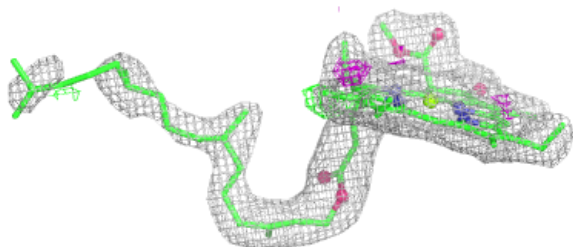
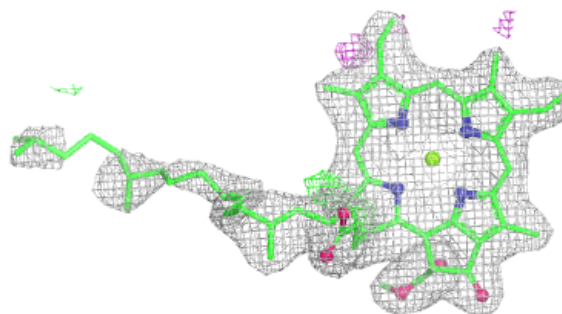


Electron density around CLA a 607:

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

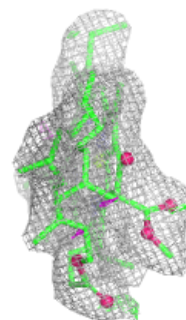
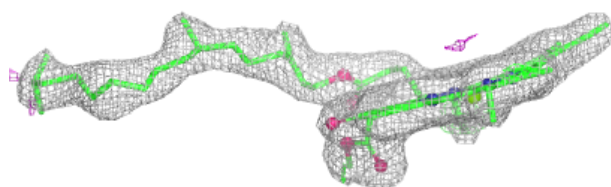
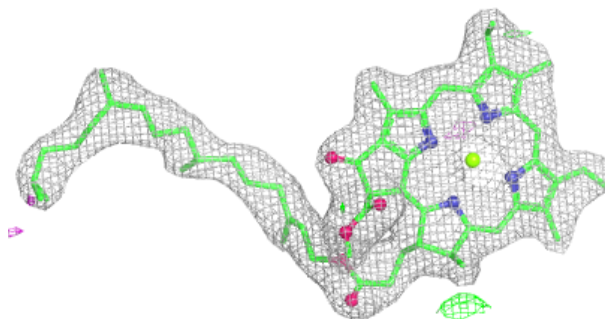
**Electron density around CLA a 608:**

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

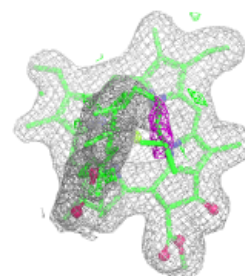
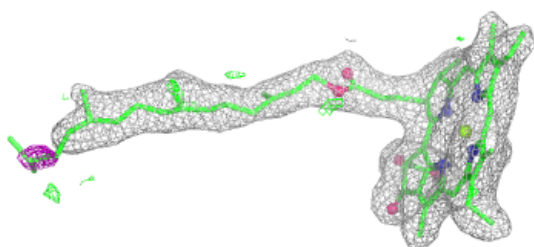
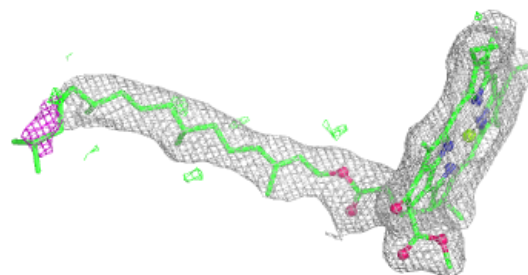


Electron density around CLA b 601:

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

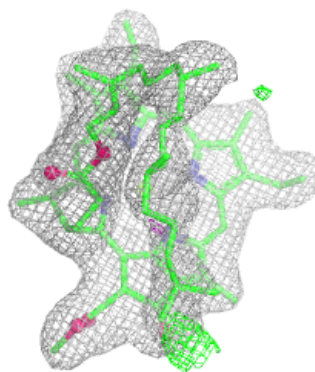
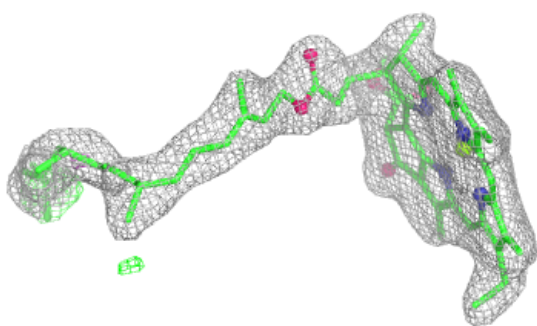
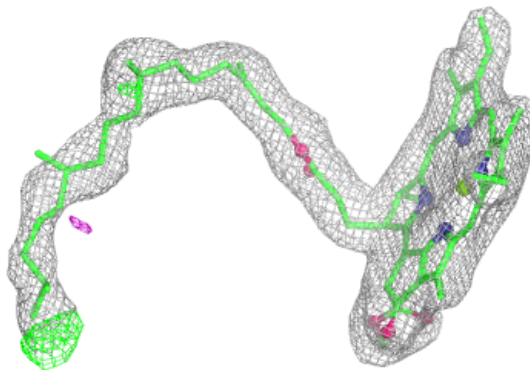
**Electron density around CLA b 603:**

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

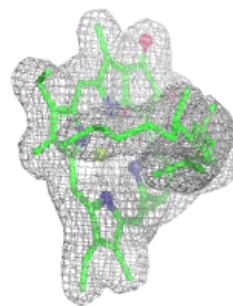
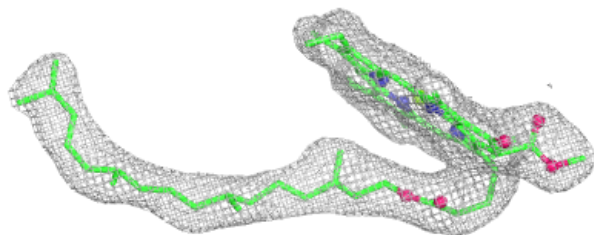
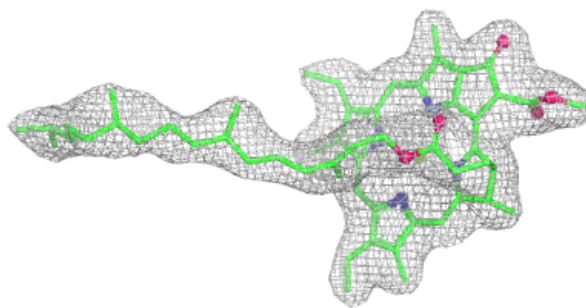


Electron density around CLA b 605:

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

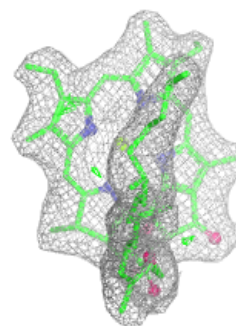
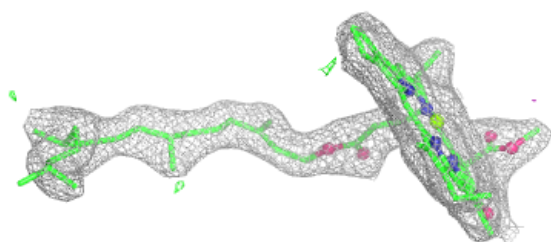
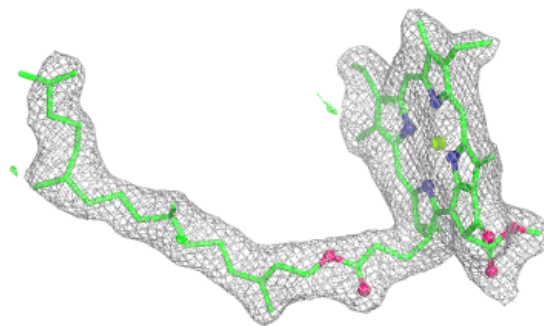
**Electron density around CLA b 607:**

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



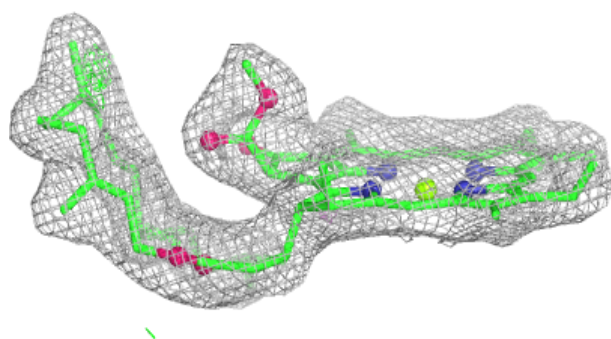
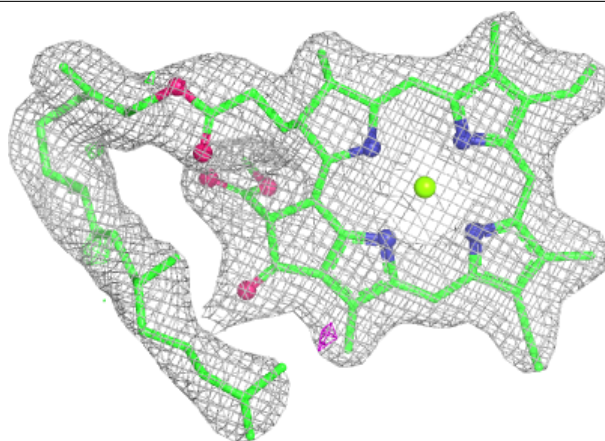
Electron density around CLA b 608:

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

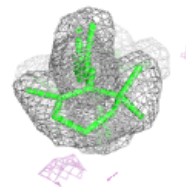
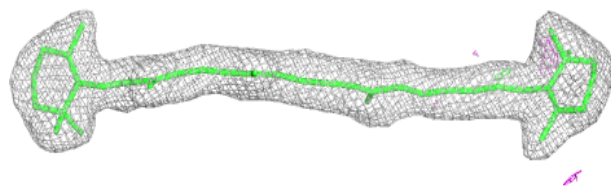
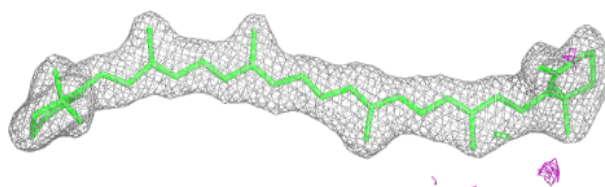


Electron density around CLA b 609:

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

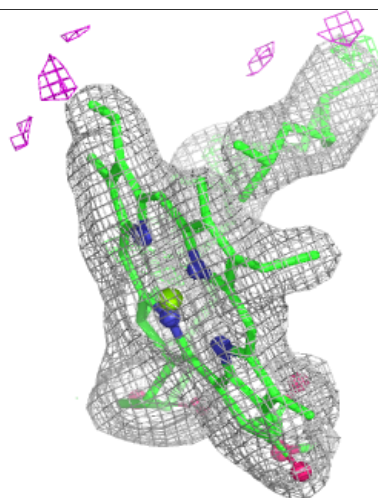
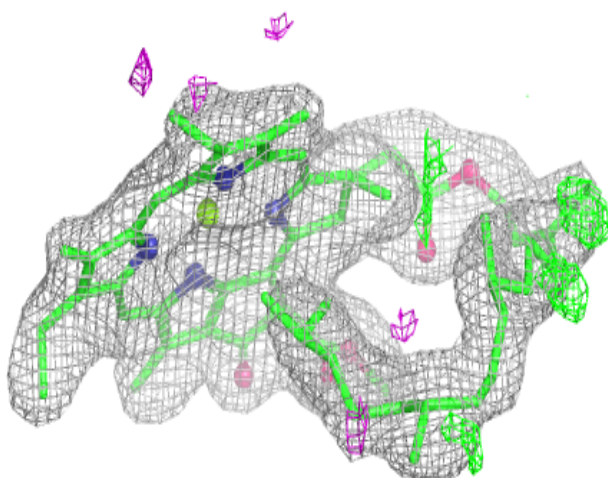
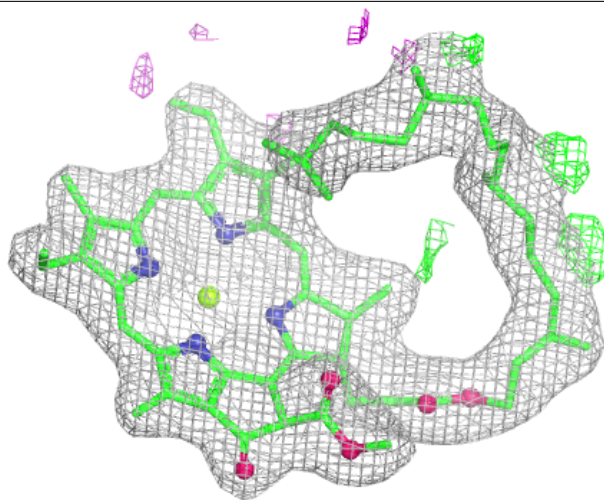
**Electron density around BCR a 611:**

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



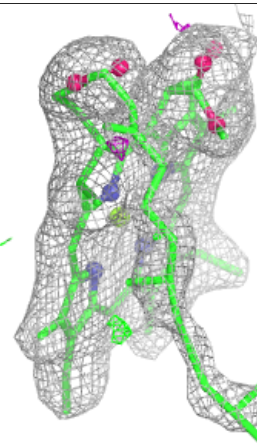
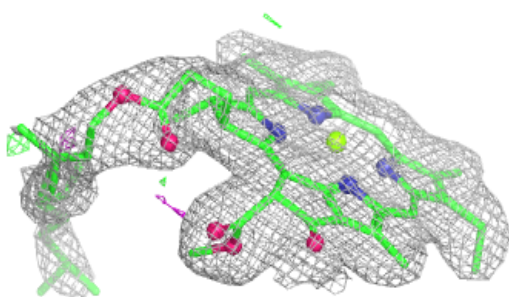
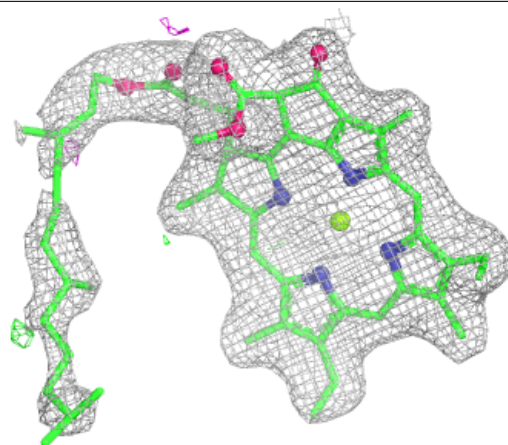
Electron density around CLA b 614:

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



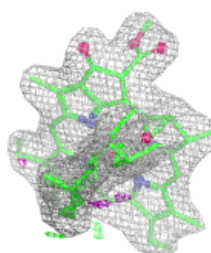
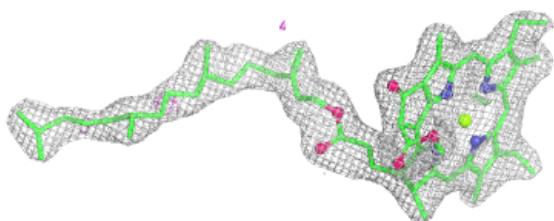
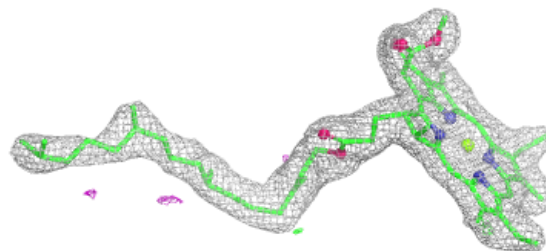
Electron density around CLA b 615:

