



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:58 AM UTC

PDB ID : 8EZ5 / pdb_00008ez5
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) 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 : 2022-10-31
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

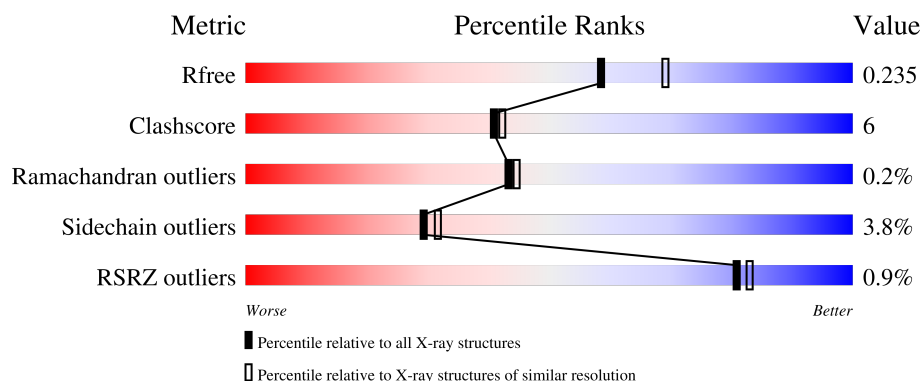
1 Overall quality at a glance

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)

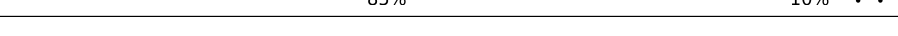
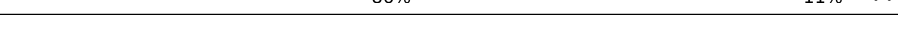
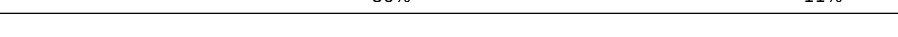
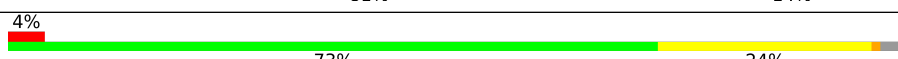
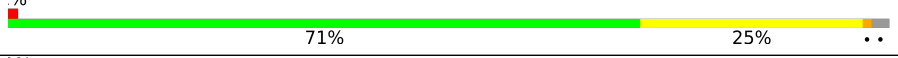
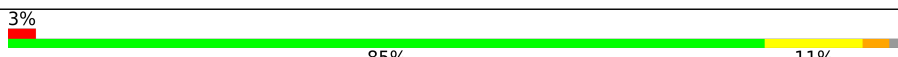
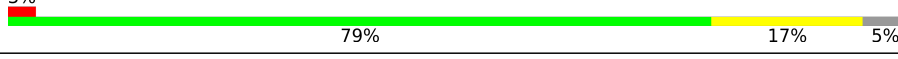
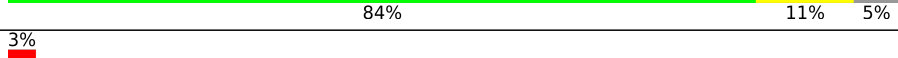
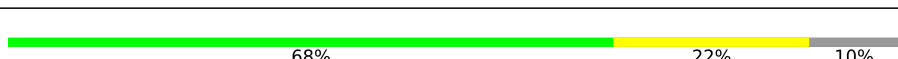
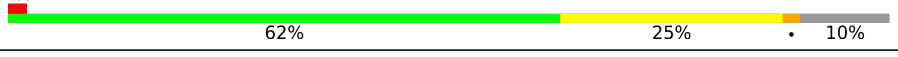
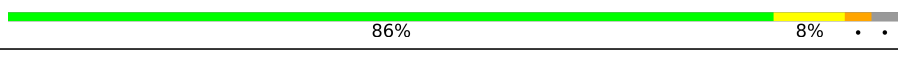
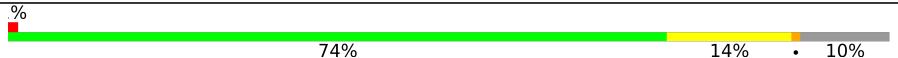
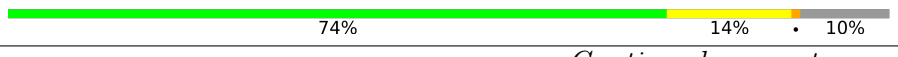
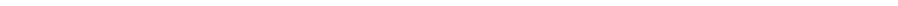
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	

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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	609	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	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	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	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
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25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 53041 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
1	A	334	Total	C	N	O	S	0	64	0
			3113	2030	513	551	19			
1	a	334	Total	C	N	O	S	0	64	0
			3110	2027	513	551	19			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3509	2302	586	607	14			
3	c	451	Total	C	N	O	S	0	12	0
			3583	2343	602	624	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2731	1809	446	464	12			
4	d	341	Total	C	N	O	S	0	3	0
			2737	1813	446	466	12			

- 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
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	32	Total	C	N	O	S	0	0	0
			251	168	36	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	1	0
			1870	1168	313	385	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			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		0	0	0
			281	188	45	48				
18	x	39	Total	C	N	O		0	0	0
			286	191	46	49				

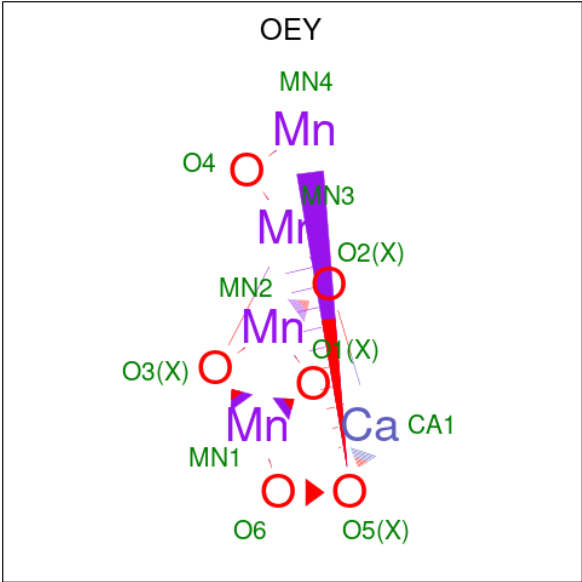
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

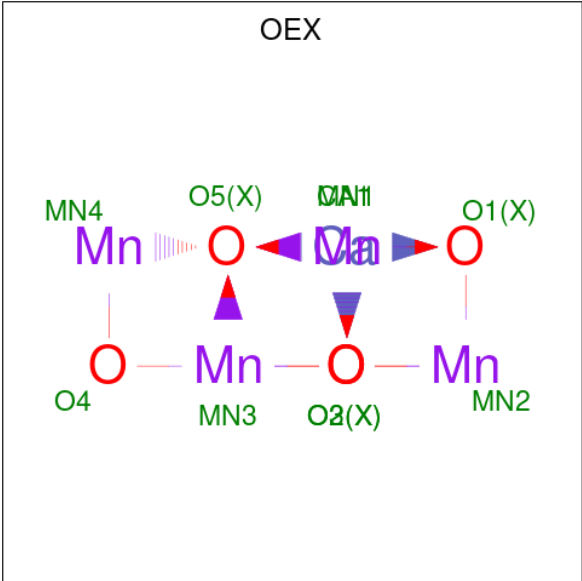
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

- 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
21	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
21	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- 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
22	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

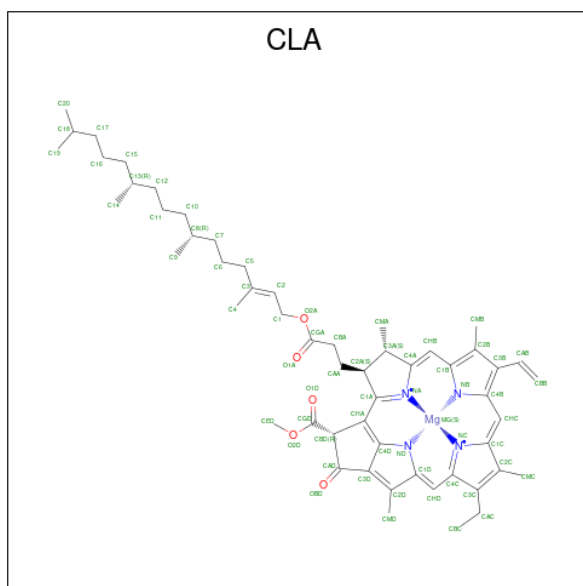
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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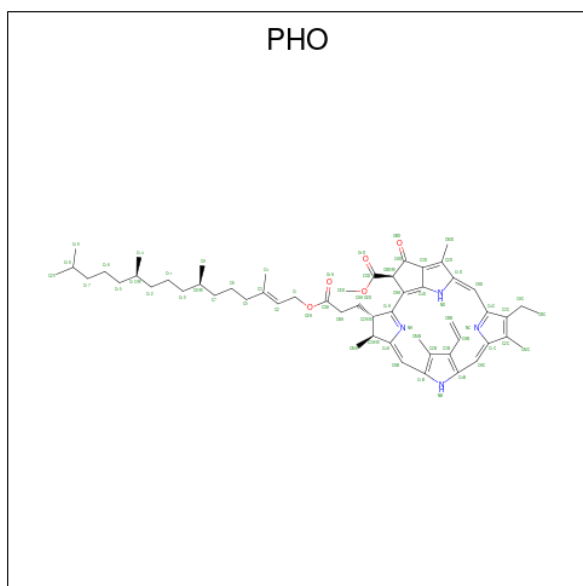
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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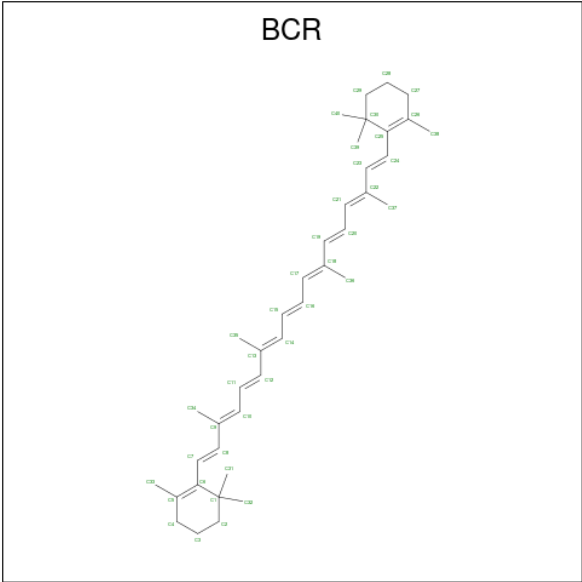
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (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	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



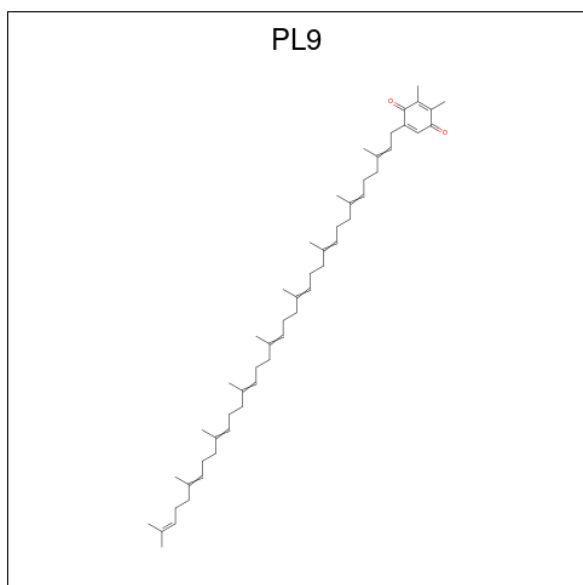
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total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

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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).



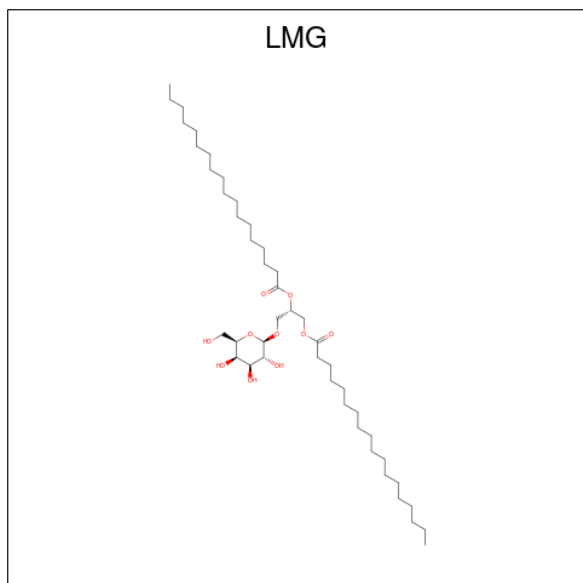
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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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-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



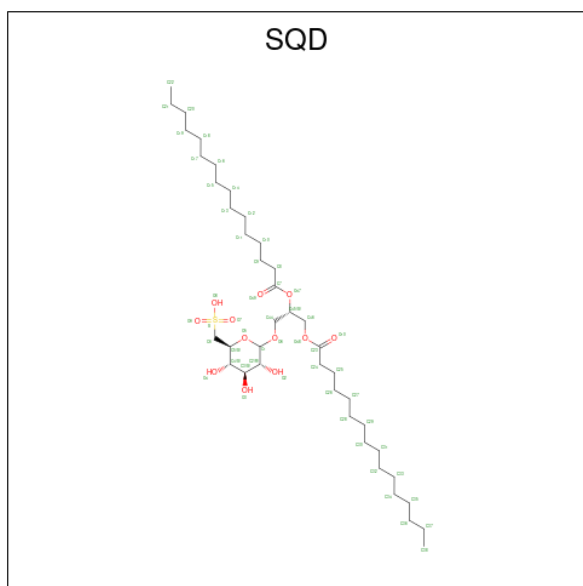
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C	O	0	0
			37	27	10		
29	c	1	Total	C	O	0	0
			48	38	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			49	39	10		
29	d	1	Total	C	O	0	0
			23	21	2		
29	d	1	Total	C	O	0	0
			44	34	10		
29	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



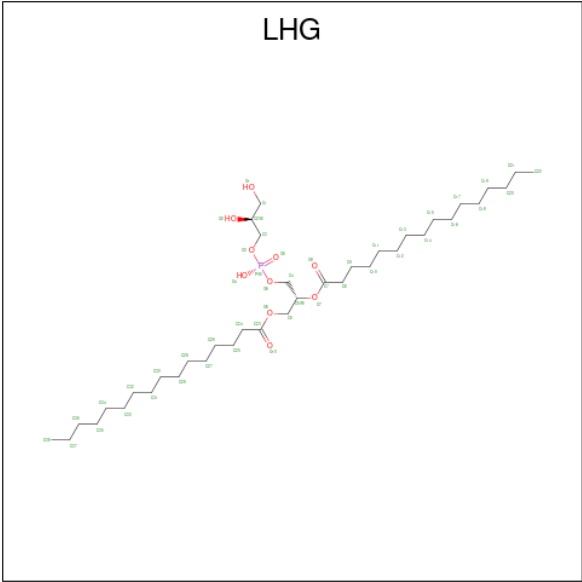
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	F	1	Total	C	O	S	0	0
			36	25	10	1		
30	L	1	Total	C	O	S	0	0
			49	36	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36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

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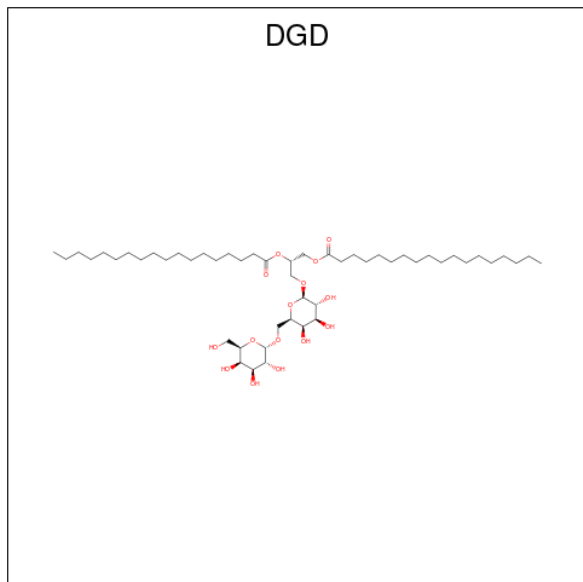
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



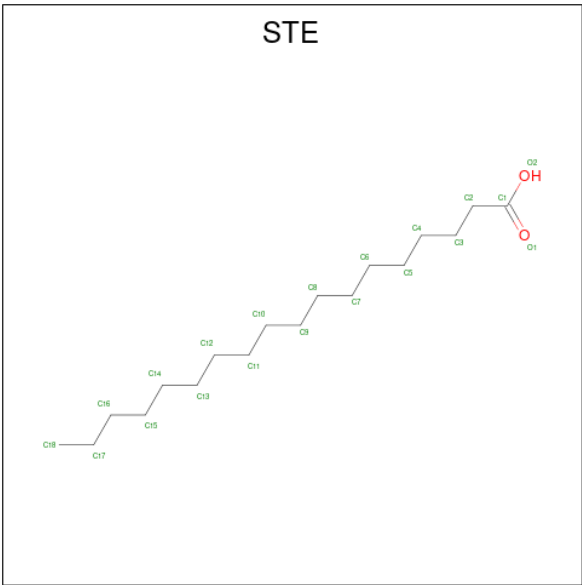
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			47	36	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



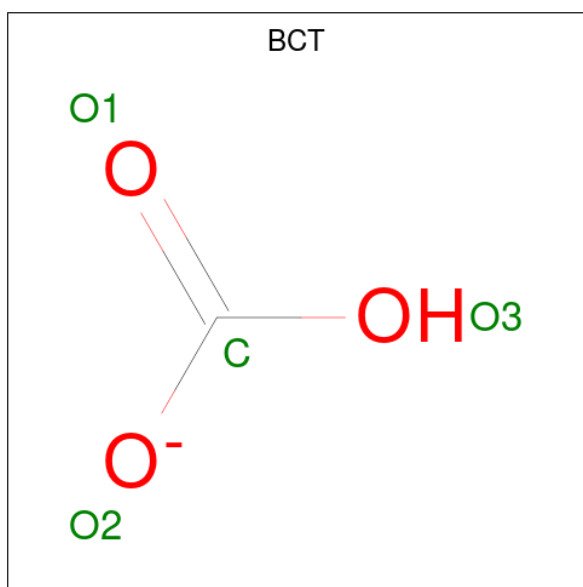
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			17	15	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C	O	0	0
			18	16	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C		0	0
			16	16			
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C		0	0
	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

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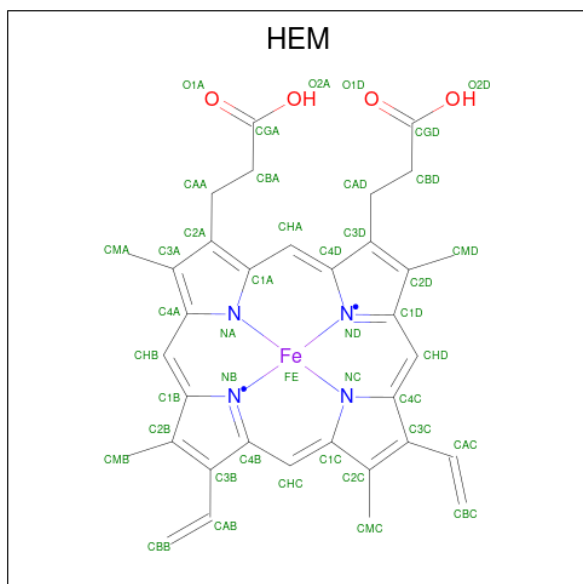
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	M	1	Total C 10 10	0	0
33	T	1	Total C 16 16	0	0
33	T	1	Total C 15 15	0	0
33	a	1	Total C 10 10	0	0
33	a	1	Total C O 12 10 2	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 10 10	0	0
33	c	1	Total C O 20 18 2	0	0
33	c	1	Total C O 12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

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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



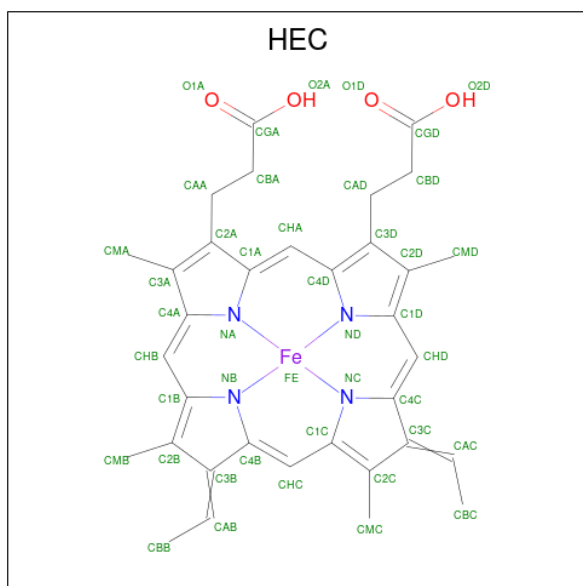
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	f	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	119	Total	O	0	4
			123	123		
37	B	197	Total	O	0	0
			197	197		
37	C	142	Total	O	0	0
			142	142		
37	D	106	Total	O	0	0
			106	106		
37	E	29	Total	O	0	0
			29	29		
37	F	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	27	Total 27	O 27	0	0
37	I	13	Total 13	O 13	0	0
37	J	12	Total 12	O 12	0	0
37	K	2	Total 2	O 2	0	0
37	L	9	Total 9	O 9	0	0
37	M	5	Total 5	O 5	0	0
37	O	73	Total 73	O 73	0	0
37	T	9	Total 9	O 9	0	0
37	U	29	Total 29	O 29	0	0
37	V	51	Total 51	O 51	0	0
37	Y	1	Total 1	O 1	0	0
37	X	8	Total 8	O 8	0	0
37	Z	3	Total 3	O 3	0	0
37	R	6	Total 6	O 6	0	0
37	a	100	Total 104	O 104	0	4
37	b	163	Total 163	O 163	0	0
37	c	160	Total 160	O 160	0	0
37	d	95	Total 95	O 95	0	0
37	e	13	Total 13	O 13	0	0
37	f	3	Total 3	O 3	0	0
37	h	20	Total 20	O 20	0	0

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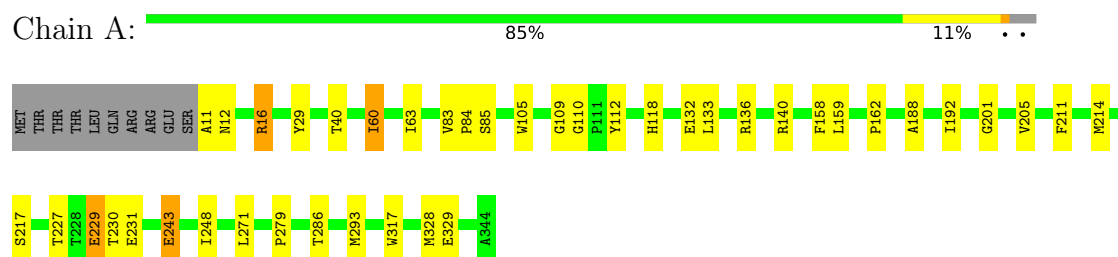
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	17	Total 17	O 17	0	0
37	j	5	Total 5	O 5	0	0
37	k	1	Total 1	O 1	0	0
37	l	12	Total 12	O 12	0	0
37	m	8	Total 8	O 8	0	0
37	o	72	Total 72	O 72	0	0
37	t	6	Total 6	O 6	0	0
37	u	50	Total 50	O 50	0	0
37	v	42	Total 42	O 42	0	0
37	x	5	Total 5	O 5	0	0
37	z	3	Total 3	O 3	0	0
37	r	7	Total 7	O 7	0	0

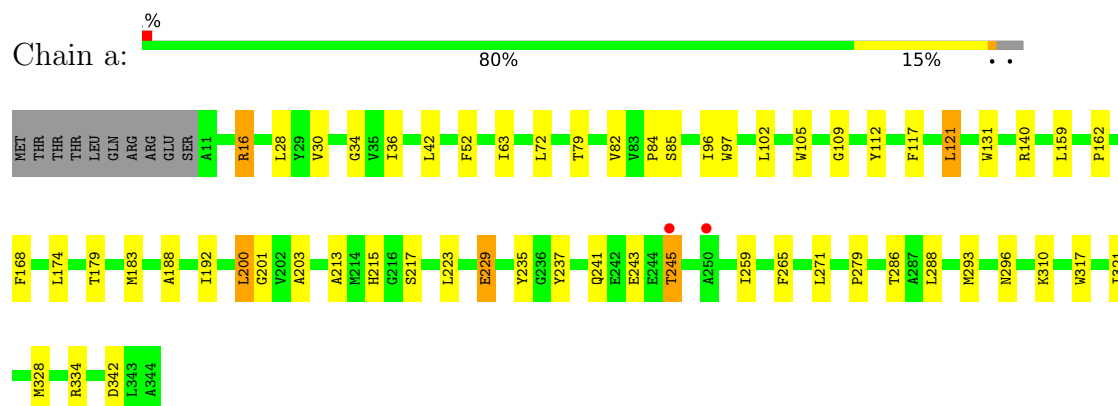
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

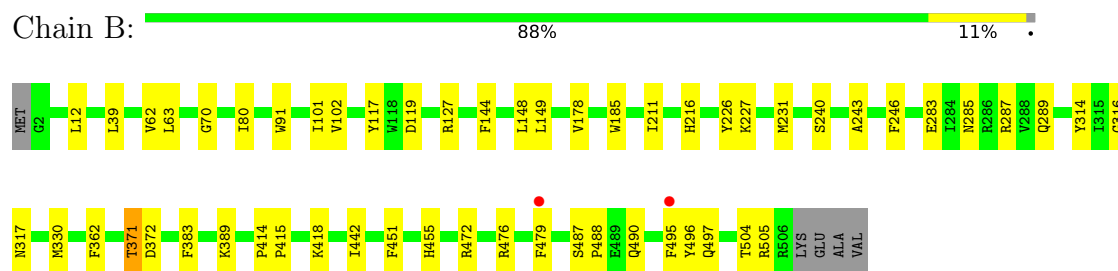
- Molecule 1: Photosystem II protein D1 1



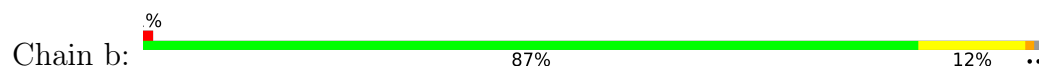
- Molecule 1: Photosystem II protein D1 1



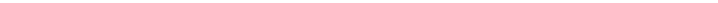
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  85% 10% . .

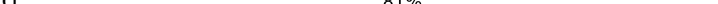
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 86% 11% ..

- Molecule 4: Photosystem II D2 protein

Chain D: 86% 11% .

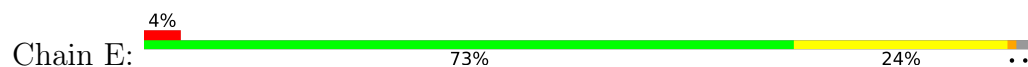
- Molecule 4: Photosystem II D2 protein

Chain d:  81% 14% ..

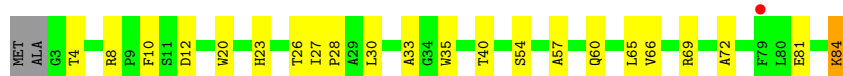




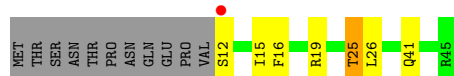
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



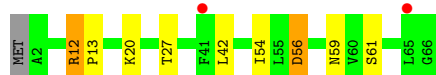
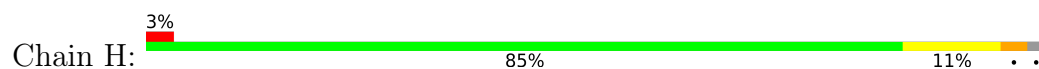
- Molecule 6: Cytochrome b559 subunit beta



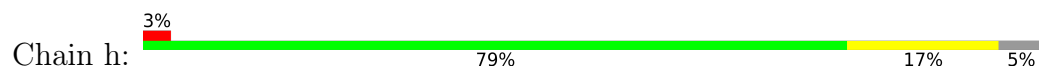
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



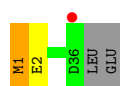
- Molecule 8: Photosystem II reaction center protein I

Chain I:  84% 11% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  89% 3% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  68% 22% 10%



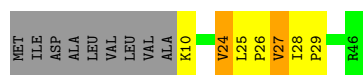
- Molecule 9: Photosystem II reaction center protein J

Chain j:  62% 25% 2% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  65% 11% 20%



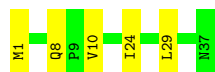
- Molecule 10: Photosystem II reaction center protein K

Chain k:  59% 22% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 8% . .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  69% 22% 8%



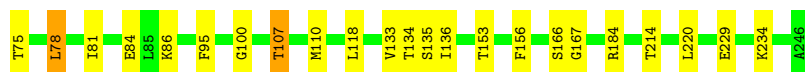
- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 11% 6% 11%



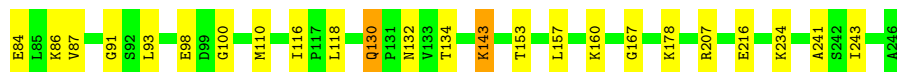
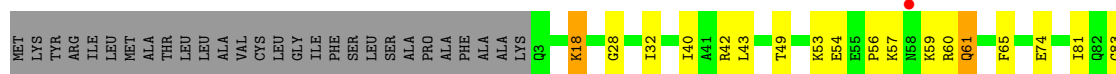
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  74% 14% . 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  74% 14% . 10%

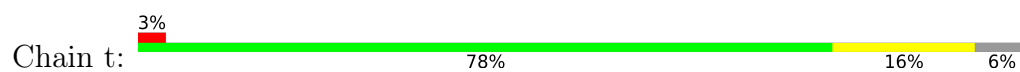


- Molecule 14: Photosystem II reaction center protein T

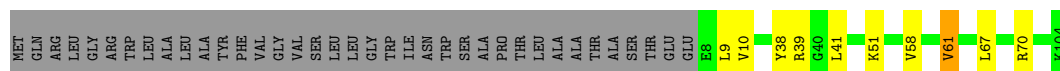
Chain T:  75% 19% 6% 3%



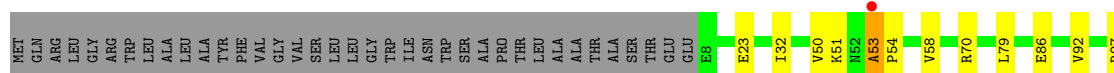
- Molecule 14: Photosystem II reaction center protein T



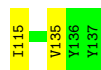
- Molecule 15: Photosystem II 12 kDa extrinsic protein



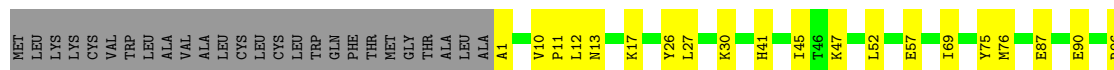
- Molecule 15: Photosystem II 12 kDa extrinsic protein



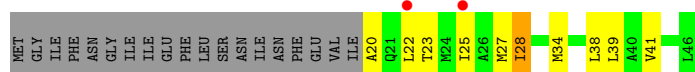
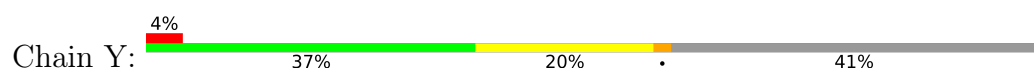
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

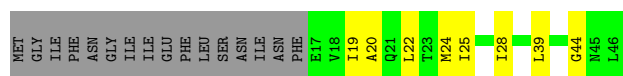


- Molecule 17: Photosystem II reaction center protein Ycf12



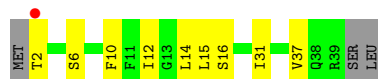
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  48% 17% 35%



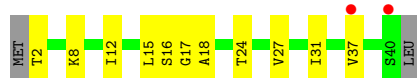
- Molecule 18: Photosystem II reaction center X protein

Chain X:  2% 71% 22% 7%



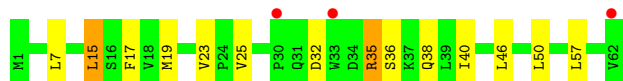
- Molecule 18: Photosystem II reaction center X protein

Chain x:  5% 68% 27% 5%



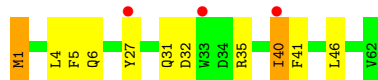
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  5% 77% 19% 5%



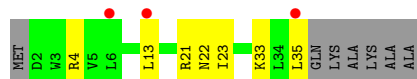
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  5% 82% 15% 5%



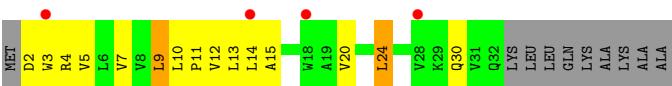
- Molecule 20: Photosystem II protein Y

Chain R:  7% 66% 17% 17%



- Molecule 20: Photosystem II protein Y

Chain r:  10% 39% 32% 5% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.65-2.09) 85.3 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.51 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.234 0.186 , 0.235	Depositor DCC
R_{free} test set	4165 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53041	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0/3212	0.50	0/4376
1	a	0.29	0/3209	0.47	0/4372
2	B	0.32	0/4155	0.49	0/5661
2	b	0.31	0/4118	0.48	0/5611
3	C	0.31	0/3625	0.47	0/4935
3	c	0.29	0/3705	0.45	0/5042
4	D	0.34	0/2825	0.50	0/3847
4	d	0.32	0/2834	0.51	0/3859
5	E	0.27	0/688	0.43	0/940
5	e	0.24	0/683	0.41	0/932
6	F	0.27	0/284	0.39	0/387
6	f	0.25	0/284	0.51	0/387
7	H	0.33	0/523	0.49	0/713
7	h	0.30	0/511	0.46	0/697
8	I	0.28	0/293	0.48	0/396
8	i	0.34	0/293	0.45	0/396
9	J	0.27	0/263	0.42	0/356
9	j	0.23	0/263	0.40	0/356
10	K	0.29	0/303	0.45	0/416
10	k	0.26	0/303	0.44	0/416
11	L	0.31	0/311	0.49	0/422
11	l	0.33	0/303	0.49	0/412
12	M	0.33	0/249	0.50	0/341
12	m	0.35	0/244	0.52	0/334
13	O	0.31	0/1904	0.50	0/2585
13	o	0.32	0/1905	0.50	0/2583
14	T	0.34	0/257	0.55	0/349
14	t	0.31	0/255	0.54	0/346
15	U	0.27	0/785	0.47	0/1064
15	u	0.30	0/785	0.48	0/1064
16	V	0.31	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.29	0/1085	0.45	0/1473
17	Y	0.21	0/197	0.36	0/264
17	y	0.20	0/219	0.39	0/294
18	X	0.26	0/284	0.39	0/384
18	x	0.23	0/289	0.32	0/391
19	Z	0.22	0/490	0.44	0/669
19	z	0.18	0/488	0.33	0/666
20	R	0.29	0/277	0.50	0/380
20	r	0.25	0/252	0.37	0/347
All	All	0.30	0/44038	0.48	0/59936

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	3113	0	2981	27	0
1	a	3110	0	2972	48	0
2	B	4005	0	3871	35	0
2	b	3978	0	3836	44	0
3	C	3509	0	3426	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	42	0
4	D	2731	0	2637	29	0
4	d	2737	0	2643	43	0
5	E	666	0	651	14	0
5	e	664	0	648	19	0
6	F	275	0	282	7	0
6	f	275	0	282	11	0
7	H	510	0	532	6	0
7	h	498	0	518	11	0
8	I	296	0	311	1	0
8	i	296	0	311	1	0
9	J	257	0	268	9	0
9	j	257	0	268	9	0
10	K	293	0	305	5	0
10	k	293	0	305	6	0
11	L	304	0	316	5	0
11	l	296	0	304	3	0
12	M	256	0	269	6	0
12	m	251	0	267	5	0
13	O	1870	0	1830	28	0
13	o	1874	0	1846	22	0
14	T	258	0	261	5	0
14	t	256	0	256	3	0
15	U	774	0	773	4	0
15	u	774	0	773	8	0
16	V	1064	0	1073	12	0
16	v	1064	0	1073	18	0
17	Y	196	0	217	8	0
17	y	218	0	241	4	0
18	X	281	0	312	8	0
18	x	286	0	314	10	0
19	Z	479	0	516	6	0
19	z	477	0	509	6	0
20	R	271	0	298	2	0
20	r	246	0	263	9	0
21	A	11	0	0	1	0
21	a	11	0	0	0	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	184	0	192	4	0
25	B	1035	0	1139	37	0
25	C	839	0	922	25	0
25	D	195	0	216	5	0
25	a	260	0	288	8	0
25	b	1035	0	1139	38	0
25	c	839	0	919	33	0
25	d	130	0	144	5	0
26	A	64	0	74	2	0
26	D	64	0	74	3	0
26	d	128	0	148	1	0
27	A	40	0	56	4	0
27	B	120	0	168	6	0
27	C	40	0	56	4	0
27	D	40	0	56	2	0
27	H	40	0	56	3	0
27	K	80	0	112	6	0
27	T	40	0	56	4	0
27	Y	40	0	56	2	0
27	a	40	0	56	3	0
27	b	120	0	168	3	0
27	c	120	0	168	7	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	4	0
28	D	55	0	80	2	0
28	a	55	0	80	6	0
28	d	55	0	80	3	0
29	A	48	0	66	2	0
29	B	28	0	40	1	0
29	C	48	0	66	2	0
29	D	84	0	117	2	0
29	M	51	0	72	1	0
29	b	55	0	86	2	0
29	c	134	0	181	6	0
29	d	67	0	92	1	0
29	m	51	0	72	3	0
30	A	91	0	136	5	0
30	B	54	0	78	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	F	36	0	46	2	0
30	L	49	0	65	4	0
30	a	90	0	134	6	0
30	f	41	0	49	3	0
31	A	98	0	148	2	0
31	D	145	0	215	6	0
31	d	137	0	199	8	0
31	e	42	0	57	2	0
31	l	49	0	74	2	0
32	A	66	0	96	7	0
32	C	186	0	246	6	0
32	H	62	0	82	2	0
32	a	44	0	75	5	0
32	c	186	0	246	3	0
32	h	62	0	82	2	0
33	B	75	0	114	5	0
33	C	40	0	60	0	0
33	D	20	0	35	1	0
33	E	12	0	16	0	0
33	H	18	0	35	2	0
33	I	15	0	26	2	0
33	J	12	0	16	0	0
33	M	25	0	38	0	0
33	T	31	0	54	2	0
33	a	22	0	32	2	0
33	b	50	0	86	2	0
33	c	32	0	51	0	0
33	d	33	0	50	1	0
33	j	12	0	16	0	0
33	l	18	0	35	1	0
33	m	12	0	16	0	0
33	t	14	0	20	1	0
33	x	20	0	35	6	0
34	D	4	0	0	0	0
34	a	4	0	0	0	0
35	E	43	0	30	2	0
35	f	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	1	0
37	A	123	0	0	2	0
37	B	197	0	0	0	0
37	C	142	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	106	0	0	0	0
37	E	29	0	0	0	0
37	F	3	0	0	1	0
37	H	27	0	0	0	0
37	I	13	0	0	0	0
37	J	12	0	0	4	0
37	K	2	0	0	0	0
37	L	9	0	0	0	0
37	M	5	0	0	2	0
37	O	73	0	0	3	0
37	R	6	0	0	0	0
37	T	9	0	0	0	0
37	U	29	0	0	0	0
37	V	51	0	0	1	0
37	X	8	0	0	0	0
37	Y	1	0	0	0	0
37	Z	3	0	0	0	0
37	a	104	0	0	4	0
37	b	163	0	0	1	0
37	c	160	0	0	3	0
37	d	95	0	0	0	0
37	e	13	0	0	0	0
37	f	3	0	0	0	0
37	h	20	0	0	0	0
37	i	17	0	0	0	0
37	j	5	0	0	1	0
37	k	1	0	0	0	0
37	l	12	0	0	1	0
37	m	8	0	0	0	0
37	o	72	0	0	1	0
37	r	7	0	0	1	0
37	t	6	0	0	0	0
37	u	50	0	0	1	0
37	v	42	0	0	2	0
37	x	5	0	0	2	0
37	z	3	0	0	0	0
All	All	53041	0	52739	673	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 (673) 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)
28:A:611:PL9:H361	6:F:25:THR:HG21	1.47	0.96
17:Y:20:ALA:N	17:Y:23:THR:HG1	1.64	0.94
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.61	0.82
35:E:101:HEM:HBC2	35:E:101:HEM:HHD	1.62	0.80
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.47	0.79
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.65	0.78
1:a:102:LEU:HD12	32:a:615:DGD:HB22	1.65	0.77
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.03	0.75
4:d:141:TYR:OH	31:d:407:LHG:O4	2.04	0.73
1:a:200:LEU:HD13	32:c:519:DGD:HAW2	1.68	0.73
28:a:611:PL9:H48	4:d:39:PRO:HG3	1.71	0.73
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.71	0.72
9:J:15:THR:O	37:J:201:HOH:O	2.07	0.72
19:z:32:ASP:HB2	19:z:35:ARG:HB2	1.72	0.71
25:B:601:CLA:H61	33:H:103:STE:H183	1.73	0.69
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.27	0.69
16:v:104:MET:HA	16:v:107:LEU:HD22	1.73	0.69
19:z:1:MET:SD	19:z:1:MET:N	2.65	0.69
1:a:97:TRP:HA	8:i:1:FME:HG2	1.75	0.68
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.74	0.68
29:C:518:LMG:H191	10:K:27:VAL:HG11	1.75	0.68
32:a:615:DGD:HAW2	32:a:615:DGD:HB72	1.77	0.66
9:j:36:LEU:O	37:j:201:HOH:O	2.12	0.66
5:e:8:ARG:NH1	5:e:12:ASP:OD2	2.29	0.65
25:B:607:CLA:H203	31:D:412:LHG:H142	1.78	0.65
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.78	0.65
7:H:56:ASP:OD2	18:X:2:THR:N	2.29	0.65
2:B:185:TRP:HB2	33:B:623:STE:H21	1.79	0.64
32:A:617:DGD:HBN1	8:I:7:THR:HG21	1.80	0.64
9:J:36:LEU:O	37:J:202:HOH:O	2.15	0.64
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.79	0.64
3:C:148:GLY:O	3:C:156:LYS:NZ	2.30	0.64
13:O:84:GLU:OE1	13:O:86:LYS:NZ	2.30	0.64
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.80	0.63
9:J:18:GLY:HA3	27:Y:101:BCR:H371	1.80	0.63
28:d:406:PL9:H201	31:l:101:LHG:H202	1.80	0.63
12:m:4:ASN:ND2	29:m:101:LMG:O10	2.31	0.63
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.80	0.63
3:c:166:ILE:HG21	25:c:512:CLA:H202	1.79	0.62
26:D:402:PHO:HBA2	25:D:404:CLA:H142	1.80	0.62
31:d:408:LHG:H321	14:t:21:ILE:HD11	1.82	0.62
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:259:ILE:HD12	31:d:408:LHG:H291	1.82	0.61
32:A:617:DGD:HD5	2:b:75:TRP:HB3	1.81	0.61
1:A:85:SER:HA	1:A:109:GLY:HA3	1.83	0.61
13:O:36:GLN:HE21	13:O:37:THR:H	1.48	0.61
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.83	0.60
32:A:617:DGD:HB61	33:I:101:STE:H51	1.83	0.60
2:B:495:PHE:HD1	2:B:505:ARG:HH12	1.49	0.60
25:c:503:CLA:H203	25:c:510:CLA:HAB	1.81	0.60
2:B:211:ILE:HG23	33:B:625:STE:H51	1.83	0.60
29:A:612:LMG:H391	3:C:281:MET:HG3	1.83	0.60
25:B:615:CLA:H2	25:B:616:CLA:HBB2	1.82	0.60
12:M:5:GLN:O	37:M:201:HOH:O	2.16	0.60
4:d:79:SER:HA	4:d:172:SER:HB3	1.82	0.60
20:r:2:ASP:N	37:r:101:HOH:O	2.35	0.60
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.82	0.60
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.83	0.59
15:U:58:VAL:O	15:U:61:VAL:HG22	2.02	0.59
1:a:217:SER:HA	4:d:272:LEU:HD12	1.83	0.59
13:o:28:GLY:O	37:o:301:HOH:O	2.16	0.59
2:B:39:LEU:HD13	33:a:616:STE:H22	1.85	0.59
2:B:371:THR:HG23	2:B:372:ASP:O	2.02	0.59
2:b:127:ARG:NH2	7:h:18:TYR:O	2.35	0.59
20:r:2:ASP:HB3	20:r:5:VAL:HG23	1.83	0.59
2:b:65:PHE:HE1	25:b:604:CLA:HED2	1.66	0.59
6:f:24:HIS:O	6:f:28:VAL:HG13	2.03	0.59
1:A:227:THR:HB	1:A:231:GLU:HG3	1.84	0.59
3:C:95:LEU:HD21	25:C:501:CLA:OBD	2.03	0.59
25:C:510:CLA:H193	25:C:510:CLA:HBC3	1.83	0.59
25:C:508:CLA:HBC3	25:C:510:CLA:H92	1.84	0.59
27:B:619:BCR:H382	30:a:614:SQD:H82	1.84	0.59
15:U:39:ARG:NH2	16:V:60:ALA:O	2.36	0.58
27:t:101:BCR:H321	27:t:101:BCR:HC8	1.83	0.58
3:C:42:LEU:HD21	25:C:511:CLA:H2A	1.85	0.58
10:k:17:ILE:HD11	19:z:6:GLN:HG2	1.84	0.58
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.68	0.58
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.36	0.58
13:o:84:GLU:OE2	13:o:86:LYS:NZ	2.36	0.58
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.86	0.58
1:a:215:HIS:ND1	28:a:611:PL9:O1	2.35	0.58
18:x:16:SER:HB3	33:x:102:STE:H71	1.85	0.58
3:C:141:GLU:H	3:C:141:GLU:CD	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:40:ILE:HD13	13:o:243:ILE:HG12	1.85	0.58
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.85	0.58
31:d:408:LHG:H281	14:t:17:PHE:CD1	2.39	0.57
9:J:19:MET:N	37:J:201:HOH:O	2.15	0.57
14:T:1:FME:HE2	33:T:103:STE:H22	1.86	0.57
25:B:615:CLA:H52	25:B:616:CLA:HBB1	1.86	0.57
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.86	0.57
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.87	0.57
1:a:84:PRO:HA	1:a:112:TYR:CG	2.40	0.57
2:b:235:GLU:OE2	2:b:469:HIS:ND1	2.29	0.57
31:A:615:LHG:H321	25:B:611:CLA:H71	1.87	0.56
3:c:44:ASN:O	37:c:601:HOH:O	2.18	0.56
32:A:617:DGD:HE4	2:b:76:SER:HB3	1.87	0.56
4:D:141:TYR:OH	31:D:412:LHG:O4	2.13	0.56
13:O:156:PHE:O	37:O:301:HOH:O	2.18	0.56
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.87	0.56
1:a:235:TYR:OH	11:l:11:GLU:OE2	2.21	0.56
28:a:611:PL9:H151	31:e:101:LHG:H292	1.87	0.56
10:K:26:PRO:O	10:K:29:PRO:HD2	2.05	0.56
3:c:45:LEU:HA	3:c:139:THR:HG22	1.88	0.56
26:A:608:PHO:H41	30:A:616:SQD:H191	1.88	0.56
25:D:405:CLA:H18	18:X:15:LEU:HD11	1.88	0.56
25:b:615:CLA:H2	25:b:616:CLA:CBB	2.35	0.55
16:v:10:VAL:HG23	16:v:69:ILE:HD11	1.87	0.55
1:A:211:PHE:CD1	28:A:611:PL9:H111	2.41	0.55
18:x:27:VAL:O	18:x:31:ILE:HG13	2.06	0.55
3:c:391[A]:ARG:HD2	3:c:395:TYR:CZ	2.42	0.55
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.36	0.55
4:d:241:GLU:CD	4:d:241:GLU:H	2.14	0.55
2:B:490:GLN:HG3	2:B:496:TYR:HE2	1.71	0.55
1:a:36:ILE:HG23	25:a:609:CLA:HBB1	1.89	0.55
3:c:78:GLU:OE1	16:v:106:ASN:ND2	2.39	0.55
15:U:70:ARG:NH2	16:V:85:GLU:OE2	2.33	0.55
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.88	0.55
13:O:184:ARG:NH2	13:O:229[A]:GLU:OE2	2.40	0.55
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.89	0.55
7:H:59:ASN:ND2	7:H:61:SER:HB3	2.22	0.54
25:b:607:CLA:H191	31:d:407:LHG:H141	1.90	0.54
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.20	0.54
2:b:39:LEU:HD22	33:b:622:STE:H72	1.89	0.54
25:b:604:CLA:H42	25:b:605:CLA:H2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:127:LEU:HD13	33:d:413:STE:H71	1.88	0.54
27:D:406:BCR:H392	27:D:406:BCR:H23C	1.89	0.54
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.89	0.54
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.89	0.54
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.40	0.54
3:c:391[A]:ARG:NH1	37:c:605:HOH:O	2.40	0.54
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.89	0.54
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.73	0.54
3:c:406:SER:HA	3:c:420:VAL:HG23	1.89	0.54
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.90	0.54
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.43	0.53
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.91	0.53
25:b:605:CLA:HHC	25:b:605:CLA:HBB1	1.90	0.53
29:D:408:LMG:H402	6:F:26:LEU:HB3	1.91	0.53
2:b:383:PHE:N	4:d:344:GLU:O	2.39	0.53
10:k:28:ILE:HD11	17:y:28:ILE:HD13	1.90	0.53
11:l:7:ARG:HH12	33:l:102:STE:C1	2.22	0.53
4:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.90	0.53
1:a:63[B]:ILE:HB	3:c:335:THR:HG21	1.89	0.53
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.09	0.53
2:b:283:GLU:OE2	2:b:287:ARG:NE	2.37	0.53
25:c:508:CLA:HMB3	25:c:508:CLA:HBB1	1.89	0.53
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.74	0.53
3:c:178:LYS:NZ	3:c:184:GLY:O	2.39	0.52
3:C:406:SER:HA	3:C:420:VAL:HG23	1.91	0.52
13:o:130:GLN:OE1	13:o:143:LYS:NZ	2.43	0.52
12:M:6:LEU:HD12	29:M:101:LMG:HC92	1.90	0.52
25:B:606:CLA:H72	27:B:619:BCR:H311	1.92	0.52
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.92	0.52
25:d:404:CLA:HBA2	33:x:102:STE:H21	1.90	0.52
16:v:41:HIS:HA	16:v:45:ILE:O	2.09	0.52
25:d:404:CLA:H92	18:x:18:ALA:HB2	1.91	0.52
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.92	0.52
16:v:13:ASN:ND2	16:v:17:LYS:HB3	2.25	0.52
25:a:608:CLA:HAB	25:d:403:CLA:H61	1.91	0.52
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.90	0.52
5:e:40:THR:HB	20:r:4:ARG:HD2	1.92	0.52
5:E:68:ASP:O	5:E:72:ALA:HB2	2.10	0.51
30:L:101:SQD:H222	2:b:29:LEU:HD23	1.92	0.51
5:e:57:ALA:H	5:e:60:GLN:HE21	1.58	0.51
35:f:101:HEM:HBC2	35:f:101:HEM:HMC1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:x:12:ILE:HG21	33:x:102:STE:H141	1.91	0.51
33:a:617:STE:O2	37:a:701:HOH:O	2.19	0.51
3:C:203:THR:O	3:C:235:GLY:HA3	2.11	0.51
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.46	0.51
4:D:279:LEU:HD22	26:D:402:PHO:HBC3	1.92	0.51
28:a:611:PL9:H513	30:f:102:SQD:H311	1.91	0.51
25:b:604:CLA:HBB1	25:b:613:CLA:HBC2	1.92	0.51
13:O:133:VAL:O	13:O:135:SER:N	2.40	0.51
25:c:501:CLA:C19	25:c:507:CLA:HBB1	2.36	0.51
2:B:497:GLN:HB2	2:B:504:THR:HB	1.93	0.51
25:B:601:CLA:H121	27:H:101:BCR:H402	1.93	0.50
25:a:608:CLA:H151	29:d:411:LMG:H362	1.93	0.50
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.46	0.50
25:c:512:CLA:H171	29:c:522:LMG:H452	1.91	0.50
16:v:11:PRO:O	16:v:69:ILE:HD12	2.11	0.50
2:B:117:TYR:HA	11:L:1:MET:HE1	1.93	0.50
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.92	0.50
1:a:321:ILE:HD11	4:d:179:PHE:HB2	1.93	0.50
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.93	0.50
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.46	0.50
19:Z:15:LEU:HD22	19:Z:19:MET:HG3	1.94	0.50
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.94	0.50
2:b:182:ALA:HB2	29:b:621:LMG:HC3	1.93	0.50
3:c:71:GLU:HB3	3:c:86:LEU:HD22	1.93	0.50
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.94	0.50
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.93	0.50
1:A:11:ALA:O	1:A:16:ARG:NH2	2.44	0.50
9:j:15:THR:HG22	9:j:19:MET:HE2	1.93	0.49
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.11	0.49
1:a:334[B]:ARG:HG3	13:o:157:LEU:HB2	1.94	0.49
2:B:149[A]:LEU:HD21	25:B:606:CLA:HBB2	1.94	0.49
3:c:438:LEU:HD11	25:c:505:CLA:HBB1	1.93	0.49
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.47	0.49
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.93	0.49
14:T:18:PHE:HD1	27:T:101:BCR:HC7	1.77	0.49
1:a:82:VAL:HB	1:a:174[B]:LEU:HB2	1.94	0.49
1:a:200:LEU:HD12	30:a:613:SQD:H223	1.94	0.49
13:o:110:MET:HE2	13:o:116:ILE:HD11	1.95	0.49
32:A:617:DGD:HB52	33:I:101:STE:H42	1.95	0.49
19:Z:23:VAL:HG22	19:Z:40:ILE:HD12	1.94	0.49
25:B:603:CLA:C3D	25:B:605:CLA:H2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149[B]:LEU:HG	25:B:604:CLA:H18	1.93	0.49
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.94	0.49
25:a:612:CLA:H52	28:d:406:PL9:H151	1.94	0.49
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.48	0.49
6:F:12:SER:N	37:F:201:HOH:O	2.45	0.49
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.95	0.49
2:b:137:LYS:HG2	7:h:14:LEU:O	2.13	0.49
26:d:402:PHO:HHD	26:d:402:PHO:HBC2	1.95	0.49
1:a:72:LEU:HD21	33:t:102:STE:H41	1.95	0.49
25:c:508:CLA:H192	32:c:518:DGD:HA72	1.95	0.49
7:H:59:ASN:HD21	7:H:61:SER:HB3	1.78	0.48
25:d:404:CLA:H2	18:x:17:GLY:HA3	1.94	0.48
2:B:91:TRP:HE1	33:B:620:STE:H32	1.77	0.48
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.49	0.48
1:A:271:LEU:HD11	28:A:611:PL9:HC71	1.95	0.48
28:D:407:PL9:H412	11:L:29:LEU:HD23	1.94	0.48
35:E:101:HEM:HMB1	35:E:101:HEM:HBB2	1.95	0.48
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.94	0.48
2:B:119:ASP:H	11:L:1:MET:CE	2.26	0.48
25:B:603:CLA:H91	25:B:603:CLA:H111	1.60	0.48
27:B:619:BCR:H363	30:a:614:SQD:H142	1.95	0.48
2:b:505:ARG:HG3	2:b:506:ARG:N	2.28	0.48
1:A:243:GLU:H	1:A:243:GLU:CD	2.21	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.14	0.48
4:d:24:ARG:HD2	37:x:201:HOH:O	2.14	0.48
5:e:57:ALA:H	5:e:60:GLN:HG2	1.79	0.48
16:v:75:TYR:OH	37:v:301:HOH:O	2.20	0.48
2:b:161:LEU:HA	2:b:161:LEU:HD23	1.69	0.48
2:B:495:PHE:HD1	2:B:505:ARG:NH1	2.12	0.48
25:C:502:CLA:H51	25:C:503:CLA:C4C	2.44	0.48
31:D:410:LHG:H191	31:D:410:LHG:H372	1.96	0.48
2:B:285:ASN:O	2:B:289:GLN:HG2	2.13	0.47
2:B:414:PRO:O	2:B:418:LYS:HG3	2.13	0.47
14:T:29:ILE:HG22	14:T:30:THR:HG23	1.95	0.47
16:V:57:GLU:H	16:V:57:GLU:CD	2.22	0.47
18:X:12:ILE:O	18:X:16:SER:OG	2.30	0.47
2:b:67:ALA:HA	2:b:71:VAL:O	2.14	0.47
2:b:498:LYS:HE3	4:d:23:LYS:HB2	1.95	0.47
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.96	0.47
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.32	0.47
25:C:513:CLA:H41	25:C:513:CLA:H61	1.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:93:TRP:HB3	33:x:102:STE:H121	1.97	0.47
5:e:33:ALA:HB2	20:r:11:PRO:HG2	1.96	0.47
2:b:30:VAL:HG12	25:b:605:CLA:HHD	1.96	0.47
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.95	0.47
6:f:16:PHE:HB2	30:f:102:SQD:H82	1.97	0.47
6:f:21:VAL:O	6:f:25:THR:OG1	2.24	0.47
16:v:87:GLU:CD	16:v:96:ARG:HH12	2.22	0.47
28:A:611:PL9:H222	28:A:611:PL9:H201	1.66	0.47
4:D:59:TYR:O	5:E:65:LEU:HD12	2.13	0.47
4:D:266:TRP:CD1	31:D:409:LHG:HC31	2.50	0.47
30:L:101:SQD:H102	25:b:614:CLA:H43	1.97	0.47
13:O:133:VAL:C	13:O:135:SER:H	2.21	0.47
2:b:154:GLY:HA2	2:b:158:LEU:HD12	1.96	0.47
2:b:164:PRO:HG3	25:b:606:CLA:O1D	2.14	0.47
25:b:614:CLA:H61	25:b:614:CLA:H93	1.70	0.47
13:O:57:LYS:NZ	37:O:308:HOH:O	2.48	0.47
2:b:442:ILE:HD12	4:d:299:ILE:HG12	1.97	0.47
31:d:408:LHG:O1	31:l:101:LHG:O4	2.32	0.47
6:f:15:ILE:H	20:r:30:GLN:NE2	2.12	0.47
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.97	0.47
16:v:57:GLU:CD	16:v:57:GLU:H	2.23	0.47
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.96	0.47
2:b:287:ARG:HD3	37:b:701:HOH:O	2.15	0.47
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.96	0.47
11:l:7:ARG:NE	37:l:203:HOH:O	2.41	0.47
25:B:615:CLA:H102	25:B:615:CLA:H172	1.97	0.47
17:Y:20:ALA:N	17:Y:23:THR:OG1	2.39	0.47
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.49	0.47
1:a:279:PRO:HG2	4:d:212:ALA:HB2	1.97	0.47
2:b:159:THR:O	2:b:180:PRO:HB3	2.15	0.47
25:c:513:CLA:HBB1	25:c:513:CLA:HMB3	1.97	0.47
13:o:216:GLU:OE2	13:o:234:LYS:HD2	2.15	0.47
16:v:26:TYR:HD2	16:v:27:LEU:HD23	1.80	0.47
2:B:62:VAL:HB	25:B:605:CLA:HED3	1.97	0.46
3:C:167:VAL:HG13	25:C:512:CLA:H93	1.96	0.46
13:O:107:THR:HG22	37:O:320:HOH:O	2.15	0.46
1:a:102:LEU:H	32:a:615:DGD:HA22	1.79	0.46
25:a:609:CLA:HMA2	29:c:524:LMG:H142	1.97	0.46
4:d:126:MET:HE3	4:d:143:ALA:O	2.15	0.46
31:d:409:LHG:H242	31:d:409:LHG:H272	1.50	0.46
25:C:509:CLA:H91	25:C:509:CLA:H112	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:18:PHE:CD1	27:T:101:BCR:H343	2.50	0.46
2:b:102:VAL:HG11	25:b:606:CLA:H142	1.97	0.46
3:c:134:ILE:HD12	25:c:511:CLA:H43	1.97	0.46
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.15	0.46
25:C:506:CLA:H8	27:C:514:BCR:H12C	1.97	0.46
29:b:621:LMG:H212	29:b:621:LMG:H372	1.97	0.46
5:e:20:TRP:CD1	9:j:8:ILE:HD12	2.51	0.46
4:d:85:MET:HE1	5:e:72:ALA:HB2	1.98	0.46
32:C:516:DGD:HAE2	32:C:516:DGD:HA82	1.63	0.46
16:V:63:THR:HG22	16:V:64:PRO:CD	2.46	0.46
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.97	0.46
5:e:84:LYS:H	5:e:84:LYS:HG3	1.57	0.46
2:B:102:VAL:HG11	25:B:606:CLA:H111	1.98	0.46
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.98	0.46
25:b:616:CLA:H102	25:b:616:CLA:H13	1.79	0.46
26:A:608:PHO:HBB1	26:A:608:PHO:HMB3	1.97	0.46
25:B:606:CLA:H101	25:B:606:CLA:H161	1.97	0.46
30:B:622:SQD:H161	30:B:622:SQD:H341	1.98	0.46
3:C:363:GLY:O	3:C:367:GLU:HG2	2.15	0.46
15:u:51:LYS:HB2	15:u:51:LYS:HE2	1.75	0.46
25:B:614:CLA:H161	25:B:614:CLA:H141	1.62	0.46
29:B:621:LMG:H372	4:D:36:LEU:HB2	1.97	0.46
4:D:79:SER:HA	4:D:172:SER:HB3	1.98	0.46
27:a:610:BCR:H24C	27:a:610:BCR:H371	1.78	0.46
25:b:612:CLA:H171	25:b:613:CLA:HBB2	1.98	0.46
4:d:126:MET:HA	4:d:129:GLN:OE1	2.16	0.46
4:d:194:ASN:HA	4:d:295:SER:OG	2.16	0.46
4:d:246:MET:HE3	4:d:264:LYS:CG	2.46	0.46
25:B:611:CLA:H203	25:B:613:CLA:H8	1.98	0.45
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	1.98	0.45
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.77	0.45
25:B:602:CLA:H191	32:H:102:DGD:HBE1	1.97	0.45
25:B:603:CLA:H202	7:H:42:LEU:HD12	1.97	0.45
6:F:16:PHE:O	30:F:101:SQD:H442	2.16	0.45
28:a:611:PL9:H512	18:x:24:THR:HG23	1.98	0.45
12:m:5:GLN:HE21	12:m:5:GLN:HA	1.81	0.45
5:e:81:GLU:O	5:e:84:LYS:HE2	2.16	0.45
15:u:98:TYR:O	37:u:201:HOH:O	2.20	0.45
2:B:283:GLU:O	2:B:287:ARG:HG3	2.17	0.45
25:B:616:CLA:H112	25:B:616:CLA:H91	1.72	0.45
9:J:19:MET:O	9:J:23:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:102:LEU:HB2	32:a:615:DGD:HG2	1.97	0.45
2:b:141:ILE:HD11	7:h:14:LEU:HD22	1.98	0.45
5:e:23:HIS:HA	5:e:26:THR:OG1	2.17	0.45
27:x:101:BCR:H24C	27:x:101:BCR:H371	1.80	0.45
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.51	0.45
4:D:274:VAL:HG22	28:D:407:PL9:H222	1.99	0.45
1:a:85:SER:HA	1:a:109:GLY:HA3	1.98	0.45
1:a:342[A]:ASP:O	37:a:702:HOH:O	2.21	0.45
3:c:279:LEU:HD11	25:c:509:CLA:H11	1.98	0.45
7:h:37:LEU:HD22	27:x:101:BCR:H16C	1.97	0.45
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.97	0.45
5:e:26:THR:HA	20:r:15:ALA:HB1	1.99	0.45
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.99	0.45
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.99	0.45
20:r:4:ARG:HA	20:r:7:VAL:HG22	1.99	0.45
25:A:607:CLA:HAB	25:D:404:CLA:H72	1.98	0.45
32:C:517:DGD:HBW2	32:C:517:DGD:HBN2	1.69	0.45
9:J:20:GLY:O	9:J:24:ILE:HG13	2.17	0.45
10:K:28:ILE:HD11	17:Y:28:ILE:HD13	1.98	0.45
2:b:191:ASN:HB2	7:h:58:VAL:HG13	1.98	0.45
16:v:90:GLU:HB2	37:v:311:HOH:O	2.16	0.45
25:a:608:CLA:H171	25:a:608:CLA:H13	1.87	0.45
25:c:505:CLA:H193	29:c:524:LMG:H131	1.97	0.45
32:c:519:DGD:HAE1	32:c:519:DGD:HA82	1.43	0.45
1:A:214:MET:HE3	1:A:214:MET:HB3	1.81	0.45
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.51	0.45
25:C:507:CLA:H61	25:C:507:CLA:H92	1.74	0.45
4:D:32:TRP:CD1	29:D:411:LMG:H142	2.51	0.45
2:b:92:SER:O	2:b:96:VAL:HG23	2.17	0.45
25:b:602:CLA:H43	7:h:45:ILE:HG22	1.99	0.45
25:b:606:CLA:HBB1	25:b:606:CLA:HMB3	1.99	0.45
27:d:405:BCR:H402	9:j:21:VAL:HG21	1.99	0.45
1:A:84:PRO:HA	1:A:112:TYR:CG	2.52	0.45
25:B:603:CLA:C2D	25:B:605:CLA:H2	2.47	0.44
3:C:50:LEU:O	3:C:54:VAL:HG23	2.17	0.44
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.82	0.44
3:c:67:MET:HE2	37:c:701:HOH:O	2.18	0.44
17:y:39:LEU:O	17:y:44:GLY:N	2.50	0.44
18:x:12:ILE:HD13	33:x:102:STE:H161	1.98	0.44
33:B:624:STE:H32	33:B:624:STE:H62	1.63	0.44
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:9:PRO:O	5:E:13:ILE:HG13	2.17	0.44
5:E:26:THR:O	5:E:30:LEU:HG	2.18	0.44
27:K:101:BCR:H24C	27:K:101:BCR:H371	1.86	0.44
2:b:71:VAL:HG23	25:b:606:CLA:HMA2	1.98	0.44
2:b:201:HIS:HB2	25:b:602:CLA:CHB	2.46	0.44
25:b:606:CLA:H52	27:b:619:BCR:H311	1.99	0.44
3:c:413[A]:GLU:OE2	16:v:47:LYS:NZ	2.39	0.44
25:c:505:CLA:H43	27:c:515:BCR:HC7	1.99	0.44
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.81	0.44
30:A:616:SQD:H321	25:b:616:CLA:H62	1.99	0.44
5:E:65:LEU:O	5:E:67:THR:HG23	2.17	0.44
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.52	0.44
25:B:604:CLA:HBD	25:B:605:CLA:H43	1.99	0.44
13:o:53:LYS:HE3	13:o:65:PHE:CZ	2.53	0.44
18:x:8:LYS:HA	18:x:8:LYS:HD2	1.78	0.44
19:z:1:MET:HB2	19:z:4:LEU:HB3	2.00	0.44
30:B:622:SQD:H352	30:B:622:SQD:H382	1.67	0.44
3:c:245:ILE:HD13	29:c:522:LMG:H401	1.98	0.44
4:d:49:LEU:HD13	27:d:405:BCR:C15	2.47	0.44
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.99	0.44
25:B:602:CLA:H161	32:H:102:DGD:HAE2	2.00	0.44
16:V:41:HIS:HA	16:V:45:ILE:O	2.17	0.44
17:Y:34:MET:O	17:Y:38:LEU:HG	2.18	0.44
28:a:611:PL9:H351	28:a:611:PL9:H371	1.60	0.44
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.00	0.44
1:a:203:ALA:HB3	30:a:613:SQD:H221	2.00	0.44
25:c:501:CLA:H202	25:c:507:CLA:H152	1.99	0.44
19:z:40:ILE:HG13	19:z:41:PHE:N	2.31	0.44
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.52	0.44
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.06	0.44
25:B:606:CLA:H91	25:B:606:CLA:H112	1.54	0.44
3:C:185:LEU:HB2	3:C:230:LEU:HD13	1.98	0.44
7:H:54:ILE:H	18:X:6:SER:HG	1.62	0.44
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.99	0.44
13:O:64:GLU:H	13:O:64:GLU:CD	2.26	0.44
1:a:63[A]:ILE:HB	3:c:335:THR:HG21	1.98	0.44
4:d:40:CYS:HB3	4:d:117:HIS:O	2.18	0.44
1:A:229:GLU:H	1:A:229:GLU:HG3	1.58	0.44
33:T:102:STE:H62	33:T:102:STE:H31	1.46	0.44
2:b:247:PHE:CE2	25:b:602:CLA:H102	2.52	0.44
7:H:12:ARG:HB3	7:H:13:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:102:LEU:HD23	1:a:102:LEU:HA	1.78	0.43
3:c:175:LEU:HD22	25:c:501:CLA:C3D	2.48	0.43
25:c:504:CLA:H13	25:c:508:CLA:H143	1.99	0.43
15:u:32:ILE:HD12	15:u:50:VAL:HG21	2.00	0.43
2:B:216:HIS:HE1	25:B:609:CLA:C1A	2.31	0.43
18:X:10:PHE:CE2	18:X:14:LEU:HD22	2.54	0.43
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.99	0.43
25:b:615:CLA:H92	25:b:615:CLA:H61	1.82	0.43
16:v:41:HIS:CD2	36:v:201:HEC:NB	2.85	0.43
27:C:514:BCR:H15C	27:C:514:BCR:H351	1.81	0.43
27:T:101:BCR:H20C	27:T:101:BCR:H361	1.90	0.43
16:V:34:GLN:HA	16:V:38:ALA:HB2	1.99	0.43
16:V:87:GLU:HB3	37:V:319:HOH:O	2.18	0.43
27:a:610:BCR:H392	32:a:615:DGD:HB82	2.00	0.43
25:b:601:CLA:H202	7:h:37:LEU:HD13	2.00	0.43
1:A:329[B]:GLU:HG3	37:A:799:HOH:O	2.17	0.43
25:C:512:CLA:H93	25:C:512:CLA:H111	1.79	0.43
29:C:518:LMG:H111	29:C:518:LMG:H142	1.71	0.43
25:b:613:CLA:H143	25:b:613:CLA:H111	1.74	0.43
1:A:230:THR:HG21	11:L:8:GLN:NE2	2.33	0.43
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.01	0.43
1:a:16:ARG:HH11	1:a:16:ARG:HB3	1.83	0.43
27:H:101:BCR:H24C	27:H:101:BCR:H371	1.78	0.43
2:B:383:PHE:O	13:O:166:SER:HA	2.17	0.43
25:C:502:CLA:HBA2	25:C:503:CLA:H171	2.00	0.43
31:A:614:LHG:H131	31:A:614:LHG:H102	1.82	0.43
25:B:603:CLA:H142	25:B:603:CLA:H112	1.82	0.43
25:B:612:CLA:H122	25:B:612:CLA:H162	1.66	0.43
31:D:409:LHG:H321	14:T:21:ILE:HD11	2.00	0.43
9:J:15:THR:HG22	9:J:19:MET:HE2	2.00	0.43
19:Z:32:ASP:OD1	19:Z:35:ARG:HB2	2.19	0.43
19:Z:57:LEU:HD23	19:Z:57:LEU:HA	1.89	0.43
2:b:224:ARG:HG2	7:h:24:GLY:O	2.18	0.43
25:b:601:CLA:H141	25:b:601:CLA:H161	1.79	0.43
3:c:55:ALA:HB1	27:c:516:BCR:H373	2.01	0.43
25:c:510:CLA:H143	25:c:510:CLA:H111	1.84	0.43
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.54	0.43
1:A:40:THR:O	1:A:118:HIS:HB3	2.18	0.43
2:B:12:LEU:HB2	25:B:612:CLA:HMC2	2.00	0.43
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.54	0.43
27:B:617:BCR:H24C	27:B:617:BCR:H371	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B:625:STE:H92	33:H:103:STE:H52	1.99	0.43
25:C:502:CLA:H62	25:C:512:CLA:H42	2.01	0.43
4:D:61:HIS:HE1	4:D:80:THR:O	2.01	0.43
25:b:610:CLA:HBB1	27:x:101:BCR:HC21	2.01	0.43
25:c:510:CLA:H161	25:c:510:CLA:H193	1.82	0.43
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.54	0.43
30:A:613:SQD:H291	25:C:508:CLA:H71	2.00	0.43
3:C:92:ILE:HD11	25:C:503:CLA:HED2	2.00	0.43
5:E:36:LEU:HA	5:E:39:SER:OG	2.19	0.43
16:V:32:LEU:HB3	16:V:115:ILE:HD11	2.01	0.43
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.49	0.43
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	2.01	0.42
3:C:124:VAL:HB	27:K:101:BCR:H362	2.01	0.42
25:C:502:CLA:H112	25:C:502:CLA:H91	1.76	0.42
31:D:410:LHG:H141	31:D:410:LHG:H171	1.82	0.42
30:F:101:SQD:H242	18:X:31:ILE:HD13	2.01	0.42
25:b:602:CLA:O1D	25:b:603:CLA:HHB	2.19	0.42
25:b:611:CLA:H121	25:b:611:CLA:H162	1.92	0.42
25:b:612:CLA:H171	25:b:612:CLA:H13	1.69	0.42
30:f:102:SQD:H312	18:x:27:VAL:HG11	2.00	0.42
13:o:57:LYS:HD3	13:o:59:LYS:HE3	2.01	0.42
4:D:103:ARG:HH21	5:E:77:GLU:CG	2.31	0.42
30:a:613:SQD:H381	9:j:22:ILE:HD11	2.02	0.42
9:j:18:GLY:O	9:j:22:ILE:HD13	2.19	0.42
2:B:317:ASN:HA	2:B:330:MET:HE1	2.01	0.42
2:B:442:ILE:HD12	4:D:299:ILE:HG12	2.01	0.42
2:B:487:SER:OG	2:B:488:PRO:HD2	2.20	0.42
25:B:615:CLA:H2	25:B:616:CLA:CBB	2.47	0.42
32:C:515:DGD:HA71	32:C:515:DGD:HA42	1.90	0.42
25:D:403:CLA:H192	25:D:403:CLA:H162	1.75	0.42
1:a:342[B]:ASP:O	37:a:702:HOH:O	2.21	0.42
2:b:280:PHE:CD2	2:b:312:TYR:HB3	2.54	0.42
29:c:522:LMG:H402	29:c:522:LMG:H372	1.81	0.42
25:B:607:CLA:H61	25:B:607:CLA:H92	1.79	0.42
27:B:619:BCR:H20C	27:B:619:BCR:H361	1.75	0.42
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.54	0.42
25:C:504:CLA:HHC	25:C:504:CLA:HBB1	2.00	0.42
25:c:501:CLA:C2D	25:c:503:CLA:H2	2.49	0.42
4:D:321:LEU:O	4:D:325:ILE:HG13	2.19	0.42
5:E:45:ASP:OD2	20:R:4:ARG:NH2	2.48	0.42
10:K:24:VAL:HG21	17:Y:25:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:54:GLU:O	13:O:63:ALA:HB3	2.20	0.42
19:Z:36:SER:O	19:Z:40:ILE:HG12	2.18	0.42
2:b:264:PRO:HG2	2:b:267:LEU:HG	2.02	0.42
3:c:128:GLY:HA3	25:c:513:CLA:C3C	2.50	0.42
5:e:35:TRP:CD2	6:f:39:ALA:HB2	2.54	0.42
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.19	0.42
1:a:265:PHE:CD2	1:a:271:LEU:HD23	2.55	0.42
1:a:310:LYS:HD2	16:v:1:ALA:HB1	2.02	0.42
2:b:296:ALA:HB1	2:b:300:GLU:HB2	2.02	0.42
3:c:26:ARG:HD3	10:k:46:ARG:NH2	2.34	0.42
25:c:509:CLA:H3A	25:c:509:CLA:HBA1	1.85	0.42
6:f:15:ILE:HD12	6:f:15:ILE:HA	1.79	0.42
13:o:54:GLU:O	13:o:56:PRO:HD3	2.20	0.42
18:x:37:VAL:HG23	37:x:201:HOH:O	2.19	0.42
25:A:609:CLA:HMC2	27:A:610:BCR:H12C	2.01	0.42
32:A:617:DGD:HB31	25:b:606:CLA:H201	2.01	0.42
27:B:618:BCR:H371	27:B:618:BCR:H24C	1.71	0.42
33:D:413:STE:H91	18:X:16:SER:HB3	2.02	0.42
1:a:213:ALA:HB2	4:d:275:PRO:HG2	2.02	0.42
2:b:12:LEU:HB2	25:b:612:CLA:HMC2	2.02	0.42
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.55	0.42
25:c:512:CLA:H121	25:c:513:CLA:H151	2.01	0.42
27:c:516:BCR:H24C	27:c:516:BCR:H371	1.77	0.42
30:A:616:SQD:H383	27:b:619:BCR:HC8	2.01	0.42
2:B:472:ARG:HG3	2:B:479[B]:PHE:CE2	2.55	0.42
30:L:101:SQD:H242	30:L:101:SQD:H81	2.01	0.42
1:a:121:LEU:HD21	25:c:505:CLA:H172	2.02	0.42
25:b:606:CLA:H72	25:b:606:CLA:H111	1.55	0.42
12:m:13:LEU:HD12	12:m:13:LEU:HA	1.87	0.42
15:u:70:ARG:HD2	15:u:70:ARG:HA	1.84	0.42
3:C:143:TYR:CE2	25:C:513:CLA:HED3	2.55	0.42
3:C:279:LEU:HD12	25:C:509:CLA:HED2	2.01	0.42
25:C:509:CLA:HBB1	25:C:509:CLA:HMB1	2.01	0.42
12:M:8:LEU:HB3	37:M:201:HOH:O	2.20	0.42
13:O:110:MET:HE2	13:O:110:MET:HB3	1.76	0.42
30:a:613:SQD:H382	30:a:613:SQD:H351	1.74	0.42
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.84	0.42
5:e:10:PHE:N	31:e:101:LHG:O4	2.53	0.42
10:k:24:VAL:O	10:k:27:VAL:HG22	2.19	0.42
29:m:101:LMG:H291	29:m:101:LMG:H322	1.82	0.42
13:o:160:LYS:HA	13:o:160:LYS:HD2	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:92:VAL:HG12	15:u:97:ARG:HD2	2.01	0.42
27:H:101:BCR:H20C	27:H:101:BCR:H361	1.94	0.42
27:a:610:BCR:H20C	27:a:610:BCR:H361	1.87	0.42
25:c:503:CLA:H203	25:c:510:CLA:CAB	2.49	0.42
16:v:26:TYR:OH	16:v:122:GLU:OE1	2.33	0.42
20:r:20:VAL:O	20:r:24:LEU:HB2	2.20	0.42
27:A:610:BCR:H11C	27:A:610:BCR:H341	1.85	0.41
3:C:344:SER:O	13:O:75:THR:HG22	2.20	0.41
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.20	0.41
1:a:82:VAL:HB	1:a:174[A]:LEU:HB2	2.02	0.41
1:a:117:PHE:HD2	25:a:609:CLA:HED3	1.84	0.41
2:b:145:LEU:HD22	25:b:604:CLA:H161	2.01	0.41
4:d:56:THR:HG23	4:d:58:TRP:H	1.84	0.41
4:d:131:GLU:O	4:d:135:LEU:HG	2.19	0.41
4:d:179:PHE:HA	4:d:182:LEU:HD22	2.01	0.41
7:h:62:TRP:CD1	32:h:101:DGD:HE62	2.55	0.41
16:v:12:LEU:HD23	16:v:17:LYS:HD3	2.02	0.41
25:C:510:CLA:H2	25:C:510:CLA:H61	1.70	0.41
13:O:6:THR:HG23	13:O:8:ASP:H	1.85	0.41
27:T:101:BCR:H321	27:T:101:BCR:HC8	2.02	0.41
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.01	0.41
25:b:608:CLA:H161	25:b:608:CLA:H141	1.63	0.41
3:c:286:ALA:HB2	25:c:502:CLA:HMD2	2.02	0.41
4:d:99:GLY:HA3	33:x:102:STE:H151	2.02	0.41
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.01	0.41
27:k:101:BCR:H24C	27:k:101:BCR:H371	1.91	0.41
13:o:18:LYS:NZ	13:o:74:GLU:OE1	2.46	0.41
25:C:508:CLA:H92	25:C:510:CLA:H52	2.02	0.41
32:C:517:DGD:HA82	32:C:517:DGD:HAE2	1.88	0.41
27:K:102:BCR:H361	27:K:102:BCR:H20C	1.83	0.41
1:a:201:GLY:HA3	1:a:286:THR:HB	2.01	0.41
2:b:83:GLU:H	2:b:83:GLU:HG2	1.52	0.41
3:c:213:LEU:HD21	27:c:515:BCR:C20	2.51	0.41
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.56	0.41
7:h:62:TRP:HD1	32:h:101:DGD:HE62	1.85	0.41
13:o:42:ARG:O	13:o:241:ALA:HA	2.20	0.41
32:A:617:DGD:HB62	32:A:617:DGD:HBE1	2.02	0.41
25:C:504:CLA:H92	32:C:516:DGD:HA92	2.01	0.41
27:C:514:BCR:H371	27:C:514:BCR:H24C	1.83	0.41
10:K:25:LEU:HD22	27:Y:101:BCR:H332	2.03	0.41
2:b:91:TRP:HE1	33:b:620:STE:H111	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:84:LYS:HB2	5:e:84:LYS:HE3	1.85	0.41
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.45	0.41
11:L:24:ILE:CD1	12:M:18:PRO:HB2	2.50	0.41
3:c:443:TRP:CE2	25:c:508:CLA:HMD2	2.55	0.41
1:A:132:GLU:O	1:A:136:ARG:HG2	2.21	0.41
25:B:614:CLA:H91	25:B:614:CLA:H111	1.85	0.41
27:K:102:BCR:H24C	27:K:102:BCR:H371	1.89	0.41
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.03	0.41
3:c:242:LEU:HD21	29:c:522:LMG:H312	2.03	0.41
27:A:610:BCR:H15C	27:A:610:BCR:H351	1.87	0.41
2:B:216:HIS:CE1	25:B:609:CLA:NA	2.88	0.41
2:B:414:PRO:N	2:B:415:PRO:HD2	2.35	0.41
25:C:504:CLA:H62	25:C:504:CLA:H41	1.84	0.41
1:a:229:GLU:CD	1:a:229:GLU:H	2.27	0.41
25:a:612:CLA:H162	25:a:612:CLA:H122	1.83	0.41
25:c:505:CLA:H61	25:c:505:CLA:H2	1.88	0.41
1:A:201:GLY:HA3	1:A:286:THR:HB	2.03	0.41
3:C:330:SER:HB3	13:O:100:GLY:O	2.21	0.41
25:C:506:CLA:H111	25:C:506:CLA:H152	1.83	0.41
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.01	0.41
30:L:101:SQD:H141	30:L:101:SQD:H172	1.77	0.41
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.02	0.41
3:c:35:TRP:CD1	10:k:45:PHE:HB3	2.56	0.41
3:c:121:SER:O	3:c:124:VAL:HG13	2.21	0.41
15:u:86:GLU:OE1	15:u:86:GLU:N	2.47	0.41
1:A:158:PHE:O	1:A:162[A]:PRO:HG2	2.20	0.41
2:B:389:LYS:HA	2:B:389:LYS:HD3	1.85	0.41
25:B:605:CLA:H41	25:B:605:CLA:H61	1.71	0.41
4:D:150:ILE:O	4:D:154:VAL:HG13	2.21	0.41
9:J:5:GLY:N	37:J:204:HOH:O	2.52	0.41
27:K:101:BCR:H20C	27:K:101:BCR:H361	1.92	0.41
16:V:28:GLU:OE2	16:V:31:ARG:NH1	2.54	0.41
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.48	0.41
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.56	0.41
25:b:601:CLA:HAB	25:b:601:CLA:H162	2.02	0.41
25:b:614:CLA:H62	25:b:614:CLA:H41	1.61	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.89	0.41
3:c:334:PRO:HA	13:o:153:THR:OG1	2.21	0.41
25:c:511:CLA:H111	25:c:511:CLA:H91	1.81	0.41
27:c:514:BCR:H20C	27:c:514:BCR:H361	1.85	0.41
29:m:101:LMG:H412	29:m:101:LMG:H381	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:616:SQD:H301	27:b:619:BCR:H363	2.03	0.41
5:E:60:GLN:HG2	5:E:62:SER:H	1.86	0.41
16:V:63:THR:HG22	16:V:64:PRO:HD2	2.02	0.41
3:c:125:LEU:HD13	27:c:514:BCR:H361	2.03	0.41
3:c:342:MET:SD	3:c:356[B]:MET:HE2	2.61	0.41
4:d:192:THR:HG23	25:d:403:CLA:HBC2	2.02	0.41
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.56	0.40
13:O:51:LEU:HB2	13:O:234:LYS:HB3	2.02	0.40
3:c:385:GLN:HB2	3:c:387:TRP:CD1	2.56	0.40
25:c:507:CLA:O1D	25:c:509:CLA:H8	2.21	0.40
1:A:217:SER:HB2	4:D:142:ASN:HA	2.04	0.40
25:A:609:CLA:H61	25:A:609:CLA:H41	1.69	0.40
37:A:770:HOH:O	13:O:107:THR:HG21	2.21	0.40
26:D:402:PHO:HHD	26:D:402:PHO:HBC2	2.02	0.40
27:K:102:BCR:H15C	27:K:102:BCR:H351	1.91	0.40
1:a:52:PHE:CE2	28:d:406:PL9:H48	2.56	0.40
1:a:296:ASN:HB2	3:c:400:PRO:O	2.22	0.40
4:d:12:ARG:NH1	4:d:16:ASP:HB3	2.37	0.40
20:r:9:LEU:O	20:r:13:LEU:HG	2.21	0.40
1:A:60[A]:ILE:HB	1:A:83:VAL:HG12	2.03	0.40
25:A:606:CLA:H203	25:A:606:CLA:H162	1.74	0.40
25:B:616:CLA:H41	25:B:616:CLA:H61	1.70	0.40
3:C:126:GLY:O	3:C:130:VAL:HG13	2.21	0.40
3:C:154:LYS:HE3	3:C:266:TRP:CG	2.56	0.40
3:C:387:TRP:CE2	3:C:388:GLN:HG3	2.57	0.40
27:C:514:BCR:H20C	27:C:514:BCR:H361	1.93	0.40
4:D:241:GLU:H	4:D:241:GLU:CD	2.29	0.40
5:E:8:ARG:O	6:F:19:ARG:NH2	2.40	0.40
1:a:30:VAL:O	1:a:34:GLY:HA3	2.21	0.40
25:b:604:CLA:CBB	25:b:613:CLA:HBC2	2.51	0.40
3:c:180:MET:HE2	3:c:180:MET:HB3	1.91	0.40
3:c:257:PHE:O	3:c:261:ARG:HG3	2.21	0.40
4:d:171:PRO:HG3	4:d:181:PHE:CZ	2.56	0.40
27:A:610:BCR:H371	27:A:610:BCR:H24C	1.85	0.40
29:A:612:LMG:H341	32:C:515:DGD:HA92	2.04	0.40
25:B:614:CLA:H2A	25:B:614:CLA:O1D	2.21	0.40
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.03	0.40
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.04	0.40
5:E:81:GLU:C	5:E:83:LEU:H	2.30	0.40
13:O:32:ILE:HD11	13:O:136:ILE:HG13	2.02	0.40
13:O:220:LEU:HD23	13:O:220:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:733:HOH:O	3:c:410:VAL:HB	2.21	0.40
25:b:602:CLA:H122	25:b:602:CLA:H162	1.61	0.40
3:c:95:LEU:HD23	3:c:95:LEU:HA	1.92	0.40
3:c:163:PHE:CG	25:c:512:CLA:HAB	2.56	0.40
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.21	0.40
9:j:10:LEU:O	9:j:13:VAL:HG22	2.20	0.40
13:o:178:LYS:HA	13:o:178:LYS:HD3	1.66	0.40
17:y:20:ALA:O	17:y:24:MET:HG2	2.21	0.40
25:B:607:CLA:H91	25:B:607:CLA:H112	1.81	0.40
25:B:614:CLA:H92	25:B:614:CLA:H62	1.79	0.40
30:B:622:SQD:H442	14:t:23:PHE:CD1	2.57	0.40
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.51	0.40
27:D:406:BCR:H361	27:D:406:BCR:H20C	1.79	0.40
4:d:39:PRO:O	4:d:43:LEU:HG	2.21	0.40
31:d:408:LHG:H112	31:d:408:LHG:HC82	1.89	0.40
5:e:30:LEU:HD11	6:f:28:VAL:HB	2.03	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	395/344 (115%)	387 (98%)	8 (2%)	0	100	100
1	a	395/344 (115%)	386 (98%)	8 (2%)	1 (0%)	36	36
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	451/461 (98%)	438 (97%)	12 (3%)	1 (0%)	43	44
3	c	461/461 (100%)	449 (97%)	11 (2%)	1 (0%)	43	44
4	D	340/352 (97%)	332 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	341/352 (97%)	331 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	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%)	59 (94%)	3 (5%)	1 (2%)	7	4
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	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%)	34 (100%)	0	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%)	229 (94%)	11 (4%)	3 (1%)	10	7
13	o	242/272 (89%)	231 (96%)	10 (4%)	1 (0%)	30	28
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%)	91 (96%)	3 (3%)	1 (1%)	11	8
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	15
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	29/41 (71%)	29 (100%)	0	0	100	100
All	All	5386/5700 (94%)	5235 (97%)	141 (3%)	10 (0%)	43	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	O	59	LYS
13	o	61	GLN
15	u	53	ALA
13	O	62	GLU
13	O	134	THR
1	a	259	ILE
7	H	12	ARG

5.3.2 Protein sidechains ⓘ

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	322/280 (115%)	314 (98%)	8 (2%)	42	48
1	a	321/280 (115%)	309 (96%)	12 (4%)	30	33
2	B	407/407 (100%)	398 (98%)	9 (2%)	45	53
2	b	402/407 (99%)	390 (97%)	12 (3%)	36	41
3	C	353/362 (98%)	346 (98%)	7 (2%)	48	56
3	c	362/362 (100%)	350 (97%)	12 (3%)	33	37
4	D	277/283 (98%)	275 (99%)	2 (1%)	76	83
4	d	278/283 (98%)	270 (97%)	8 (3%)	37	42
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	28
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	34
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	4
7	H	54/55 (98%)	51 (94%)	3 (6%)	19	18
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	17
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	6
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	8
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	5
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	5
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%)	25 (89%)	3 (11%)	6	4
13	O	206/228 (90%)	200 (97%)	6 (3%)	37	42
13	o	207/228 (91%)	198 (96%)	9 (4%)	26	27
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	32
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	29
15	U	84/112 (75%)	79 (94%)	5 (6%)	17	15
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	72
16	V	117/138 (85%)	114 (97%)	3 (3%)	40	46
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	35
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	25
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	13
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
19	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
20	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
20	r	25/33 (76%)	19 (76%)	6 (24%)	1	0
All	All	4450/4654 (96%)	4283 (96%)	167 (4%)	29	32

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	16	ARG
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	205	VAL
1	A	229	GLU
1	A	243	GLU
1	A	248	ILE
2	B	63	LEU
2	B	80	ILE
2	B	101	ILE
2	B	127	ARG
2	B	227	LYS
2	B	240	SER
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	43	LEU
4	D	154	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
6	F	25	THR
7	H	20	LYS
7	H	27	THR
7	H	56	ASP
8	I	4	LEU
8	I	6	ILE
8	I	36	ASP
10	K	10	LYS
10	K	24	VAL
10	K	27	VAL
11	L	10	VAL
12	M	9	ILE
12	M	25	LEU

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Mol	Chain	Res	Type
13	O	6	THR
13	O	54	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	214	THR
14	T	25	GLU
15	U	9	LEU
15	U	10	VAL
15	U	51	LYS
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	31	ARG
17	Y	28	ILE
17	Y	41	VAL
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	35	ARG
19	Z	38	GLN
19	Z	46	LEU
19	Z	50	LEU
20	R	13	LEU
20	R	21	ARG
20	R	22	ASN
20	R	33	LYS
20	R	35	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	243	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU

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Mol	Chain	Res	Type
2	b	86	ILE
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	266	GLU
2	b	315	ILE
2	b	362	PHE
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	78	GLU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
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	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	54	SER
5	e	65	LEU
5	e	66	VAL
5	e	84	LYS
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
7	h	27	THR
7	h	43	LEU

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Mol	Chain	Res	Type
8	i	2	GLU
9	j	7	ARG
9	j	13	VAL
10	k	10	LYS
10	k	30	VAL
10	k	35	LEU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	5	GLN
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS
13	o	49	THR
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	143	LYS
13	o	207	ARG
14	t	25	GLU
15	u	23	GLU
16	v	30	LYS
16	v	52	LEU
16	v	107	LEU
16	v	128	ASP
17	y	19	ILE
18	x	2	THR
18	x	15	LEU
19	z	1	MET
19	z	27	TYR
19	z	31	GLN
19	z	40	ILE
19	z	46	LEU
20	r	3	TRP
20	r	9	LEU
20	r	10	LEU
20	r	12	VAL
20	r	14	LEU
20	r	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
3	C	385	GLN
4	D	61	HIS
7	H	59	ASN
11	L	8	GLN
12	M	5	GLN
13	O	36	GLN
13	O	88	ASN
13	O	155	ASN
13	O	231	HIS
15	U	78	ASN
15	U	81	HIS
16	V	86	GLN
17	Y	45	ASN
20	R	22	ASN
1	a	19	ASN
1	a	234	ASN
2	b	179	GLN
2	b	274	GLN
2	b	331	ASN
2	b	338	GLN
2	b	409	GLN
2	b	490	GLN
4	d	350	ASN
5	e	60	GLN
11	l	6	ASN
12	m	5	GLN
13	o	61	GLN
13	o	109	GLN
13	o	124	ASN
13	o	155	ASN
16	v	25	GLN
18	x	33	GLN
19	z	31	GLN
20	r	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	1.09	1 (12%)	8,9,11	0.86	0
12	FME	M	1	12	8,9,10	1.02	1 (12%)	8,9,11	1.02	0
8	FME	i	1	8	8,9,10	1.03	1 (12%)	8,9,11	0.76	0
8	FME	I	1	8	8,9,10	1.00	0	8,9,11	1.02	0
14	FME	t	1	14	8,9,10	1.21	1 (12%)	8,9,11	0.78	0
14	FME	T	1	14	8,9,10	1.07	0	8,9,11	1.13	0

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.46	1.43	1.46
12	m	1	FME	CA-N	-2.34	1.43	1.46
12	M	1	FME	CA-N	-2.18	1.43	1.46
8	i	1	FME	CA-N	-2.03	1.43	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	i	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 [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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	$\# Z > 2$
27	BCR	d	405	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	7 (12%)
25	CLA	c	509	-	69,73,73	1.26	7 (10%)	82,113,113	1.58	8 (9%)
29	LMG	m	101	-	51,51,55	0.87	3 (5%)	59,59,63	1.47	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	e	101	-	41,41,48	0.77	1 (2%)	44,47,54	1.29	5 (11%)
33	STE	l	102	-	17,17,19	0.34	0	16,16,19	0.96	0
36	HEC	v	201	16	46,50,50	1.86	7 (15%)	58,82,82	1.83	4 (6%)
29	LMG	D	411	-	31,31,55	0.73	1 (3%)	33,33,63	1.17	2 (6%)
33	STE	C	520	-	11,11,19	0.71	0	11,11,19	1.41	2 (18%)
25	CLA	b	606	-	69,73,73	1.32	7 (10%)	82,113,113	1.53	9 (10%)
25	CLA	C	503	-	69,73,73	1.51	9 (13%)	82,113,113	1.47	9 (10%)
27	BCR	D	406	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	5 (8%)
33	STE	b	622	-	19,19,19	0.69	0	19,19,19	0.95	1 (5%)
35	HEM	f	101	6,5	50,50,50	1.52	8 (16%)	67,82,82	1.21	7 (10%)
27	BCR	B	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	8 (14%)
33	STE	C	519	-	11,11,19	0.61	0	11,11,19	1.48	3 (27%)
25	CLA	B	606	-	69,73,73	1.29	8 (11%)	82,113,113	1.39	9 (10%)
27	BCR	B	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.32	6 (10%)
33	STE	j	101	-	11,11,19	0.70	0	11,11,19	1.40	2 (18%)
32	DGD	H	102	-	63,63,67	1.07	5 (7%)	77,77,81	1.40	8 (10%)
33	STE	C	521	-	15,15,19	0.46	0	14,14,19	0.60	0
25	CLA	C	502	-	69,73,73	1.20	8 (11%)	82,113,113	1.27	7 (8%)
25	CLA	C	505	-	69,73,73	1.31	6 (8%)	82,113,113	1.22	5 (6%)
33	STE	d	412	-	15,15,19	0.73	0	15,15,19	0.98	0
25	CLA	C	501	-	69,73,73	1.23	6 (8%)	82,113,113	1.38	6 (7%)
25	CLA	a	609	-	69,73,73	1.24	7 (10%)	82,113,113	1.12	6 (7%)
25	CLA	b	610	37	69,73,73	1.30	8 (11%)	82,113,113	1.31	9 (10%)
25	CLA	C	504	37	63,67,73	1.26	7 (11%)	74,105,113	1.27	8 (10%)
31	LHG	A	614	-	48,48,48	0.70	1 (2%)	51,54,54	1.23	7 (13%)
33	STE	H	103	-	17,17,19	0.40	0	16,16,19	0.73	0
33	STE	E	102	-	11,11,19	0.79	0	11,11,19	1.00	0
32	DGD	c	518	-	63,63,67	1.02	4 (6%)	77,77,81	1.40	10 (12%)
25	CLA	B	614	-	69,73,73	1.34	8 (11%)	82,113,113	1.23	6 (7%)
33	STE	M	103	-	9,9,19	0.40	0	8,8,19	0.72	0
25	CLA	B	610	37	69,73,73	1.18	6 (8%)	82,113,113	1.43	10 (12%)
25	CLA	c	511	3	69,73,73	1.40	6 (8%)	82,113,113	1.55	6 (7%)
25	CLA	b	609	-	69,73,73	1.22	8 (11%)	82,113,113	1.20	9 (10%)
25	CLA	c	504	37	64,68,73	1.24	8 (12%)	76,107,113	1.35	8 (10%)
31	LHG	d	408	-	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
25	CLA	B	611	-	69,73,73	1.13	6 (8%)	82,113,113	1.37	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	612	37	69,73,73	1.27	6 (8%)	82,113,113	1.34	7 (8%)
26	PHO	A	608	-	58,69,69	1.97	9 (15%)	55,99,99	1.47	6 (10%)
33	STE	a	616	-	9,9,19	0.46	0	8,8,19	0.61	0
25	CLA	c	503	-	69,73,73	1.31	9 (13%)	82,113,113	1.45	6 (7%)
25	CLA	c	508	-	68,72,73	1.25	9 (13%)	80,111,113	1.29	7 (8%)
25	CLA	c	501	-	69,73,73	1.17	6 (8%)	82,113,113	1.35	8 (9%)
29	LMG	c	520	-	37,37,55	0.85	0	45,45,63	1.37	7 (15%)
29	LMG	d	411	-	44,44,55	0.94	2 (4%)	52,52,63	1.34	6 (11%)
30	SQD	A	616	-	38,38,54	1.77	5 (13%)	40,40,65	1.28	2 (5%)
25	CLA	D	403	37	69,73,73	1.23	7 (10%)	82,113,113	1.11	7 (8%)
22	OEX	a	602[A]	37,3,1	0,15,15	-	-	-	-	-
27	BCR	c	515	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	6 (10%)
25	CLA	B	605	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	8 (9%)
30	SQD	a	613	-	52,54,54	1.52	7 (13%)	62,65,65	1.95	12 (19%)
25	CLA	C	511	3	69,73,73	1.28	7 (10%)	82,113,113	1.29	4 (4%)
25	CLA	B	603	-	69,73,73	1.22	9 (13%)	82,113,113	1.29	10 (12%)
33	STE	c	521	-	19,19,19	0.68	0	19,19,19	0.92	0
28	PL9	D	407	-	55,55,55	0.94	2 (3%)	68,69,69	1.51	13 (19%)
25	CLA	c	505	-	69,73,73	1.12	6 (8%)	82,113,113	1.24	6 (7%)
32	DGD	A	617	-	67,67,67	1.10	7 (10%)	81,81,81	1.41	15 (18%)
25	CLA	A	606	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	9 (10%)
25	CLA	c	507	37	69,73,73	1.28	5 (7%)	82,113,113	1.28	7 (8%)
33	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.23	0
25	CLA	A	607	37	69,73,73	1.21	6 (8%)	82,113,113	1.20	7 (8%)
29	LMG	M	101	-	51,51,55	0.86	1 (1%)	59,59,63	1.39	6 (10%)
30	SQD	L	101	-	47,49,54	1.62	8 (17%)	57,60,65	1.96	12 (21%)
25	CLA	c	502	-	69,73,73	1.18	9 (13%)	82,113,113	1.31	8 (9%)
25	CLA	B	615	-	69,73,73	1.34	5 (7%)	82,113,113	1.36	8 (9%)
25	CLA	B	609	-	69,73,73	1.16	6 (8%)	82,113,113	1.19	4 (4%)
27	BCR	T	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	4 (7%)
27	BCR	A	610	-	41,41,41	0.96	2 (4%)	56,56,56	1.39	10 (17%)
25	CLA	B	602	-	69,73,73	1.21	7 (10%)	82,113,113	1.39	9 (10%)
25	CLA	C	507	37	69,73,73	1.21	9 (13%)	82,113,113	1.46	7 (8%)
25	CLA	C	510	-	69,73,73	1.18	9 (13%)	82,113,113	1.25	9 (10%)
25	CLA	b	605	-	69,73,73	1.13	6 (8%)	82,113,113	1.32	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	x	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.20	5 (8%)
25	CLA	b	603	-	69,73,73	1.24	8 (11%)	82,113,113	1.37	11 (13%)
25	CLA	B	612	-	69,73,73	1.07	7 (10%)	82,113,113	1.36	12 (14%)
36	HEC	V	201	16	46,50,50	1.80	6 (13%)	58,82,82	1.95	7 (12%)
31	LHG	D	409	-	48,48,48	0.79	3 (6%)	51,54,54	1.32	7 (13%)
33	STE	b	623	-	9,9,19	0.40	0	8,8,19	0.67	0
35	HEM	E	101	6,5	50,50,50	1.39	7 (14%)	67,82,82	1.10	1 (1%)
26	PHO	D	402	-	58,69,69	2.06	10 (17%)	55,99,99	1.60	8 (14%)
33	STE	B	625	-	11,11,19	0.73	0	11,11,19	1.20	1 (9%)
33	STE	I	101	-	14,14,19	0.44	0	13,13,19	0.63	0
33	STE	a	617	-	11,11,19	0.80	0	11,11,19	1.08	1 (9%)
25	CLA	b	611	-	69,73,73	1.29	7 (10%)	82,113,113	1.42	7 (8%)
29	LMG	d	410	-	21,21,55	0.49	0	20,20,63	1.19	2 (10%)
34	BCT	a	606	23	3,3,3	3.71	1 (33%)	2,3,3	2.09	1 (50%)
33	STE	M	102	-	14,14,19	0.68	0	14,14,19	1.21	1 (7%)
27	BCR	C	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	5 (8%)
28	PL9	a	611	-	55,55,55	0.79	1 (1%)	68,69,69	1.51	13 (19%)
33	STE	T	103	-	14,14,19	0.31	0	13,13,19	0.96	0
21	OEY	a	601[B]	37,3,1	0,16,16	-	-	-		
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.40	7 (12%)
28	PL9	A	611	-	55,55,55	0.92	2 (3%)	68,69,69	1.41	11 (16%)
31	LHG	D	410	-	46,46,48	0.79	1 (2%)	49,52,54	1.23	5 (10%)
25	CLA	B	616	-	64,68,73	1.28	7 (10%)	76,107,113	1.45	6 (7%)
27	BCR	b	617	-	41,41,41	0.99	3 (7%)	56,56,56	1.31	7 (12%)
32	DGD	C	516	-	63,63,67	1.11	6 (9%)	77,77,81	1.41	13 (16%)
25	CLA	c	510	-	69,73,73	1.25	10 (14%)	82,113,113	1.39	10 (12%)
32	DGD	C	515	-	63,63,67	1.04	4 (6%)	77,77,81	1.39	12 (15%)
25	CLA	b	613	-	69,73,73	1.45	8 (11%)	82,113,113	1.36	12 (14%)
25	CLA	B	604	-	69,73,73	1.35	9 (13%)	82,113,113	1.61	11 (13%)
25	CLA	b	607	37	69,73,73	1.17	7 (10%)	82,113,113	1.28	8 (9%)
32	DGD	c	519	-	63,63,67	0.96	3 (4%)	77,77,81	1.41	8 (10%)
33	STE	B	620	-	16,16,19	0.65	0	16,16,19	1.15	0
22	OEX	A	602[A]	37,3,1	0,15,15	-	-	-		
27	BCR	t	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.34	6 (10%)
30	SQD	A	613	-	50,52,54	1.59	6 (12%)	60,63,65	1.88	12 (20%)
33	STE	B	623	-	11,11,19	0.75	0	11,11,19	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	b	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	4 (7%)
34	BCT	D	401	23	3,3,3	3.55	1 (33%)	2,3,3	2.02	1 (50%)
25	CLA	b	601	37	69,73,73	1.31	8 (11%)	82,113,113	1.41	5 (6%)
25	CLA	C	508	-	69,73,73	1.28	7 (10%)	82,113,113	1.37	9 (10%)
25	CLA	c	506	-	69,73,73	1.21	9 (13%)	82,113,113	1.31	7 (8%)
27	BCR	k	101	-	41,41,41	1.07	4 (9%)	56,56,56	1.07	3 (5%)
25	CLA	D	404	-	69,73,73	1.30	6 (8%)	82,113,113	1.30	8 (9%)
29	LMG	b	621	-	55,55,55	0.84	2 (3%)	63,63,63	1.33	8 (12%)
25	CLA	B	601	37	69,73,73	1.41	10 (14%)	82,113,113	1.33	6 (7%)
32	DGD	C	517	-	63,63,67	0.93	3 (4%)	77,77,81	1.34	7 (9%)
25	CLA	b	604	-	69,73,73	1.18	6 (8%)	82,113,113	1.61	9 (10%)
25	CLA	c	513	-	69,73,73	1.25	8 (11%)	82,113,113	1.27	8 (9%)
27	BCR	a	610	-	41,41,41	0.98	2 (4%)	56,56,56	1.28	8 (14%)
27	BCR	b	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	5 (8%)
31	LHG	A	615	-	48,48,48	0.75	3 (6%)	51,54,54	1.21	2 (3%)
27	BCR	B	617	-	41,41,41	1.04	3 (7%)	56,56,56	1.23	5 (8%)
27	BCR	c	516	-	41,41,41	1.03	2 (4%)	56,56,56	1.16	6 (10%)
25	CLA	C	513	-	69,73,73	1.28	8 (11%)	82,113,113	1.36	6 (7%)
25	CLA	D	405	-	69,73,73	1.36	9 (13%)	82,113,113	1.35	9 (10%)
29	LMG	c	522	-	48,48,55	0.88	3 (6%)	56,56,63	1.33	9 (16%)
25	CLA	d	404	-	69,73,73	1.27	8 (11%)	82,113,113	1.23	8 (9%)
33	STE	x	102	-	19,19,19	0.66	0	19,19,19	0.90	1 (5%)
25	CLA	b	615	-	69,73,73	1.35	10 (14%)	82,113,113	1.27	6 (7%)
29	LMG	A	612	-	48,48,55	0.78	2 (4%)	56,56,63	1.33	6 (10%)
30	SQD	a	614	-	35,35,54	1.74	7 (20%)	37,37,65	1.36	4 (10%)
25	CLA	B	613	-	69,73,73	1.18	8 (11%)	82,113,113	1.41	9 (10%)
25	CLA	a	608	37	69,73,73	1.20	8 (11%)	82,113,113	1.30	7 (8%)
29	LMG	c	524	-	49,49,55	0.84	2 (4%)	57,57,63	1.27	4 (7%)
33	STE	c	523	-	11,11,19	0.69	0	11,11,19	1.35	1 (9%)
26	PHO	d	402	-	58,69,69	2.15	8 (13%)	55,99,99	1.63	8 (14%)
25	CLA	a	607	-	69,73,73	1.47	10 (14%)	82,113,113	1.27	9 (10%)
25	CLA	b	616	-	64,68,73	1.13	7 (10%)	76,107,113	1.40	9 (11%)
33	STE	m	102	-	11,11,19	0.69	0	11,11,19	1.41	1 (9%)
33	STE	B	626	-	15,15,19	0.38	0	14,14,19	0.81	0
25	CLA	b	608	-	69,73,73	1.21	8 (11%)	82,113,113	1.43	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	d	409	-	38,38,48	0.77	1 (2%)	41,44,54	1.14	2 (4%)
32	DGD	a	615	-	43,43,67	0.77	2 (4%)	45,45,81	1.47	8 (17%)
25	CLA	A	609	-	58,62,73	1.24	6 (10%)	68,99,113	1.35	8 (11%)
21	OEY	A	601[B]	37,3,1	0,16,16	-	-	-		
33	STE	b	620	-	19,19,19	0.63	0	19,19,19	0.98	0
26	PHO	d	401	-	58,69,69	2.14	10 (17%)	55,99,99	1.43	10 (18%)
33	STE	t	102	-	13,13,19	0.67	0	13,13,19	1.16	1 (7%)
30	SQD	B	622	-	52,54,54	1.60	8 (15%)	62,65,65	1.51	8 (12%)
32	DGD	h	101	-	63,63,67	0.99	3 (4%)	77,77,81	1.47	10 (12%)
31	LHG	l	101	-	48,48,48	0.66	1 (2%)	51,54,54	1.20	6 (11%)
33	STE	T	102	-	15,15,19	0.40	0	14,14,19	0.73	0
25	CLA	c	512	-	69,73,73	1.28	9 (13%)	82,113,113	1.34	7 (8%)
25	CLA	C	509	-	69,73,73	1.24	8 (11%)	82,113,113	1.35	8 (9%)
29	LMG	B	621	-	26,26,55	0.59	0	26,26,63	1.35	2 (7%)
25	CLA	B	608	-	69,73,73	1.28	8 (11%)	82,113,113	1.49	8 (9%)
25	CLA	b	614	-	69,73,73	1.26	8 (11%)	82,113,113	1.14	8 (9%)
27	BCR	K	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.16	4 (7%)
30	SQD	F	101	-	34,36,54	1.60	6 (17%)	42,45,65	1.93	12 (28%)
27	BCR	H	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.24	6 (10%)
25	CLA	b	612	-	69,73,73	1.19	6 (8%)	82,113,113	1.30	8 (9%)
30	SQD	f	102	-	39,41,54	1.70	8 (20%)	49,52,65	1.67	11 (22%)
29	LMG	C	518	-	48,48,55	0.82	1 (2%)	56,56,63	1.37	10 (17%)
33	STE	d	413	-	16,16,19	0.63	0	16,16,19	1.13	1 (6%)
25	CLA	d	403	-	69,73,73	1.21	8 (11%)	82,113,113	1.14	5 (6%)
25	CLA	B	607	37	69,73,73	1.36	9 (13%)	82,113,113	1.32	6 (7%)
31	LHG	d	407	-	48,48,48	0.81	2 (4%)	51,54,54	1.36	6 (11%)
32	DGD	c	517	-	63,63,67	0.97	3 (4%)	77,77,81	1.36	7 (9%)
31	LHG	D	412	-	48,48,48	0.92	2 (4%)	51,54,54	1.37	6 (11%)
33	STE	B	624	-	17,17,19	0.63	0	17,17,19	1.03	0
28	PL9	d	406	-	55,55,55	1.06	4 (7%)	68,69,69	1.59	16 (23%)
25	CLA	C	512	-	69,73,73	1.41	10 (14%)	82,113,113	1.31	9 (10%)
33	STE	D	413	-	19,19,19	0.59	0	19,19,19	1.15	0
27	BCR	Y	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.19	4 (7%)
29	LMG	D	408	-	51,51,55	0.89	3 (5%)	59,59,63	1.34	6 (10%)
27	BCR	c	514	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	7 (12%)
25	CLA	C	506	-	69,73,73	1.24	9 (13%)	82,113,113	1.31	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	602	-	69,73,73	1.08	5 (7%)	82,113,113	1.31	10 (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
27	BCR	d	405	-	-	7/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	10/39/115/115	-
29	LMG	m	101	-	-	12/46/66/70	0/1/1/1
31	LHG	e	101	-	-	22/46/46/53	-
33	STE	l	102	-	-	9/15/15/17	-
36	HEC	v	201	16	-	6/14/54/54	-
29	LMG	D	411	-	-	20/33/33/70	-
33	STE	C	520	-	-	5/9/9/17	-
25	CLA	b	606	-	1/1/15/20	11/39/115/115	-
25	CLA	C	503	-	1/1/15/20	8/39/115/115	-
27	BCR	D	406	-	-	6/29/63/63	0/2/2/2
33	STE	b	622	-	-	8/17/17/17	-
35	HEM	f	101	6,5	-	5/14/54/54	-
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2
33	STE	C	519	-	-	5/9/9/17	-
25	CLA	B	606	-	1/1/15/20	14/39/115/115	-
27	BCR	B	619	-	-	5/29/63/63	0/2/2/2
33	STE	j	101	-	-	4/9/9/17	-
32	DGD	H	102	-	-	18/51/91/95	0/2/2/2
33	STE	C	521	-	-	7/13/13/17	-
25	CLA	C	502	-	1/1/15/20	9/39/115/115	-
25	CLA	C	505	-	1/1/15/20	17/39/115/115	-
33	STE	d	412	-	-	6/13/13/17	-
25	CLA	C	501	-	1/1/15/20	5/39/115/115	-
25	CLA	a	609	-	1/1/15/20	7/39/115/115	-
25	CLA	b	610	37	1/1/15/20	5/39/115/115	-
25	CLA	C	504	37	1/1/13/20	7/32/108/115	-
31	LHG	A	614	-	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	H	103	-	-	6/15/15/17	-
33	STE	E	102	-	-	4/9/9/17	-
32	DGD	c	518	-	-	22/51/91/95	0/2/2/2
25	CLA	B	614	-	1/1/15/20	10/39/115/115	-
33	STE	M	103	-	-	3/7/7/17	-
25	CLA	B	610	37	1/1/15/20	7/39/115/115	-
25	CLA	c	511	3	1/1/15/20	11/39/115/115	-
25	CLA	b	609	-	1/1/15/20	8/39/115/115	-
25	CLA	c	504	37	1/1/14/20	7/33/109/115	-
31	LHG	d	408	-	-	20/53/53/53	-
25	CLA	B	611	-	1/1/15/20	7/39/115/115	-
25	CLA	a	612	37	1/1/15/20	2/39/115/115	-
26	PHO	A	608	-	-	5/37/103/103	0/5/6/6
33	STE	a	616	-	-	3/7/7/17	-
25	CLA	c	503	-	-	7/39/115/115	-
25	CLA	c	508	-	-	3/38/114/115	-
25	CLA	c	501	-	1/1/15/20	5/39/115/115	-
29	LMG	c	520	-	-	10/31/51/70	0/1/1/1
29	LMG	d	411	-	-	11/39/59/70	0/1/1/1
30	SQD	A	616	-	-	18/39/39/69	-
25	CLA	D	403	37	1/1/15/20	11/39/115/115	-
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
25	CLA	B	605	-	1/1/15/20	13/39/115/115	-
30	SQD	a	613	-	-	25/49/69/69	0/1/1/1
25	CLA	C	511	3	1/1/15/20	6/39/115/115	-
25	CLA	B	603	-	1/1/15/20	11/39/115/115	-
33	STE	c	521	-	-	8/17/17/17	-
28	PL9	D	407	-	-	7/53/73/73	0/1/1/1
25	CLA	c	505	-	1/1/15/20	12/39/115/115	-
32	DGD	A	617	-	-	28/55/95/95	0/2/2/2
25	CLA	A	606	-	1/1/15/20	6/39/115/115	-
25	CLA	c	507	37	1/1/15/20	10/39/115/115	-
33	STE	J	101	-	-	2/9/9/17	-
25	CLA	A	607	37	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	M	101	-	-	21/46/66/70	0/1/1/1
30	SQD	L	101	-	-	17/44/64/69	0/1/1/1
25	CLA	c	502	-	1/1/15/20	12/39/115/115	-
25	CLA	B	615	-	1/1/15/20	10/39/115/115	-
25	CLA	B	609	-	-	2/39/115/115	-
27	BCR	T	101	-	-	8/29/63/63	0/2/2/2
27	BCR	A	610	-	-	2/29/63/63	0/2/2/2
25	CLA	B	602	-	1/1/15/20	9/39/115/115	-
25	CLA	C	507	37	1/1/15/20	6/39/115/115	-
25	CLA	C	510	-	1/1/15/20	11/39/115/115	-
25	CLA	b	605	-	1/1/15/20	7/39/115/115	-
27	BCR	x	101	-	-	9/29/63/63	0/2/2/2
25	CLA	b	603	-	1/1/15/20	6/39/115/115	-
25	CLA	B	612	-	1/1/15/20	8/39/115/115	-
36	HEC	V	201	16	-	6/14/54/54	-
31	LHG	D	409	-	-	22/53/53/53	-
33	STE	b	623	-	-	5/7/7/17	-
35	HEM	E	101	6,5	-	3/14/54/54	-
26	PHO	D	402	-	-	3/37/103/103	0/5/6/6
33	STE	B	625	-	-	8/9/9/17	-
33	STE	I	101	-	-	6/12/12/17	-
33	STE	a	617	-	-	4/9/9/17	-
25	CLA	b	611	-	1/1/15/20	5/39/115/115	-
29	LMG	d	410	-	-	11/17/17/70	-
33	STE	M	102	-	-	5/12/12/17	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
28	PL9	a	611	-	-	15/53/73/73	0/1/1/1
33	STE	T	103	-	-	8/12/12/17	-
27	BCR	K	101	-	-	7/29/63/63	0/2/2/2
28	PL9	A	611	-	-	26/53/73/73	0/1/1/1
31	LHG	D	410	-	-	16/51/51/53	-
25	CLA	B	616	-	1/1/14/20	13/33/109/115	-
27	BCR	b	617	-	-	6/29/63/63	0/2/2/2
32	DGD	C	516	-	-	21/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	510	-	1/1/15/20	14/39/115/115	-
32	DGD	C	515	-	-	22/51/91/95	0/2/2/2
25	CLA	b	613	-	1/1/15/20	8/39/115/115	-
25	CLA	B	604	-	1/1/15/20	11/39/115/115	-
25	CLA	b	607	37	1/1/15/20	16/39/115/115	-
32	DGD	c	519	-	-	21/51/91/95	0/2/2/2
33	STE	B	620	-	-	8/14/14/17	-
27	BCR	t	101	-	-	7/29/63/63	0/2/2/2
30	SQD	A	613	-	-	16/47/67/69	0/1/1/1
33	STE	B	623	-	-	7/9/9/17	-
27	BCR	b	619	-	-	3/29/63/63	0/2/2/2
25	CLA	b	601	37	1/1/15/20	16/39/115/115	-
25	CLA	c	506	-	1/1/15/20	12/39/115/115	-
25	CLA	C	508	-	-	8/39/115/115	-
27	BCR	k	101	-	-	10/29/63/63	0/2/2/2
25	CLA	D	404	-	1/1/15/20	8/39/115/115	-
29	LMG	b	621	-	-	26/50/70/70	0/1/1/1
25	CLA	B	601	37	1/1/15/20	15/39/115/115	-
32	DGD	C	517	-	-	14/51/91/95	0/2/2/2
25	CLA	b	604	-	1/1/15/20	8/39/115/115	-
25	CLA	c	513	-	1/1/15/20	10/39/115/115	-
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2
27	BCR	b	618	-	-	4/29/63/63	0/2/2/2
31	LHG	A	615	-	-	17/53/53/53	-
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
27	BCR	c	516	-	-	3/29/63/63	0/2/2/2
25	CLA	C	513	-	1/1/15/20	16/39/115/115	-
25	CLA	D	405	-	-	7/39/115/115	-
29	LMG	c	522	-	-	23/43/63/70	0/1/1/1
25	CLA	d	404	-	1/1/15/20	6/39/115/115	-
33	STE	x	102	-	-	10/17/17/17	-
25	CLA	b	615	-	1/1/15/20	11/39/115/115	-
29	LMG	A	612	-	-	23/43/63/70	0/1/1/1
30	SQD	a	614	-	-	17/37/37/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	613	-	1/1/15/20	14/39/115/115	-
25	CLA	a	608	37	-	14/39/115/115	-
29	LMG	c	524	-	-	19/44/64/70	0/1/1/1
33	STE	c	523	-	-	4/9/9/17	-
26	PHO	d	402	-	-	7/37/103/103	0/5/6/6
25	CLA	a	607	-	1/1/15/20	4/39/115/115	-
25	CLA	b	616	-	1/1/14/20	7/33/109/115	-
33	STE	m	102	-	-	4/9/9/17	-
33	STE	B	626	-	-	7/13/13/17	-
25	CLA	b	608	-	1/1/15/20	8/39/115/115	-
31	LHG	d	409	-	-	11/43/43/53	-
32	DGD	a	615	-	-	28/45/45/95	-
25	CLA	A	609	-	1/1/12/20	3/26/102/115	-
33	STE	b	620	-	-	9/17/17/17	-
26	PHO	d	401	-	-	6/37/103/103	0/5/6/6
33	STE	t	102	-	-	5/11/11/17	-
30	SQD	B	622	-	-	25/49/69/69	0/1/1/1
32	DGD	h	101	-	-	16/51/91/95	0/2/2/2
31	LHG	l	101	-	-	20/53/53/53	-
33	STE	T	102	-	-	7/13/13/17	-
25	CLA	c	512	-	1/1/15/20	22/39/115/115	-
25	CLA	C	509	-	1/1/15/20	11/39/115/115	-
29	LMG	B	621	-	-	14/22/22/70	-
25	CLA	B	608	-	1/1/15/20	4/39/115/115	-
25	CLA	b	614	-	1/1/15/20	12/39/115/115	-
27	BCR	K	102	-	-	10/29/63/63	0/2/2/2
30	SQD	F	101	-	-	12/28/48/69	0/1/1/1
27	BCR	H	101	-	-	6/29/63/63	0/2/2/2
25	CLA	b	612	-	1/1/15/20	4/39/115/115	-
30	SQD	f	102	-	-	12/36/56/69	0/1/1/1
29	LMG	C	518	-	-	20/43/63/70	0/1/1/1
33	STE	d	413	-	-	9/14/14/17	-
25	CLA	d	403	-	1/1/15/20	8/39/115/115	-
25	CLA	B	607	37	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	d	407	-	-	22/53/53/53	-
32	DGD	c	517	-	-	30/51/91/95	0/2/2/2
31	LHG	D	412	-	-	15/53/53/53	-
33	STE	B	624	-	-	9/15/15/17	-
28	PL9	d	406	-	-	12/53/73/73	0/1/1/1
25	CLA	C	512	-	1/1/15/20	15/39/115/115	-
33	STE	D	413	-	-	9/17/17/17	-
27	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
29	LMG	D	408	-	-	17/46/66/70	0/1/1/1
27	BCR	c	514	-	-	10/29/63/63	0/2/2/2
25	CLA	C	506	-	1/1/15/20	10/39/115/115	-
25	CLA	b	602	-	-	13/39/115/115	-

