



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 12:33 AM EDT

PDB ID : 8F4F / pdb_00008f4f
Title : RT XFEL structure of Photosystem II 500 microseconds after the third illumination at 2.03 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.03 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

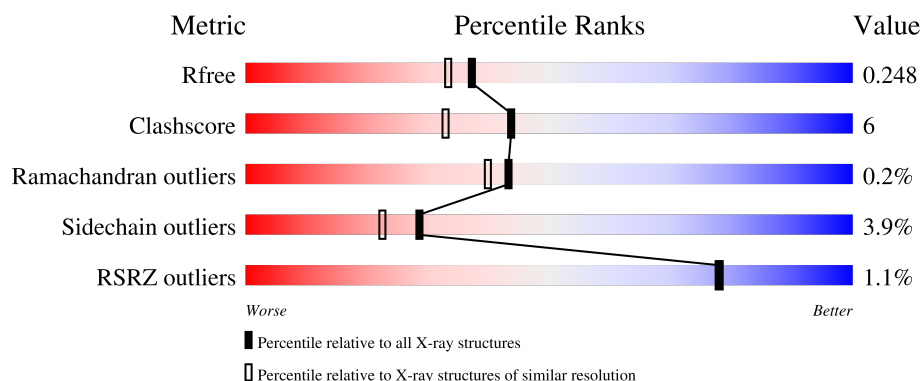
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

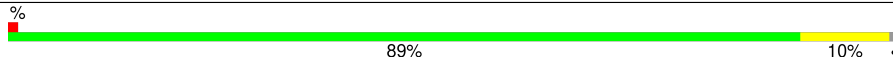
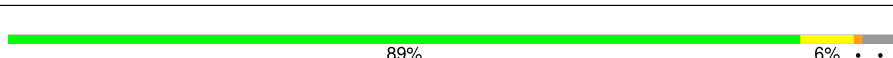
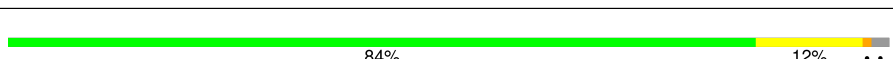
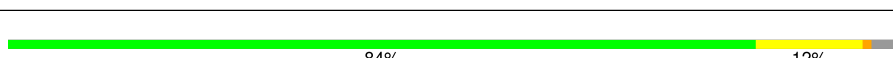
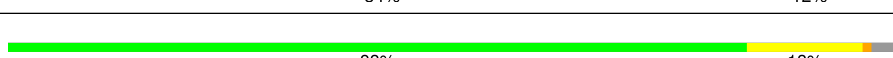
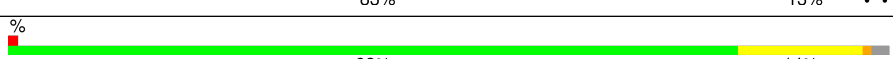
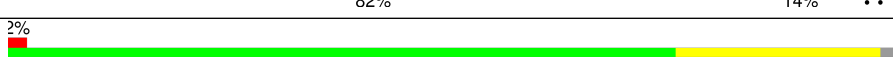
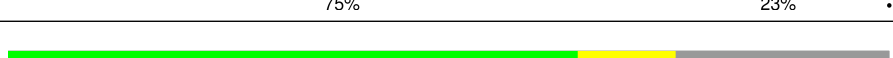
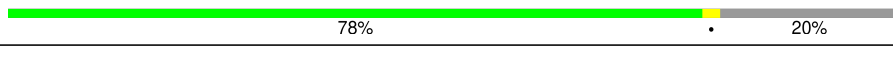
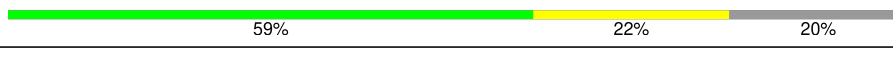
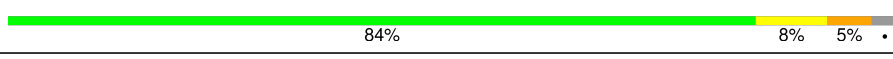
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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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
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 53209 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				

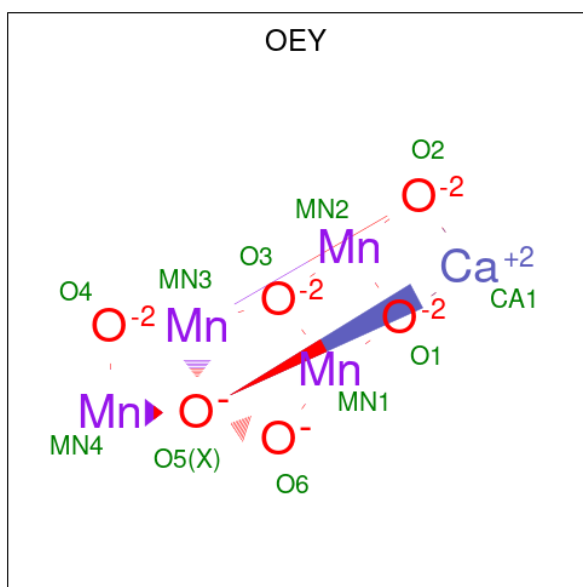
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			22	2	8	12		
21	a	1	Total	Ca	Mn	O	0	1
			22	2	8	12		

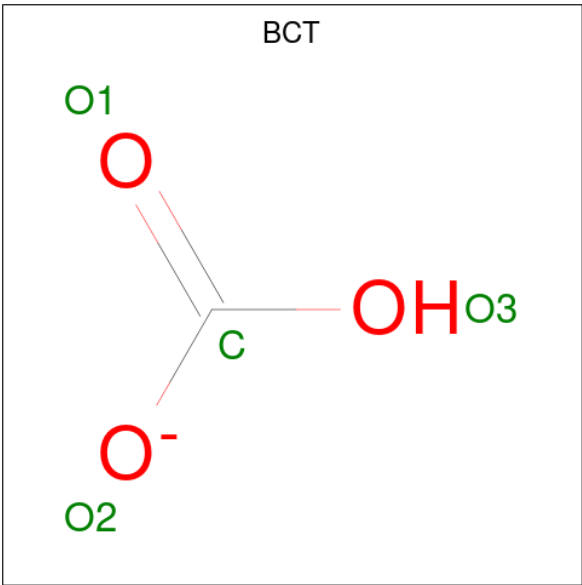
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

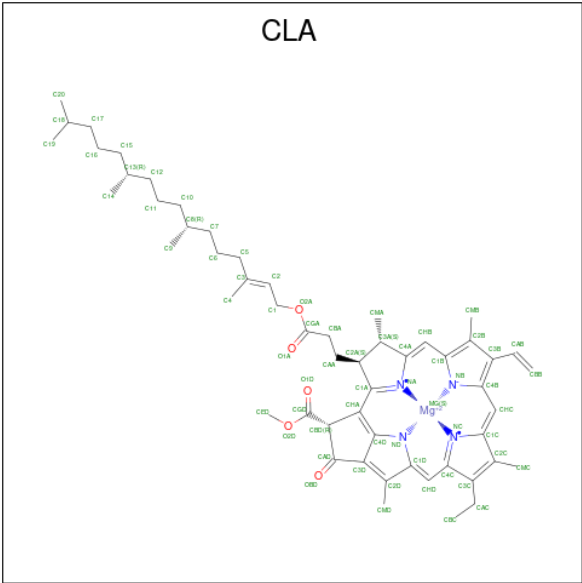
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O		0	0
			4	1	3			
24	d	1	Total	C	O		0	0
			4	1	3			

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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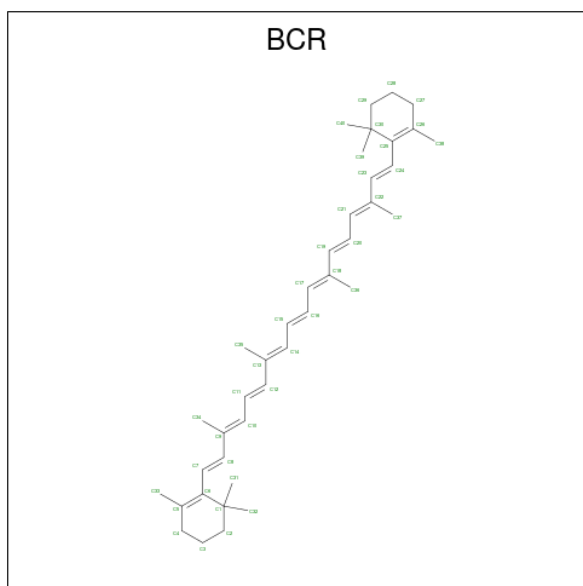
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 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 BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



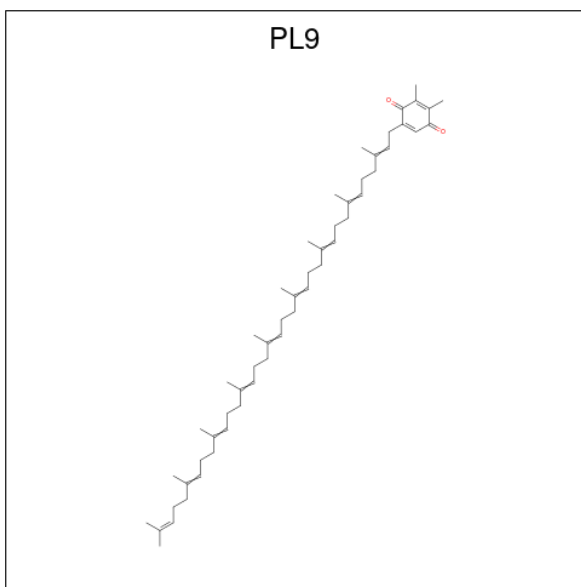
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		

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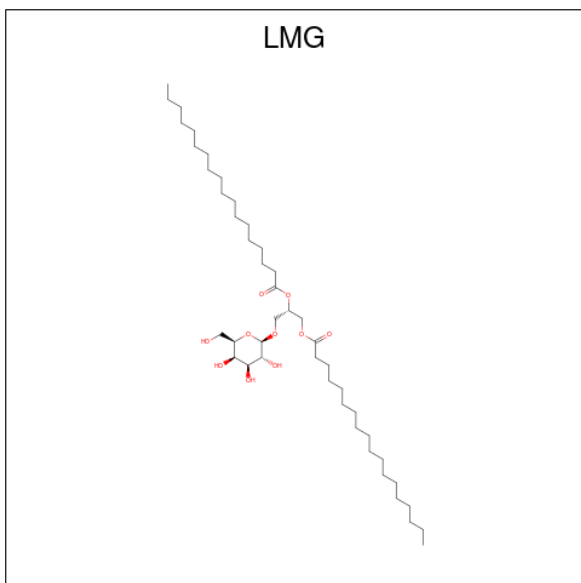
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total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

- Molecule 27 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).



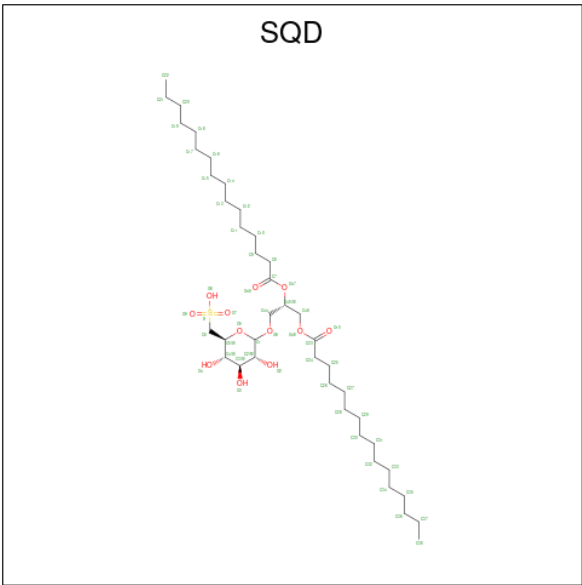
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



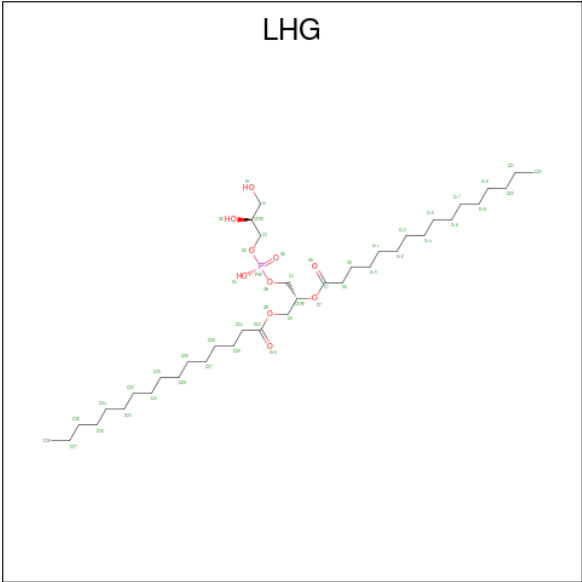
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			48	38	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			28	24	4		
28	C	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			51	41	10		
28	D	1	Total	C	O	0	0
			33	27	6		
28	b	1	Total	C	O	0	0
			55	45	10		
28	c	1	Total	C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

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



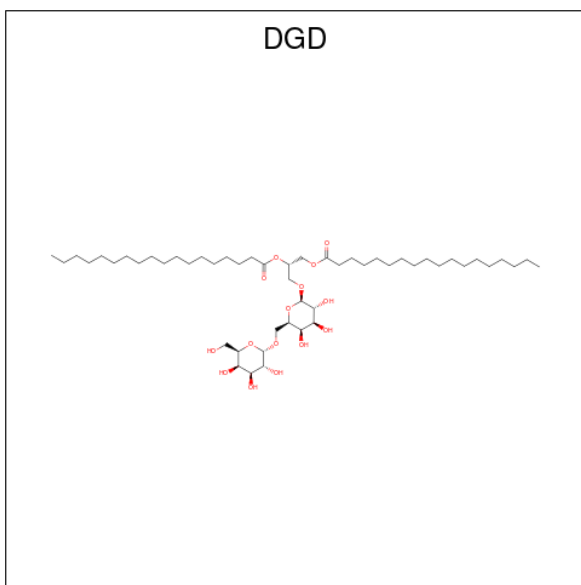
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			39	35	4			
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			36	25	10	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O		0	0
			36	31	5			
29	b	1	Total	C	O	S	0	0
			49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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



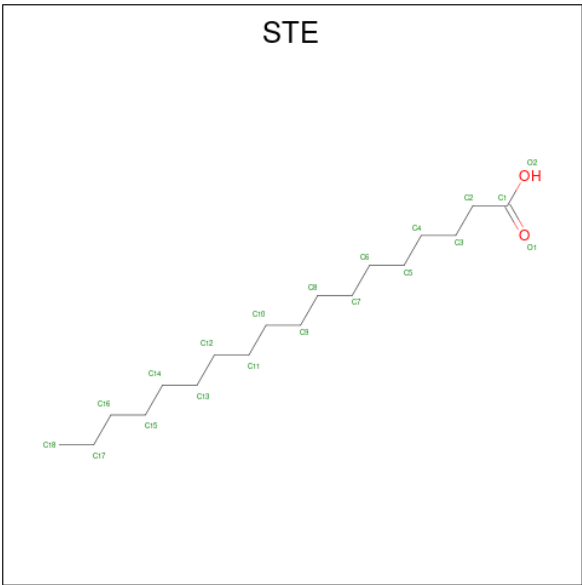
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			47	36	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



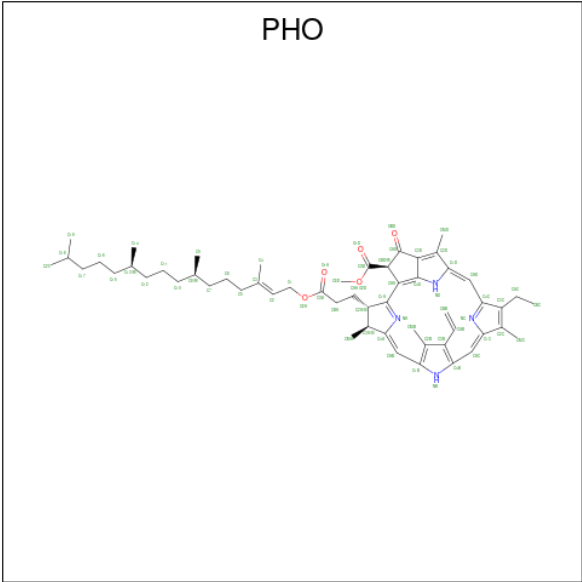
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			20	18	2		
32	B	1	Total	C	O	0	0
			17	15	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C	O	0	0
			18	16	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C		0	0
			16	16			
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C	O	0	0
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

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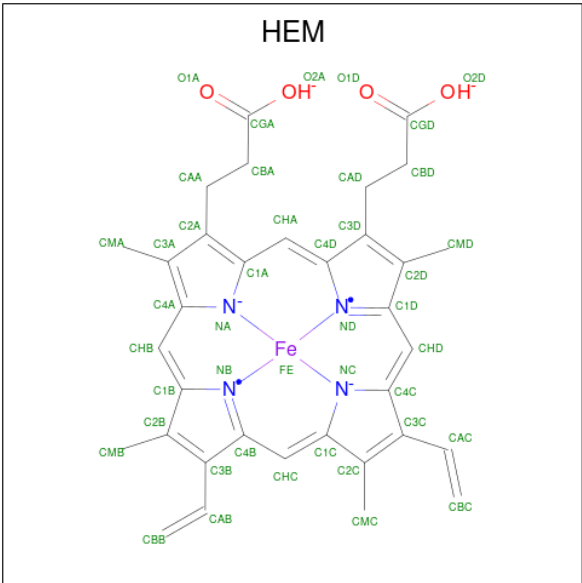
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	L	1	Total C O 12 10 2	0	0
32	M	1	Total C O 15 13 2	0	0
32	M	1	Total C 10 10	0	0
32	T	1	Total C 16 16	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 15 15	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 2	0	0
32	d	1	Total C O 17 15 2	0	0
32	d	1	Total C O 20 18 2	0	0
32	j	1	Total C O 12 10 2	0	0
32	k	1	Total C O 12 10 2	0	0
32	m	1	Total C 18 18	0	0
32	t	1	Total C O 14 12 2	0	0
32	t	1	Total C 10 10	0	0

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



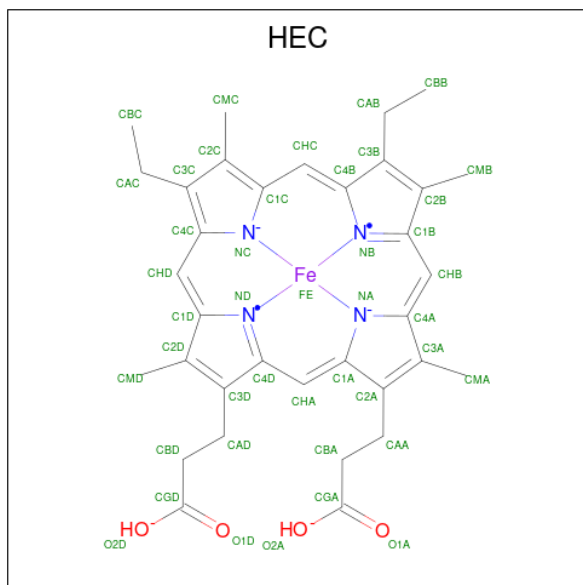
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	N	O	0	0
			64	55	4	5		
33	D	1	Total	C	N	O	0	0
			64	55	4	5		
33	a	1	Total	C	N	O	0	0
			64	55	4	5		
33	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	124	Total	O		
			128	128	0	4
36	B	185	Total	O		
			185	185	0	0
36	C	160	Total	O		
			160	160	0	0
36	D	123	Total	O		
			123	123	0	0
36	E	17	Total	O		
			17	17	0	0
36	F	2	Total	O		
			2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	H	32	Total O 32 32	0	0
36	I	9	Total O 9 9	0	0
36	J	11	Total O 11 11	0	0
36	K	10	Total O 10 10	0	0
36	L	7	Total O 7 7	0	0
36	M	8	Total O 8 8	0	0
36	O	108	Total O 108 108	0	0
36	T	9	Total O 9 9	0	0
36	U	33	Total O 33 33	0	0
36	V	74	Total O 74 74	0	0
36	Y	10	Total O 10 10	0	0
36	X	11	Total O 11 11	0	0
36	Z	4	Total O 4 4	0	0
36	R	4	Total O 4 4	0	0
36	a	107	Total O 111 111	0	4
36	b	171	Total O 171 171	0	0
36	c	150	Total O 150 150	0	0
36	d	94	Total O 94 94	0	0
36	e	16	Total O 16 16	0	0
36	f	3	Total O 3 3	0	0
36	h	16	Total O 16 16	0	0

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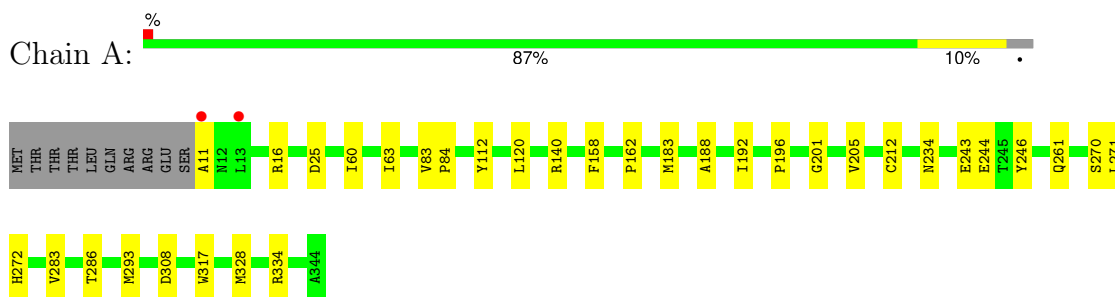
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	i	16	Total 16	O 16	0	0
36	j	11	Total 11	O 11	0	0
36	k	6	Total 6	O 6	0	0
36	l	14	Total 14	O 14	0	0
36	m	8	Total 8	O 8	0	0
36	o	96	Total 96	O 96	0	0
36	t	9	Total 9	O 9	0	0
36	u	58	Total 58	O 58	0	0
36	v	44	Total 44	O 44	0	0
36	y	11	Total 11	O 11	0	0
36	x	11	Total 11	O 11	0	0
36	r	10	Total 10	O 10	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.

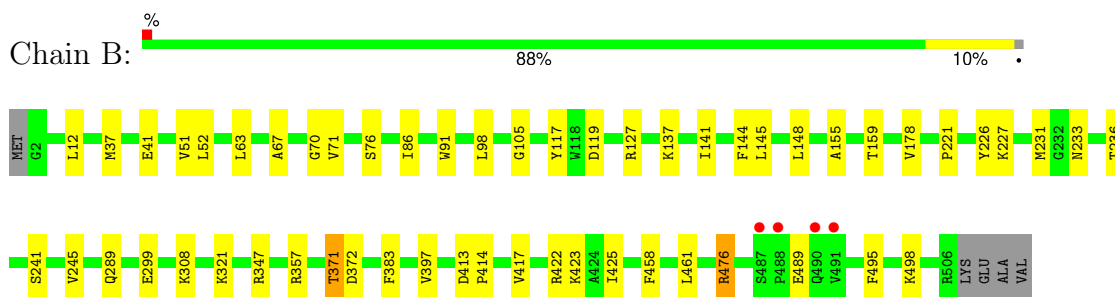
- Molecule 1: Photosystem II protein D1 1



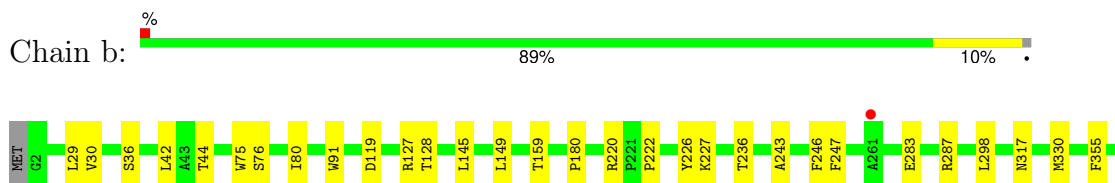
- Molecule 1: Photosystem II protein D1 1

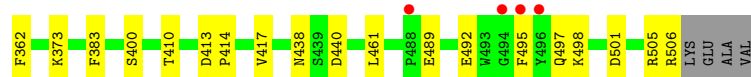


- Molecule 2: Photosystem II CP47 reaction center protein



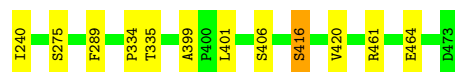
- Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 89% 6% . .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 84% 12% . .



- Molecule 4: Photosystem II D2 protein

Chain D: 84% 12% . .

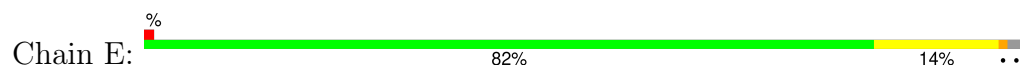


- Molecule 4: Photosystem II D2 protein

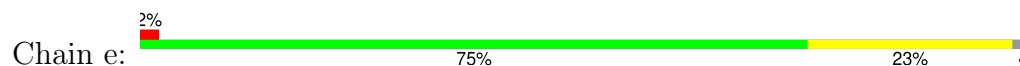
Chain d: 83% 13% . .



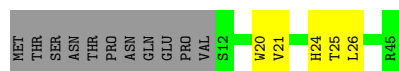
- Molecule 5: Cytochrome b559 subunit alpha



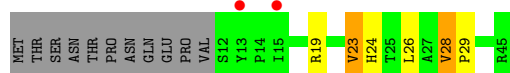
- Molecule 5: Cytochrome b559 subunit alpha



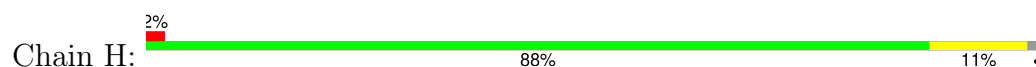
- Molecule 6: Cytochrome b559 subunit beta



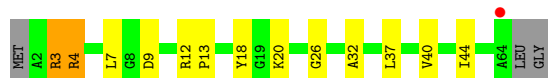
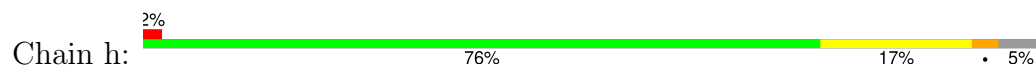
- Molecule 6: Cytochrome b559 subunit beta



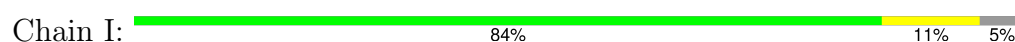
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  79% 16% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  2% 78% 12% 10%



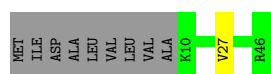
- Molecule 9: Photosystem II reaction center protein J

Chain j:  8% 65% 22% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  78% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  59% 22% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  84% 16%



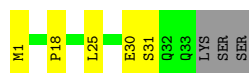
- Molecule 11: Photosystem II reaction center protein L

Chain l:  84% 8% 5% 5%



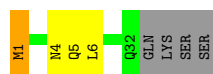
- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 14% 8%



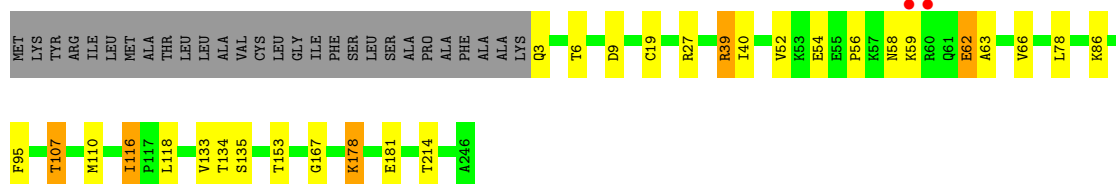
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 8% 11%



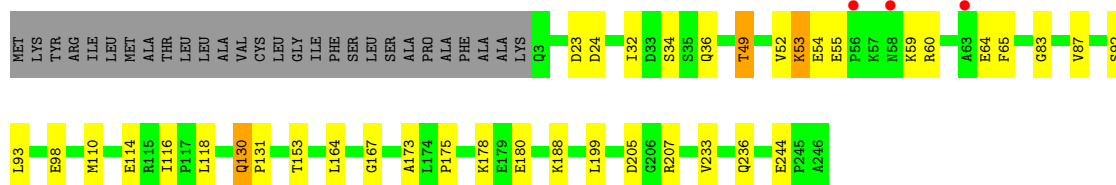
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  79% 9% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  75% 13% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 6% 6%



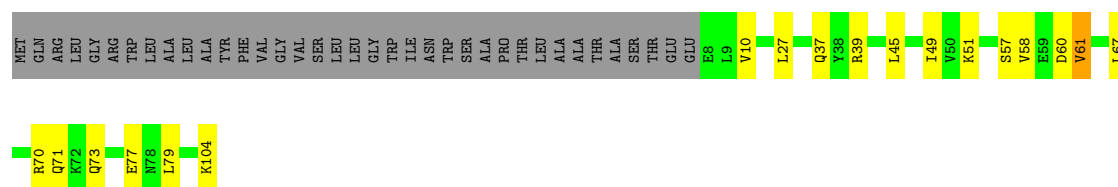
- Molecule 14: Photosystem II reaction center protein T

Chain t:  88% 6% 6%



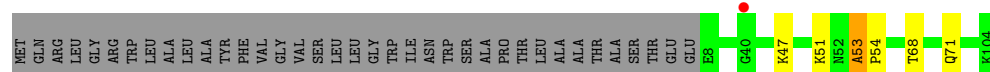
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 



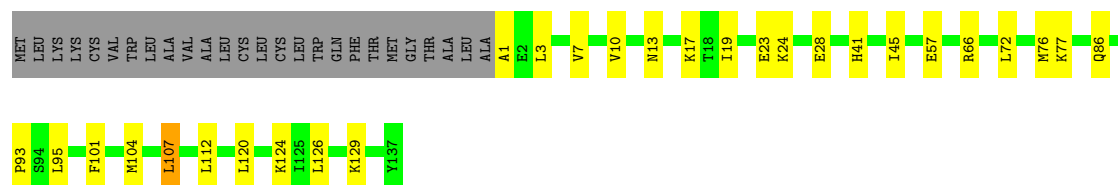
- Molecule 16: Cytochrome c-550

Chain V: 

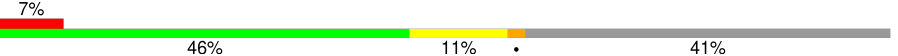


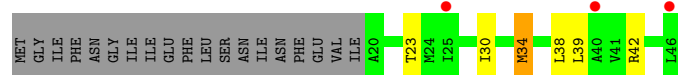
- Molecule 16: Cytochrome c-550

Chain v: 



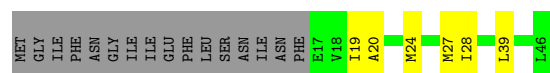
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 

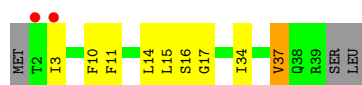


- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 



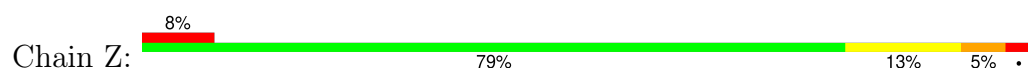
- Molecule 18: Photosystem II reaction center X protein



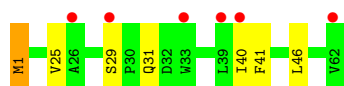
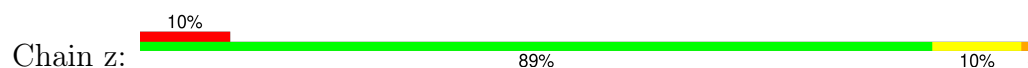
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



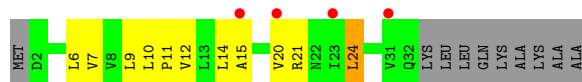
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.53Å 222.83Å 309.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.23 – 2.03 31.23 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.9 (31.23-2.03) 85.2 (31.23-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.199 , 0.248 0.200 , 0.248	Depositor DCC
R_{free} test set	4617 reflections (0.74%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53209	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, LMG, HEM, BCR, LHG, SQD, CL, OEY, PHO, HEC, PL9, CLA, FE2, BCT, STE, FME

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	0.32	0/3212	0.49	0/4376
1	a	0.31	0/3209	0.48	0/4372
2	B	0.33	0/4155	0.48	0/5661
2	b	0.31	0/4118	0.46	0/5611
3	C	0.31	0/3625	0.47	0/4935
3	c	0.29	0/3705	0.45	0/5042
4	D	0.35	0/2825	0.50	0/3847
4	d	0.34	0/2834	0.51	0/3859
5	E	0.25	0/688	0.41	0/940
5	e	0.22	0/683	0.42	0/932
6	F	0.27	0/284	0.42	0/387
6	f	0.27	0/284	0.49	0/387
7	H	0.31	0/523	0.47	0/713
7	h	0.28	0/511	0.44	0/697
8	I	0.31	0/293	0.46	0/396
8	i	0.32	0/293	0.46	0/396
9	J	0.26	0/263	0.38	0/356
9	j	0.25	0/263	0.40	0/356
10	K	0.26	0/303	0.43	0/416
10	k	0.25	0/303	0.41	0/416
11	L	0.34	0/311	0.44	0/422
11	l	0.33	0/303	0.49	0/412
12	M	0.33	0/249	0.45	0/341
12	m	0.34	0/244	0.47	0/334
13	O	0.30	0/1904	0.52	0/2585
13	o	0.31	0/1905	0.50	0/2583
14	T	0.32	0/257	0.48	0/349
14	t	0.30	0/255	0.44	0/346
15	U	0.27	0/785	0.45	0/1064
15	u	0.31	0/785	0.49	0/1064
16	V	0.30	0/1085	0.50	0/1473
16	v	0.26	0/1085	0.43	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.25	0/197	0.38	0/264
17	y	0.19	0/219	0.40	0/294
18	X	0.25	0/284	0.39	0/384
18	x	0.22	0/289	0.28	0/391
19	Z	0.20	0/490	0.41	0/669
19	z	0.18	0/488	0.30	0/666
20	R	0.25	0/277	0.40	0/380
20	r	0.21	0/252	0.36	0/347
All	All	0.31	0/44038	0.47	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	2981	29	0
1	a	3110	0	2972	36	0
2	B	4005	0	3871	36	0
2	b	3978	0	3836	38	0
3	C	3509	0	3426	22	0
3	c	3583	0	3499	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2731	0	2637	35	0
4	d	2737	0	2643	31	0
5	E	666	0	651	11	0
5	e	664	0	648	12	0
6	F	275	0	282	3	0
6	f	275	0	282	4	0
7	H	510	0	532	4	0
7	h	498	0	518	11	0
8	I	296	0	311	1	0
8	i	296	0	311	6	0
9	J	257	0	268	3	0
9	j	257	0	268	7	0
10	K	293	0	305	0	0
10	k	293	0	305	4	0
11	L	304	0	316	8	0
11	l	296	0	304	3	0
12	M	256	0	269	5	0
12	m	251	0	267	4	0
13	O	1870	0	1830	20	0
13	o	1874	0	1846	21	0
14	T	258	0	261	4	0
14	t	256	0	256	1	0
15	U	774	0	773	8	0
15	u	774	0	773	5	0
16	V	1064	0	1073	13	0
16	v	1064	0	1073	15	0
17	Y	196	0	217	4	0
17	y	218	0	241	4	0
18	X	281	0	312	6	0
18	x	286	0	314	9	0
19	Z	479	0	516	10	0
19	z	477	0	509	4	0
20	R	271	0	298	4	0
20	r	246	0	263	4	0
21	A	22	0	0	2	0
21	a	22	0	0	1	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	4	0	1	1	0
24	d	4	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	249	0	264	6	0
25	B	1035	0	1139	30	0
25	C	839	0	922	30	0
25	D	130	0	144	6	0
25	a	260	0	288	8	0
25	b	1035	0	1139	37	0
25	c	839	0	919	36	0
25	d	130	0	144	3	0
26	A	40	0	56	0	0
26	B	120	0	168	5	0
26	C	40	0	56	2	0
26	D	40	0	56	1	0
26	H	40	0	56	5	0
26	K	120	0	168	4	0
26	T	40	0	56	3	0
26	a	40	0	56	0	0
26	b	120	0	168	6	0
26	c	40	0	56	4	0
26	d	40	0	56	1	0
26	h	40	0	56	5	0
26	k	120	0	168	4	0
26	t	40	0	56	4	0
27	A	55	0	80	6	0
27	D	55	0	80	2	0
27	a	55	0	80	5	0
27	d	55	0	80	3	0
28	A	48	0	66	0	0
28	B	79	0	112	7	0
28	C	48	0	66	1	0
28	D	84	0	116	4	0
28	b	55	0	86	1	0
28	c	134	0	181	6	0
28	d	67	0	92	1	0
28	m	51	0	72	4	0
29	A	91	0	136	2	0
29	B	54	0	78	5	0
29	D	36	0	46	1	0
29	a	90	0	134	4	0
29	b	49	0	65	5	0
29	f	41	0	49	3	0
30	A	49	0	74	1	0
30	D	145	0	215	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	L	49	0	74	1	0
30	d	137	0	199	6	0
30	e	42	0	57	5	0
30	l	49	0	74	5	0
31	A	66	0	96	4	0
31	C	124	0	164	2	0
31	H	62	0	82	2	0
31	J	62	0	82	5	0
31	a	44	0	75	3	0
31	c	186	0	246	12	0
31	h	62	0	82	0	0
32	A	20	0	35	0	0
32	B	75	0	117	5	0
32	C	40	0	63	1	0
32	D	20	0	35	6	0
32	E	12	0	16	0	0
32	H	18	0	35	2	0
32	I	15	0	26	2	0
32	J	12	0	16	0	0
32	L	12	0	16	1	0
32	M	25	0	38	0	0
32	T	16	0	31	2	0
32	a	12	0	16	0	0
32	b	61	0	104	4	0
32	c	20	0	35	1	0
32	d	37	0	61	7	0
32	j	12	0	16	1	0
32	k	12	0	16	0	0
32	m	18	0	35	2	0
32	t	24	0	36	0	0
33	D	128	0	148	1	0
33	a	64	0	74	1	0
33	d	64	0	74	3	0
34	E	43	0	30	2	0
34	f	43	0	30	3	0
35	V	43	0	30	0	0
35	v	43	0	30	1	0
36	A	128	0	0	6	0
36	B	185	0	0	2	0
36	C	160	0	0	1	0
36	D	123	0	0	2	0
36	E	17	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	F	2	0	0	0	0
36	H	32	0	0	0	0
36	I	9	0	0	0	0
36	J	11	0	0	0	0
36	K	10	0	0	0	0
36	L	7	0	0	0	0
36	M	8	0	0	1	0
36	O	108	0	0	5	0
36	R	4	0	0	0	0
36	T	9	0	0	0	0
36	U	33	0	0	1	0
36	V	74	0	0	2	0
36	X	11	0	0	0	0
36	Y	10	0	0	1	0
36	Z	4	0	0	0	0
36	a	111	0	0	3	0
36	b	171	0	0	3	0
36	c	150	0	0	2	0
36	d	94	0	0	0	0
36	e	16	0	0	0	0
36	f	3	0	0	0	0
36	h	16	0	0	0	0
36	i	16	0	0	3	0
36	j	11	0	0	2	0
36	k	6	0	0	0	0
36	l	14	0	0	1	0
36	m	8	0	0	1	0
36	o	96	0	0	3	0
36	r	10	0	0	1	0
36	t	9	0	0	0	0
36	u	58	0	0	2	0
36	v	44	0	0	1	0
36	x	11	0	0	0	0
36	y	11	0	0	0	0
All	All	53209	0	52752	630	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 (630) 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)
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	1.93	0.85
32:D:413:STE:H142	18:X:17:GLY:HA2	1.60	0.83
25:C:513:CLA:HBB1	26:K:101:BCR:H24C	1.58	0.83
15:u:53:ALA:O	36:u:201:HOH:O	1.95	0.82
2:B:357:ARG:NH1	36:D:501:HOH:O	2.15	0.79
17:Y:34:MET:SD	36:Y:101:HOH:O	2.40	0.78
21:a:601[B]:OEY:O5	21:a:601[B]:OEY:O6	2.01	0.78
2:B:91:TRP:HE1	32:B:621:STE:H32	1.47	0.77
2:b:29:LEU:HD23	29:b:620:SQD:H222	1.66	0.77
21:A:601[A]:OEY:O6	21:A:601[A]:OEY:O5	2.02	0.76
25:b:614:CLA:H43	29:b:620:SQD:H102	1.68	0.75
27:A:610:PL9:H28	30:A:614:LHG:H202	1.68	0.74
4:d:246:MET:HE3	4:d:264:LYS:HD2	1.68	0.74
3:c:275:SER:HB3	25:c:509:CLA:HED3	1.70	0.73
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.53	0.72
25:B:606:CLA:H72	26:B:619:BCR:H311	1.71	0.71
16:v:77:LYS:HG2	16:v:95:LEU:HD12	1.73	0.70
31:a:614:DGD:O3G	36:a:701:HOH:O	2.10	0.70
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.73	0.70
9:J:15:THR:HG22	9:J:19:MET:HE2	1.72	0.70
13:O:39:ARG:NH2	36:O:303:HOH:O	2.24	0.70
25:b:614:CLA:H121	32:m:102:STE:H182	1.74	0.70
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.75	0.69
2:b:226:TYR:OH	36:b:701:HOH:O	2.10	0.68
7:h:4:ARG:NH2	7:h:9:ASP:OD2	2.27	0.68
24:A:605:BCT:O2	36:A:701:HOH:O	2.12	0.68
25:C:506:CLA:H8	26:C:514:BCR:H12C	1.75	0.67
3:c:315:MET:HE3	3:c:365:TRP:HZ3	1.57	0.67
4:D:338:ASN:O	36:D:501:HOH:O	2.13	0.67
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.74	0.67
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.76	0.66
13:O:27:ARG:NH1	36:O:305:HOH:O	2.29	0.66
2:b:127:ARG:NH2	7:h:18:TYR:O	2.27	0.66
32:d:413:STE:H31	18:x:17:GLY:HA2	1.76	0.66
31:c:516:DGD:HB22	28:c:518:LMG:H311	1.78	0.65
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.76	0.65
1:a:102:LEU:HD12	31:a:614:DGD:HB22	1.78	0.65
9:j:16:VAL:HA	9:j:19:MET:HE2	1.79	0.65
32:d:413:STE:H172	18:x:12:ILE:HD13	1.79	0.65
2:b:91:TRP:HE1	32:b:621:STE:H141	1.61	0.64
31:A:616:DGD:HD5	2:b:75:TRP:HB3	1.80	0.64
2:B:119:ASP:H	11:L:1:MET:HE1	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:614:CLA:H192	28:m:101:LMG:H421	1.80	0.64
16:V:87:GLU:CD	16:V:96:ARG:HH12	2.07	0.63
34:f:101:HEM:HBC2	34:f:101:HEM:HMC2	1.80	0.63
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.62	0.63
34:E:101:HEM:HBC2	34:E:101:HEM:HHD	1.81	0.63
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.62	0.63
28:B:620:LMG:HC5	32:B:625:STE:H31	1.80	0.62
32:I:101:STE:H131	25:b:606:CLA:H192	1.81	0.62
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.81	0.62
1:A:244:GLU:OE2	4:D:264:LYS:NZ	2.33	0.62
25:C:504:CLA:H143	25:C:508:CLA:H152	1.80	0.62
16:v:24:LYS:NZ	16:v:28:GLU:OE1	2.32	0.62
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.81	0.62
25:B:601:CLA:HBA1	25:B:601:CLA:HBD	1.80	0.62
1:A:25:ASP:OD1	36:A:702:HOH:O	2.16	0.61
2:B:117:TYR:HA	11:L:1:MET:HE2	1.82	0.61
4:D:279:LEU:HD22	33:D:402:PHO:HBC3	1.83	0.61
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.81	0.61
16:v:104:MET:HA	16:v:107:LEU:HD22	1.81	0.61
15:U:70:ARG:NH2	36:U:202:HOH:O	2.33	0.61
2:b:400:SER:OG	2:b:410:THR:OG1	2.15	0.61
25:b:613:CLA:H203	30:d:407:LHG:H212	1.82	0.60
1:a:200:LEU:HD13	31:c:517:DGD:HAW2	1.84	0.60
25:A:606:CLA:H201	30:D:409:LHG:H162	1.84	0.60
2:b:247:PHE:HE1	25:b:602:CLA:H102	1.66	0.60
29:f:102:SQD:H312	18:x:27:VAL:HG11	1.84	0.60
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.83	0.60
14:T:15:ALA:HB2	26:T:101:BCR:H14C	1.84	0.59
4:d:100:ASP:OD2	5:e:73:LYS:NZ	2.33	0.59
15:U:104:LYS:NZ	16:V:131:GLY:O	2.30	0.59
27:d:406:PL9:H201	30:l:101:LHG:H202	1.83	0.59
25:B:601:CLA:H51	32:H:103:STE:H171	1.84	0.59
6:f:24:HIS:O	6:f:28:VAL:HG13	2.02	0.59
32:D:413:STE:H92	18:X:16:SER:HB3	1.85	0.59
2:b:440:ASP:OD2	36:b:702:HOH:O	2.17	0.59
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.85	0.59
25:A:607:CLA:HED1	31:J:101:DGD:HAH2	1.85	0.58
25:B:615:CLA:H162	7:H:7:LEU:HD21	1.84	0.58
15:U:70:ARG:NH2	16:V:85:GLU:OE2	2.33	0.58
3:c:26:ARG:NH2	36:c:607:HOH:O	2.36	0.58
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299[A]:GLU:OE2	36:B:901:HOH:O	2.16	0.58
13:o:205:ASP:HA	13:o:207:ARG:HH21	1.68	0.58
3:C:406:SER:HA	3:C:420:VAL:HG23	1.85	0.58
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.86	0.58
3:C:178:LYS:NZ	3:C:184:GLY:O	2.36	0.58
5:E:7:GLU:OE2	36:E:201:HOH:O	2.17	0.58
3:c:281:MET:HG3	28:c:521:LMG:H402	1.86	0.58
17:Y:42:ARG:HH22	19:Z:31:GLN:NE2	2.02	0.58
3:c:146:PHE:O	3:c:156:LYS:NZ	2.33	0.58
8:i:34:ARG:NH2	36:i:102:HOH:O	2.36	0.58
1:A:246:TYR:OH	36:A:701:HOH:O	2.17	0.57
13:o:36:GLN:NE2	36:o:304:HOH:O	2.32	0.57
25:c:505:CLA:H43	26:c:514:BCR:HC7	1.86	0.57
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.86	0.57
27:a:610:PL9:H28	30:e:101:LHG:H171	1.85	0.57
19:z:1:MET:SD	19:z:1:MET:N	2.73	0.57
32:d:413:STE:H71	18:x:16:SER:HB3	1.87	0.57
26:k:102:BCR:H10C	17:y:28:ILE:HG23	1.85	0.57
3:C:148:GLY:O	3:C:156:LYS:NZ	2.38	0.57
3:c:315:MET:HE3	3:c:365:TRP:CZ3	2.39	0.57
17:y:39:LEU:HD21	19:z:25:VAL:HA	1.86	0.56
5:E:60:GLN:NE2	5:E:62:SER:O	2.36	0.56
13:O:52:VAL:HG11	13:O:116:ILE:HD12	1.87	0.56
2:B:371:THR:HG23	2:B:372:ASP:O	2.06	0.56
11:L:14:ARG:HB3	14:T:25:GLU:HG2	1.87	0.56
25:a:606:CLA:H202	27:a:610:PL9:H262	1.88	0.56
25:B:614:CLA:H143	29:B:623:SQD:H382	1.87	0.56
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.86	0.56
9:j:26:GLY:HA2	32:j:101:STE:H82	1.85	0.56
12:M:30:GLU:O	36:M:201:HOH:O	2.18	0.56
1:a:45:THR:HG23	25:a:611:CLA:H201	1.87	0.56
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.88	0.56
25:B:614:CLA:HBA1	29:B:623:SQD:H91	1.88	0.55
13:o:23:ASP:OD1	13:o:24:ASP:N	2.39	0.55
3:c:213:LEU:HD23	25:c:506:CLA:H192	1.88	0.55
31:c:516:DGD:HA41	28:c:518:LMG:H322	1.86	0.55
17:y:20:ALA:O	17:y:24:MET:HG2	2.06	0.55
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.06	0.55
1:a:42:LEU:HD13	29:a:613:SQD:H321	1.89	0.55
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.39	0.55
25:b:603:CLA:HMD3	25:b:606:CLA:HBB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:247:PHE:CE1	25:b:602:CLA:H102	2.42	0.54
19:Z:31:GLN:CD	19:Z:32:ASP:H	2.16	0.54
25:B:615:CLA:H2	25:B:616:CLA:HBB2	1.89	0.54
5:e:57:ALA:H	5:e:60:GLN:NE2	2.05	0.54
2:b:355:PHE:HE2	2:b:373:LYS:HG2	1.72	0.54
1:A:261:GLN:NE2	36:A:709:HOH:O	2.40	0.54
3:c:256:PRO:O	3:c:261:ARG:NH1	2.41	0.54
1:A:11:ALA:O	1:A:16:ARG:NH2	2.41	0.54
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.90	0.54
17:Y:38:LEU:HD12	19:Z:25:VAL:HG21	1.88	0.54
1:a:245:THR:HB	4:d:265:ARG:HE	1.72	0.54
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.88	0.54
15:U:27:LEU:HD22	15:U:49:ILE:HG21	1.89	0.53
31:c:517:DGD:HE4	9:j:40:LEU:HD21	1.89	0.53
5:e:33:ALA:HB2	20:r:11:PRO:HG2	1.90	0.53
25:C:502:CLA:H61	25:C:512:CLA:H42	1.90	0.53
19:Z:34:ASP:O	19:Z:37:LYS:HG2	2.07	0.53
1:a:300:PHE:HZ	31:c:517:DGD:HB62	1.72	0.53
4:D:23:LYS:NZ	28:D:411:LMG:H122	2.23	0.53
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.24	0.53
4:d:79:SER:HA	4:d:172:SER:HB3	1.89	0.53
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.91	0.53
16:v:3:LEU:HD23	16:v:23:GLU:HG3	1.91	0.53
7:H:59:ASN:ND2	7:H:61:SER:HB3	2.24	0.53
5:E:17:VAL:HG23	9:J:7:ARG:HG3	1.91	0.53
32:T:102:STE:H61	2:b:44:THR:HG22	1.91	0.53
9:j:18:GLY:O	9:j:22:ILE:HG12	2.09	0.53
16:V:4:THR:OG1	36:V:301:HOH:O	2.18	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
28:b:622:LMG:H292	28:b:622:LMG:H112	1.91	0.52
25:A:608:CLA:H43	25:C:505:CLA:H191	1.92	0.52
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.89	0.52
2:b:498:LYS:HE3	4:d:20:ASP:HA	1.91	0.52
2:b:489:GLU:HA	2:b:495:PHE:HD2	1.74	0.52
25:B:607:CLA:H122	28:B:620:LMG:H241	1.92	0.52
28:d:410:LMG:H412	7:h:32:ALA:HB1	1.92	0.52
25:B:601:CLA:H92	26:H:101:BCR:H21C	1.90	0.52
26:T:101:BCR:H321	26:T:101:BCR:HC8	1.92	0.52
31:c:517:DGD:HA72	31:c:517:DGD:HB92	1.92	0.52
4:d:93:TRP:CZ3	32:d:413:STE:H62	2.45	0.52
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:455:PHE:HD2	8:i:33:LYS:HG3	1.75	0.52
25:C:511:CLA:O1A	36:C:601:HOH:O	2.18	0.52
4:D:150:ILE:O	4:D:154:VAL:HG13	2.10	0.52
4:d:279:LEU:HD22	33:d:402:PHO:HBC3	1.91	0.52
30:d:407:LHG:HC91	30:l:101:LHG:HC81	1.91	0.52
25:b:608:CLA:H8	25:b:609:CLA:H142	1.91	0.51
30:d:407:LHG:H111	30:l:101:LHG:H102	1.92	0.51
29:A:615:SQD:H301	26:b:619:BCR:H363	1.92	0.51
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.45	0.51
1:a:16:ARG:HB3	1:a:16:ARG:NH1	2.26	0.51
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.46	0.51
2:B:137:LYS:NZ	7:H:17:GLU:OE1	2.39	0.51
4:D:23:LYS:HZ2	28:D:411:LMG:H122	1.76	0.51
1:a:163[B]:ILE:HD11	31:c:515:DGD:HA21	1.93	0.51
25:a:608:CLA:H111	25:a:608:CLA:H52	1.93	0.51
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.45	0.51
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.93	0.51
27:D:406:PL9:H412	11:L:29:LEU:HD23	1.93	0.51
2:b:30:VAL:HG12	25:b:605:CLA:HHD	1.92	0.51
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.92	0.51
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.45	0.51
1:A:234:ASN:ND2	30:D:412:LHG:HC11	2.26	0.51
28:B:622:LMG:H341	4:D:127:LEU:HD13	1.93	0.51
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.46	0.51
25:b:604:CLA:H42	25:b:605:CLA:H2	1.92	0.51
5:e:14:ILE:O	5:e:20:TRP:NE1	2.44	0.51
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.51
1:a:202:VAL:HG11	25:a:606:CLA:C3D	2.41	0.51
4:D:92:LEU:HD23	32:D:413:STE:H62	1.94	0.50
29:B:623:SQD:H161	29:B:623:SQD:H342	1.93	0.50
1:A:183[B]:MET:HA	25:A:606:CLA:HMD1	1.93	0.50
13:O:3:GLN:NE2	36:O:315:HOH:O	2.42	0.50
13:O:19:CYS:O	36:O:301:HOH:O	2.18	0.50
4:d:192:THR:HG23	25:d:403:CLA:HBC2	1.92	0.50
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.93	0.50
25:B:614:CLA:H42	32:L:102:STE:H22	1.94	0.50
16:V:28:GLU:CD	16:V:31:ARG:HH12	2.19	0.50
7:h:40:VAL:O	7:h:44:ILE:HG13	2.12	0.50
2:B:155:ALA:O	2:B:159:THR:OG1	2.27	0.50
5:e:13:ILE:HG22	5:e:19:TYR:CD2	2.47	0.50
10:k:28:ILE:HD11	17:y:28:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:29:SER:HB3	19:z:31:GLN:HG2	1.94	0.50
13:O:56:PRO:HG3	13:O:62:GLU:HA	1.94	0.50
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.44	0.50
3:c:455:PHE:CD2	8:i:33:LYS:HG3	2.46	0.50
4:d:78:VAL:HG11	4:d:114:ILE:HD12	1.93	0.50
9:j:34:ALA:O	36:j:201:HOH:O	2.19	0.50
5:e:56:TYR:HA	5:e:60:GLN:HE21	1.76	0.49
25:B:613:CLA:H192	30:D:412:LHG:H211	1.93	0.49
3:c:45:LEU:HA	3:c:139:THR:HG22	1.95	0.49
30:d:408:LHG:H281	14:t:17:PHE:CD1	2.48	0.49
4:d:126:MET:HE3	4:d:143:ALA:O	2.12	0.49
6:f:19:ARG:O	6:f:23:VAL:HG13	2.13	0.49
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.48	0.49
14:T:1:FME:HE1	12:m:6:LEU:HD21	1.93	0.49
15:U:58:VAL:O	15:U:61:VAL:HG22	2.13	0.49
3:c:433:LEU:HD22	25:c:502:CLA:HMC3	1.93	0.49
2:B:233:ASN:HD21	2:B:476:ARG:NH1	2.11	0.49
25:B:609:CLA:HBC1	32:H:103:STE:H52	1.94	0.49
25:b:616:CLA:H91	26:b:619:BCR:H14C	1.95	0.49
3:c:42:LEU:HD22	3:c:48:LYS:HB3	1.94	0.49
16:v:41:HIS:HA	16:v:45:ILE:O	2.12	0.49
13:O:39:ARG:NH1	36:O:310:HOH:O	2.38	0.49
1:a:217:SER:HA	4:d:272:LEU:HD12	1.93	0.49
12:m:5:GLN:O	36:m:201:HOH:O	2.20	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.49
2:b:145:LEU:HD22	25:b:604:CLA:H161	1.95	0.49
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.49
1:a:159[B]:LEU:C	1:a:162[B]:PRO:HD2	2.37	0.49
3:c:117:VAL:HG12	32:c:519:STE:H152	1.94	0.49
4:d:131:GLU:HB2	32:d:412:STE:H42	1.94	0.49
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.95	0.49
3:c:221:GLU:OE2	36:c:601:HOH:O	2.19	0.49
8:i:33:LYS:O	8:i:35:LYS:NZ	2.40	0.49
1:a:334[A]:ARG:NH2	36:a:707:HOH:O	2.45	0.48
25:b:612:CLA:H13	25:b:612:CLA:H171	1.63	0.48
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.95	0.48
3:C:42:LEU:HD21	25:C:511:CLA:H2A	1.94	0.48
3:C:141:GLU:H	3:C:141:GLU:CD	2.20	0.48
3:c:110:PRO:O	3:c:114:VAL:HG23	2.13	0.48
25:D:403:CLA:H192	28:D:407:LMG:H232	1.96	0.48
1:a:266:ASN:N	1:a:266:ASN:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:503:CLA:H203	25:c:510:CLA:HAB	1.96	0.48
2:b:91:TRP:HD1	32:b:621:STE:H162	1.78	0.48
8:i:26:GLY:N	36:i:103:HOH:O	2.46	0.48
4:D:141:TYR:OH	30:D:412:LHG:O4	2.23	0.48
16:V:57:GLU:CD	16:V:57:GLU:H	2.21	0.48
2:b:501:ASP:OD2	18:x:39:ARG:NH2	2.34	0.48
3:c:26:ARG:HA	25:c:511:CLA:OBD	2.12	0.48
25:c:512:CLA:H101	25:c:513:CLA:H151	1.95	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.94	0.48
5:E:26:THR:HA	20:R:15:ALA:HB1	1.96	0.48
30:l:101:LHG:H241	30:l:101:LHG:H101	1.96	0.48
3:C:48:LYS:NZ	3:C:133:ALA:O	2.46	0.48
16:V:87:GLU:HB3	36:V:325:HOH:O	2.14	0.48
13:o:110:MET:HE2	13:o:116:ILE:HD11	1.96	0.48
29:f:102:SQD:H331	18:x:27:VAL:HG11	1.96	0.47
12:m:4:ASN:ND2	28:m:101:LMG:O10	2.47	0.47
31:C:516:DGD:HA42	31:J:101:DGD:HB41	1.96	0.47
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.66	0.47
25:b:601:CLA:C9	26:h:101:BCR:H23C	2.43	0.47
25:B:607:CLA:H102	28:B:620:LMG:H221	1.95	0.47
25:b:615:CLA:H151	25:b:615:CLA:H112	1.78	0.47
15:U:57:SER:OG	15:U:60:ASP:OD1	2.31	0.47
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.47
25:c:508:CLA:H92	25:c:510:CLA:H52	1.96	0.47
3:C:139:THR:HB	3:C:141:GLU:OE2	2.13	0.47
3:C:464:GLU:OE2	4:D:245:SER:OG	2.30	0.47
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.95	0.47
25:C:508:CLA:HBC3	25:C:510:CLA:H71	1.96	0.47
1:A:234:ASN:HD21	30:D:412:LHG:HC11	1.78	0.47
4:D:162:LEU:HD13	31:H:102:DGD:HBT2	1.96	0.47
4:D:241:GLU:CD	4:D:241:GLU:H	2.23	0.47
1:a:286:THR:HG23	25:a:605:CLA:HED3	1.95	0.47
2:b:36:SER:OG	26:b:618:BCR:H362	2.14	0.47
3:c:134:ILE:HD12	25:c:511:CLA:H43	1.96	0.47
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.70	0.47
7:h:12:ARG:HB3	7:h:13:PRO:HD3	1.97	0.47
25:C:508:CLA:H122	25:C:508:CLA:H162	1.63	0.47
2:b:159:THR:O	2:b:180:PRO:HB3	2.14	0.47
25:b:614:CLA:H93	25:b:614:CLA:H61	1.76	0.47
19:z:40:ILE:HG13	19:z:41:PHE:N	2.30	0.47
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:603:CLA:H142	25:B:603:CLA:H112	1.67	0.47
13:O:133:VAL:C	13:O:135:SER:H	2.23	0.47
15:u:47:LYS:NZ	36:u:207:HOH:O	2.48	0.47
25:B:614:CLA:H62	25:B:614:CLA:H41	1.75	0.46
32:B:625:STE:H52	32:B:625:STE:H21	1.71	0.46
20:r:20:VAL:O	20:r:24:LEU:HB2	2.15	0.46
2:B:105:GLY:HA3	26:B:618:BCR:H402	1.96	0.46
25:B:601:CLA:H162	25:B:601:CLA:H141	1.63	0.46
25:a:605:CLA:H162	25:a:605:CLA:H193	1.73	0.46
25:c:509:CLA:H141	25:c:509:CLA:H161	1.73	0.46
3:C:38:GLY:HA3	25:C:511:CLA:HMD2	1.97	0.46
25:C:513:CLA:HBB1	26:K:101:BCR:H371	1.97	0.46
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.51	0.46
1:a:227:THR:HB	1:a:231:GLU:HG3	1.98	0.46
13:O:54:GLU:O	13:O:63:ALA:HB3	2.16	0.46
1:a:85:SER:HA	1:a:109:GLY:HA3	1.98	0.46
25:b:611:CLA:H121	25:b:611:CLA:H162	1.70	0.46
29:b:620:SQD:H151	29:b:620:SQD:H122	1.52	0.46
20:r:21:ARG:NH2	36:r:101:HOH:O	2.39	0.46
2:B:91:TRP:NE1	32:B:621:STE:H32	2.22	0.46
25:B:601:CLA:HAA1	32:B:624:STE:H82	1.97	0.46
28:D:407:LMG:H402	6:F:26:LEU:HB3	1.98	0.46
8:i:3:THR:OG1	36:i:101:HOH:O	2.20	0.46
29:D:408:SQD:H242	6:F:21:VAL:HG21	1.98	0.46
13:O:56:PRO:O	13:O:58:ASN:N	2.40	0.46
2:b:119:ASP:HB3	7:h:3:ARG:NH2	2.30	0.46
25:c:509:CLA:H142	25:c:509:CLA:H111	1.60	0.46
4:D:123:ILE:HD11	31:H:102:DGD:HAH1	1.98	0.46
2:B:221:PRO:HA	25:B:609:CLA:HED3	1.97	0.46
25:D:403:CLA:H112	25:D:403:CLA:H142	1.68	0.46
31:c:515:DGD:HB61	28:c:521:LMG:H392	1.97	0.46
28:c:521:LMG:H162	28:c:521:LMG:H192	1.54	0.46
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.98	0.46
29:A:613:SQD:H331	29:A:613:SQD:H302	1.42	0.46
30:D:412:LHG:H222	12:M:18:PRO:HG3	1.98	0.46
2:b:283:GLU:O	2:b:287:ARG:HG3	2.16	0.46
25:b:606:CLA:H72	25:b:606:CLA:H111	1.40	0.46
3:c:67:MET:O	3:c:71:GLU:HG3	2.15	0.46
7:h:4:ARG:HE	7:h:4:ARG:HB3	1.27	0.46
26:K:102:BCR:H322	19:Z:17:PHE:CE2	2.51	0.45
25:b:602:CLA:H193	25:b:602:CLA:H161	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:612:CLA:H122	25:b:612:CLA:H8	1.75	0.45
3:c:457:LYS:HD3	4:d:228:GLY:O	2.16	0.45
28:m:101:LMG:H371	28:m:101:LMG:H342	1.55	0.45
2:B:37:MET:O	2:B:41:GLU:HG3	2.16	0.45
11:L:14:ARG:HH22	29:b:620:SQD:H3	1.81	0.45
13:O:6:THR:HG22	13:O:9:ASP:CG	2.41	0.45
20:R:34:LEU:C	20:R:35:LEU:HG	2.41	0.45
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.51	0.45
13:o:178:LYS:HA	13:o:178:LYS:HD3	1.77	0.45
15:U:73:GLN:O	15:U:77:GLU:HG3	2.15	0.45
1:a:279:PRO:HG2	4:d:212:ALA:HB2	1.97	0.45
25:b:601:CLA:HBB2	26:h:101:BCR:H351	1.97	0.45
25:c:511:CLA:H143	25:c:511:CLA:H161	1.79	0.45
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.82	0.45
20:R:27:ALA:O	20:R:31:VAL:HG23	2.17	0.45
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.98	0.45
27:A:610:PL9:H471	27:A:610:PL9:H451	1.70	0.45
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.05	0.45
25:b:608:CLA:H161	25:b:608:CLA:H141	1.67	0.45
3:c:167:VAL:HG13	25:c:512:CLA:H102	1.98	0.45
3:c:391[B]:ARG:HH21	3:c:394:GLU:HG2	1.80	0.45
25:c:506:CLA:H51	25:c:507:CLA:H191	1.98	0.45
3:C:59:LEU:HD13	25:C:510:CLA:HMD2	1.99	0.45
25:C:501:CLA:HMD1	25:C:502:CLA:H101	1.99	0.45
19:Z:31:GLN:NE2	19:Z:32:ASP:H	2.14	0.45
25:b:615:CLA:H141	25:b:615:CLA:H161	1.76	0.45
3:c:464:GLU:HB3	3:c:467:LEU:HD12	1.99	0.45
25:c:506:CLA:H51	25:c:506:CLA:H12	1.70	0.45
10:k:26:PRO:O	10:k:29:PRO:HD2	2.17	0.45
28:m:101:LMG:H361	28:m:101:LMG:H392	1.83	0.45
16:v:57:GLU:CD	16:v:57:GLU:H	2.24	0.45
19:Z:31:GLN:O	19:Z:33:TRP:N	2.47	0.45
1:a:201:GLY:HA3	1:a:286:THR:HB	1.97	0.45
2:b:373:LYS:NZ	36:b:720:HOH:O	2.50	0.45
13:o:244:GLU:OE1	36:o:301:HOH:O	2.20	0.45
3:C:45:LEU:HA	3:C:139:THR:HG22	1.97	0.45
25:C:502:CLA:H161	25:C:502:CLA:H141	1.61	0.45
34:E:101:HEM:HMB1	34:E:101:HEM:HBB2	1.99	0.45
16:V:26:TYR:OH	16:V:122:GLU:OE1	2.31	0.45
32:d:413:STE:H22	32:d:413:STE:H51	1.67	0.45
25:C:507:CLA:H141	25:C:507:CLA:H161	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:242:LEU:HD21	28:c:520:LMG:H311	1.99	0.45
13:o:164:LEU:HD13	13:o:188:LYS:O	2.17	0.45
15:u:51:LYS:HB2	15:u:51:LYS:HE2	1.63	0.45
28:B:620:LMG:H392	28:B:620:LMG:H362	1.79	0.44
3:C:461:ARG:HG2	4:D:223:PHE:CD1	2.52	0.44
1:a:58[A]:VAL:HB	1:a:83:VAL:HB	1.99	0.44
27:a:610:PL9:H513	29:f:102:SQD:H311	1.98	0.44
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.99	0.44
2:b:497:GLN:HE21	4:d:24:ARG:HH12	1.64	0.44
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.52	0.44
13:o:92:SER:HB3	13:o:131:PRO:HA	1.99	0.44
36:A:761:HOH:O	13:O:107:THR:HG21	2.16	0.44
26:B:618:BCR:H15C	26:B:618:BCR:H351	1.86	0.44
9:J:20:GLY:O	9:J:24:ILE:HG13	2.18	0.44
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.99	0.44
13:o:130:GLN:HB2	36:o:345:HOH:O	2.16	0.44
1:A:60[A]:ILE:HB	1:A:83:VAL:HG12	1.98	0.44
2:B:289:GLN:HB2	36:B:909:HOH:O	2.16	0.44
13:O:178:LYS:HD2	13:O:181:GLU:OE2	2.17	0.44
36:a:728:HOH:O	3:c:410:VAL:HB	2.16	0.44
6:f:26:LEU:O	6:f:29:PRO:HD2	2.17	0.44
32:C:518:STE:H71	32:C:518:STE:H42	1.58	0.44
4:D:261:PHE:CE1	30:D:409:LHG:HC81	2.52	0.44
2:b:91:TRP:CD1	32:b:621:STE:H162	2.52	0.44
26:c:514:BCR:H15C	26:c:514:BCR:H351	1.87	0.44
25:C:513:CLA:H121	25:C:513:CLA:H162	1.77	0.44
16:V:3:LEU:HD23	16:V:3:LEU:HA	1.81	0.44
1:a:46:ILE:HD13	31:a:614:DGD:HBN2	2.00	0.44
32:b:621:STE:H141	32:b:621:STE:H111	1.58	0.44
3:c:279:LEU:HD11	25:c:509:CLA:H11	2.00	0.44
25:c:504:CLA:H92	25:c:504:CLA:H62	1.86	0.44
26:B:619:BCR:H361	26:B:619:BCR:H20C	1.79	0.44
31:C:516:DGD:HAE2	31:C:516:DGD:HA82	1.55	0.44
2:b:222:PRO:HB3	7:h:26:GLY:HA3	1.99	0.44
25:c:503:CLA:HMC2	25:c:512:CLA:H12	1.99	0.44
2:B:422:ARG:O	2:B:425:ILE:HG12	2.18	0.44
16:v:120:LEU:O	36:v:301:HOH:O	2.20	0.44
27:A:610:PL9:H351	27:A:610:PL9:H371	1.68	0.44
2:B:458:PHE:HB3	25:B:604:CLA:HBC2	2.00	0.44
25:D:404:CLA:H141	18:X:15:LEU:HD12	1.98	0.44
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:413:ASP:O	2:b:417:VAL:HG23	2.18	0.44
30:e:101:LHG:H262	30:e:101:LHG:H291	1.85	0.44
10:k:17:ILE:HG13	10:k:18:PHE:CD1	2.52	0.44
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.44
25:b:612:CLA:H43	25:b:615:CLA:H12	1.99	0.44
3:c:286:ALA:HB2	25:c:502:CLA:HMD2	1.98	0.44
25:c:503:CLA:HBB1	25:c:512:CLA:H62	1.99	0.44
4:d:48:TRP:CE2	33:d:402:PHO:H162	2.53	0.44
16:v:7:VAL:O	16:v:124:LYS:NZ	2.43	0.44
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.53	0.43
32:T:102:STE:H52	32:T:102:STE:H81	1.76	0.43
19:Z:50:LEU:HD12	19:Z:50:LEU:HA	1.80	0.43
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.99	0.43
29:a:613:SQD:H92	29:a:613:SQD:H241	1.99	0.43
25:b:607:CLA:HMB1	25:b:607:CLA:HBB1	2.00	0.43
2:B:397:VAL:HG12	2:B:417:VAL:HG11	2.00	0.43
25:B:607:CLA:H193	11:L:27:LEU:HD11	1.99	0.43
25:C:505:CLA:H2	25:C:505:CLA:H61	1.80	0.43
25:C:506:CLA:H111	25:C:506:CLA:H91	1.78	0.43
31:c:517:DGD:HBH2	31:c:517:DGD:HBT2	1.79	0.43
4:d:62:GLY:HA2	5:e:63:ILE:HG21	1.99	0.43
32:d:413:STE:H171	32:d:413:STE:H142	1.69	0.43
4:d:141:TYR:OH	30:d:407:LHG:O4	2.22	0.43
2:B:52:LEU:HD12	13:o:59:LYS:HE2	2.01	0.43
3:C:203:THR:O	3:C:235:GLY:HA3	2.19	0.43
4:D:99:GLY:HA3	32:D:413:STE:H21	1.99	0.43
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.53	0.43
31:A:616:DGD:HAT1	31:A:616:DGD:HAH2	1.75	0.43
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.53	0.43
2:B:233:ASN:O	2:B:236:THR:HG22	2.19	0.43
3:C:334:PRO:HA	13:O:153:THR:OG1	2.18	0.43
25:D:404:CLA:C4B	32:D:413:STE:H151	2.48	0.43
11:L:24:ILE:HG12	12:M:18:PRO:HB2	1.99	0.43
18:X:10:PHE:CE2	18:X:14:LEU:HD22	2.53	0.43
18:x:14:LEU:HD12	18:x:14:LEU:HA	1.83	0.43
25:C:511:CLA:H141	25:C:511:CLA:H162	1.76	0.43
1:a:16:ARG:HB3	1:a:16:ARG:HH11	1.82	0.43
29:a:613:SQD:H81	29:a:613:SQD:H112	1.85	0.43
2:b:317:ASN:HA	2:b:330:MET:HE1	2.00	0.43
25:c:508:CLA:H111	25:c:508:CLA:H142	1.67	0.43
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:LEU:HD11	25:B:614:CLA:HMA1	2.00	0.43
1:a:95:PRO:HD2	1:a:98:GLU:HG3	2.01	0.43
25:b:614:CLA:H92	26:b:617:BCR:H362	1.99	0.43
31:c:515:DGD:HA42	31:c:515:DGD:HA72	1.72	0.43
26:B:617:BCR:H24C	26:B:617:BCR:H371	1.82	0.43
29:b:620:SQD:H101	29:b:620:SQD:H131	1.84	0.43
1:A:158:PHE:O	1:A:162[B]:PRO:HG2	2.18	0.43
28:C:517:LMG:H361	28:C:517:LMG:H331	1.74	0.43
25:a:605:CLA:HBD	25:a:611:CLA:HAC2	2.01	0.43
25:b:611:CLA:H142	25:b:611:CLA:H111	1.71	0.43
3:c:213:LEU:HD21	26:c:514:BCR:C20	2.49	0.43
16:v:76:MET:HE3	35:v:201:HEC:HBB3	2.01	0.43
25:B:601:CLA:H92	26:H:101:BCR:C21	2.49	0.42
25:C:509:CLA:H62	25:C:509:CLA:H92	1.76	0.42
25:c:512:CLA:H121	25:c:513:CLA:H151	2.00	0.42
4:d:103:ARG:NE	4:d:106:GLN:OE1	2.50	0.42
25:c:504:CLA:H142	25:c:508:CLA:H121	1.99	0.42
2:B:67:ALA:HA	2:B:71:VAL:O	2.19	0.42
28:B:620:LMG:H321	28:B:620:LMG:H352	1.67	0.42
25:d:404:CLA:H92	18:x:18:ALA:HB2	2.01	0.42
9:j:36:LEU:O	36:j:201:HOH:O	2.22	0.42
13:o:53:LYS:HG3	13:o:65:PHE:CE2	2.54	0.42
2:b:461:LEU:HD21	4:d:284:ILE:HD11	2.00	0.42
25:c:509:CLA:H3A	25:c:509:CLA:HBA1	1.86	0.42
2:B:489:GLU:HG3	2:B:495:PHE:CE2	2.54	0.42
4:D:131:GLU:O	4:D:135:LEU:HG	2.19	0.42
16:V:77:LYS:HG2	16:V:95:LEU:HD12	2.00	0.42
2:b:298:LEU:HD23	2:b:298:LEU:HA	1.91	0.42
26:b:618:BCR:H15C	26:b:618:BCR:H351	1.81	0.42
3:c:318:LEU:C	3:c:318:LEU:HD23	2.44	0.42
30:e:101:LHG:HC61	30:e:101:LHG:H241	1.62	0.42
26:h:101:BCR:H20C	26:h:101:BCR:H361	1.85	0.42
26:k:101:BCR:H371	26:k:101:BCR:H24C	1.74	0.42
25:A:607:CLA:H141	25:A:607:CLA:H161	1.91	0.42
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.02	0.42
27:a:610:PL9:H48	4:d:39:PRO:HG3	2.02	0.42
25:c:503:CLA:H102	25:c:503:CLA:H62	1.71	0.42
26:c:514:BCR:H20C	26:c:514:BCR:H361	1.88	0.42
13:o:59:LYS:H	13:o:59:LYS:HG3	1.50	0.42
1:A:158:PHE:O	1:A:162[A]:PRO:HG2	2.20	0.42
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:LEU:HD12	3:C:213:LEU:HA	1.85	0.42
12:M:31:SER:HB3	32:m:102:STE:H22	2.01	0.42
7:h:37:LEU:HD22	26:h:101:BCR:H16C	2.01	0.42
9:j:18:GLY:O	9:j:21:VAL:HG13	2.20	0.42
25:B:613:CLA:HHC	25:B:613:CLA:HAB	1.90	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.42
25:C:513:CLA:H61	25:C:513:CLA:H41	1.85	0.42
5:E:60:GLN:HG2	5:E:62:SER:H	1.85	0.42
11:L:27:LEU:HD23	11:L:27:LEU:HA	1.89	0.42
3:c:248:GLY:O	3:c:252:ILE:HG13	2.20	0.42
11:l:16:SER:OG	30:l:101:LHG:HC62	2.19	0.42
12:m:1:FME:HE2	12:m:1:FME:HB2	1.88	0.42
26:T:101:BCR:H20C	26:T:101:BCR:H361	1.88	0.42
13:o:205:ASP:OD1	13:o:207:ARG:NE	2.48	0.42
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.01	0.42
1:A:271:LEU:HD11	27:A:610:PL9:HC71	2.02	0.42
2:B:498:LYS:NZ	4:D:19:ASP:OD2	2.40	0.42
25:B:602:CLA:H92	25:B:602:CLA:H62	1.82	0.42
25:B:614:CLA:H43	29:B:623:SQD:H132	2.02	0.42
25:b:601:CLA:H171	26:h:101:BCR:C16	2.50	0.42
25:C:512:CLA:H141	25:C:512:CLA:H162	1.79	0.41
25:a:605:CLA:CBD	25:a:611:CLA:HAC2	2.50	0.41
25:b:609:CLA:H62	25:b:609:CLA:H2	1.82	0.41
4:d:194:ASN:HA	4:d:295:SER:OG	2.20	0.41
27:d:406:PL9:H372	27:d:406:PL9:H351	1.85	0.41
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	2.02	0.41
2:B:141:ILE:O	2:B:145:LEU:HG	2.20	0.41
2:B:241:SER:O	2:B:245:VAL:HG23	2.20	0.41
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.91	0.41
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.01	0.41
26:D:405:BCR:H15C	26:D:405:BCR:H351	1.89	0.41
13:O:66:VAL:HG21	13:O:110:MET:HE3	2.02	0.41
19:Z:29:SER:HB3	19:Z:31:GLN:HG3	2.03	0.41
25:b:601:CLA:H91	25:b:601:CLA:H111	1.70	0.41
31:c:516:DGD:HAH2	26:d:405:BCR:H271	2.02	0.41
5:e:26:THR:HA	20:r:15:ALA:HB1	2.02	0.41
13:o:32:ILE:HG21	13:o:93:LEU:HD21	2.02	0.41
1:A:201:GLY:HA3	1:A:286:THR:HB	2.02	0.41
2:B:12:LEU:HB2	25:B:612:CLA:HMC2	2.02	0.41
25:C:504:CLA:H101	31:J:101:DGD:HBF2	2.03	0.41
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:603:CLA:C4D	25:b:605:CLA:H43	2.50	0.41
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.02	0.41
26:K:103:BCR:H20C	26:K:103:BCR:H361	1.81	0.41
1:a:182[B]:PHE:O	1:a:186[B]:PHE:HB2	2.21	0.41
1:a:215:HIS:HA	27:a:610:PL9:O1	2.21	0.41
2:b:317:ASN:HA	2:b:330:MET:CE	2.50	0.41
25:B:602:CLA:H92	7:H:46:LEU:HD13	2.02	0.41
3:C:399:ALA:O	3:C:401:LEU:N	2.47	0.41
30:L:101:LHG:HC42	30:L:101:LHG:HC32	2.03	0.41
25:c:501:CLA:H92	25:c:501:CLA:H62	1.89	0.41
31:c:516:DGD:HA91	31:c:517:DGD:HB91	2.02	0.41
1:A:196:PRO:HB3	31:J:101:DGD:HA92	2.02	0.41
27:A:610:PL9:H161	27:A:610:PL9:H121	1.84	0.41
25:B:614:CLA:H152	25:B:614:CLA:H18	1.49	0.41
3:C:275:SER:HB3	25:C:509:CLA:HED3	2.02	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.41
25:b:603:CLA:CAD	25:b:605:CLA:H12	2.51	0.41
4:d:259:ILE:HD12	30:d:408:LHG:H291	2.01	0.41
13:o:110:MET:HE3	13:o:114:GLU:HB3	2.02	0.41
15:u:68:THR:OG1	15:u:71:GLN:HG3	2.21	0.41
16:v:66:ARG:O	16:v:72:LEU:HG	2.21	0.41
28:B:622:LMG:H391	4:D:36:LEU:HB2	2.03	0.41
26:C:514:BCR:H15C	26:C:514:BCR:H351	1.81	0.41
4:D:186:GLN:HB2	25:D:403:CLA:HBC1	2.03	0.41
31:J:101:DGD:HA82	31:J:101:DGD:HAE2	1.67	0.41
2:b:119:ASP:HB3	7:h:3:ARG:HH22	1.86	0.41
25:c:507:CLA:H61	25:c:507:CLA:H92	1.77	0.41
5:e:30:LEU:HD11	34:f:101:HEM:CBB	2.50	0.41
11:l:2:GLU:HB2	36:l:201:HOH:O	2.21	0.41
26:t:101:BCR:HC7	26:t:101:BCR:H331	1.82	0.41
1:A:334[B]:ARG:NH2	36:A:726:HOH:O	2.54	0.41
25:B:605:CLA:H41	25:B:612:CLA:H161	2.03	0.41
13:O:178:LYS:H	13:O:178:LYS:HG3	1.49	0.41
16:V:61:LEU:HD23	16:V:61:LEU:HA	1.90	0.41
2:b:42:LEU:HA	2:b:42:LEU:HD23	1.82	0.41
3:c:334:PRO:HA	13:o:153:THR:OG1	2.21	0.41
25:c:505:CLA:H92	25:c:505:CLA:HAB	2.02	0.41
25:A:606:CLA:H162	25:A:606:CLA:H203	1.83	0.41
2:B:347:ARG:O	2:B:397:VAL:HA	2.21	0.41
25:C:504:CLA:H143	25:C:508:CLA:H141	2.02	0.41
26:H:101:BCR:H15C	26:H:101:BCR:H351	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:321:ASP:OD2	3:c:340:TYR:OH	2.23	0.41
25:c:510:CLA:HMB1	25:c:510:CLA:HBB1	2.03	0.41
5:e:11:SER:CB	30:e:101:LHG:HC12	2.51	0.41
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:CB	2.51	0.41
25:C:508:CLA:H142	25:C:508:CLA:H101	2.02	0.41
27:D:406:PL9:H512	14:T:10:PHE:HB2	2.03	0.41
12:M:1:FME:HE2	12:M:1:FME:HB2	1.86	0.41
25:b:610:CLA:H203	25:b:610:CLA:H162	1.71	0.41
3:c:124:VAL:HG13	26:k:101:BCR:H362	2.01	0.41
13:o:173:ALA:C	13:o:175:PRO:HD3	2.46	0.41
1:A:120:LEU:HA	1:A:120:LEU:HD23	1.85	0.40
27:A:610:PL9:H422	27:A:610:PL9:H401	1.63	0.40
2:B:321:LYS:HD2	2:B:321:LYS:HA	1.92	0.40
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.56	0.40
3:C:95:LEU:HD13	25:C:502:CLA:H143	2.03	0.40
16:V:4:THR:O	16:V:7:VAL:HG13	2.21	0.40
1:a:310:LYS:HD2	16:v:1:ALA:HB1	2.03	0.40
3:c:131:TYR:OH	25:c:513:CLA:HED2	2.22	0.40
3:c:461:ARG:HG2	4:d:223:PHE:CD1	2.56	0.40
25:c:502:CLA:H141	25:c:502:CLA:H161	1.71	0.40
26:k:103:BCR:H24C	26:k:103:BCR:H371	1.86	0.40
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.93	0.40
4:D:194:ASN:HA	4:D:295:SER:OG	2.21	0.40
1:a:112:TYR:O	1:a:116:ILE:HG12	2.21	0.40
29:a:613:SQD:H282	26:t:101:BCR:HC41	2.04	0.40
25:d:404:CLA:H111	25:d:404:CLA:H91	1.83	0.40
26:t:101:BCR:H11C	26:t:101:BCR:H341	1.99	0.40
1:A:283:VAL:HA	1:A:286:THR:HG22	2.03	0.40
31:A:616:DGD:HB62	32:I:101:STE:H51	2.03	0.40
31:A:616:DGD:HBF2	8:I:7:THR:HG21	2.02	0.40
29:B:623:SQD:H292	29:B:623:SQD:H322	1.83	0.40
25:C:506:CLA:H61	25:C:506:CLA:H2	1.82	0.40
25:C:512:CLA:H161	25:C:512:CLA:H193	1.67	0.40
18:X:11:PHE:O	18:X:15:LEU:HD13	2.21	0.40
2:b:413:ASP:HA	2:b:414:PRO:HD3	1.89	0.40
25:b:616:CLA:H142	25:b:616:CLA:H111	1.86	0.40
26:b:619:BCR:H361	26:b:619:BCR:H20C	1.88	0.40
30:e:101:LHG:H151	30:e:101:LHG:H182	1.88	0.40
13:o:52:VAL:HG22	13:o:233:VAL:HG22	2.02	0.40
25:C:506:CLA:C2	25:C:507:CLA:H201	2.52	0.40
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:607:PHO:HMB3	33:a:607:PHO:HBB1	2.03	0.40
4:d:18:LEU:HD11	18:x:28:LEU:HB3	2.03	0.40
27:d:406:PL9:H421	27:d:406:PL9:H401	1.83	0.40
1:A:308:ASP:HB2	5:E:52:PRO:O	2.22	0.40
25:B:611:CLA:H203	25:B:613:CLA:C10	2.50	0.40
25:D:404:CLA:H43	32:D:413:STE:H182	2.02	0.40
5:E:22[A]:ILE:HD13	5:E:23:HIS:CE1	2.57	0.40
5:E:53:ASP:O	16:V:1:ALA:N	2.54	0.40
26:H:101:BCR:H20C	26:H:101:BCR:H361	1.85	0.40
13:O:110:MET:HE2	13:O:110:MET:HB3	1.87	0.40
1:a:214:MET:SD	33:d:402:PHO:HED3	2.61	0.40
25:b:608:CLA:H61	25:b:609:CLA:H142	2.04	0.40
25:c:510:CLA:H191	10:k:33:LEU:HD22	2.03	0.40
11:l:21:LEU:HD12	11:l:21:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/344 (115%)	391 (99%)	4 (1%)	0	100	100
1	a	395/344 (115%)	390 (99%)	5 (1%)	0	100	100
2	B	507/510 (99%)	502 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	495 (98%)	8 (2%)	0	100	100
3	C	451/461 (98%)	439 (97%)	11 (2%)	1 (0%)	43	40
3	c	461/461 (100%)	448 (97%)	12 (3%)	1 (0%)	43	40
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	331 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/84 (95%)	79 (99%)	1 (1%)	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%)	4 (6%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	230 (95%)	10 (4%)	3 (1%)	10	4
13	o	242/272 (89%)	234 (97%)	8 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	5
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	10
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	3	1
19	z	60/62 (97%)	60 (100%)	0	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5386/5700 (94%)	5252 (98%)	125 (2%)	9 (0%)	43 40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
19	Z	31	GLN
3	c	416	SER
13	O	59	LYS
15	u	53	ALA
13	O	62	GLU
19	Z	32	ASP
13	O	134	THR