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

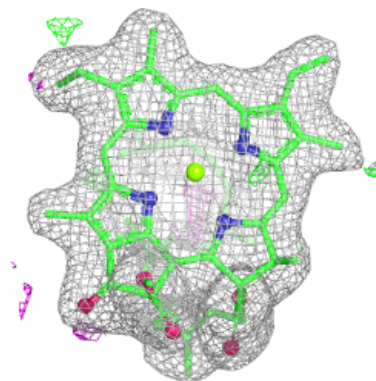
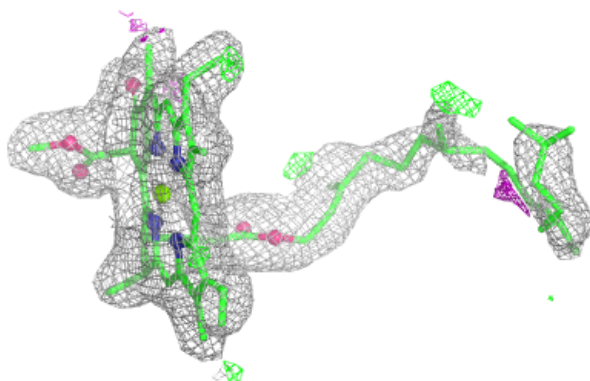
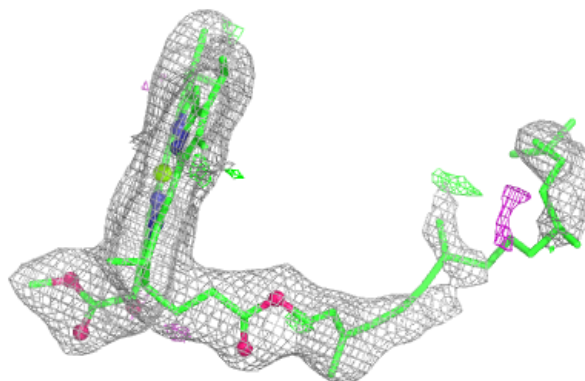


Electron density around CLA c 502:

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

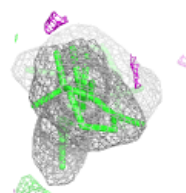
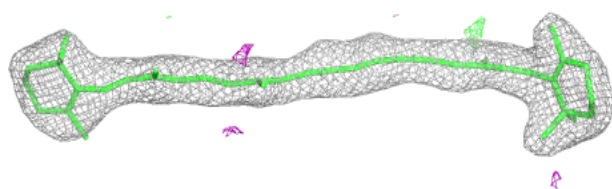
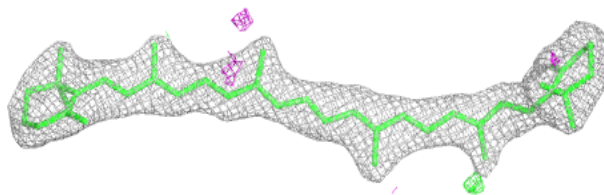
**Electron density around CLA C 506:**

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

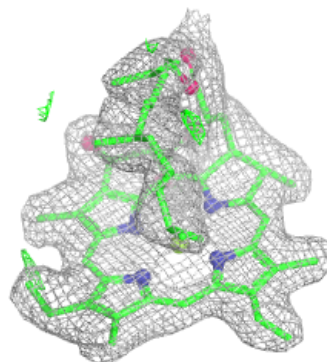
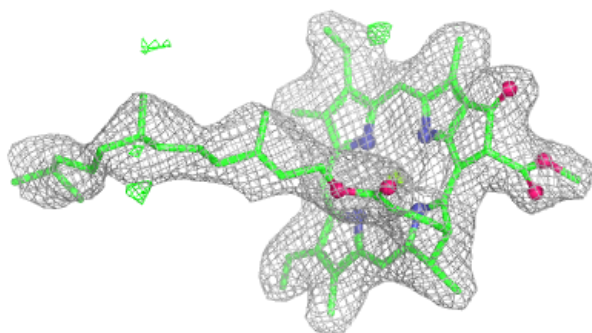
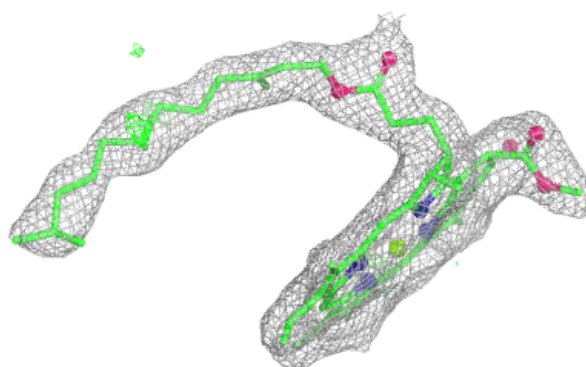


Electron density around BCR c 515:

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

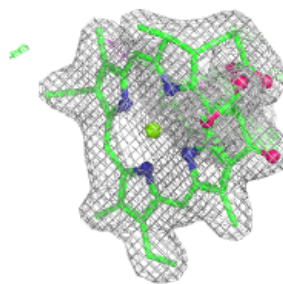
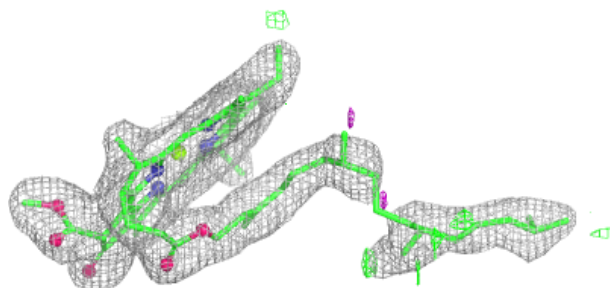
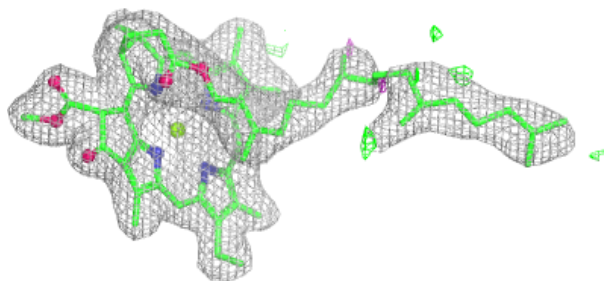
**Electron density around CLA c 504:**

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

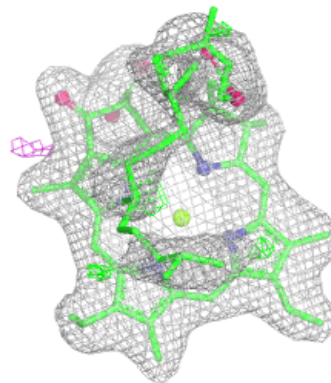
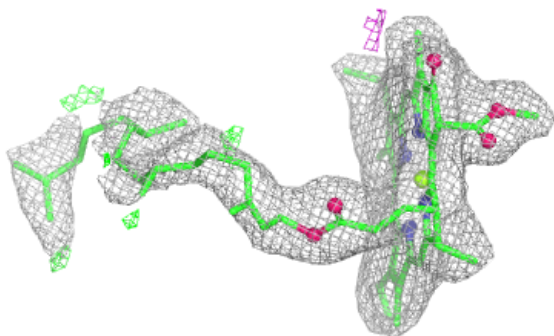
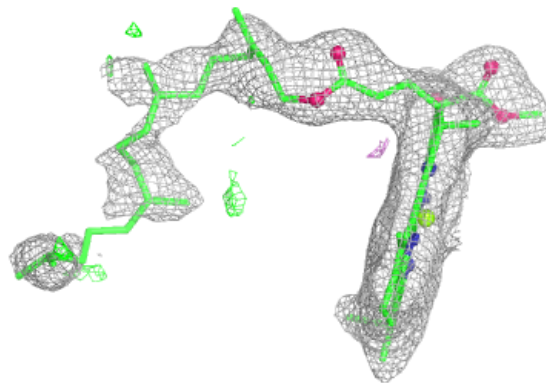


Electron density around CLA c 505:

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

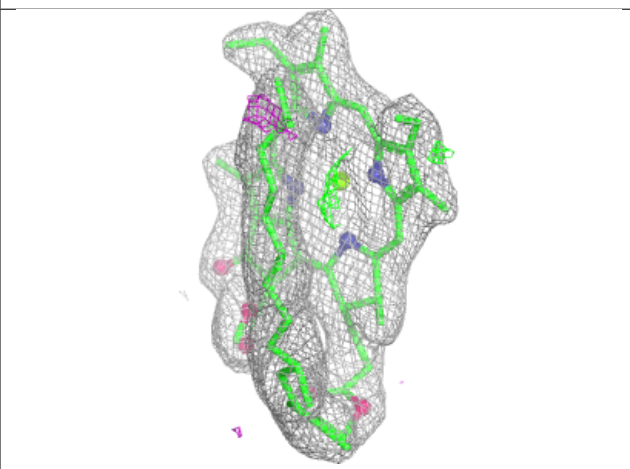
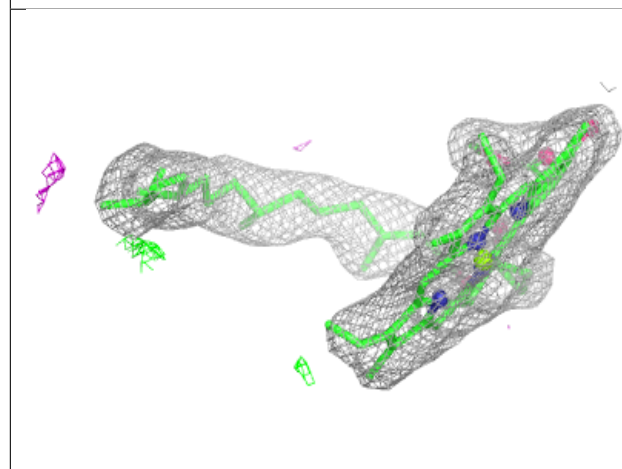
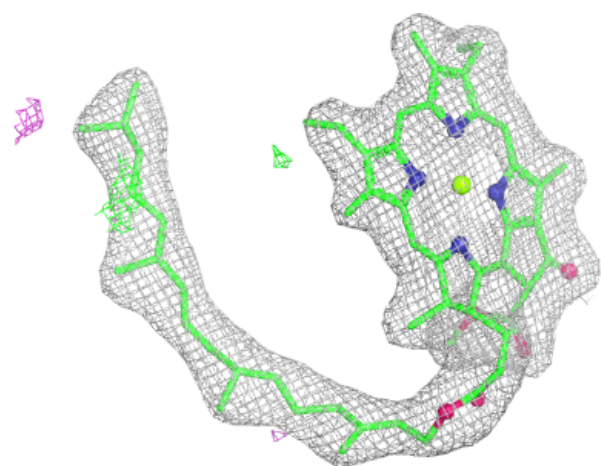
**Electron density around CLA c 506:**

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



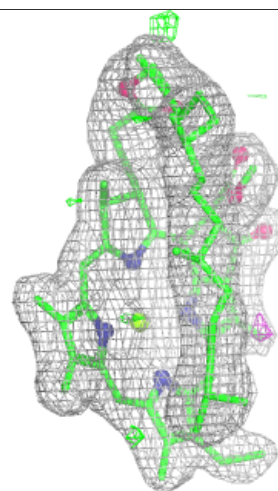
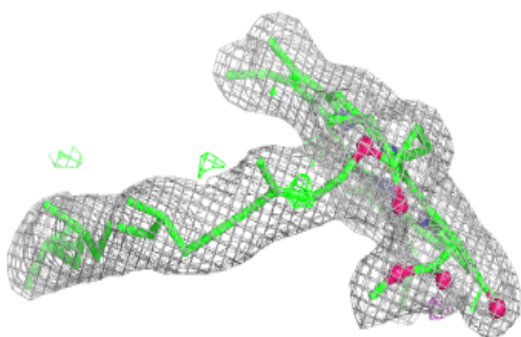
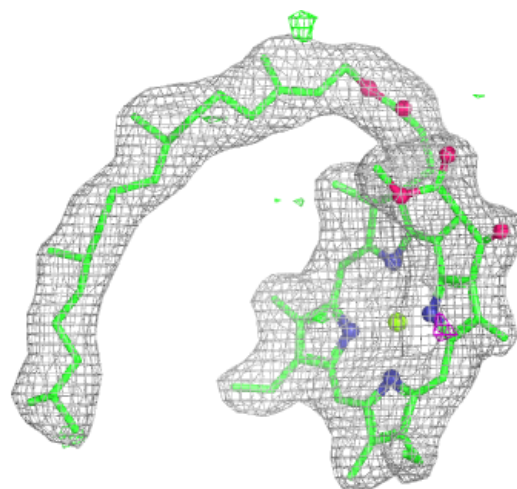
Electron density around CLA c 507:

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



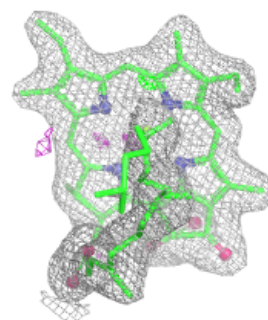
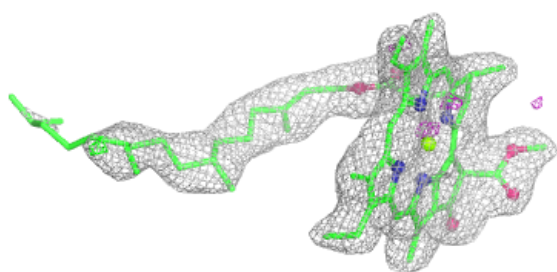
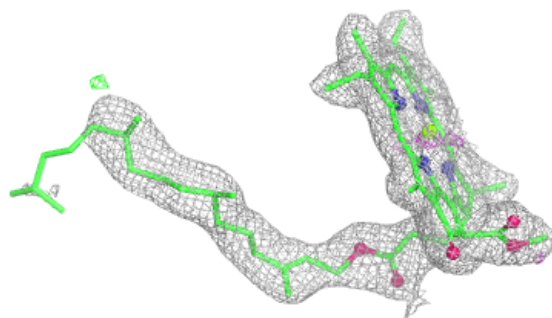
Electron density around CLA C 507:

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

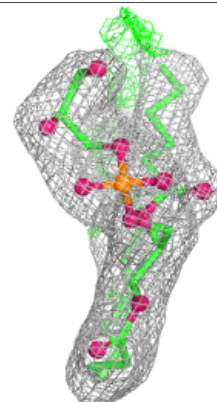
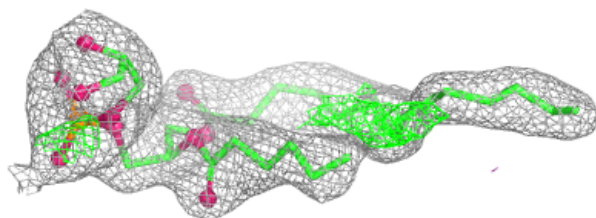
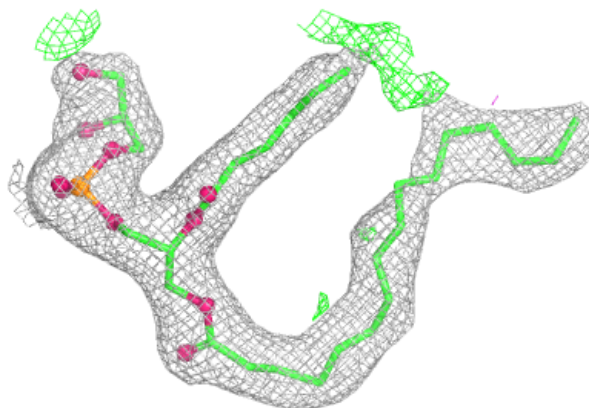


Electron density around CLA C 508:

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

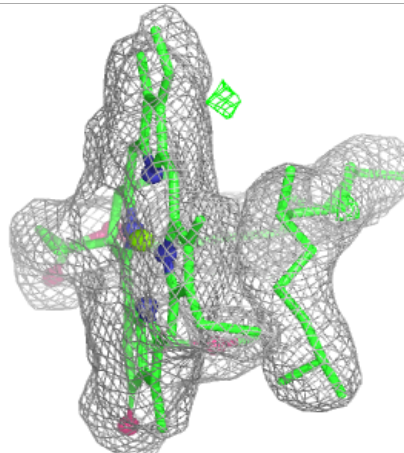
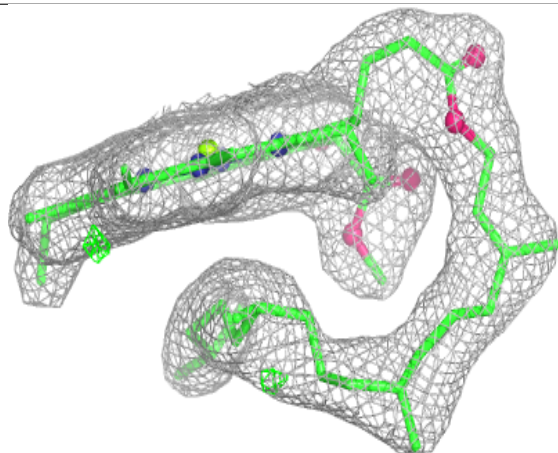
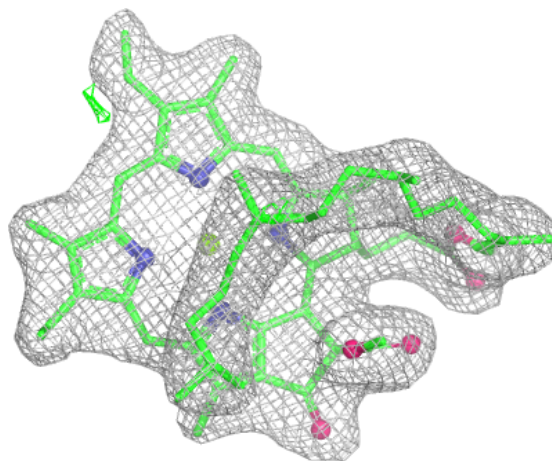
**Electron density around LHG d 408:**

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



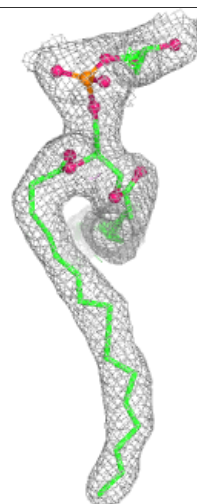
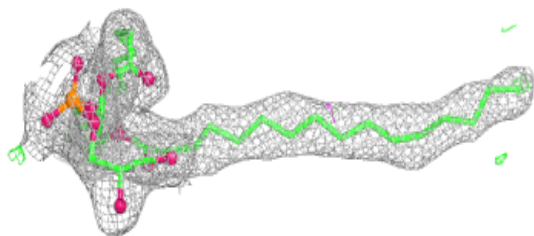
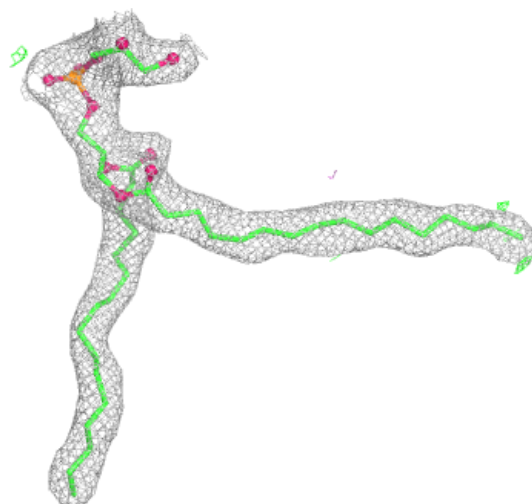
Electron density around CLA c 510:

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



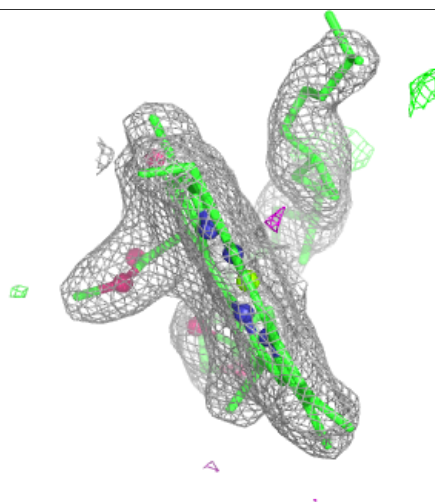
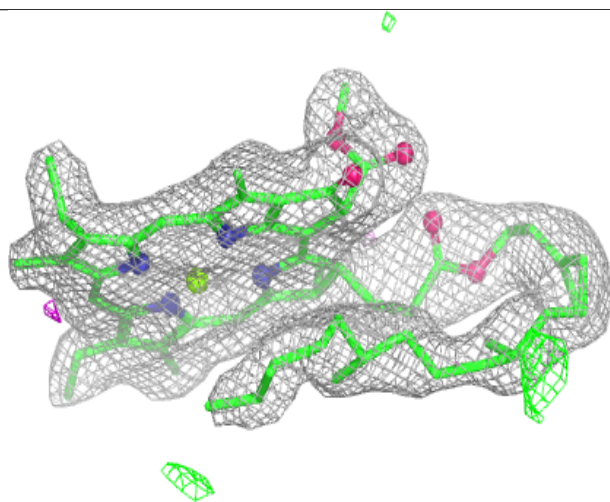
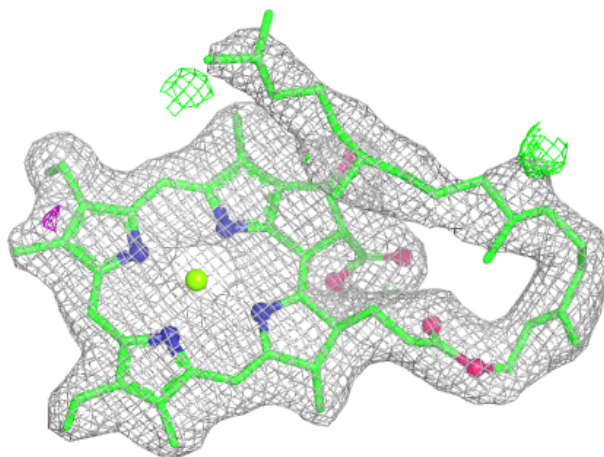
Electron density around LHG 1 102:

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



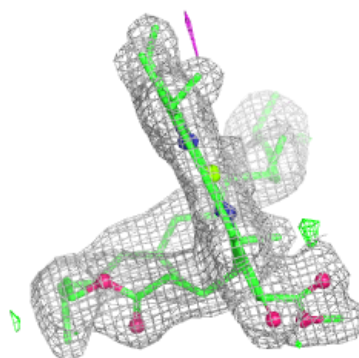
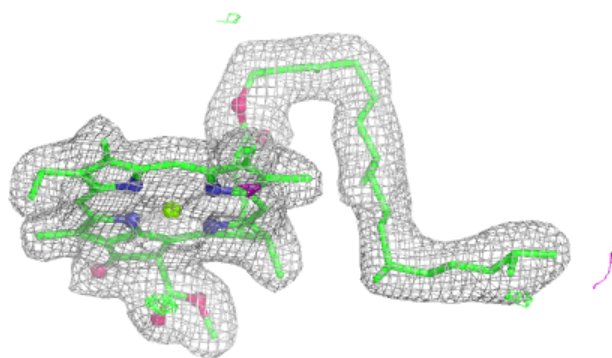
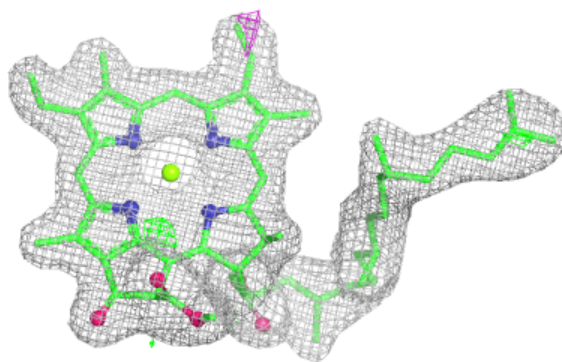
Electron density around CLA C 509:

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

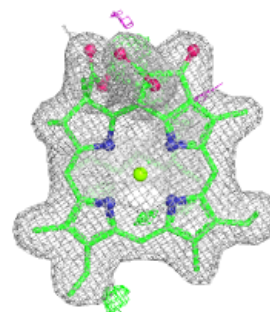
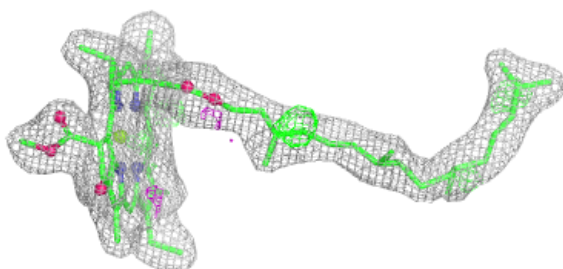
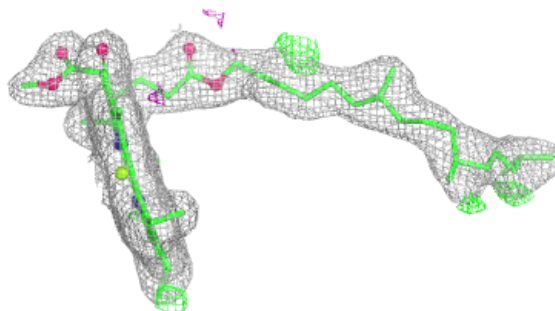


Electron density around CLA a 613:

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

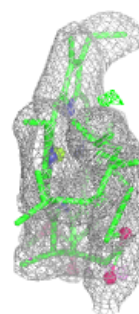
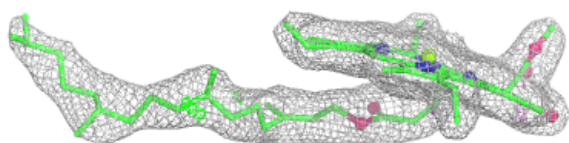
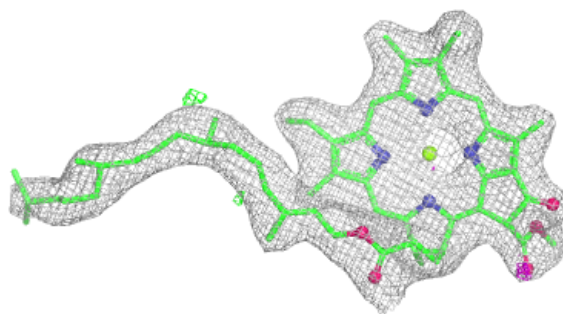
**Electron density around CLA B 604:**

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

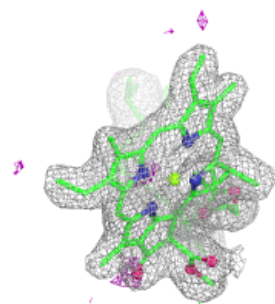
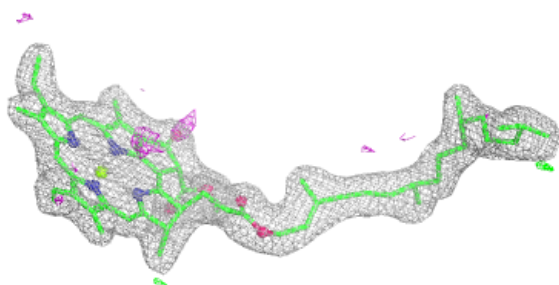
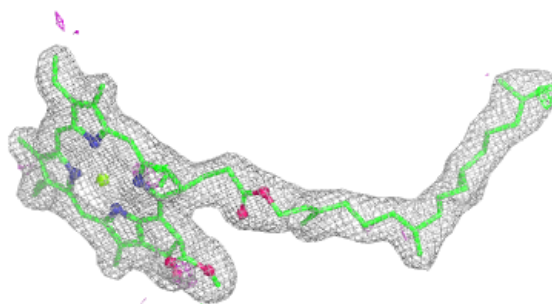


Electron density around CLA b 602:

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

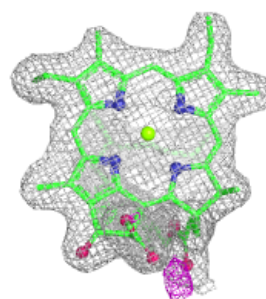
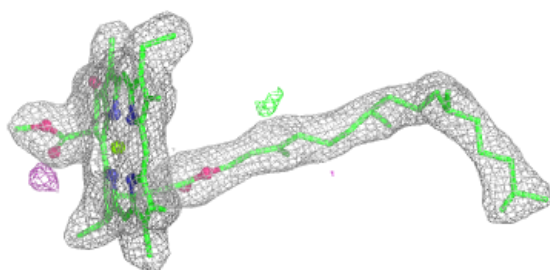
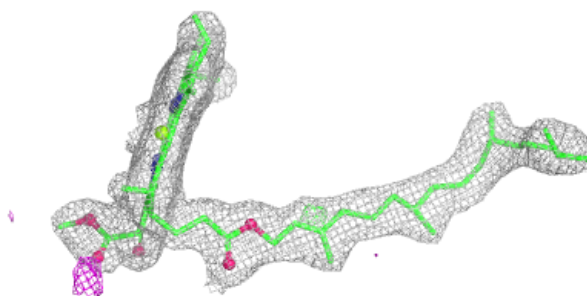
**Electron density around CLA A 606:**