All (787) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	402	PHO	C1B-C2B	10.06	1.50	1.39
26	d	401	PHO	C1B-C2B	9.64	1.50	1.39
26	A	608	PHO	C1B-C2B	9.04	1.49	1.39
26	D	402	PHO	C1B-C2B	8.81	1.49	1.39
26	D	402	PHO	C3B-C4B	8.61	1.50	1.41
26	d	402	PHO	C3B-C4B	8.53	1.50	1.41
26	d	401	PHO	C3B-C4B	8.44	1.50	1.41
26	A	608	PHO	C3B-C4B	6.84	1.48	1.41
25	b	613	CLA	MG-NA	6.80	2.22	2.06
36	V	201	HEC	CAC-C3C	6.50	1.56	1.35
25	c	511	CLA	MG-NA	6.31	2.21	2.06
36	v	201	HEC	CAC-C3C	6.30	1.55	1.35
34	a	606	BCT	O1-C	6.24	1.47	1.25
36	v	201	HEC	CAB-C3B	6.22	1.55	1.35
25	b	606	CLA	MG-NA	6.14	2.20	2.06
25	C	503	CLA	MG-NA	6.01	2.20	2.06
25	C	505	CLA	MG-NA	6.00	2.20	2.06
36	V	201	HEC	CAB-C3B	5.98	1.54	1.35
34	D	401	BCT	O1-C	5.97	1.46	1.25
25	B	601	CLA	MG-NA	5.74	2.19	2.06
25	B	604	CLA	MG-NC	5.62	2.19	2.06
36	v	201	HEC	C3D-C2D	5.55	1.53	1.38
25	B	615	CLA	MG-NA	5.46	2.19	2.06
25	B	607	CLA	MG-NB	-5.41	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	404	CLA	MG-NA	5.28	2.18	2.06
30	A	616	SQD	O47-C45	-5.26	1.38	1.47
25	b	611	CLA	MG-NA	5.21	2.18	2.06
25	C	508	CLA	MG-NA	5.05	2.18	2.06
30	F	101	SQD	O48-C23	5.00	1.47	1.33
36	V	201	HEC	C3D-C2D	4.96	1.51	1.38
25	C	511	CLA	MG-NA	4.96	2.18	2.06
30	B	622	SQD	O48-C23	4.83	1.47	1.33
25	C	512	CLA	MG-NB	4.83	2.15	2.05
25	D	405	CLA	MG-NB	-4.83	1.96	2.05
35	f	101	HEM	FE-NB	4.83	2.09	1.94
30	L	101	SQD	O48-C23	4.79	1.47	1.33
30	a	614	SQD	O48-C23	4.77	1.47	1.33
30	A	613	SQD	O48-C23	4.76	1.47	1.33
30	A	616	SQD	O48-C23	4.75	1.47	1.33
25	a	612	CLA	MG-NA	4.72	2.17	2.06
30	f	102	SQD	O48-C23	4.71	1.47	1.33
25	B	614	CLA	MG-NA	4.70	2.17	2.06
25	c	507	CLA	MG-NA	4.69	2.17	2.06
25	b	615	CLA	MG-NA	4.66	2.17	2.06
35	f	101	HEM	FE-NA	4.63	2.10	1.95
25	C	503	CLA	MG-ND	4.61	2.14	2.05
25	b	610	CLA	MG-NB	-4.59	1.96	2.05
30	a	613	SQD	O48-C23	4.56	1.46	1.33
25	a	607	CLA	MG-NC	4.55	2.17	2.06
25	b	601	CLA	MG-NA	4.48	2.16	2.06
25	B	606	CLA	MG-NA	4.46	2.16	2.06
25	a	609	CLA	MG-ND	-4.42	1.97	2.05
26	d	401	PHO	C1D-C2D	4.40	1.44	1.39
25	d	404	CLA	MG-NB	-4.36	1.97	2.05
25	a	607	CLA	C1D-ND	4.28	1.43	1.37
25	b	612	CLA	MG-ND	-4.24	1.97	2.05
25	a	607	CLA	MG-ND	-4.13	1.97	2.05
25	b	615	CLA	MG-NB	4.07	2.13	2.05
25	C	512	CLA	MG-ND	-4.06	1.97	2.05
25	d	403	CLA	C1D-ND	4.03	1.43	1.37
27	b	618	BCR	C30-C25	-4.03	1.48	1.53
25	b	614	CLA	C4B-NB	4.01	1.43	1.37
25	B	609	CLA	C1D-ND	3.97	1.43	1.37
25	c	503	CLA	MG-NB	3.96	2.13	2.05
25	B	607	CLA	C1D-ND	3.95	1.43	1.37
25	A	606	CLA	MG-NA	3.95	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	101	BCR	C1-C6	-3.91	1.48	1.53
25	a	608	CLA	C1D-ND	3.89	1.43	1.37
30	B	622	SQD	O47-C7	3.89	1.45	1.34
25	D	405	CLA	C1D-ND	3.87	1.42	1.37
26	D	402	PHO	C1D-C2D	3.87	1.43	1.39
26	d	402	PHO	C1D-C2D	3.87	1.43	1.39
27	B	618	BCR	C30-C25	-3.86	1.48	1.53
28	d	406	PL9	C3-C4	-3.86	1.43	1.49
25	C	512	CLA	MG-NA	3.86	2.15	2.06
25	B	616	CLA	MG-NA	3.83	2.15	2.06
25	b	613	CLA	C1D-ND	3.82	1.42	1.37
27	C	514	BCR	C1-C6	-3.80	1.48	1.53
25	c	510	CLA	C1D-ND	3.80	1.42	1.37
25	a	607	CLA	MG-NA	3.79	2.15	2.06
25	C	513	CLA	C1D-ND	3.79	1.42	1.37
25	C	506	CLA	C1D-ND	3.79	1.42	1.37
25	B	615	CLA	C4B-NB	3.79	1.42	1.37
25	B	608	CLA	MG-NA	3.78	2.15	2.06
27	c	515	BCR	C1-C6	-3.78	1.48	1.53
25	b	607	CLA	MG-NA	3.77	2.15	2.06
30	L	101	SQD	O47-C7	3.76	1.44	1.34
25	B	601	CLA	C1D-ND	3.74	1.42	1.37
31	D	412	LHG	O7-C5	-3.74	1.37	1.46
30	a	614	SQD	O47-C7	3.72	1.44	1.34
25	B	613	CLA	MG-ND	-3.71	1.98	2.05
25	b	601	CLA	C1D-ND	3.71	1.42	1.37
25	B	614	CLA	C1D-ND	3.70	1.42	1.37
30	A	613	SQD	O47-C45	-3.66	1.38	1.46
25	b	612	CLA	C1D-ND	3.66	1.42	1.37
25	c	501	CLA	C1D-ND	3.66	1.42	1.37
25	C	509	CLA	MG-NA	3.65	2.14	2.06
25	A	607	CLA	C1D-ND	3.64	1.42	1.37
27	c	514	BCR	C1-C6	-3.63	1.49	1.53
35	E	101	HEM	FE-NB	3.63	2.06	1.94
25	B	608	CLA	MG-NC	3.63	2.14	2.06
25	b	603	CLA	C1D-ND	3.63	1.42	1.37
25	c	513	CLA	C1D-ND	3.63	1.42	1.37
25	A	609	CLA	C1D-ND	3.62	1.42	1.37
25	b	604	CLA	C4B-NB	3.62	1.42	1.37
25	c	508	CLA	MG-NC	3.62	2.14	2.06
25	c	507	CLA	C1D-ND	3.60	1.42	1.37
25	D	404	CLA	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	612	CLA	C1D-ND	3.60	1.42	1.37
25	c	504	CLA	C4B-NB	3.57	1.42	1.37
25	c	506	CLA	C1D-ND	3.57	1.42	1.37
25	C	503	CLA	C1D-ND	3.56	1.42	1.37
25	b	614	CLA	C1D-ND	3.56	1.42	1.37
25	c	512	CLA	C1D-ND	3.56	1.42	1.37
30	f	102	SQD	O47-C7	3.55	1.44	1.34
30	a	613	SQD	O47-C45	-3.54	1.38	1.46
30	A	616	SQD	O47-C7	3.54	1.44	1.34
25	c	512	CLA	MG-NA	3.53	2.14	2.06
26	d	401	PHO	C4D-CHA	3.53	1.44	1.39
29	D	408	LMG	C4-C5	3.51	1.60	1.53
26	A	608	PHO	C1D-C2D	3.51	1.43	1.39
25	C	509	CLA	C1D-ND	3.50	1.42	1.37
25	B	616	CLA	C1D-ND	3.50	1.42	1.37
25	B	608	CLA	C1D-ND	3.48	1.42	1.37
27	Y	101	BCR	C1-C6	-3.48	1.49	1.53
25	b	616	CLA	C1D-ND	3.47	1.42	1.37
25	C	501	CLA	C1D-ND	3.47	1.42	1.37
32	c	517	DGD	O2G-C2G	-3.47	1.38	1.46
25	B	605	CLA	C1B-C2B	3.47	1.51	1.43
25	B	606	CLA	C1D-ND	3.46	1.42	1.37
25	c	502	CLA	C1D-ND	3.46	1.42	1.37
25	B	614	CLA	MG-ND	-3.44	1.99	2.05
25	B	607	CLA	MG-NA	3.44	2.14	2.06
25	B	602	CLA	C4B-NB	3.43	1.42	1.37
25	b	606	CLA	C1D-ND	3.42	1.42	1.37
25	d	404	CLA	C1D-ND	3.42	1.42	1.37
25	C	505	CLA	C1B-C2B	3.42	1.51	1.43
25	D	403	CLA	C1D-ND	3.42	1.42	1.37
28	D	407	PL9	C6-C1	-3.40	1.42	1.48
25	c	509	CLA	C1B-C2B	3.40	1.51	1.43
25	B	602	CLA	C1D-ND	3.40	1.42	1.37
30	f	102	SQD	O47-C45	-3.39	1.38	1.46
30	F	101	SQD	C24-C23	3.39	1.60	1.50
25	C	504	CLA	MG-NA	3.39	2.14	2.06
25	b	602	CLA	C1D-ND	3.39	1.42	1.37
25	C	504	CLA	C1D-ND	3.37	1.42	1.37
27	d	405	BCR	C1-C6	-3.37	1.49	1.53
25	c	511	CLA	C1D-ND	3.37	1.42	1.37
25	B	611	CLA	C1D-ND	3.37	1.42	1.37
30	a	614	SQD	C24-C23	3.36	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	405	BCR	C30-C25	-3.36	1.49	1.53
25	c	503	CLA	C1D-ND	3.36	1.42	1.37
25	B	601	CLA	C1B-C2B	3.35	1.51	1.43
25	C	503	CLA	C4B-NB	3.35	1.42	1.37
25	b	610	CLA	C1D-ND	3.35	1.42	1.37
25	b	608	CLA	C1D-ND	3.35	1.42	1.37
26	A	608	PHO	C4D-CHA	3.34	1.44	1.39
25	C	506	CLA	MG-ND	-3.34	1.99	2.05
25	C	513	CLA	MG-NB	3.34	2.12	2.05
27	D	406	BCR	C1-C6	-3.34	1.49	1.53
25	c	509	CLA	C1D-ND	3.33	1.42	1.37
25	B	615	CLA	C1D-ND	3.33	1.42	1.37
27	D	406	BCR	C30-C25	-3.33	1.49	1.53
25	C	508	CLA	C1D-ND	3.32	1.42	1.37
25	b	604	CLA	C1D-ND	3.31	1.42	1.37
25	B	604	CLA	C1D-ND	3.31	1.42	1.37
25	B	603	CLA	MG-NA	3.31	2.14	2.06
25	C	504	CLA	C4B-NB	3.31	1.42	1.37
25	b	609	CLA	C4B-NB	3.30	1.42	1.37
25	B	614	CLA	C4B-NB	3.29	1.42	1.37
25	D	404	CLA	C1B-C2B	3.29	1.50	1.43
26	d	402	PHO	C4D-CHA	3.29	1.44	1.39
25	c	509	CLA	MG-ND	3.28	2.12	2.05
32	C	516	DGD	C4D-C3D	3.27	1.60	1.52
27	b	618	BCR	C1-C6	-3.27	1.49	1.53
27	c	514	BCR	C30-C25	-3.27	1.49	1.53
30	B	622	SQD	O5-C1	3.26	1.50	1.41
30	F	101	SQD	O5-C1	3.26	1.50	1.41
25	C	501	CLA	MG-NA	3.25	2.14	2.06
30	B	622	SQD	O47-C45	-3.25	1.38	1.46
27	k	101	BCR	C1-C6	-3.25	1.49	1.53
25	c	503	CLA	C1B-C2B	3.25	1.50	1.43
25	b	611	CLA	C1B-C2B	3.25	1.50	1.43
25	b	601	CLA	C4B-NB	3.24	1.42	1.37
25	b	609	CLA	MG-ND	-3.24	1.99	2.05
25	B	603	CLA	MG-ND	3.23	2.12	2.05
27	B	617	BCR	C1-C6	-3.23	1.49	1.53
25	C	512	CLA	C1D-ND	3.22	1.42	1.37
27	K	101	BCR	C30-C25	-3.22	1.49	1.53
30	f	102	SQD	C24-C23	3.22	1.60	1.50
25	d	403	CLA	MG-NA	3.21	2.13	2.06
25	b	613	CLA	MG-ND	-3.21	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	613	SQD	C24-C23	3.19	1.60	1.50
25	c	508	CLA	C1D-ND	3.19	1.42	1.37
25	A	607	CLA	MG-NA	3.18	2.13	2.06
25	b	609	CLA	C1D-ND	3.18	1.42	1.37
25	C	502	CLA	MG-ND	-3.18	1.99	2.05
25	c	513	CLA	C4B-NB	3.18	1.42	1.37
32	A	617	DGD	O5D-C6D	-3.17	1.38	1.43
25	b	607	CLA	C1D-ND	3.17	1.42	1.37
25	C	501	CLA	C4B-NB	3.17	1.42	1.37
25	B	615	CLA	C1B-C2B	3.17	1.50	1.43
25	b	610	CLA	C1B-C2B	3.16	1.50	1.43
25	c	511	CLA	C4B-NB	3.15	1.42	1.37
25	B	610	CLA	C4B-NB	3.15	1.42	1.37
25	C	511	CLA	C1D-ND	3.14	1.42	1.37
25	A	606	CLA	C1D-ND	3.14	1.42	1.37
30	a	614	SQD	O47-C45	-3.14	1.39	1.46
25	a	607	CLA	C4B-NB	3.13	1.42	1.37
25	b	611	CLA	C1D-ND	3.13	1.42	1.37
25	b	610	CLA	MG-NA	3.13	2.13	2.06
25	B	601	CLA	C4B-NB	3.12	1.42	1.37
25	C	510	CLA	C1D-ND	3.12	1.42	1.37
25	c	509	CLA	C4B-NB	3.12	1.42	1.37
25	C	507	CLA	C1D-ND	3.12	1.42	1.37
27	B	619	BCR	C1-C6	-3.11	1.49	1.53
25	c	509	CLA	MG-NC	3.11	2.13	2.06
25	c	512	CLA	C4B-NB	3.10	1.41	1.37
25	c	511	CLA	C1B-C2B	3.10	1.50	1.43
25	C	502	CLA	C1D-ND	3.10	1.41	1.37
25	C	507	CLA	C1B-C2B	3.10	1.50	1.43
25	d	404	CLA	C4B-NB	3.09	1.41	1.37
35	E	101	HEM	FE-NA	3.09	2.05	1.95
25	a	609	CLA	C1B-C2B	3.09	1.50	1.43
25	b	608	CLA	MG-NA	3.09	2.13	2.06
25	B	609	CLA	C1B-C2B	3.08	1.50	1.43
31	d	407	LHG	O7-C5	-3.08	1.39	1.46
25	C	511	CLA	C1B-C2B	3.08	1.50	1.43
31	D	410	LHG	P-O6	3.08	1.71	1.59
25	D	403	CLA	MG-NB	-3.08	1.99	2.05
27	H	101	BCR	C30-C25	-3.08	1.49	1.53
25	c	503	CLA	MG-NA	3.07	2.13	2.06
25	B	606	CLA	C4B-NB	3.07	1.41	1.37
27	K	102	BCR	C30-C25	-3.07	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	101	SQD	O47-C45	-3.06	1.39	1.46
27	b	619	BCR	C1-C6	-3.06	1.49	1.53
30	A	616	SQD	C24-C23	3.05	1.59	1.50
25	b	601	CLA	C1B-C2B	3.05	1.50	1.43
25	C	513	CLA	C4B-NB	3.05	1.41	1.37
25	C	505	CLA	C1D-ND	3.05	1.41	1.37
25	b	603	CLA	MG-NB	-3.04	1.99	2.05
27	b	619	BCR	C30-C25	-3.04	1.49	1.53
30	A	613	SQD	O47-C7	3.04	1.42	1.34
25	B	612	CLA	C1D-ND	3.04	1.41	1.37
25	c	513	CLA	MG-NC	3.04	2.13	2.06
25	b	604	CLA	C1B-C2B	3.03	1.50	1.43
25	c	512	CLA	C1B-C2B	3.03	1.50	1.43
32	C	515	DGD	O2G-C2G	-3.03	1.39	1.46
30	f	102	SQD	O5-C1	3.03	1.49	1.41
30	B	622	SQD	C24-C23	3.03	1.59	1.50
25	a	612	CLA	C1B-C2B	3.03	1.50	1.43
25	C	503	CLA	C1B-C2B	3.03	1.50	1.43
25	b	608	CLA	C4B-NB	3.03	1.41	1.37
30	a	613	SQD	O47-C7	3.03	1.42	1.34
25	D	405	CLA	MG-NA	3.02	2.13	2.06
30	a	613	SQD	C24-C23	3.02	1.59	1.50
26	d	401	PHO	C3D-C4D	3.01	1.45	1.41
25	C	513	CLA	C1B-C2B	3.01	1.50	1.43
27	c	516	BCR	C1-C6	-3.01	1.49	1.53
25	D	403	CLA	C4B-NB	3.00	1.41	1.37
25	C	508	CLA	C4B-NB	2.99	1.41	1.37
35	E	101	HEM	CAB-C3B	2.99	1.55	1.47
25	b	615	CLA	C1D-ND	2.98	1.41	1.37
30	L	101	SQD	O5-C1	2.98	1.49	1.41
25	b	603	CLA	MG-NA	2.98	2.13	2.06
25	a	607	CLA	C1B-C2B	2.98	1.50	1.43
25	b	605	CLA	C3B-C4B	2.98	1.51	1.42
25	b	605	CLA	C4B-NB	2.98	1.41	1.37
32	c	519	DGD	C6D-C5D	2.97	1.60	1.51
27	x	101	BCR	C30-C25	-2.97	1.50	1.53
27	K	101	BCR	C1-C6	-2.96	1.50	1.53
26	d	402	PHO	CMC-C2C	-2.96	1.46	1.50
25	c	501	CLA	C4B-NB	2.96	1.41	1.37
25	C	508	CLA	C1B-C2B	2.96	1.50	1.43
25	B	610	CLA	C1B-C2B	2.95	1.50	1.43
25	c	508	CLA	C4B-NB	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	MG-ND	-2.94	1.99	2.05
25	c	507	CLA	C1B-C2B	2.94	1.50	1.43
35	E	101	HEM	FE-NC	2.93	2.04	1.95
27	k	101	BCR	C30-C25	-2.93	1.50	1.53
25	b	605	CLA	C1D-ND	2.93	1.41	1.37
25	C	510	CLA	C4B-NB	2.92	1.41	1.37
27	b	617	BCR	C1-C6	-2.92	1.50	1.53
27	A	610	BCR	C1-C6	-2.92	1.50	1.53
25	c	506	CLA	MG-NC	2.92	2.13	2.06
32	H	102	DGD	O5D-C1E	2.92	1.45	1.40
25	B	602	CLA	C1B-C2B	2.91	1.50	1.43
25	c	505	CLA	C4B-NB	2.91	1.41	1.37
25	B	603	CLA	C3B-C4B	2.91	1.51	1.42
25	C	505	CLA	C4B-NB	2.91	1.41	1.37
25	c	504	CLA	MG-ND	-2.91	2.00	2.05
35	f	101	HEM	CAC-C3C	2.91	1.55	1.47
25	B	613	CLA	C1D-ND	2.90	1.41	1.37
25	B	610	CLA	C3B-C4B	2.90	1.51	1.42
25	B	608	CLA	C4B-NB	2.90	1.41	1.37
25	c	505	CLA	C1B-C2B	2.89	1.49	1.43
25	B	610	CLA	C1D-ND	2.89	1.41	1.37
25	B	616	CLA	C1B-C2B	2.89	1.49	1.43
27	c	516	BCR	C30-C25	-2.89	1.50	1.53
25	C	509	CLA	C4B-NB	2.88	1.41	1.37
25	a	609	CLA	C1D-ND	2.87	1.41	1.37
25	c	507	CLA	C4B-NB	2.86	1.41	1.37
27	c	515	BCR	C30-C25	-2.86	1.50	1.53
25	b	605	CLA	C1B-C2B	2.86	1.49	1.43
32	a	615	DGD	O1G-C1A	2.86	1.41	1.33
30	L	101	SQD	C24-C23	2.86	1.59	1.50
25	B	611	CLA	CHC-C1C	2.85	1.44	1.38
25	a	609	CLA	C4B-NB	2.85	1.41	1.37
25	B	610	CLA	CHC-C1C	2.83	1.44	1.38
25	c	505	CLA	C1D-ND	2.82	1.41	1.37
25	c	510	CLA	MG-NC	2.82	2.13	2.06
25	b	603	CLA	C4B-NB	2.82	1.41	1.37
25	C	510	CLA	MG-NA	2.82	2.13	2.06
25	C	507	CLA	MG-NA	2.81	2.13	2.06
26	A	608	PHO	C3D-C4D	2.81	1.45	1.41
25	C	507	CLA	C4B-NB	2.81	1.41	1.37
25	C	511	CLA	C4B-NB	2.80	1.41	1.37
25	c	508	CLA	C1B-C2B	2.80	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	CMC-C2C	-2.78	1.46	1.50
25	b	607	CLA	C4B-NB	2.78	1.41	1.37
27	Y	101	BCR	C30-C25	-2.78	1.50	1.53
25	b	608	CLA	CHC-C1C	2.78	1.44	1.38
25	A	606	CLA	C1B-C2B	2.77	1.49	1.43
27	K	102	BCR	C1-C6	-2.77	1.50	1.53
25	C	510	CLA	C1B-C2B	2.77	1.49	1.43
25	c	502	CLA	C4B-NB	2.77	1.41	1.37
25	c	501	CLA	C1B-C2B	2.77	1.49	1.43
30	A	613	SQD	O5-C1	2.77	1.49	1.41
25	A	607	CLA	C4B-NB	2.77	1.41	1.37
26	D	402	PHO	CMC-C2C	-2.76	1.46	1.50
25	B	605	CLA	MG-NA	2.76	2.12	2.06
25	B	613	CLA	MG-NA	2.76	2.12	2.06
25	b	615	CLA	C4B-NB	2.76	1.41	1.37
28	D	407	PL9	C52-C5	-2.75	1.45	1.50
25	b	608	CLA	C3B-C4B	2.75	1.50	1.42
25	C	513	CLA	MG-NA	2.75	2.12	2.06
32	h	101	DGD	O2G-C2G	-2.74	1.40	1.46
25	a	608	CLA	C4B-NB	2.74	1.41	1.37
25	B	613	CLA	C4B-NB	2.74	1.41	1.37
25	c	506	CLA	C4B-NB	2.74	1.41	1.37
29	m	101	LMG	C4-C3	2.73	1.59	1.52
25	C	506	CLA	C4B-NB	2.73	1.41	1.37
25	A	607	CLA	C1B-C2B	2.73	1.49	1.43
25	d	403	CLA	C1B-C2B	2.72	1.49	1.43
25	c	504	CLA	C1D-ND	2.72	1.41	1.37
25	b	615	CLA	C1B-C2B	2.72	1.49	1.43
25	c	505	CLA	C3B-C4B	2.72	1.50	1.42
25	a	608	CLA	MG-ND	-2.72	2.00	2.05
25	C	512	CLA	C1B-C2B	2.71	1.49	1.43
25	a	612	CLA	C4B-NB	2.70	1.41	1.37
25	B	608	CLA	C1B-C2B	2.70	1.49	1.43
27	a	610	BCR	C1-C6	-2.70	1.50	1.53
25	B	605	CLA	C1D-ND	2.70	1.41	1.37
25	c	503	CLA	C4B-NB	2.70	1.41	1.37
25	b	614	CLA	C1B-C2B	2.69	1.49	1.43
26	D	402	PHO	C4D-CHA	2.69	1.43	1.39
25	c	513	CLA	C1B-C2B	2.69	1.49	1.43
25	C	506	CLA	MG-NA	2.69	2.12	2.06
27	T	101	BCR	C30-C25	-2.69	1.50	1.53
25	c	504	CLA	CHC-C1C	2.69	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	403	CLA	C1B-C2B	2.69	1.49	1.43
25	c	510	CLA	C1B-C2B	2.68	1.49	1.43
25	b	613	CLA	C4B-NB	2.68	1.41	1.37
25	D	405	CLA	C1B-C2B	2.68	1.49	1.43
32	A	617	DGD	C1E-C2E	2.67	1.60	1.52
26	d	402	PHO	CAC-C3C	-2.67	1.47	1.51
35	f	101	HEM	CAB-C3B	2.67	1.54	1.47
25	b	602	CLA	C1B-C2B	2.67	1.49	1.43
25	B	614	CLA	MG-NB	2.66	2.11	2.05
25	B	611	CLA	C4B-NB	2.66	1.41	1.37
25	c	511	CLA	CHC-C1C	2.66	1.43	1.38
25	C	502	CLA	MG-NA	2.66	2.12	2.06
25	B	616	CLA	C4B-NB	2.66	1.41	1.37
31	d	409	LHG	P-O6	2.66	1.69	1.59
25	C	509	CLA	CHC-C1C	2.66	1.43	1.38
27	B	617	BCR	C30-C25	-2.65	1.50	1.53
25	B	612	CLA	MG-NA	2.65	2.12	2.06
25	C	509	CLA	C1B-C2B	2.65	1.49	1.43
25	b	603	CLA	C1B-C2B	2.65	1.49	1.43
25	b	613	CLA	C1B-C2B	2.64	1.49	1.43
25	C	502	CLA	C3B-C4B	2.63	1.50	1.42
25	a	608	CLA	CHC-C1C	2.63	1.43	1.38
25	C	511	CLA	C3B-C4B	2.63	1.50	1.42
29	c	524	LMG	C4-C5	2.63	1.58	1.53
28	A	611	PL9	C7-C3	-2.63	1.47	1.51
25	D	405	CLA	C4B-NB	2.63	1.41	1.37
25	B	604	CLA	C1B-C2B	2.63	1.49	1.43
25	b	601	CLA	CHC-C1C	2.62	1.43	1.38
30	A	616	SQD	C46-C45	2.62	1.56	1.50
25	c	505	CLA	CHC-C1C	2.62	1.43	1.38
25	B	613	CLA	C1B-C2B	2.61	1.49	1.43
31	D	412	LHG	C24-C23	2.61	1.58	1.50
25	C	504	CLA	CHC-C1C	2.61	1.43	1.38
25	C	512	CLA	C4B-NB	2.61	1.41	1.37
25	C	504	CLA	C3B-C4B	2.61	1.50	1.42
25	b	608	CLA	C1B-C2B	2.61	1.49	1.43
32	h	101	DGD	C1E-C2E	2.61	1.60	1.52
25	B	606	CLA	CHC-C1C	2.60	1.43	1.38
25	B	605	CLA	C3B-C4B	2.60	1.50	1.42
29	d	411	LMG	C4-C5	2.60	1.58	1.53
31	A	614	LHG	P-O6	2.60	1.69	1.59
25	B	609	CLA	C4B-NB	2.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	611	PL9	C53-C6	-2.60	1.45	1.50
26	D	402	PHO	C4D-ND	-2.59	1.34	1.38
25	B	610	CLA	CMB-C2B	-2.59	1.45	1.50
29	b	621	LMG	C3-C2	2.59	1.59	1.52
25	C	508	CLA	C3B-C4B	2.59	1.50	1.42
25	D	405	CLA	MG-NC	2.59	2.12	2.06
25	B	603	CLA	CHC-C1C	2.58	1.43	1.38
25	c	513	CLA	C3B-C4B	2.58	1.50	1.42
26	D	402	PHO	CMB-C2B	-2.57	1.46	1.51
25	b	614	CLA	MG-ND	-2.57	2.00	2.05
27	b	617	BCR	C30-C25	-2.57	1.50	1.53
27	C	514	BCR	C30-C25	-2.57	1.50	1.53
25	c	510	CLA	MG-NA	2.57	2.12	2.06
25	B	606	CLA	C1B-C2B	2.56	1.49	1.43
25	D	404	CLA	C4B-NB	2.56	1.41	1.37
25	b	606	CLA	C1B-C2B	2.56	1.49	1.43
25	B	605	CLA	C4B-NB	2.56	1.41	1.37
25	c	513	CLA	MG-ND	-2.56	2.00	2.05
25	a	609	CLA	C3B-C4B	2.56	1.50	1.42
35	E	101	HEM	CAC-C3C	2.56	1.54	1.47
25	A	609	CLA	MG-ND	-2.55	2.00	2.05
25	B	603	CLA	CMC-C2C	-2.55	1.45	1.50
32	A	617	DGD	C3E-C2E	2.55	1.58	1.52
31	D	409	LHG	P-O6	2.55	1.69	1.59
32	A	617	DGD	C4D-C5D	2.55	1.58	1.53
25	c	512	CLA	C3B-C4B	2.55	1.50	1.42
32	c	519	DGD	O2G-C2G	-2.54	1.40	1.46
25	B	604	CLA	C3B-C4B	2.54	1.50	1.42
25	B	611	CLA	C1B-C2B	2.54	1.49	1.43
25	B	607	CLA	C3B-C4B	2.54	1.50	1.42
25	c	502	CLA	C1B-C2B	2.53	1.49	1.43
25	B	615	CLA	CHC-C1C	2.53	1.43	1.38
25	c	510	CLA	MG-ND	-2.52	2.00	2.05
29	m	101	LMG	O7-C8	-2.52	1.40	1.46
32	H	102	DGD	O1G-C1G	-2.52	1.39	1.45
25	b	611	CLA	C4B-NB	2.52	1.41	1.37
25	C	513	CLA	C3B-C4B	2.52	1.50	1.42
25	C	505	CLA	CHC-C1C	2.51	1.43	1.38
30	a	613	SQD	O5-C1	2.51	1.48	1.41
26	d	402	PHO	CMD-C2D	-2.51	1.46	1.51
25	B	602	CLA	CHC-C1C	2.51	1.43	1.38
25	b	609	CLA	CMB-C2B	-2.50	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	e	101	LHG	P-O6	2.50	1.69	1.59
25	c	502	CLA	MG-NB	-2.49	2.00	2.05
27	t	101	BCR	C1-C6	-2.49	1.50	1.53
26	D	402	PHO	CMD-C2D	-2.49	1.46	1.51
25	b	605	CLA	CHC-C1C	2.49	1.43	1.38
25	C	510	CLA	CHC-C1C	2.49	1.43	1.38
25	C	502	CLA	C4B-NB	2.48	1.41	1.37
26	A	608	PHO	CMD-C2D	-2.48	1.46	1.51
25	B	601	CLA	C3B-C4B	2.48	1.50	1.42
29	D	411	LMG	C7-C8	2.48	1.57	1.51
25	B	604	CLA	CHC-C1C	2.48	1.43	1.38
32	A	617	DGD	C6E-C5E	2.47	1.60	1.51
25	B	602	CLA	C3B-C4B	2.47	1.49	1.42
25	B	612	CLA	CHC-C1C	2.47	1.43	1.38
25	B	612	CLA	C1B-C2B	2.47	1.48	1.43
25	b	615	CLA	C3B-C4B	2.47	1.49	1.42
25	c	508	CLA	CHC-C1C	2.47	1.43	1.38
25	d	404	CLA	CHC-C1C	2.47	1.43	1.38
25	b	602	CLA	C4B-NB	2.47	1.41	1.37
25	D	403	CLA	CHC-C1C	2.47	1.43	1.38
25	A	606	CLA	C4B-NB	2.46	1.41	1.37
25	C	503	CLA	C3B-C4B	2.46	1.49	1.42
32	C	516	DGD	C1E-C2E	2.46	1.59	1.52
25	c	508	CLA	C3B-C4B	2.46	1.49	1.42
25	b	614	CLA	CHC-C1C	2.46	1.43	1.38
25	b	616	CLA	C1B-C2B	2.46	1.48	1.43
25	b	602	CLA	C3B-C4B	2.46	1.49	1.42
25	C	506	CLA	C1B-C2B	2.46	1.48	1.43
25	C	503	CLA	CHC-C1C	2.45	1.43	1.38
25	c	513	CLA	CHC-C1C	2.45	1.43	1.38
25	C	512	CLA	CHC-C1C	2.45	1.43	1.38
25	C	504	CLA	C1B-C2B	2.45	1.48	1.43
25	C	512	CLA	C3B-C4B	2.45	1.49	1.42
25	c	510	CLA	CMD-C2D	-2.44	1.45	1.50
28	d	406	PL9	C6-C1	-2.44	1.44	1.48
25	C	502	CLA	CHC-C1C	2.44	1.43	1.38
25	a	607	CLA	CHC-C1C	2.43	1.43	1.38
30	a	613	SQD	O7-S	2.43	1.52	1.45
25	c	503	CLA	CHC-C1C	2.43	1.43	1.38
25	b	615	CLA	CMD-C2D	-2.43	1.45	1.50
25	C	513	CLA	CHC-C1C	2.42	1.43	1.38
25	C	510	CLA	C3B-C4B	2.42	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C1B-C2B	2.42	1.48	1.43
25	b	601	CLA	C3B-C4B	2.42	1.49	1.42
32	C	515	DGD	C4D-C3D	2.42	1.58	1.52
25	A	609	CLA	C4B-NB	2.41	1.41	1.37
25	b	614	CLA	MG-NA	2.41	2.12	2.06
25	c	506	CLA	CHC-C1C	2.41	1.43	1.38
25	C	507	CLA	C3B-C4B	2.41	1.49	1.42
30	B	622	SQD	O9-S	2.41	1.51	1.45
26	D	402	PHO	CAC-C3C	-2.40	1.47	1.51
25	B	603	CLA	C1D-ND	2.40	1.41	1.37
25	b	604	CLA	CHC-C1C	2.40	1.43	1.38
25	C	502	CLA	C1B-C2B	2.40	1.48	1.43
30	A	613	SQD	O9-S	2.40	1.51	1.45
27	B	618	BCR	C1-C6	-2.40	1.50	1.53
25	b	606	CLA	C4B-NB	2.39	1.41	1.37
25	b	615	CLA	MG-ND	-2.39	2.01	2.05
25	D	405	CLA	CMC-C2C	-2.38	1.45	1.50
25	D	403	CLA	C1D-C2D	2.38	1.50	1.45
25	C	509	CLA	C3B-C4B	2.38	1.49	1.42
30	F	101	SQD	O7-S	2.38	1.51	1.45
25	B	603	CLA	CMD-C2D	-2.38	1.45	1.50
25	A	607	CLA	C3B-C4B	2.38	1.49	1.42
25	c	504	CLA	C1B-C2B	2.38	1.48	1.43
32	c	518	DGD	C4D-C3D	2.38	1.58	1.52
25	C	501	CLA	C1B-C2B	2.37	1.48	1.43
29	M	101	LMG	C4-C5	2.37	1.58	1.53
32	H	102	DGD	C4D-C5D	2.37	1.58	1.53
30	F	101	SQD	O9-S	2.37	1.51	1.45
25	C	501	CLA	C3B-C4B	2.36	1.49	1.42
25	b	616	CLA	C4B-NB	2.36	1.41	1.37
25	b	613	CLA	CMB-C2B	-2.36	1.45	1.50
25	B	614	CLA	CHC-C1C	2.36	1.43	1.38
25	A	606	CLA	C3B-C4B	2.35	1.49	1.42
25	b	607	CLA	CMD-C2D	-2.35	1.45	1.50
25	c	506	CLA	C3B-C4B	2.35	1.49	1.42
25	c	506	CLA	MG-ND	-2.35	2.01	2.05
32	C	516	DGD	C1G-C2G	2.35	1.58	1.50
26	d	401	PHO	C4D-ND	-2.35	1.35	1.38
25	b	614	CLA	CMC-C2C	-2.35	1.45	1.50
25	C	508	CLA	CHC-C1C	2.35	1.43	1.38
25	B	605	CLA	CHC-C1C	2.35	1.43	1.38
25	C	506	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	609	CLA	CMC-C2C	-2.35	1.46	1.50
25	b	604	CLA	C3B-C4B	2.35	1.49	1.42
25	d	404	CLA	C3B-C4B	2.34	1.49	1.42
30	L	101	SQD	O9-S	2.34	1.51	1.45
28	d	406	PL9	C46-C44	-2.34	1.46	1.51
25	c	512	CLA	CHC-C1C	2.34	1.43	1.38
30	F	101	SQD	O5-C5	2.33	1.50	1.44
25	D	404	CLA	CMD-C2D	-2.33	1.46	1.50
30	f	102	SQD	O9-S	2.33	1.51	1.45
25	b	615	CLA	CMB-C2B	-2.32	1.46	1.50
25	d	403	CLA	C3B-C4B	2.32	1.49	1.42
25	B	607	CLA	C1B-C2B	2.32	1.48	1.43
32	C	515	DGD	C4E-C3E	2.32	1.58	1.52
32	c	518	DGD	C3D-C2D	2.32	1.58	1.52
25	B	616	CLA	CMC-C2C	-2.32	1.46	1.50
25	d	403	CLA	CMB-C2B	-2.32	1.46	1.50
25	B	601	CLA	CMC-C2C	-2.31	1.46	1.50
25	B	604	CLA	C4B-NB	2.31	1.40	1.37
25	B	609	CLA	CMD-C2D	-2.31	1.46	1.50
25	c	510	CLA	CMB-C2B	-2.31	1.46	1.50
25	B	616	CLA	MG-NC	2.30	2.11	2.06
25	b	610	CLA	C4B-NB	2.30	1.40	1.37
25	C	507	CLA	CHC-C1C	2.30	1.43	1.38
25	c	506	CLA	C1B-C2B	2.30	1.48	1.43
36	V	201	HEC	CMC-C2C	2.30	1.55	1.50
25	A	607	CLA	CHC-C1C	2.30	1.43	1.38
32	C	517	DGD	C6D-C5D	2.29	1.58	1.51
25	a	607	CLA	CMB-C2B	-2.29	1.46	1.50
25	b	612	CLA	MG-NC	2.29	2.11	2.06
26	d	401	PHO	O2D-CGD	2.29	1.38	1.33
25	a	612	CLA	MG-NB	-2.29	2.01	2.05
25	b	611	CLA	CMD-C2D	-2.29	1.46	1.50
25	b	603	CLA	CMD-C2D	-2.28	1.46	1.50
25	c	509	CLA	C3B-C4B	2.28	1.49	1.42
25	c	510	CLA	C4B-NB	2.28	1.40	1.37
25	B	612	CLA	C4B-NB	2.28	1.40	1.37
25	b	604	CLA	MG-NC	2.28	2.11	2.06
25	c	504	CLA	C3B-C4B	2.28	1.49	1.42
25	B	608	CLA	CMD-C2D	-2.28	1.46	1.50
31	A	615	LHG	O8-C23	2.27	1.40	1.33
25	b	614	CLA	C3B-C4B	2.27	1.49	1.42
25	B	612	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	622	SQD	O7-S	2.26	1.51	1.45
25	B	608	CLA	C1D-C2D	2.26	1.49	1.45
25	B	604	CLA	MG-NA	2.26	2.11	2.06
29	c	522	LMG	C3-C2	2.25	1.58	1.52
25	d	403	CLA	CHC-C1C	2.25	1.43	1.38
25	b	610	CLA	C3B-C4B	2.25	1.49	1.42
25	a	608	CLA	C1B-C2B	2.25	1.48	1.43
27	x	101	BCR	C1-C6	-2.25	1.50	1.53
25	c	503	CLA	C3B-C4B	2.25	1.49	1.42
25	c	504	CLA	CMD-C2D	-2.24	1.46	1.50
25	b	606	CLA	CHC-C1C	2.24	1.43	1.38
25	B	604	CLA	MG-NB	2.24	2.10	2.05
32	c	519	DGD	O1G-C1G	-2.24	1.40	1.45
25	b	613	CLA	CMD-C2D	-2.24	1.46	1.50
25	B	607	CLA	CHC-C1C	2.24	1.43	1.38
25	b	609	CLA	MG-NA	2.24	2.11	2.06
25	c	503	CLA	CMC-C2C	-2.24	1.46	1.50
25	B	601	CLA	CMB-C2B	-2.24	1.46	1.50
25	c	501	CLA	CHC-C1C	2.24	1.43	1.38
28	d	406	PL9	C41-C39	-2.24	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.24	1.46	1.50
25	C	506	CLA	CHC-C1C	2.24	1.43	1.38
30	f	102	SQD	O7-S	2.24	1.51	1.45
29	c	522	LMG	C4-C3	2.23	1.58	1.52
25	b	609	CLA	C1B-C2B	2.23	1.48	1.43
25	B	601	CLA	CHC-C1C	2.23	1.43	1.38
31	A	615	LHG	O7-C5	-2.23	1.41	1.46
32	c	518	DGD	O6D-C5D	-2.23	1.38	1.44
25	b	616	CLA	C3B-C4B	2.23	1.49	1.42
32	c	517	DGD	C4D-C3D	2.22	1.58	1.52
25	C	511	CLA	CMB-C2B	-2.22	1.46	1.50
25	B	613	CLA	CMD-C2D	-2.22	1.46	1.50
25	D	405	CLA	C3B-C4B	2.22	1.49	1.42
25	b	616	CLA	CMC-C2C	-2.22	1.46	1.50
25	b	607	CLA	CHC-C1C	2.22	1.42	1.38
25	C	513	CLA	CMC-C2C	-2.22	1.46	1.50
25	C	506	CLA	C1B-NB	-2.22	1.34	1.37
32	H	102	DGD	C1E-C2E	2.22	1.59	1.52
27	a	610	BCR	C30-C25	-2.22	1.50	1.53
29	d	411	LMG	O1-C7	-2.21	1.39	1.43
25	A	606	CLA	CHC-C1C	2.21	1.42	1.38
29	A	612	LMG	C4-C5	2.21	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	CMB-C2B	-2.21	1.47	1.51
25	d	404	CLA	C1B-C2B	2.21	1.48	1.43
25	c	502	CLA	C3B-C4B	2.21	1.49	1.42
25	B	613	CLA	CHC-C1C	2.21	1.42	1.38
32	c	518	DGD	O2G-C2G	-2.21	1.41	1.46
25	b	609	CLA	C3B-C4B	2.20	1.49	1.42
25	b	602	CLA	CHC-C1C	2.20	1.42	1.38
25	b	607	CLA	C1B-C2B	2.20	1.48	1.43
29	C	518	LMG	O7-C8	-2.20	1.41	1.46
25	d	403	CLA	CMD-C2D	-2.20	1.46	1.50
25	A	609	CLA	C1B-C2B	2.20	1.48	1.43
27	H	101	BCR	C1-C6	-2.20	1.51	1.53
25	c	502	CLA	CMD-C2D	-2.20	1.46	1.50
25	c	506	CLA	CMC-C2C	-2.20	1.46	1.50
30	B	622	SQD	C8-C7	2.20	1.57	1.50
26	A	608	PHO	C4D-ND	-2.20	1.35	1.38
35	f	101	HEM	CMA-C3A	2.20	1.55	1.50
25	c	510	CLA	CHC-C1C	2.20	1.42	1.38
26	d	401	PHO	CMB-C2B	-2.19	1.47	1.51
25	c	508	CLA	MG-ND	2.19	2.10	2.05
26	D	402	PHO	C3D-C4D	2.19	1.44	1.41
26	d	401	PHO	CMC-C2C	-2.19	1.47	1.50
25	b	615	CLA	CHC-C1C	2.19	1.42	1.38
32	C	516	DGD	O2G-C2G	-2.19	1.41	1.46
25	c	511	CLA	C3B-C4B	2.19	1.49	1.42
35	f	101	HEM	C3B-C2B	-2.18	1.32	1.37
29	b	621	LMG	C1-C2	2.18	1.58	1.52
25	b	612	CLA	C1B-C2B	2.18	1.48	1.43
32	h	101	DGD	C4D-C3D	2.18	1.58	1.52
30	f	102	SQD	O5-C5	2.18	1.49	1.44
25	C	509	CLA	O2D-CGD	2.18	1.38	1.33
25	C	510	CLA	MG-NC	2.18	2.11	2.06
25	B	611	CLA	CMD-C2D	-2.17	1.46	1.50
25	B	613	CLA	C3B-C4B	2.17	1.49	1.42
25	B	607	CLA	C4B-NB	2.17	1.40	1.37
25	B	606	CLA	C3B-C4B	2.17	1.49	1.42
25	c	512	CLA	C1D-C2D	2.16	1.49	1.45
25	b	608	CLA	C3C-C2C	2.16	1.41	1.36
29	m	101	LMG	O1-C7	-2.16	1.40	1.43
25	D	404	CLA	C3B-C4B	2.16	1.49	1.42
36	v	201	HEC	C3B-C2B	-2.15	1.33	1.41
25	c	509	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	C3B-C4B	2.15	1.49	1.42
25	A	606	CLA	MG-ND	-2.15	2.01	2.05
25	a	609	CLA	CMD-C2D	-2.15	1.46	1.50
35	f	101	HEM	CMC-C2C	2.15	1.55	1.50
30	L	101	SQD	O7-S	2.15	1.51	1.45
36	v	201	HEC	CMC-C2C	2.14	1.55	1.50
27	B	619	BCR	C30-C25	-2.14	1.51	1.53
25	C	512	CLA	CMD-C2D	-2.14	1.46	1.50
32	c	517	DGD	C4D-C5D	2.14	1.57	1.53
29	D	408	LMG	O2-C2	-2.14	1.37	1.43
25	c	504	CLA	CMC-C2C	-2.14	1.46	1.50
25	d	404	CLA	MG-NA	2.14	2.11	2.06
25	C	503	CLA	MG-NC	2.14	2.11	2.06
31	d	408	LHG	O7-C5	-2.14	1.41	1.46
36	V	201	HEC	CMB-C2B	2.14	1.55	1.50
32	C	517	DGD	O1G-C1G	-2.13	1.40	1.45
25	B	607	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	603	CLA	C4B-NB	2.13	1.40	1.37
25	c	508	CLA	CMD-C2D	-2.13	1.46	1.50
25	a	608	CLA	CMB-C2B	-2.13	1.46	1.50
25	b	612	CLA	CMC-C2C	-2.12	1.46	1.50
30	a	614	SQD	C44-C45	2.12	1.56	1.51
32	A	617	DGD	C4E-C5E	2.12	1.57	1.53
25	D	403	CLA	MG-NC	2.12	2.11	2.06
25	C	504	CLA	C1B-NB	-2.12	1.35	1.37
25	C	511	CLA	CHC-C1C	2.12	1.42	1.38
25	B	606	CLA	CMB-C2B	-2.12	1.46	1.50
29	c	524	LMG	C1-C2	2.12	1.58	1.52
25	a	608	CLA	C3B-C4B	2.12	1.48	1.42
36	v	201	HEC	CMB-C2B	2.12	1.55	1.50
25	a	612	CLA	CMB-C2B	-2.12	1.46	1.50
32	C	517	DGD	O2G-C2G	-2.12	1.41	1.46
27	t	101	BCR	C30-C25	-2.11	1.51	1.53
29	c	522	LMG	C1-C2	2.11	1.58	1.52
25	b	607	CLA	C3B-C4B	2.11	1.48	1.42
27	B	617	BCR	C33-C5	-2.11	1.47	1.50
27	k	101	BCR	C33-C5	-2.11	1.47	1.50
25	C	506	CLA	CMC-C2C	-2.11	1.46	1.50
25	b	612	CLA	C3B-C4B	2.11	1.48	1.42
25	c	501	CLA	CMB-C2B	-2.11	1.46	1.50
35	E	101	HEM	CMD-C2D	2.11	1.55	1.50
25	B	604	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	O5D-C6D	-2.10	1.40	1.43
31	d	407	LHG	C24-C23	2.10	1.56	1.50
25	B	612	CLA	CMC-C2C	-2.10	1.46	1.50
32	H	102	DGD	O2G-C2G	-2.09	1.41	1.46
25	C	508	CLA	C1D-C2D	2.09	1.49	1.45
31	A	615	LHG	P-O6	2.09	1.67	1.59
25	c	502	CLA	CHC-C1C	2.09	1.42	1.38
25	B	614	CLA	C1B-C2B	2.09	1.48	1.43
32	A	617	DGD	O2G-C2G	-2.09	1.41	1.46
25	C	512	CLA	C1D-C2D	2.09	1.49	1.45
25	A	609	CLA	MG-NA	-2.09	2.01	2.06
25	c	508	CLA	CMC-C2C	-2.08	1.46	1.50
25	b	609	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	606	CLA	C3B-C4B	2.08	1.48	1.42
31	l	101	LHG	P-O6	2.08	1.67	1.59
30	a	613	SQD	O9-S	2.08	1.51	1.45
25	B	605	CLA	CMC-C2C	-2.08	1.46	1.50
25	C	501	CLA	CHC-C1C	2.08	1.42	1.38
25	A	609	CLA	CMD-C2D	-2.08	1.46	1.50
25	a	607	CLA	C3B-C4B	2.08	1.48	1.42
25	b	616	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	616	CLA	C3B-C4B	2.07	1.48	1.42
25	D	405	CLA	CMB-C2B	-2.07	1.46	1.50
25	b	603	CLA	CMB-C2B	-2.07	1.46	1.50
32	C	516	DGD	C4D-C5D	2.07	1.57	1.53
25	C	507	CLA	CMB-C2B	-2.07	1.46	1.50
26	d	401	PHO	CMD-C2D	-2.07	1.47	1.51
25	c	501	CLA	MG-NC	2.07	2.11	2.06
25	B	607	CLA	C3D-C4D	2.06	1.48	1.44
25	b	611	CLA	CHC-C1C	2.06	1.42	1.38
25	a	608	CLA	CMC-C2C	-2.06	1.46	1.50
25	B	608	CLA	CMB-C2B	-2.06	1.46	1.50
32	a	615	DGD	C1G-C2G	2.06	1.57	1.50
25	b	613	CLA	C3B-C4B	2.06	1.48	1.42
25	B	611	CLA	C3B-C4B	2.05	1.48	1.42
25	B	614	CLA	CMB-C2B	-2.05	1.46	1.50
25	b	610	CLA	CMD-C2D	-2.05	1.46	1.50
27	d	405	BCR	C38-C26	-2.05	1.47	1.50
25	b	601	CLA	C3D-C4D	2.05	1.48	1.44
25	B	606	CLA	CMD-C2D	-2.05	1.46	1.50
25	c	512	CLA	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	C3B-C4B	2.05	1.48	1.42
25	c	502	CLA	CMB-C2B	-2.05	1.46	1.50
29	A	612	LMG	C4-C3	2.05	1.57	1.52
25	C	505	CLA	C3B-C4B	2.05	1.48	1.42
29	D	408	LMG	C7-C8	2.05	1.57	1.50
28	A	611	PL9	C25-C24	-2.04	1.45	1.50
25	d	403	CLA	C4B-NB	2.04	1.40	1.37
25	A	606	CLA	CMD-C2D	-2.04	1.46	1.50
25	c	502	CLA	CMC-C2C	-2.04	1.46	1.50
27	k	101	BCR	C38-C26	-2.04	1.47	1.50
31	D	409	LHG	O8-C6	-2.04	1.40	1.45
32	C	515	DGD	C3E-C2E	2.04	1.57	1.52
30	a	614	SQD	C25-C24	2.03	1.59	1.52
25	b	606	CLA	MG-ND	2.03	2.09	2.05
35	E	101	HEM	CMC-C2C	2.03	1.54	1.50
25	C	510	CLA	CMC-C2C	-2.03	1.46	1.50
30	a	614	SQD	C46-C45	2.03	1.57	1.50
25	d	404	CLA	CMB-C2B	-2.03	1.46	1.50
25	b	601	CLA	CMC-C2C	-2.03	1.46	1.50
25	c	503	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	601	CLA	MG-ND	-2.03	2.01	2.05
25	c	513	CLA	CMB-C2B	-2.03	1.46	1.50
31	D	409	LHG	O7-C5	-2.03	1.41	1.46
25	a	607	CLA	C3D-C4D	2.02	1.48	1.44
25	C	510	CLA	CMD-C2D	-2.02	1.46	1.50
36	v	201	HEC	CMA-C3A	2.02	1.54	1.50
36	V	201	HEC	C3B-C2B	-2.02	1.34	1.41
26	d	402	PHO	CMB-C2B	-2.02	1.47	1.51
25	C	509	CLA	CMB-C2B	-2.02	1.46	1.50
25	c	505	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	605	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	605	CLA	CMD-C2D	-2.02	1.46	1.50
25	c	507	CLA	CMB-C2B	-2.02	1.46	1.50
35	f	101	HEM	FE-ND	2.02	2.01	1.94
25	b	610	CLA	C3D-C4D	2.02	1.48	1.44
25	B	609	CLA	O2D-CGD	2.02	1.38	1.33
25	B	609	CLA	C3B-C4B	2.02	1.48	1.42
25	B	601	CLA	CMD-C2D	-2.02	1.46	1.50
27	b	617	BCR	C33-C5	-2.01	1.47	1.50
25	C	502	CLA	CMC-C2C	-2.01	1.46	1.50
25	c	512	CLA	CMD-C2D	-2.01	1.46	1.50
30	L	101	SQD	O6-C44	2.01	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	610	BCR	C33-C5	-2.01	1.47	1.50
25	C	507	CLA	MG-NC	2.01	2.11	2.06
25	b	616	CLA	CMB-C2B	-2.00	1.46	1.50
25	B	602	CLA	C1D-C2D	2.00	1.49	1.45
25	b	611	CLA	CMC-C2C	-2.00	1.46	1.50
25	C	503	CLA	MG-NB	-2.00	2.01	2.05
25	b	608	CLA	C1D-C2D	2.00	1.49	1.45

All (1106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	C4A-NA-C1A	10.11	111.29	106.68
25	c	509	CLA	C4A-NA-C1A	9.52	111.02	106.68
36	V	201	HEC	CBB-CAB-C3B	-9.36	108.73	127.43
25	c	503	CLA	C4A-NA-C1A	8.89	110.74	106.68
25	B	604	CLA	C4A-NA-C1A	8.88	110.73	106.68
36	v	201	HEC	CBB-CAB-C3B	-8.23	110.99	127.43
25	b	601	CLA	C4A-NA-C1A	8.20	110.42	106.68
25	b	606	CLA	C4A-NA-C1A	8.11	110.38	106.68
25	C	513	CLA	C4A-NA-C1A	7.99	110.33	106.68
25	b	604	CLA	C4A-NA-C1A	7.83	110.25	106.68
36	v	201	HEC	CBC-CAC-C3C	-7.70	112.04	127.43
25	C	507	CLA	C4A-NA-C1A	7.68	110.18	106.68
25	B	601	CLA	C4A-NA-C1A	7.57	110.13	106.68
25	C	503	CLA	C4A-NA-C1A	7.34	110.03	106.68
25	B	616	CLA	C4A-NA-C1A	7.32	110.02	106.68
25	B	607	CLA	C4A-NA-C1A	7.30	110.01	106.68
25	C	511	CLA	C4A-NA-C1A	7.17	109.95	106.68
25	B	615	CLA	C4A-NA-C1A	7.13	109.93	106.68
25	C	501	CLA	C4A-NA-C1A	7.13	109.93	106.68
30	L	101	SQD	O6-C1-C2	7.04	118.97	108.27
25	C	508	CLA	C4A-NA-C1A	6.92	109.83	106.68
25	b	611	CLA	C4A-NA-C1A	6.89	109.82	106.68
36	V	201	HEC	CBC-CAC-C3C	-6.76	113.92	127.43
30	a	613	SQD	O6-C1-C2	6.73	118.50	108.27
25	D	405	CLA	C4A-NA-C1A	6.66	109.72	106.68
25	c	501	CLA	C4A-NA-C1A	6.66	109.72	106.68
25	c	506	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	c	510	CLA	C4A-NA-C1A	6.47	109.63	106.68
25	C	505	CLA	C4A-NA-C1A	6.46	109.62	106.68
30	a	613	SQD	C1-O5-C5	-6.32	101.38	113.72
25	B	608	CLA	C4A-NA-C1A	6.15	109.49	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	506	CLA	C4A-NA-C1A	6.14	109.48	106.68
30	A	613	SQD	O6-C1-C2	6.13	117.59	108.27
25	c	508	CLA	C4A-NA-C1A	6.10	109.46	106.68
25	B	606	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	c	512	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	c	507	CLA	C4A-NA-C1A	5.91	109.38	106.68
25	C	509	CLA	C4A-NA-C1A	5.89	109.37	106.68
25	b	615	CLA	C4A-NA-C1A	5.75	109.30	106.68
25	D	404	CLA	C4A-NA-C1A	5.72	109.29	106.68
25	b	607	CLA	C4A-NA-C1A	5.71	109.29	106.68
25	c	504	CLA	C4A-NA-C1A	5.64	109.25	106.68
25	c	505	CLA	C4A-NA-C1A	5.62	109.24	106.68
25	a	612	CLA	C4A-NA-C1A	5.61	109.24	106.68
25	B	609	CLA	C4A-NA-C1A	5.60	109.23	106.68
25	b	608	CLA	C4A-NA-C1A	5.50	109.19	106.68
28	a	611	PL9	C7-C3-C4	5.48	121.43	116.91
25	C	512	CLA	C4A-NA-C1A	5.48	109.18	106.68
25	b	616	CLA	C4A-NA-C1A	5.43	109.16	106.68
28	D	407	PL9	C7-C3-C4	5.38	121.34	116.91
25	c	502	CLA	C4A-NA-C1A	5.33	109.11	106.68
25	b	604	CLA	C1-C2-C3	-5.33	117.46	126.20
30	A	613	SQD	C1-O5-C5	-5.30	103.36	113.72
25	B	613	CLA	C1-C2-C3	-5.26	117.57	126.20
25	c	513	CLA	C4A-NA-C1A	5.24	109.07	106.68
25	B	605	CLA	C4A-NA-C1A	5.21	109.06	106.68
25	C	510	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	B	602	CLA	C4A-NA-C1A	5.12	109.02	106.68
26	A	608	PHO	C4D-CHA-CBD	-5.12	106.00	108.45
25	a	607	CLA	C4A-NA-C1A	5.05	108.98	106.68
25	b	613	CLA	C4A-NA-C1A	5.00	108.96	106.68
25	b	603	CLA	C4A-NA-C1A	4.99	108.95	106.68
26	D	402	PHO	C2B-C1B-NB	-4.75	106.00	109.43
26	D	402	PHO	C1-C2-C3	-4.74	118.43	126.20
25	B	612	CLA	C4A-NA-C1A	4.70	108.83	106.68
25	a	608	CLA	C4A-NA-C1A	4.70	108.82	106.68
25	B	608	CLA	O2D-CGD-O1D	-4.69	114.71	123.85
28	A	611	PL9	C7-C3-C4	4.64	120.73	116.91
30	F	101	SQD	C1-O5-C5	-4.64	104.66	113.72
26	d	402	PHO	C1-C2-C3	-4.64	118.60	126.20
31	A	615	LHG	O4-P-O5	4.58	133.76	112.44
30	a	614	SQD	O47-C7-C8	4.58	121.38	111.48
25	B	610	CLA	C4A-NA-C1A	4.57	108.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	622	SQD	O47-C7-C8	4.57	121.37	111.48
25	B	614	CLA	C4A-NA-C1A	4.52	108.74	106.68
30	A	613	SQD	C1-C2-C3	-4.50	100.54	110.01
25	B	611	CLA	C4A-NA-C1A	4.47	108.72	106.68
25	B	610	CLA	O2D-CGD-O1D	-4.44	115.20	123.85
30	F	101	SQD	O9-S-C6	4.44	113.39	106.76
31	e	101	LHG	O4-P-O5	4.43	133.03	112.44
31	D	412	LHG	O4-P-O5	4.40	132.92	112.44
28	a	611	PL9	C7-C3-C2	-4.40	118.20	123.39
25	d	403	CLA	C4A-NA-C1A	4.39	108.68	106.68
27	K	101	BCR	C11-C10-C9	-4.38	121.14	127.28
31	A	614	LHG	O4-P-O5	4.37	132.76	112.44
28	d	406	PL9	C7-C3-C4	4.35	120.50	116.91
25	b	606	CLA	O2D-CGD-O1D	-4.35	115.38	123.85
31	d	408	LHG	O4-P-O5	4.33	132.61	112.44
31	D	409	LHG	O4-P-O5	4.33	132.59	112.44
25	B	614	CLA	C3B-C4B-NB	-4.33	106.67	110.53
30	L	101	SQD	O47-C7-C8	4.32	120.82	111.48
25	b	605	CLA	C4A-NA-C1A	4.30	108.64	106.68
26	d	402	PHO	O1D-CGD-CBD	4.29	131.23	124.72
31	d	407	LHG	O4-P-O5	4.28	132.37	112.44
25	B	603	CLA	C3B-C4B-NB	-4.28	106.71	110.53
25	C	502	CLA	C4A-NA-C1A	4.27	108.63	106.68
32	a	615	DGD	O3G-C3G-C2G	-4.27	100.80	111.77
25	b	603	CLA	O2D-CGD-O1D	-4.27	115.54	123.85
30	A	613	SQD	O47-C7-C8	4.26	120.70	111.48
26	d	402	PHO	C4D-CHA-CBD	-4.26	106.41	108.45
25	b	612	CLA	C4A-NA-C1A	4.25	108.62	106.68
30	B	622	SQD	O9-S-O7	-4.25	100.00	113.82
25	c	501	CLA	O2D-CGD-O1D	-4.25	115.58	123.85
25	b	608	CLA	C3B-C4B-NB	-4.24	106.75	110.53
30	L	101	SQD	O7-S-C6	4.22	113.06	106.76
25	c	512	CLA	C1-C2-C3	-4.21	119.30	126.20
31	D	410	LHG	O4-P-O5	4.20	131.98	112.44
25	B	611	CLA	O2D-CGD-O1D	-4.19	115.68	123.85
31	d	409	LHG	O4-P-O5	4.19	131.93	112.44
30	B	622	SQD	O7-S-C6	4.18	113.00	106.76
25	C	504	CLA	C4A-NA-C1A	4.17	108.58	106.68
25	B	603	CLA	C4A-NA-C1A	4.13	108.56	106.68
32	c	518	DGD	O3G-C3G-C2G	-4.11	100.83	110.82
32	H	102	DGD	O3G-C3G-C2G	-4.10	100.85	110.82
25	B	613	CLA	C4A-NA-C1A	4.09	108.55	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	611	CLA	O2D-CGD-O1D	-4.08	115.90	123.85
25	B	608	CLA	O2D-CGD-CBD	4.07	118.35	111.23
25	B	602	CLA	O2D-CGD-CBD	4.05	118.30	111.23
31	l	101	LHG	O4-P-O5	4.04	131.23	112.44
25	A	606	CLA	C4A-NA-C1A	4.04	108.52	106.68
25	b	612	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
25	A	609	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
25	B	606	CLA	C3B-C4B-NB	-3.98	106.98	110.53
26	d	402	PHO	C2B-C1B-NB	-3.98	106.55	109.43
25	A	607	CLA	C4A-NA-C1A	3.95	108.48	106.68
30	a	613	SQD	O9-S-O7	-3.95	100.98	113.82
30	f	102	SQD	O9-S-O7	-3.95	100.99	113.82
30	a	613	SQD	O47-C7-C8	3.93	119.98	111.48
30	f	102	SQD	O7-S-C6	3.92	112.61	106.76
26	d	402	PHO	O2D-CGD-O1D	-3.89	116.28	123.85
32	C	515	DGD	O3G-C3G-C2G	-3.89	101.36	110.82
25	c	509	CLA	O2A-CGA-O1A	-3.87	113.94	123.63
32	h	101	DGD	O3G-C3G-C2G	-3.86	101.42	110.82
25	b	609	CLA	C4A-NA-C1A	3.86	108.44	106.68
30	A	613	SQD	O9-S-O7	-3.85	101.29	113.82
30	F	101	SQD	C44-O6-C1	3.85	120.25	113.68
25	C	507	CLA	O2D-CGD-O1D	-3.83	116.38	123.85
25	c	505	CLA	C3B-C4B-NB	-3.83	107.11	110.53
25	b	602	CLA	C4A-NA-C1A	3.81	108.42	106.68
25	B	610	CLA	CHB-C4A-NA	3.81	129.90	124.40
32	c	519	DGD	O3G-C3G-C2G	-3.80	101.58	110.82
27	b	617	BCR	C2-C1-C6	3.79	115.94	110.44
30	A	616	SQD	O47-C7-C8	3.79	119.67	111.48
25	b	616	CLA	O2D-CGD-O1D	-3.79	116.48	123.85
25	A	609	CLA	C4A-NA-C1A	3.78	108.40	106.68
32	C	516	DGD	O3G-C3G-C2G	-3.75	101.69	110.82
25	d	404	CLA	C3B-C4B-NB	-3.75	107.18	110.53
25	b	610	CLA	C4A-NA-C1A	3.74	108.39	106.68
30	L	101	SQD	O48-C23-C24	3.73	123.20	111.83
26	A	608	PHO	O2D-CGD-CBD	3.72	115.04	110.95
25	c	510	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
25	b	602	CLA	C1-C2-C3	-3.71	120.12	126.20
25	D	403	CLA	C3B-C4B-NB	-3.70	107.23	110.53
26	d	401	PHO	C4D-CHA-CBD	-3.63	106.71	108.45
30	L	101	SQD	O9-S-O7	-3.62	102.05	113.82
25	B	602	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
30	a	613	SQD	O7-S-C6	3.59	112.12	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	C1-C2-C3	-3.59	120.31	126.20
30	a	614	SQD	O48-C23-C24	3.58	122.75	111.83
25	b	614	CLA	C4A-NA-C1A	3.58	108.31	106.68
25	b	611	CLA	O2D-CGD-CBD	3.57	117.48	111.23
32	A	617	DGD	O3G-C3G-C2G	-3.56	102.17	110.82
30	B	622	SQD	O48-C23-C24	3.55	122.67	111.83
30	F	101	SQD	O9-S-O7	-3.55	102.27	113.82
25	B	611	CLA	C3B-C4B-NB	-3.55	107.36	110.53
25	d	404	CLA	C4A-NA-C1A	3.55	108.30	106.68
27	B	617	BCR	C2-C1-C6	3.54	115.59	110.44
25	b	602	CLA	CHB-C4A-NA	3.54	129.51	124.40
36	v	201	HEC	C4D-ND-C1D	3.54	111.60	105.82
25	B	604	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
30	F	101	SQD	O5-C1-O6	3.54	118.41	110.04
25	b	606	CLA	O2D-CGD-CBD	3.54	117.42	111.23
30	a	613	SQD	C44-O6-C1	-3.53	106.22	113.80
25	B	611	CLA	O2D-CGD-CBD	3.51	117.37	111.23
25	B	612	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
25	D	404	CLA	O2D-CGD-CBD	3.50	117.34	111.23
28	A	611	PL9	C7-C3-C2	-3.49	119.27	123.39
26	A	608	PHO	C2B-C1B-NB	-3.47	106.92	109.43
30	f	102	SQD	O6-C1-C2	3.46	113.53	108.27
25	b	604	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
25	b	612	CLA	C1-C2-C3	-3.45	120.55	126.20
25	B	616	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
30	f	102	SQD	O5-C5-C4	3.41	115.85	109.70
32	A	617	DGD	C4E-C3E-C2E	-3.40	104.85	110.83
27	A	610	BCR	C11-C10-C9	-3.40	122.52	127.28
25	b	605	CLA	C3B-C4B-NB	-3.39	107.50	110.53
32	C	517	DGD	O3G-C3G-C2G	-3.38	102.59	110.82
27	B	619	BCR	C2-C1-C6	3.38	115.35	110.44
30	L	101	SQD	C1-C2-C3	-3.38	102.90	110.01
25	b	616	CLA	CMB-C2B-C1B	-3.37	120.28	125.42
26	A	608	PHO	CMB-C2B-C3B	3.37	131.42	124.68
30	L	101	SQD	O5-C5-C4	3.37	115.77	109.70
30	A	616	SQD	O48-C23-C24	3.37	122.10	111.83
32	c	517	DGD	O3G-C3G-C2G	-3.36	102.63	110.82
25	c	513	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
25	B	610	CLA	C1-C2-C3	-3.35	120.72	126.20
25	C	509	CLA	C3B-C4B-NB	-3.34	107.54	110.53
31	D	412	LHG	O8-C23-C24	3.34	122.02	111.83
28	d	406	PL9	C40-C39-C41	3.34	121.02	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	101	BCR	C15-C16-C17	-3.33	116.71	123.52
26	D	402	PHO	C4D-CHA-CBD	-3.33	106.86	108.45
36	V	201	HEC	CBD-CAD-C3D	-3.32	103.35	112.53
25	B	607	CLA	C3B-C4B-NB	-3.32	107.57	110.53
25	B	610	CLA	O2A-CGA-O1A	-3.31	115.34	123.63
25	B	601	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
25	b	602	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
32	H	102	DGD	C3E-C4E-C5E	-3.31	104.23	110.23
25	B	613	CLA	CAC-C3C-C4C	3.30	129.09	124.79
30	a	613	SQD	C1-C2-C3	-3.30	103.07	110.01
25	c	507	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
25	b	610	CLA	CAC-C3C-C4C	3.30	129.08	124.79
31	d	407	LHG	O8-C23-O10	-3.30	115.39	123.63
25	C	508	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	D	404	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
31	d	408	LHG	O8-C23-C24	3.28	121.85	111.83
25	B	604	CLA	C3B-C4B-NB	-3.27	107.61	110.53
25	b	613	CLA	C1-C2-C3	-3.27	120.84	126.20
30	A	613	SQD	O8-S-C6	3.27	112.28	105.97
25	b	601	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
31	d	407	LHG	O8-C23-C24	3.25	121.76	111.83
25	B	610	CLA	O2D-CGD-CBD	3.25	116.91	111.23
25	B	615	CLA	C3B-C4B-NB	-3.25	107.63	110.53
25	B	615	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
25	a	608	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
25	c	511	CLA	C3B-C4B-NB	-3.23	107.65	110.53
25	C	502	CLA	C3B-C4B-NB	-3.22	107.65	110.53
30	A	613	SQD	O5-C1-C2	-3.22	103.75	110.37
25	D	405	CLA	CMB-C2B-C1B	-3.22	120.52	125.42
25	C	503	CLA	C3B-C4B-NB	-3.22	107.66	110.53
25	b	601	CLA	C3B-C4B-NB	-3.22	107.66	110.53
25	B	610	CLA	C3B-C4B-NB	-3.21	107.66	110.53
30	F	101	SQD	O48-C23-C24	3.20	121.60	111.83
25	a	609	CLA	C4A-NA-C1A	3.19	108.14	106.68
25	b	605	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
25	c	502	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
25	c	504	CLA	CMB-C2B-C1B	-3.18	120.57	125.42
25	C	506	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	c	513	CLA	C3B-C4B-NB	-3.18	107.69	110.53
29	c	522	LMG	O1-C1-C2	-3.17	103.46	108.27
25	B	605	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
26	d	401	PHO	C2B-C1B-NB	-3.16	107.15	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
25	c	502	CLA	C1-C2-C3	-3.15	121.03	126.20
25	b	604	CLA	CHB-C4A-NA	3.15	128.95	124.40
28	D	407	PL9	C7-C3-C2	-3.15	119.67	123.39
27	T	101	BCR	C7-C8-C9	-3.14	121.59	126.23
25	C	510	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
25	C	506	CLA	C1-C2-C3	-3.14	121.06	126.20
25	c	511	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
25	A	606	CLA	C3B-C4B-NB	-3.13	107.74	110.53
25	d	404	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
25	A	607	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	C	513	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
26	D	402	PHO	O2D-CGD-O1D	-3.11	117.79	123.85
25	c	507	CLA	C3B-C4B-NB	-3.11	107.75	110.53
26	D	402	PHO	CMB-C2B-C3B	3.11	130.90	124.68
25	c	505	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
28	d	406	PL9	C37-C38-C39	-3.10	120.52	127.62
25	B	613	CLA	O2A-CGA-O1A	-3.10	115.88	123.63
29	d	411	LMG	O2-C2-C1	-3.10	102.69	110.08
25	D	405	CLA	O2D-CGD-O1D	-3.09	117.82	123.85
29	m	101	LMG	O1-C7-C8	-3.09	103.29	110.82
32	c	519	DGD	O6D-C1D-O3G	-3.09	102.74	110.04
25	a	612	CLA	O2D-CGD-CBD	3.09	116.63	111.23
30	a	613	SQD	O48-C23-C24	3.09	121.24	111.83
25	C	510	CLA	C3B-C4B-NB	-3.08	107.78	110.53
26	A	608	PHO	O2D-CGD-O1D	-3.08	117.86	123.85
25	a	607	CLA	C3B-C4B-NB	-3.07	107.78	110.53
35	f	101	HEM	C3B-C2B-C1B	3.07	108.72	106.41
25	C	504	CLA	O2A-CGA-O1A	-3.07	115.95	123.63
26	D	402	PHO	O1D-CGD-CBD	3.07	129.37	124.72
27	a	610	BCR	C2-C1-C6	3.06	114.89	110.44
25	b	613	CLA	O2D-CGD-CBD	3.06	116.58	111.23
30	L	101	SQD	O9-S-C6	3.06	111.32	106.76
27	d	405	BCR	C27-C26-C25	3.05	126.83	122.70
25	B	608	CLA	CMB-C2B-C1B	-3.05	120.77	125.42
25	A	606	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
32	C	515	DGD	O6D-C1D-O3G	-3.05	102.84	110.04
25	C	507	CLA	CHB-C4A-NA	3.05	128.80	124.40
25	b	603	CLA	O2D-CGD-CBD	3.04	116.55	111.23
25	a	612	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
32	C	516	DGD	O6D-C1D-O3G	-3.04	102.85	110.04
25	b	610	CLA	O2D-CGD-O1D	-3.04	117.92	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	516	DGD	O5D-C6D-C5D	-3.04	102.57	109.42
25	C	512	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
29	D	408	LMG	O6-C1-O1	-3.03	102.87	110.04
25	c	503	CLA	CHB-C4A-NA	3.03	128.78	124.40
29	M	101	LMG	C38-C37-C36	-3.03	99.04	114.37
27	C	514	BCR	C2-C1-C6	3.03	114.84	110.44
35	E	101	HEM	CBD-CAD-C3D	-3.03	104.16	112.53
25	b	601	CLA	CHB-C4A-NA	3.03	128.77	124.40
25	C	502	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
27	B	618	BCR	C24-C23-C22	-3.02	121.77	126.23
28	d	406	PL9	C7-C3-C2	-3.01	119.84	123.39
25	c	509	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
25	B	602	CLA	CHB-C4A-NA	3.01	128.74	124.40
25	A	607	CLA	C1-C2-C3	-3.01	121.27	126.20
25	D	403	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
25	c	504	CLA	C3B-C4B-NB	-3.00	107.85	110.53
25	b	615	CLA	C3B-C4B-NB	-3.00	107.85	110.53
25	B	614	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
32	c	518	DGD	O6D-C1D-O3G	-2.99	102.97	110.04
25	A	606	CLA	CHB-C4A-NA	2.99	128.72	124.40
25	B	602	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
25	C	513	CLA	C3B-C4B-NB	-2.99	107.86	110.53
32	C	517	DGD	O6D-C1D-O3G	-2.99	102.98	110.04
27	K	101	BCR	C15-C14-C13	-2.99	123.09	127.28
25	b	613	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	T	101	BCR	C27-C26-C25	2.98	126.73	122.70
25	C	512	CLA	CHB-C4A-NA	2.97	128.69	124.40
25	C	509	CLA	CHB-C4A-NA	2.95	128.66	124.40
28	d	406	PL9	C42-C43-C44	-2.95	120.86	127.62
33	m	102	STE	O2-C1-C2	2.95	123.33	114.00
25	b	608	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
25	b	610	CLA	CAA-CBA-CGA	-2.95	104.83	113.21
27	Y	101	BCR	C27-C26-C25	2.94	126.68	122.70
25	C	508	CLA	C3B-C4B-NB	-2.94	107.91	110.53
25	B	611	CLA	C1-C2-C3	-2.94	121.39	126.20
25	B	604	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	C	513	CLA	CHB-C4A-NA	2.93	128.63	124.40
29	C	518	LMG	O1-C7-C8	-2.93	103.68	110.82
25	b	605	CLA	O2A-CGA-O1A	-2.93	116.31	123.63
32	H	102	DGD	O2D-C2D-C1D	-2.93	103.10	110.08
30	B	622	SQD	O6-C1-C2	2.93	112.72	108.27
33	j	101	STE	O2-C1-C2	2.92	123.24	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	607	CLA	C3B-C4B-NB	-2.92	107.93	110.53
29	d	411	LMG	O6-C1-O1	-2.91	103.17	110.04
27	B	618	BCR	C15-C14-C13	-2.91	123.20	127.28
25	a	608	CLA	CHB-C4A-NA	2.90	128.59	124.40
27	D	406	BCR	C7-C8-C9	-2.90	121.94	126.23
25	c	504	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
36	V	201	HEC	C4D-ND-C1D	2.90	110.55	105.82
25	b	602	CLA	O2D-CGD-CBD	2.90	116.29	111.23
25	c	508	CLA	C1-C2-C3	-2.89	121.46	126.20
33	C	520	STE	C3-C2-C1	-2.89	106.97	114.51
25	A	609	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
25	a	607	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
27	A	610	BCR	C27-C26-C25	2.88	126.60	122.70
25	C	504	CLA	C3B-C4B-NB	-2.88	107.96	110.53
25	C	511	CLA	CHB-C4A-NA	2.87	128.54	124.40
27	t	101	BCR	C15-C14-C13	-2.86	123.26	127.28
27	c	515	BCR	C7-C8-C9	-2.86	122.00	126.23
27	d	405	BCR	C38-C26-C25	-2.86	121.37	124.48
25	b	608	CLA	O2D-CGD-CBD	2.85	116.22	111.23
25	b	612	CLA	CHB-C4A-NA	2.85	128.52	124.40
25	d	403	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
28	d	406	PL9	C22-C23-C24	-2.85	121.10	127.62
27	D	406	BCR	C27-C26-C25	2.85	126.55	122.70
25	C	501	CLA	C3B-C4B-NB	-2.85	107.99	110.53
25	b	616	CLA	CMB-C2B-C3B	2.84	133.24	126.55
25	B	612	CLA	O2A-CGA-O1A	-2.84	116.52	123.63
32	c	519	DGD	CDB-CCB-CBB	-2.84	100.00	114.37
27	D	406	BCR	C2-C1-C6	2.84	114.57	110.44
32	c	517	DGD	O3G-C1D-C2D	-2.84	103.96	108.27
25	B	612	CLA	C11-C12-C13	-2.84	106.53	115.97
29	b	621	LMG	C1-O6-C5	-2.84	108.18	113.72
26	D	402	PHO	C3B-C4B-NB	-2.84	105.62	107.46
25	C	503	CLA	C7-C6-C5	-2.83	105.71	113.26
25	B	603	CLA	CHD-C4C-NC	2.83	128.62	124.23
30	f	102	SQD	C1-O5-C5	-2.83	108.19	113.72
25	B	602	CLA	C3B-C4B-NB	-2.83	108.00	110.53
25	c	509	CLA	CHB-C4A-NA	2.83	128.49	124.40
30	A	613	SQD	O48-C23-C24	2.83	120.46	111.83
28	d	406	PL9	O1-C4-C3	-2.83	117.75	120.73
27	C	514	BCR	C15-C16-C17	-2.83	117.74	123.52
25	A	609	CLA	O2D-CGD-CBD	2.82	116.17	111.23
25	b	607	CLA	CHB-C4A-NA	2.82	128.47	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	407	PL9	C22-C23-C24	-2.82	121.17	127.62
27	k	101	BCR	C33-C5-C6	-2.82	121.41	124.48
26	d	401	PHO	CMB-C2B-C3B	2.82	130.31	124.68
25	c	503	CLA	C3B-C4B-NB	-2.82	108.02	110.53
25	B	612	CLA	C1-C2-C3	-2.82	121.58	126.20
25	A	606	CLA	C7-C6-C5	-2.82	105.76	113.26
25	d	404	CLA	CHB-C1B-NB	2.81	128.27	124.05
28	A	611	PL9	C22-C23-C24	-2.81	121.18	127.62
32	H	102	DGD	CDB-CCB-CBB	-2.81	100.14	114.37
25	B	613	CLA	C3B-C4B-NB	-2.81	108.02	110.53
27	H	101	BCR	C27-C26-C25	2.81	126.50	122.70
27	B	617	BCR	C29-C30-C25	2.81	114.52	110.44
25	a	609	CLA	CHB-C4A-NA	2.81	128.45	124.40
29	m	101	LMG	O3-C3-C2	-2.81	103.76	110.38
25	C	508	CLA	CHD-C1D-ND	-2.80	120.86	124.80
28	D	407	PL9	C12-C13-C14	-2.80	121.21	127.62
29	M	101	LMG	C1-C2-C3	-2.80	104.11	110.01
34	a	606	BCT	O2-C-O1	-2.80	112.51	119.68
32	A	617	DGD	CDB-CCB-CBB	-2.80	100.23	114.37
29	b	621	LMG	C3-C4-C5	-2.79	105.17	110.23
25	B	616	CLA	CAA-CBA-CGA	-2.79	105.28	113.21
25	c	506	CLA	CHB-C4A-NA	2.79	128.43	124.40
30	L	101	SQD	C3-C4-C5	2.79	115.30	110.23
25	b	609	CLA	C3B-C4B-NB	-2.79	108.04	110.53
27	c	515	BCR	C27-C26-C25	2.79	126.48	122.70
25	c	508	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
27	k	101	BCR	C27-C26-C25	2.79	126.47	122.70
25	C	509	CLA	CED-O2D-CGD	2.78	122.22	115.92
25	a	607	CLA	O1D-CGD-CBD	2.78	130.00	124.52
25	c	501	CLA	O2D-CGD-CBD	2.78	116.09	111.23
32	a	615	DGD	CDB-CCB-CBB	-2.78	100.33	114.37
27	c	514	BCR	C15-C14-C13	-2.78	123.39	127.28
25	b	606	CLA	C3B-C4B-NB	-2.77	108.06	110.53
30	f	102	SQD	O5-C1-C2	-2.77	104.68	110.37
25	a	608	CLA	O2D-CGD-CBD	2.77	116.07	111.23
27	B	618	BCR	C3-C4-C5	-2.77	109.12	114.06
30	f	102	SQD	C1-C2-C3	-2.77	104.19	110.01
27	c	516	BCR	C27-C26-C25	2.76	126.44	122.70
27	x	101	BCR	C2-C1-C6	2.76	114.45	110.44
25	d	404	CLA	CMB-C2B-C3B	2.76	133.04	126.55
25	B	605	CLA	C3B-C4B-NB	-2.76	108.07	110.53
29	b	621	LMG	O7-C10-O9	-2.75	117.26	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	503	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
25	b	616	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	A	607	CLA	C3B-C4B-NB	-2.75	108.08	110.53
25	B	602	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
25	C	509	CLA	CMB-C2B-C1B	-2.75	121.24	125.42
25	B	612	CLA	CHB-C4A-NA	2.75	128.36	124.40
27	b	618	BCR	C8-C7-C6	-2.75	119.67	127.00
27	B	619	BCR	C29-C30-C25	2.74	114.42	110.44
25	a	608	CLA	C3B-C4B-NB	-2.74	108.08	110.53
25	C	501	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
25	B	606	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
25	a	607	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
25	c	510	CLA	C3B-C4B-NB	-2.74	108.09	110.53
25	c	509	CLA	C3B-C4B-NB	-2.73	108.09	110.53
25	b	603	CLA	CHD-C1D-ND	-2.73	120.96	124.80
27	c	515	BCR	C35-C13-C14	-2.73	118.39	122.82
27	Y	101	BCR	C33-C5-C6	-2.73	121.51	124.48
25	c	508	CLA	C3B-C4B-NB	-2.73	108.09	110.53
27	a	610	BCR	C24-C23-C22	-2.73	122.20	126.23
25	b	604	CLA	C3B-C4B-NB	-2.73	108.10	110.53
32	c	517	DGD	CDB-CCB-CBB	-2.73	100.59	114.37
27	K	102	BCR	C27-C26-C25	2.72	126.38	122.70
25	b	609	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
25	b	608	CLA	CHB-C4A-NA	2.72	128.33	124.40
29	m	101	LMG	O7-C10-O9	-2.72	117.35	123.70
25	b	612	CLA	O1D-CGD-CBD	2.72	129.88	124.52
25	D	405	CLA	CMB-C2B-C3B	2.72	132.94	126.55
27	x	101	BCR	C27-C26-C25	2.71	126.37	122.70
25	B	612	CLA	C3B-C4B-NB	-2.71	108.11	110.53
25	c	513	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
25	b	615	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
27	b	617	BCR	C27-C26-C25	2.71	126.36	122.70
31	D	409	LHG	C18-C17-C16	-2.71	100.69	114.37
26	d	401	PHO	OBD-CAD-CBD	-2.70	121.86	125.82
25	B	605	CLA	CHD-C1D-ND	-2.70	121.00	124.80
26	d	402	PHO	CMB-C2B-C3B	2.70	130.08	124.68
27	c	514	BCR	C24-C23-C22	-2.70	122.24	126.23
25	A	609	CLA	CHB-C4A-NA	2.70	128.30	124.40
25	c	512	CLA	C3B-C4B-NB	-2.70	108.12	110.53
32	C	517	DGD	CDB-CCB-CBB	-2.70	100.72	114.37
31	A	614	LHG	O8-C23-C24	2.70	120.06	111.83
25	c	513	CLA	CMB-C2B-C1B	-2.70	121.31	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	O2D-CGD-CBD	2.70	115.94	111.23
26	A	608	PHO	C1-C2-C3	-2.69	121.78	126.20
28	d	406	PL9	C36-C34-C33	-2.68	115.14	121.17
25	C	501	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
29	c	522	LMG	C6-C5-C4	-2.68	106.44	113.02
29	m	101	LMG	O6-C1-O1	-2.68	103.71	110.04
28	a	611	PL9	C7-C8-C9	-2.68	122.22	126.83
27	D	406	BCR	C3-C4-C5	-2.67	109.29	114.06
28	D	407	PL9	C20-C19-C21	2.67	119.87	115.23
30	A	613	SQD	O7-S-C6	2.67	110.74	106.76
33	c	523	STE	C3-C2-C1	-2.67	107.54	114.51
29	b	621	LMG	O8-C28-O10	-2.67	116.95	123.63
25	c	508	CLA	CHB-C4A-NA	2.67	128.25	124.40
32	C	515	DGD	CDB-CCB-CBB	-2.67	100.88	114.37
32	C	516	DGD	CDB-CCB-CBB	-2.67	100.88	114.37
27	a	610	BCR	C27-C26-C25	2.67	126.31	122.70
27	b	618	BCR	C15-C14-C13	-2.67	123.54	127.28
25	D	403	CLA	C4A-NA-C1A	2.67	107.89	106.68
25	C	511	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
27	b	618	BCR	C27-C26-C25	2.66	126.30	122.70
25	b	613	CLA	O2A-CGA-O1A	-2.66	116.96	123.63
25	b	606	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	A	609	CLA	CMB-C2B-C3B	2.66	132.81	126.55
25	B	602	CLA	CMB-C2B-C3B	2.66	132.81	126.55
27	b	619	BCR	C11-C10-C9	-2.66	123.55	127.28
30	a	613	SQD	O8-S-C6	2.65	111.10	105.97
28	D	407	PL9	C7-C8-C9	-2.65	122.26	126.83
25	c	505	CLA	O2D-CGD-CBD	2.65	115.86	111.23
25	B	606	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
25	B	605	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
29	c	520	LMG	O6-C1-O1	-2.64	103.80	110.04
28	d	406	PL9	C7-C8-C9	-2.64	122.28	126.83
25	c	512	CLA	CHB-C4A-NA	2.64	128.21	124.40
31	d	408	LHG	O8-C23-O10	-2.64	117.03	123.63
35	f	101	HEM	CBD-CAD-C3D	-2.64	105.24	112.53
28	A	611	PL9	C36-C34-C33	-2.64	115.25	121.17
25	B	609	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
32	h	101	DGD	CDB-CCB-CBB	-2.63	101.06	114.37
25	c	502	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
27	c	515	BCR	C2-C1-C6	2.63	114.26	110.44
32	A	617	DGD	C3G-C2G-C1G	-2.63	105.65	111.78
30	a	613	SQD	C3-C4-C5	2.63	115.00	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	612	CLA	CMB-C2B-C3B	2.63	132.73	126.55
25	a	612	CLA	CHC-C4B-NB	2.63	127.99	124.05
25	C	512	CLA	C3B-C4B-NB	-2.62	108.19	110.53
27	B	618	BCR	C2-C1-C6	2.62	114.25	110.44
25	B	609	CLA	O2A-CGA-O1A	-2.62	117.08	123.63
25	B	611	CLA	CHB-C4A-NA	2.61	128.17	124.40
32	h	101	DGD	O3E-C3E-C2E	-2.61	104.22	110.38
32	C	516	DGD	C1D-O6D-C5D	-2.61	108.63	113.72
25	b	615	CLA	CHB-C4A-NA	2.60	128.16	124.40
25	A	606	CLA	C6-C5-C3	2.60	119.80	113.47
26	d	401	PHO	O2A-CGA-O1A	-2.60	117.12	123.63
32	A	617	DGD	O6D-C1D-O3G	-2.60	103.90	110.04
25	a	609	CLA	O2D-CGD-CBD	2.60	115.77	111.23
30	f	102	SQD	O48-C23-C24	2.60	119.75	111.83
25	a	609	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
25	D	404	CLA	C3B-C4B-NB	-2.59	108.21	110.53
28	A	611	PL9	C20-C19-C21	2.59	119.73	115.23
27	c	514	BCR	C33-C5-C6	-2.59	121.66	124.48
29	M	101	LMG	C1-O6-C5	-2.59	108.66	113.72
32	A	617	DGD	O5D-C6D-C5D	-2.59	103.59	109.42
25	b	614	CLA	C3B-C4B-NB	-2.59	108.22	110.53
32	c	517	DGD	O6D-C1D-O3G	-2.58	103.94	110.04
32	C	516	DGD	O2D-C2D-C1D	-2.58	103.92	110.08
28	D	407	PL9	C37-C38-C39	-2.58	121.71	127.62
25	c	506	CLA	C3B-C4B-NB	-2.58	108.22	110.53
25	a	612	CLA	C3B-C4B-NB	-2.58	108.23	110.53
25	c	510	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
31	e	101	LHG	O8-C23-C24	2.58	119.70	111.83
27	b	617	BCR	C33-C5-C6	-2.58	121.67	124.48
28	a	611	PL9	C22-C23-C24	-2.58	121.72	127.62
25	C	506	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
30	F	101	SQD	C46-C45-C44	-2.58	105.34	113.67
25	B	615	CLA	O2D-CGD-CBD	2.58	115.73	111.23
25	b	616	CLA	O2D-CGD-CBD	2.58	115.73	111.23
25	c	504	CLA	CMB-C2B-C3B	2.57	132.60	126.55
27	C	514	BCR	C15-C14-C13	-2.57	123.67	127.28
25	B	614	CLA	CHC-C4B-NB	2.57	127.91	124.05
25	b	605	CLA	O1D-CGD-CBD	2.57	129.59	124.52
30	f	102	SQD	O9-S-C6	2.57	110.59	106.76
25	B	615	CLA	CHB-C4A-NA	2.57	128.10	124.40
25	b	614	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
25	c	506	CLA	C1-O2A-CGA	2.56	122.86	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	102	SQD	O47-C7-C8	2.56	120.33	110.93
25	c	510	CLA	C1-C2-C3	-2.55	122.01	126.20
32	h	101	DGD	C1D-C2D-C3D	-2.55	104.64	110.01
31	D	412	LHG	C18-C17-C16	-2.55	101.47	114.37
32	c	518	DGD	O2D-C2D-C1D	-2.55	104.00	110.08
30	L	101	SQD	O5-C1-C2	-2.55	105.13	110.37
25	C	508	CLA	O2D-CGD-CBD	2.55	115.68	111.23
27	K	101	BCR	C24-C23-C22	-2.54	122.47	126.23
25	b	616	CLA	CHD-C1D-ND	-2.54	121.22	124.80
31	d	408	LHG	C20-C19-C18	-2.54	101.53	114.37
30	F	101	SQD	O5-C5-C4	2.54	114.27	109.70
31	D	409	LHG	O8-C23-C24	2.54	119.58	111.83
29	c	524	LMG	C1-O6-C5	-2.54	108.76	113.72
25	b	613	CLA	C16-C15-C13	-2.54	107.53	115.97
25	b	616	CLA	C3B-C4B-NB	-2.53	108.27	110.53
29	C	518	LMG	O2-C2-C1	-2.53	104.05	110.08
25	c	502	CLA	CHD-C1D-ND	-2.53	121.24	124.80
26	d	401	PHO	C1-C2-C3	-2.53	122.05	126.20
27	H	101	BCR	C16-C15-C14	-2.53	118.35	123.52
25	C	509	CLA	CMB-C2B-C3B	2.53	132.49	126.55
25	b	606	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
29	M	101	LMG	C40-C39-C38	-2.52	101.61	114.37
31	l	101	LHG	C20-C19-C18	-2.52	101.61	114.37
31	D	410	LHG	O8-C6-C5	-2.52	101.12	108.40
27	b	617	BCR	C3-C4-C5	-2.52	109.56	114.06
32	a	615	DGD	C5B-C4B-C3B	-2.52	101.62	114.37
25	b	605	CLA	CHD-C1D-ND	-2.52	121.25	124.80
30	F	101	SQD	O5-C1-C2	-2.52	105.19	110.37
27	c	514	BCR	C15-C16-C17	-2.52	118.36	123.52
25	B	612	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
25	b	608	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
31	d	409	LHG	O8-C23-C24	2.52	119.51	111.83
27	H	101	BCR	C24-C23-C22	-2.52	122.51	126.23
27	c	515	BCR	C15-C16-C17	-2.52	118.37	123.52
29	c	524	LMG	O6-C1-O1	-2.51	104.10	110.04
25	d	404	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
25	c	513	CLA	CHB-C4A-NA	2.51	128.03	124.40
25	c	502	CLA	C3B-C4B-NB	-2.51	108.29	110.53
29	m	101	LMG	O1-C1-C2	-2.51	104.46	108.27
25	B	612	CLA	C16-C15-C13	-2.51	107.62	115.97
25	B	613	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
31	D	409	LHG	C11-C10-C9	-2.51	101.70	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	BCR	C2-C1-C6	2.51	114.08	110.44
32	C	515	DGD	O5D-C6D-C5D	-2.51	103.77	109.42
27	c	514	BCR	C27-C26-C25	2.51	126.09	122.70
25	a	607	CLA	CHC-C4B-NB	2.51	127.81	124.05
25	c	507	CLA	O2A-CGA-O1A	-2.50	117.36	123.63
28	d	406	PL9	C27-C28-C29	-2.50	121.89	127.62
32	a	615	DGD	C1G-C2G-C3G	-2.50	106.03	111.80
25	D	405	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	B	604	CLA	C2D-C1D-ND	-2.50	107.66	110.13
25	C	512	CLA	CAA-CBA-CGA	-2.49	106.13	113.21
32	C	515	DGD	C7B-C6B-C5B	-2.49	101.77	114.37
25	c	504	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	B	603	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	b	611	CLA	CHB-C4A-NA	2.49	127.99	124.40
25	d	403	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
31	D	409	LHG	C27-C26-C25	-2.49	101.79	114.37
25	b	609	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
32	C	517	DGD	C3G-C2G-C1G	-2.49	105.98	111.78
25	b	613	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
25	b	610	CLA	CHB-C4A-NA	2.49	127.99	124.40
27	B	619	BCR	C34-C9-C10	-2.48	118.79	122.82
29	c	520	LMG	O8-C28-O10	-2.48	117.42	123.63
30	F	101	SQD	O8-S-C6	2.48	110.76	105.97
30	f	102	SQD	C3-C4-C5	2.48	114.72	110.23
33	b	622	STE	C3-C2-C1	-2.48	108.04	114.51
29	C	518	LMG	O6-C1-O1	-2.47	104.20	110.04
25	b	613	CLA	CHA-C1A-NA	-2.47	120.79	126.39
32	c	517	DGD	C3G-C2G-C1G	-2.47	106.03	111.78
25	B	608	CLA	CHB-C1B-NB	2.47	127.75	124.05
25	B	608	CLA	C3B-C4B-NB	-2.47	108.33	110.53
32	c	518	DGD	CDB-CCB-CBB	-2.47	101.91	114.37
31	l	101	LHG	C11-C10-C9	-2.46	101.91	114.37
25	B	602	CLA	C16-C15-C13	-2.46	107.78	115.97
25	D	403	CLA	CHB-C4A-NA	2.46	127.95	124.40
28	a	611	PL9	C40-C39-C41	2.45	119.49	115.23
25	B	605	CLA	O1D-CGD-CBD	2.45	129.36	124.52
25	c	511	CLA	O2D-CGD-CBD	2.45	115.52	111.23
25	B	603	CLA	O2D-CGD-CBD	2.45	115.51	111.23
25	B	613	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
25	a	612	CLA	CHB-C4A-NA	2.45	127.93	124.40
27	x	101	BCR	C15-C16-C17	-2.45	118.52	123.52
25	A	607	CLA	O2A-CGA-O1A	-2.44	117.51	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	101	BCR	C7-C8-C9	-2.44	122.62	126.23
31	D	409	LHG	C20-C19-C18	-2.44	102.02	114.37
25	a	607	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	b	614	CLA	CHD-C1D-ND	-2.44	121.37	124.80
25	b	608	CLA	C1-C2-C3	-2.44	122.20	126.20
29	c	520	LMG	C40-C39-C38	-2.44	102.04	114.37
27	a	610	BCR	C29-C30-C25	2.44	113.98	110.44
25	b	609	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	C	506	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
25	c	505	CLA	CHB-C4A-NA	2.43	127.91	124.40
31	e	101	LHG	C11-C10-C9	-2.43	102.08	114.37
32	A	617	DGD	O2D-C2D-C1D	-2.43	104.29	110.08
29	C	518	LMG	O1-C1-C2	-2.43	104.58	108.27
29	A	612	LMG	C40-C39-C38	-2.43	102.09	114.37
27	a	610	BCR	C11-C10-C9	-2.43	123.87	127.28
26	d	402	PHO	O2A-CGA-O1A	-2.43	117.56	123.63
27	B	617	BCR	C3-C4-C5	-2.43	109.73	114.06
25	C	505	CLA	C3B-C4B-NB	-2.43	108.36	110.53
30	a	613	SQD	O9-S-C6	2.42	110.37	106.76
25	b	608	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
33	M	102	STE	C3-C2-C1	-2.42	108.20	114.51
31	D	412	LHG	C11-C10-C9	-2.42	102.15	114.37
32	h	101	DGD	O6D-C1D-O3G	-2.41	104.34	110.04
25	c	513	CLA	C1-C2-C3	-2.41	122.25	126.20
27	B	619	BCR	C11-C10-C9	-2.41	123.90	127.28
25	C	509	CLA	CHD-C1D-ND	-2.41	121.41	124.80
27	t	101	BCR	C7-C8-C9	-2.41	122.67	126.23
29	m	101	LMG	O8-C28-O10	-2.41	117.61	123.63
25	b	609	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
25	c	501	CLA	CHB-C4A-NA	2.40	127.87	124.40
30	A	613	SQD	O9-S-C6	2.40	110.34	106.76
31	d	408	LHG	C18-C17-C16	-2.40	102.23	114.37
25	B	614	CLA	CHB-C4A-NA	2.40	127.87	124.40
27	A	610	BCR	C15-C14-C13	-2.40	123.91	127.28
25	b	610	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
25	B	604	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
28	a	611	PL9	O2-C1-C2	-2.40	116.38	121.83
29	D	408	LMG	C38-C37-C36	-2.40	102.26	114.37
25	C	512	CLA	C1-C2-C3	-2.40	122.27	126.20
25	c	501	CLA	C3B-C4B-NB	-2.39	108.39	110.53
29	d	411	LMG	C40-C39-C38	-2.39	102.27	114.37
30	L	101	SQD	C25-C24-C23	-2.39	104.93	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	510	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
25	D	404	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
25	b	614	CLA	C1-C2-C3	-2.39	122.28	126.20
27	d	405	BCR	C33-C5-C6	-2.39	121.88	124.48
25	A	607	CLA	O2D-CGD-CBD	2.39	115.41	111.23
29	m	101	LMG	C38-C37-C36	-2.39	102.30	114.37
32	C	516	DGD	C1D-C2D-C3D	-2.39	104.99	110.01
31	l	101	LHG	O8-C23-C24	2.38	119.11	111.83
25	C	501	CLA	CHB-C1B-NB	2.38	127.62	124.05
25	C	512	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
27	b	617	BCR	C15-C14-C13	-2.38	123.94	127.28
27	b	619	BCR	C15-C16-C17	-2.38	118.65	123.52
33	d	413	STE	O2-C1-C2	2.38	121.51	114.00
27	A	610	BCR	C15-C16-C17	-2.38	118.66	123.52
30	a	614	SQD	O48-C23-O10	-2.37	117.69	123.63
27	c	516	BCR	C33-C5-C6	-2.37	121.89	124.48
31	d	407	LHG	C11-C10-C9	-2.37	102.38	114.37
25	c	510	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
27	d	405	BCR	C16-C15-C14	-2.37	118.67	123.52
25	b	604	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
27	c	516	BCR	C2-C1-C6	2.36	113.87	110.44
25	C	504	CLA	CHB-C1B-NB	2.36	127.58	124.05
27	c	516	BCR	C24-C23-C22	-2.36	122.75	126.23
25	c	503	CLA	C11-C12-C13	-2.36	108.14	115.97
29	c	520	LMG	C38-C37-C36	-2.35	102.46	114.37
27	A	610	BCR	C33-C5-C6	-2.35	121.92	124.48
25	b	605	CLA	CHB-C4A-NA	2.35	127.79	124.40
27	K	101	BCR	C27-C26-C25	2.35	125.88	122.70
25	C	510	CLA	CMB-C2B-C3B	2.35	132.07	126.55
25	B	606	CLA	O2D-CGD-CBD	2.35	115.33	111.23
25	b	607	CLA	C6-C7-C8	-2.35	108.16	115.97
31	D	412	LHG	C20-C19-C18	-2.35	102.51	114.37
25	b	603	CLA	CHB-C4A-NA	2.35	127.78	124.40
29	A	612	LMG	O1-C7-C8	-2.35	105.11	110.82
27	K	102	BCR	C3-C4-C5	-2.34	109.88	114.06
32	A	617	DGD	CBB-CAB-C9B	-2.34	102.52	114.37
25	C	507	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
29	d	410	LMG	O7-C10-O9	-2.34	117.31	123.33
29	c	522	LMG	O6-C1-O1	-2.34	104.51	110.04
25	b	607	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
28	d	406	PL9	C50-C49-C48	-2.34	115.64	122.66
32	h	101	DGD	C7B-C6B-C5B	-2.34	102.56	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	512	CLA	O2D-CGD-CBD	2.34	115.31	111.23
27	C	514	BCR	C27-C26-C25	2.34	125.86	122.70
32	a	615	DGD	CFB-CEB-CDB	-2.33	102.57	114.37
25	B	613	CLA	CMB-C2B-C3B	2.33	132.04	126.55
25	b	606	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
25	c	506	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
25	B	608	CLA	CMB-C2B-C3B	2.33	132.03	126.55
25	B	610	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
33	C	519	STE	C3-C2-C1	-2.33	108.43	114.51
26	d	401	PHO	C3D-C4D-ND	2.33	110.69	107.71
31	A	614	LHG	C11-C10-C9	-2.33	102.59	114.37
32	C	515	DGD	CAB-C9B-C8B	-2.33	102.60	114.37
25	D	403	CLA	O2D-CGD-CBD	2.33	115.30	111.23
28	d	406	PL9	C20-C19-C21	2.33	119.27	115.23
28	A	611	PL9	C7-C8-C9	-2.33	122.82	126.83
27	b	618	BCR	C24-C23-C22	-2.33	122.79	126.23
25	b	612	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
25	c	509	CLA	C1-O2A-CGA	-2.33	111.02	116.65
32	A	617	DGD	C3E-C4E-C5E	-2.32	106.02	110.23
25	c	511	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	m	101	LMG	C40-C39-C38	-2.32	102.62	114.37
29	b	621	LMG	O2-C2-C1	-2.32	104.54	110.08
27	B	619	BCR	C15-C16-C17	-2.32	118.77	123.52
27	d	405	BCR	C30-C25-C26	-2.32	119.47	122.64
25	C	504	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
28	a	611	PL9	O2-C1-C6	2.31	124.16	120.48
28	d	406	PL9	O2-C1-C6	2.31	124.16	120.48
28	A	611	PL9	C12-C13-C14	-2.31	122.34	127.62
28	D	407	PL9	C32-C33-C34	-2.31	122.34	127.62
25	B	607	CLA	CHB-C1B-NB	2.31	127.51	124.05
33	C	519	STE	C4-C3-C2	-2.31	104.66	113.13
25	B	611	CLA	CHD-C4C-NC	2.30	127.80	124.23
32	C	517	DGD	O3E-C3E-C2E	-2.30	104.95	110.38
25	c	512	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
25	C	501	CLA	O2D-CGD-CBD	2.30	115.25	111.23
25	a	609	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
27	t	101	BCR	C33-C5-C6	-2.29	121.98	124.48
25	B	604	CLA	C1D-ND-C4D	2.29	107.92	106.31
27	T	101	BCR	C33-C5-C6	-2.29	121.98	124.48
31	D	412	LHG	O8-C23-O10	-2.29	117.89	123.63
27	B	618	BCR	C27-C26-C25	2.29	125.80	122.70
31	D	410	LHG	C27-C26-C25	-2.29	102.78	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	619	BCR	C29-C30-C25	2.29	113.76	110.44
25	b	613	CLA	CHB-C4A-NA	2.29	127.70	124.40
25	b	602	CLA	CMB-C2B-C3B	2.29	131.93	126.55
25	C	507	CLA	C2A-C1A-CHA	2.28	127.83	123.87
31	D	409	LHG	O8-C23-O10	-2.28	117.92	123.63
25	b	603	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
25	C	503	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	c	504	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	b	605	CLA	CHD-C4C-NC	2.28	127.77	124.23
27	c	516	BCR	C11-C10-C9	-2.28	124.08	127.28
32	C	515	DGD	C6D-O5D-C1E	2.28	118.69	113.80
25	A	607	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	a	612	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
29	D	408	LMG	O1-C1-C2	-2.28	104.81	108.27
25	b	603	CLA	CHD-C1D-C2D	2.28	130.22	125.49
25	C	504	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
29	c	522	LMG	C40-C39-C38	-2.27	102.88	114.37
32	a	615	DGD	CAB-C9B-C8B	-2.27	102.88	114.37
27	t	101	BCR	C27-C26-C25	2.27	125.78	122.70
27	A	610	BCR	C2-C1-C6	2.27	113.74	110.44
27	c	514	BCR	C11-C10-C9	-2.27	124.09	127.28
25	b	607	CLA	CHB-C1B-NB	2.27	127.45	124.05
25	c	510	CLA	CHB-C4A-NA	2.27	127.67	124.40
25	B	615	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
25	b	604	CLA	C11-C12-C13	-2.27	108.43	115.97
25	b	614	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
30	B	622	SQD	C25-C24-C23	-2.27	105.39	113.69
25	b	608	CLA	CHB-C1B-NB	2.26	127.45	124.05
25	a	608	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
31	D	410	LHG	C11-C10-C9	-2.26	102.95	114.37
25	b	605	CLA	C1-C2-C3	-2.26	122.50	126.20
25	D	404	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	b	608	CLA	C6-C7-C8	-2.26	108.46	115.97
25	b	603	CLA	C3B-C4B-NB	-2.26	108.52	110.53
32	a	615	DGD	C7B-C6B-C5B	-2.26	102.96	114.37
30	B	622	SQD	O8-S-C6	2.26	110.33	105.97
30	B	622	SQD	O9-S-C6	2.25	110.12	106.76
27	B	619	BCR	C1-C6-C5	-2.25	119.56	122.64
25	C	508	CLA	CHB-C1B-NB	2.25	127.43	124.05
25	c	507	CLA	CHB-C4A-NA	2.25	127.65	124.40
34	D	401	BCT	O2-C-O1	-2.25	113.92	119.68
35	f	101	HEM	CAB-C3B-C2B	-2.25	121.12	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	H	102	DGD	C3G-C2G-C1G	-2.25	106.54	111.78
27	c	514	BCR	C2-C1-C6	2.25	113.70	110.44
29	D	408	LMG	C3-C4-C5	-2.25	106.16	110.23
29	c	522	LMG	O7-C10-O9	-2.25	118.45	123.70
27	t	101	BCR	C35-C13-C12	2.25	121.52	118.09
25	B	604	CLA	C11-C10-C8	-2.25	108.50	115.97
29	D	408	LMG	O1-C7-C8	-2.24	105.36	110.82
25	b	603	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
25	c	512	CLA	CHD-C1D-ND	-2.24	121.64	124.80
25	C	510	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
26	d	401	PHO	CMA-C3A-C4A	-2.24	109.78	114.61
25	b	610	CLA	O1D-CGD-CBD	2.24	128.94	124.52
25	c	507	CLA	CHA-C1A-NA	-2.24	121.31	126.39
26	D	402	PHO	C4B-NB-C1B	2.24	112.08	108.82
25	c	513	CLA	CMB-C2B-C3B	2.24	131.81	126.55
25	C	506	CLA	CHB-C4A-NA	2.24	127.63	124.40
32	H	102	DGD	C1D-C2D-C3D	-2.24	105.31	110.01
25	B	601	CLA	C3B-C4B-NB	-2.23	108.53	110.53
25	b	602	CLA	C3B-C4B-NB	-2.23	108.53	110.53
25	c	509	CLA	O2D-CGD-CBD	2.23	115.13	111.23
29	b	621	LMG	O6-C5-C6	2.23	111.97	106.44
25	b	601	CLA	O2D-CGD-CBD	2.23	115.13	111.23
29	c	524	LMG	C9-C8-C7	-2.23	106.58	111.78
25	B	611	CLA	CHD-C1D-ND	-2.23	121.66	124.80
25	C	506	CLA	O1D-CGD-CBD	2.23	128.92	124.52
27	x	101	BCR	C3-C4-C5	-2.23	110.08	114.06
25	b	604	CLA	C11-C10-C8	-2.23	108.55	115.97
28	D	407	PL9	C27-C28-C29	-2.23	122.52	127.62
25	b	604	CLA	C6-C7-C8	-2.23	108.56	115.97
32	H	102	DGD	O6D-C1D-O3G	-2.23	104.78	110.04
25	c	502	CLA	CHB-C4A-NA	2.23	127.61	124.40
32	h	101	DGD	C5B-C4B-C3B	-2.22	103.13	114.37
31	e	101	LHG	C20-C19-C18	-2.22	103.13	114.37
32	A	617	DGD	C5B-C4B-C3B	-2.22	103.15	114.37
25	c	511	CLA	C2A-C1A-CHA	2.22	127.72	123.87
28	A	611	PL9	O1-C4-C3	-2.22	118.39	120.73
31	A	615	LHG	C20-C19-C18	-2.22	103.16	114.37
25	B	612	CLA	CHD-C1D-ND	-2.22	121.68	124.80
32	c	519	DGD	C1D-C2D-C3D	-2.22	105.35	110.01
25	c	508	CLA	CHD-C1D-ND	-2.22	121.68	124.80
29	A	612	LMG	O6-C1-O1	-2.22	104.81	110.04
32	c	517	DGD	CBB-CAB-C9B	-2.22	103.17	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	516	DGD	CAB-C9B-C8B	-2.21	103.17	114.37
25	B	613	CLA	CHB-C4A-NA	2.21	127.60	124.40
25	C	513	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
27	d	405	BCR	C24-C23-C22	-2.21	122.96	126.23
32	c	519	DGD	CBB-CAB-C9B	-2.21	103.18	114.37
32	H	102	DGD	CAB-C9B-C8B	-2.21	103.19	114.37
32	A	617	DGD	O3G-C1D-C2D	-2.21	104.92	108.27
32	C	515	DGD	C5B-C4B-C3B	-2.21	103.19	114.37
28	A	611	PL9	C40-C39-C38	-2.21	117.95	123.63
33	x	102	STE	C3-C2-C1	-2.21	108.74	114.51
25	B	605	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	A	606	CLA	O1D-CGD-CBD	2.21	128.87	124.52
25	C	502	CLA	CHB-C1B-NB	2.21	127.36	124.05
32	A	617	DGD	C8B-C7B-C6B	-2.21	103.22	114.37
32	h	101	DGD	C1D-O6D-C5D	-2.20	109.42	113.72
25	D	405	CLA	CHB-C1B-NB	2.20	127.36	124.05
27	b	619	BCR	C27-C26-C25	2.20	125.68	122.70
27	B	617	BCR	C15-C14-C13	-2.20	124.19	127.28
25	c	501	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
28	a	611	PL9	C36-C34-C33	-2.20	116.22	121.17
32	h	101	DGD	CBB-CAB-C9B	-2.20	103.24	114.37
25	c	508	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
29	c	524	LMG	O7-C10-O9	-2.20	118.56	123.70
25	b	602	CLA	CHD-C1D-ND	-2.20	121.70	124.80
25	D	403	CLA	CHD-C1D-ND	-2.20	121.71	124.80
32	c	519	DGD	CAB-C9B-C8B	-2.20	103.26	114.37
25	c	510	CLA	CMB-C2B-C3B	2.20	131.72	126.55
25	B	606	CLA	CHB-C4A-NA	2.20	127.57	124.40
31	d	407	LHG	C5-O7-C7	-2.20	112.54	117.80
25	B	604	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
25	B	605	CLA	CHD-C1D-C2D	2.19	130.05	125.49
35	f	101	HEM	C3B-C4B-NB	-2.19	107.89	109.47
29	c	522	LMG	C38-C37-C36	-2.19	103.28	114.37
25	d	404	CLA	C1-C2-C3	-2.19	122.61	126.20
25	C	510	CLA	CHB-C4A-NA	2.19	127.56	124.40
25	A	609	CLA	CHD-C1D-ND	-2.19	121.72	124.80
29	C	518	LMG	C38-C37-C36	-2.19	103.30	114.37
29	D	408	LMG	O2-C2-C1	-2.19	104.86	110.08
32	C	517	DGD	O3G-C1D-C2D	-2.19	104.95	108.27
29	C	518	LMG	O7-C10-O9	-2.19	118.59	123.70
27	H	101	BCR	C2-C1-C6	2.19	113.61	110.44
27	x	101	BCR	C15-C14-C13	-2.18	124.22	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	609	CLA	C3B-C4B-NB	-2.18	108.58	110.53
25	b	608	CLA	CHD-C4C-NC	2.18	127.61	124.23
25	B	603	CLA	CHD-C1D-ND	-2.18	121.73	124.80
32	c	517	DGD	C5B-C4B-C3B	-2.18	103.35	114.37
25	C	503	CLA	CHB-C1B-NB	2.18	127.32	124.05
31	A	614	LHG	C20-C19-C18	-2.18	103.37	114.37
25	c	501	CLA	C1-C2-C3	-2.18	122.63	126.20
29	b	621	LMG	C40-C39-C38	-2.17	103.38	114.37
32	a	615	DGD	CBB-CAB-C9B	-2.17	103.38	114.37
27	b	617	BCR	C29-C30-C25	2.17	113.59	110.44
29	A	612	LMG	C38-C37-C36	-2.17	103.40	114.37
29	B	621	LMG	O7-C10-O9	-2.17	117.75	123.33
25	b	615	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
28	d	406	PL9	O2-C1-C2	-2.17	116.89	121.83
27	B	618	BCR	C35-C13-C14	-2.17	119.30	122.82
27	H	101	BCR	C35-C13-C14	-2.17	119.30	122.82
25	B	604	CLA	C16-C15-C13	-2.16	108.77	115.97
29	M	101	LMG	O3-C3-C2	-2.16	105.28	110.38
28	a	611	PL9	C32-C33-C34	-2.16	122.67	127.62
29	c	520	LMG	C6-C5-C4	-2.16	107.71	113.02
25	b	607	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
29	m	101	LMG	O2-C2-C1	-2.16	104.93	110.08
25	C	508	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
25	a	608	CLA	CAC-C3C-C4C	2.16	127.60	124.79
29	A	612	LMG	C1-C2-C3	-2.16	105.47	110.01
25	d	403	CLA	CMB-C2B-C3B	2.16	131.63	126.55
29	d	411	LMG	O1-C1-C2	-2.16	105.00	108.27
29	d	411	LMG	C38-C37-C36	-2.16	103.46	114.37
29	C	518	LMG	C40-C39-C38	-2.16	103.47	114.37
28	D	407	PL9	C42-C43-C44	-2.16	122.69	127.62
27	b	617	BCR	C11-C10-C9	-2.15	124.26	127.28
32	c	519	DGD	C8B-C7B-C6B	-2.15	103.48	114.37
25	b	605	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	t	101	BCR	C1-C6-C5	-2.15	119.69	122.64
25	b	602	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
25	B	616	CLA	O2D-CGD-CBD	2.15	114.99	111.23
31	d	407	LHG	C20-C19-C18	-2.15	103.50	114.37
26	d	402	PHO	C3B-C4B-NB	-2.15	106.06	107.46
32	C	516	DGD	C3E-C4E-C5E	-2.15	106.34	110.23
25	C	502	CLA	C1-C2-C3	-2.15	122.68	126.20
29	C	518	LMG	C6-C5-C4	-2.15	107.75	113.02
25	b	612	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	515	DGD	O1G-C1A-C2A	-2.14	105.30	111.83
25	c	510	CLA	O1D-CGD-CBD	2.14	128.75	124.52
25	b	614	CLA	CHB-C4A-NA	2.14	127.49	124.40
29	M	101	LMG	O2-C2-C1	-2.14	104.97	110.08
30	F	101	SQD	C3-C4-C5	2.14	114.12	110.23
32	c	519	DGD	C6B-C5B-C4B	-2.14	103.54	114.37
36	V	201	HEC	CHB-C4A-NA	2.14	126.78	124.45
25	c	505	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
27	C	514	BCR	C33-C5-C6	-2.14	122.15	124.48
25	C	504	CLA	CHA-C1A-NA	-2.14	121.55	126.39
29	A	612	LMG	O7-C10-O9	-2.14	118.71	123.70
25	b	612	CLA	C11-C10-C8	-2.14	108.86	115.97
28	A	611	PL9	O2-C1-C6	2.14	123.88	120.48
25	C	510	CLA	O2D-CGD-CBD	2.14	114.96	111.23
27	D	406	BCR	C30-C25-C26	-2.13	119.72	122.64
25	C	505	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
29	c	522	LMG	O2-C2-C1	-2.13	104.99	110.08
25	B	603	CLA	CHB-C4A-NA	2.13	127.48	124.40
32	C	516	DGD	C6D-C5D-C4D	2.13	116.53	112.07
25	c	507	CLA	CHC-C4B-NB	2.13	127.24	124.05
28	a	611	PL9	O1-C4-C3	-2.13	118.49	120.73
32	c	518	DGD	C5B-C4B-C3B	-2.13	103.62	114.37
36	v	201	HEC	CHA-C4D-ND	2.13	127.72	123.86
25	B	604	CLA	O2D-CGD-CBD	2.13	114.94	111.23
25	b	608	CLA	C11-C10-C8	-2.12	108.91	115.97
25	B	607	CLA	CHB-C4A-NA	2.12	127.46	124.40
32	A	617	DGD	CFB-CEB-CDB	-2.12	103.64	114.37
25	C	508	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	C	505	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
26	d	401	PHO	O1D-CGD-CBD	2.12	127.94	124.72
25	B	616	CLA	C3B-C4B-NB	-2.12	108.64	110.53
27	B	618	BCR	C38-C26-C25	-2.12	122.17	124.48
25	C	504	CLA	CHD-C1D-ND	-2.12	121.82	124.80
25	B	606	CLA	CHB-C1B-NB	2.12	127.22	124.05
30	A	613	SQD	O47-C7-O49	-2.12	118.76	123.70
25	b	603	CLA	CMB-C2B-C3B	2.12	131.53	126.55
25	C	502	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
33	a	617	STE	C3-C2-C1	-2.11	108.99	114.51
25	B	609	CLA	CAC-C3C-C4C	2.11	127.54	124.79
27	Y	101	BCR	C16-C15-C14	-2.11	119.20	123.52
33	B	625	STE	O2-C1-C2	2.11	120.67	114.00
30	L	101	SQD	C9-C8-C7	-2.11	105.96	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	602	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
25	B	612	CLA	O1D-CGD-CBD	2.11	128.68	124.52
25	B	606	CLA	CHD-C4C-NC	2.11	127.50	124.23
25	D	405	CLA	CHC-C4B-NB	2.11	127.21	124.05
28	d	406	PL9	C32-C33-C34	-2.11	122.80	127.62
28	D	407	PL9	C36-C34-C33	-2.11	116.44	121.17
31	A	614	LHG	O8-C23-O10	-2.11	118.36	123.63
35	f	101	HEM	CHD-C4C-NC	2.11	126.75	124.45
28	a	611	PL9	C27-C28-C29	-2.11	122.80	127.62
25	B	601	CLA	C4-C3-C5	2.11	118.88	115.23
30	a	614	SQD	C9-C8-C7	-2.10	105.98	113.69
25	a	607	CLA	C4-C3-C5	2.10	118.88	115.23
29	b	621	LMG	C8-O7-C10	2.10	122.83	117.80
25	B	615	CLA	CHC-C4B-NB	2.10	127.20	124.05
25	B	601	CLA	CHB-C4A-NA	2.10	127.44	124.40
31	A	614	LHG	C18-C17-C16	-2.10	103.74	114.37
28	D	407	PL9	C8-C7-C3	2.10	117.46	112.03
25	b	613	CLA	CHA-C4D-ND	2.10	136.88	132.55
25	c	504	CLA	CHB-C1B-NB	2.10	127.20	124.05
25	b	610	CLA	CHD-C1D-ND	-2.10	121.85	124.80
25	B	610	CLA	CHD-C1D-ND	-2.10	121.85	124.80
25	C	503	CLA	C4D-CHA-C1A	2.10	123.74	121.24
25	B	616	CLA	CHC-C4B-NB	2.10	127.19	124.05
36	V	201	HEC	CMD-C2D-C1D	2.10	128.61	125.42
25	C	505	CLA	C1-C2-C3	-2.09	122.77	126.20
29	c	520	LMG	O1-C7-C8	-2.09	105.72	110.82
32	h	101	DGD	CAB-C9B-C8B	-2.09	103.78	114.37
25	B	603	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
32	C	516	DGD	O6E-C1E-O5D	-2.09	105.10	110.04
25	c	510	CLA	C2D-C1D-ND	-2.09	108.06	110.13
25	c	509	CLA	CHD-C1D-ND	-2.09	121.86	124.80
27	B	618	BCR	C33-C5-C6	-2.09	122.20	124.48
27	A	610	BCR	C16-C15-C14	-2.09	119.24	123.52
25	b	609	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	c	501	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	b	603	CLA	C11-C12-C13	-2.09	109.03	115.97
25	C	512	CLA	CHD-C1D-ND	-2.09	121.87	124.80
25	B	601	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
32	A	617	DGD	CAB-C9B-C8B	-2.09	103.82	114.37
27	A	610	BCR	C8-C7-C6	-2.09	121.43	127.00
31	l	101	LHG	C18-C17-C16	-2.08	103.83	114.37
31	D	410	LHG	O8-C23-C24	2.08	118.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	606	CLA	C11-C12-C13	-2.08	109.04	115.97
25	D	405	CLA	O2D-CGD-CBD	2.08	114.87	111.23
29	C	518	LMG	O3-C3-C2	-2.08	105.47	110.38
25	C	509	CLA	C1-C2-C3	-2.08	122.79	126.20
25	a	607	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
25	A	606	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	b	605	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
25	C	510	CLA	C16-C15-C13	-2.08	109.05	115.97
25	C	503	CLA	O1D-CGD-CBD	2.08	128.62	124.52
30	A	613	SQD	O5-C5-C4	2.08	113.45	109.70
29	D	411	LMG	O7-C10-O9	-2.08	118.85	123.70
29	c	522	LMG	C42-C41-C40	-2.08	103.86	114.37
25	b	613	CLA	C2A-C1A-CHA	2.08	127.47	123.87
25	B	606	CLA	CGD-CBD-CAD	-2.08	104.13	110.85
25	C	511	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	b	611	CLA	CHC-C1C-NC	2.07	127.43	124.31
28	d	406	PL9	C8-C7-C3	2.07	117.39	112.03
25	b	607	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
29	D	411	LMG	C38-C37-C36	-2.07	103.91	114.37
28	A	611	PL9	O2-C1-C2	-2.07	117.12	121.83
27	A	610	BCR	C7-C8-C9	-2.07	123.17	126.23
25	b	616	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	B	615	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	b	611	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	b	605	CLA	C7-C6-C5	-2.07	107.75	113.26
35	f	101	HEM	CHB-C1B-NB	2.07	126.92	124.37
31	e	101	LHG	C18-C17-C16	-2.07	103.92	114.37
33	t	102	STE	O2-C1-C2	2.07	120.53	114.00
25	a	609	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	b	606	CLA	CHB-C1B-NB	2.06	127.14	124.05
33	C	520	STE	O2-C1-C2	2.06	120.52	114.00
27	a	610	BCR	C40-C30-C25	2.06	113.48	110.24
36	V	201	HEC	CMC-C2C-C1C	-2.06	122.28	125.42
27	d	405	BCR	C11-C10-C9	-2.06	124.39	127.28
25	b	614	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
28	a	611	PL9	C42-C43-C44	-2.06	122.91	127.62
25	B	603	CLA	CHD-C1D-C2D	2.06	129.77	125.49
25	D	403	CLA	CHC-C4B-NB	2.06	127.14	124.05
25	b	611	CLA	CHD-C1D-C2D	2.06	129.77	125.49
25	b	608	CLA	CMB-C2B-C3B	2.06	131.39	126.55
27	B	617	BCR	C33-C5-C6	-2.05	122.24	124.48
27	T	101	BCR	C15-C14-C13	-2.05	124.40	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	517	DGD	CBB-CAB-C9B	-2.05	103.99	114.37
32	c	518	DGD	CBB-CAB-C9B	-2.05	103.99	114.37
29	c	520	LMG	O2-C2-C1	-2.05	105.19	110.08
25	d	404	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
29	d	411	LMG	C3-C4-C5	-2.05	106.52	110.23
29	c	522	LMG	O3-C3-C2	-2.05	105.55	110.38
25	b	613	CLA	CMB-C2B-C3B	2.05	131.37	126.55
32	c	518	DGD	O6E-C1E-O5D	-2.05	105.21	110.04
25	C	513	CLA	O1D-CGD-CBD	2.05	128.56	124.52
31	A	614	LHG	C27-C26-C25	-2.05	104.03	114.37
25	c	503	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	C	503	CLA	C1-C2-C3	2.04	129.55	126.20
27	A	610	BCR	C38-C26-C25	-2.04	122.25	124.48
33	j	101	STE	C3-C2-C1	-2.04	109.17	114.51
27	a	610	BCR	C21-C20-C19	-2.04	117.28	123.20
27	a	610	BCR	C39-C30-C25	-2.04	107.04	110.24
32	C	515	DGD	O3E-C3E-C2E	-2.04	105.56	110.38
32	C	515	DGD	CBB-CAB-C9B	-2.04	104.05	114.37
25	b	606	CLA	CMB-C2B-C3B	2.04	131.35	126.55
30	F	101	SQD	C1-C2-C3	-2.04	105.72	110.01
25	c	503	CLA	C7-C6-C5	-2.04	107.83	113.26
29	B	621	LMG	C38-C37-C36	-2.04	104.07	114.37
30	a	613	SQD	O47-C7-O49	-2.03	118.95	123.70
27	Y	101	BCR	C10-C11-C12	-2.03	117.31	123.20
33	C	519	STE	C6-C5-C4	-2.03	104.09	114.37
25	c	502	CLA	CED-O2D-CGD	2.03	120.53	115.92
32	c	518	DGD	C7B-C6B-C5B	-2.03	104.11	114.37
29	d	410	LMG	C38-C37-C36	-2.03	104.12	114.37
27	c	516	BCR	C38-C26-C25	-2.03	122.27	124.48
28	D	407	PL9	C40-C39-C41	2.03	118.75	115.23
31	l	101	LHG	C27-C26-C25	-2.03	104.13	114.37
27	c	515	BCR	C33-C5-C6	-2.03	122.27	124.48
25	D	404	CLA	C11-C12-C13	-2.02	109.23	115.97
25	D	405	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
25	C	507	CLA	CHA-C1A-NA	-2.02	121.81	126.39
25	C	508	CLA	CHD-C1D-C2D	2.02	129.70	125.49
25	B	607	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	c	506	CLA	CMB-C2B-C3B	2.02	131.31	126.55
32	c	518	DGD	C1D-C2D-C3D	-2.02	105.76	110.01
25	B	614	CLA	CHB-C1B-NB	2.02	127.08	124.05
31	d	408	LHG	C27-C26-C25	-2.02	104.17	114.37
25	d	403	CLA	O2A-CGA-O1A	-2.02	118.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	516	DGD	C3D-C4D-C5D	-2.02	106.57	110.23
25	B	607	CLA	CMB-C2B-C3B	2.02	131.29	126.55
32	c	518	DGD	O2E-C2E-C1E	-2.02	105.27	110.08
27	b	618	BCR	C35-C13-C14	-2.02	119.55	122.82
25	b	615	CLA	CHC-C1C-NC	2.02	127.35	124.31
27	k	101	BCR	C38-C26-C25	-2.02	122.28	124.48
32	C	516	DGD	C6D-O5D-C1E	2.01	118.11	113.80
27	K	102	BCR	C11-C10-C9	-2.01	124.46	127.28
25	C	502	CLA	C16-C15-C13	-2.01	109.28	115.97
25	b	609	CLA	C1-C2-C3	-2.01	122.90	126.20
28	a	611	PL9	C20-C19-C21	2.01	118.72	115.23
32	A	617	DGD	C1D-C2D-C3D	-2.01	105.78	110.01
25	C	506	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
25	c	506	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
27	K	101	BCR	C33-C5-C6	-2.01	122.29	124.48
25	B	603	CLA	CHB-C1B-NB	2.01	127.06	124.05
25	D	404	CLA	C1-C2-C3	-2.01	122.91	126.20
25	B	608	CLA	C11-C12-C13	-2.01	109.30	115.97
25	b	609	CLA	CMB-C2B-C3B	2.01	131.27	126.55
26	d	401	PHO	CED-O2D-CGD	2.00	120.46	115.92
35	f	101	HEM	C1B-NB-C4B	2.00	107.58	105.21
27	H	101	BCR	C1-C6-C5	-2.00	119.90	122.64
32	C	515	DGD	C3G-C2G-C1G	-2.00	107.11	111.78
29	C	518	LMG	O8-C28-O10	-2.00	118.62	123.63
25	B	610	CLA	C4-C3-C5	2.00	118.70	115.23