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%)	319 (99%)	3 (1%)	70 73
1	a	321/280 (115%)	309 (96%)	12 (4%)	30 24
2	B	407/407 (100%)	399 (98%)	8 (2%)	48 48
2	b	402/407 (99%)	393 (98%)	9 (2%)	45 45
3	C	353/362 (98%)	347 (98%)	6 (2%)	53 53
3	c	362/362 (100%)	345 (95%)	17 (5%)	23 16
4	D	277/283 (98%)	271 (98%)	6 (2%)	45 45
4	d	278/283 (98%)	266 (96%)	12 (4%)	26 19
5	E	72/73 (99%)	69 (96%)	3 (4%)	26 20
5	e	71/73 (97%)	67 (94%)	4 (6%)	19 12
6	F	28/39 (72%)	27 (96%)	1 (4%)	31 26
6	f	28/39 (72%)	26 (93%)	2 (7%)	13 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/55 (98%)	52 (96%)	2 (4%)	30	24
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	11
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	9
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	5
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	29
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	34
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	1
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	26
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	206/228 (90%)	198 (96%)	8 (4%)	28	22
13	o	207/228 (91%)	195 (94%)	12 (6%)	18	11
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	23
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	22
15	U	84/112 (75%)	77 (92%)	7 (8%)	10	5
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	53
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	28
17	Y	19/37 (51%)	16 (84%)	3 (16%)	2	0
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	4
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	2
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	2
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	0
19	z	51/52 (98%)	49 (96%)	2 (4%)	28	22
20	R	28/33 (85%)	23 (82%)	5 (18%)	2	0
20	r	25/33 (76%)	18 (72%)	7 (28%)	0	0
All	All	4450/4654 (96%)	4278 (96%)	172 (4%)	28	22

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
1	A	243	GLU
1	A	270	SER
2	B	63	LEU
2	B	76	SER
2	B	86	ILE
2	B	98	LEU
2	B	127	ARG
2	B	227	LYS
2	B	371	THR
2	B	476	ARG
3	C	141	GLU
3	C	170	ILE
3	C	213	LEU
3	C	240	ILE
3	C	289	PHE
3	C	416	SER
4	D	43	LEU
4	D	154	VAL
4	D	241	GLU
4	D	259	ILE
4	D	264	LYS
4	D	345	VAL
5	E	4	THR
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	10	ILE
7	H	56	ASP
8	I	4	LEU
8	I	35	LYS
10	K	27	VAL
11	L	7	ARG
12	M	25	LEU
13	O	39	ARG
13	O	78	LEU
13	O	86	LYS
13	O	107	THR
13	O	116	ILE
13	O	118	LEU
13	O	178	LYS
13	O	214	THR
14	T	25	GLU

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Mol	Chain	Res	Type
15	U	10	VAL
15	U	37	GLN
15	U	39	ARG
15	U	51	LYS
15	U	61	VAL
15	U	67	LEU
15	U	79	LEU
16	V	7	VAL
16	V	57	GLU
17	Y	23	THR
17	Y	30	ILE
17	Y	34	MET
18	X	3	ILE
18	X	34	ILE
18	X	37	VAL
19	Z	15	LEU
19	Z	17	PHE
19	Z	31	GLN
19	Z	32	ASP
19	Z	34	ASP
19	Z	35	ARG
19	Z	46	LEU
19	Z	50	LEU
19	Z	51	VAL
20	R	6	LEU
20	R	10	LEU
20	R	12	VAL
20	R	21	ARG
20	R	35	LEU
1	a	16	ARG
1	a	42	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	242	GLU
1	a	243	GLU
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	76	SER

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Mol	Chain	Res	Type
2	b	80	ILE
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	362	PHE
2	b	438	ASN
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	142	GLU
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	355[A]	THR
3	c	355[B]	THR
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	396	MET
3	c	416	SER
4	d	90	LEU
4	d	144	ILE
4	d	150	ILE
4	d	182	LEU
4	d	230	SER
4	d	233	ARG
4	d	238	THR
4	d	259	ILE
4	d	264	LYS
4	d	291	LEU
4	d	307	GLU
4	d	321	LEU
5	e	17	VAL
5	e	66	VAL
5	e	83	LEU
5	e	84	LYS
6	f	23	VAL

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Mol	Chain	Res	Type
6	f	28	VAL
7	h	3	ARG
7	h	4	ARG
7	h	7	LEU
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	24	VAL
10	k	27	VAL
10	k	30	VAL
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
13	o	34	SER
13	o	49	THR
13	o	53	LYS
13	o	54	GLU
13	o	55	GLU
13	o	60	ARG
13	o	64	GLU
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	180	GLU
13	o	199	LEU
14	t	25	GLU
16	v	10	VAL
16	v	19	ILE
16	v	86	GLN
16	v	107	LEU
17	y	19	ILE
17	y	27	MET
18	x	2	THR
18	x	15	LEU
18	x	21	LEU
19	z	1	MET
19	z	46	LEU
20	r	6	LEU
20	r	7	VAL
20	r	9	LEU
20	r	10	LEU

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Mol	Chain	Res	Type
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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	261	GLN
2	B	331	ASN
2	B	374	ASN
4	D	334	GLN
6	F	44	GLN
7	H	59	ASN
13	O	88	ASN
16	V	86	GLN
18	X	38	GLN
19	Z	31	GLN
1	a	234	ASN
1	a	296	ASN
2	b	179	GLN
2	b	338	GLN
2	b	409	GLN
2	b	497	GLN
3	c	25	ASN
3	c	311	GLN
5	e	60	GLN
5	e	82	GLN
7	h	59	ASN
13	o	130	GLN
13	o	132	ASN
13	o	219	GLN
16	v	25	GLN
19	z	31	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	0.99	0	8,9,11	1.01	0
12	FME	m	1	12	8,9,10	1.04	1 (12%)	8,9,11	0.90	0
14	FME	t	1	14	8,9,10	1.10	0	8,9,11	0.80	0
14	FME	T	1	14	8,9,10	1.28	1 (12%)	8,9,11	1.10	1 (12%)
8	FME	i	1	8	8,9,10	1.00	0	8,9,11	1.04	1 (12%)
8	FME	I	1	8	8,9,10	1.06	1 (12%)	8,9,11	0.69	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	-	1/7/9/11	-
12	FME	m	1	12	-	3/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.87	1.42	1.46
8	I	1	FME	CA-N	-2.10	1.43	1.46
12	m	1	FME	CA-N	-2.04	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.58	114.48	109.50
8	i	1	FME	CA-N-CN	-2.01	119.73	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	1	0
12	m	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
25	CLA	B	606	2	69,73,73	1.36	7 (10%)	82,113,113	1.51	8 (9%)
35	HEC	v	201	16	50,50,50	1.80	7 (14%)	68,82,82	1.32	4 (5%)
25	CLA	b	610	36	69,73,73	1.26	6 (8%)	82,113,113	1.21	8 (9%)
28	LMG	D	411	-	31,31,55	0.69	1 (3%)	33,33,63	1.24	3 (9%)
29	SQD	a	613	-	35,35,54	1.73	5 (14%)	37,37,65	1.37	3 (8%)
25	CLA	b	616	2	64,68,73	1.30	8 (12%)	76,107,113	1.56	7 (9%)
25	CLA	b	615	2	69,73,73	1.40	7 (10%)	82,113,113	1.29	5 (6%)
25	CLA	C	504	36	63,67,73	1.50	10 (15%)	74,105,113	1.36	10 (13%)
25	CLA	C	511	3	69,73,73	1.34	8 (11%)	82,113,113	1.44	5 (6%)
31	DGD	a	614	-	43,43,67	0.69	2 (4%)	45,45,81	1.40	6 (13%)
25	CLA	b	608	2	69,73,73	1.26	9 (13%)	82,113,113	1.32	8 (9%)
25	CLA	C	502	3	69,73,73	1.12	6 (8%)	82,113,113	1.23	5 (6%)
32	STE	C	519	-	11,11,19	0.72	0	11,11,19	1.10	0
24	BCT	d	401	22	3,3,3	1.16	0	2,3,3	2.97	1 (50%)
26	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	7 (12%)
26	BCR	H	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.22	6 (10%)
32	STE	C	518	-	11,11,19	0.71	0	11,11,19	1.38	1 (9%)
28	LMG	B	620	-	51,51,55	0.83	2 (3%)	59,59,63	1.36	5 (8%)
21	OEY	A	601[A]	36,3,1	0,16,16	-	-	-	-	-
31	DGD	H	102	-	63,63,67	1.10	7 (11%)	77,77,81	1.44	9 (11%)
32	STE	b	625	-	9,9,19	0.40	0	8,8,19	0.63	0
28	LMG	c	518	-	37,37,55	0.95	2 (5%)	45,45,63	1.31	5 (11%)
25	CLA	B	601	36	69,73,73	1.34	7 (10%)	82,113,113	1.53	8 (9%)
25	CLA	C	513	3	69,73,73	1.39	9 (13%)	82,113,113	1.30	8 (9%)
32	STE	B	625	-	17,17,19	0.68	0	17,17,19	1.00	0
25	CLA	c	503	3	69,73,73	1.26	8 (11%)	82,113,113	1.49	7 (8%)
26	BCR	k	102	-	41,41,41	1.06	3 (7%)	56,56,56	1.09	2 (3%)
32	STE	C	520	-	15,15,19	0.38	0	14,14,19	0.80	0
29	SQD	A	613	-	50,52,54	1.58	7 (14%)	60,63,65	1.95	12 (20%)
31	DGD	A	616	-	67,67,67	1.09	9 (13%)	81,81,81	1.33	10 (12%)
29	SQD	D	408	-	34,36,54	1.50	6 (17%)	42,45,65	1.84	11 (26%)
28	LMG	c	520	-	48,48,55	0.82	1 (2%)	56,56,63	1.39	9 (16%)
26	BCR	a	609	-	41,41,41	0.96	2 (4%)	56,56,56	1.17	4 (7%)
32	STE	d	413	-	19,19,19	0.56	0	19,19,19	1.19	1 (5%)
26	BCR	B	617	-	41,41,41	1.00	3 (7%)	56,56,56	1.24	3 (5%)
25	CLA	b	601	36	69,73,73	1.40	7 (10%)	82,113,113	1.40	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	d	407	-	48,48,48	0.82	3 (6%)	51,54,54	1.30	5 (9%)
25	CLA	C	510	3	69,73,73	1.29	10 (14%)	82,113,113	1.48	7 (8%)
30	LHG	D	410	-	46,46,48	0.82	3 (6%)	49,52,54	1.28	6 (12%)
32	STE	B	621	-	16,16,19	0.70	0	16,16,19	1.04	0
31	DGD	c	517	-	63,63,67	0.92	3 (4%)	77,77,81	1.39	10 (12%)
25	CLA	b	606	2	69,73,73	1.29	7 (10%)	82,113,113	1.45	7 (8%)
26	BCR	b	619	-	41,41,41	0.97	2 (4%)	56,56,56	1.16	3 (5%)
25	CLA	d	403	4	69,73,73	1.20	8 (11%)	82,113,113	1.26	6 (7%)
25	CLA	c	506	3	69,73,73	1.33	8 (11%)	82,113,113	1.27	6 (7%)
29	SQD	A	615	-	38,38,54	1.74	5 (13%)	40,40,65	1.13	2 (5%)
26	BCR	k	103	-	41,41,41	1.02	2 (4%)	56,56,56	1.09	2 (3%)
25	CLA	a	611	36	69,73,73	1.39	7 (10%)	82,113,113	1.41	11 (13%)
27	PL9	A	610	-	55,55,55	0.71	0	68,69,69	1.50	10 (14%)
33	PHO	D	401	-	58,69,69	1.91	10 (17%)	55,99,99	1.39	4 (7%)
25	CLA	B	616	2	64,68,73	1.27	7 (10%)	76,107,113	1.36	6 (7%)
26	BCR	b	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
25	CLA	b	602	2	69,73,73	1.20	7 (10%)	82,113,113	1.34	8 (9%)
25	CLA	c	508	3	68,72,73	1.35	9 (13%)	80,111,113	1.30	7 (8%)
25	CLA	B	608	2	69,73,73	1.22	10 (14%)	82,113,113	1.35	7 (8%)
31	DGD	h	102	-	63,63,67	0.96	4 (6%)	77,77,81	1.45	12 (15%)
32	STE	B	627	-	15,15,19	0.33	0	14,14,19	0.87	0
25	CLA	D	403	4	69,73,73	1.20	7 (10%)	82,113,113	1.36	10 (12%)
25	CLA	c	505	3	69,73,73	1.29	8 (11%)	82,113,113	1.37	8 (9%)
25	CLA	a	608	1	69,73,73	1.23	6 (8%)	82,113,113	1.17	4 (4%)
21	OEY	A	601[B]	36,3,1	0,16,16	-	-	-	-	-
25	CLA	B	605	2	69,73,73	1.21	7 (10%)	82,113,113	1.32	9 (10%)
28	LMG	C	517	-	48,48,55	0.82	1 (2%)	56,56,63	1.33	6 (10%)
31	DGD	J	101	-	63,63,67	0.84	3 (4%)	77,77,81	1.41	11 (14%)
32	STE	J	102	-	11,11,19	0.72	0	11,11,19	1.16	0
32	STE	b	624	-	14,14,19	0.30	0	13,13,19	0.97	0
35	HEC	V	201	16	50,50,50	1.70	8 (16%)	68,82,82	1.37	8 (11%)
32	STE	d	412	-	16,16,19	0.65	0	16,16,19	1.10	0
25	CLA	d	404	4	69,73,73	1.22	9 (13%)	82,113,113	1.29	8 (9%)
26	BCR	B	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.37	9 (16%)
32	STE	t	102	-	13,13,19	0.70	0	13,13,19	1.16	2 (15%)
32	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	c	514	-	41,41,41	1.09	3 (7%)	56,56,56	1.17	5 (8%)
26	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.32	8 (14%)
30	LHG	d	409	-	38,38,48	0.71	1 (2%)	41,44,54	1.14	3 (7%)
26	BCR	K	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.16	2 (3%)
32	STE	D	413	-	19,19,19	0.59	0	19,19,19	1.14	0
32	STE	j	101	-	11,11,19	0.74	0	11,11,19	1.19	1 (9%)
25	CLA	C	501	3	69,73,73	1.49	10 (14%)	82,113,113	1.48	7 (8%)
27	PL9	D	406	-	55,55,55	0.98	4 (7%)	68,69,69	1.48	15 (22%)
28	LMG	d	410	-	21,21,55	0.52	0	20,20,63	1.19	2 (10%)
25	CLA	C	505	3	69,73,73	1.20	7 (10%)	82,113,113	1.21	7 (8%)
28	LMG	b	622	-	55,55,55	0.87	4 (7%)	63,63,63	1.43	11 (17%)
28	LMG	d	411	-	44,44,55	0.90	2 (4%)	52,52,63	1.33	6 (11%)
25	CLA	b	604	2	69,73,73	1.32	8 (11%)	82,113,113	1.49	11 (13%)
25	CLA	B	603	2	69,73,73	1.35	6 (8%)	82,113,113	1.37	9 (10%)
25	CLA	c	511	3	69,73,73	1.44	6 (8%)	82,113,113	1.46	7 (8%)
25	CLA	b	603	2	69,73,73	1.29	9 (13%)	82,113,113	1.33	10 (12%)
25	CLA	b	613	2	69,73,73	1.24	7 (10%)	82,113,113	1.34	10 (12%)
26	BCR	h	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.26	6 (10%)
28	LMG	B	622	-	26,26,55	0.76	2 (7%)	26,26,63	1.21	1 (3%)
25	CLA	C	512	3	69,73,73	1.36	9 (13%)	82,113,113	1.38	10 (12%)
33	PHO	a	607	-	58,69,69	2.03	10 (17%)	55,99,99	1.39	6 (10%)
28	LMG	A	612	-	48,48,55	0.70	0	56,56,63	1.36	6 (10%)
25	CLA	C	503	3	69,73,73	1.39	9 (13%)	82,113,113	1.54	10 (12%)
25	CLA	c	502	3	69,73,73	1.25	6 (8%)	82,113,113	1.31	7 (8%)
30	LHG	D	409	-	48,48,48	0.74	3 (6%)	51,54,54	1.25	7 (13%)
32	STE	T	102	-	15,15,19	0.38	0	14,14,19	0.75	0
25	CLA	B	614	2	69,73,73	1.38	9 (13%)	82,113,113	1.27	10 (12%)
30	LHG	l	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.23	4 (7%)
27	PL9	d	406	-	55,55,55	0.90	1 (1%)	68,69,69	1.58	14 (20%)
25	CLA	c	507	36	69,73,73	1.24	9 (13%)	82,113,113	1.37	7 (8%)
30	LHG	D	412	-	48,48,48	0.82	1 (2%)	51,54,54	1.38	7 (13%)
26	BCR	d	405	-	41,41,41	1.05	3 (7%)	56,56,56	1.17	5 (8%)
25	CLA	B	607	36	69,73,73	1.14	6 (8%)	82,113,113	1.26	6 (7%)
25	CLA	c	504	36	64,68,73	1.32	7 (10%)	76,107,113	1.31	8 (10%)
21	OXY	a	601[A]	36,3,1	0,16,16	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	e	101	-	41,41,48	0.78	1 (2%)	44,47,54	1.31	6 (13%)
25	CLA	b	614	2	69,73,73	1.38	7 (10%)	82,113,113	1.29	10 (12%)
26	BCR	A	609	-	41,41,41	0.92	1 (2%)	56,56,56	1.23	5 (8%)
32	STE	I	101	-	14,14,19	0.35	0	13,13,19	0.88	0
25	CLA	a	605	1	69,73,73	1.44	10 (14%)	82,113,113	1.46	8 (9%)
32	STE	M	101	-	14,14,19	0.67	0	14,14,19	1.25	1 (7%)
30	LHG	L	101	-	48,48,48	0.64	1 (2%)	51,54,54	1.27	4 (7%)
25	CLA	B	602	2	69,73,73	1.21	5 (7%)	82,113,113	1.36	8 (9%)
25	CLA	C	509	3	69,73,73	1.20	8 (11%)	82,113,113	1.28	8 (9%)
25	CLA	A	608	1	58,62,73	1.27	8 (13%)	68,99,113	1.40	12 (17%)
25	CLA	a	606	36	69,73,73	1.26	6 (8%)	82,113,113	1.37	9 (10%)
30	LHG	d	408	-	48,48,48	0.69	0	51,54,54	1.26	6 (11%)
25	CLA	b	611	2	69,73,73	1.33	6 (8%)	82,113,113	1.35	9 (10%)
25	CLA	c	501	3	69,73,73	1.31	9 (13%)	82,113,113	1.38	6 (7%)
26	BCR	C	514	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	6 (10%)
32	STE	B	626	-	11,11,19	0.66	0	11,11,19	1.55	2 (18%)
32	STE	c	519	-	19,19,19	0.64	0	19,19,19	0.89	0
26	BCR	K	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	3 (5%)
25	CLA	B	609	2	69,73,73	1.24	8 (11%)	82,113,113	1.36	6 (7%)
32	STE	M	102	-	9,9,19	0.37	0	8,8,19	0.83	0
34	HEM	E	101	5,6	50,50,50	1.54	6 (12%)	67,82,82	1.15	5 (7%)
25	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.51	11 (13%)
32	STE	k	104	-	11,11,19	0.76	0	11,11,19	1.07	0
32	STE	L	102	-	11,11,19	0.67	0	11,11,19	1.19	1 (9%)
26	BCR	T	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.27	6 (10%)
25	CLA	B	615	2	69,73,73	1.29	6 (8%)	82,113,113	1.41	7 (8%)
29	SQD	b	620	-	47,49,54	1.65	9 (19%)	57,60,65	1.88	11 (19%)
29	SQD	f	102	-	39,41,54	1.65	7 (17%)	49,52,65	1.70	10 (20%)
29	SQD	a	612	-	52,54,54	1.60	7 (13%)	62,65,65	1.77	9 (14%)
25	CLA	c	513	3	69,73,73	1.20	7 (10%)	82,113,113	1.24	6 (7%)
25	CLA	A	607	36	69,73,73	1.44	8 (11%)	82,113,113	1.41	14 (17%)
32	STE	a	615	-	11,11,19	0.80	0	11,11,19	1.01	0
32	STE	m	102	-	17,17,19	0.36	0	16,16,19	0.90	0
27	PL9	a	610	-	55,55,55	0.75	0	68,69,69	1.47	11 (16%)
29	SQD	B	623	-	52,54,54	1.57	8 (15%)	62,65,65	1.56	8 (12%)
30	LHG	A	614	-	48,48,48	0.79	2 (4%)	51,54,54	1.20	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	605	2	69,73,73	1.21	6 (8%)	82,113,113	1.35	10 (12%)
25	CLA	C	506	3	69,73,73	1.23	7 (10%)	82,113,113	1.35	7 (8%)
32	STE	b	623	-	15,15,19	0.67	0	15,15,19	1.12	0
31	DGD	C	515	-	63,63,67	1.02	5 (7%)	77,77,81	1.30	10 (12%)
32	STE	t	103	-	9,9,19	0.32	0	8,8,19	0.84	0
25	CLA	A	606	1	69,73,73	1.35	8 (11%)	82,113,113	1.34	7 (8%)
25	CLA	B	604	2	69,73,73	1.45	7 (10%)	82,113,113	1.58	9 (10%)
25	CLA	B	610	36	69,73,73	1.18	7 (10%)	82,113,113	1.39	10 (12%)
25	CLA	B	613	2	69,73,73	1.34	7 (10%)	82,113,113	1.41	6 (7%)
28	LMG	D	407	-	51,51,55	0.94	3 (5%)	59,59,63	1.36	8 (13%)
21	OEY	a	601[B]	36,3,1	0,16,16	-	-	-		
26	BCR	D	405	-	41,41,41	0.99	2 (4%)	56,56,56	1.24	4 (7%)
28	LMG	c	521	-	49,49,55	0.89	3 (6%)	57,57,63	1.26	7 (12%)
31	DGD	c	515	-	63,63,67	0.99	4 (6%)	77,77,81	1.40	11 (14%)
25	CLA	B	612	2	69,73,73	1.24	8 (11%)	82,113,113	1.36	9 (10%)
32	STE	A	617	-	19,19,19	0.62	0	19,19,19	0.95	0
25	CLA	b	612	2	69,73,73	1.14	5 (7%)	82,113,113	1.37	11 (13%)
25	CLA	A	611	36	69,73,73	1.19	6 (8%)	82,113,113	1.41	7 (8%)
33	PHO	D	402	-	58,69,69	2.14	9 (15%)	55,99,99	1.48	6 (10%)
25	CLA	D	404	4	69,73,73	1.26	8 (11%)	82,113,113	1.20	4 (4%)
24	BCT	A	605	22	3,3,3	1.15	0	2,3,3	2.84	1 (50%)
25	CLA	b	609	2	69,73,73	1.27	7 (10%)	82,113,113	1.38	9 (10%)
26	BCR	b	617	-	41,41,41	1.07	3 (7%)	56,56,56	1.34	7 (12%)
34	HEM	f	101	5,6	50,50,50	1.58	11 (22%)	67,82,82	1.34	8 (11%)
25	CLA	b	607	36	69,73,73	1.10	5 (7%)	82,113,113	1.26	10 (12%)
32	STE	B	624	-	11,11,19	0.75	0	11,11,19	1.40	2 (18%)
32	STE	b	621	-	19,19,19	0.59	0	19,19,19	1.14	0
26	BCR	B	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	c	512	3	69,73,73	1.33	12 (17%)	82,113,113	1.35	7 (8%)
25	CLA	B	611	2	69,73,73	1.16	7 (10%)	82,113,113	1.40	9 (10%)
31	DGD	C	516	-	63,63,67	1.04	5 (7%)	77,77,81	1.36	10 (12%)
25	CLA	c	509	3	69,73,73	1.17	8 (11%)	82,113,113	1.47	7 (8%)
25	CLA	C	507	36	69,73,73	1.27	7 (10%)	82,113,113	1.48	9 (10%)
25	CLA	c	510	3	69,73,73	1.35	7 (10%)	82,113,113	1.26	8 (9%)
26	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.28	6 (10%)
33	PHO	d	402	-	58,69,69	2.07	10 (17%)	55,99,99	1.54	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DGD	c	516	-	63,63,67	1.03	7 (11%)	77,77,81	1.45	15 (19%)
28	LMG	m	101	-	51,51,55	0.91	3 (5%)	59,59,63	1.39	7 (11%)
32	STE	E	102	-	11,11,19	0.77	0	11,11,19	1.13	1 (9%)

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
25	CLA	B	606	2	-	14/39/115/115	-
35	HEC	v	201	16	1/1/3/7	6/14/54/54	-
25	CLA	b	610	36	-	9/39/115/115	-
28	LMG	D	411	-	-	13/33/33/70	-
29	SQD	a	613	-	-	22/37/37/69	-
25	CLA	b	616	2	-	4/33/109/115	-
25	CLA	b	615	2	-	9/39/115/115	-
25	CLA	C	504	36	-	8/32/108/115	-
25	CLA	C	511	3	-	6/39/115/115	-
31	DGD	a	614	-	-	26/45/45/95	-
25	CLA	b	608	2	-	5/39/115/115	-
25	CLA	C	502	3	-	6/39/115/115	-
32	STE	C	519	-	-	5/9/9/17	-
26	BCR	k	101	-	-	7/29/63/63	0/2/2/2
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
32	STE	C	518	-	-	5/9/9/17	-
28	LMG	B	620	-	-	14/46/66/70	0/1/1/1
31	DGD	H	102	-	-	17/51/91/95	0/2/2/2
32	STE	b	625	-	-	4/7/7/17	-
28	LMG	c	518	-	-	13/31/51/70	0/1/1/1
25	CLA	B	601	36	-	18/39/115/115	-
25	CLA	C	513	3	-	13/39/115/115	-
32	STE	B	625	-	-	5/15/15/17	-
25	CLA	c	503	3	-	13/39/115/115	-
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
32	STE	C	520	-	-	5/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	A	613	-	-	19/47/67/69	0/1/1/1
31	DGD	A	616	-	-	28/55/95/95	0/2/2/2
29	SQD	D	408	-	-	15/28/48/69	0/1/1/1
28	LMG	c	520	-	-	20/43/63/70	0/1/1/1
26	BCR	a	609	-	-	0/29/63/63	0/2/2/2
32	STE	d	413	-	-	10/17/17/17	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
25	CLA	b	601	36	-	17/39/115/115	-
30	LHG	d	407	-	-	15/53/53/53	-
25	CLA	C	510	3	-	7/39/115/115	-
30	LHG	D	410	-	-	21/51/51/53	-
32	STE	B	621	-	-	6/14/14/17	-
31	DGD	c	517	-	-	22/51/91/95	0/2/2/2
25	CLA	b	606	2	-	12/39/115/115	-
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	CLA	d	403	4	-	10/39/115/115	-
25	CLA	c	506	3	-	11/39/115/115	-
29	SQD	A	615	-	-	15/39/39/69	-
26	BCR	k	103	-	-	5/29/63/63	0/2/2/2
25	CLA	a	611	36	-	3/39/115/115	-
27	PL9	A	610	-	-	20/53/73/73	0/1/1/1
33	PHO	D	401	-	-	3/37/103/103	0/5/6/6
25	CLA	B	616	2	-	12/33/109/115	-
26	BCR	b	618	-	-	5/29/63/63	0/2/2/2
25	CLA	b	602	2	-	9/39/115/115	-
25	CLA	c	508	3	-	8/38/114/115	-
25	CLA	B	608	2	-	1/39/115/115	-
31	DGD	h	102	-	-	16/51/91/95	0/2/2/2
32	STE	B	627	-	-	7/13/13/17	-
25	CLA	D	403	4	-	7/39/115/115	-
25	CLA	c	505	3	-	9/39/115/115	-
25	CLA	a	608	1	-	8/39/115/115	-
25	CLA	B	605	2	-	10/39/115/115	-
28	LMG	C	517	-	-	18/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEC	V	201	16	1/1/3/7	6/14/54/54	-
31	DGD	J	101	-	-	15/51/91/95	0/2/2/2
32	STE	J	102	-	-	3/9/9/17	-
32	STE	b	624	-	-	10/12/12/17	-
32	STE	d	412	-	-	8/14/14/17	-
25	CLA	d	404	4	-	7/39/115/115	-
26	BCR	B	619	-	-	3/29/63/63	0/2/2/2
32	STE	t	102	-	-	7/11/11/17	-
32	STE	H	103	-	-	11/15/15/17	-
26	BCR	c	514	-	-	2/29/63/63	0/2/2/2
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2
30	LHG	d	409	-	-	13/43/43/53	-
26	BCR	K	103	-	-	7/29/63/63	0/2/2/2
32	STE	D	413	-	-	12/17/17/17	-
32	STE	j	101	-	-	5/9/9/17	-
25	CLA	C	501	3	-	5/39/115/115	-
27	PL9	D	406	-	-	10/53/73/73	0/1/1/1
28	LMG	d	410	-	-	11/17/17/70	-
25	CLA	C	505	3	-	6/39/115/115	-
28	LMG	b	622	-	-	27/50/70/70	0/1/1/1
28	LMG	d	411	-	-	15/39/59/70	0/1/1/1
25	CLA	b	604	2	-	8/39/115/115	-
25	CLA	B	603	2	-	10/39/115/115	-
25	CLA	c	511	3	-	5/39/115/115	-
25	CLA	b	603	2	-	6/39/115/115	-
25	CLA	b	613	2	-	8/39/115/115	-
26	BCR	h	101	-	-	7/29/63/63	0/2/2/2
28	LMG	B	622	-	-	12/22/22/70	-
25	CLA	C	512	3	-	10/39/115/115	-
33	PHO	a	607	-	-	4/37/103/103	0/5/6/6
28	LMG	A	612	-	-	20/43/63/70	0/1/1/1
25	CLA	C	503	3	-	7/39/115/115	-
25	CLA	c	502	3	-	10/39/115/115	-
30	LHG	D	409	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	T	102	-	-	8/13/13/17	-
25	CLA	B	614	2	-	16/39/115/115	-
30	LHG	l	101	-	-	15/53/53/53	-
27	PL9	d	406	-	-	13/53/73/73	0/1/1/1
25	CLA	c	507	36	-	10/39/115/115	-
30	LHG	D	412	-	-	14/53/53/53	-
26	BCR	d	405	-	-	7/29/63/63	0/2/2/2
25	CLA	B	607	36	-	9/39/115/115	-
25	CLA	c	504	36	-	7/33/109/115	-
30	LHG	e	101	-	-	22/46/46/53	-
25	CLA	b	614	2	-	13/39/115/115	-
26	BCR	A	609	-	-	4/29/63/63	0/2/2/2
32	STE	I	101	-	-	4/12/12/17	-
25	CLA	a	605	1	-	1/39/115/115	-
32	STE	M	101	-	-	3/12/12/17	-
30	LHG	L	101	-	-	15/53/53/53	-
25	CLA	B	602	2	-	10/39/115/115	-
25	CLA	C	509	3	-	13/39/115/115	-
25	CLA	A	608	1	-	5/26/102/115	-
25	CLA	a	606	36	-	8/39/115/115	-
30	LHG	d	408	-	-	19/53/53/53	-
25	CLA	b	611	2	-	11/39/115/115	-
25	CLA	c	501	3	-	4/39/115/115	-
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
32	STE	B	626	-	-	3/9/9/17	-
32	STE	c	519	-	-	11/17/17/17	-
26	BCR	K	102	-	-	7/29/63/63	0/2/2/2
25	CLA	B	609	2	-	7/39/115/115	-
32	STE	M	102	-	-	2/7/7/17	-
34	HEM	E	101	5,6	-	2/14/54/54	-
25	CLA	C	508	3	-	6/39/115/115	-
32	STE	k	104	-	-	4/9/9/17	-
32	STE	L	102	-	-	4/9/9/17	-
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	615	2	-	7/39/115/115	-
29	SQD	b	620	-	-	22/44/64/69	0/1/1/1
29	SQD	f	102	-	-	14/36/56/69	0/1/1/1
29	SQD	a	612	-	-	29/49/69/69	0/1/1/1
25	CLA	c	513	3	-	12/39/115/115	-
25	CLA	A	607	36	-	7/39/115/115	-
32	STE	a	615	-	-	5/9/9/17	-
32	STE	m	102	-	-	8/15/15/17	-
27	PL9	a	610	-	-	16/53/73/73	0/1/1/1
29	SQD	B	623	-	-	25/49/69/69	0/1/1/1
30	LHG	A	614	-	-	24/53/53/53	-
25	CLA	b	605	2	-	8/39/115/115	-
25	CLA	C	506	3	-	12/39/115/115	-
32	STE	b	623	-	-	9/13/13/17	-
31	DGD	C	515	-	-	17/51/91/95	0/2/2/2
32	STE	t	103	-	-	5/7/7/17	-
25	CLA	A	606	1	-	3/39/115/115	-
25	CLA	B	604	2	-	13/39/115/115	-
25	CLA	B	610	36	-	7/39/115/115	-
25	CLA	B	613	2	-	13/39/115/115	-
28	LMG	D	407	-	-	19/46/66/70	0/1/1/1
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
28	LMG	c	521	-	-	27/44/64/70	0/1/1/1
31	DGD	c	515	-	-	27/51/91/95	0/2/2/2
25	CLA	B	612	2	-	10/39/115/115	-
32	STE	A	617	-	-	10/17/17/17	-
25	CLA	b	612	2	-	12/39/115/115	-
25	CLA	A	611	36	-	4/39/115/115	-
33	PHO	D	402	-	-	1/37/103/103	0/5/6/6
25	CLA	D	404	4	-	9/39/115/115	-
25	CLA	b	609	2	-	12/39/115/115	-
26	BCR	b	617	-	-	4/29/63/63	0/2/2/2
34	HEM	f	101	5,6	-	2/14/54/54	-
25	CLA	b	607	36	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	B	624	-	-	5/9/9/17	-
32	STE	b	621	-	-	11/17/17/17	-
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	CLA	c	512	3	-	16/39/115/115	-
25	CLA	B	611	2	-	2/39/115/115	-
31	DGD	C	516	-	-	17/51/91/95	0/2/2/2
25	CLA	c	509	3	-	13/39/115/115	-
25	CLA	C	507	36	-	9/39/115/115	-
25	CLA	c	510	3	-	11/39/115/115	-
26	BCR	t	101	-	-	4/29/63/63	0/2/2/2
33	PHO	d	402	-	-	11/37/103/103	0/5/6/6
31	DGD	c	516	-	-	23/51/91/95	0/2/2/2
28	LMG	m	101	-	-	24/46/66/70	0/1/1/1
32	STE	E	102	-	-	5/9/9/17	-