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

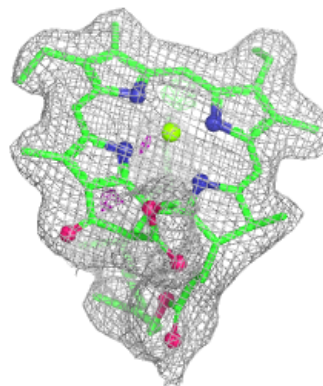
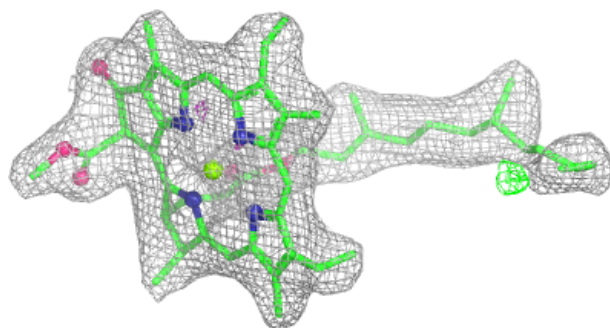
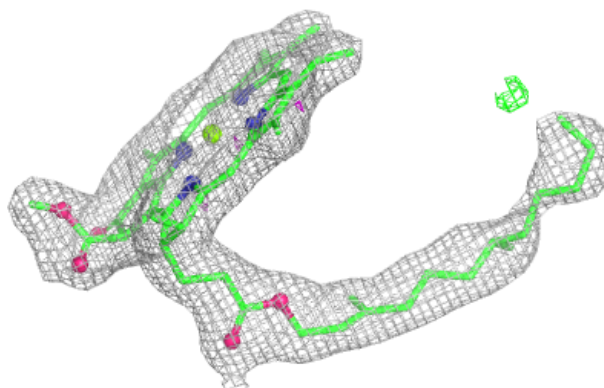


Electron density around CLA b 604:

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

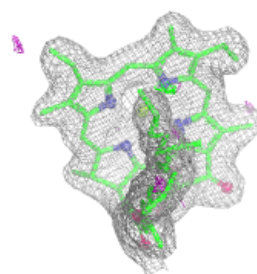
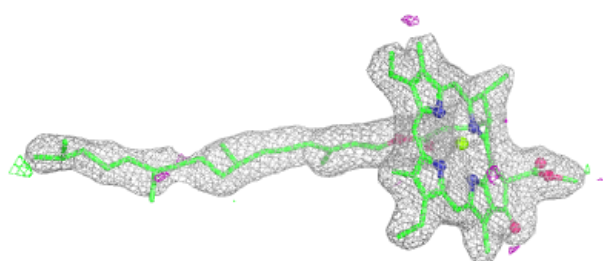
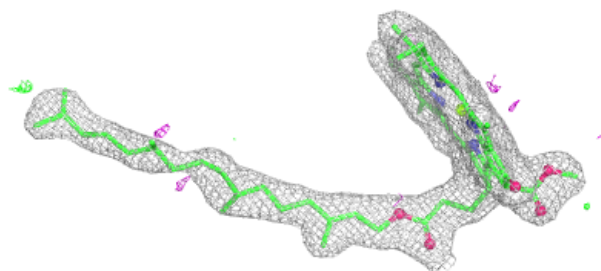
**Electron density around CLA C 504:**

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

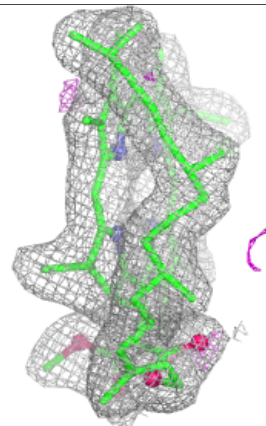
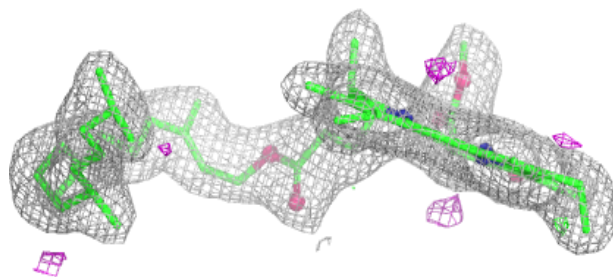
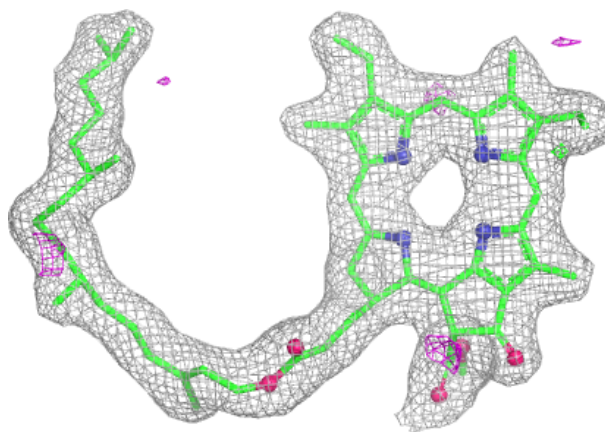


Electron density around CLA b 606:

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

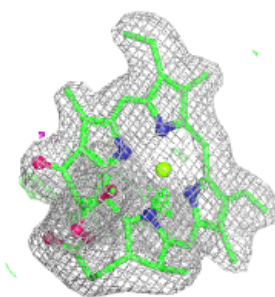
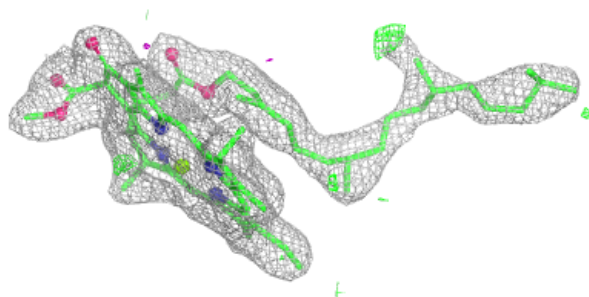
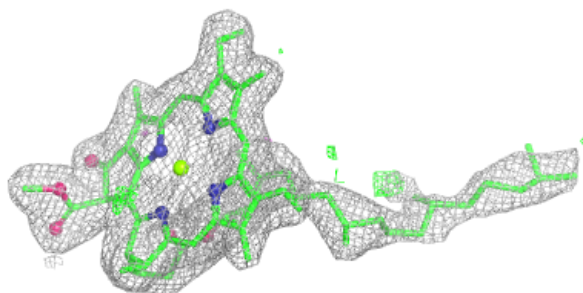
**Electron density around PHO A 608:**

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

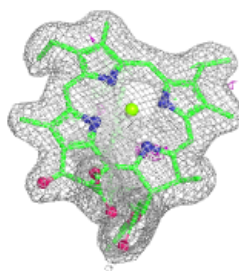
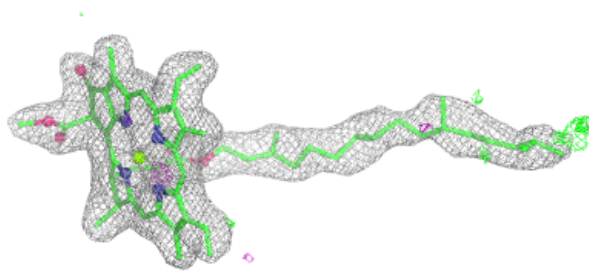
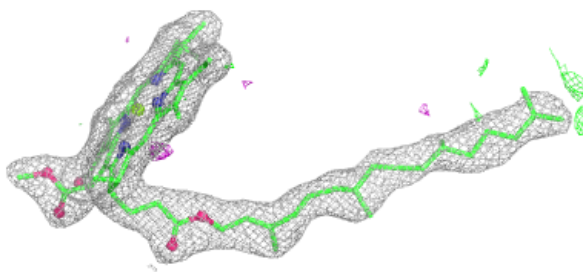


Electron density around CLA C 505:

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

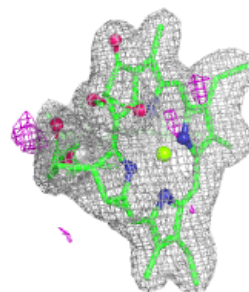
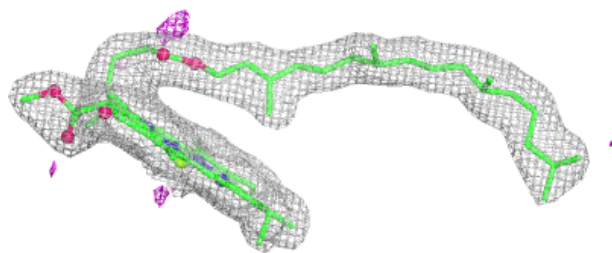
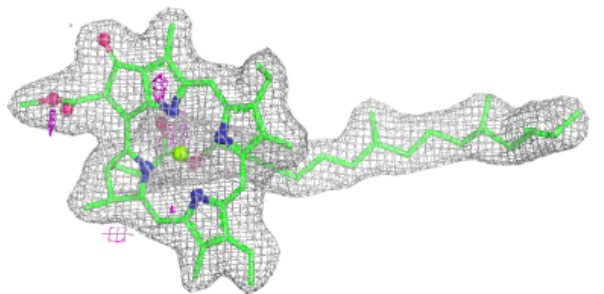
**Electron density around CLA B 606:**

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



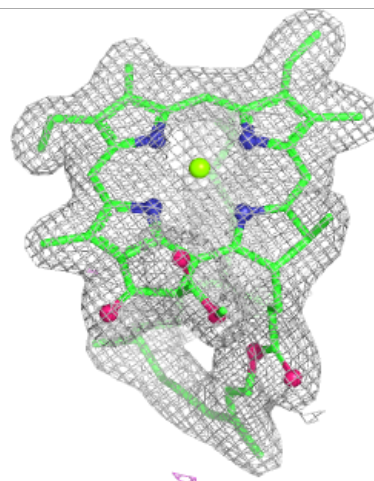
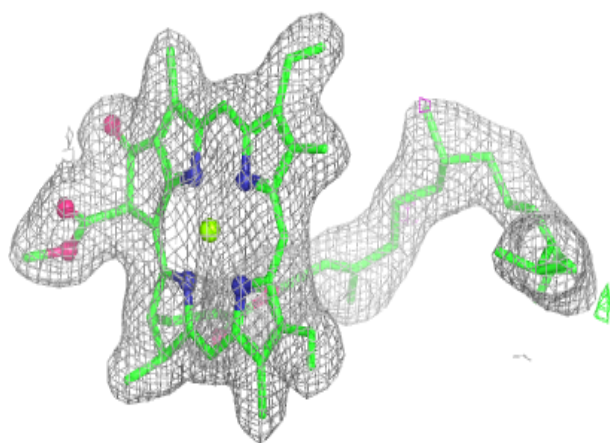
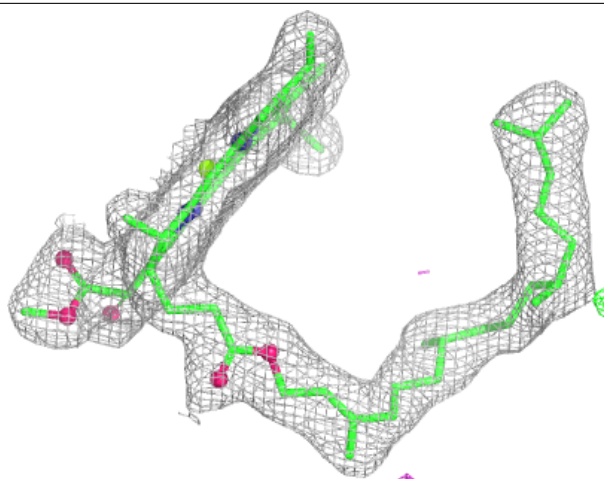
Electron density around CLA B 607:

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



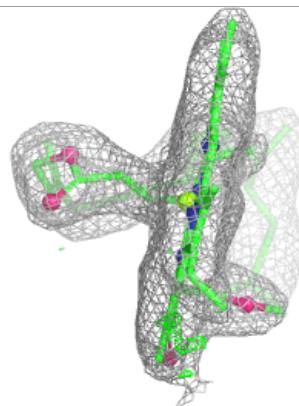
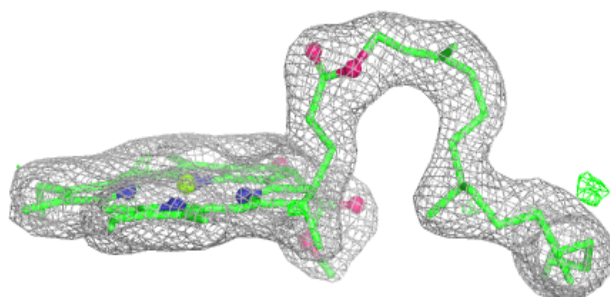
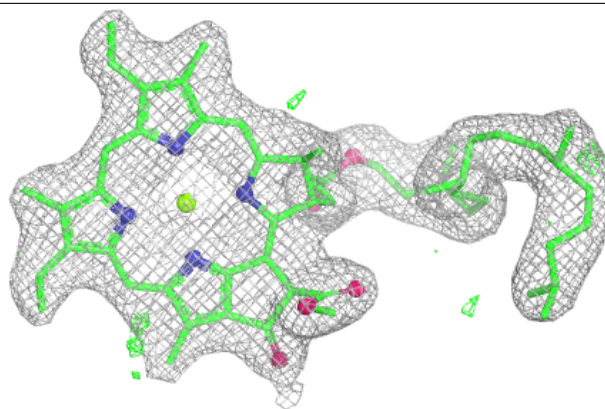
Electron density around CLA b 610:

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

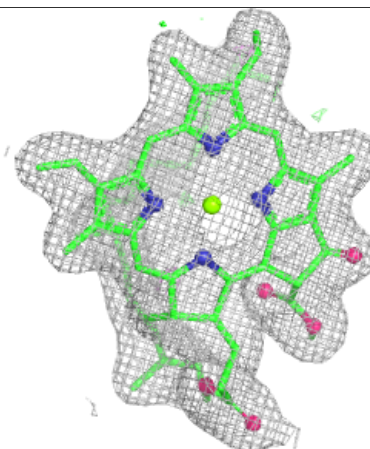
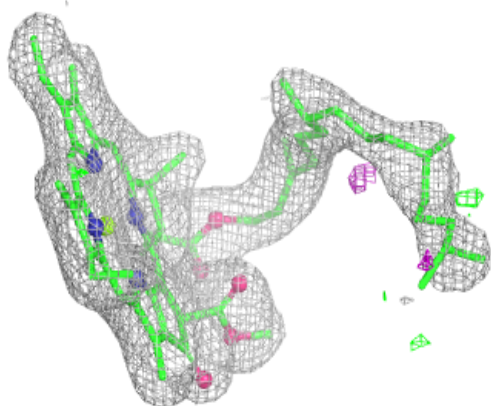
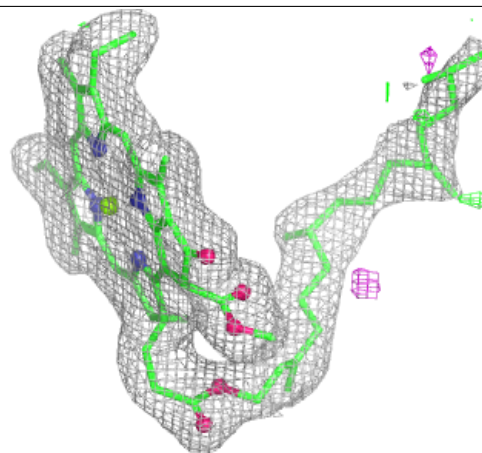


Electron density around CLA b 611:

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

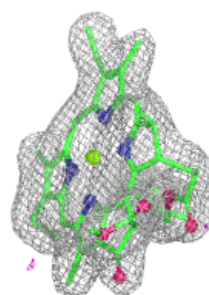
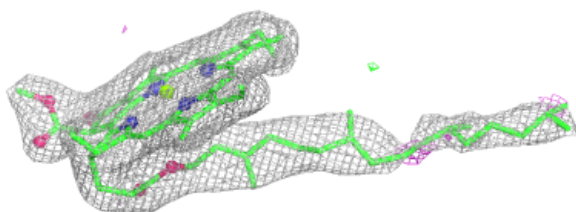
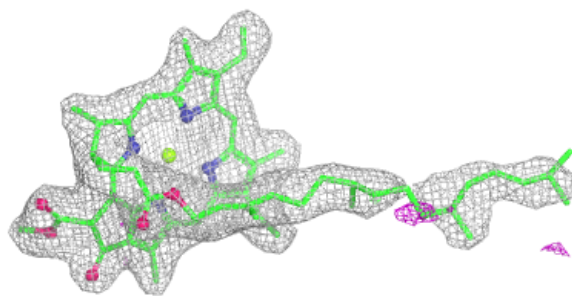
**Electron density around CLA b 612:**

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

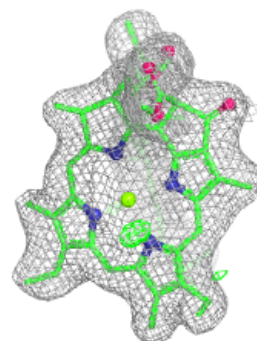
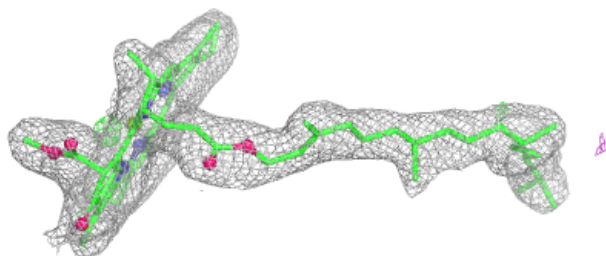
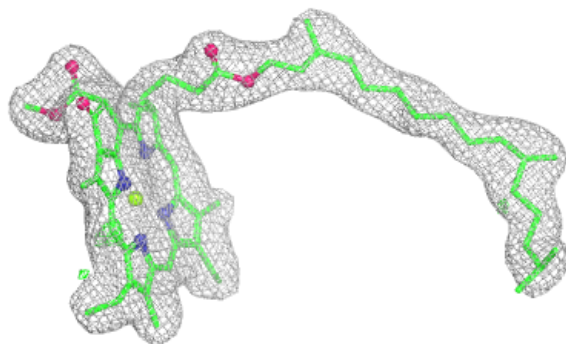


Electron density around CLA b 613:

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

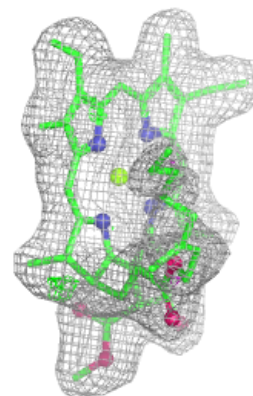
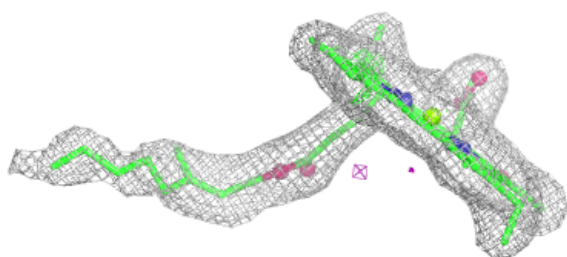
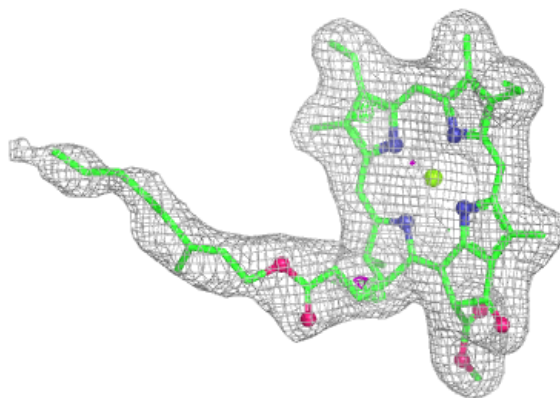
**Electron density around CLA B 608:**

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

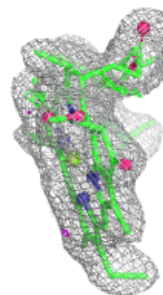
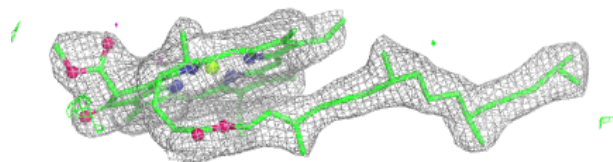
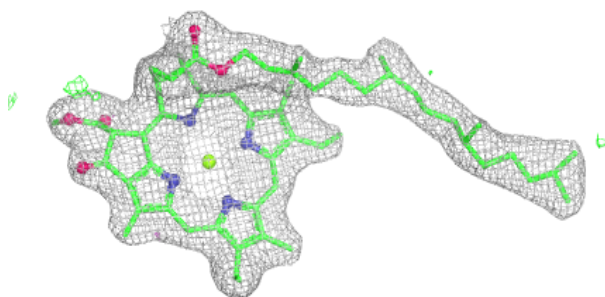


Electron density around CLA A 610:

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

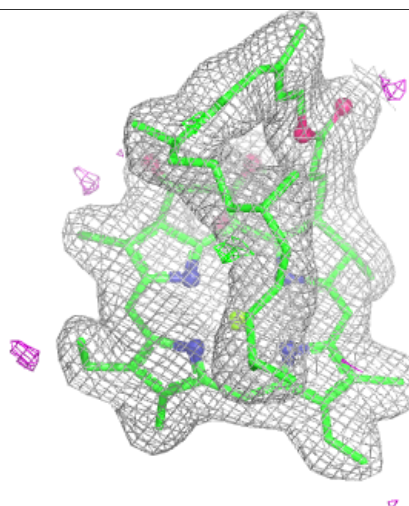
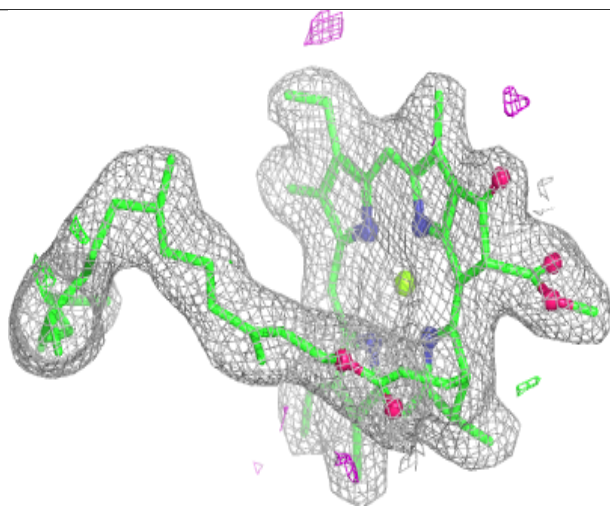
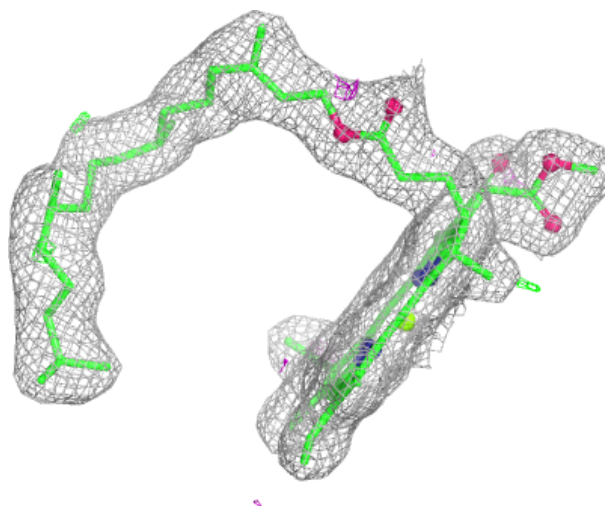
**Electron density around CLA c 501:**

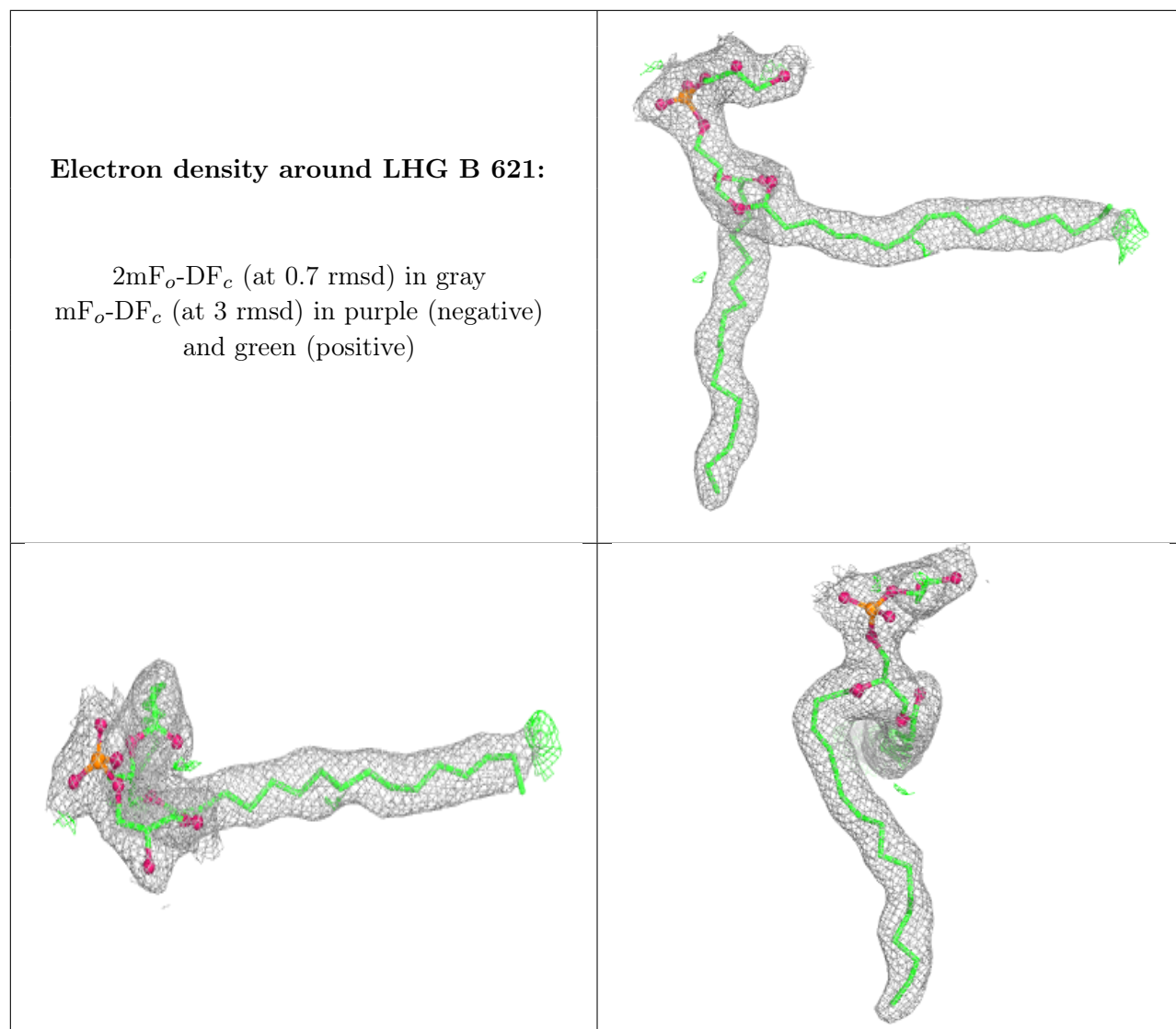
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 610:

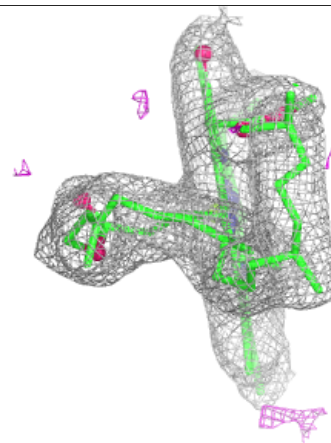
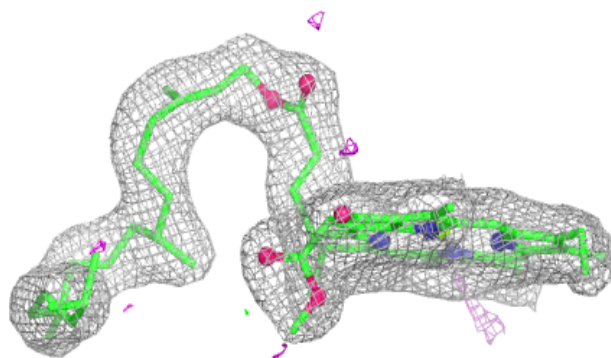
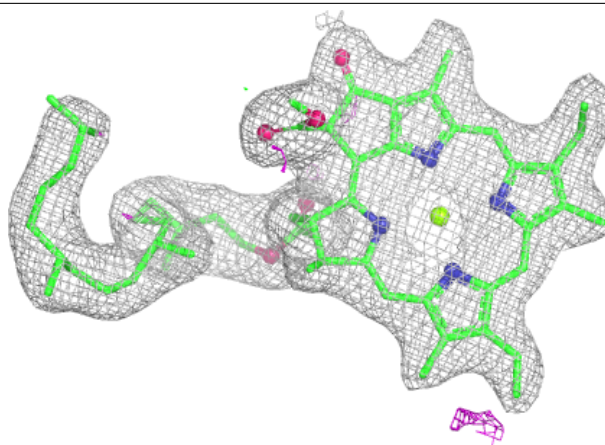
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



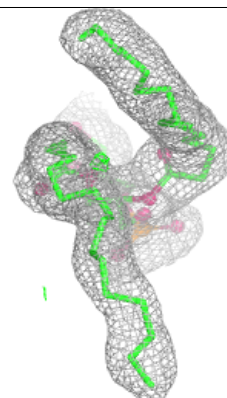
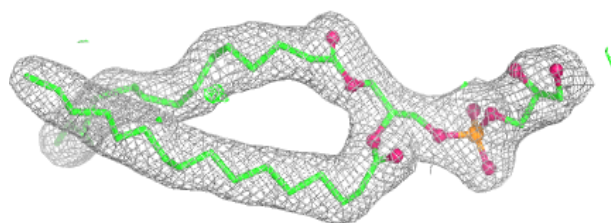
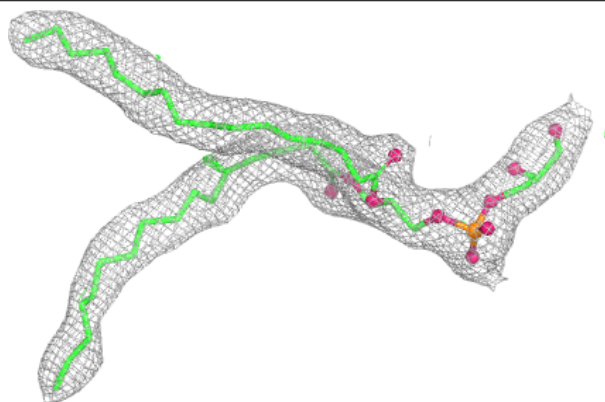


Electron density around CLA B 611:

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

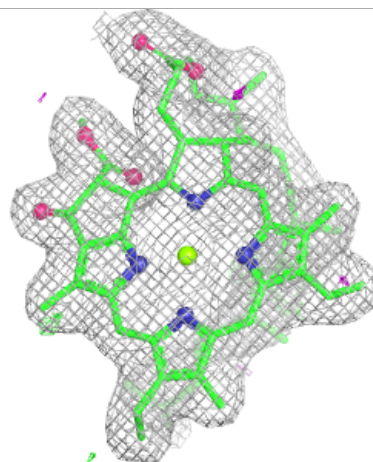
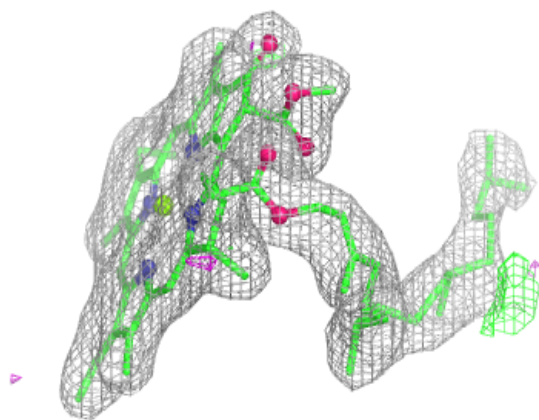
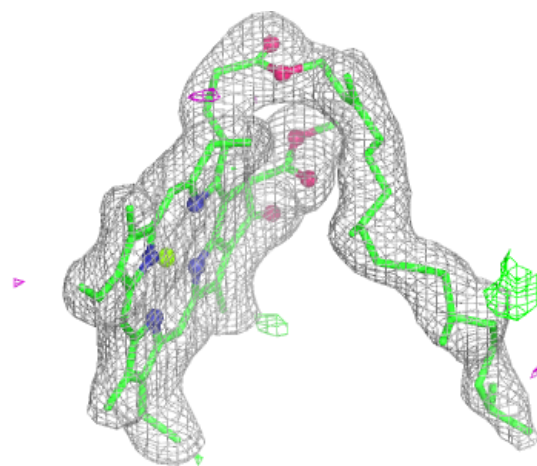
**Electron density around LHG D 407:**

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



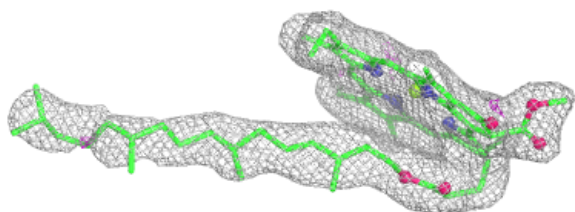
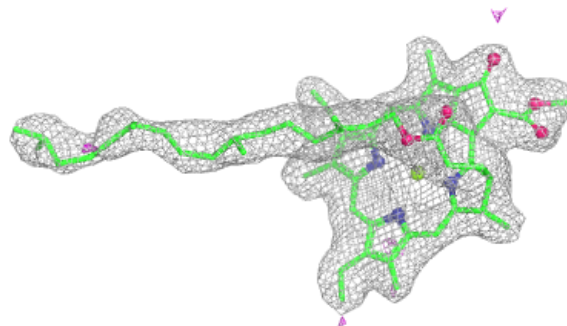
Electron density around CLA B 612:

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

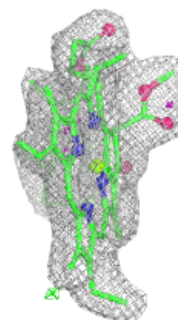
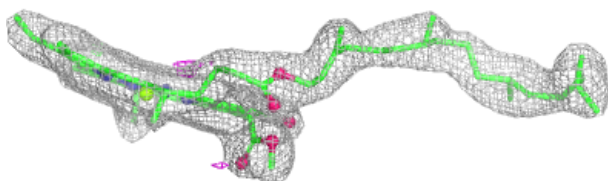
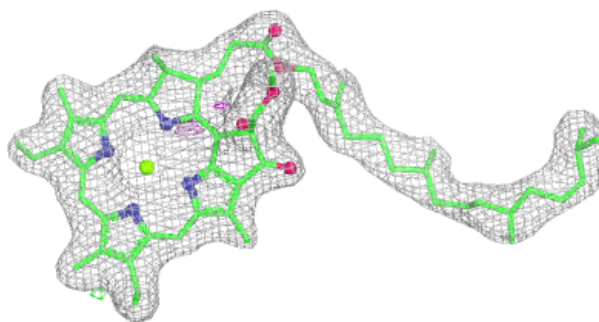


Electron density around CLA B 613:

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

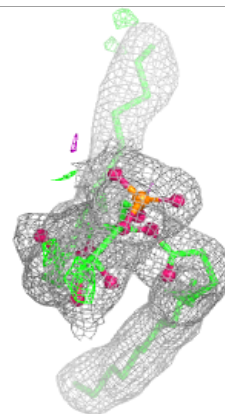
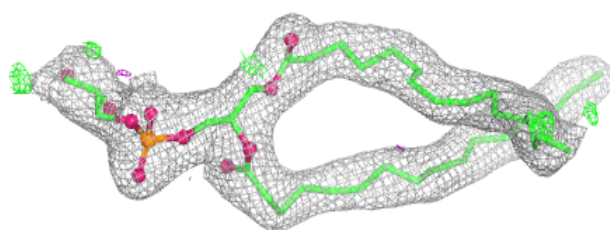
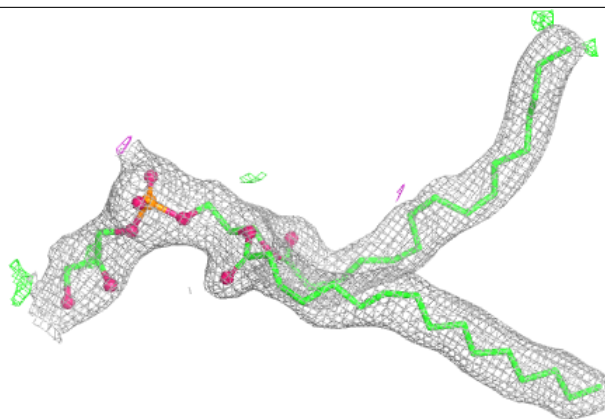
**Electron density around CLA B 601:**

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

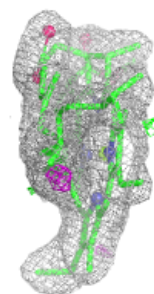
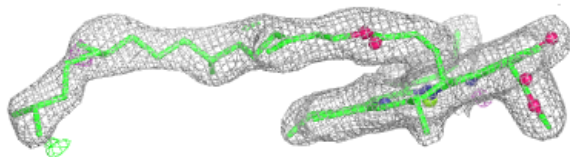
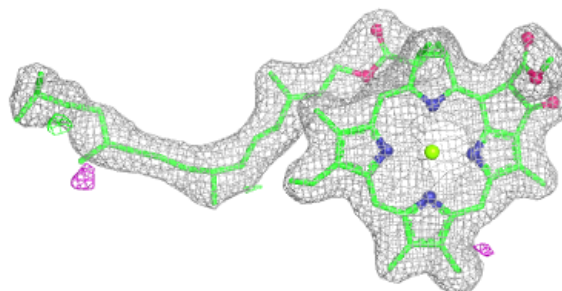


Electron density around LHG d 407:

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

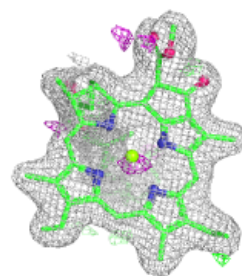
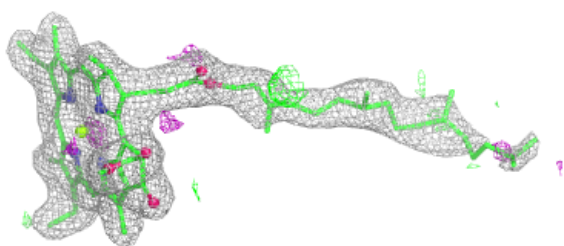
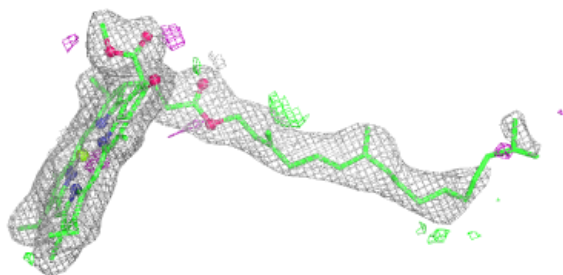
**Electron density around CLA B 602:**

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

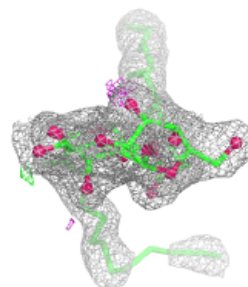
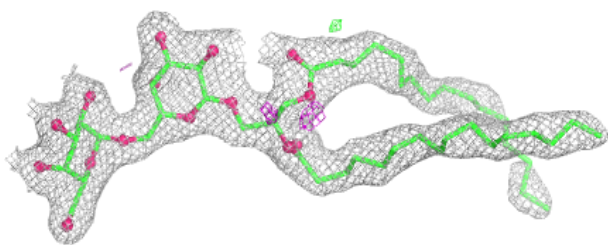
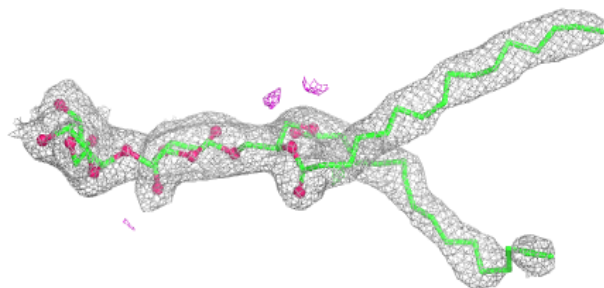


Electron density around CLA B 603:

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

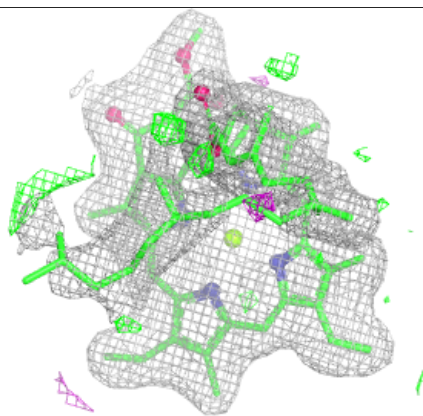
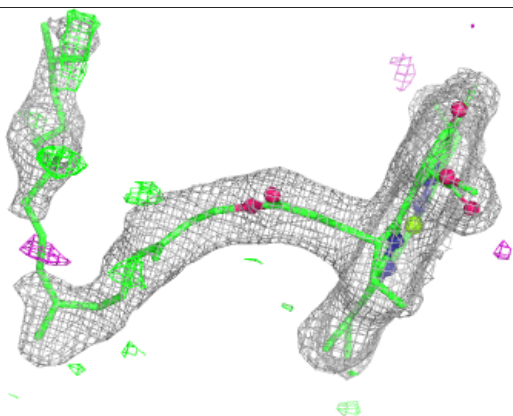
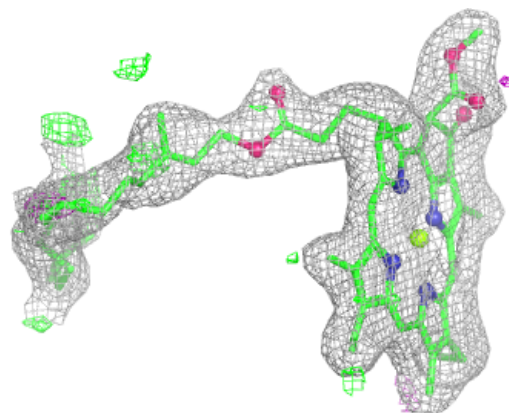
**Electron density around DGD c 517:**

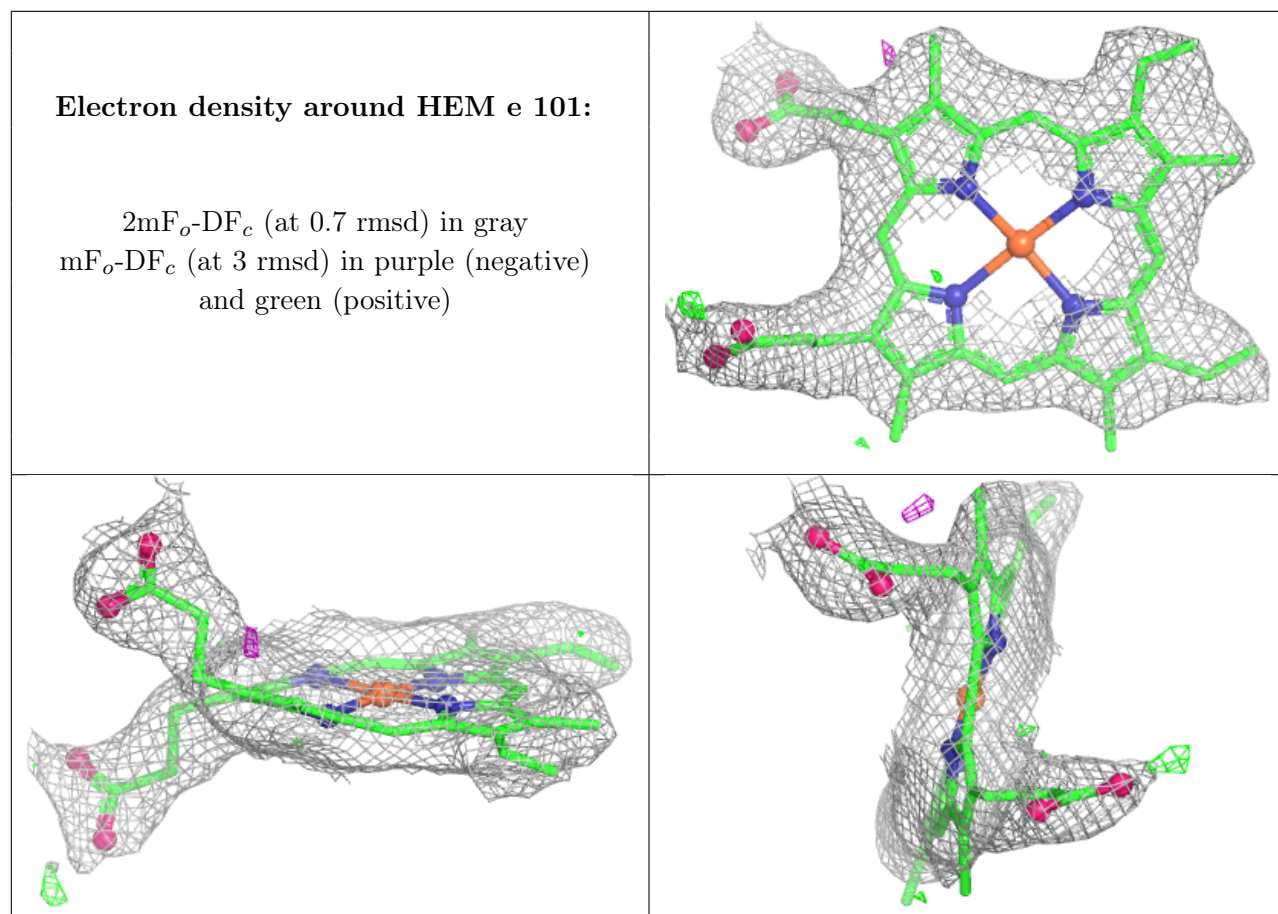
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA a 610:

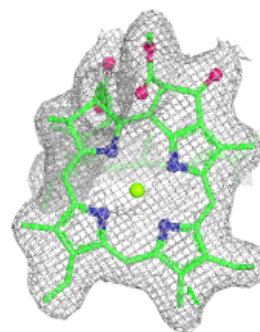
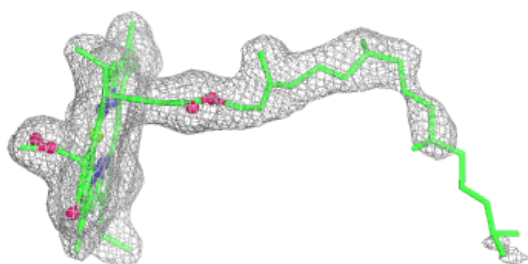
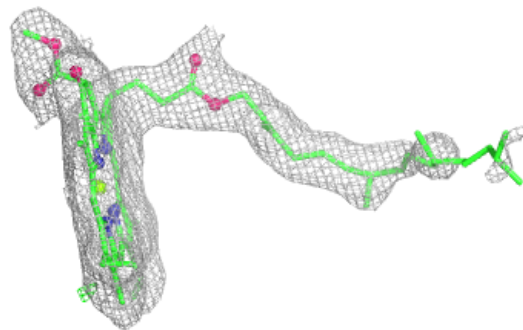
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



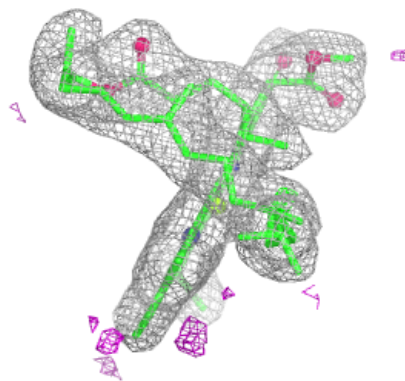
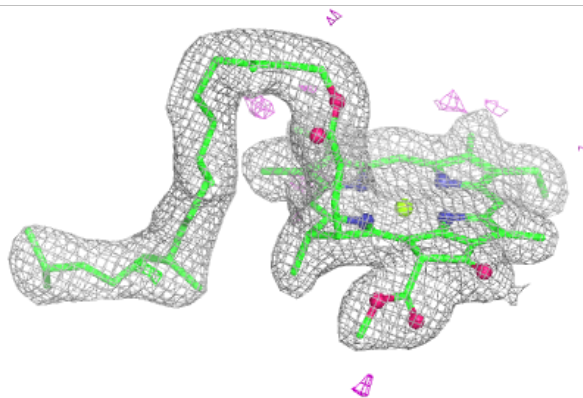
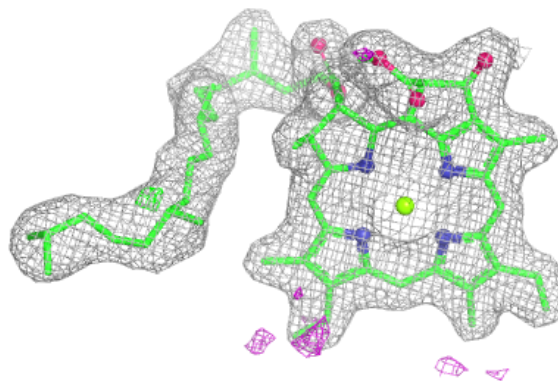


Electron density around CLA D 403:

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

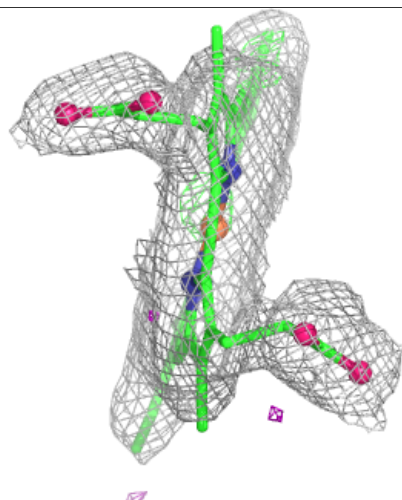
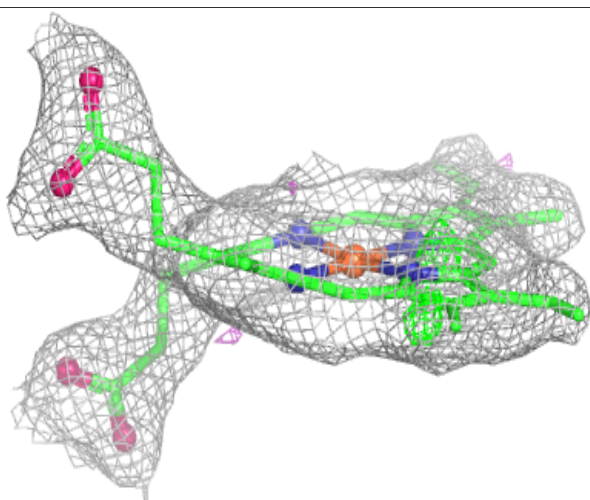
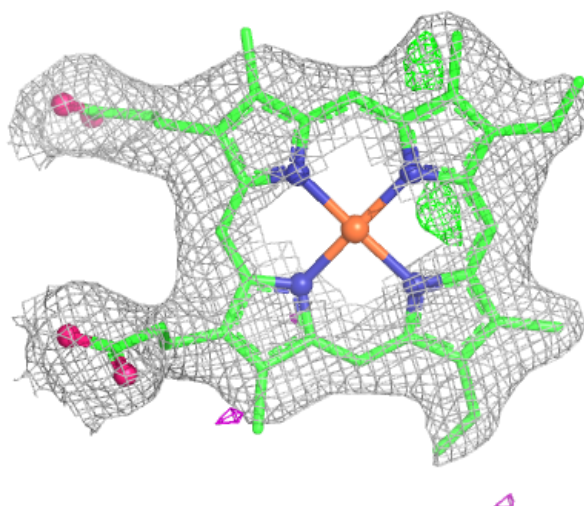
**Electron density around CLA A 613:**

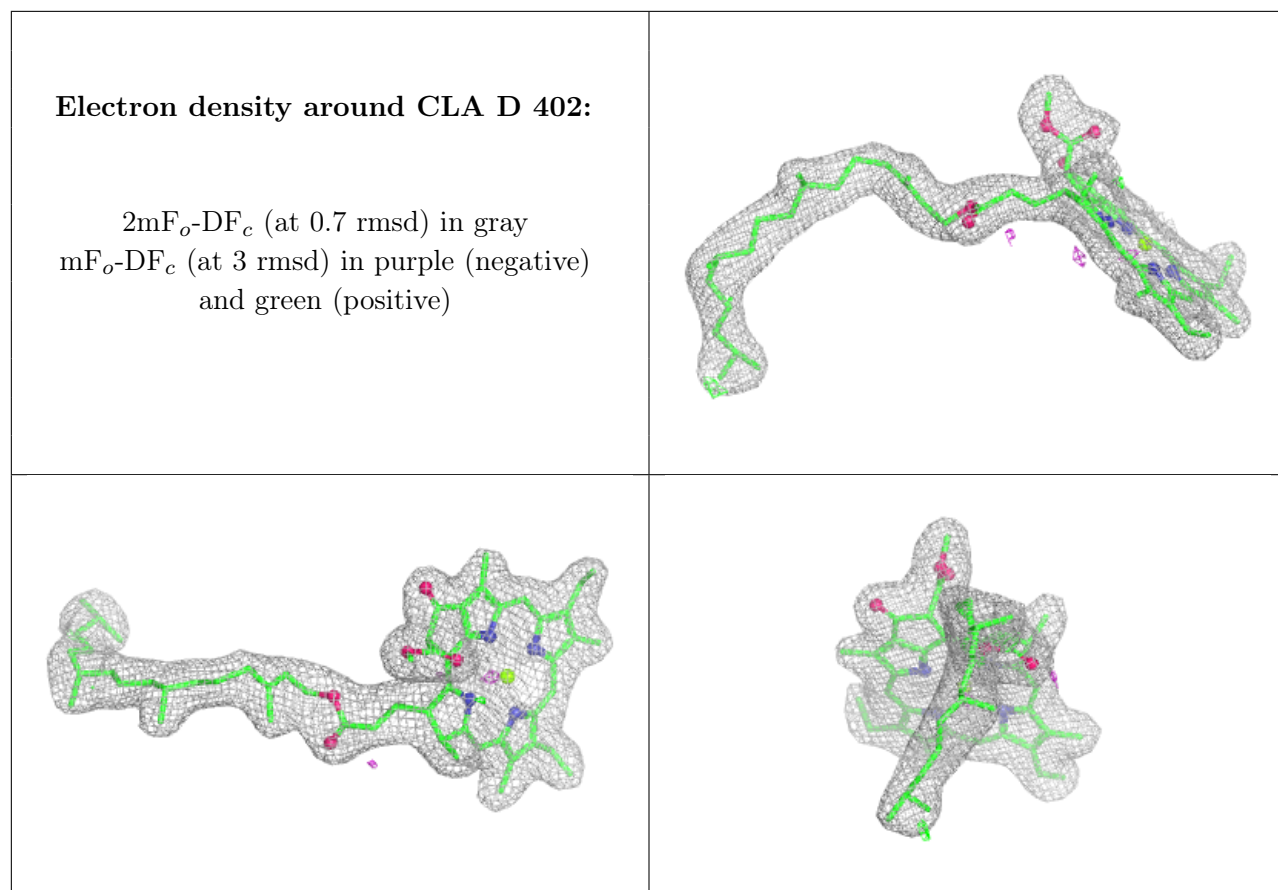
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM F 101:

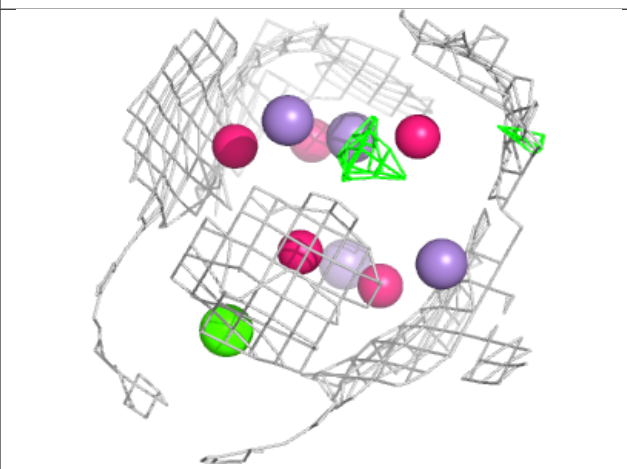
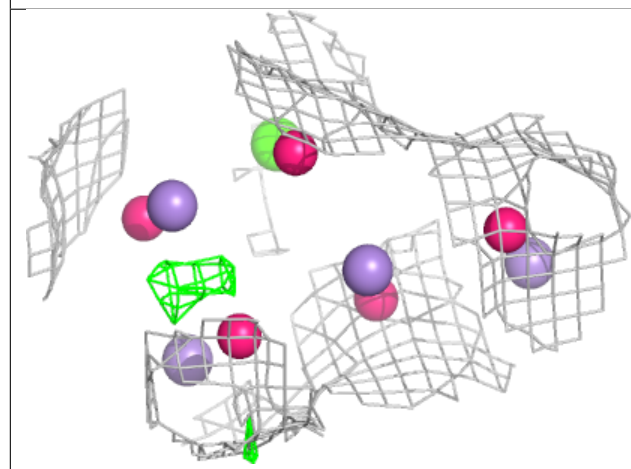
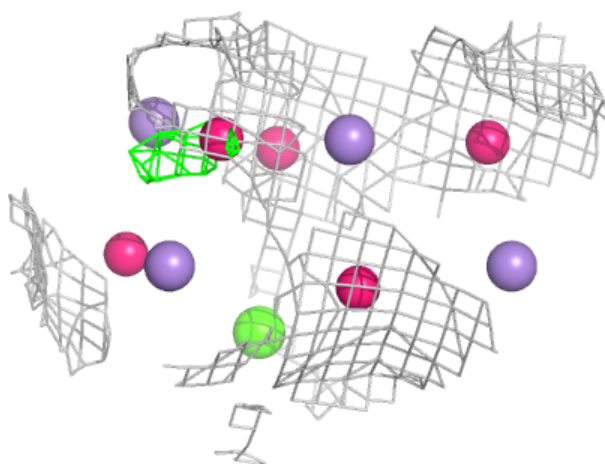
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





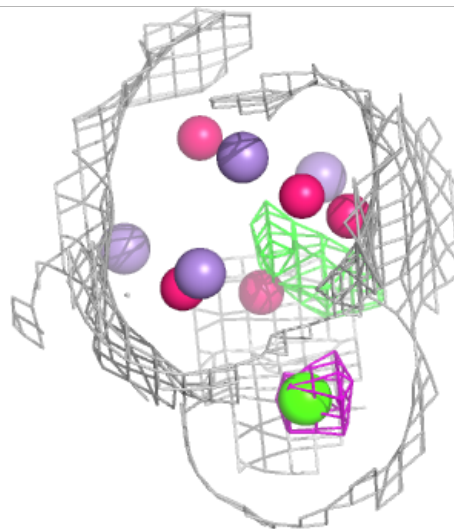
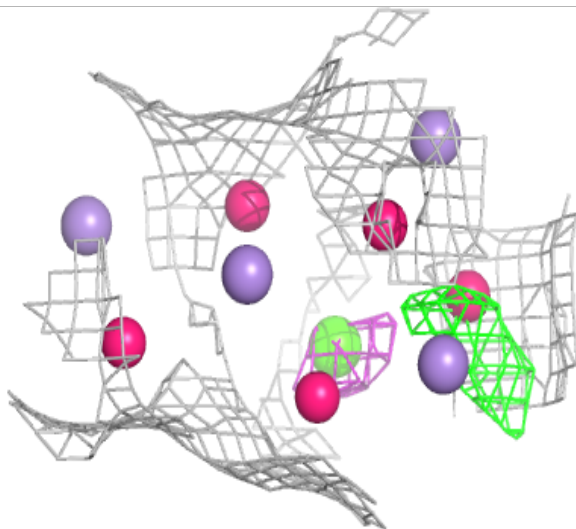
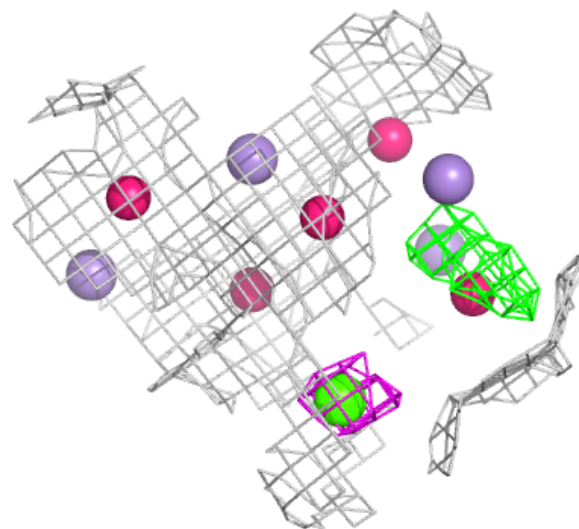
Electron density around OEX a 602 (A):