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	609	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	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	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
25	D	403	CLA	ND
25	D	404	CLA	ND
25	a	607	CLA	ND
25	a	609	CLA	ND
25	a	612	CLA	ND
25	b	601	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	b	616	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND

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Mol	Chain	Res	Type	Atom
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	403	CLA	ND
25	d	404	CLA	ND

All (1862) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	605	CLA	C4B-C3B-CAB-CBB
25	B	606	CLA	C11-C10-C8-C9
25	B	607	CLA	C4-C3-C5-C6
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	615	CLA	C2B-C3B-CAB-CBB
25	B	615	CLA	C4B-C3B-CAB-CBB
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C4B-C3B-CAB-CBB
25	C	513	CLA	C12-C13-C15-C16
25	a	608	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C4B-C3B-CAB-CBB
25	b	607	CLA	C4-C3-C5-C6
25	b	607	CLA	C11-C10-C8-C9
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C6-C7-C8-C9
25	c	511	CLA	C14-C13-C15-C16
25	c	512	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
27	B	618	BCR	C20-C21-C22-C37
27	C	514	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
27	D	406	BCR	C22-C23-C24-C25
27	D	406	BCR	C23-C24-C25-C26
27	D	406	BCR	C23-C24-C25-C30
27	H	101	BCR	C11-C12-C13-C35
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	T	101	BCR	C7-C8-C9-C10
27	Y	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C37-C22-C23-C24
27	b	617	BCR	C20-C21-C22-C37
27	d	405	BCR	C7-C8-C9-C34
27	d	405	BCR	C21-C22-C23-C24
27	k	101	BCR	C7-C8-C9-C34
27	k	101	BCR	C17-C18-C19-C20
27	k	101	BCR	C20-C21-C22-C37
28	A	611	PL9	C12-C13-C14-C15
28	A	611	PL9	C12-C13-C14-C16
28	A	611	PL9	C22-C23-C24-C25
28	A	611	PL9	C32-C33-C34-C36
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C40-C39-C41-C42
28	D	407	PL9	C32-C33-C34-C36
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C35-C34-C36-C37
28	a	611	PL9	C42-C43-C44-C46
28	a	611	PL9	C44-C46-C47-C48
28	d	406	PL9	C42-C43-C44-C46
28	d	406	PL9	C47-C48-C49-C51
29	A	612	LMG	O6-C1-O1-C7
29	A	612	LMG	O1-C7-C8-O7
29	A	612	LMG	O9-C10-O7-C8
29	A	612	LMG	C11-C10-O7-C8
29	c	524	LMG	O6-C1-O1-C7
30	A	616	SQD	C44-C45-C46-O48
30	A	616	SQD	C46-C45-O47-C7
30	B	622	SQD	C2-C1-O6-C44
30	B	622	SQD	O5-C1-O6-C44
30	B	622	SQD	O49-C7-O47-C45
30	B	622	SQD	C8-C7-O47-C45
30	B	622	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
30	F	101	SQD	C45-C44-O6-C1
30	L	101	SQD	C8-C7-O47-C45
30	L	101	SQD	O10-C23-O48-C46
30	L	101	SQD	C24-C23-O48-C46
30	a	614	SQD	C8-C7-O47-C45
30	f	102	SQD	O5-C1-O6-C44
31	A	614	LHG	C3-O3-P-O5
31	A	614	LHG	O10-C23-O8-C6
31	A	615	LHG	C3-O3-P-O4
31	A	615	LHG	C4-O6-P-O4
31	D	409	LHG	C1-C2-C3-O3
31	D	409	LHG	O2-C2-C3-O3
31	D	409	LHG	C3-O3-P-O5
31	D	409	LHG	C3-O3-P-O6
31	D	409	LHG	C4-O6-P-O3
31	D	409	LHG	C4-O6-P-O4
31	D	412	LHG	O1-C1-C2-C3
31	D	412	LHG	C1-C2-C3-O3
31	D	412	LHG	C3-O3-P-O4
31	D	412	LHG	C3-O3-P-O5
31	D	412	LHG	C3-O3-P-O6
31	d	407	LHG	O1-C1-C2-O2
31	d	407	LHG	O1-C1-C2-C3
31	d	407	LHG	C3-O3-P-O6
31	d	408	LHG	O1-C1-C2-C3
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O4
31	e	101	LHG	O1-C1-C2-O2
31	e	101	LHG	O1-C1-C2-C3
31	e	101	LHG	C3-O3-P-O4
31	e	101	LHG	C3-O3-P-O6
31	e	101	LHG	O6-C4-C5-O7
31	e	101	LHG	O10-C23-O8-C6
31	l	101	LHG	C3-O3-P-O4
31	l	101	LHG	C4-O6-P-O3
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
32	A	617	DGD	O1B-C1B-O2G-C2G
36	V	201	HEC	C2B-C3B-CAB-CBB
36	V	201	HEC	C4B-C3B-CAB-CBB
36	V	201	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
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	b	601	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
26	d	402	PHO	CBD-CGD-O2D-CED
25	B	601	CLA	O1A-CGA-O2A-C1
30	F	101	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
28	D	407	PL9	C47-C48-C49-C50
28	d	406	PL9	C47-C48-C49-C50
25	B	601	CLA	CBA-CGA-O2A-C1
30	F	101	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
31	A	614	LHG	C24-C23-O8-C6
31	e	101	LHG	C24-C23-O8-C6
25	c	510	CLA	CBD-CGD-O2D-CED
29	D	411	LMG	O9-C10-O7-C8
29	b	621	LMG	O9-C10-O7-C8
29	c	522	LMG	O9-C10-O7-C8
30	L	101	SQD	O49-C7-O47-C45
30	a	614	SQD	O49-C7-O47-C45
32	a	615	DGD	O1B-C1B-O2G-C2G
25	B	605	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	c	511	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
32	A	617	DGD	C2B-C1B-O2G-C2G
32	a	615	DGD	C2B-C1B-O2G-C2G
25	b	601	CLA	O1D-CGD-O2D-CED
25	A	609	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
28	d	406	PL9	C40-C39-C41-C42
25	A	609	CLA	C2-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	B	607	CLA	C2-C3-C5-C6
25	b	607	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	C2-C3-C5-C6
28	D	407	PL9	C47-C48-C49-C51
29	M	101	LMG	O10-C28-O8-C9
25	b	614	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7
30	B	622	SQD	C24-C23-O48-C46
28	A	611	PL9	C27-C28-C29-C30
28	A	611	PL9	C22-C23-C24-C26
28	A	611	PL9	C37-C38-C39-C41
29	c	524	LMG	O10-C28-O8-C9
30	B	622	SQD	O10-C23-O48-C46
29	c	522	LMG	O6-C5-C6-O5
25	B	608	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
25	b	606	CLA	C3-C5-C6-C7
26	d	402	PHO	O1D-CGD-O2D-CED
30	a	614	SQD	C24-C23-O48-C46
32	c	519	DGD	O1A-C1A-O1G-C1G
29	C	518	LMG	C11-C10-O7-C8
29	b	621	LMG	C11-C10-O7-C8
25	c	509	CLA	O1D-CGD-O2D-CED
29	b	621	LMG	O10-C28-O8-C9
25	c	513	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	C4-C3-C5-C6
25	C	513	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
28	A	611	PL9	C18-C19-C21-C22
28	A	611	PL9	C38-C39-C41-C42
28	A	611	PL9	C43-C44-C46-C47
28	d	406	PL9	C38-C39-C41-C42
28	A	611	PL9	C34-C36-C37-C38
28	D	407	PL9	C44-C46-C47-C48
29	c	524	LMG	C4-C5-C6-O5
29	c	522	LMG	C4-C5-C6-O5
30	F	101	SQD	O5-C1-O6-C44
29	M	101	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
30	a	614	SQD	O10-C23-O48-C46
31	D	412	LHG	C28-C29-C30-C31
25	C	501	CLA	CBD-CGD-O2D-CED
29	D	411	LMG	C11-C10-O7-C8
25	C	509	CLA	C3-C5-C6-C7
25	a	609	CLA	CBA-CGA-O2A-C1
29	C	518	LMG	C29-C28-O8-C9
29	c	524	LMG	C29-C28-O8-C9
32	a	615	DGD	C2A-C1A-O1G-C1G
25	B	610	CLA	CBD-CGD-O2D-CED
30	L	101	SQD	C12-C13-C14-C15
31	d	409	LHG	C24-C25-C26-C27
25	c	510	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	C4-C3-C5-C6
28	A	611	PL9	C20-C19-C21-C22
28	A	611	PL9	C45-C44-C46-C47
28	a	611	PL9	C33-C34-C36-C37
25	B	604	CLA	C3-C5-C6-C7
25	C	513	CLA	C3-C5-C6-C7
25	A	607	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C14
25	B	607	CLA	C14-C13-C15-C16
25	B	613	CLA	C11-C12-C13-C14
25	B	614	CLA	C14-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	C	513	CLA	C6-C7-C8-C9
25	a	608	CLA	C11-C12-C13-C14
25	b	601	CLA	C14-C13-C15-C16
25	b	606	CLA	C14-C13-C15-C16
25	b	616	CLA	C11-C10-C8-C9
25	c	502	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C10-C8-C9
25	c	512	CLA	C6-C7-C8-C9
26	A	608	PHO	C14-C13-C15-C16
32	A	617	DGD	C4E-C5E-C6E-O5E
30	A	616	SQD	C44-C45-O47-C7
30	f	102	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
31	D	412	LHG	O2-C2-C3-O3
29	c	524	LMG	O6-C5-C6-O5
33	b	622	STE	C4-C5-C6-C7
32	a	615	DGD	O1A-C1A-O1G-C1G
25	D	404	CLA	CBD-CGD-O2D-CED
27	B	619	BCR	C7-C8-C9-C34
27	B	619	BCR	C37-C22-C23-C24
27	D	406	BCR	C37-C22-C23-C24
27	K	101	BCR	C7-C8-C9-C34
27	K	101	BCR	C37-C22-C23-C24
27	K	102	BCR	C11-C12-C13-C35
27	T	101	BCR	C7-C8-C9-C34
27	b	618	BCR	C7-C8-C9-C34
27	b	619	BCR	C37-C22-C23-C24
27	d	405	BCR	C37-C22-C23-C24
27	t	101	BCR	C7-C8-C9-C34
32	A	617	DGD	O6E-C5E-C6E-O5E
29	c	522	LMG	O7-C8-C9-O8
30	a	613	SQD	O6-C44-C45-O47
25	c	506	CLA	CBA-CGA-O2A-C1
28	d	406	PL9	C42-C43-C44-C45
25	B	611	CLA	C8-C10-C11-C12
25	C	510	CLA	C13-C15-C16-C17
25	b	615	CLA	C5-C6-C7-C8
32	C	515	DGD	O6E-C5E-C6E-O5E
30	A	616	SQD	C7-C8-C9-C10
25	a	609	CLA	O1A-CGA-O2A-C1
25	D	405	CLA	C10-C11-C12-C13
25	B	611	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C7
25	b	615	CLA	C11-C12-C13-C15
30	a	613	SQD	C11-C12-C13-C14
33	T	102	STE	C3-C4-C5-C6
25	c	503	CLA	C5-C6-C7-C8
32	H	102	DGD	C1A-C2A-C3A-C4A
33	B	624	STE	C1-C2-C3-C4
28	A	611	PL9	C19-C21-C22-C23
28	d	406	PL9	C44-C46-C47-C48
25	C	503	CLA	C5-C6-C7-C8
25	C	513	CLA	C13-C15-C16-C17
29	A	612	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
29	D	411	LMG	C10-C11-C12-C13
30	A	613	SQD	C7-C8-C9-C10
32	c	518	DGD	C1B-C2B-C3B-C4B
25	c	506	CLA	O1A-CGA-O2A-C1
25	B	607	CLA	C8-C10-C11-C12
25	B	607	CLA	C10-C11-C12-C13
25	C	506	CLA	C8-C10-C11-C12
25	C	506	CLA	C13-C15-C16-C17
25	C	509	CLA	C8-C10-C11-C12
25	b	602	CLA	C13-C15-C16-C17
25	c	509	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
27	c	514	BCR	C18-C19-C20-C21
25	D	403	CLA	C15-C16-C17-C18
25	a	609	CLA	C5-C6-C7-C8
25	c	506	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17
29	d	411	LMG	C28-C29-C30-C31
30	B	622	SQD	C23-C24-C25-C26
30	L	101	SQD	C23-C24-C25-C26
31	A	614	LHG	C7-C8-C9-C10
31	d	407	LHG	C7-C8-C9-C10
31	d	407	LHG	C23-C24-C25-C26
31	d	409	LHG	C23-C24-C25-C26
31	e	101	LHG	C23-C24-C25-C26
32	C	515	DGD	C1A-C2A-C3A-C4A
33	E	102	STE	C1-C2-C3-C4
29	C	518	LMG	O6-C1-O1-C7
32	C	516	DGD	O6E-C1E-O5D-C6D
32	c	519	DGD	C8A-C9A-CAA-CBA
25	B	603	CLA	C15-C16-C17-C18
25	B	607	CLA	C5-C6-C7-C8
25	C	509	CLA	C5-C6-C7-C8
25	b	611	CLA	C8-C10-C11-C12
25	b	614	CLA	C13-C15-C16-C17
25	c	503	CLA	C8-C10-C11-C12
31	d	407	LHG	O2-C2-C3-O3
31	e	101	LHG	O2-C2-C3-O3
29	b	621	LMG	C10-C11-C12-C13
32	a	615	DGD	C1A-C2A-C3A-C4A
32	c	518	DGD	C1A-C2A-C3A-C4A
25	B	606	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	c	511	CLA	O1D-CGD-O2D-CED
25	B	613	CLA	C5-C6-C7-C8
25	c	510	CLA	C15-C16-C17-C18
29	m	101	LMG	C29-C28-O8-C9
32	c	519	DGD	C2A-C1A-O1G-C1G
25	B	613	CLA	C8-C10-C11-C12
25	b	601	CLA	C10-C11-C12-C13
30	L	101	SQD	C11-C10-C9-C8
31	A	614	LHG	C1-C2-C3-O3
31	d	407	LHG	C1-C2-C3-O3
31	e	101	LHG	C1-C2-C3-O3
25	B	606	CLA	C2A-CAA-CBA-CGA
29	b	621	LMG	C29-C28-O8-C9
25	B	603	CLA	C8-C10-C11-C12
25	C	513	CLA	C5-C6-C7-C8
25	a	607	CLA	C15-C16-C17-C18
25	b	615	CLA	C15-C16-C17-C18
25	c	511	CLA	C15-C16-C17-C18
25	c	512	CLA	C13-C15-C16-C17
33	B	620	STE	C1-C2-C3-C4
25	B	607	CLA	C13-C15-C16-C17
25	D	403	CLA	C13-C15-C16-C17
25	b	601	CLA	C13-C15-C16-C17
25	c	511	CLA	C13-C15-C16-C17
29	b	621	LMG	O6-C5-C6-O5
25	C	509	CLA	C10-C11-C12-C13
25	b	603	CLA	C13-C15-C16-C17
25	b	614	CLA	C8-C10-C11-C12
25	d	404	CLA	C8-C10-C11-C12
29	M	101	LMG	C28-C29-C30-C31
28	d	406	PL9	C33-C34-C36-C37
25	b	607	CLA	C8-C10-C11-C12
29	c	522	LMG	C11-C10-O7-C8
29	A	612	LMG	C2-C1-O1-C7
29	C	518	LMG	C2-C1-O1-C7
29	c	524	LMG	C2-C1-O1-C7
32	C	516	DGD	C2E-C1E-O5D-C6D
32	c	518	DGD	C2E-C1E-O5D-C6D
25	B	606	CLA	C10-C11-C12-C13
25	C	505	CLA	C10-C11-C12-C13
28	A	611	PL9	C24-C26-C27-C28
25	c	512	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C20
28	a	611	PL9	C32-C33-C34-C36
27	H	101	BCR	C20-C21-C22-C37
27	K	101	BCR	C16-C17-C18-C36
27	K	102	BCR	C16-C17-C18-C36
27	T	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C16-C17-C18-C36
27	b	617	BCR	C11-C10-C9-C34
27	b	618	BCR	C20-C21-C22-C37
27	b	619	BCR	C35-C13-C14-C15
27	b	619	BCR	C20-C21-C22-C37
27	c	514	BCR	C16-C17-C18-C36
27	k	101	BCR	C16-C17-C18-C36
27	t	101	BCR	C20-C21-C22-C37
29	c	522	LMG	C10-C11-C12-C13
32	a	615	DGD	C1B-C2B-C3B-C4B
25	C	512	CLA	C13-C15-C16-C17
25	b	607	CLA	C10-C11-C12-C13
27	c	515	BCR	C7-C8-C9-C34
27	x	101	BCR	C7-C8-C9-C34
27	Y	101	BCR	C21-C22-C23-C24
27	b	617	BCR	C21-C22-C23-C24
27	k	101	BCR	C7-C8-C9-C10
25	b	606	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	C	512	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
31	D	409	LHG	O1-C1-C2-C3
31	D	410	LHG	O1-C1-C2-C3
31	d	409	LHG	O1-C1-C2-C3
30	L	101	SQD	C46-C45-O47-C7
25	b	604	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C20
27	C	514	BCR	C20-C21-C22-C23
27	K	101	BCR	C20-C21-C22-C23
27	b	618	BCR	C11-C10-C9-C8
27	c	514	BCR	C12-C13-C14-C15
27	c	514	BCR	C16-C17-C18-C19
27	k	101	BCR	C20-C21-C22-C23
27	x	101	BCR	C11-C10-C9-C8
27	x	101	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	M	101	LMG	O6-C1-O1-C7
25	C	510	CLA	C15-C16-C17-C18
25	c	506	CLA	C2-C1-O2A-CGA
25	B	602	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C20
25	a	608	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C19
32	c	517	DGD	O6E-C5E-C6E-O5E
29	C	518	LMG	C17-C18-C19-C20
32	c	517	DGD	C4B-C5B-C6B-C7B
33	B	626	STE	C3-C4-C5-C6
33	H	103	STE	C11-C12-C13-C14
27	D	406	BCR	C14-C15-C16-C17
27	K	101	BCR	C14-C15-C16-C17
29	A	612	LMG	C33-C34-C35-C36
29	D	408	LMG	C14-C15-C16-C17
29	c	522	LMG	C39-C40-C41-C42
31	e	101	LHG	C27-C28-C29-C30
32	C	515	DGD	C7B-C8B-C9B-CAB
32	a	615	DGD	C8B-C9B-CAB-CBB
33	B	625	STE	C5-C6-C7-C8
33	I	101	STE	C10-C11-C12-C13
33	M	102	STE	C9-C10-C11-C12
33	l	102	STE	C3-C4-C5-C6
25	C	505	CLA	C15-C16-C17-C18
29	M	101	LMG	C37-C38-C39-C40
29	m	101	LMG	C39-C40-C41-C42
30	F	101	SQD	C25-C26-C27-C28
31	D	409	LHG	C10-C11-C12-C13
31	D	410	LHG	C25-C26-C27-C28
31	d	408	LHG	C29-C30-C31-C32
32	c	517	DGD	CBB-CCB-CDB-CEB
32	h	101	DGD	C6B-C7B-C8B-C9B
33	d	413	STE	C10-C11-C12-C13
33	x	102	STE	C2-C3-C4-C5
29	B	621	LMG	C33-C34-C35-C36
29	d	410	LMG	C35-C36-C37-C38
30	A	613	SQD	C16-C17-C18-C19
30	a	613	SQD	C17-C18-C19-C20
30	a	614	SQD	C10-C11-C12-C13
30	a	614	SQD	C18-C19-C20-C21
31	d	407	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C32-C33-C34-C35
32	c	518	DGD	C2A-C3A-C4A-C5A
33	H	103	STE	C5-C6-C7-C8
33	a	616	STE	C2-C3-C4-C5
33	b	622	STE	C12-C13-C14-C15
33	b	622	STE	C14-C15-C16-C17
33	m	102	STE	C5-C6-C7-C8
33	x	102	STE	C12-C13-C14-C15
31	D	412	LHG	O1-C1-C2-O2
31	d	408	LHG	O1-C1-C2-O2
29	B	621	LMG	C32-C33-C34-C35
29	D	411	LMG	C34-C35-C36-C37
31	D	410	LHG	C29-C30-C31-C32
31	d	409	LHG	C26-C27-C28-C29
25	B	606	CLA	C4B-C3B-CAB-CBB
25	C	502	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
32	C	515	DGD	C1B-C2B-C3B-C4B
29	C	518	LMG	C13-C14-C15-C16
33	x	102	STE	C7-C8-C9-C10
25	B	602	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C20
28	A	611	PL9	C27-C28-C29-C31
32	c	517	DGD	C7A-C8A-C9A-CAA
33	d	413	STE	C11-C12-C13-C14
25	B	616	CLA	C5-C6-C7-C8
25	b	613	CLA	C13-C15-C16-C17
31	A	614	LHG	C8-C7-O7-C5
29	c	522	LMG	C16-C17-C18-C19
31	D	410	LHG	C34-C35-C36-C37
33	a	617	STE	C4-C5-C6-C7
25	D	404	CLA	C12-C13-C15-C16
29	D	408	LMG	C36-C37-C38-C39
29	b	621	LMG	C11-C12-C13-C14
30	A	616	SQD	C28-C29-C30-C31
30	a	614	SQD	C14-C15-C16-C17
31	D	410	LHG	C27-C28-C29-C30
32	c	518	DGD	CCA-CDA-CEA-CFA
33	C	520	STE	C3-C4-C5-C6
31	A	614	LHG	C23-C24-C25-C26
25	d	404	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	C	518	LMG	C31-C32-C33-C34
29	M	101	LMG	C14-C15-C16-C17
29	c	520	LMG	C31-C32-C33-C34
30	A	613	SQD	C11-C10-C9-C8
30	A	616	SQD	C18-C19-C20-C21
30	f	102	SQD	C29-C30-C31-C32
31	d	407	LHG	C16-C17-C18-C19
32	c	517	DGD	C9B-CAB-CBB-CCB
32	c	519	DGD	CCA-CDA-CEA-CFA
33	B	620	STE	C9-C10-C11-C12
25	c	512	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	C3A-C2A-CAA-CBA
29	D	411	LMG	C14-C15-C16-C17
30	A	613	SQD	C10-C11-C12-C13
31	A	614	LHG	C17-C18-C19-C20
33	E	102	STE	C3-C4-C5-C6
33	b	620	STE	C14-C15-C16-C17
25	B	603	CLA	O1D-CGD-O2D-CED
25	B	612	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
31	d	408	LHG	C32-C33-C34-C35
32	H	102	DGD	CAB-CBB-CCB-CDB
32	c	518	DGD	C8A-C9A-CAA-CBA
33	J	101	STE	C3-C4-C5-C6
33	c	521	STE	C9-C10-C11-C12
31	l	101	LHG	C24-C25-C26-C27
29	D	408	LMG	C31-C32-C33-C34
29	b	621	LMG	C16-C17-C18-C19
31	A	615	LHG	C12-C13-C14-C15
31	A	615	LHG	C32-C33-C34-C35
31	l	101	LHG	C11-C12-C13-C14
32	C	516	DGD	C5A-C6A-C7A-C8A
33	T	103	STE	C11-C10-C9-C8
33	t	102	STE	C11-C10-C9-C8
29	D	408	LMG	C10-C11-C12-C13
30	F	101	SQD	C23-C24-C25-C26
32	c	519	DGD	C1A-C2A-C3A-C4A
33	d	412	STE	C1-C2-C3-C4
33	d	413	STE	C1-C2-C3-C4
29	A	612	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
29	d	410	LMG	C33-C34-C35-C36
30	a	613	SQD	C26-C27-C28-C29
31	A	615	LHG	C17-C18-C19-C20
31	D	410	LHG	C15-C16-C17-C18
31	d	407	LHG	C32-C33-C34-C35
31	d	408	LHG	C34-C35-C36-C37
31	e	101	LHG	C17-C18-C19-C20
31	l	101	LHG	C16-C17-C18-C19
32	H	102	DGD	C8B-C9B-CAB-CBB
32	a	615	DGD	C5A-C6A-C7A-C8A
32	c	517	DGD	C5B-C6B-C7B-C8B
32	h	101	DGD	C5B-C6B-C7B-C8B
33	x	102	STE	C3-C4-C5-C6
29	A	612	LMG	O6-C5-C6-O5
29	A	612	LMG	C38-C39-C40-C41
29	c	524	LMG	C12-C13-C14-C15
29	c	524	LMG	C15-C16-C17-C18
31	A	614	LHG	C25-C26-C27-C28
33	d	413	STE	C2-C3-C4-C5
32	c	517	DGD	O6D-C5D-C6D-O5D
29	B	621	LMG	C31-C32-C33-C34
32	A	617	DGD	C2B-C3B-C4B-C5B
32	a	615	DGD	C6A-C7A-C8A-C9A
33	D	413	STE	C4-C5-C6-C7
30	a	614	SQD	C11-C10-C9-C8
33	B	625	STE	C4-C5-C6-C7
25	B	601	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
25	c	506	CLA	C16-C17-C18-C20
25	B	605	CLA	C2B-C3B-CAB-CBB
25	a	608	CLA	C2B-C3B-CAB-CBB
25	b	601	CLA	C2B-C3B-CAB-CBB
27	Y	101	BCR	C1-C6-C7-C8
27	Y	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C5-C6-C7-C8
29	b	621	LMG	C12-C13-C14-C15
32	C	516	DGD	C8B-C9B-CAB-CBB
32	h	101	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
33	d	413	STE	C5-C6-C7-C8
25	C	505	CLA	CBD-CGD-O2D-CED
31	e	101	LHG	C8-C7-O7-C5
32	C	515	DGD	C9B-CAB-CBB-CCB
33	C	519	STE	C6-C7-C8-C9
29	M	101	LMG	C33-C34-C35-C36
29	m	101	LMG	C17-C18-C19-C20
30	B	622	SQD	C11-C12-C13-C14
31	A	615	LHG	C18-C19-C20-C21
31	d	408	LHG	C12-C13-C14-C15
32	c	517	DGD	C4A-C5A-C6A-C7A
32	c	517	DGD	CCB-CDB-CEB-CFB
33	l	102	STE	C7-C8-C9-C10
33	x	102	STE	C1-C2-C3-C4
29	M	101	LMG	C38-C39-C40-C41
29	b	621	LMG	C37-C38-C39-C40
29	c	522	LMG	C32-C33-C34-C35
30	B	622	SQD	C18-C19-C20-C21
31	A	614	LHG	C33-C34-C35-C36
31	d	407	LHG	C11-C10-C9-C8
32	C	517	DGD	C8A-C9A-CAA-CBA
32	H	102	DGD	C6A-C7A-C8A-C9A
28	A	611	PL9	C4-C3-C7-C8
29	B	621	LMG	C34-C35-C36-C37
29	c	522	LMG	C15-C16-C17-C18
29	d	410	LMG	C36-C37-C38-C39
31	e	101	LHG	O9-C7-O7-C5
31	D	410	LHG	C11-C12-C13-C14
32	A	617	DGD	C2A-C3A-C4A-C5A
32	H	102	DGD	C6B-C7B-C8B-C9B
32	c	517	DGD	C6B-C7B-C8B-C9B
27	K	101	BCR	C10-C11-C12-C13
27	d	405	BCR	C10-C11-C12-C13
25	c	507	CLA	C8-C10-C11-C12
25	a	608	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C19
32	C	517	DGD	C8B-C9B-CAB-CBB
33	D	413	STE	C6-C7-C8-C9
33	x	102	STE	C5-C6-C7-C8
25	B	611	CLA	C11-C12-C13-C14
25	b	601	CLA	C6-C7-C8-C9
25	b	614	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	b	621	LMG	C40-C41-C42-C43
31	e	101	LHG	C11-C12-C13-C14
31	A	614	LHG	C15-C16-C17-C18
31	A	615	LHG	C27-C28-C29-C30
31	d	407	LHG	C15-C16-C17-C18
32	A	617	DGD	CCA-CDA-CEA-CFA
32	C	517	DGD	C4B-C5B-C6B-C7B
33	B	624	STE	C12-C13-C14-C15
33	b	620	STE	C2-C3-C4-C5
32	c	518	DGD	O6D-C1D-O3G-C3G
32	c	518	DGD	O6E-C1E-O5D-C6D
29	M	101	LMG	C15-C16-C17-C18
31	D	410	LHG	C9-C10-C11-C12
32	C	515	DGD	C4B-C5B-C6B-C7B
33	C	521	STE	C3-C4-C5-C6
33	D	413	STE	C7-C8-C9-C10
25	B	614	CLA	C13-C15-C16-C17
25	B	616	CLA	C8-C10-C11-C12
25	c	509	CLA	C13-C15-C16-C17
29	M	101	LMG	C13-C14-C15-C16
29	c	520	LMG	C38-C39-C40-C41
31	A	614	LHG	C29-C30-C31-C32
32	c	519	DGD	C9A-CAA-CBA-CCA
33	T	103	STE	C2-C3-C4-C5
31	l	101	LHG	C33-C34-C35-C36
33	D	413	STE	C14-C15-C16-C17
29	D	408	LMG	C15-C16-C17-C18
29	D	408	LMG	C17-C18-C19-C20
31	A	614	LHG	C13-C14-C15-C16
31	D	410	LHG	C33-C34-C35-C36
32	c	519	DGD	CBA-CCA-CDA-CEA
33	B	624	STE	C5-C6-C7-C8
25	B	601	CLA	C15-C16-C17-C18
27	k	101	BCR	C19-C20-C21-C22
33	d	413	STE	C12-C13-C14-C15
25	c	511	CLA	C16-C17-C18-C19
29	d	411	LMG	C39-C40-C41-C42
30	A	616	SQD	C8-C7-O47-C45
30	A	613	SQD	C23-C24-C25-C26
29	C	518	LMG	C14-C15-C16-C17
29	c	522	LMG	C30-C31-C32-C33
30	B	622	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	d	407	LHG	C27-C28-C29-C30
33	T	102	STE	C5-C6-C7-C8
25	b	604	CLA	C15-C16-C17-C18
29	C	518	LMG	C30-C31-C32-C33
32	c	519	DGD	C1B-C2B-C3B-C4B
29	b	621	LMG	C13-C14-C15-C16
31	D	409	LHG	C28-C29-C30-C31
31	l	101	LHG	C14-C15-C16-C17
27	d	405	BCR	C7-C8-C9-C10
33	c	523	STE	C5-C6-C7-C8
25	B	601	CLA	C16-C17-C18-C19
25	C	513	CLA	C16-C17-C18-C20
25	C	508	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
29	c	524	LMG	C33-C34-C35-C36
30	A	613	SQD	C12-C13-C14-C15
30	F	101	SQD	C26-C27-C28-C29
32	H	102	DGD	C5A-C6A-C7A-C8A
28	a	611	PL9	C20-C19-C21-C22
29	c	524	LMG	C28-C29-C30-C31
33	C	521	STE	C5-C6-C7-C8
33	I	101	STE	C4-C5-C6-C7
33	j	101	STE	C4-C5-C6-C7
29	D	408	LMG	C12-C13-C14-C15
30	f	102	SQD	C24-C25-C26-C27
33	B	626	STE	C4-C5-C6-C7
33	c	521	STE	C2-C3-C4-C5
29	b	621	LMG	C23-C24-C25-C26
30	a	614	SQD	C11-C12-C13-C14
31	D	409	LHG	C17-C18-C19-C20
32	A	617	DGD	C8B-C9B-CAB-CBB
33	m	102	STE	C6-C7-C8-C9
25	b	601	CLA	C15-C16-C17-C18
25	b	603	CLA	C5-C6-C7-C8
25	b	608	CLA	C5-C6-C7-C8
30	a	613	SQD	C34-C35-C36-C37
31	A	614	LHG	C18-C19-C20-C21
32	a	615	DGD	C3A-C4A-C5A-C6A
32	c	517	DGD	C5A-C6A-C7A-C8A
32	c	517	DGD	O1B-C1B-O2G-C2G
29	d	410	LMG	C38-C39-C40-C41
29	d	410	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
33	d	413	STE	C9-C10-C11-C12
30	A	616	SQD	C10-C11-C12-C13
33	B	625	STE	C1-C2-C3-C4
29	c	524	LMG	C18-C19-C20-C21
32	c	517	DGD	C3B-C4B-C5B-C6B
33	x	102	STE	C4-C5-C6-C7
29	d	411	LMG	O6-C5-C6-O5
25	C	512	CLA	C3-C5-C6-C7
30	B	622	SQD	O6-C44-C45-O47
32	A	617	DGD	O2G-C2G-C3G-O3G
30	a	613	SQD	C19-C20-C21-C22
29	D	408	LMG	C32-C33-C34-C35
30	a	613	SQD	C13-C14-C15-C16
31	D	409	LHG	C30-C31-C32-C33
31	d	409	LHG	C27-C28-C29-C30
32	H	102	DGD	CCB-CDB-CEB-CFB
32	c	517	DGD	C8B-C9B-CAB-CBB
25	C	505	CLA	C5-C6-C7-C8
25	c	505	CLA	C5-C6-C7-C8
30	L	101	SQD	C29-C30-C31-C32
32	C	516	DGD	C6A-C7A-C8A-C9A
33	B	620	STE	C6-C7-C8-C9
33	T	103	STE	C3-C4-C5-C6
33	a	617	STE	C5-C6-C7-C8
33	c	521	STE	C11-C12-C13-C14
25	a	608	CLA	CBD-CGD-O2D-CED
31	d	408	LHG	C14-C15-C16-C17
32	a	615	DGD	CEB-CFB-CGB-CHB
32	c	519	DGD	C4A-C5A-C6A-C7A
33	b	620	STE	C6-C7-C8-C9
25	C	502	CLA	C16-C17-C18-C20
25	a	609	CLA	C10-C11-C12-C13
25	b	606	CLA	C10-C11-C12-C13
25	b	614	CLA	C5-C6-C7-C8
31	A	615	LHG	C13-C14-C15-C16
31	e	101	LHG	C11-C10-C9-C8
32	C	516	DGD	CAA-CBA-CCA-CDA
32	C	516	DGD	C6B-C7B-C8B-C9B
31	D	410	LHG	C14-C15-C16-C17
32	a	615	DGD	C7B-C8B-C9B-CAB
33	D	413	STE	C13-C14-C15-C16
25	b	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	C	518	LMG	O9-C10-O7-C8
31	d	408	LHG	O9-C7-O7-C5
32	c	519	DGD	C8B-C9B-CAB-CBB
29	A	612	LMG	C12-C13-C14-C15
30	L	101	SQD	C24-C25-C26-C27
25	D	404	CLA	O1D-CGD-O2D-CED
29	c	522	LMG	C35-C36-C37-C38
31	D	412	LHG	C26-C27-C28-C29
25	B	611	CLA	C13-C15-C16-C17
25	a	608	CLA	C13-C15-C16-C17
29	b	621	LMG	C18-C19-C20-C21
31	A	615	LHG	C30-C31-C32-C33
30	B	622	SQD	C13-C14-C15-C16
32	a	615	DGD	C6B-C7B-C8B-C9B
31	D	409	LHG	O1-C1-C2-O2
32	C	516	DGD	C9B-CAB-CBB-CCB
25	b	601	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C5-C6-C7-C8
29	D	408	LMG	C39-C40-C41-C42
32	c	519	DGD	C2B-C3B-C4B-C5B
29	M	101	LMG	C35-C36-C37-C38
30	A	613	SQD	C27-C28-C29-C30
31	A	615	LHG	C11-C12-C13-C14
30	a	613	SQD	C15-C16-C17-C18
32	c	517	DGD	C8A-C9A-CAA-CBA
32	c	517	DGD	CCA-CDA-CEA-CFA
32	c	518	DGD	CCB-CDB-CEB-CFB
33	c	521	STE	C10-C11-C12-C13
33	t	102	STE	C2-C3-C4-C5
30	A	616	SQD	O49-C7-O47-C45
29	A	612	LMG	C16-C17-C18-C19
29	c	520	LMG	C36-C37-C38-C39
25	B	601	CLA	C3-C5-C6-C7
25	B	601	CLA	C11-C10-C8-C7
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C11-C10-C8-C7
25	B	604	CLA	C11-C12-C13-C15
25	B	604	CLA	C12-C13-C15-C16
25	B	608	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C15
25	B	616	CLA	C6-C7-C8-C10
25	C	503	CLA	C12-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C10
25	C	507	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C10-C8-C7
25	b	602	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C10-C8-C7
25	c	504	CLA	C11-C10-C8-C7
25	c	509	CLA	C6-C7-C8-C10
31	A	614	LHG	C32-C33-C34-C35
32	a	615	DGD	C4A-C5A-C6A-C7A
33	T	103	STE	C10-C11-C12-C13
32	a	615	DGD	CEA-CFA-CGA-CHA
31	d	409	LHG	C31-C32-C33-C34
31	e	101	LHG	C16-C17-C18-C19
33	I	101	STE	C7-C8-C9-C10
28	D	407	PL9	C30-C29-C31-C32
25	C	505	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
29	c	520	LMG	C33-C34-C35-C36
31	D	409	LHG	C18-C19-C20-C21
32	c	519	DGD	C5A-C6A-C7A-C8A
30	a	613	SQD	C12-C13-C14-C15
32	c	518	DGD	C4A-C5A-C6A-C7A
25	b	602	CLA	C15-C16-C17-C18
32	H	102	DGD	C4E-C5E-C6E-O5E
25	c	501	CLA	C2A-CAA-CBA-CGA
25	B	602	CLA	C11-C12-C13-C14
25	B	604	CLA	C14-C13-C15-C16
25	C	503	CLA	C14-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C12-C13-C14
25	b	602	CLA	C6-C7-C8-C9
25	b	615	CLA	C11-C10-C8-C9
25	c	504	CLA	C11-C10-C8-C9
25	c	505	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	C	504	CLA	C11-C12-C13-C14
29	b	621	LMG	C19-C20-C21-C22
33	M	102	STE	C11-C10-C9-C8
33	d	412	STE	C6-C7-C8-C9
33	l	102	STE	C13-C14-C15-C16
29	d	410	LMG	C31-C32-C33-C34
31	d	409	LHG	C33-C34-C35-C36
25	C	503	CLA	C15-C16-C17-C18
28	A	611	PL9	C32-C33-C34-C35
29	c	524	LMG	C35-C36-C37-C38
31	d	409	LHG	C30-C31-C32-C33
29	M	101	LMG	C2-C1-O1-C7
25	b	606	CLA	C15-C16-C17-C18
29	A	612	LMG	O1-C7-C8-C9
29	C	518	LMG	O1-C7-C8-C9
29	M	101	LMG	O1-C7-C8-C9
29	M	101	LMG	C7-C8-C9-O8
30	B	622	SQD	O6-C44-C45-C46
30	a	613	SQD	O6-C44-C45-C46
31	A	614	LHG	C4-C5-C6-O8
32	A	617	DGD	C1G-C2G-C3G-O3G
31	D	409	LHG	C29-C30-C31-C32
31	D	412	LHG	C12-C13-C14-C15
25	b	616	CLA	C10-C11-C12-C13
30	A	616	SQD	C30-C31-C32-C33
32	C	515	DGD	C8A-C9A-CAA-CBA
25	B	610	CLA	O1D-CGD-O2D-CED
29	c	522	LMG	C29-C28-O8-C9
25	c	506	CLA	C16-C17-C18-C19
29	c	522	LMG	C34-C35-C36-C37
32	C	515	DGD	C2A-C3A-C4A-C5A
25	B	615	CLA	C13-C15-C16-C17
31	A	614	LHG	C34-C35-C36-C37
25	A	606	CLA	C2C-C3C-CAC-CBC
32	h	101	DGD	O6E-C5E-C6E-O5E
32	a	615	DGD	C4B-C5B-C6B-C7B
28	d	406	PL9	C32-C33-C34-C36
27	c	514	BCR	C35-C13-C14-C15
27	c	515	BCR	C20-C21-C22-C37
25	C	513	CLA	C8-C10-C11-C12
25	b	613	CLA	C10-C11-C12-C13
29	m	101	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	c	518	DGD	O6E-C5E-C6E-O5E
32	C	515	DGD	CCB-CDB-CEB-CFB
32	C	517	DGD	C2A-C3A-C4A-C5A
32	h	101	DGD	CBA-CCA-CDA-CEA
33	B	620	STE	C11-C12-C13-C14
25	C	505	CLA	C4-C3-C5-C6
25	B	605	CLA	C8-C10-C11-C12
27	K	102	BCR	C37-C22-C23-C24
29	D	411	LMG	C35-C36-C37-C38
31	A	614	LHG	C27-C28-C29-C30
29	D	408	LMG	O6-C5-C6-O5
25	B	605	CLA	C13-C15-C16-C17
25	B	612	CLA	C13-C15-C16-C17
25	C	509	CLA	C13-C15-C16-C17
32	H	102	DGD	CBA-CCA-CDA-CEA
25	b	615	CLA	C13-C15-C16-C17
25	c	503	CLA	C15-C16-C17-C18
32	c	518	DGD	CAB-CBB-CCB-CDB
33	B	620	STE	C7-C8-C9-C10
29	B	621	LMG	C16-C17-C18-C19
31	A	614	LHG	C11-C10-C9-C8
25	C	501	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	O2A-C1-C2-C3
29	A	612	LMG	C9-C8-O7-C10
30	A	613	SQD	C14-C15-C16-C17
31	l	101	LHG	C18-C19-C20-C21
27	K	102	BCR	C18-C19-C20-C21
27	c	515	BCR	C18-C19-C20-C21
29	D	411	LMG	C16-C17-C18-C19
29	d	411	LMG	C37-C38-C39-C40
32	h	101	DGD	CAB-CBB-CCB-CDB
33	C	519	STE	C3-C4-C5-C6
29	C	518	LMG	C11-C12-C13-C14
30	f	102	SQD	C28-C29-C30-C31
32	c	517	DGD	CAB-CBB-CCB-CDB
27	B	619	BCR	C11-C10-C9-C8
27	b	618	BCR	C20-C21-C22-C23
31	A	615	LHG	C31-C32-C33-C34
30	L	101	SQD	O5-C1-O6-C44
29	d	410	LMG	C39-C40-C41-C42
30	f	102	SQD	C34-C35-C36-C37
32	A	617	DGD	CEB-CFB-CGB-CHB

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Mol	Chain	Res	Type	Atoms
30	a	614	SQD	C15-C16-C17-C18
33	B	624	STE	C3-C4-C5-C6
30	L	101	SQD	C19-C20-C21-C22
25	B	616	CLA	C4-C3-C5-C6
25	C	510	CLA	C2-C3-C5-C6
29	c	520	LMG	C39-C40-C41-C42
29	c	522	LMG	C11-C12-C13-C14
30	L	101	SQD	C11-C12-C13-C14
32	a	615	DGD	CBA-CCA-CDA-CEA
33	C	521	STE	C7-C8-C9-C10
33	l	102	STE	C4-C5-C6-C7
25	a	607	CLA	C16-C17-C18-C20
29	b	621	LMG	C38-C39-C40-C41
30	a	613	SQD	C30-C31-C32-C33
32	A	617	DGD	CBB-CCB-CDB-CEB
33	B	620	STE	C4-C5-C6-C7
33	C	520	STE	C6-C7-C8-C9
29	B	621	LMG	C37-C38-C39-C40
30	A	613	SQD	C17-C18-C19-C20
32	C	516	DGD	CDA-CEA-CFA-CGA
33	M	103	STE	C1-C2-C3-C4
30	L	101	SQD	C7-C8-C9-C10
29	A	612	LMG	C14-C15-C16-C17
31	D	409	LHG	C11-C10-C9-C8
29	b	621	LMG	O1-C7-C8-O7
32	C	517	DGD	CDA-CEA-CFA-CGA
32	c	519	DGD	CDA-CEA-CFA-CGA
32	A	617	DGD	C8A-C9A-CAA-CBA
33	B	624	STE	C7-C8-C9-C10
33	b	620	STE	C13-C14-C15-C16
29	m	101	LMG	C31-C32-C33-C34
25	C	510	CLA	C3-C5-C6-C7
25	c	502	CLA	C3-C5-C6-C7
29	D	408	LMG	C38-C39-C40-C41
25	B	606	CLA	C15-C16-C17-C18
31	d	408	LHG	C35-C36-C37-C38
33	I	101	STE	C2-C3-C4-C5
32	c	517	DGD	C4D-C5D-C6D-O5D
30	A	616	SQD	C17-C18-C19-C20
32	C	515	DGD	C6B-C7B-C8B-C9B
29	D	411	LMG	C37-C38-C39-C40
29	C	518	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C28-C29-C30-C31
30	A	616	SQD	C31-C32-C33-C34
32	H	102	DGD	C7B-C8B-C9B-CAB
32	A	617	DGD	C5B-C6B-C7B-C8B
29	b	621	LMG	C24-C25-C26-C27
25	C	513	CLA	C15-C16-C17-C18
28	A	611	PL9	C15-C14-C16-C17
33	c	523	STE	C6-C7-C8-C9
25	b	608	CLA	C13-C15-C16-C17
30	F	101	SQD	C30-C31-C32-C33
31	A	614	LHG	C24-C25-C26-C27
32	C	516	DGD	CCA-CDA-CEA-CFA
33	B	623	STE	C6-C7-C8-C9
33	B	626	STE	C6-C7-C8-C9
33	b	620	STE	C12-C13-C14-C15
33	T	103	STE	C6-C7-C8-C9
31	A	614	LHG	O9-C7-O7-C5
25	A	607	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C10-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	608	CLA	C6-C7-C8-C9
25	B	610	CLA	C14-C13-C15-C16
25	B	613	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	D	403	CLA	C11-C12-C13-C14
25	D	405	CLA	C6-C7-C8-C9
25	b	604	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C14
25	A	606	CLA	C13-C15-C16-C17
25	C	503	CLA	C4B-C3B-CAB-CBB
29	c	522	LMG	C13-C14-C15-C16
29	d	411	LMG	C34-C35-C36-C37
29	d	410	LMG	C37-C38-C39-C40
25	a	607	CLA	C16-C17-C18-C19
33	B	624	STE	C13-C14-C15-C16
29	d	411	LMG	C14-C15-C16-C17
29	m	101	LMG	C14-C15-C16-C17
29	m	101	LMG	C18-C19-C20-C21
25	b	613	CLA	C8-C10-C11-C12
31	D	409	LHG	C25-C26-C27-C28
31	e	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	D	411	LMG	C33-C34-C35-C36
25	A	607	CLA	C11-C12-C13-C15
25	B	607	CLA	C12-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C7
25	C	505	CLA	C12-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C15
25	D	403	CLA	C11-C12-C13-C15
25	D	405	CLA	C6-C7-C8-C10
25	b	607	CLA	C6-C7-C8-C10
25	b	607	CLA	C11-C12-C13-C15
25	b	616	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10
25	c	511	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C7
25	B	605	CLA	C10-C11-C12-C13
33	b	623	STE	C7-C8-C9-C10
28	a	611	PL9	C47-C48-C49-C51
31	D	412	LHG	C9-C10-C11-C12
31	d	408	LHG	C11-C12-C13-C14
32	A	617	DGD	CFA-CGA-CHA-CIA
33	B	623	STE	C7-C8-C9-C10
33	T	102	STE	C13-C14-C15-C16
29	D	411	LMG	C32-C33-C34-C35
30	B	622	SQD	C29-C30-C31-C32
33	B	625	STE	C3-C4-C5-C6
33	D	413	STE	C12-C13-C14-C15
33	j	101	STE	C5-C6-C7-C8
32	a	615	DGD	CFA-CGA-CHA-CIA
25	C	510	CLA	C4-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6
26	d	402	PHO	C3A-C2A-CAA-CBA
33	b	623	STE	C3-C4-C5-C6
32	H	102	DGD	O2G-C1B-C2B-C3B
26	A	608	PHO	C2-C3-C5-C6
29	A	612	LMG	C17-C18-C19-C20
33	C	521	STE	C12-C13-C14-C15
30	a	614	SQD	C31-C32-C33-C34
31	l	101	LHG	C17-C18-C19-C20
29	C	518	LMG	O10-C28-O8-C9
25	C	508	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	D	410	LHG	C30-C31-C32-C33
25	B	612	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C19
27	B	619	BCR	C11-C12-C13-C35
31	d	407	LHG	C14-C15-C16-C17
30	a	613	SQD	C31-C32-C33-C34
32	c	518	DGD	CBA-CCA-CDA-CEA
33	b	623	STE	C4-C5-C6-C7
25	B	613	CLA	C10-C11-C12-C13
25	C	508	CLA	C8-C10-C11-C12
32	c	519	DGD	C2A-C3A-C4A-C5A
30	B	622	SQD	C19-C20-C21-C22
29	b	621	LMG	O1-C7-C8-C9
29	c	522	LMG	C7-C8-C9-O8
30	A	613	SQD	O6-C44-C45-C46
30	a	614	SQD	C44-C45-C46-O48
33	B	620	STE	C11-C10-C9-C8
33	B	624	STE	C10-C11-C12-C13
32	A	617	DGD	CCB-CDB-CEB-CFB
25	C	505	CLA	C16-C17-C18-C20
25	B	615	CLA	C5-C6-C7-C8
25	c	502	CLA	C13-C15-C16-C17
30	B	622	SQD	C27-C28-C29-C30
31	e	101	LHG	C14-C15-C16-C17
31	D	410	LHG	C11-C10-C9-C8
32	c	519	DGD	C7B-C8B-C9B-CAB
33	H	103	STE	C7-C8-C9-C10
32	C	516	DGD	C4A-C5A-C6A-C7A
33	C	519	STE	C2-C3-C4-C5
33	a	617	STE	C2-C3-C4-C5
25	b	609	CLA	C4-C3-C5-C6
26	A	608	PHO	C4-C3-C5-C6
30	A	616	SQD	C33-C34-C35-C36
30	a	613	SQD	C29-C30-C31-C32
31	d	407	LHG	C29-C30-C31-C32
32	a	615	DGD	CDA-CEA-CFA-CGA
28	d	406	PL9	C13-C14-C16-C17
25	C	502	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
25	c	502	CLA	CBD-CGD-O2D-CED
33	J	101	STE	C2-C3-C4-C5
30	A	616	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C16-C17-C18-C19
25	D	405	CLA	C16-C17-C18-C19
29	D	411	LMG	C31-C32-C33-C34
30	A	616	SQD	C12-C13-C14-C15
32	c	519	DGD	C5B-C6B-C7B-C8B
27	H	101	BCR	C23-C24-C25-C30
27	K	102	BCR	C1-C6-C7-C8
27	b	617	BCR	C1-C6-C7-C8
27	d	405	BCR	C23-C24-C25-C30
29	M	101	LMG	C17-C18-C19-C20
29	c	520	LMG	C4-C5-C6-O5
32	C	516	DGD	C4B-C5B-C6B-C7B
30	B	622	SQD	C9-C10-C11-C12
33	H	103	STE	C13-C14-C15-C16
33	T	102	STE	C10-C11-C12-C13
25	D	405	CLA	C13-C15-C16-C17
30	F	101	SQD	C33-C34-C35-C36
33	a	616	STE	C5-C6-C7-C8
32	C	515	DGD	O1G-C1A-C2A-C3A
29	M	101	LMG	O7-C8-C9-O8
30	A	613	SQD	O6-C44-C45-O47
30	a	613	SQD	O47-C45-C46-O48
32	c	517	DGD	C6A-C7A-C8A-C9A
29	C	518	LMG	C15-C16-C17-C18
32	A	617	DGD	C7B-C8B-C9B-CAB
33	m	102	STE	C1-C2-C3-C4
28	d	406	PL9	C15-C14-C16-C17
29	A	612	LMG	C31-C32-C33-C34
29	b	621	LMG	C39-C40-C41-C42
30	A	613	SQD	C29-C30-C31-C32
31	l	101	LHG	C30-C31-C32-C33
27	C	514	BCR	C18-C19-C20-C21
25	A	606	CLA	C15-C16-C17-C18
32	H	102	DGD	C3A-C4A-C5A-C6A
32	h	101	DGD	CCA-CDA-CEA-CFA
31	D	409	LHG	C32-C33-C34-C35
31	e	101	LHG	C28-C29-C30-C31
25	C	510	CLA	C11-C10-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	510	CLA	C11-C12-C13-C14
25	c	502	CLA	O1D-CGD-O2D-CED
30	a	613	SQD	C35-C36-C37-C38
33	D	413	STE	C11-C12-C13-C14
33	M	102	STE	C4-C5-C6-C7
25	B	603	CLA	C10-C11-C12-C13
26	d	402	PHO	C5-C6-C7-C8
32	a	615	DGD	C9B-CAB-CBB-CCB
33	C	520	STE	C4-C5-C6-C7
32	C	516	DGD	O6D-C1D-O3G-C3G
32	c	517	DGD	O6E-C1E-O5D-C6D
30	B	622	SQD	C35-C36-C37-C38
28	A	611	PL9	C29-C31-C32-C33
28	d	406	PL9	C34-C36-C37-C38
31	A	614	LHG	C9-C10-C11-C12
30	a	614	SQD	O6-C44-C45-O47
31	A	614	LHG	C14-C15-C16-C17
30	a	613	SQD	C27-C28-C29-C30
29	C	518	LMG	C40-C41-C42-C43
25	b	615	CLA	C10-C11-C12-C13
31	d	409	LHG	O1-C1-C2-O2
32	H	102	DGD	CDA-CEA-CFA-CGA
25	b	609	CLA	C2-C3-C5-C6
25	B	610	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
33	B	626	STE	C2-C3-C4-C5
31	d	408	LHG	C15-C16-C17-C18
27	T	101	BCR	C11-C10-C9-C34
27	a	610	BCR	C35-C13-C14-C15
27	c	515	BCR	C16-C17-C18-C36
27	t	101	BCR	C11-C10-C9-C34
27	x	101	BCR	C20-C21-C22-C37
25	c	507	CLA	C5-C6-C7-C8
29	A	612	LMG	C40-C41-C42-C43
31	l	101	LHG	O6-C4-C5-C6
25	b	602	CLA	C10-C11-C12-C13
25	b	607	CLA	C13-C15-C16-C17
27	t	101	BCR	C11-C12-C13-C35
32	c	517	DGD	CDB-CEB-CFB-CGB
25	B	606	CLA	C11-C12-C13-C15
25	B	611	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	C6-C7-C8-C10
25	C	510	CLA	C11-C10-C8-C7
25	C	513	CLA	C6-C7-C8-C10
25	a	609	CLA	C12-C13-C15-C16
25	b	603	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	c	505	CLA	C6-C7-C8-C10
25	c	509	CLA	C11-C12-C13-C15
33	C	520	STE	C1-C2-C3-C4
33	c	521	STE	C1-C2-C3-C4
29	d	411	LMG	C36-C37-C38-C39
32	c	518	DGD	C7B-C8B-C9B-CAB
29	b	621	LMG	C22-C23-C24-C25
32	C	517	DGD	C3B-C4B-C5B-C6B
33	d	412	STE	C11-C10-C9-C8
33	m	102	STE	C4-C5-C6-C7
25	C	512	CLA	C10-C11-C12-C13
25	A	606	CLA	C4C-C3C-CAC-CBC
27	D	406	BCR	C7-C8-C9-C10
27	T	101	BCR	C21-C22-C23-C24
25	B	612	CLA	CBA-CGA-O2A-C1
32	A	617	DGD	C2A-C1A-O1G-C1G
29	M	101	LMG	C39-C40-C41-C42
30	A	613	SQD	C30-C31-C32-C33
32	c	518	DGD	C5D-C6D-O5D-C1E
30	A	613	SQD	C32-C33-C34-C35
25	c	509	CLA	C8-C10-C11-C12
25	b	610	CLA	C2A-CAA-CBA-CGA
33	I	101	STE	C12-C13-C14-C15
30	L	101	SQD	C26-C27-C28-C29
33	B	625	STE	C6-C7-C8-C9
25	B	606	CLA	C16-C17-C18-C19
25	D	405	CLA	C16-C17-C18-C20
25	a	612	CLA	CBD-CGD-O2D-CED
32	c	519	DGD	C4B-C5B-C6B-C7B
25	C	506	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
29	c	524	LMG	O8-C28-C29-C30
33	B	626	STE	C9-C10-C11-C12
30	B	622	SQD	C16-C17-C18-C19
25	B	601	CLA	C5-C6-C7-C8
25	b	605	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	D	411	LMG	C9-C8-O7-C10
32	a	615	DGD	C1G-C2G-O2G-C1B
32	a	615	DGD	C8A-C9A-CAA-CBA
27	H	101	BCR	C11-C10-C9-C8
31	l	101	LHG	O6-C4-C5-O7
29	D	411	LMG	C15-C16-C17-C18
31	d	407	LHG	C31-C32-C33-C34
25	A	609	CLA	C6-C7-C8-C9
28	a	611	PL9	C34-C36-C37-C38
29	c	524	LMG	C7-C8-C9-O8
30	a	613	SQD	C44-C45-C46-O48
35	E	101	HEM	C4C-C3C-CAC-CBC
31	D	410	LHG	O10-C23-O8-C6
25	c	512	CLA	C4-C3-C5-C6
25	b	601	CLA	C2A-CAA-CBA-CGA
29	b	621	LMG	C14-C15-C16-C17
33	C	520	STE	C5-C6-C7-C8
25	B	603	CLA	C5-C6-C7-C8
25	B	603	CLA	C13-C15-C16-C17
25	B	607	CLA	C15-C16-C17-C18
32	a	615	DGD	C5B-C6B-C7B-C8B
33	H	103	STE	C10-C11-C12-C13
29	C	518	LMG	O1-C7-C8-O7
29	M	101	LMG	O1-C7-C8-O7
29	c	524	LMG	O7-C8-C9-O8
32	C	515	DGD	O1G-C1G-C2G-O2G
32	c	517	DGD	O1G-C1G-C2G-O2G
25	B	603	CLA	C11-C12-C13-C14
25	B	605	CLA	C6-C7-C8-C9
25	B	606	CLA	C11-C12-C13-C14
25	C	513	CLA	C11-C12-C13-C14
25	b	603	CLA	C11-C12-C13-C14
25	b	607	CLA	C14-C13-C15-C16
25	b	616	CLA	C6-C7-C8-C9
25	B	611	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C20
29	D	408	LMG	C34-C35-C36-C37
29	b	621	LMG	C33-C34-C35-C36
29	b	621	LMG	C31-C32-C33-C34
32	C	516	DGD	C3A-C4A-C5A-C6A
32	C	517	DGD	C2B-C3B-C4B-C5B
33	x	102	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	d	402	PHO	C2C-C3C-CAC-CBC
32	C	517	DGD	O1A-C1A-O1G-C1G
29	C	518	LMG	C18-C19-C20-C21
25	c	511	CLA	C8-C10-C11-C12
32	C	516	DGD	C7B-C8B-C9B-CAB
31	e	101	LHG	C7-C8-C9-C10
25	A	607	CLA	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C19
25	b	608	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C20
25	B	602	CLA	C15-C16-C17-C18
31	d	407	LHG	C17-C18-C19-C20
32	a	615	DGD	CAB-CBB-CCB-CDB
32	h	101	DGD	CAA-CBA-CCA-CDA
32	A	617	DGD	C4A-C5A-C6A-C7A
32	c	519	DGD	C7A-C8A-C9A-CAA
25	B	613	CLA	C4-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
31	A	614	LHG	O2-C2-C3-O3
25	B	616	CLA	CBD-CGD-O2D-CED
26	d	401	PHO	CBD-CGD-O2D-CED
32	C	516	DGD	C8A-C9A-CAA-CBA
33	B	625	STE	C2-C3-C4-C5
29	M	101	LMG	O6-C5-C6-O5
25	c	501	CLA	CBD-CGD-O2D-CED
25	a	608	CLA	O1D-CGD-O2D-CED
31	A	615	LHG	C10-C11-C12-C13
32	h	101	DGD	C9A-CAA-CBA-CCA
32	h	101	DGD	CDB-CEB-CFB-CGB
25	B	601	CLA	C4B-C3B-CAB-CBB
25	B	604	CLA	C1A-C2A-CAA-CBA
25	c	505	CLA	C4B-C3B-CAB-CBB
25	c	511	CLA	C1A-C2A-CAA-CBA
25	B	616	CLA	O1D-CGD-O2D-CED
25	C	511	CLA	O1D-CGD-O2D-CED
25	C	511	CLA	CBA-CGA-O2A-C1
29	A	612	LMG	C36-C37-C38-C39
31	l	101	LHG	C10-C11-C12-C13
25	B	610	CLA	C16-C17-C18-C20
33	c	523	STE	C2-C3-C4-C5
29	m	101	LMG	C32-C33-C34-C35
32	c	517	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
33	d	412	STE	C9-C10-C11-C12
33	x	102	STE	C9-C10-C11-C12
25	A	607	CLA	C6-C7-C8-C10
25	B	613	CLA	C6-C7-C8-C10
25	B	613	CLA	C11-C12-C13-C15
25	B	614	CLA	C12-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C7
25	C	505	CLA	C6-C7-C8-C10
25	C	506	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C7
25	C	509	CLA	C12-C13-C15-C16
25	b	601	CLA	C12-C13-C15-C16
25	b	602	CLA	C11-C12-C13-C15
25	b	605	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C12-C13-C15
25	b	608	CLA	C11-C10-C8-C7
25	b	608	CLA	C11-C12-C13-C15
25	c	502	CLA	C6-C7-C8-C10
25	c	512	CLA	C6-C7-C8-C10
25	c	512	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
25	B	606	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C19
25	C	505	CLA	O1D-CGD-O2D-CED
26	d	401	PHO	O1D-CGD-O2D-CED
29	c	520	LMG	C35-C36-C37-C38
32	A	617	DGD	C7A-C8A-C9A-CAA
32	C	517	DGD	C9A-CAA-CBA-CCA
32	H	102	DGD	C4B-C5B-C6B-C7B
25	B	604	CLA	CBA-CGA-O2A-C1
30	B	622	SQD	C15-C16-C17-C18
33	b	620	STE	C4-C5-C6-C7
32	a	615	DGD	CFB-CGB-CHB-CIB
25	C	511	CLA	O1A-CGA-O2A-C1
29	B	621	LMG	C11-C12-C13-C14
32	A	617	DGD	CDB-CEB-CFB-CGB
33	l	102	STE	C10-C11-C12-C13
25	B	605	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C19
29	m	101	LMG	C37-C38-C39-C40
32	C	516	DGD	C3B-C4B-C5B-C6B
33	a	617	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
35	f	101	HEM	C2A-CAA-CBA-CGA
25	B	614	CLA	C8-C10-C11-C12
31	D	412	LHG	C29-C30-C31-C32
32	h	101	DGD	C2B-C3B-C4B-C5B
33	d	412	STE	C3-C4-C5-C6
25	A	607	CLA	C6-C7-C8-C9
25	C	510	CLA	C6-C7-C8-C9
25	a	609	CLA	C14-C13-C15-C16
31	d	407	LHG	C33-C34-C35-C36
33	M	103	STE	C6-C7-C8-C9
25	C	508	CLA	O1D-CGD-O2D-CED
32	C	516	DGD	CBB-CCB-CDB-CEB
25	B	604	CLA	O1A-CGA-O2A-C1
25	B	612	CLA	O1A-CGA-O2A-C1
30	a	614	SQD	O47-C45-C46-O48
31	A	614	LHG	O7-C5-C6-O8
31	d	407	LHG	C25-C26-C27-C28
29	D	408	LMG	C30-C31-C32-C33
25	D	404	CLA	C2C-C3C-CAC-CBC
29	D	411	LMG	C7-C8-C9-O8
25	c	512	CLA	C2-C3-C5-C6
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
29	c	522	LMG	C31-C32-C33-C34
31	l	101	LHG	C25-C26-C27-C28
25	B	605	CLA	C16-C17-C18-C19
25	C	501	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C20
33	M	102	STE	C10-C11-C12-C13
25	B	616	CLA	O1A-CGA-O2A-C1
31	D	410	LHG	C12-C13-C14-C15
25	B	609	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
25	b	607	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	c	510	CLA	CAD-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O2D
27	K	102	BCR	C20-C21-C22-C37
31	D	409	LHG	C3-O3-P-O4
31	d	407	LHG	C3-O3-P-O5
33	b	622	STE	C2-C3-C4-C5
33	d	413	STE	C6-C7-C8-C9
28	a	611	PL9	C15-C14-C16-C17
25	B	606	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
32	a	615	DGD	C3B-C4B-C5B-C6B
25	c	509	CLA	CAA-CBA-CGA-O2A
28	A	611	PL9	C13-C14-C16-C17
32	c	519	DGD	CAB-CBB-CCB-CDB
33	t	102	STE	C3-C4-C5-C6
25	C	507	CLA	C5-C6-C7-C8
32	h	101	DGD	C7A-C8A-C9A-CAA
25	b	612	CLA	C16-C17-C18-C20
29	c	522	LMG	C41-C42-C43-C44
28	a	611	PL9	C4-C3-C7-C8
31	D	412	LHG	C19-C20-C21-C22
33	B	623	STE	C4-C5-C6-C7
25	c	504	CLA	C8-C10-C11-C12
29	b	621	LMG	C9-C8-O7-C10
31	D	409	LHG	C16-C17-C18-C19
31	D	412	LHG	C16-C17-C18-C19
33	b	620	STE	C3-C4-C5-C6
33	B	626	STE	C1-C2-C3-C4
31	D	412	LHG	C27-C28-C29-C30
27	x	101	BCR	C15-C16-C17-C18
25	B	611	CLA	C16-C17-C18-C19
31	d	409	LHG	C35-C36-C37-C38
30	A	616	SQD	C19-C20-C21-C22
25	B	606	CLA	C8-C10-C11-C12
25	C	510	CLA	C8-C10-C11-C12
25	B	601	CLA	C11-C10-C8-C9
25	B	607	CLA	C11-C10-C8-C9
25	B	615	CLA	C11-C12-C13-C14
25	B	616	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	a	608	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C11-C12-C13-C14
25	c	505	CLA	C6-C7-C8-C9
25	c	512	CLA	C11-C12-C13-C14
33	C	519	STE	C7-C8-C9-C10
25	a	608	CLA	C11-C12-C13-C15
25	b	606	CLA	C12-C13-C15-C16
25	c	513	CLA	C6-C7-C8-C10
27	c	514	BCR	C20-C21-C22-C23
32	h	101	DGD	C1A-C2A-C3A-C4A
33	E	102	STE	C4-C5-C6-C7
25	C	505	CLA	O1A-CGA-O2A-C1
33	B	626	STE	C5-C6-C7-C8
31	A	615	LHG	O10-C23-O8-C6
32	C	515	DGD	C5B-C6B-C7B-C8B
29	D	411	LMG	C29-C30-C31-C32
30	a	613	SQD	C24-C23-O48-C46
25	A	606	CLA	C16-C17-C18-C20
25	b	610	CLA	C5-C6-C7-C8
32	A	617	DGD	C5A-C6A-C7A-C8A
25	b	615	CLA	C8-C10-C11-C12
30	F	101	SQD	O6-C44-C45-C46
27	a	610	BCR	C19-C20-C21-C22
27	c	516	BCR	C13-C14-C15-C16
33	l	102	STE	C1-C2-C3-C4
33	j	101	STE	C2-C3-C4-C5
30	f	102	SQD	C35-C36-C37-C38
25	c	513	CLA	C5-C6-C7-C8
30	a	613	SQD	C24-C25-C26-C27
25	b	616	CLA	C2-C1-O2A-CGA
33	d	412	STE	C7-C8-C9-C10
25	B	615	CLA	C16-C17-C18-C20
30	a	614	SQD	C30-C31-C32-C33
28	A	611	PL9	C9-C11-C12-C13
25	A	607	CLA	C16-C17-C18-C19
31	A	615	LHG	C14-C15-C16-C17
32	C	515	DGD	C5D-C6D-O5D-C1E
29	c	522	LMG	O10-C28-O8-C9
27	c	516	BCR	C19-C20-C21-C22
30	B	622	SQD	C14-C15-C16-C17
30	L	101	SQD	C16-C17-C18-C19
32	H	102	DGD	O6E-C5E-C6E-O5E
25	B	610	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	H	102	DGD	C3B-C4B-C5B-C6B
30	a	613	SQD	O10-C23-O48-C46
25	B	613	CLA	C6-C7-C8-C9
25	C	505	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C10-C8-C9
25	b	602	CLA	C11-C12-C13-C14
25	c	512	CLA	C11-C10-C8-C9
33	x	102	STE	C15-C16-C17-C18
25	b	603	CLA	C4B-C3B-CAB-CBB
25	c	502	CLA	C4B-C3B-CAB-CBB
25	b	611	CLA	C13-C15-C16-C17
31	A	615	LHG	C19-C20-C21-C22
25	B	608	CLA	C16-C17-C18-C19
25	B	609	CLA	C16-C17-C18-C19
25	c	502	CLA	C16-C17-C18-C20
25	c	513	CLA	C16-C17-C18-C19
25	B	616	CLA	CBA-CGA-O2A-C1
29	c	520	LMG	C29-C28-O8-C9
32	C	517	DGD	C5B-C6B-C7B-C8B
33	B	623	STE	C5-C6-C7-C8
25	B	616	CLA	C2-C3-C5-C6
25	C	513	CLA	C11-C10-C8-C7
25	c	504	CLA	O1D-CGD-O2D-CED
30	a	613	SQD	C23-C24-C25-C26
25	C	505	CLA	CBA-CGA-O2A-C1
25	C	508	CLA	C16-C17-C18-C19
29	B	621	LMG	C15-C16-C17-C18
31	l	101	LHG	C29-C30-C31-C32
25	b	609	CLA	C13-C15-C16-C17
25	c	504	CLA	CBD-CGD-O2D-CED
29	c	524	LMG	C13-C14-C15-C16
32	H	102	DGD	C9B-CAB-CBB-CCB
32	c	517	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	C8B-C9B-CAB-CBB
27	c	516	BCR	C20-C21-C22-C37
27	x	101	BCR	C35-C13-C14-C15
25	B	613	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
30	B	622	SQD	C34-C35-C36-C37
30	F	101	SQD	C27-C28-C29-C30
31	d	408	LHG	C28-C29-C30-C31
29	D	408	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	d	408	LHG	C1-C2-C3-O3
29	c	524	LMG	C38-C39-C40-C41
31	D	409	LHG	C15-C16-C17-C18
32	c	518	DGD	CBB-CCB-CDB-CEB
25	B	603	CLA	C11-C10-C8-C9
25	C	501	CLA	C14-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C9
25	b	605	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C10-C8-C9
25	c	512	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
33	B	620	STE	C5-C6-C7-C8
33	T	103	STE	C5-C6-C7-C8
32	A	617	DGD	CFB-CGB-CHB-CIB
29	B	621	LMG	O7-C10-C11-C12
33	c	521	STE	O1-C1-C2-C3
26	d	402	PHO	C1A-C2A-CAA-CBA
29	D	411	LMG	O1-C7-C8-C9
30	a	613	SQD	C28-C29-C30-C31
29	d	411	LMG	C10-C11-C12-C13
29	B	621	LMG	O9-C10-C11-C12
33	B	623	STE	O2-C1-C2-C3
25	B	603	CLA	C2A-CAA-CBA-CGA
29	d	411	LMG	C11-C12-C13-C14
27	t	101	BCR	C20-C21-C22-C23
27	x	101	BCR	C20-C21-C22-C23
25	D	403	CLA	C2C-C3C-CAC-CBC
33	B	623	STE	O1-C1-C2-C3
33	c	521	STE	O2-C1-C2-C3
25	B	601	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C2B-C3B-CAB-CBB
27	A	610	BCR	C1-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C23-C24-C25-C30
27	H	101	BCR	C23-C24-C25-C26
27	K	102	BCR	C5-C6-C7-C8
27	b	617	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C26
33	l	102	STE	C12-C13-C14-C15
29	d	411	LMG	C15-C16-C17-C18
25	c	510	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	d	404	CLA	C4-C3-C5-C6
30	A	616	SQD	C34-C35-C36-C37
31	d	408	LHG	C33-C34-C35-C36
32	A	617	DGD	CEA-CFA-CGA-CHA
33	b	620	STE	C5-C6-C7-C8
25	A	607	CLA	C11-C10-C8-C7
25	B	615	CLA	C12-C13-C15-C16
25	D	403	CLA	C12-C13-C15-C16
25	a	608	CLA	C6-C7-C8-C10
25	a	608	CLA	C12-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C10-C8-C7
25	c	508	CLA	C11-C10-C8-C7
25	c	512	CLA	C11-C12-C13-C15
30	f	102	SQD	C32-C33-C34-C35
28	a	611	PL9	C19-C21-C22-C23
25	C	501	CLA	C2A-CAA-CBA-CGA
29	D	411	LMG	O7-C8-C9-O8
30	f	102	SQD	O6-C44-C45-O47
35	E	101	HEM	CAD-CBD-CGD-O1D
32	C	516	DGD	CCB-CDB-CEB-CFB
25	b	613	CLA	CBD-CGD-O2D-CED
29	d	410	LMG	O9-C10-C11-C12
33	b	622	STE	O2-C1-C2-C3
29	M	101	LMG	C12-C13-C14-C15
33	a	616	STE	C7-C8-C9-C10
25	B	603	CLA	C16-C17-C18-C19
29	d	411	LMG	C30-C31-C32-C33
33	b	620	STE	C7-C8-C9-C10
33	b	622	STE	O1-C1-C2-C3
31	A	615	LHG	C15-C16-C17-C18
33	M	103	STE	C4-C5-C6-C7
33	E	102	STE	C7-C8-C9-C10
33	D	413	STE	O2-C1-C2-C3
25	a	608	CLA	C6-C7-C8-C9
33	T	102	STE	C4-C5-C6-C7
25	b	611	CLA	C10-C11-C12-C13
33	H	103	STE	C6-C7-C8-C9
33	t	102	STE	C6-C7-C8-C9
27	K	101	BCR	C22-C23-C24-C25
29	m	101	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C35-C36-C37-C38
25	B	604	CLA	C2C-C3C-CAC-CBC
25	C	502	CLA	C4-C3-C5-C6
25	d	403	CLA	C4-C3-C5-C6
31	D	410	LHG	C2-C3-O3-P
31	d	409	LHG	C2-C3-O3-P
25	c	510	CLA	C2-C3-C5-C6
30	a	614	SQD	C29-C30-C31-C32
32	C	515	DGD	C2B-C3B-C4B-C5B
25	B	612	CLA	C10-C11-C12-C13
33	B	625	STE	O1-C1-C2-C3
29	C	518	LMG	C33-C34-C35-C36
29	d	410	LMG	C11-C12-C13-C14
32	c	519	DGD	O6D-C5D-C6D-O5D
29	A	612	LMG	C13-C14-C15-C16
29	B	621	LMG	C36-C37-C38-C39
32	C	515	DGD	O1G-C1G-C2G-C3G
35	E	101	HEM	CAD-CBD-CGD-O2D
35	f	101	HEM	CAD-CBD-CGD-O1D
29	D	411	LMG	O1-C7-C8-O7
25	B	614	CLA	C2A-CAA-CBA-CGA
36	V	201	HEC	CAD-CBD-CGD-O2D
30	B	622	SQD	C28-C29-C30-C31
30	A	616	SQD	C11-C12-C13-C14
33	b	622	STE	C5-C6-C7-C8
25	D	404	CLA	C4B-C3B-CAB-CBB
26	A	608	PHO	C10-C11-C12-C13
25	d	404	CLA	C16-C17-C18-C19
26	d	401	PHO	CHA-CBD-CGD-O1D
25	b	612	CLA	C8-C10-C11-C12
32	h	101	DGD	O2G-C1B-C2B-C3B
29	d	410	LMG	O7-C10-C11-C12
32	C	515	DGD	C4D-C5D-C6D-O5D
25	D	403	CLA	C4C-C3C-CAC-CBC
33	T	103	STE	C9-C10-C11-C12
26	D	402	PHO	C2C-C3C-CAC-CBC
25	C	506	CLA	C16-C17-C18-C20
29	M	101	LMG	C18-C19-C20-C21
25	C	502	CLA	C2-C3-C5-C6
25	A	607	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C10-C8-C7
29	C	518	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	D	413	STE	O1-C1-C2-C3
32	a	615	DGD	C2B-C3B-C4B-C5B
25	C	505	CLA	C11-C10-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	D	404	CLA	C14-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C9
26	d	401	PHO	C14-C13-C15-C16
30	L	101	SQD	C10-C11-C12-C13
29	c	524	LMG	C11-C12-C13-C14
33	b	623	STE	C5-C6-C7-C8
33	l	102	STE	C15-C16-C17-C18
25	C	506	CLA	C2-C1-O2A-CGA
25	b	608	CLA	C2-C1-O2A-CGA
32	C	515	DGD	O6D-C5D-C6D-O5D
25	c	505	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C20
33	b	623	STE	C1-C2-C3-C4
25	B	610	CLA	C8-C10-C11-C12
25	c	512	CLA	C5-C6-C7-C8
29	B	621	LMG	C30-C31-C32-C33
31	D	409	LHG	C9-C10-C11-C12
36	v	201	HEC	CAD-CBD-CGD-O2D
25	B	613	CLA	C2-C3-C5-C6
36	V	201	HEC	CAD-CBD-CGD-O1D
33	t	102	STE	C4-C5-C6-C7
32	C	516	DGD	C2D-C1D-O3G-C3G
32	c	517	DGD	C2E-C1E-O5D-C6D
25	B	616	CLA	O2A-C1-C2-C3
31	D	409	LHG	C11-C12-C13-C14
27	H	101	BCR	C10-C11-C12-C13
27	T	101	BCR	C18-C19-C20-C21
25	b	602	CLA	CBD-CGD-O2D-CED
33	l	102	STE	C14-C15-C16-C17
30	a	613	SQD	C33-C34-C35-C36
36	v	201	HEC	CAD-CBD-CGD-O1D
25	c	503	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	O1A-CGA-O2A-C1
33	b	622	STE	C6-C7-C8-C9
32	C	517	DGD	O6E-C5E-C6E-O5E
29	A	612	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
33	C	521	STE	C6-C7-C8-C9
29	A	612	LMG	C7-C8-C9-O8
32	A	617	DGD	O1G-C1G-C2G-C3G
32	c	517	DGD	O1G-C1G-C2G-C3G
32	C	515	DGD	CDB-CEB-CFB-CGB
25	c	503	CLA	O1A-CGA-O2A-C1
29	D	411	LMG	O10-C28-O8-C9
25	b	610	CLA	C3-C5-C6-C7
29	c	520	LMG	C29-C30-C31-C32
25	A	607	CLA	C10-C11-C12-C13
25	b	609	CLA	C15-C16-C17-C18
31	d	408	LHG	C31-C32-C33-C34
32	C	517	DGD	C3A-C4A-C5A-C6A
32	h	101	DGD	C7B-C8B-C9B-CAB
25	b	613	CLA	CAA-CBA-CGA-O2A
31	D	410	LHG	C17-C18-C19-C20
25	C	504	CLA	C11-C10-C8-C9
25	D	403	CLA	C14-C13-C15-C16
25	b	608	CLA	C11-C10-C8-C9
25	b	613	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C10-C8-C9
33	T	103	STE	C11-C12-C13-C14
25	B	613	CLA	CAA-CBA-CGA-O2A
31	A	614	LHG	O6-C4-C5-C6
33	B	625	STE	O2-C1-C2-C3
28	D	407	PL9	C32-C33-C34-C35
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	612	CLA	CAA-CBA-CGA-O2A
30	a	613	SQD	O47-C7-C8-C9
25	B	602	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C15
25	B	606	CLA	C11-C10-C8-C7
25	C	512	CLA	C6-C7-C8-C10
25	D	403	CLA	C6-C7-C8-C10
25	b	602	CLA	C12-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C10
25	d	404	CLA	C11-C12-C13-C15
32	h	101	DGD	O1B-C1B-C2B-C3B
25	C	503	CLA	C2B-C3B-CAB-CBB
25	D	404	CLA	C2B-C3B-CAB-CBB
25	D	405	CLA	C2B-C3B-CAB-CBB
25	b	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	c	502	CLA	C2B-C3B-CAB-CBB
25	c	507	CLA	C2B-C3B-CAB-CBB
27	A	610	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	C	514	BCR	C1-C6-C7-C8
27	C	514	BCR	C23-C24-C25-C26
27	K	102	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
27	c	514	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C26
27	k	101	BCR	C23-C24-C25-C30
27	x	101	BCR	C23-C24-C25-C26
27	x	101	BCR	C23-C24-C25-C30
32	c	518	DGD	CDA-CEA-CFA-CGA
32	A	617	DGD	CBA-CCA-CDA-CEA
25	A	606	CLA	C2-C1-O2A-CGA
25	D	404	CLA	C2-C1-O2A-CGA
29	c	522	LMG	C42-C43-C44-C45
32	c	518	DGD	C5B-C6B-C7B-C8B
29	m	101	LMG	O8-C28-C29-C30
35	f	101	HEM	CAD-CBD-CGD-O2D
25	c	513	CLA	C8-C10-C11-C12
32	a	615	DGD	C9A-CAA-CBA-CCA
25	b	604	CLA	C13-C15-C16-C17
25	c	510	CLA	C5-C6-C7-C8
25	b	601	CLA	CAA-CBA-CGA-O2A
26	D	402	PHO	O1D-CGD-O2D-CED
31	d	407	LHG	C26-C27-C28-C29
33	B	623	STE	C3-C4-C5-C6
32	C	517	DGD	O6D-C5D-C6D-O5D
25	c	501	CLA	O1D-CGD-O2D-CED
29	D	408	LMG	C18-C19-C20-C21
32	c	519	DGD	C9B-CAB-CBB-CCB
30	B	622	SQD	C4-C5-C6-S
27	B	618	BCR	C18-C19-C20-C21
25	c	506	CLA	C2-C3-C5-C6
28	a	611	PL9	C23-C24-C26-C27
25	a	608	CLA	C3-C5-C6-C7
25	b	609	CLA	C16-C17-C18-C19
32	c	518	DGD	C5A-C6A-C7A-C8A
33	B	624	STE	C11-C12-C13-C14
33	c	521	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	C	515	DGD	C4E-C5E-C6E-O5E
25	B	614	CLA	C6-C7-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	C	506	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C9
25	c	501	CLA	C11-C12-C13-C14
33	j	101	STE	C7-C8-C9-C10
29	A	612	LMG	C28-C29-C30-C31
26	D	402	PHO	CBD-CGD-O2D-CED
32	c	517	DGD	C1G-C2G-C3G-O3G
25	b	602	CLA	C8-C10-C11-C12
25	B	602	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	c	502	CLA	CBA-CGA-O2A-C1
31	A	614	LHG	O7-C7-C8-C9
27	K	102	BCR	C17-C18-C19-C20
35	f	101	HEM	CAA-CBA-CGA-O2A
32	A	617	DGD	O2G-C1B-C2B-C3B
25	b	610	CLA	C10-C11-C12-C13
29	c	522	LMG	C36-C37-C38-C39
32	C	517	DGD	C6A-C7A-C8A-C9A
25	a	612	CLA	O1D-CGD-O2D-CED
29	B	621	LMG	O8-C28-C29-C30
25	c	505	CLA	C15-C16-C17-C18
29	B	621	LMG	C29-C30-C31-C32
25	B	601	CLA	C11-C12-C13-C15
25	C	505	CLA	C11-C10-C8-C7
25	C	511	CLA	C6-C7-C8-C10
25	C	512	CLA	O2A-C1-C2-C3
26	d	401	PHO	O2A-C1-C2-C3
33	B	624	STE	C4-C5-C6-C7
33	I	101	STE	C11-C12-C13-C14
25	C	510	CLA	C10-C11-C12-C13
29	c	520	LMG	O6-C5-C6-O5
28	A	611	PL9	C44-C46-C47-C48
29	D	411	LMG	C29-C28-O8-C9
25	B	602	CLA	C3A-C2A-CAA-CBA
25	C	512	CLA	C3A-C2A-CAA-CBA
25	a	609	CLA	C15-C16-C17-C18
25	B	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	d	408	LHG	C7-C8-C9-C10
27	B	618	BCR	C20-C21-C22-C23
27	B	619	BCR	C12-C13-C14-C15
27	b	617	BCR	C12-C13-C14-C15
25	b	613	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	CAA-CBA-CGA-O1A
29	m	101	LMG	O10-C28-O8-C9
32	H	102	DGD	C8A-C9A-CAA-CBA
25	B	606	CLA	C5-C6-C7-C8
31	A	615	LHG	O7-C7-C8-C9
25	b	612	CLA	CAA-CBA-CGA-O1A
25	b	610	CLA	C13-C15-C16-C17
25	A	607	CLA	C11-C10-C8-C9
25	B	601	CLA	C11-C12-C13-C14
25	b	606	CLA	C11-C12-C13-C14
31	A	614	LHG	C10-C11-C12-C13
30	A	613	SQD	C9-C10-C11-C12
31	d	408	LHG	O2-C2-C3-O3
33	d	413	STE	O1-C1-C2-C3
35	f	101	HEM	CAA-CBA-CGA-O1A
31	e	101	LHG	O10-C23-C24-C25
27	K	102	BCR	C11-C12-C13-C14
25	b	613	CLA	CAA-CBA-CGA-O1A
29	c	524	LMG	C14-C15-C16-C17
32	C	516	DGD	C5D-C6D-O5D-C1E
32	c	517	DGD	C5D-C6D-O5D-C1E
32	c	518	DGD	C2D-C1D-O3G-C3G
25	B	613	CLA	CAA-CBA-CGA-O1A
30	a	613	SQD	O49-C7-C8-C9
31	A	614	LHG	O9-C7-C8-C9
32	A	617	DGD	O1B-C1B-C2B-C3B
31	d	407	LHG	O8-C23-C24-C25
32	c	517	DGD	O1G-C1A-C2A-C3A
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
33	C	521	STE	C11-C12-C13-C14
25	c	512	CLA	C15-C16-C17-C18
30	f	102	SQD	O6-C44-C45-C46
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	605	CLA	C15-C16-C17-C18
25	d	404	CLA	C2-C3-C5-C6
29	c	522	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
33	C	521	STE	C2-C3-C4-C5
30	F	101	SQD	C34-C35-C36-C37
25	B	607	CLA	CAD-CBD-CGD-O2D
25	a	607	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
26	d	401	PHO	CAD-CBD-CGD-O2D
25	b	604	CLA	C5-C6-C7-C8
30	A	613	SQD	O47-C7-C8-C9
32	C	515	DGD	O1B-C1B-C2B-C3B
33	T	102	STE	C1-C2-C3-C4
29	b	621	LMG	O6-C1-O1-C7
32	C	515	DGD	O6E-C1E-O5D-C6D
25	c	513	CLA	C2-C1-O2A-CGA
32	c	517	DGD	O1B-C1B-C2B-C3B
30	a	614	SQD	O6-C44-C45-C46
28	D	407	PL9	C46-C47-C48-C49
32	c	518	DGD	C3B-C4B-C5B-C6B
33	c	523	STE	O2-C1-C2-C3
33	C	519	STE	O2-C1-C2-C3
29	D	408	LMG	C28-C29-C30-C31
28	A	611	PL9	C2-C3-C7-C8
33	T	102	STE	C11-C10-C9-C8
29	D	408	LMG	C22-C23-C24-C25
33	M	102	STE	O2-C1-C2-C3

There are no ring outliers.

150 monomers are involved in 304 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	d	405	BCR	2	0
25	c	509	CLA	3	0
29	m	101	LMG	3	0
31	e	101	LHG	2	0
33	l	102	STE	1	0
36	v	201	HEC	1	0
29	D	411	LMG	1	0
25	b	606	CLA	7	0
25	C	503	CLA	3	0
27	D	406	BCR	2	0
33	b	622	STE	1	0
35	f	101	HEM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	618	BCR	1	0
25	B	606	CLA	5	0
27	B	619	BCR	4	0
32	H	102	DGD	2	0
25	C	502	CLA	4	0
25	C	501	CLA	1	0
25	a	609	CLA	3	0
25	b	610	CLA	1	0
25	C	504	CLA	3	0
31	A	614	LHG	1	0
33	H	103	STE	2	0
32	c	518	DGD	1	0
25	B	614	CLA	4	0
25	c	511	CLA	3	0
25	c	504	CLA	1	0
31	d	408	LHG	5	0
25	B	611	CLA	2	0
25	a	612	CLA	2	0
26	A	608	PHO	2	0
33	a	616	STE	1	0
25	c	503	CLA	4	0
25	c	508	CLA	4	0
25	c	501	CLA	6	0
29	d	411	LMG	1	0
30	A	616	SQD	4	0
25	D	403	CLA	1	0
27	c	515	BCR	2	0
25	B	605	CLA	5	0
30	a	613	SQD	4	0
25	C	511	CLA	1	0
25	B	603	CLA	5	0
28	D	407	PL9	2	0
25	c	505	CLA	6	0
32	A	617	DGD	7	0
25	A	606	CLA	1	0
25	c	507	CLA	4	0
25	A	607	CLA	1	0
29	M	101	LMG	1	0
30	L	101	SQD	4	0
25	c	502	CLA	1	0
25	B	615	CLA	4	0
25	B	609	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	T	101	BCR	4	0
27	A	610	BCR	4	0
25	B	602	CLA	2	0
25	C	507	CLA	1	0
25	C	510	CLA	4	0
25	b	605	CLA	3	0
27	x	101	BCR	3	0
25	b	603	CLA	1	0
25	B	612	CLA	2	0
31	D	409	LHG	2	0
35	E	101	HEM	2	0
26	D	402	PHO	3	0
33	B	625	STE	2	0
33	I	101	STE	2	0
33	a	617	STE	1	0
25	b	611	CLA	1	0
27	C	514	BCR	4	0
28	a	611	PL9	6	0
33	T	103	STE	1	0
27	K	101	BCR	3	0
28	A	611	PL9	4	0
31	D	410	LHG	2	0
25	B	616	CLA	5	0
32	C	516	DGD	2	0
25	c	510	CLA	4	0
32	C	515	DGD	2	0
25	b	613	CLA	4	0
25	B	604	CLA	2	0
25	b	607	CLA	1	0
32	c	519	DGD	2	0
33	B	620	STE	1	0
27	t	101	BCR	1	0
30	A	613	SQD	1	0
33	B	623	STE	1	0
27	b	619	BCR	3	0
25	b	601	CLA	3	0
25	C	508	CLA	3	0
27	k	101	BCR	1	0
25	D	404	CLA	3	0
29	b	621	LMG	2	0
25	B	601	CLA	2	0
32	C	517	DGD	2	0

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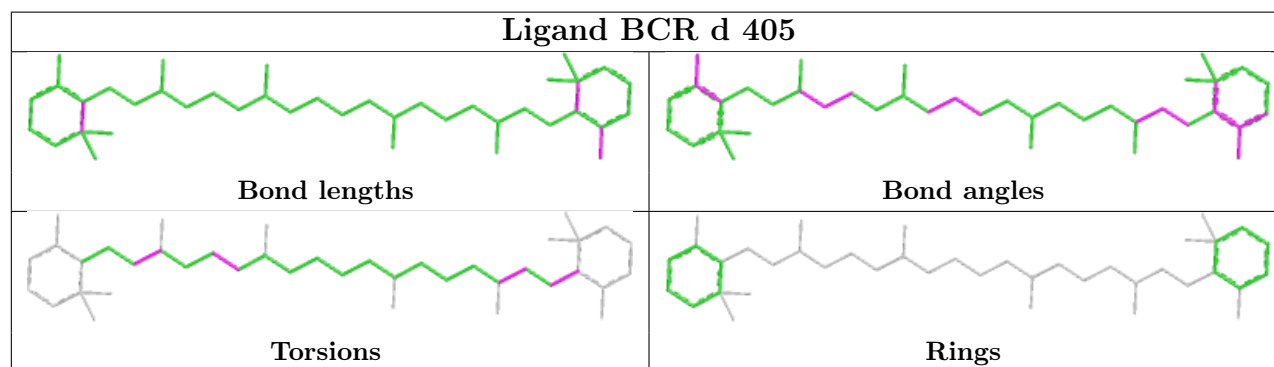
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	604	CLA	5	0
25	c	513	CLA	3	0
27	a	610	BCR	3	0
31	A	615	LHG	1	0
27	B	617	BCR	1	0
27	c	516	BCR	2	0
25	C	513	CLA	2	0
25	D	405	CLA	1	0
29	c	522	LMG	4	0
25	d	404	CLA	3	0
33	x	102	STE	6	0
25	b	615	CLA	3	0
29	A	612	LMG	2	0
30	a	614	SQD	2	0
25	B	613	CLA	1	0
25	a	608	CLA	3	0
29	c	524	LMG	2	0
26	d	402	PHO	1	0
25	b	616	CLA	4	0
25	b	608	CLA	1	0
31	d	409	LHG	1	0
32	a	615	DGD	5	0
25	A	609	CLA	2	0
21	A	601[B]	OEY	1	0
33	b	620	STE	1	0
33	t	102	STE	1	0
30	B	622	SQD	3	0
32	h	101	DGD	2	0
31	l	101	LHG	2	0
33	T	102	STE	1	0
25	c	512	CLA	4	0
25	C	509	CLA	3	0
29	B	621	LMG	1	0
25	b	614	CLA	3	0
27	K	102	BCR	3	0
30	F	101	SQD	2	0
27	H	101	BCR	3	0
25	b	612	CLA	3	0
30	f	102	SQD	3	0
29	C	518	LMG	2	0
33	d	413	STE	1	0
25	d	403	CLA	2	0

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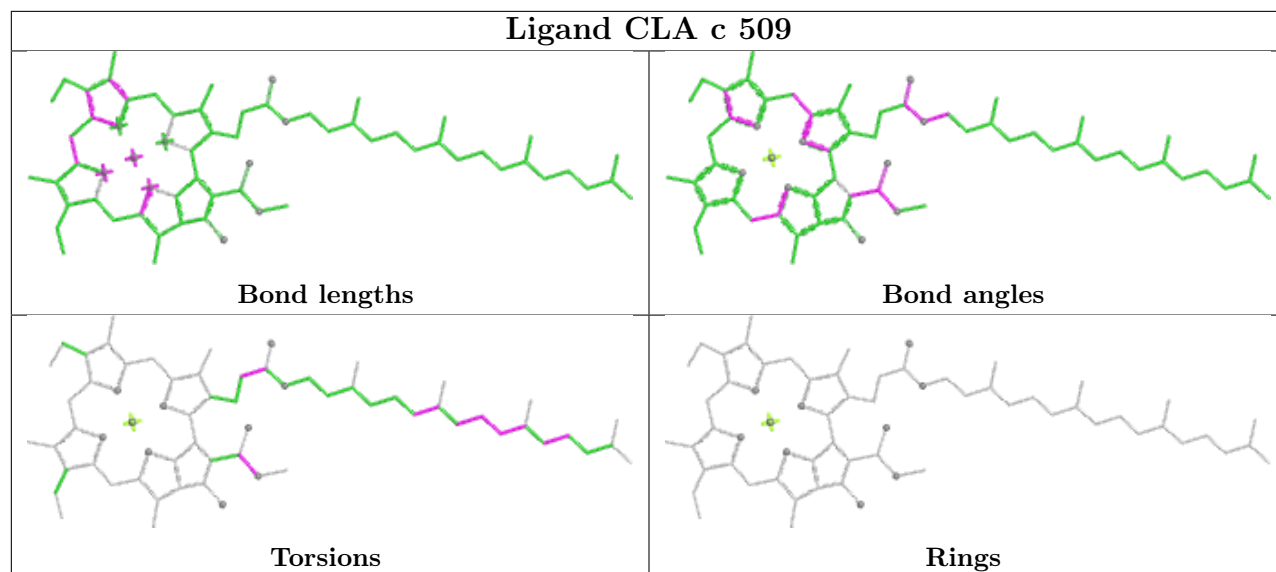
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	607	CLA	3	0
31	d	407	LHG	2	0
31	D	412	LHG	2	0
33	B	624	STE	1	0
28	d	406	PL9	3	0
25	C	512	CLA	3	0
33	D	413	STE	1	0
27	Y	101	BCR	2	0
29	D	408	LMG	1	0
27	c	514	BCR	3	0
25	C	506	CLA	2	0
25	b	602	CLA	5	0

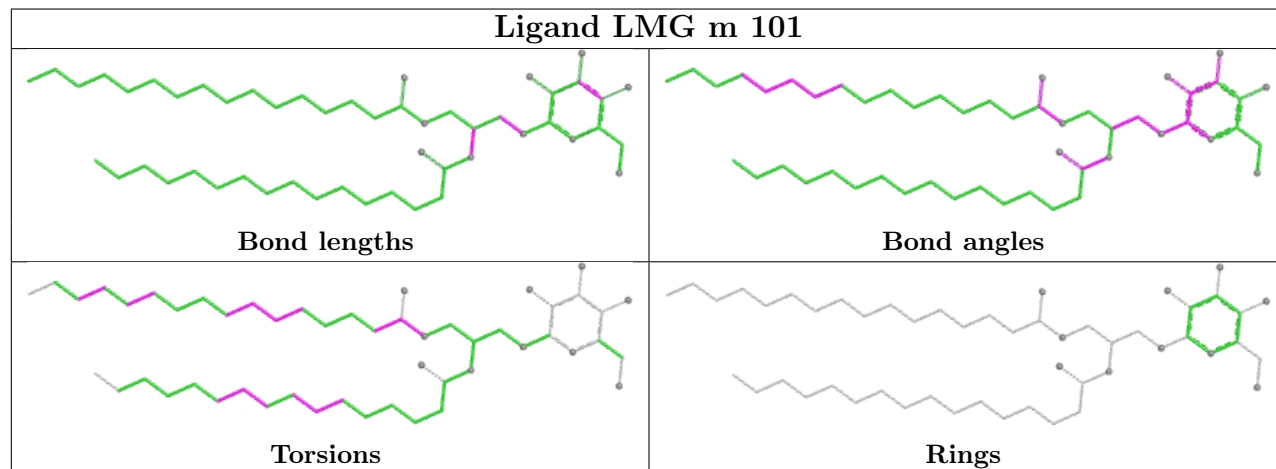
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

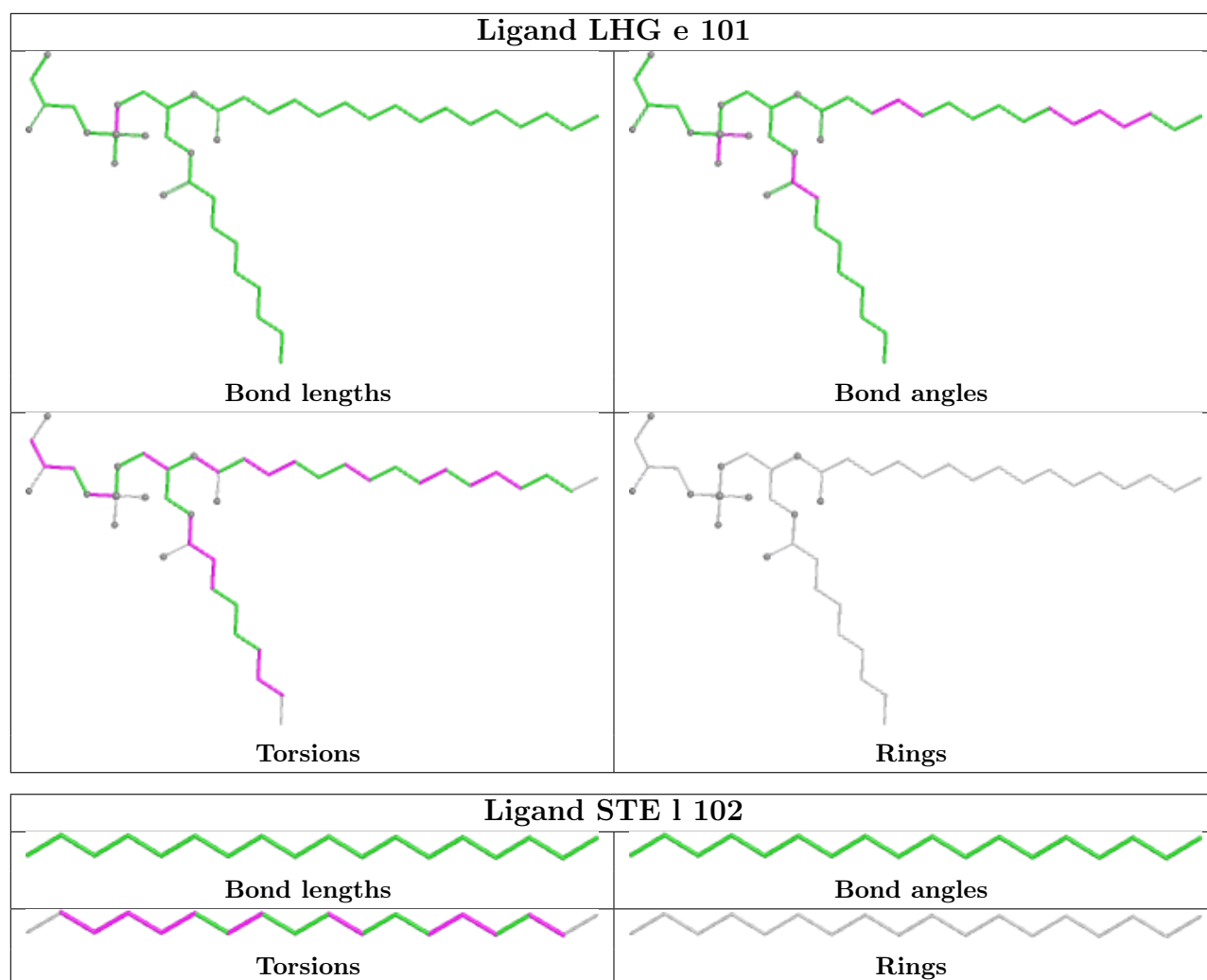


Ligand CLA c 509

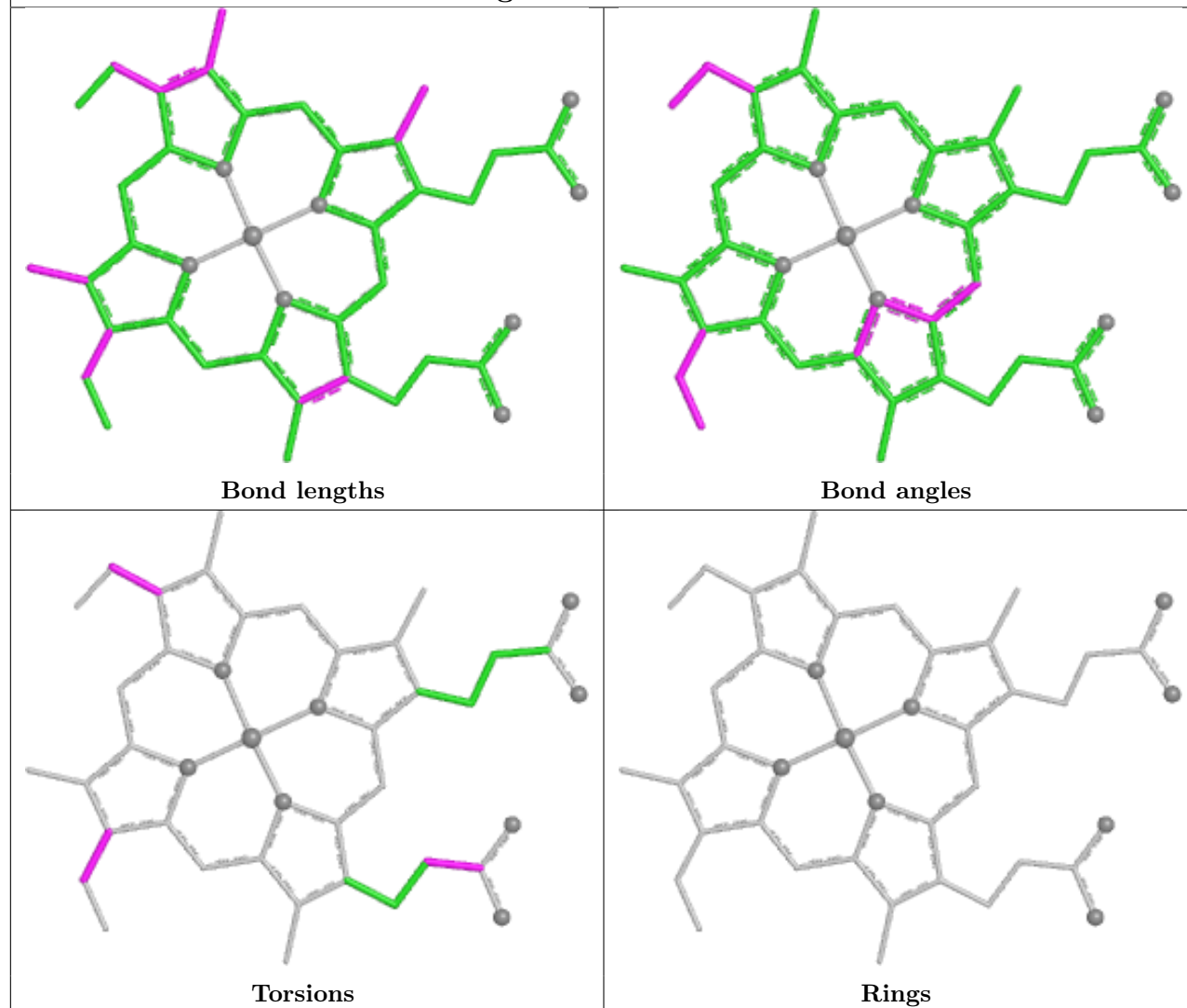


Ligand LMG m 101

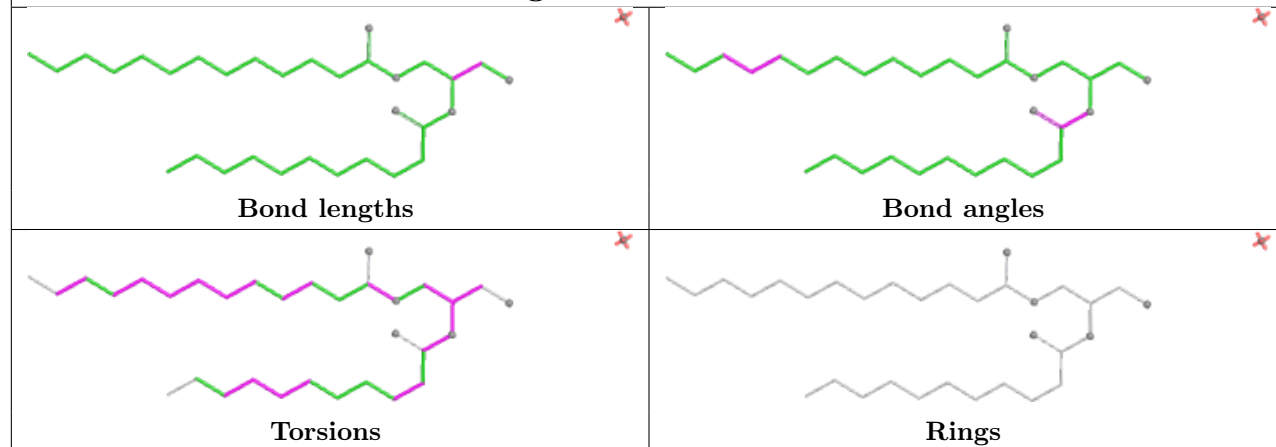


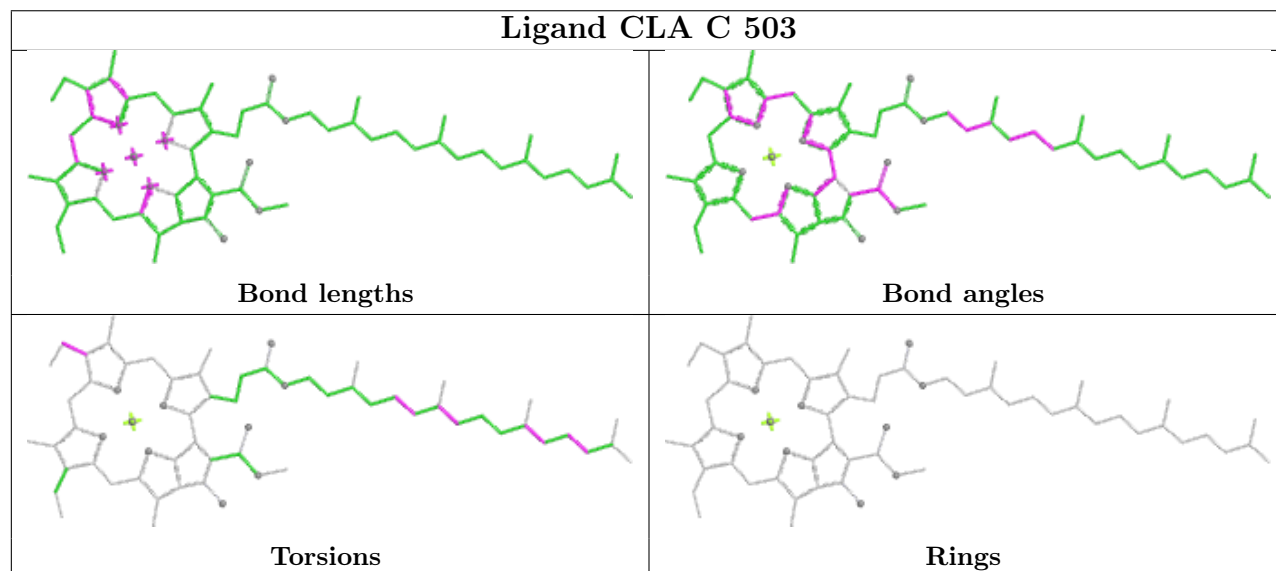
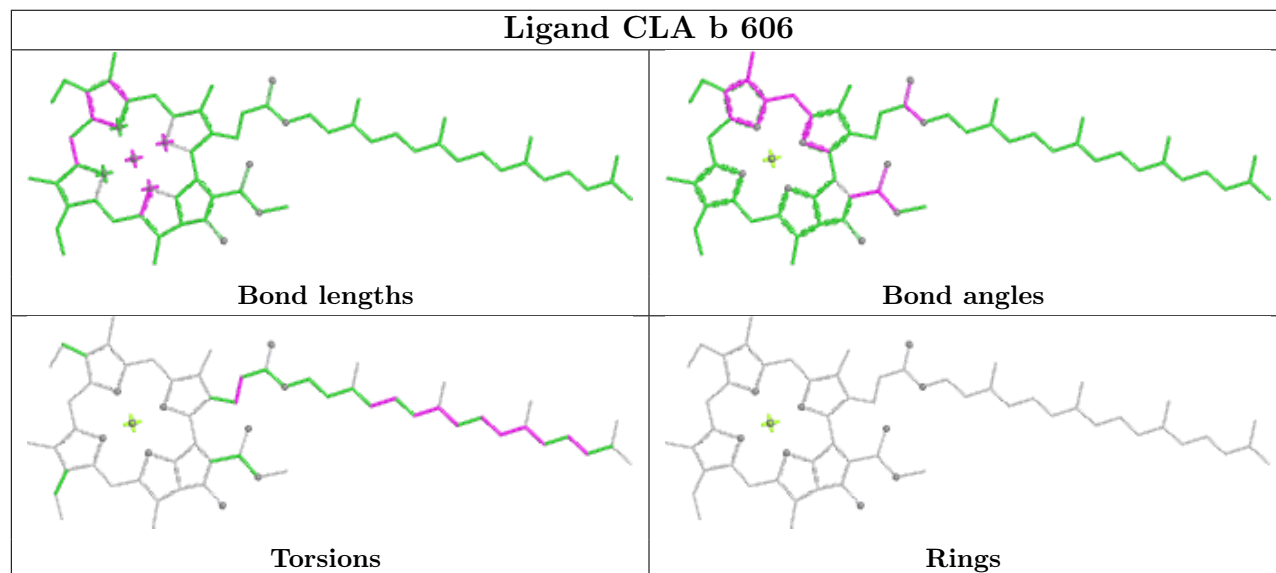
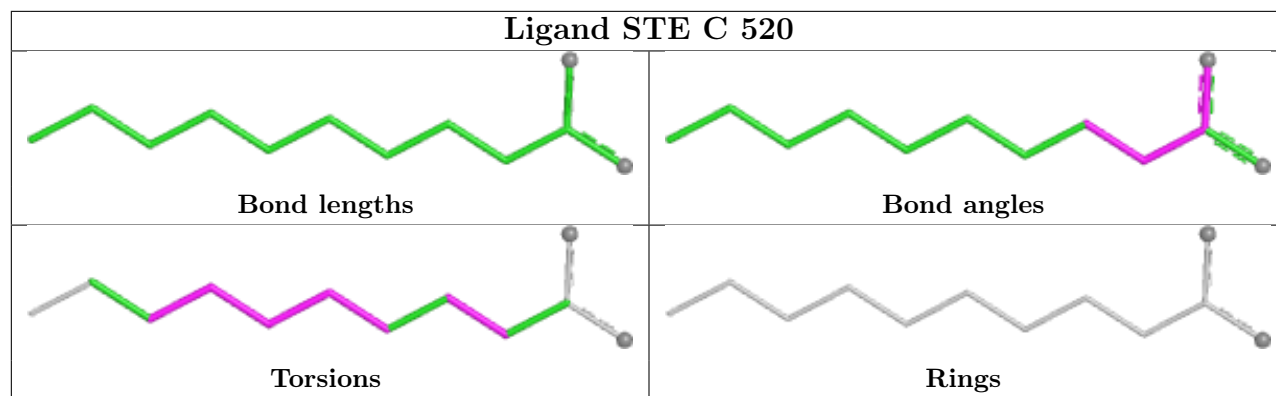