All (797) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	402	PHO	C1B-C2B	9.21	1.49	1.39
33	d	402	PHO	C1B-C2B	9.12	1.49	1.39
33	D	402	PHO	C3B-C4B	8.87	1.50	1.41
33	a	607	PHO	C1B-C2B	8.76	1.49	1.39
33	d	402	PHO	C3B-C4B	8.22	1.49	1.41
35	v	201	HEC	C3D-C2D	7.84	1.53	1.36
33	D	401	PHO	C1B-C2B	7.69	1.48	1.39
33	a	607	PHO	C3B-C4B	7.32	1.48	1.41
35	V	201	HEC	C3D-C2D	7.23	1.52	1.36
33	D	401	PHO	C3B-C4B	7.22	1.48	1.41
25	c	511	CLA	MG-NA	7.01	2.22	2.06
25	C	501	CLA	MG-NA	6.92	2.22	2.06
25	b	615	CLA	MG-NA	6.89	2.22	2.06
25	b	611	CLA	MG-NA	6.48	2.21	2.06
25	a	611	CLA	MG-NA	6.31	2.21	2.06
25	B	606	CLA	MG-NA	6.30	2.21	2.06
25	B	604	CLA	MG-NA	6.17	2.20	2.06
25	B	603	CLA	MG-NA	6.15	2.20	2.06
25	b	614	CLA	MG-NA	5.81	2.20	2.06
25	c	510	CLA	MG-NA	5.64	2.19	2.06
25	b	601	CLA	MG-NA	5.56	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	MG-NC	5.56	2.19	2.06
25	C	513	CLA	MG-NA	5.55	2.19	2.06
25	b	606	CLA	MG-NA	5.38	2.19	2.06
25	C	512	CLA	MG-NA	5.32	2.18	2.06
29	A	615	SQD	O47-C45	-5.32	1.37	1.47
25	A	607	CLA	MG-NA	5.31	2.18	2.06
25	C	511	CLA	MG-NA	5.21	2.18	2.06
35	V	201	HEC	FE-ND	5.14	2.10	1.94
29	a	612	SQD	O48-C23	5.04	1.48	1.33
29	b	620	SQD	O48-C23	4.92	1.47	1.33
25	C	507	CLA	MG-NA	4.82	2.17	2.06
25	a	605	CLA	MG-NA	4.77	2.17	2.06
29	D	408	SQD	O48-C23	4.76	1.47	1.33
33	D	402	PHO	C1D-C2D	4.74	1.44	1.39
25	A	607	CLA	MG-NB	-4.72	1.96	2.05
29	A	615	SQD	O48-C23	4.72	1.47	1.33
25	c	506	CLA	MG-ND	-4.70	1.96	2.05
25	c	501	CLA	MG-ND	-4.70	1.96	2.05
29	B	623	SQD	O48-C23	4.70	1.47	1.33
34	E	101	HEM	FE-NB	4.68	2.09	1.94
29	a	613	SQD	O48-C23	4.67	1.47	1.33
25	b	609	CLA	MG-NA	4.67	2.17	2.06
34	E	101	HEM	FE-NA	4.62	2.10	1.95
33	a	607	PHO	C1D-C2D	4.62	1.44	1.39
29	f	102	SQD	O48-C23	4.61	1.46	1.33
25	b	603	CLA	MG-NA	4.56	2.17	2.06
25	c	502	CLA	MG-NB	-4.53	1.96	2.05
25	B	601	CLA	MG-NA	4.51	2.17	2.06
25	b	610	CLA	MG-NB	-4.51	1.96	2.05
35	v	201	HEC	FE-NA	4.49	2.10	1.95
25	B	615	CLA	MG-NA	4.47	2.16	2.06
29	A	613	SQD	O48-C23	4.44	1.46	1.33
25	b	604	CLA	C1D-ND	4.37	1.43	1.37
25	C	504	CLA	MG-ND	-4.33	1.97	2.05
25	C	503	CLA	MG-NA	4.32	2.16	2.06
25	B	604	CLA	C1D-ND	4.30	1.43	1.37
25	A	606	CLA	MG-NA	4.30	2.16	2.06
34	f	101	HEM	FE-NB	4.28	2.08	1.94
25	b	608	CLA	MG-NA	4.27	2.16	2.06
34	f	101	HEM	FE-NA	4.23	2.09	1.95
25	b	613	CLA	MG-NA	4.21	2.16	2.06
25	B	609	CLA	MG-NC	4.21	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	FE-ND	4.17	2.07	1.94
25	B	614	CLA	MG-ND	-4.17	1.97	2.05
25	A	606	CLA	MG-NB	4.16	2.14	2.05
25	c	507	CLA	MG-NA	4.15	2.16	2.06
25	a	605	CLA	C1D-ND	4.09	1.43	1.37
25	C	501	CLA	C1D-ND	4.07	1.43	1.37
25	B	613	CLA	MG-ND	-4.06	1.97	2.05
25	B	604	CLA	MG-NC	4.01	2.15	2.06
25	a	606	CLA	MG-NB	3.99	2.13	2.05
25	B	612	CLA	MG-ND	-3.98	1.97	2.05
25	c	506	CLA	MG-NC	3.98	2.15	2.06
25	B	601	CLA	C1D-ND	3.97	1.43	1.37
25	B	614	CLA	MG-NC	3.97	2.15	2.06
33	d	402	PHO	C1D-C2D	3.96	1.43	1.39
25	D	403	CLA	MG-NC	3.95	2.15	2.06
25	A	607	CLA	C1D-ND	3.94	1.43	1.37
25	a	608	CLA	C1D-ND	3.93	1.43	1.37
25	c	504	CLA	MG-ND	-3.92	1.98	2.05
25	B	613	CLA	C1D-ND	3.92	1.43	1.37
29	A	613	SQD	O47-C45	-3.91	1.37	1.46
25	b	604	CLA	MG-ND	-3.90	1.98	2.05
25	D	404	CLA	C1D-ND	3.90	1.43	1.37
25	C	513	CLA	MG-ND	3.90	2.13	2.05
25	C	504	CLA	MG-NB	3.89	2.13	2.05
25	B	614	CLA	C1D-ND	3.88	1.43	1.37
25	c	508	CLA	MG-NA	3.88	2.15	2.06
25	B	616	CLA	C1D-ND	3.87	1.42	1.37
25	C	510	CLA	MG-NB	3.87	2.13	2.05
33	a	607	PHO	C4D-CHA	3.87	1.45	1.39
25	c	504	CLA	MG-NC	3.85	2.15	2.06
25	c	505	CLA	MG-NB	3.84	2.13	2.05
25	b	612	CLA	C1D-ND	3.82	1.42	1.37
25	C	508	CLA	MG-NA	3.81	2.15	2.06
30	D	412	LHG	O7-C5	-3.80	1.37	1.46
25	B	609	CLA	C1D-ND	3.80	1.42	1.37
26	B	618	BCR	C30-C25	-3.79	1.48	1.53
25	A	606	CLA	C1D-ND	3.79	1.42	1.37
25	C	503	CLA	MG-ND	3.79	2.13	2.05
25	C	507	CLA	MG-NB	3.77	2.13	2.05
33	D	401	PHO	C4D-CHA	3.75	1.45	1.39
25	b	614	CLA	C1D-ND	3.74	1.42	1.37
25	c	511	CLA	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	611	CLA	C1D-ND	3.73	1.42	1.37
25	a	608	CLA	MG-ND	-3.73	1.98	2.05
25	C	504	CLA	C4B-NB	3.72	1.42	1.37
25	B	611	CLA	MG-NA	3.72	2.15	2.06
25	c	512	CLA	C1D-ND	3.72	1.42	1.37
26	k	101	BCR	C30-C25	-3.71	1.49	1.53
25	b	610	CLA	C1D-ND	3.69	1.42	1.37
25	B	614	CLA	C4B-NB	3.68	1.42	1.37
25	a	605	CLA	MG-NC	3.68	2.15	2.06
25	B	608	CLA	MG-NA	3.68	2.15	2.06
25	C	511	CLA	C1D-ND	3.67	1.42	1.37
25	B	605	CLA	C1D-ND	3.66	1.42	1.37
35	V	201	HEC	FE-NC	3.65	2.07	1.95
25	B	610	CLA	C4B-NB	3.65	1.42	1.37
25	C	503	CLA	MG-NC	3.65	2.14	2.06
25	c	501	CLA	C1D-ND	3.64	1.42	1.37
25	b	616	CLA	MG-ND	3.63	2.13	2.05
26	K	102	BCR	C1-C6	-3.63	1.49	1.53
26	c	514	BCR	C1-C6	-3.61	1.49	1.53
29	a	612	SQD	O47-C45	-3.61	1.38	1.46
26	C	514	BCR	C1-C6	-3.60	1.49	1.53
25	B	601	CLA	C4B-NB	3.60	1.42	1.37
25	C	510	CLA	MG-NA	3.60	2.14	2.06
25	c	503	CLA	C1D-ND	3.59	1.42	1.37
25	B	602	CLA	C1D-ND	3.59	1.42	1.37
29	b	620	SQD	O47-C7	3.57	1.44	1.34
25	A	611	CLA	MG-NA	3.56	2.14	2.06
25	b	602	CLA	C1D-ND	3.56	1.42	1.37
29	A	615	SQD	O47-C7	3.56	1.44	1.34
25	b	613	CLA	C1D-ND	3.55	1.42	1.37
26	b	618	BCR	C30-C25	-3.54	1.49	1.53
29	B	623	SQD	O47-C7	3.54	1.44	1.34
25	c	509	CLA	C1D-ND	3.54	1.42	1.37
25	C	505	CLA	C1D-ND	3.53	1.42	1.37
29	a	613	SQD	O47-C45	-3.50	1.38	1.46
29	f	102	SQD	O47-C7	3.50	1.44	1.34
25	c	507	CLA	C1D-ND	3.49	1.42	1.37
25	b	605	CLA	C4B-NB	3.48	1.42	1.37
25	c	503	CLA	MG-NA	3.48	2.14	2.06
25	b	614	CLA	C4B-NB	3.48	1.42	1.37
35	v	201	HEC	FE-ND	3.47	2.05	1.94
25	B	606	CLA	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	C4B-NB	3.47	1.42	1.37
25	C	506	CLA	C1D-ND	3.46	1.42	1.37
25	a	606	CLA	C1D-ND	3.46	1.42	1.37
25	A	607	CLA	C4B-NB	3.45	1.42	1.37
25	b	606	CLA	C1D-ND	3.45	1.42	1.37
25	B	615	CLA	C4B-NB	3.45	1.42	1.37
25	B	606	CLA	C4B-NB	3.45	1.42	1.37
30	D	410	LHG	P-O6	3.45	1.72	1.59
25	b	602	CLA	MG-NC	3.44	2.14	2.06
25	b	601	CLA	C1D-ND	3.43	1.42	1.37
26	K	103	BCR	C1-C6	-3.43	1.49	1.53
25	C	509	CLA	MG-NB	-3.43	1.99	2.05
29	D	408	SQD	C24-C23	3.42	1.60	1.50
25	c	513	CLA	C1D-ND	3.42	1.42	1.37
25	d	404	CLA	C1D-ND	3.42	1.42	1.37
25	B	615	CLA	C1D-ND	3.42	1.42	1.37
27	D	406	PL9	C6-C1	-3.42	1.42	1.48
25	C	513	CLA	C1D-ND	3.41	1.42	1.37
25	B	603	CLA	C1D-ND	3.41	1.42	1.37
25	c	512	CLA	MG-NC	3.41	2.14	2.06
25	a	611	CLA	C1D-ND	3.40	1.42	1.37
33	d	402	PHO	C4D-CHA	3.40	1.44	1.39
29	a	612	SQD	O47-C7	3.40	1.43	1.34
25	c	504	CLA	C4B-NB	3.39	1.42	1.37
31	H	102	DGD	O5D-C1E	3.39	1.45	1.40
25	d	403	CLA	MG-NC	3.39	2.14	2.06
26	b	617	BCR	C1-C6	-3.39	1.49	1.53
25	C	504	CLA	C1D-ND	3.38	1.42	1.37
25	b	615	CLA	C1D-ND	3.37	1.42	1.37
26	k	103	BCR	C1-C6	-3.36	1.49	1.53
25	b	616	CLA	C1B-C2B	3.36	1.51	1.43
25	c	512	CLA	C4B-NB	3.36	1.42	1.37
25	C	512	CLA	C1D-ND	3.35	1.42	1.37
25	b	601	CLA	C4B-NB	3.35	1.42	1.37
29	f	102	SQD	O47-C45	-3.35	1.38	1.46
25	b	616	CLA	C1D-ND	3.34	1.42	1.37
25	d	403	CLA	C1D-ND	3.34	1.42	1.37
29	B	623	SQD	O47-C45	-3.33	1.38	1.46
25	c	510	CLA	C1D-ND	3.33	1.42	1.37
25	C	508	CLA	C1D-ND	3.32	1.42	1.37
25	b	609	CLA	C1D-ND	3.32	1.42	1.37
25	A	606	CLA	C1B-C2B	3.32	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	613	SQD	O47-C7	3.31	1.43	1.34
25	B	605	CLA	MG-NB	3.31	2.12	2.05
25	c	505	CLA	C4B-NB	3.31	1.42	1.37
25	a	605	CLA	CHC-C1C	3.30	1.45	1.38
35	v	201	HEC	FE-NB	3.30	2.05	1.94
25	C	504	CLA	MG-NA	3.29	2.14	2.06
29	b	620	SQD	O5-C1	3.28	1.50	1.41
26	d	405	BCR	C30-C25	-3.27	1.49	1.53
25	b	603	CLA	C1D-ND	3.27	1.42	1.37
26	k	102	BCR	C1-C6	-3.26	1.49	1.53
25	b	609	CLA	C4B-NB	3.26	1.42	1.37
25	b	605	CLA	CHC-C1C	3.25	1.45	1.38
25	a	611	CLA	MG-NB	3.24	2.12	2.05
25	c	508	CLA	MG-NB	3.24	2.12	2.05
25	c	505	CLA	MG-NC	3.24	2.14	2.06
25	C	509	CLA	C1D-ND	3.23	1.42	1.37
33	D	402	PHO	C4D-CHA	3.23	1.44	1.39
25	C	506	CLA	C4B-NB	3.23	1.42	1.37
33	D	401	PHO	C1D-C2D	3.21	1.43	1.39
25	c	502	CLA	C1D-ND	3.21	1.42	1.37
29	a	612	SQD	C24-C23	3.21	1.60	1.50
26	B	618	BCR	C1-C6	-3.19	1.49	1.53
26	b	617	BCR	C30-C25	-3.19	1.49	1.53
25	C	501	CLA	C4B-NB	3.19	1.42	1.37
29	A	613	SQD	O47-C7	3.18	1.43	1.34
25	b	605	CLA	C1B-C2B	3.17	1.50	1.43
34	f	101	HEM	CAC-C3C	3.17	1.55	1.47
25	B	607	CLA	C1D-ND	3.17	1.42	1.37
29	a	613	SQD	C24-C23	3.17	1.59	1.50
25	c	506	CLA	C1D-ND	3.16	1.42	1.37
29	A	615	SQD	C24-C23	3.16	1.59	1.50
25	b	604	CLA	MG-NA	3.16	2.13	2.06
26	H	101	BCR	C30-C25	-3.16	1.49	1.53
26	B	617	BCR	C1-C6	-3.15	1.49	1.53
25	B	607	CLA	MG-ND	-3.14	1.99	2.05
25	c	508	CLA	C1D-ND	3.13	1.42	1.37
25	B	615	CLA	C1B-C2B	3.12	1.50	1.43
25	B	610	CLA	MG-NB	-3.12	1.99	2.05
25	c	502	CLA	MG-NA	3.12	2.13	2.06
25	b	611	CLA	C1D-ND	3.11	1.41	1.37
26	h	101	BCR	C30-C25	-3.10	1.49	1.53
25	D	404	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	101	HEM	FE-NC	3.10	2.05	1.95
25	C	505	CLA	MG-NA	3.10	2.13	2.06
26	K	102	BCR	C30-C25	-3.10	1.49	1.53
25	d	404	CLA	MG-NC	3.10	2.13	2.06
25	b	606	CLA	C1B-C2B	3.10	1.50	1.43
25	c	503	CLA	MG-NC	3.09	2.13	2.06
25	c	508	CLA	C4B-NB	3.09	1.41	1.37
28	d	411	LMG	O7-C8	-3.09	1.39	1.46
25	c	506	CLA	C4B-NB	3.08	1.41	1.37
25	B	611	CLA	C1D-ND	3.08	1.41	1.37
29	A	613	SQD	C24-C23	3.08	1.59	1.50
25	a	605	CLA	C1B-C2B	3.08	1.50	1.43
25	a	606	CLA	C4B-NB	3.06	1.41	1.37
25	c	512	CLA	C1B-C2B	3.05	1.50	1.43
25	a	608	CLA	C4B-NB	3.05	1.41	1.37
31	c	515	DGD	O2G-C2G	-3.05	1.39	1.46
25	D	403	CLA	C1B-C2B	3.05	1.50	1.43
29	A	613	SQD	O5-C1	3.04	1.49	1.41
25	d	404	CLA	C4B-NB	3.04	1.41	1.37
25	B	612	CLA	C1D-ND	3.04	1.41	1.37
31	c	517	DGD	C4D-C5D	3.03	1.59	1.53
25	b	601	CLA	C1B-C2B	3.03	1.50	1.43
25	c	508	CLA	C1B-C2B	3.03	1.50	1.43
25	c	509	CLA	MG-NA	3.03	2.13	2.06
25	b	608	CLA	C1D-ND	3.03	1.41	1.37
34	E	101	HEM	CAC-C3C	3.03	1.55	1.47
25	B	608	CLA	C1D-ND	3.03	1.41	1.37
26	K	103	BCR	C30-C25	-3.03	1.49	1.53
26	K	101	BCR	C1-C6	-3.01	1.49	1.53
30	A	614	LHG	P-O6	3.01	1.71	1.59
25	c	511	CLA	C4B-NB	3.01	1.41	1.37
25	B	611	CLA	C1B-C2B	3.00	1.50	1.43
25	b	615	CLA	C4B-NB	3.00	1.41	1.37
25	c	505	CLA	C3B-C4B	2.99	1.51	1.42
25	c	507	CLA	C1B-C2B	2.98	1.50	1.43
25	C	511	CLA	C1B-C2B	2.98	1.50	1.43
25	c	508	CLA	CHC-C1C	2.98	1.44	1.38
26	b	618	BCR	C1-C6	-2.97	1.50	1.53
25	d	404	CLA	MG-ND	-2.97	1.99	2.05
26	K	101	BCR	C30-C25	-2.97	1.50	1.53
25	A	608	CLA	C4B-NB	2.97	1.41	1.37
31	C	516	DGD	C1E-C2E	2.97	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	623	SQD	O5-C1	2.97	1.49	1.41
25	c	509	CLA	C1B-C2B	2.96	1.50	1.43
29	f	102	SQD	C24-C23	2.96	1.59	1.50
26	k	102	BCR	C30-C25	-2.96	1.50	1.53
25	b	614	CLA	CHC-C1C	2.96	1.44	1.38
25	b	610	CLA	C1B-C2B	2.96	1.50	1.43
25	b	611	CLA	C1B-C2B	2.95	1.50	1.43
25	a	608	CLA	C1B-C2B	2.95	1.50	1.43
25	b	608	CLA	C4B-NB	2.95	1.41	1.37
25	c	511	CLA	C1B-C2B	2.94	1.50	1.43
25	B	610	CLA	C1D-ND	2.94	1.41	1.37
29	a	612	SQD	O5-C1	2.94	1.49	1.41
25	C	503	CLA	C1D-ND	2.94	1.41	1.37
25	A	606	CLA	C4B-NB	2.93	1.41	1.37
25	C	502	CLA	C1D-ND	2.93	1.41	1.37
26	A	609	BCR	C1-C6	-2.93	1.50	1.53
30	l	101	LHG	O7-C5	-2.93	1.39	1.46
26	t	101	BCR	C30-C25	-2.93	1.50	1.53
25	B	603	CLA	C1B-C2B	2.93	1.50	1.43
25	b	608	CLA	C1B-C2B	2.93	1.50	1.43
25	C	506	CLA	MG-NC	2.92	2.13	2.06
25	C	507	CLA	C1B-C2B	2.92	1.50	1.43
31	A	616	DGD	C4D-C5D	2.92	1.59	1.53
25	B	601	CLA	C1B-C2B	2.92	1.50	1.43
25	a	605	CLA	MG-NB	2.92	2.11	2.05
25	c	503	CLA	C4B-NB	2.92	1.41	1.37
25	A	608	CLA	MG-ND	2.91	2.11	2.05
25	B	616	CLA	C1B-C2B	2.91	1.50	1.43
25	B	605	CLA	CHC-C1C	2.91	1.44	1.38
26	k	101	BCR	C1-C6	-2.91	1.50	1.53
25	b	603	CLA	C4B-NB	2.91	1.41	1.37
34	E	101	HEM	CAB-C3B	2.90	1.55	1.47
25	B	616	CLA	MG-NA	2.90	2.13	2.06
25	c	504	CLA	C1D-ND	2.90	1.41	1.37
28	b	622	LMG	C4-C3	2.90	1.59	1.52
25	C	509	CLA	C4B-NB	2.90	1.41	1.37
25	D	403	CLA	C4B-NB	2.90	1.41	1.37
29	b	620	SQD	O47-C45	-2.90	1.39	1.46
31	c	515	DGD	O1G-C1G	-2.89	1.38	1.45
25	b	615	CLA	C1B-C2B	2.89	1.49	1.43
25	C	510	CLA	C1B-C2B	2.89	1.49	1.43
25	b	607	CLA	C1D-ND	2.88	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	623	SQD	C24-C23	2.88	1.59	1.50
25	b	602	CLA	C1B-C2B	2.87	1.49	1.43
26	D	405	BCR	C30-C25	-2.87	1.50	1.53
25	C	508	CLA	C1B-C2B	2.87	1.49	1.43
25	d	403	CLA	C1B-C2B	2.86	1.49	1.43
29	b	620	SQD	C24-C23	2.86	1.59	1.50
25	c	505	CLA	C1D-ND	2.86	1.41	1.37
25	B	602	CLA	C1B-C2B	2.86	1.49	1.43
25	b	601	CLA	MG-ND	2.86	2.11	2.05
31	h	102	DGD	C4D-C5D	2.85	1.59	1.53
25	C	510	CLA	C1D-ND	2.85	1.41	1.37
25	c	501	CLA	C1B-C2B	2.85	1.49	1.43
25	C	502	CLA	C1B-C2B	2.85	1.49	1.43
25	b	605	CLA	C3B-C4B	2.84	1.51	1.42
30	d	407	LHG	C24-C23	2.84	1.59	1.50
25	c	505	CLA	C1B-C2B	2.84	1.49	1.43
25	b	616	CLA	MG-NA	2.83	2.13	2.06
25	b	604	CLA	MG-NC	2.83	2.13	2.06
25	a	611	CLA	C1B-C2B	2.82	1.49	1.43
26	B	619	BCR	C1-C6	-2.82	1.50	1.53
25	B	608	CLA	C4B-NB	2.82	1.41	1.37
25	b	602	CLA	C4B-NB	2.82	1.41	1.37
29	f	102	SQD	O5-C1	2.81	1.49	1.41
25	C	505	CLA	CHC-C1C	2.81	1.44	1.38
25	B	612	CLA	C4B-NB	2.81	1.41	1.37
25	C	509	CLA	C1B-C2B	2.81	1.49	1.43
25	c	510	CLA	C1B-C2B	2.81	1.49	1.43
25	C	501	CLA	MG-ND	-2.80	2.00	2.05
25	C	511	CLA	C4B-NB	2.80	1.41	1.37
25	c	513	CLA	C4B-NB	2.80	1.41	1.37
25	D	403	CLA	C1D-ND	2.80	1.41	1.37
25	C	507	CLA	C1D-ND	2.80	1.41	1.37
25	B	605	CLA	C3B-C4B	2.79	1.50	1.42
25	C	503	CLA	C1B-C2B	2.79	1.49	1.43
25	d	403	CLA	C4B-NB	2.79	1.41	1.37
25	C	513	CLA	C4B-NB	2.79	1.41	1.37
25	c	513	CLA	C1B-C2B	2.78	1.49	1.43
26	d	405	BCR	C1-C6	-2.78	1.50	1.53
31	C	515	DGD	C4E-C3E	2.78	1.59	1.52
25	c	505	CLA	CHC-C1C	2.77	1.44	1.38
25	d	404	CLA	C1B-C2B	2.77	1.49	1.43
25	D	404	CLA	MG-NA	2.77	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	MG-NB	2.77	2.11	2.05
31	H	102	DGD	C6D-C5D	2.77	1.59	1.51
25	c	509	CLA	C4B-NB	2.77	1.41	1.37
25	b	609	CLA	C1B-C2B	2.77	1.49	1.43
25	C	508	CLA	C4B-NB	2.77	1.41	1.37
25	C	508	CLA	C3B-C4B	2.76	1.50	1.42
33	D	401	PHO	C4D-ND	-2.76	1.34	1.38
25	c	513	CLA	MG-NA	2.75	2.12	2.06
25	C	513	CLA	C3B-C4B	2.75	1.50	1.42
33	a	607	PHO	CMC-C2C	-2.74	1.46	1.50
25	C	505	CLA	C1B-C2B	2.74	1.49	1.43
25	c	507	CLA	C4B-NB	2.74	1.41	1.37
25	c	510	CLA	CHC-C1C	2.74	1.44	1.38
25	b	605	CLA	MG-ND	2.74	2.11	2.05
28	D	407	LMG	C4-C5	2.73	1.58	1.53
25	C	501	CLA	CHC-C1C	2.73	1.44	1.38
26	a	609	BCR	C1-C6	-2.73	1.50	1.53
25	C	512	CLA	C4B-NB	2.73	1.41	1.37
33	D	402	PHO	C3D-C4D	2.73	1.44	1.41
25	C	506	CLA	CHC-C1C	2.72	1.43	1.38
25	B	606	CLA	C1B-C2B	2.72	1.49	1.43
26	T	101	BCR	C1-C6	-2.72	1.50	1.53
31	C	516	DGD	O2G-C2G	-2.72	1.40	1.46
30	d	409	LHG	P-O6	2.71	1.70	1.59
25	B	604	CLA	C1B-C2B	2.71	1.49	1.43
26	T	101	BCR	C30-C25	-2.71	1.50	1.53
30	l	101	LHG	O8-C23	2.71	1.41	1.33
25	C	513	CLA	C1B-C2B	2.70	1.49	1.43
33	D	401	PHO	C3D-C4D	2.70	1.44	1.41
25	c	510	CLA	C4B-NB	2.70	1.41	1.37
25	A	608	CLA	C1B-C2B	2.70	1.49	1.43
25	B	608	CLA	MG-NB	-2.69	2.00	2.05
25	b	614	CLA	C1B-C2B	2.69	1.49	1.43
25	c	508	CLA	C3B-C4B	2.69	1.50	1.42
34	f	101	HEM	CAB-C3B	2.69	1.54	1.47
26	b	619	BCR	C1-C6	-2.69	1.50	1.53
25	D	404	CLA	C1B-C2B	2.69	1.49	1.43
25	B	605	CLA	C1B-C2B	2.69	1.49	1.43
26	a	609	BCR	C30-C25	-2.68	1.50	1.53
25	C	506	CLA	C1B-C2B	2.68	1.49	1.43
33	d	402	PHO	CMD-C2D	-2.68	1.46	1.51
25	B	605	CLA	C4B-NB	2.68	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	620	LMG	C4-C5	2.67	1.58	1.53
25	b	613	CLA	C4B-NB	2.67	1.41	1.37
25	A	607	CLA	C1B-C2B	2.67	1.49	1.43
25	b	612	CLA	C3B-C4B	2.67	1.50	1.42
25	C	503	CLA	C4B-NB	2.67	1.41	1.37
25	a	611	CLA	C3B-C4B	2.66	1.50	1.42
25	C	504	CLA	C3B-C4B	2.66	1.50	1.42
25	c	501	CLA	C4B-NB	2.66	1.41	1.37
25	c	513	CLA	CHC-C1C	2.66	1.43	1.38
25	B	612	CLA	MG-NA	2.66	2.12	2.06
25	C	505	CLA	C4B-NB	2.65	1.41	1.37
33	a	607	PHO	CAC-C3C	-2.65	1.47	1.51
25	a	605	CLA	C4B-NB	2.64	1.41	1.37
25	C	512	CLA	C1B-C2B	2.64	1.49	1.43
31	c	517	DGD	C6D-C5D	2.64	1.59	1.51
25	c	506	CLA	C1B-C2B	2.64	1.49	1.43
25	c	506	CLA	CHC-C1C	2.64	1.43	1.38
25	C	506	CLA	MG-NA	2.64	2.12	2.06
25	a	606	CLA	CHC-C1C	2.63	1.43	1.38
25	B	613	CLA	C1B-C2B	2.62	1.49	1.43
28	m	101	LMG	C4-C5	2.62	1.58	1.53
25	B	608	CLA	C1B-C2B	2.62	1.49	1.43
25	b	608	CLA	CHC-C1C	2.62	1.43	1.38
25	c	511	CLA	CHC-C1C	2.62	1.43	1.38
25	b	611	CLA	C4B-NB	2.62	1.41	1.37
28	c	518	LMG	C4-C5	2.61	1.58	1.53
25	B	610	CLA	C1B-C2B	2.61	1.49	1.43
25	c	504	CLA	C1B-C2B	2.61	1.49	1.43
25	b	601	CLA	CHC-C1C	2.61	1.43	1.38
28	D	407	LMG	O2-C2	-2.61	1.36	1.43
25	b	615	CLA	C3B-C4B	2.60	1.50	1.42
25	B	614	CLA	CHC-C1C	2.60	1.43	1.38
25	B	603	CLA	C4B-NB	2.60	1.41	1.37
25	C	504	CLA	C1B-C2B	2.60	1.49	1.43
25	c	503	CLA	C1B-C2B	2.60	1.49	1.43
25	C	512	CLA	C3B-C4B	2.60	1.50	1.42
25	B	609	CLA	C1B-C2B	2.60	1.49	1.43
35	v	201	HEC	FE-NC	2.59	2.03	1.95
25	b	612	CLA	C1B-C2B	2.59	1.49	1.43
25	A	611	CLA	C1B-C2B	2.58	1.49	1.43
31	C	516	DGD	C1G-C2G	2.58	1.58	1.50
25	a	606	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	616	CLA	C4B-NB	2.57	1.41	1.37
33	a	607	PHO	C3D-C4D	2.57	1.44	1.41
25	B	612	CLA	C1B-C2B	2.57	1.49	1.43
25	C	501	CLA	C3B-C4B	2.57	1.50	1.42
25	C	512	CLA	CHC-C1C	2.57	1.43	1.38
25	b	614	CLA	C3B-C4B	2.56	1.50	1.42
25	C	504	CLA	CHC-C1C	2.56	1.43	1.38
25	c	513	CLA	C3B-C4B	2.56	1.50	1.42
25	D	404	CLA	MG-NB	-2.56	2.00	2.05
29	D	408	SQD	O5-C1	2.55	1.48	1.41
25	B	616	CLA	C4B-NB	2.54	1.41	1.37
30	e	101	LHG	P-O6	2.54	1.69	1.59
25	c	512	CLA	C3B-C4B	2.54	1.50	1.42
28	B	622	LMG	O8-C28	2.53	1.39	1.30
26	c	514	BCR	C30-C25	-2.53	1.50	1.53
25	c	502	CLA	C1B-C2B	2.53	1.49	1.43
29	A	615	SQD	C46-C45	2.53	1.56	1.50
25	A	606	CLA	CHC-C1C	2.53	1.43	1.38
25	b	603	CLA	C1B-C2B	2.52	1.49	1.43
25	C	506	CLA	C3B-C4B	2.51	1.50	1.42
26	b	619	BCR	C30-C25	-2.51	1.50	1.53
31	A	616	DGD	C4D-C3D	2.51	1.58	1.52
33	D	401	PHO	CMC-C2C	-2.51	1.46	1.50
25	a	608	CLA	C3B-C4B	2.51	1.50	1.42
25	A	608	CLA	CHC-C1C	2.50	1.43	1.38
25	c	506	CLA	C3B-C4B	2.50	1.50	1.42
25	b	607	CLA	C4B-NB	2.50	1.41	1.37
25	C	509	CLA	C3B-C4B	2.49	1.50	1.42
25	d	403	CLA	CMB-C2B	-2.49	1.45	1.50
25	b	605	CLA	C1D-ND	2.49	1.41	1.37
28	B	622	LMG	O7-C10	2.49	1.39	1.30
28	c	520	LMG	C4-C3	2.48	1.58	1.52
25	b	601	CLA	C3B-C4B	2.48	1.49	1.42
25	B	607	CLA	C1B-C2B	2.48	1.48	1.43
25	a	606	CLA	C3B-C4B	2.48	1.49	1.42
28	b	622	LMG	C3-C2	2.47	1.58	1.52
25	b	606	CLA	C4B-NB	2.47	1.41	1.37
25	b	607	CLA	C1B-C2B	2.47	1.48	1.43
25	c	508	CLA	MG-NC	2.47	2.12	2.06
25	B	603	CLA	C3B-C4B	2.46	1.49	1.42
25	a	605	CLA	C3B-C4B	2.46	1.49	1.42
25	B	613	CLA	C4B-NB	2.46	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	MG-NC	2.46	2.12	2.06
25	c	510	CLA	C3B-C4B	2.46	1.49	1.42
25	B	601	CLA	C3B-C4B	2.46	1.49	1.42
25	C	503	CLA	CHC-C1C	2.46	1.43	1.38
31	a	614	DGD	O1G-C1A	2.46	1.40	1.33
25	c	512	CLA	CHC-C1C	2.45	1.43	1.38
33	D	401	PHO	O2D-CGD	2.44	1.39	1.33
25	b	612	CLA	CHC-C1C	2.44	1.43	1.38
25	C	501	CLA	C1B-C2B	2.44	1.48	1.43
25	C	508	CLA	C1D-C2D	2.44	1.50	1.45
25	C	502	CLA	MG-NA	2.44	2.12	2.06
31	h	102	DGD	O2E-C2E	-2.43	1.36	1.43
25	c	502	CLA	C4B-NB	2.43	1.41	1.37
25	d	403	CLA	C3B-C4B	2.42	1.49	1.42
30	D	409	LHG	P-O3	2.42	1.68	1.59
33	d	402	PHO	C3D-C4D	2.42	1.44	1.41
25	b	602	CLA	C3B-C4B	2.41	1.49	1.42
25	A	611	CLA	CHC-C1C	2.41	1.43	1.38
25	C	508	CLA	MG-NB	2.41	2.10	2.05
25	B	616	CLA	CMC-C2C	-2.41	1.45	1.50
25	B	614	CLA	MG-NA	2.41	2.12	2.06
33	a	607	PHO	CMB-C2B	-2.41	1.46	1.51
25	C	510	CLA	MG-ND	-2.40	2.01	2.05
25	D	404	CLA	CMD-C2D	-2.40	1.45	1.50
31	a	614	DGD	C3G-C2G	2.40	1.56	1.51
25	C	511	CLA	MG-NC	2.40	2.12	2.06
29	f	102	SQD	O7-S	2.40	1.51	1.45
25	b	610	CLA	C3B-C4B	2.40	1.49	1.42
25	D	403	CLA	C3B-C4B	2.40	1.49	1.42
28	D	407	LMG	C4-C3	2.40	1.58	1.52
25	B	607	CLA	MG-NA	2.40	2.12	2.06
25	c	501	CLA	MG-NA	2.39	2.12	2.06
28	d	411	LMG	C4-C5	2.39	1.58	1.53
31	A	616	DGD	C3E-C2E	2.39	1.58	1.52
25	b	603	CLA	C3B-C4B	2.39	1.49	1.42
28	b	622	LMG	C9-C8	2.39	1.58	1.50
26	D	405	BCR	C1-C6	-2.39	1.50	1.53
25	b	608	CLA	C3B-C4B	2.39	1.49	1.42
25	B	604	CLA	CHC-C1C	2.38	1.43	1.38
25	c	503	CLA	C3B-C4B	2.38	1.49	1.42
25	B	610	CLA	C3B-C4B	2.38	1.49	1.42
31	A	616	DGD	C1E-C2E	2.37	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	517	LMG	O7-C8	-2.36	1.41	1.46
26	k	103	BCR	C30-C25	-2.36	1.50	1.53
25	C	507	CLA	CHC-C1C	2.36	1.43	1.38
25	C	507	CLA	C3B-C4B	2.36	1.49	1.42
25	B	604	CLA	C4B-NB	2.36	1.41	1.37
25	A	606	CLA	C3B-C4B	2.35	1.49	1.42
25	c	509	CLA	C3B-C4B	2.35	1.49	1.42
25	b	603	CLA	CMD-C2D	-2.35	1.45	1.50
25	c	503	CLA	CHC-C1C	2.35	1.43	1.38
25	B	606	CLA	C3B-C4B	2.35	1.49	1.42
25	B	611	CLA	CMD-C2D	-2.35	1.46	1.50
25	b	613	CLA	CMD-C2D	-2.34	1.46	1.50
25	C	512	CLA	MG-ND	-2.34	2.01	2.05
29	f	102	SQD	O9-S	2.34	1.51	1.45
25	B	606	CLA	CHC-C1C	2.34	1.43	1.38
25	C	509	CLA	CMD-C2D	-2.34	1.46	1.50
31	c	516	DGD	O2G-C2G	-2.34	1.41	1.46
25	B	601	CLA	CHC-C1C	2.34	1.43	1.38
25	C	510	CLA	C3B-C4B	2.34	1.49	1.42
33	d	402	PHO	C4D-ND	-2.33	1.35	1.38
25	B	608	CLA	C3B-C4B	2.33	1.49	1.42
34	f	101	HEM	C3B-C2B	-2.33	1.32	1.37
25	b	604	CLA	C1B-C2B	2.33	1.48	1.43
25	c	512	CLA	MG-NA	2.33	2.11	2.06
29	B	623	SQD	O9-S	2.32	1.51	1.45
25	C	511	CLA	CHC-C1C	2.32	1.43	1.38
25	d	403	CLA	CMC-C2C	-2.32	1.46	1.50
25	b	610	CLA	MG-NC	2.32	2.11	2.06
31	A	616	DGD	C3G-C2G	2.32	1.58	1.50
25	a	611	CLA	CHC-C1C	2.32	1.43	1.38
31	h	102	DGD	C6D-C5D	2.32	1.58	1.51
25	b	604	CLA	CMD-C2D	-2.31	1.46	1.50
29	a	613	SQD	C44-C45	2.31	1.56	1.51
25	B	610	CLA	C1D-C2D	2.31	1.49	1.45
25	B	605	CLA	MG-NA	2.30	2.11	2.06
25	C	508	CLA	CHC-C1C	2.30	1.43	1.38
25	b	608	CLA	CMB-C2B	-2.30	1.46	1.50
25	B	615	CLA	CHC-C1C	2.30	1.43	1.38
29	b	620	SQD	O9-S	2.30	1.51	1.45
25	b	607	CLA	CMD-C2D	-2.30	1.46	1.50
25	b	612	CLA	CMC-C2C	-2.30	1.46	1.50
25	B	607	CLA	CMB-C2B	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	v	201	HEC	CMA-C3A	2.29	1.55	1.50
25	b	609	CLA	C3B-C4B	2.29	1.49	1.42
25	c	507	CLA	MG-NB	-2.29	2.01	2.05
33	D	402	PHO	CMD-C2D	-2.29	1.47	1.51
35	V	201	HEC	CAC-C3C	2.28	1.56	1.51
31	J	101	DGD	O2G-C2G	-2.28	1.41	1.46
25	d	403	CLA	CHC-C1C	2.28	1.43	1.38
26	B	619	BCR	C30-C25	-2.28	1.50	1.53
25	C	511	CLA	C3B-C4B	2.28	1.49	1.42
25	C	510	CLA	C4B-NB	2.28	1.40	1.37
31	A	616	DGD	C6E-C5E	2.28	1.59	1.51
35	V	201	HEC	CMB-C2B	2.28	1.55	1.50
26	B	617	BCR	C33-C5	-2.28	1.47	1.50
25	C	505	CLA	MG-NC	2.27	2.11	2.06
25	B	602	CLA	MG-NC	2.27	2.11	2.06
33	d	402	PHO	CAC-C3C	-2.27	1.47	1.51
28	m	101	LMG	C4-C3	2.27	1.58	1.52
25	D	403	CLA	CHC-C1C	2.27	1.43	1.38
25	B	609	CLA	MG-NA	2.27	2.11	2.06
34	f	101	HEM	CMC-C2C	2.27	1.55	1.50
25	b	607	CLA	C3B-C4B	2.27	1.49	1.42
25	C	503	CLA	C1D-C2D	2.26	1.49	1.45
31	c	516	DGD	C3E-C2E	2.26	1.58	1.52
31	c	516	DGD	C1E-C2E	2.26	1.59	1.52
30	d	407	LHG	O7-C5	-2.26	1.41	1.46
26	H	101	BCR	C1-C6	-2.26	1.50	1.53
25	b	613	CLA	CHC-C1C	2.26	1.43	1.38
33	D	402	PHO	CMC-C2C	-2.26	1.47	1.50
31	c	515	DGD	C3G-C2G	2.26	1.57	1.50
25	C	503	CLA	C3B-C4B	2.25	1.49	1.42
25	B	614	CLA	C1B-C2B	2.25	1.48	1.43
25	B	611	CLA	C4B-NB	2.25	1.40	1.37
25	C	502	CLA	C4B-NB	2.24	1.40	1.37
25	B	603	CLA	CMD-C2D	-2.24	1.46	1.50
25	B	609	CLA	C4B-NB	2.24	1.40	1.37
29	a	612	SQD	O7-S	2.24	1.51	1.45
25	b	609	CLA	CHC-C1C	2.23	1.43	1.38
25	b	604	CLA	C4B-NB	2.23	1.40	1.37
31	H	102	DGD	C1E-C2E	2.23	1.59	1.52
33	D	402	PHO	CMB-C2B	-2.23	1.47	1.51
25	C	513	CLA	CHC-C1C	2.23	1.42	1.38
25	B	615	CLA	CMB-C2B	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	CMB-C2B	-2.23	1.46	1.50
25	C	504	CLA	CMB-C2B	-2.23	1.46	1.50
25	C	502	CLA	C3B-C4B	2.22	1.49	1.42
27	d	406	PL9	C3-C4	-2.21	1.46	1.49
25	b	602	CLA	CHC-C1C	2.21	1.42	1.38
25	c	504	CLA	C3B-C4B	2.21	1.49	1.42
31	A	616	DGD	O1G-C1G	-2.21	1.40	1.45
31	J	101	DGD	C1G-C2G	2.21	1.57	1.50
25	c	507	CLA	CMC-C2C	-2.21	1.46	1.50
25	B	609	CLA	C3B-C4B	2.20	1.49	1.42
33	d	402	PHO	CMC-C2C	-2.20	1.47	1.50
29	A	613	SQD	C8-C7	2.20	1.57	1.50
25	B	608	CLA	C1D-C2D	2.20	1.49	1.45
25	B	612	CLA	CHC-C1C	2.20	1.42	1.38
25	C	509	CLA	MG-NA	2.19	2.11	2.06
25	c	512	CLA	CMC-C2C	-2.19	1.46	1.50
29	D	408	SQD	O9-S	2.19	1.51	1.45
30	A	614	LHG	O8-C23	2.19	1.39	1.33
25	b	615	CLA	CHC-C1C	2.19	1.42	1.38
25	B	614	CLA	MG-NB	2.19	2.10	2.05
25	c	513	CLA	CMD-C2D	-2.18	1.46	1.50
27	D	406	PL9	C3-C4	-2.18	1.46	1.49
25	B	610	CLA	CHC-C1C	2.18	1.42	1.38
25	D	404	CLA	C3D-C4D	2.18	1.49	1.44
30	D	410	LHG	O7-C7	2.18	1.40	1.34
28	c	518	LMG	C7-C8	2.18	1.57	1.50
25	A	608	CLA	C1D-ND	2.18	1.40	1.37
25	b	613	CLA	C3B-C4B	2.18	1.49	1.42
25	B	601	CLA	CMB-C2B	-2.17	1.46	1.50
26	C	514	BCR	C30-C25	-2.17	1.51	1.53
25	B	608	CLA	CMD-C2D	-2.17	1.46	1.50
25	B	614	CLA	C3B-C4B	2.17	1.49	1.42
28	c	521	LMG	O1-C7	-2.17	1.40	1.43
29	b	620	SQD	O5-C5	2.17	1.49	1.44
25	C	501	CLA	CMD-C2D	-2.17	1.46	1.50
25	c	509	CLA	CHC-C1C	2.17	1.42	1.38
25	A	608	CLA	C1D-C2D	2.17	1.49	1.45
25	A	608	CLA	C1B-NB	-2.17	1.35	1.37
25	C	507	CLA	C4B-NB	2.17	1.40	1.37
29	B	623	SQD	C8-C7	2.17	1.57	1.50
31	H	102	DGD	C1G-C2G	2.17	1.57	1.50
31	C	516	DGD	C6D-C5D	2.17	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	C3B-C4B	2.16	1.49	1.42
25	B	611	CLA	CHC-C1C	2.16	1.42	1.38
25	b	606	CLA	C3B-C4B	2.16	1.49	1.42
25	b	615	CLA	CMD-C2D	-2.16	1.46	1.50
27	D	406	PL9	C11-C9	-2.16	1.46	1.51
31	C	516	DGD	C4D-C3D	2.16	1.57	1.52
25	c	501	CLA	CMD-C2D	-2.16	1.46	1.50
25	c	501	CLA	C3B-C4B	2.16	1.49	1.42
34	f	101	HEM	CMA-C3A	2.15	1.55	1.50
25	C	501	CLA	MG-NB	2.15	2.10	2.05
35	v	201	HEC	CAB-C3B	2.15	1.56	1.51
25	a	605	CLA	C3D-C4D	2.15	1.49	1.44
25	B	612	CLA	C3D-C4D	2.15	1.49	1.44
25	C	505	CLA	C3B-C4B	2.15	1.49	1.42
25	b	609	CLA	CMC-C2C	-2.15	1.46	1.50
25	A	607	CLA	C3B-C4B	2.15	1.49	1.42
25	c	507	CLA	CMB-C2B	-2.15	1.46	1.50
31	C	515	DGD	C6D-C5D	2.15	1.58	1.51
29	D	408	SQD	O7-S	2.15	1.51	1.45
25	C	513	CLA	C1D-C2D	2.15	1.49	1.45
25	b	611	CLA	CHC-C1C	2.15	1.42	1.38
29	b	620	SQD	C46-C45	2.15	1.57	1.50
25	b	608	CLA	MG-ND	2.15	2.10	2.05
25	B	612	CLA	CMC-C2C	-2.14	1.46	1.50
31	C	515	DGD	C3D-C2D	2.14	1.57	1.52
30	D	409	LHG	P-O6	2.14	1.67	1.59
31	A	616	DGD	O3G-C1D	2.14	1.43	1.40
25	B	613	CLA	CMD-C2D	-2.14	1.46	1.50
25	c	512	CLA	MG-NB	2.14	2.10	2.05
31	H	102	DGD	O2G-C2G	-2.14	1.41	1.46
25	d	404	CLA	C3B-C4B	2.13	1.49	1.42
31	c	516	DGD	C4D-C5D	2.13	1.57	1.53
25	A	611	CLA	CMD-C2D	-2.13	1.46	1.50
31	c	517	DGD	O2G-C2G	-2.13	1.41	1.46
29	A	613	SQD	O9-S	2.13	1.51	1.45
25	c	509	CLA	CMB-C2B	-2.13	1.46	1.50
25	b	616	CLA	C3B-C4B	2.13	1.48	1.42
25	B	616	CLA	C3B-C4B	2.13	1.48	1.42
25	c	504	CLA	CHC-C1C	2.13	1.42	1.38
25	b	610	CLA	C4B-NB	2.12	1.40	1.37
28	c	521	LMG	C1-C2	2.12	1.58	1.52
25	b	616	CLA	CMC-C2C	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	CLA	CMD-C2D	-2.12	1.46	1.50
25	D	403	CLA	MG-NB	2.12	2.10	2.05
25	b	611	CLA	C3B-C4B	2.12	1.48	1.42
25	b	603	CLA	CMC-C2C	-2.11	1.46	1.50
25	a	611	CLA	C1D-C2D	2.11	1.49	1.45
35	V	201	HEC	FE-NA	2.11	2.02	1.95
25	b	614	CLA	C1D-C2D	2.11	1.49	1.45
31	A	616	DGD	O2G-C1B	2.11	1.40	1.34
26	B	617	BCR	C30-C25	-2.11	1.51	1.53
25	c	505	CLA	MG-ND	-2.11	2.01	2.05
28	D	411	LMG	C9-C8	2.11	1.57	1.50
25	c	506	CLA	CMC-C2C	-2.11	1.46	1.50
25	c	508	CLA	CMD-C2D	-2.11	1.46	1.50
25	c	507	CLA	C3D-C4D	2.10	1.48	1.44
25	c	502	CLA	CMC-C2C	-2.10	1.46	1.50
33	a	607	PHO	O2D-CGD	2.10	1.38	1.33
26	t	101	BCR	C1-C6	-2.10	1.51	1.53
25	B	611	CLA	C1B-NB	-2.10	1.35	1.37
25	b	606	CLA	CMD-C2D	-2.09	1.46	1.50
31	c	516	DGD	O3D-C3D	-2.09	1.37	1.43
26	b	617	BCR	C33-C5	-2.09	1.47	1.50
29	B	623	SQD	O7-S	2.09	1.51	1.45
25	b	603	CLA	CMB-C2B	-2.09	1.46	1.50
25	B	604	CLA	C3B-C4B	2.09	1.48	1.42
25	C	501	CLA	C3D-C4D	2.09	1.48	1.44
25	c	512	CLA	CMB-C2B	-2.09	1.46	1.50
25	B	609	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	510	CLA	CMB-C2B	-2.08	1.46	1.50
25	B	602	CLA	CHC-C1C	2.08	1.42	1.38
25	c	501	CLA	CMB-C2B	-2.08	1.46	1.50
25	A	606	CLA	CMC-C2C	-2.08	1.46	1.50
26	d	405	BCR	C33-C5	-2.08	1.47	1.50
31	c	516	DGD	C3D-C2D	2.08	1.57	1.52
30	L	101	LHG	P-O6	2.08	1.67	1.59
25	D	404	CLA	CMB-C2B	-2.08	1.46	1.50
30	d	407	LHG	O8-C23	2.08	1.39	1.33
25	A	611	CLA	C3B-C4B	2.07	1.48	1.42
31	c	515	DGD	C4D-C3D	2.07	1.57	1.52
25	C	510	CLA	CHC-C1C	2.07	1.42	1.38
25	b	606	CLA	MG-ND	2.07	2.09	2.05
25	c	501	CLA	MG-NC	2.07	2.11	2.06
34	f	101	HEM	FE-NC	2.07	2.02	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	410	LHG	O3-C3	-2.07	1.36	1.44
34	f	101	HEM	C2A-C3A	-2.07	1.33	1.38
30	D	409	LHG	O7-C5	-2.07	1.41	1.46
25	c	507	CLA	CHC-C1C	2.07	1.42	1.38
35	V	201	HEC	CMD-C2D	2.07	1.55	1.50
26	h	101	BCR	C1-C6	-2.07	1.51	1.53
25	B	609	CLA	C3D-C4D	2.07	1.48	1.44
26	k	102	BCR	C33-C5	-2.07	1.47	1.50
25	A	607	CLA	CHC-C1C	2.07	1.42	1.38
25	B	606	CLA	CMC-C2C	-2.06	1.46	1.50
25	d	404	CLA	CMB-C2B	-2.06	1.46	1.50
31	C	515	DGD	C1D-C2D	2.06	1.58	1.52
35	V	201	HEC	CMC-C2C	2.06	1.55	1.50
31	J	101	DGD	C4D-C5D	2.06	1.57	1.53
33	D	401	PHO	CMB-C2B	-2.06	1.47	1.51
33	D	401	PHO	CMD-C2D	-2.05	1.47	1.51
31	H	102	DGD	O1G-C1G	-2.05	1.40	1.45
25	c	503	CLA	C1D-C2D	2.05	1.49	1.45
25	b	608	CLA	CMD-C2D	-2.05	1.46	1.50
34	E	101	HEM	CMA-C3A	2.05	1.55	1.50
25	C	502	CLA	CHC-C1C	2.05	1.42	1.38
31	H	102	DGD	C4D-C3D	2.05	1.57	1.52
25	B	607	CLA	CHC-C1C	2.05	1.42	1.38
31	C	515	DGD	C3G-C2G	2.05	1.57	1.50
33	d	402	PHO	CMB-C2B	-2.05	1.47	1.51
25	c	512	CLA	C3D-C4D	2.05	1.48	1.44
25	C	511	CLA	CMC-C2C	-2.05	1.46	1.50
25	b	616	CLA	CMB-C2B	-2.04	1.46	1.50
25	b	602	CLA	CMD-C2D	-2.04	1.46	1.50
25	C	504	CLA	CMD-C2D	-2.04	1.46	1.50
25	d	404	CLA	CMC-C2C	-2.04	1.46	1.50
25	a	605	CLA	CMD-C2D	-2.04	1.46	1.50
31	h	102	DGD	C4D-C3D	2.04	1.57	1.52
25	C	510	CLA	CMD-C2D	-2.04	1.46	1.50
28	b	622	LMG	C7-C8	2.03	1.57	1.50
33	a	607	PHO	C4D-ND	-2.03	1.35	1.38
25	B	613	CLA	CMB-C2B	-2.03	1.46	1.50
25	A	608	CLA	CMC-C2C	-2.03	1.46	1.50
25	a	608	CLA	CMC-C2C	-2.03	1.46	1.50
25	C	513	CLA	CMB-C2B	-2.02	1.46	1.50
25	b	603	CLA	CHC-C1C	2.02	1.42	1.38
25	B	608	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	509	CLA	C3C-C2C	2.02	1.41	1.36
26	c	514	BCR	C33-C5	-2.02	1.47	1.50
33	D	402	PHO	C4D-ND	-2.02	1.35	1.38
28	m	101	LMG	O7-C8	-2.02	1.41	1.46
28	B	620	LMG	C9-C8	2.02	1.57	1.50
25	c	512	CLA	CMD-C2D	-2.02	1.46	1.50
25	B	616	CLA	O2D-CGD	2.02	1.38	1.33
28	c	521	LMG	C3-C2	2.02	1.57	1.52
25	B	608	CLA	C3C-C2C	2.02	1.41	1.36
29	a	612	SQD	C8-C7	2.02	1.56	1.50
25	A	607	CLA	C4C-C3C	2.01	1.48	1.45
25	C	510	CLA	O2D-CGD	2.01	1.38	1.33
29	b	620	SQD	O7-S	2.01	1.50	1.45
25	b	613	CLA	C1B-C2B	2.01	1.47	1.43
31	c	516	DGD	O6D-C5D	-2.01	1.39	1.44
25	C	509	CLA	CMB-C2B	-2.00	1.46	1.50
29	D	408	SQD	C25-C24	2.00	1.59	1.52
27	D	406	PL9	C52-C5	-2.00	1.46	1.50
25	b	604	CLA	MG-NB	2.00	2.09	2.05
34	f	101	HEM	CMB-C2B	2.00	1.54	1.50