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



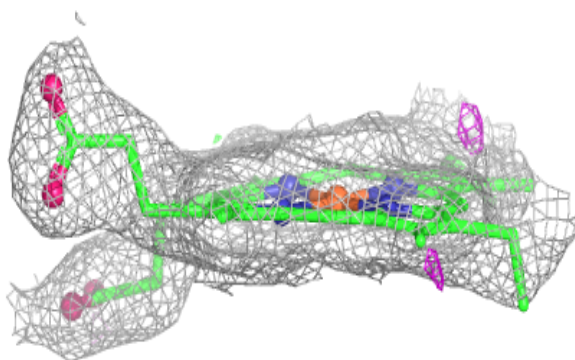
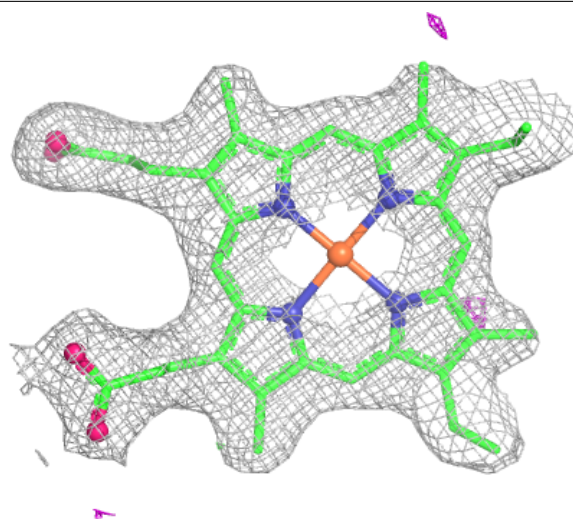
Electron density around OEX A 602 (A):

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



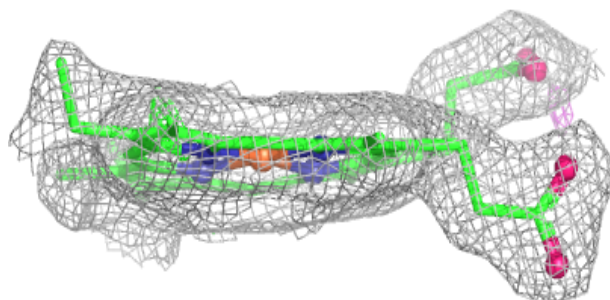
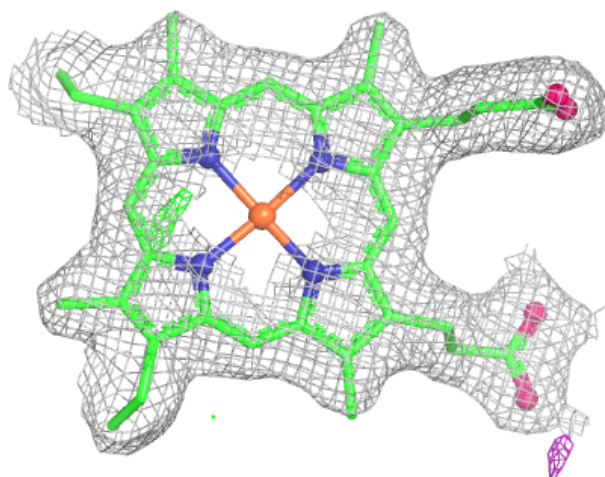
Electron density around HEC V 201:

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



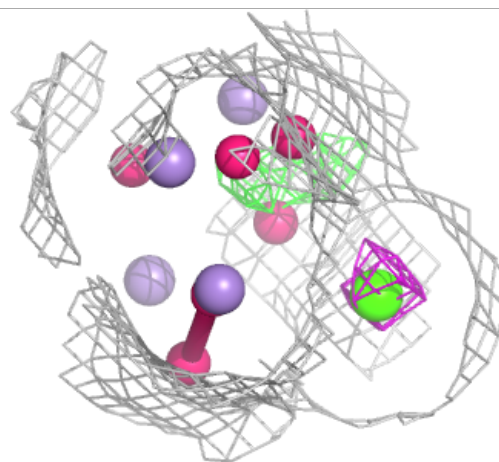
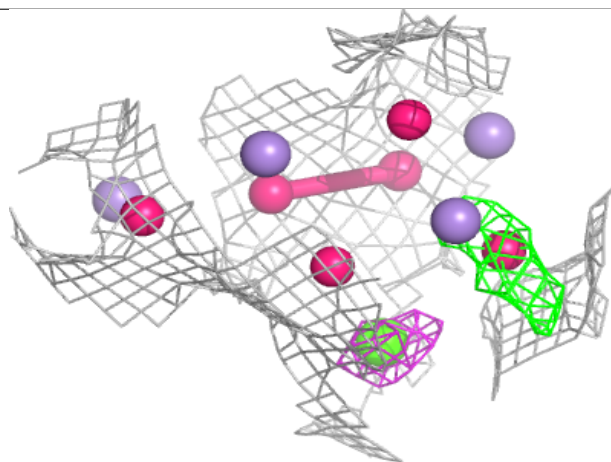
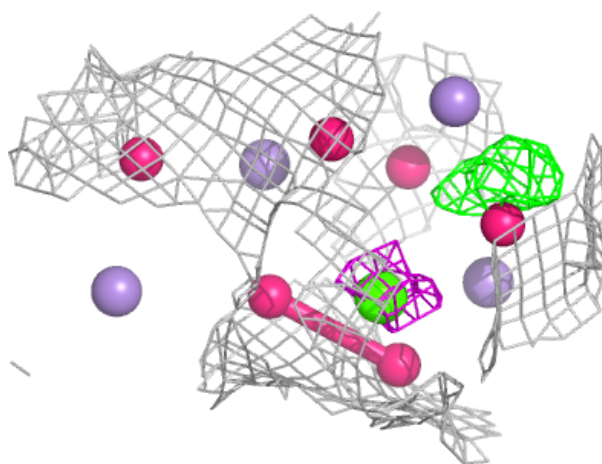
Electron density around HEC v 201:

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



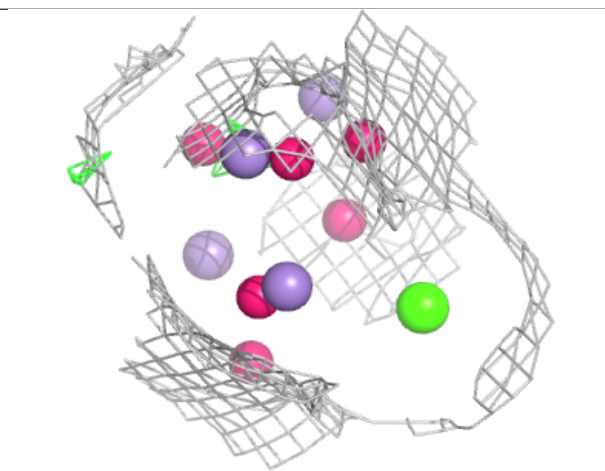
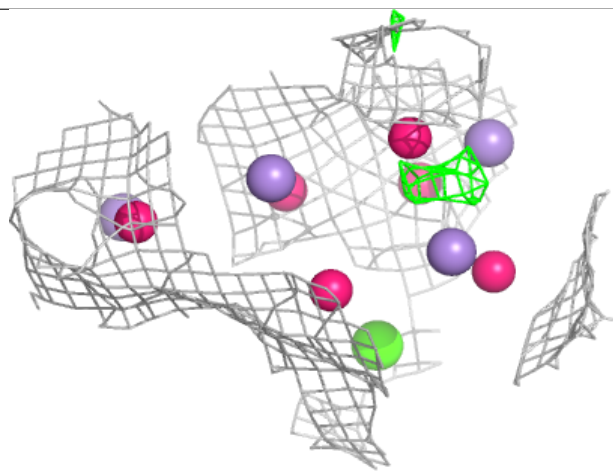
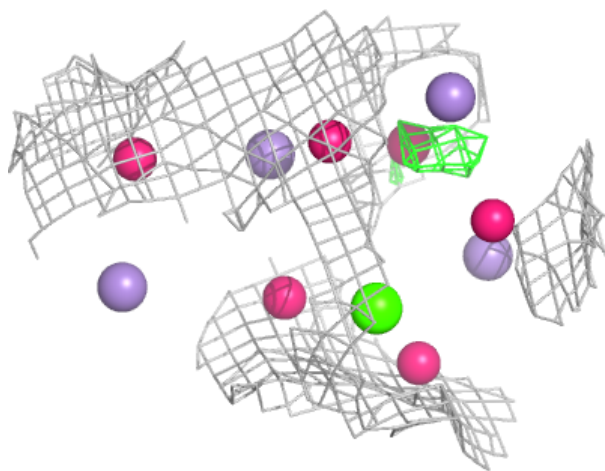
Electron density around OEY A 601 (C):

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



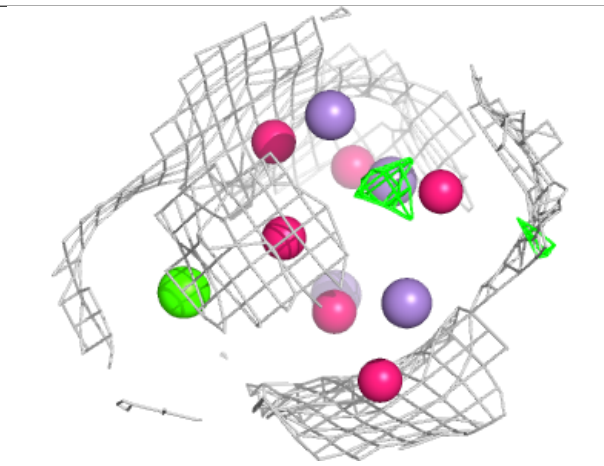
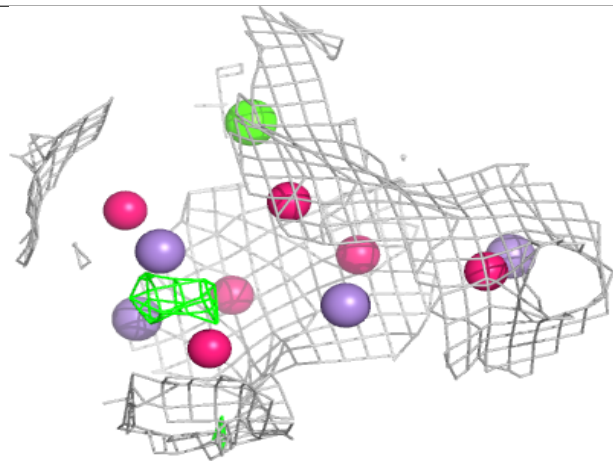
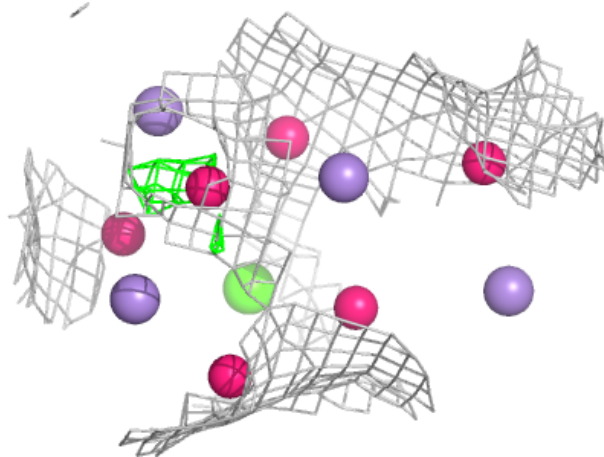
Electron density around OEY a 601 (B):

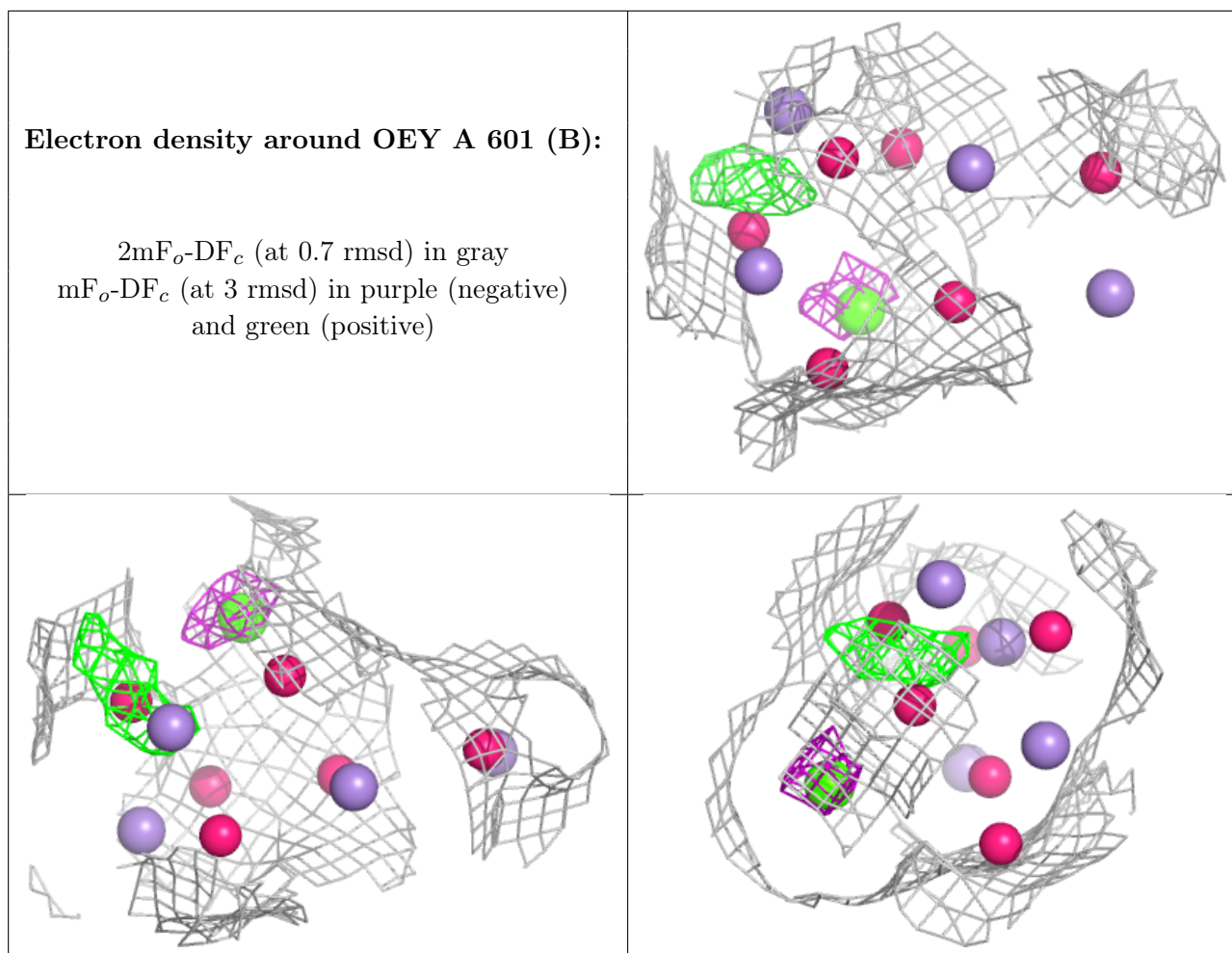
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEY a 601 (C):

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





6.5 Other polymers [i](#)

There are no such residues in this entry.