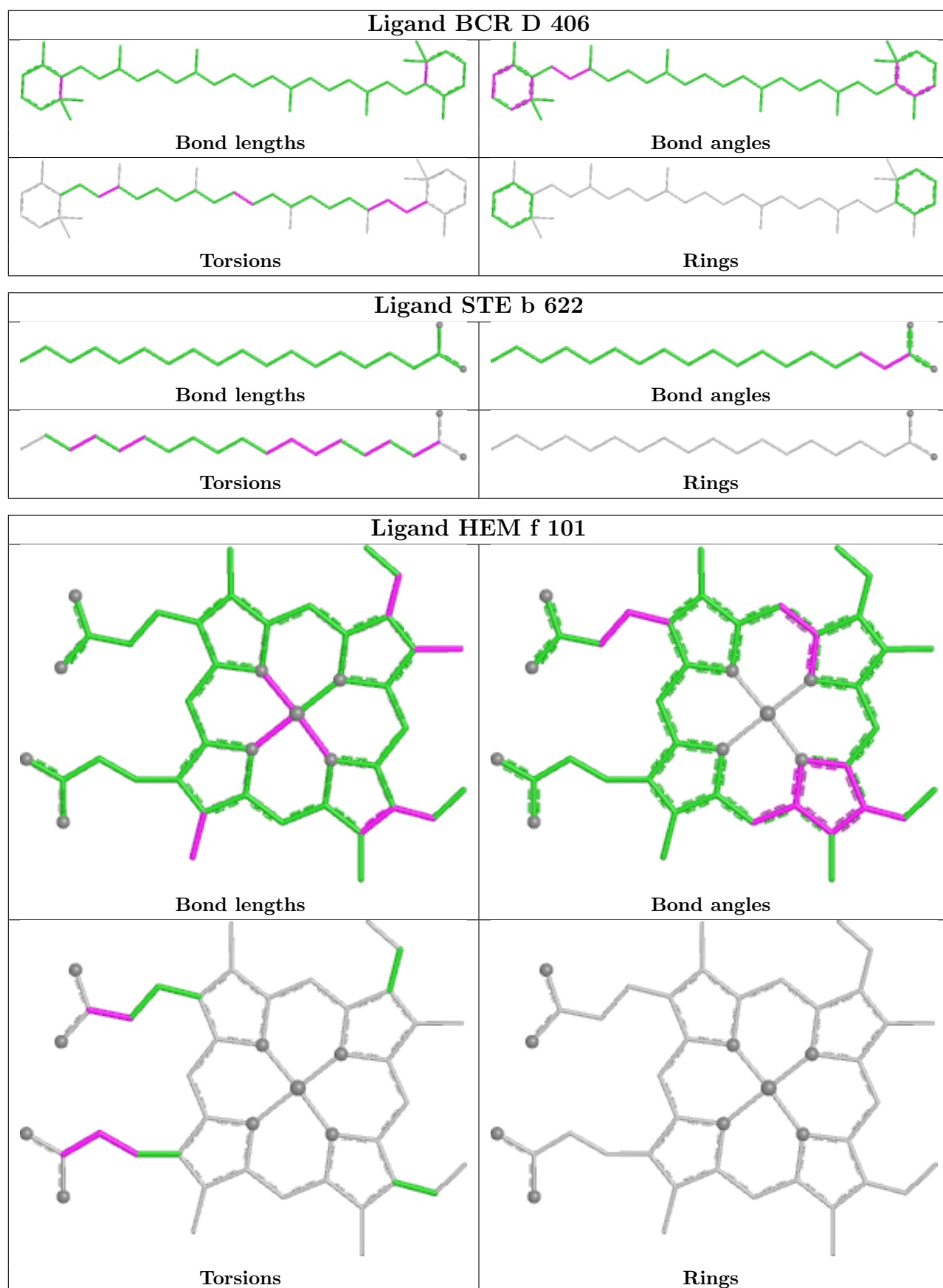
Ligand HEC v 201



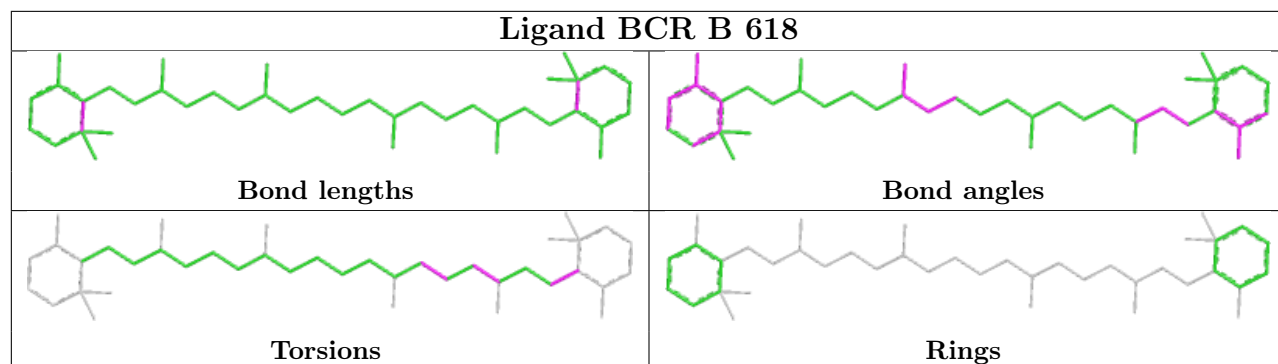
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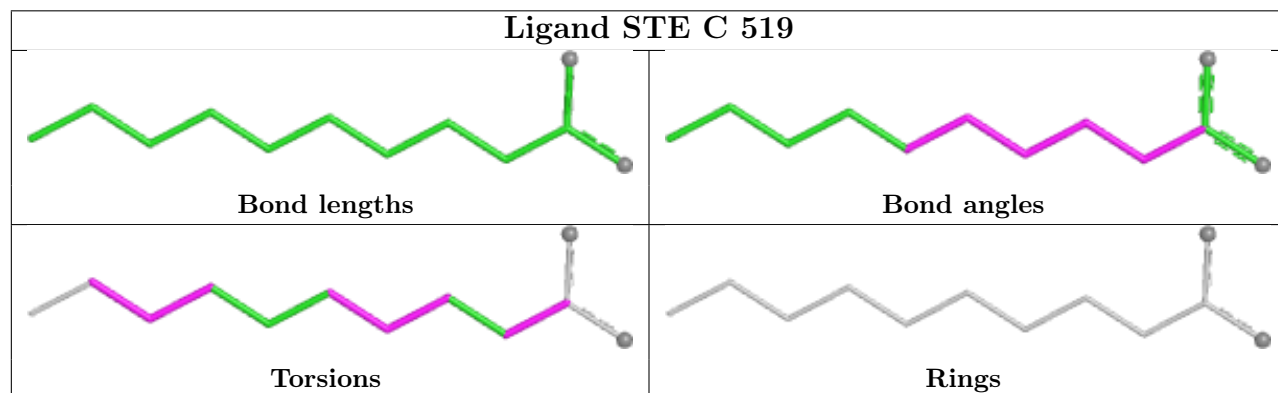




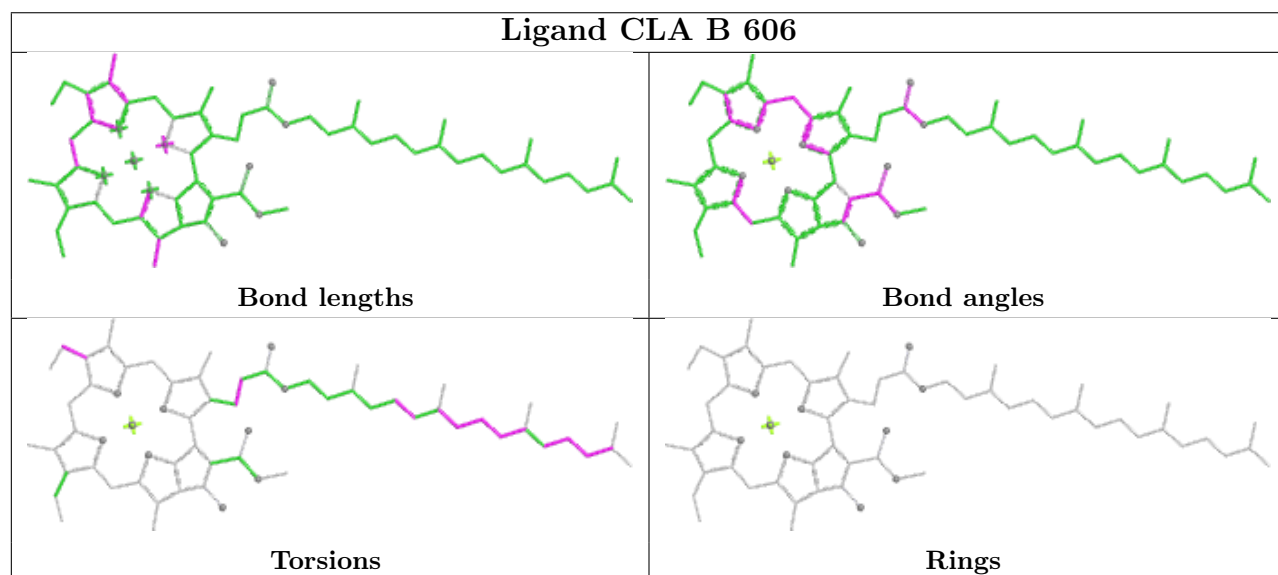
Ligand BCR B 618



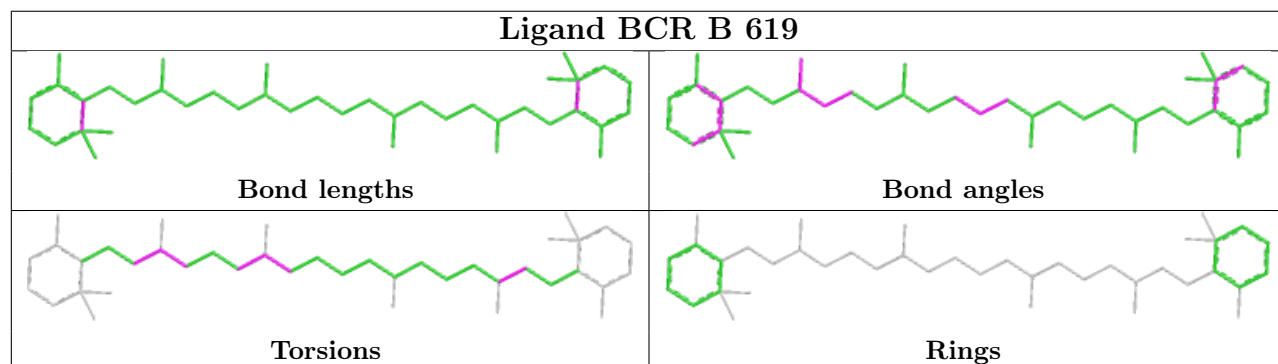
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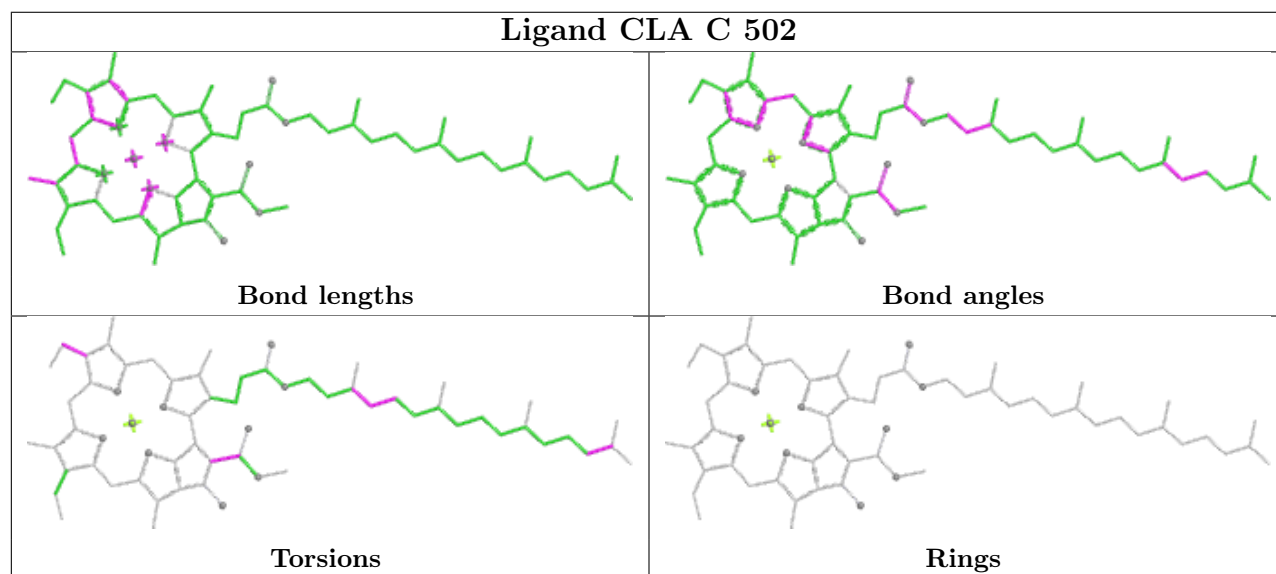
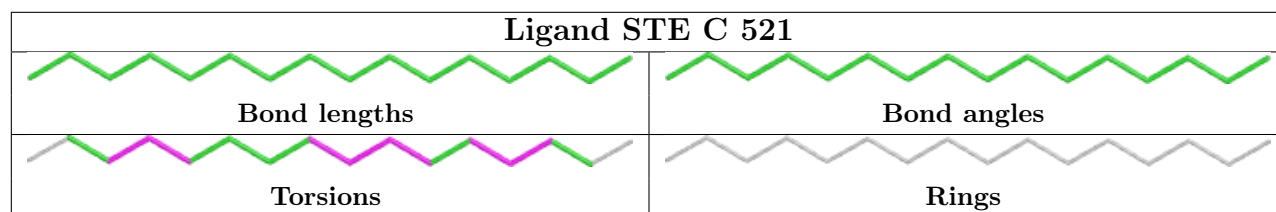
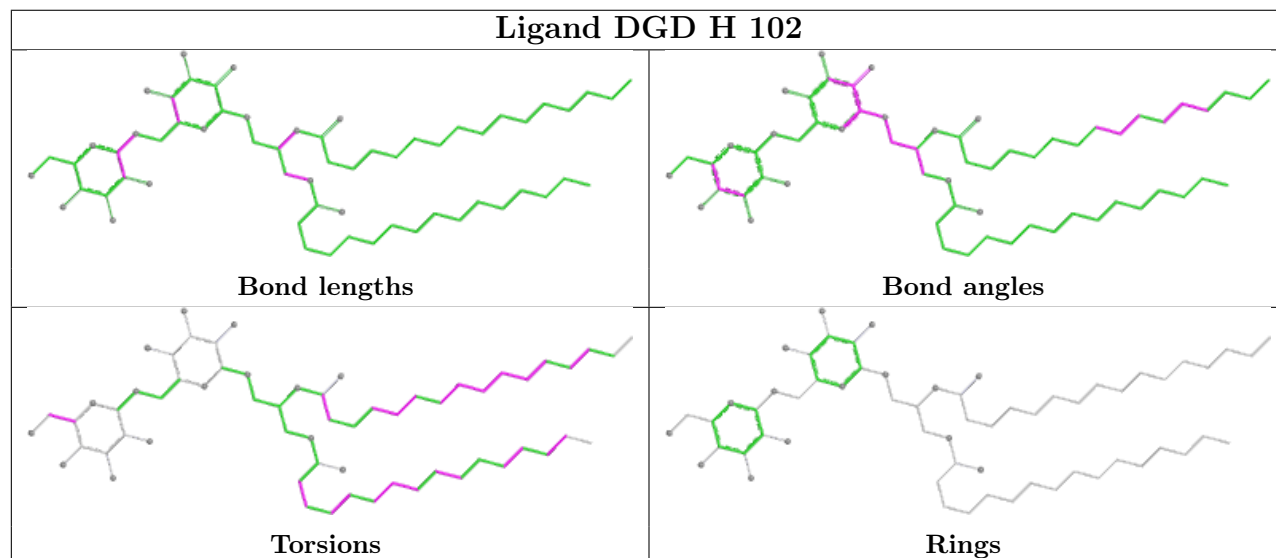
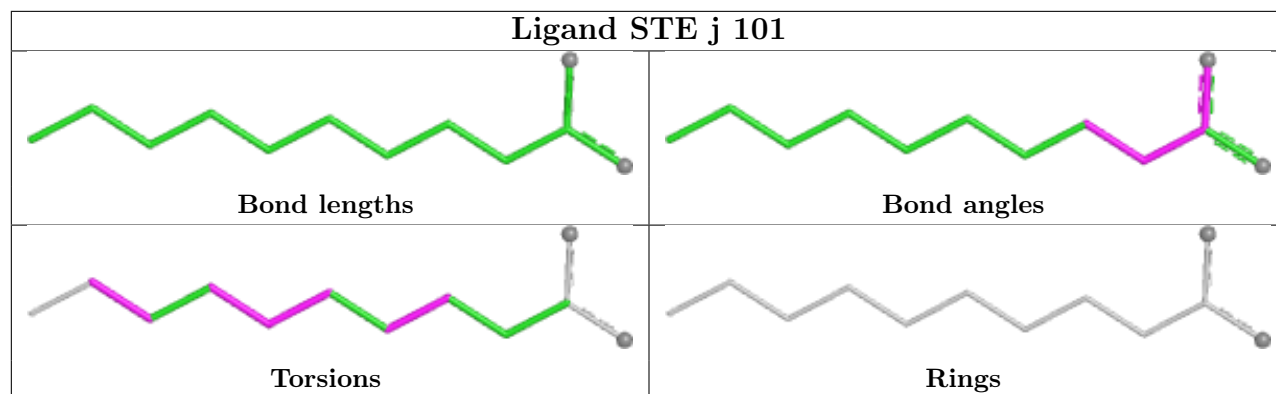


Ligand CLA B 606

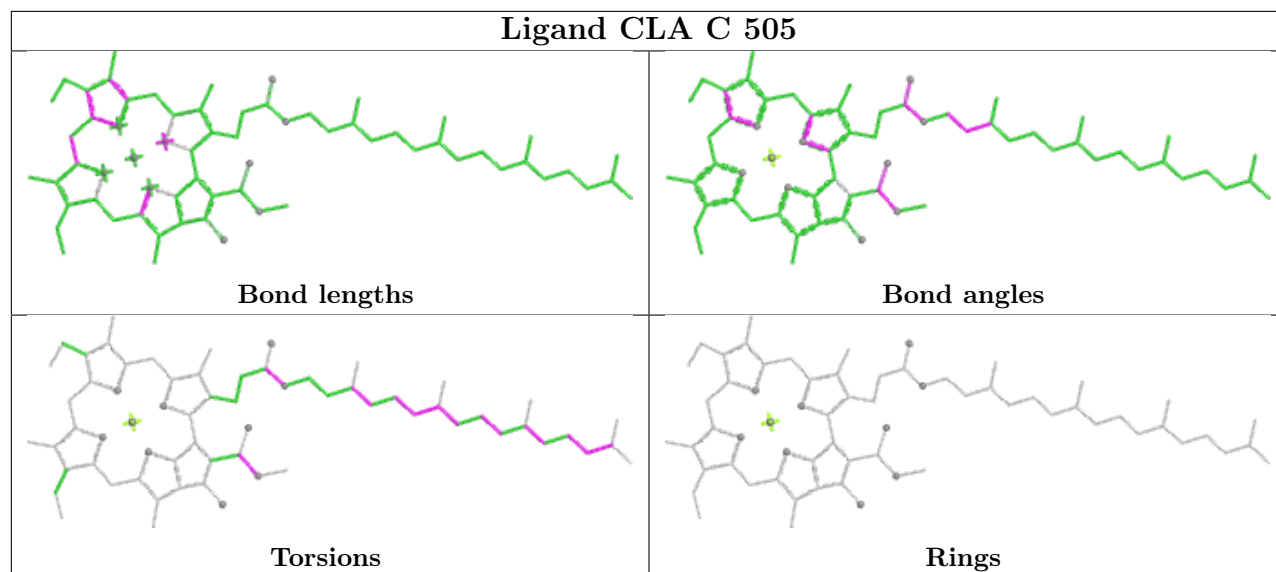


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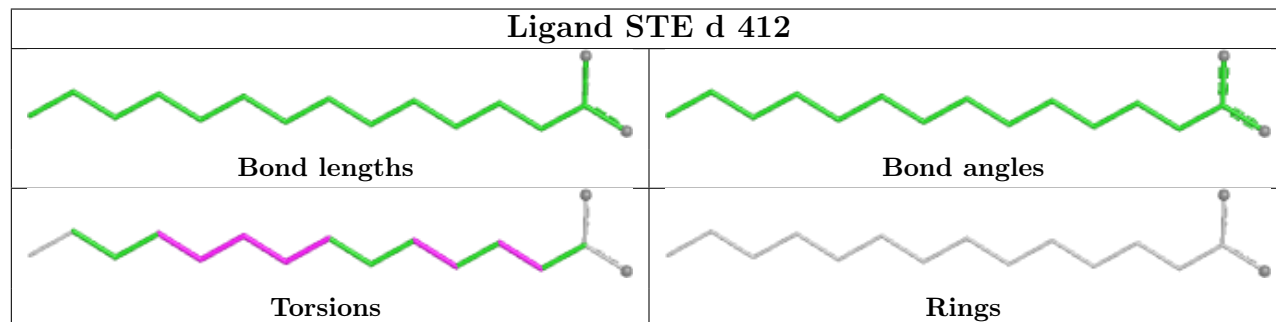




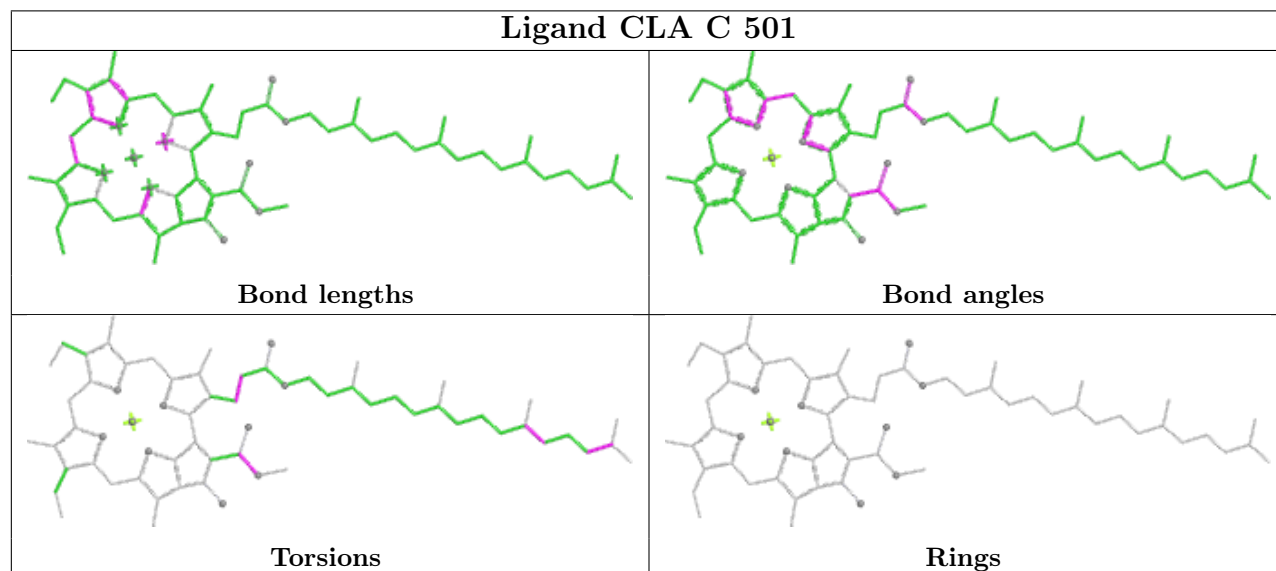
Ligand CLA C 505

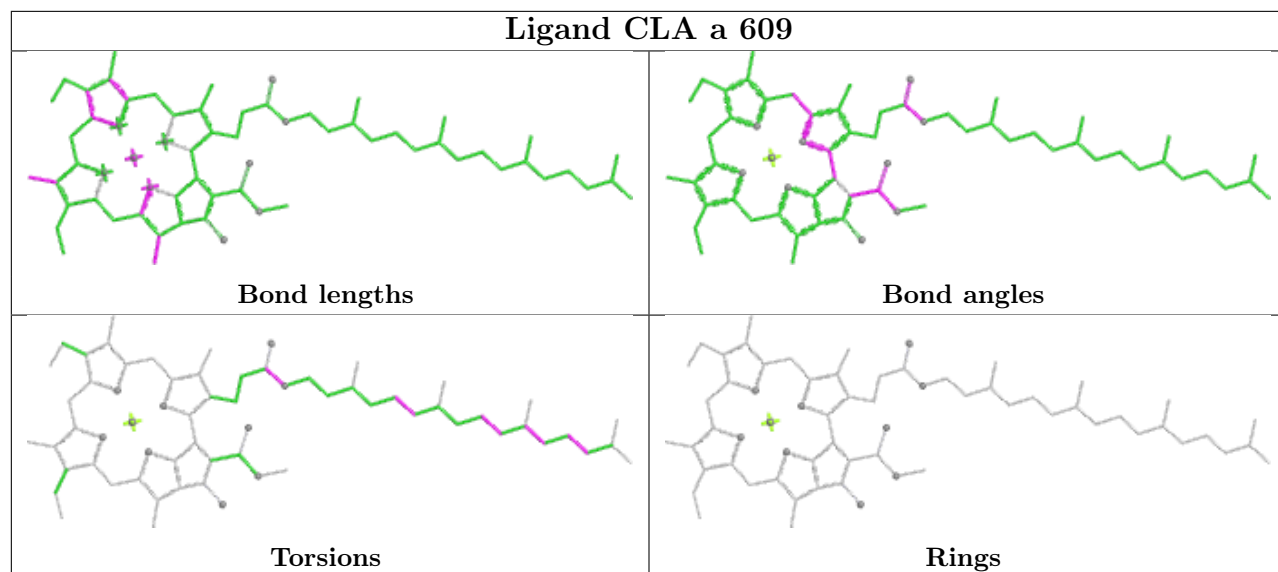
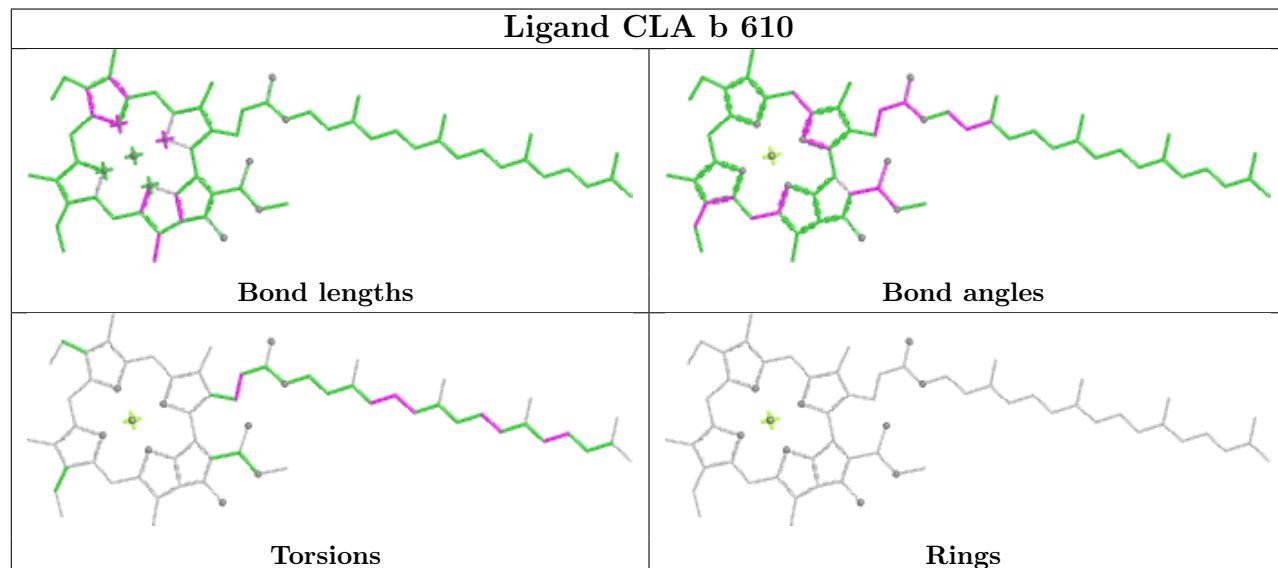


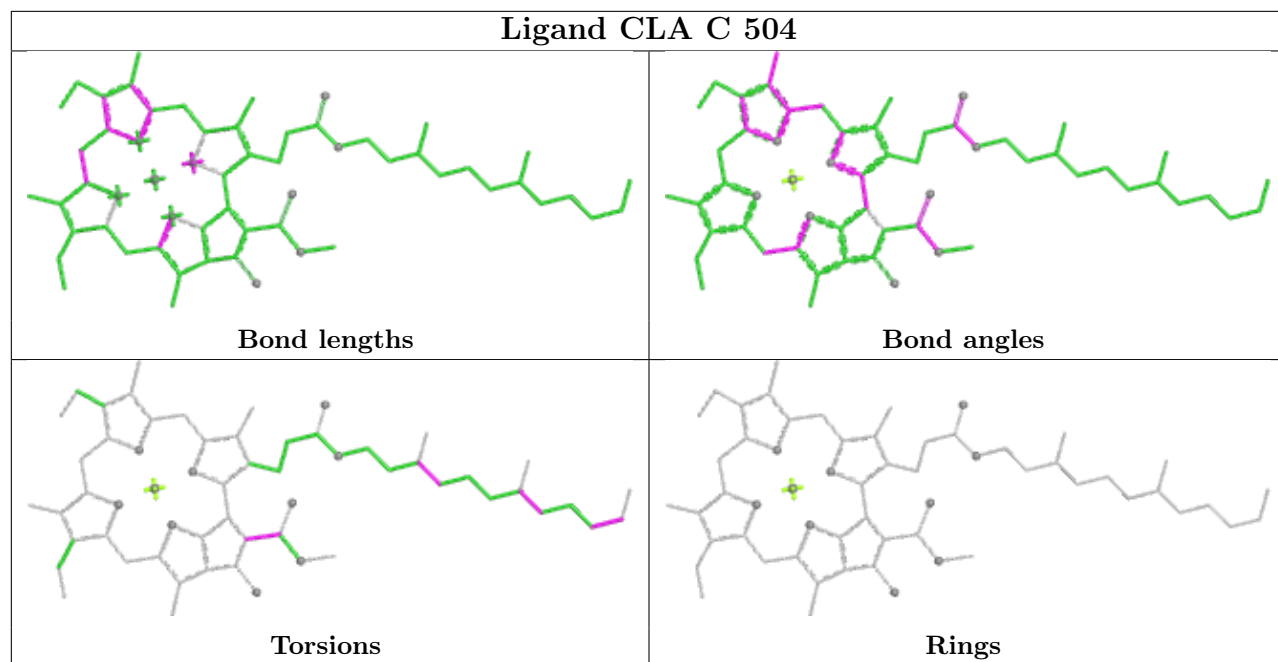
Ligand STE d 412

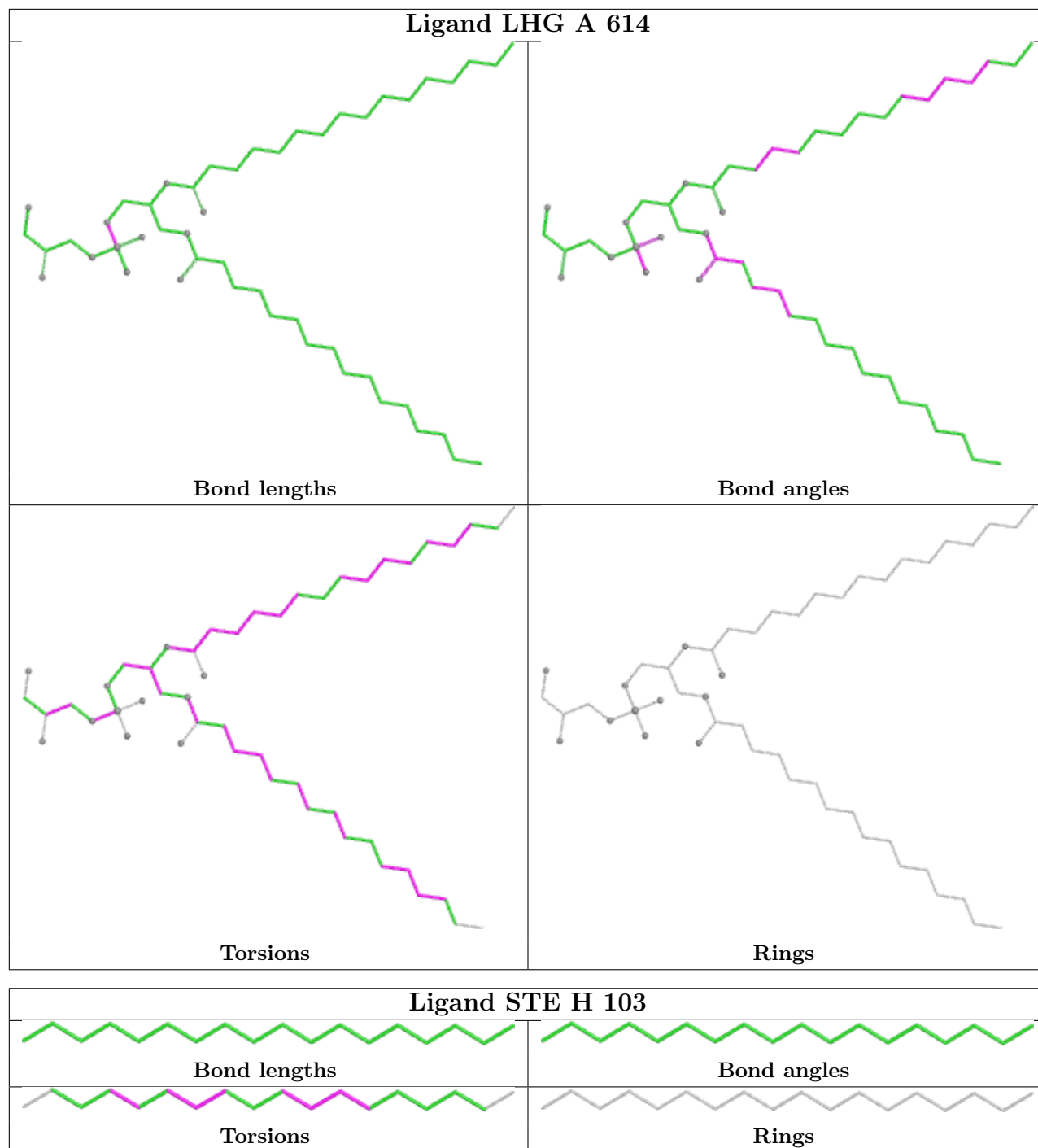


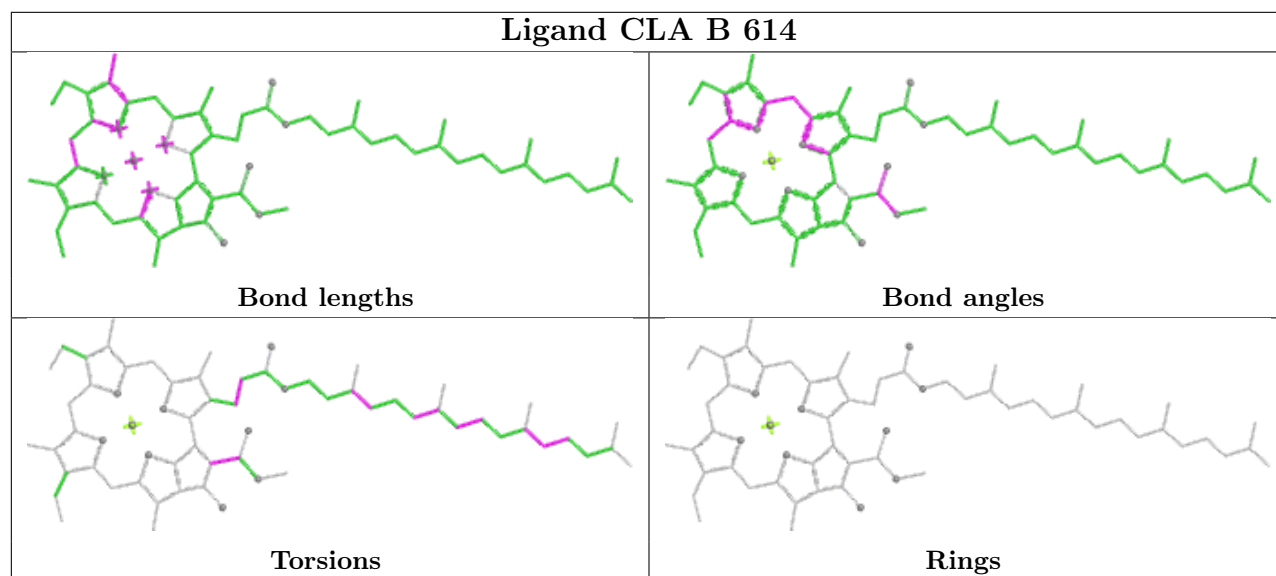
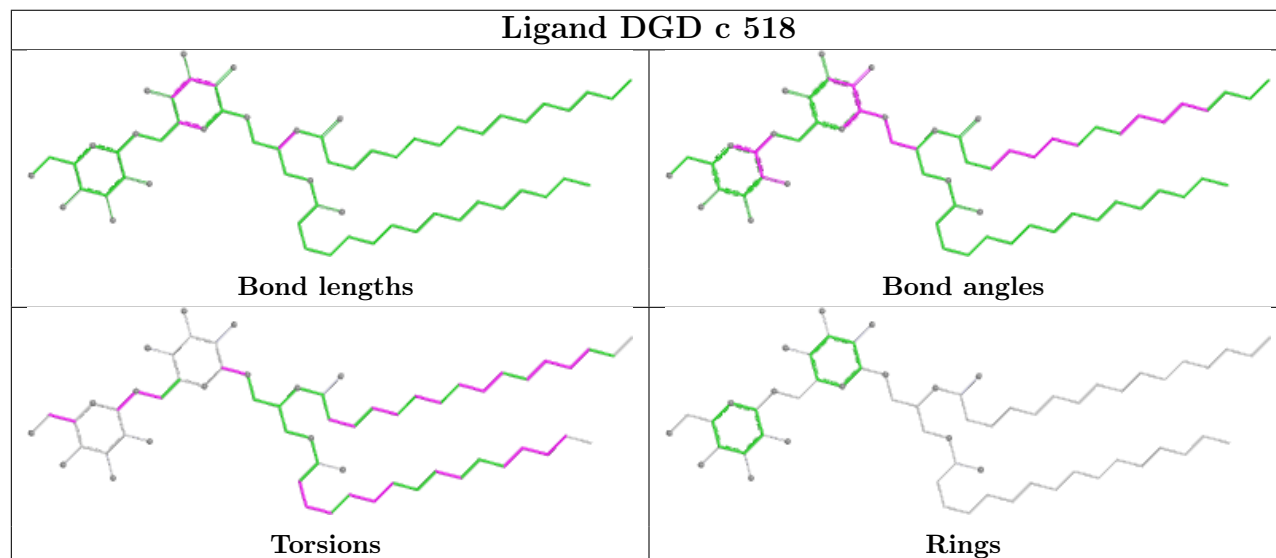
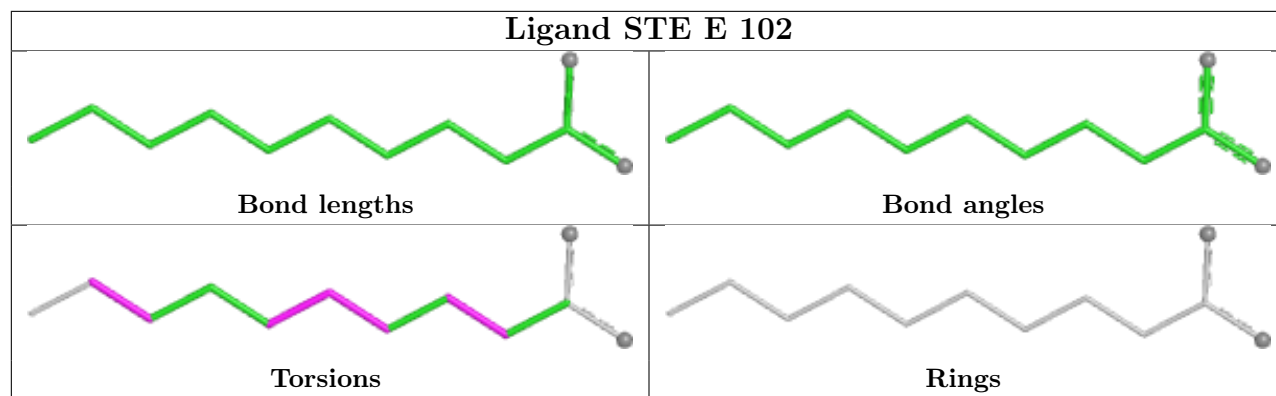
Ligand CLA C 501

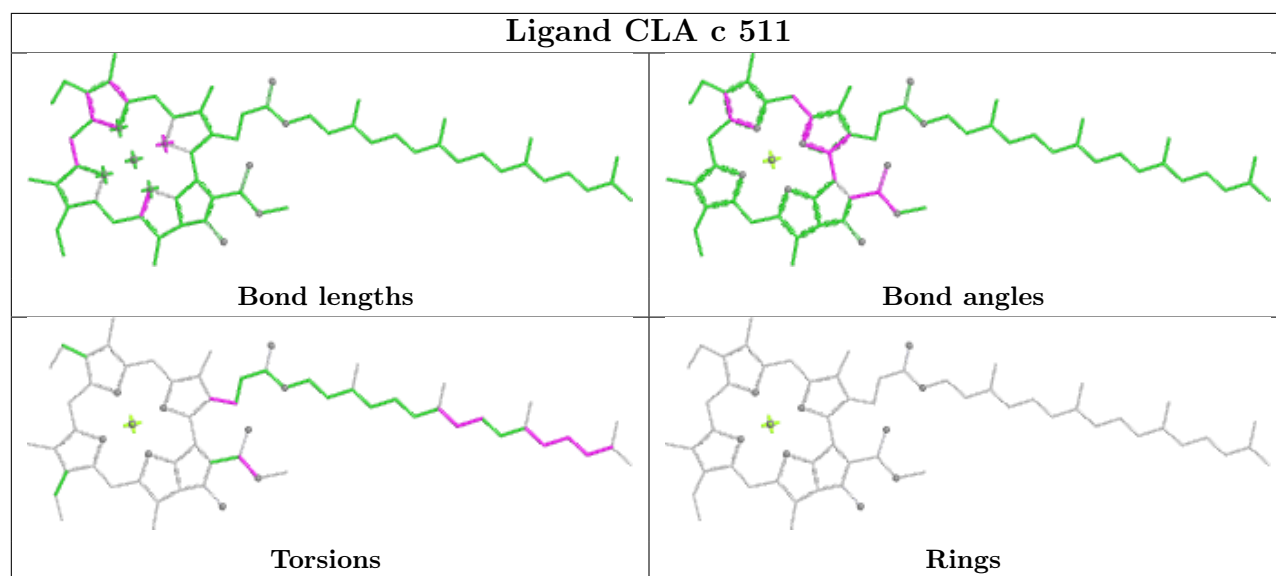
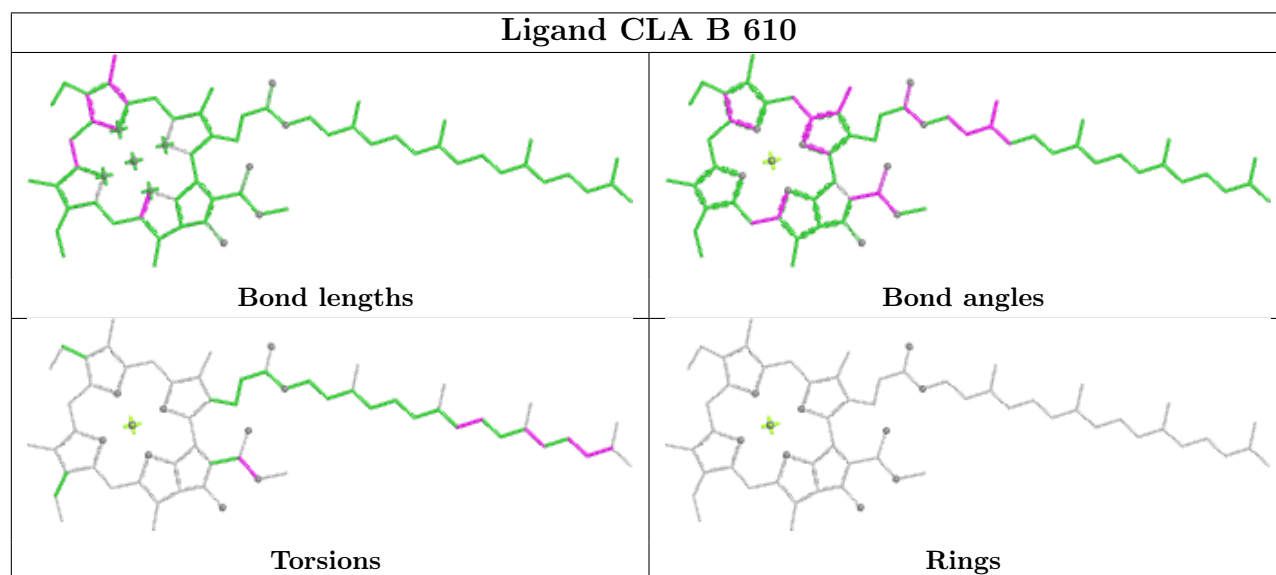
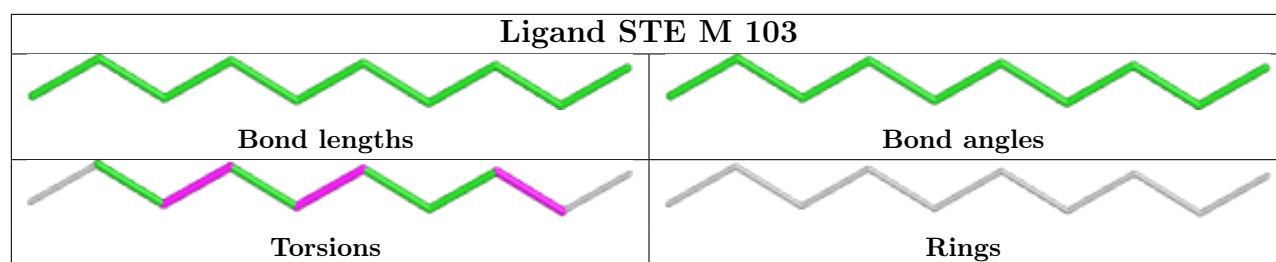


Ligand CLA a 609**Ligand CLA b 610**

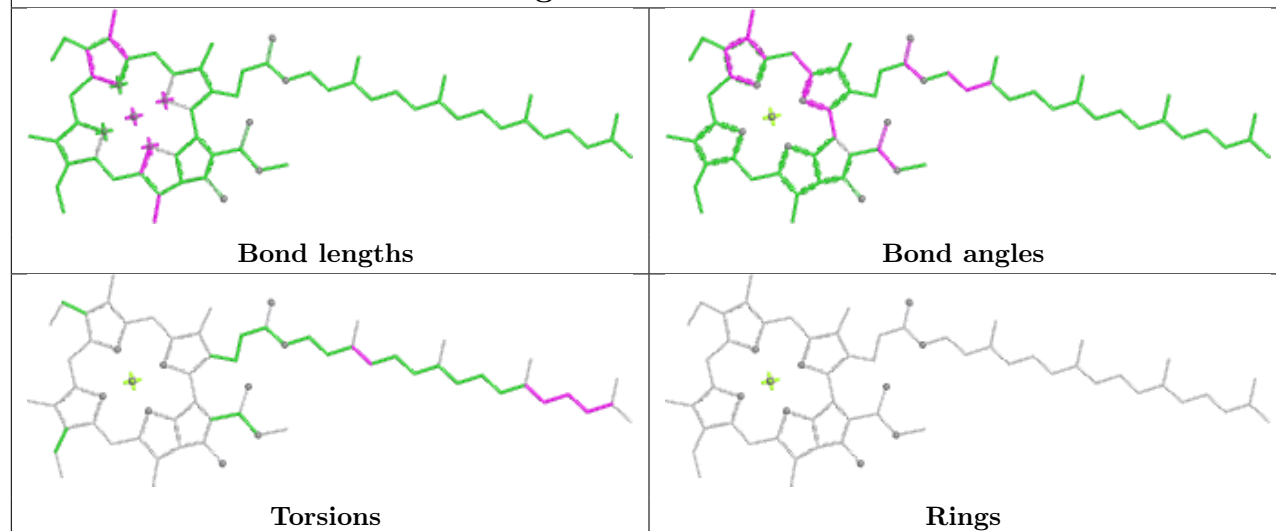




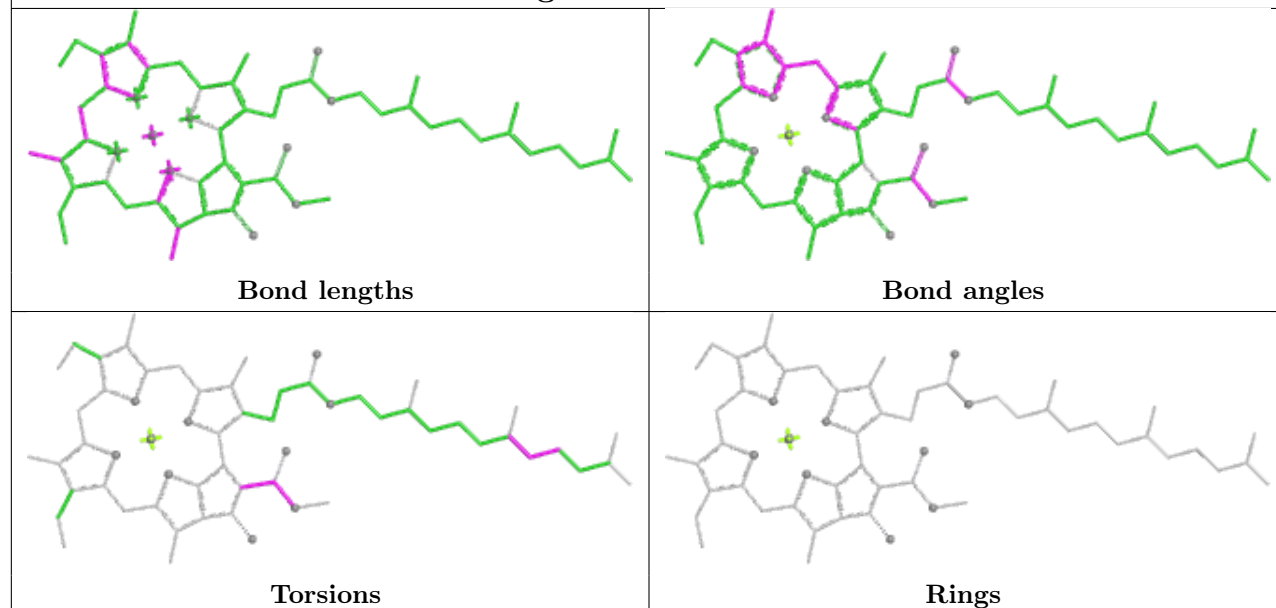


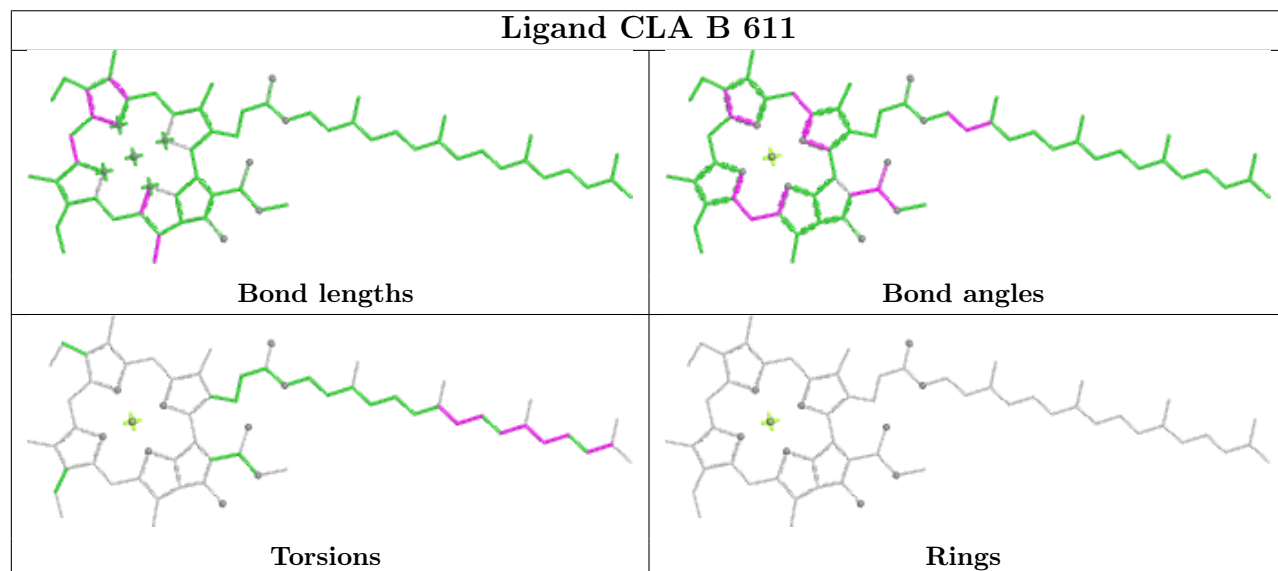
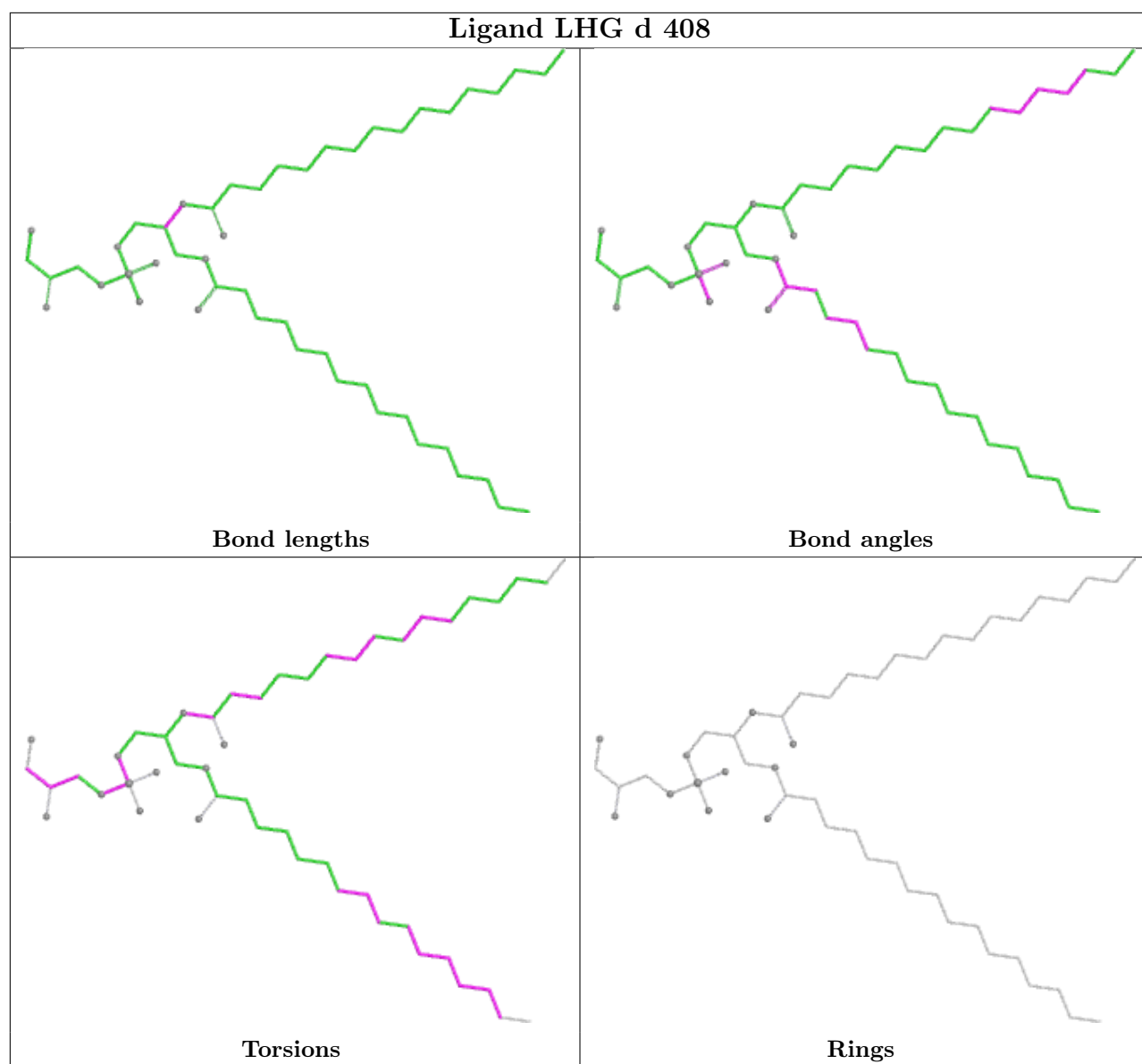


Ligand CLA b 609

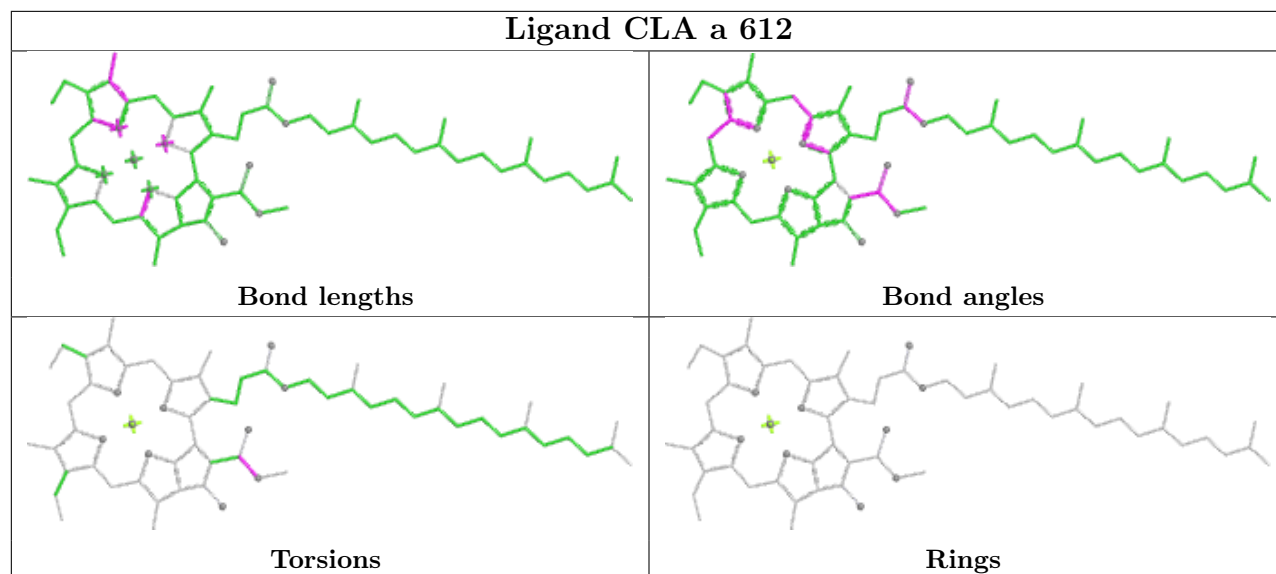


Ligand CLA c 504

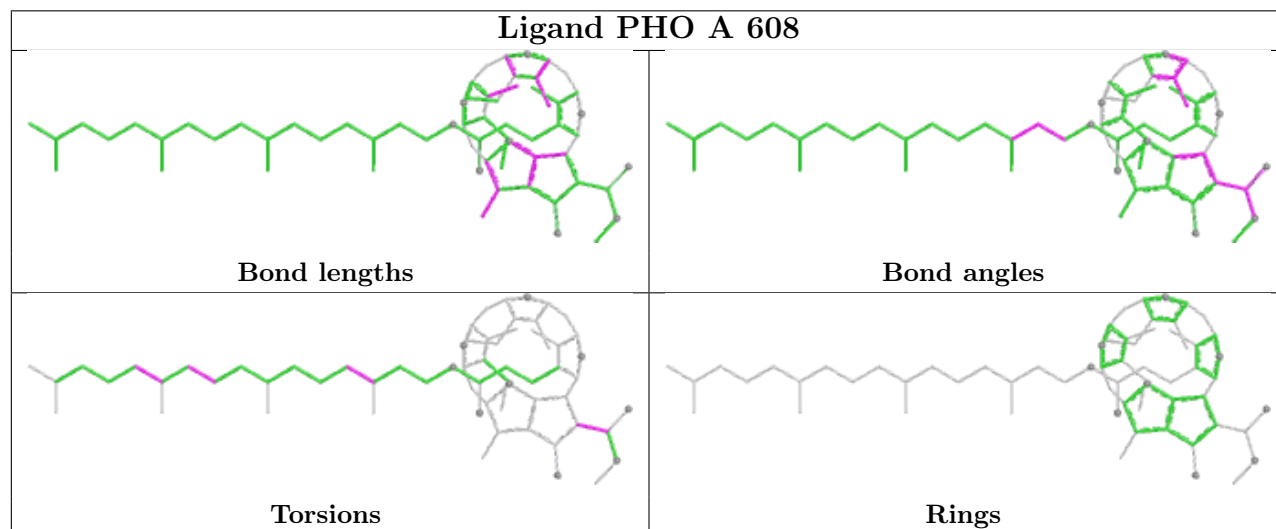




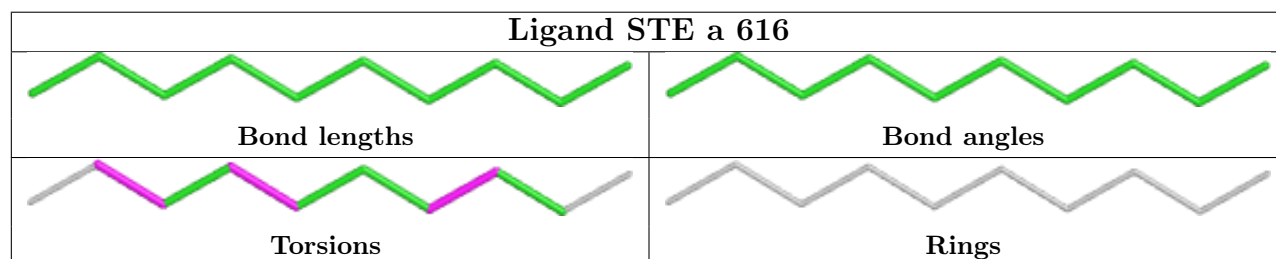
Ligand CLA a 612



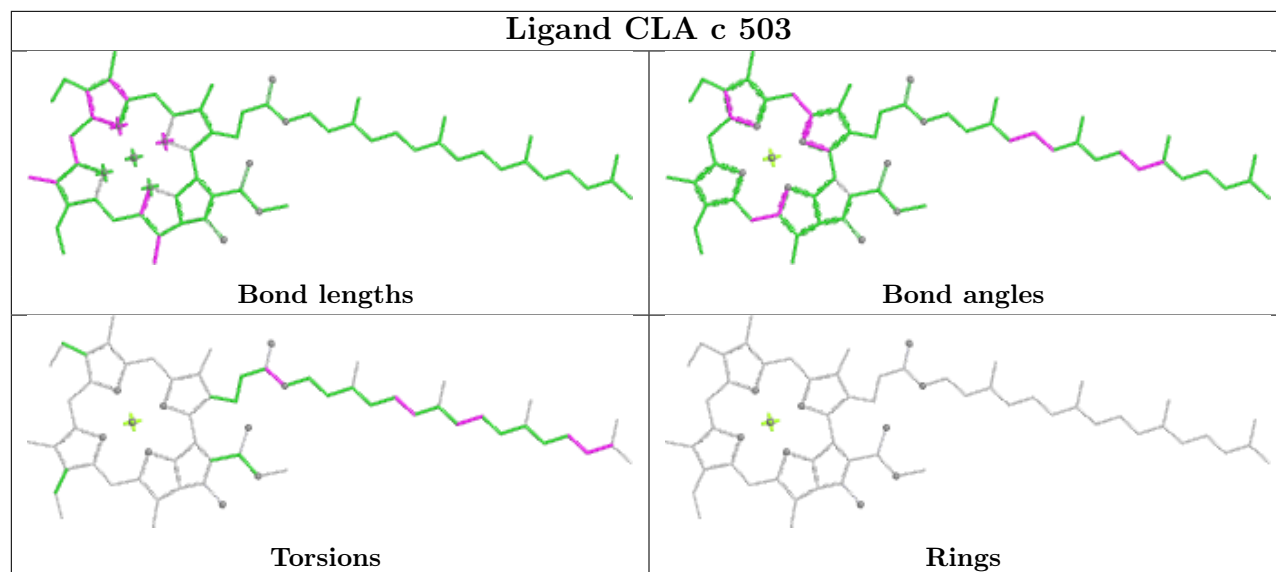
Ligand PHO A 608



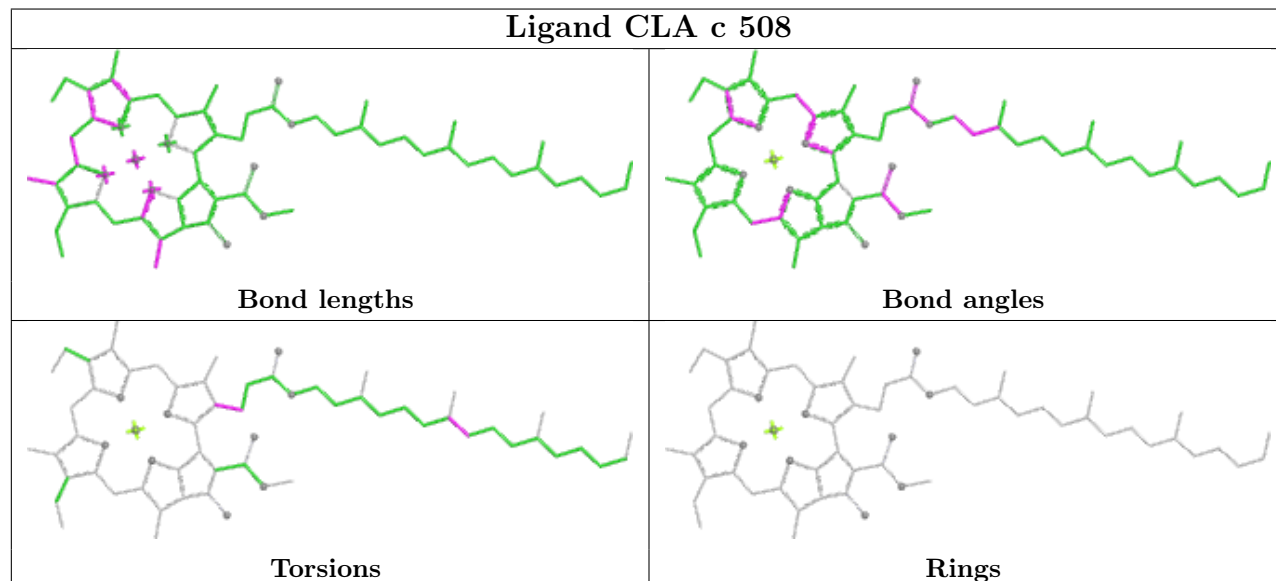
Ligand STE a 616



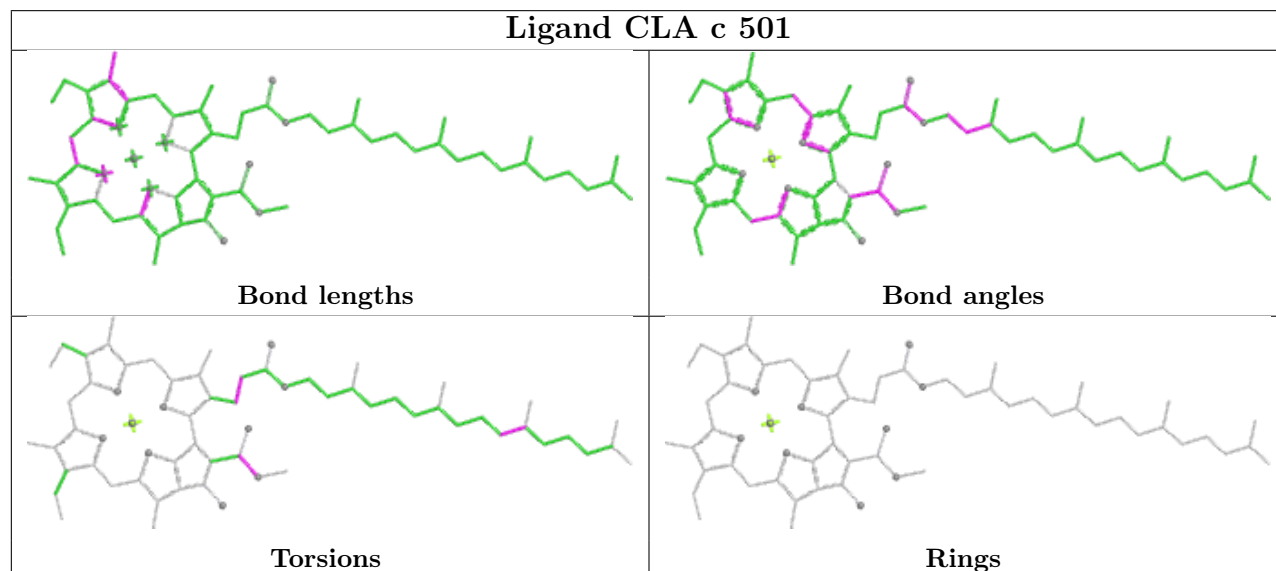
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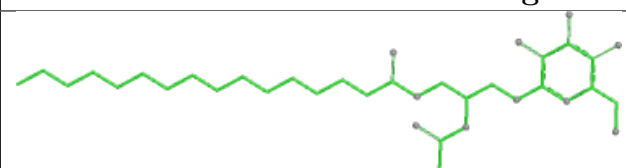
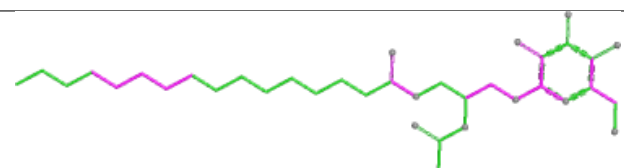
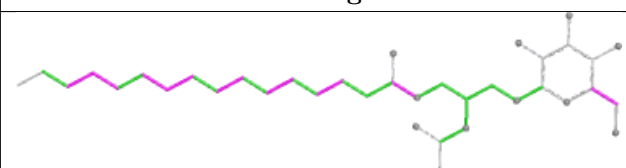
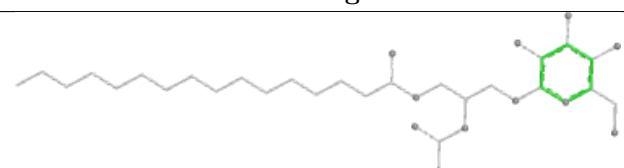


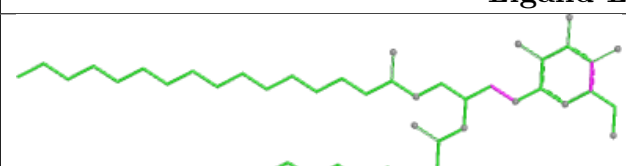
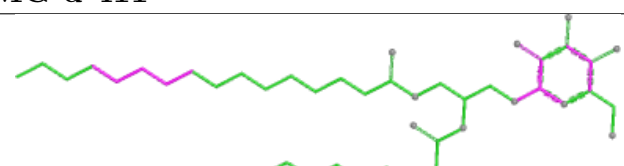
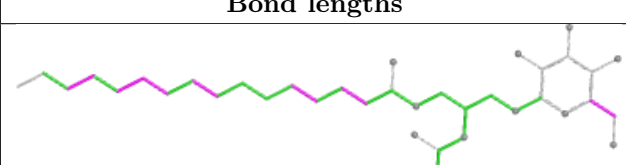
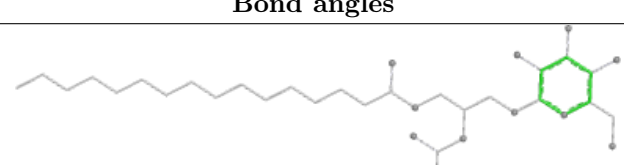
Ligand CLA c 508



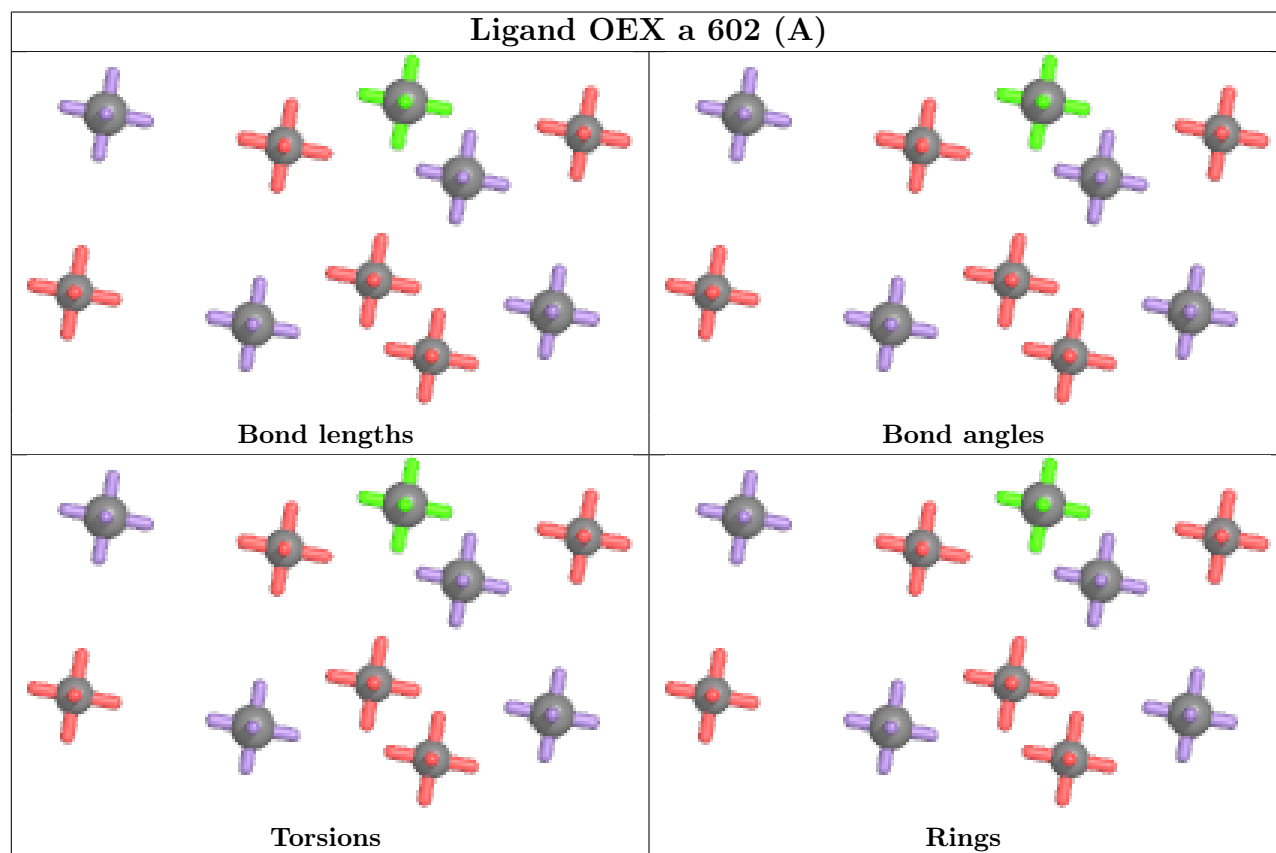
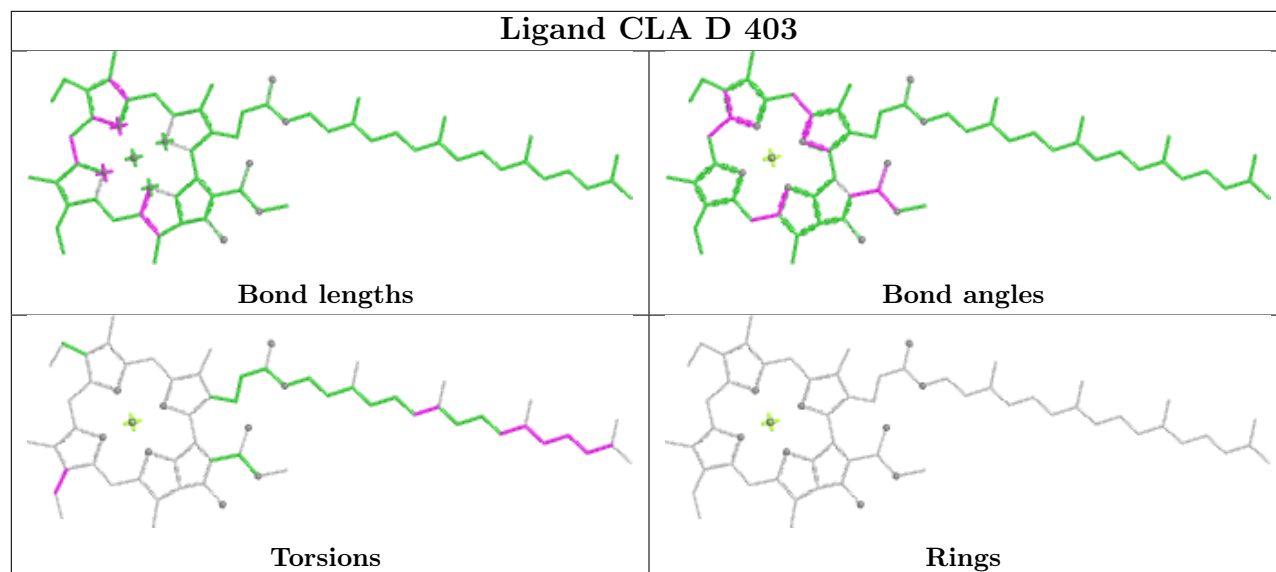
Ligand CLA c 501



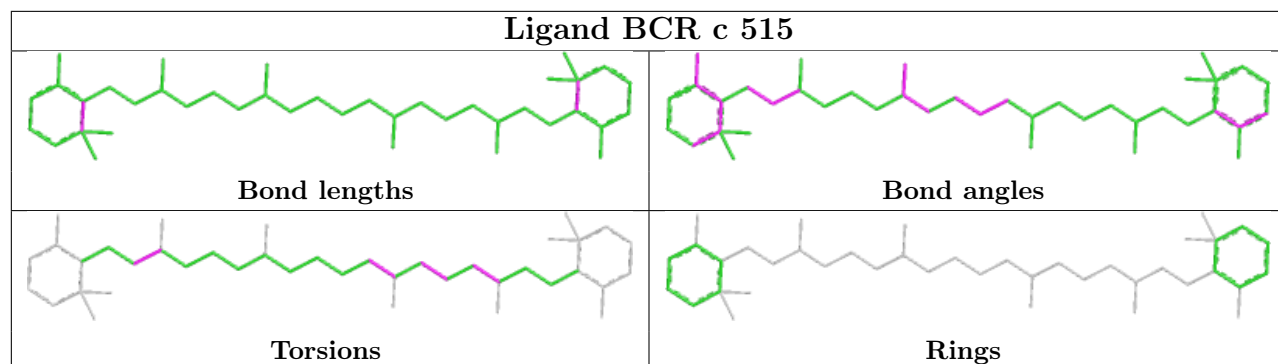
Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

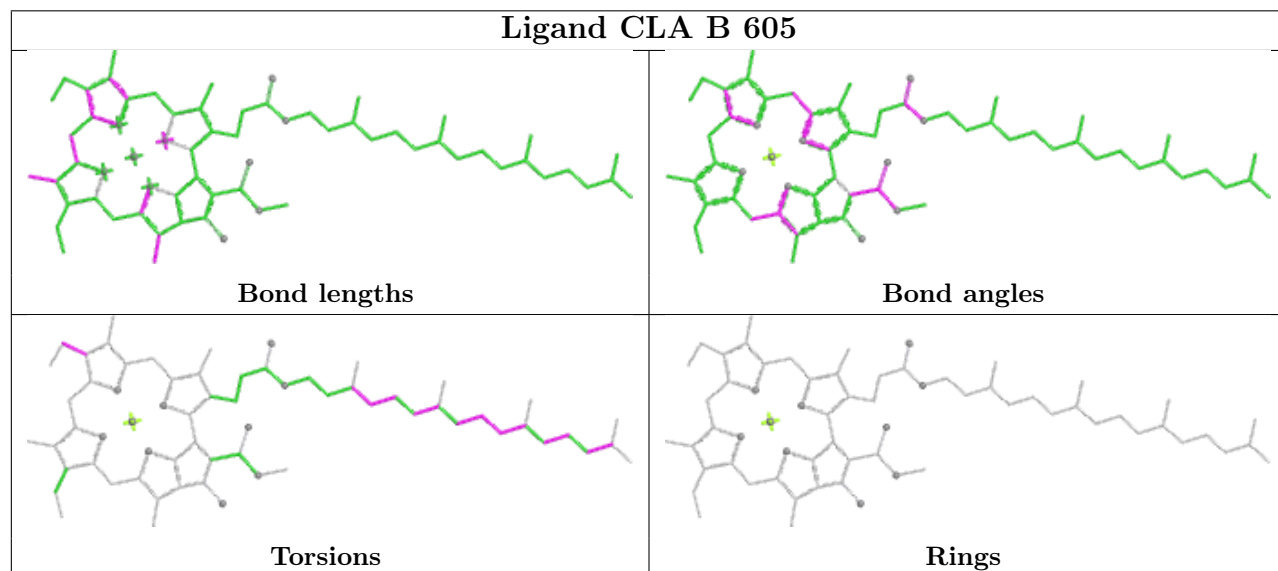
Ligand SQD A 616	
	
Bond lengths	Bond angles
	
Torsions	Rings



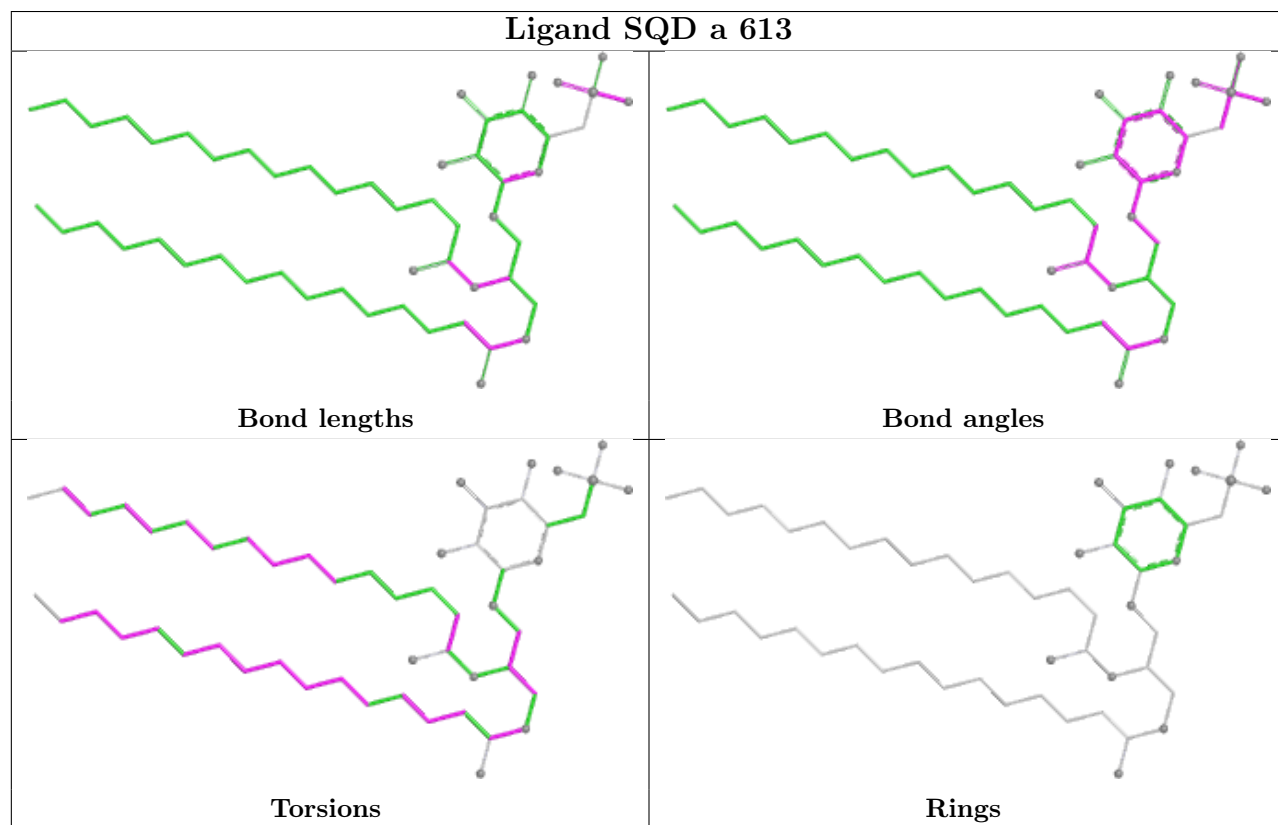
Ligand BCR c 515

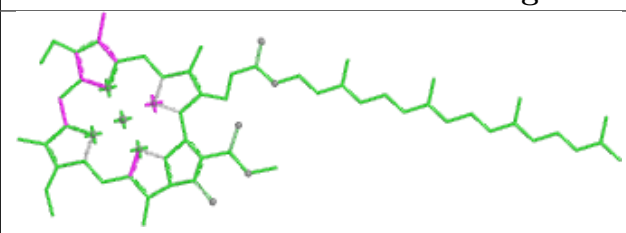
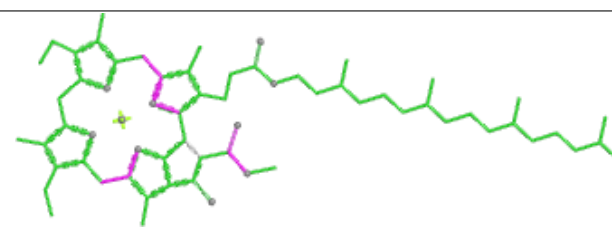
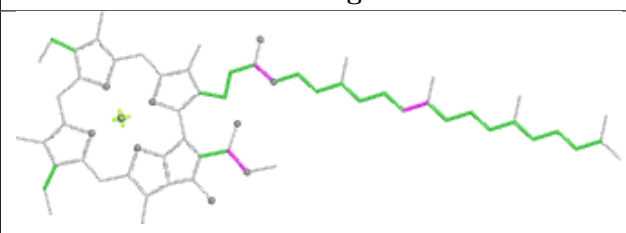
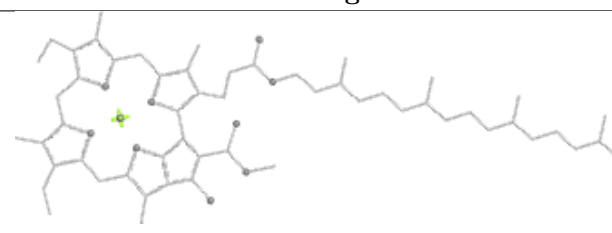


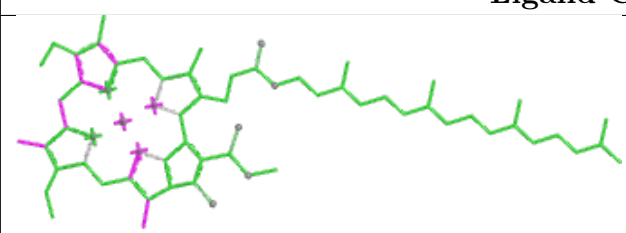
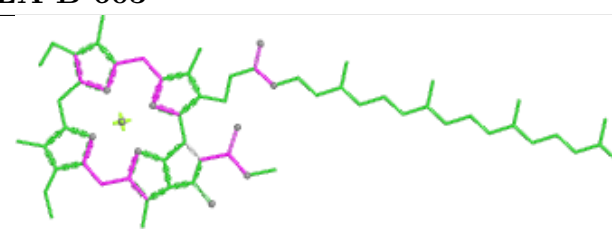
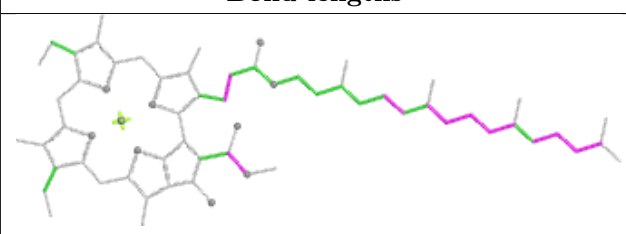
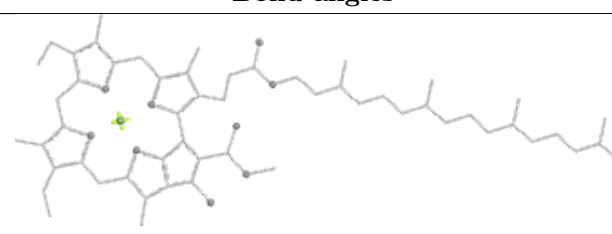
Ligand CLA B 605

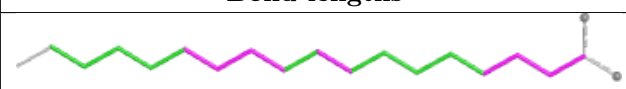
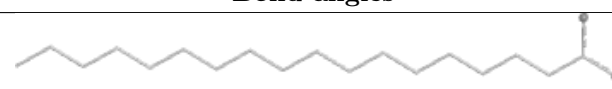


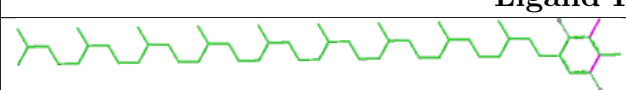
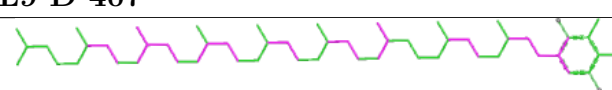
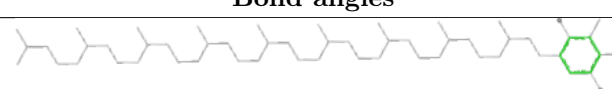
Ligand SQD a 613

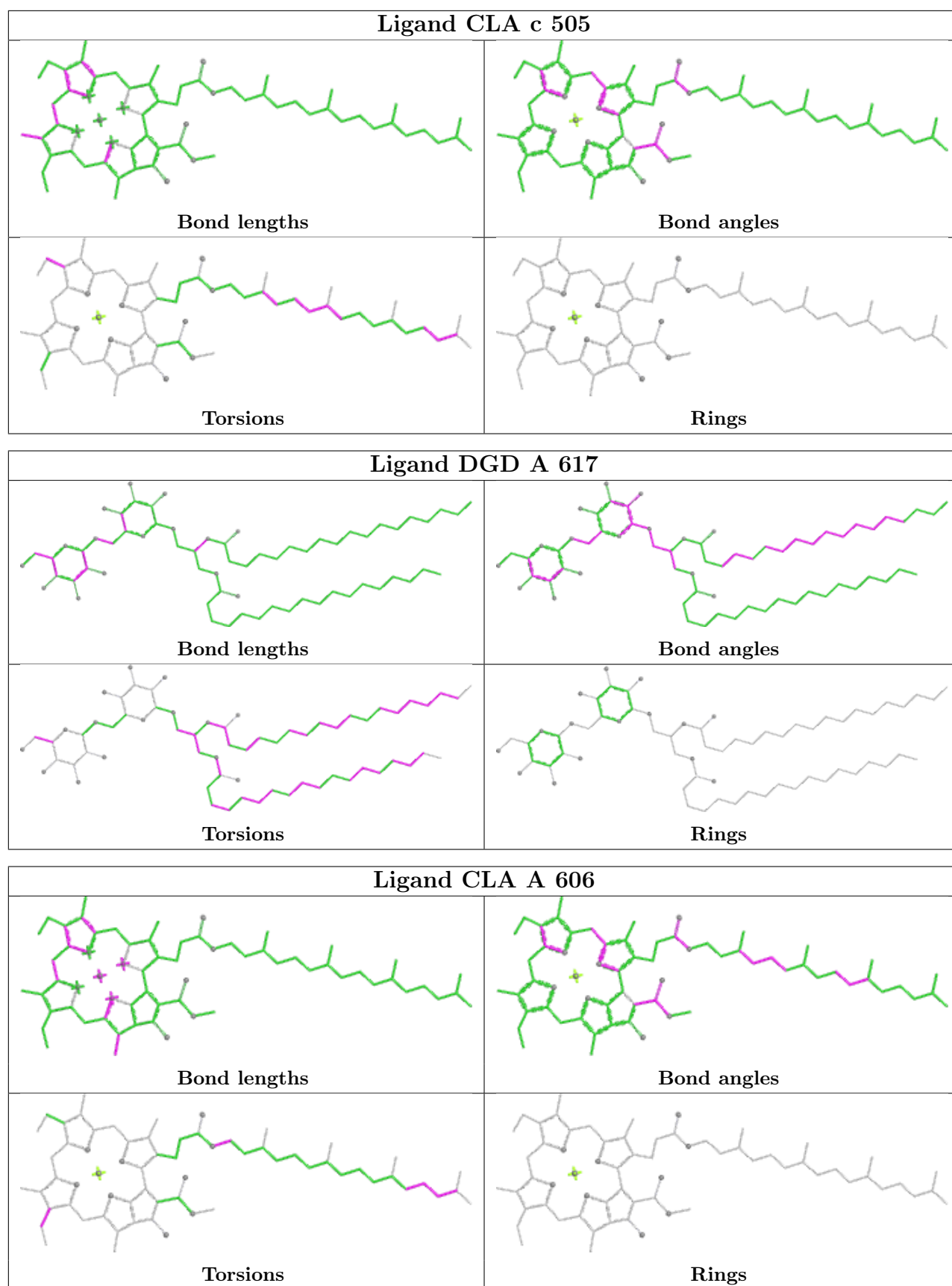


Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

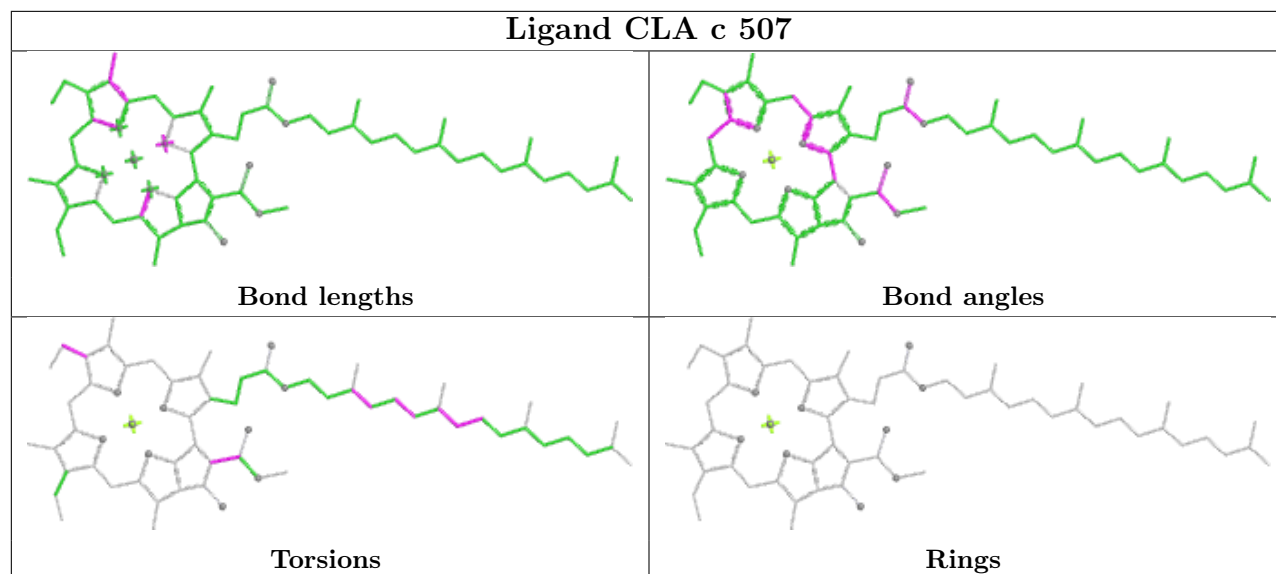
Ligand CLA B 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

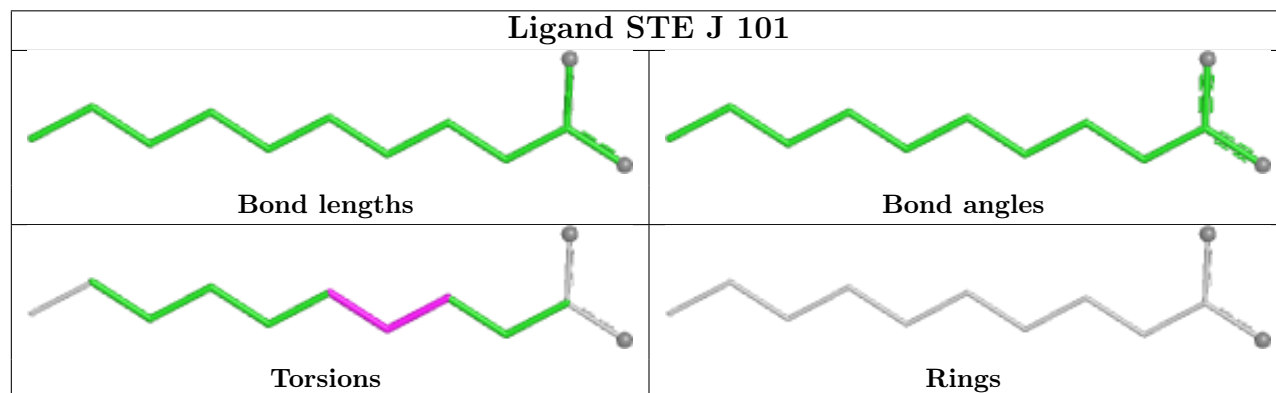
Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



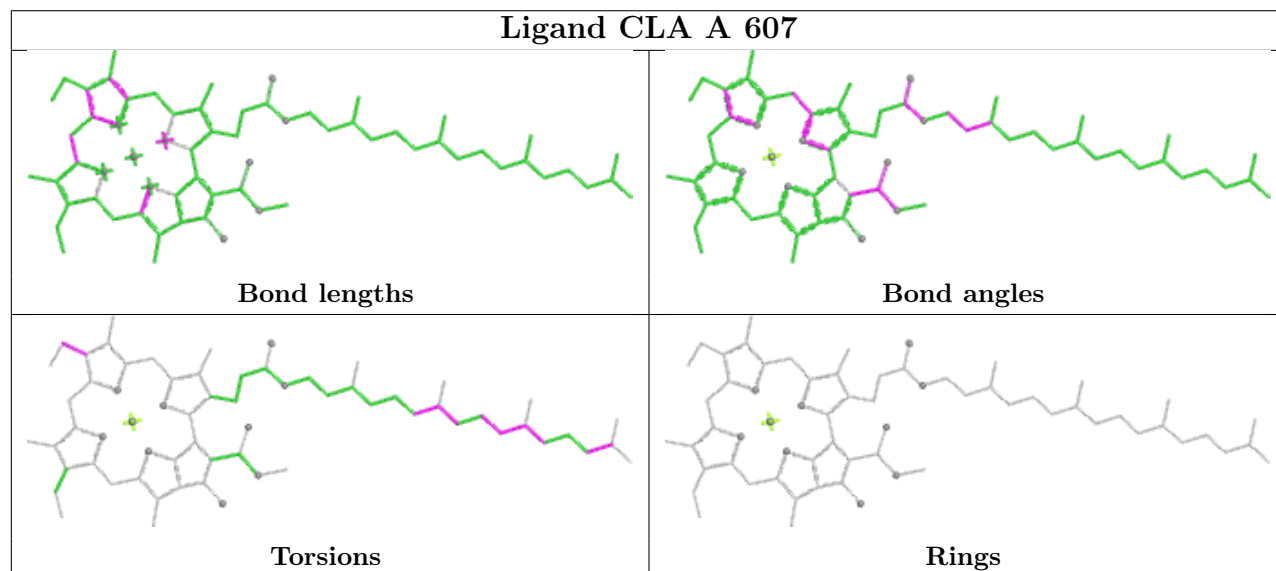
Ligand CLA c 507

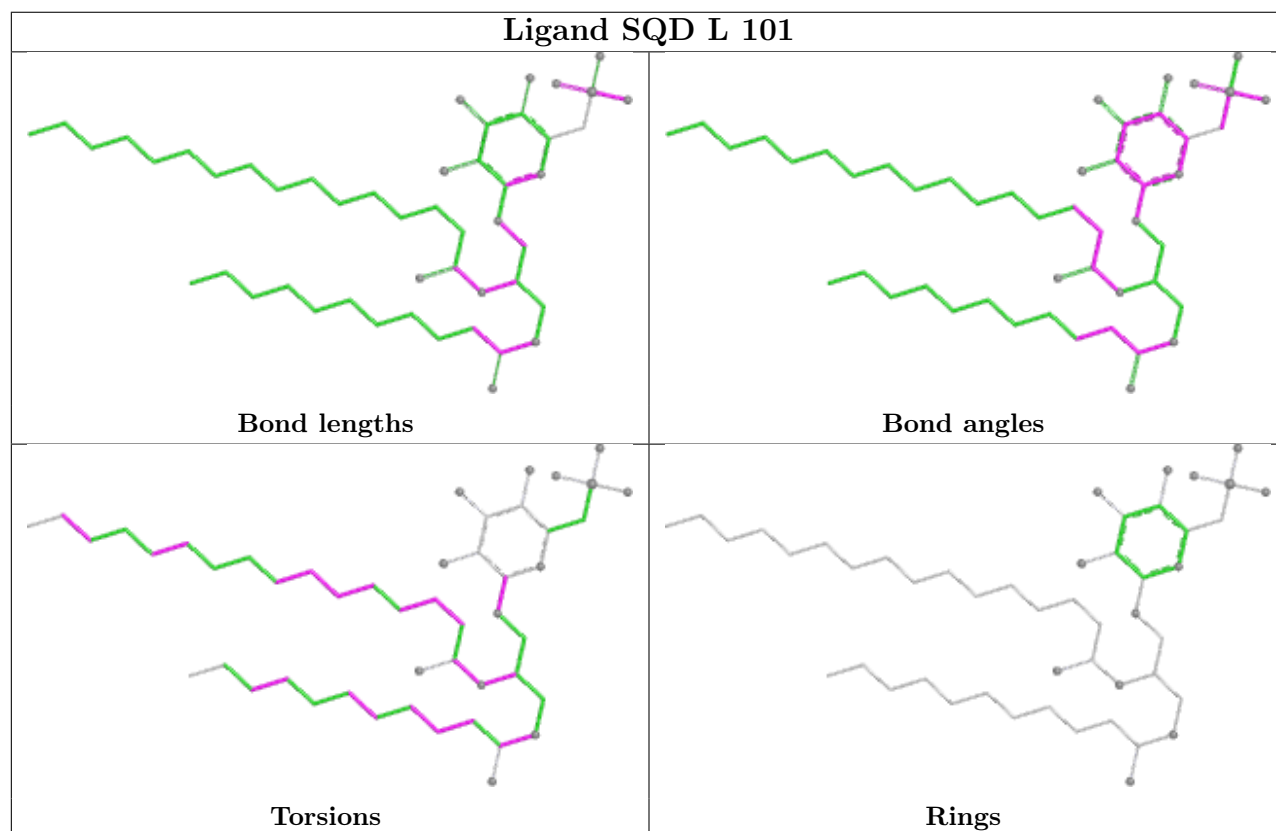
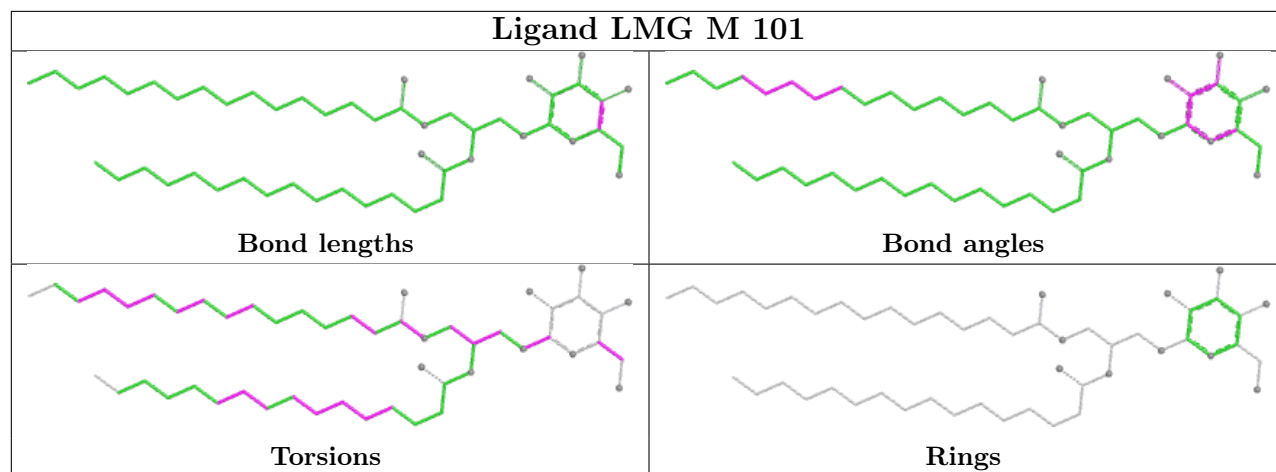


Ligand STE J 101

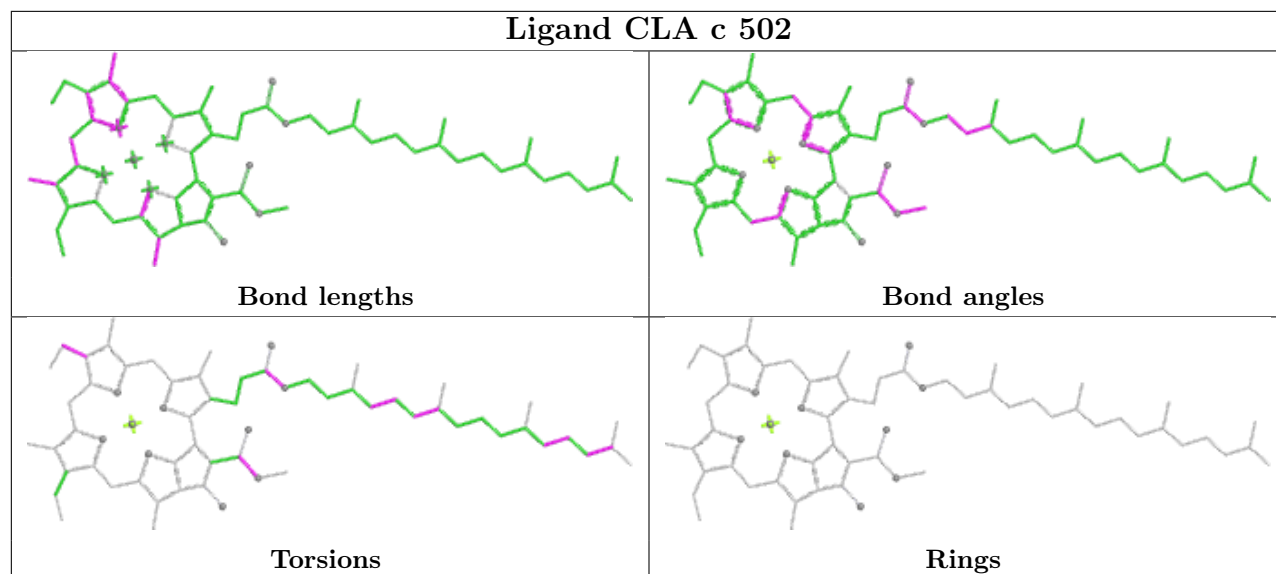


Ligand CLA A 607

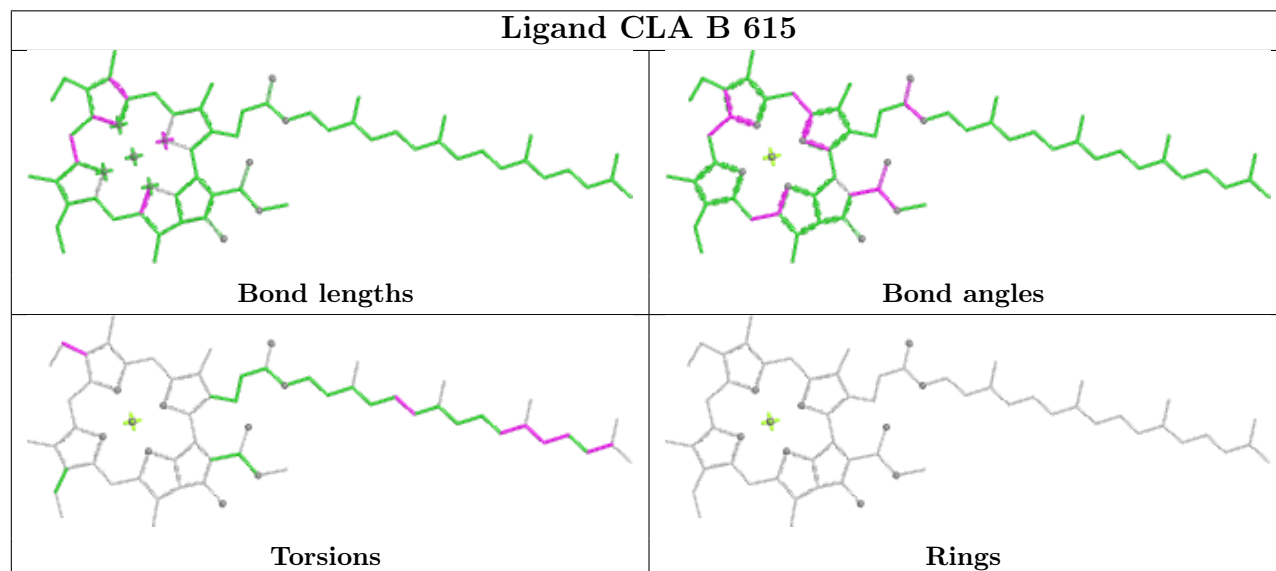




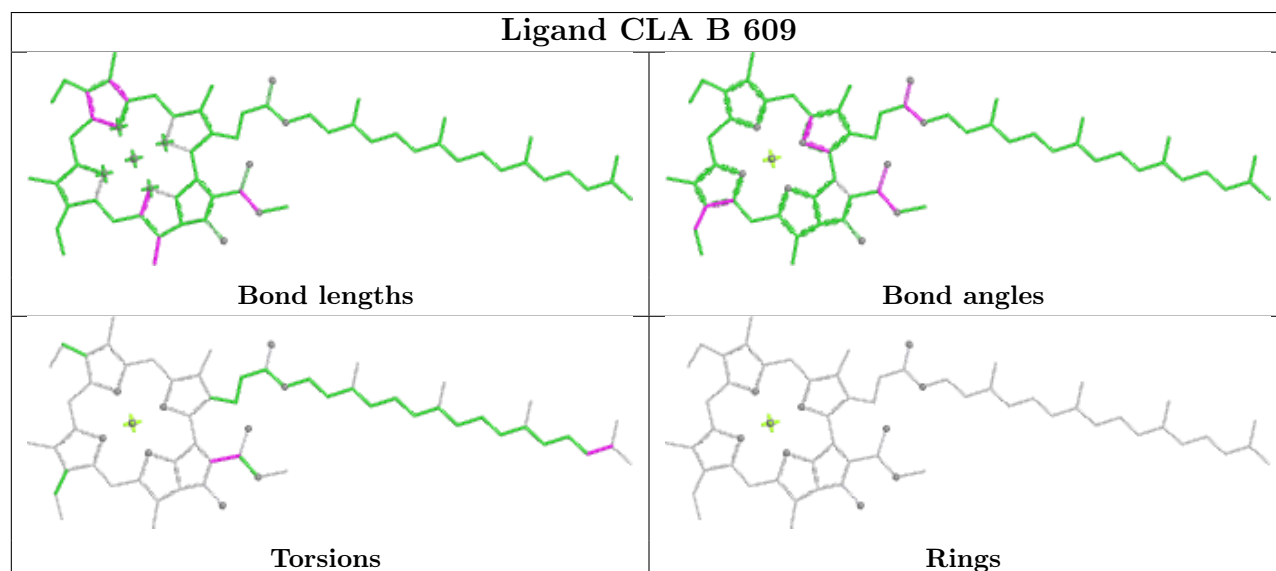
Ligand CLA c 502

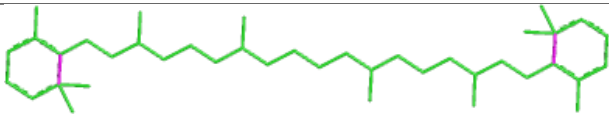
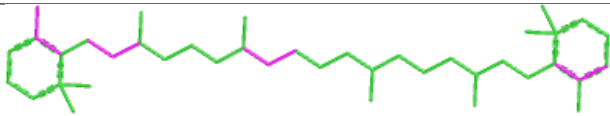
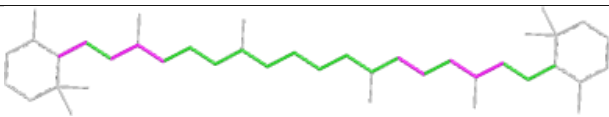
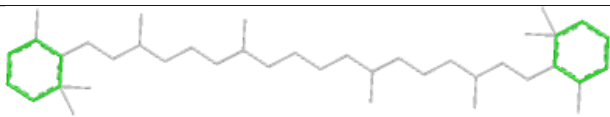