All (1086) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C4A-NA-C1A	9.64	111.08	106.68
25	b	616	CLA	C4A-NA-C1A	9.10	110.83	106.68
25	B	601	CLA	C4A-NA-C1A	9.04	110.80	106.68
25	c	511	CLA	C4A-NA-C1A	8.69	110.64	106.68
25	C	503	CLA	C4A-NA-C1A	8.49	110.55	106.68
25	C	510	CLA	C4A-NA-C1A	8.48	110.55	106.68
25	b	606	CLA	C4A-NA-C1A	8.23	110.43	106.68
25	a	605	CLA	C4A-NA-C1A	8.10	110.37	106.68
25	C	508	CLA	C4A-NA-C1A	8.07	110.36	106.68
25	c	503	CLA	C4A-NA-C1A	8.00	110.33	106.68
25	C	511	CLA	C4A-NA-C1A	7.98	110.32	106.68
25	c	509	CLA	C4A-NA-C1A	7.85	110.26	106.68
25	C	507	CLA	C4A-NA-C1A	7.81	110.24	106.68
25	B	606	CLA	C4A-NA-C1A	7.74	110.21	106.68
25	c	507	CLA	C4A-NA-C1A	7.70	110.19	106.68
25	b	601	CLA	C4A-NA-C1A	7.48	110.09	106.68
25	B	615	CLA	C4A-NA-C1A	7.43	110.07	106.68
25	C	501	CLA	C4A-NA-C1A	7.39	110.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	506	CLA	C4A-NA-C1A	7.31	110.01	106.68
25	b	615	CLA	C4A-NA-C1A	7.05	109.90	106.68
25	A	606	CLA	C4A-NA-C1A	6.89	109.82	106.68
25	A	611	CLA	C4A-NA-C1A	6.81	109.78	106.68
25	B	609	CLA	C4A-NA-C1A	6.79	109.78	106.68
29	A	613	SQD	O6-C1-C2	6.75	118.53	108.27
25	b	609	CLA	C4A-NA-C1A	6.72	109.74	106.68
25	a	606	CLA	C4A-NA-C1A	6.69	109.73	106.68
25	B	607	CLA	C4A-NA-C1A	6.60	109.69	106.68
25	c	512	CLA	C4A-NA-C1A	6.57	109.67	106.68
25	B	612	CLA	C4A-NA-C1A	6.55	109.67	106.68
25	c	502	CLA	C4A-NA-C1A	6.51	109.65	106.68
25	b	611	CLA	C4A-NA-C1A	6.35	109.58	106.68
25	B	613	CLA	C4A-NA-C1A	6.29	109.55	106.68
25	c	501	CLA	C4A-NA-C1A	6.23	109.52	106.68
33	D	401	PHO	C4D-CHA-CBD	-6.21	105.47	108.45
25	b	602	CLA	C4A-NA-C1A	6.18	109.50	106.68
25	d	403	CLA	C4A-NA-C1A	6.16	109.49	106.68
27	A	610	PL9	C7-C3-C4	6.11	121.94	116.91
25	D	403	CLA	C4A-NA-C1A	6.00	109.42	106.68
25	C	513	CLA	C4A-NA-C1A	5.95	109.39	106.68
25	C	509	CLA	C4A-NA-C1A	5.95	109.39	106.68
25	c	506	CLA	C4A-NA-C1A	5.90	109.37	106.68
25	c	513	CLA	C4A-NA-C1A	5.89	109.37	106.68
29	A	613	SQD	C1-O5-C5	-5.87	102.26	113.72
25	B	608	CLA	C4A-NA-C1A	5.83	109.34	106.68
25	c	505	CLA	C4A-NA-C1A	5.82	109.33	106.68
29	a	612	SQD	C1-O5-C5	-5.75	102.50	113.72
25	B	616	CLA	C4A-NA-C1A	5.58	109.22	106.68
29	b	620	SQD	O6-C1-C2	5.55	116.70	108.27
25	c	510	CLA	C4A-NA-C1A	5.55	109.21	106.68
25	C	512	CLA	C4A-NA-C1A	5.53	109.20	106.68
33	a	607	PHO	C4D-CHA-CBD	-5.50	105.82	108.45
25	B	611	CLA	C4A-NA-C1A	5.49	109.18	106.68
29	a	612	SQD	O6-C1-C2	5.48	116.59	108.27
25	B	602	CLA	C4A-NA-C1A	5.48	109.18	106.68
35	v	201	HEC	C1D-ND-C4D	5.44	111.65	105.21
25	C	502	CLA	C4A-NA-C1A	5.43	109.16	106.68
25	C	505	CLA	C4A-NA-C1A	5.42	109.15	106.68
25	c	508	CLA	C4A-NA-C1A	5.41	109.15	106.68
25	b	613	CLA	C4A-NA-C1A	5.36	109.12	106.68
25	b	604	CLA	C4A-NA-C1A	5.34	109.12	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	C4A-NA-C1A	5.34	109.11	106.68
25	d	404	CLA	C4A-NA-C1A	5.34	109.11	106.68
29	a	613	SQD	O47-C7-C8	5.30	122.94	111.48
25	B	605	CLA	C4A-NA-C1A	5.30	109.10	106.68
25	A	607	CLA	C4A-NA-C1A	5.28	109.09	106.68
27	a	610	PL9	C7-C3-C4	5.21	121.20	116.91
25	C	504	CLA	C4A-NA-C1A	5.11	109.01	106.68
25	b	605	CLA	C4A-NA-C1A	5.09	109.00	106.68
25	B	613	CLA	C1-C2-C3	-5.07	117.89	126.20
25	b	603	CLA	C4A-NA-C1A	5.06	108.99	106.68
29	D	408	SQD	O6-C1-C2	5.04	115.93	108.27
25	B	603	CLA	C4A-NA-C1A	5.03	108.98	106.68
29	A	613	SQD	O7-S-C6	5.03	114.27	106.76
25	a	611	CLA	C4A-NA-C1A	5.03	108.97	106.68
25	b	608	CLA	C4A-NA-C1A	5.03	108.97	106.68
35	V	201	HEC	C1D-ND-C4D	5.00	111.13	105.21
25	b	604	CLA	C1-C2-C3	-4.95	118.09	126.20
25	D	404	CLA	C4A-NA-C1A	4.93	108.93	106.68
25	B	610	CLA	O2D-CGD-O1D	-4.86	114.40	123.85
25	c	501	CLA	O2D-CGD-O1D	-4.82	114.46	123.85
29	b	620	SQD	O9-S-O7	-4.71	98.49	113.82
25	B	614	CLA	C3B-C4B-NB	-4.62	106.40	110.53
25	b	607	CLA	C4A-NA-C1A	4.60	108.78	106.68
25	C	501	CLA	C3B-C4B-NB	-4.59	106.43	110.53
29	A	613	SQD	O9-S-O7	-4.54	99.07	113.82
25	c	505	CLA	C3B-C4B-NB	-4.53	106.49	110.53
25	B	606	CLA	O2D-CGD-O1D	-4.52	115.05	123.85
30	D	410	LHG	O4-P-O5	4.50	133.40	112.44
29	b	620	SQD	O5-C5-C4	4.49	117.79	109.70
25	a	608	CLA	C4A-NA-C1A	4.45	108.71	106.68
29	a	612	SQD	O9-S-O7	-4.45	99.36	113.82
25	b	610	CLA	C4A-NA-C1A	4.41	108.69	106.68
33	d	402	PHO	C4D-CHA-CBD	-4.40	106.35	108.45
25	A	608	CLA	C4A-NA-C1A	4.38	108.68	106.68
31	H	102	DGD	O3G-C3G-C2G	-4.37	100.18	110.82
30	e	101	LHG	O4-P-O5	4.36	132.72	112.44
33	D	402	PHO	O1D-CGD-CBD	4.36	131.33	124.72
25	b	612	CLA	C4A-NA-C1A	4.34	108.66	106.68
25	B	610	CLA	C4A-NA-C1A	4.32	108.65	106.68
30	d	408	LHG	O4-P-O5	4.31	132.49	112.44
29	f	102	SQD	O9-S-O7	-4.29	99.87	113.82
30	D	412	LHG	O4-P-O5	4.26	132.28	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	623	SQD	O6-C1-C2	4.25	114.72	108.27
25	a	605	CLA	C3B-C4B-NB	-4.21	106.77	110.53
30	A	614	LHG	O4-P-O5	4.21	132.03	112.44
29	B	623	SQD	O47-C7-C8	4.21	120.59	111.48
30	L	101	LHG	O4-P-O5	4.21	132.01	112.44
30	d	407	LHG	O4-P-O5	4.20	131.97	112.44
29	f	102	SQD	O6-C1-C2	4.19	114.64	108.27
30	D	409	LHG	O4-P-O5	4.18	131.89	112.44
25	B	611	CLA	O2D-CGD-O1D	-4.17	115.73	123.85
30	d	409	LHG	O4-P-O5	4.16	131.80	112.44
29	a	612	SQD	O7-S-C6	4.13	112.92	106.76
29	A	613	SQD	C1-C2-C3	-4.11	101.37	110.01
25	b	614	CLA	C4A-NA-C1A	4.09	108.55	106.68
27	A	610	PL9	C7-C3-C2	-4.09	118.56	123.39
25	b	603	CLA	O2D-CGD-O1D	-4.08	115.91	123.85
33	D	402	PHO	C1-C2-C3	-4.07	119.52	126.20
26	b	617	BCR	C2-C1-C6	4.06	116.33	110.44
27	d	406	PL9	C7-C3-C4	4.01	120.21	116.91
29	D	408	SQD	C1-O5-C5	-3.97	105.97	113.72
30	l	101	LHG	O4-P-O5	3.96	130.88	112.44
29	A	613	SQD	O47-C7-C8	3.96	120.05	111.48
24	d	401	BCT	O2-C-O1	3.95	129.77	119.68
26	T	101	BCR	C7-C8-C9	-3.94	120.40	126.23
25	b	608	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
26	B	617	BCR	C2-C1-C6	3.93	116.15	110.44
33	a	607	PHO	C2B-C1B-NB	-3.92	106.60	109.43
25	B	614	CLA	C4A-NA-C1A	3.91	108.46	106.68
31	c	516	DGD	O3G-C3G-C2G	-3.91	101.31	110.82
27	a	610	PL9	C7-C3-C2	-3.90	118.79	123.39
29	B	623	SQD	O7-S-C6	3.90	112.58	106.76
25	b	606	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
31	c	515	DGD	O3G-C3G-C2G	-3.88	101.39	110.82
25	C	506	CLA	C3B-C4B-NB	-3.88	107.07	110.53
25	A	611	CLA	O2D-CGD-O1D	-3.87	116.31	123.85
25	C	508	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
25	B	603	CLA	O2D-CGD-O1D	-3.86	116.34	123.85
24	A	605	BCT	O2-C-O1	3.85	129.53	119.68
25	B	606	CLA	O2D-CGD-CBD	3.85	117.96	111.23
31	c	517	DGD	O3G-C3G-C2G	-3.84	101.48	110.82
29	b	620	SQD	O7-S-C6	3.82	112.47	106.76
25	b	615	CLA	C3B-C4B-NB	-3.77	107.17	110.53
29	b	620	SQD	C3-C4-C5	3.77	117.06	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	402	PHO	C2B-C1B-NB	-3.76	106.71	109.43
25	a	611	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
29	f	102	SQD	O7-S-C6	3.75	112.35	106.76
25	b	610	CLA	O2D-CGD-O1D	-3.74	116.58	123.85
29	B	623	SQD	O9-S-O7	-3.73	101.68	113.82
25	A	607	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
25	a	606	CLA	C3B-C4B-NB	-3.69	107.23	110.53
25	b	605	CLA	C3B-C4B-NB	-3.69	107.24	110.53
25	c	509	CLA	O2A-CGA-O1A	-3.67	114.46	123.63
31	C	516	DGD	O3G-C3G-C2G	-3.67	101.90	110.82
25	B	614	CLA	O2D-CGD-O1D	-3.66	116.73	123.85
31	h	102	DGD	O3G-C3G-C2G	-3.66	101.92	110.82
25	B	608	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
26	D	405	BCR	C2-C1-C6	3.63	115.72	110.44
25	B	610	CLA	C1-C2-C3	-3.63	120.25	126.20
25	b	612	CLA	CHB-C4A-NA	3.62	129.63	124.40
33	d	402	PHO	O1D-CGD-CBD	3.62	130.22	124.72
25	c	501	CLA	O2D-CGD-CBD	3.62	117.56	111.23
33	D	402	PHO	O2D-CGD-O1D	-3.62	116.80	123.85
25	c	506	CLA	C3B-C4B-NB	-3.61	107.30	110.53
33	D	401	PHO	CMB-C2B-C3B	3.61	131.90	124.68
25	C	501	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
27	d	406	PL9	C40-C39-C41	3.60	121.48	115.23
25	C	507	CLA	CHB-C4A-NA	3.59	129.57	124.40
29	a	612	SQD	O47-C7-C8	3.58	119.23	111.48
31	a	614	DGD	O3G-C3G-C2G	-3.56	102.62	111.77
25	C	503	CLA	C3B-C4B-NB	-3.56	107.35	110.53
25	B	604	CLA	C3B-C4B-NB	-3.55	107.36	110.53
25	b	605	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
25	c	503	CLA	C3B-C4B-NB	-3.53	107.38	110.53
29	f	102	SQD	O9-S-C6	3.53	112.02	106.76
27	d	406	PL9	C7-C8-C9	-3.52	120.77	126.83
25	b	611	CLA	O2D-CGD-CBD	3.51	117.37	111.23
29	b	620	SQD	O47-C7-C8	3.51	119.07	111.48
28	b	622	LMG	O1-C1-C2	-3.51	102.94	108.27
25	b	601	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
25	a	611	CLA	O2D-CGD-CBD	3.49	117.33	111.23
26	h	101	BCR	C2-C1-C6	3.49	115.51	110.44
27	D	406	PL9	C7-C3-C4	3.48	119.78	116.91
25	b	612	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
25	C	507	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
25	C	512	CLA	C1-C2-C3	-3.47	120.51	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	412	LHG	O8-C23-C24	3.47	122.40	111.83
25	B	611	CLA	O2D-CGD-CBD	3.46	117.28	111.23
25	c	512	CLA	C1-C2-C3	-3.45	120.54	126.20
25	c	505	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
31	J	101	DGD	O3G-C3G-C2G	-3.45	102.44	110.82
26	B	619	BCR	C2-C1-C6	3.42	115.41	110.44
25	b	613	CLA	C3B-C4B-NB	-3.42	107.48	110.53
25	B	602	CLA	O2D-CGD-CBD	3.41	117.20	111.23
25	C	512	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
25	B	610	CLA	O2A-CGA-O1A	-3.41	115.11	123.63
31	H	102	DGD	C1D-C2D-C3D	-3.40	102.87	110.01
25	b	606	CLA	O2D-CGD-CBD	3.38	117.14	111.23
26	b	618	BCR	C15-C14-C13	-3.38	122.54	127.28
25	d	403	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
27	d	406	PL9	C7-C3-C2	-3.37	119.41	123.39
25	a	606	CLA	CHB-C4A-NA	3.37	129.27	124.40
25	c	511	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	A	608	CLA	CHB-C4A-NA	3.36	129.25	124.40
25	A	608	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
25	b	608	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	b	616	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
29	A	615	SQD	O47-C7-C8	3.35	118.73	111.48
29	D	408	SQD	O8-S-C6	3.35	112.44	105.97
25	B	611	CLA	C1-C2-C3	-3.35	120.71	126.20
31	A	616	DGD	C3G-C2G-C1G	-3.34	103.99	111.78
25	b	603	CLA	O2D-CGD-CBD	3.33	117.06	111.23
34	f	101	HEM	CBA-CAA-C2A	-3.32	103.37	112.53
29	D	408	SQD	C1-C2-C3	-3.31	103.05	110.01
28	d	411	LMG	O6-C1-O1	-3.31	102.22	110.04
25	b	605	CLA	C1-C2-C3	-3.31	120.78	126.20
29	b	620	SQD	C1-C2-C3	-3.31	103.05	110.01
25	B	603	CLA	C3B-C4B-NB	-3.30	107.58	110.53
33	D	402	PHO	CMB-C2B-C3B	3.30	131.28	124.68
25	b	603	CLA	C3B-C4B-NB	-3.30	107.58	110.53
25	A	611	CLA	C3B-C4B-NB	-3.29	107.59	110.53
29	D	408	SQD	O9-S-O7	-3.29	103.11	113.82
25	B	606	CLA	C1-C2-C3	-3.28	120.82	126.20
25	C	502	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
25	A	606	CLA	CHB-C4A-NA	3.27	129.12	124.40
25	b	604	CLA	C3B-C4B-NB	-3.27	107.61	110.53
33	D	401	PHO	C2B-C1B-NB	-3.27	107.07	109.43
25	D	403	CLA	C3B-C4B-NB	-3.27	107.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	102	SQD	O5-C5-C4	3.26	115.58	109.70
31	C	515	DGD	O6D-C1D-O3G	-3.26	102.34	110.04
25	a	611	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	d	404	CLA	CHB-C4A-NA	3.25	129.10	124.40
25	A	606	CLA	C3B-C4B-NB	-3.25	107.63	110.53
25	B	602	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
25	b	602	CLA	CHB-C4A-NA	3.23	129.06	124.40
25	b	601	CLA	C3B-C4B-NB	-3.23	107.65	110.53
29	a	612	SQD	O48-C23-C24	3.22	121.66	111.83
25	C	510	CLA	CHB-C4A-NA	3.22	129.04	124.40
25	B	601	CLA	C3B-C4B-NB	-3.21	107.66	110.53
33	d	402	PHO	CMB-C2B-C3B	3.21	131.09	124.68
25	B	615	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
25	B	616	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
25	c	505	CLA	O2D-CGD-CBD	3.19	116.81	111.23
35	V	201	HEC	CAD-CBD-CGD	-3.19	105.19	113.67
25	B	601	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
31	J	101	DGD	O6D-C1D-O3G	-3.19	102.50	110.04
29	b	620	SQD	O48-C23-C24	3.19	121.56	111.83
25	b	608	CLA	CHB-C4A-NA	3.19	129.00	124.40
25	C	513	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
25	b	602	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
32	M	101	STE	C3-C2-C1	-3.18	106.22	114.51
25	B	602	CLA	CHB-C4A-NA	3.17	128.98	124.40
26	T	101	BCR	C33-C5-C6	-3.17	121.02	124.48
35	V	201	HEC	CHB-C1B-NB	3.17	127.84	124.42
27	d	406	PL9	C22-C23-C24	-3.17	120.36	127.62
25	c	510	CLA	C3B-C4B-NB	-3.17	107.70	110.53
25	c	507	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
29	a	612	SQD	C3-C4-C5	3.17	115.97	110.23
25	B	605	CLA	C3B-C4B-NB	-3.16	107.70	110.53
25	c	513	CLA	C3B-C4B-NB	-3.16	107.70	110.53
25	c	504	CLA	CMB-C2B-C1B	-3.16	120.60	125.42
28	c	521	LMG	O6-C1-O1	-3.16	102.57	110.04
25	A	606	CLA	O2A-CGA-O1A	-3.16	115.72	123.63
25	b	614	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
25	c	513	CLA	O2D-CGD-O1D	-3.16	117.71	123.85
27	D	406	PL9	C37-C38-C39	-3.15	120.42	127.62
25	c	512	CLA	C3B-C4B-NB	-3.15	107.72	110.53
31	C	516	DGD	O6D-C1D-O3G	-3.13	102.64	110.04
29	D	408	SQD	O9-S-C6	3.12	111.42	106.76
25	B	610	CLA	O2D-CGD-CBD	3.12	116.69	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	608	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
25	A	611	CLA	O2D-CGD-CBD	3.12	116.68	111.23
25	b	612	CLA	C1-C2-C3	-3.12	121.09	126.20
29	b	620	SQD	O9-S-C6	3.10	111.39	106.76
25	c	512	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
28	m	101	LMG	O1-C7-C8	-3.10	103.28	110.82
27	D	406	PL9	C22-C23-C24	-3.10	120.54	127.62
25	C	512	CLA	C3B-C4B-NB	-3.09	107.78	110.53
25	c	508	CLA	C3B-C4B-NB	-3.08	107.78	110.53
25	c	503	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
26	c	514	BCR	C27-C26-C25	3.07	126.85	122.70
25	b	611	CLA	C3B-C4B-NB	-3.07	107.79	110.53
26	A	609	BCR	C27-C26-C25	3.06	126.84	122.70
25	C	504	CLA	C3B-C4B-NB	-3.06	107.80	110.53
26	A	609	BCR	C2-C1-C6	3.06	114.88	110.44
26	b	617	BCR	C11-C10-C9	-3.04	123.02	127.28
25	C	511	CLA	CAC-C3C-C4C	3.04	128.74	124.79
25	C	510	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
25	C	503	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
25	B	606	CLA	C3B-C4B-NB	-3.03	107.82	110.53
25	B	612	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
26	K	101	BCR	C11-C10-C9	-3.02	123.04	127.28
25	C	509	CLA	C1-C2-C3	-3.02	121.25	126.20
25	b	612	CLA	O2A-CGA-O1A	-3.02	116.07	123.63
31	c	517	DGD	O6D-C1D-O3G	-3.02	102.91	110.04
25	B	605	CLA	CHD-C1D-ND	-3.02	120.55	124.80
29	a	613	SQD	O48-C23-C24	3.02	121.03	111.83
25	B	608	CLA	C3B-C4B-NB	-3.01	107.84	110.53
26	K	101	BCR	C15-C14-C13	-3.01	123.05	127.28
28	b	622	LMG	C1-O6-C5	-3.01	107.84	113.72
25	B	616	CLA	O2D-CGD-CBD	3.01	116.49	111.23
26	B	619	BCR	C29-C30-C25	3.01	114.81	110.44
25	b	607	CLA	C3B-C4B-NB	-3.01	107.85	110.53
25	b	613	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
25	B	605	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
25	c	507	CLA	CHB-C4A-NA	3.00	128.74	124.40
27	D	406	PL9	C27-C28-C29	-3.00	120.75	127.62
25	B	615	CLA	CHB-C4A-NA	3.00	128.73	124.40
34	f	101	HEM	C3B-C4B-NB	-3.00	107.31	109.47
25	B	610	CLA	CHB-C4A-NA	3.00	128.73	124.40
28	c	520	LMG	O1-C1-C2	-2.99	103.73	108.27
26	a	609	BCR	C27-C26-C25	2.99	126.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	626	STE	C3-C2-C1	-2.99	106.71	114.51
25	b	612	CLA	CAC-C3C-C4C	2.99	128.68	124.79
26	K	101	BCR	C27-C26-C25	2.98	126.74	122.70
29	B	623	SQD	C1-O5-C5	-2.98	107.90	113.72
31	C	515	DGD	CDB-CCB-CBB	-2.98	99.32	114.37
26	T	101	BCR	C27-C26-C25	2.98	126.72	122.70
25	C	505	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	C	503	CLA	O1D-CGD-CBD	2.97	130.38	124.52
26	a	609	BCR	C2-C1-C6	2.97	114.75	110.44
26	b	617	BCR	C27-C26-C25	2.96	126.70	122.70
25	C	501	CLA	O2D-CGD-CBD	2.96	116.41	111.23
25	d	403	CLA	O2A-CGA-O1A	-2.96	116.23	123.63
30	l	101	LHG	O8-C23-C24	2.95	120.83	111.83
26	d	405	BCR	C27-C26-C25	2.95	126.69	122.70
25	c	512	CLA	O2A-CGA-O1A	-2.94	116.26	123.63
25	A	608	CLA	CHD-C1D-ND	-2.94	120.66	124.80
27	D	406	PL9	C42-C43-C44	-2.94	120.89	127.62
26	k	101	BCR	C7-C8-C9	-2.94	121.89	126.23
25	D	403	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
26	k	101	BCR	C2-C1-C6	2.93	114.69	110.44
31	h	102	DGD	C4E-C3E-C2E	-2.92	105.70	110.83
25	b	611	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
30	L	101	LHG	C5-O7-C7	-2.90	110.84	117.80
25	a	606	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
28	b	622	LMG	O3-C3-C2	-2.90	103.53	110.38
25	B	610	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	B	623	SQD	O48-C23-C24	2.90	120.68	111.83
33	d	402	PHO	C1-C2-C3	-2.90	121.45	126.20
25	c	506	CLA	C1-C2-C3	-2.89	121.45	126.20
25	B	615	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	C	504	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
26	b	619	BCR	C29-C30-C25	2.89	114.63	110.44
31	C	515	DGD	O3G-C3G-C2G	-2.89	103.80	110.82
26	D	405	BCR	C27-C26-C25	2.88	126.60	122.70
26	B	618	BCR	C27-C26-C25	2.88	126.60	122.70
25	C	511	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
25	C	513	CLA	C3B-C4B-NB	-2.88	107.96	110.53
25	b	603	CLA	CHB-C1B-NB	2.88	128.37	124.05
25	b	614	CLA	C3B-C4B-NB	-2.88	107.96	110.53
26	k	101	BCR	C27-C26-C25	2.88	126.59	122.70
25	A	611	CLA	CHB-C4A-NA	2.88	128.55	124.40
27	D	406	PL9	C12-C13-C14	-2.88	121.04	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	612	CLA	O1D-CGD-CBD	2.87	130.18	124.52
25	c	505	CLA	C1-C2-C3	-2.87	121.50	126.20
31	a	614	DGD	CDB-CCB-CBB	-2.86	99.89	114.37
25	b	616	CLA	CHB-C4A-NA	2.86	128.53	124.40
30	d	407	LHG	O8-C23-C24	2.86	120.56	111.83
31	c	516	DGD	O6D-C1D-O3G	-2.86	103.28	110.04
25	b	604	CLA	CHB-C4A-NA	2.86	128.53	124.40
25	C	508	CLA	O2D-CGD-CBD	2.86	116.23	111.23
33	d	402	PHO	O2D-CGD-O1D	-2.85	118.30	123.85
29	f	102	SQD	C1-O5-C5	-2.85	108.15	113.72
25	C	507	CLA	C3B-C4B-NB	-2.85	107.99	110.53
30	A	614	LHG	O8-C23-C24	2.84	120.51	111.83
26	B	617	BCR	C3-C4-C5	-2.84	108.98	114.06
31	h	102	DGD	CDB-CCB-CBB	-2.84	100.00	114.37
30	D	409	LHG	O8-C23-C24	2.84	120.49	111.83
25	C	509	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
25	c	508	CLA	C7-C6-C5	-2.83	105.71	113.26
28	D	407	LMG	O1-C7-C8	-2.83	103.93	110.82
25	C	513	CLA	CHD-C1D-ND	-2.82	120.83	124.80
29	D	408	SQD	O48-C23-C24	2.82	120.42	111.83
26	b	618	BCR	C8-C7-C6	-2.81	119.48	127.00
25	D	403	CLA	C4-C3-C5	2.81	120.11	115.23
26	K	101	BCR	C15-C16-C17	-2.81	117.77	123.52
25	c	504	CLA	C1-C2-C3	-2.81	121.60	126.20
25	C	506	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
30	e	101	LHG	O8-C23-C24	2.81	120.39	111.83
25	b	602	CLA	O2D-CGD-CBD	2.80	116.13	111.23
25	B	612	CLA	CHB-C4A-NA	2.80	128.44	124.40
25	c	504	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
27	d	406	PL9	C20-C19-C21	2.79	120.07	115.23
28	D	407	LMG	O6-C1-O1	-2.79	103.46	110.04
26	K	103	BCR	C27-C26-C25	2.78	126.47	122.70
25	b	614	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
26	k	102	BCR	C33-C5-C6	-2.78	121.45	124.48
25	A	606	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
33	a	607	PHO	CMB-C2B-C3B	2.78	130.23	124.68
25	b	612	CLA	C3B-C4B-NB	-2.77	108.05	110.53
26	t	101	BCR	C33-C5-C6	-2.77	121.46	124.48
33	D	402	PHO	C2B-C1B-NB	-2.77	107.43	109.43
35	v	201	HEC	CHD-C1D-ND	2.77	127.79	124.37
28	m	101	LMG	C1-C2-C3	-2.77	104.18	110.01
31	C	516	DGD	CDB-CCB-CBB	-2.77	100.38	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	607	CLA	O2D-CGD-CBD	2.76	116.06	111.23
25	B	615	CLA	C6-C7-C8	-2.76	106.78	115.97
25	b	609	CLA	C3B-C4B-NB	-2.76	108.06	110.53
26	k	101	BCR	C24-C23-C22	-2.76	122.15	126.23
28	C	517	LMG	O6-C1-O1	-2.76	103.52	110.04
27	a	610	PL9	C7-C8-C9	-2.76	122.08	126.83
25	b	613	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
25	c	511	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
25	C	512	CLA	CHB-C4A-NA	2.75	128.38	124.40
31	H	102	DGD	CDB-CCB-CBB	-2.75	100.45	114.37
31	H	102	DGD	C3E-C4E-C5E	-2.75	105.24	110.23
26	H	101	BCR	C27-C26-C25	2.75	126.42	122.70
25	b	609	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
25	c	509	CLA	CHB-C4A-NA	2.74	128.35	124.40
25	B	611	CLA	C3B-C4B-NB	-2.74	108.08	110.53
26	h	101	BCR	C27-C26-C25	2.74	126.40	122.70
25	B	603	CLA	O2D-CGD-CBD	2.74	116.01	111.23
29	f	102	SQD	O5-C1-C2	-2.74	104.75	110.37
26	H	101	BCR	C2-C1-C6	2.73	114.41	110.44
25	C	508	CLA	C3B-C4B-NB	-2.73	108.09	110.53
25	c	504	CLA	O2A-CGA-O1A	-2.73	116.80	123.63
26	K	101	BCR	C2-C1-C6	2.73	114.40	110.44
27	A	610	PL9	C22-C23-C24	-2.72	121.40	127.62
30	d	407	LHG	O8-C23-O10	-2.72	116.83	123.63
31	h	102	DGD	O6D-C1D-O3G	-2.72	103.62	110.04
26	b	619	BCR	C7-C8-C9	-2.72	122.22	126.23
25	c	507	CLA	C3B-C4B-NB	-2.72	108.11	110.53
28	C	517	LMG	O1-C7-C8	-2.71	104.23	110.82
25	B	602	CLA	O2A-CGA-O1A	-2.71	116.86	123.63
25	C	505	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	c	513	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
30	d	408	LHG	O8-C23-C24	2.70	120.07	111.83
25	B	604	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	b	609	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
25	a	611	CLA	CHB-C4A-NA	2.69	128.29	124.40
25	C	504	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
25	B	612	CLA	C3B-C4B-NB	-2.69	108.13	110.53
35	v	201	HEC	CBD-CAD-C3D	-2.69	105.09	112.53
25	b	614	CLA	C1-C2-C3	-2.69	121.79	126.20
25	b	607	CLA	CHD-C1D-ND	-2.69	121.02	124.80
28	b	622	LMG	C8-O7-C10	2.69	124.23	117.80
26	B	619	BCR	C38-C26-C25	-2.68	121.56	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	502	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	B	602	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
25	B	613	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
26	B	618	BCR	C7-C8-C9	-2.68	122.27	126.23
26	K	102	BCR	C33-C5-C6	-2.68	121.56	124.48
25	a	611	CLA	C1D-ND-C4D	2.68	108.19	106.31
31	J	101	DGD	CDB-CCB-CBB	-2.68	100.83	114.37
31	h	102	DGD	C6D-C5D-C4D	2.68	117.68	112.07
25	A	607	CLA	O2A-CGA-O1A	-2.68	116.94	123.63
25	a	608	CLA	CHB-C4A-NA	2.67	128.26	124.40
25	c	503	CLA	CHB-C4A-NA	2.67	128.26	124.40
31	c	517	DGD	CDB-CCB-CBB	-2.67	100.86	114.37
25	C	510	CLA	C3B-C4B-NB	-2.67	108.15	110.53
26	C	514	BCR	C15-C16-C17	-2.67	118.06	123.52
27	A	610	PL9	C36-C34-C33	-2.66	115.19	121.17
26	t	101	BCR	C27-C26-C25	2.66	126.30	122.70
25	b	610	CLA	C3B-C4B-NB	-2.65	108.16	110.53
29	A	613	SQD	O9-S-C6	2.65	110.72	106.76
29	B	623	SQD	O9-S-C6	2.65	110.71	106.76
29	a	612	SQD	O8-S-C6	2.65	111.08	105.97
26	k	102	BCR	C27-C26-C25	2.65	126.28	122.70
25	b	604	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
25	B	601	CLA	CHB-C4A-NA	2.64	128.22	124.40
25	c	512	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	a	608	CLA	O2D-CGD-CBD	2.64	115.84	111.23
26	k	103	BCR	C27-C26-C25	2.64	126.27	122.70
34	f	101	HEM	CAB-C3B-C2B	-2.64	119.86	128.43
34	f	101	HEM	C3B-C2B-C1B	2.64	108.39	106.41
25	C	510	CLA	O2D-CGD-CBD	2.64	115.84	111.23
25	b	602	CLA	C3B-C4B-NB	-2.64	108.18	110.53
25	c	513	CLA	CHB-C4A-NA	2.63	128.20	124.40
25	C	504	CLA	CHB-C1B-NB	2.63	128.00	124.05
30	D	412	LHG	C11-C10-C9	-2.63	101.07	114.37
25	A	607	CLA	C1-C2-C3	-2.63	121.89	126.20
26	b	618	BCR	C27-C26-C25	2.63	126.25	122.70
31	c	515	DGD	C3G-C2G-C1G	-2.62	105.67	111.78
25	C	501	CLA	CHB-C1B-NB	2.62	127.99	124.05
27	a	610	PL9	O1-C4-C3	-2.62	117.96	120.73
25	B	607	CLA	C3B-C4B-NB	-2.62	108.19	110.53
30	d	407	LHG	C11-C10-C9	-2.62	101.13	114.37
25	C	508	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
25	C	501	CLA	C1-C2-C3	-2.62	121.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	413	STE	C3-C2-C1	-2.61	107.69	114.51
25	D	404	CLA	CHB-C4A-NA	2.61	128.17	124.40
25	C	501	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
25	A	607	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
31	h	102	DGD	C1E-O6E-C5E	2.61	118.81	113.72
29	A	613	SQD	O5-C1-C2	-2.60	105.02	110.37
25	c	501	CLA	CHB-C4A-NA	2.60	128.16	124.40
25	b	610	CLA	C1-C2-C3	-2.60	121.93	126.20
25	c	510	CLA	C16-C15-C13	-2.60	107.31	115.97
25	c	502	CLA	C1-C2-C3	-2.60	121.94	126.20
25	B	607	CLA	CED-O2D-CGD	2.60	121.81	115.92
25	C	505	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
25	a	606	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
31	c	516	DGD	CDB-CCB-CBB	-2.60	101.25	114.37
26	C	514	BCR	C15-C14-C13	-2.60	123.64	127.28
25	b	607	CLA	CHB-C4A-NA	2.59	128.14	124.40
25	b	605	CLA	CHD-C1D-ND	-2.59	121.16	124.80
25	D	403	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
25	c	511	CLA	CHB-C4A-NA	2.58	128.13	124.40
25	b	606	CLA	C1-C2-C3	-2.58	121.98	126.20
25	C	513	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
26	b	619	BCR	C2-C1-C6	2.57	114.17	110.44
26	b	617	BCR	C3-C4-C5	-2.57	109.47	114.06
25	d	403	CLA	C3B-C4B-NB	-2.57	108.24	110.53
25	a	605	CLA	CHB-C4A-NA	2.57	128.10	124.40
31	c	516	DGD	O3D-C3D-C4D	-2.57	104.33	110.38
25	c	509	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
30	D	412	LHG	O8-C23-O10	-2.56	117.22	123.63
25	c	505	CLA	CHB-C4A-NA	2.56	128.10	124.40
28	m	101	LMG	C38-C37-C36	-2.56	101.45	114.37
25	B	614	CLA	C1-C2-C3	-2.56	122.01	126.20
25	d	404	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
27	A	610	PL9	O2-C1-C6	2.55	124.54	120.48
25	A	607	CLA	C3B-C4B-NB	-2.55	108.26	110.53
25	A	608	CLA	C3B-C4B-NB	-2.54	108.26	110.53
27	A	610	PL9	O2-C1-C2	-2.54	116.05	121.83
27	D	406	PL9	C8-C7-C3	2.54	118.60	112.03
25	a	605	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
25	d	404	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
25	c	506	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
25	C	509	CLA	C3B-C4B-NB	-2.54	108.26	110.53
25	c	508	CLA	O2A-CGA-O1A	-2.54	117.28	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	521	LMG	O7-C10-O9	-2.53	117.78	123.70
31	c	516	DGD	O6E-C1E-O5D	-2.53	104.06	110.04
27	d	406	PL9	C37-C38-C39	-2.53	121.83	127.62
25	B	606	CLA	CGD-CBD-CAD	-2.53	102.66	110.85
31	h	102	DGD	O6E-C5E-C4E	2.53	114.26	109.70
27	D	406	PL9	C36-C34-C33	-2.53	115.49	121.17
25	a	611	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
29	D	408	SQD	C3-C4-C5	2.53	114.81	110.23
26	H	101	BCR	C16-C15-C14	-2.53	118.35	123.52
25	D	403	CLA	C1-C2-C3	-2.53	122.06	126.20
35	v	201	HEC	CHA-C4D-ND	2.52	127.14	124.42
27	a	610	PL9	C37-C38-C39	-2.52	121.84	127.62
26	B	619	BCR	C15-C16-C17	-2.52	118.35	123.52
27	D	406	PL9	C40-C39-C41	2.52	119.61	115.23
25	C	508	CLA	C1-C2-C3	-2.52	122.06	126.20
31	c	516	DGD	O2D-C2D-C1D	-2.52	104.06	110.08
27	A	610	PL9	C7-C8-C9	-2.52	122.49	126.83
25	b	608	CLA	O2D-CGD-CBD	2.52	115.64	111.23
25	b	604	CLA	C6-C7-C8	-2.52	107.59	115.97
32	B	624	STE	C3-C2-C1	-2.52	107.94	114.51
25	B	609	CLA	C7-C6-C5	-2.52	106.55	113.26
28	m	101	LMG	C40-C39-C38	-2.52	101.65	114.37
25	b	606	CLA	C3B-C4B-NB	-2.51	108.28	110.53
25	b	602	CLA	C1-C2-C3	-2.51	122.08	126.20
26	C	514	BCR	C2-C1-C6	2.51	114.09	110.44
25	A	608	CLA	O2D-CGD-CBD	2.51	115.62	111.23
29	f	102	SQD	O47-C7-C8	2.51	120.15	110.93
34	E	101	HEM	CBD-CAD-C3D	-2.51	105.59	112.53
26	A	609	BCR	C7-C8-C9	-2.51	122.52	126.23
26	a	609	BCR	C7-C8-C9	-2.51	122.52	126.23
25	c	510	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
29	b	620	SQD	O8-S-C6	2.51	110.81	105.97
32	B	626	STE	O2-C1-C2	2.51	121.92	114.00
25	a	606	CLA	CHD-C1D-ND	-2.51	121.28	124.80
28	D	411	LMG	O1-C7-C8	-2.50	105.33	111.77
25	D	403	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	B	601	CLA	CAA-C2A-C3A	-2.50	106.24	113.00
31	A	616	DGD	CDB-CCB-CBB	-2.50	101.73	114.37
25	b	607	CLA	CMB-C2B-C1B	-2.50	121.62	125.42
29	b	620	SQD	O2-C2-C1	2.50	116.02	110.08
25	b	607	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
26	a	609	BCR	C3-C4-C5	-2.49	109.61	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	407	LMG	O8-C28-O10	-2.49	117.39	123.63
27	d	406	PL9	C8-C7-C3	2.49	118.47	112.03
31	C	516	DGD	C3E-C4E-C5E	-2.49	105.72	110.23
27	A	610	PL9	C40-C39-C41	2.49	119.55	115.23
28	c	518	LMG	O6-C1-O1	-2.49	104.16	110.04
25	A	608	CLA	CHD-C4C-NC	2.49	128.09	124.23
25	B	606	CLA	CHB-C4A-NA	2.49	127.99	124.40
27	d	406	PL9	C27-C28-C29	-2.48	121.94	127.62
30	A	614	LHG	C11-C10-C9	-2.48	101.83	114.37
27	a	610	PL9	C40-C39-C41	2.48	119.53	115.23
25	b	613	CLA	CED-O2D-CGD	2.48	121.53	115.92
34	f	101	HEM	CBD-CAD-C3D	-2.47	105.69	112.53
27	D	406	PL9	C20-C19-C21	2.47	119.52	115.23
31	c	515	DGD	O3E-C3E-C2E	-2.47	104.55	110.38
27	D	406	PL9	C7-C8-C9	-2.47	122.57	126.83
33	D	402	PHO	OBD-CAD-CBD	-2.47	122.20	125.82
26	B	619	BCR	C15-C14-C13	-2.47	123.81	127.28
27	a	610	PL9	C12-C13-C14	-2.47	121.97	127.62
31	h	102	DGD	O5E-C6E-C5E	-2.47	102.93	111.33
25	b	610	CLA	CAA-CBA-CGA	-2.47	106.20	113.21
28	d	411	LMG	C40-C39-C38	-2.47	101.89	114.37
25	B	608	CLA	O2D-CGD-CBD	2.47	115.54	111.23
30	D	410	LHG	C11-C10-C9	-2.47	101.90	114.37
25	b	604	CLA	CAC-C3C-C4C	2.47	128.00	124.79
25	C	512	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
25	b	615	CLA	C1-C2-C3	-2.47	122.16	126.20
31	c	515	DGD	CDB-CCB-CBB	-2.46	101.91	114.37
25	B	609	CLA	C3B-C4B-NB	-2.46	108.33	110.53
31	C	516	DGD	C4E-C3E-C2E	-2.46	106.51	110.83
28	c	520	LMG	C38-C37-C36	-2.46	101.93	114.37
30	d	408	LHG	C11-C10-C9	-2.46	101.93	114.37
28	D	407	LMG	O3-C3-C2	-2.46	104.59	110.38
25	A	611	CLA	C11-C12-C13	-2.46	107.80	115.97
32	L	102	STE	O2-C1-C2	2.45	121.76	114.00
28	c	520	LMG	O3-C3-C2	-2.45	104.59	110.38
25	B	613	CLA	CHC-C4B-NB	2.45	127.73	124.05
27	A	610	PL9	C20-C19-C21	2.45	119.48	115.23
28	A	612	LMG	C40-C39-C38	-2.45	101.99	114.37
29	D	408	SQD	C44-O6-C1	-2.44	109.51	113.68
30	L	101	LHG	C20-C19-C18	-2.44	102.02	114.37
27	d	406	PL9	O2-C1-C6	2.44	124.36	120.48
25	b	601	CLA	CHB-C4A-NA	2.44	127.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	611	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	C	502	CLA	CHD-C1D-ND	-2.44	121.37	124.80
25	c	504	CLA	CMB-C2B-C3B	2.43	132.27	126.55
31	C	515	DGD	C6D-O5D-C1E	2.43	119.00	113.80
25	C	504	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
25	d	404	CLA	C1-C2-C3	-2.42	122.23	126.20
33	d	402	PHO	OBD-CAD-CBD	-2.42	122.27	125.82
25	B	611	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
25	A	607	CLA	C1D-ND-C4D	2.42	108.01	106.31
25	B	601	CLA	C2A-C1A-CHA	2.42	128.06	123.87
28	B	620	LMG	O7-C10-O9	-2.41	118.06	123.70
25	B	605	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
27	D	406	PL9	O1-C4-C3	-2.41	118.19	120.73
25	b	601	CLA	O2D-CGD-CBD	2.41	115.44	111.23
25	b	605	CLA	O1D-CGD-CBD	2.41	129.26	124.52
30	D	412	LHG	C18-C17-C16	-2.40	102.21	114.37
31	c	515	DGD	O6D-C1D-O3G	-2.40	104.36	110.04
31	h	102	DGD	CBB-CAB-C9B	-2.40	102.22	114.37
25	b	612	CLA	CMB-C2B-C3B	2.40	132.20	126.55
30	l	101	LHG	C11-C10-C9	-2.40	102.23	114.37
25	c	504	CLA	C3B-C4B-NB	-2.40	108.39	110.53
25	A	607	CLA	C2A-C1A-CHA	2.40	128.03	123.87
26	D	405	BCR	C24-C23-C22	-2.40	122.68	126.23
30	A	614	LHG	C20-C19-C18	-2.40	102.25	114.37
31	H	102	DGD	C3G-C2G-C1G	-2.40	106.20	111.78
25	B	609	CLA	CHC-C4B-NB	2.39	127.64	124.05
25	C	513	CLA	CHB-C4A-NA	2.39	127.85	124.40
31	c	517	DGD	CAB-C9B-C8B	-2.39	102.27	114.37
25	C	508	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	C	509	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
28	C	517	LMG	C40-C39-C38	-2.39	102.30	114.37
30	l	101	LHG	C20-C19-C18	-2.39	102.30	114.37
25	b	607	CLA	CHD-C4C-NC	2.38	127.93	124.23
35	V	201	HEC	C1D-C2D-C3D	-2.38	104.47	106.98
25	C	508	CLA	CHB-C4A-NA	2.38	127.84	124.40
30	D	409	LHG	C20-C19-C18	-2.38	102.32	114.37
25	B	603	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
28	A	612	LMG	C38-C37-C36	-2.38	102.33	114.37
25	C	510	CLA	C11-C10-C8	-2.38	108.05	115.97
28	c	520	LMG	O2-C2-C1	-2.38	104.40	110.08
25	C	506	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	B	605	CLA	CHD-C1D-C2D	2.38	130.44	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
25	B	602	CLA	CMB-C2B-C3B	2.38	132.14	126.55
25	c	509	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
27	d	406	PL9	O1-C4-C3	-2.37	118.23	120.73
28	b	622	LMG	C40-C39-C38	-2.37	102.37	114.37
25	B	609	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
25	B	614	CLA	CHB-C1B-NB	2.37	127.61	124.05
25	B	608	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
31	a	614	DGD	CBB-CAB-C9B	-2.37	102.39	114.37
25	b	612	CLA	C11-C12-C13	-2.37	108.09	115.97
25	c	502	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
29	f	102	SQD	C3-C4-C5	2.37	114.52	110.23
31	c	516	DGD	CBB-CAB-C9B	-2.37	102.41	114.37
25	B	612	CLA	C11-C12-C13	-2.36	108.11	115.97
25	b	606	CLA	CHB-C4A-NA	2.36	127.81	124.40
25	B	616	CLA	C1-O2A-CGA	2.36	122.37	116.65
25	b	601	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
25	c	506	CLA	CHB-C4A-NA	2.36	127.81	124.40
25	D	403	CLA	O2D-CGD-CBD	2.36	115.36	111.23
26	K	102	BCR	C27-C26-C25	2.36	125.89	122.70
32	j	101	STE	O2-C1-C2	2.36	121.45	114.00
28	c	520	LMG	O7-C10-O9	-2.36	118.19	123.70
30	D	410	LHG	O8-C6-C5	-2.36	101.60	108.40
25	b	605	CLA	CHB-C4A-NA	2.35	127.80	124.40
28	d	411	LMG	O1-C7-C8	-2.35	105.10	110.82
25	C	509	CLA	CED-O2D-CGD	2.35	121.25	115.92
31	c	516	DGD	O3G-C1D-C2D	-2.35	104.70	108.27
31	c	516	DGD	C3G-C2G-C1G	-2.35	106.30	111.78
25	B	603	CLA	C4-C3-C5	2.35	119.31	115.23
25	C	502	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
30	d	409	LHG	O8-C23-C24	2.35	118.99	111.83
26	D	405	BCR	C7-C8-C9	-2.34	122.77	126.23
25	C	511	CLA	C3B-C4B-NB	-2.34	108.44	110.53
25	B	616	CLA	CHB-C4A-NA	2.34	127.78	124.40
31	A	616	DGD	CAB-C9B-C8B	-2.34	102.52	114.37
33	a	607	PHO	C3B-C4B-NB	-2.34	105.94	107.46
25	b	604	CLA	O2D-CGD-CBD	2.34	115.33	111.23
27	a	610	PL9	O2-C1-C2	-2.34	116.50	121.83
27	a	610	PL9	C27-C28-C29	-2.34	122.26	127.62
25	D	404	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
25	A	608	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
25	c	510	CLA	O2D-CGD-O1D	-2.34	119.29	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	517	LMG	C38-C37-C36	-2.34	102.54	114.37
26	B	617	BCR	C27-C26-C25	2.34	125.86	122.70
25	B	615	CLA	O2D-CGD-CBD	2.34	115.32	111.23
27	d	406	PL9	C42-C43-C44	-2.34	122.27	127.62
25	C	507	CLA	C1-C2-C3	-2.34	122.37	126.20
25	A	611	CLA	C1-C2-C3	-2.34	122.37	126.20
25	B	603	CLA	CHB-C4A-NA	2.33	127.77	124.40
31	C	516	DGD	O5D-C1E-C2E	2.33	111.82	108.27
25	A	606	CLA	O1D-CGD-CBD	2.33	129.12	124.52
31	h	102	DGD	O3E-C3E-C2E	-2.33	104.88	110.38
31	C	516	DGD	CBB-CAB-C9B	-2.33	102.59	114.37
25	C	513	CLA	CHD-C1D-C2D	2.33	130.33	125.49
30	d	409	LHG	C27-C26-C25	-2.33	102.60	114.37
30	e	101	LHG	C11-C10-C9	-2.33	102.60	114.37
25	c	505	CLA	C1D-ND-C4D	2.33	107.94	106.31
26	B	618	BCR	C15-C14-C13	-2.32	124.02	127.28
25	b	603	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
31	H	102	DGD	CAB-C9B-C8B	-2.32	102.64	114.37
28	d	411	LMG	O3-C3-C2	-2.32	104.91	110.38
28	c	520	LMG	C40-C39-C38	-2.32	102.64	114.37
31	a	614	DGD	C1G-C2G-C3G	-2.32	106.45	111.80
28	D	407	LMG	O2-C2-C1	-2.32	104.56	110.08
25	C	507	CLA	O2D-CGD-CBD	2.31	115.28	111.23
25	b	612	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
25	B	612	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
25	b	613	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	D	403	CLA	C6-C5-C3	2.31	119.09	113.47
31	h	102	DGD	C3G-C2G-C1G	-2.31	106.40	111.78
30	d	408	LHG	C20-C19-C18	-2.31	102.69	114.37
28	c	520	LMG	O6-C1-O1	-2.31	104.59	110.04
25	B	613	CLA	CED-O2D-CGD	2.31	121.15	115.92
25	B	604	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	c	507	CLA	CHC-C4B-NB	2.30	127.50	124.05
31	C	516	DGD	C1D-C2D-C3D	-2.30	105.17	110.01
28	A	612	LMG	O1-C7-C8	-2.30	105.22	110.82
28	d	411	LMG	C38-C37-C36	-2.30	102.73	114.37
28	b	622	LMG	O6-C1-O1	-2.30	104.61	110.04
25	c	508	CLA	C1-C2-C3	-2.30	122.43	126.20
25	b	605	CLA	CHD-C4C-NC	2.30	127.80	124.23
25	c	507	CLA	C4-C3-C5	2.30	119.22	115.23
25	C	510	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
25	B	610	CLA	CHD-C1D-ND	-2.30	121.57	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C33-C5-C6	-2.29	121.98	124.48
25	a	605	CLA	O1D-CGD-CBD	2.29	129.04	124.52
25	C	505	CLA	O2D-CGD-CBD	2.29	115.24	111.23
25	C	506	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
25	b	614	CLA	CHB-C4A-NA	2.29	127.71	124.40
25	b	615	CLA	CHB-C4A-NA	2.29	127.71	124.40
29	f	102	SQD	O48-C23-C24	2.29	118.82	111.83
25	b	609	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
27	a	610	PL9	O2-C1-C6	2.29	124.12	120.48
25	b	613	CLA	CMB-C2B-C3B	2.29	131.93	126.55
25	c	511	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
26	C	514	BCR	C27-C26-C25	2.29	125.79	122.70
25	B	614	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
31	c	517	DGD	C6D-C5D-C4D	2.28	116.86	112.07
28	B	620	LMG	O1-C7-C8	-2.28	105.26	110.82
25	c	502	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
31	C	515	DGD	O1G-C1A-C2A	-2.28	104.87	111.83
31	J	101	DGD	O5E-C6E-C5E	-2.28	103.56	111.33
29	A	613	SQD	O47-C7-O49	-2.28	118.37	123.70
28	c	518	LMG	C40-C39-C38	-2.28	102.84	114.37
27	a	610	PL9	C22-C23-C24	-2.28	122.40	127.62
26	K	103	BCR	C24-C23-C22	-2.28	122.86	126.23
31	C	515	DGD	O3E-C3E-C2E	-2.28	105.00	110.38
31	c	517	DGD	C3G-C2G-C1G	-2.28	106.47	111.78
30	D	409	LHG	O8-C23-O10	-2.28	117.93	123.63
28	m	101	LMG	C1-O6-C5	-2.28	109.27	113.72
25	C	508	CLA	CHD-C1D-C2D	2.28	130.22	125.49
25	A	607	CLA	CMB-C2B-C3B	2.27	131.90	126.55
30	D	409	LHG	C11-C10-C9	-2.27	102.89	114.37
30	e	101	LHG	C20-C19-C18	-2.27	102.91	114.37
25	B	612	CLA	C1-C2-C3	-2.27	122.48	126.20
25	B	614	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
29	D	408	SQD	O7-S-C6	2.27	110.14	106.76
28	c	521	LMG	C38-C37-C36	-2.26	102.92	114.37
25	b	613	CLA	C7-C6-C5	-2.26	107.23	113.26
25	B	602	CLA	C16-C15-C13	-2.26	108.44	115.97
32	t	102	STE	O2-C1-C2	2.26	121.15	114.00
25	c	503	CLA	O1D-CGD-CBD	2.26	128.98	124.52
28	D	407	LMG	O1-C1-C2	-2.26	104.84	108.27
25	B	614	CLA	CHC-C4B-NB	2.26	127.44	124.05
25	a	606	CLA	CHD-C1D-C2D	2.26	130.19	125.49
25	B	605	CLA	CHB-C4A-NA	2.26	127.66	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
28	B	620	LMG	C40-C39-C38	-2.26	102.96	114.37
25	b	611	CLA	CHD-C1D-ND	-2.26	121.63	124.80
26	b	617	BCR	C15-C14-C13	-2.25	124.12	127.28
26	k	103	BCR	C33-C5-C6	-2.25	122.03	124.48
28	c	518	LMG	C38-C37-C36	-2.25	102.99	114.37
30	D	410	LHG	C27-C26-C25	-2.25	102.99	114.37
25	b	610	CLA	O1D-CGD-CBD	2.25	128.95	124.52
25	a	605	CLA	C4-C3-C5	2.25	119.13	115.23
31	A	616	DGD	C8B-C7B-C6B	-2.25	103.01	114.37
31	A	616	DGD	O6D-C1D-O3G	-2.25	104.74	110.04
25	b	616	CLA	CHD-C1D-ND	-2.25	121.64	124.80
25	A	608	CLA	CHD-C1D-C2D	2.25	130.16	125.49
28	D	411	LMG	C38-C37-C36	-2.24	103.02	114.37
25	C	503	CLA	CHB-C4A-NA	2.24	127.64	124.40
26	h	101	BCR	C7-C8-C9	-2.24	122.92	126.23
31	c	515	DGD	O5D-C6D-C5D	-2.24	104.36	109.42
29	A	615	SQD	O48-C23-C24	2.24	118.67	111.83
25	B	614	CLA	O2D-CGD-CBD	2.24	115.15	111.23
29	B	623	SQD	C45-O47-C7	-2.24	112.43	117.80
25	b	609	CLA	C7-C6-C5	-2.24	107.30	113.26
25	A	607	CLA	CHC-C4B-NB	2.24	127.40	124.05
26	d	405	BCR	C7-C8-C9	-2.23	122.93	126.23
25	c	509	CLA	C3B-C4B-NB	-2.23	108.54	110.53
30	D	409	LHG	C27-C26-C25	-2.23	103.10	114.37
32	E	102	STE	O2-C1-C2	2.23	121.04	114.00
25	c	508	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
28	b	622	LMG	C42-C41-C40	-2.23	103.11	114.37
25	a	611	CLA	CHD-C1D-C2D	2.22	130.11	125.49
25	B	608	CLA	CHB-C4A-NA	2.22	127.61	124.40
30	D	412	LHG	C20-C19-C18	-2.22	103.14	114.37
25	b	611	CLA	CHD-C1D-C2D	2.22	130.10	125.49
25	C	503	CLA	C16-C15-C13	-2.22	108.59	115.97
25	B	610	CLA	O1D-CGD-CBD	2.22	128.89	124.52
30	D	410	LHG	O8-C23-C24	2.22	118.59	111.83
31	H	102	DGD	C8B-C7B-C6B	-2.22	103.16	114.37
27	d	406	PL9	C32-C33-C34	-2.22	122.55	127.62
28	D	407	LMG	C38-C37-C36	-2.21	103.18	114.37
25	B	606	CLA	CHD-C4C-NC	2.21	127.66	124.23
25	a	605	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
31	J	101	DGD	O3G-C1D-C2D	-2.21	104.92	108.27
26	K	101	BCR	C24-C23-C22	-2.21	122.97	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	607	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
25	C	507	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
25	C	505	CLA	CMB-C2B-C3B	2.21	131.74	126.55
25	b	610	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
25	b	614	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
25	B	609	CLA	C1-C2-C3	-2.21	122.58	126.20
31	C	515	DGD	C3D-C4D-C5D	-2.20	106.24	110.23
31	c	516	DGD	C7B-C6B-C5B	-2.20	103.25	114.37
31	H	102	DGD	O6D-C1D-O3G	-2.20	104.85	110.04
26	c	514	BCR	C11-C10-C9	-2.20	124.20	127.28
29	A	613	SQD	O48-C23-C24	2.20	118.53	111.83
28	b	622	LMG	C38-C37-C36	-2.20	103.27	114.37
25	c	509	CLA	CMB-C2B-C3B	2.19	131.71	126.55
31	J	101	DGD	CBB-CAB-C9B	-2.19	103.28	114.37
25	b	610	CLA	CHB-C4A-NA	2.19	127.56	124.40
28	c	521	LMG	C40-C39-C38	-2.19	103.29	114.37
25	B	601	CLA	O2D-CGD-CBD	2.19	115.06	111.23
34	E	101	HEM	CHD-C4C-C3C	2.19	128.90	125.21
25	b	613	CLA	CHB-C1B-NB	2.19	127.33	124.05
26	k	101	BCR	C33-C5-C6	-2.19	122.10	124.48
25	B	604	CLA	C1-C2-C3	-2.19	122.61	126.20
35	V	201	HEC	CBB-CAB-C3B	-2.18	106.50	112.42
31	h	102	DGD	O5D-C1E-C2E	2.18	111.59	108.27
25	B	615	CLA	CHC-C4B-NB	2.18	127.32	124.05
26	b	618	BCR	C30-C25-C26	-2.18	119.65	122.64
26	c	514	BCR	C33-C5-C6	-2.18	122.10	124.48
31	c	517	DGD	C7A-C6A-C5A	-2.18	103.34	114.37
25	C	503	CLA	C1-O2A-CGA	2.18	121.93	116.65
26	t	101	BCR	C35-C13-C14	-2.18	119.28	122.82
25	B	603	CLA	C5-C3-C2	-2.18	116.27	121.17
26	d	405	BCR	C30-C25-C26	-2.18	119.66	122.64
34	E	101	HEM	C4D-ND-C1D	2.18	107.79	105.21
25	C	512	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
25	a	611	CLA	CMB-C2B-C3B	2.18	131.67	126.55
26	A	609	BCR	C15-C16-C17	-2.18	119.06	123.52
31	a	614	DGD	C5B-C4B-C3B	-2.18	103.37	114.37
25	a	611	CLA	CHD-C1D-ND	-2.18	121.74	124.80
25	b	601	CLA	CHD-C1D-ND	-2.17	121.74	124.80
25	A	608	CLA	CMB-C2B-C3B	2.17	131.66	126.55
30	D	410	LHG	C18-C17-C16	-2.17	103.39	114.37
31	A	616	DGD	O5D-C6D-C5D	-2.17	104.52	109.42
25	B	604	CLA	CHC-C4B-NB	2.17	127.31	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	515	DGD	CBB-CAB-C9B	-2.17	103.40	114.37
26	C	514	BCR	C33-C5-C6	-2.17	122.12	124.48
25	c	502	CLA	CHD-C1D-ND	-2.17	121.75	124.80
25	d	403	CLA	CHB-C4A-NA	2.17	127.53	124.40
31	C	515	DGD	CBB-CAB-C9B	-2.17	103.41	114.37
26	T	101	BCR	C30-C25-C26	-2.17	119.67	122.64
31	c	517	DGD	C5B-C4B-C3B	-2.17	103.41	114.37
26	d	405	BCR	C1-C6-C5	-2.17	119.67	122.64
25	C	511	CLA	CHB-C4A-NA	2.17	127.53	124.40
28	C	517	LMG	O8-C28-O10	-2.17	118.21	123.63
26	T	101	BCR	C38-C26-C27	-2.17	108.98	113.60
25	A	607	CLA	CHB-C4A-NA	2.16	127.52	124.40
25	B	604	CLA	CAA-CBA-CGA	-2.16	107.07	113.21
25	b	614	CLA	O1D-CGD-CBD	2.16	128.78	124.52
25	C	507	CLA	C2A-C1A-CHA	2.16	127.61	123.87
30	D	412	LHG	C15-C14-C13	-2.16	103.45	114.37
30	e	101	LHG	C27-C26-C25	-2.16	103.47	114.37
26	b	617	BCR	C33-C5-C6	-2.15	122.13	124.48
31	J	101	DGD	C7B-C6B-C5B	-2.15	103.48	114.37
28	C	517	LMG	O7-C10-O9	-2.15	118.67	123.70
25	B	613	CLA	CHB-C4A-NA	2.15	127.51	124.40
25	c	503	CLA	C11-C12-C13	-2.15	108.81	115.97
25	c	510	CLA	CHB-C4A-NA	2.15	127.51	124.40
28	B	622	LMG	C38-C37-C36	-2.15	103.49	114.37
31	A	616	DGD	O2D-C2D-C1D	-2.15	104.95	110.08
25	B	607	CLA	CHC-C4B-NB	2.15	127.28	124.05
25	C	509	CLA	CMB-C2B-C3B	2.15	131.61	126.55
34	f	101	HEM	C4D-ND-C1D	2.15	107.75	105.21
25	C	508	CLA	CMB-C2B-C3B	2.15	131.61	126.55
26	b	618	BCR	C2-C1-C6	2.15	113.56	110.44
28	c	518	LMG	O1-C7-C8	-2.15	105.60	110.82
25	b	604	CLA	C2D-C1D-ND	-2.15	108.00	110.13
25	b	609	CLA	O1D-CGD-CBD	2.14	128.75	124.52
26	h	101	BCR	C24-C23-C22	-2.14	123.06	126.23
26	t	101	BCR	C2-C1-C6	2.14	113.55	110.44
25	B	616	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
28	b	622	LMG	C4-C3-C2	2.14	114.59	110.83
25	B	607	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
28	A	612	LMG	O8-C28-O10	-2.14	118.27	123.63
29	A	613	SQD	C44-O6-C1	-2.14	109.21	113.80
25	b	613	CLA	C16-C15-C13	-2.14	108.85	115.97
31	H	102	DGD	O1G-C1A-O1A	-2.14	118.28	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	607	PHO	O2A-CGA-O1A	-2.14	118.28	123.63
26	t	101	BCR	C1-C6-C5	-2.14	119.71	122.64
25	B	608	CLA	CMB-C2B-C3B	2.14	131.58	126.55
32	C	518	STE	C3-C2-C1	-2.14	108.93	114.51
26	d	405	BCR	C38-C26-C25	-2.14	122.15	124.48
26	t	101	BCR	C7-C8-C9	-2.14	123.08	126.23
29	a	612	SQD	O5-C1-C2	-2.13	105.98	110.37
28	B	620	LMG	C38-C37-C36	-2.13	103.58	114.37
31	c	516	DGD	O5D-C6D-C5D	-2.13	104.61	109.42
25	b	611	CLA	C1-C2-C3	-2.13	122.70	126.20
25	c	512	CLA	CHA-C1A-NA	-2.13	121.56	126.39
28	m	101	LMG	O6-C1-O1	-2.13	105.01	110.04
31	c	515	DGD	C7A-C6A-C5A	-2.13	103.59	114.37
35	V	201	HEC	CMD-C2D-C1D	2.13	128.36	125.03
25	b	616	CLA	C3B-C4B-NB	-2.13	108.63	110.53
31	C	515	DGD	O5D-C6D-C5D	-2.13	104.62	109.42
25	B	605	CLA	CHD-C4C-NC	2.13	127.53	124.23
32	t	102	STE	O2-C1-O1	-2.13	117.86	123.33
26	k	101	BCR	C15-C14-C13	-2.12	124.30	127.28
25	B	605	CLA	O1D-CGD-CBD	2.12	128.71	124.52
26	B	619	BCR	C27-C26-C25	2.12	125.57	122.70
30	e	101	LHG	C5-O7-C7	-2.12	112.72	117.80
25	b	609	CLA	CHB-C4A-NA	2.12	127.46	124.40
25	C	513	CLA	CHD-C4C-NC	2.12	127.52	124.23
27	D	406	PL9	C50-C49-C48	-2.12	116.29	122.66
25	c	503	CLA	C4-C3-C5	2.12	118.91	115.23
25	c	513	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
25	a	605	CLA	C1-C2-C3	-2.12	122.73	126.20
31	c	516	DGD	C1D-O6D-C5D	-2.12	109.58	113.72
25	C	504	CLA	C1-C2-C3	-2.12	122.73	126.20
26	B	619	BCR	C3-C4-C5	-2.12	110.28	114.06
31	J	101	DGD	O6E-C5E-C4E	2.12	113.51	109.70
25	C	504	CLA	CHD-C1D-ND	-2.12	121.83	124.80
28	c	521	LMG	O8-C28-O10	-2.12	118.34	123.63
25	C	503	CLA	CHD-C1D-C2D	2.11	129.88	125.49
27	D	406	PL9	C35-C34-C36	2.11	118.90	115.23
28	A	612	LMG	O6-C1-O1	-2.11	105.05	110.04
30	D	409	LHG	C18-C17-C16	-2.11	103.69	114.37
25	c	508	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
25	b	604	CLA	C11-C10-C8	-2.11	108.95	115.97
25	b	607	CLA	CMB-C2B-C3B	2.11	131.51	126.55
34	f	101	HEM	C1B-NB-C4B	2.11	107.70	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	512	CLA	O2D-CGD-CBD	2.11	114.91	111.23
25	b	603	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
26	b	618	BCR	C15-C16-C17	-2.11	119.21	123.52
34	E	101	HEM	CHC-C1C-NC	2.10	126.74	124.45
34	E	101	HEM	C2D-C1D-ND	-2.10	107.48	109.90
26	B	619	BCR	C10-C11-C12	-2.10	117.12	123.20
25	C	509	CLA	CHB-C4A-NA	2.10	127.43	124.40
31	A	616	DGD	O3G-C3G-C2G	-2.10	105.72	110.82
30	d	408	LHG	C18-C17-C16	-2.10	103.78	114.37
25	b	609	CLA	CHC-C4B-NB	2.09	127.19	124.05
31	C	515	DGD	CAB-C9B-C8B	-2.09	103.78	114.37
26	K	102	BCR	C1-C6-C5	-2.09	119.78	122.64
31	c	516	DGD	CAB-C9B-C8B	-2.09	103.79	114.37
29	D	408	SQD	C46-C45-C44	-2.09	106.91	113.67
26	h	101	BCR	C11-C10-C9	-2.09	124.34	127.28
31	C	516	DGD	O2D-C2D-C1D	-2.09	105.09	110.08
25	c	504	CLA	O2D-CGD-CBD	2.09	114.89	111.23
33	D	401	PHO	CMA-C3A-C4A	-2.09	110.11	114.61
25	B	610	CLA	CHB-C1B-NB	2.09	127.19	124.05
25	b	608	CLA	CHD-C4C-NC	2.09	127.47	124.23
26	b	617	BCR	C38-C26-C25	-2.09	122.20	124.48
28	b	622	LMG	O7-C10-O9	-2.09	118.82	123.70
31	a	614	DGD	CFB-CEB-CDB	-2.09	103.81	114.37
30	d	407	LHG	C20-C19-C18	-2.09	103.81	114.37
25	A	607	CLA	CHA-C4D-ND	2.09	136.86	132.55
25	A	608	CLA	C1-C2-C3	-2.09	122.78	126.20
26	H	101	BCR	C3-C4-C5	-2.09	110.33	114.06
28	d	410	LMG	C38-C37-C36	-2.08	103.83	114.37
31	J	101	DGD	C5B-C4B-C3B	-2.08	103.84	114.37
33	a	607	PHO	CBC-CAC-C3C	-2.08	109.89	112.87
25	B	603	CLA	CMB-C2B-C3B	2.08	131.45	126.55
31	c	517	DGD	O3E-C3E-C2E	-2.08	105.47	110.38
25	c	511	CLA	C1-C2-C3	-2.08	122.79	126.20
25	C	505	CLA	CHB-C4A-NA	2.08	127.40	124.40
31	A	616	DGD	CBB-CAB-C9B	-2.08	103.88	114.37
25	b	603	CLA	CMB-C2B-C3B	2.08	131.43	126.55
25	d	404	CLA	CMB-C2B-C3B	2.07	131.43	126.55
25	C	506	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
28	m	101	LMG	O2-C2-C1	-2.07	105.14	110.08
25	b	605	CLA	CHD-C1D-C2D	2.07	129.79	125.49
26	B	618	BCR	C29-C30-C25	2.07	113.45	110.44
31	c	516	DGD	C5B-C4B-C3B	-2.07	103.91	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C7-C8-C9	-2.07	123.17	126.23
25	B	612	CLA	CMB-C2B-C3B	2.07	131.41	126.55
25	d	404	CLA	C3B-C4B-NB	-2.07	108.68	110.53
25	b	607	CLA	C16-C15-C13	-2.07	109.09	115.97
26	K	101	BCR	C3-C4-C5	-2.07	110.37	114.06
25	C	503	CLA	CHD-C1D-ND	-2.06	121.90	124.80
25	C	507	CLA	CHD-C1D-ND	-2.06	121.90	124.80
25	d	403	CLA	O1D-CGD-CBD	2.06	128.59	124.52
25	b	616	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	b	602	CLA	C16-C15-C13	-2.06	109.11	115.97
25	C	512	CLA	C6-C5-C3	-2.06	108.44	113.47
28	c	521	LMG	C20-C19-C18	-2.06	103.94	114.37
25	b	602	CLA	C6-C7-C8	-2.06	109.12	115.97
34	f	101	HEM	CHC-C1C-NC	2.06	126.69	124.45
26	C	514	BCR	C35-C13-C14	-2.06	119.48	122.82
28	b	622	LMG	O2-C2-C1	-2.06	105.17	110.08
31	c	515	DGD	O2D-C2D-C1D	-2.06	105.17	110.08
25	C	508	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
25	B	611	CLA	CHD-C1D-C2D	2.05	129.76	125.49
26	c	514	BCR	C30-C25-C26	-2.05	119.83	122.64
25	b	611	CLA	C11-C10-C8	-2.05	109.14	115.97
31	J	101	DGD	O3E-C3E-C2E	-2.05	105.53	110.38
25	A	606	CLA	CHC-C1C-NC	2.05	127.41	124.31
28	c	518	LMG	O8-C28-O10	-2.05	118.49	123.63
25	A	607	CLA	CHA-C1A-NA	-2.05	121.74	126.39
27	d	406	PL9	C35-C34-C36	2.05	118.79	115.23
29	A	613	SQD	O8-S-C6	2.05	109.93	105.97
31	c	517	DGD	C8B-C7B-C6B	-2.05	104.01	114.37
25	c	506	CLA	O1D-CGD-CBD	2.05	128.56	124.52
26	A	609	BCR	C38-C26-C25	-2.05	122.25	124.48
25	b	608	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	B	612	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
25	B	604	CLA	C2D-C1D-ND	-2.05	108.10	110.13
25	c	502	CLA	CHB-C4A-NA	2.05	127.36	124.40
25	c	510	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	C	504	CLA	CHB-C4A-NA	2.05	127.35	124.40
25	b	605	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
25	b	608	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	b	601	CLA	CHD-C1D-C2D	2.05	129.74	125.49
25	B	614	CLA	CMB-C2B-C3B	2.04	131.36	126.55
26	B	619	BCR	C1-C6-C5	-2.04	119.84	122.64
25	c	510	CLA	CMB-C2B-C3B	2.04	131.36	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	410	LMG	C40-C39-C38	-2.04	104.04	114.37
28	c	520	LMG	C42-C41-C40	-2.04	104.04	114.37
25	C	506	CLA	O1D-CGD-CBD	2.04	128.55	124.52
25	b	616	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
30	d	408	LHG	O8-C23-O10	-2.04	118.52	123.63
31	c	516	DGD	C9B-C8B-C7B	-2.04	104.06	114.37
25	D	403	CLA	CED-O2D-CGD	2.04	120.54	115.92
25	c	511	CLA	C2A-C1A-CHA	2.04	127.40	123.87
28	c	521	LMG	O1-C7-C8	-2.04	105.86	110.82
25	B	604	CLA	CHA-C4D-ND	2.04	136.75	132.55
26	c	514	BCR	C2-C1-C6	2.04	113.40	110.44
31	A	616	DGD	C5B-C4B-C3B	-2.03	104.09	114.37
25	C	502	CLA	C3B-C4B-NB	-2.03	108.72	110.53
25	b	615	CLA	CHB-C1B-NB	2.03	127.10	124.05
28	D	411	LMG	O7-C10-O9	-2.03	118.95	123.70
26	T	101	BCR	C4-C5-C6	2.03	125.45	122.70
26	h	101	BCR	C3-C4-C5	-2.03	110.44	114.06
27	D	406	PL9	C7-C3-C2	-2.03	120.99	123.39
25	c	501	CLA	CHA-C4D-ND	2.03	136.73	132.55
28	B	620	LMG	C1-O6-C5	-2.03	109.76	113.72
25	C	504	CLA	CHD-C4C-NC	2.03	127.38	124.23
25	b	603	CLA	CHC-C4B-NB	2.03	127.09	124.05
28	d	411	LMG	O7-C10-O9	-2.03	118.97	123.70
25	C	512	CLA	CHA-C1A-NA	-2.03	121.81	126.39
25	b	611	CLA	CHB-C4A-NA	2.02	127.32	124.40
35	V	201	HEC	C2A-C1A-NA	-2.02	108.37	110.32
30	A	614	LHG	C27-C26-C25	-2.02	104.14	114.37
26	k	101	BCR	C30-C25-C26	-2.02	119.87	122.64
25	b	601	CLA	C16-C15-C13	-2.02	109.24	115.97
35	V	201	HEC	C3B-C4B-NB	-2.02	107.95	110.17
25	b	606	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
25	b	607	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
27	A	610	PL9	C12-C13-C14	-2.02	123.00	127.62
25	b	614	CLA	C1D-ND-C4D	2.02	107.73	106.31
25	c	505	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
31	c	515	DGD	C1D-C2D-C3D	-2.02	105.76	110.01
25	C	503	CLA	C1D-ND-C4D	2.02	107.73	106.31
25	a	606	CLA	O2D-CGD-CBD	2.02	114.76	111.23
25	B	601	CLA	CAA-C2A-C1A	2.02	118.59	111.97
31	C	516	DGD	CAB-C9B-C8B	-2.02	104.18	114.37
25	c	507	CLA	O2D-CGD-CBD	2.02	114.75	111.23
25	b	603	CLA	CHB-C1B-C2B	-2.02	121.58	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	612	LMG	O7-C10-O9	-2.01	119.00	123.70
30	L	101	LHG	C27-C26-C25	-2.01	104.19	114.37
28	D	407	LMG	C40-C39-C38	-2.01	104.20	114.37
26	H	101	BCR	C16-C17-C18	-2.01	124.46	127.28
25	c	501	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
32	B	624	STE	C6-C5-C4	-2.01	104.22	114.37
25	d	404	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
25	A	608	CLA	CHC-C1C-NC	2.01	127.33	124.31
33	d	402	PHO	CMD-C2D-C3D	2.01	128.69	124.68
31	J	101	DGD	C7A-C6A-C5A	-2.01	104.23	114.37
25	b	614	CLA	CHD-C1D-ND	-2.00	121.98	124.80
31	c	515	DGD	O3D-C3D-C4D	-2.00	105.65	110.38
25	B	611	CLA	CHD-C1D-ND	-2.00	121.98	124.80
26	H	101	BCR	C24-C23-C22	-2.00	123.27	126.23
25	a	611	CLA	C2D-C1D-ND	-2.00	108.14	110.13
29	a	613	SQD	C9-C8-C7	-2.00	106.36	113.69
28	c	520	LMG	C9-C8-C7	-2.00	107.12	111.78
25	a	606	CLA	CHC-C1C-NC	2.00	127.32	124.31