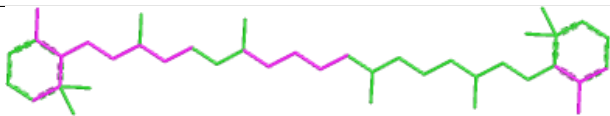
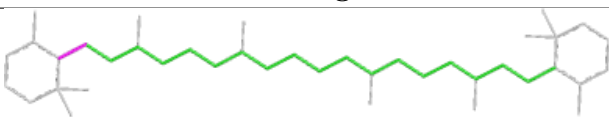
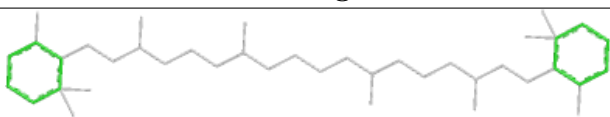
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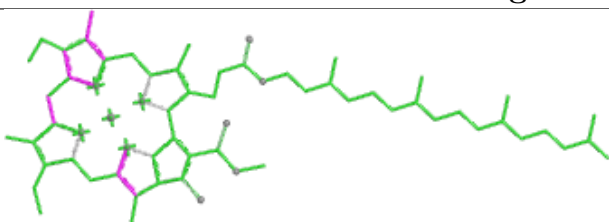
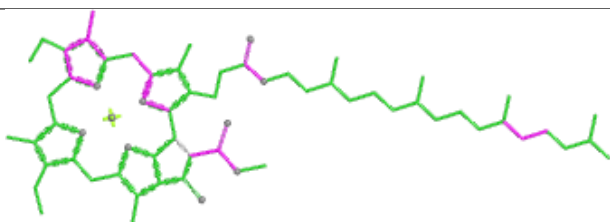
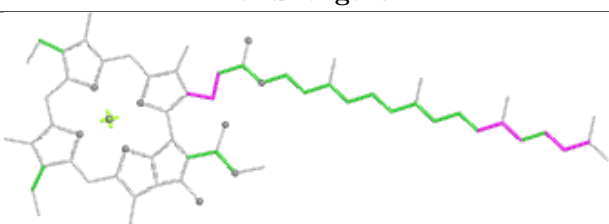
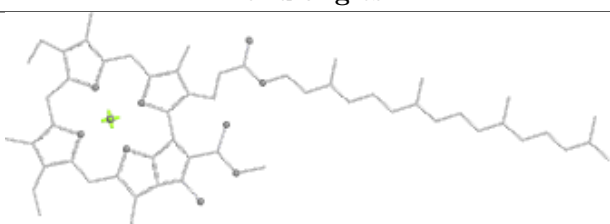


Ligand CLA B 609

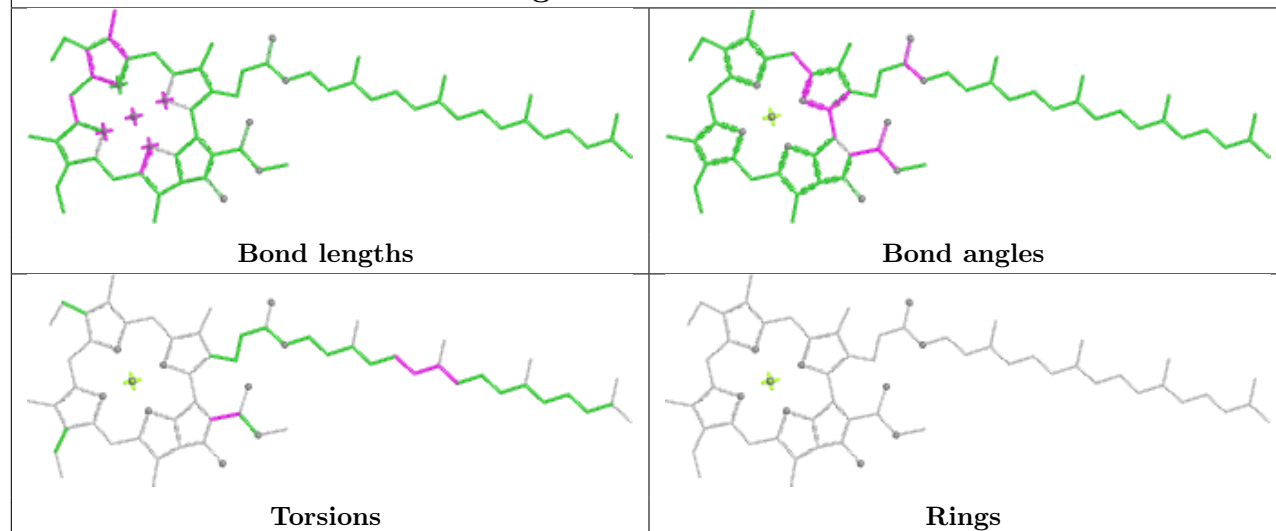


Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

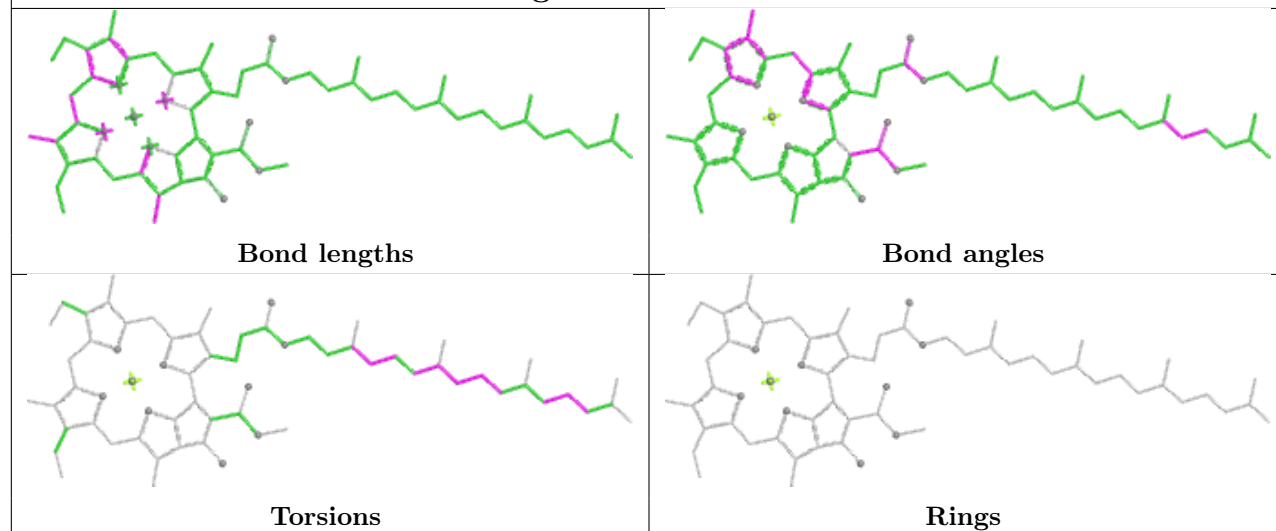
Ligand BCR A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

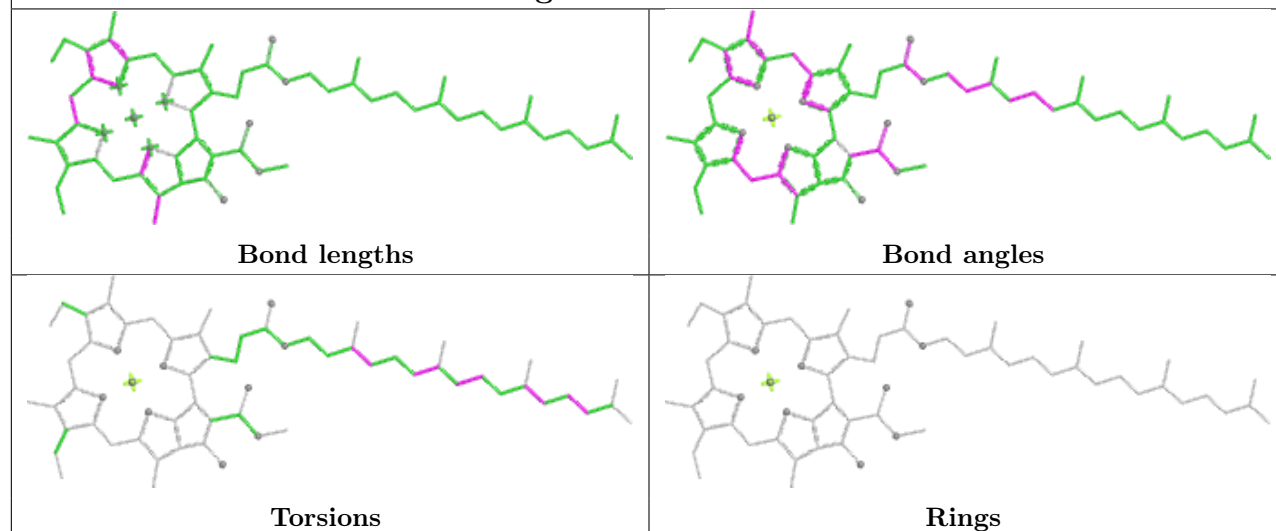
Ligand CLA C 507



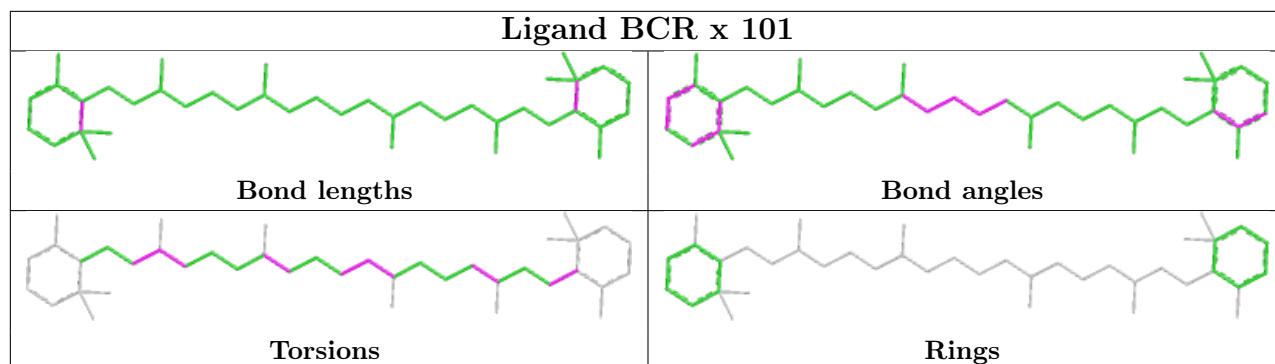
Ligand CLA C 510



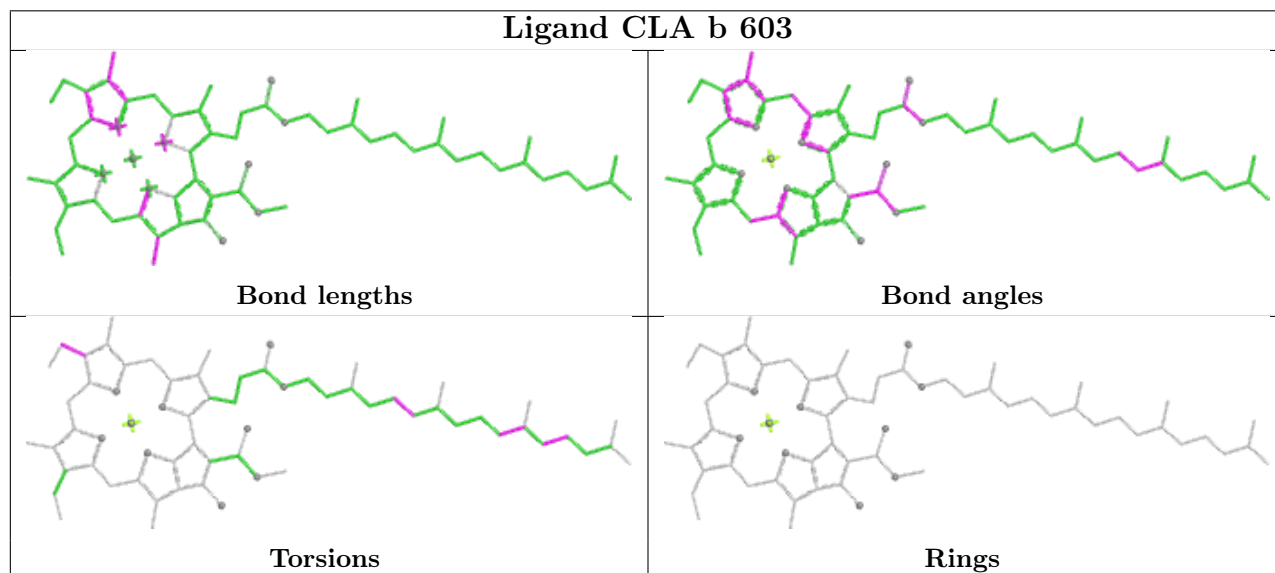
Ligand CLA b 605



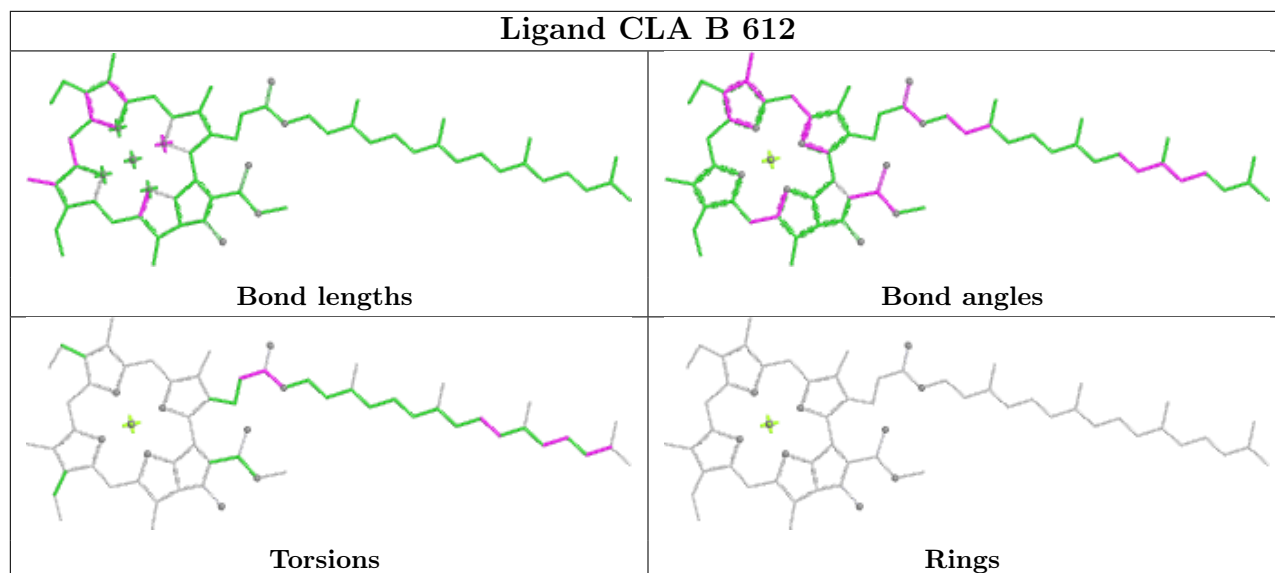
Ligand BCR x 101



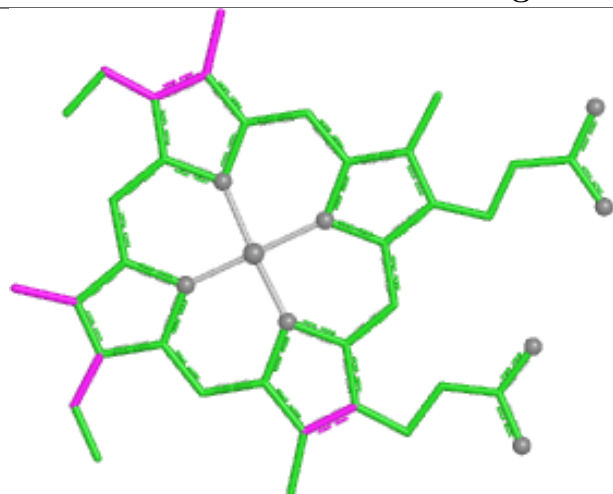
Ligand CLA b 603



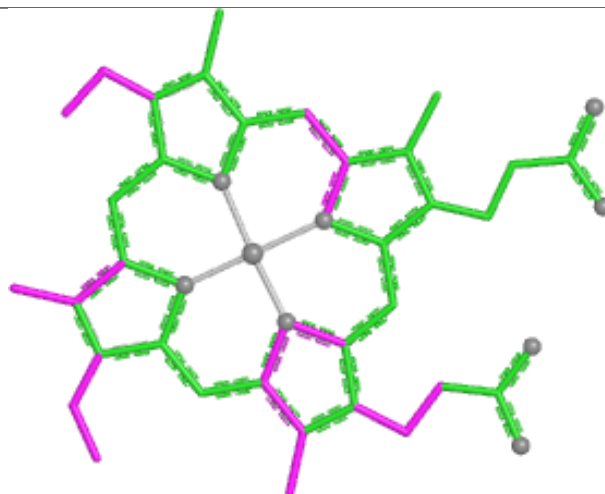
Ligand CLA B 612



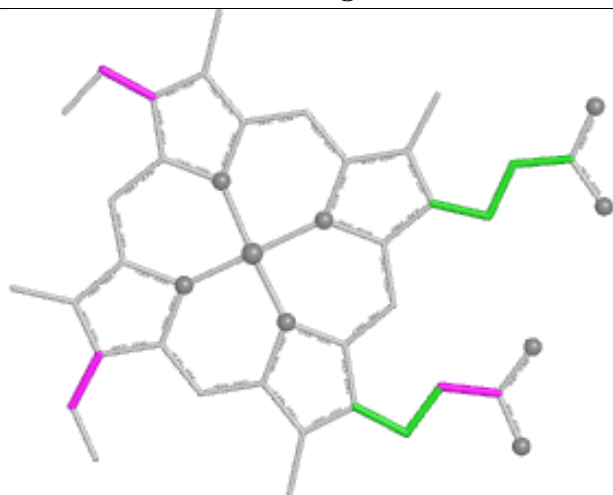
Ligand HEC V 201



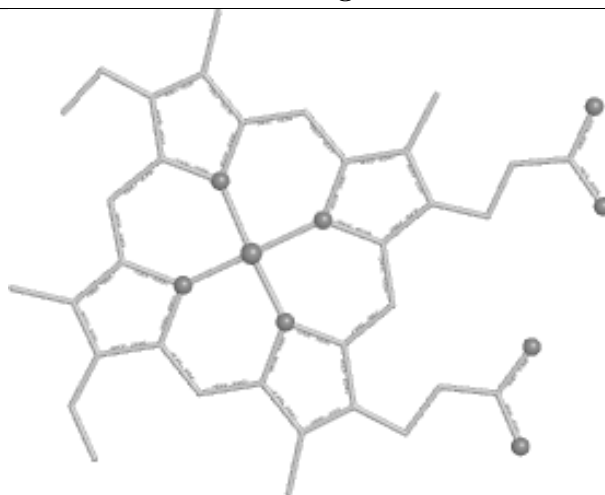
Bond lengths



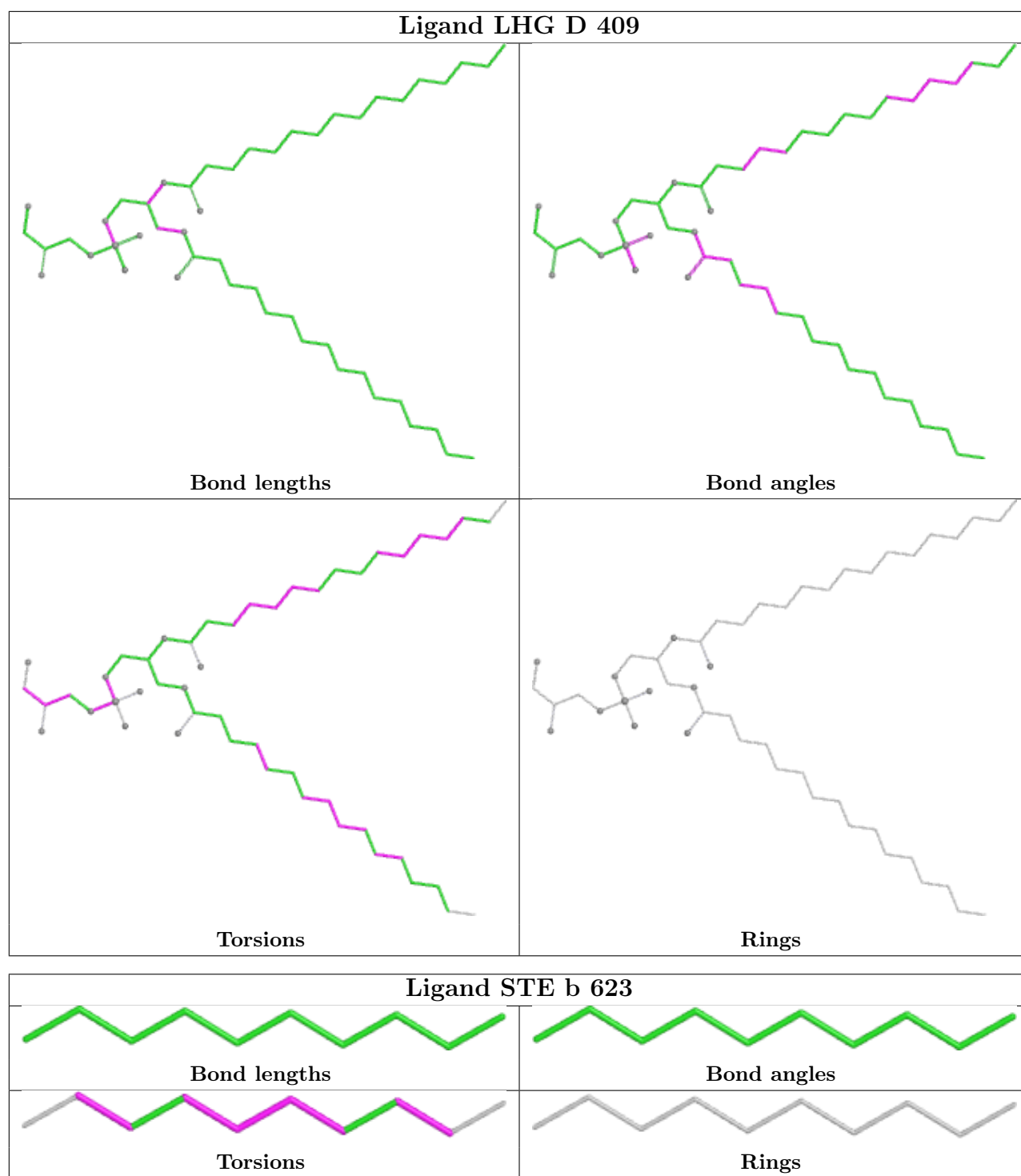
Bond angles

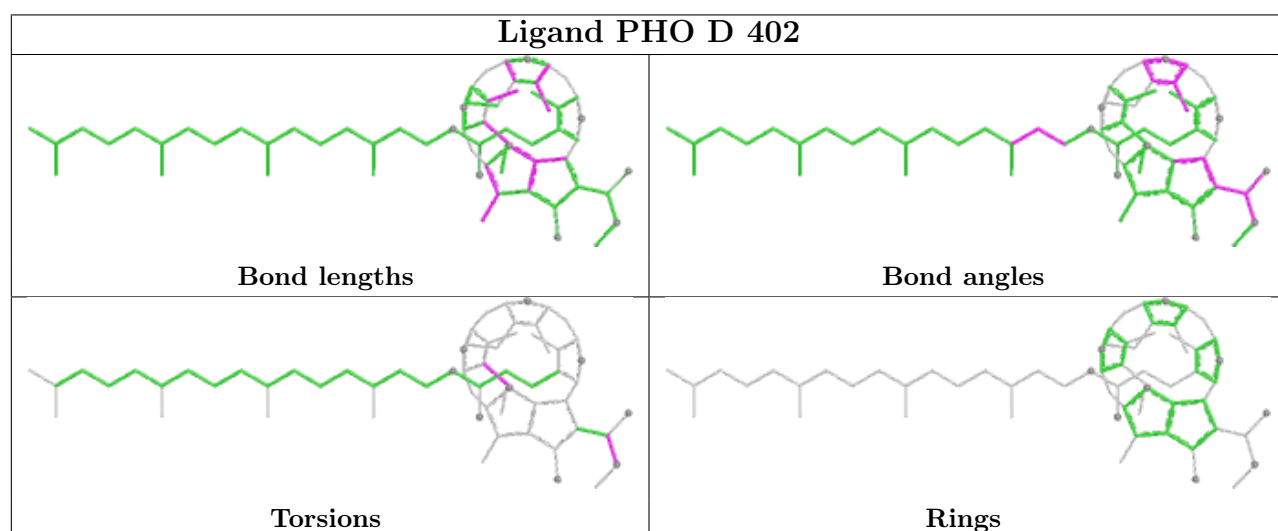
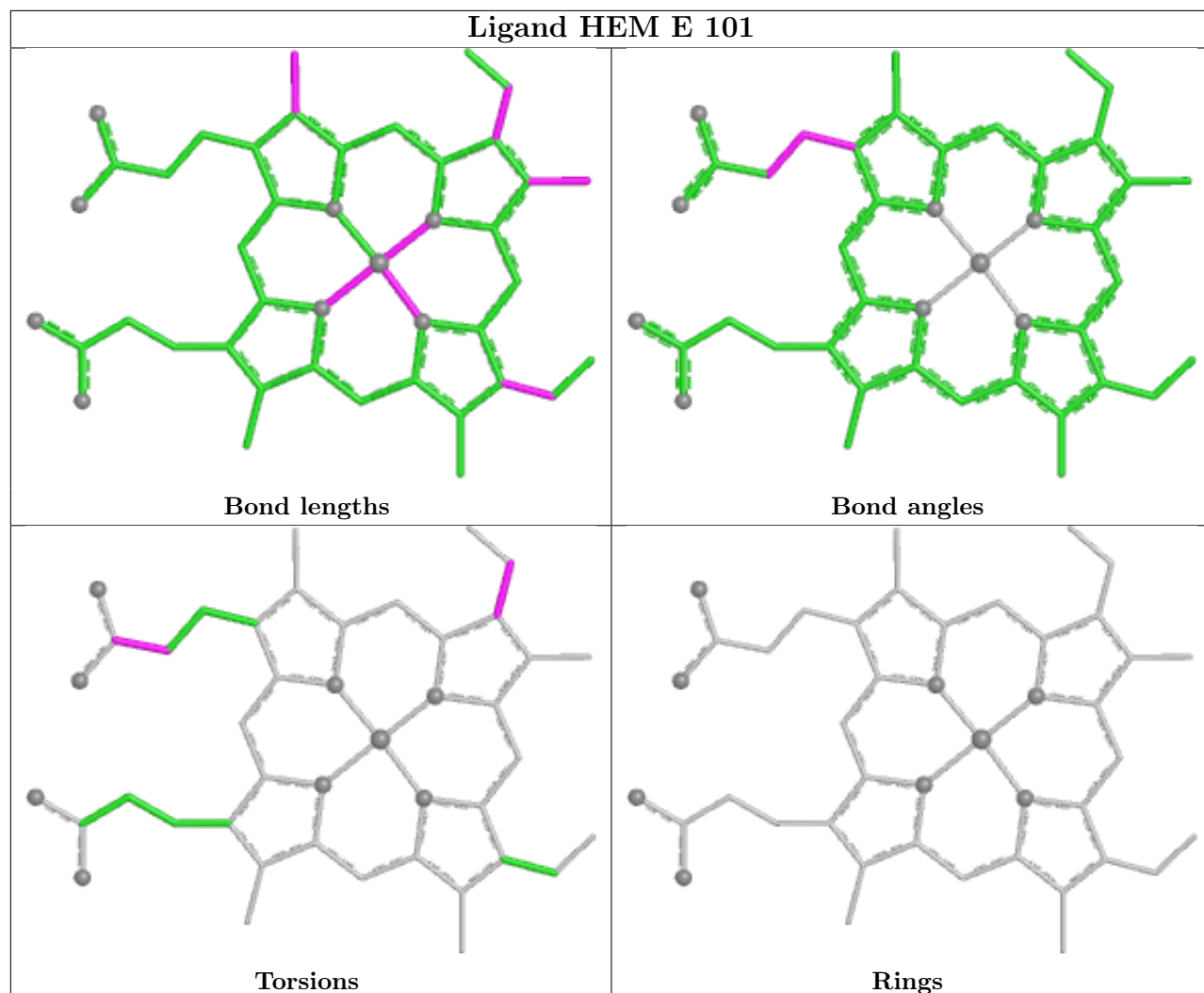


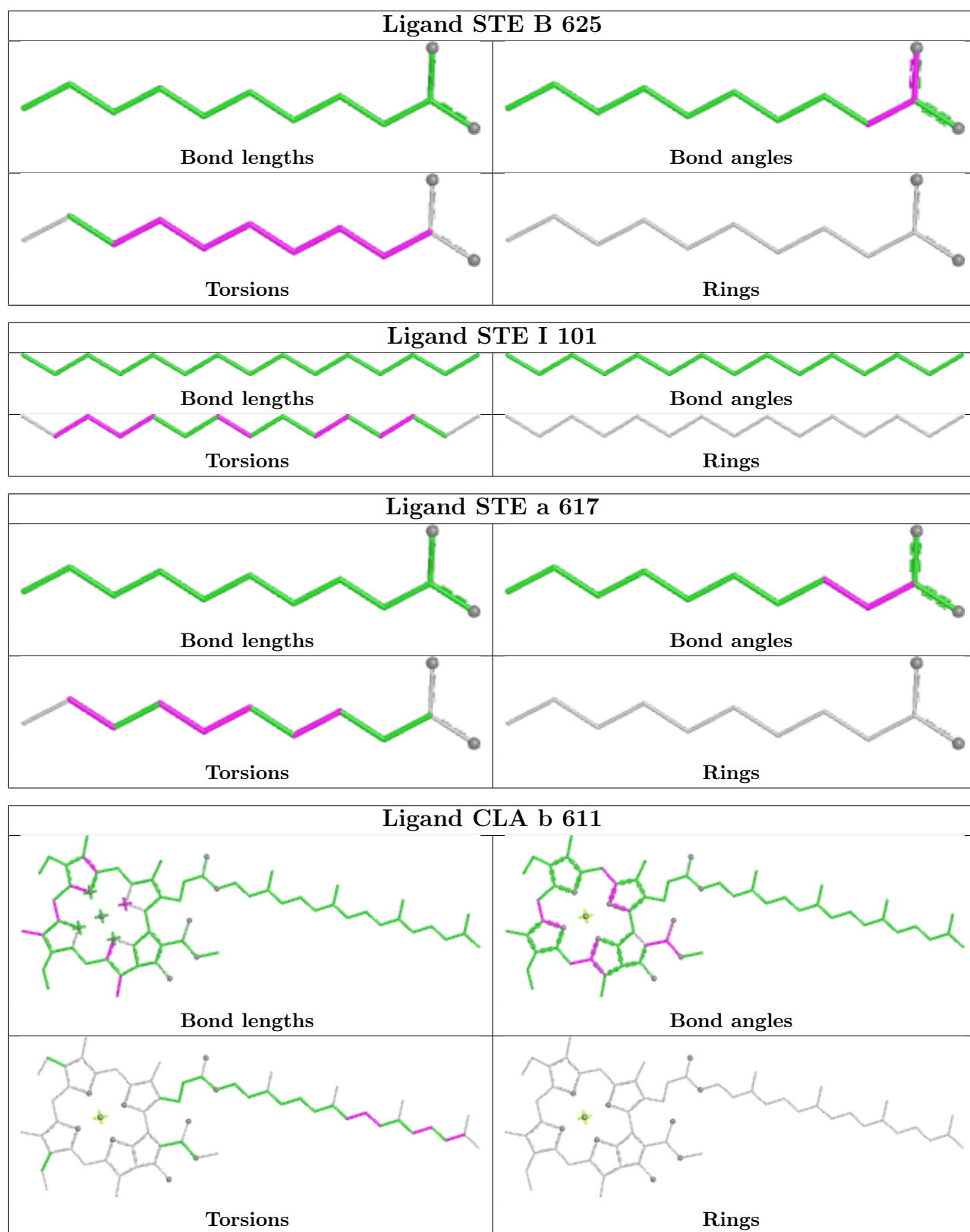
Torsions

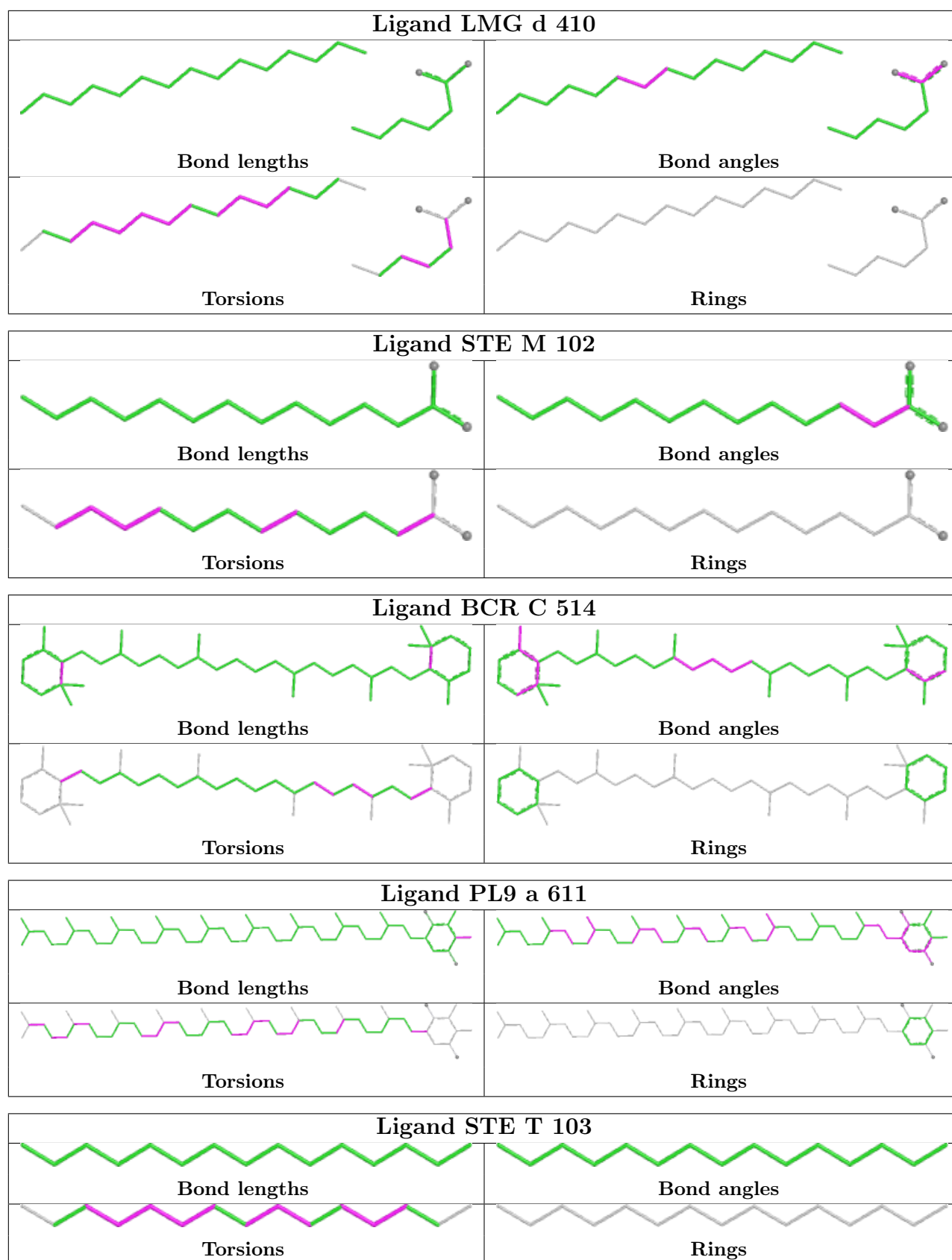


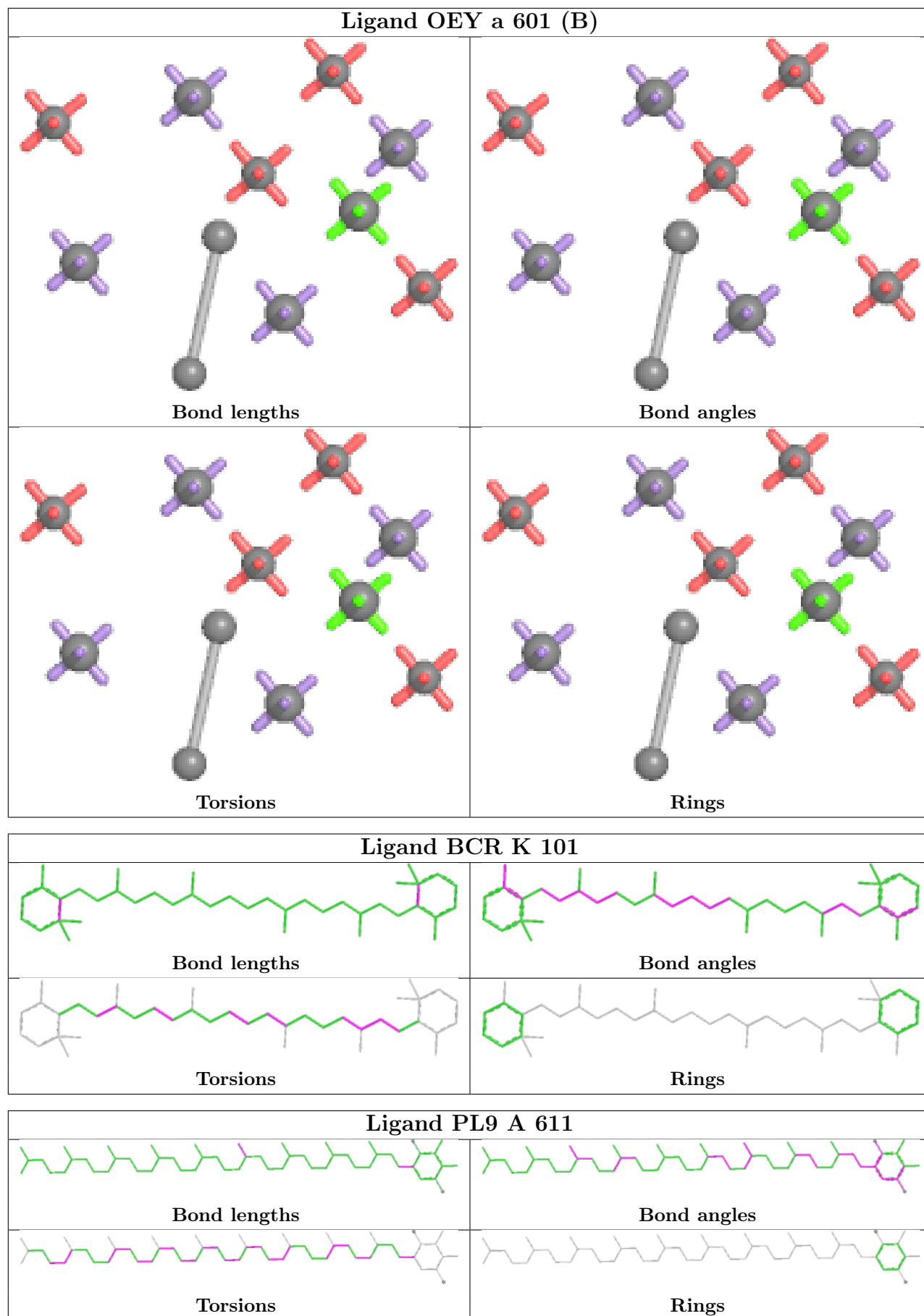
Rings

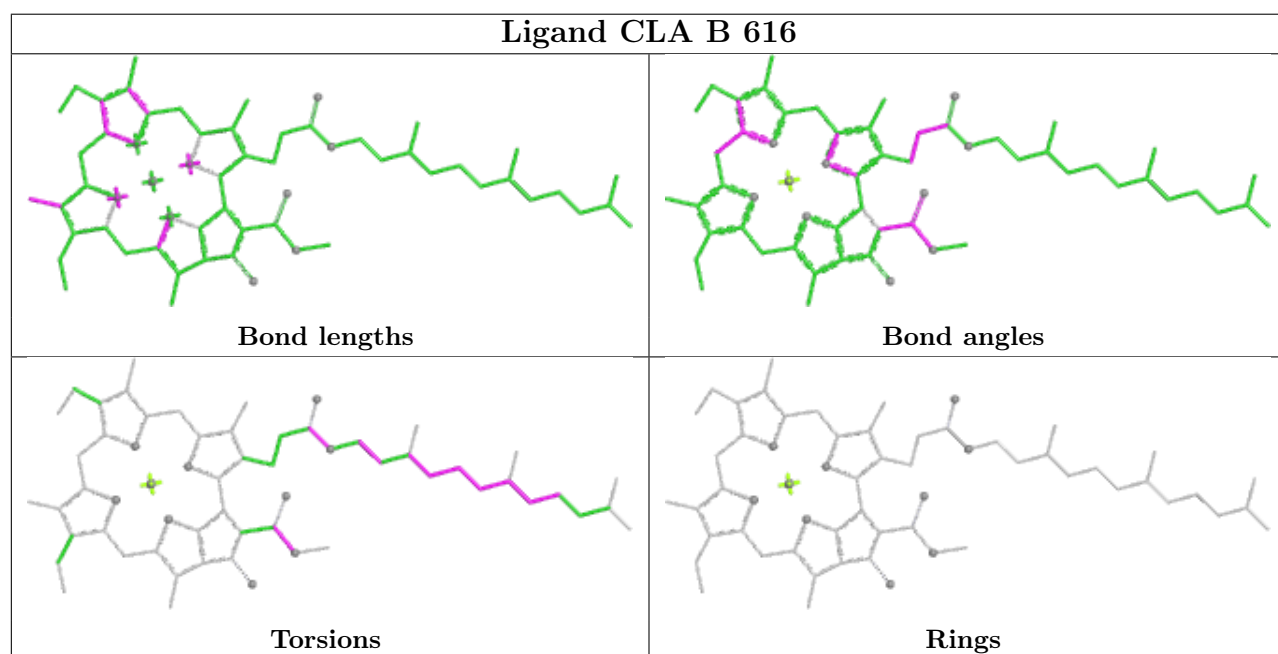
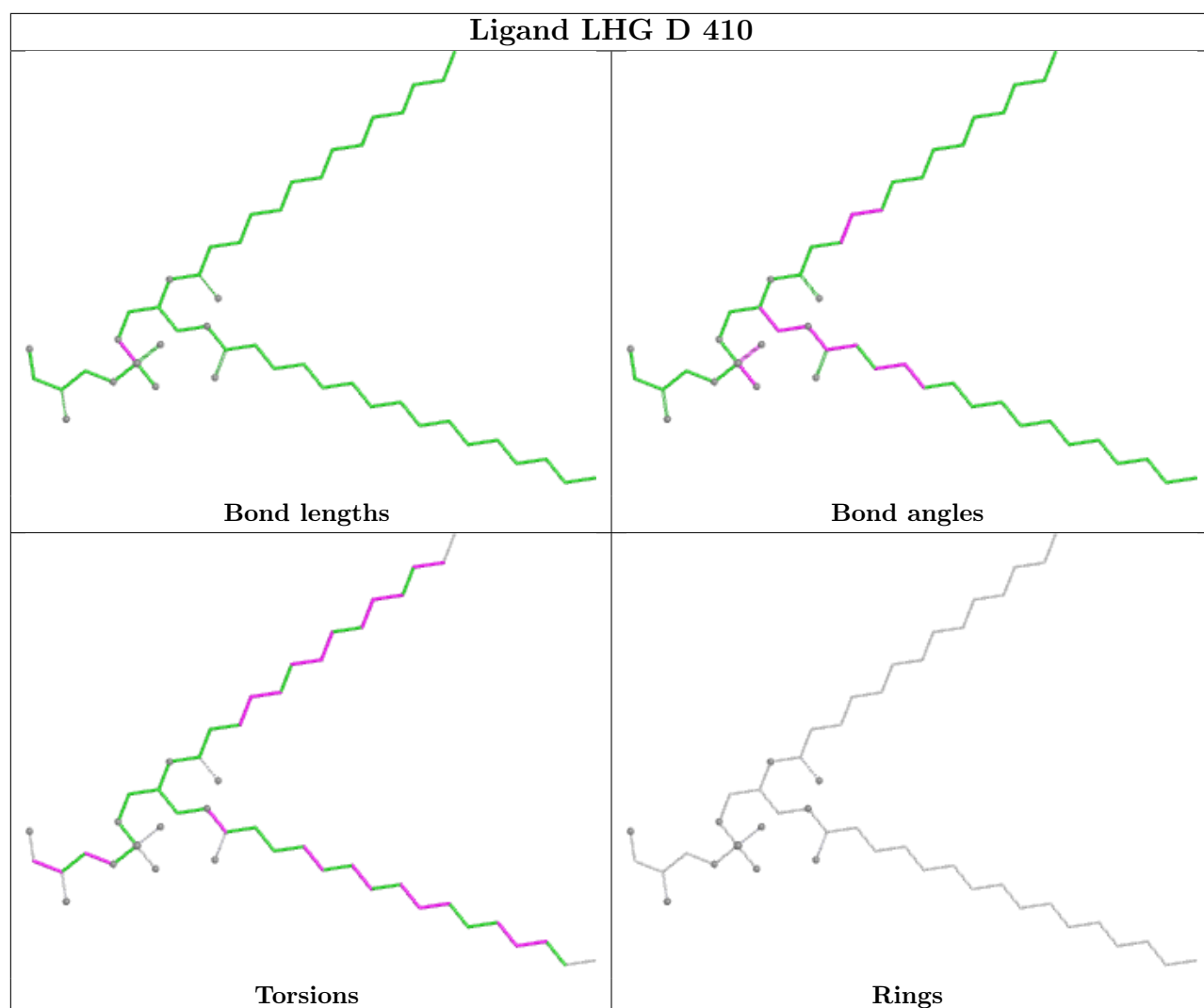


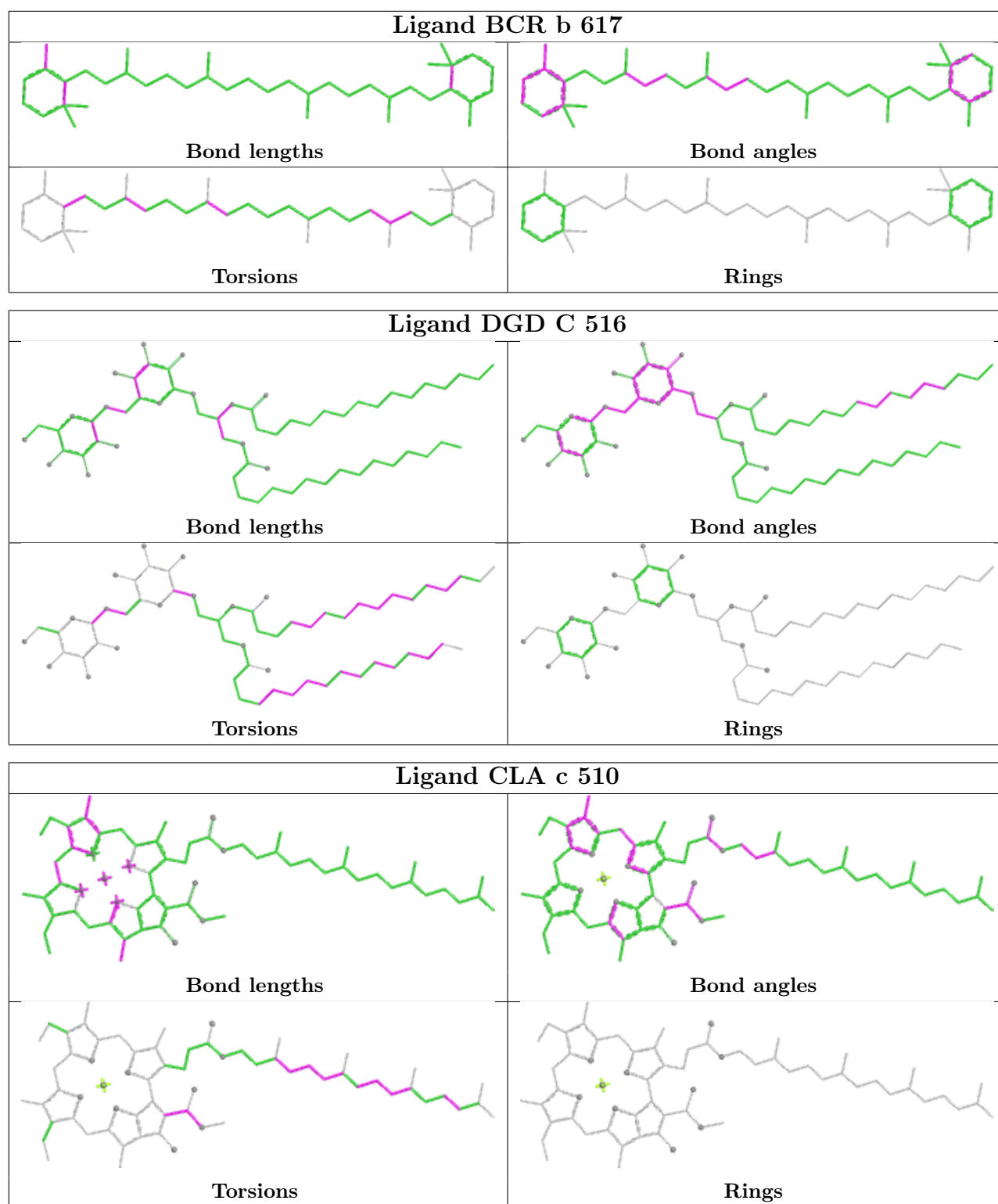


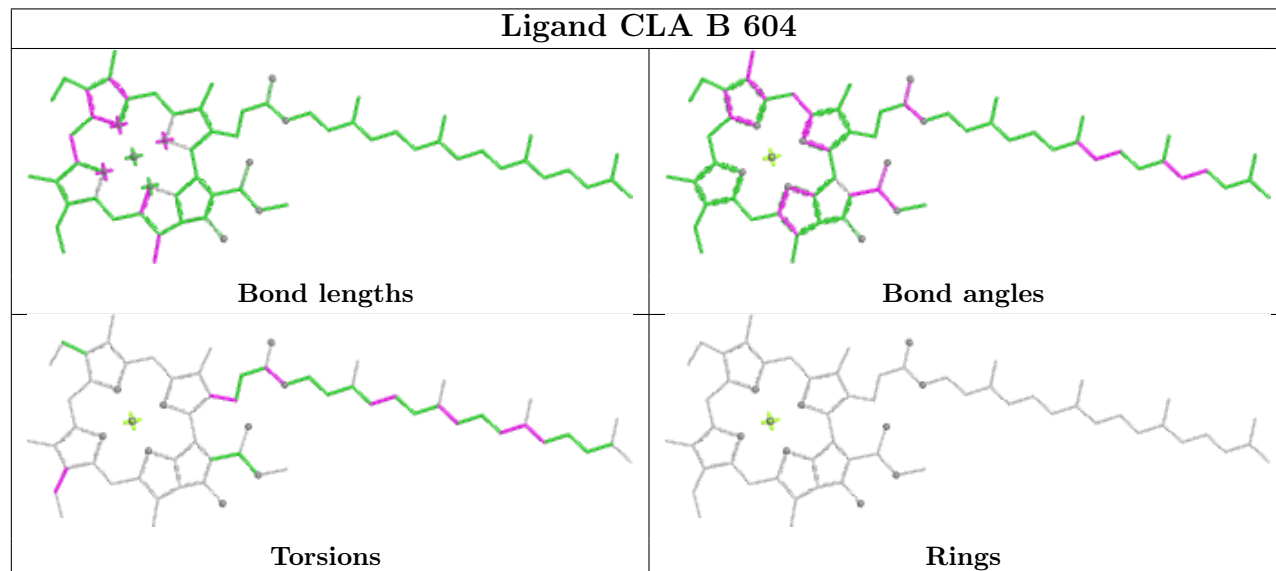
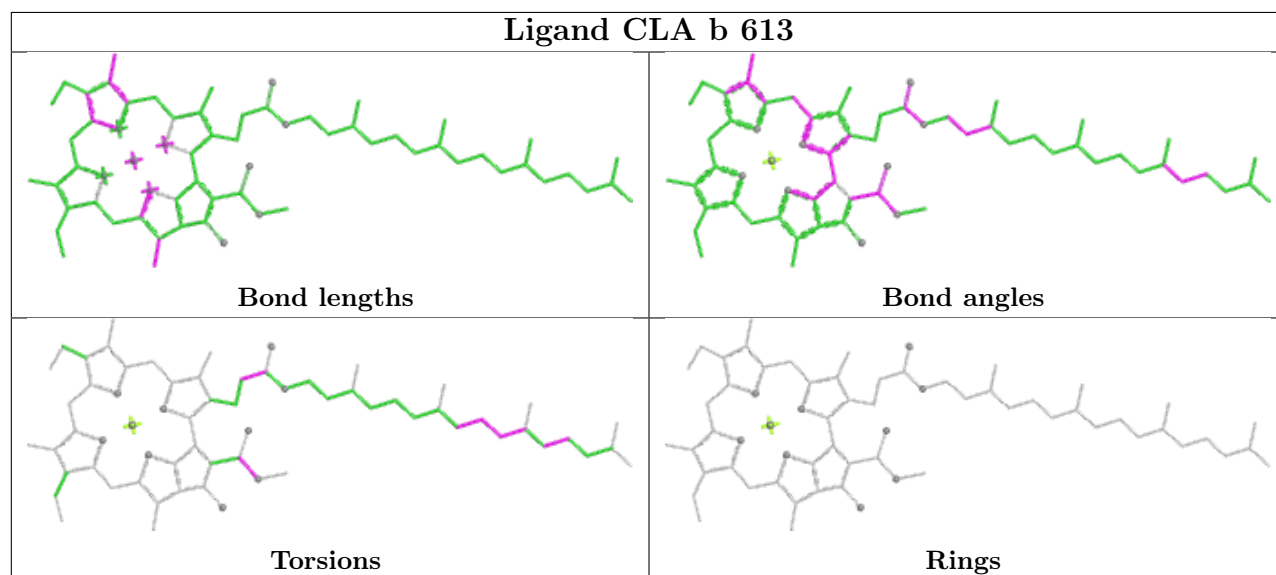
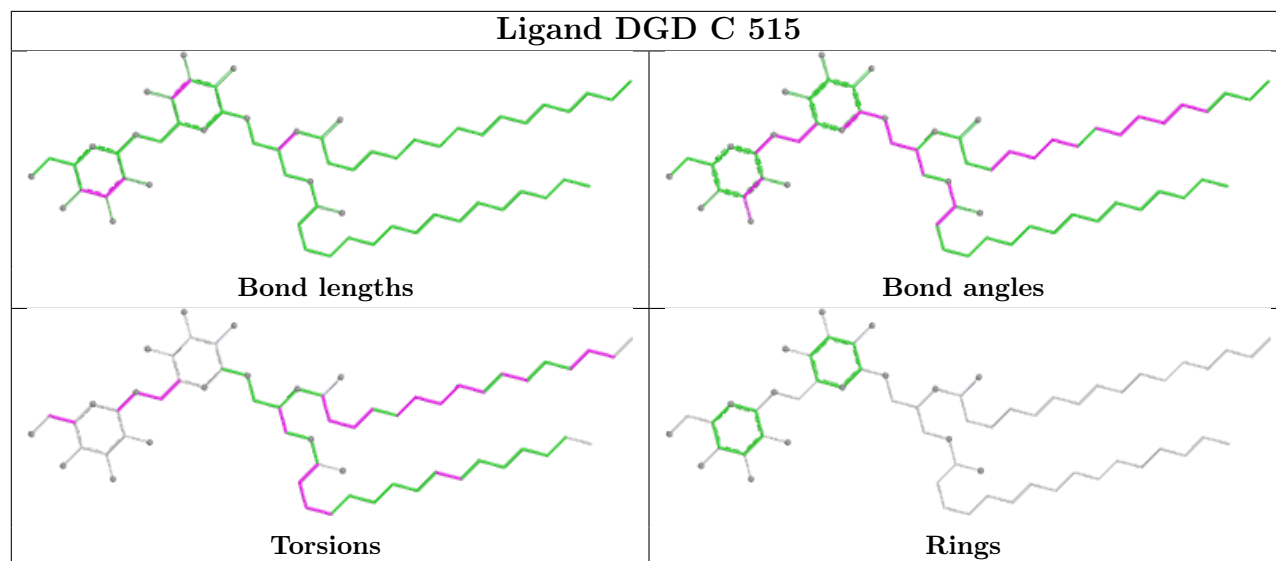


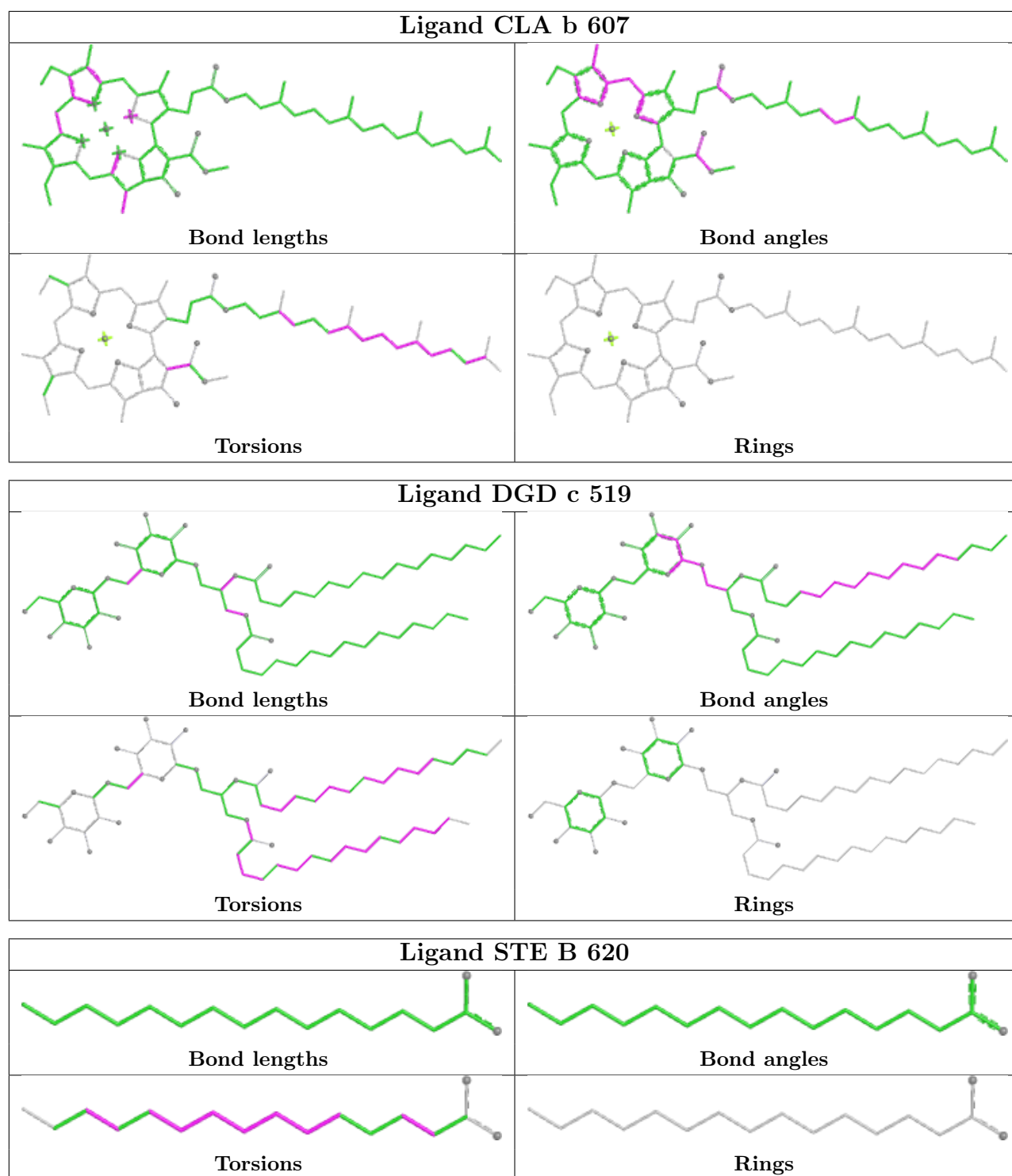


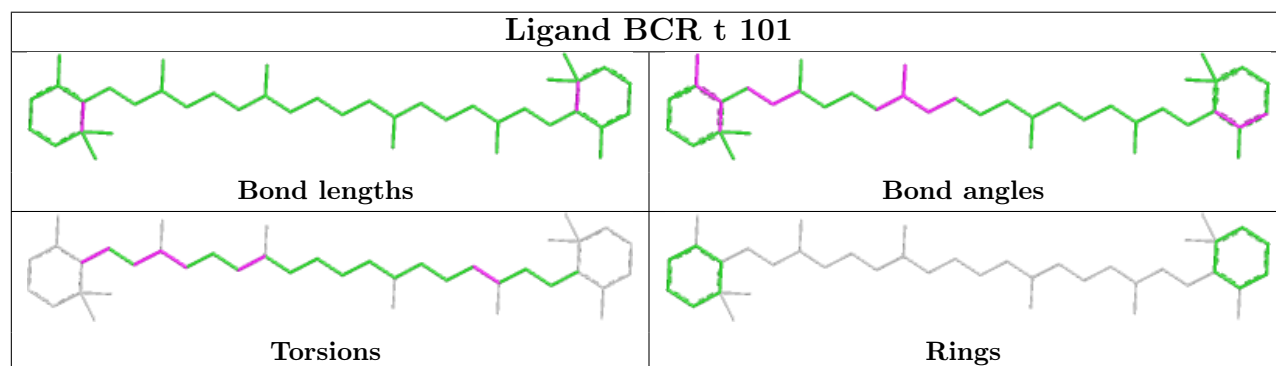
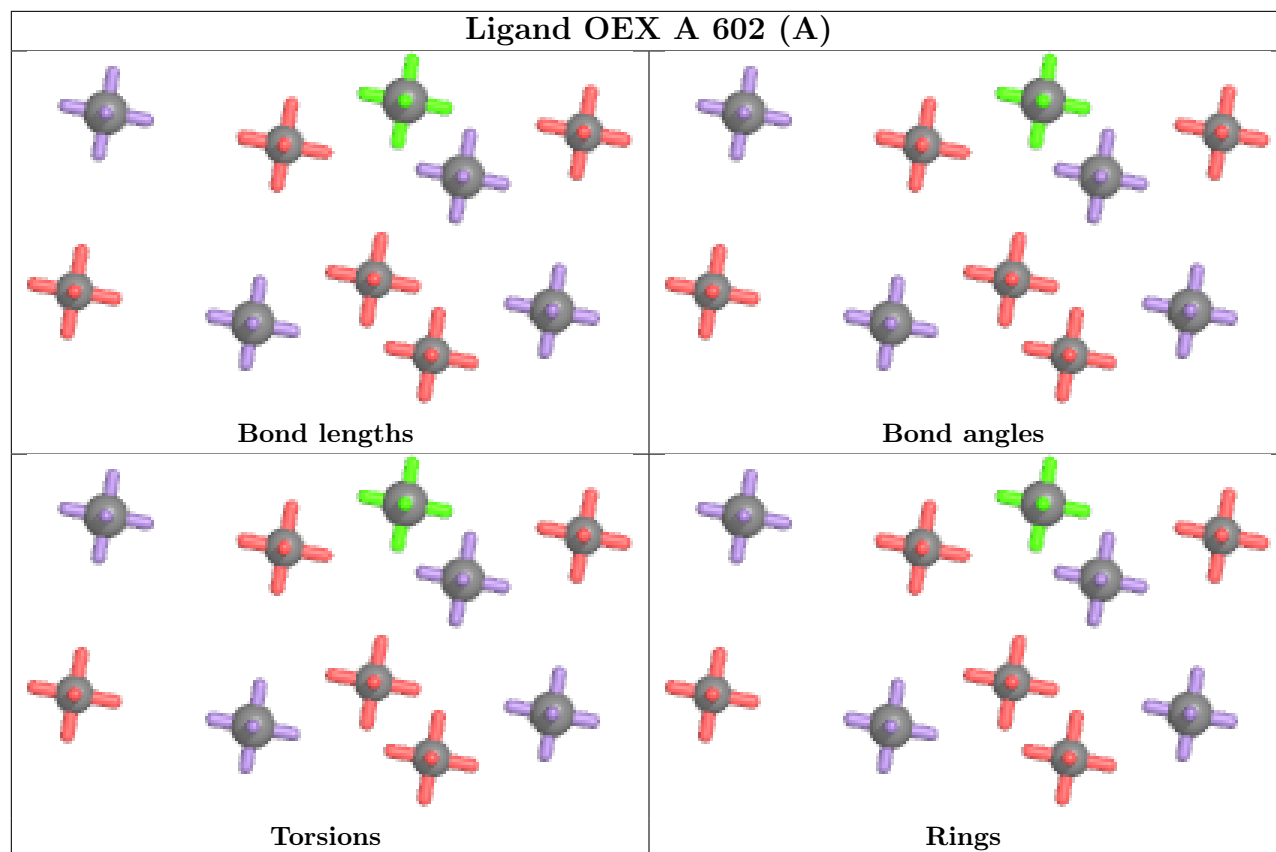




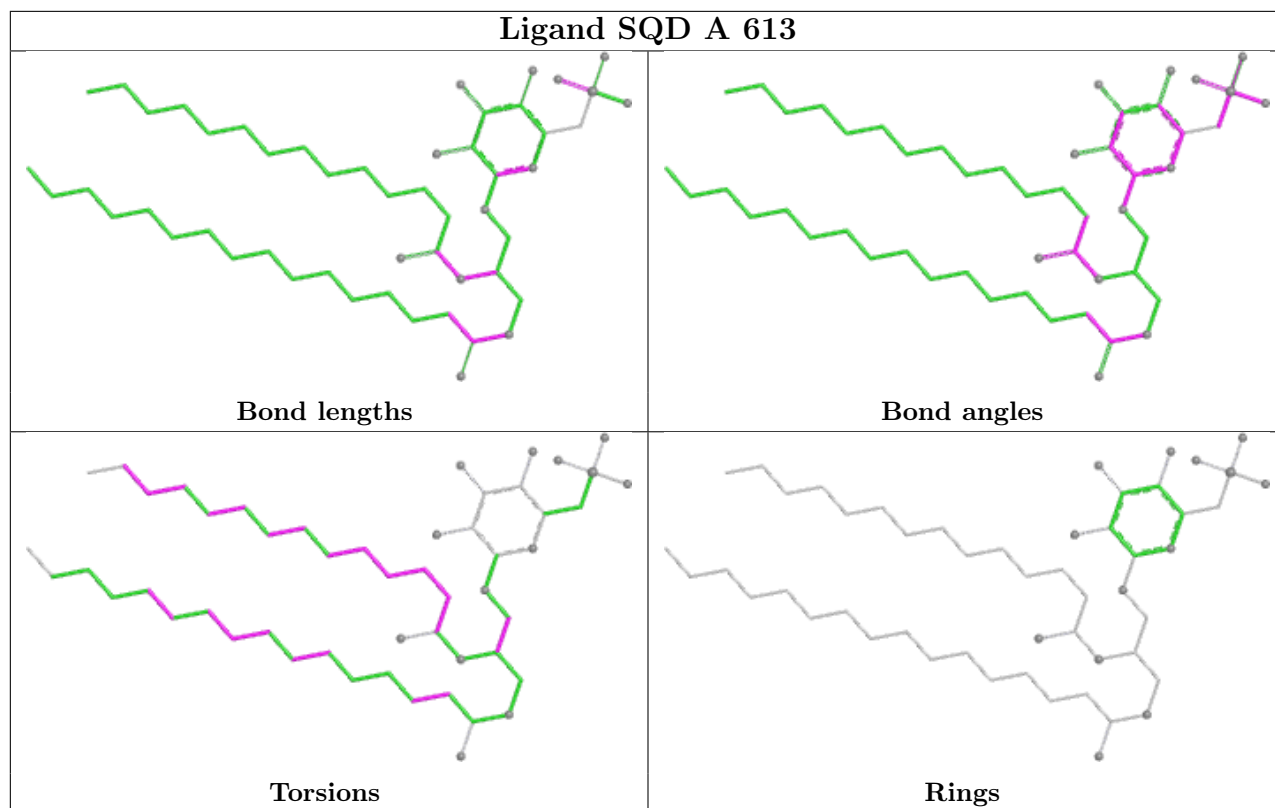




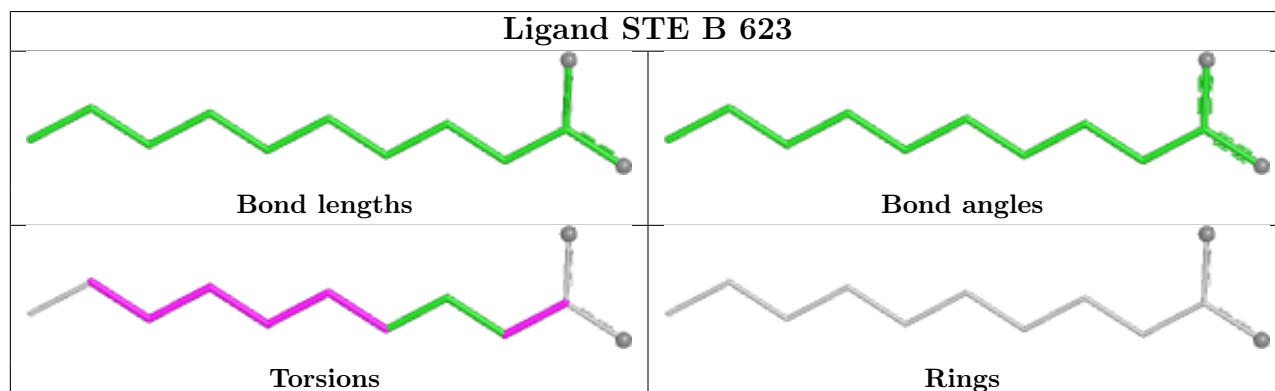




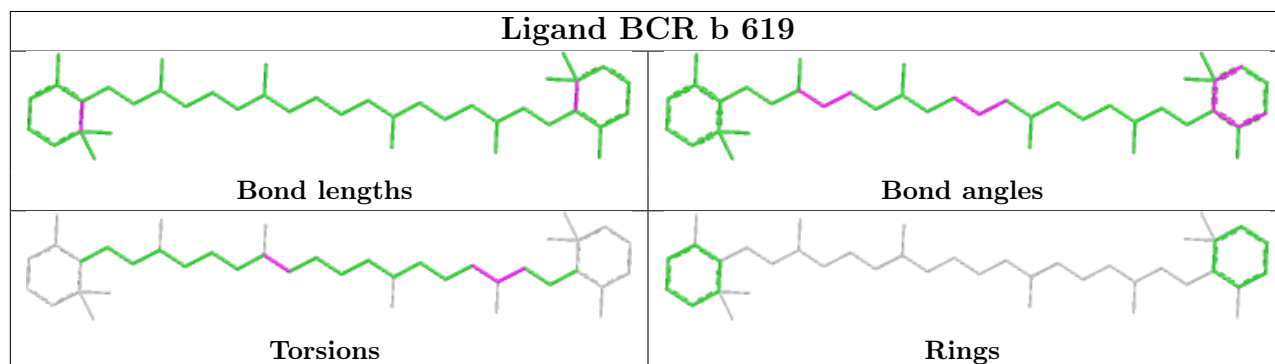
Ligand SQD A 613



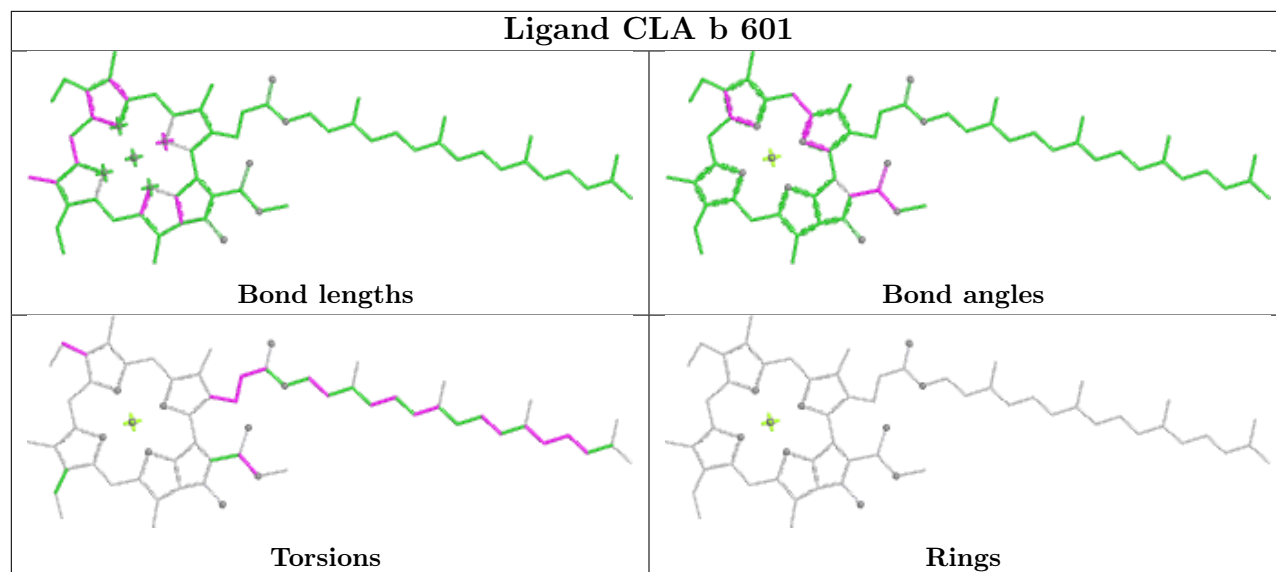
Ligand STE B 623



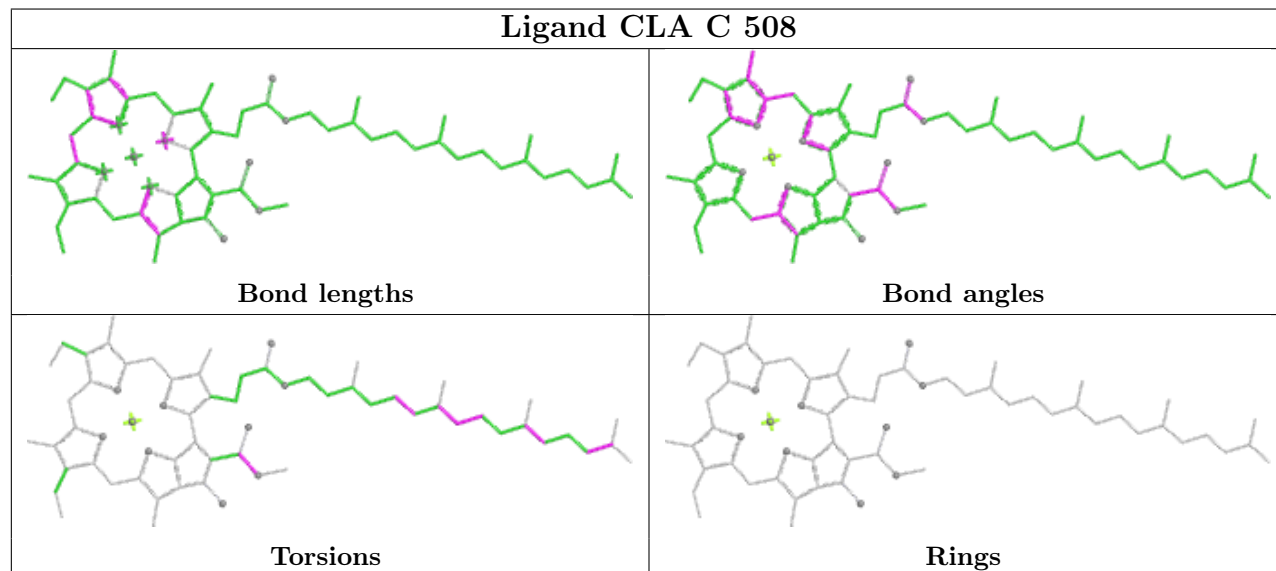
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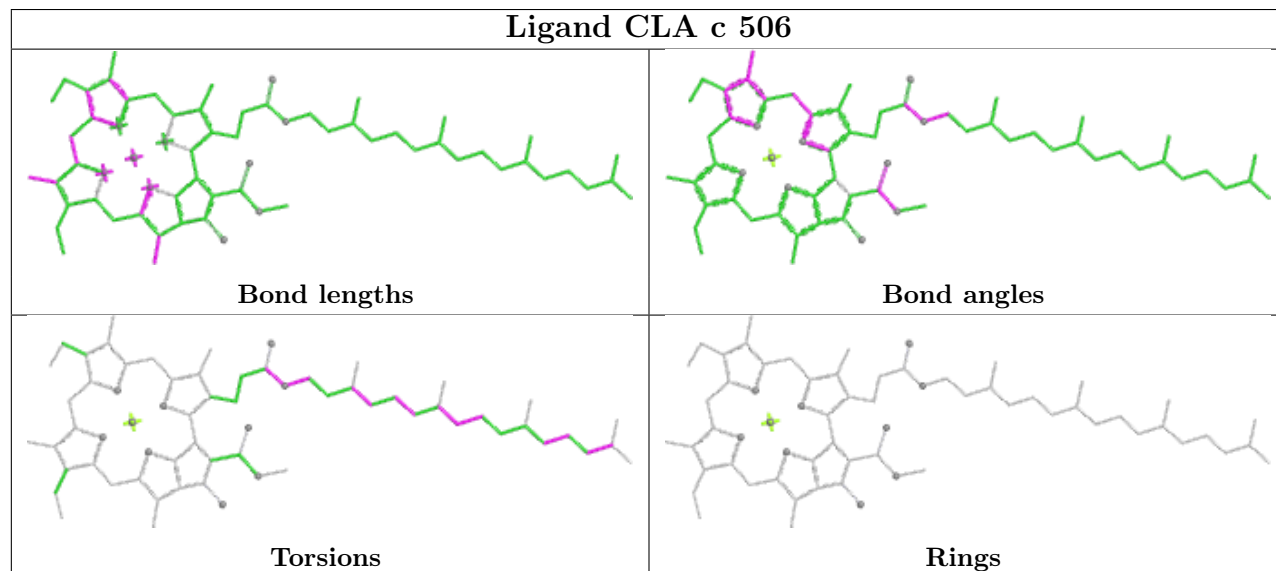
Ligand CLA b 601

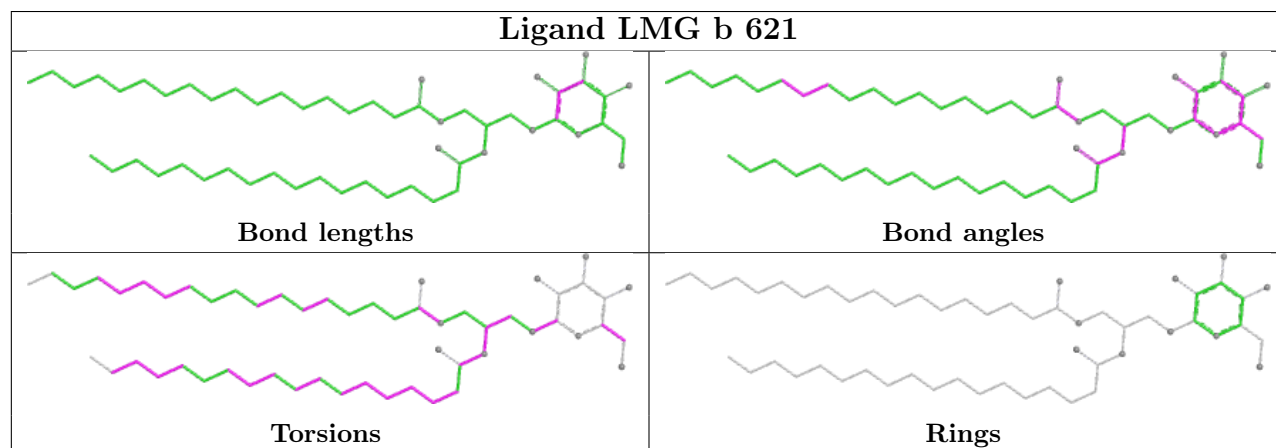
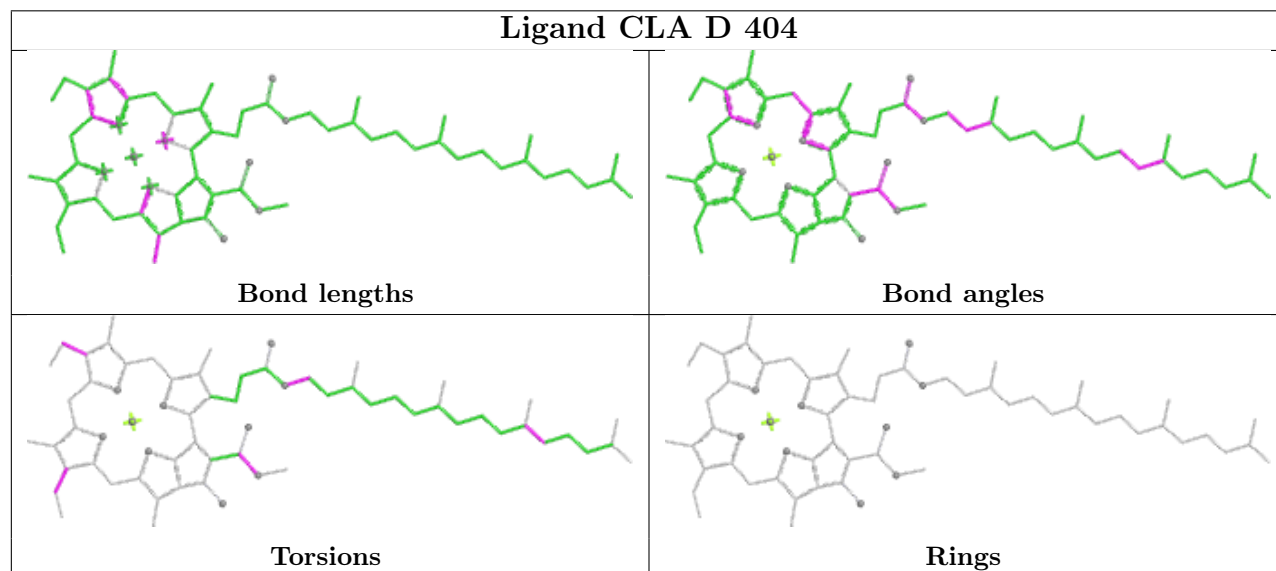
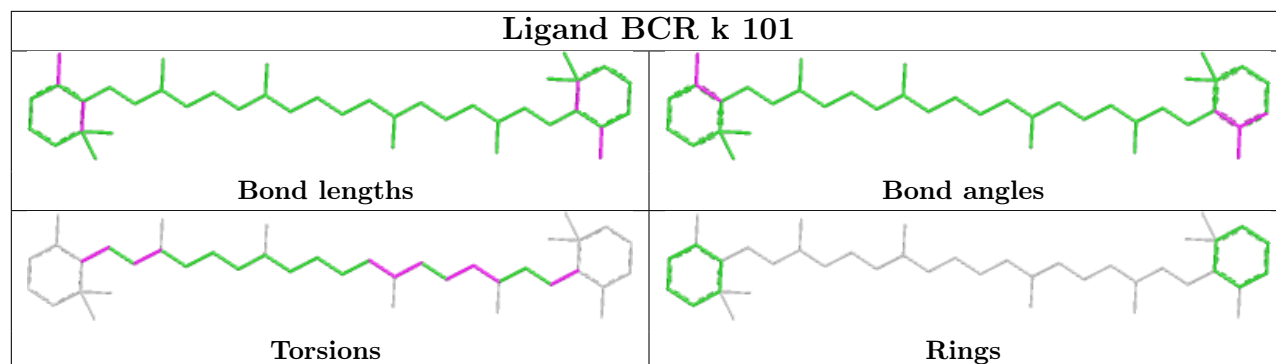


Ligand CLA C 508

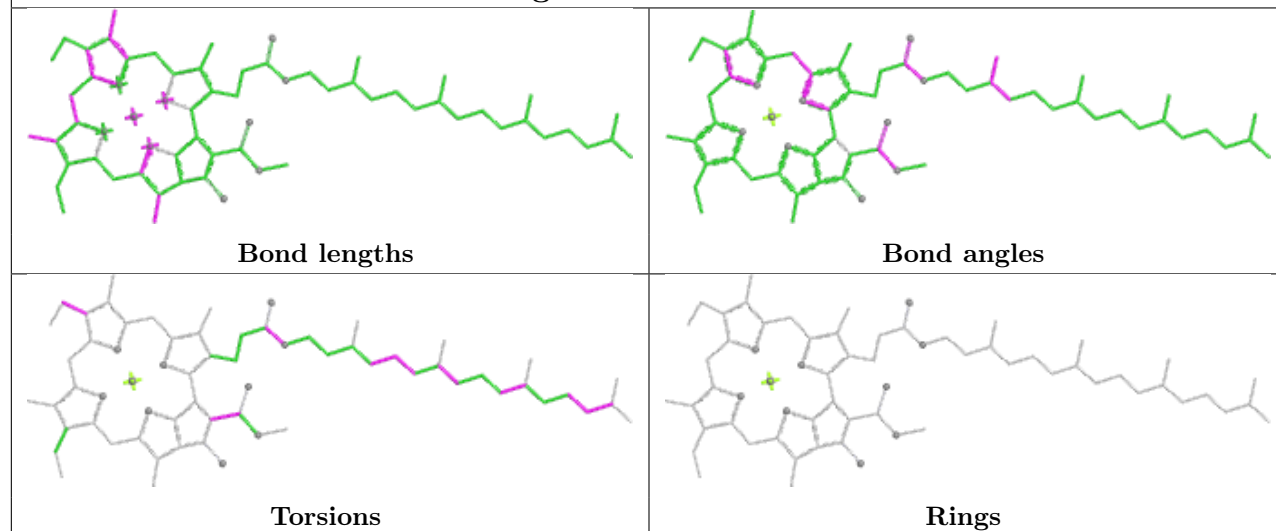


Ligand CLA c 506

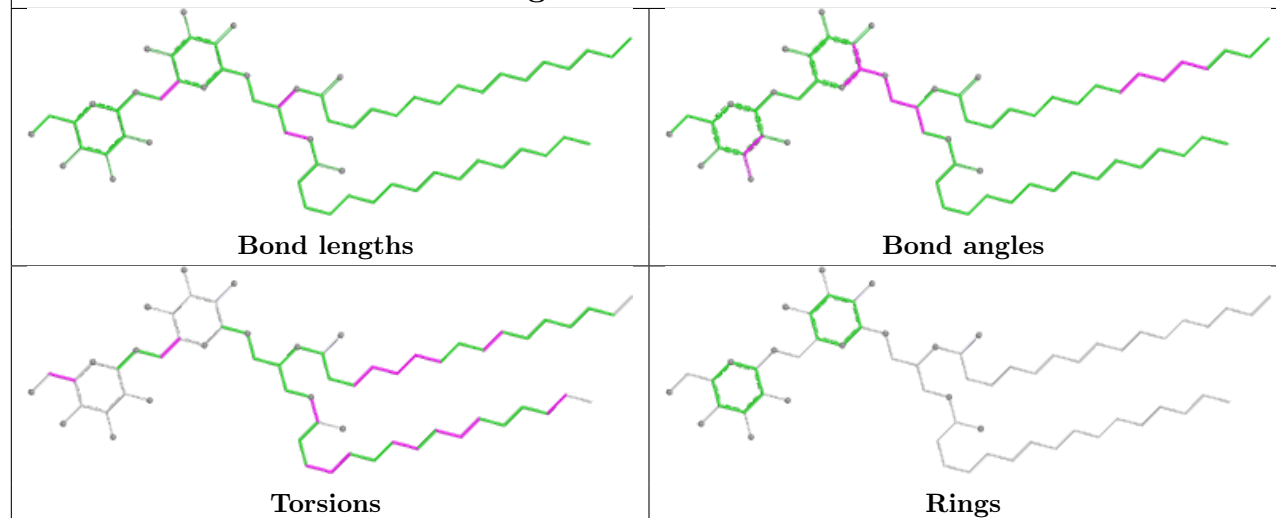




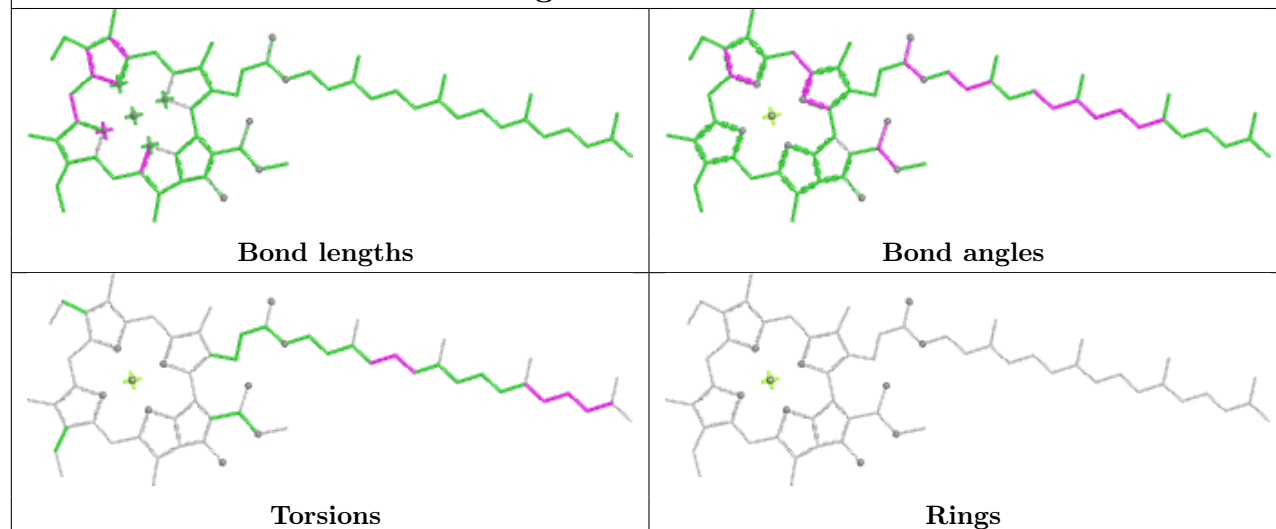
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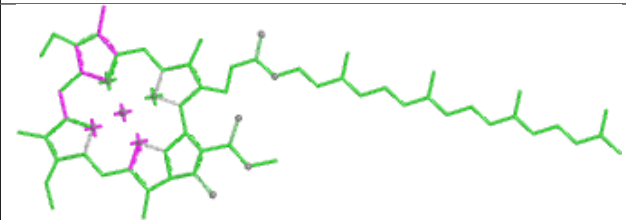
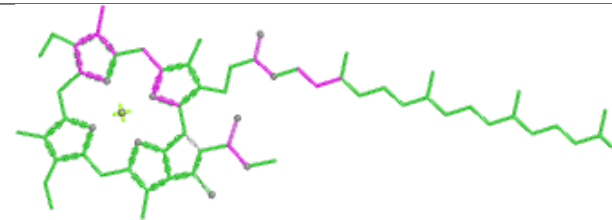
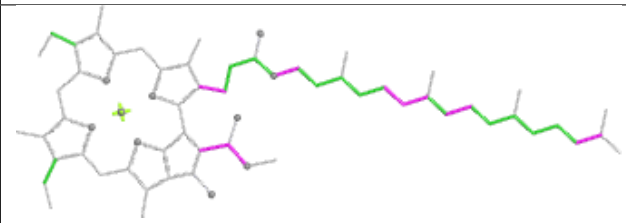
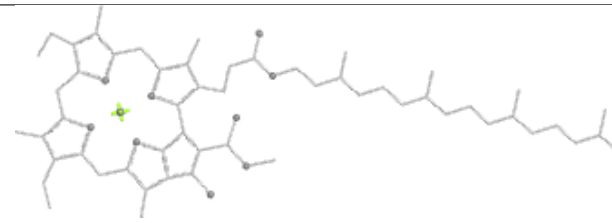


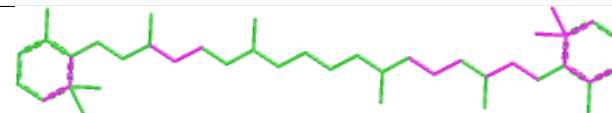
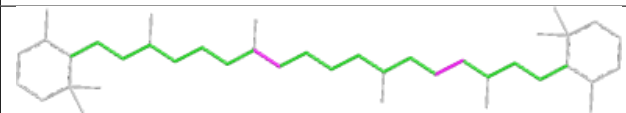
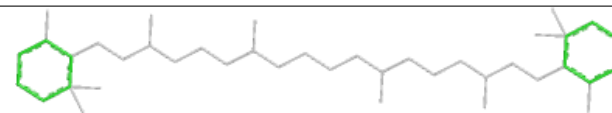
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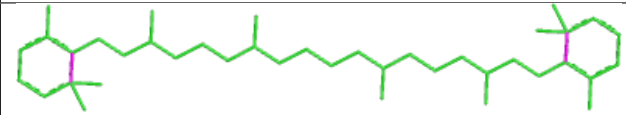
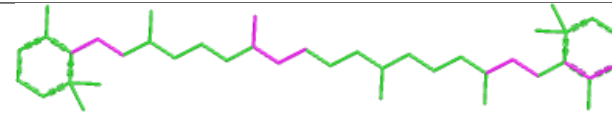
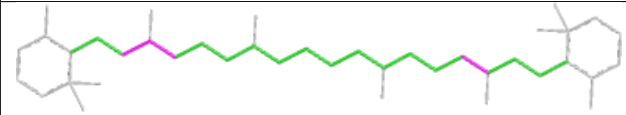
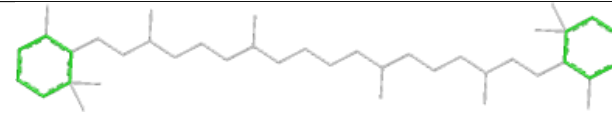


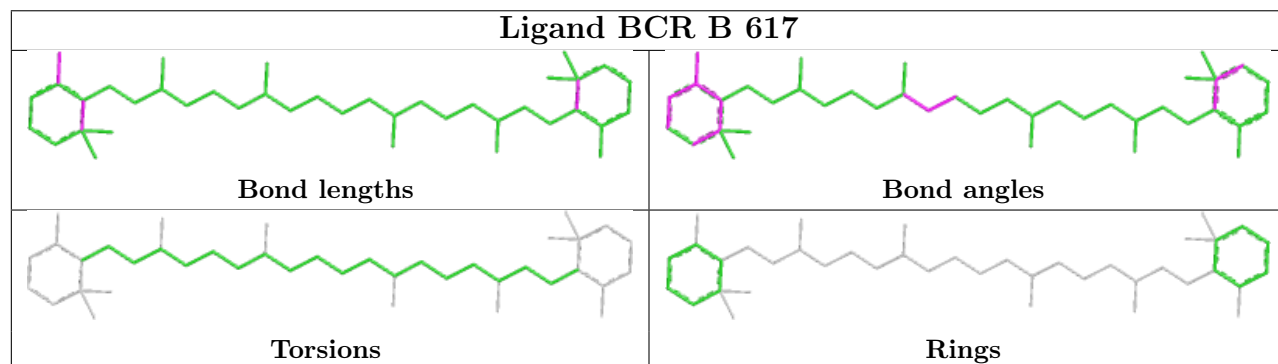
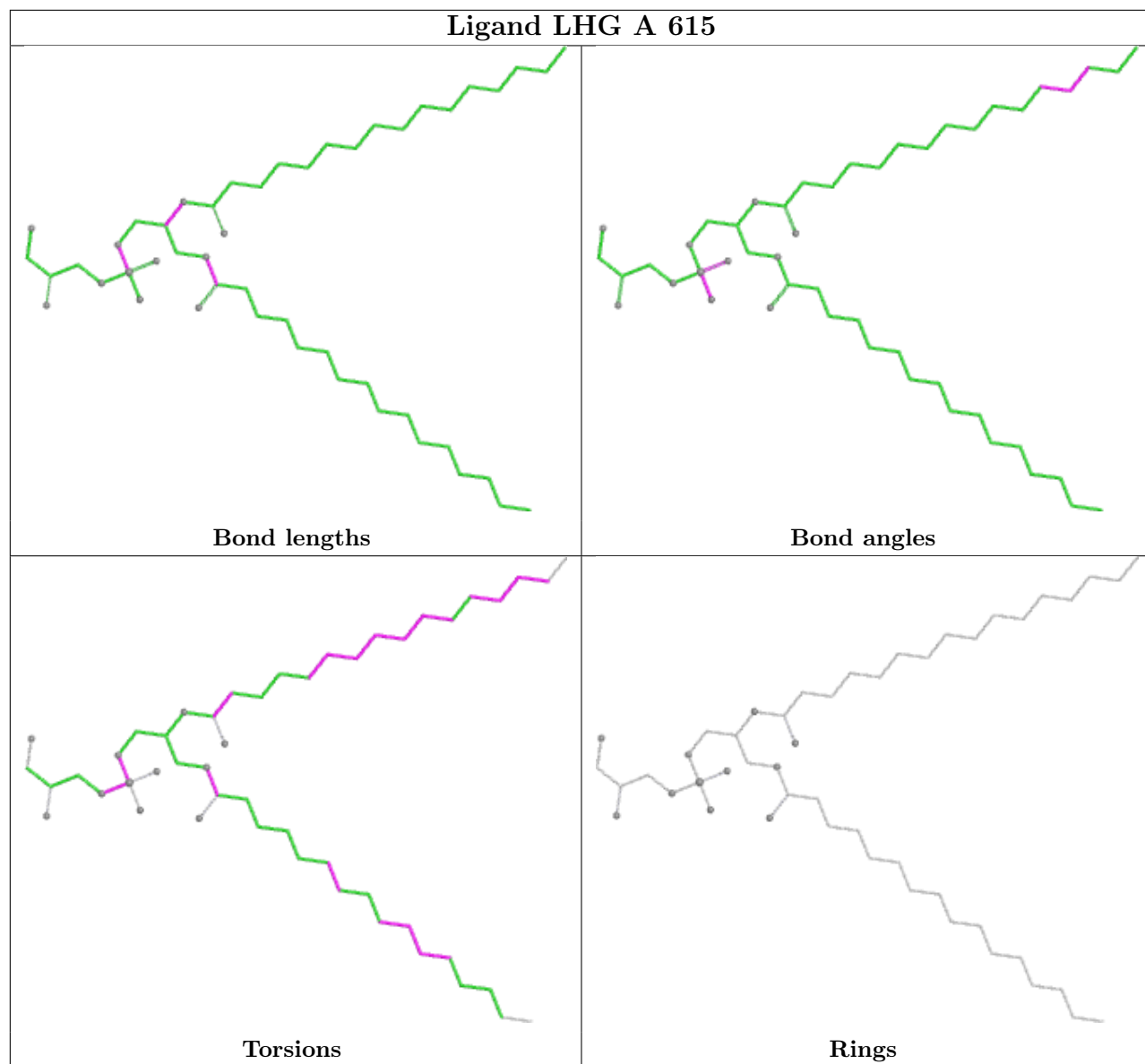
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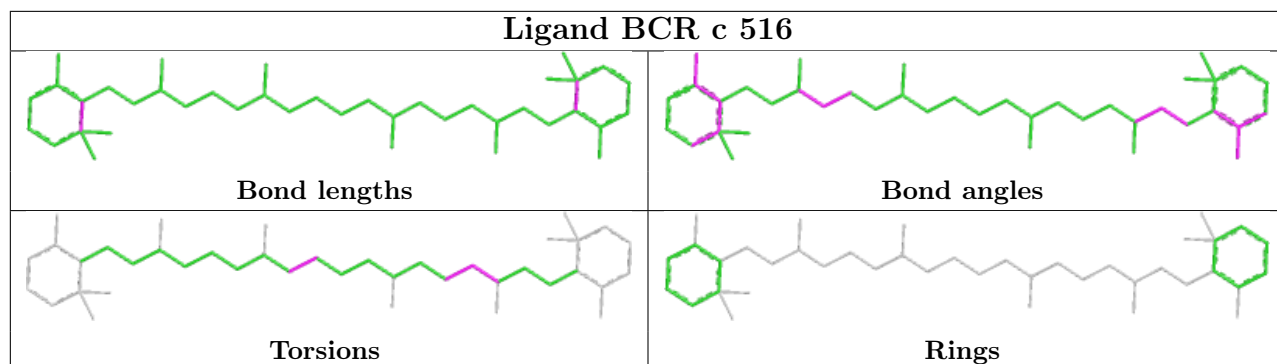
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

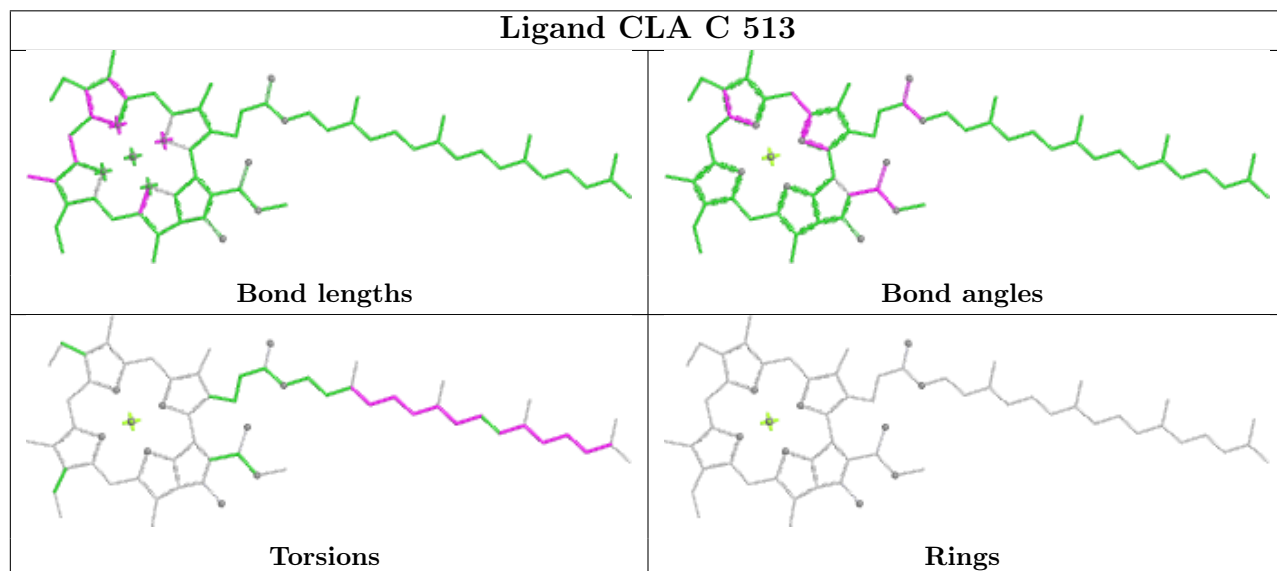
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



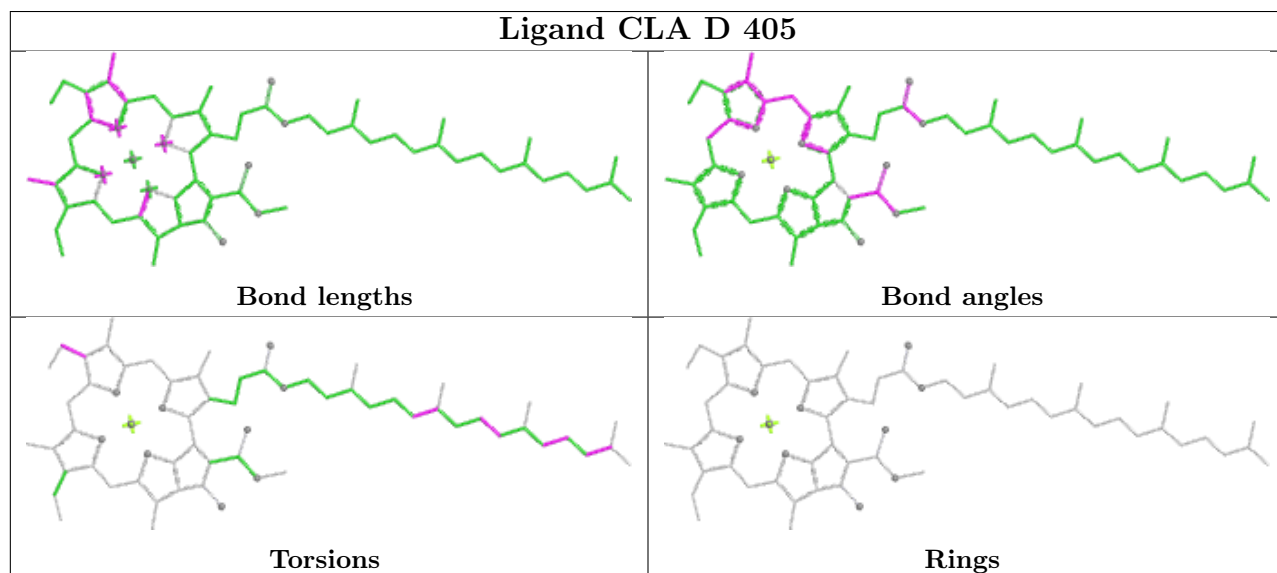
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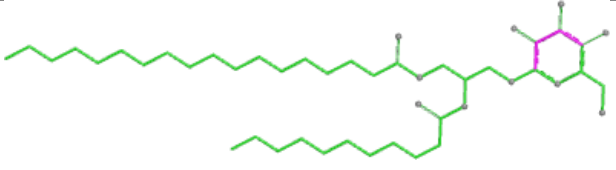
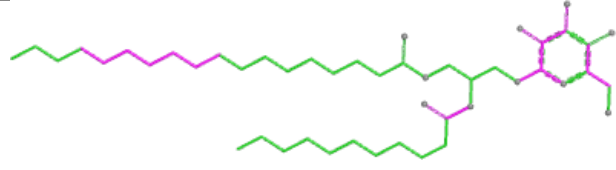
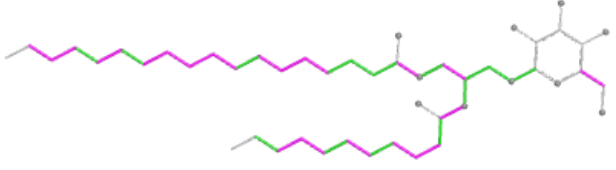
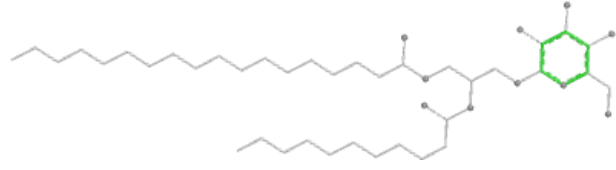


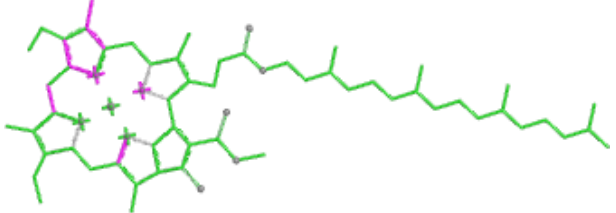
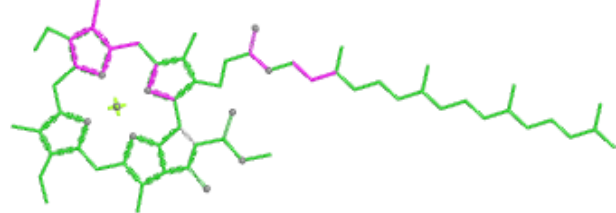
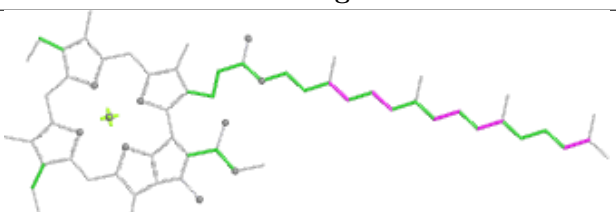
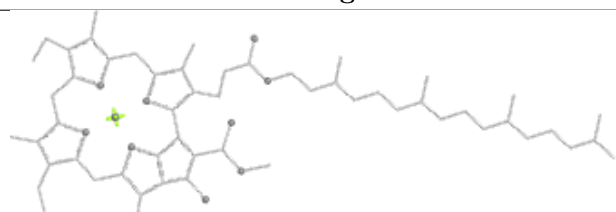
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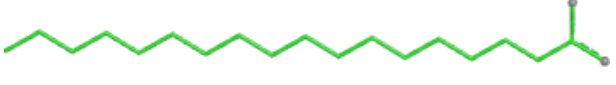
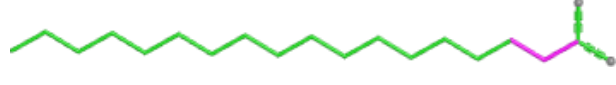
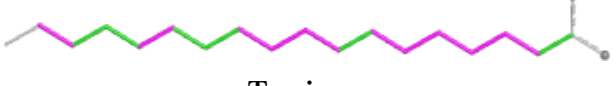
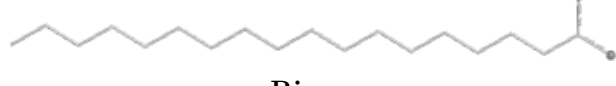


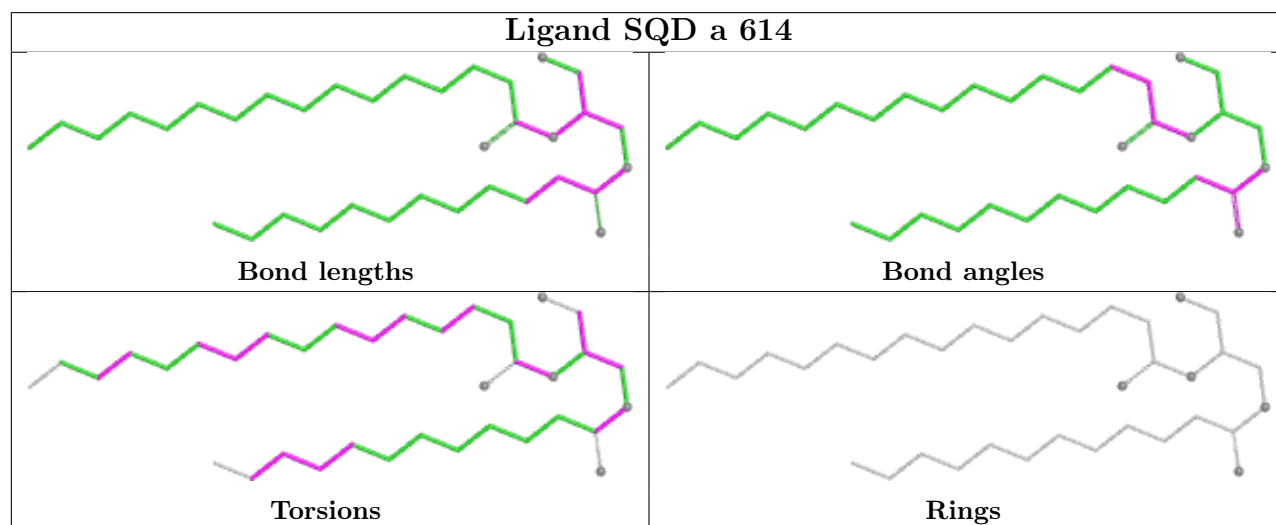
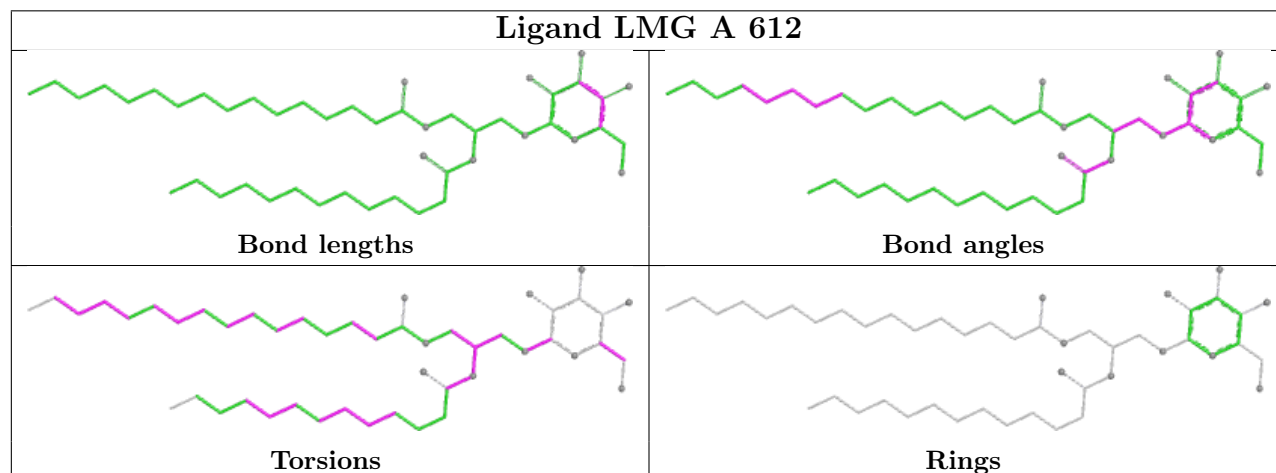
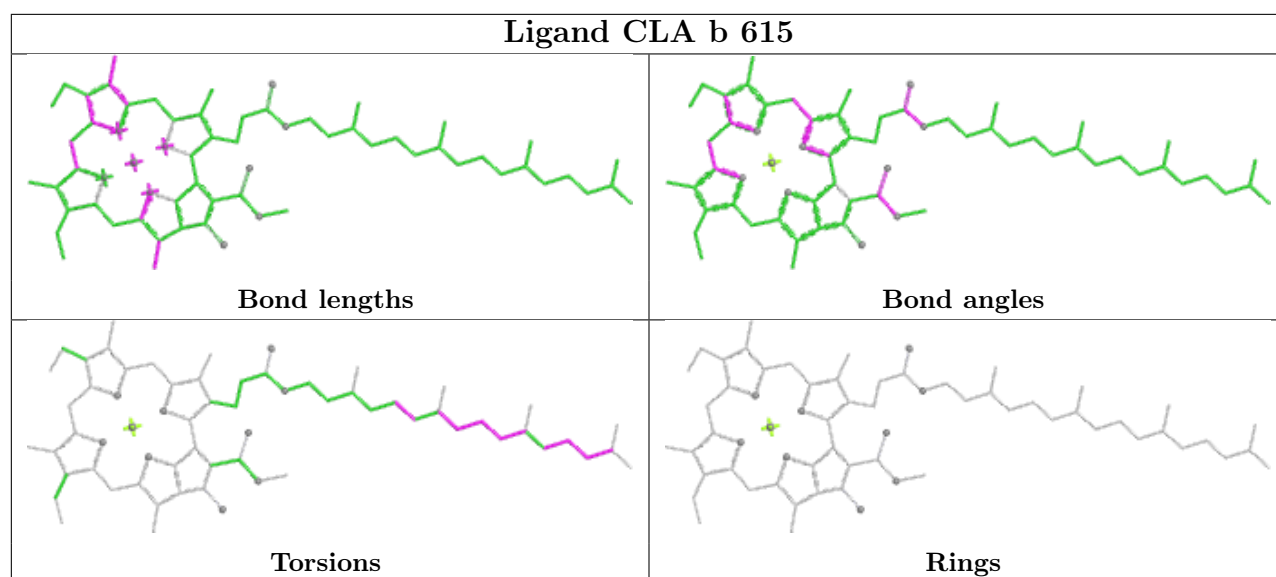
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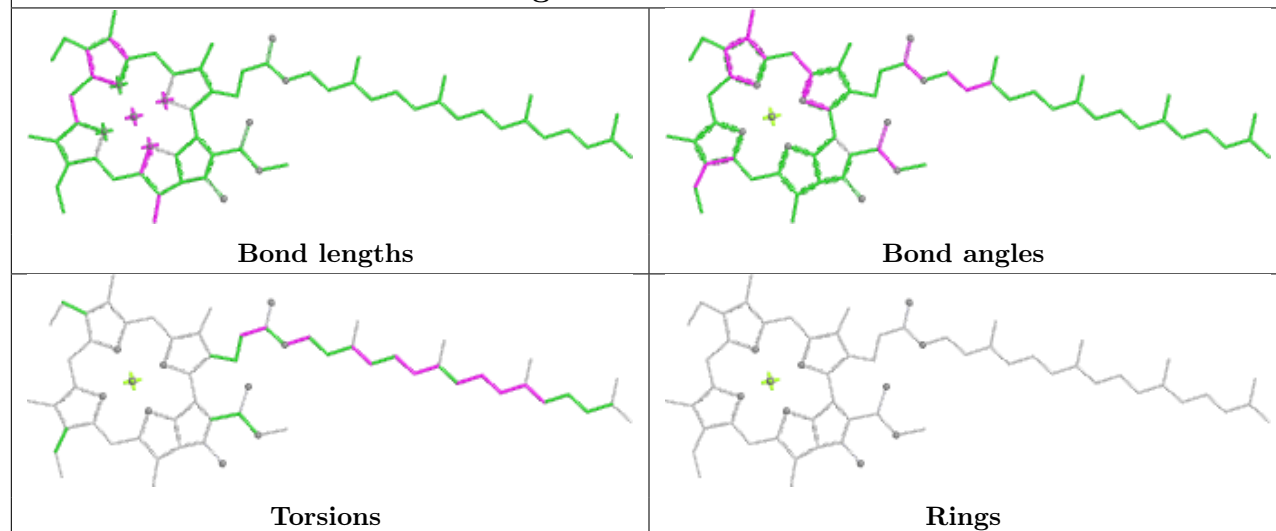
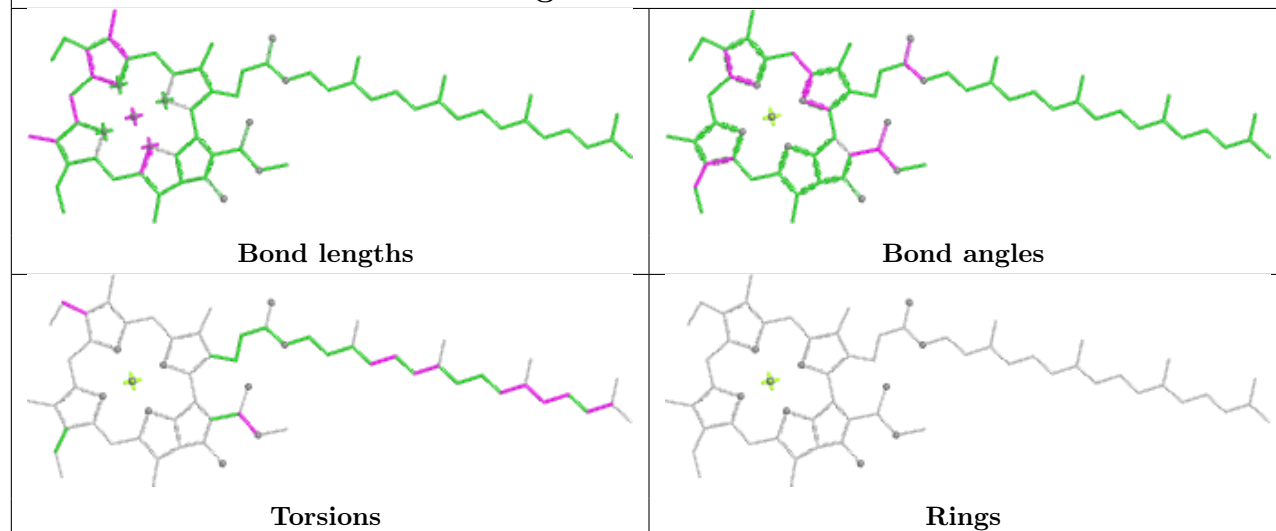
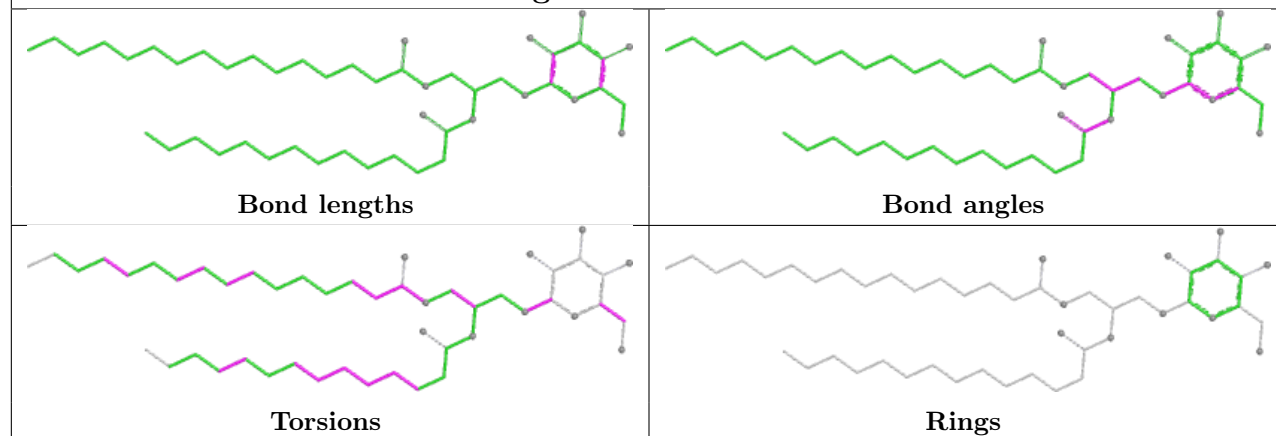


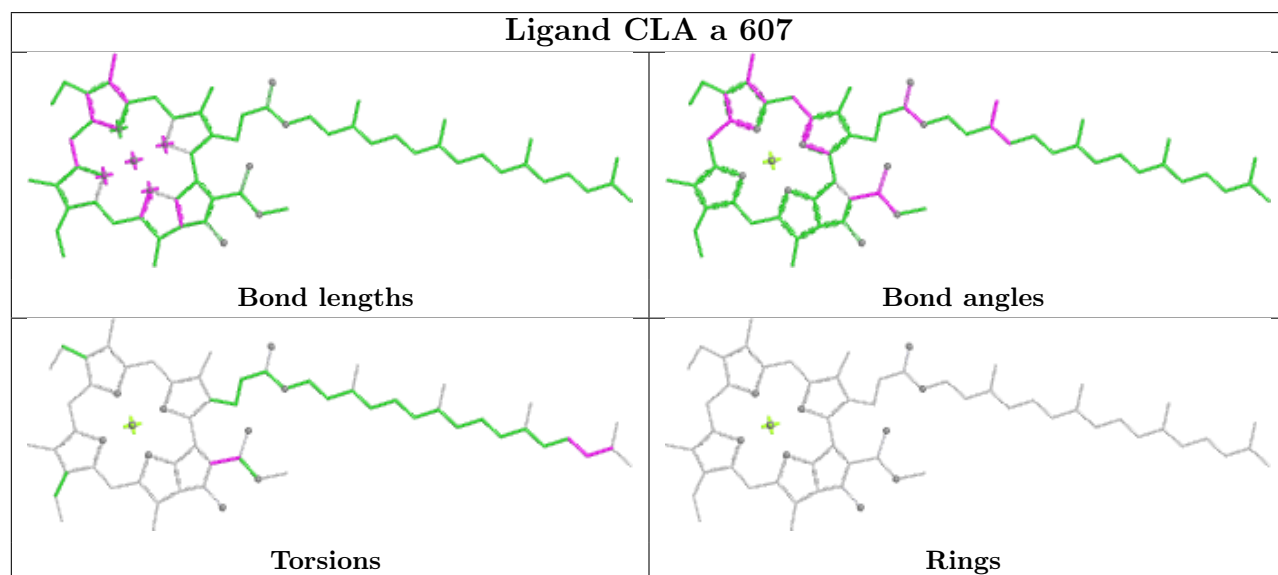
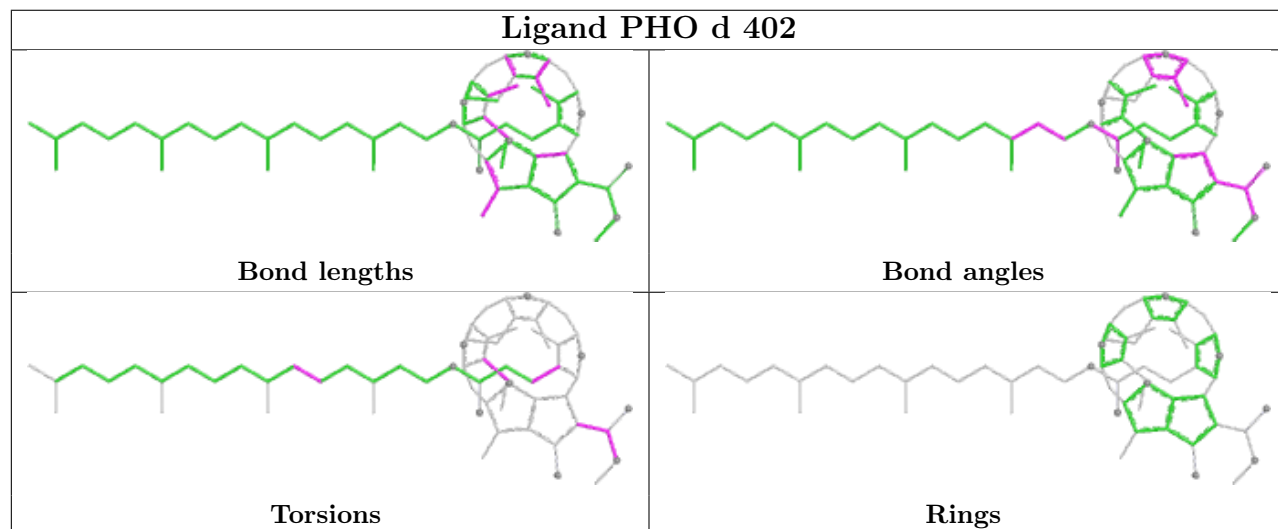
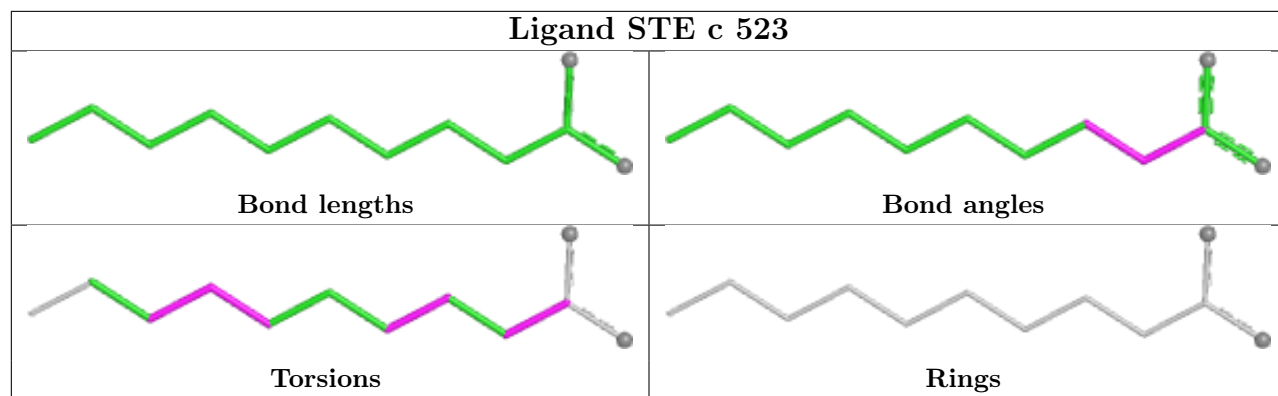
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

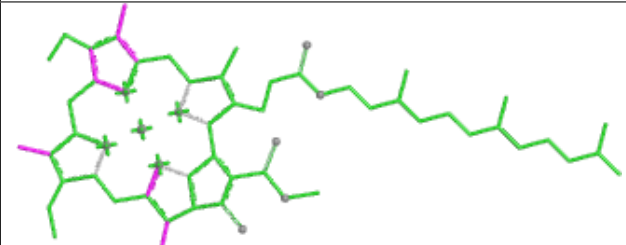
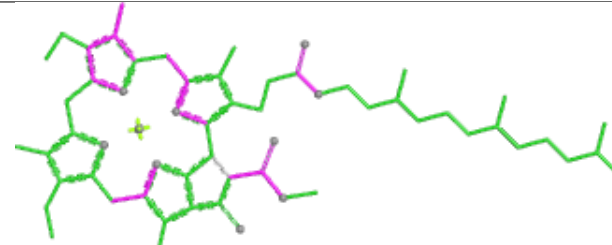
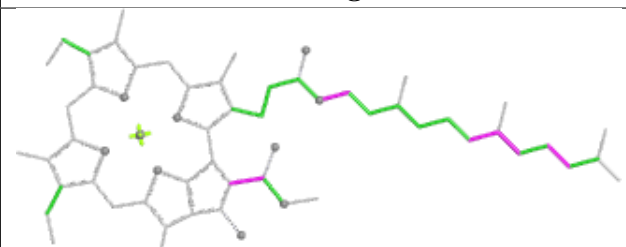
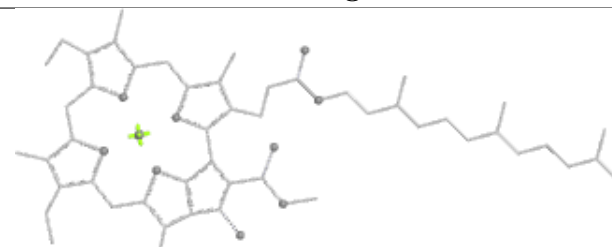
Ligand CLA d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

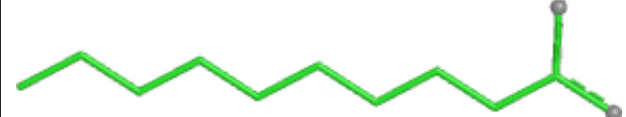
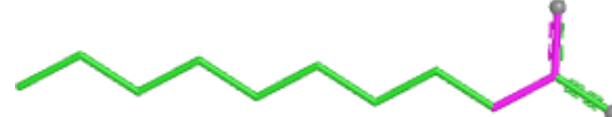
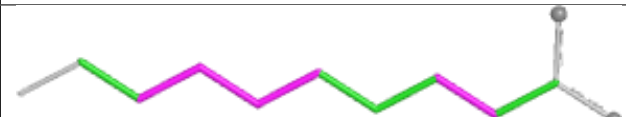
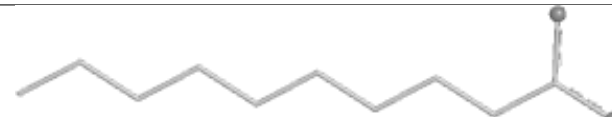
Ligand STE x 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

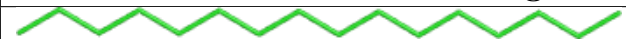
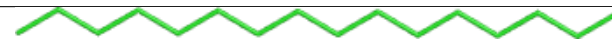


Ligand CLA B 613**Ligand CLA a 608****Ligand LMG c 524**

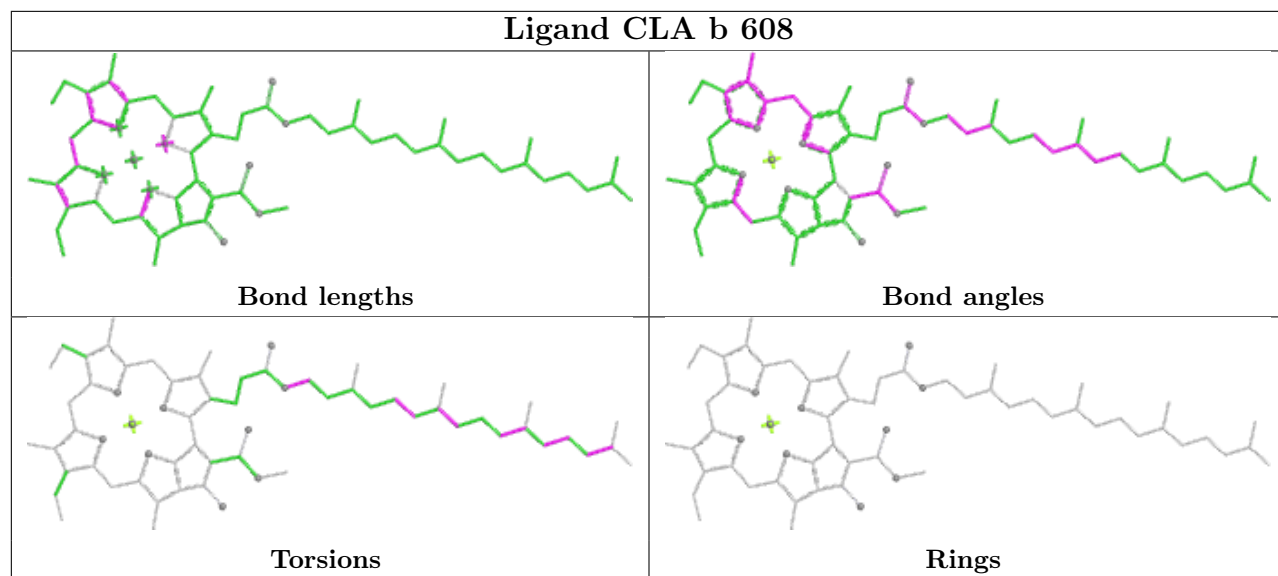


Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

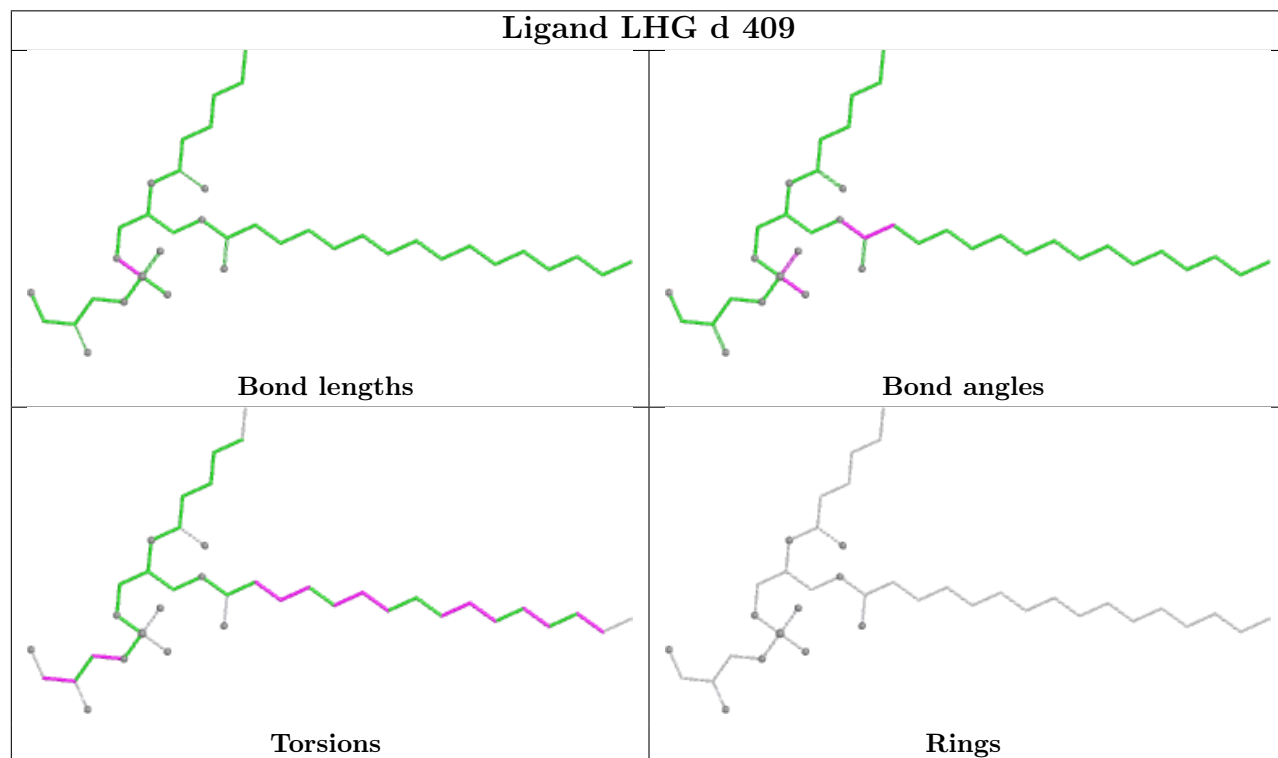
Ligand STE m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

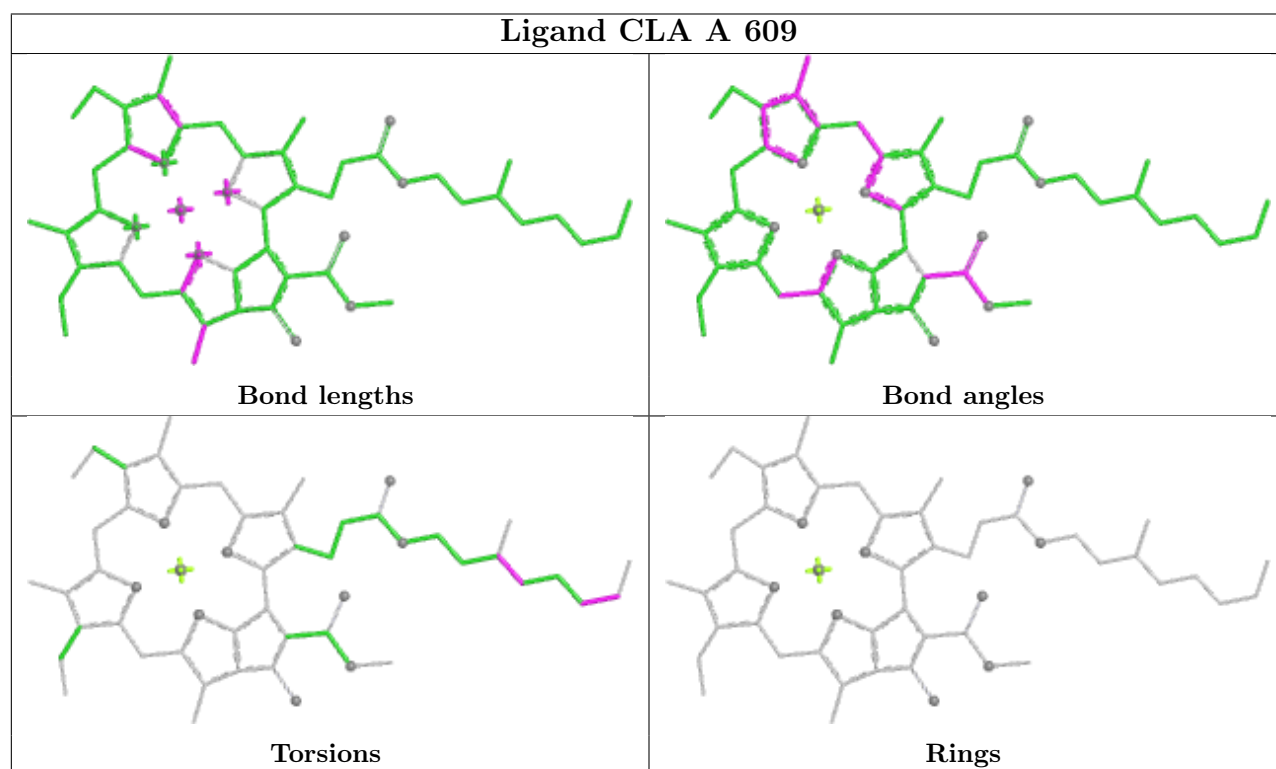
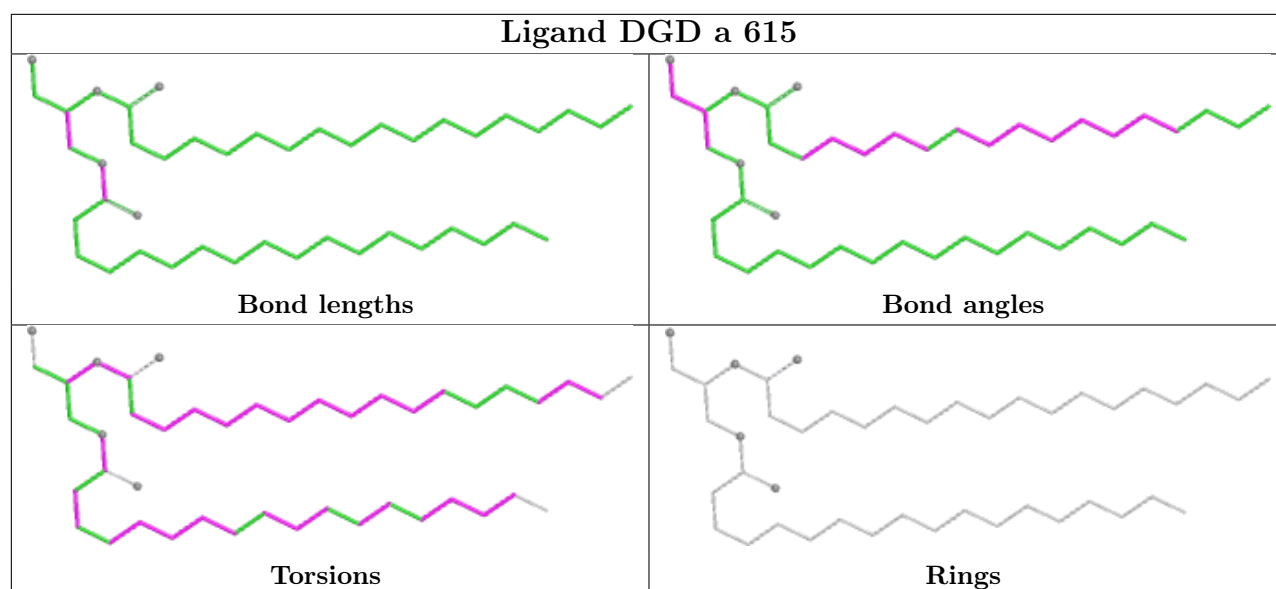
Ligand STE B 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 608

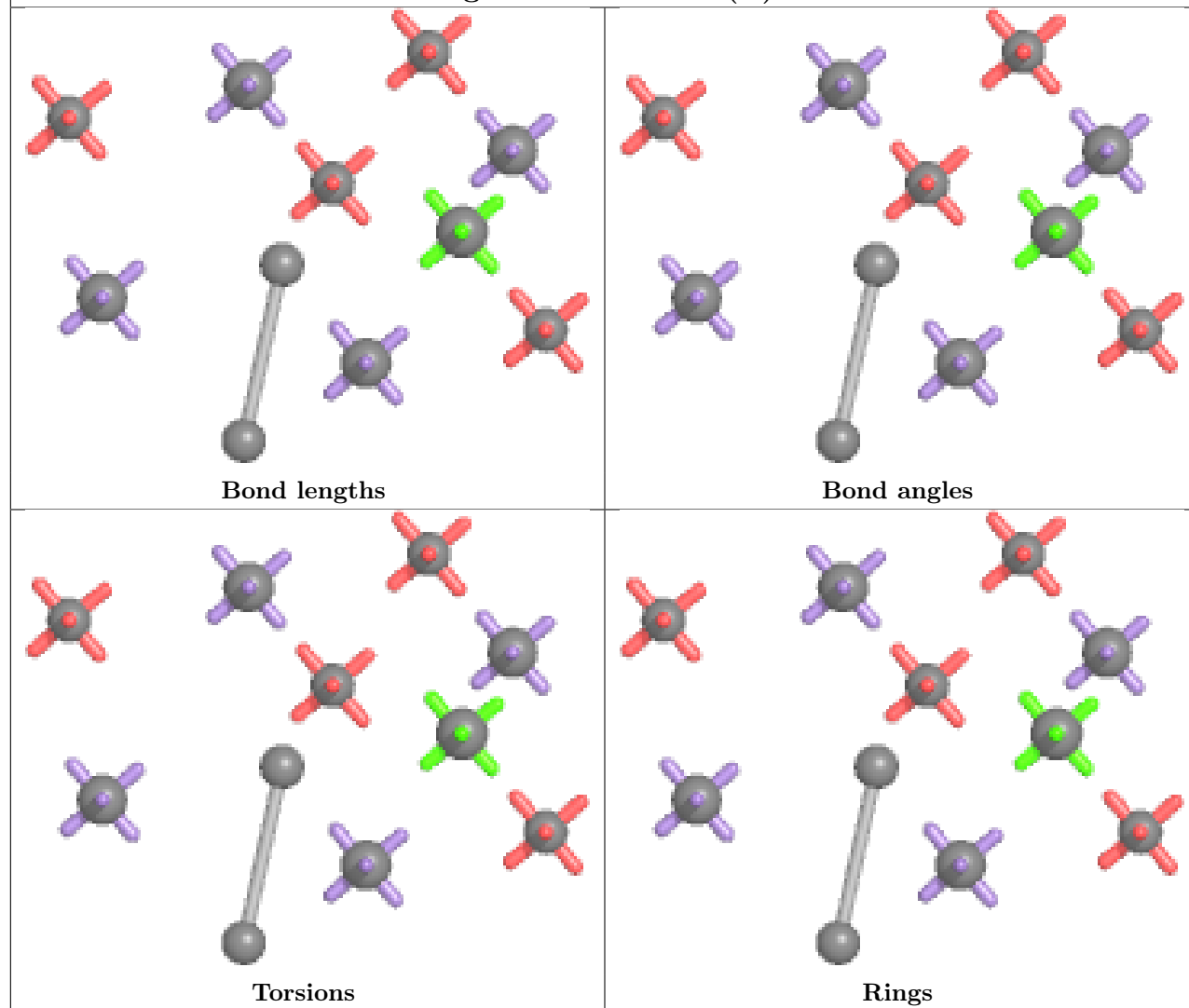


Ligand LHG d 409

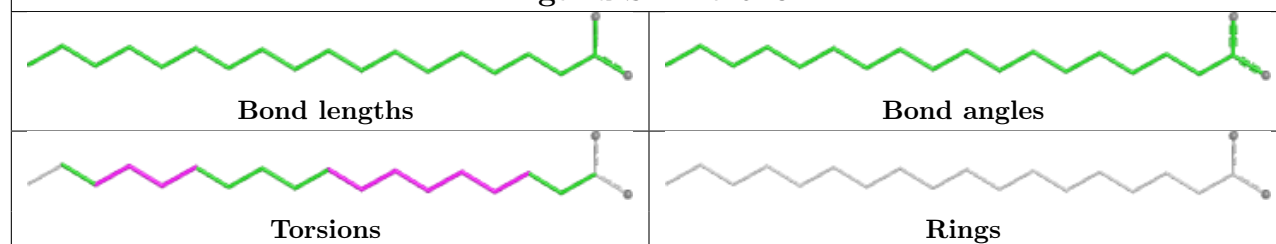


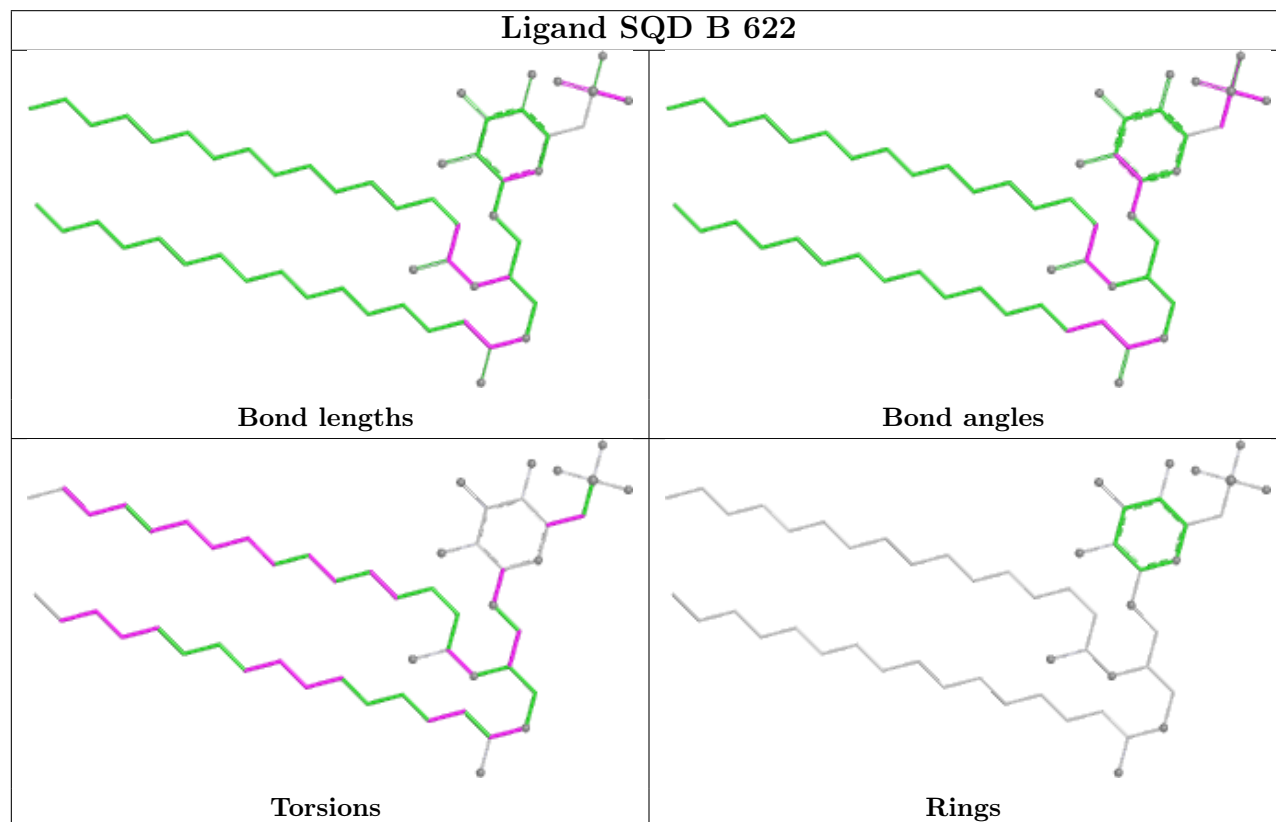
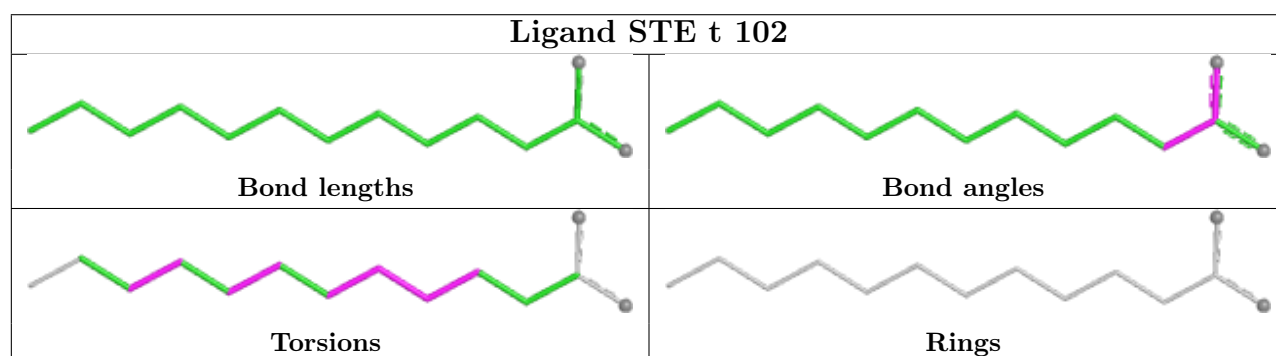
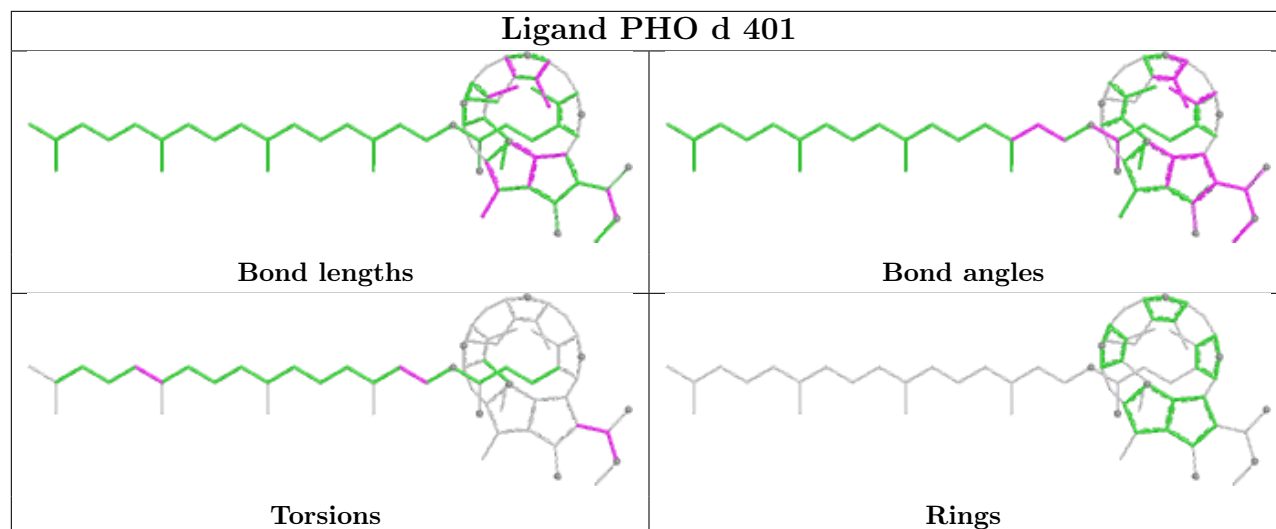


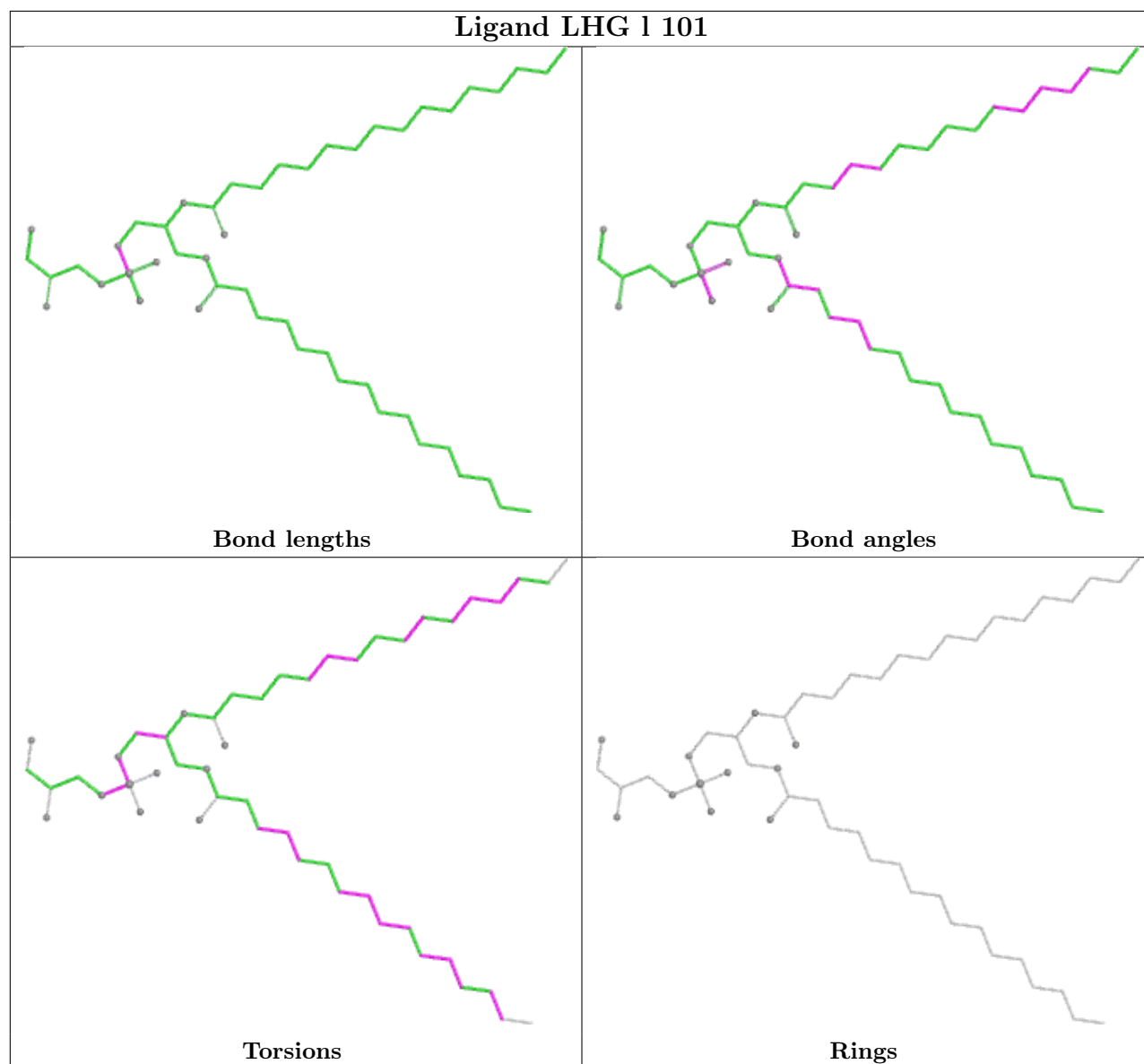
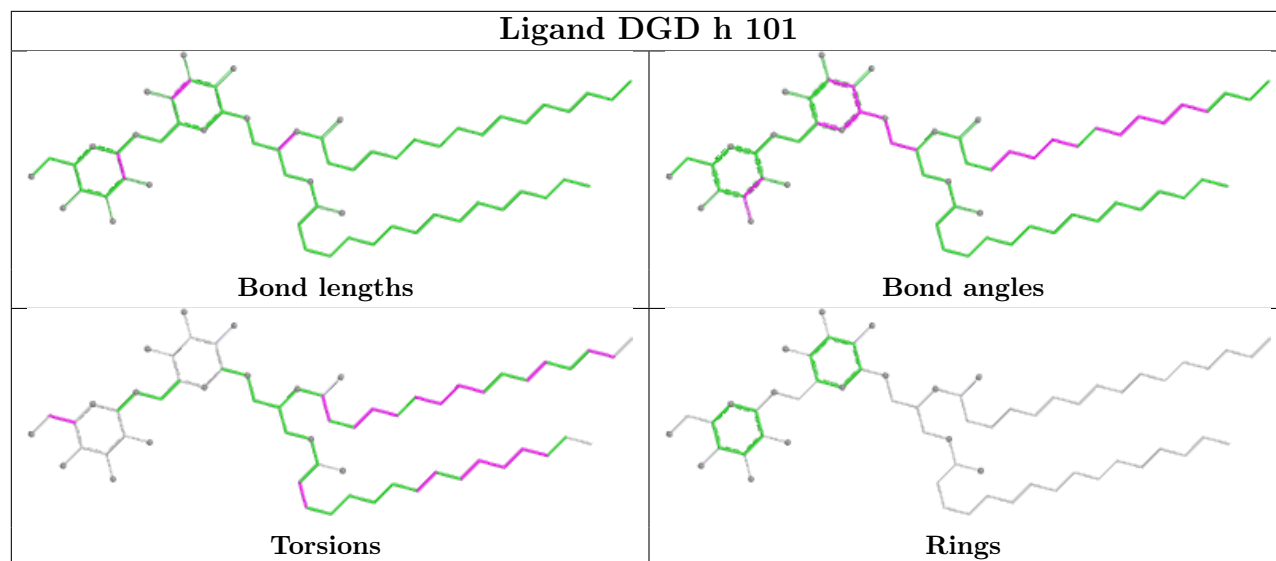
Ligand OEY A 601 (B)

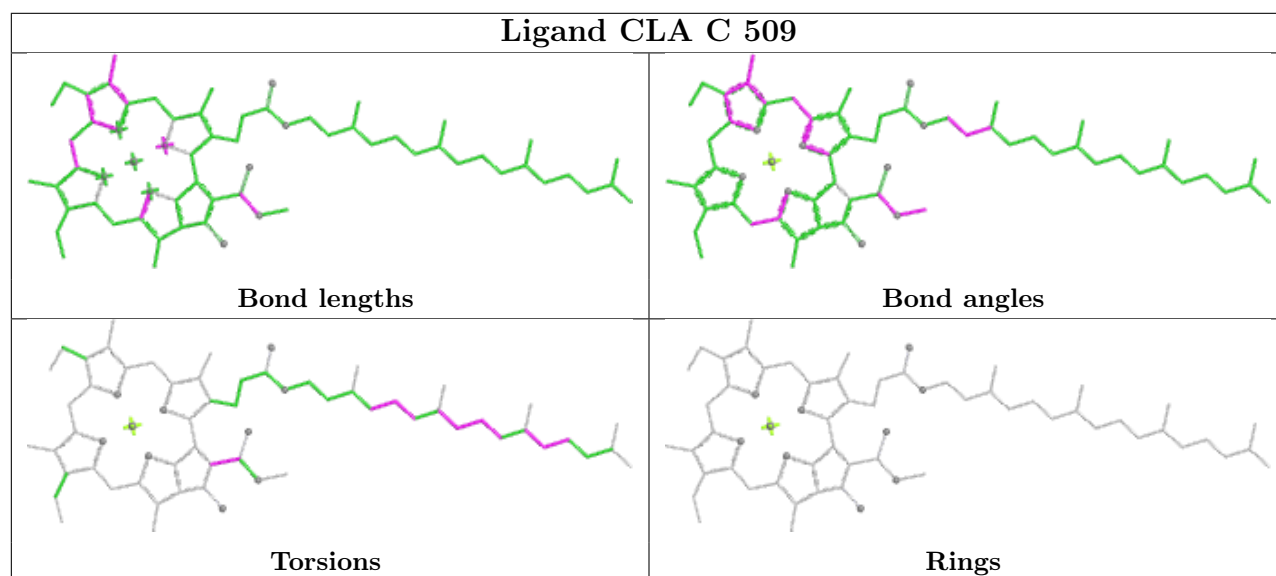
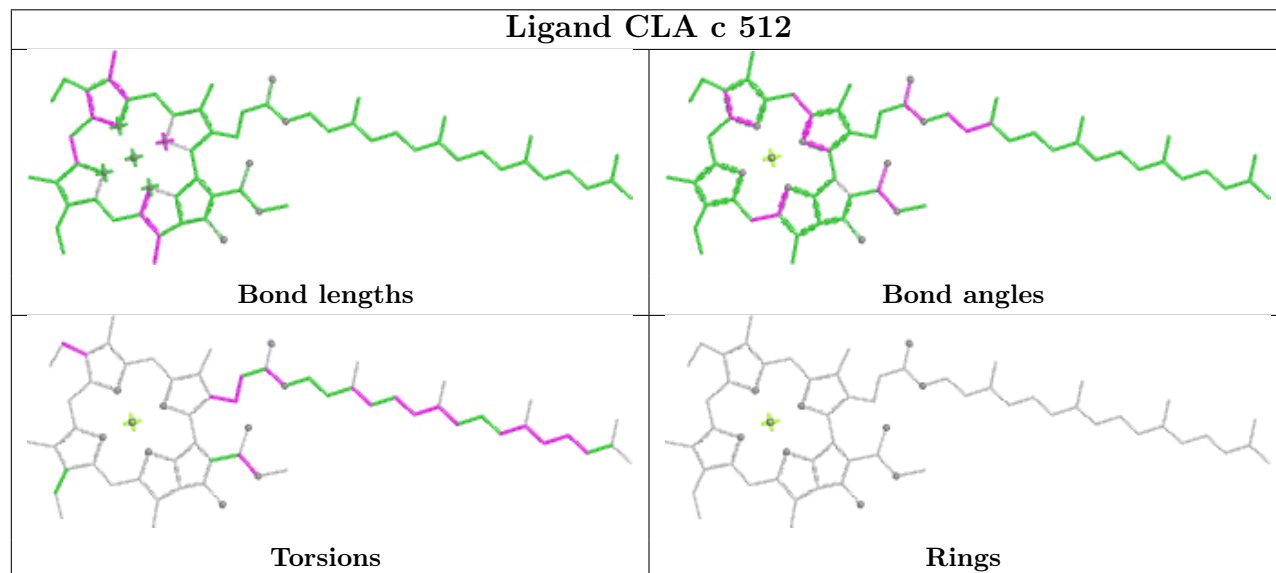
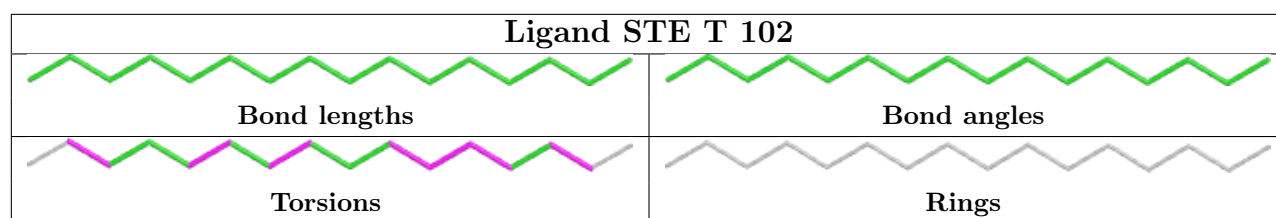


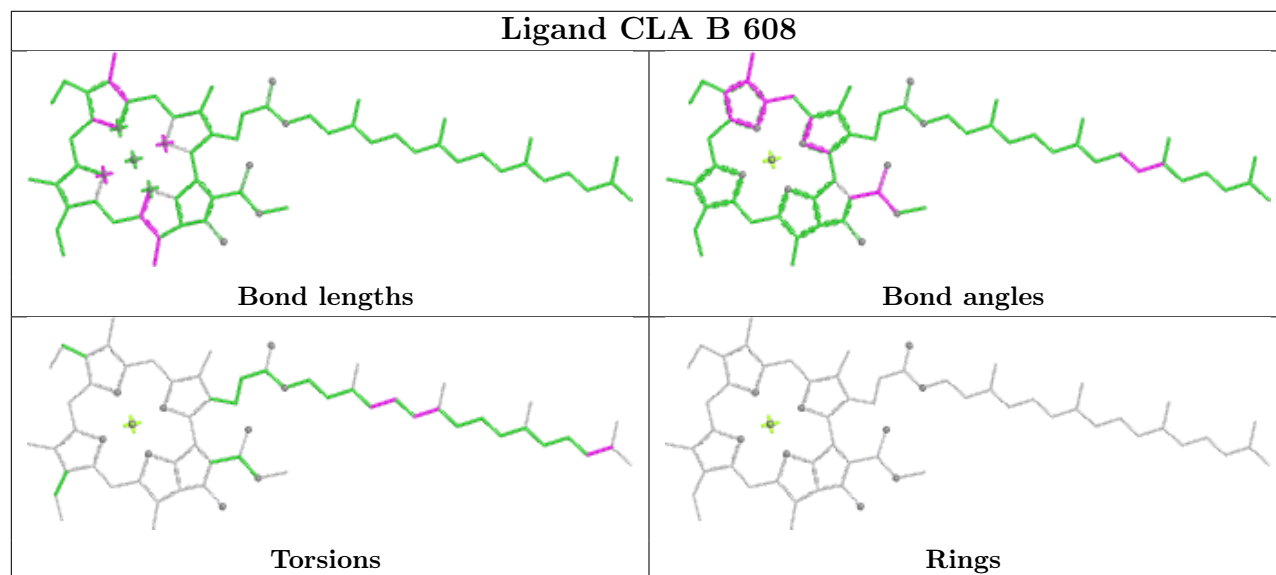
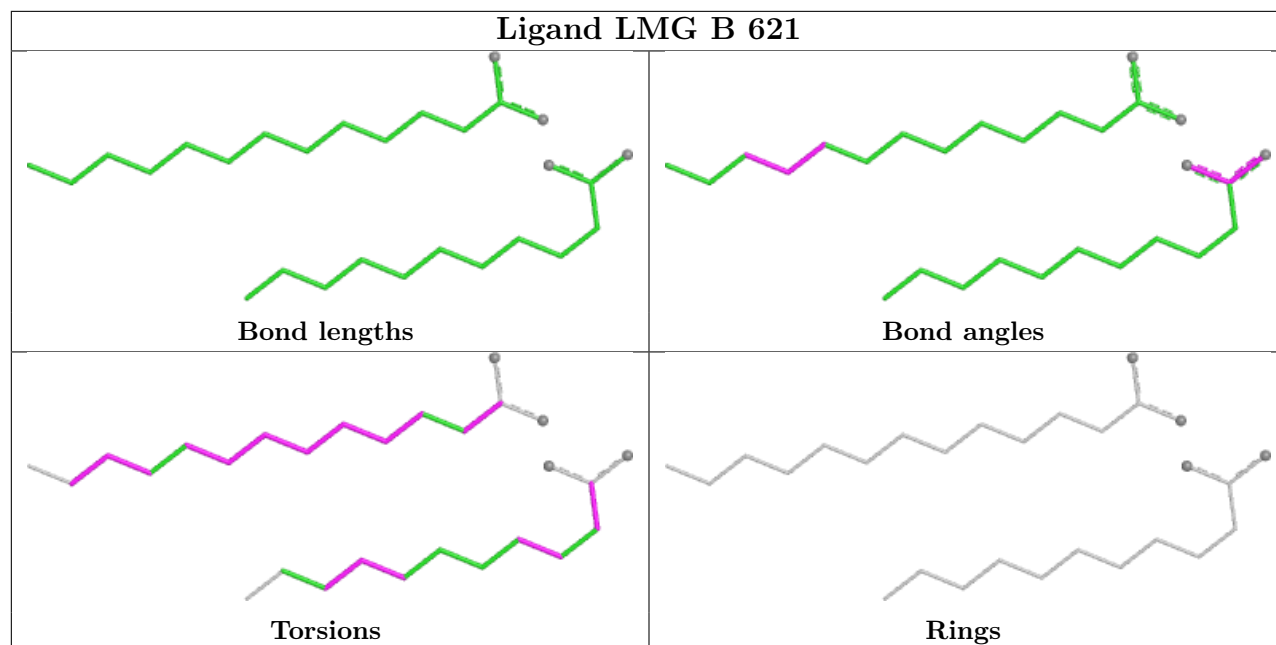
Ligand STE b 620

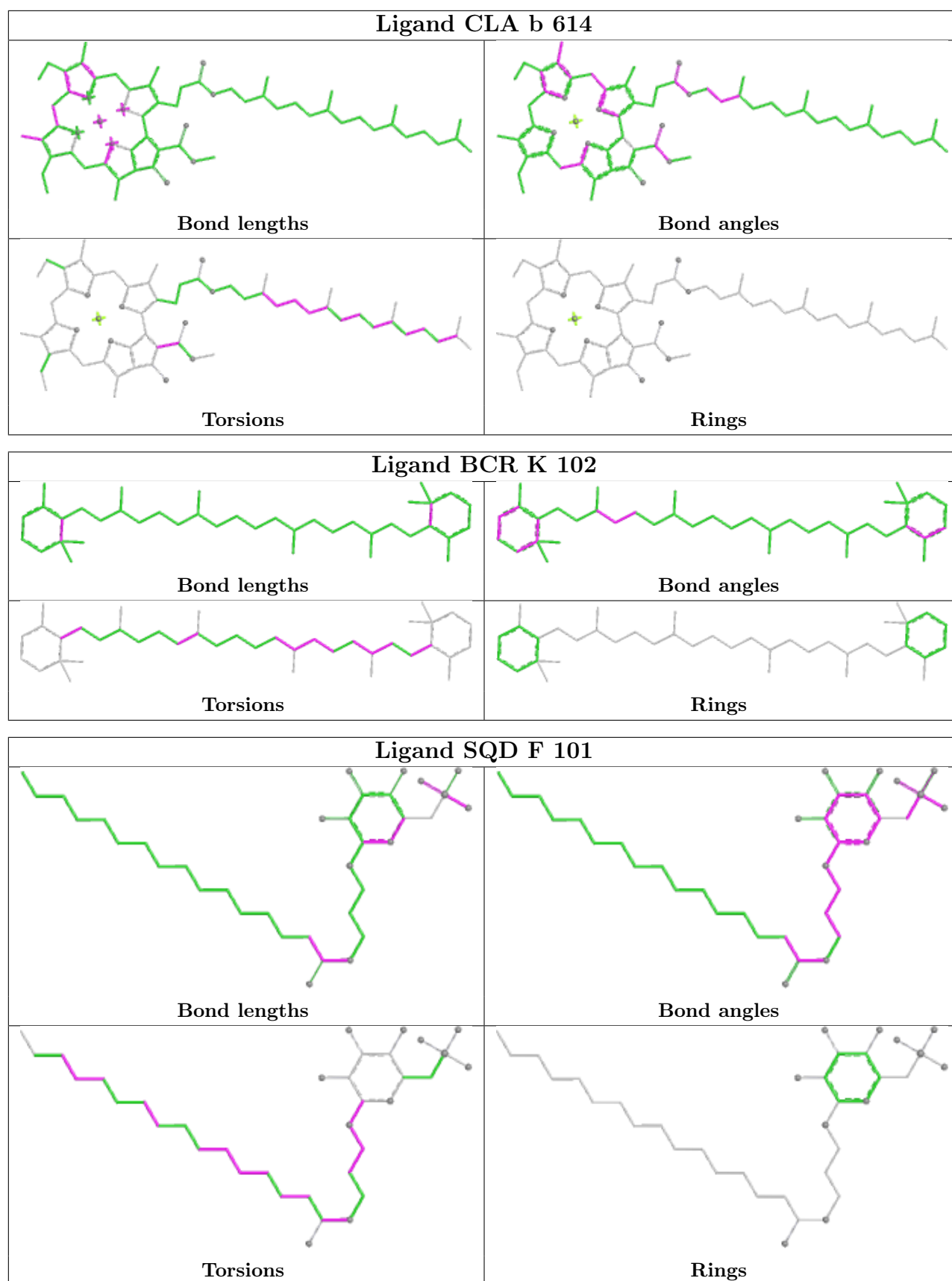


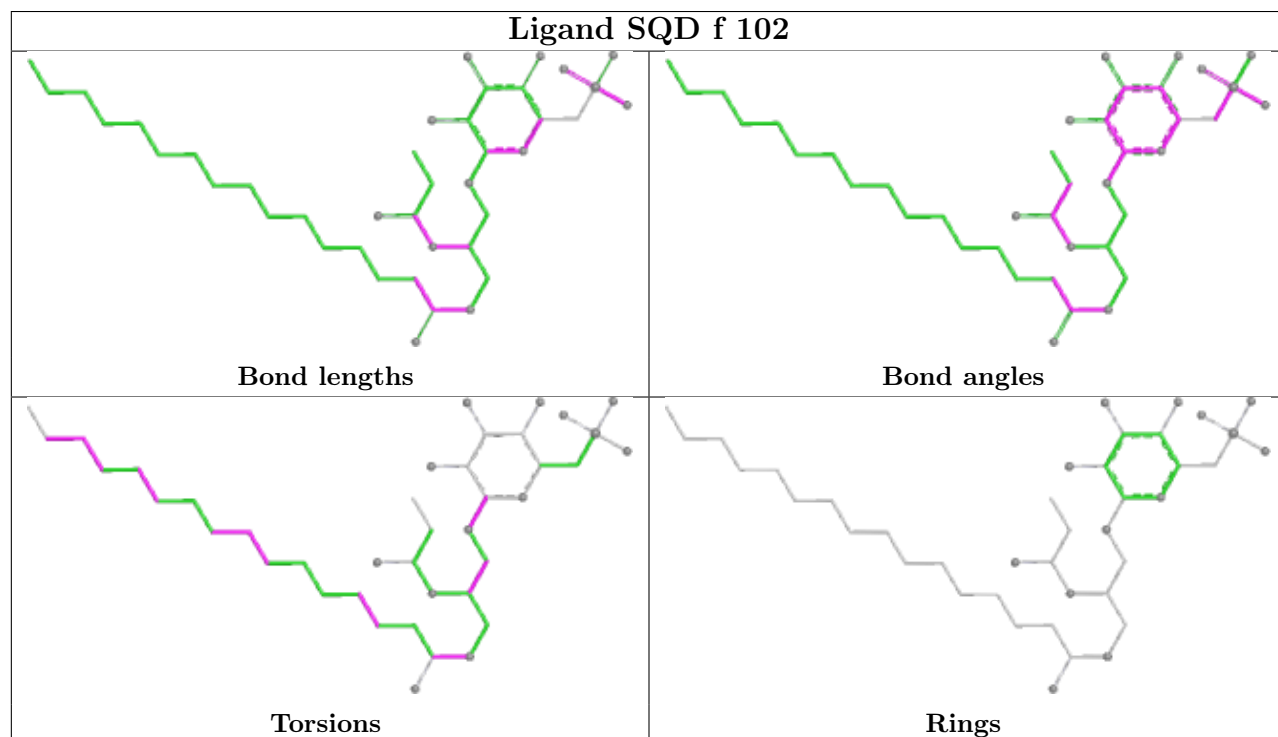
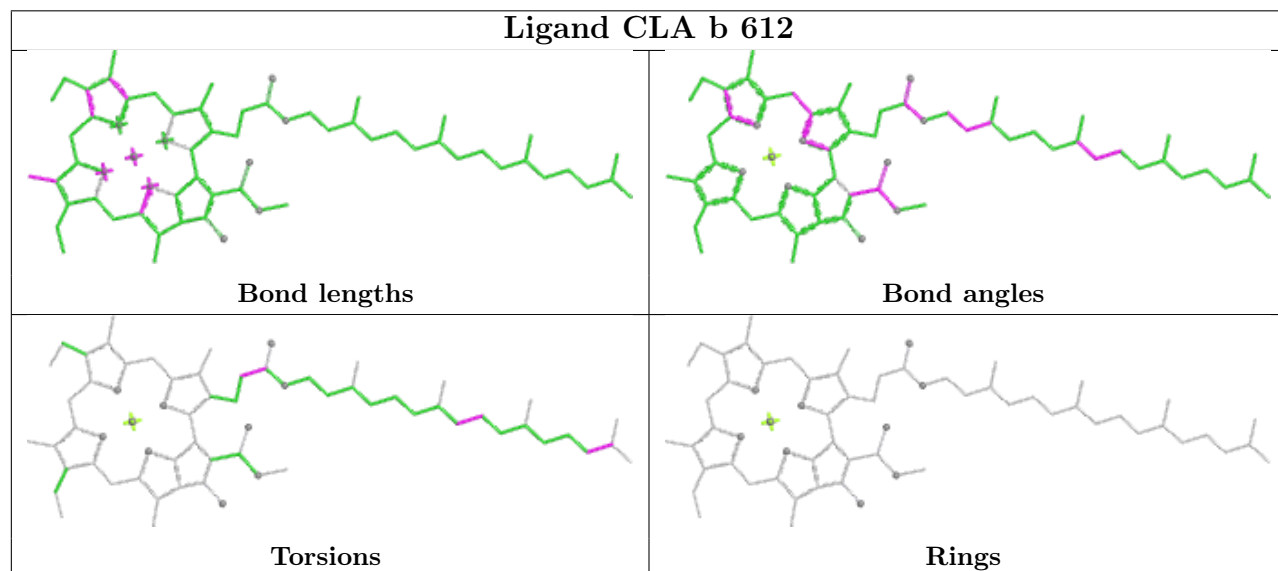
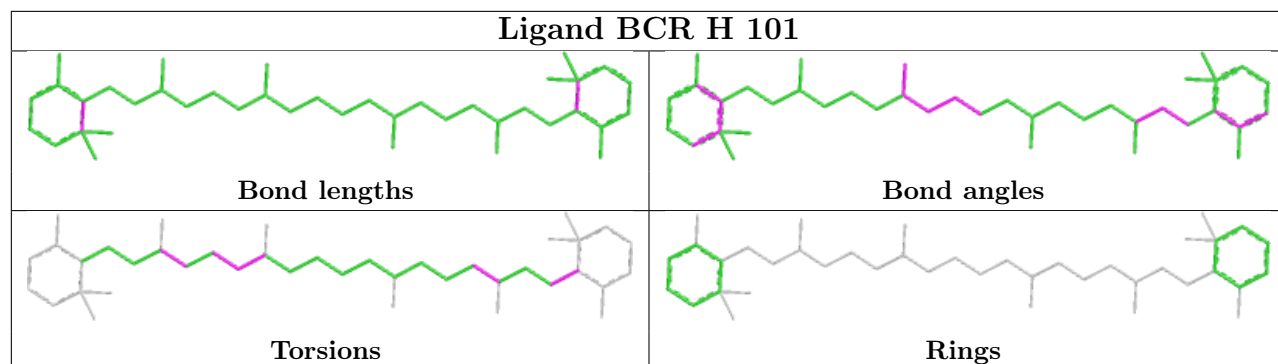


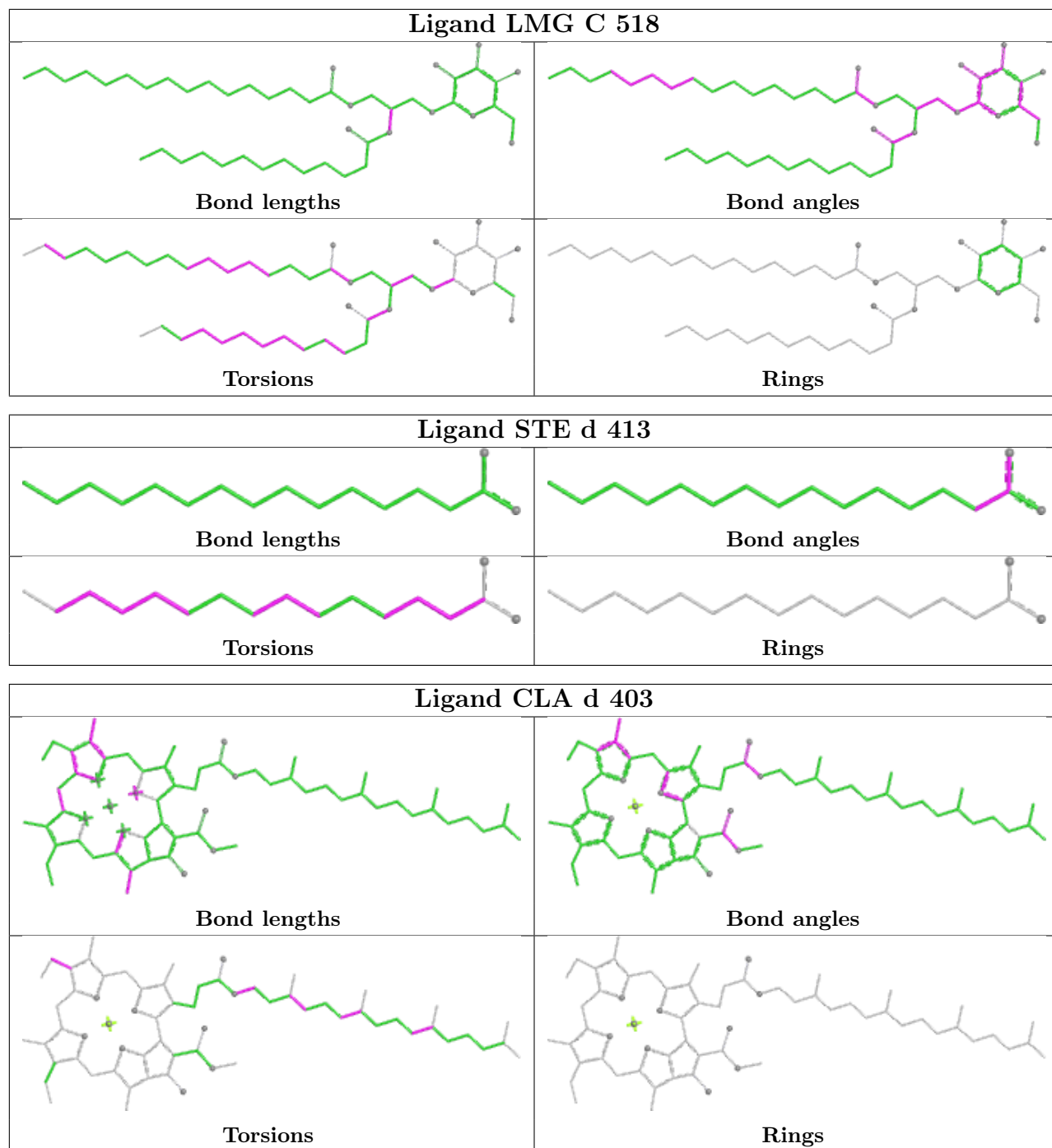


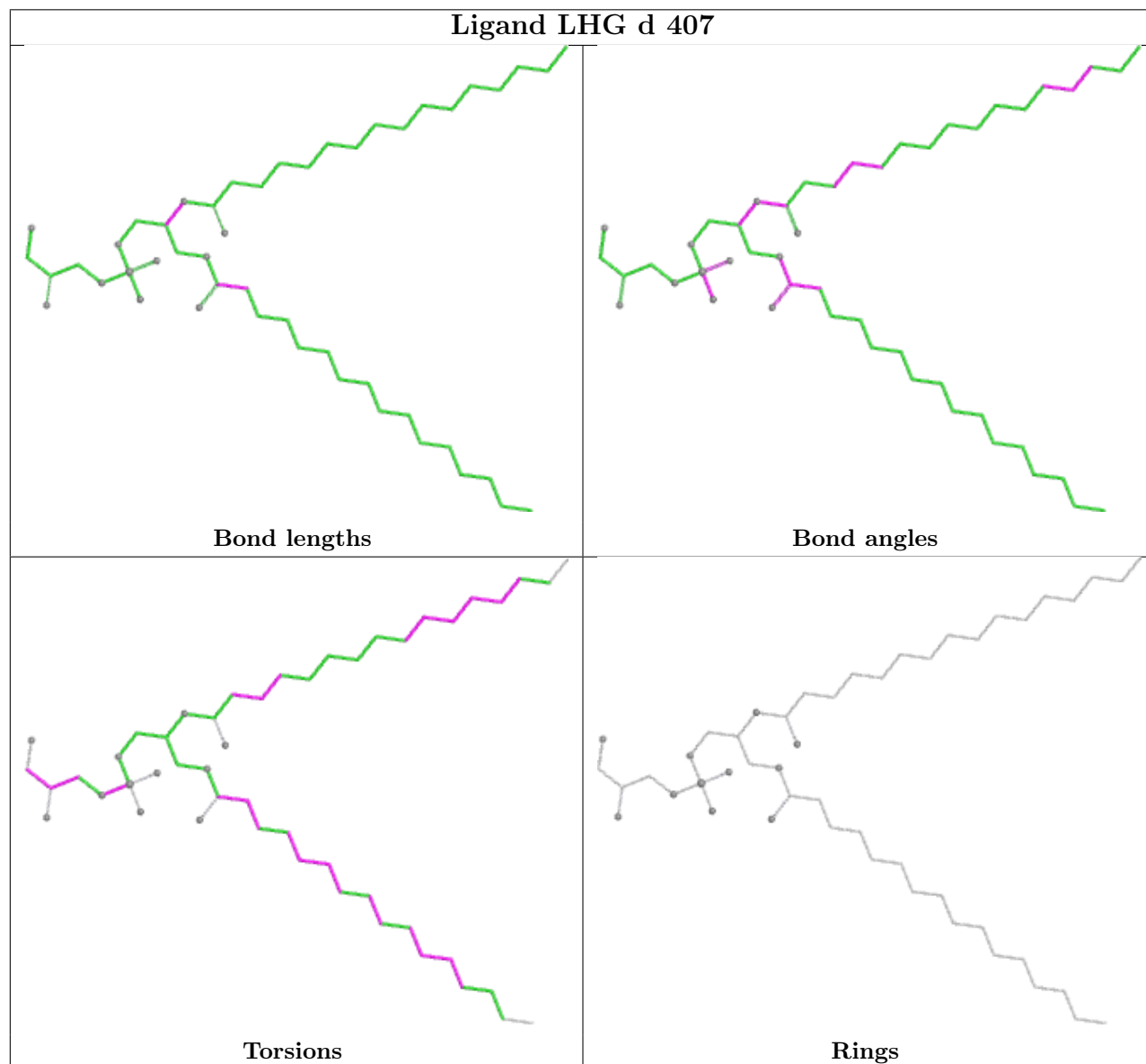
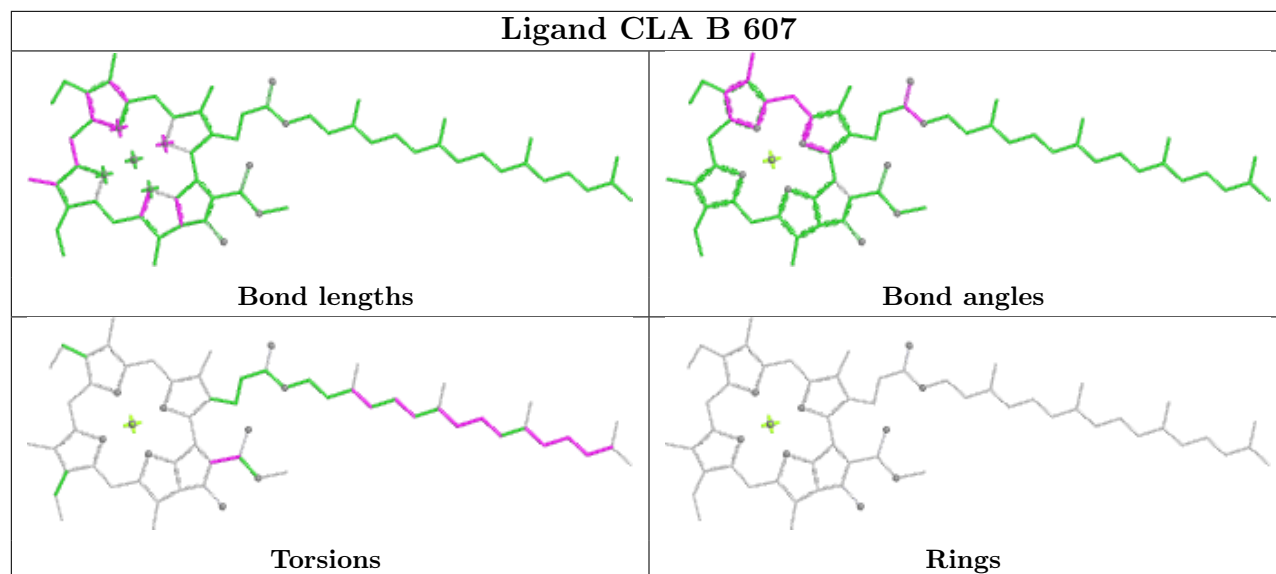


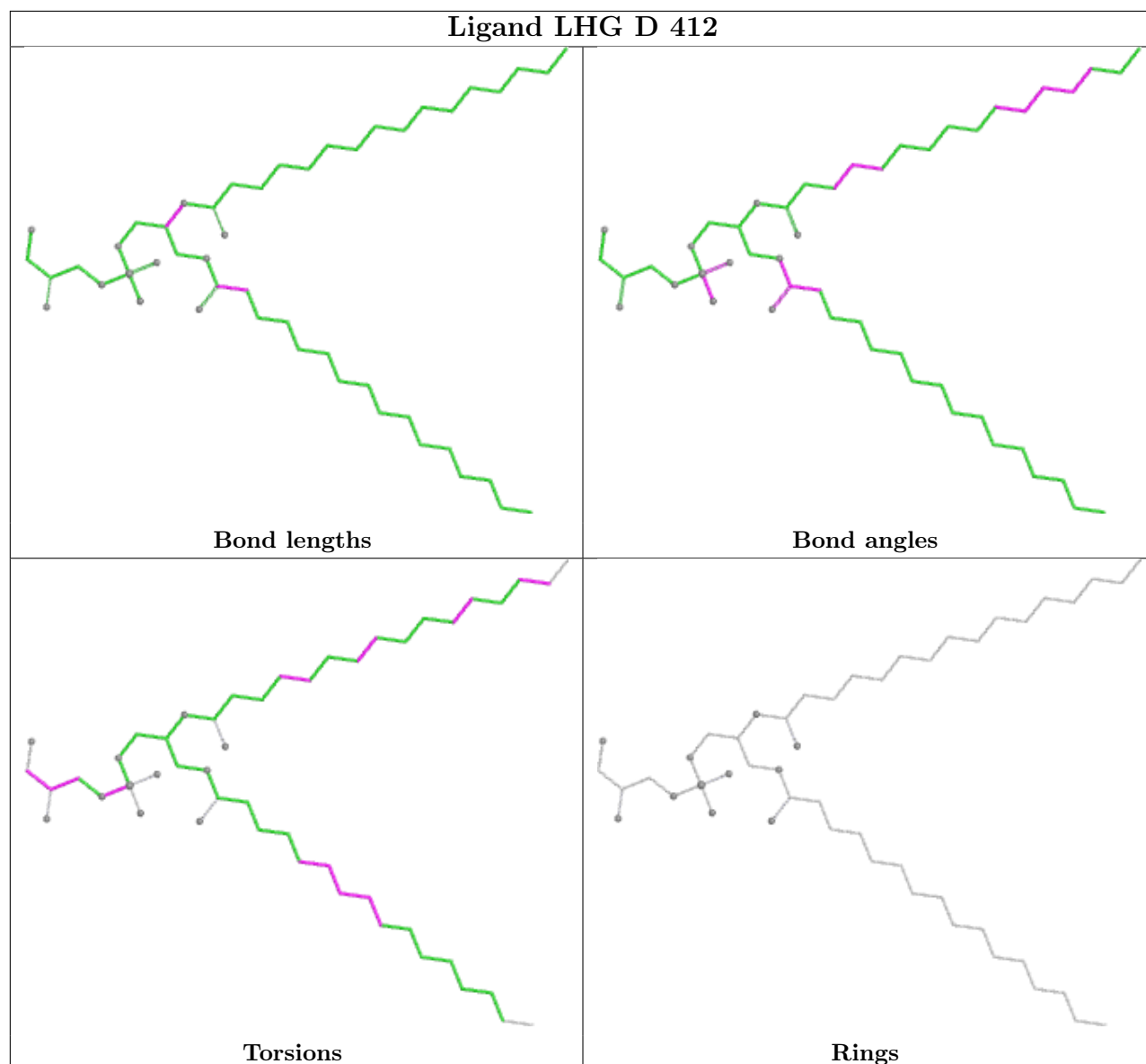
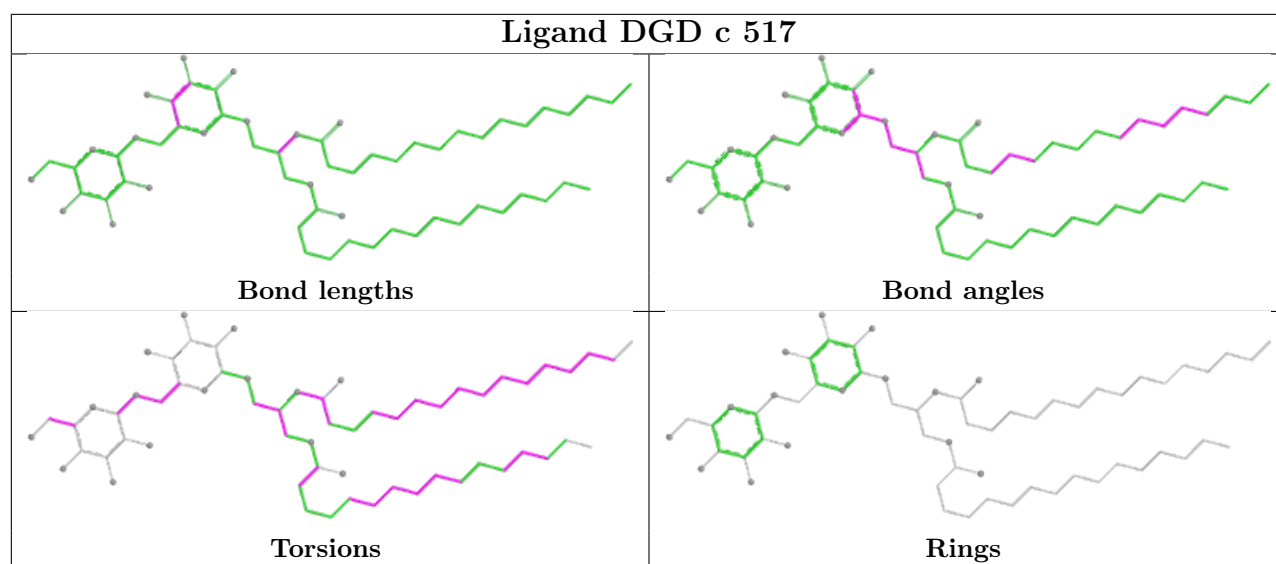


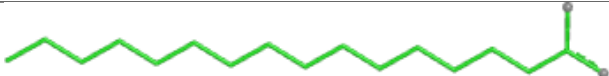
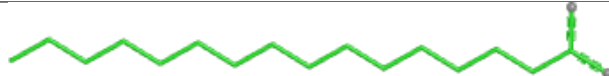
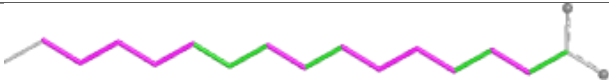
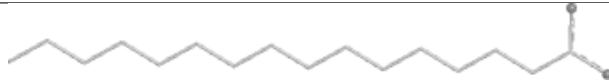


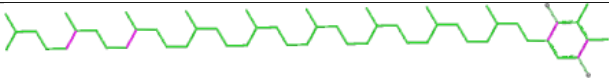
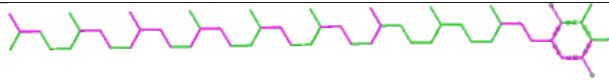
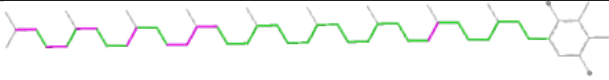
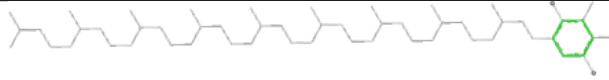


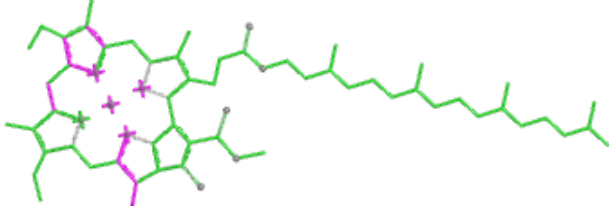
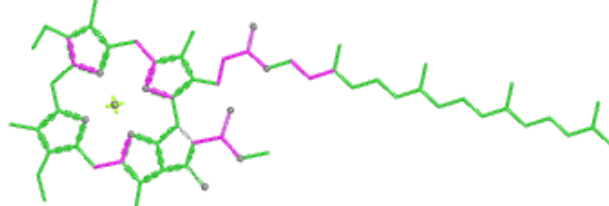
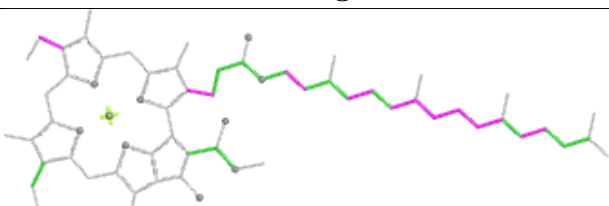
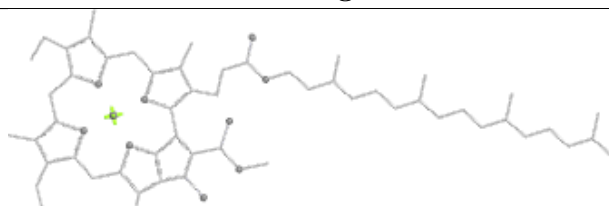


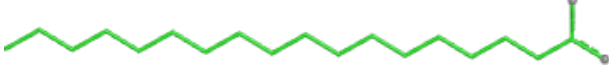
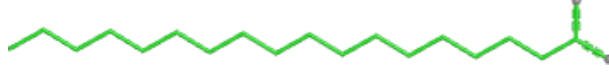
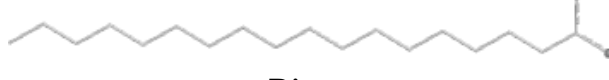


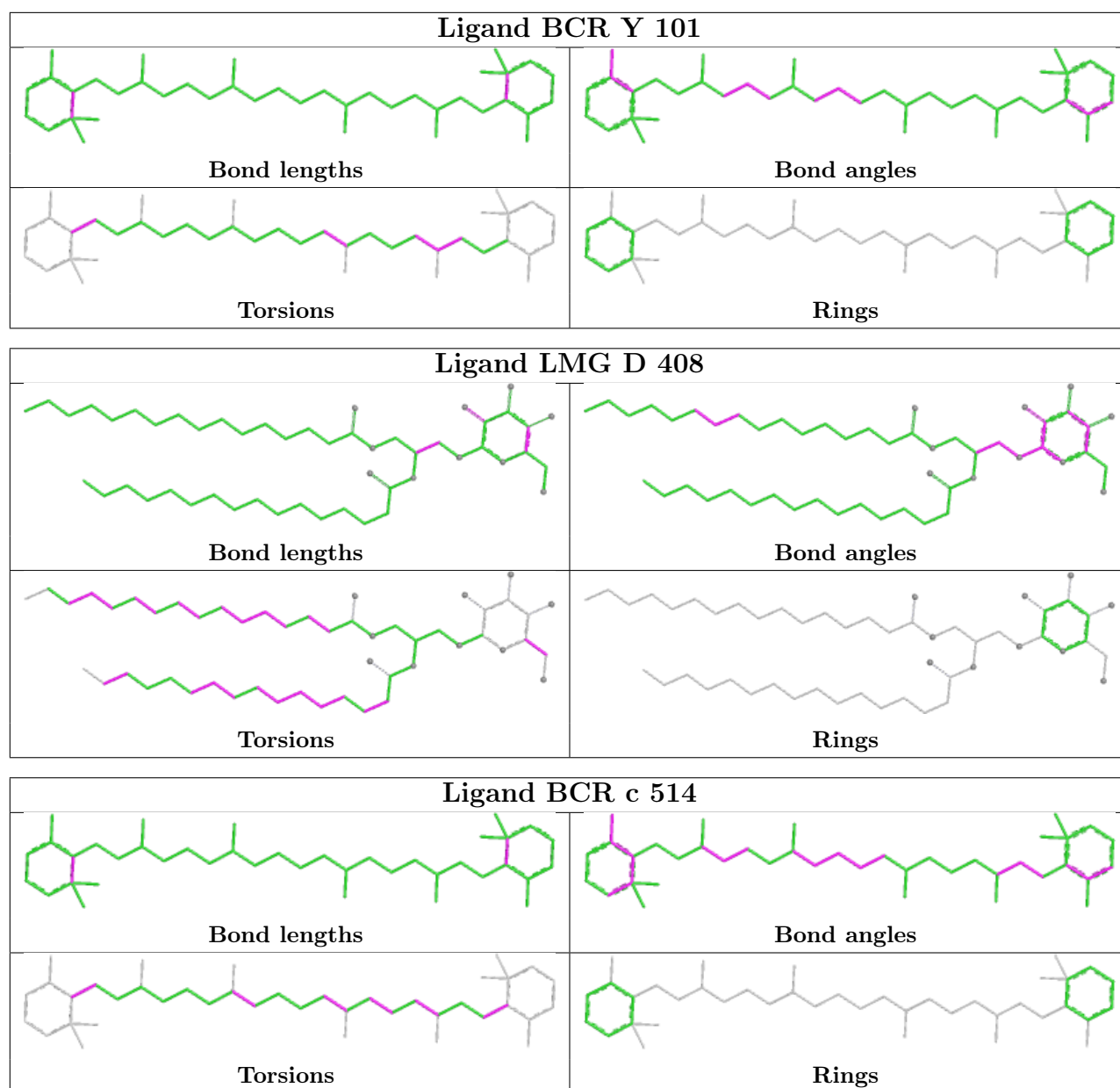


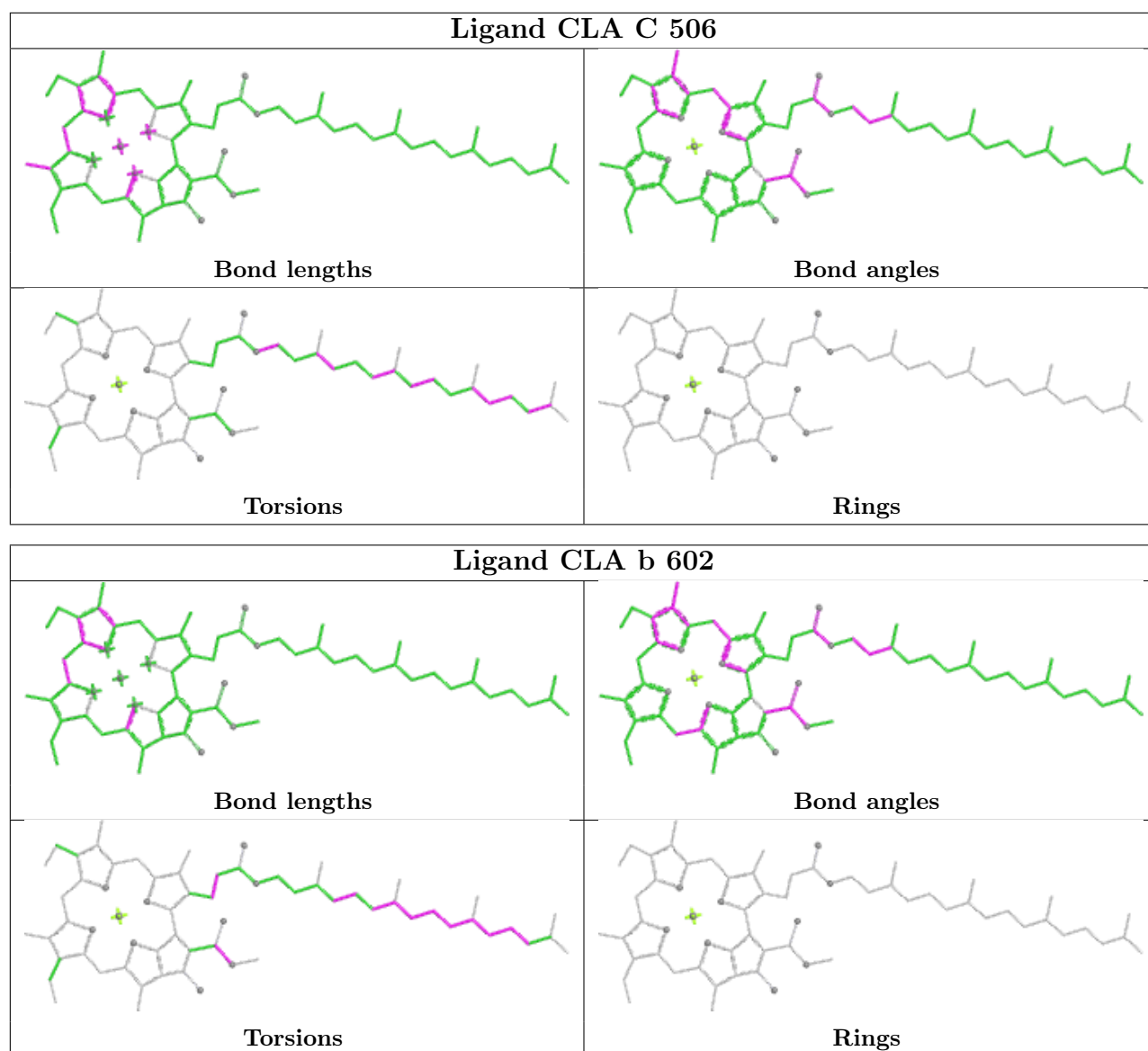
Ligand STE B 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE D 413	
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.40	0 100 100	13, 31, 52, 80	64 (19%)
1	a	334/344 (97%)	-0.30	2 (0%) 85 87	13, 33, 58, 76	64 (19%)
2	B	505/510 (99%)	-0.33	2 (0%) 88 90	19, 35, 62, 88	4 (0%)
2	b	505/510 (99%)	-0.18	5 (0%) 79 81	27, 38, 71, 111	0
3	C	442/461 (95%)	-0.25	0 100 100	15, 38, 54, 79	11 (2%)
3	c	451/461 (97%)	-0.14	1 (0%) 91 92	15, 41, 62, 97	12 (2%)
4	D	341/352 (96%)	-0.40	1 (0%) 90 91	15, 33, 50, 78	2 (0%)
4	d	341/352 (96%)	-0.29	0 100 100	16, 36, 59, 81	3 (0%)
5	E	82/84 (97%)	0.44	3 (3%) 45 47	36, 53, 69, 85	1 (1%)
5	e	82/84 (97%)	0.43	1 (1%) 76 78	41, 59, 79, 85	0
6	F	34/45 (75%)	0.08	1 (2%) 53 56	41, 47, 63, 85	0
6	f	34/45 (75%)	0.24	0 100 100	44, 52, 78, 94	0
7	H	65/66 (98%)	-0.08	2 (3%) 51 54	36, 42, 58, 75	0
7	h	63/66 (95%)	0.21	2 (3%) 50 53	41, 50, 61, 64	0
8	I	35/38 (92%)	-0.22	0 100 100	34, 40, 67, 83	0
8	i	35/38 (92%)	-0.10	1 (2%) 53 56	33, 42, 72, 80	0
9	J	36/40 (90%)	0.00	0 100 100	36, 51, 78, 88	0
9	j	36/40 (90%)	0.39	1 (2%) 55 57	42, 53, 86, 98	0
10	K	37/46 (80%)	0.16	0 100 100	46, 54, 71, 83	0
10	k	37/46 (80%)	0.34	0 100 100	49, 56, 70, 83	0
11	L	37/37 (100%)	-0.42	0 100 100	27, 32, 63, 68	0
11	l	36/37 (97%)	-0.51	0 100 100	28, 33, 66, 88	0
12	M	32/36 (88%)	-0.40	0 100 100	30, 36, 58, 70	0
12	m	31/36 (86%)	-0.41	0 100 100	28, 35, 52, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.09	2 (0%) 82 84	29, 43, 79, 132	1 (0%)
13	o	244/272 (89%)	-0.07	1 (0%) 88 90	29, 42, 82, 123	0
14	T	29/32 (90%)	-0.40	1 (3%) 48 50	29, 34, 60, 72	0
14	t	29/32 (90%)	-0.36	1 (3%) 48 50	29, 34, 73, 89	0
15	U	97/134 (72%)	-0.06	0 100 100	33, 45, 69, 86	0
15	u	97/134 (72%)	-0.15	1 (1%) 79 81	32, 42, 58, 87	0
16	V	137/163 (84%)	-0.18	0 100 100	32, 42, 55, 80	0
16	v	137/163 (84%)	-0.01	0 100 100	35, 48, 67, 85	0
17	Y	27/46 (58%)	0.96	2 (7%) 20 22	55, 72, 92, 96	0
17	y	30/46 (65%)	0.76	0 100 100	62, 75, 88, 94	0
18	X	38/41 (92%)	0.06	1 (2%) 57 60	42, 52, 69, 78	0
18	x	39/41 (95%)	0.32	2 (5%) 33 35	51, 61, 87, 99	0
19	Z	62/62 (100%)	0.85	3 (4%) 35 38	55, 69, 108, 124	0
19	z	62/62 (100%)	0.73	3 (4%) 35 38	61, 71, 112, 117	0
20	R	34/41 (82%)	0.96	3 (8%) 15 16	64, 75, 84, 93	0
20	r	31/41 (75%)	1.36	4 (12%) 7 8	75, 94, 112, 117	0
All	All	5302/5700 (93%)	-0.14	46 (0%) 81 83	13, 40, 74, 132	162 (3%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	35	LEU	4.3
9	j	6	GLY	3.9
14	t	30	THR	3.5
19	Z	62	VAL	3.5
13	O	60	ARG	3.1
20	r	14	LEU	3.1
5	e	79	PHE	3.1
13	o	58	ASN	3.0
7	H	41	PHE	2.9
19	z	27	TYR	2.9
3	c	23	ALA	2.8
19	Z	33	TRP	2.8
17	Y	25	ILE	2.8
19	z	33	TRP	2.8
7	H	65	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
13	O	59	LYS	2.6
5	E	3	GLY	2.6
6	F	12	SER	2.6
20	r	3	TRP	2.6
17	Y	22	LEU	2.5
20	r	18	TRP	2.5
18	X	2	THR	2.5
7	h	64	ALA	2.5
1	a	250	ALA	2.4
15	u	53	ALA	2.4
2	b	499	VAL	2.4
2	b	495	PHE	2.3
18	x	40	SER	2.3
19	z	40	ILE	2.3
14	T	30	THR	2.3
4	D	227	GLU	2.3
19	Z	30	PRO	2.2
5	E	79	PHE	2.2
5	E	4	THR	2.2
20	R	6	LEU	2.2
2	B	479[A]	PHE	2.1
7	h	41	PHE	2.1
20	r	28	VAL	2.1
2	B	495	PHE	2.1
18	x	37	VAL	2.1
2	b	486	LEU	2.1
20	R	13	LEU	2.1
2	b	488	PRO	2.0
2	b	496	TYR	2.0
8	i	36	ASP	2.0
1	a	245	THR	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
14	FME	t	1	10/11	0.92	0.09	33,40,56,70	0
14	FME	T	1	10/11	0.94	0.09	29,41,54,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	I	1	10/11	0.94	0.09	38,46,49,50	0
12	FME	M	1	10/11	0.95	0.09	39,47,62,64	0
12	FME	m	1	10/11	0.96	0.09	30,46,64,66	0
8	FME	i	1	10/11	0.96	0.08	36,49,53,53	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($\text{\AA}^2$)	Q<0.9
33	STE	b	622	20/20	0.74	0.17	47,58,69,70	0
33	STE	H	103	18/20	0.75	0.19	47,63,69,73	0
31	LHG	A	614	49/49	0.76	0.16	54,76,98,103	0
29	LMG	b	621	55/55	0.78	0.17	53,65,77,85	0
33	STE	x	102	20/20	0.78	0.15	45,53,60,64	0
29	LMG	c	522	48/55	0.80	0.15	45,69,89,93	0
33	STE	m	102	12/20	0.80	0.18	50,56,67,69	0
33	STE	a	616	10/20	0.80	0.15	37,55,60,62	0
32	DGD	a	615	44/66	0.81	0.14	36,51,70,72	0
33	STE	B	626	16/20	0.81	0.15	42,59,71,72	0
28	PL9	A	611	55/55	0.81	0.17	42,61,74,85	0
33	STE	I	101	15/20	0.81	0.16	39,48,61,65	0
29	LMG	d	410	23/55	0.82	0.17	41,59,69,72	0
33	STE	E	102	12/20	0.82	0.15	60,67,83,84	0
33	STE	b	623	10/20	0.82	0.13	43,50,62,63	0
33	STE	c	521	20/20	0.82	0.13	42,54,83,83	0
33	STE	c	523	12/20	0.82	0.12	54,62,72,77	0
31	LHG	e	101	42/49	0.82	0.14	57,77,97,102	0
30	SQD	a	614	36/54	0.82	0.14	35,55,66,72	0
29	LMG	A	612	48/55	0.83	0.12	45,57,68,75	0
33	STE	J	101	12/20	0.83	0.14	46,54,61,64	0
33	STE	T	102	16/20	0.83	0.14	36,47,61,66	0
33	STE	d	412	16/20	0.83	0.14	48,54,75,77	0
29	LMG	D	411	33/55	0.83	0.14	41,52,69,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	PL9	a	611	55/55	0.83	0.16	43,64,79,85	0
32	DGD	A	617	66/66	0.84	0.12	45,57,67,74	0
33	STE	a	617	12/20	0.84	0.12	52,58,64,66	0
25	CLA	b	601	65/65	0.84	0.12	49,64,78,89	0
33	STE	B	620	17/20	0.85	0.12	38,47,64,66	0
30	SQD	A	616	39/54	0.86	0.13	39,49,72,77	0
30	SQD	f	102	41/54	0.86	0.14	63,78,89,92	0
33	STE	j	101	12/20	0.86	0.13	49,55,61,67	0
33	STE	T	103	15/20	0.86	0.14	44,53,64,66	0
33	STE	C	521	16/20	0.86	0.13	37,49,64,65	0
33	STE	D	413	20/20	0.87	0.12	37,46,70,81	0
33	STE	b	620	20/20	0.87	0.11	38,52,71,73	0
29	LMG	c	520	37/55	0.87	0.12	45,64,74,77	0
33	STE	C	519	12/20	0.87	0.12	34,42,52,53	0
33	STE	B	624	18/20	0.87	0.12	40,49,78,85	0
33	STE	C	520	12/20	0.88	0.11	43,49,57,58	0
29	LMG	c	524	49/55	0.88	0.10	40,56,68,73	0
33	STE	B	625	12/20	0.88	0.12	44,59,64,67	0
30	SQD	B	622	54/54	0.88	0.11	40,57,82,93	0
25	CLA	B	601	65/65	0.88	0.11	37,53,75,87	0
29	LMG	M	101	51/55	0.89	0.10	31,46,62,65	0
29	LMG	B	621	28/55	0.89	0.12	38,48,58,70	0
29	LMG	m	101	51/55	0.89	0.10	34,49,64,70	0
29	LMG	C	518	48/55	0.89	0.12	45,63,73,78	0
27	BCR	d	405	40/40	0.89	0.12	39,49,78,87	0
30	SQD	F	101	36/54	0.89	0.12	49,66,74,77	0
30	SQD	L	101	49/54	0.89	0.10	37,55,73,77	0
33	STE	t	102	14/20	0.89	0.11	36,49,54,61	0
33	STE	B	623	12/20	0.89	0.12	41,51,60,68	0
27	BCR	x	101	40/40	0.90	0.11	42,54,65,71	0
33	STE	l	102	18/20	0.90	0.12	36,44,63,66	0
33	STE	M	103	10/20	0.90	0.11	41,44,50,50	0
30	SQD	a	613	54/54	0.90	0.10	40,57,71,73	0
33	STE	d	413	17/20	0.90	0.12	46,51,62,65	0
27	BCR	Y	101	40/40	0.91	0.10	46,52,61,64	0
32	DGD	h	101	62/66	0.91	0.09	38,45,53,53	0
27	BCR	c	514	40/40	0.91	0.10	44,55,64,66	0
25	CLA	C	513	65/65	0.91	0.10	44,56,83,89	0
27	BCR	k	101	40/40	0.91	0.11	47,57,64,68	0
27	BCR	B	618	40/40	0.91	0.09	29,36,47,50	0
27	BCR	D	406	40/40	0.91	0.10	34,41,66,70	0
27	BCR	H	101	40/40	0.91	0.09	35,43,50,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	DGD	c	518	62/66	0.92	0.09	37,48,74,80	0
27	BCR	K	102	40/40	0.92	0.11	39,49,63,65	0
27	BCR	C	514	40/40	0.92	0.09	32,39,47,47	0
33	STE	M	102	15/20	0.92	0.10	37,46,62,67	0
32	DGD	C	516	62/66	0.92	0.10	38,47,83,95	0
32	DGD	H	102	62/66	0.92	0.09	34,42,49,53	0
27	BCR	K	101	40/40	0.92	0.11	49,56,60,61	0
25	CLA	c	513	65/65	0.93	0.10	47,61,81,86	0
27	BCR	A	610	40/40	0.93	0.08	27,34,40,43	0
32	DGD	C	515	62/66	0.93	0.10	27,37,65,71	0
27	BCR	T	101	40/40	0.93	0.07	31,37,49,53	0
30	SQD	A	613	52/54	0.93	0.10	32,53,75,79	0
25	CLA	C	503	65/65	0.93	0.08	33,42,47,53	0
27	BCR	b	618	40/40	0.93	0.07	28,38,48,53	0
29	LMG	D	408	51/55	0.93	0.10	33,47,64,71	0
27	BCR	B	619	40/40	0.93	0.08	32,40,46,49	0
27	BCR	c	516	40/40	0.93	0.11	45,53,58,66	0
25	CLA	C	512	65/65	0.93	0.09	35,51,68,77	0
25	CLA	c	509	65/65	0.93	0.10	38,45,55,58	0
25	CLA	c	512	65/65	0.93	0.10	45,53,76,81	0
34	BCT	a	606	4/4	0.93	0.08	34,40,44,49	0
27	BCR	t	101	40/40	0.94	0.07	28,36,46,47	0
25	CLA	c	508	64/65	0.94	0.09	32,43,73,90	0
31	LHG	d	407	49/49	0.94	0.10	32,46,58,65	0
31	LHG	d	409	39/49	0.94	0.09	32,43,54,58	0
25	CLA	B	606	65/65	0.94	0.08	26,36,57,62	0
28	PL9	D	407	55/55	0.94	0.07	23,32,38,45	0
27	BCR	b	617	40/40	0.94	0.07	30,38,43,43	0
25	CLA	c	511	65/65	0.94	0.09	40,52,61,64	0
32	DGD	C	517	62/66	0.94	0.08	34,43,66,71	0
27	BCR	b	619	40/40	0.94	0.08	33,42,57,60	0
25	CLA	C	510	65/65	0.94	0.08	32,42,51,54	0
27	BCR	c	515	40/40	0.94	0.08	34,41,48,55	0
25	CLA	C	511	65/65	0.94	0.09	36,48,57,65	0
25	CLA	c	506	65/65	0.94	0.08	36,44,74,78	0
27	BCR	B	617	40/40	0.94	0.07	32,38,49,50	0
25	CLA	a	608	65/65	0.95	0.09	31,38,79,85	0
25	CLA	B	604	65/65	0.95	0.07	23,31,58,61	0
25	CLA	b	606	65/65	0.95	0.07	28,38,58,64	0
25	CLA	b	608	65/65	0.95	0.07	33,41,51,53	0
25	CLA	b	614	65/65	0.95	0.08	25,37,60,65	0
25	CLA	b	615	65/65	0.95	0.08	29,40,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	616	60/65	0.95	0.08	32,40,70,73	0
29	LMG	d	411	44/55	0.95	0.08	39,45,71,76	0
25	CLA	c	501	65/65	0.95	0.07	30,38,45,50	0
27	BCR	a	610	40/40	0.95	0.06	24,31,40,44	0
25	CLA	c	502	65/65	0.95	0.07	32,41,53,60	0
25	CLA	c	503	65/65	0.95	0.07	33,44,49,53	0
25	CLA	c	504	60/65	0.95	0.07	35,42,72,73	0
25	CLA	c	505	65/65	0.95	0.07	29,39,54,58	0
25	CLA	C	506	65/65	0.95	0.08	29,42,72,76	0
25	CLA	c	507	65/65	0.95	0.08	30,40,50,56	0
25	CLA	C	507	65/65	0.95	0.07	28,36,48,51	0
25	CLA	C	508	65/65	0.95	0.08	30,39,82,89	0
31	LHG	D	410	47/49	0.95	0.09	28,39,66,77	0
31	LHG	D	412	49/49	0.95	0.09	30,40,54,58	0
25	CLA	c	510	65/65	0.95	0.08	37,47,53,61	0
25	CLA	C	509	65/65	0.95	0.08	31,39,52,58	0
25	CLA	B	610	65/65	0.95	0.07	23,30,38,41	0
31	LHG	l	101	49/49	0.95	0.08	31,42,48,53	0
25	CLA	B	616	60/65	0.95	0.09	26,36,74,85	0
25	CLA	d	404	65/65	0.95	0.08	32,41,75,81	0
28	PL9	d	406	55/55	0.95	0.07	27,33,37,41	0
26	PHO	d	401	64/64	0.95	0.06	24,31,36,38	0
25	CLA	C	501	65/65	0.95	0.07	25,33,44,48	0
25	CLA	C	502	65/65	0.95	0.07	32,39,48,53	0
32	DGD	c	517	62/66	0.95	0.08	29,38,60,66	0
25	CLA	a	607	65/65	0.95	0.07	23,30,38,50	0
34	BCT	D	401	4/4	0.95	0.08	34,39,39,40	0
32	DGD	c	519	62/66	0.95	0.08	32,45,68,76	0
25	CLA	b	610	65/65	0.96	0.07	29,37,42,46	0
25	CLA	b	611	65/65	0.96	0.06	26,33,46,53	0
25	CLA	b	612	65/65	0.96	0.07	27,33,43,51	0
25	CLA	b	613	65/65	0.96	0.07	23,31,61,67	0
25	CLA	C	505	65/65	0.96	0.08	27,36,59,61	0
25	CLA	B	608	65/65	0.96	0.06	24,31,45,50	0
25	CLA	B	609	65/65	0.96	0.07	28,37,43,48	0
25	CLA	B	602	65/65	0.96	0.07	29,37,48,53	0
25	CLA	B	611	65/65	0.96	0.06	22,29,41,46	0
25	CLA	B	612	65/65	0.96	0.07	24,31,39,44	0
25	CLA	B	613	65/65	0.96	0.06	22,30,55,60	0
25	CLA	B	614	65/65	0.96	0.07	27,35,61,74	0
25	CLA	B	615	65/65	0.96	0.07	29,36,53,63	0
25	CLA	D	405	65/65	0.96	0.07	28,36,81,92	0

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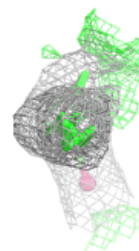
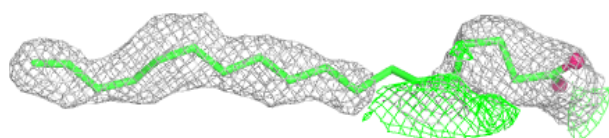
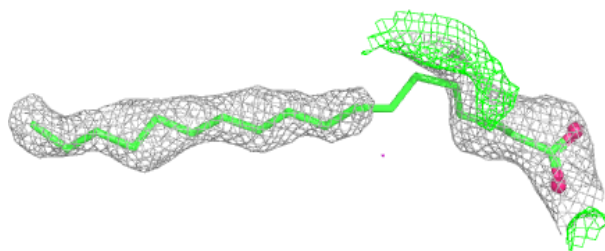
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LHG	A	615	49/49	0.96	0.07	30,37,47,57	0
31	LHG	D	409	49/49	0.96	0.07	27,36,44,52	0
25	CLA	B	603	65/65	0.96	0.07	24,31,49,53	0
25	CLA	A	607	65/65	0.96	0.09	26,32,83,88	0
25	CLA	a	609	65/65	0.96	0.08	23,30,63,67	0
31	LHG	d	408	49/49	0.96	0.07	30,40,47,57	0
25	CLA	a	612	65/65	0.96	0.06	22,30,36,42	0
25	CLA	B	605	65/65	0.96	0.06	23,31,40,42	0
25	CLA	b	602	65/65	0.96	0.07	30,39,51,55	0
25	CLA	d	403	65/65	0.96	0.07	25,33,46,55	0
25	CLA	b	603	65/65	0.96	0.07	25,33,55,62	0
26	PHO	A	608	64/64	0.96	0.05	20,28,33,39	0
26	PHO	D	402	64/64	0.96	0.06	25,32,38,42	0
25	CLA	b	604	65/65	0.96	0.08	25,33,63,76	0
26	PHO	d	402	64/64	0.96	0.06	29,38,43,49	0
25	CLA	b	605	65/65	0.96	0.07	22,35,43,46	0
25	CLA	A	606	65/65	0.96	0.06	22,27,37,43	0
25	CLA	C	504	59/65	0.96	0.07	32,39,66,71	0
25	CLA	b	609	65/65	0.96	0.07	33,41,55,63	0
35	HEM	f	101	43/43	0.96	0.09	47,59,75,85	0
25	CLA	b	607	65/65	0.97	0.07	22,32,50,58	0
25	CLA	D	404	65/65	0.97	0.06	21,29,45,48	0
25	CLA	A	609	54/65	0.97	0.06	21,28,58,62	0
25	CLA	B	607	65/65	0.97	0.07	20,29,52,58	0
35	HEM	E	101	43/43	0.97	0.08	44,50,62,68	0
25	CLA	D	403	65/65	0.97	0.05	21,27,38,44	0
24	CL	a	604	1/1	0.98	0.05	32,32,32,32	0
36	HEC	V	201	43/43	0.98	0.07	27,34,41,45	0
36	HEC	v	201	43/43	0.98	0.07	31,38,43,50	0
22	OEX	a	602[A]	10/10	0.99	0.03	29,32,36,37	10
23	FE2	a	603	1/1	0.99	0.02	38,38,38,38	0
24	CL	A	604	1/1	0.99	0.04	33,33,33,33	0
24	CL	A	605	1/1	0.99	0.08	34,34,34,34	0
21	OEY	A	601[B]	11/11	0.99	0.03	26,29,33,34	11
24	CL	a	605	1/1	0.99	0.08	33,33,33,33	0
21	OEY	a	601[B]	11/11	0.99	0.03	27,30,33,38	11
22	OEX	A	602[A]	10/10	0.99	0.03	31,32,36,38	10
23	FE2	A	603	1/1	1.00	0.01	32,32,32,32	0

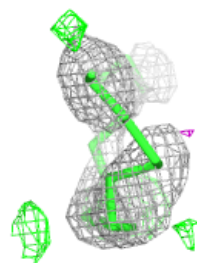
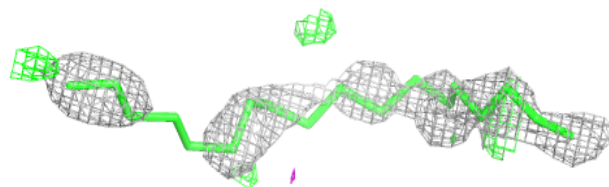
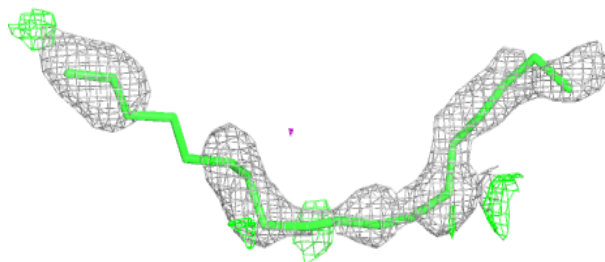
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

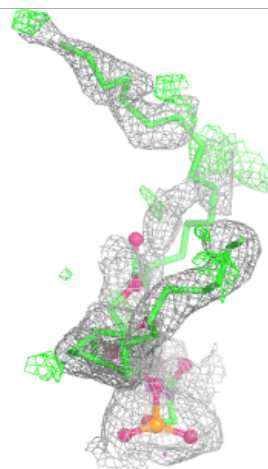
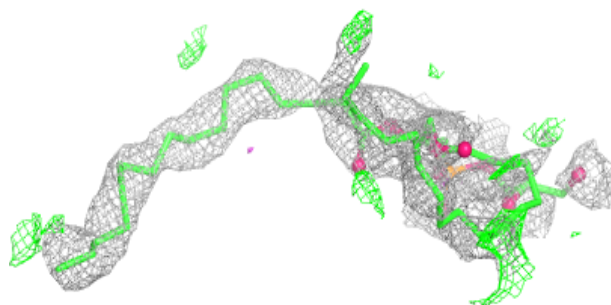
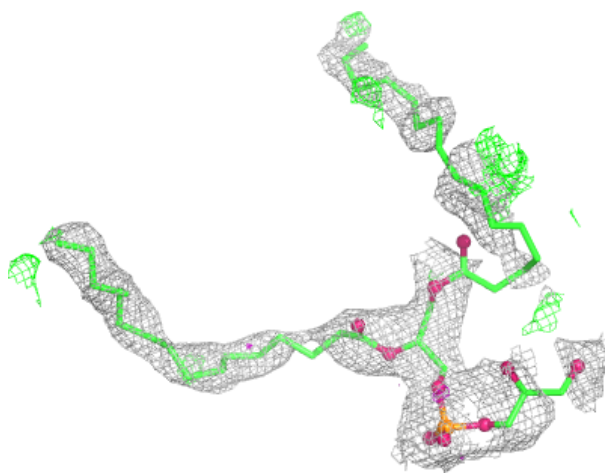
**Electron density around STE H 103:**

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



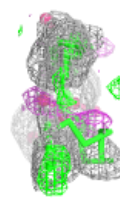
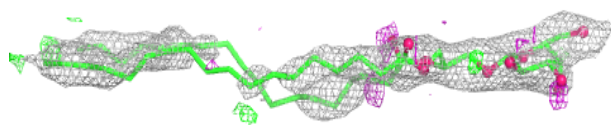
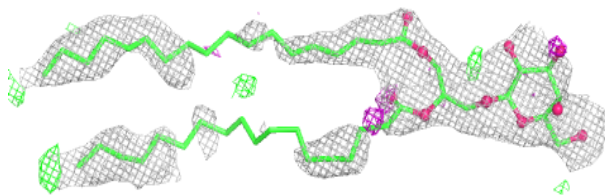
Electron density around LHG A 614:

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

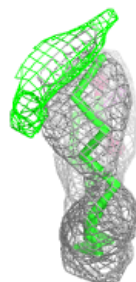
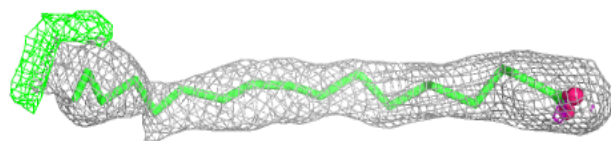
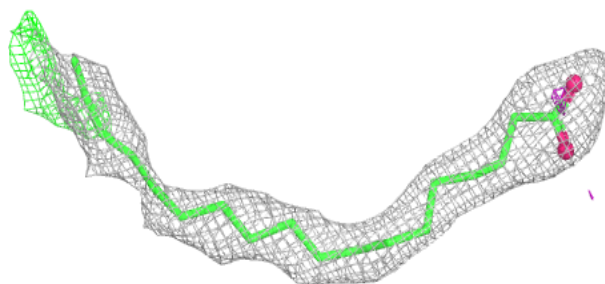


Electron density around LMG b 621:

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

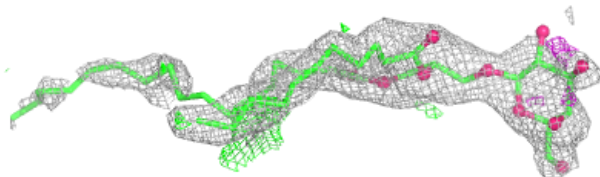
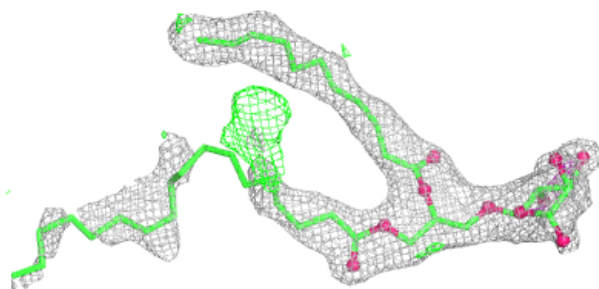
**Electron density around STE x 102:**

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

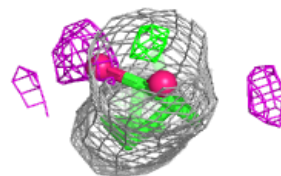
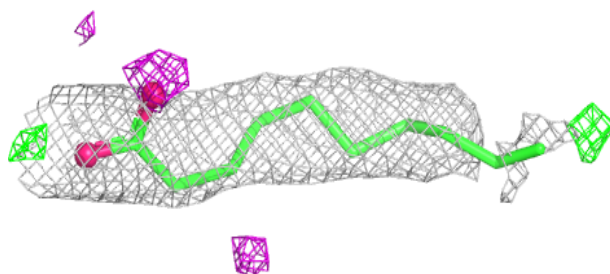
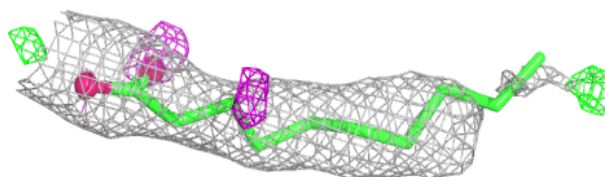


Electron density around LMG c 522:

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

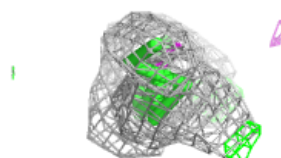
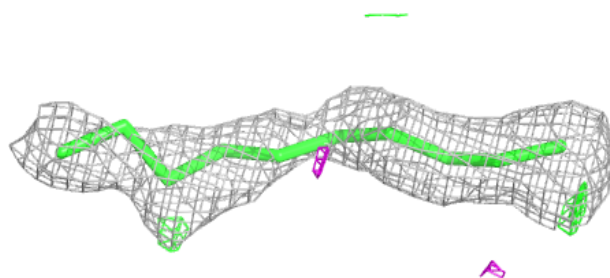
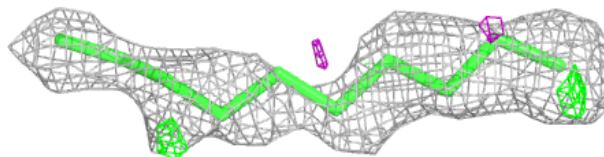
**Electron density around STE m 102:**

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

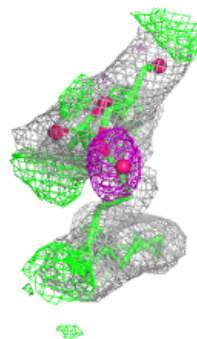
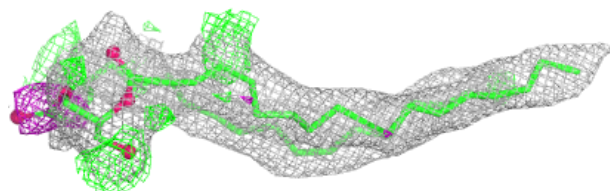
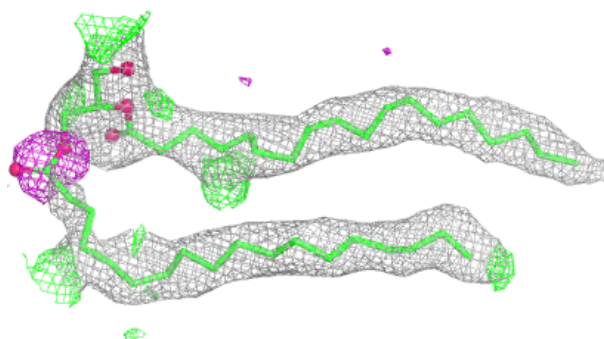


Electron density around STE a 616:

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

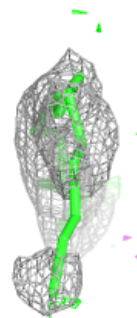
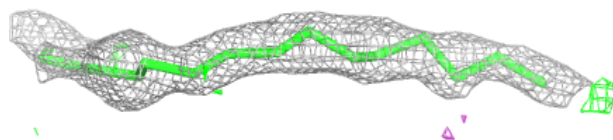
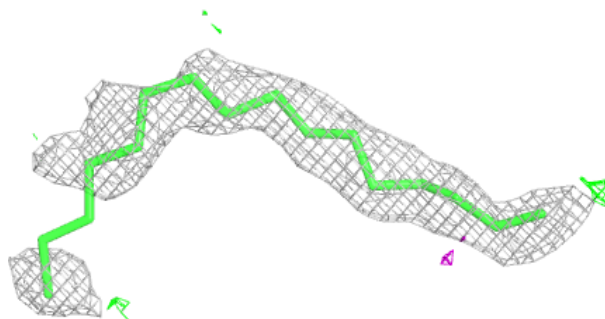
**Electron density around DGD a 615:**

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

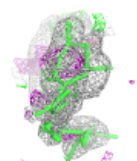
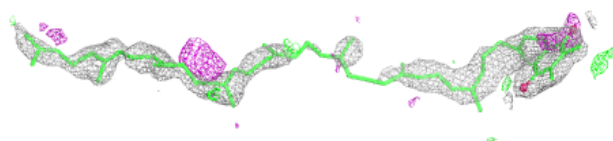
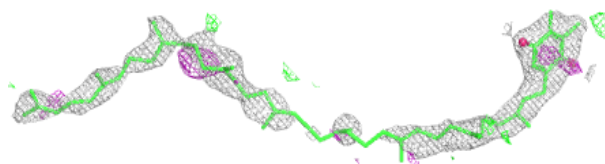


Electron density around STE B 626:

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

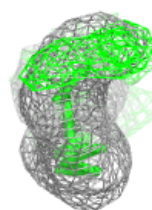
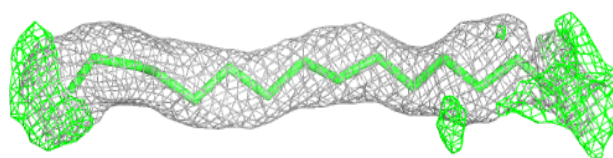
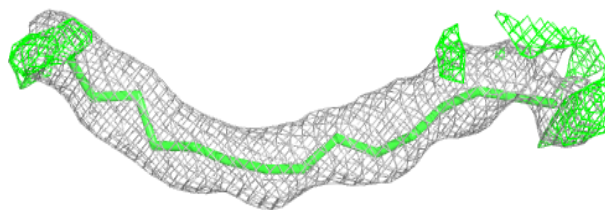
**Electron density around PL9 A 611:**

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

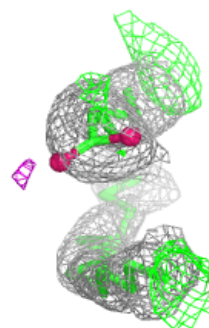
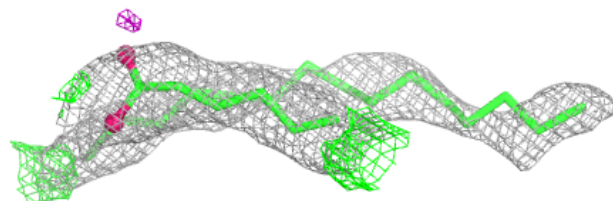
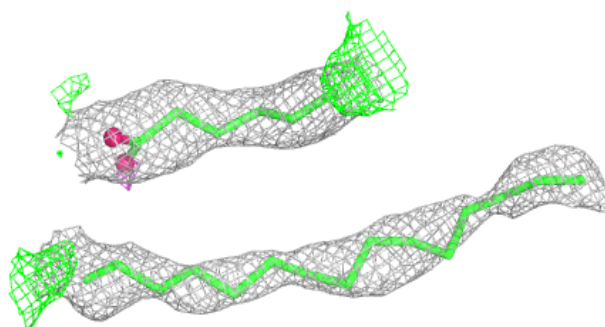


Electron density around STE I 101:

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

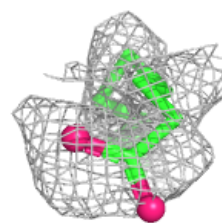
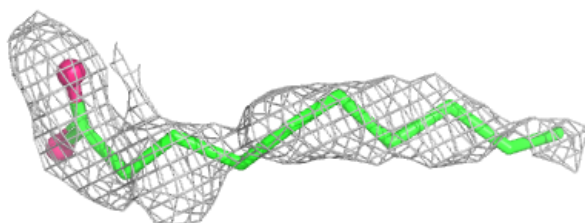
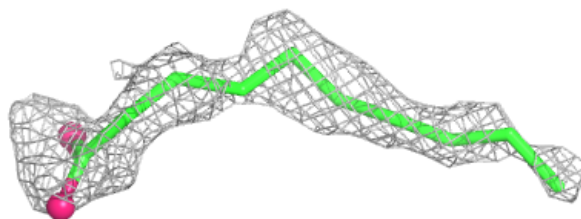
**Electron density around LMG d 410:**