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	V	201	HEC	NA
35	v	201	HEC	NA

All (1807) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C4-C3-C5-C6
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
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	b	601	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C11-C10-C8-C9
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	C2-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	b	616	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	503	CLA	C2B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
25	c	506	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C3A-C2A-CAA-CBA
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	513	CLA	CBD-CGD-O2D-CED
26	A	609	BCR	C20-C21-C22-C37
26	B	619	BCR	C37-C22-C23-C24
26	D	405	BCR	C37-C22-C23-C24
26	K	101	BCR	C11-C10-C9-C8
26	K	102	BCR	C5-C6-C7-C8
26	T	101	BCR	C7-C8-C9-C10
26	c	514	BCR	C7-C8-C9-C34
26	d	405	BCR	C21-C22-C23-C24
26	d	405	BCR	C37-C22-C23-C24
26	d	405	BCR	C22-C23-C24-C25
26	h	101	BCR	C22-C23-C24-C25
26	k	101	BCR	C6-C7-C8-C9
26	k	102	BCR	C20-C21-C22-C37
26	k	103	BCR	C17-C18-C19-C20
27	A	610	PL9	C37-C38-C39-C40
27	A	610	PL9	C37-C38-C39-C41
27	a	610	PL9	C12-C13-C14-C16
27	a	610	PL9	C32-C33-C34-C35
27	d	406	PL9	C32-C33-C34-C35
27	d	406	PL9	C35-C34-C36-C37
28	A	612	LMG	O6-C1-O1-C7
28	A	612	LMG	O9-C10-O7-C8
28	A	612	LMG	C11-C10-O7-C8
28	C	517	LMG	O9-C10-O7-C8
28	C	517	LMG	C11-C10-O7-C8
28	D	411	LMG	C11-C10-O7-C8
28	b	622	LMG	O7-C8-C9-O8
28	c	521	LMG	O6-C1-O1-C7
29	B	623	SQD	C2-C1-O6-C44
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
29	B	623	SQD	O49-C7-O47-C45
29	a	613	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
29	a	613	SQD	O6-C44-C45-O47
29	a	613	SQD	C8-C7-O47-C45
29	b	620	SQD	O5-C1-O6-C44
29	b	620	SQD	C8-C7-O47-C45
29	b	620	SQD	C24-C23-O48-C46
29	b	620	SQD	C5-C6-S-O7
29	b	620	SQD	C5-C6-S-O8
29	b	620	SQD	C5-C6-S-O9
29	f	102	SQD	C2-C1-O6-C44
29	f	102	SQD	O5-C1-O6-C44
29	f	102	SQD	O10-C23-O48-C46
30	A	614	LHG	C4-O6-P-O3
30	A	614	LHG	C4-O6-P-O4
30	D	409	LHG	C3-O3-P-O4
30	D	409	LHG	C4-O6-P-O3
30	D	409	LHG	C4-O6-P-O4
30	D	410	LHG	C3-O3-P-O6
30	L	101	LHG	C3-O3-P-O4
30	d	407	LHG	C4-O6-P-O5
30	d	408	LHG	C3-O3-P-O4
30	d	408	LHG	C4-O6-P-O3
30	d	408	LHG	C4-O6-P-O4
30	d	409	LHG	O1-C1-C2-C3
30	e	101	LHG	O1-C1-C2-O2
30	e	101	LHG	O1-C1-C2-C3
30	e	101	LHG	C3-O3-P-O4
30	e	101	LHG	C3-O3-P-O6
30	e	101	LHG	C4-O6-P-O3
30	e	101	LHG	C4-O6-P-O5
30	e	101	LHG	O10-C23-O8-C6
30	e	101	LHG	C24-C23-O8-C6
31	A	616	DGD	O1B-C1B-O2G-C2G
31	A	616	DGD	O2G-C2G-C3G-O3G
31	a	614	DGD	C2B-C1B-O2G-C2G
33	d	402	PHO	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	CBD-CGD-O2D-CED
28	m	101	LMG	O10-C28-O8-C9
29	b	620	SQD	O10-C23-O48-C46
27	a	610	PL9	C47-C48-C49-C50
27	a	610	PL9	C47-C48-C49-C51
31	a	614	DGD	C2G-C1G-O1G-C1A

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Mol	Chain	Res	Type	Atoms
25	b	601	CLA	O1D-CGD-O2D-CED
28	m	101	LMG	C29-C28-O8-C9
29	f	102	SQD	C24-C23-O48-C46
28	c	520	LMG	O10-C28-O8-C9
29	a	613	SQD	O10-C23-O48-C46
33	d	402	PHO	O1D-CGD-O2D-CED
31	H	102	DGD	O6E-C5E-C6E-O5E
28	D	411	LMG	O9-C10-O7-C8
28	c	520	LMG	O9-C10-O7-C8
29	a	613	SQD	O49-C7-O47-C45
31	a	614	DGD	O1B-C1B-O2G-C2G
25	A	608	CLA	C3-C5-C6-C7
25	B	604	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
25	b	606	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
29	a	613	SQD	C24-C23-O48-C46
25	B	606	CLA	CBD-CGD-O2D-CED
28	c	520	LMG	C11-C10-O7-C8
29	B	623	SQD	C8-C7-O47-C45
31	A	616	DGD	C2B-C1B-O2G-C2G
25	c	513	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	C4-C3-C5-C6
27	A	610	PL9	C20-C19-C21-C22
27	A	610	PL9	C35-C34-C36-C37
27	A	610	PL9	C40-C39-C41-C42
27	D	406	PL9	C35-C34-C36-C37
27	d	406	PL9	C40-C39-C41-C42
25	B	603	CLA	C2-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
27	A	610	PL9	C18-C19-C21-C22
27	A	610	PL9	C23-C24-C26-C27
28	c	520	LMG	C29-C28-O8-C9
27	D	406	PL9	C32-C33-C34-C35
28	c	521	LMG	O10-C28-O8-C9
29	b	620	SQD	O49-C7-O47-C45
25	C	511	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7
25	b	609	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
30	d	408	LHG	O2-C2-C3-O3
28	c	521	LMG	C29-C28-O8-C9
29	D	408	SQD	C24-C23-O48-C46
31	H	102	DGD	C4E-C5E-C6E-O5E
28	B	620	LMG	O10-C28-O8-C9
35	V	201	HEC	C2C-C3C-CAC-CBC
25	b	607	CLA	CBD-CGD-O2D-CED
25	C	513	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
27	A	610	PL9	C33-C34-C36-C37
27	A	610	PL9	C43-C44-C46-C47
27	d	406	PL9	C38-C39-C41-C42
29	D	408	SQD	O10-C23-O48-C46
31	a	614	DGD	O1A-C1A-O1G-C1G
28	c	518	LMG	O6-C5-C6-O5
27	A	610	PL9	C9-C11-C12-C13
27	A	610	PL9	C29-C31-C32-C33
27	a	610	PL9	C24-C26-C27-C28
27	a	610	PL9	C39-C41-C42-C43
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
28	b	622	LMG	O6-C5-C6-O5
28	b	622	LMG	O10-C28-O8-C9
28	b	622	LMG	O6-C1-O1-C7
28	m	101	LMG	O6-C1-O1-C7
25	C	509	CLA	CBD-CGD-O2D-CED
28	d	411	LMG	C10-C11-C12-C13
31	h	102	DGD	O6E-C5E-C6E-O5E
27	a	610	PL9	C22-C23-C24-C25
25	B	614	CLA	C15-C16-C17-C18
27	a	610	PL9	C22-C23-C24-C26
27	a	610	PL9	C42-C43-C44-C46
28	A	612	LMG	C4-C5-C6-O5
25	C	503	CLA	CBD-CGD-O2D-CED
27	d	406	PL9	C47-C48-C49-C51
28	B	620	LMG	C29-C28-O8-C9
28	b	622	LMG	C29-C28-O8-C9
29	A	613	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	A	616	DGD	O6E-C5E-C6E-O5E
25	B	606	CLA	O1D-CGD-O2D-CED
29	A	613	SQD	C30-C31-C32-C33
30	A	614	LHG	C32-C33-C34-C35
28	C	517	LMG	C4-C5-C6-O5
27	D	406	PL9	C33-C34-C36-C37
25	A	607	CLA	C14-C13-C15-C16
25	B	605	CLA	C6-C7-C8-C9
25	B	606	CLA	C11-C10-C8-C9
25	B	610	CLA	C14-C13-C15-C16
25	B	613	CLA	C11-C12-C13-C14
25	B	614	CLA	C14-C13-C15-C16
25	C	501	CLA	C14-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C9
25	C	507	CLA	C14-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C12-C13-C14
25	D	404	CLA	C11-C12-C13-C14
25	a	611	CLA	C14-C13-C15-C16
25	b	605	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	b	610	CLA	C14-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C14
25	b	615	CLA	C6-C7-C8-C9
25	c	513	CLA	C6-C7-C8-C9
28	b	622	LMG	C2-C1-O1-C7
31	A	616	DGD	C4E-C5E-C6E-O5E
26	B	618	BCR	C37-C22-C23-C24
26	B	619	BCR	C11-C12-C13-C35
26	K	101	BCR	C7-C8-C9-C34
26	T	101	BCR	C7-C8-C9-C34
26	b	618	BCR	C7-C8-C9-C34
26	b	619	BCR	C37-C22-C23-C24
26	d	405	BCR	C7-C8-C9-C34
26	h	101	BCR	C11-C12-C13-C35
26	k	102	BCR	C37-C22-C23-C24
26	k	103	BCR	C36-C18-C19-C20
35	V	201	HEC	C4C-C3C-CAC-CBC
32	B	624	STE	C1-C2-C3-C4
31	c	517	DGD	O1A-C1A-O1G-C1G
25	b	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	A	612	LMG	O6-C5-C6-O5
31	a	614	DGD	C2A-C1A-O1G-C1G
29	a	612	SQD	C7-C8-C9-C10
29	a	612	SQD	C23-C24-C25-C26
25	b	602	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	C8-C10-C11-C12
25	a	611	CLA	C15-C16-C17-C18
25	b	607	CLA	C8-C10-C11-C12
27	D	406	PL9	C47-C48-C49-C51
27	D	406	PL9	C32-C33-C34-C36
28	C	517	LMG	O6-C5-C6-O5
25	C	508	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C7
25	b	615	CLA	C11-C12-C13-C15
29	B	623	SQD	C10-C11-C12-C13
28	c	520	LMG	C10-C11-C12-C13
26	K	101	BCR	C15-C16-C17-C18
27	A	610	PL9	C44-C46-C47-C48
25	b	608	CLA	C13-C15-C16-C17
28	c	518	LMG	C4-C5-C6-O5
28	c	521	LMG	C4-C5-C6-O5
30	e	101	LHG	C23-C24-C25-C26
31	c	516	DGD	C1A-C2A-C3A-C4A
25	B	607	CLA	C13-C15-C16-C17
25	b	605	CLA	C15-C16-C17-C18
25	b	607	CLA	C5-C6-C7-C8
25	c	503	CLA	C5-C6-C7-C8
25	c	509	CLA	C10-C11-C12-C13
25	B	601	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	B	601	CLA	C15-C16-C17-C18
25	C	507	CLA	C15-C16-C17-C18
25	D	404	CLA	C10-C11-C12-C13
25	b	614	CLA	C13-C15-C16-C17
25	b	615	CLA	C15-C16-C17-C18
25	c	513	CLA	C8-C10-C11-C12
28	B	622	LMG	C28-C29-C30-C31
28	C	517	LMG	C28-C29-C30-C31
28	c	521	LMG	C10-C11-C12-C13
28	d	411	LMG	C28-C29-C30-C31
28	m	101	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	A	615	SQD	C23-C24-C25-C26
30	d	407	LHG	C7-C8-C9-C10
30	d	407	LHG	C23-C24-C25-C26
30	e	101	LHG	C7-C8-C9-C10
31	c	517	DGD	C1B-C2B-C3B-C4B
25	c	512	CLA	O1D-CGD-O2D-CED
25	A	606	CLA	C15-C16-C17-C18
25	B	601	CLA	C5-C6-C7-C8
25	B	603	CLA	C13-C15-C16-C17
25	B	607	CLA	C5-C6-C7-C8
25	C	509	CLA	C10-C11-C12-C13
25	b	602	CLA	C15-C16-C17-C18
25	b	605	CLA	C5-C6-C7-C8
25	c	510	CLA	C5-C6-C7-C8
25	c	510	CLA	C10-C11-C12-C13
25	c	511	CLA	C13-C15-C16-C17
29	B	623	SQD	C29-C30-C31-C32
30	e	101	LHG	O2-C2-C3-O3
25	c	512	CLA	CBA-CGA-O2A-C1
32	A	617	STE	C1-C2-C3-C4
25	C	507	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
25	c	507	CLA	C5-C6-C7-C8
25	B	606	CLA	C15-C16-C17-C18
25	C	502	CLA	C13-C15-C16-C17
25	b	601	CLA	C8-C10-C11-C12
25	c	513	CLA	C5-C6-C7-C8
32	C	519	STE	C1-C2-C3-C4
32	t	102	STE	C1-C2-C3-C4
25	b	614	CLA	O1D-CGD-O2D-CED
31	C	515	DGD	O6E-C5E-C6E-O5E
25	C	510	CLA	C15-C16-C17-C18
31	c	517	DGD	C2A-C1A-O1G-C1G
29	f	102	SQD	C23-C24-C25-C26
32	B	626	STE	C1-C2-C3-C4
25	C	509	CLA	C13-C15-C16-C17
29	b	620	SQD	C12-C13-C14-C15
30	d	408	LHG	C1-C2-C3-O3
30	e	101	LHG	C1-C2-C3-O3
25	B	606	CLA	C2A-CAA-CBA-CGA
25	B	616	CLA	C5-C6-C7-C8
25	C	503	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C8-C10-C11-C12
25	a	608	CLA	C5-C6-C7-C8
25	b	608	CLA	C8-C10-C11-C12
25	b	613	CLA	C13-C15-C16-C17
25	c	507	CLA	C8-C10-C11-C12
25	C	504	CLA	C8-C10-C11-C12
25	c	511	CLA	C15-C16-C17-C18
28	b	622	LMG	C4-C5-C6-O5
25	A	607	CLA	C15-C16-C17-C18
25	B	603	CLA	C8-C10-C11-C12
25	C	512	CLA	C8-C10-C11-C12
25	a	606	CLA	C8-C10-C11-C12
25	b	613	CLA	C10-C11-C12-C13
25	b	614	CLA	C5-C6-C7-C8
25	b	615	CLA	C10-C11-C12-C13
25	c	508	CLA	C10-C11-C12-C13
25	B	601	CLA	CBD-CGD-O2D-CED
29	b	620	SQD	C10-C11-C12-C13
25	c	503	CLA	O1D-CGD-O2D-CED
28	A	612	LMG	C2-C1-O1-C7
28	m	101	LMG	C2-C1-O1-C7
31	C	516	DGD	C2E-C1E-O5D-C6D
31	c	516	DGD	C2E-C1E-O5D-C6D
25	c	509	CLA	O1D-CGD-O2D-CED
30	A	614	LHG	O2-C2-C3-O3
25	B	609	CLA	C16-C17-C18-C20
26	D	405	BCR	C20-C21-C22-C37
26	K	101	BCR	C20-C21-C22-C37
26	K	102	BCR	C20-C21-C22-C37
26	T	101	BCR	C35-C13-C14-C15
26	T	101	BCR	C16-C17-C18-C36
26	b	619	BCR	C35-C13-C14-C15
26	b	619	BCR	C16-C17-C18-C36
26	b	619	BCR	C20-C21-C22-C37
26	h	101	BCR	C11-C10-C9-C34
26	h	101	BCR	C20-C21-C22-C37
26	t	101	BCR	C20-C21-C22-C37
30	D	410	LHG	C7-C8-C9-C10
25	C	513	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	C8-C10-C11-C12
26	K	102	BCR	C7-C8-C9-C34
26	b	617	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	D	410	LHG	O1-C1-C2-C3
30	D	412	LHG	O1-C1-C2-C3
32	d	412	STE	C1-C2-C3-C4
25	b	607	CLA	O1D-CGD-O2D-CED
28	D	411	LMG	C9-C8-O7-C10
29	b	620	SQD	C46-C45-O47-C7
25	B	602	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
33	d	402	PHO	C16-C17-C18-C19
25	c	509	CLA	C13-C15-C16-C17
25	c	510	CLA	C8-C10-C11-C12
31	h	102	DGD	C4E-C5E-C6E-O5E
26	A	609	BCR	C16-C17-C18-C19
26	K	101	BCR	C16-C17-C18-C19
26	K	101	BCR	C20-C21-C22-C23
26	T	101	BCR	C12-C13-C14-C15
26	h	101	BCR	C11-C10-C9-C8
26	h	101	BCR	C20-C21-C22-C23
30	e	101	LHG	O9-C7-O7-C5
31	c	516	DGD	O6E-C1E-O5D-C6D
31	c	515	DGD	C1A-C2A-C3A-C4A
25	b	604	CLA	C15-C16-C17-C18
28	A	612	LMG	O1-C7-C8-O7
25	b	601	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
25	d	403	CLA	C16-C17-C18-C20
25	c	503	CLA	C15-C16-C17-C18
29	A	615	SQD	C14-C15-C16-C17
29	a	612	SQD	C12-C13-C14-C15
31	J	101	DGD	C5B-C6B-C7B-C8B
28	c	518	LMG	O9-C10-O7-C8
28	d	410	LMG	C33-C34-C35-C36
28	d	410	LMG	C37-C38-C39-C40
30	L	101	LHG	C28-C29-C30-C31
31	H	102	DGD	C7A-C8A-C9A-CAA
31	H	102	DGD	CAB-CBB-CCB-CDB
32	B	621	STE	C9-C10-C11-C12
32	B	624	STE	C2-C3-C4-C5
32	C	518	STE	C2-C3-C4-C5
32	H	103	STE	C6-C7-C8-C9
32	I	101	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	a	615	STE	C3-C4-C5-C6
32	b	621	STE	C10-C11-C12-C13
32	d	412	STE	C10-C11-C12-C13
25	c	504	CLA	C8-C10-C11-C12
28	D	407	LMG	C17-C18-C19-C20
29	a	612	SQD	C13-C14-C15-C16
29	a	613	SQD	C10-C11-C12-C13
30	D	410	LHG	C34-C35-C36-C37
30	l	101	LHG	C31-C32-C33-C34
31	H	102	DGD	C9A-CAA-CBA-CCA
32	B	621	STE	C6-C7-C8-C9
32	B	627	STE	C7-C8-C9-C10
32	D	413	STE	C7-C8-C9-C10
28	c	518	LMG	C35-C36-C37-C38
28	d	410	LMG	C35-C36-C37-C38
28	m	101	LMG	C32-C33-C34-C35
29	D	408	SQD	C33-C34-C35-C36
31	A	616	DGD	C5B-C6B-C7B-C8B
31	c	515	DGD	C3B-C4B-C5B-C6B
31	h	102	DGD	C3B-C4B-C5B-C6B
31	h	102	DGD	C5B-C6B-C7B-C8B
32	b	623	STE	C11-C10-C9-C8
28	m	101	LMG	C17-C18-C19-C20
30	A	614	LHG	C24-C25-C26-C27
30	D	409	LHG	C10-C11-C12-C13
30	L	101	LHG	C17-C18-C19-C20
31	A	616	DGD	C2B-C3B-C4B-C5B
31	C	515	DGD	C4B-C5B-C6B-C7B
32	D	413	STE	C4-C5-C6-C7
25	C	509	CLA	O1D-CGD-O2D-CED
25	B	604	CLA	C10-C11-C12-C13
25	b	615	CLA	C8-C10-C11-C12
25	b	609	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
30	A	614	LHG	C15-C16-C17-C18
30	d	407	LHG	C15-C16-C17-C18
30	d	408	LHG	C29-C30-C31-C32
31	c	517	DGD	C9B-CAB-CBB-CCB
28	c	521	LMG	O6-C5-C6-O5
25	B	602	CLA	C16-C17-C18-C20
25	B	612	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	B	615	CLA	C16-C17-C18-C19
25	B	615	CLA	C16-C17-C18-C20
25	D	403	CLA	C16-C17-C18-C20
25	c	512	CLA	O1A-CGA-O2A-C1
29	B	623	SQD	C12-C13-C14-C15
30	d	407	LHG	C30-C31-C32-C33
31	J	101	DGD	CBB-CCB-CDB-CEB
32	D	413	STE	C5-C6-C7-C8
32	D	413	STE	C9-C10-C11-C12
25	B	614	CLA	C13-C15-C16-C17
31	c	516	DGD	C6A-C7A-C8A-C9A
32	b	624	STE	C11-C10-C9-C8
25	B	601	CLA	C6-C7-C8-C10
25	B	606	CLA	C12-C13-C15-C16
25	b	611	CLA	C12-C13-C15-C16
30	A	614	LHG	C27-C28-C29-C30
32	H	103	STE	C9-C10-C11-C12
32	H	103	STE	C14-C15-C16-C17
30	D	409	LHG	O2-C2-C3-O3
30	D	410	LHG	O2-C2-C3-O3
25	B	606	CLA	C13-C15-C16-C17
25	B	607	CLA	C15-C16-C17-C18
25	b	601	CLA	C10-C11-C12-C13
31	c	516	DGD	O6E-C5E-C6E-O5E
28	D	407	LMG	C16-C17-C18-C19
30	D	410	LHG	C9-C10-C11-C12
30	l	101	LHG	C9-C10-C11-C12
31	c	516	DGD	CBA-CCA-CDA-CEA
32	c	519	STE	C9-C10-C11-C12
25	c	512	CLA	C3A-C2A-CAA-CBA
29	D	408	SQD	C29-C30-C31-C32
31	A	616	DGD	C4B-C5B-C6B-C7B
25	b	601	CLA	C15-C16-C17-C18
30	d	408	LHG	C17-C18-C19-C20
26	K	103	BCR	C19-C20-C21-C22
25	B	612	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
31	a	614	DGD	C5A-C6A-C7A-C8A
28	A	612	LMG	C16-C17-C18-C19
29	B	623	SQD	C25-C26-C27-C28
28	B	620	LMG	C37-C38-C39-C40
29	b	620	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
30	d	409	LHG	C26-C27-C28-C29
31	A	616	DGD	CEB-CFB-CGB-CHB
31	a	614	DGD	C2B-C3B-C4B-C5B
25	B	606	CLA	C8-C10-C11-C12
28	C	517	LMG	C31-C32-C33-C34
29	a	612	SQD	C30-C31-C32-C33
29	a	612	SQD	C34-C35-C36-C37
29	b	620	SQD	C26-C27-C28-C29
30	d	407	LHG	C16-C17-C18-C19
30	l	101	LHG	C25-C26-C27-C28
31	J	101	DGD	CCB-CDB-CEB-CFB
31	c	515	DGD	C4B-C5B-C6B-C7B
32	C	519	STE	C5-C6-C7-C8
32	T	102	STE	C7-C8-C9-C10
32	T	102	STE	C14-C15-C16-C17
28	c	518	LMG	C36-C37-C38-C39
28	c	521	LMG	C33-C34-C35-C36
29	a	612	SQD	C32-C33-C34-C35
30	L	101	LHG	C27-C28-C29-C30
31	A	616	DGD	C6B-C7B-C8B-C9B
32	H	103	STE	C5-C6-C7-C8
28	B	622	LMG	C36-C37-C38-C39
28	D	407	LMG	C18-C19-C20-C21
31	J	101	DGD	C6A-C7A-C8A-C9A
32	T	102	STE	C11-C10-C9-C8
32	m	102	STE	C3-C4-C5-C6
28	C	517	LMG	C17-C18-C19-C20
29	B	623	SQD	C15-C16-C17-C18
30	d	407	LHG	C17-C18-C19-C20
30	d	407	LHG	C25-C26-C27-C28
30	d	409	LHG	C29-C30-C31-C32
31	J	101	DGD	C5A-C6A-C7A-C8A
32	A	617	STE	C4-C5-C6-C7
30	l	101	LHG	C23-C24-C25-C26
31	J	101	DGD	C1B-C2B-C3B-C4B
31	c	517	DGD	C1A-C2A-C3A-C4A
25	b	601	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C2B-C3B-CAB-CBB
26	D	405	BCR	C23-C24-C25-C26
26	D	405	BCR	C23-C24-C25-C30
26	K	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	k	102	BCR	C1-C6-C7-C8
26	k	102	BCR	C5-C6-C7-C8
30	D	412	LHG	C11-C12-C13-C14
31	A	616	DGD	CBB-CCB-CDB-CEB
31	c	515	DGD	C9B-CAB-CBB-CCB
31	h	102	DGD	C6B-C7B-C8B-C9B
32	b	624	STE	C12-C13-C14-C15
32	j	101	STE	C2-C3-C4-C5
29	f	102	SQD	C8-C7-O47-C45
25	a	606	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
25	C	509	CLA	C3-C5-C6-C7
28	B	620	LMG	C12-C13-C14-C15
28	D	407	LMG	C13-C14-C15-C16
28	D	411	LMG	C11-C12-C13-C14
32	A	617	STE	C14-C15-C16-C17
28	A	612	LMG	C35-C36-C37-C38
28	c	520	LMG	C30-C31-C32-C33
29	A	613	SQD	C11-C12-C13-C14
30	L	101	LHG	C12-C13-C14-C15
31	c	515	DGD	CCB-CDB-CEB-CFB
31	c	517	DGD	C3B-C4B-C5B-C6B
28	b	622	LMG	C30-C31-C32-C33
29	a	612	SQD	C25-C26-C27-C28
30	A	614	LHG	C16-C17-C18-C19
32	b	625	STE	C6-C7-C8-C9
28	D	407	LMG	C36-C37-C38-C39
29	f	102	SQD	C25-C26-C27-C28
31	a	614	DGD	C8A-C9A-CAA-CBA
31	c	517	DGD	C9A-CAA-CBA-CCA
32	T	102	STE	C5-C6-C7-C8
32	J	102	STE	C5-C6-C7-C8
26	d	405	BCR	C18-C19-C20-C21
26	k	101	BCR	C10-C11-C12-C13
26	k	101	BCR	C18-C19-C20-C21
25	c	505	CLA	C10-C11-C12-C13
27	A	610	PL9	C38-C39-C41-C42
25	b	602	CLA	C16-C17-C18-C20
28	b	622	LMG	C19-C20-C21-C22
29	D	408	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	D	410	LHG	C24-C25-C26-C27
31	A	616	DGD	CCA-CDA-CEA-CFA
31	c	515	DGD	C2A-C3A-C4A-C5A
32	A	617	STE	C9-C10-C11-C12
32	t	103	STE	C3-C4-C5-C6
32	L	102	STE	C1-C2-C3-C4
28	b	622	LMG	C32-C33-C34-C35
28	d	411	LMG	C38-C39-C40-C41
28	m	101	LMG	C15-C16-C17-C18
30	e	101	LHG	C11-C10-C9-C8
30	l	101	LHG	C32-C33-C34-C35
31	H	102	DGD	C6B-C7B-C8B-C9B
32	b	624	STE	C10-C11-C12-C13
28	d	410	LMG	C32-C33-C34-C35
28	m	101	LMG	C19-C20-C21-C22
29	A	615	SQD	C18-C19-C20-C21
29	a	613	SQD	C11-C12-C13-C14
30	A	614	LHG	C11-C12-C13-C14
30	A	614	LHG	C30-C31-C32-C33
32	b	623	STE	C6-C7-C8-C9
31	C	516	DGD	O6E-C1E-O5D-C6D
28	c	521	LMG	C32-C33-C34-C35
28	m	101	LMG	C14-C15-C16-C17
30	L	101	LHG	C24-C25-C26-C27
30	L	101	LHG	C32-C33-C34-C35
31	C	515	DGD	C5A-C6A-C7A-C8A
31	c	515	DGD	C5B-C6B-C7B-C8B
30	D	410	LHG	C29-C30-C31-C32
30	l	101	LHG	C16-C17-C18-C19
31	C	515	DGD	C5B-C6B-C7B-C8B
31	J	101	DGD	CBA-CCA-CDA-CEA
32	L	102	STE	C6-C7-C8-C9
32	b	625	STE	C5-C6-C7-C8
28	d	410	LMG	C31-C32-C33-C34
29	A	615	SQD	C30-C31-C32-C33
32	b	624	STE	C13-C14-C15-C16
29	A	615	SQD	C10-C11-C12-C13
29	D	408	SQD	C32-C33-C34-C35
30	e	101	LHG	C8-C7-O7-C5
31	a	614	DGD	C4A-C5A-C6A-C7A
25	B	605	CLA	C15-C16-C17-C18
28	c	518	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
28	c	521	LMG	C38-C39-C40-C41
32	T	102	STE	C13-C14-C15-C16
32	b	623	STE	C3-C4-C5-C6
29	a	612	SQD	C26-C27-C28-C29
31	c	516	DGD	CCB-CDB-CEB-CFB
25	c	508	CLA	C13-C15-C16-C17
28	D	407	LMG	C28-C29-C30-C31
29	a	612	SQD	C16-C17-C18-C19
28	B	620	LMG	C38-C39-C40-C41
29	b	620	SQD	C17-C18-C19-C20
31	A	616	DGD	CEA-CFA-CGA-CHA
31	H	102	DGD	C3A-C4A-C5A-C6A
33	d	402	PHO	C16-C17-C18-C20
25	b	613	CLA	CBD-CGD-O2D-CED
30	d	409	LHG	C27-C28-C29-C30
31	H	102	DGD	CBB-CCB-CDB-CEB
31	c	515	DGD	C8B-C9B-CAB-CBB
32	B	625	STE	C10-C11-C12-C13
27	A	610	PL9	C25-C24-C26-C27
28	c	521	LMG	C39-C40-C41-C42
31	J	101	DGD	C4B-C5B-C6B-C7B
25	c	502	CLA	C15-C16-C17-C18
28	B	620	LMG	C13-C14-C15-C16
29	b	620	SQD	C29-C30-C31-C32
32	H	103	STE	C7-C8-C9-C10
29	a	612	SQD	C14-C15-C16-C17
32	d	412	STE	C12-C13-C14-C15
25	C	512	CLA	C13-C15-C16-C17
32	D	413	STE	C2-C3-C4-C5
31	c	516	DGD	C1B-C2B-C3B-C4B
30	e	101	LHG	O6-C4-C5-O7
28	c	520	LMG	O6-C5-C6-O5
28	D	407	LMG	C20-C21-C22-C23
29	b	620	SQD	C25-C26-C27-C28
32	D	413	STE	C3-C4-C5-C6
32	c	519	STE	C2-C3-C4-C5
34	E	101	HEM	C4C-C3C-CAC-CBC
25	b	601	CLA	C16-C17-C18-C19
28	D	407	LMG	C38-C39-C40-C41
30	D	410	LHG	C16-C17-C18-C19
31	a	614	DGD	C3B-C4B-C5B-C6B
31	a	614	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
32	c	519	STE	C4-C5-C6-C7
30	D	409	LHG	C12-C13-C14-C15
31	h	102	DGD	C2B-C3B-C4B-C5B
28	C	517	LMG	C10-C11-C12-C13
25	B	615	CLA	C15-C16-C17-C18
25	C	503	CLA	O1D-CGD-O2D-CED
28	c	520	LMG	C40-C41-C42-C43
29	A	613	SQD	C34-C35-C36-C37
30	D	410	LHG	C10-C11-C12-C13
31	A	616	DGD	C8A-C9A-CAA-CBA
31	c	515	DGD	CBB-CCB-CDB-CEB
29	a	612	SQD	O47-C45-C46-O48
28	C	517	LMG	C32-C33-C34-C35
28	d	411	LMG	C37-C38-C39-C40
30	D	412	LHG	C27-C28-C29-C30
30	d	408	LHG	C12-C13-C14-C15
32	a	615	STE	C5-C6-C7-C8
29	f	102	SQD	C29-C30-C31-C32
30	D	409	LHG	C15-C16-C17-C18
31	C	516	DGD	C9B-CAB-CBB-CCB
31	a	614	DGD	CEB-CFB-CGB-CHB
28	c	520	LMG	C15-C16-C17-C18
28	c	520	LMG	C35-C36-C37-C38
30	D	412	LHG	C28-C29-C30-C31
28	c	520	LMG	C36-C37-C38-C39
30	d	408	LHG	C11-C12-C13-C14
32	b	623	STE	C7-C8-C9-C10
25	B	609	CLA	C16-C17-C18-C19
25	D	404	CLA	C16-C17-C18-C19
28	c	520	LMG	C31-C32-C33-C34
30	L	101	LHG	C13-C14-C15-C16
31	H	102	DGD	C7B-C8B-C9B-CAB
31	c	515	DGD	C7A-C8A-C9A-CAA
29	B	623	SQD	C33-C34-C35-C36
29	f	102	SQD	O49-C7-O47-C45
30	d	408	LHG	O9-C7-O7-C5
31	c	515	DGD	O1B-C1B-O2G-C2G
30	A	614	LHG	C1-C2-C3-O3
28	B	622	LMG	C15-C16-C17-C18
30	D	410	LHG	C32-C33-C34-C35
31	c	516	DGD	C5A-C6A-C7A-C8A
32	c	519	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	c	519	STE	C14-C15-C16-C17
25	B	614	CLA	CBD-CGD-O2D-CED
31	c	515	DGD	O6E-C5E-C6E-O5E
28	D	407	LMG	C15-C16-C17-C18
28	c	521	LMG	C31-C32-C33-C34
32	b	621	STE	C5-C6-C7-C8
28	B	620	LMG	C17-C18-C19-C20
30	A	614	LHG	C11-C10-C9-C8
25	c	503	CLA	C16-C17-C18-C19
25	c	504	CLA	C11-C12-C13-C15
30	D	410	LHG	C25-C26-C27-C28
32	A	617	STE	C3-C4-C5-C6
32	d	412	STE	C9-C10-C11-C12
25	B	601	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	C	505	CLA	C5-C6-C7-C8
28	C	517	LMG	C37-C38-C39-C40
29	b	620	SQD	C11-C12-C13-C14
31	H	102	DGD	C5A-C6A-C7A-C8A
29	a	612	SQD	C11-C10-C9-C8
29	f	102	SQD	C27-C28-C29-C30
31	H	102	DGD	CCA-CDA-CEA-CFA
31	h	102	DGD	C9B-CAB-CBB-CCB
30	A	614	LHG	O6-C4-C5-C6
32	I	101	STE	C1-C2-C3-C4
31	a	614	DGD	C4B-C5B-C6B-C7B
31	c	517	DGD	C4A-C5A-C6A-C7A
31	c	517	DGD	C5B-C6B-C7B-C8B
32	A	617	STE	C2-C3-C4-C5
25	A	607	CLA	C12-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C15
25	B	614	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C10-C8-C7
25	C	503	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
25	C	506	CLA	C6-C7-C8-C10
25	C	511	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C12-C13-C15
25	a	606	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C6-C7-C8-C10
25	b	606	CLA	C12-C13-C15-C16
25	b	610	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C10-C8-C7
25	c	508	CLA	C12-C13-C15-C16
32	H	103	STE	C2-C3-C4-C5
32	t	102	STE	C7-C8-C9-C10
29	B	623	SQD	C24-C23-O48-C46
31	C	516	DGD	C3B-C4B-C5B-C6B
25	B	605	CLA	C8-C10-C11-C12
25	C	510	CLA	C10-C11-C12-C13
25	b	611	CLA	C15-C16-C17-C18
29	A	613	SQD	C23-C24-C25-C26
27	a	610	PL9	C13-C14-C16-C17
27	d	406	PL9	C43-C44-C46-C47
32	B	627	STE	C13-C14-C15-C16
28	D	407	LMG	O6-C5-C6-O5
25	B	604	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C9
25	C	505	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	D	404	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C12-C13-C14
25	b	606	CLA	C6-C7-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	b	615	CLA	C11-C12-C13-C14
25	c	506	CLA	C11-C10-C8-C9
25	c	508	CLA	C14-C13-C15-C16
25	c	510	CLA	C14-C13-C15-C16
31	C	516	DGD	C6B-C7B-C8B-C9B
32	b	621	STE	C4-C5-C6-C7
25	A	608	CLA	CBA-CGA-O2A-C1
29	f	102	SQD	C24-C25-C26-C27
30	l	101	LHG	O9-C7-O7-C5
27	A	610	PL9	C39-C41-C42-C43
28	B	620	LMG	C7-C8-C9-O8
28	D	411	LMG	C7-C8-C9-O8
28	b	622	LMG	C7-C8-C9-O8
28	c	520	LMG	C7-C8-C9-O8
28	c	521	LMG	C7-C8-C9-O8
29	A	613	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	O6-C44-C45-C46
29	a	612	SQD	O6-C44-C45-C46
29	a	613	SQD	C44-C45-C46-O48
31	A	616	DGD	C1G-C2G-C3G-O3G
31	A	616	DGD	C4A-C5A-C6A-C7A
28	c	521	LMG	C15-C16-C17-C18
29	A	615	SQD	C12-C13-C14-C15
32	d	412	STE	C11-C12-C13-C14
25	B	608	CLA	C15-C16-C17-C18
25	C	513	CLA	C13-C15-C16-C17
31	C	516	DGD	C8B-C9B-CAB-CBB
32	d	413	STE	C10-C11-C12-C13
25	b	609	CLA	CBA-CGA-O2A-C1
28	c	518	LMG	C29-C28-O8-C9
29	f	102	SQD	C30-C31-C32-C33
31	A	616	DGD	C5A-C6A-C7A-C8A
31	J	101	DGD	C3A-C4A-C5A-C6A
29	A	615	SQD	C9-C10-C11-C12
26	K	101	BCR	C11-C10-C9-C34
35	V	201	HEC	C2B-C3B-CAB-CBB
30	L	101	LHG	C18-C19-C20-C21
31	c	517	DGD	C6A-C7A-C8A-C9A
28	c	521	LMG	C13-C14-C15-C16
28	d	411	LMG	C34-C35-C36-C37
32	B	624	STE	C4-C5-C6-C7
32	L	102	STE	C5-C6-C7-C8
30	D	412	LHG	C29-C30-C31-C32
30	d	408	LHG	C16-C17-C18-C19
32	m	102	STE	C7-C8-C9-C10
28	c	518	LMG	C39-C40-C41-C42
32	B	624	STE	C6-C7-C8-C9
28	d	411	LMG	O6-C5-C6-O5
26	K	103	BCR	C21-C22-C23-C24
26	c	514	BCR	C7-C8-C9-C10
25	c	506	CLA	C13-C15-C16-C17
30	D	409	LHG	C25-C26-C27-C28
32	t	102	STE	C5-C6-C7-C8
30	d	408	LHG	C33-C34-C35-C36
31	C	516	DGD	CCB-CDB-CEB-CFB
30	L	101	LHG	C11-C12-C13-C14
30	d	407	LHG	C10-C11-C12-C13
32	b	624	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	CBA-CGA-O2A-C1
25	B	616	CLA	O2A-C1-C2-C3
28	A	612	LMG	C9-C8-O7-C10
30	d	409	LHG	C30-C31-C32-C33
31	A	616	DGD	CBA-CCA-CDA-CEA
31	c	515	DGD	C6A-C7A-C8A-C9A
25	C	508	CLA	C10-C11-C12-C13
29	A	613	SQD	C9-C10-C11-C12
29	A	613	SQD	C31-C32-C33-C34
29	D	408	SQD	C28-C29-C30-C31
30	D	410	LHG	C27-C28-C29-C30
32	b	621	STE	C9-C10-C11-C12
25	D	404	CLA	C16-C17-C18-C20
28	b	622	LMG	C35-C36-C37-C38
29	B	623	SQD	C34-C35-C36-C37
31	C	515	DGD	C7A-C8A-C9A-CAA
31	c	516	DGD	C8A-C9A-CAA-CBA
26	A	609	BCR	C20-C21-C22-C23
26	K	103	BCR	C11-C10-C9-C8
26	k	102	BCR	C20-C21-C22-C23
28	b	622	LMG	C40-C41-C42-C43
31	c	516	DGD	CBB-CCB-CDB-CEB
25	b	607	CLA	CBA-CGA-O2A-C1
32	B	625	STE	C11-C10-C9-C8
28	m	101	LMG	C18-C19-C20-C21
29	f	102	SQD	C32-C33-C34-C35
25	C	505	CLA	C2-C3-C5-C6
31	a	614	DGD	CFA-CGA-CHA-CIA
25	A	608	CLA	C5-C6-C7-C8
28	A	612	LMG	C37-C38-C39-C40
30	d	409	LHG	C25-C26-C27-C28
32	b	621	STE	C7-C8-C9-C10
32	c	519	STE	C10-C11-C12-C13
32	d	412	STE	C2-C3-C4-C5
25	B	603	CLA	C16-C17-C18-C20
28	d	410	LMG	C36-C37-C38-C39
28	m	101	LMG	C38-C39-C40-C41
30	A	614	LHG	C12-C13-C14-C15
31	C	516	DGD	C4A-C5A-C6A-C7A
30	D	409	LHG	C11-C12-C13-C14
32	d	413	STE	C13-C14-C15-C16
28	m	101	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
29	A	613	SQD	O6-C44-C45-O47
29	a	612	SQD	O6-C44-C45-O47
29	A	615	SQD	C19-C20-C21-C22
31	c	517	DGD	C4B-C5B-C6B-C7B
32	B	625	STE	C12-C13-C14-C15
32	C	520	STE	C11-C10-C9-C8
32	m	102	STE	C12-C13-C14-C15
25	B	604	CLA	CBA-CGA-O2A-C1
32	d	413	STE	C11-C10-C9-C8
25	b	602	CLA	O1D-CGD-O2D-CED
28	B	622	LMG	C31-C32-C33-C34
29	B	623	SQD	C13-C14-C15-C16
32	A	617	STE	C11-C12-C13-C14
32	D	413	STE	C14-C15-C16-C17
32	b	625	STE	C2-C3-C4-C5
25	c	501	CLA	C2A-CAA-CBA-CGA
25	C	506	CLA	C3-C5-C6-C7
32	D	413	STE	C11-C12-C13-C14
31	A	616	DGD	C3A-C4A-C5A-C6A
29	B	623	SQD	O10-C23-O48-C46
31	c	517	DGD	C2A-C3A-C4A-C5A
31	h	102	DGD	CBB-CCB-CDB-CEB
25	c	502	CLA	CBA-CGA-O2A-C1
31	J	101	DGD	CCA-CDA-CEA-CFA
32	J	102	STE	C3-C4-C5-C6
32	b	623	STE	C11-C12-C13-C14
29	A	615	SQD	C28-C29-C30-C31
30	D	410	LHG	C11-C10-C9-C8
32	B	621	STE	C2-C3-C4-C5
25	c	510	CLA	C3-C5-C6-C7
30	d	407	LHG	C18-C19-C20-C21
31	c	517	DGD	C2B-C3B-C4B-C5B
28	B	622	LMG	C37-C38-C39-C40
25	B	616	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
31	A	616	DGD	CDA-CEA-CFA-CGA
32	B	621	STE	C11-C10-C9-C8
28	c	521	LMG	C40-C41-C42-C43
32	a	615	STE	C4-C5-C6-C7
32	b	621	STE	C3-C4-C5-C6
30	D	412	LHG	O1-C1-C2-O2
25	B	602	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C11-C12-C13-C14
25	C	504	CLA	C11-C10-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	a	606	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	609	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C10-C8-C9
25	c	511	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C10-C8-C9
30	e	101	LHG	C16-C17-C18-C19
32	B	627	STE	C11-C10-C9-C8
25	B	601	CLA	O1D-CGD-O2D-CED
25	b	602	CLA	C5-C6-C7-C8
25	b	610	CLA	C15-C16-C17-C18
25	C	504	CLA	C4B-C3B-CAB-CBB
25	a	606	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	C4B-C3B-CAB-CBB
28	m	101	LMG	C12-C13-C14-C15
29	B	623	SQD	C27-C28-C29-C30
30	A	614	LHG	C29-C30-C31-C32
30	D	409	LHG	C18-C19-C20-C21
30	d	407	LHG	C28-C29-C30-C31
31	C	516	DGD	CDA-CEA-CFA-CGA
25	B	616	CLA	C11-C12-C13-C14
29	B	623	SQD	C28-C29-C30-C31
32	m	102	STE	C4-C5-C6-C7
28	A	612	LMG	C17-C18-C19-C20
28	D	407	LMG	C14-C15-C16-C17
29	a	612	SQD	C27-C28-C29-C30
29	a	613	SQD	C15-C16-C17-C18
30	D	409	LHG	C16-C17-C18-C19
30	l	101	LHG	C26-C27-C28-C29
31	c	517	DGD	CCA-CDA-CEA-CFA
31	h	102	DGD	C7A-C8A-C9A-CAA
32	E	102	STE	C6-C7-C8-C9
28	d	411	LMG	C12-C13-C14-C15
29	a	612	SQD	C28-C29-C30-C31
30	A	614	LHG	C10-C11-C12-C13
30	l	101	LHG	C28-C29-C30-C31
29	a	613	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C11-C10-C8-C7
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	605	CLA	C11-C10-C8-C7
25	B	606	CLA	C11-C10-C8-C7
25	B	613	CLA	C12-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	C	513	CLA	C11-C10-C8-C7
25	D	404	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C12-C13-C15
25	b	603	CLA	C11-C10-C8-C7
25	b	606	CLA	C11-C12-C13-C15
25	b	607	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C15
25	c	509	CLA	C6-C7-C8-C10
25	B	602	CLA	C8-C10-C11-C12
32	B	621	STE	C12-C13-C14-C15
28	b	622	LMG	C15-C16-C17-C18
32	d	412	STE	C5-C6-C7-C8
28	d	411	LMG	C35-C36-C37-C38
29	A	615	SQD	C11-C10-C9-C8
32	b	624	STE	C7-C8-C9-C10
25	A	608	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1
27	d	406	PL9	C45-C44-C46-C47
33	D	402	PHO	C2C-C3C-CAC-CBC
32	t	102	STE	C3-C4-C5-C6
25	c	505	CLA	C2-C3-C5-C6
27	d	406	PL9	C13-C14-C16-C17
31	J	101	DGD	C1A-C2A-C3A-C4A
28	B	622	LMG	C17-C18-C19-C20
25	B	603	CLA	C10-C11-C12-C13
25	a	605	CLA	C15-C16-C17-C18
31	C	516	DGD	C8A-C9A-CAA-CBA
29	a	613	SQD	C29-C30-C31-C32
32	M	102	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	K	102	BCR	C37-C22-C23-C24
26	k	102	BCR	C7-C8-C9-C34
25	b	609	CLA	O1A-CGA-O2A-C1
32	B	621	STE	C11-C12-C13-C14
28	c	521	LMG	C16-C17-C18-C19
30	e	101	LHG	C11-C12-C13-C14
30	D	409	LHG	C1-C2-C3-O3
31	c	517	DGD	CDA-CEA-CFA-CGA
27	A	610	PL9	C24-C26-C27-C28
28	A	612	LMG	O1-C7-C8-C9
28	b	622	LMG	O1-C7-C8-C9
28	m	101	LMG	O1-C7-C8-C9
28	m	101	LMG	C7-C8-C9-O8
29	a	612	SQD	C44-C45-C46-O48
31	a	614	DGD	O1G-C1G-C2G-C3G
30	L	101	LHG	C30-C31-C32-C33
28	D	411	LMG	C31-C32-C33-C34
28	c	520	LMG	C41-C42-C43-C44
32	M	101	STE	C10-C11-C12-C13
28	C	517	LMG	C30-C31-C32-C33
31	C	515	DGD	C3A-C4A-C5A-C6A
25	C	505	CLA	C4-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6
27	d	406	PL9	C15-C14-C16-C17
31	J	101	DGD	C3B-C4B-C5B-C6B
32	b	624	STE	C9-C10-C11-C12
25	c	510	CLA	C2-C3-C5-C6
28	m	101	LMG	C11-C12-C13-C14
30	D	412	LHG	C19-C20-C21-C22
31	c	516	DGD	CDA-CEA-CFA-CGA
31	c	515	DGD	CBA-CCA-CDA-CEA
31	C	515	DGD	C8B-C9B-CAB-CBB
25	C	504	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C1-C6-C7-C8
26	B	618	BCR	C23-C24-C25-C30
26	b	617	BCR	C1-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C30
25	d	404	CLA	C5-C6-C7-C8
29	B	623	SQD	C26-C27-C28-C29
30	L	101	LHG	C31-C32-C33-C34
30	l	101	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
31	A	616	DGD	CCB-CDB-CEB-CFB
28	D	407	LMG	C33-C34-C35-C36
25	B	606	CLA	C5-C6-C7-C8
25	B	612	CLA	C10-C11-C12-C13
25	C	506	CLA	C15-C16-C17-C18
25	b	606	CLA	C8-C10-C11-C12
27	A	610	PL9	C47-C48-C49-C50
25	B	603	CLA	C16-C17-C18-C19
31	h	102	DGD	O2G-C1B-C2B-C3B
25	C	507	CLA	C5-C6-C7-C8
28	m	101	LMG	O1-C7-C8-O7
29	a	613	SQD	O47-C45-C46-O48
31	c	515	DGD	CDB-CEB-CFB-CGB
27	A	610	PL9	C4-C3-C7-C8
27	a	610	PL9	C4-C3-C7-C8
27	d	406	PL9	C4-C3-C7-C8
25	b	611	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
29	a	613	SQD	C9-C10-C11-C12
31	a	614	DGD	CAA-CBA-CCA-CDA
32	D	413	STE	C10-C11-C12-C13
32	m	102	STE	C9-C10-C11-C12
26	b	617	BCR	C18-C19-C20-C21
29	a	612	SQD	C9-C10-C11-C12
31	c	516	DGD	CAA-CBA-CCA-CDA
25	B	616	CLA	C11-C12-C13-C15
25	c	509	CLA	C16-C17-C18-C20
28	b	622	LMG	C18-C19-C20-C21
29	A	613	SQD	C13-C14-C15-C16
32	j	101	STE	C3-C4-C5-C6
32	m	102	STE	C2-C3-C4-C5
30	D	409	LHG	C23-C24-C25-C26
25	b	604	CLA	C3-C5-C6-C7
25	B	601	CLA	C11-C10-C8-C9
25	B	604	CLA	C6-C7-C8-C9
25	B	607	CLA	C11-C10-C8-C9
25	B	613	CLA	C14-C13-C15-C16
25	C	513	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C12-C13-C14
25	c	504	CLA	C11-C10-C8-C9
25	c	512	CLA	C6-C7-C8-C9
28	c	521	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
31	h	102	DGD	C6A-C7A-C8A-C9A
32	C	518	STE	C5-C6-C7-C8
26	b	618	BCR	C22-C23-C24-C25
30	d	409	LHG	C9-C10-C11-C12
28	A	612	LMG	C36-C37-C38-C39
32	b	623	STE	C5-C6-C7-C8
26	A	609	BCR	C14-C15-C16-C17
25	b	602	CLA	C16-C17-C18-C19
25	b	612	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C19
31	c	516	DGD	C8B-C9B-CAB-CBB
32	H	103	STE	C11-C12-C13-C14
28	c	518	LMG	C40-C41-C42-C43
28	c	521	LMG	C2-C1-O1-C7
32	B	625	STE	C13-C14-C15-C16
27	A	610	PL9	C34-C36-C37-C38
30	d	408	LHG	C32-C33-C34-C35
32	H	103	STE	C15-C16-C17-C18
28	A	612	LMG	C32-C33-C34-C35
30	D	412	LHG	C18-C19-C20-C21
29	D	408	SQD	C26-C27-C28-C29
25	b	607	CLA	O1A-CGA-O2A-C1
28	c	518	LMG	C38-C39-C40-C41
30	d	408	LHG	O1-C1-C2-O2
25	c	504	CLA	CBA-CGA-O2A-C1
32	H	103	STE	C1-C2-C3-C4
27	d	406	PL9	C28-C29-C31-C32
25	b	612	CLA	C16-C17-C18-C20
28	c	520	LMG	C14-C15-C16-C17
25	B	610	CLA	C15-C16-C17-C18
30	A	614	LHG	C9-C10-C11-C12
29	A	613	SQD	C17-C18-C19-C20
25	c	505	CLA	C13-C15-C16-C17
27	d	406	PL9	C27-C28-C29-C31
28	c	518	LMG	C31-C32-C33-C34
32	C	520	STE	C10-C11-C12-C13
26	B	617	BCR	C35-C13-C14-C15
26	C	514	BCR	C20-C21-C22-C37
26	H	101	BCR	C20-C21-C22-C37
26	K	103	BCR	C35-C13-C14-C15
26	T	101	BCR	C11-C10-C9-C34
26	b	618	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
25	c	502	CLA	O1A-CGA-O2A-C1
30	d	409	LHG	O10-C23-O8-C6
25	B	616	CLA	CBA-CGA-O2A-C1
25	B	607	CLA	C8-C10-C11-C12
32	d	413	STE	C9-C10-C11-C12
30	e	101	LHG	O6-C4-C5-C6
25	b	610	CLA	C16-C17-C18-C20
32	C	520	STE	C12-C13-C14-C15
25	c	511	CLA	C8-C10-C11-C12
26	K	101	BCR	C37-C22-C23-C24
25	A	607	CLA	C11-C12-C13-C15
25	B	603	CLA	C12-C13-C15-C16
25	B	604	CLA	C6-C7-C8-C10
25	B	607	CLA	C11-C10-C8-C7
25	B	616	CLA	C6-C7-C8-C10
25	D	404	CLA	C6-C7-C8-C10
25	a	606	CLA	C12-C13-C15-C16
25	a	608	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C12-C13-C15
25	b	611	CLA	C11-C12-C13-C15
25	c	504	CLA	C11-C10-C8-C7
25	c	505	CLA	C6-C7-C8-C10
25	c	513	CLA	C6-C7-C8-C10
28	b	622	LMG	C13-C14-C15-C16
29	a	612	SQD	C31-C32-C33-C34
28	c	521	LMG	C12-C13-C14-C15
32	t	103	STE	C4-C5-C6-C7
25	B	604	CLA	O1A-CGA-O2A-C1
31	C	516	DGD	C2G-C3G-O3G-C1D
31	C	516	DGD	C5D-C6D-O5D-C1E
29	D	408	SQD	C27-C28-C29-C30
25	b	601	CLA	C2A-CAA-CBA-CGA
30	l	101	LHG	C14-C15-C16-C17
25	A	611	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C20
28	B	620	LMG	C15-C16-C17-C18
29	a	612	SQD	C29-C30-C31-C32
30	A	614	LHG	C31-C32-C33-C34
25	B	616	CLA	O1A-CGA-O2A-C1
28	D	407	LMG	C37-C38-C39-C40
29	a	612	SQD	C17-C18-C19-C20
32	m	102	STE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	607	CLA	C10-C11-C12-C13
30	D	412	LHG	C24-C25-C26-C27
31	C	515	DGD	C3B-C4B-C5B-C6B
32	B	626	STE	C6-C7-C8-C9
29	B	623	SQD	C24-C25-C26-C27
29	a	612	SQD	C10-C11-C12-C13
31	C	516	DGD	C9A-CAA-CBA-CCA
25	D	403	CLA	C3-C5-C6-C7
31	a	614	DGD	C1B-C2B-C3B-C4B
32	d	412	STE	C3-C4-C5-C6
26	k	103	BCR	C11-C10-C9-C8
35	v	201	HEC	C2C-C3C-CAC-CBC
31	c	517	DGD	C7A-C8A-C9A-CAA
30	D	410	LHG	O6-C4-C5-O7
31	C	516	DGD	CBB-CCB-CDB-CEB
32	C	518	STE	C3-C4-C5-C6
32	t	103	STE	C5-C6-C7-C8
28	c	518	LMG	O6-C1-O1-C7
31	C	515	DGD	O1G-C1G-C2G-C3G
29	A	613	SQD	C7-C8-C9-C10
25	a	608	CLA	C13-C15-C16-C17
25	b	612	CLA	C10-C11-C12-C13
25	c	505	CLA	C5-C6-C7-C8
25	C	513	CLA	O1D-CGD-O2D-CED
32	b	621	STE	C2-C3-C4-C5
25	b	604	CLA	C5-C6-C7-C8
28	d	411	LMG	C15-C16-C17-C18
28	B	620	LMG	O7-C8-C9-O8
28	C	517	LMG	O1-C7-C8-O7
28	b	622	LMG	O1-C7-C8-O7
28	c	518	LMG	O1-C7-C8-O7
28	c	521	LMG	O7-C8-C9-O8
31	C	515	DGD	O1G-C1G-C2G-O2G
31	a	614	DGD	O1G-C1G-C2G-O2G
25	B	614	CLA	C6-C7-C8-C9
25	C	508	CLA	C6-C7-C8-C9
25	c	502	CLA	C6-C7-C8-C9
25	B	610	CLA	C16-C17-C18-C19
29	A	615	SQD	C15-C16-C17-C18
28	d	411	LMG	C40-C41-C42-C43
32	T	102	STE	C10-C11-C12-C13
25	c	504	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	D	407	LMG	C30-C31-C32-C33
31	c	517	DGD	C6B-C7B-C8B-C9B
25	C	512	CLA	C10-C11-C12-C13
28	D	407	LMG	C32-C33-C34-C35
25	A	608	CLA	C6-C7-C8-C9
25	d	404	CLA	C16-C17-C18-C19
25	B	604	CLA	C13-C15-C16-C17
32	b	621	STE	C11-C12-C13-C14
28	D	411	LMG	C36-C37-C38-C39
31	c	515	DGD	CAA-CBA-CCA-CDA
25	B	610	CLA	O1D-CGD-O2D-CED
32	b	623	STE	C9-C10-C11-C12
25	c	512	CLA	C4-C3-C5-C6
29	A	613	SQD	C16-C17-C18-C19
25	c	510	CLA	C15-C16-C17-C18
35	v	201	HEC	C2B-C3B-CAB-CBB
29	a	613	SQD	C14-C15-C16-C17
25	A	611	CLA	C13-C15-C16-C17
32	a	615	STE	C2-C3-C4-C5
31	A	616	DGD	C1A-C2A-C3A-C4A
28	d	411	LMG	C32-C33-C34-C35
32	B	627	STE	C9-C10-C11-C12
28	c	521	LMG	C20-C21-C22-C23
29	D	408	SQD	C23-C24-C25-C26
28	d	411	LMG	C39-C40-C41-C42
26	D	405	BCR	C18-C19-C20-C21
25	c	503	CLA	CBA-CGA-O2A-C1
32	C	520	STE	C7-C8-C9-C10
32	c	519	STE	C12-C13-C14-C15
32	t	102	STE	C11-C10-C9-C8
25	b	613	CLA	O1D-CGD-O2D-CED
31	A	616	DGD	CFB-CGB-CHB-CIB
32	J	102	STE	C6-C7-C8-C9
25	C	501	CLA	C4B-C3B-CAB-CBB
25	a	608	CLA	C1A-C2A-CAA-CBA
29	D	408	SQD	O48-C23-C24-C25
31	H	102	DGD	O2G-C1B-C2B-C3B
26	K	101	BCR	C21-C22-C23-C24
26	K	102	BCR	C7-C8-C9-C10
30	e	101	LHG	C25-C26-C27-C28
30	D	410	LHG	O6-C4-C5-C6
29	b	620	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	d	409	LHG	C31-C32-C33-C34
31	a	614	DGD	C7B-C8B-C9B-CAB
25	B	602	CLA	C12-C13-C15-C16
25	B	605	CLA	C12-C13-C15-C16
25	B	613	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C10-C8-C7
25	C	507	CLA	C12-C13-C15-C16
25	C	509	CLA	C12-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C7
25	b	602	CLA	C11-C10-C8-C7
25	b	607	CLA	C6-C7-C8-C10
25	b	608	CLA	C11-C10-C8-C7
25	c	501	CLA	C11-C12-C13-C15
25	c	510	CLA	C12-C13-C15-C16
25	c	512	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
30	d	408	LHG	C18-C19-C20-C21
25	c	503	CLA	O1A-CGA-O2A-C1
30	D	409	LHG	C31-C32-C33-C34
31	h	102	DGD	C4A-C5A-C6A-C7A
28	c	521	LMG	C37-C38-C39-C40
31	C	515	DGD	CAB-CBB-CCB-CDB
25	B	601	CLA	C3A-C2A-CAA-CBA
25	A	611	CLA	C16-C17-C18-C20
25	B	613	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C19
28	d	410	LMG	C40-C41-C42-C43
30	D	409	LHG	O9-C7-O7-C5
25	B	614	CLA	O1D-CGD-O2D-CED
30	A	614	LHG	O6-C4-C5-O7
32	b	623	STE	C1-C2-C3-C4
25	B	603	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	508	CLA	C14-C13-C15-C16
25	b	603	CLA	C11-C10-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	611	CLA	C14-C13-C15-C16
29	D	408	SQD	C34-C35-C36-C37
31	c	516	DGD	C7A-C8A-C9A-CAA
26	K	101	BCR	C9-C10-C11-C12
28	A	612	LMG	C12-C13-C14-C15
32	C	518	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	c	519	STE	C11-C12-C13-C14
30	D	412	LHG	C33-C34-C35-C36
31	c	515	DGD	O6D-C5D-C6D-O5D
28	D	411	LMG	O7-C8-C9-O8
28	c	520	LMG	O7-C8-C9-O8
25	C	512	CLA	C15-C16-C17-C18
25	B	613	CLA	C16-C17-C18-C19
28	C	517	LMG	O1-C7-C8-C9
28	c	520	LMG	O1-C7-C8-C9
32	a	615	STE	C7-C8-C9-C10
29	a	613	SQD	C13-C14-C15-C16
31	a	614	DGD	CCB-CDB-CEB-CFB
25	B	601	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O2D
28	m	101	LMG	C20-C21-C22-C23
29	a	612	SQD	O10-C23-O48-C46
25	c	513	CLA	CBA-CGA-O2A-C1
29	a	612	SQD	C24-C23-O48-C46
25	a	608	CLA	C10-C11-C12-C13
25	b	610	CLA	C16-C17-C18-C19
30	D	409	LHG	C35-C36-C37-C38
28	m	101	LMG	C4-C5-C6-O5
28	d	410	LMG	C34-C35-C36-C37
29	f	102	SQD	C28-C29-C30-C31
31	H	102	DGD	CCB-CDB-CEB-CFB
32	b	621	STE	C14-C15-C16-C17
25	B	601	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O2D
30	A	614	LHG	C3-O3-P-O4
30	A	614	LHG	C3-O3-P-O5
30	D	409	LHG	C4-O6-P-O5
30	D	410	LHG	C3-O3-P-O5
30	d	408	LHG	C4-O6-P-O5
30	e	101	LHG	C4-O6-P-O4
33	d	402	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
33	d	402	PHO	CHA-CBD-CGD-O2D
25	b	604	CLA	C16-C17-C18-C20
32	B	627	STE	C15-C16-C17-C18
26	h	101	BCR	C14-C15-C16-C17
25	a	606	CLA	C2B-C3B-CAB-CBB
25	b	609	CLA	C2B-C3B-CAB-CBB
32	d	413	STE	C4-C5-C6-C7
25	C	504	CLA	C2-C3-C5-C6
25	C	506	CLA	C13-C15-C16-C17
31	c	517	DGD	C8A-C9A-CAA-CBA
28	A	612	LMG	C14-C15-C16-C17
32	t	102	STE	C4-C5-C6-C7
28	d	411	LMG	C36-C37-C38-C39
30	D	412	LHG	C32-C33-C34-C35
31	a	614	DGD	CDB-CEB-CFB-CGB
32	k	104	STE	C2-C3-C4-C5
25	d	404	CLA	C8-C10-C11-C12
28	A	612	LMG	C31-C32-C33-C34
30	e	101	LHG	C14-C15-C16-C17
27	D	406	PL9	C4-C3-C7-C8
31	h	102	DGD	CDA-CEA-CFA-CGA
25	b	602	CLA	C10-C11-C12-C13
28	b	622	LMG	C7-C8-O7-C10
28	b	622	LMG	C34-C35-C36-C37
29	B	623	SQD	C14-C15-C16-C17
31	C	515	DGD	O6D-C5D-C6D-O5D
25	b	615	CLA	C13-C15-C16-C17
33	d	402	PHO	C13-C15-C16-C17
27	d	406	PL9	C33-C34-C36-C37
30	D	410	LHG	C14-C15-C16-C17
31	c	516	DGD	C2A-C3A-C4A-C5A
25	B	610	CLA	C16-C17-C18-C20
30	d	408	LHG	C35-C36-C37-C38
32	I	101	STE	C12-C13-C14-C15
25	c	512	CLA	C13-C15-C16-C17
25	A	607	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C10-C8-C9
25	B	606	CLA	C14-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C14
25	C	502	CLA	C6-C7-C8-C9
25	C	505	CLA	C11-C12-C13-C14
25	C	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	D	404	CLA	C6-C7-C8-C9
25	a	606	CLA	C14-C13-C15-C16
25	a	608	CLA	C14-C13-C15-C16
25	b	609	CLA	C11-C10-C8-C9
25	c	505	CLA	C6-C7-C8-C9
25	d	404	CLA	C11-C12-C13-C14
33	D	401	PHO	C14-C13-C15-C16
33	a	607	PHO	C14-C13-C15-C16
25	C	506	CLA	C11-C12-C13-C15
26	K	102	BCR	C20-C21-C22-C23
26	k	101	BCR	C20-C21-C22-C23
28	D	411	LMG	C28-C29-C30-C31
28	B	620	LMG	C39-C40-C41-C42
31	a	614	DGD	C9A-CAA-CBA-CCA
28	B	622	LMG	C14-C15-C16-C17
32	C	519	STE	C3-C4-C5-C6
25	B	612	CLA	C13-C15-C16-C17
28	b	622	LMG	C16-C17-C18-C19
25	c	513	CLA	O1A-CGA-O2A-C1
28	b	622	LMG	C42-C43-C44-C45
25	B	610	CLA	CBD-CGD-O2D-CED
25	B	602	CLA	C15-C16-C17-C18
25	B	613	CLA	C10-C11-C12-C13
27	D	406	PL9	C15-C14-C16-C17
33	D	401	PHO	C4-C3-C5-C6
25	b	611	CLA	C2-C3-C5-C6
25	c	512	CLA	C2-C3-C5-C6
32	B	626	STE	C7-C8-C9-C10
28	D	407	LMG	C31-C32-C33-C34
28	d	411	LMG	C30-C31-C32-C33
30	D	412	LHG	C25-C26-C27-C28
31	A	616	DGD	C7B-C8B-C9B-CAB
28	D	411	LMG	C33-C34-C35-C36
25	B	609	CLA	C3-C5-C6-C7
30	d	407	LHG	C32-C33-C34-C35
32	B	627	STE	C5-C6-C7-C8
25	B	601	CLA	CAA-CBA-CGA-O2A
25	c	509	CLA	CAA-CBA-CGA-O2A
29	a	613	SQD	C11-C10-C9-C8
29	A	615	SQD	C7-C8-C9-C10
31	C	515	DGD	O1G-C1A-C2A-C3A
26	K	103	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C16-C17-C18-C20
31	C	515	DGD	C4D-C5D-C6D-O5D
26	t	101	BCR	C21-C22-C23-C24
32	b	624	STE	C4-C5-C6-C7
31	c	515	DGD	C5D-C6D-O5D-C1E
25	b	611	CLA	C10-C11-C12-C13
25	c	502	CLA	C13-C15-C16-C17
31	h	102	DGD	C9A-CAA-CBA-CCA
28	B	622	LMG	C34-C35-C36-C37
28	m	101	LMG	C31-C32-C33-C34
32	T	102	STE	C11-C12-C13-C14
28	B	620	LMG	C28-C29-C30-C31
30	l	101	LHG	C24-C25-C26-C27
27	A	610	PL9	C45-C44-C46-C47
28	C	517	LMG	C18-C19-C20-C21
25	B	601	CLA	C6-C7-C8-C9
25	B	605	CLA	C14-C13-C15-C16
25	C	509	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C9
25	b	608	CLA	C11-C10-C8-C9
25	c	501	CLA	C11-C12-C13-C14
25	B	612	CLA	CBA-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
25	B	612	CLA	C8-C10-C11-C12
25	B	609	CLA	C4B-C3B-CAB-CBB
25	b	605	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
30	l	101	LHG	C13-C14-C15-C16
32	T	102	STE	C12-C13-C14-C15
31	c	517	DGD	CCB-CDB-CEB-CFB
30	A	614	LHG	C28-C29-C30-C31
32	A	617	STE	C13-C14-C15-C16
32	m	102	STE	C10-C11-C12-C13
25	C	511	CLA	O1A-CGA-O2A-C1
26	k	102	BCR	C19-C20-C21-C22
31	A	616	DGD	C2A-C1A-O1G-C1G
25	b	609	CLA	O1D-CGD-O2D-CED
25	C	506	CLA	C12-C13-C15-C16
25	C	512	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	609	CLA	C6-C7-C8-C10
30	D	410	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	c	517	DGD	CBB-CCB-CDB-CEB
28	m	101	LMG	C34-C35-C36-C37
29	A	615	SQD	C32-C33-C34-C35
28	D	411	LMG	C34-C35-C36-C37
32	c	519	STE	C7-C8-C9-C10
25	C	510	CLA	C4-C3-C5-C6
33	d	402	PHO	C3A-C2A-CAA-CBA
30	D	412	LHG	C23-C24-C25-C26
32	t	103	STE	C7-C8-C9-C10
25	c	513	CLA	C15-C16-C17-C18
32	b	624	STE	C11-C12-C13-C14
29	D	408	SQD	C24-C25-C26-C27
30	d	407	LHG	C14-C15-C16-C17
25	D	403	CLA	C2-C1-O2A-CGA
32	D	413	STE	O2-C1-C2-C3
32	b	621	STE	O2-C1-C2-C3
31	H	102	DGD	C6A-C7A-C8A-C9A
32	t	103	STE	C6-C7-C8-C9
25	b	612	CLA	C8-C10-C11-C12
25	B	609	CLA	C4-C3-C5-C6
27	D	406	PL9	C39-C41-C42-C43
28	c	521	LMG	O1-C7-C8-C9
28	B	622	LMG	O9-C10-C11-C12
25	A	611	CLA	C14-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C14
25	b	604	CLA	C14-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C9
25	b	614	CLA	C6-C7-C8-C9
25	c	507	CLA	C6-C7-C8-C9
28	c	521	LMG	C18-C19-C20-C21
28	c	521	LMG	C30-C31-C32-C33
30	A	614	LHG	C17-C18-C19-C20
30	d	409	LHG	C32-C33-C34-C35
32	b	624	STE	C6-C7-C8-C9
29	b	620	SQD	C19-C20-C21-C22
32	C	519	STE	O2-C1-C2-C3
32	D	413	STE	O1-C1-C2-C3
32	k	104	STE	O2-C1-C2-C3
29	B	623	SQD	C44-C45-O47-C7
29	B	623	SQD	C46-C45-O47-C7
29	a	613	SQD	C46-C45-O47-C7
31	a	614	DGD	C1G-C2G-O2G-C1B