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

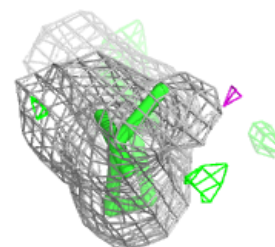
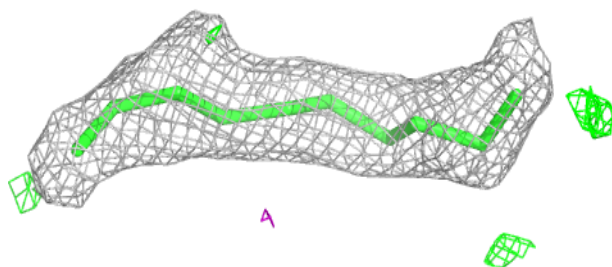
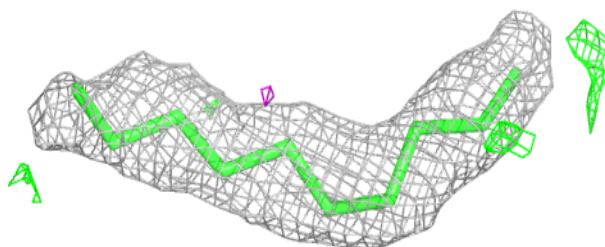


Electron density around STE E 102:

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

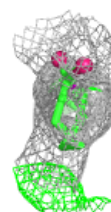
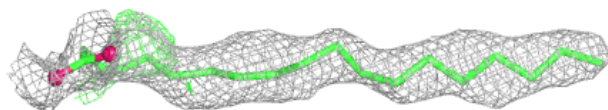
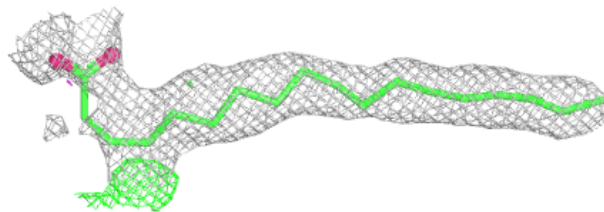
**Electron density around STE b 623:**

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

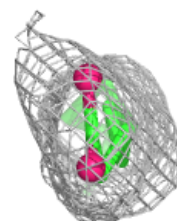
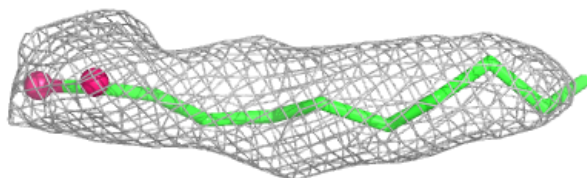
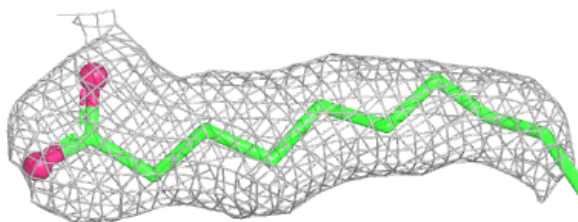


Electron density around STE c 521:

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

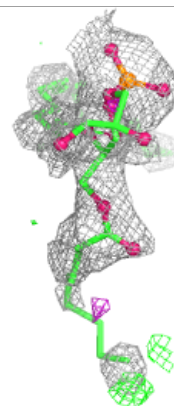
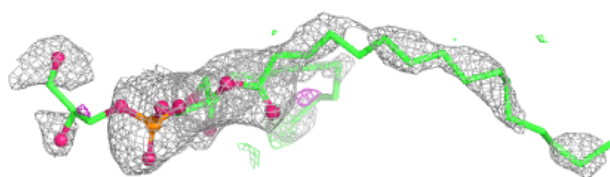
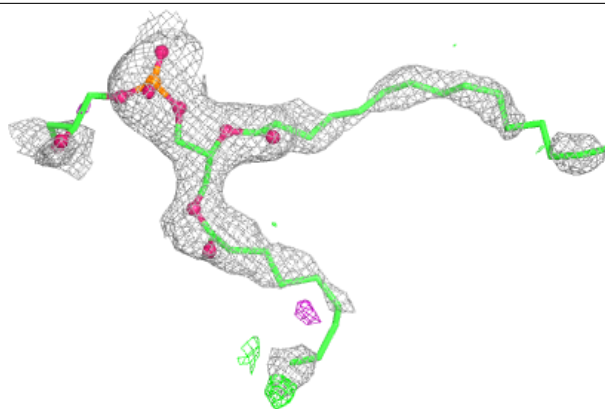
**Electron density around STE c 523:**

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



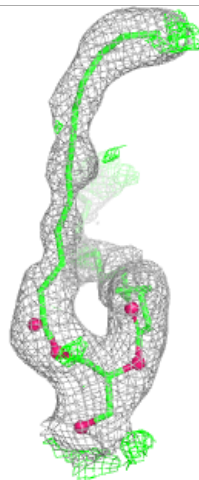
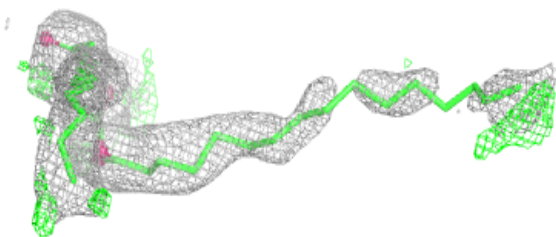
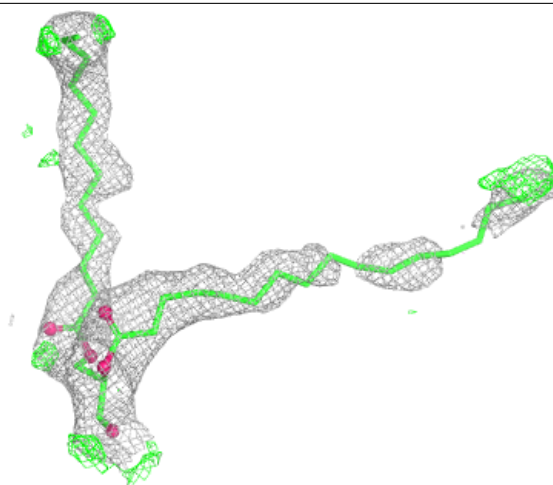
Electron density around LHG e 101:

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



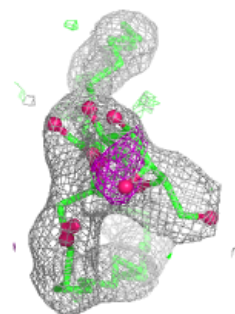
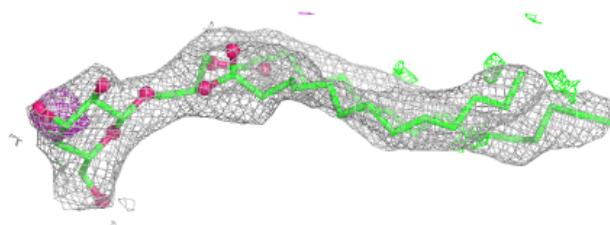
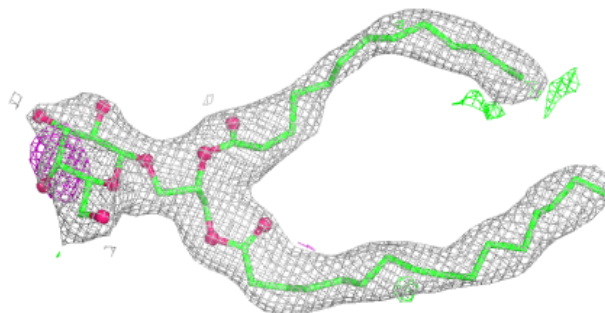
Electron density around SQD a 614:

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

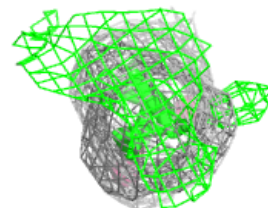
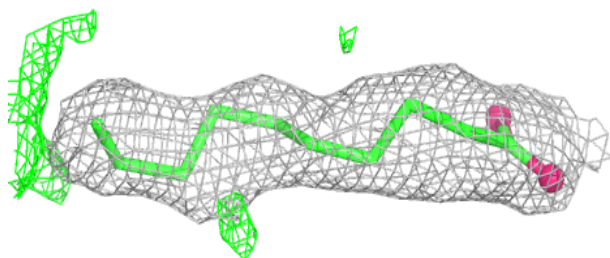
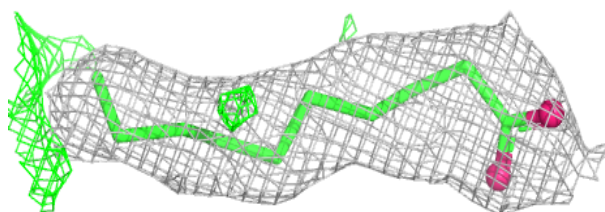


Electron density around LMG A 612:

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

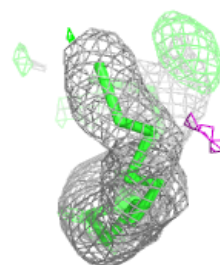
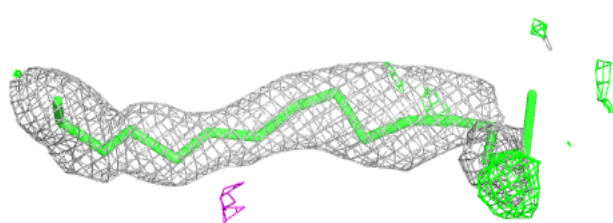
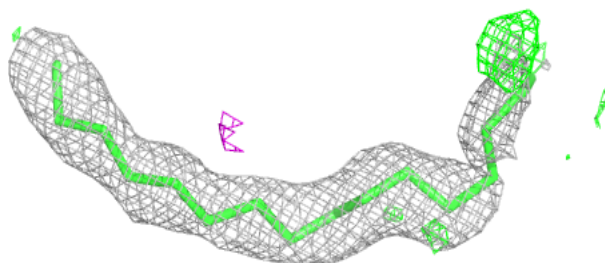
**Electron density around STE J 101:**

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

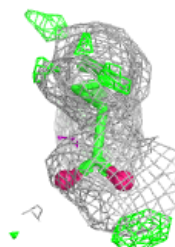
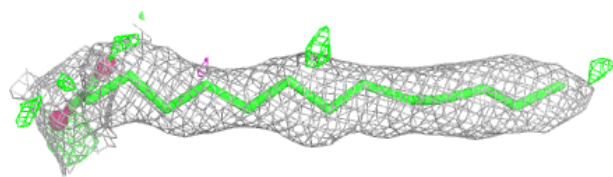
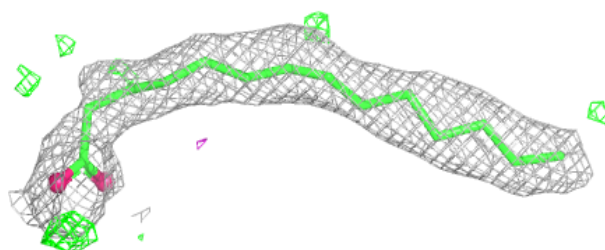


Electron density around STE T 102:

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

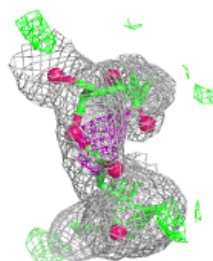
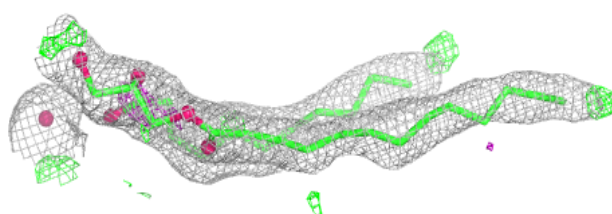
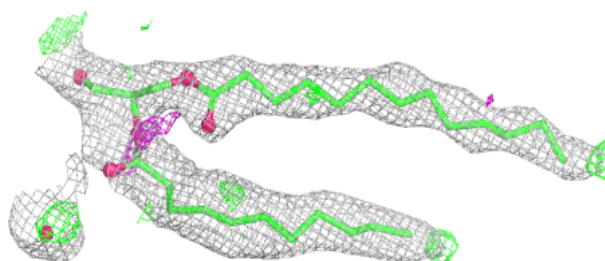
**Electron density around STE d 412:**

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

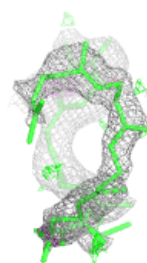
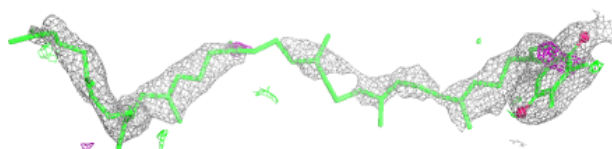
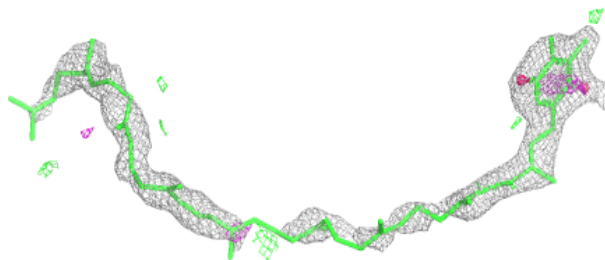


Electron density around LMG D 411:

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

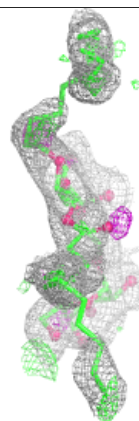
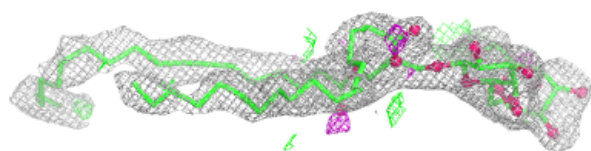
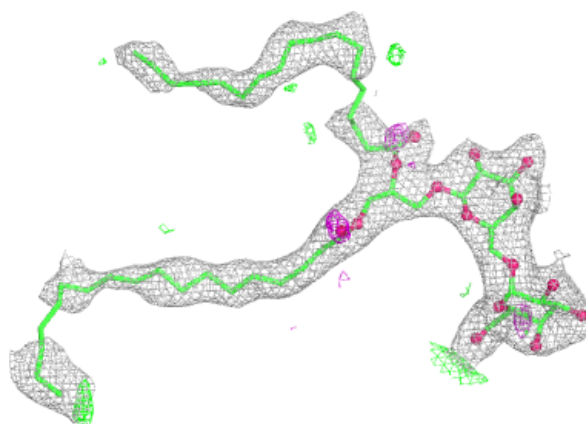
**Electron density around PL9 a 611:**

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

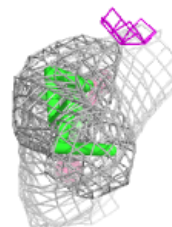
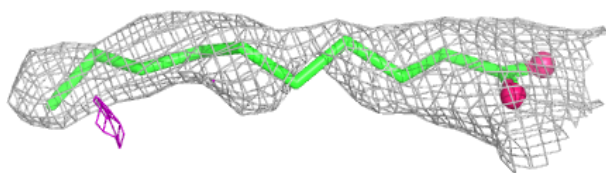
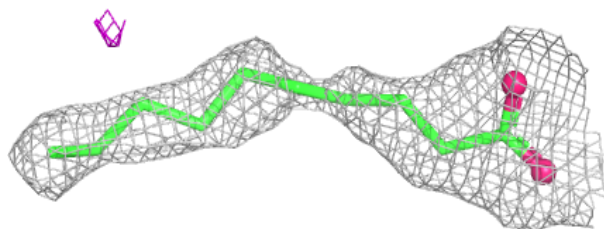


Electron density around DGD A 617:

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

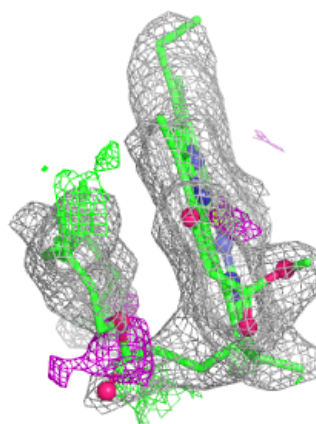
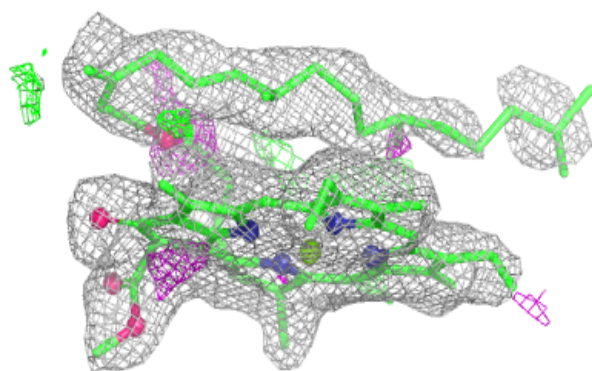
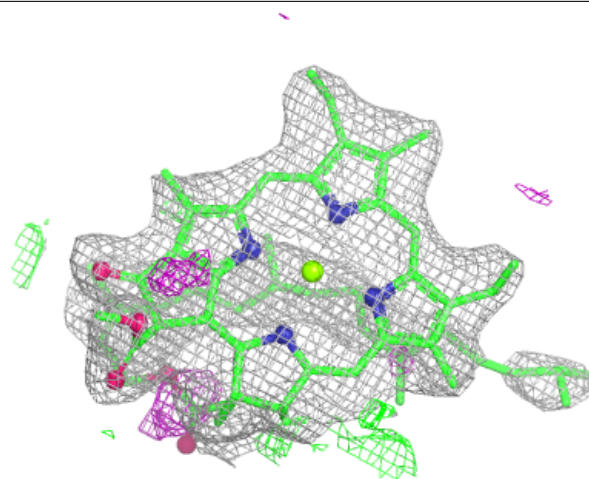
**Electron density around STE a 617:**

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



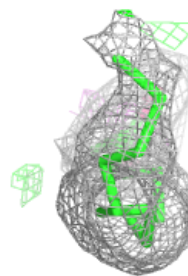
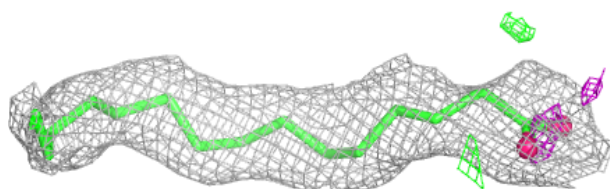
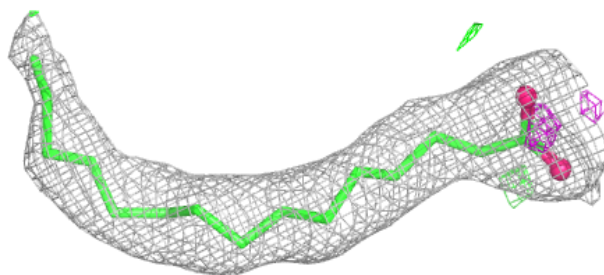
Electron density around CLA b 601:

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



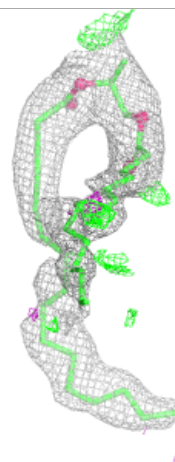
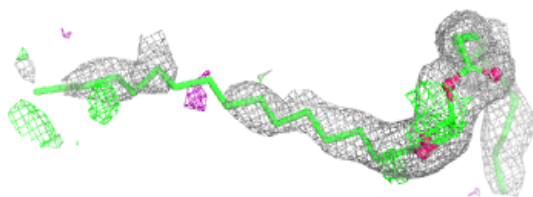
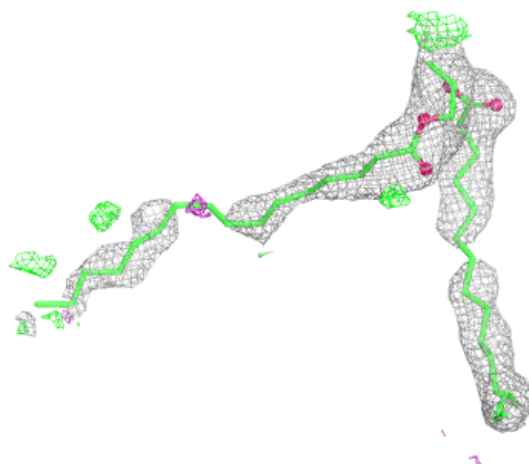
Electron density around STE B 620:

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



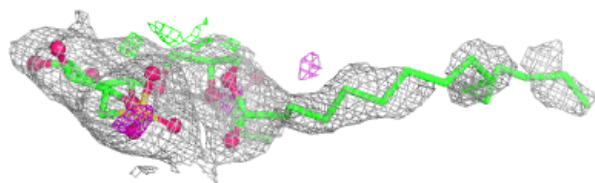
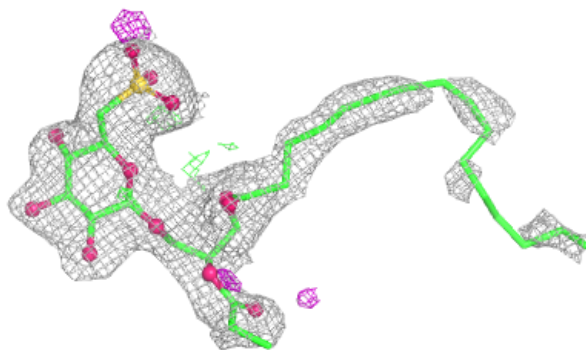
Electron density around SQD A 616:

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

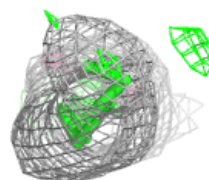
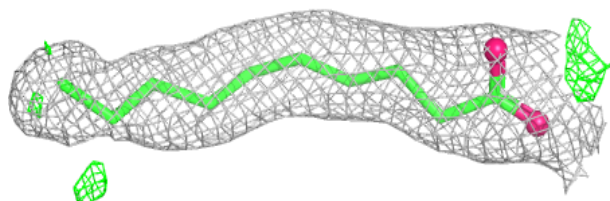
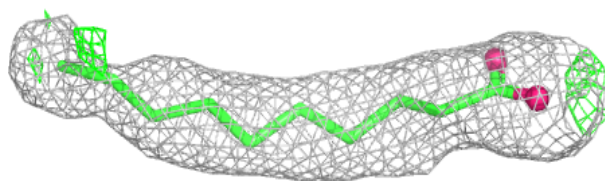


Electron density around SQD f 102:

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

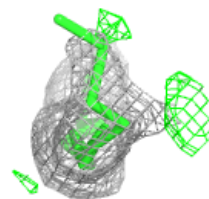
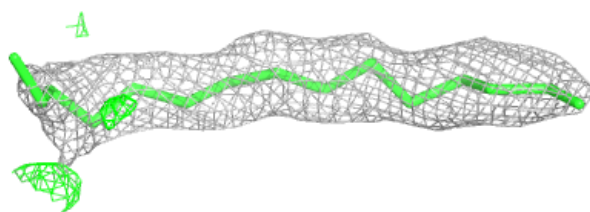
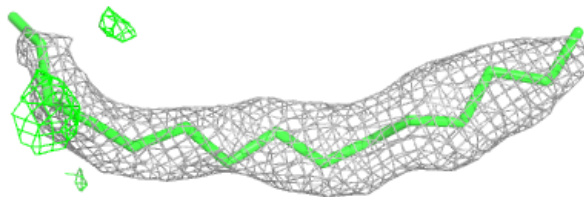
**Electron density around STE j 101:**

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

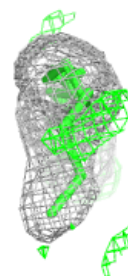
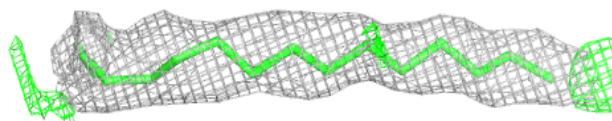
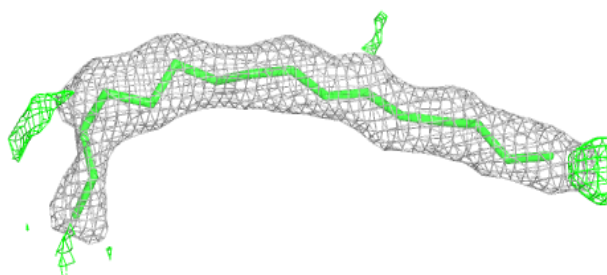


Electron density around STE T 103:

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

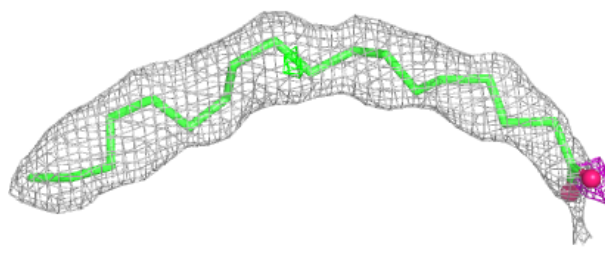
**Electron density around STE C 521:**

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

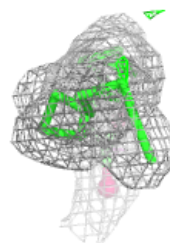
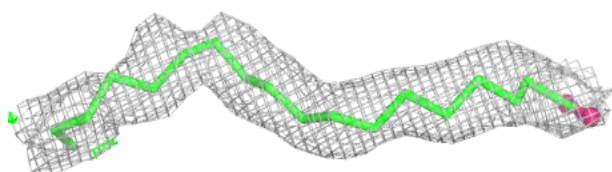
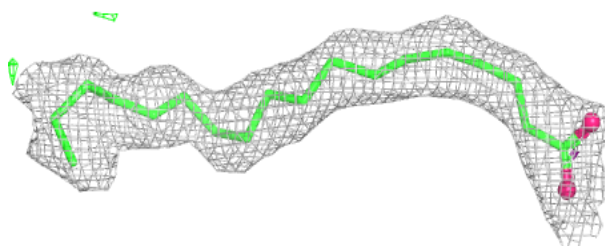


Electron density around STE D 413:

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

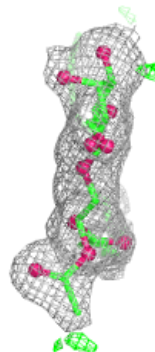
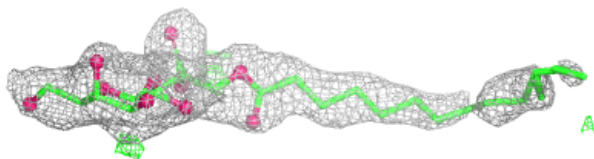
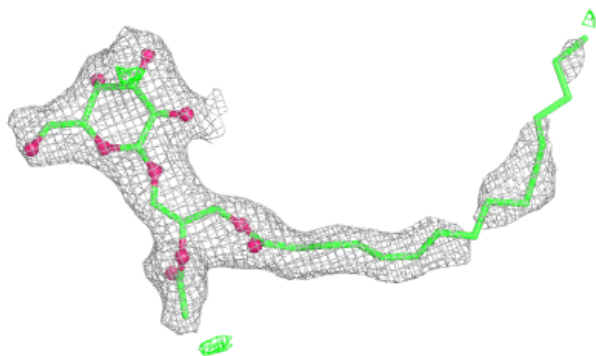
**Electron density around STE b 620:**

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

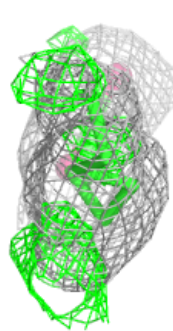
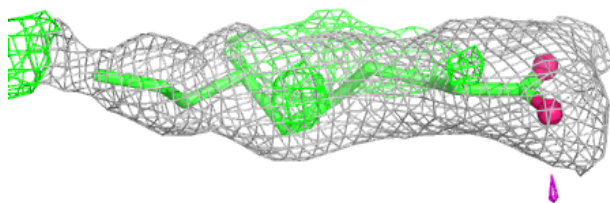
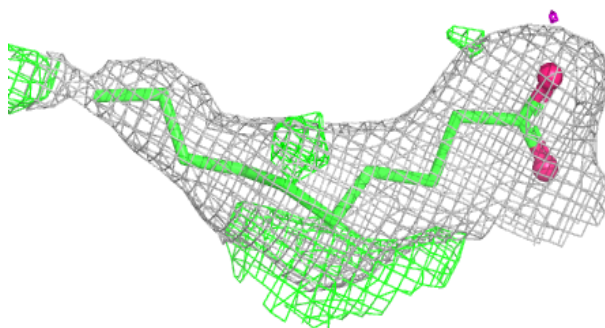


Electron density around LMG c 520:

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

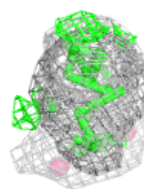
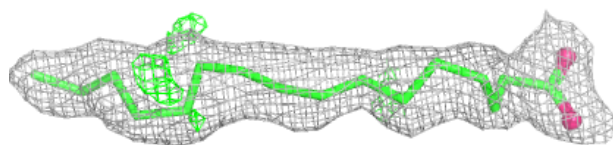
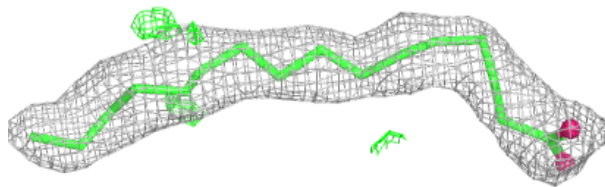
**Electron density around STE C 519:**

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

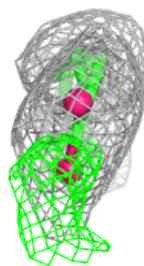
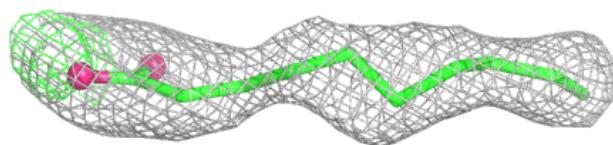
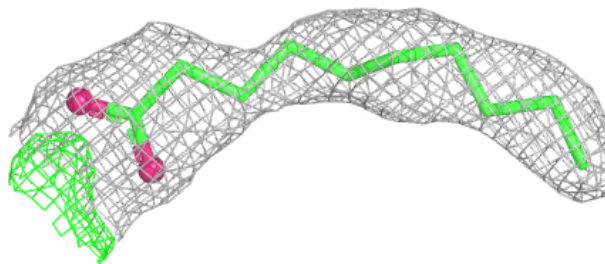


Electron density around STE B 624:

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

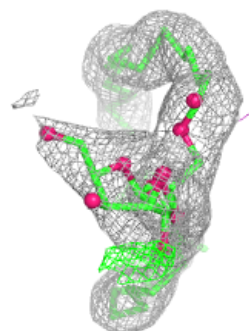
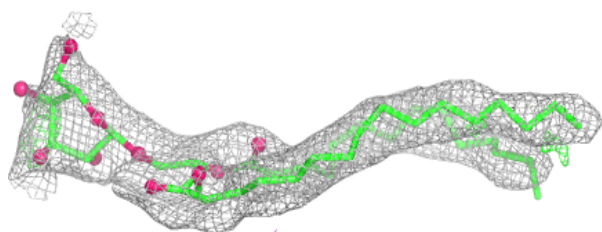
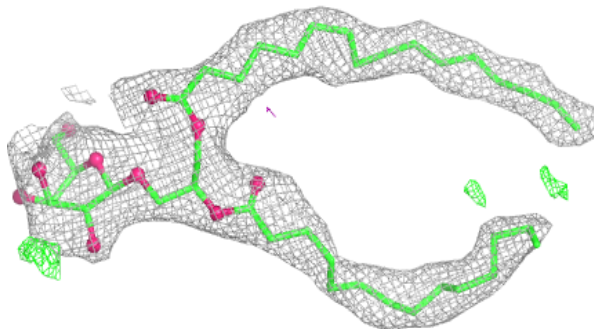
**Electron density around STE C 520:**

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

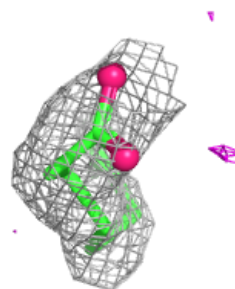
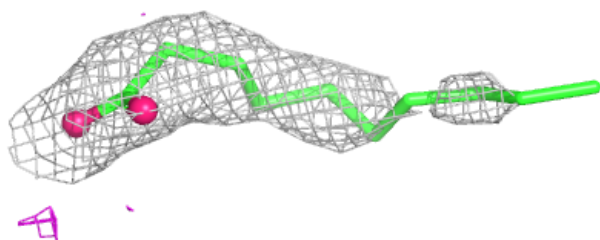


Electron density around LMG c 524:

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

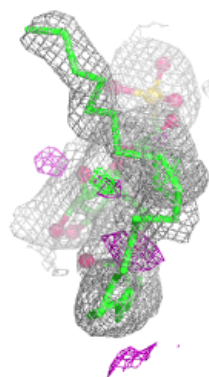
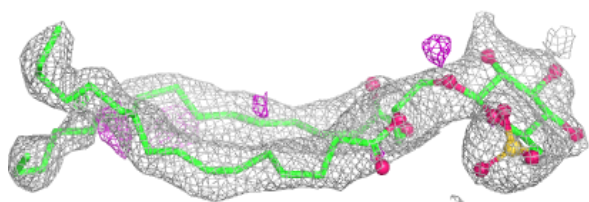
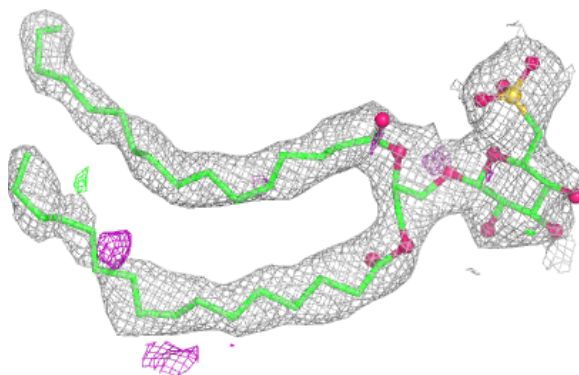
**Electron density around STE B 625:**

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

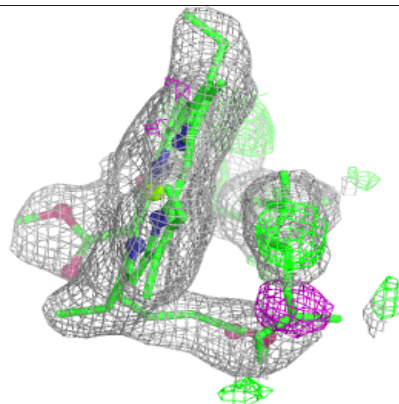
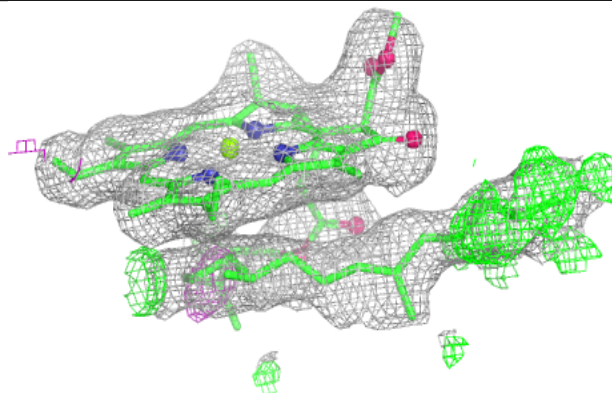
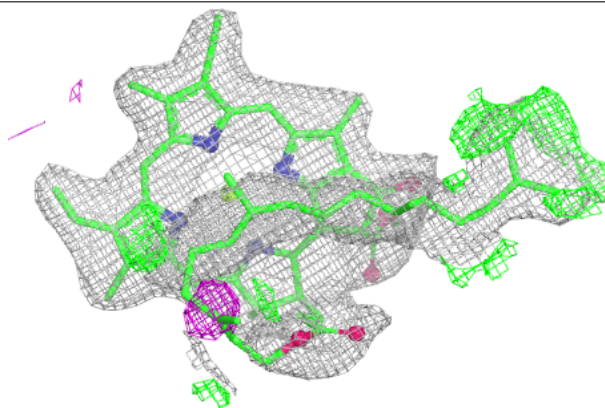


Electron density around SQD B 622:

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

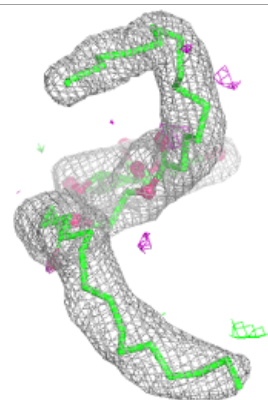
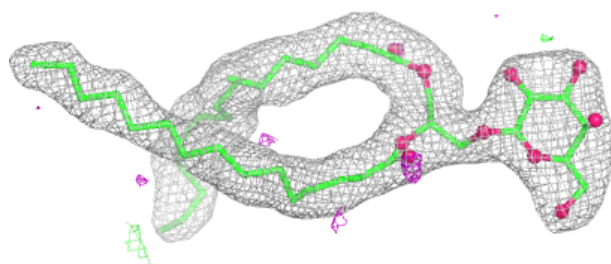
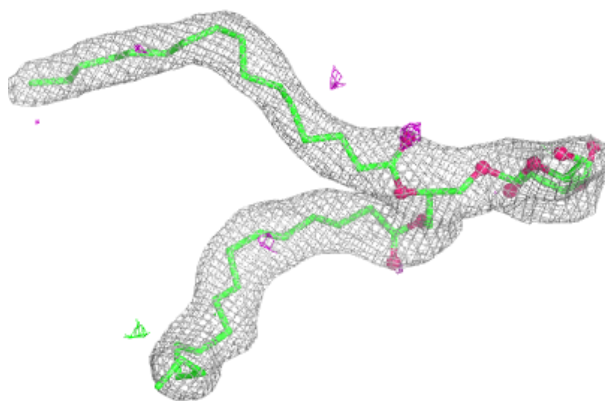
**Electron density around CLA B 601:**

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

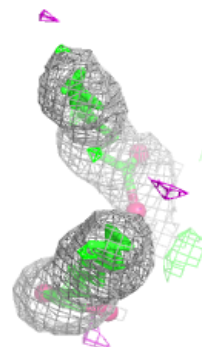
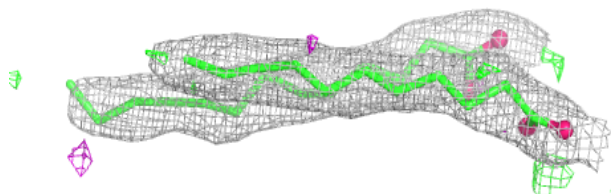
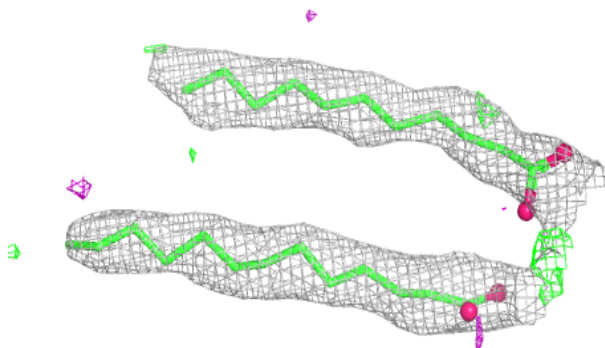


Electron density around LMG M 101:

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

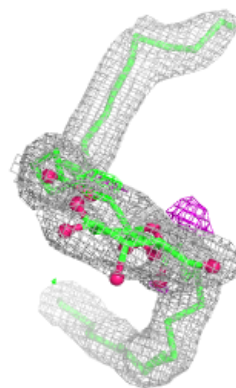
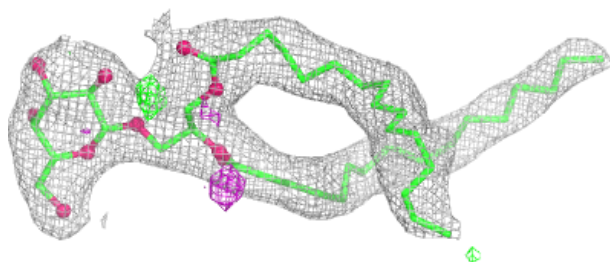
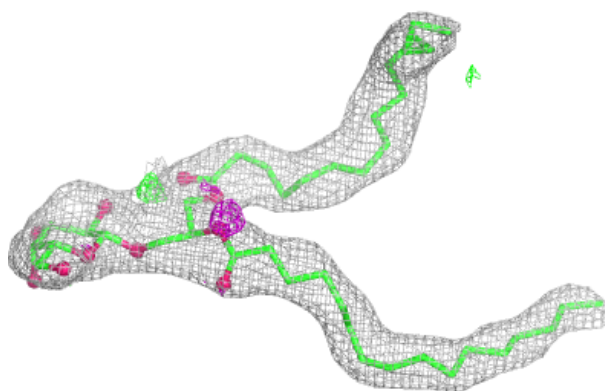
**Electron density around LMG B 621:**

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

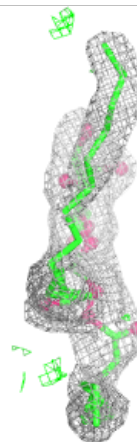
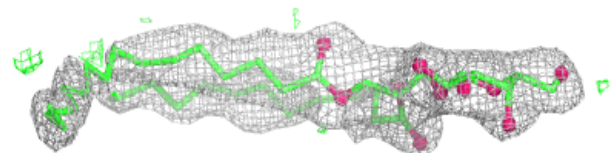
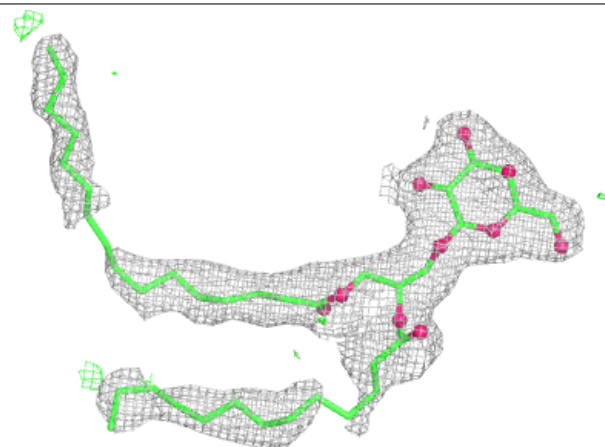


Electron density around LMG m 101:

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

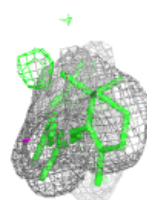
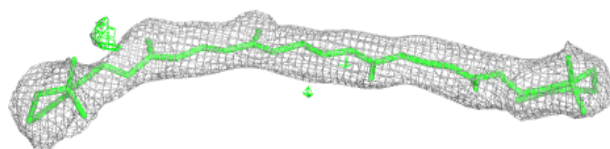
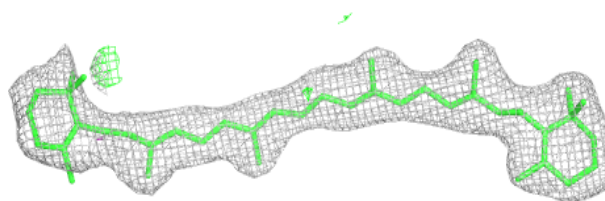
**Electron density around LMG C 518:**

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

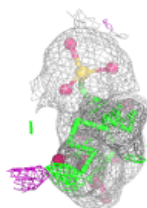
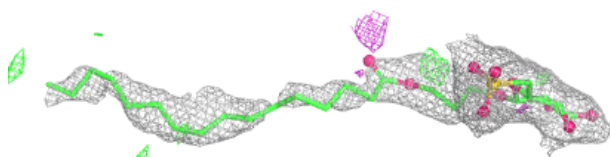
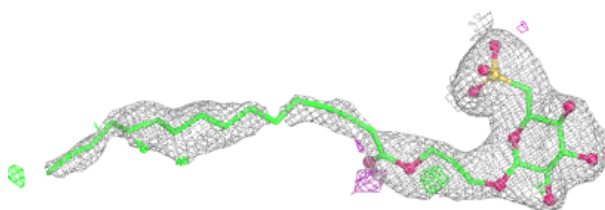


Electron density around BCR d 405:

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

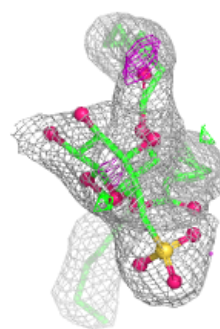
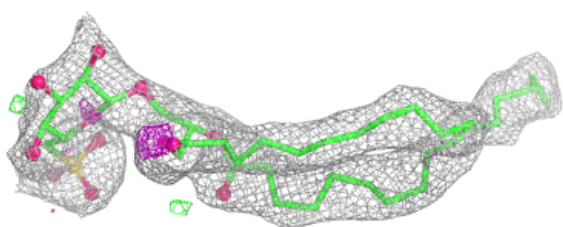
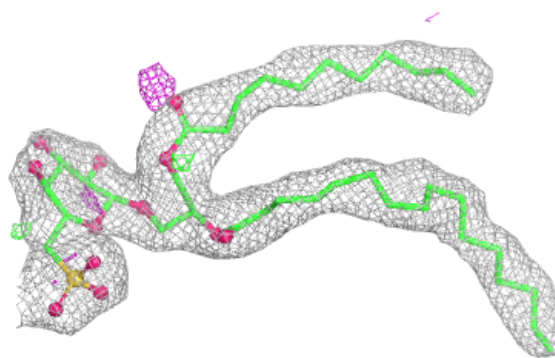
**Electron density around SQD F 101:**

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

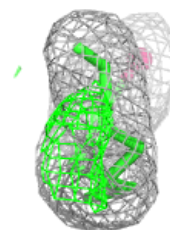
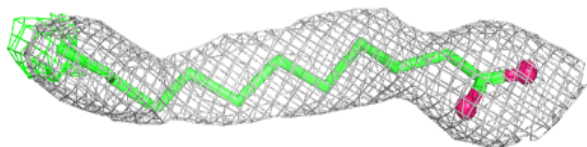
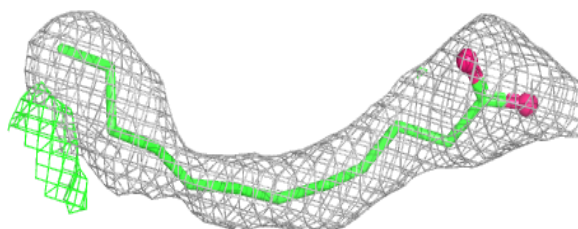


Electron density around SQD L 101:

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

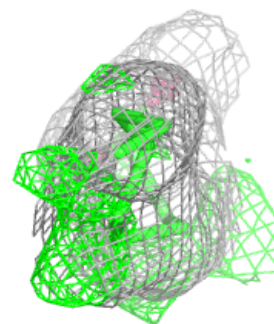
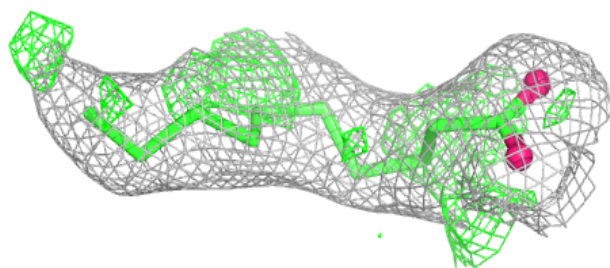
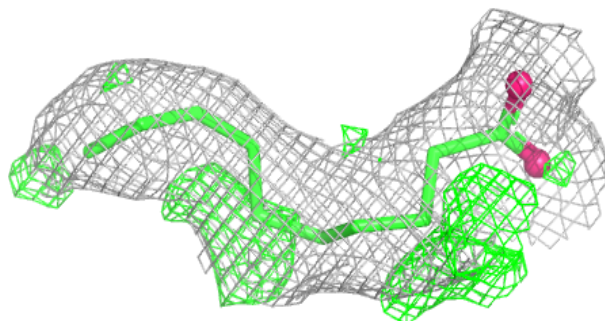
**Electron density around STE t 102:**

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

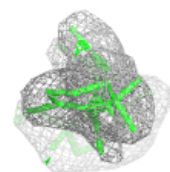
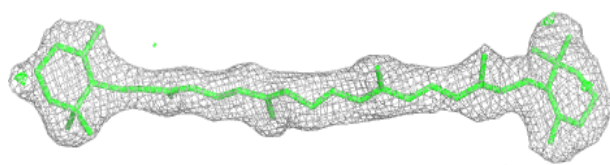
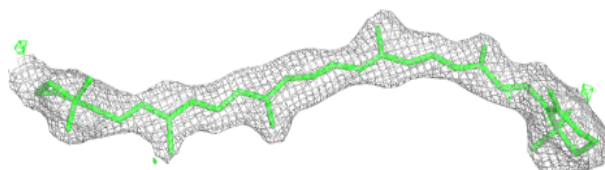


Electron density around STE B 623:

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

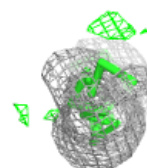
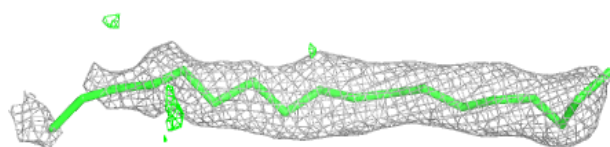
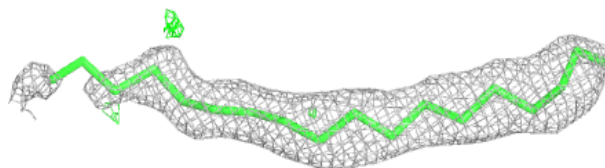
**Electron density around BCR x 101:**

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

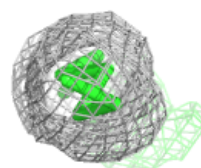
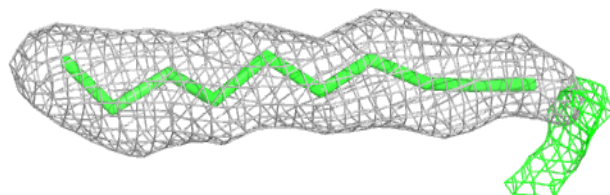
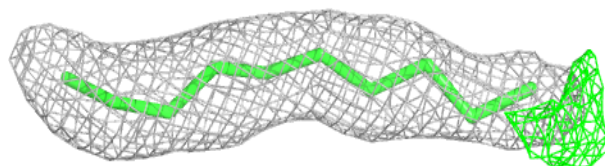


Electron density around STE I 102:

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

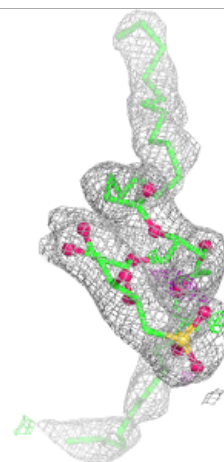
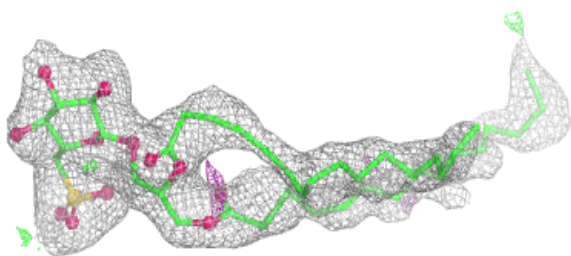
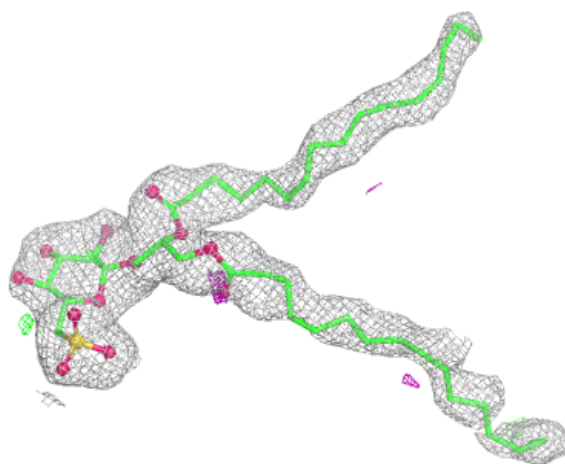
**Electron density around STE M 103:**

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



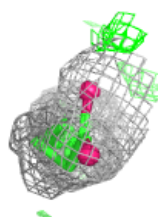
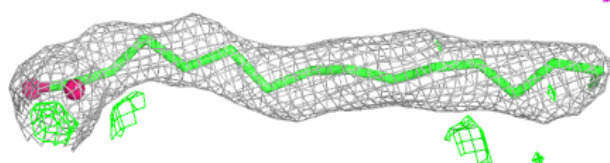
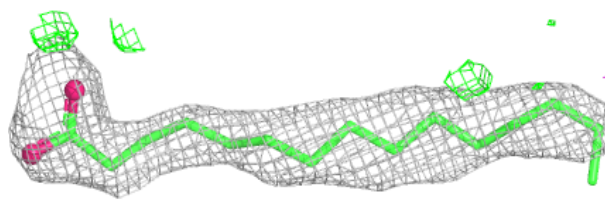
Electron density around SQD a 613:

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

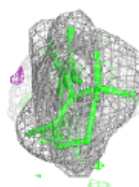
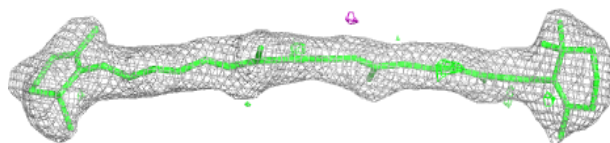
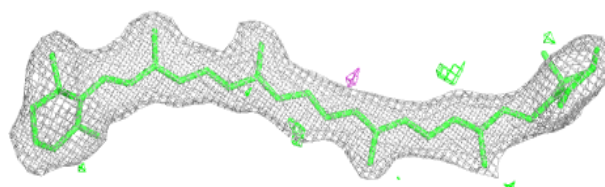


Electron density around STE d 413:

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

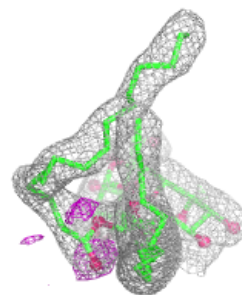
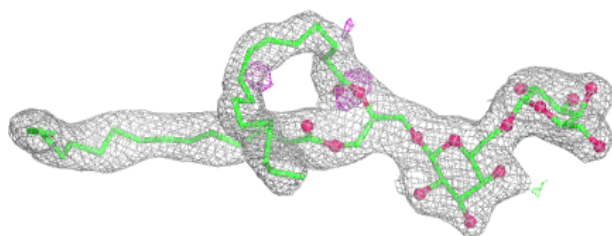
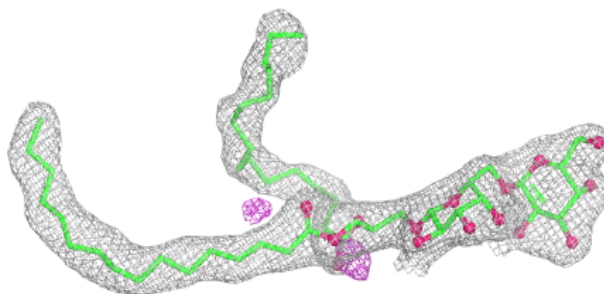
**Electron density around BCR Y 101:**

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

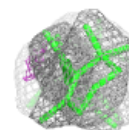
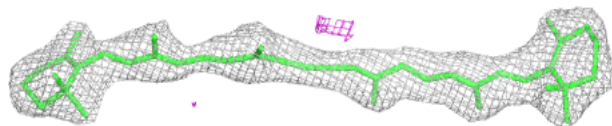
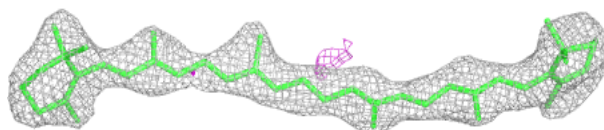


Electron density around DGD h 101:

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

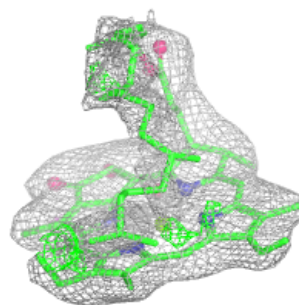
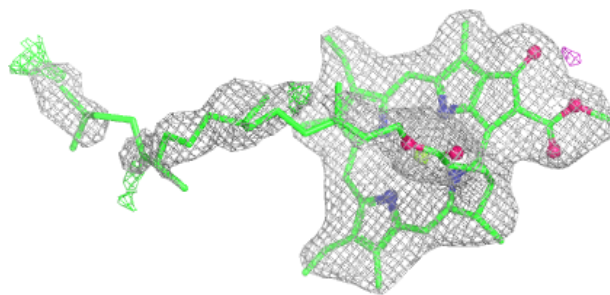
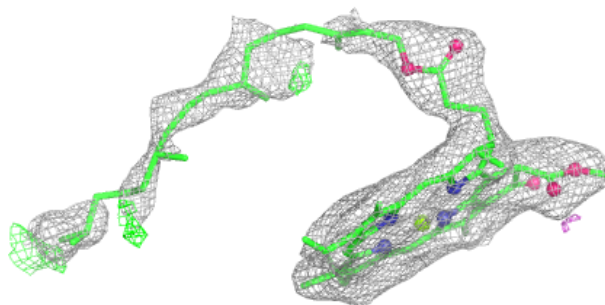
**Electron density around BCR c 514:**

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

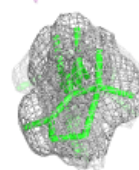
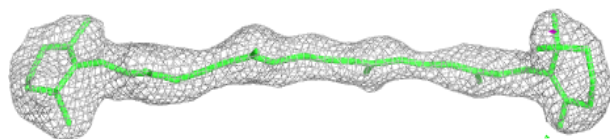
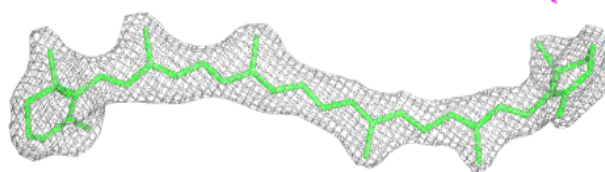


Electron density around CLA C 513:

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

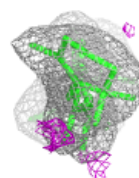
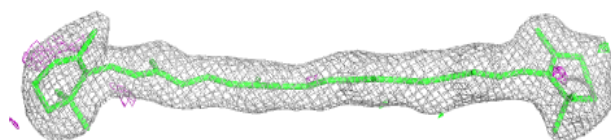
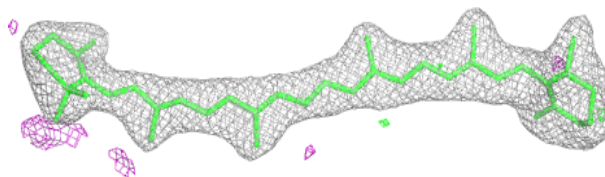
**Electron density around BCR k 101:**

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

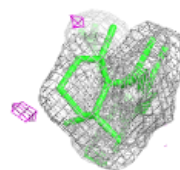
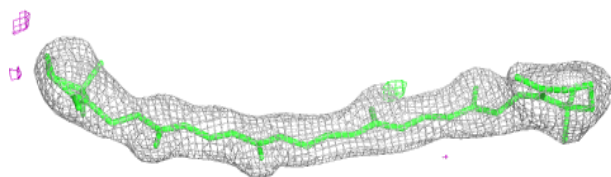
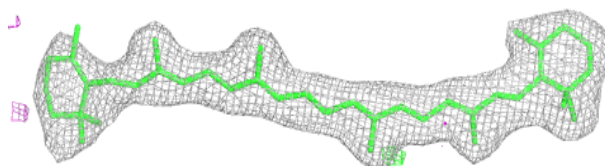


Electron density around BCR B 618:

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

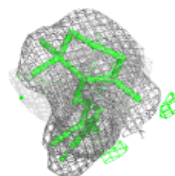
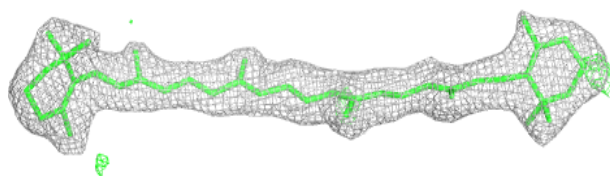
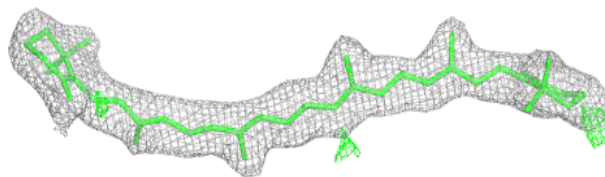
**Electron density around BCR D 406:**

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

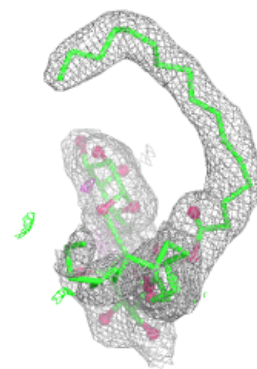
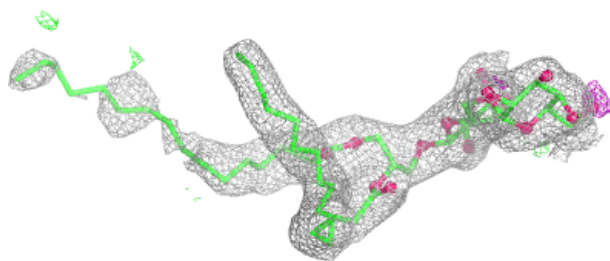
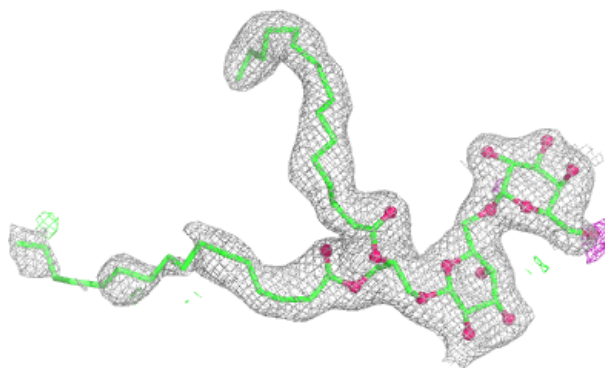


Electron density around BCR H 101:

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

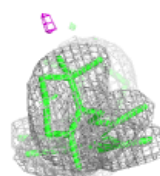
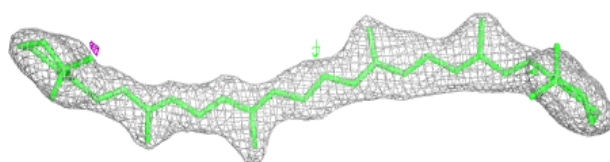
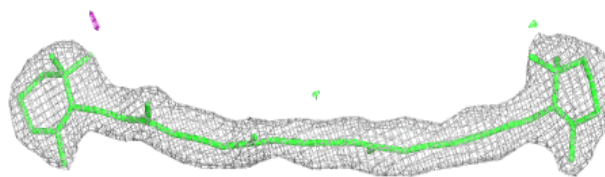
**Electron density around DGD c 518:**

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

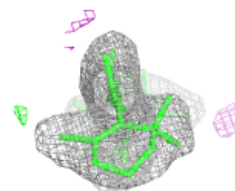
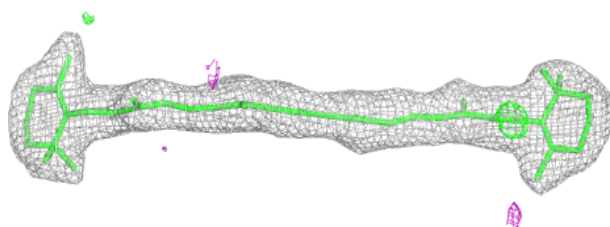
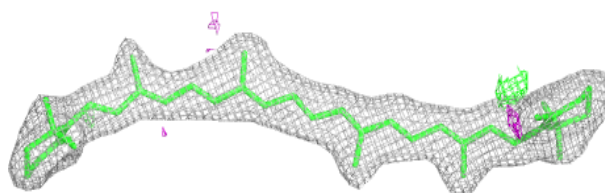


Electron density around BCR K 102:

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

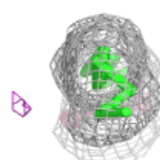
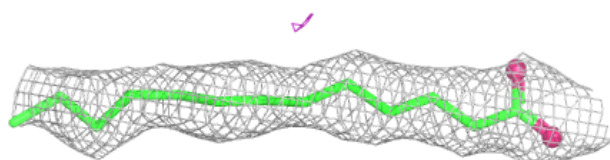
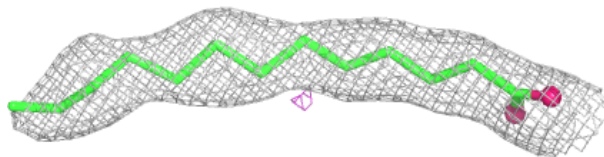
**Electron density around BCR C 514:**

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

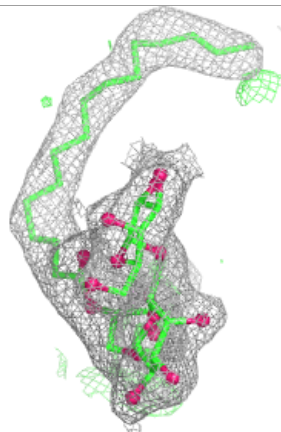
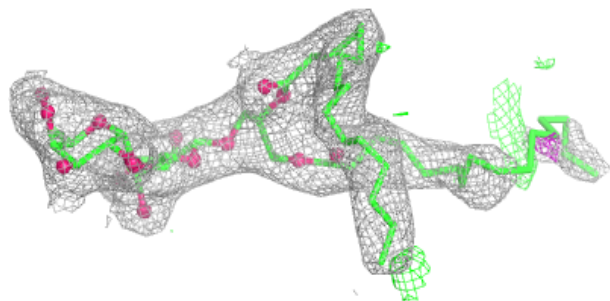
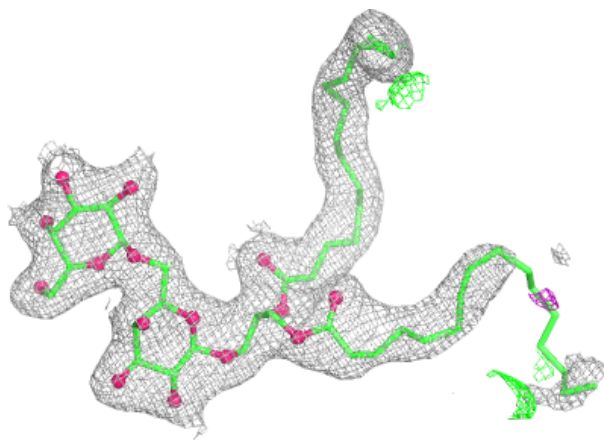


Electron density around STE M 102:

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

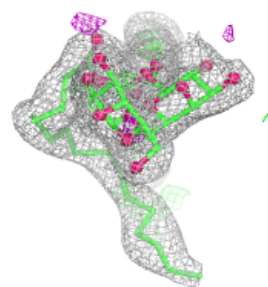
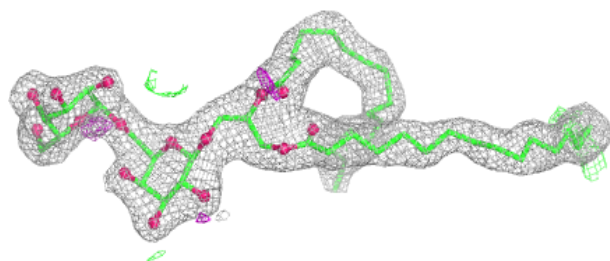
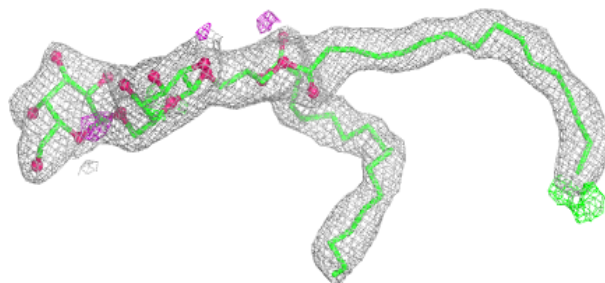
**Electron density around DGD C 516:**

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

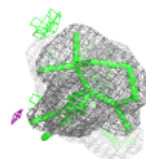
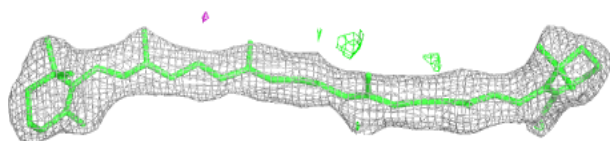
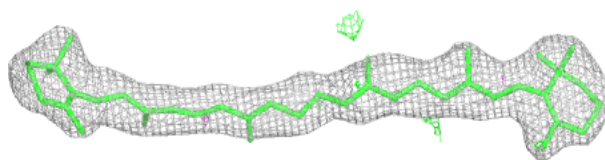


Electron density around DGD H 102:

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

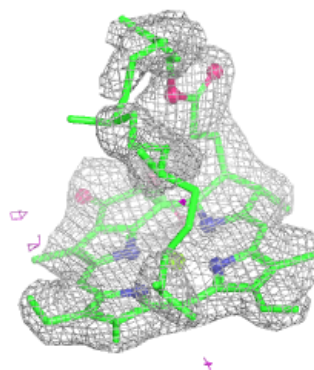
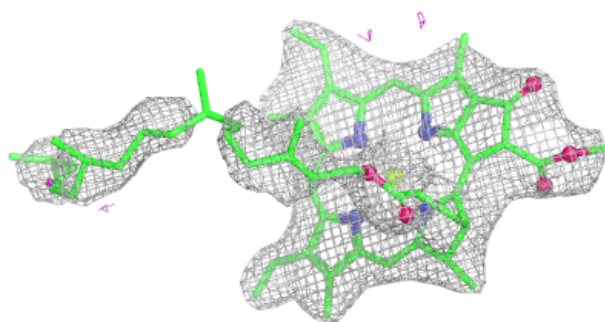
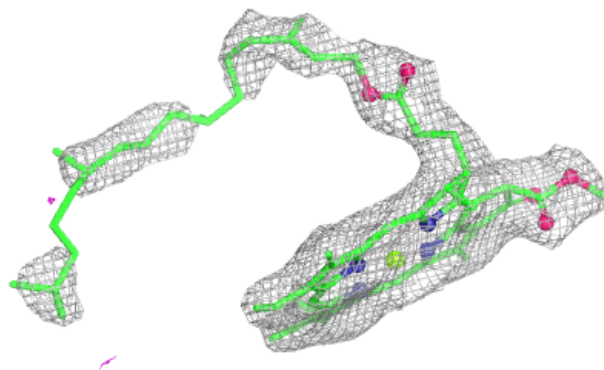
**Electron density around BCR K 101:**

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

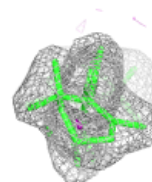
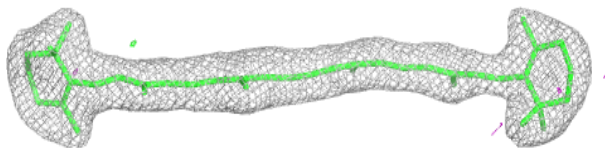
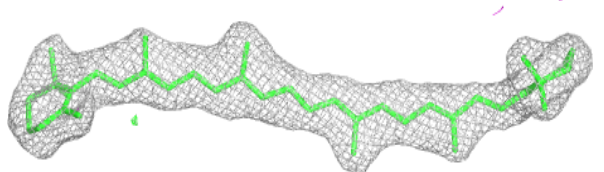


Electron density around CLA c 513:

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

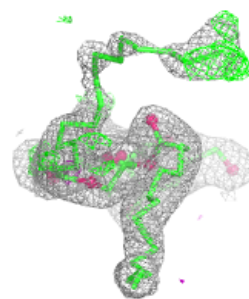
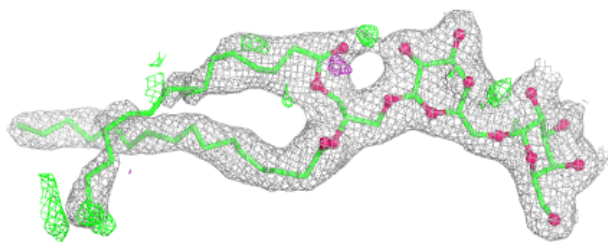
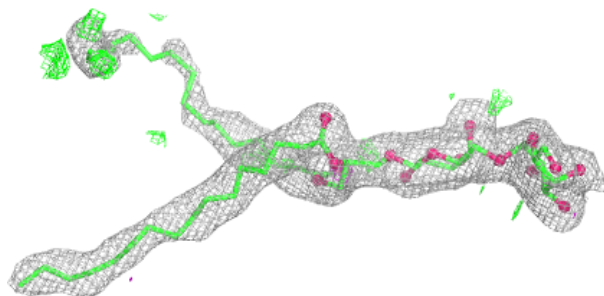
**Electron density around BCR A 610:**

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

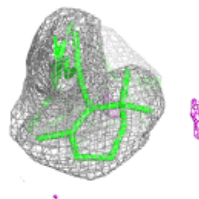
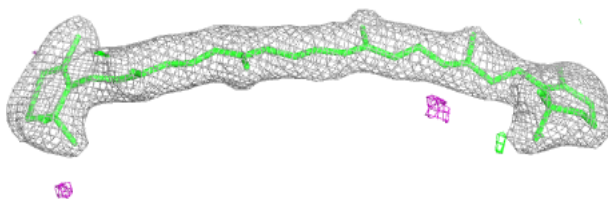
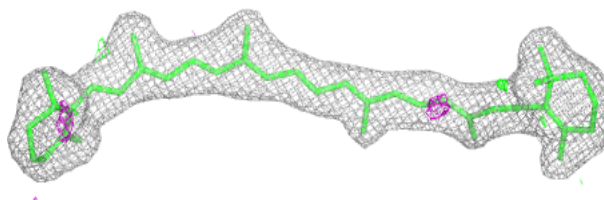


Electron density around DGD C 515:

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

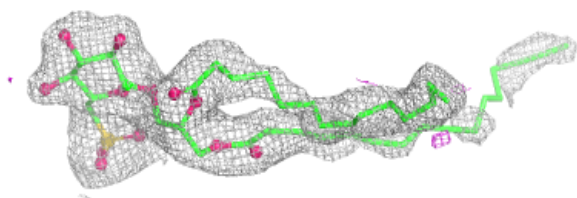
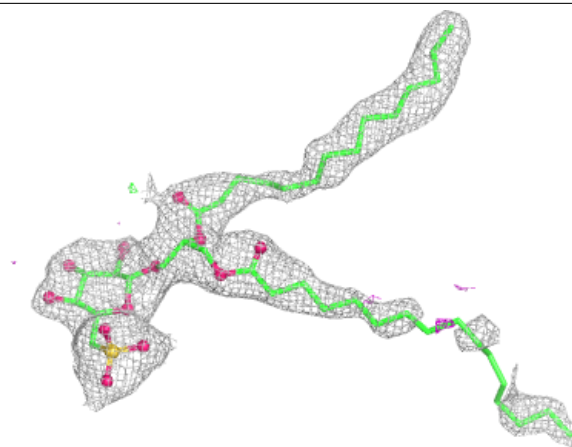
**Electron density around BCR T 101:**

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



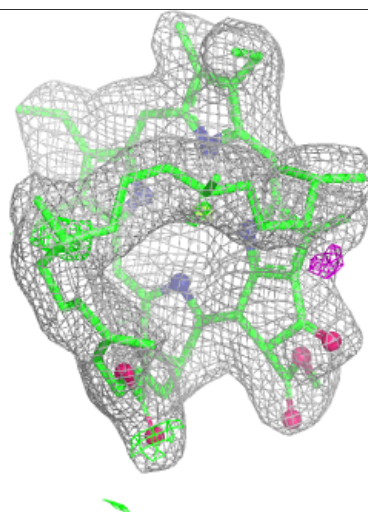
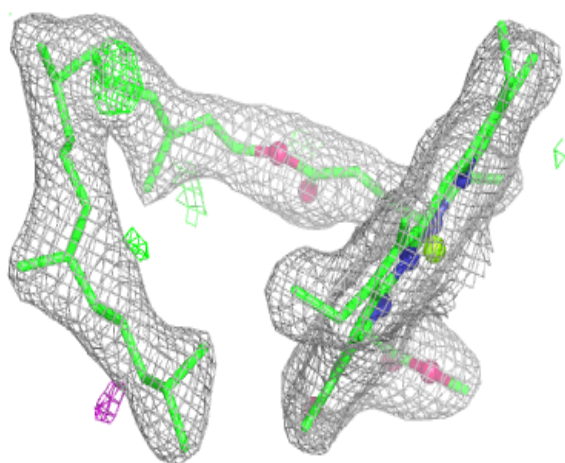
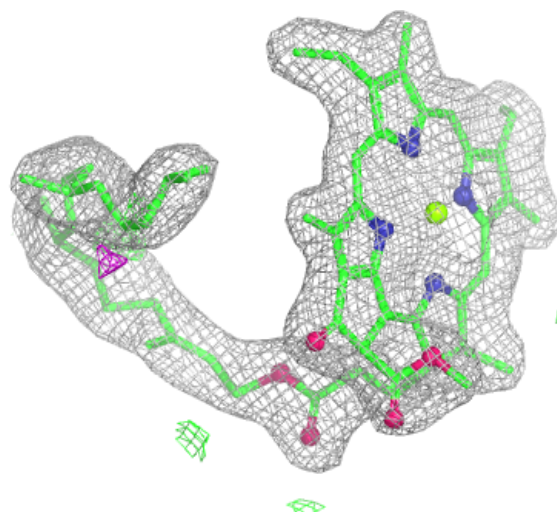
Electron density around SQD A 613:

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



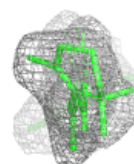
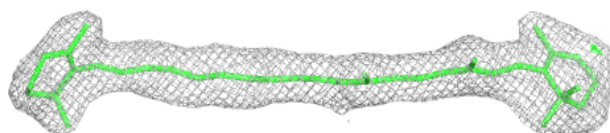
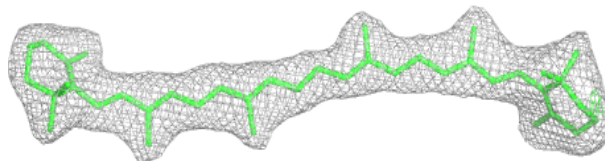
Electron density around CLA C 503:

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

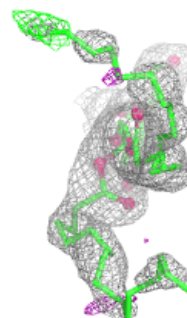
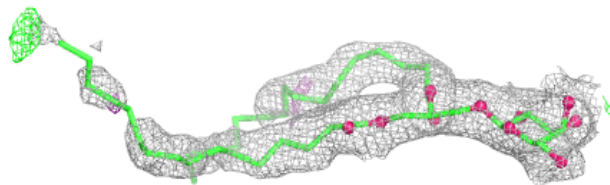
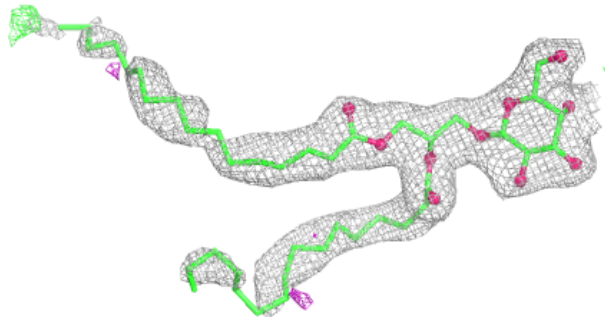


Electron density around BCR b 618:

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

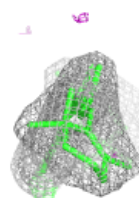
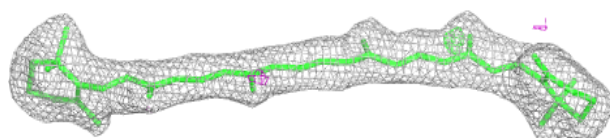
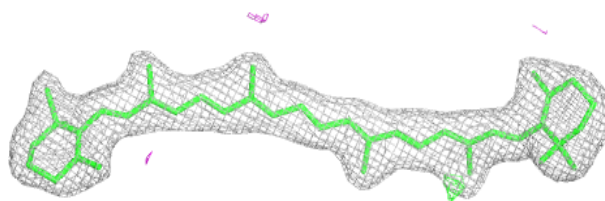
**Electron density around LMG D 408:**

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

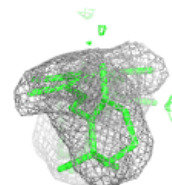
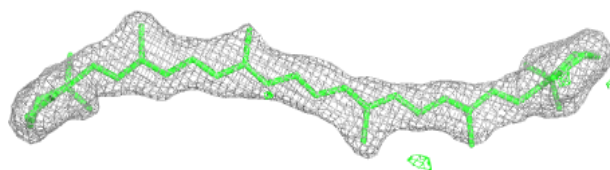
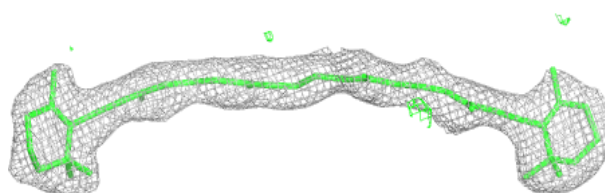


Electron density around BCR B 619:

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

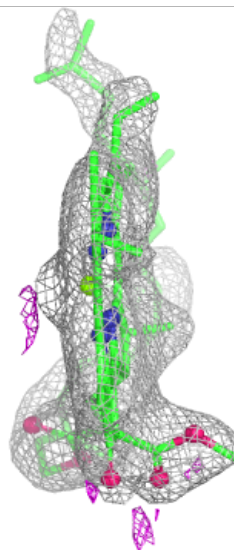
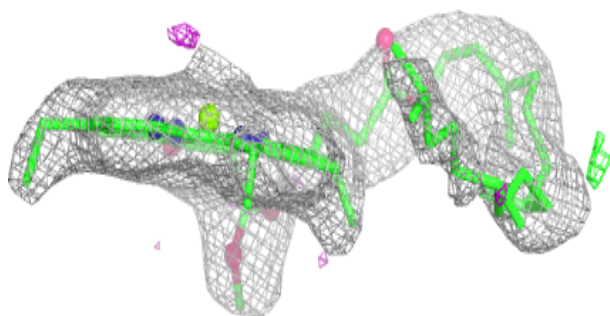
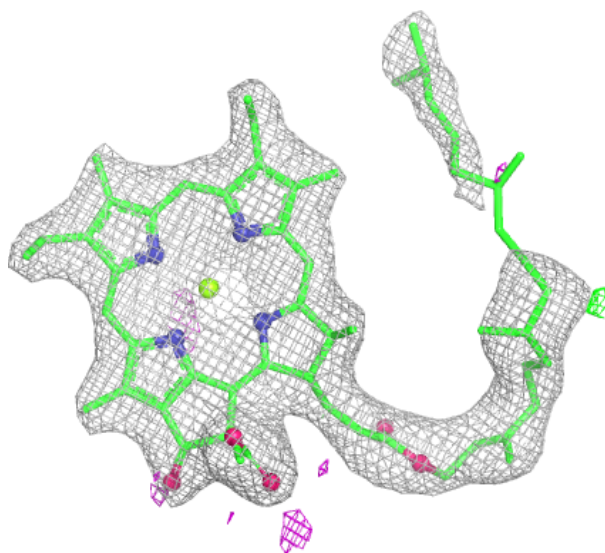
**Electron density around BCR c 516:**

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



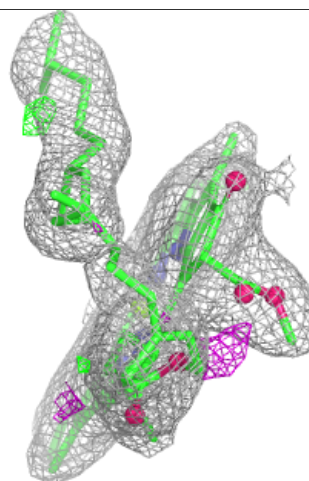
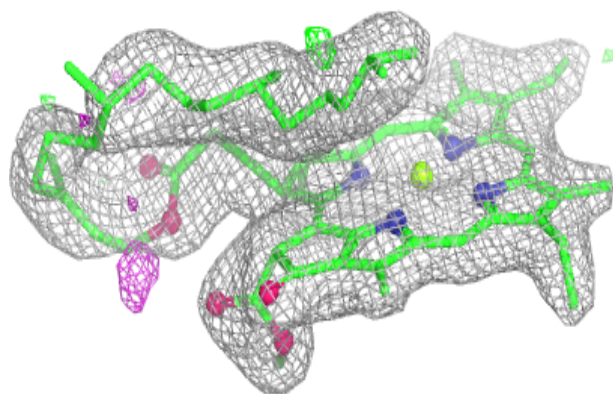
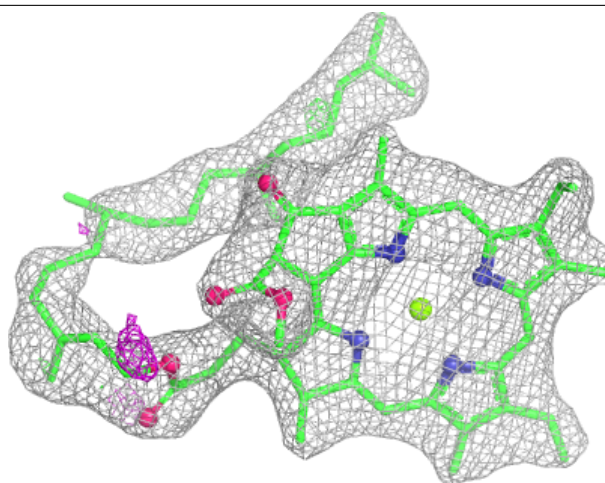
Electron density around CLA C 512:

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



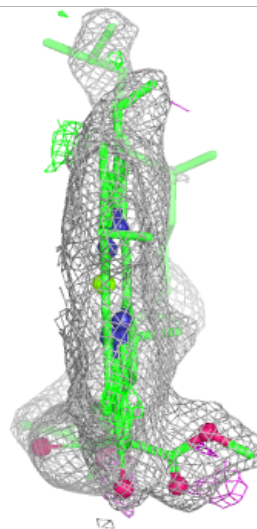
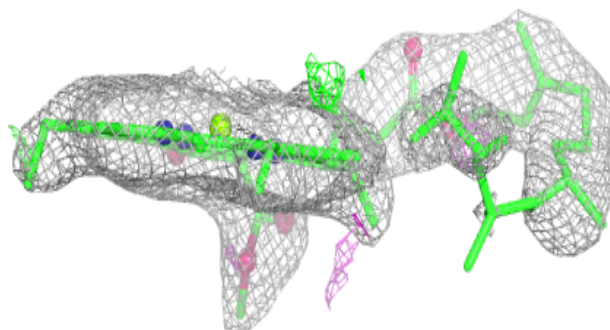
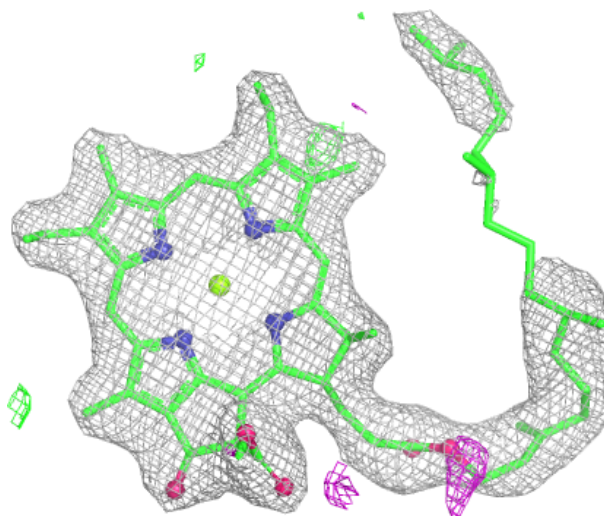
Electron density around CLA c 509:

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



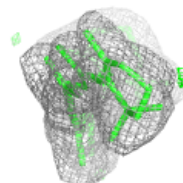
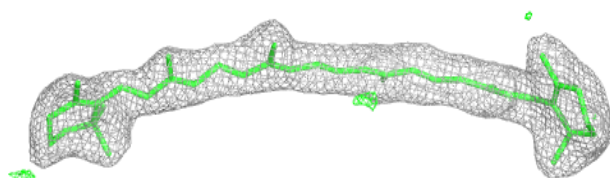
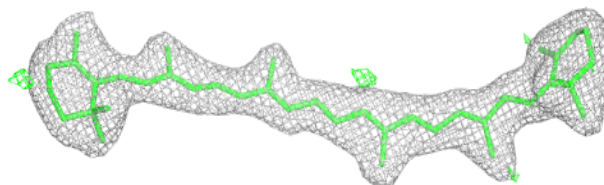
Electron density around CLA c 512:

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

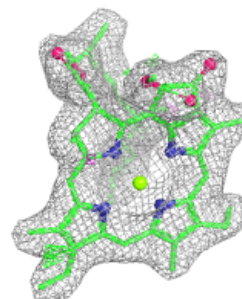
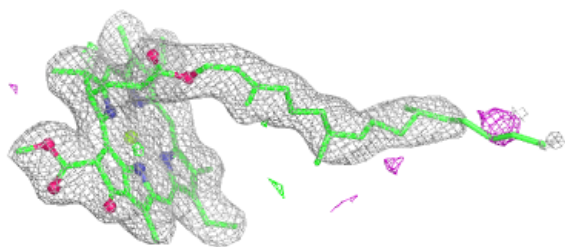
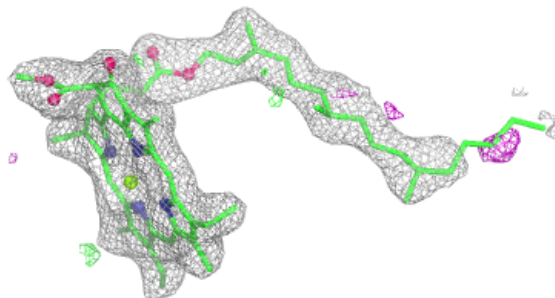


Electron density around BCR t 101:

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

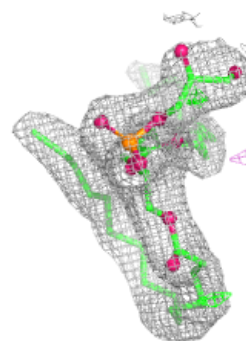
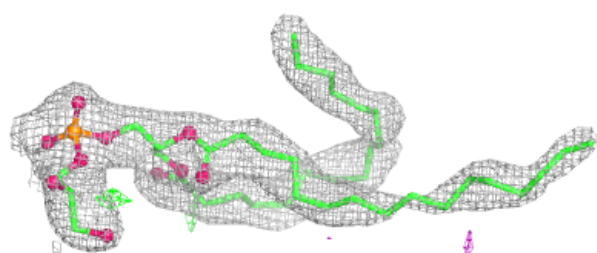
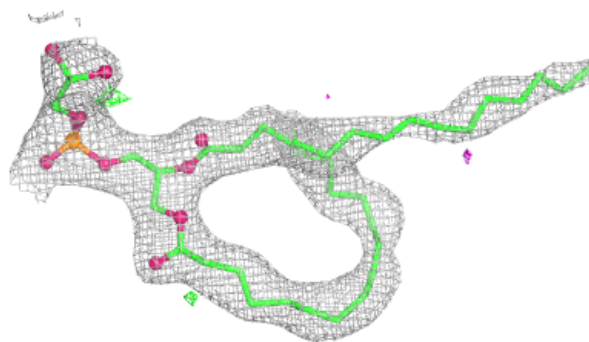
**Electron density around CLA c 508:**

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

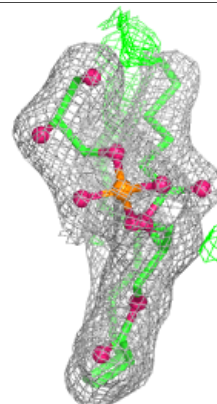
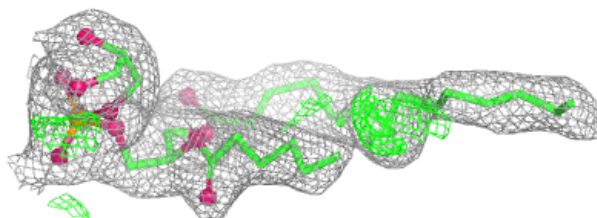
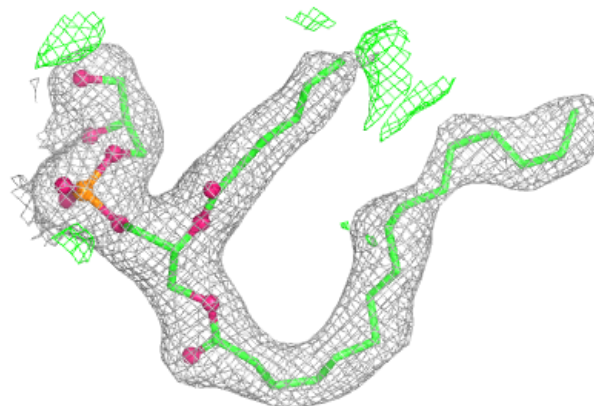


Electron density around LHG d 407:

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

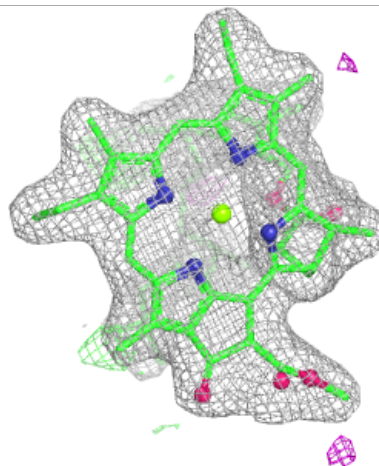
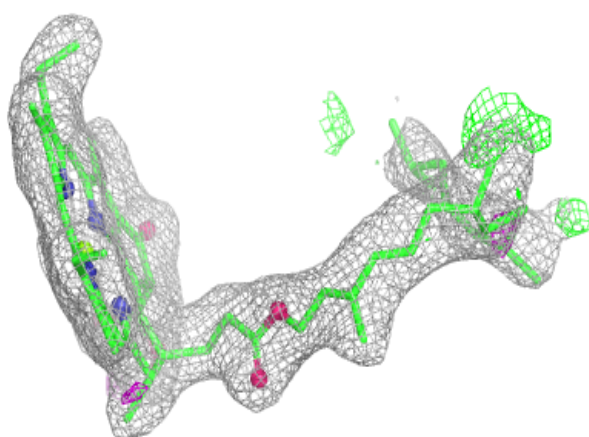
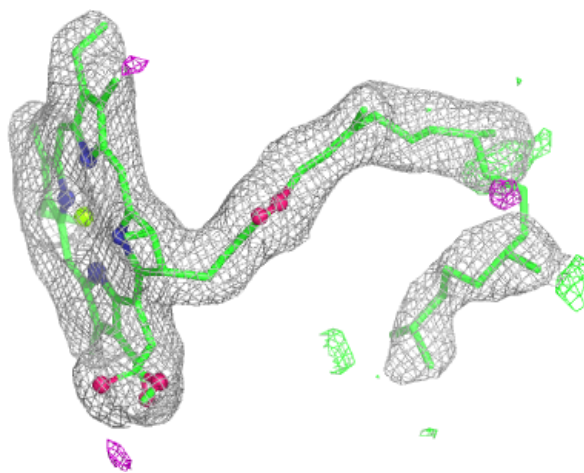
**Electron density around LHG d 409:**

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



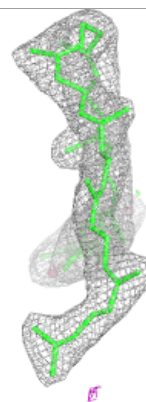
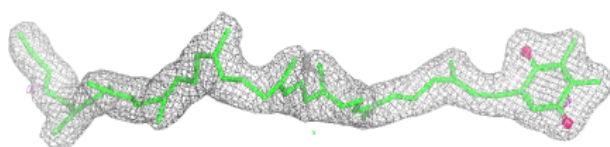
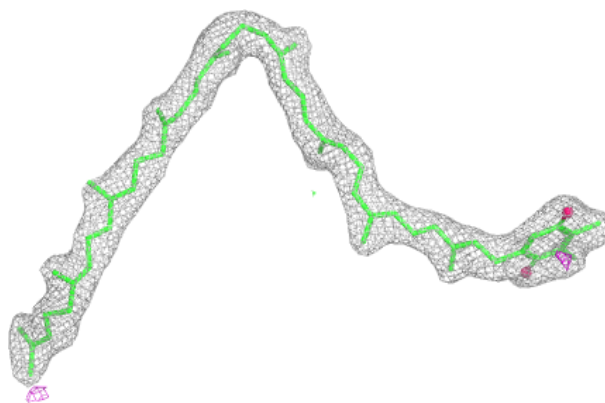
Electron density around CLA B 606:

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

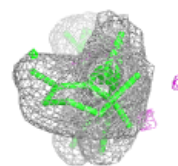
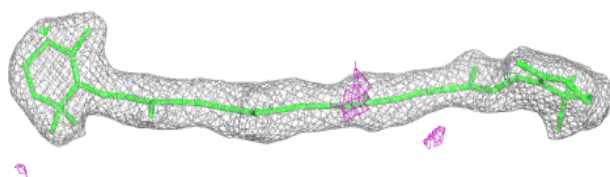
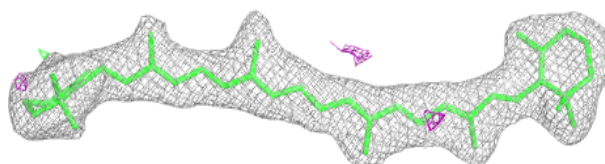


Electron density around PL9 D 407:

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

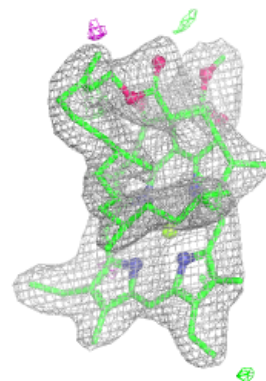
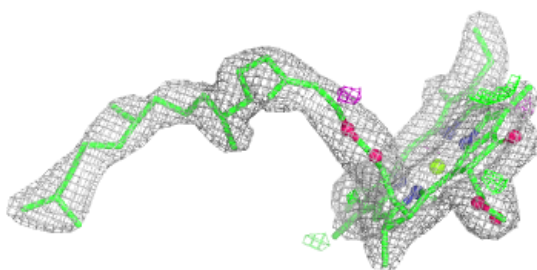
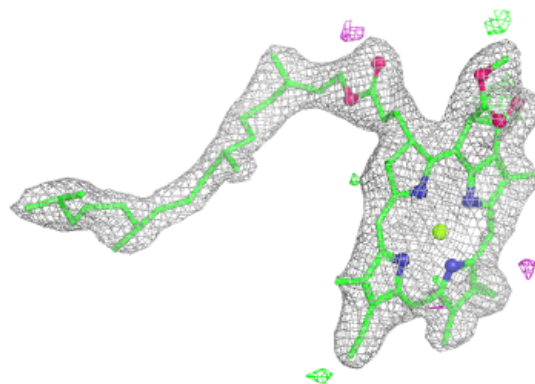
**Electron density around BCR b 617:**

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

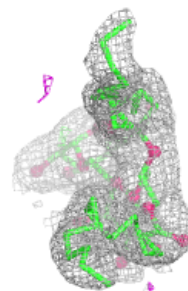
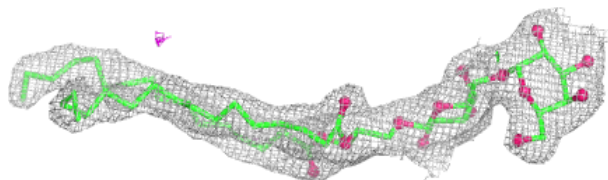
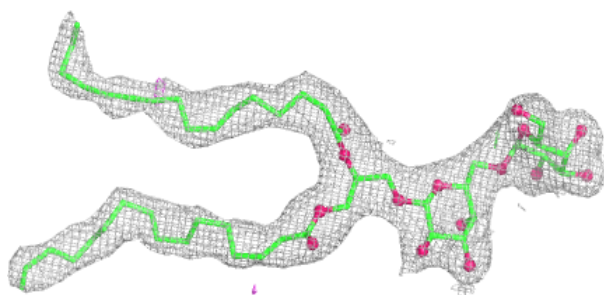


Electron density around CLA c 511:

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

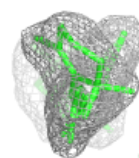
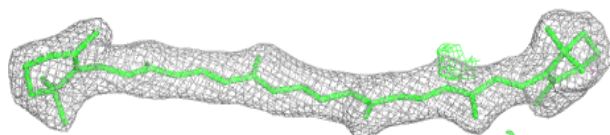
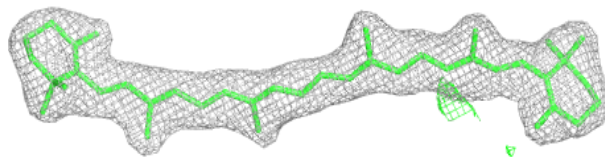
**Electron density around DGD C 517:**

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

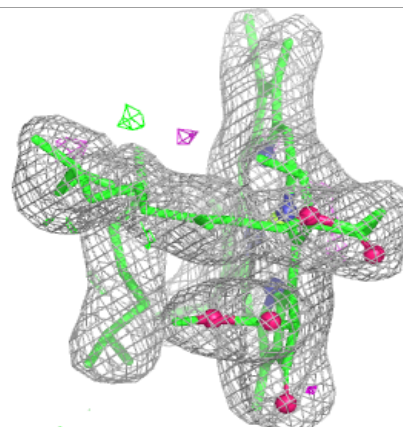
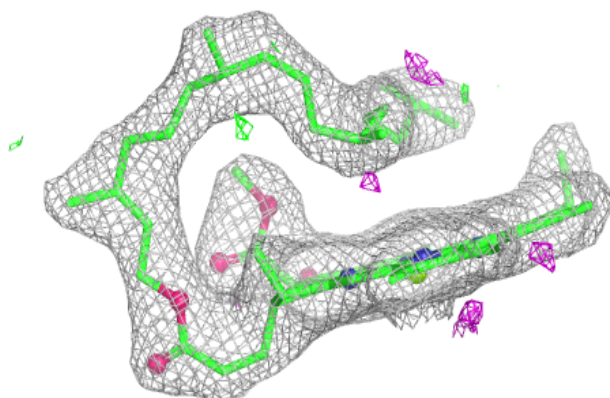
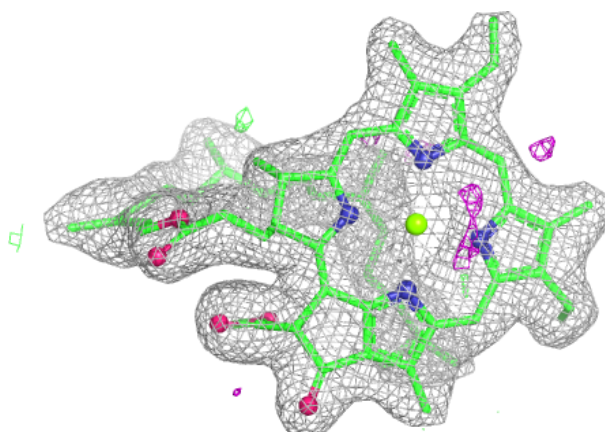


Electron density around BCR b 619:

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

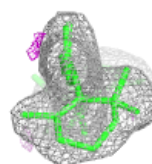
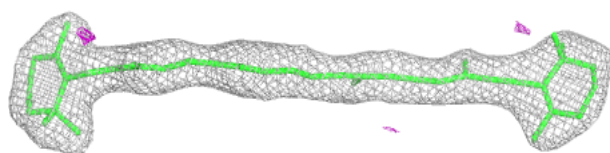
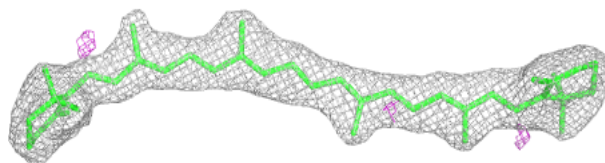
**Electron density around CLA C 510:**

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

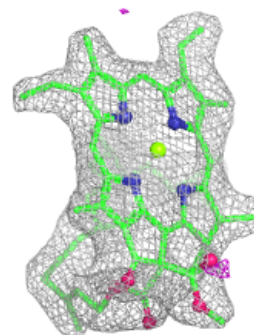
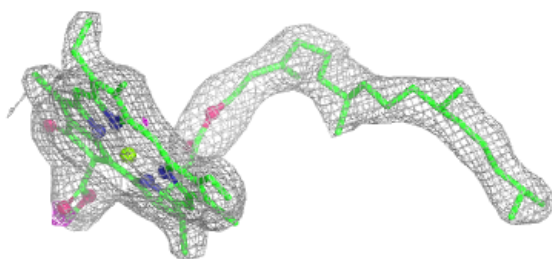
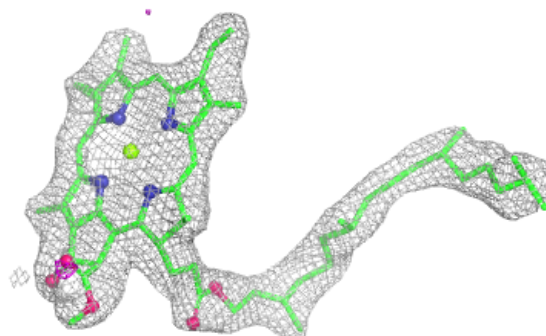


Electron density around BCR c 515:

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

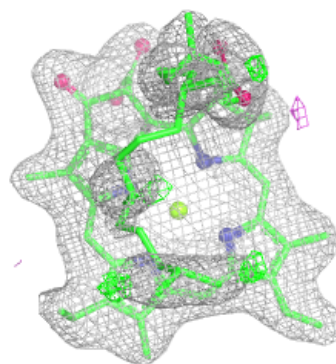
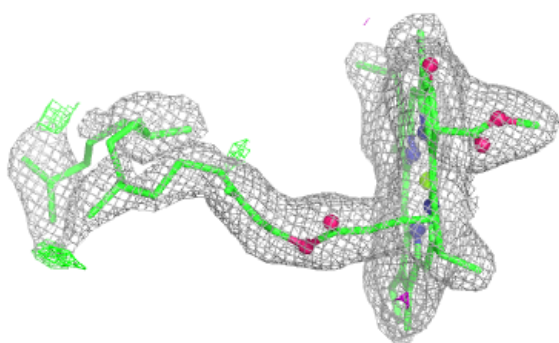
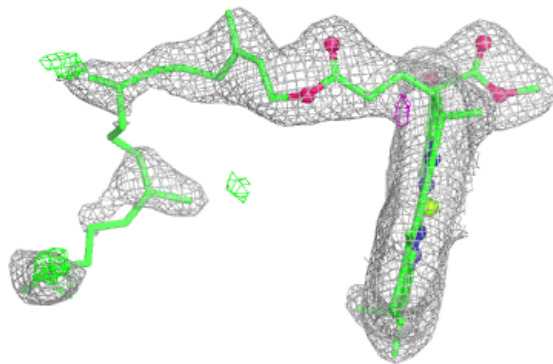
**Electron density around CLA C 511:**

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

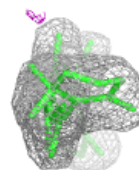
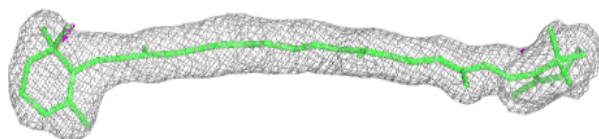
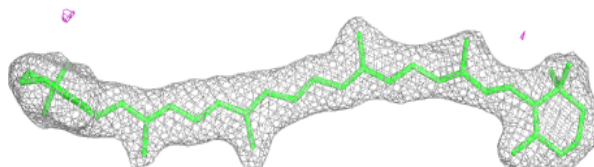


Electron density around CLA c 506:

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

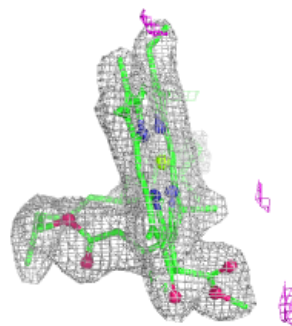
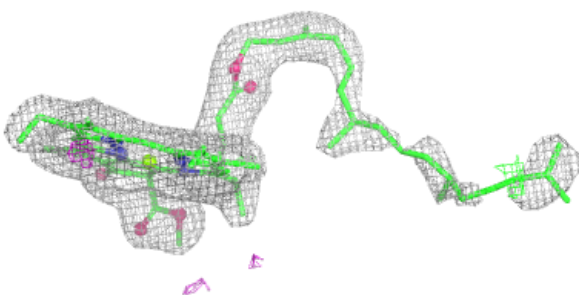
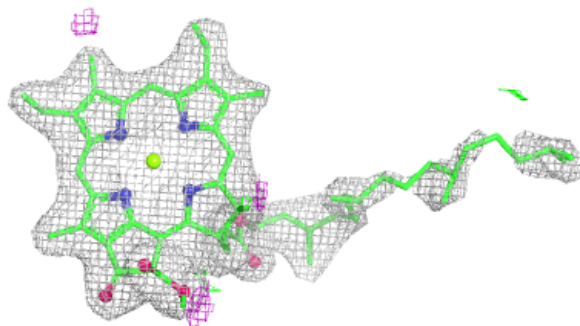
**Electron density around BCR B 617:**

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

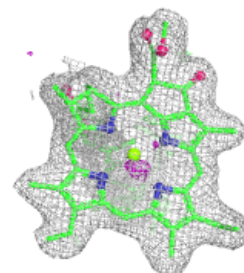
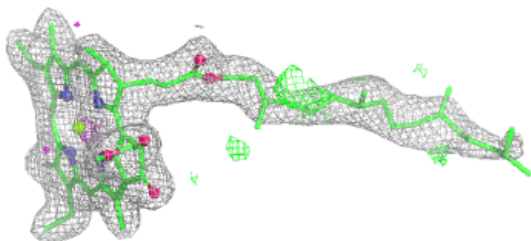
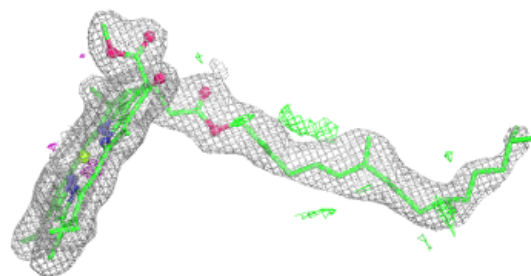


Electron density around CLA a 608:

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

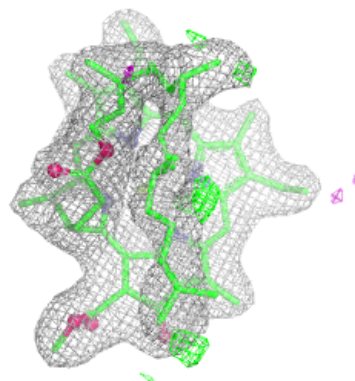
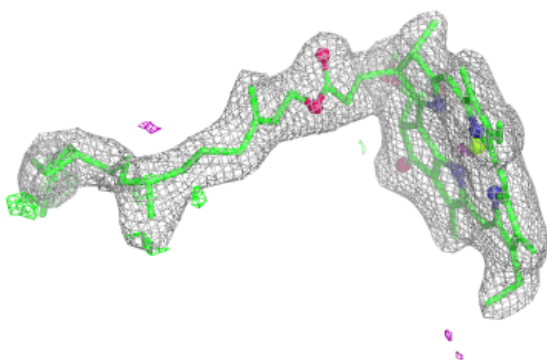
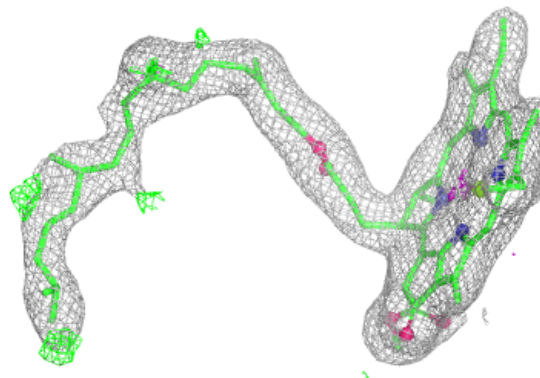
**Electron density around CLA B 604:**

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

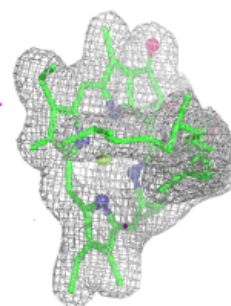
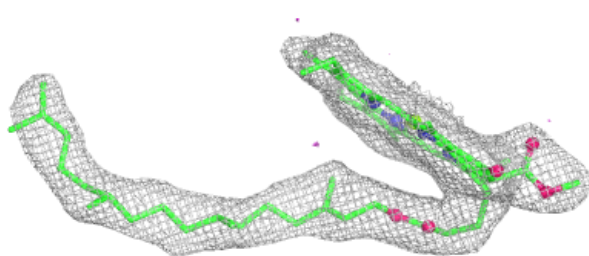
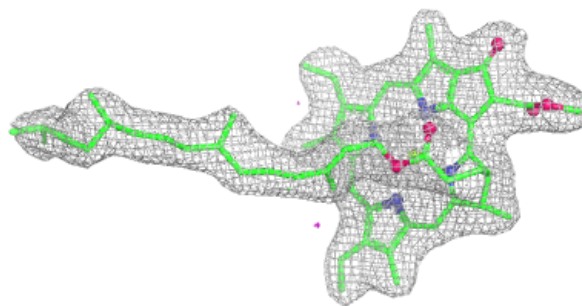


Electron density around CLA b 606:

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

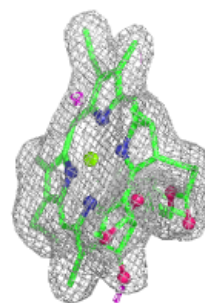
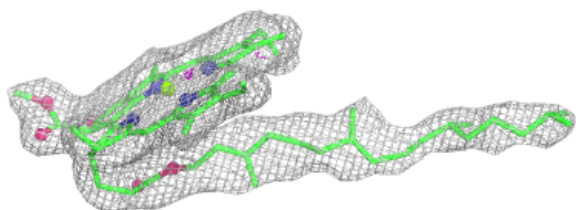
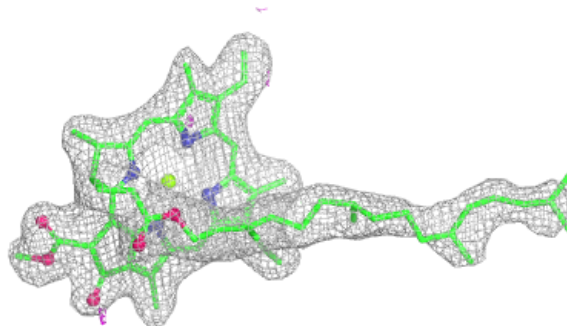
**Electron density around CLA b 608:**

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



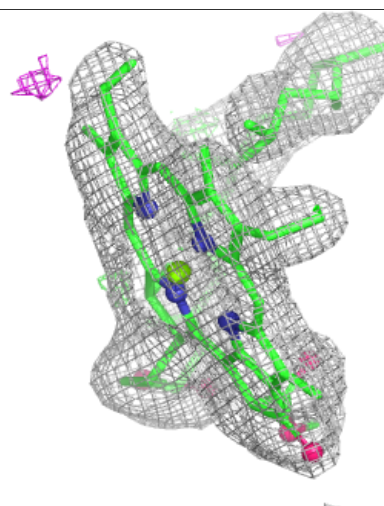
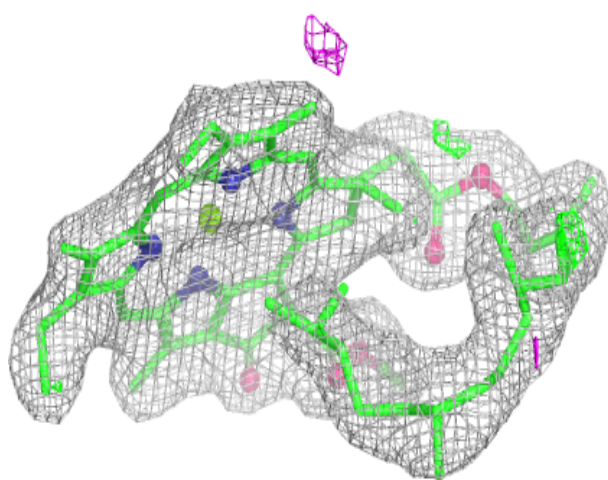
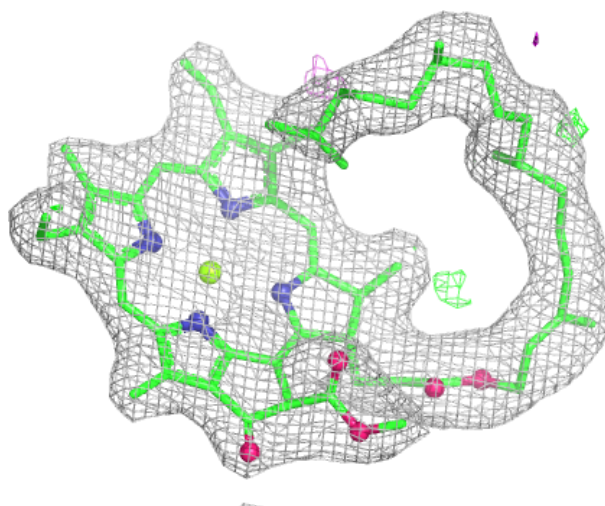
Electron density around CLA b 614:

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



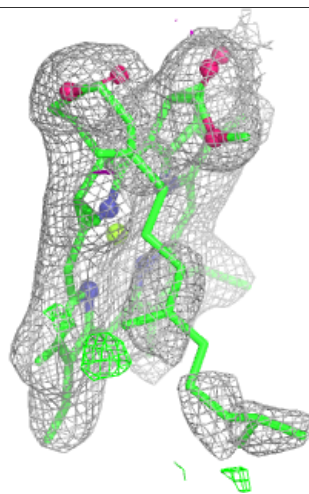
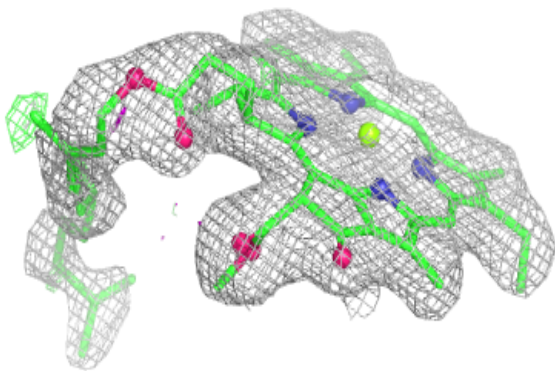
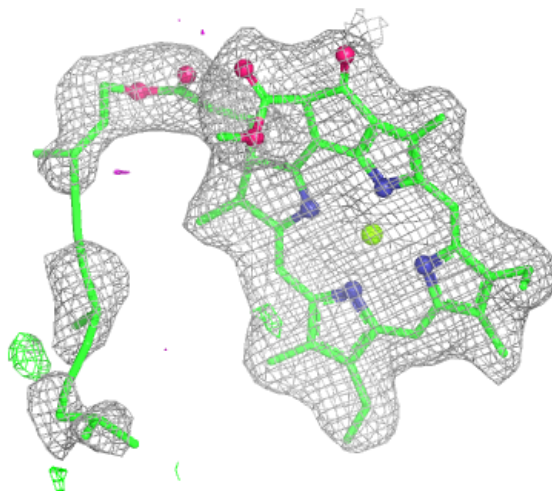
Electron density around CLA b 615:

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



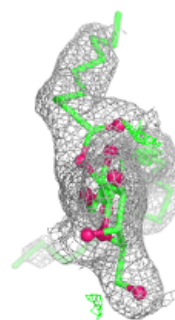
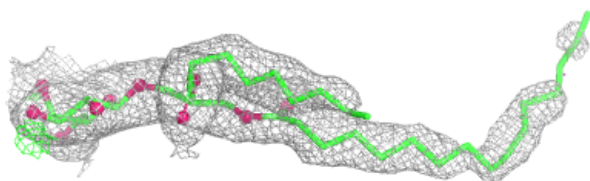
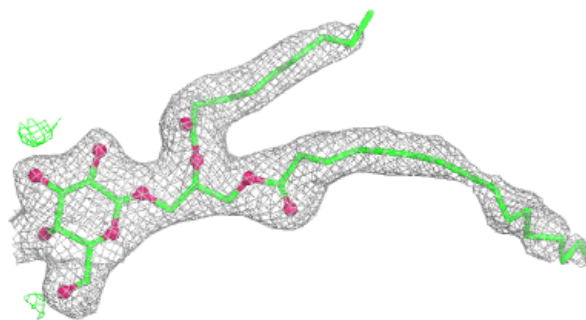
Electron density around CLA b 616:

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

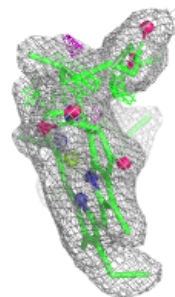
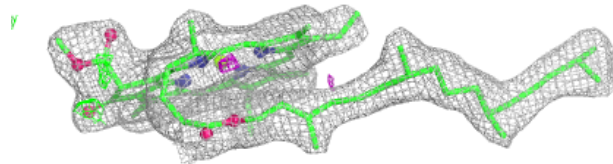
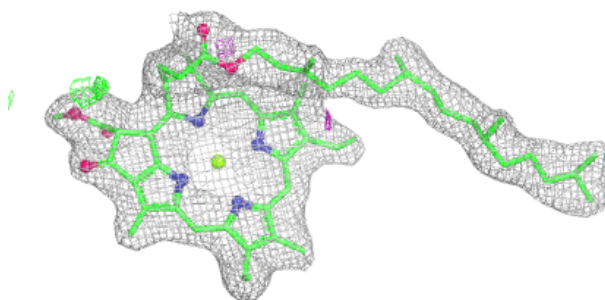


Electron density around LMG d 411:

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

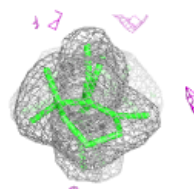
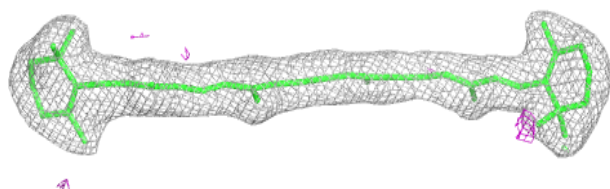
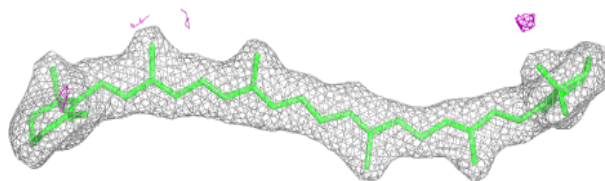
**Electron density around CLA c 501:**

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

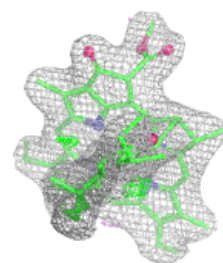
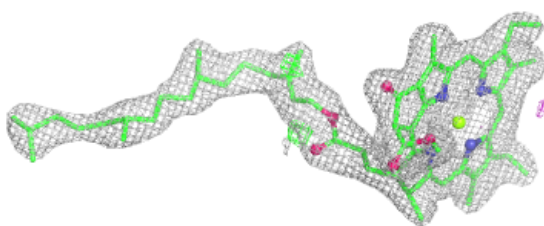
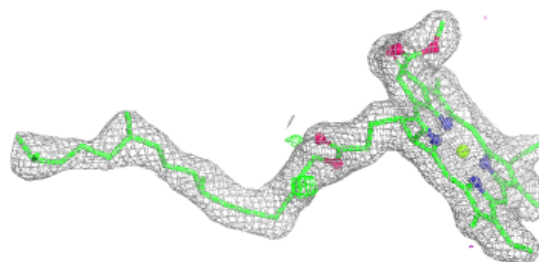


Electron density around BCR a 610:

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

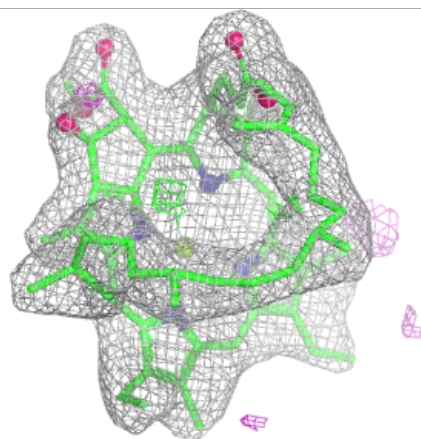
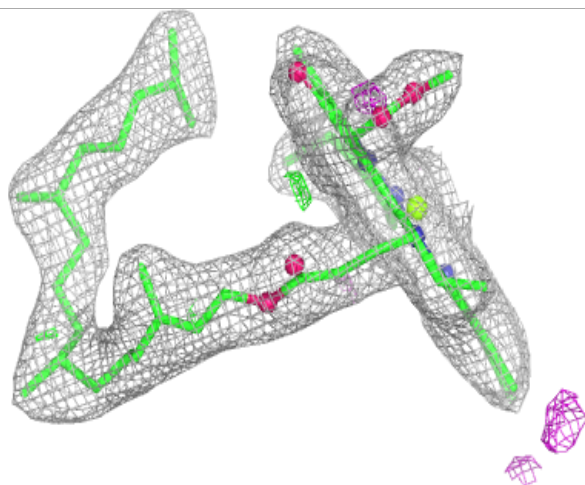
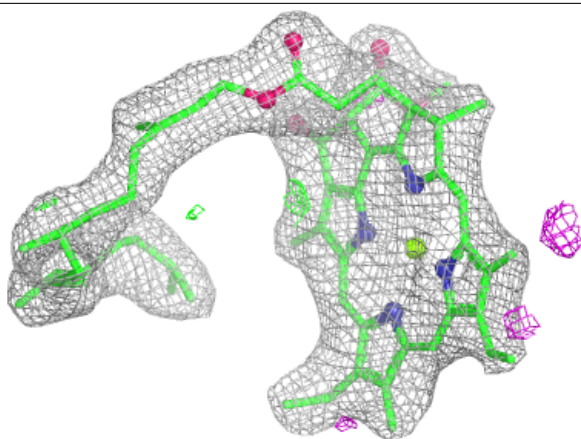
**Electron density around CLA c 502:**

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



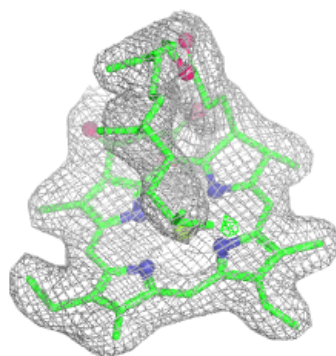
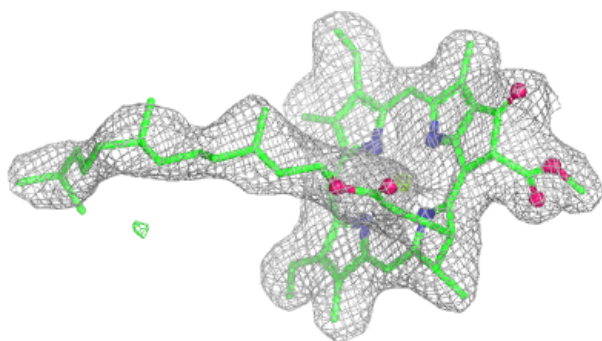
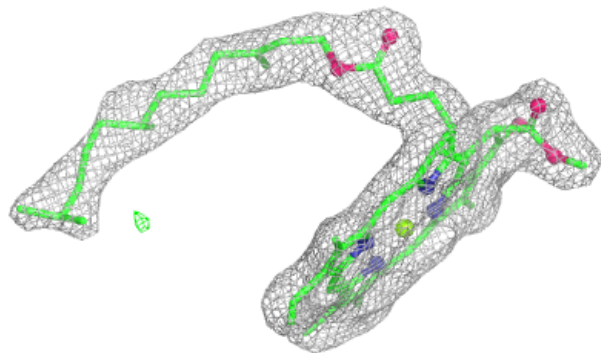
Electron density around CLA c 503:

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

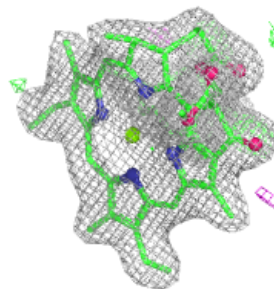
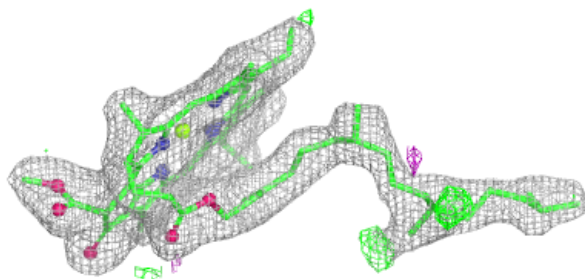
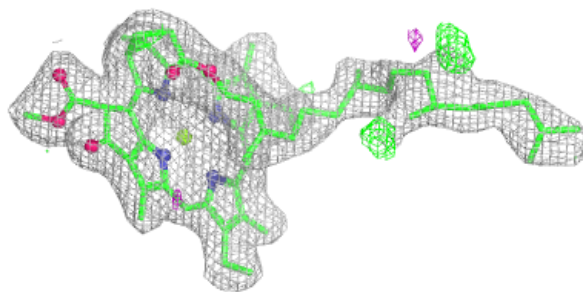


Electron density around CLA c 504:

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

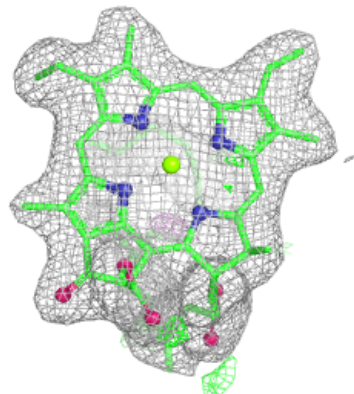
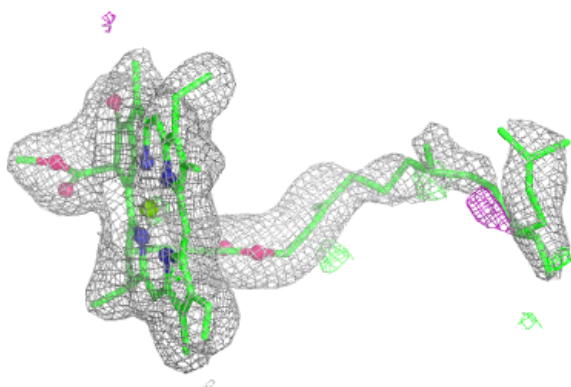
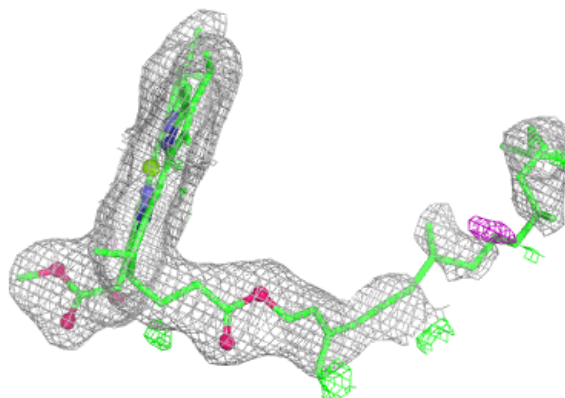
**Electron density around CLA c 505:**

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



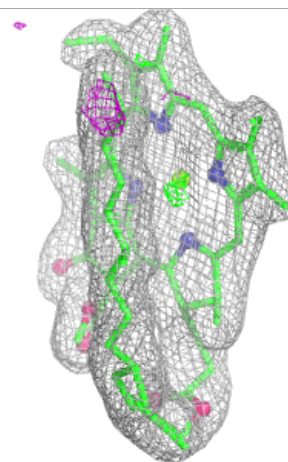
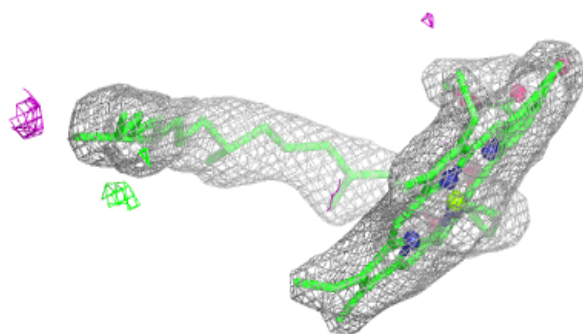
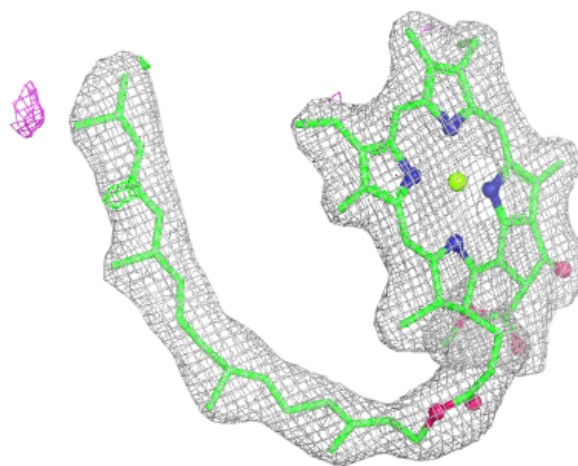
Electron density around CLA C 506:

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



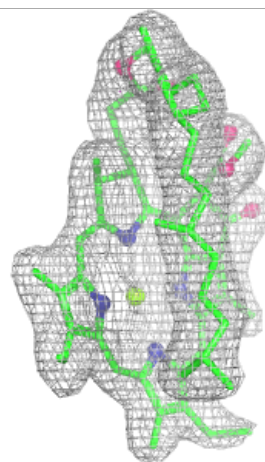
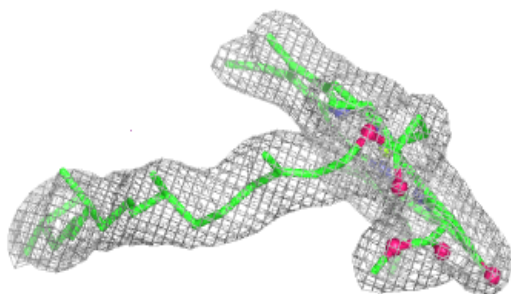
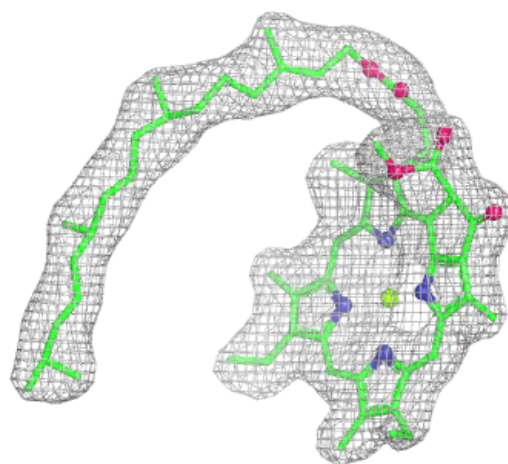
Electron density around CLA c 507:

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



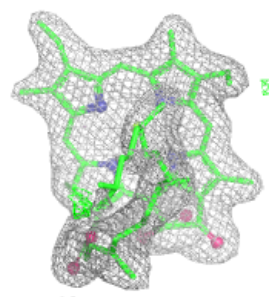
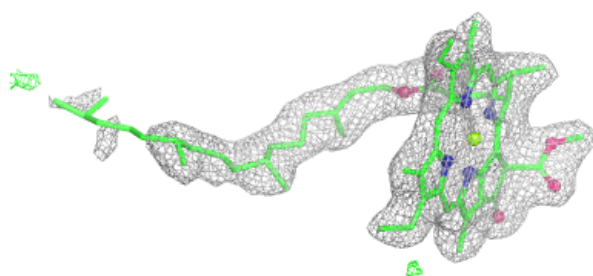
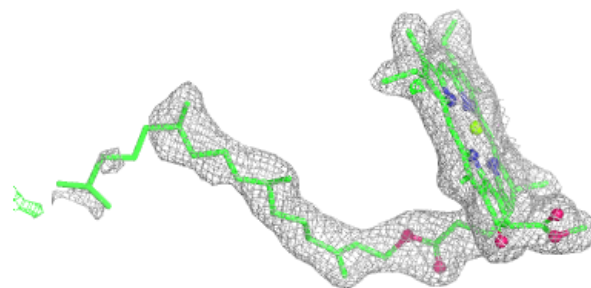
Electron density around CLA C 507:

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

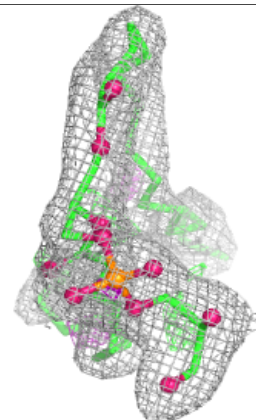
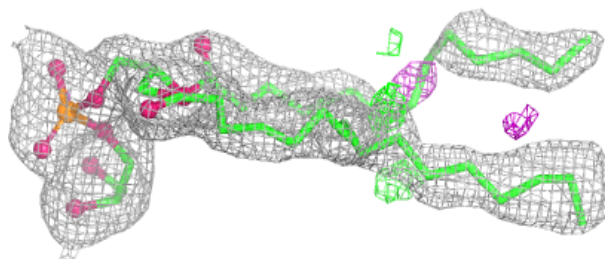
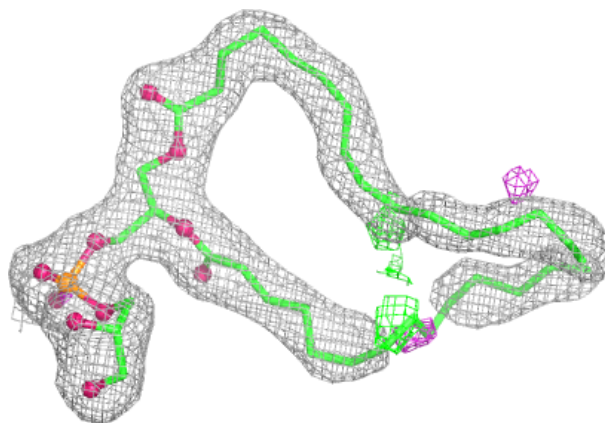


Electron density around CLA C 508:

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

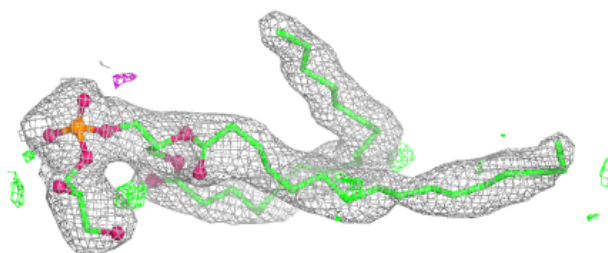
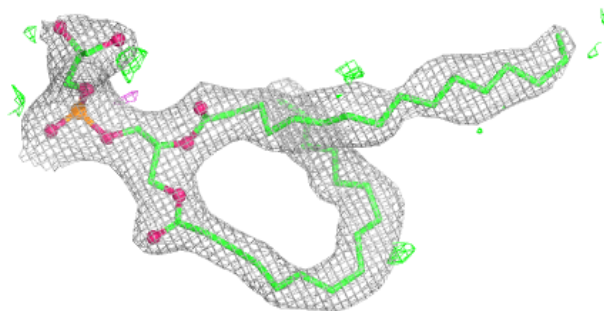
**Electron density around LHG D 410:**

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

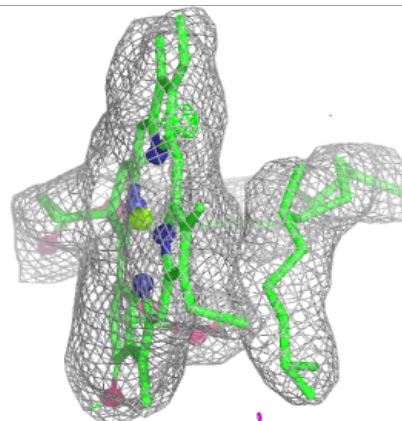
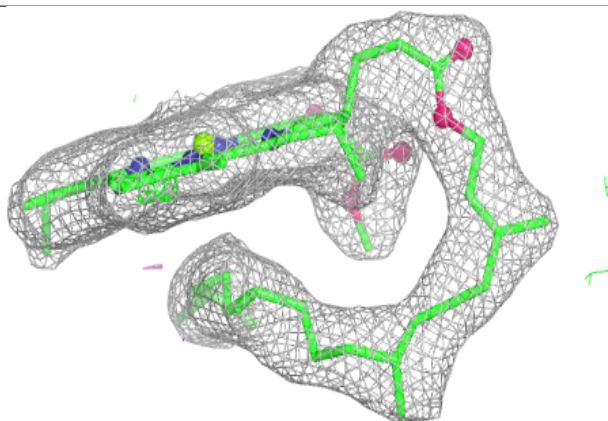
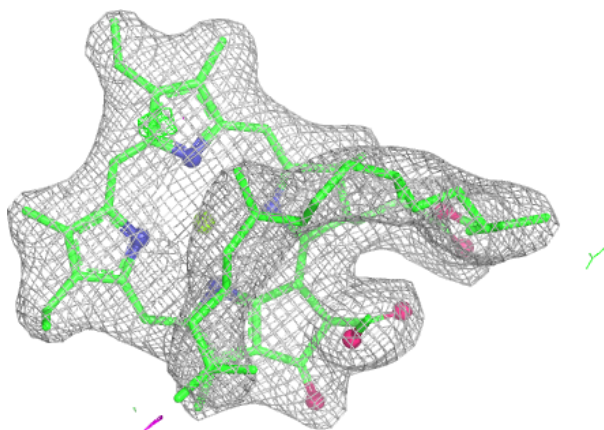


Electron density around LHG D 412:

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

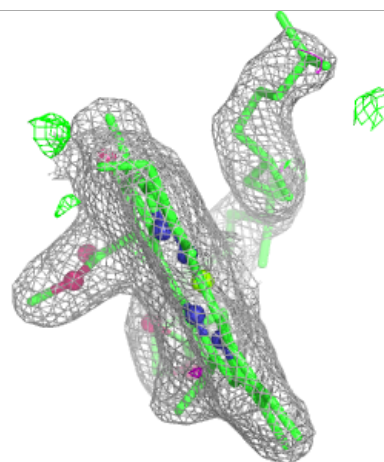
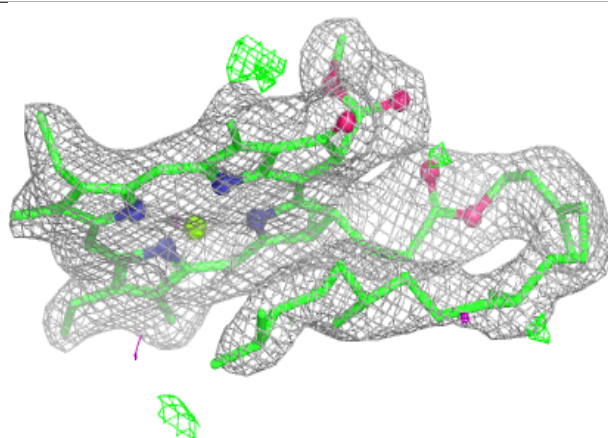
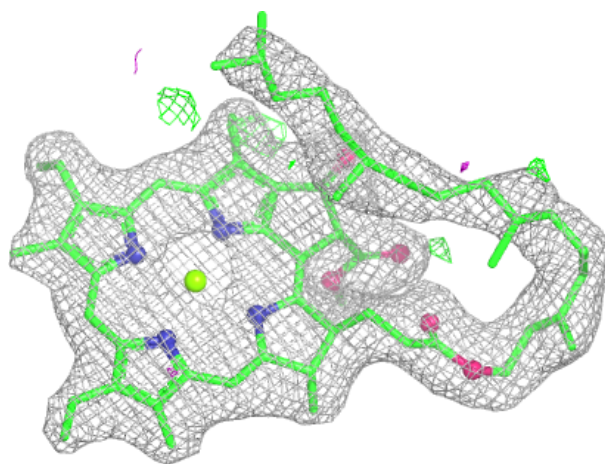
**Electron density around CLA c 510:**

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



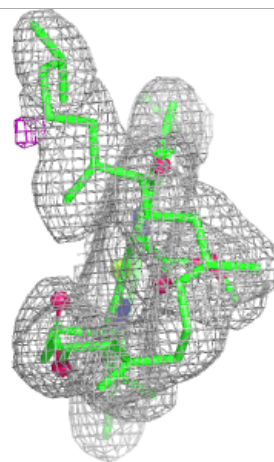
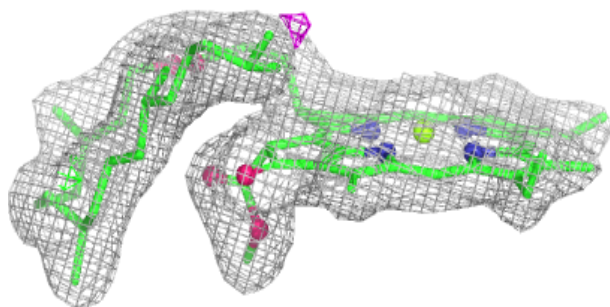
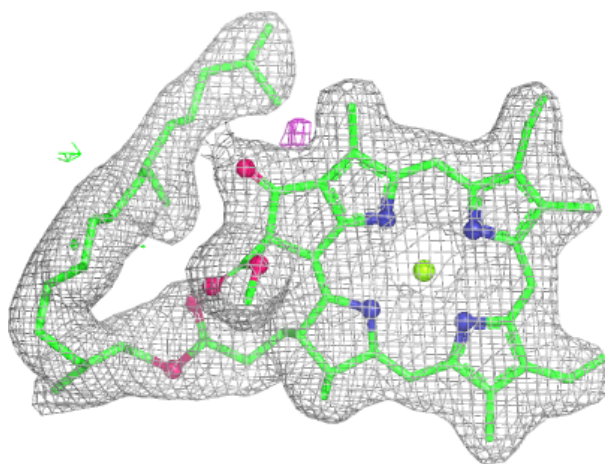
Electron density around CLA C 509:

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



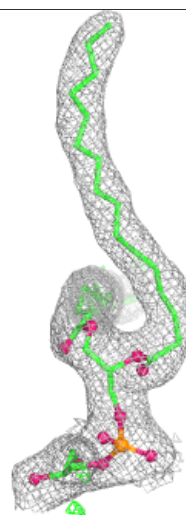
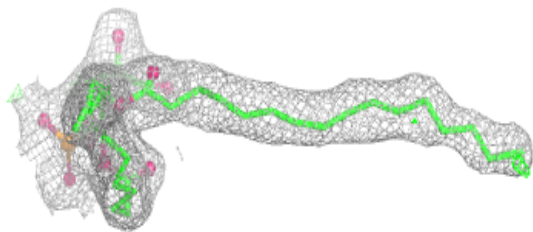
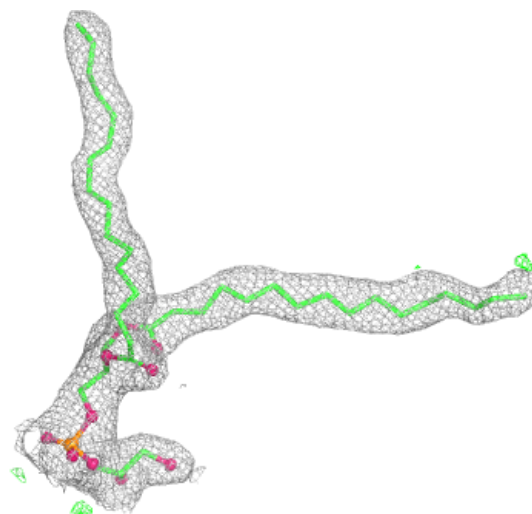
Electron density around CLA B 610:

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



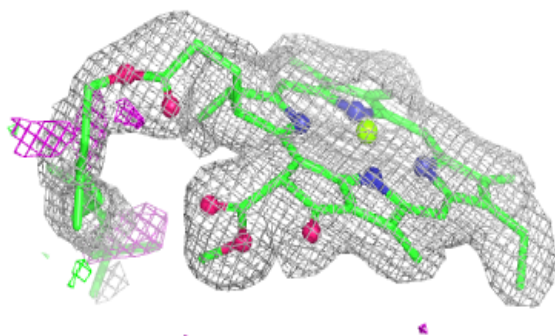
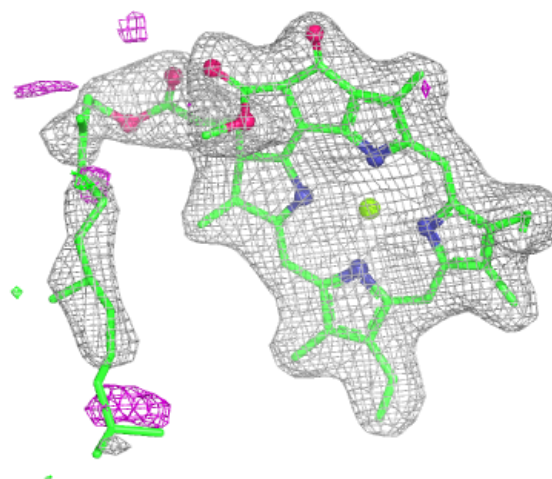
Electron density around LHG 1 101:

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



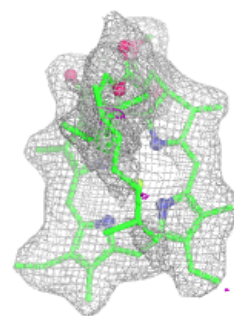
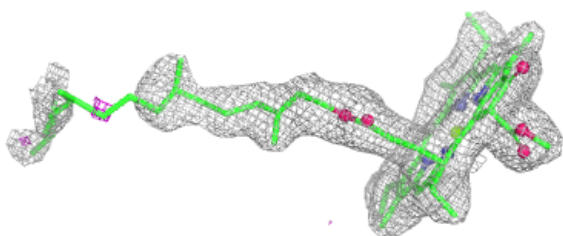
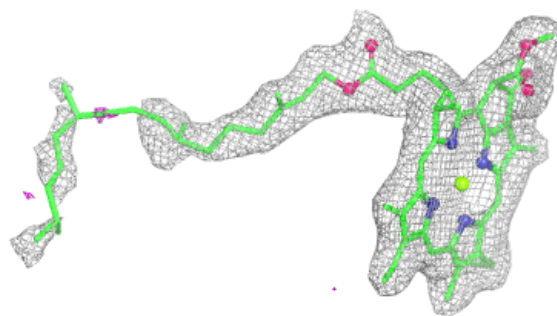
Electron density around CLA B 616:

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

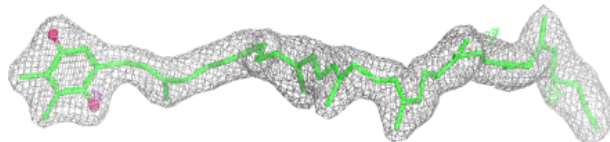
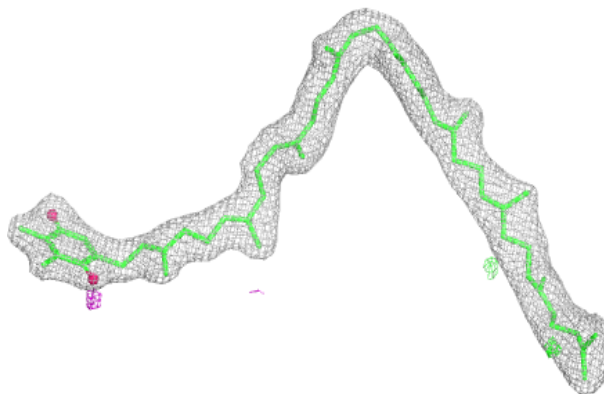


Electron density around CLA d 404:

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

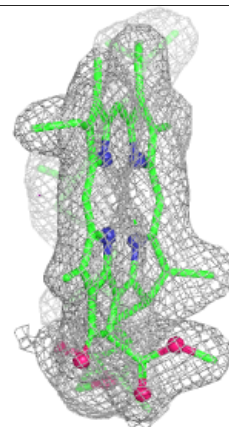
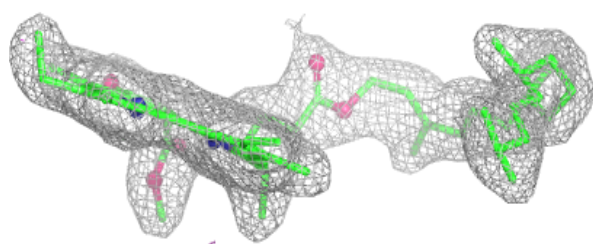
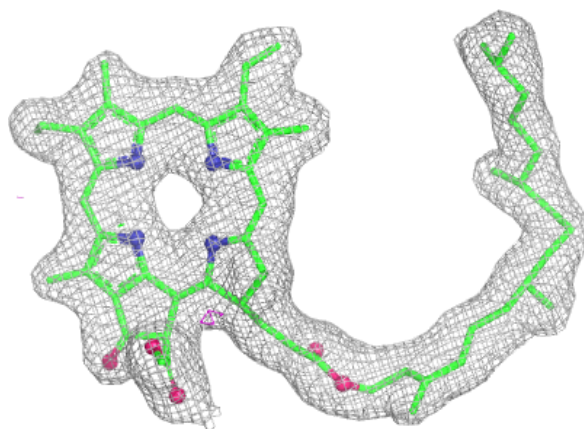
**Electron density around PL9 d 406:**

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

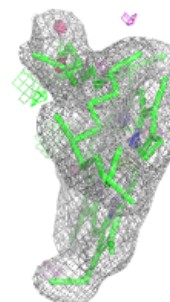
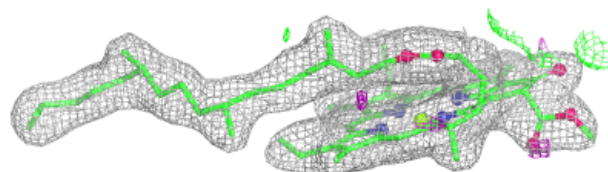
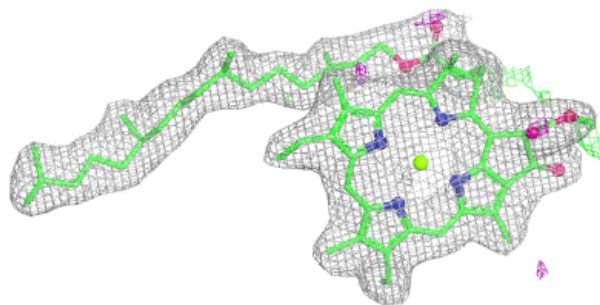


Electron density around PHO d 401:

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

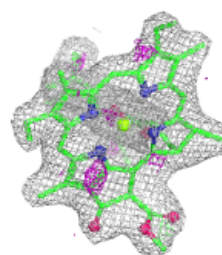
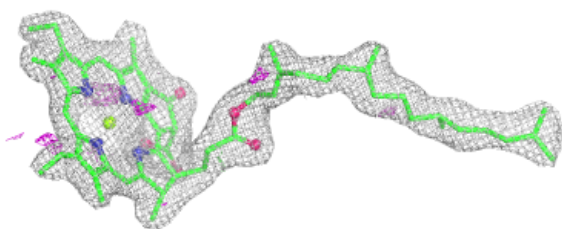
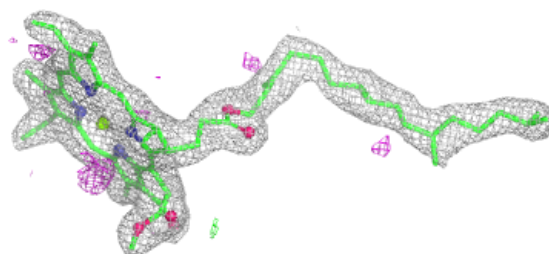
**Electron density around CLA C 501:**

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

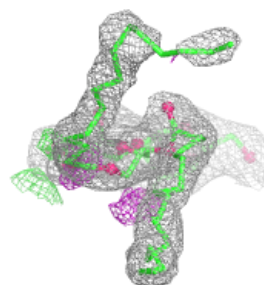
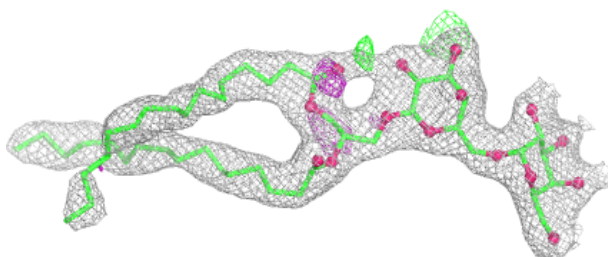
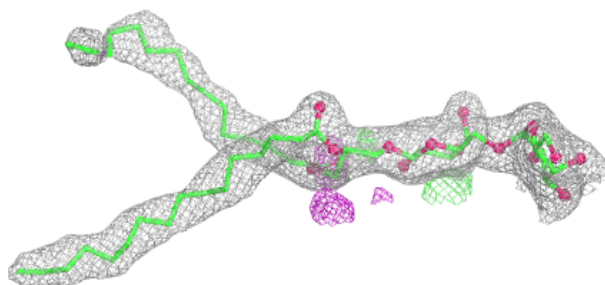


Electron density around CLA C 502:

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

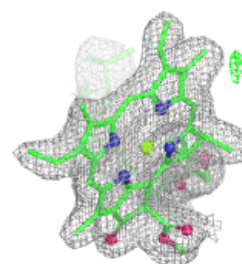
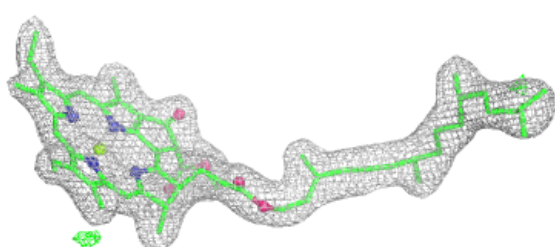
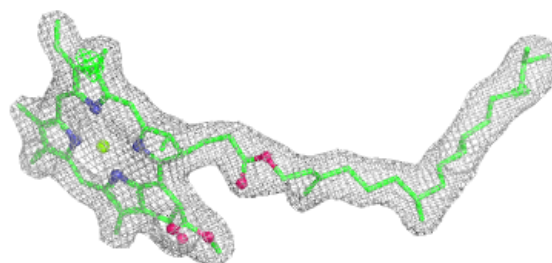
**Electron density around DGD c 517:**

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

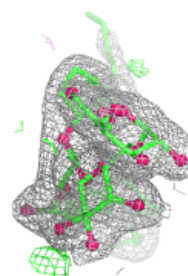
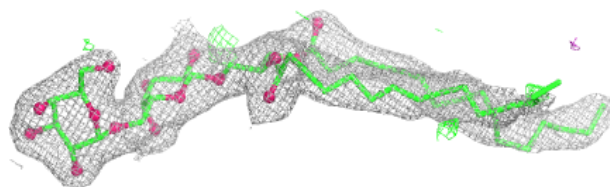
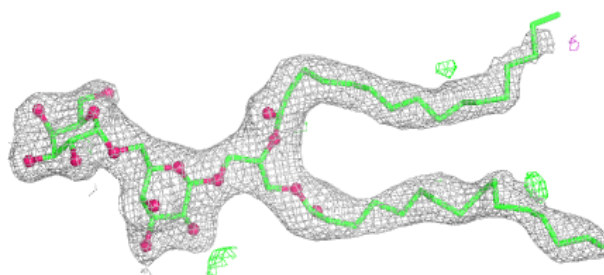


Electron density around CLA a 607:

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

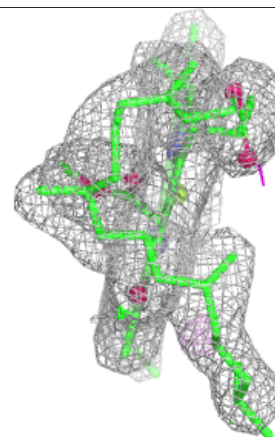
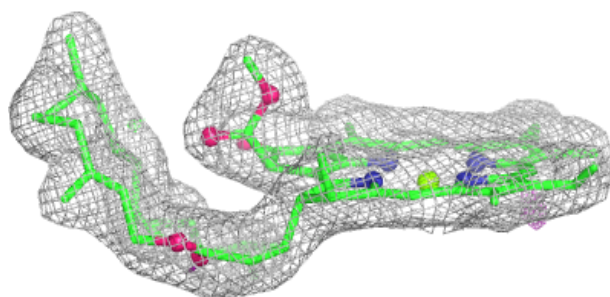
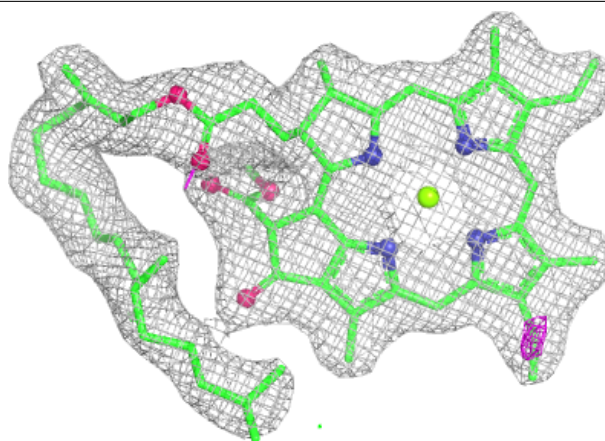
**Electron density around DGD c 519:**

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



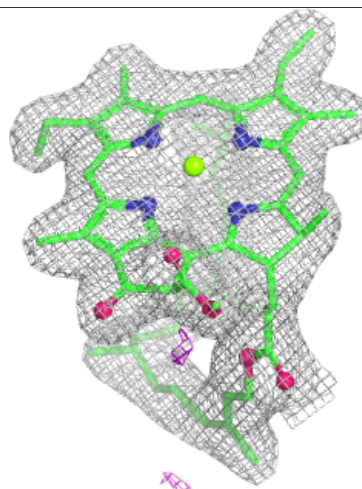
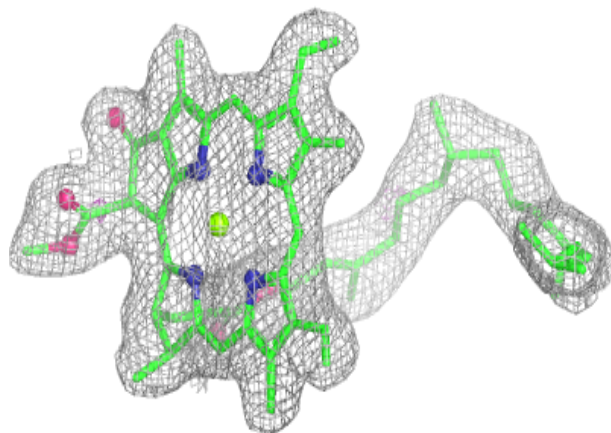
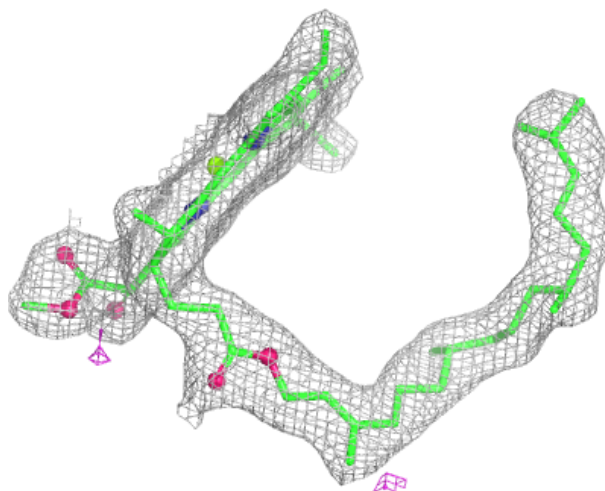
Electron density around CLA b 610:

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



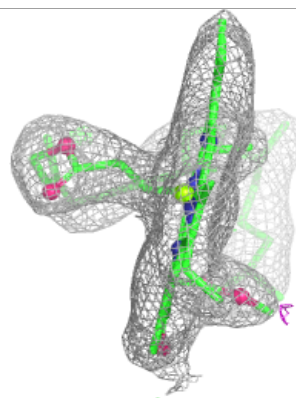
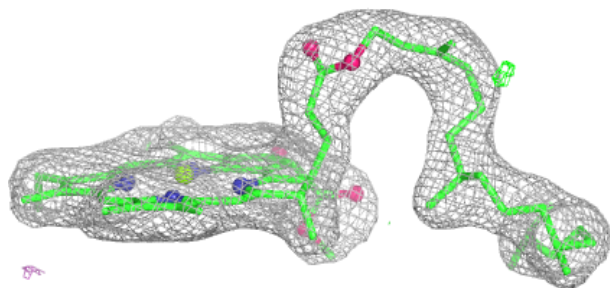
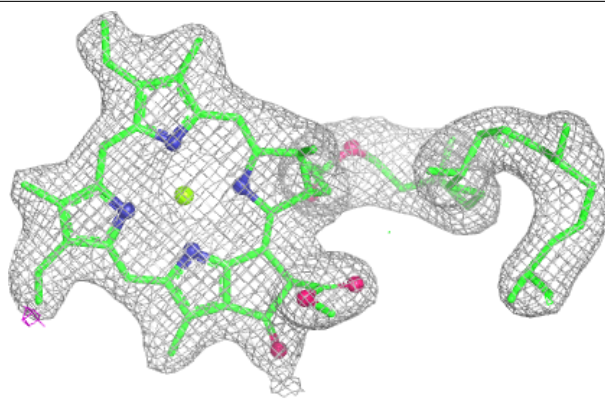
Electron density around CLA b 611:

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



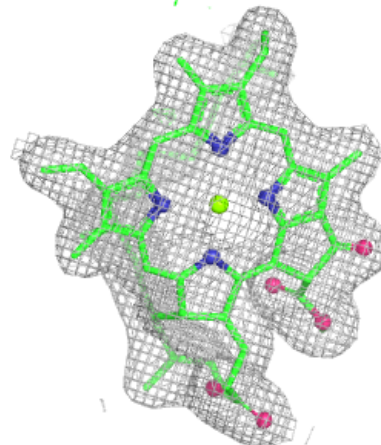
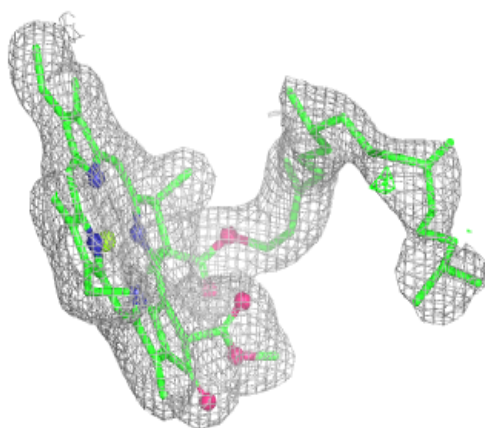
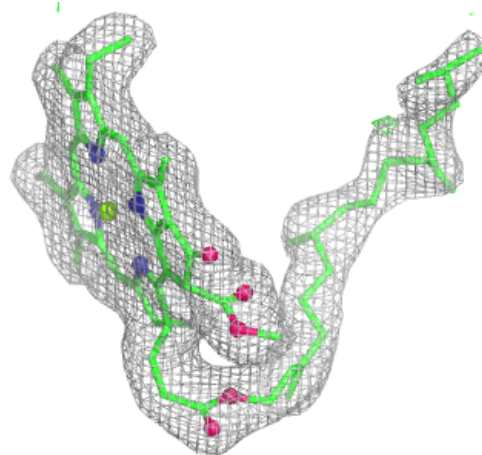
Electron density around CLA b 612:

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



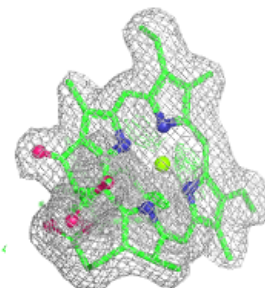
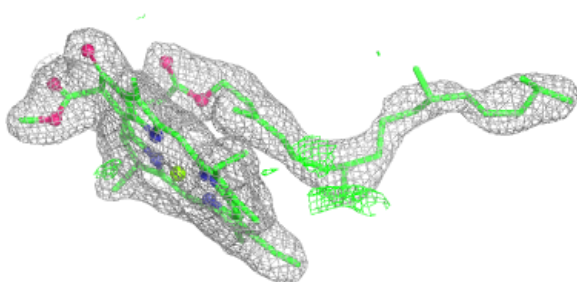
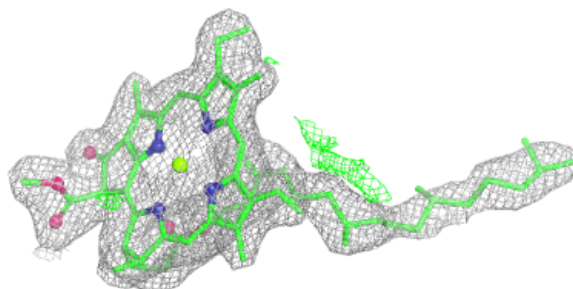
Electron density around CLA b 613:

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

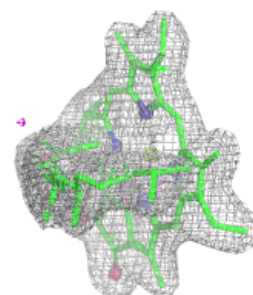
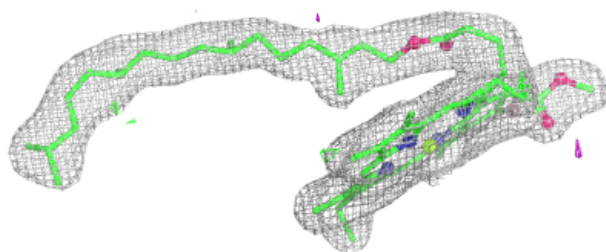
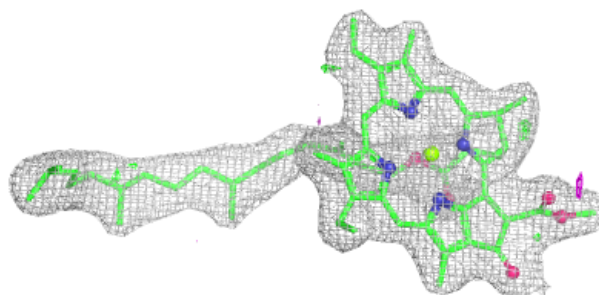


Electron density around CLA C 505:

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

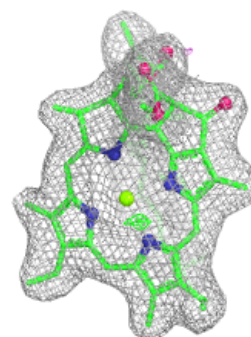
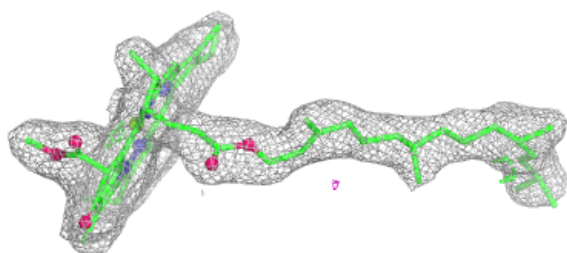
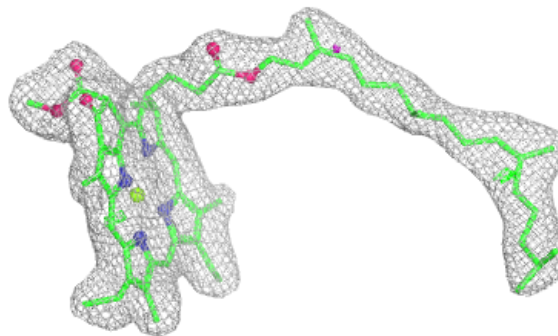
**Electron density around CLA B 608:**

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

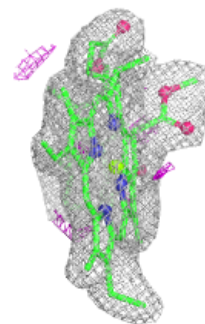
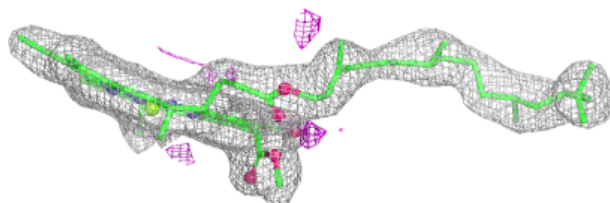
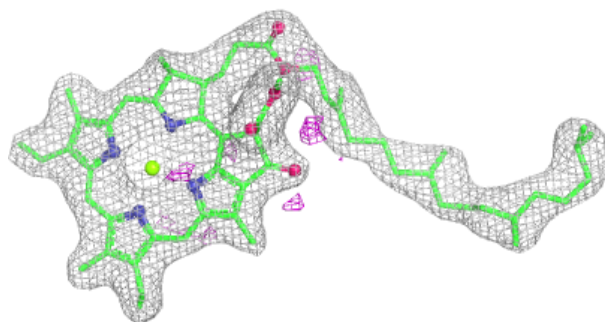


Electron density around CLA B 609:

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

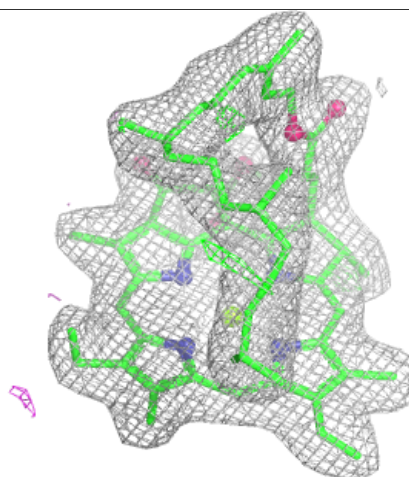
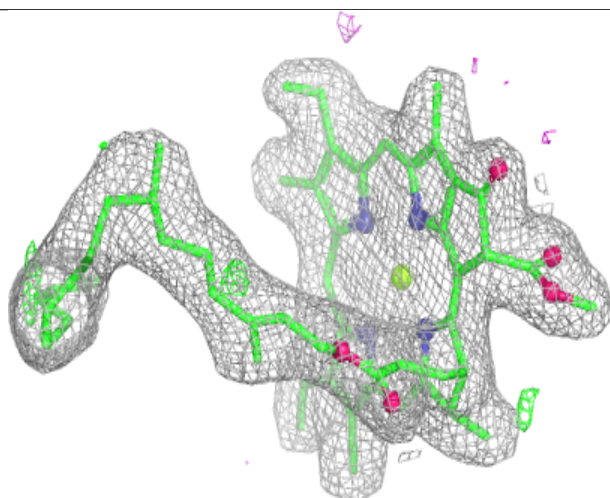
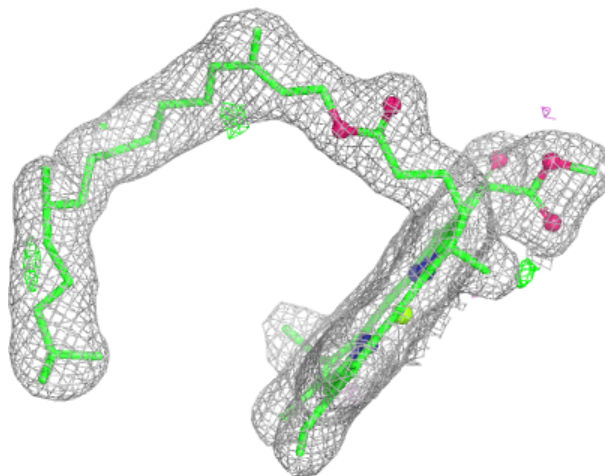
**Electron density around CLA B 602:**

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



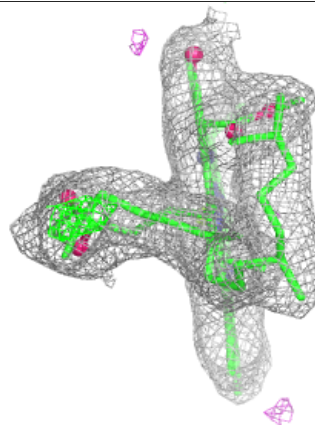
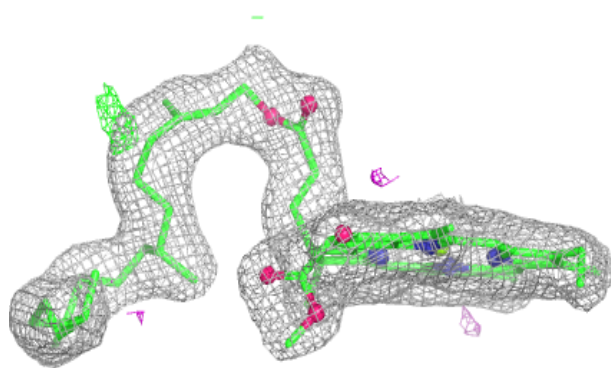
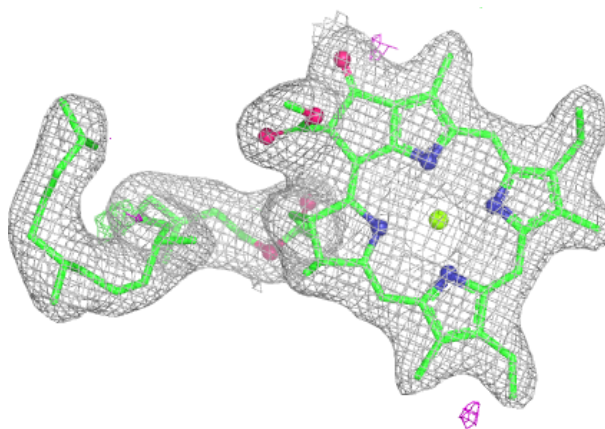
Electron density around CLA B 611:

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



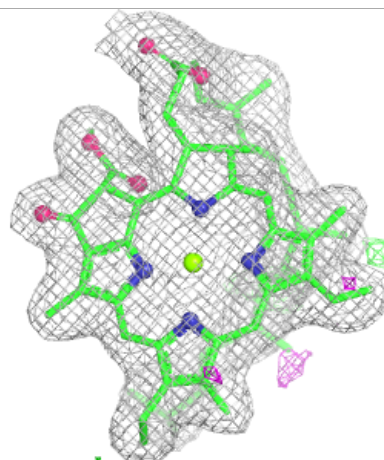
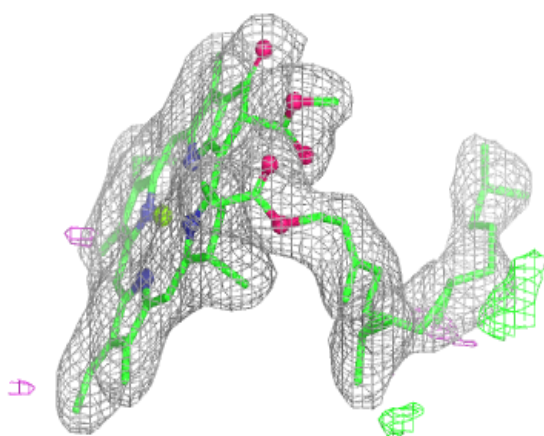
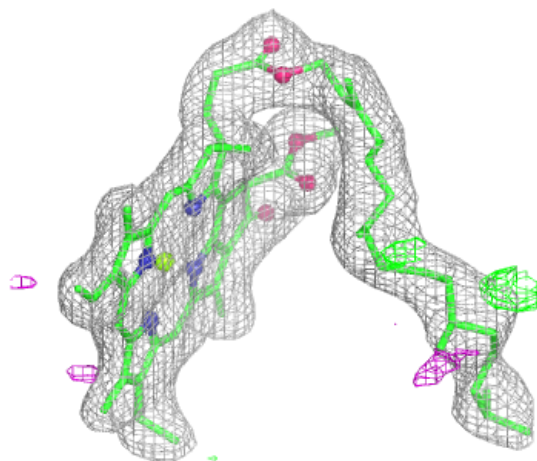
Electron density around CLA B 612:

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



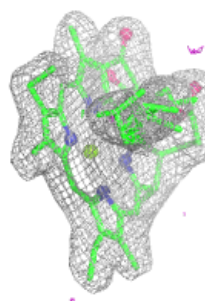
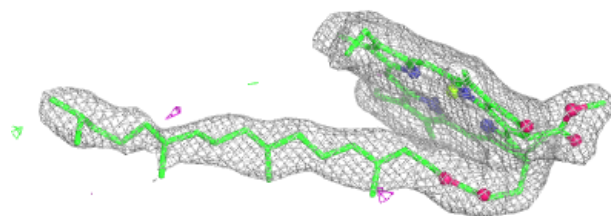
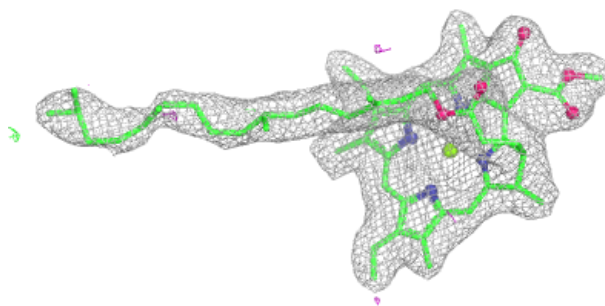
Electron density around CLA B 613:

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



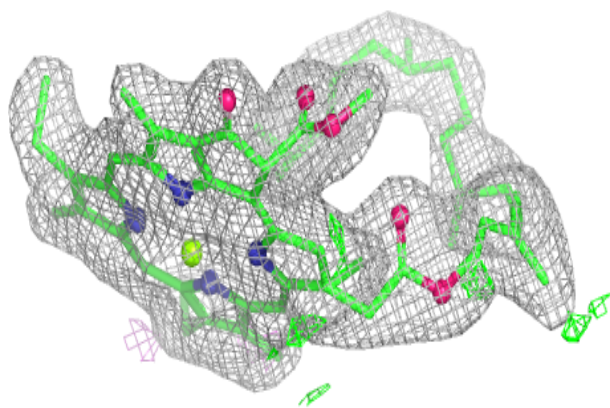
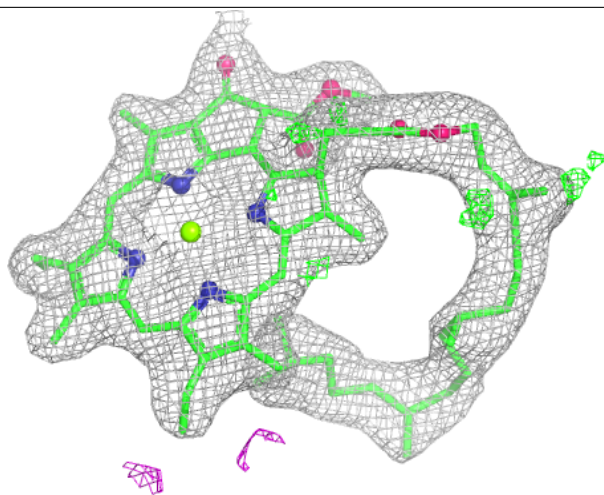
Electron density around CLA B 614:

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



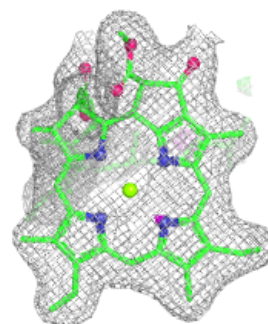
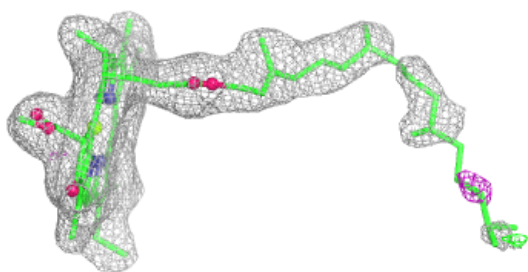
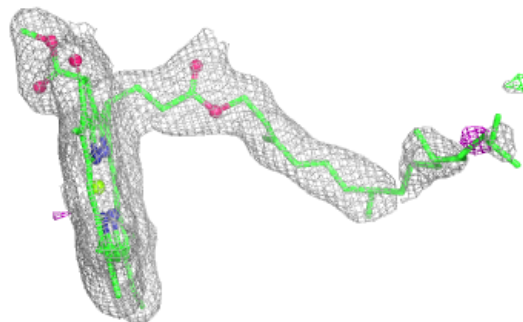
Electron density around CLA B 615:

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



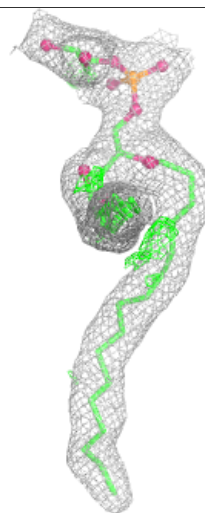
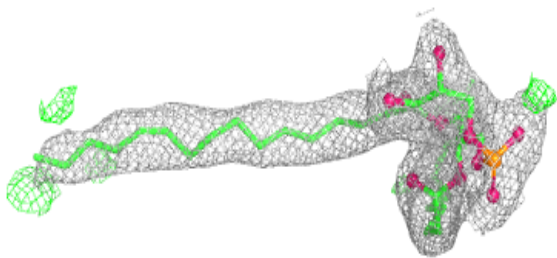
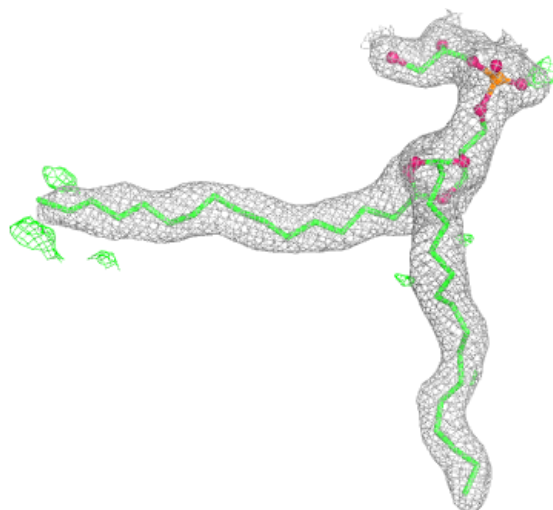
Electron density around CLA D 405:

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



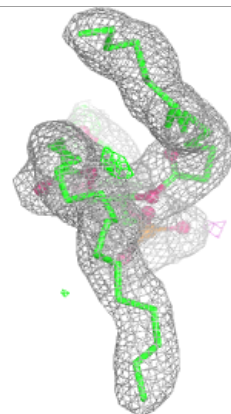
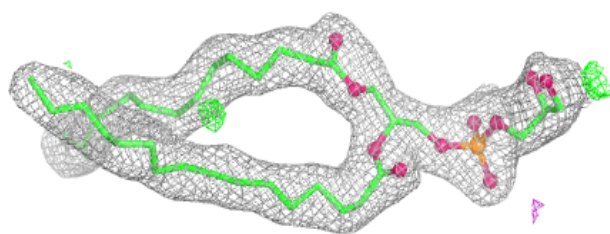
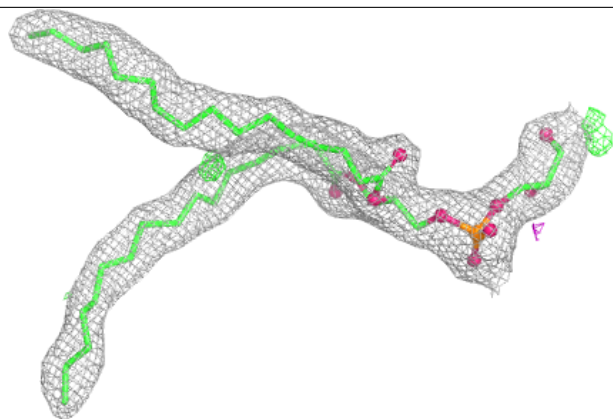
Electron density around LHG A 615:

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

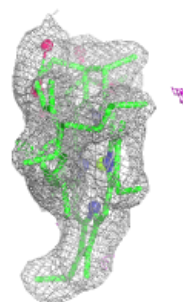
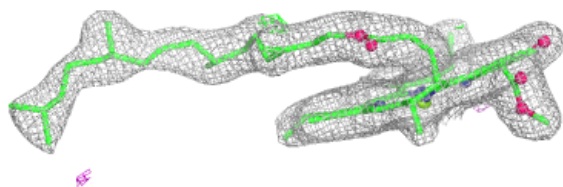
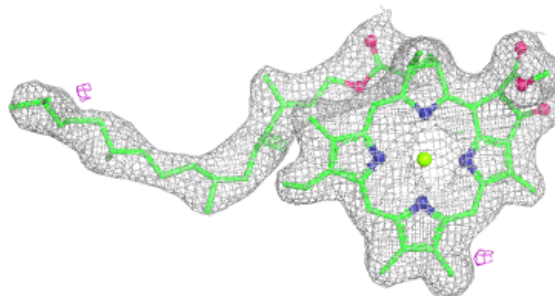


Electron density around LHG D 409:

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

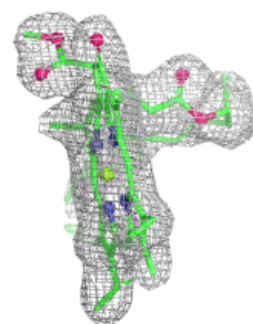
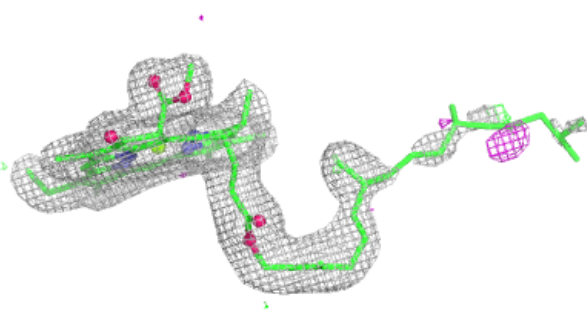
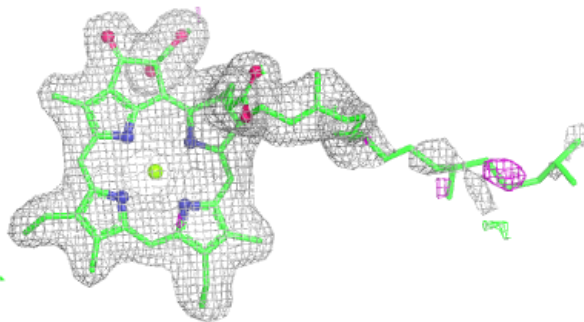
**Electron density around CLA B 603:**

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

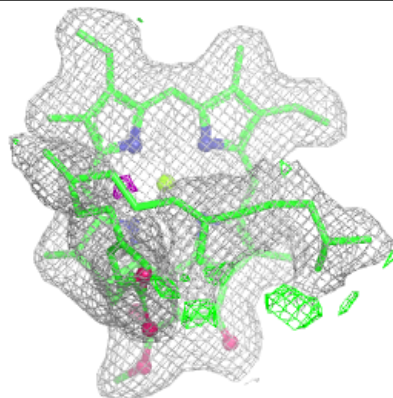
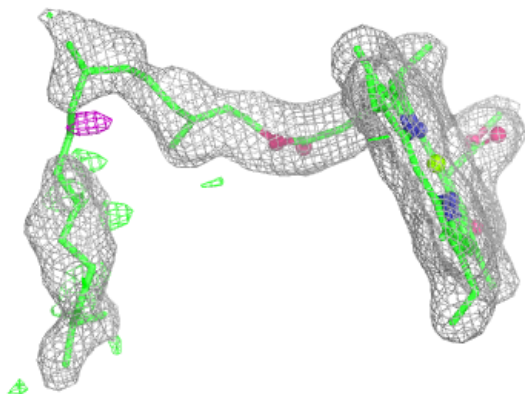
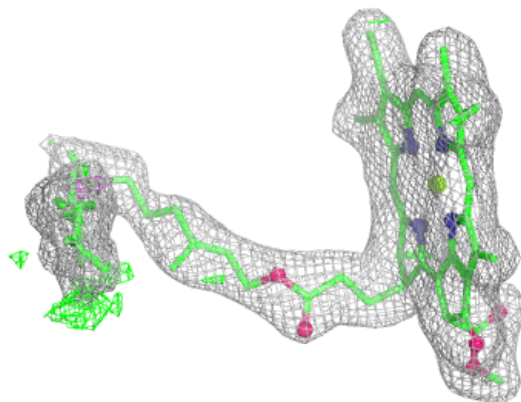


Electron density around CLA A 607:

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

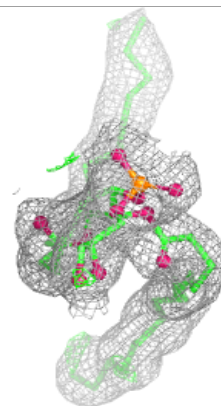
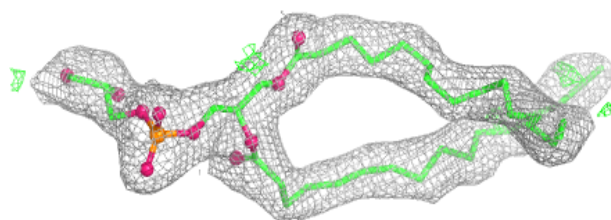
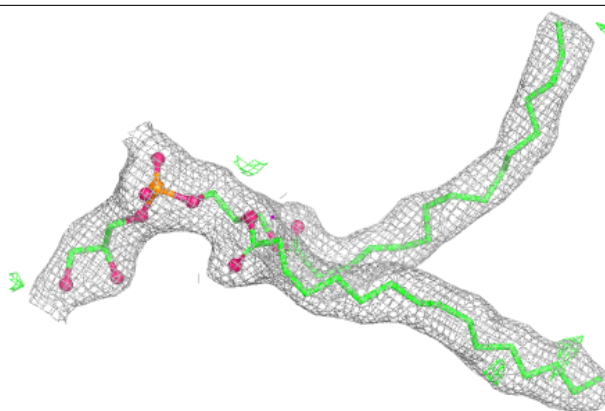
**Electron density around CLA a 609:**

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

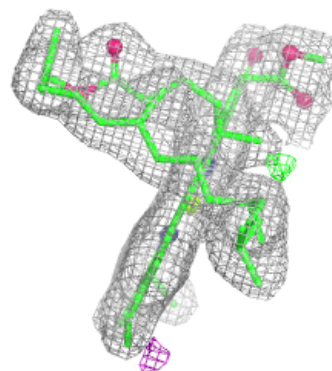
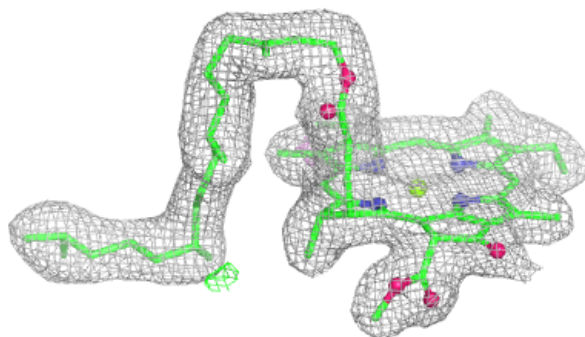
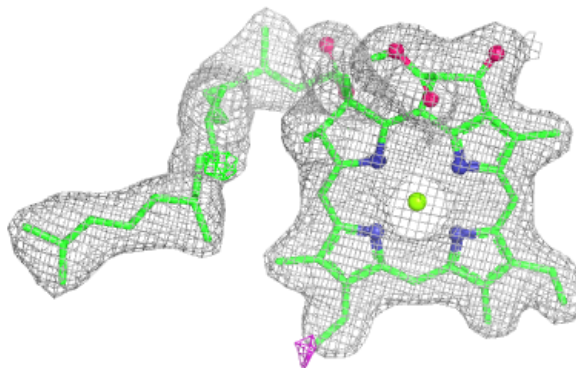


Electron density around LHG d 408:

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

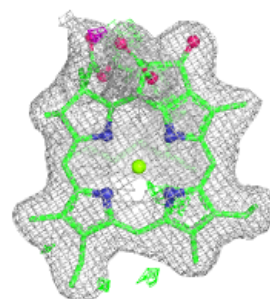
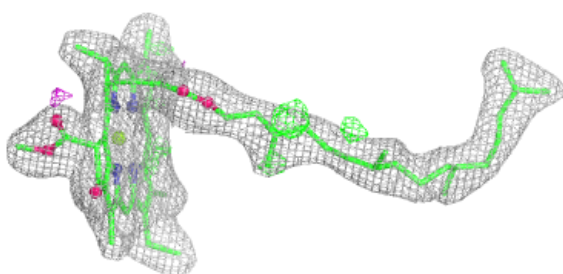
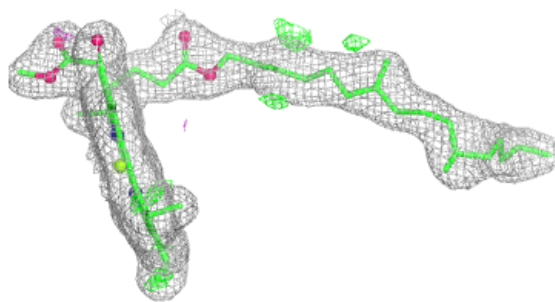
**Electron density around CLA a 612:**

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

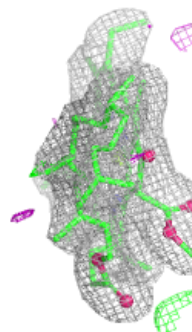
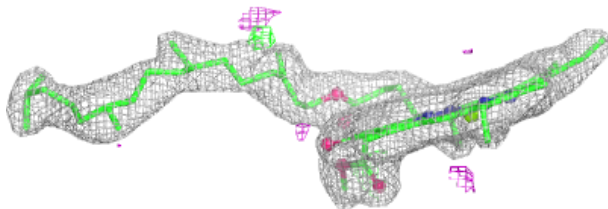
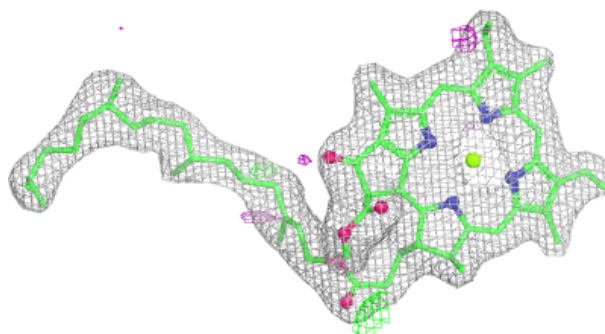


Electron density around CLA B 605:

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

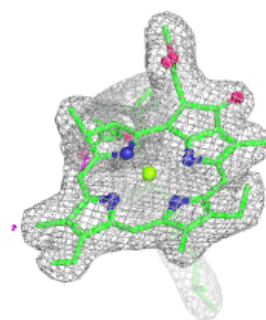
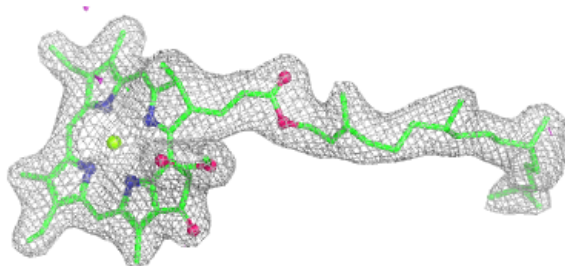
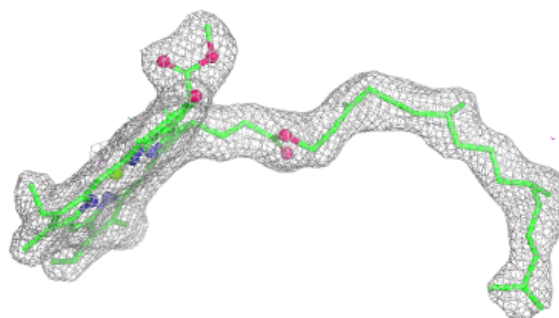
**Electron density around CLA b 602:**

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

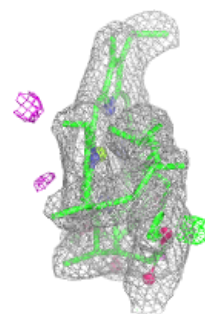
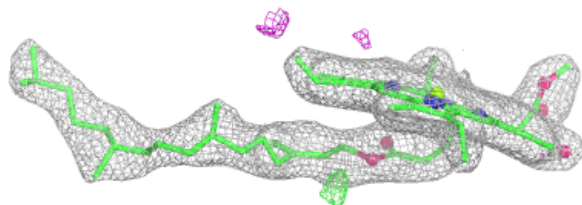
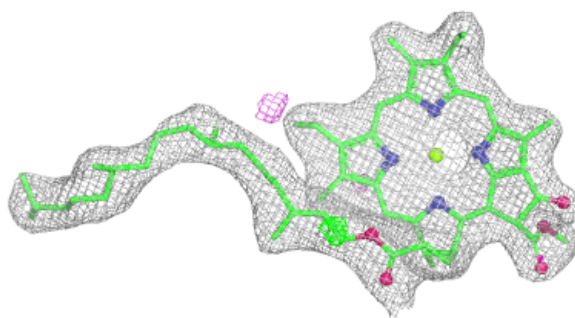


Electron density around CLA d 403:

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

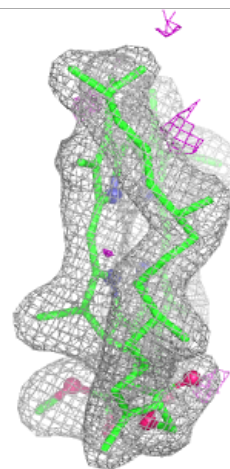
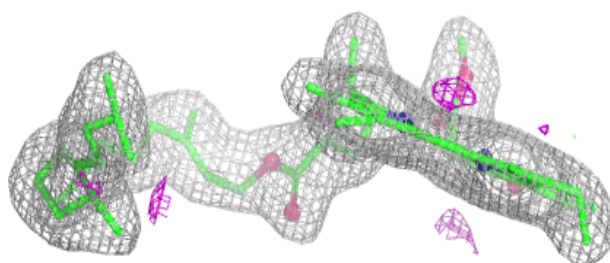
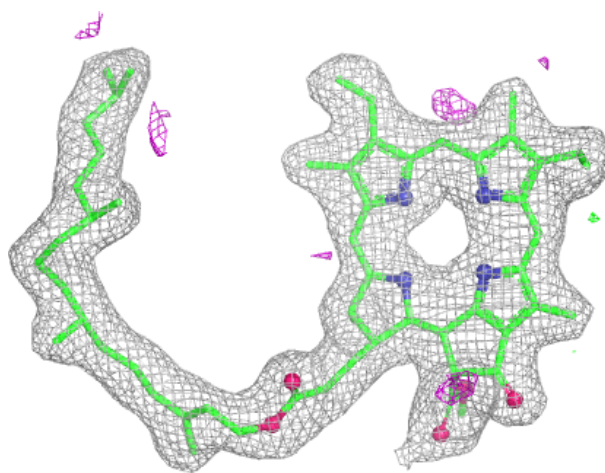
**Electron density around CLA b 603:**

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



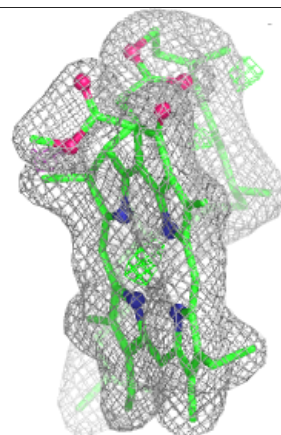
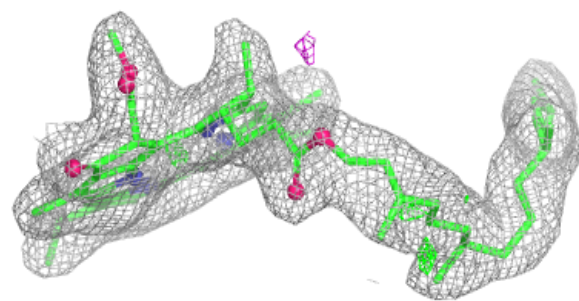
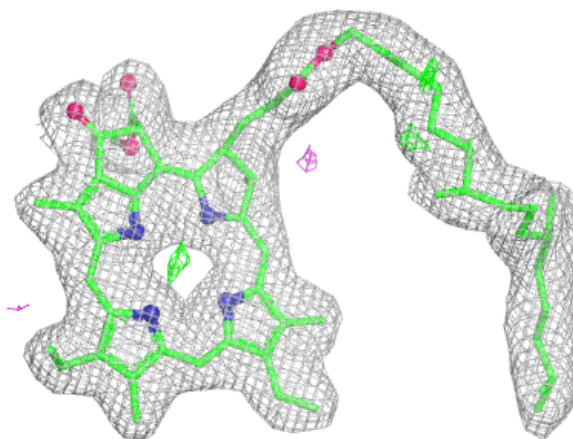
Electron density around PHO A 608:

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



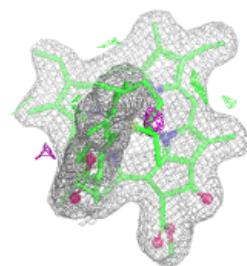
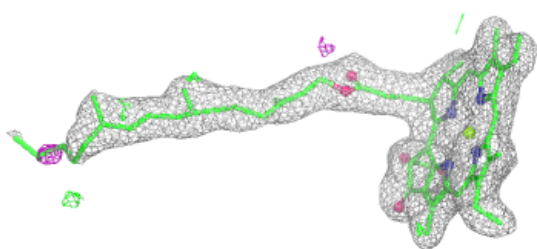
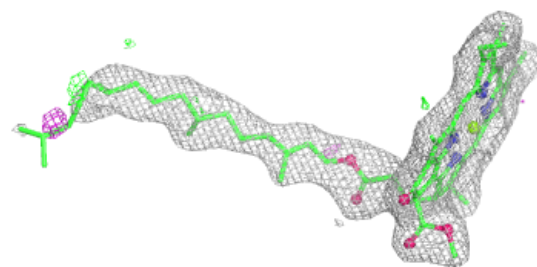
Electron density around PHO D 402:

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



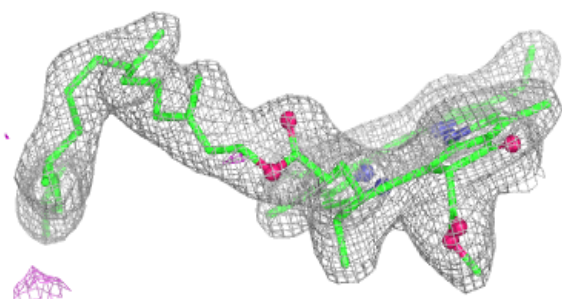
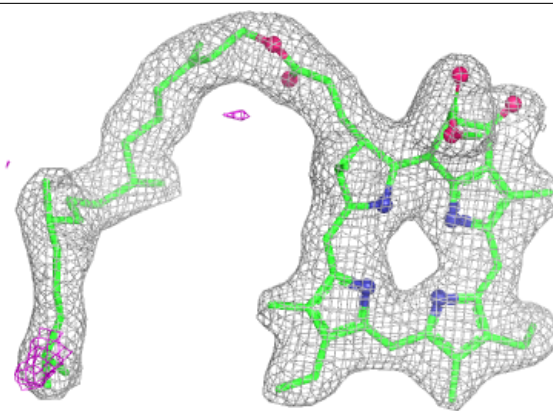
Electron density around CLA b 604:

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



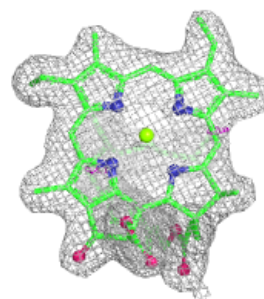
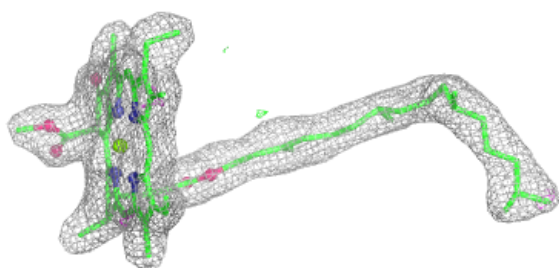
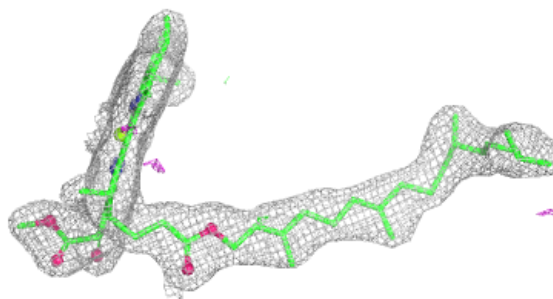
Electron density around PHO d 402:

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

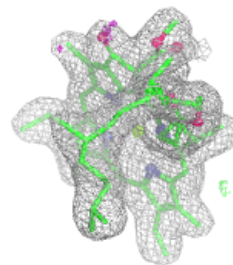
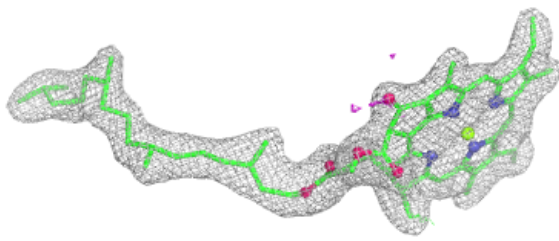
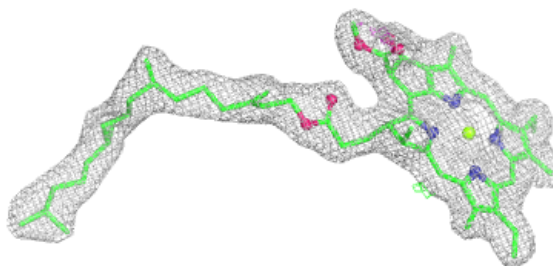


Electron density around CLA b 605:

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

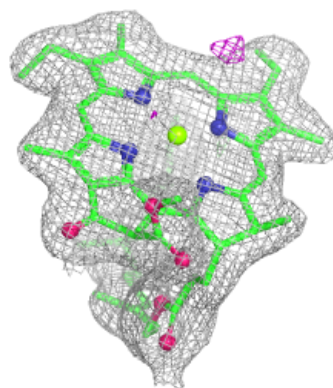
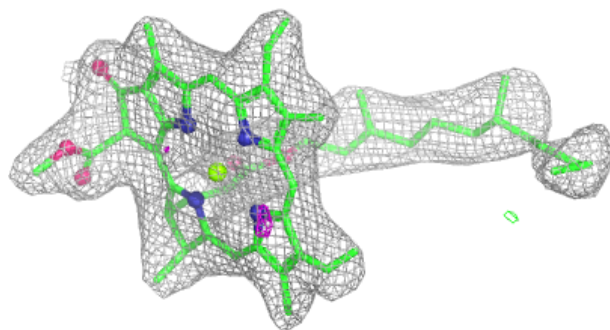
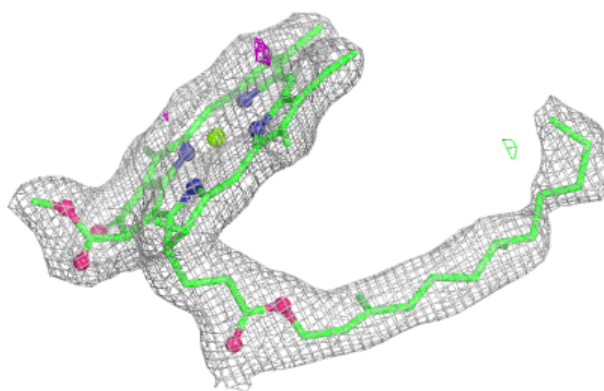
**Electron density around CLA A 606:**

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

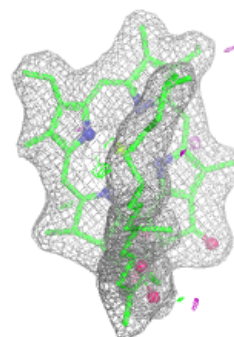
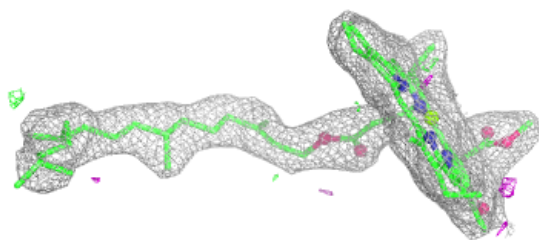
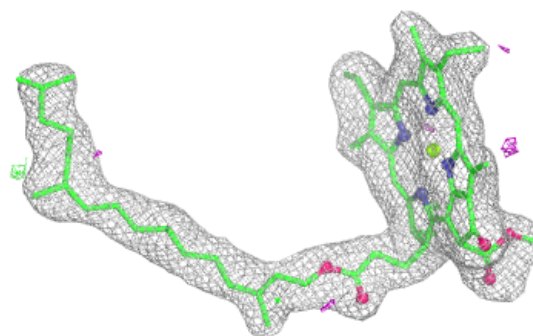


Electron density around CLA C 504:

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

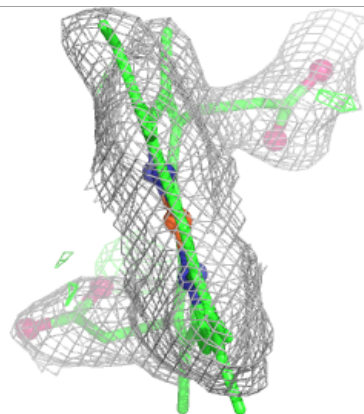
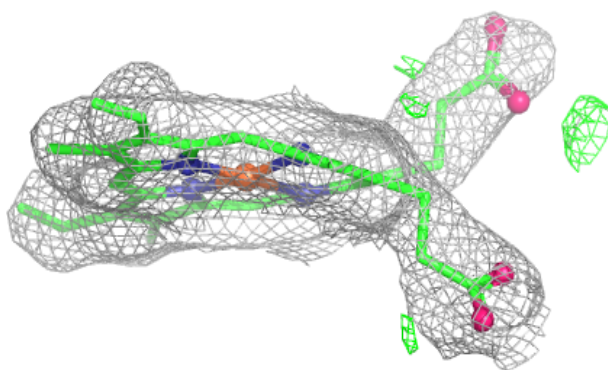
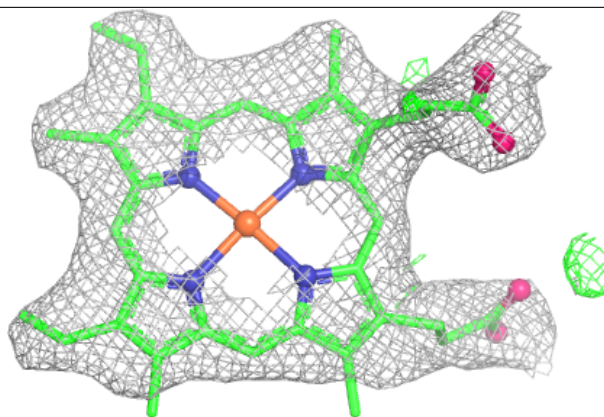
**Electron density around CLA b 609:**

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

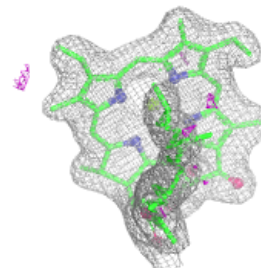
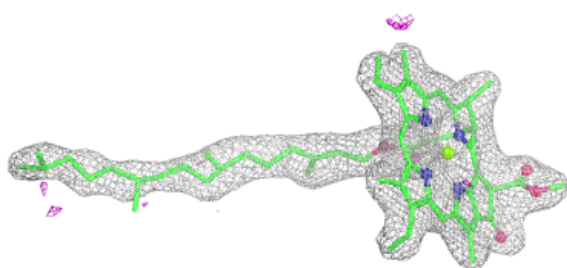
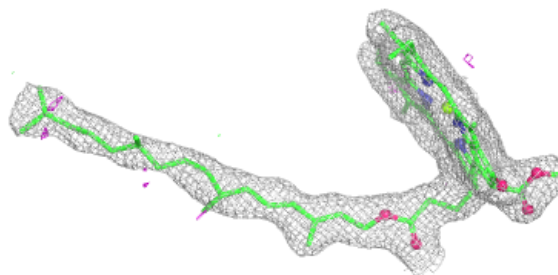


Electron density around HEM f 101:

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

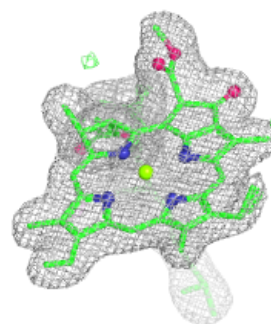
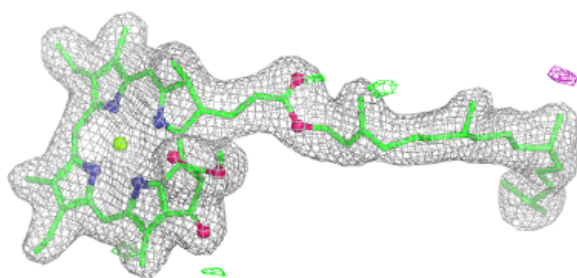
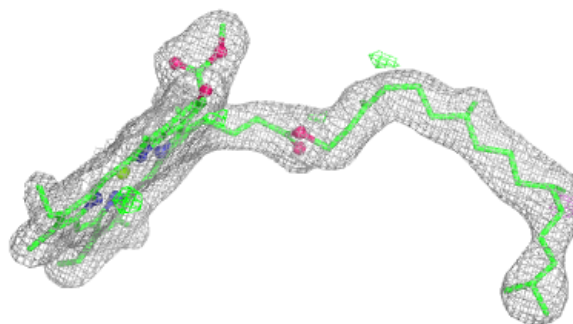
**Electron density around CLA b 607:**

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

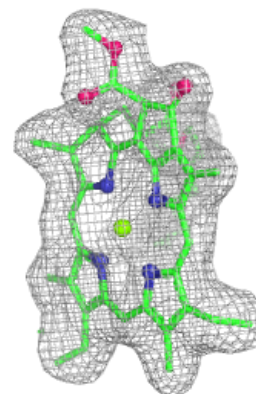
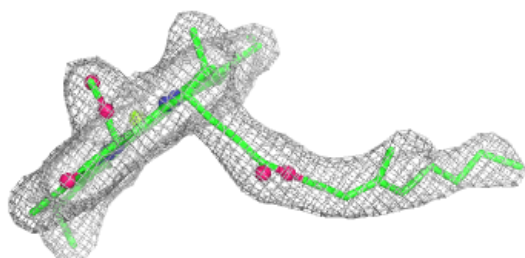
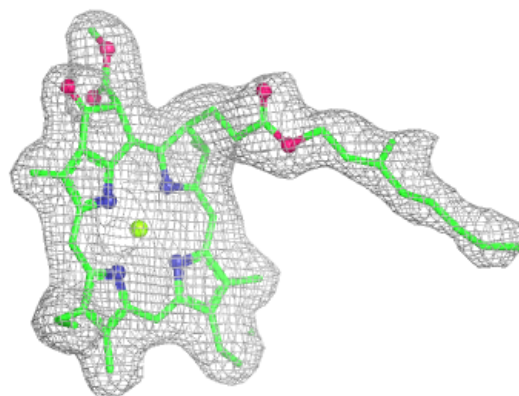


Electron density around CLA D 404:

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

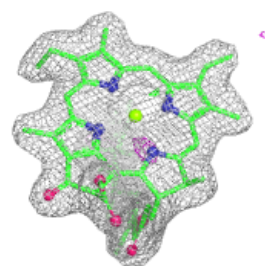
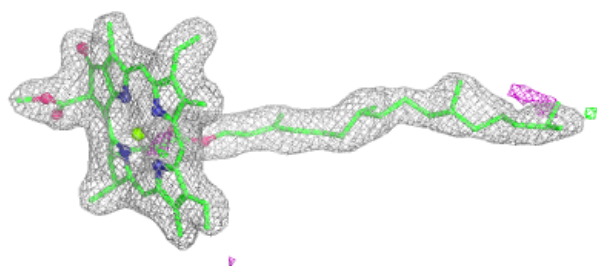
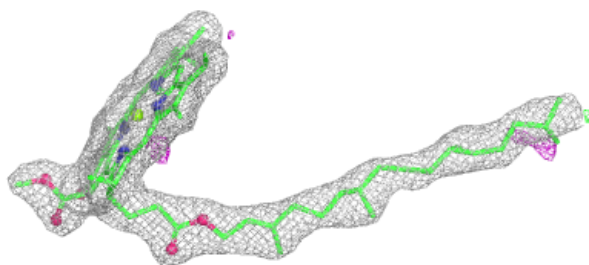
**Electron density around CLA A 609:**

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



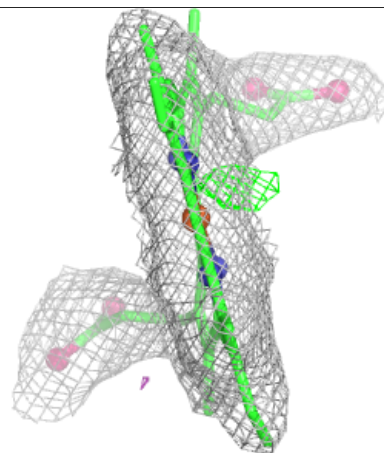
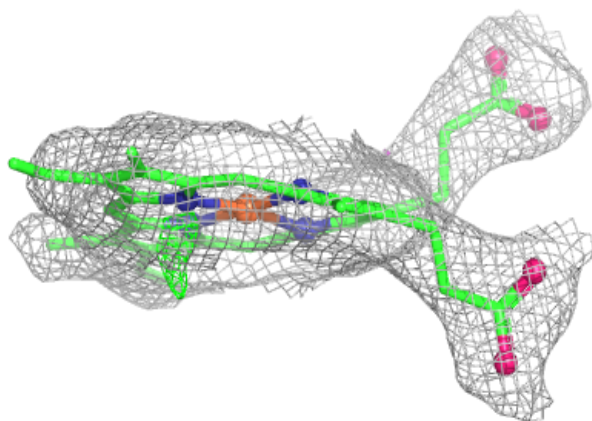
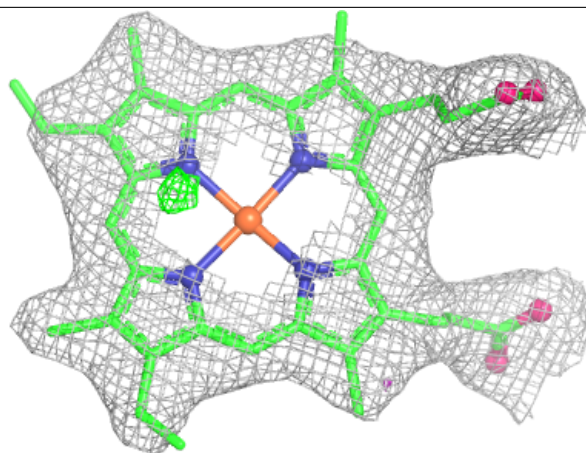
Electron density around CLA B 607:

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



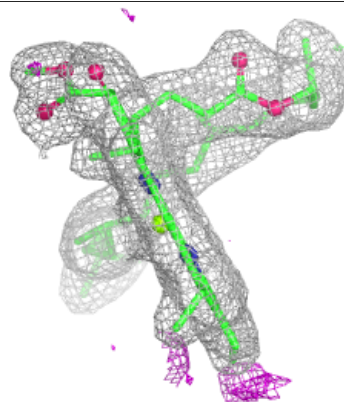
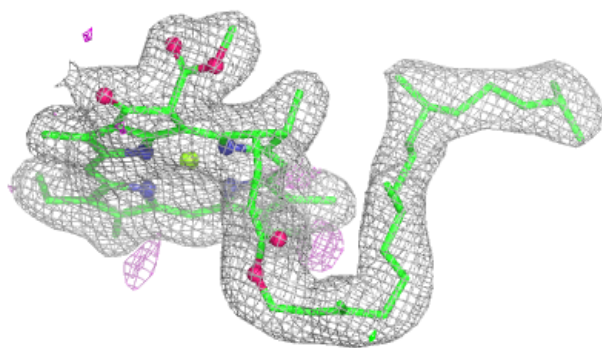
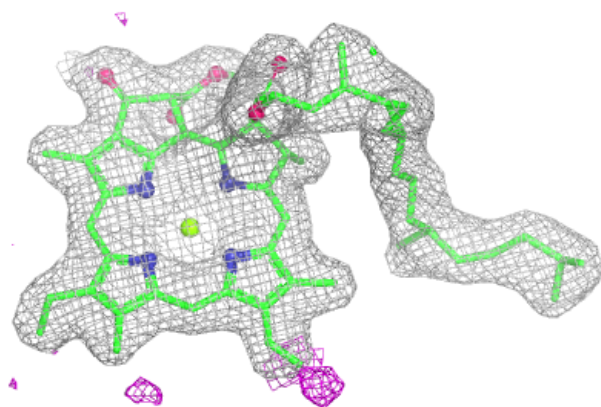
Electron density around HEM E 101:

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



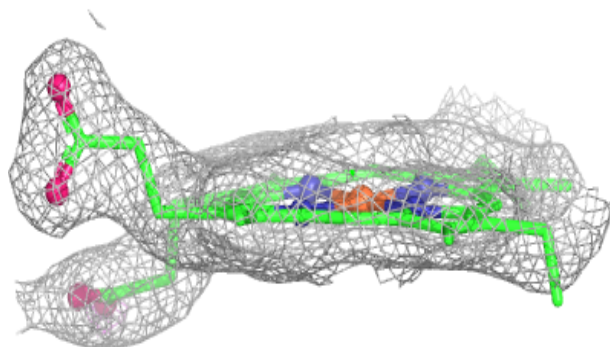
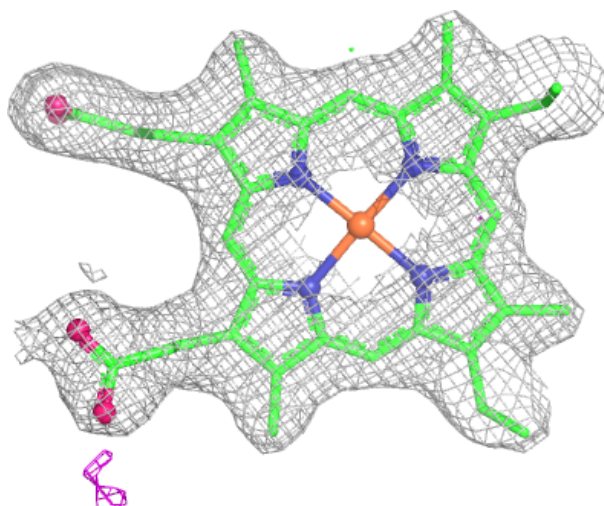
Electron density around CLA D 403:

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



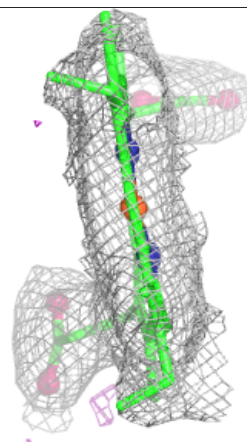
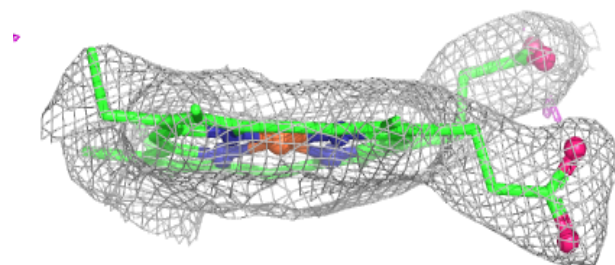
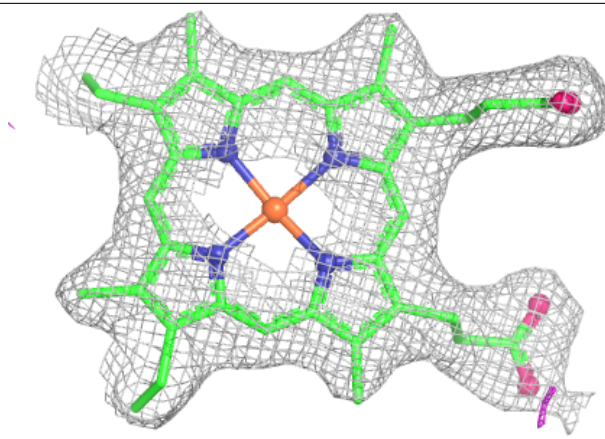
Electron density around HEC V 201:

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



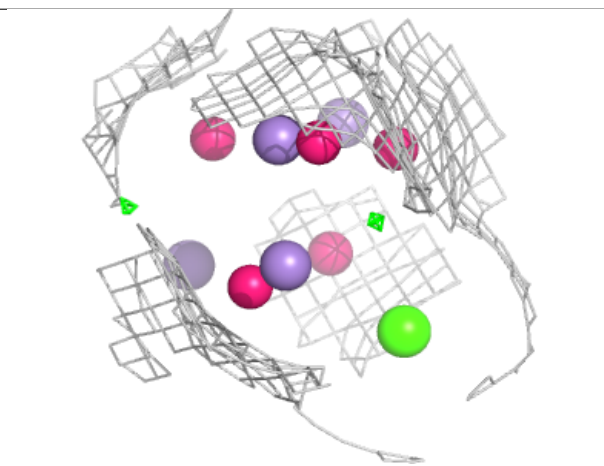
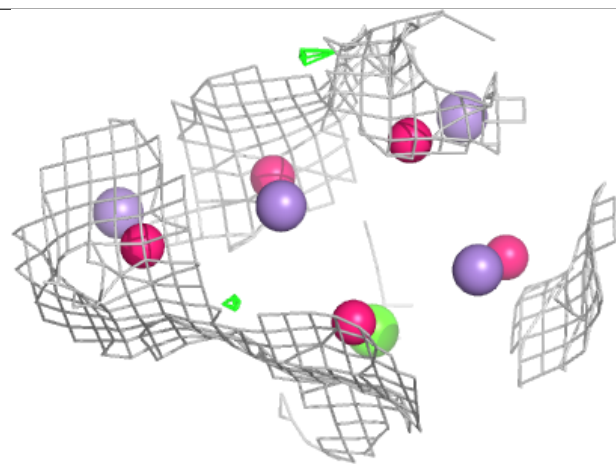
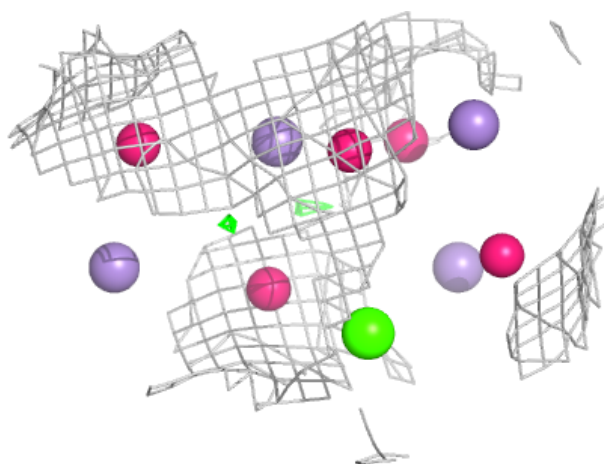
Electron density around HEC v 201:

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



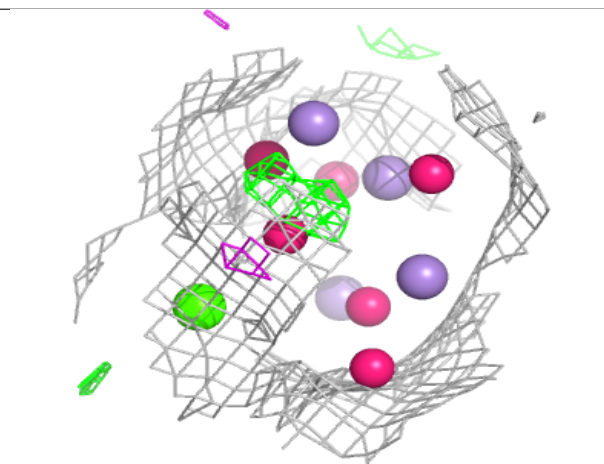
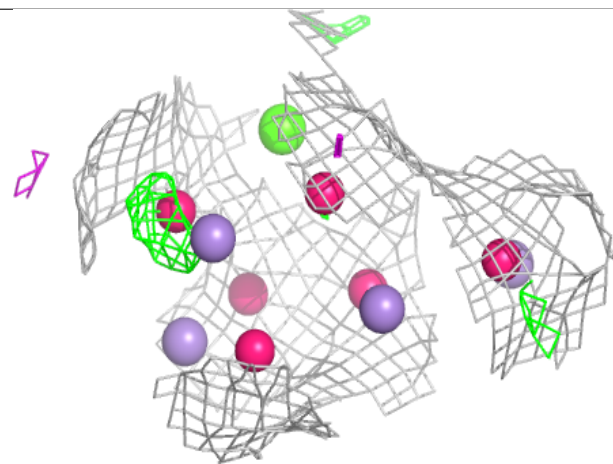
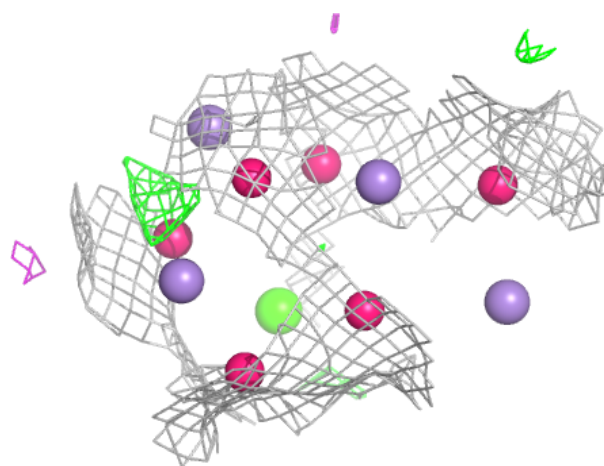
Electron density around OEX a 602 (A):

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



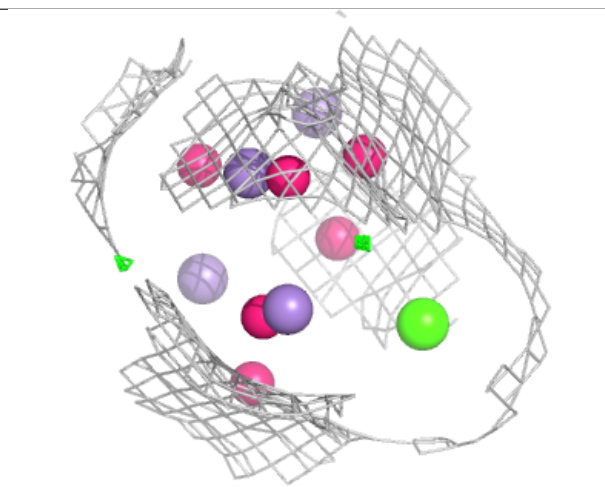
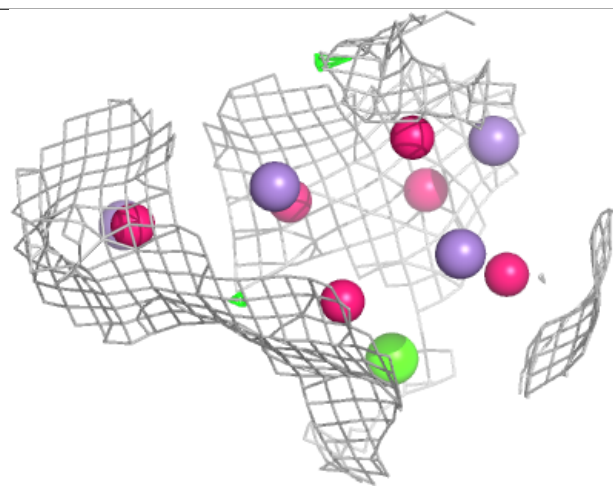
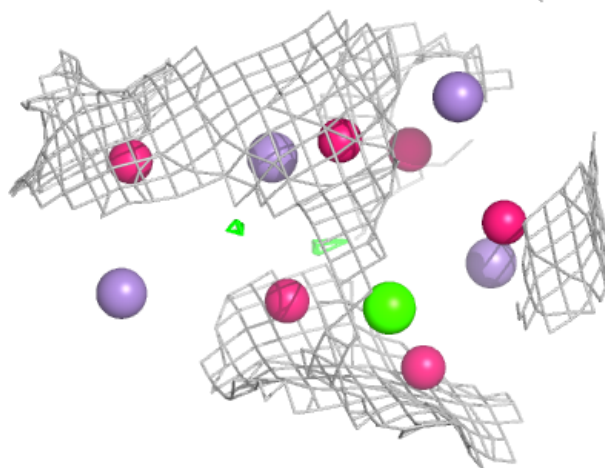
Electron density around OEY A 601 (B):

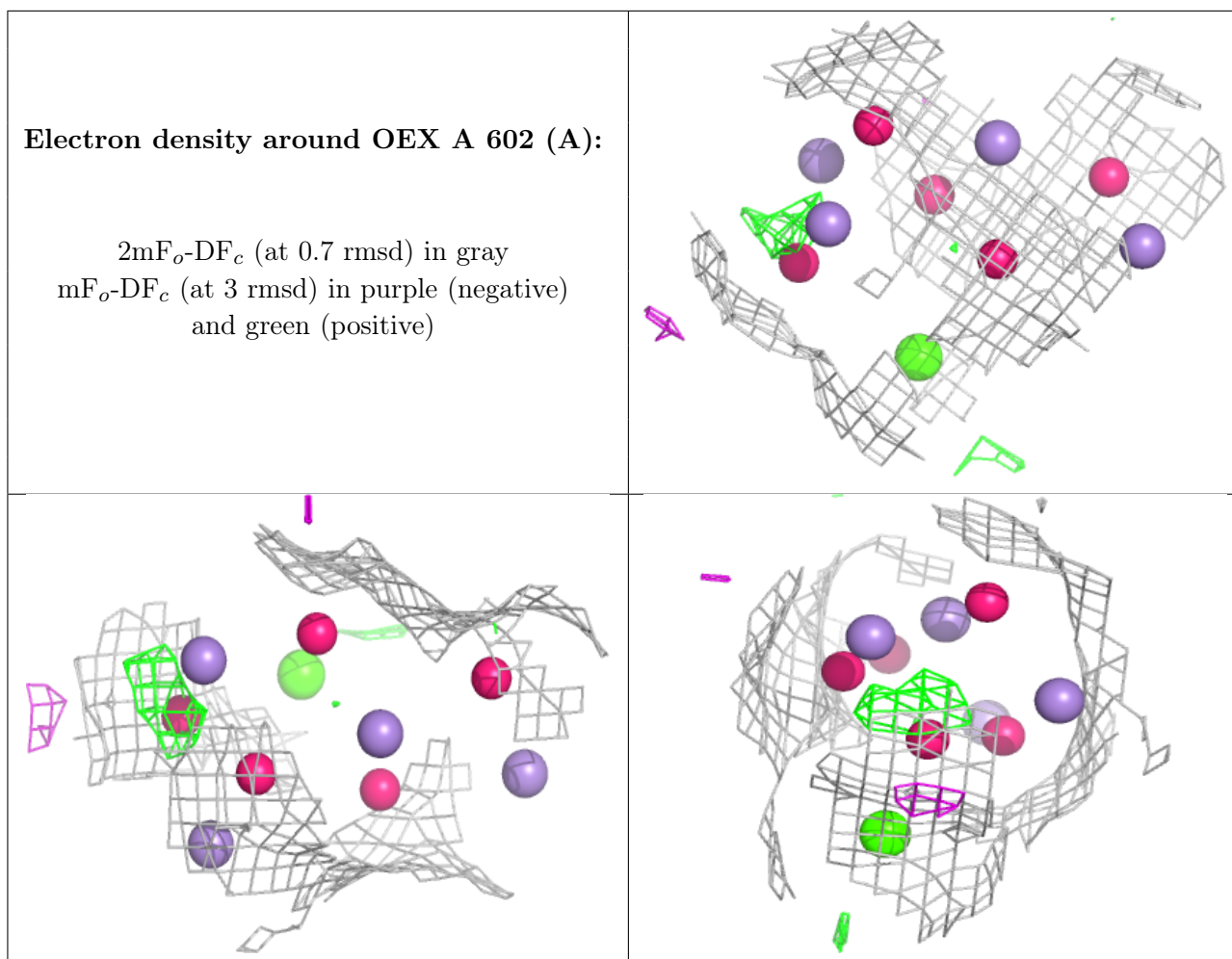
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEY a 601 (B):

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





6.5 Other polymers ⓘ

There are no such residues in this entry.