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Mol	Chain	Res	Type	Atoms
32	d	413	STE	C2-C3-C4-C5
31	c	515	DGD	C4D-C5D-C6D-O5D
25	B	612	CLA	O1A-CGA-O2A-C1
31	c	515	DGD	O1A-C1A-O1G-C1G
32	C	519	STE	O1-C1-C2-C3
25	b	610	CLA	C2A-CAA-CBA-CGA
25	C	508	CLA	C13-C15-C16-C17
25	B	602	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
35	V	201	HEC	C4B-C3B-CAB-CBB
25	B	607	CLA	CBA-CGA-O2A-C1
28	A	612	LMG	C38-C39-C40-C41
25	B	614	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C19
35	v	201	HEC	C4B-C3B-CAB-CBB
32	E	102	STE	C4-C5-C6-C7
25	C	501	CLA	C2B-C3B-CAB-CBB
25	b	610	CLA	C2B-C3B-CAB-CBB
25	c	502	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C5-C6-C7-C8
26	B	619	BCR	C23-C24-C25-C30
26	K	103	BCR	C23-C24-C25-C30
26	b	617	BCR	C5-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
26	k	101	BCR	C23-C24-C25-C30
28	b	622	LMG	C14-C15-C16-C17
32	c	519	STE	O2-C1-C2-C3
25	b	610	CLA	C13-C15-C16-C17
30	d	407	LHG	C29-C30-C31-C32
31	h	102	DGD	CCA-CDA-CEA-CFA
30	d	408	LHG	C19-C20-C21-C22
32	c	519	STE	O1-C1-C2-C3
25	B	601	CLA	C4-C3-C5-C6
25	d	403	CLA	C4-C3-C5-C6
32	M	102	STE	C1-C2-C3-C4
25	D	403	CLA	C2C-C3C-CAC-CBC
31	c	515	DGD	C8A-C9A-CAA-CBA
32	I	101	STE	C5-C6-C7-C8
25	B	613	CLA	C11-C12-C13-C15
25	B	615	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	C11-C10-C8-C7
25	b	605	CLA	C11-C12-C13-C15
25	c	509	CLA	C11-C12-C13-C15
25	c	510	CLA	C11-C10-C8-C7
32	b	623	STE	C2-C3-C4-C5
27	a	610	PL9	C19-C21-C22-C23
25	C	501	CLA	C2A-CAA-CBA-CGA
28	c	520	LMG	O1-C7-C8-O7
31	c	515	DGD	O1G-C1G-C2G-O2G
29	A	615	SQD	C24-C25-C26-C27
32	k	104	STE	C6-C7-C8-C9
25	b	616	CLA	C10-C11-C12-C13
28	C	517	LMG	C16-C17-C18-C19
31	a	614	DGD	C6B-C7B-C8B-C9B
31	c	516	DGD	C4B-C5B-C6B-C7B
28	D	411	LMG	C16-C17-C18-C19
32	B	627	STE	C4-C5-C6-C7
29	a	613	SQD	C19-C20-C21-C22
25	B	614	CLA	C16-C17-C18-C20
25	C	502	CLA	C16-C17-C18-C20
32	D	413	STE	C6-C7-C8-C9
25	D	403	CLA	C13-C15-C16-C17
35	V	201	HEC	CAD-CBD-CGD-O2D
25	B	601	CLA	C2-C3-C5-C6
25	B	616	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6
25	b	612	CLA	C2C-C3C-CAC-CBC
31	C	516	DGD	C2B-C3B-C4B-C5B
25	c	508	CLA	O1A-CGA-O2A-C1
25	B	602	CLA	C14-C13-C15-C16
25	C	506	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	b	605	CLA	C11-C12-C13-C14
25	C	509	CLA	C5-C6-C7-C8
31	c	515	DGD	C3A-C4A-C5A-C6A
32	t	102	STE	C6-C7-C8-C9
32	k	104	STE	O1-C1-C2-C3
31	H	102	DGD	C9B-CAB-CBB-CCB
31	J	101	DGD	C9A-CAA-CBA-CCA
28	B	622	LMG	C29-C30-C31-C32
30	A	614	LHG	C2-C3-O3-P
30	d	409	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
26	K	101	BCR	C14-C15-C16-C17
25	B	609	CLA	C2-C3-C5-C6
25	C	510	CLA	C2-C3-C5-C6
30	D	409	LHG	C30-C31-C32-C33
25	B	601	CLA	C13-C15-C16-C17
25	B	607	CLA	O1A-CGA-O2A-C1
29	A	613	SQD	C35-C36-C37-C38
29	b	620	SQD	C16-C17-C18-C19
28	c	520	LMG	C11-C12-C13-C14
32	E	102	STE	C7-C8-C9-C10
32	b	621	STE	O1-C1-C2-C3
34	f	101	HEM	CAD-CBD-CGD-O1D
25	B	614	CLA	C2A-CAA-CBA-CGA
29	A	613	SQD	C26-C27-C28-C29
25	C	511	CLA	C2C-C3C-CAC-CBC
28	d	410	LMG	O7-C10-C11-C12
32	A	617	STE	O2-C1-C2-C3
33	D	401	PHO	C2-C3-C5-C6
25	B	606	CLA	C4B-C3B-CAB-CBB
25	b	611	CLA	C4B-C3B-CAB-CBB
25	c	502	CLA	C4B-C3B-CAB-CBB
32	E	102	STE	O2-C1-C2-C3
35	V	201	HEC	CAD-CBD-CGD-O1D
29	A	615	SQD	C17-C18-C19-C20
33	a	607	PHO	CHA-CBD-CGD-O1D
25	C	513	CLA	C5-C6-C7-C8
28	C	517	LMG	C40-C41-C42-C43
28	D	407	LMG	C34-C35-C36-C37
32	B	624	STE	C5-C6-C7-C8
30	L	101	LHG	C25-C26-C27-C28
30	l	101	LHG	O6-C4-C5-C6
25	b	605	CLA	C4-C3-C5-C6
27	a	610	PL9	C35-C34-C36-C37
25	C	504	CLA	C11-C12-C13-C14
31	C	516	DGD	O6D-C1D-O3G-C3G
31	c	516	DGD	C4A-C5A-C6A-C7A
25	C	501	CLA	C12-C13-C15-C16
25	b	616	CLA	C11-C10-C8-C7
25	c	512	CLA	C11-C10-C8-C7
28	B	622	LMG	O7-C10-C11-C12
28	c	521	LMG	C34-C35-C36-C37
30	D	409	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C11-C12-C13-C14
25	B	613	CLA	C6-C7-C8-C9
25	B	614	CLA	C11-C10-C8-C9
25	b	614	CLA	C11-C10-C8-C9
25	c	512	CLA	C14-C13-C15-C16
33	d	402	PHO	C14-C13-C15-C16
31	c	516	DGD	C2G-C3G-O3G-C1D
31	H	102	DGD	C2A-C3A-C4A-C5A
25	C	512	CLA	C2A-CAA-CBA-CGA
25	B	612	CLA	C2-C1-O2A-CGA
25	b	613	CLA	C2-C1-O2A-CGA
27	a	610	PL9	C27-C28-C29-C31
25	c	508	CLA	CBA-CGA-O2A-C1
25	B	602	CLA	C3A-C2A-CAA-CBA
25	d	404	CLA	C3A-C2A-CAA-CBA
27	a	610	PL9	C40-C39-C41-C42
35	v	201	HEC	CAD-CBD-CGD-O1D
35	v	201	HEC	CAD-CBD-CGD-O2D
32	j	101	STE	C4-C5-C6-C7
25	d	404	CLA	C3-C5-C6-C7
28	D	411	LMG	O10-C28-O8-C9
31	c	517	DGD	C3A-C4A-C5A-C6A
26	B	617	BCR	C10-C11-C12-C13
31	c	516	DGD	CAB-CBB-CCB-CDB
30	D	410	LHG	C31-C32-C33-C34
32	A	617	STE	O1-C1-C2-C3
32	E	102	STE	O1-C1-C2-C3
29	B	623	SQD	C32-C33-C34-C35
25	C	510	CLA	C13-C15-C16-C17
25	c	503	CLA	C10-C11-C12-C13
29	a	613	SQD	C24-C25-C26-C27
31	C	515	DGD	CCB-CDB-CEB-CFB
29	A	613	SQD	C25-C26-C27-C28
26	b	618	BCR	C11-C10-C9-C8
30	D	410	LHG	C1-C2-C3-O3
30	l	101	LHG	O6-C4-C5-O7
28	A	612	LMG	C7-C8-C9-O8
31	A	616	DGD	O1G-C1G-C2G-C3G
31	c	515	DGD	C1G-C2G-C3G-O3G
25	b	616	CLA	C5-C6-C7-C8
28	D	407	LMG	C39-C40-C41-C42
32	H	103	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	b	620	SQD	C27-C28-C29-C30
31	J	101	DGD	C7B-C8B-C9B-CAB
32	j	101	STE	C5-C6-C7-C8
30	d	409	LHG	C34-C35-C36-C37
31	A	616	DGD	C6A-C7A-C8A-C9A
26	k	101	BCR	C9-C10-C11-C12
30	D	409	LHG	C33-C34-C35-C36
32	C	520	STE	C3-C4-C5-C6
28	b	622	LMG	C38-C39-C40-C41
31	A	616	DGD	O1G-C1G-C2G-O2G
25	c	506	CLA	C10-C11-C12-C13
25	B	611	CLA	C11-C12-C13-C14
25	a	608	CLA	C11-C12-C13-C14
25	b	612	CLA	C11-C10-C8-C9
25	c	508	CLA	C11-C12-C13-C14
25	d	403	CLA	C11-C12-C13-C14
25	d	403	CLA	C14-C13-C15-C16
29	D	408	SQD	C30-C31-C32-C33
25	b	613	CLA	CAA-CBA-CGA-O2A
32	d	413	STE	C6-C7-C8-C9
27	D	406	PL9	C30-C29-C31-C32
25	C	502	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C12-C13-C15
25	a	611	CLA	C12-C13-C15-C16
25	b	609	CLA	C11-C12-C13-C15
25	b	612	CLA	C11-C10-C8-C7
32	b	625	STE	C1-C2-C3-C4
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	609	CLA	C2B-C3B-CAB-CBB
25	b	611	CLA	C2B-C3B-CAB-CBB
25	b	612	CLA	C2B-C3B-CAB-CBB
25	c	507	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
26	B	618	BCR	C23-C24-C25-C26
26	C	514	BCR	C23-C24-C25-C30
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	K	103	BCR	C23-C24-C25-C26
26	b	618	BCR	C23-C24-C25-C30
26	k	101	BCR	C23-C24-C25-C26
26	k	103	BCR	C1-C6-C7-C8
26	k	103	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	t	101	BCR	C1-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
25	B	613	CLA	C2-C1-O2A-CGA
25	A	607	CLA	C16-C17-C18-C20
28	c	520	LMG	C16-C17-C18-C19
28	b	622	LMG	O7-C10-C11-C12
30	D	412	LHG	C24-C23-O8-C6
31	h	102	DGD	C1A-C2A-C3A-C4A
34	f	101	HEM	CAD-CBD-CGD-O2D
29	a	612	SQD	O49-C7-O47-C45
28	b	622	LMG	C33-C34-C35-C36
29	A	613	SQD	C29-C30-C31-C32
29	a	612	SQD	C8-C7-O47-C45
29	B	623	SQD	C23-C24-C25-C26
28	C	517	LMG	O7-C10-C11-C12
31	a	614	DGD	O1G-C1A-C2A-C3A
30	d	408	LHG	C28-C29-C30-C31
32	M	101	STE	C4-C5-C6-C7
31	C	516	DGD	C1A-C2A-C3A-C4A
32	H	103	STE	C13-C14-C15-C16
25	B	612	CLA	CAA-CBA-CGA-O2A
25	B	613	CLA	CAA-CBA-CGA-O2A
32	C	518	STE	C4-C5-C6-C7
25	b	608	CLA	C2C-C3C-CAC-CBC
28	B	622	LMG	O8-C28-C29-C30
25	B	615	CLA	C11-C10-C8-C9
25	d	404	CLA	C6-C7-C8-C9
30	d	409	LHG	O8-C23-C24-C25
25	c	513	CLA	C13-C15-C16-C17
25	A	607	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
31	c	516	DGD	O6D-C1D-O3G-C3G
28	d	411	LMG	O7-C10-C11-C12
27	D	406	PL9	C42-C43-C44-C46
25	c	510	CLA	CAA-CBA-CGA-O2A
28	m	101	LMG	O8-C28-C29-C30
29	a	612	SQD	O47-C7-C8-C9
31	C	515	DGD	O2G-C1B-C2B-C3B
31	c	515	DGD	C9A-CAA-CBA-CCA
31	a	614	DGD	CCA-CDA-CEA-CFA
31	c	517	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	CDA-CEA-CFA-CGA
28	C	517	LMG	C12-C13-C14-C15
30	D	409	LHG	C34-C35-C36-C37
32	L	102	STE	C3-C4-C5-C6
25	A	606	CLA	C5-C6-C7-C8
25	C	506	CLA	C4-C3-C5-C6
25	A	606	CLA	C2-C1-O2A-CGA
25	B	601	CLA	C2-C1-O2A-CGA
25	c	502	CLA	C2-C1-O2A-CGA
29	A	613	SQD	O47-C7-C8-C9
25	B	605	CLA	C6-C7-C8-C10
25	B	606	CLA	C11-C12-C13-C15
25	B	610	CLA	C12-C13-C15-C16
25	b	615	CLA	C6-C7-C8-C10
25	c	506	CLA	C16-C17-C18-C20
30	D	409	LHG	C9-C10-C11-C12
29	a	613	SQD	C44-C45-O47-C7
33	a	607	PHO	O2A-C1-C2-C3
29	a	613	SQD	C27-C28-C29-C30
32	B	625	STE	C3-C4-C5-C6
28	d	410	LMG	O9-C10-C11-C12
31	c	516	DGD	CCA-CDA-CEA-CFA
27	a	610	PL9	C14-C16-C17-C18
32	M	101	STE	O1-C1-C2-C3
25	b	601	CLA	C3A-C2A-CAA-CBA
30	L	101	LHG	O10-C23-O8-C6
25	B	611	CLA	C13-C15-C16-C17
29	b	620	SQD	C11-C10-C9-C8
33	d	402	PHO	C2C-C3C-CAC-CBC
32	d	413	STE	O1-C1-C2-C3
31	c	516	DGD	O1B-C1B-C2B-C3B
28	c	521	LMG	C28-C29-C30-C31
25	b	612	CLA	C15-C16-C17-C18
25	C	502	CLA	C11-C10-C8-C9
25	D	403	CLA	C11-C10-C8-C9
25	a	608	CLA	C6-C7-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	b	615	CLA	C11-C10-C8-C9
25	C	509	CLA	C8-C10-C11-C12
32	d	413	STE	C14-C15-C16-C17
25	b	612	CLA	CAA-CBA-CGA-O2A
32	j	101	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	d	413	STE	C12-C13-C14-C15
30	d	407	LHG	O1-C1-C2-O2
28	B	620	LMG	C8-C7-O1-C1
28	b	622	LMG	C8-C7-O1-C1
25	b	613	CLA	CAA-CBA-CGA-O1A
25	B	605	CLA	C10-C11-C12-C13
34	E	101	HEM	CAD-CBD-CGD-O2D
25	B	613	CLA	CAA-CBA-CGA-O1A
29	A	613	SQD	O49-C7-C8-C9
29	a	612	SQD	O49-C7-C8-C9
31	C	515	DGD	O1B-C1B-C2B-C3B
25	B	616	CLA	CAD-CBD-CGD-O2D
33	a	607	PHO	CAD-CBD-CGD-O2D
28	m	101	LMG	O10-C28-C29-C30
31	c	515	DGD	O1B-C1B-C2B-C3B
25	d	403	CLA	C2-C1-O2A-CGA
28	d	410	LMG	C38-C39-C40-C41
25	B	612	CLA	CAA-CBA-CGA-O1A
33	d	402	PHO	C1A-C2A-CAA-CBA
29	D	408	SQD	C31-C32-C33-C34
31	J	101	DGD	C4A-C5A-C6A-C7A
25	c	501	CLA	CAA-CBA-CGA-O2A
31	c	515	DGD	O2G-C1B-C2B-C3B
25	C	506	CLA	C2-C3-C5-C6
28	B	620	LMG	C18-C19-C20-C21
25	b	612	CLA	CAA-CBA-CGA-O1A
28	D	407	LMG	O7-C10-C11-C12
35	v	201	HEC	C4C-C3C-CAC-CBC
30	L	101	LHG	C34-C35-C36-C37

There are no ring outliers.

149 monomers are involved in 312 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	606	CLA	1	0
35	v	201	HEC	1	0
25	b	610	CLA	1	0
28	D	411	LMG	2	0
29	a	613	SQD	4	0
25	b	616	CLA	3	0
25	b	615	CLA	4	0
25	C	504	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	511	CLA	4	0
31	a	614	DGD	3	0
25	b	608	CLA	3	0
25	C	502	CLA	4	0
26	k	101	BCR	2	0
26	H	101	BCR	5	0
32	C	518	STE	1	0
28	B	620	LMG	5	0
21	A	601[A]	OEY	1	0
31	H	102	DGD	2	0
28	c	518	LMG	2	0
25	B	601	CLA	6	0
25	C	513	CLA	4	0
32	B	625	STE	2	0
25	c	503	CLA	5	0
26	k	102	BCR	1	0
29	A	613	SQD	1	0
31	A	616	DGD	4	0
29	D	408	SQD	1	0
28	c	520	LMG	1	0
32	d	413	STE	6	0
26	B	617	BCR	1	0
25	b	601	CLA	4	0
30	d	407	LHG	4	0
25	C	510	CLA	2	0
32	B	621	STE	2	0
31	c	517	DGD	6	0
25	b	606	CLA	3	0
26	b	619	BCR	3	0
25	d	403	CLA	1	0
25	c	506	CLA	3	0
29	A	615	SQD	1	0
26	k	103	BCR	1	0
25	a	611	CLA	3	0
27	A	610	PL9	6	0
25	B	616	CLA	1	0
26	b	618	BCR	2	0
25	b	602	CLA	3	0
25	c	508	CLA	3	0
25	D	403	CLA	3	0
25	c	505	CLA	3	0
25	a	608	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	601[B]	OEY	1	0
25	B	605	CLA	1	0
28	C	517	LMG	1	0
31	J	101	DGD	5	0
32	d	412	STE	1	0
25	d	404	CLA	2	0
26	B	619	BCR	2	0
32	H	103	STE	2	0
26	c	514	BCR	4	0
26	K	101	BCR	2	0
26	K	103	BCR	1	0
32	D	413	STE	6	0
32	j	101	STE	1	0
25	C	501	CLA	1	0
27	D	406	PL9	2	0
28	d	410	LMG	1	0
25	C	505	CLA	2	0
28	b	622	LMG	1	0
25	b	604	CLA	2	0
25	B	603	CLA	1	0
25	c	511	CLA	4	0
25	b	603	CLA	3	0
25	b	613	CLA	1	0
26	h	101	BCR	5	0
28	B	622	LMG	2	0
25	C	512	CLA	3	0
33	a	607	PHO	1	0
25	c	502	CLA	3	0
30	D	409	LHG	2	0
32	T	102	STE	2	0
25	B	614	CLA	7	0
30	l	101	LHG	5	0
27	d	406	PL9	3	0
25	c	507	CLA	3	0
30	D	412	LHG	5	0
26	d	405	BCR	1	0
25	B	607	CLA	3	0
25	c	504	CLA	2	0
30	e	101	LHG	5	0
25	b	614	CLA	5	0
32	I	101	STE	2	0
25	a	605	CLA	4	0

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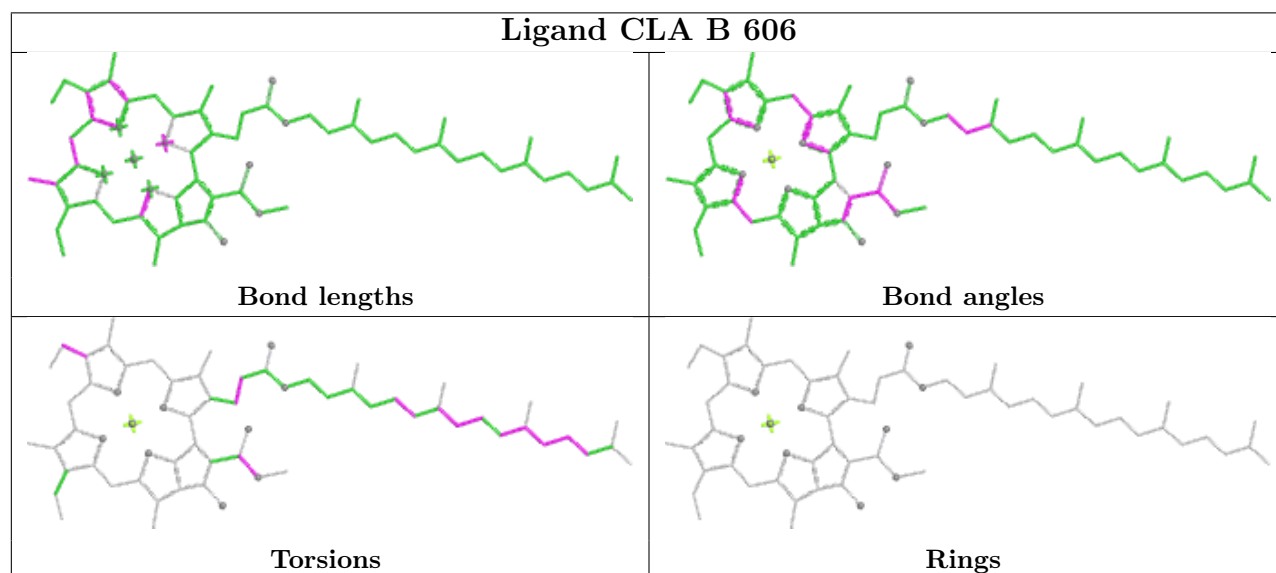
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	L	101	LHG	1	0
25	B	602	CLA	2	0
25	C	509	CLA	2	0
25	A	608	CLA	1	0
25	a	606	CLA	2	0
30	d	408	LHG	2	0
25	b	611	CLA	2	0
25	c	501	CLA	3	0
26	C	514	BCR	2	0
32	c	519	STE	1	0
26	K	102	BCR	1	0
25	B	609	CLA	2	0
34	E	101	HEM	2	0
25	C	508	CLA	5	0
32	L	102	STE	1	0
26	T	101	BCR	3	0
25	B	615	CLA	2	0
29	b	620	SQD	5	0
29	f	102	SQD	3	0
25	c	513	CLA	3	0
25	A	607	CLA	2	0
32	m	102	STE	2	0
27	a	610	PL9	5	0
29	B	623	SQD	5	0
30	A	614	LHG	1	0
25	b	605	CLA	4	0
25	C	506	CLA	4	0
25	A	606	CLA	3	0
25	B	604	CLA	1	0
25	B	613	CLA	3	0
28	D	407	LMG	2	0
21	a	601[B]	OEY	1	0
26	D	405	BCR	1	0
28	c	521	LMG	3	0
31	c	515	DGD	3	0
25	B	612	CLA	2	0
25	b	612	CLA	3	0
33	D	402	PHO	1	0
25	D	404	CLA	3	0
24	A	605	BCT	1	0
25	b	609	CLA	3	0
26	b	617	BCR	1	0

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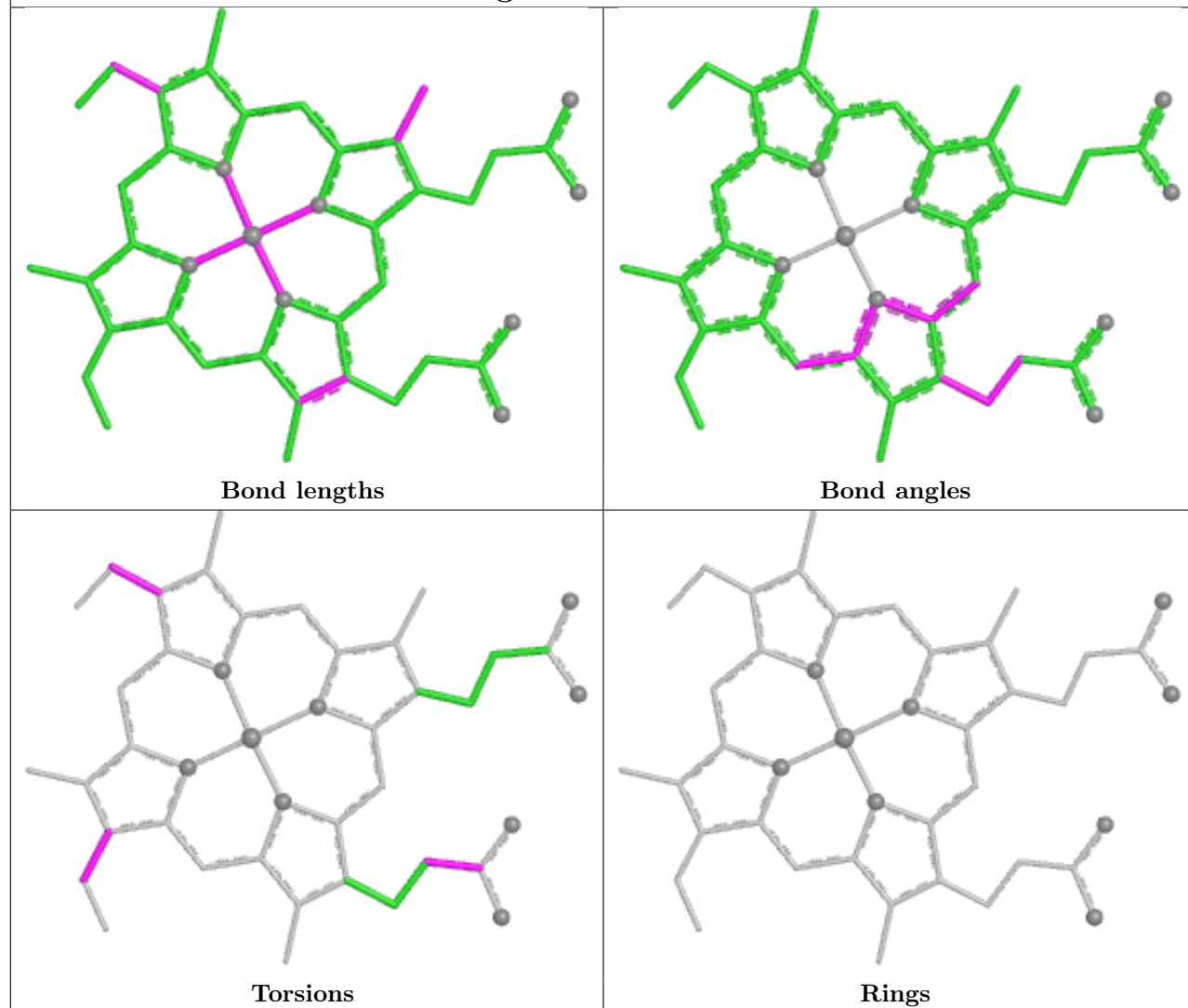
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	f	101	HEM	3	0
25	b	607	CLA	1	0
32	B	624	STE	1	0
32	b	621	STE	4	0
26	B	618	BCR	2	0
25	c	512	CLA	5	0
25	B	611	CLA	1	0
31	C	516	DGD	2	0
25	c	509	CLA	5	0
25	C	507	CLA	2	0
25	c	510	CLA	4	0
26	t	101	BCR	4	0
33	d	402	PHO	3	0
31	c	516	DGD	4	0
28	m	101	LMG	4	0

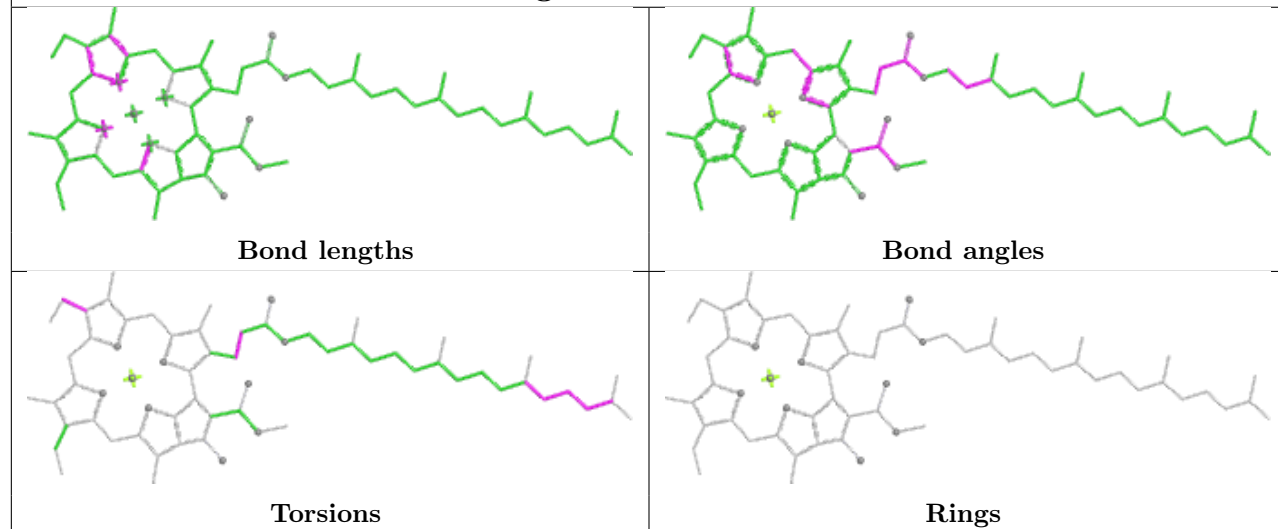
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

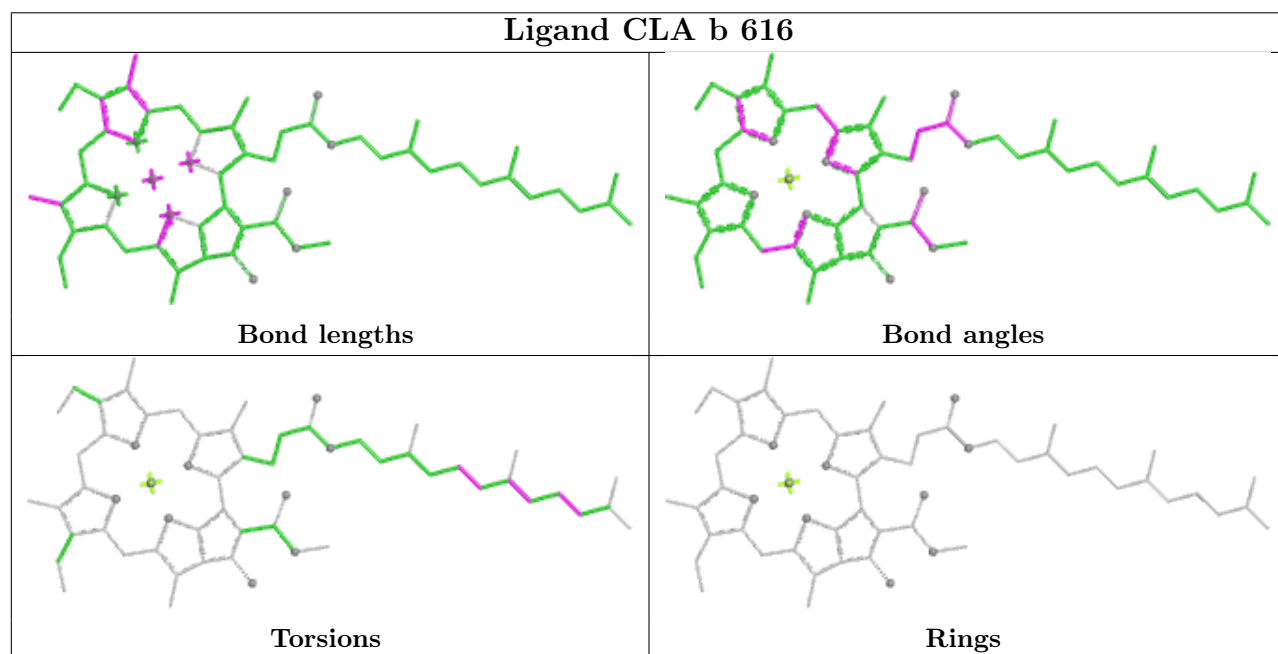
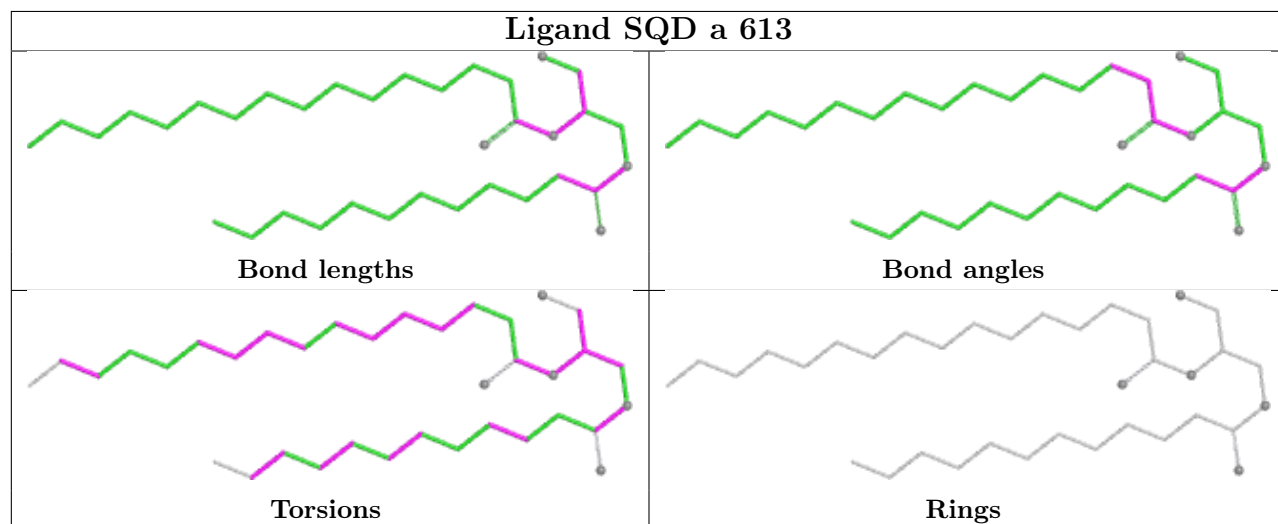
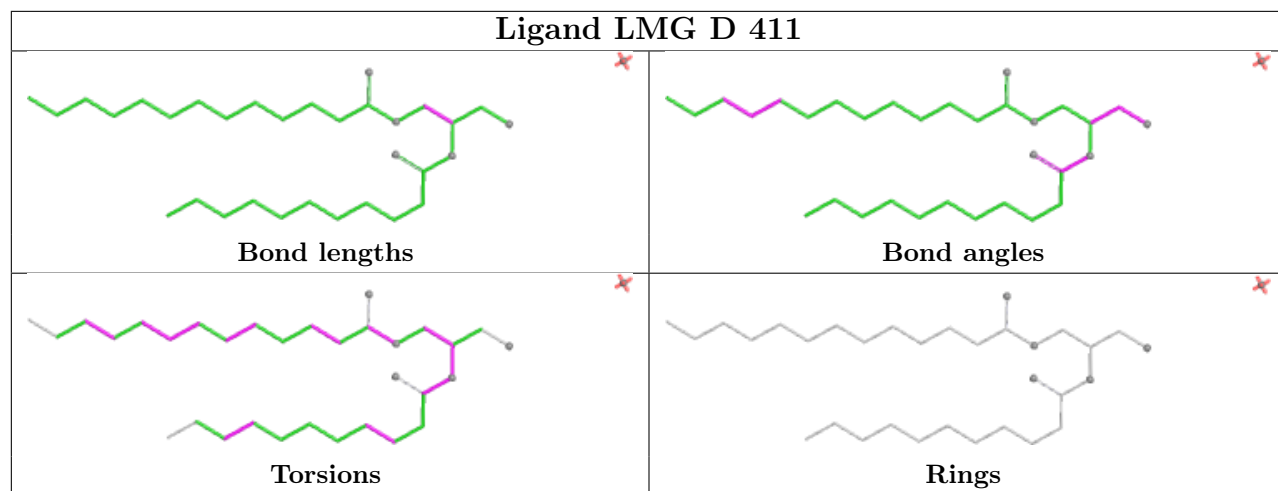


Ligand HEC v 201

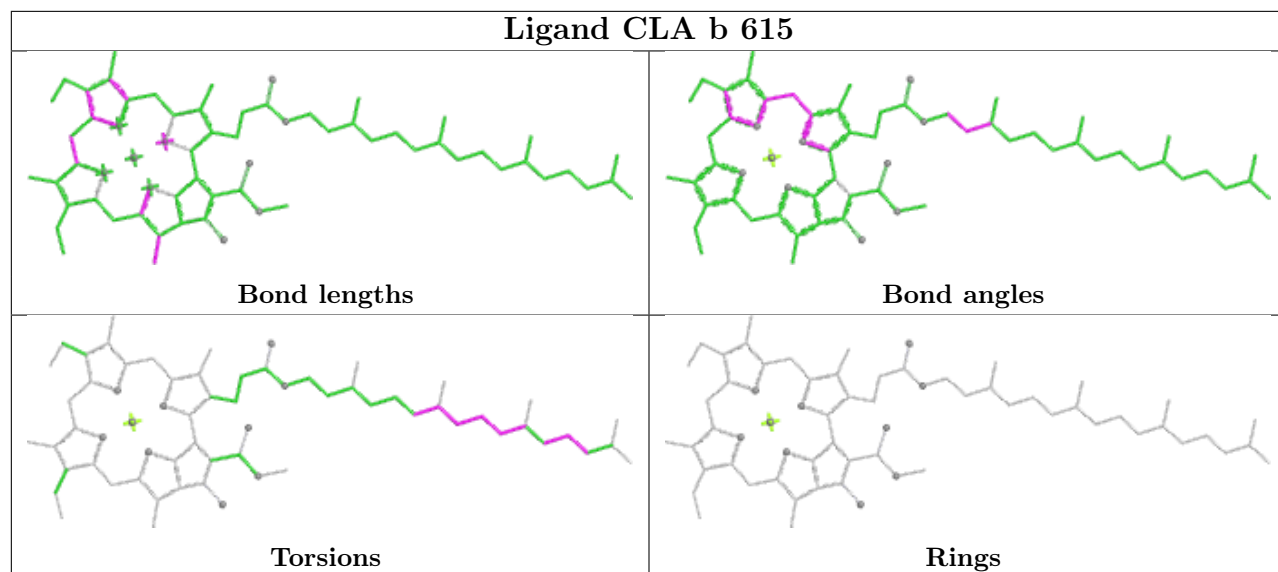


Ligand CLA b 610

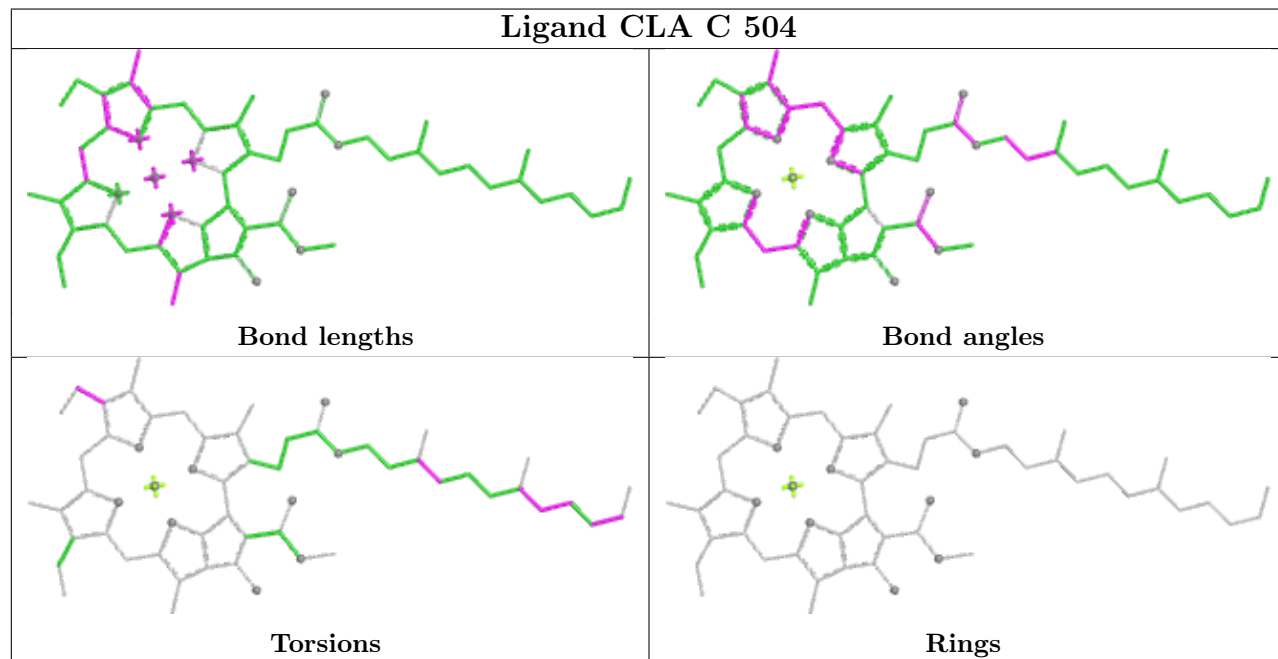




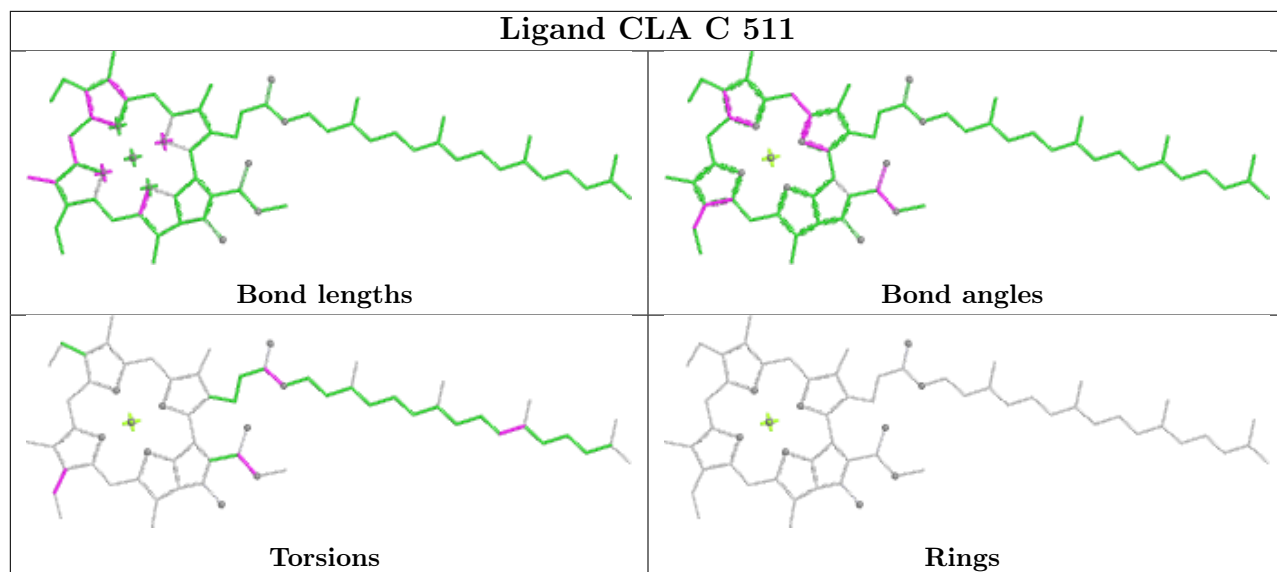
Ligand CLA b 615



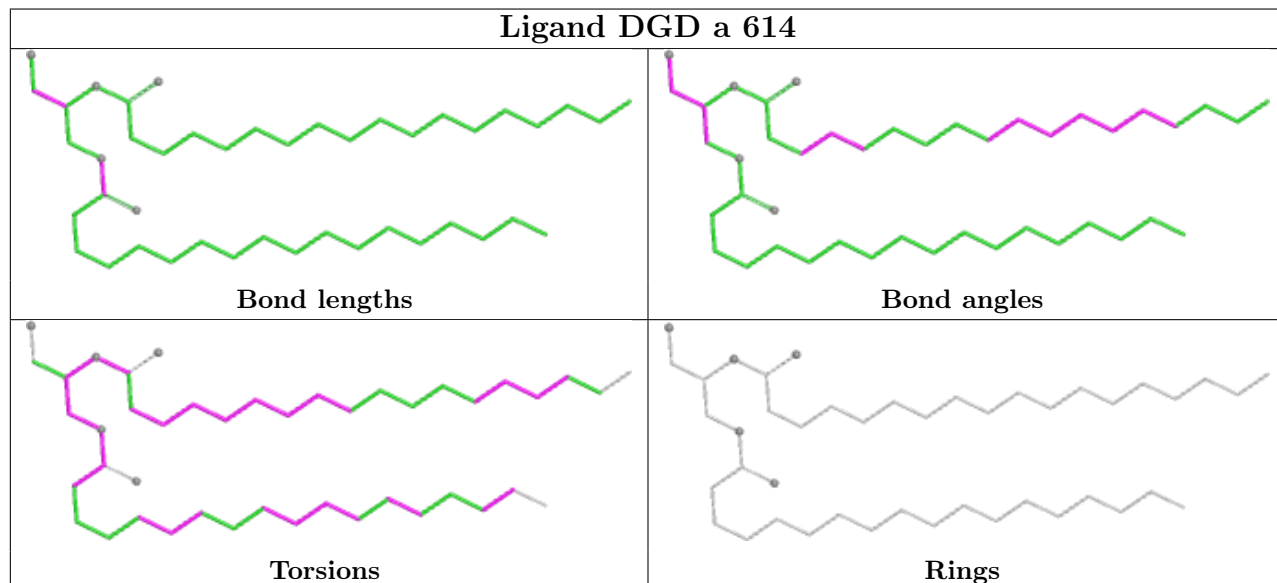
Ligand CLA C 504



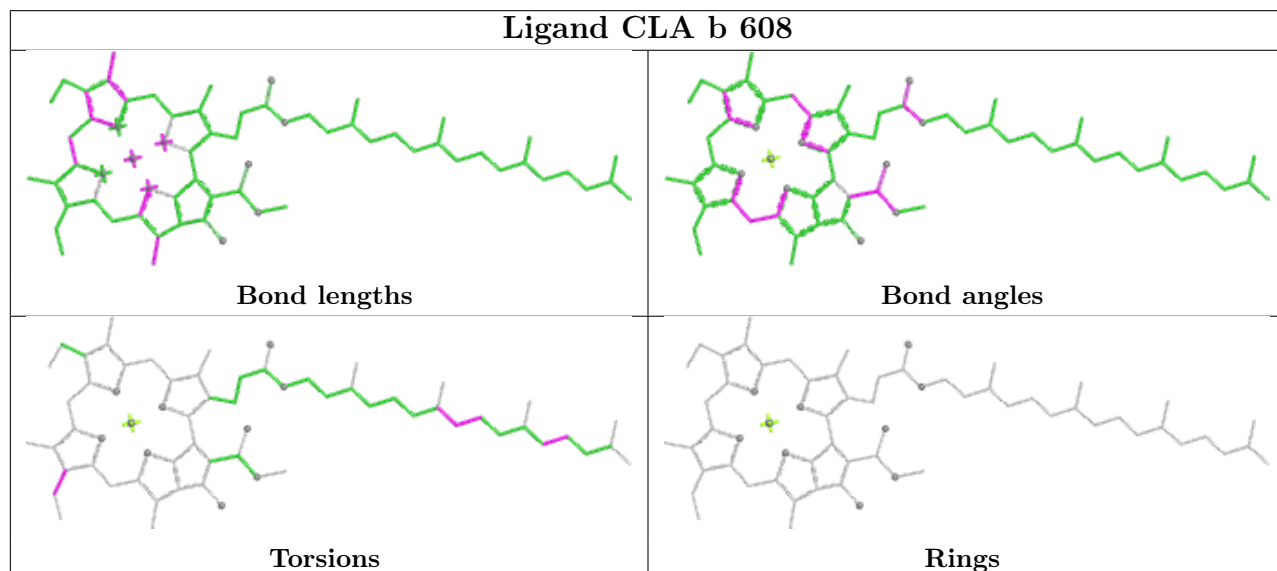
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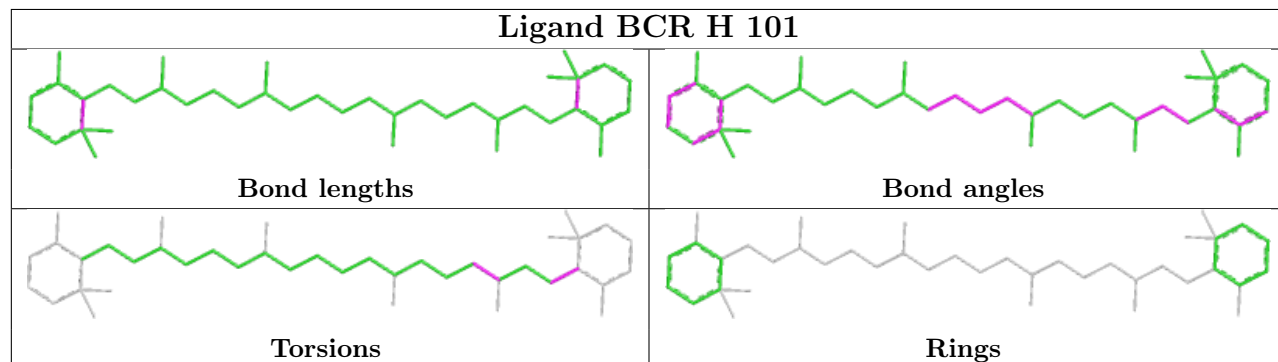
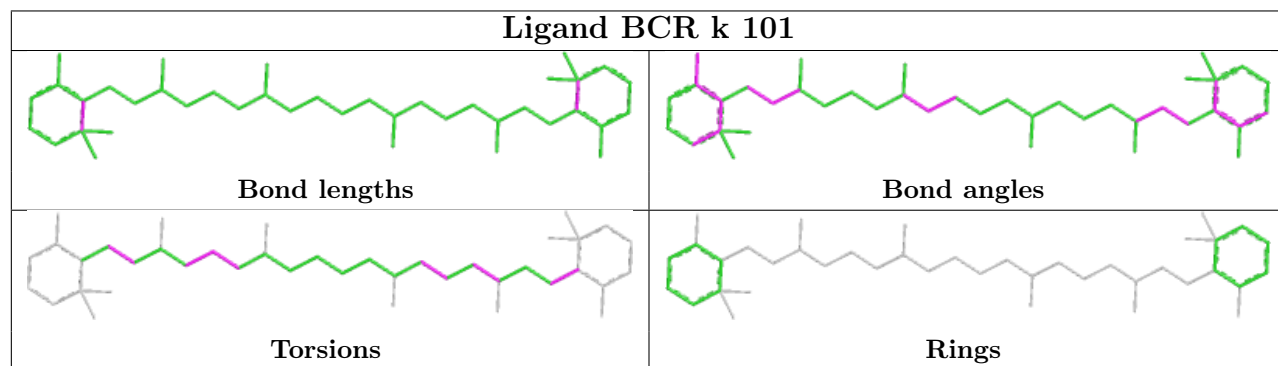
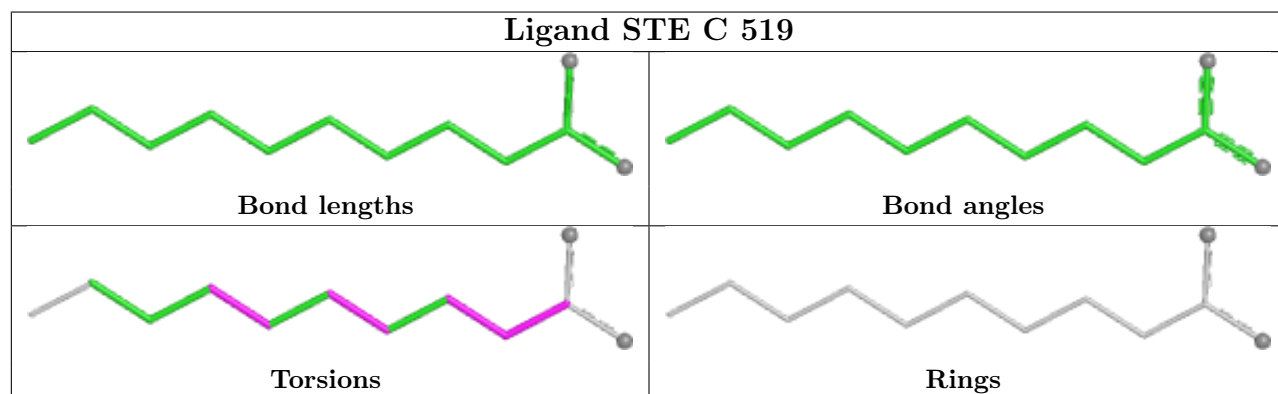
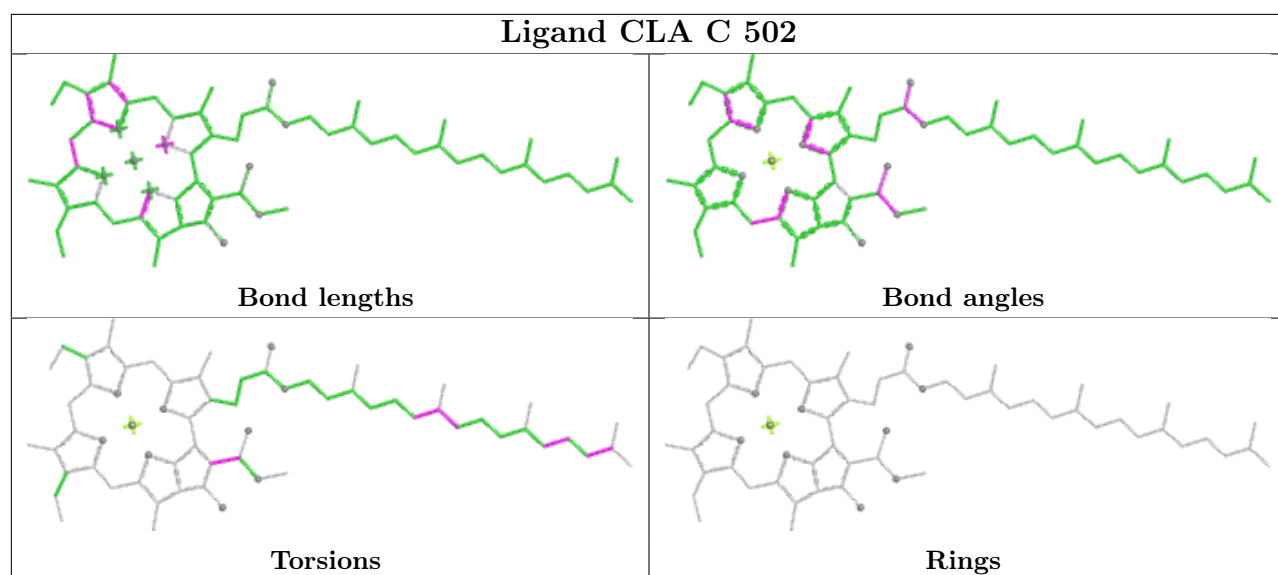


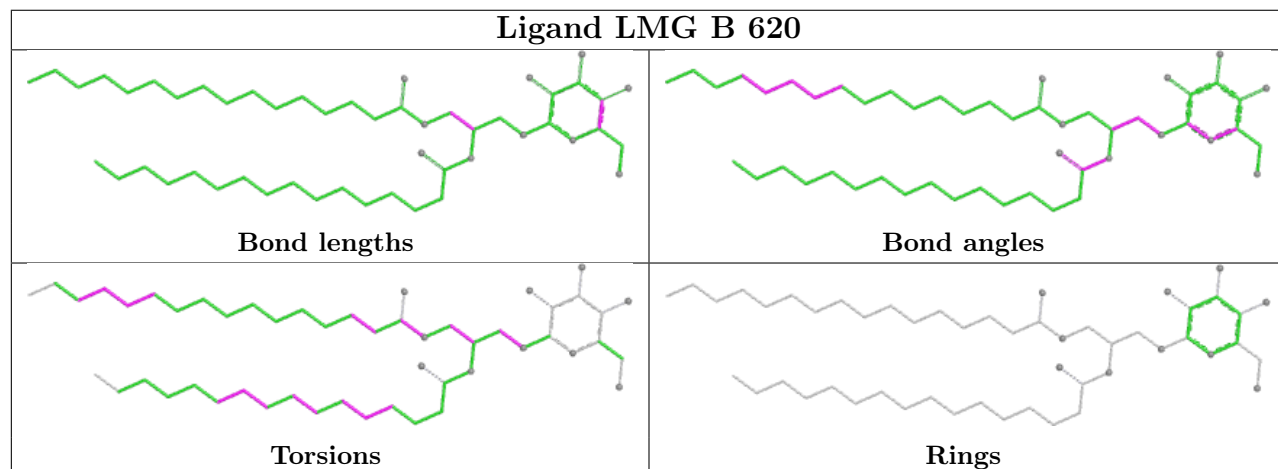
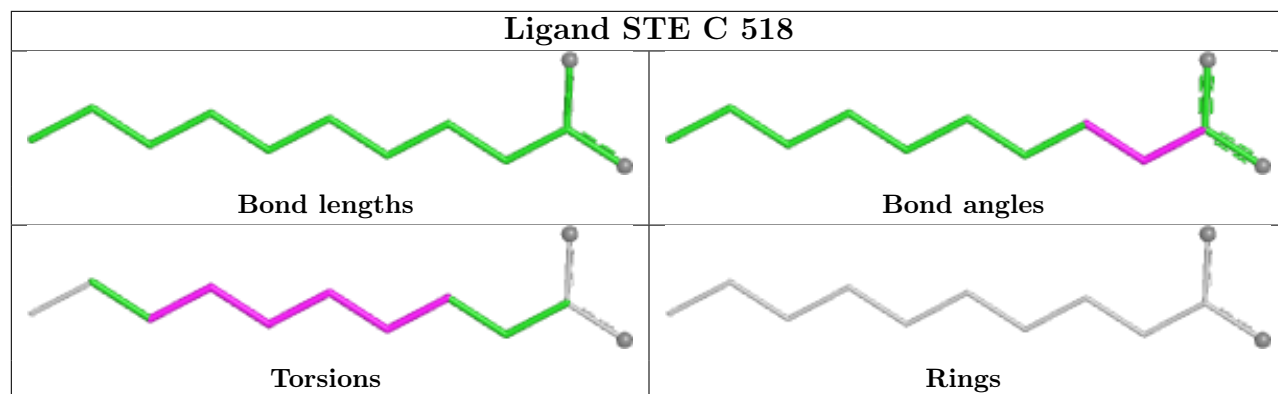
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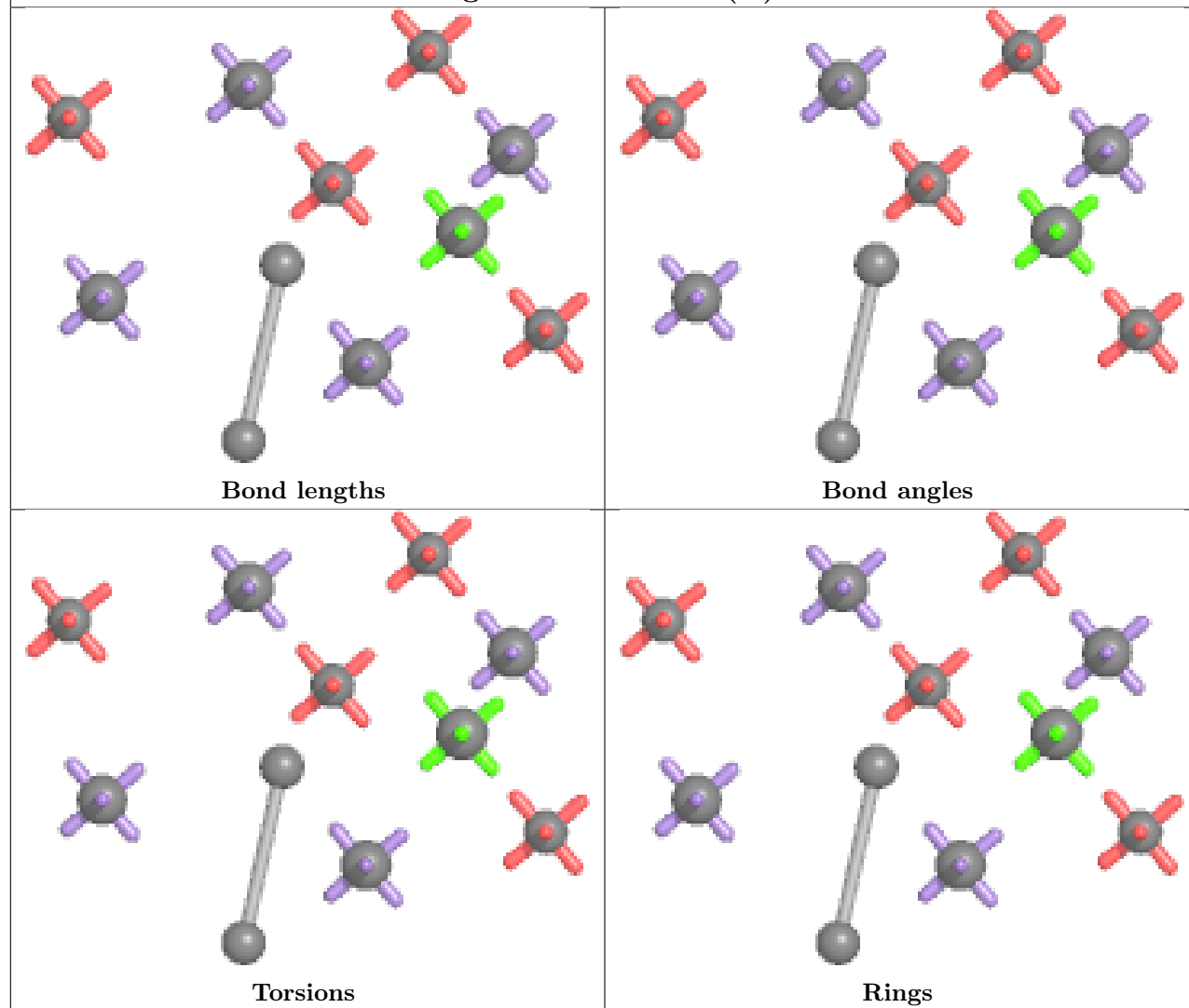
Ligand CLA b 608



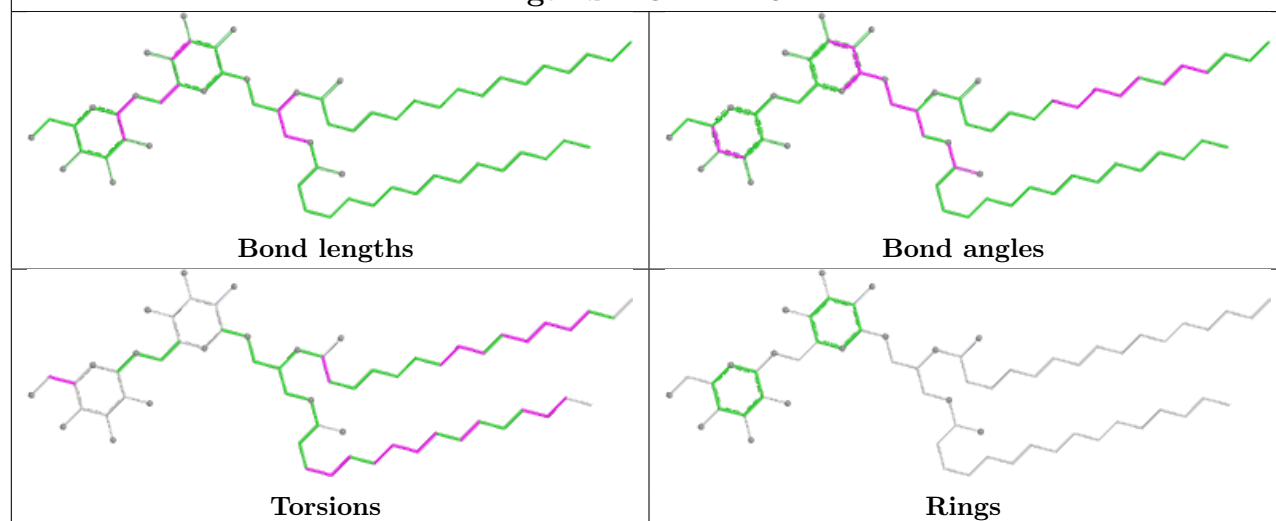


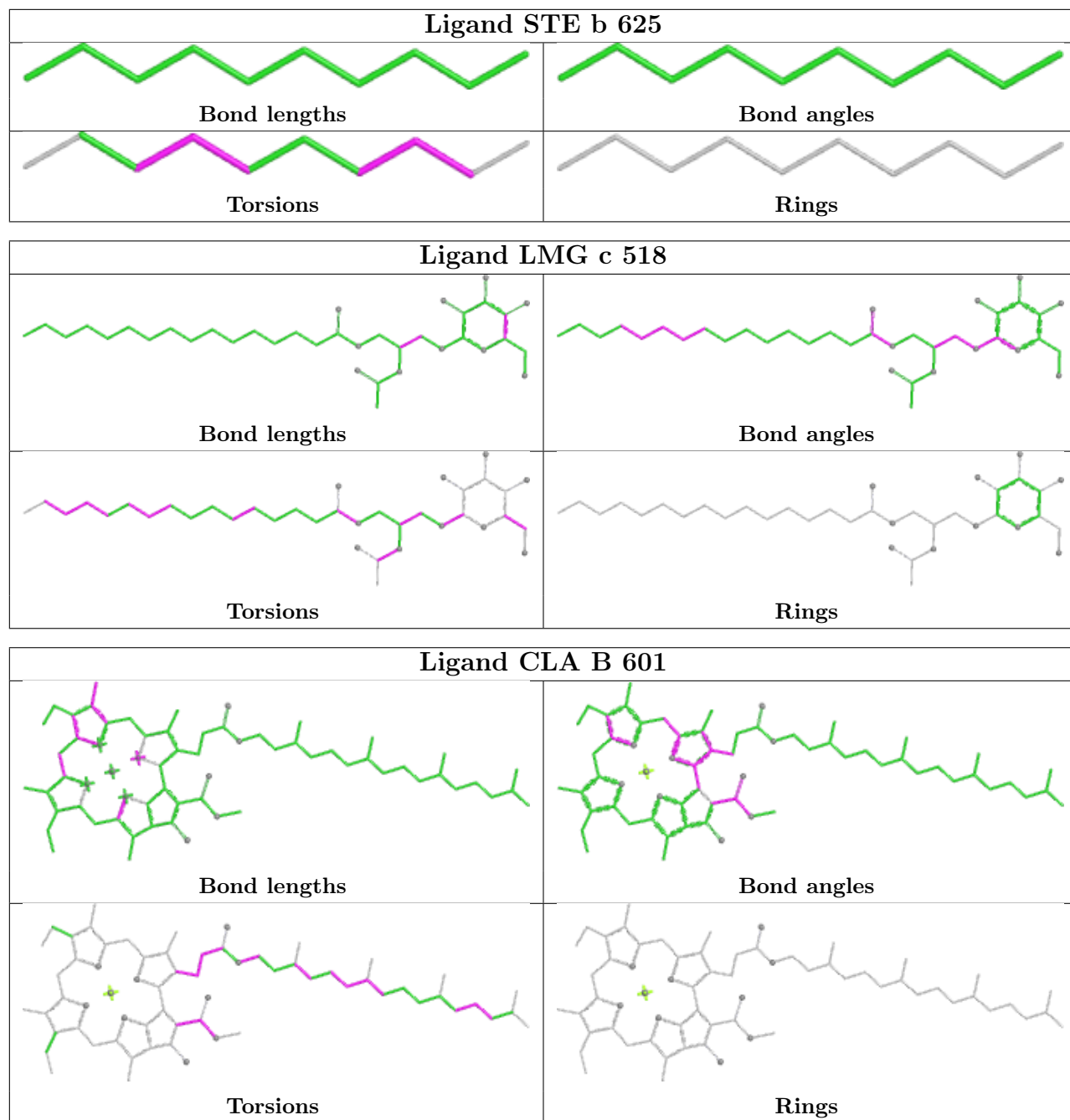


Ligand OEY A 601 (A)

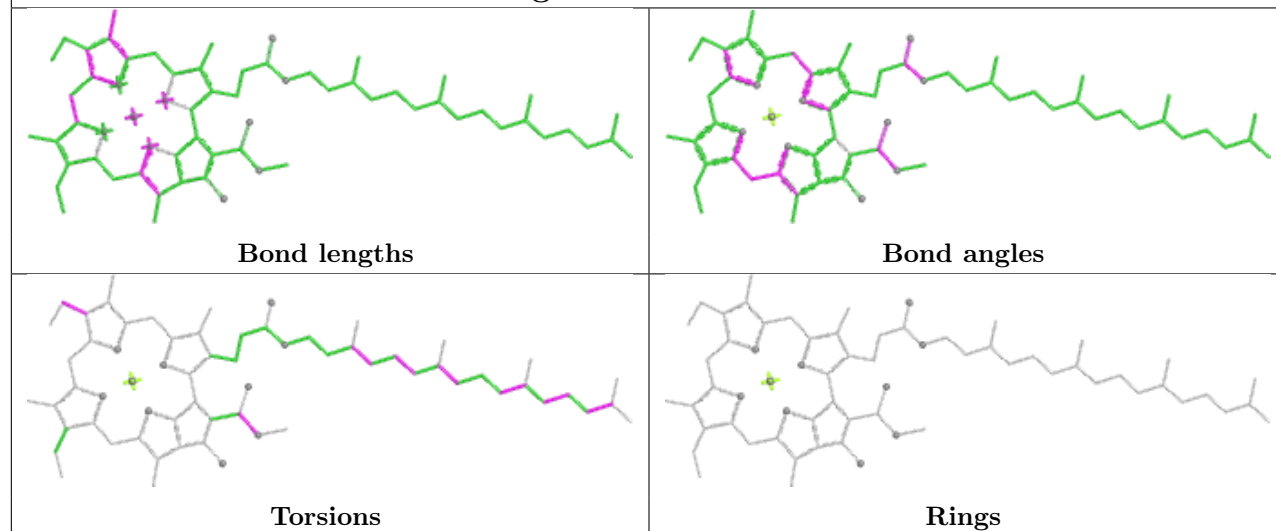


Ligand DGD H 102

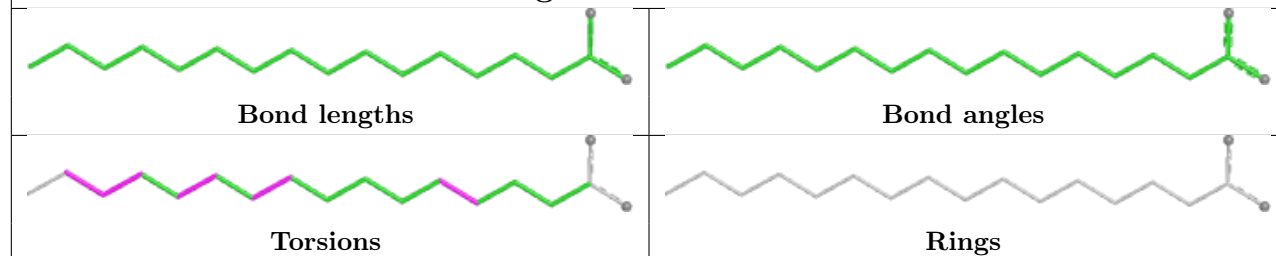




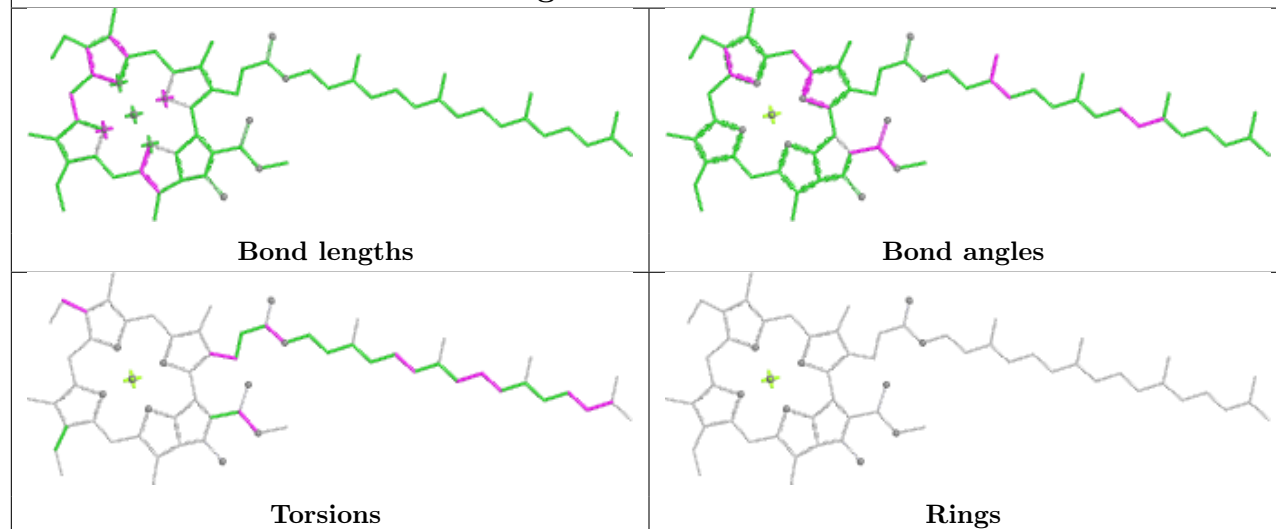
Ligand CLA C 513

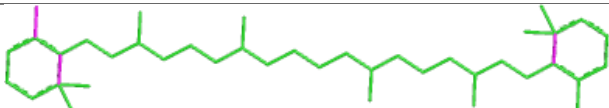
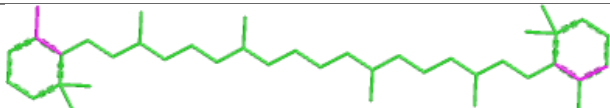
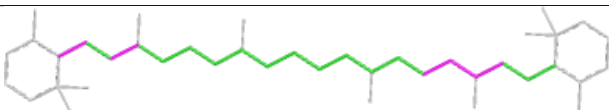
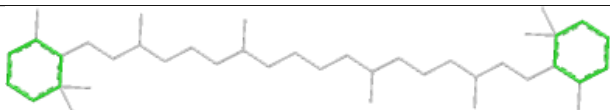


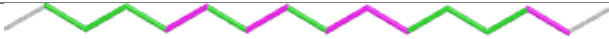
Ligand STE B 625

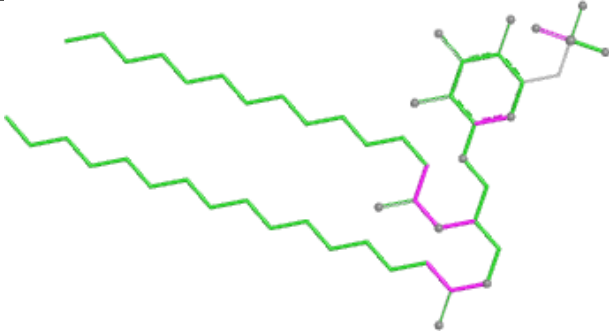
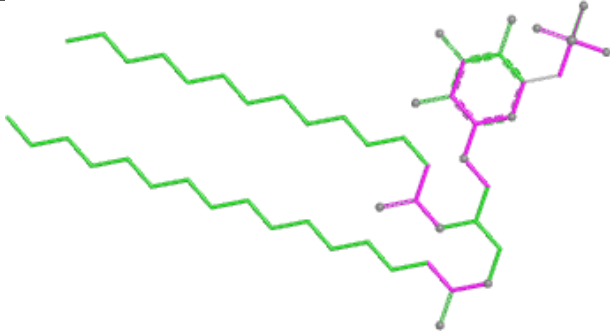
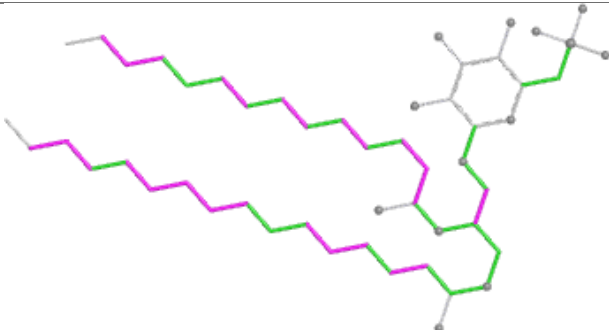
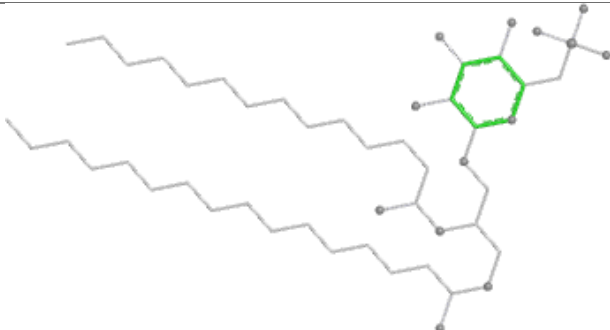


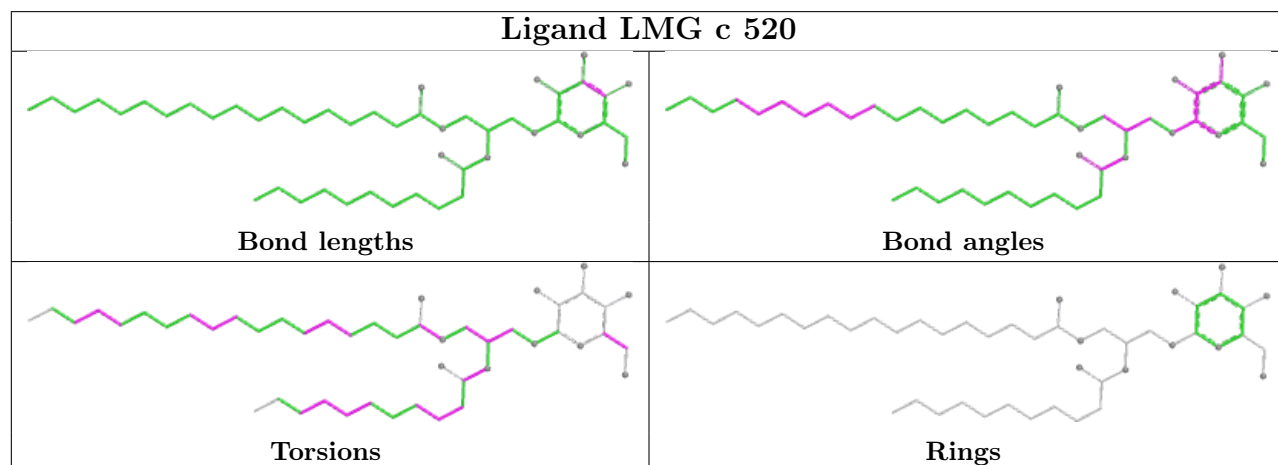
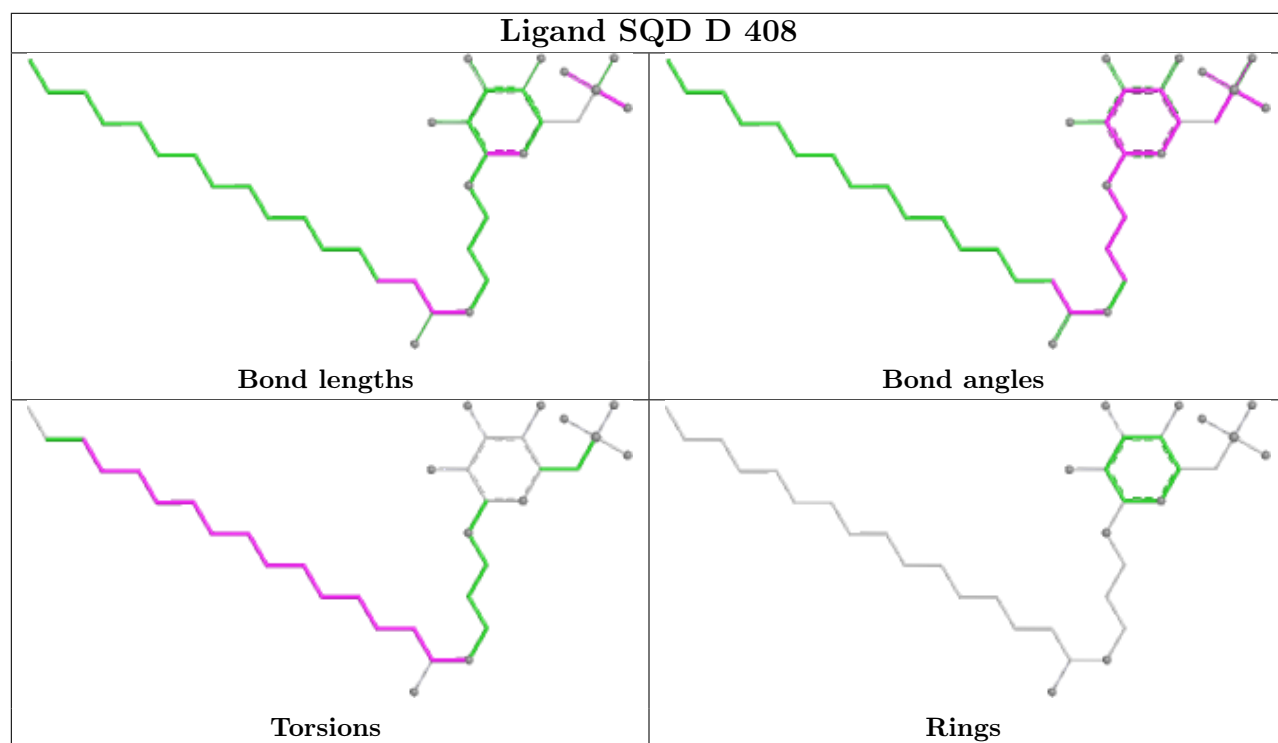
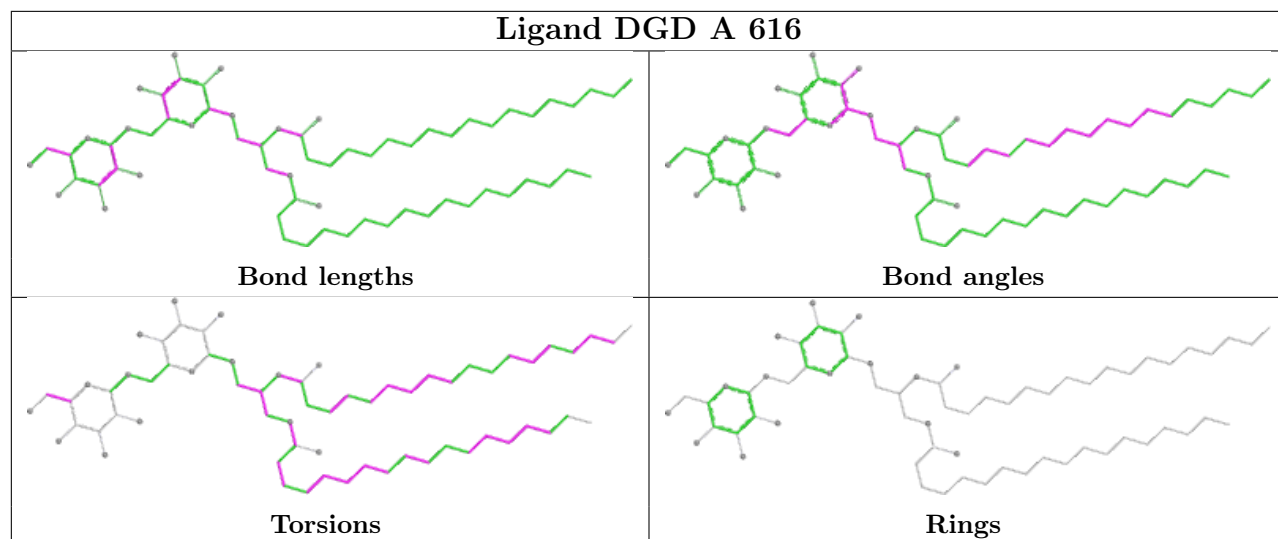
Ligand CLA c 503

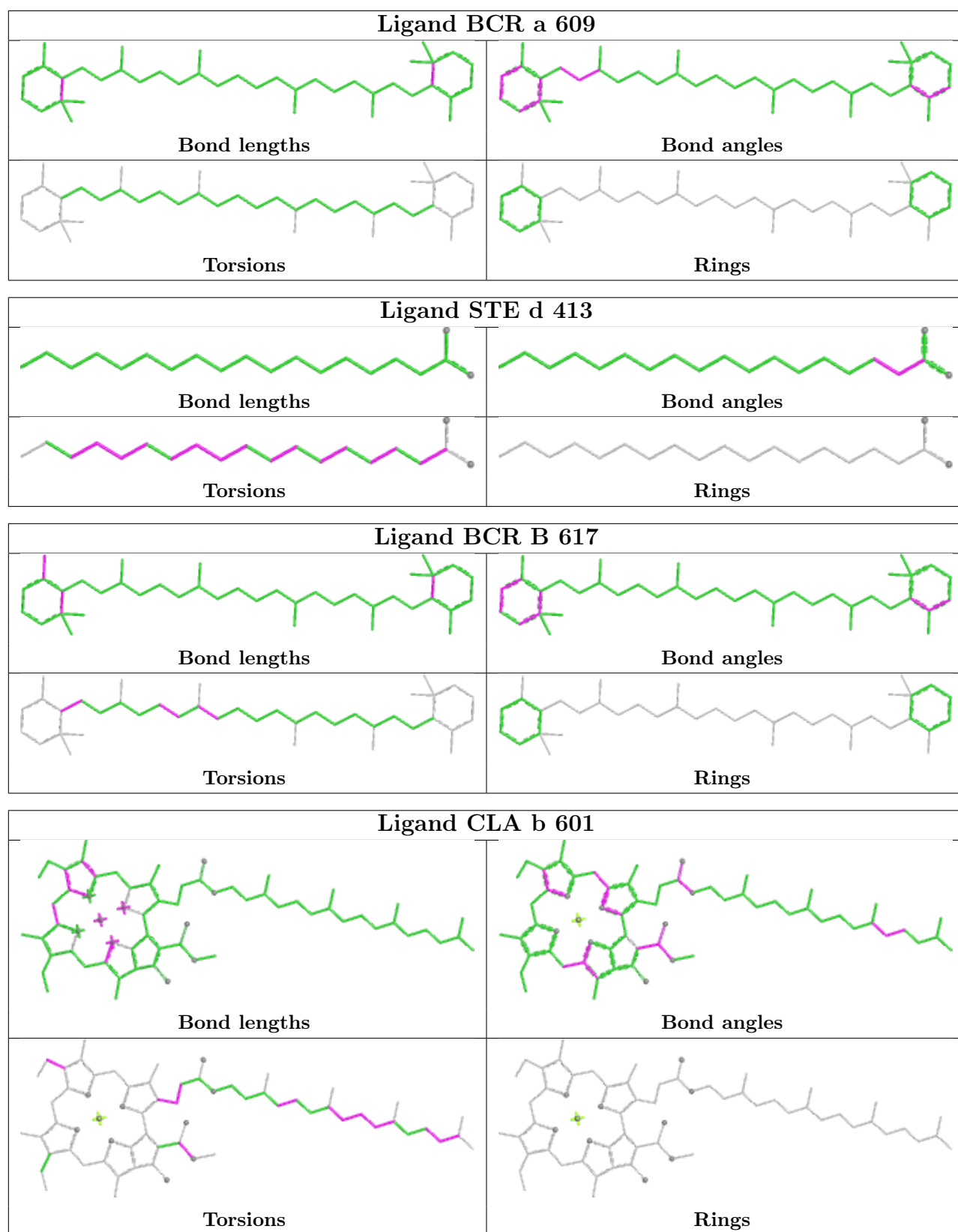


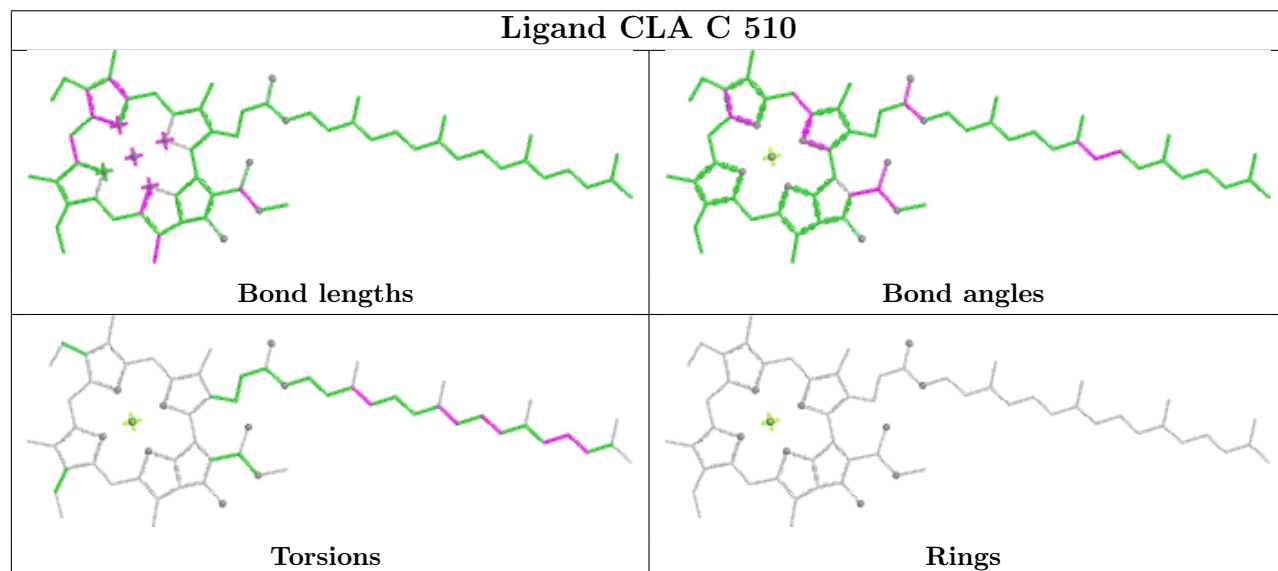
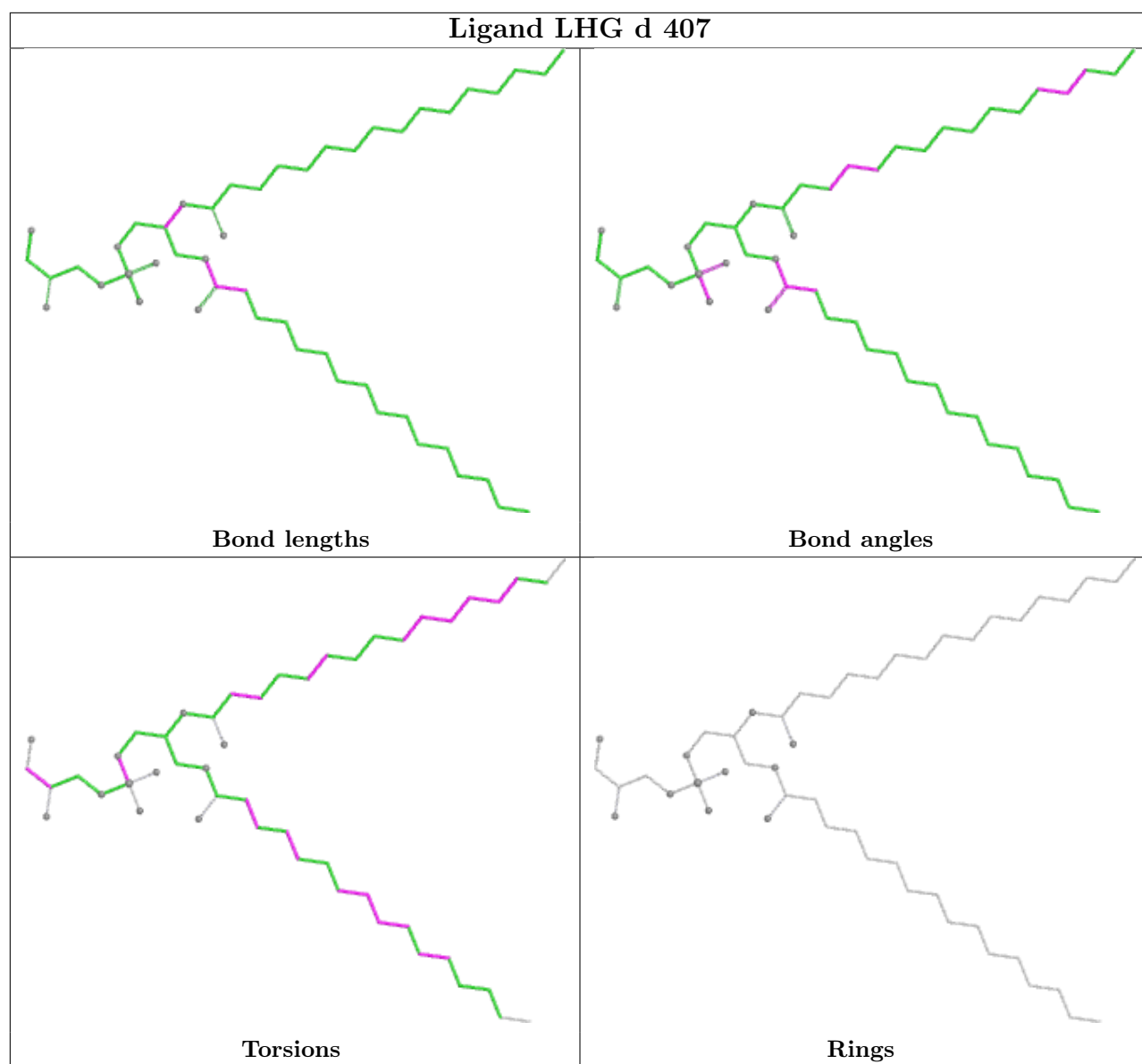
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

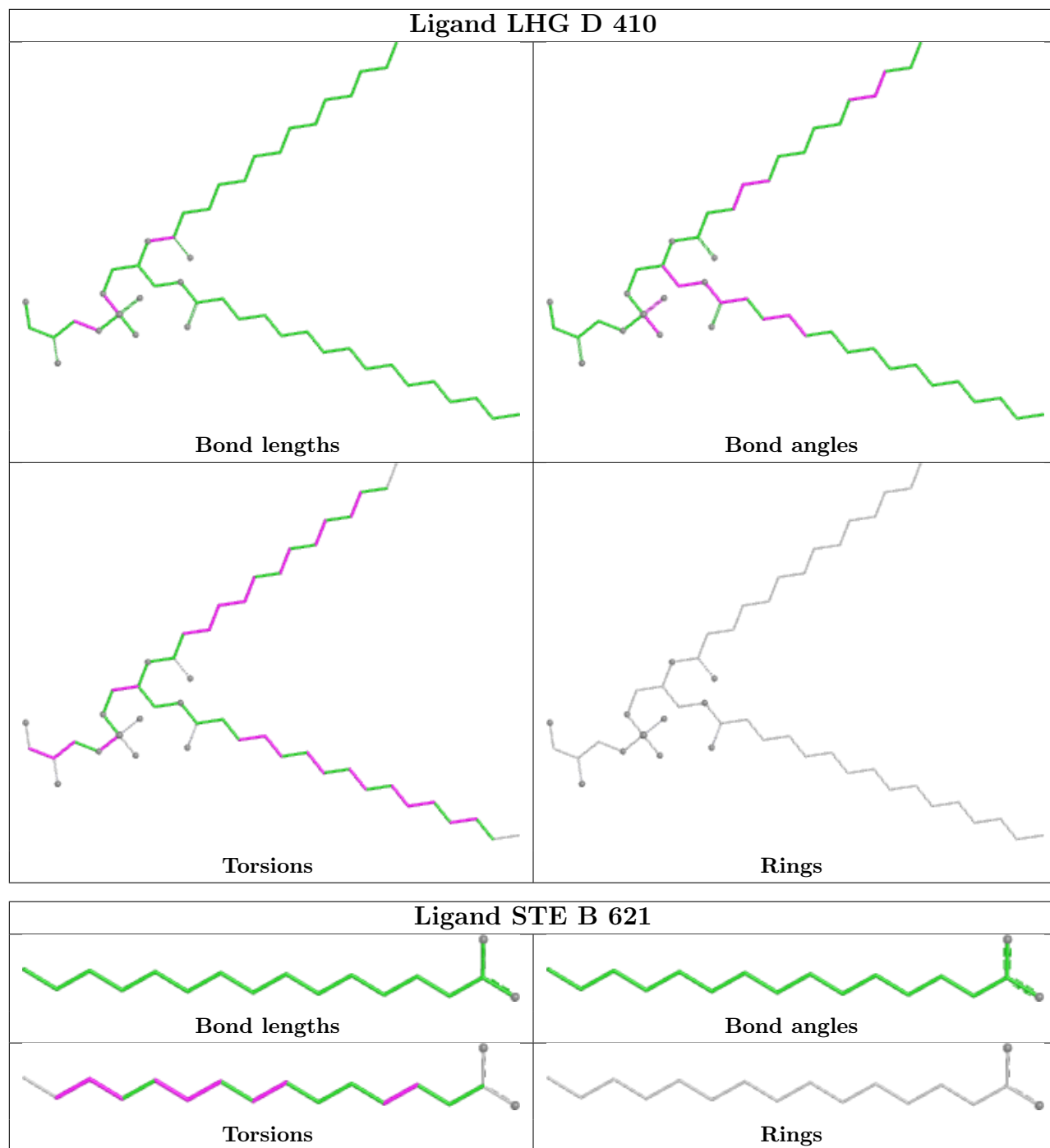
Ligand STE C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SQD A 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

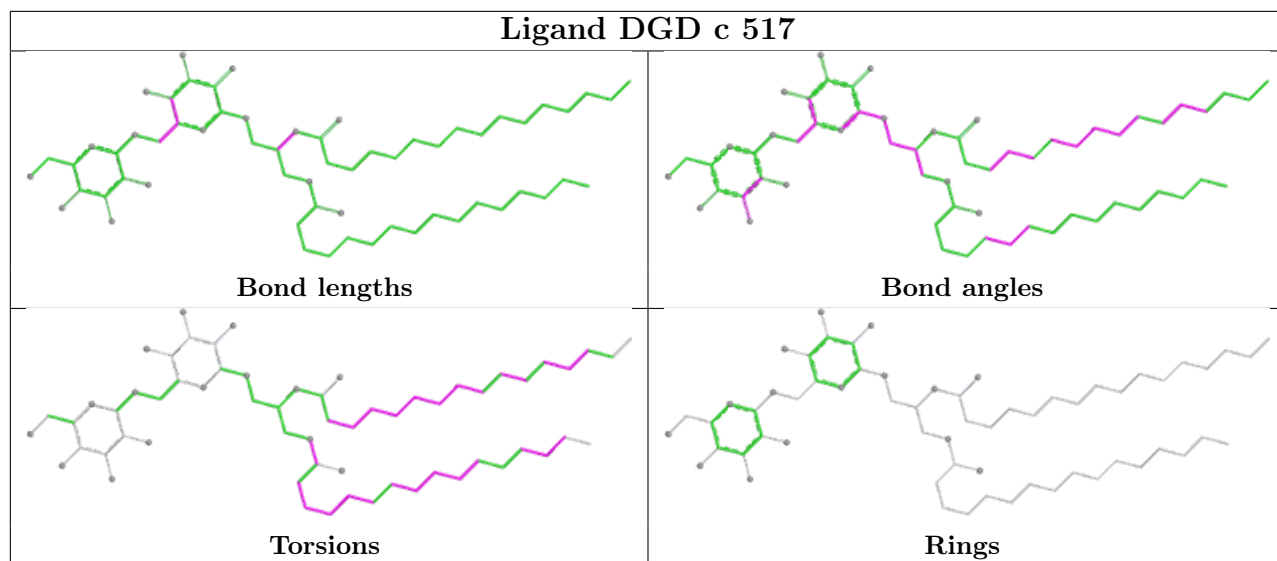




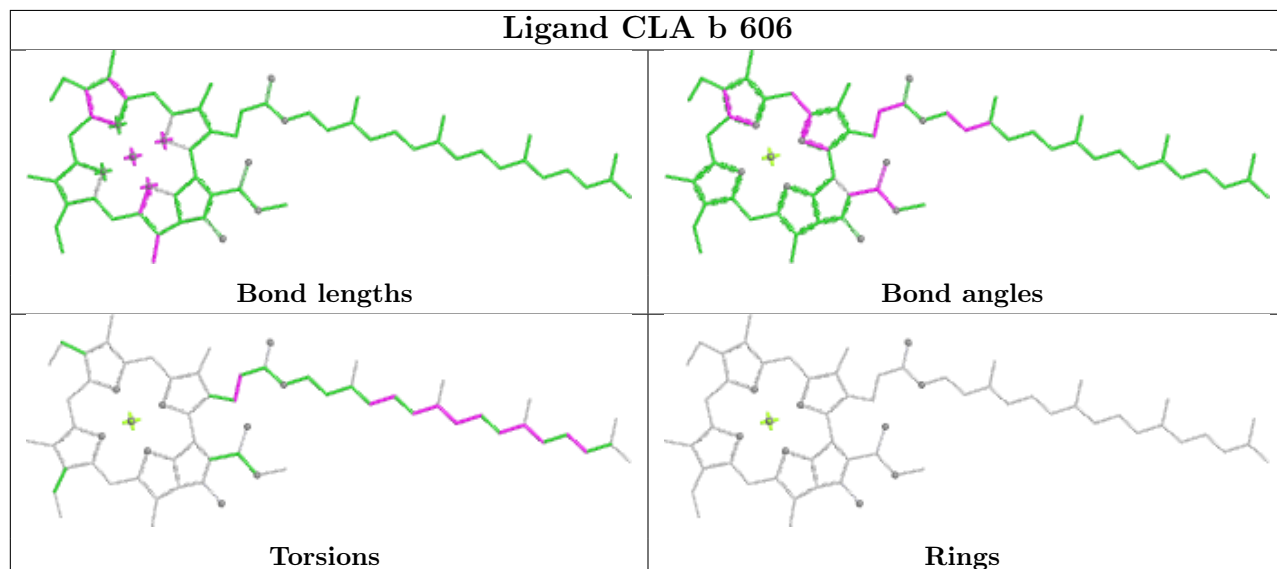




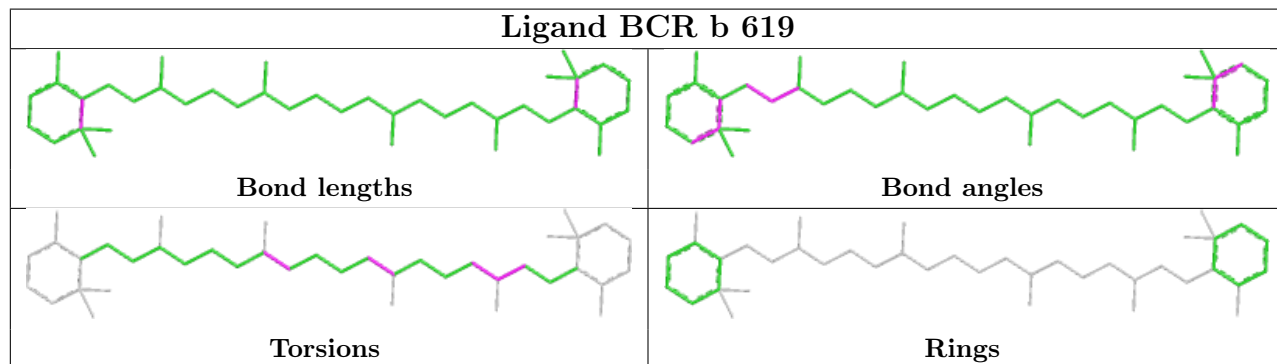
Ligand DGD c 517



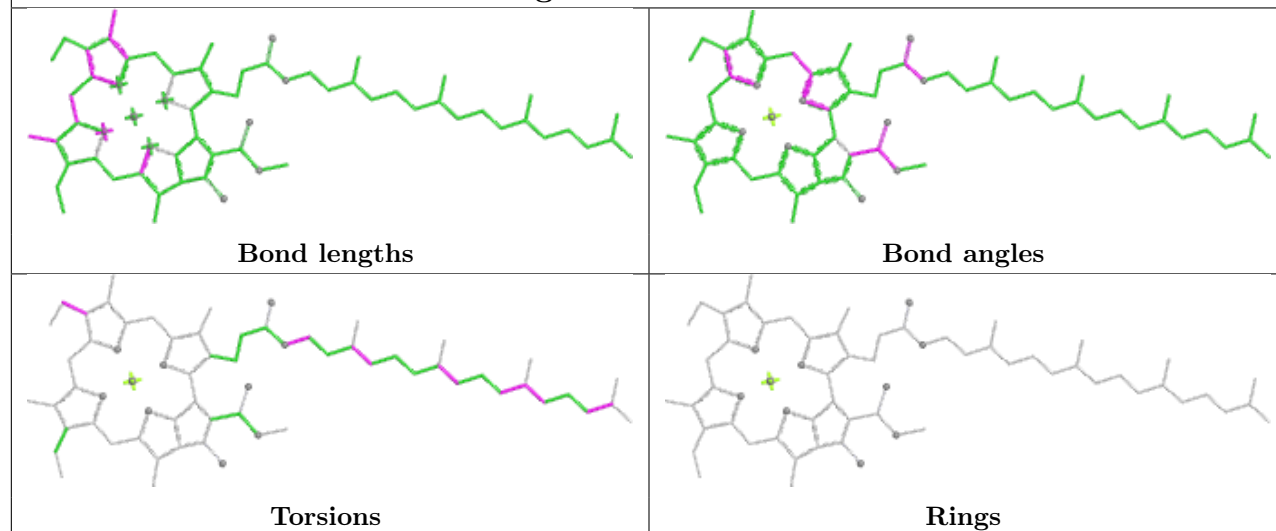
Ligand CLA b 606



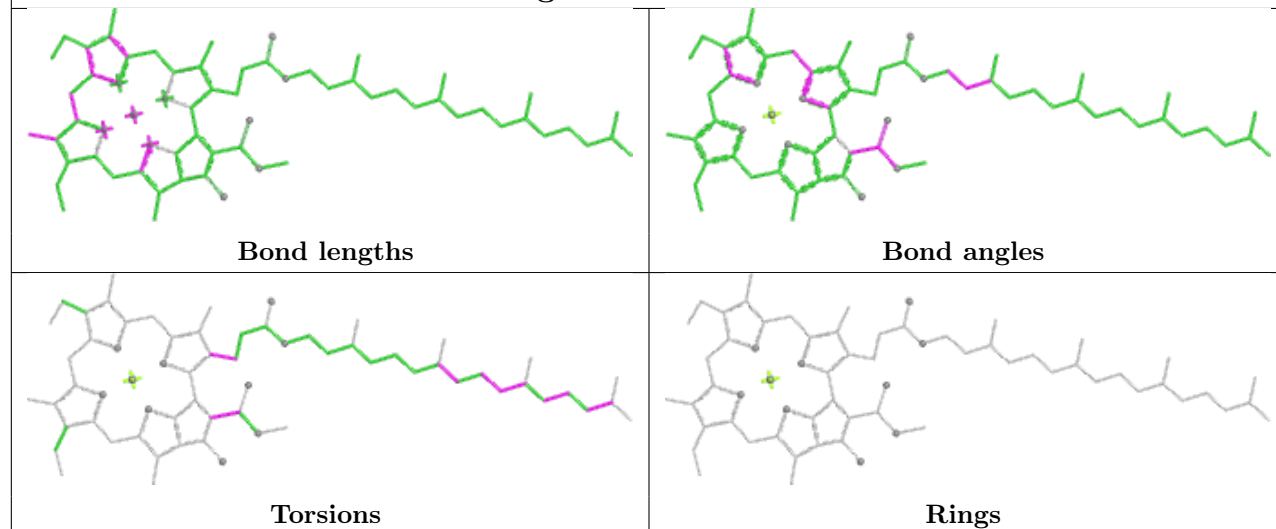
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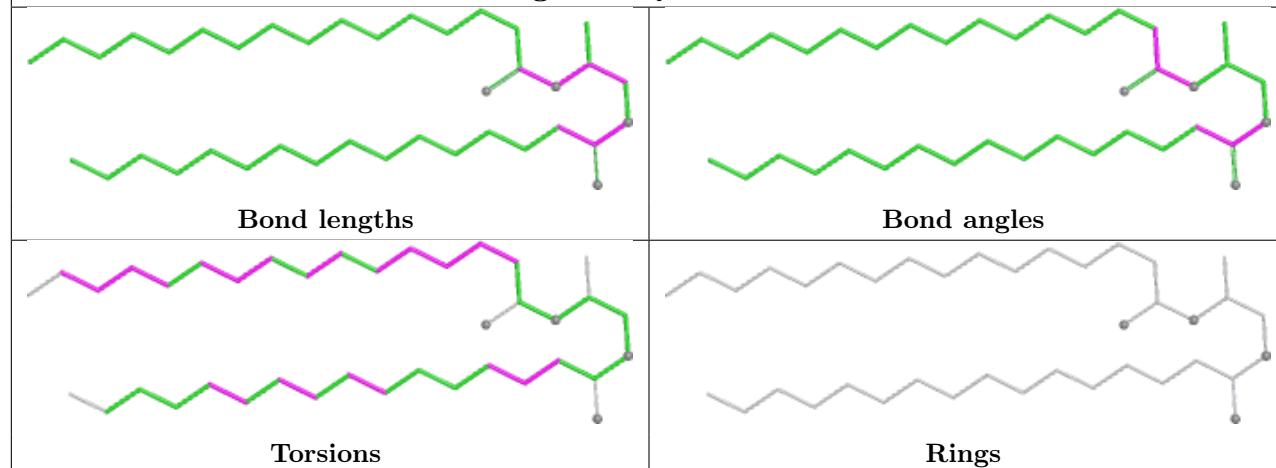
Ligand CLA d 403



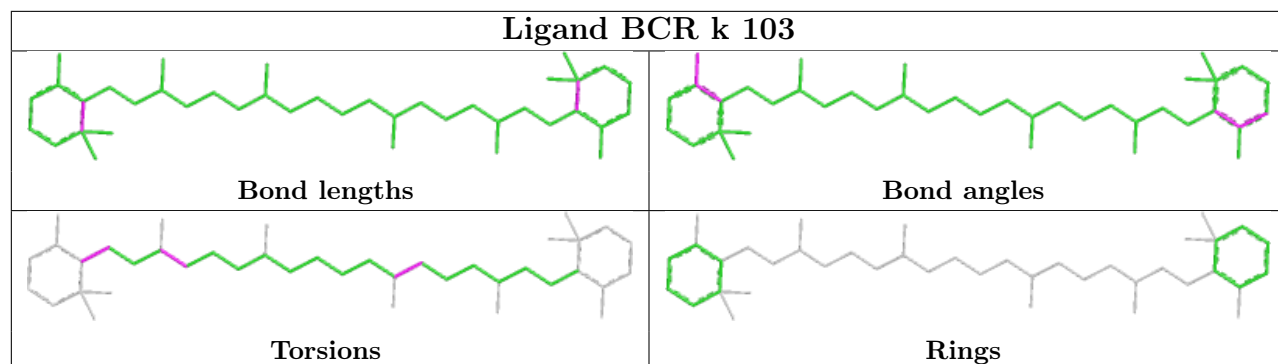
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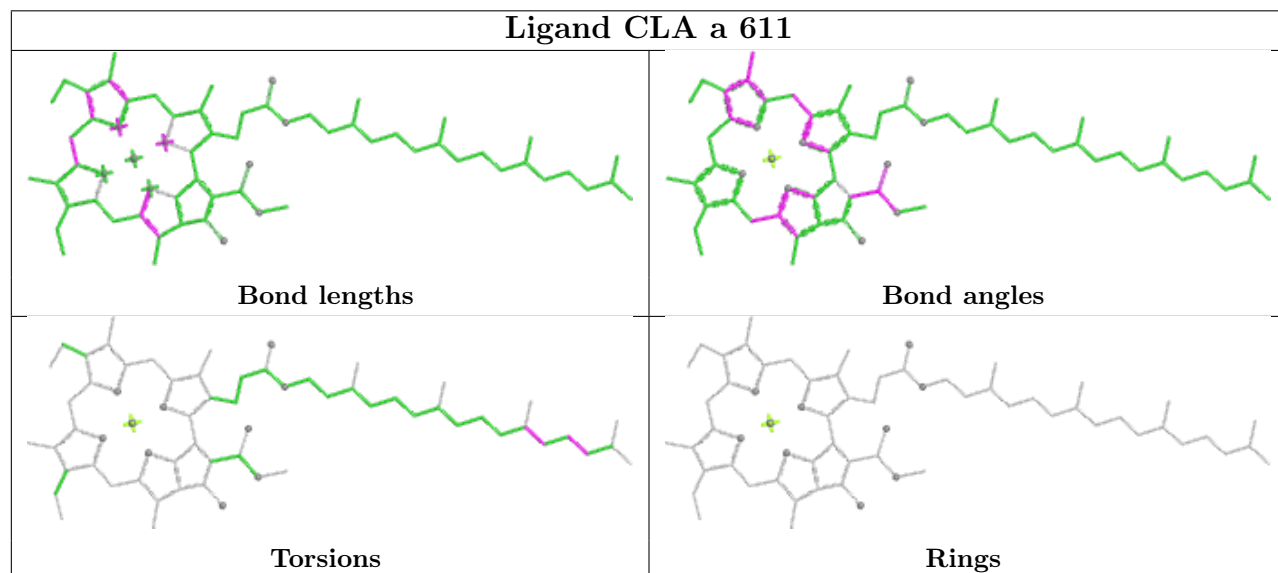
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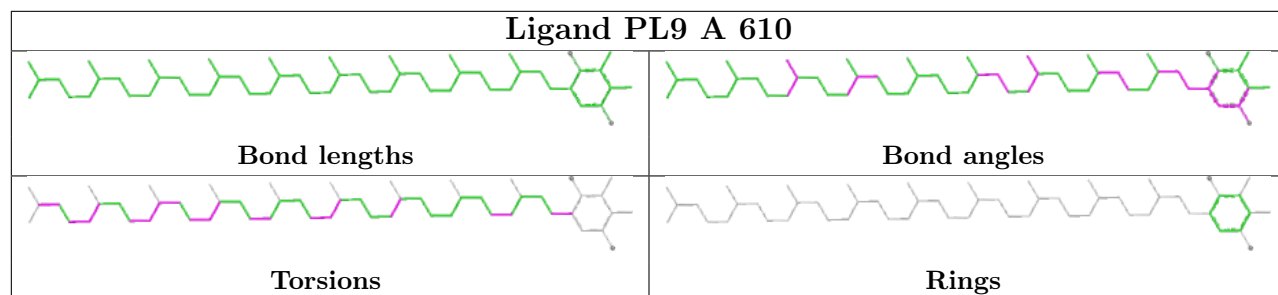
Ligand BCR k 103



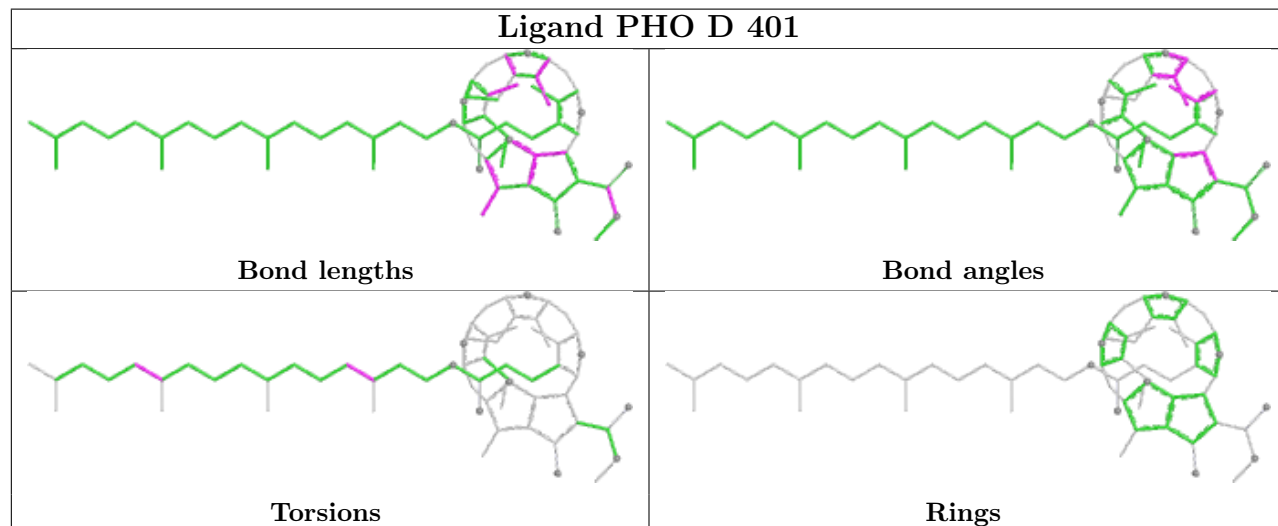
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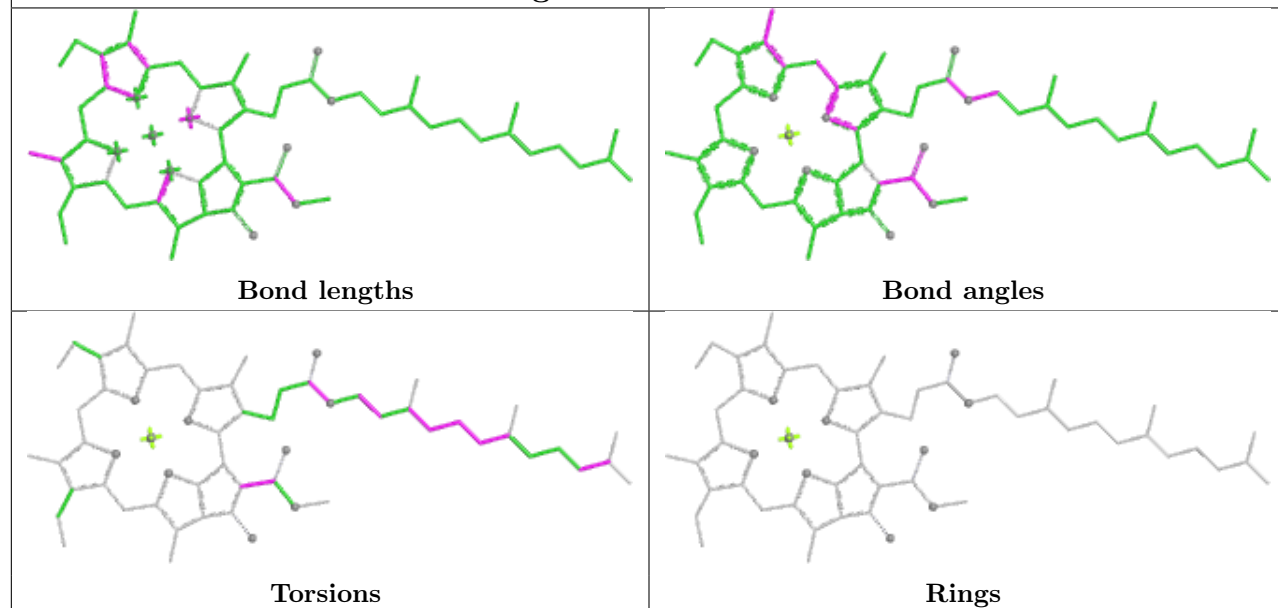
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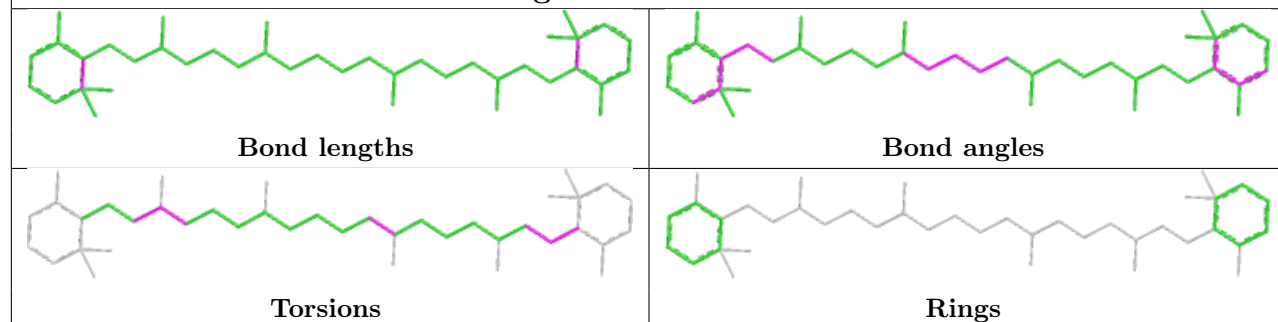
Ligand PHO D 401



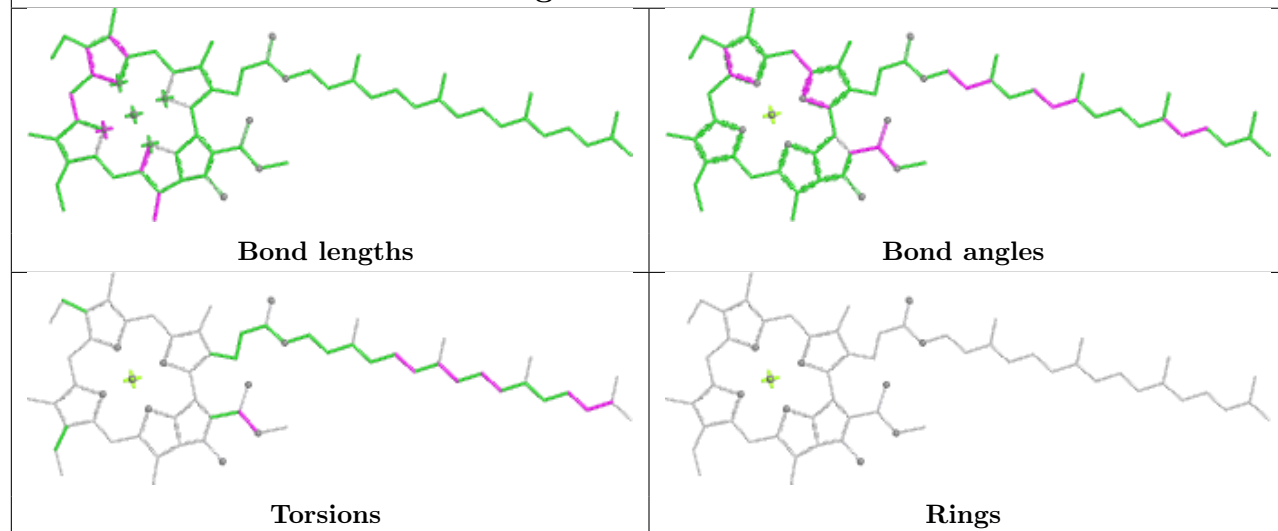
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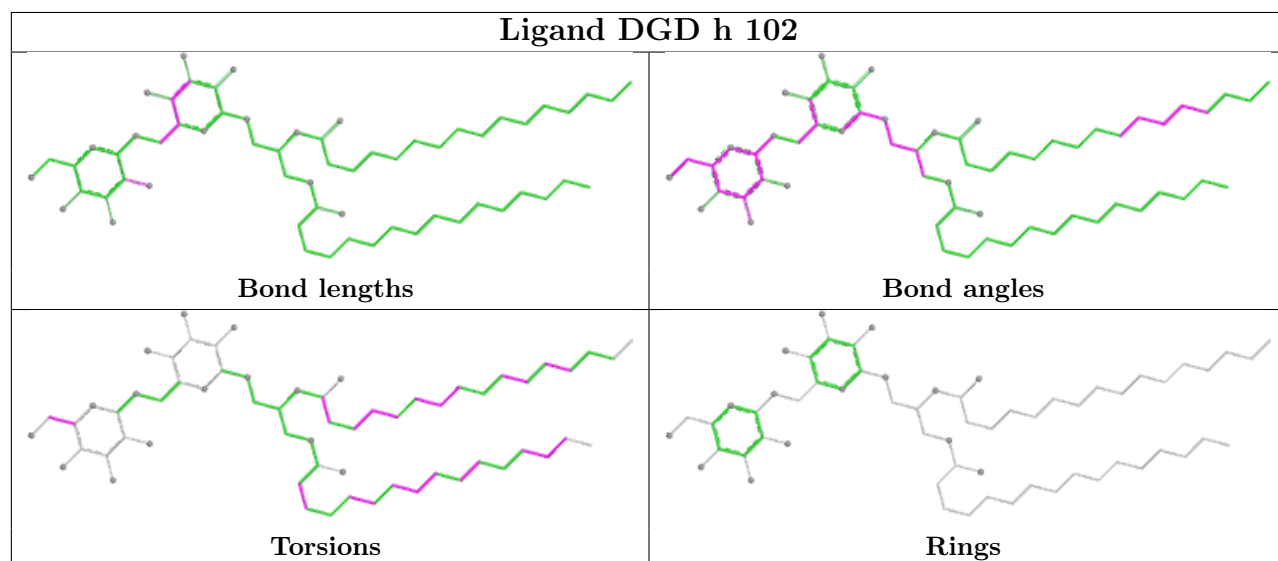
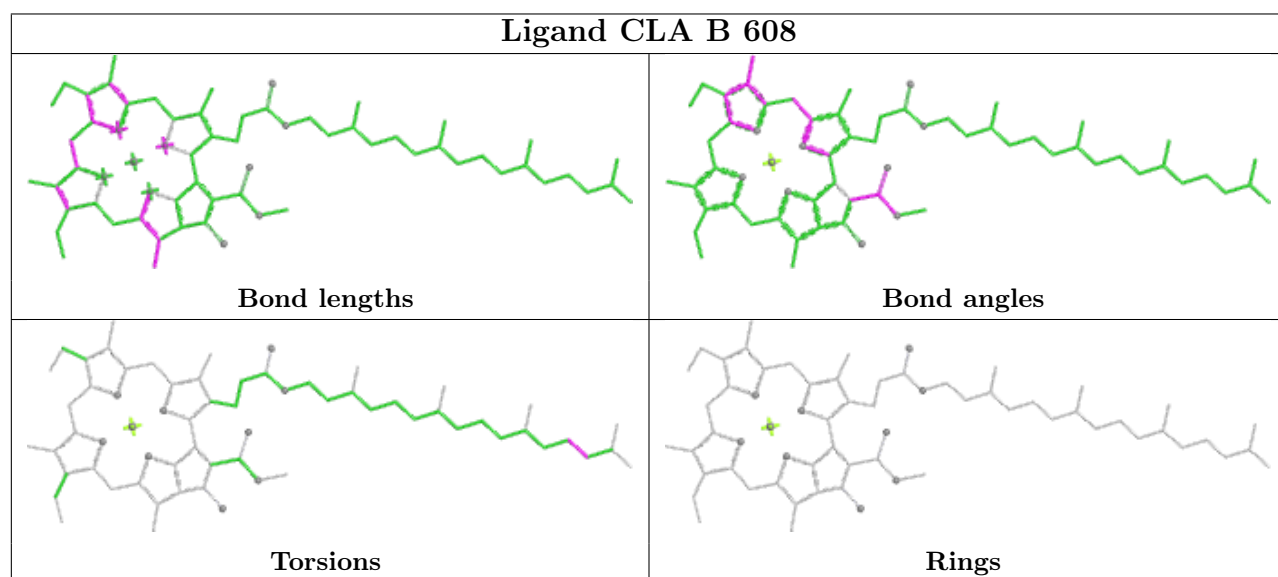
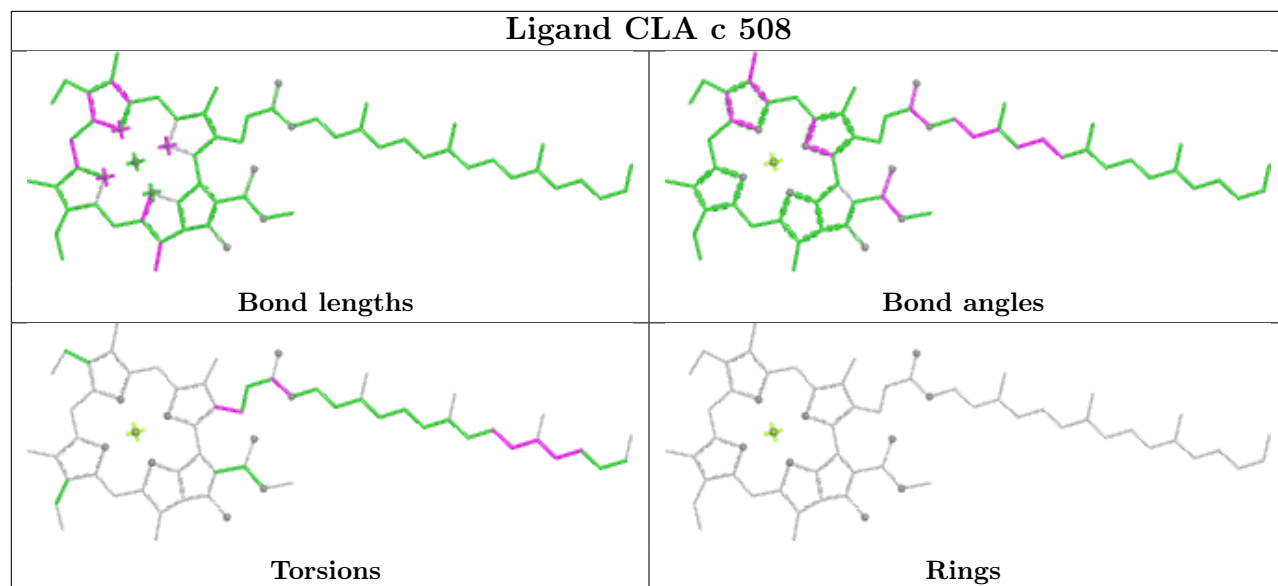


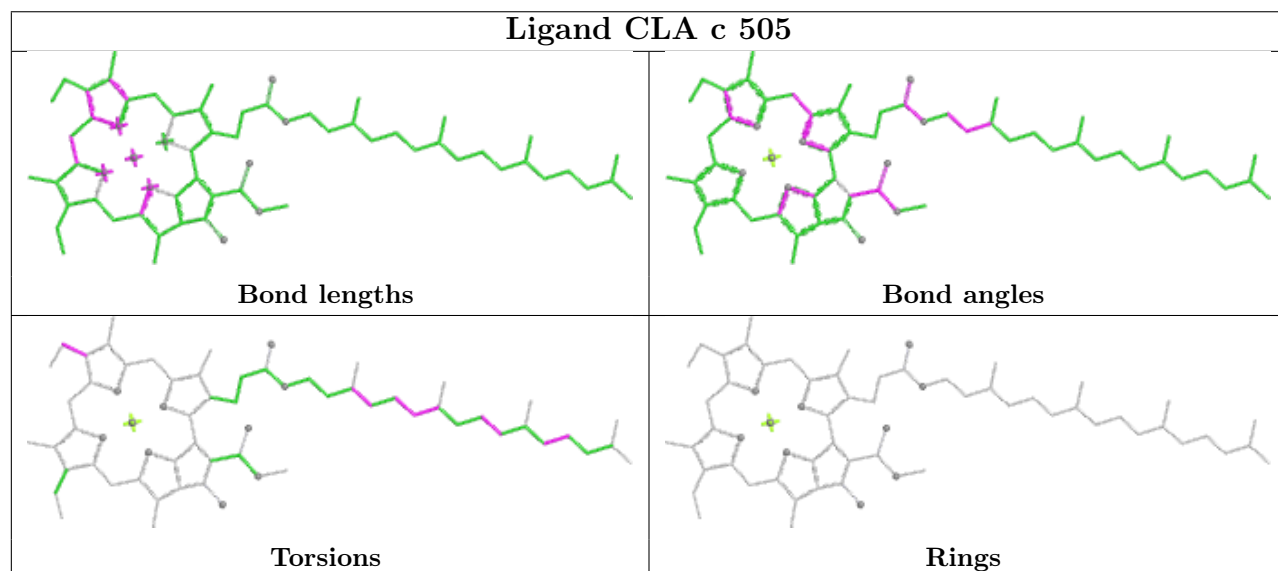
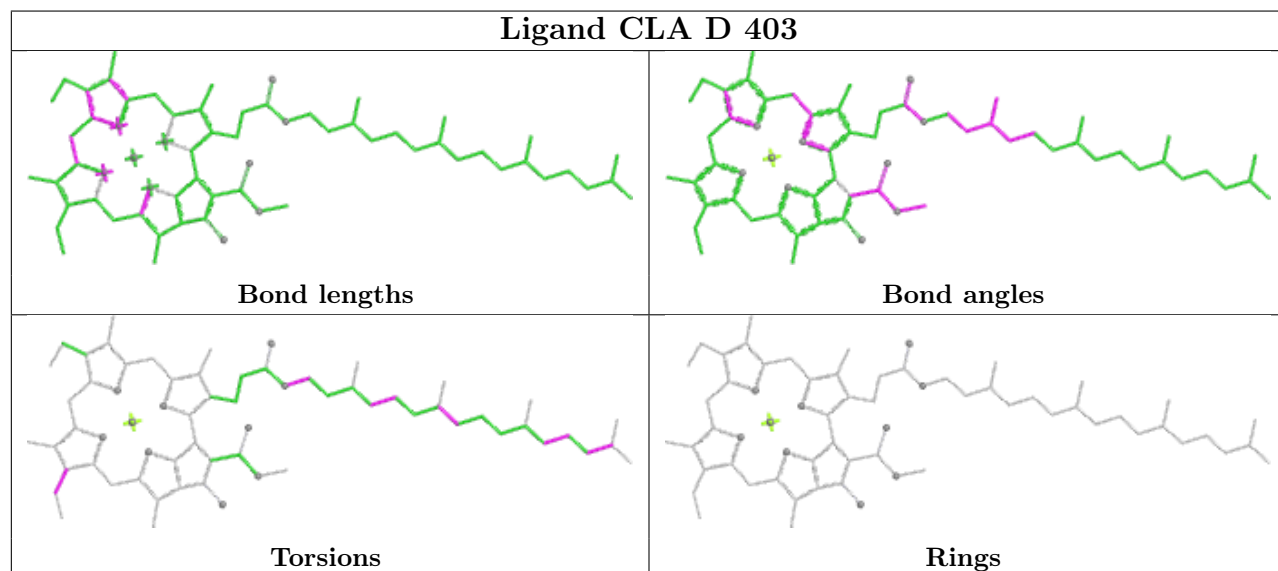
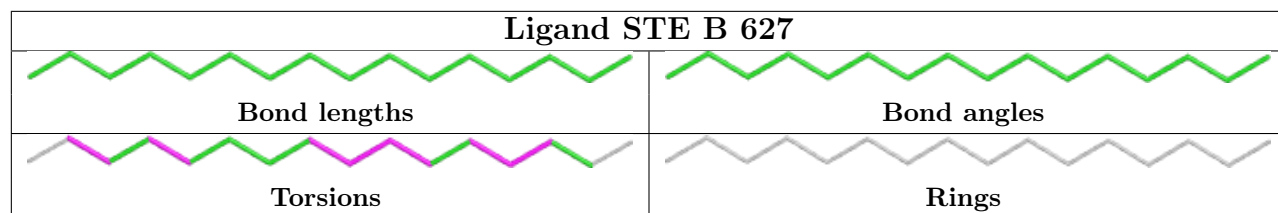
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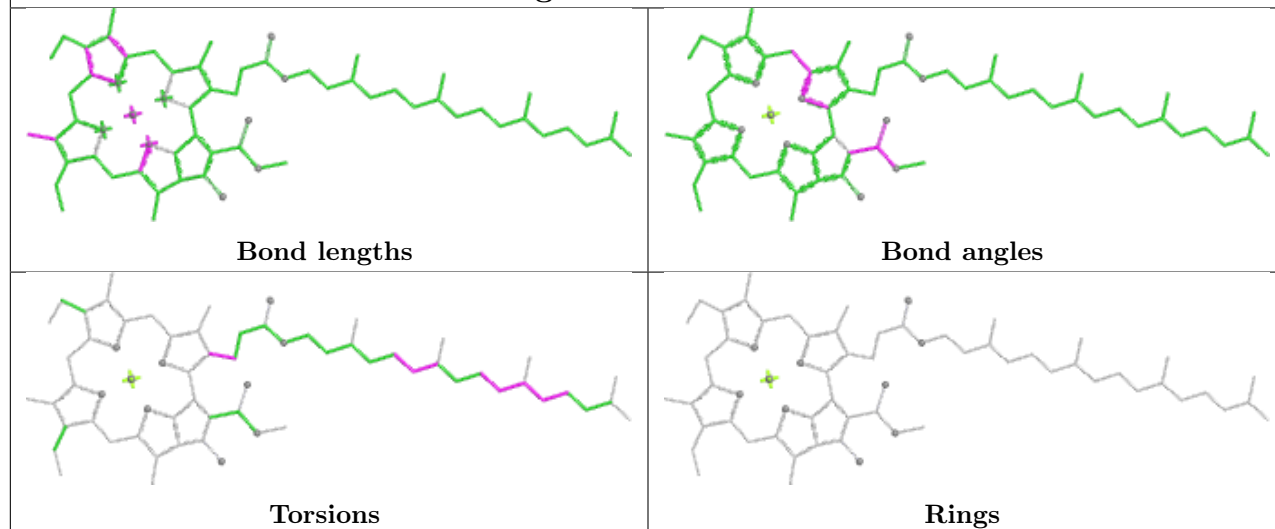
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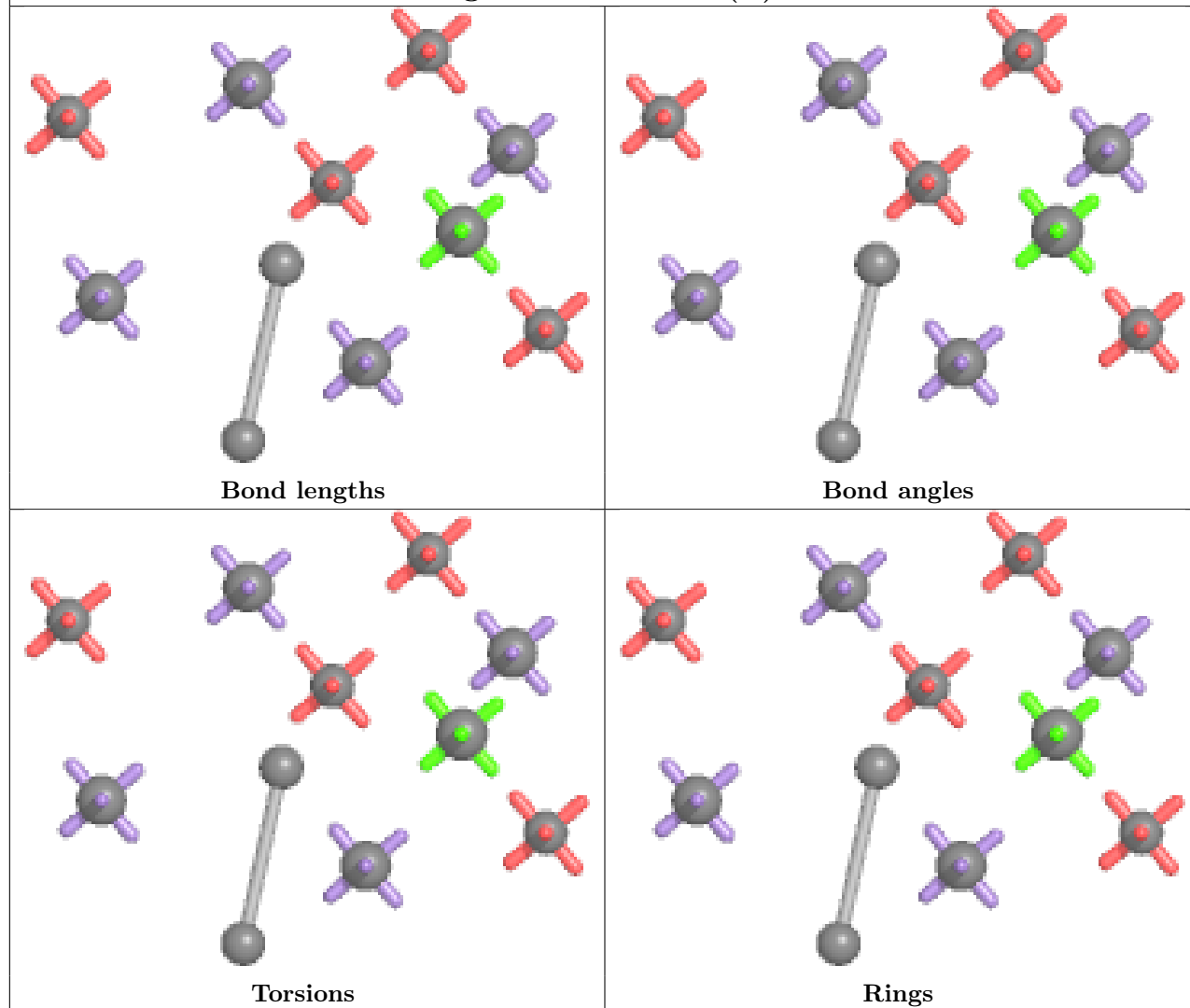




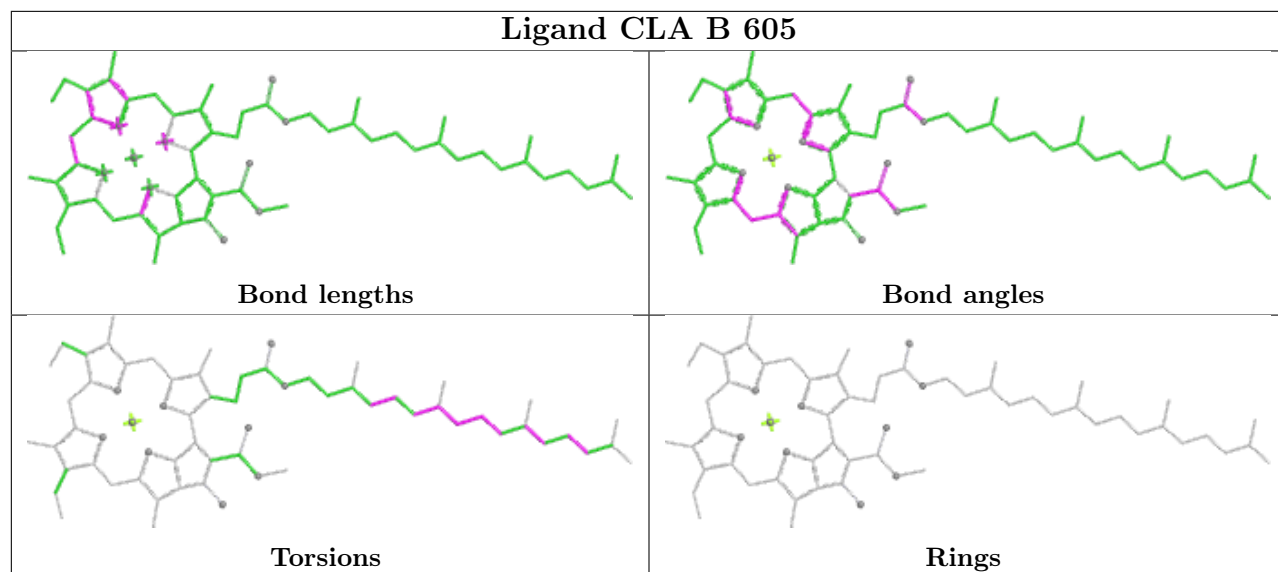
Ligand CLA a 608



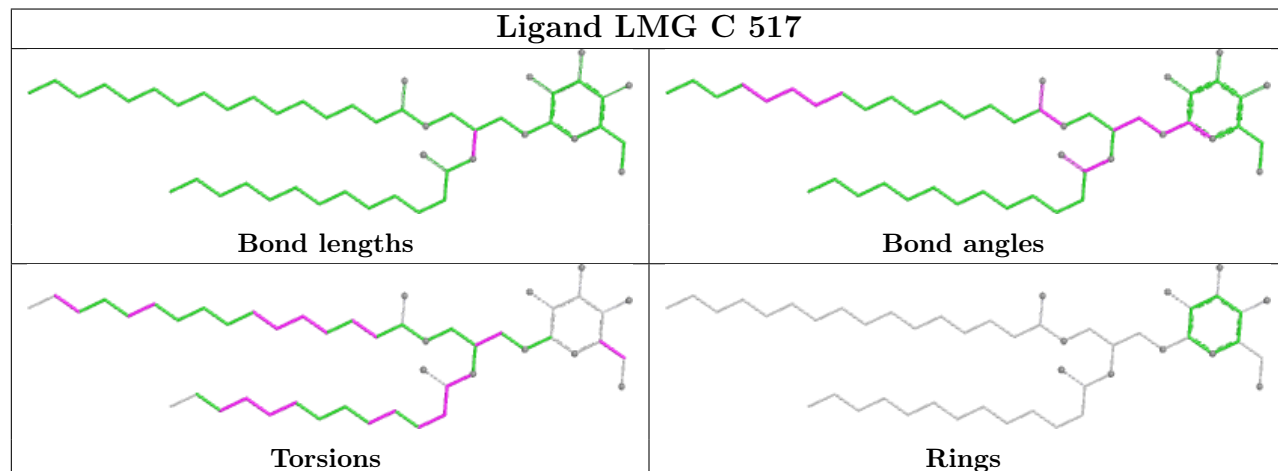
Ligand OEY A 601 (B)



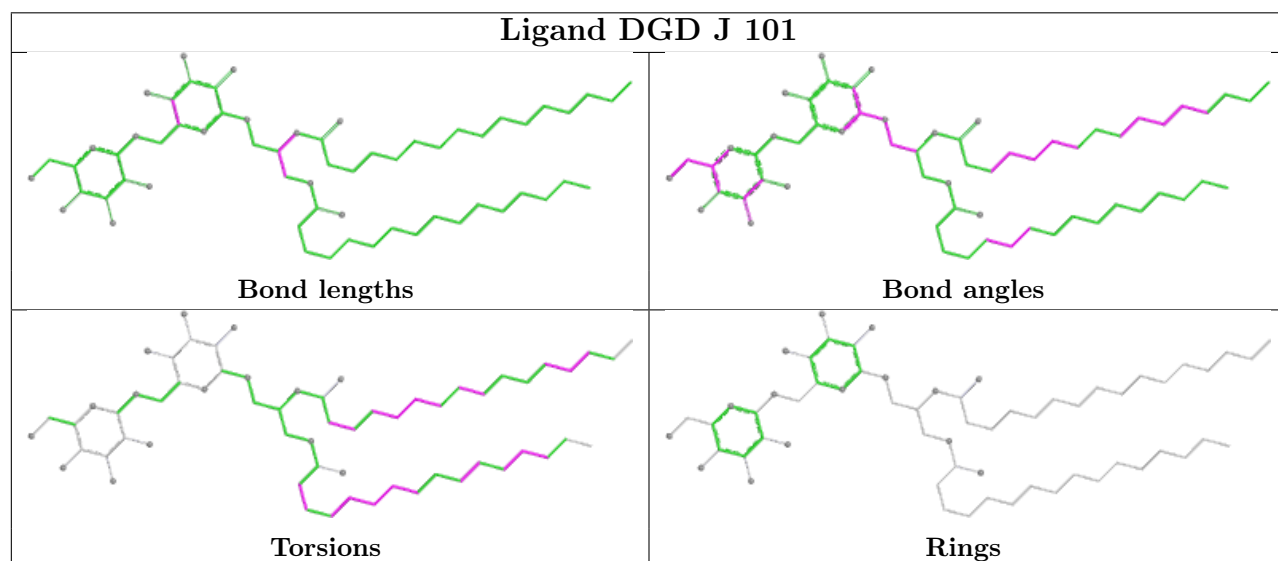
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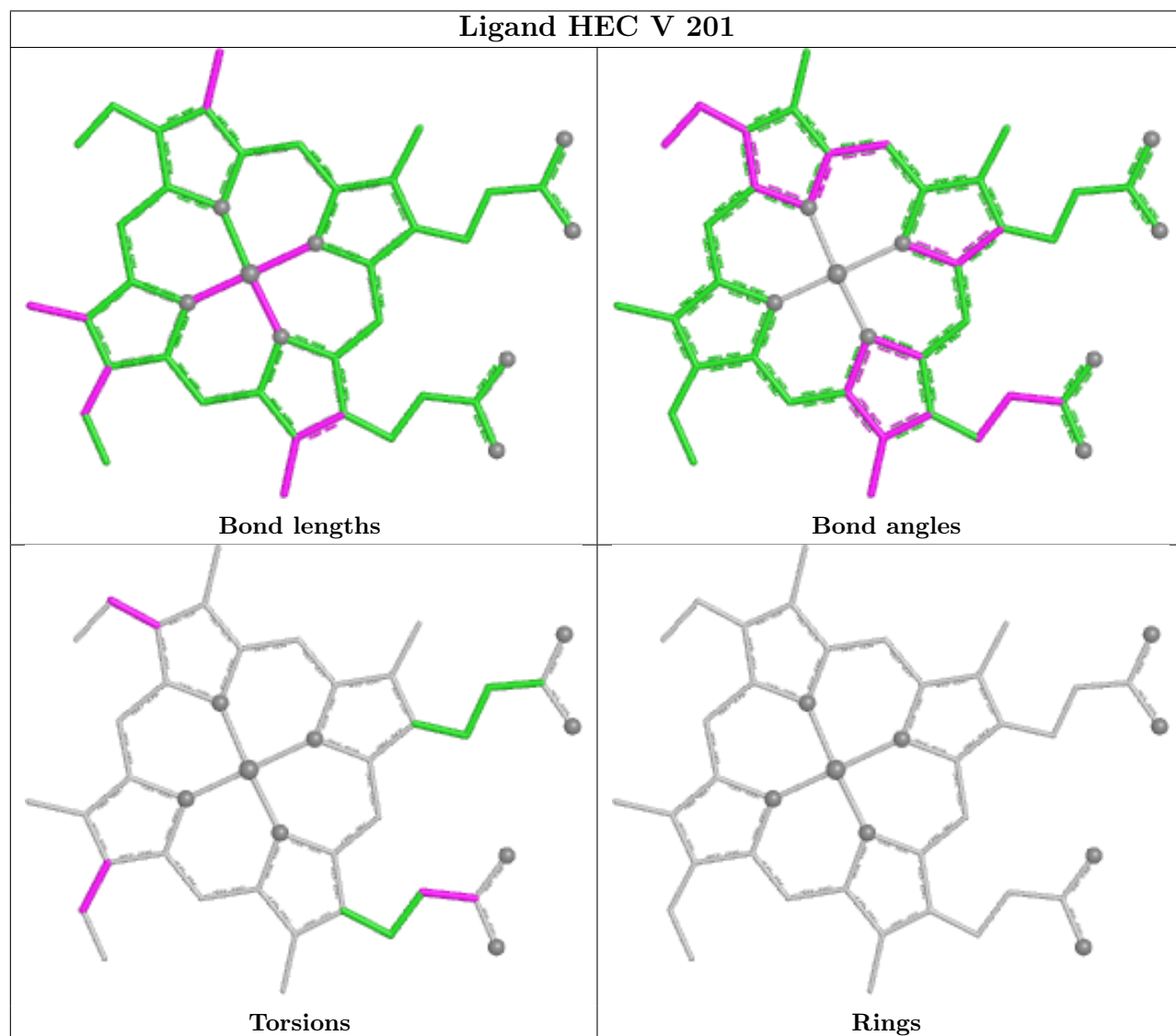
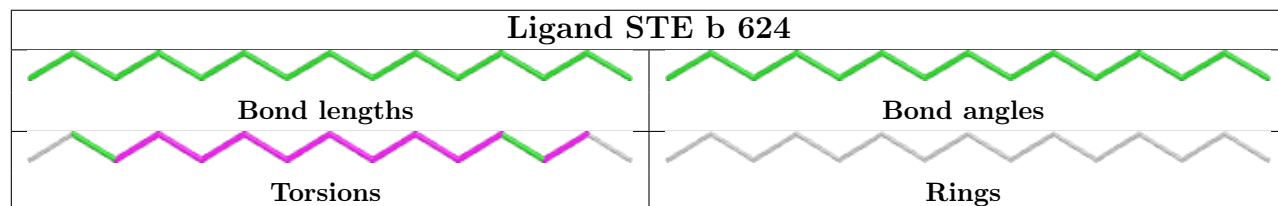
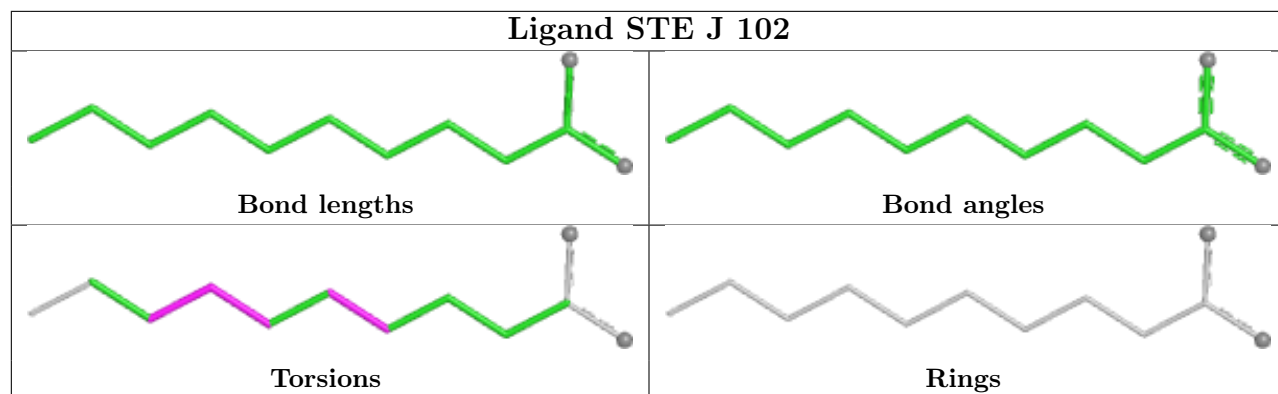


Ligand LMG C 517

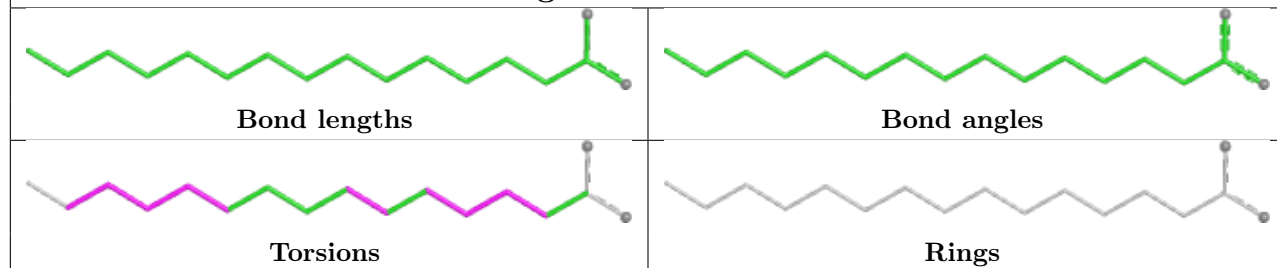


Ligand DGD J 101

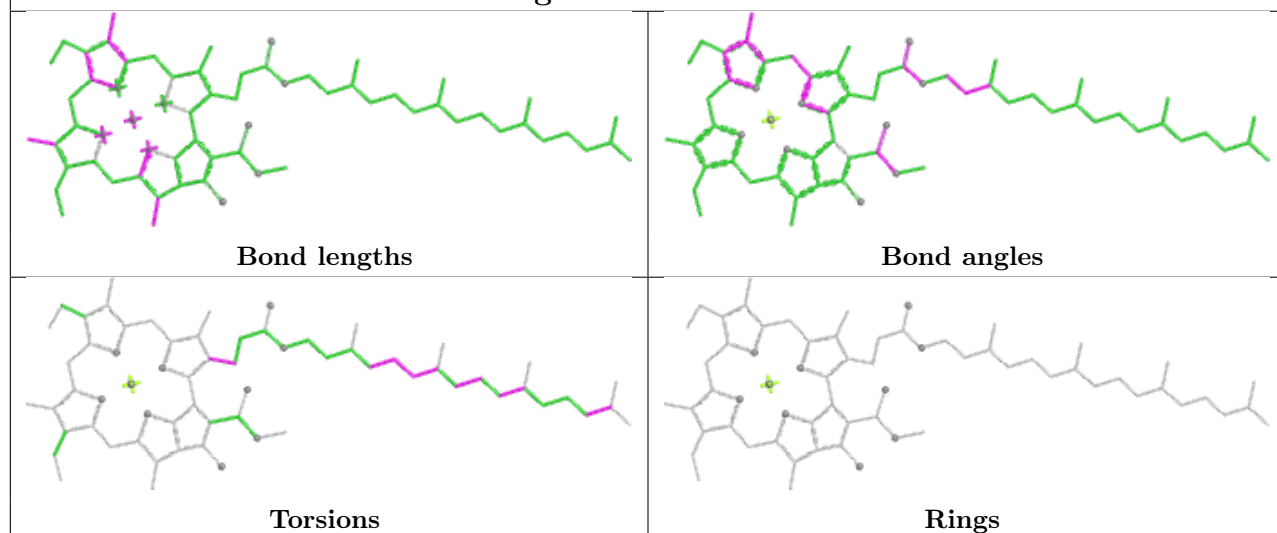




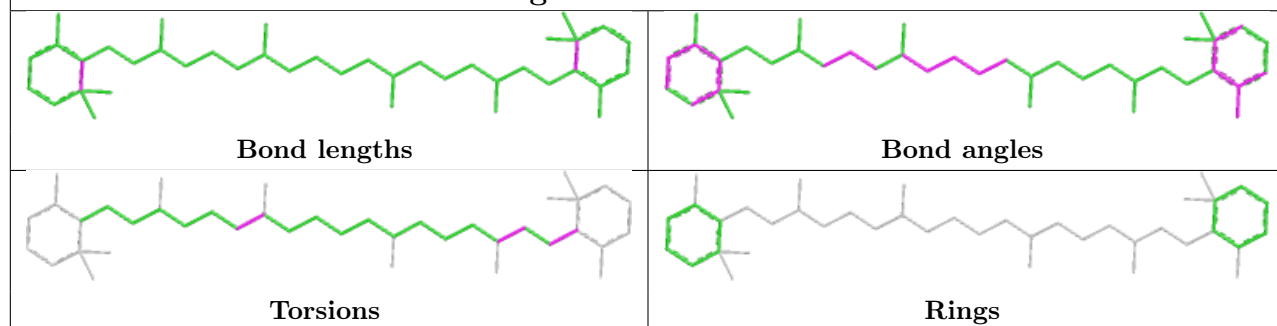
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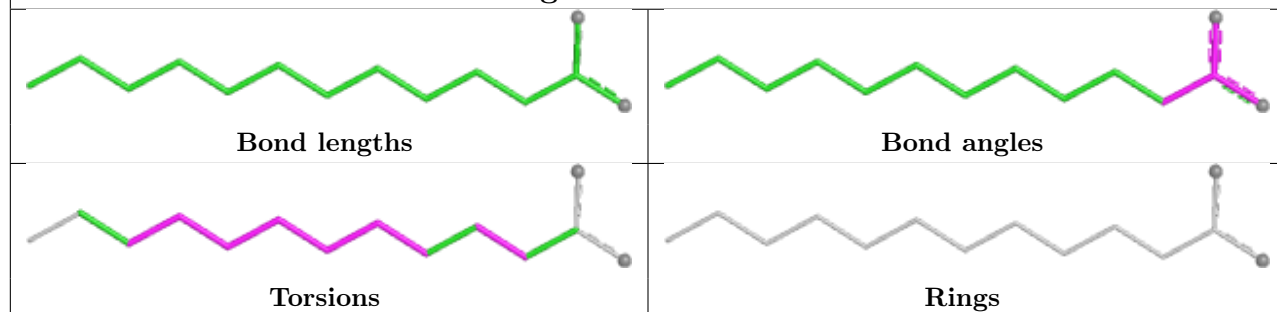
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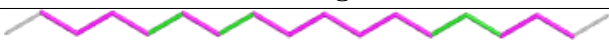
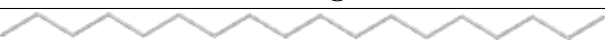


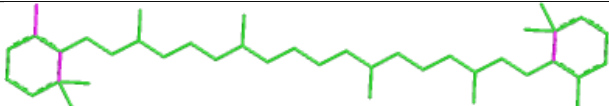
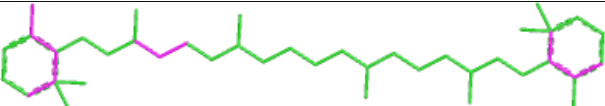
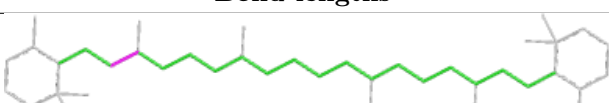
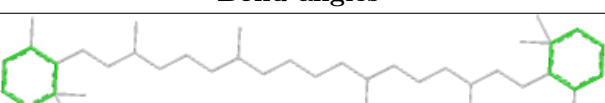
Ligand BCR B 619

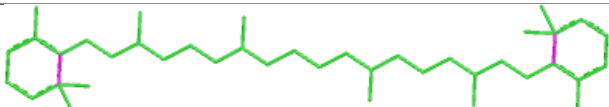
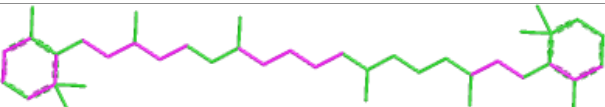
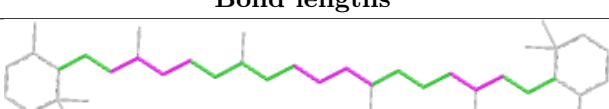
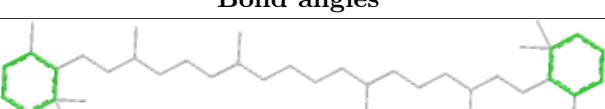


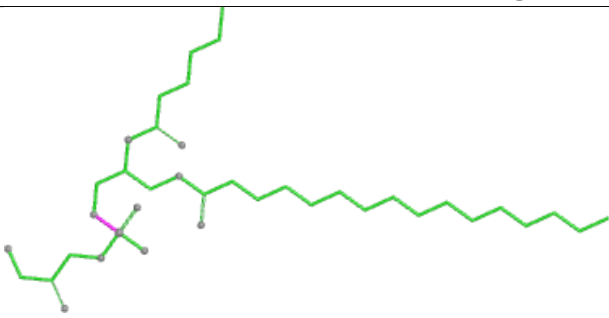
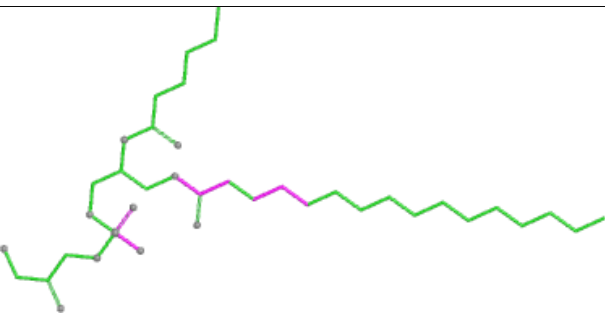
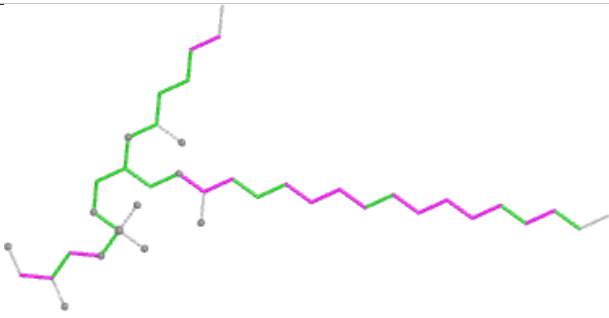
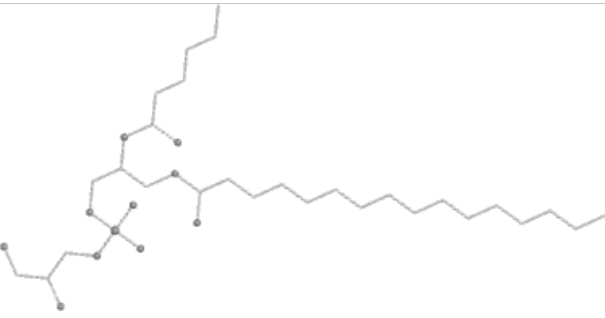
Ligand STE t 102

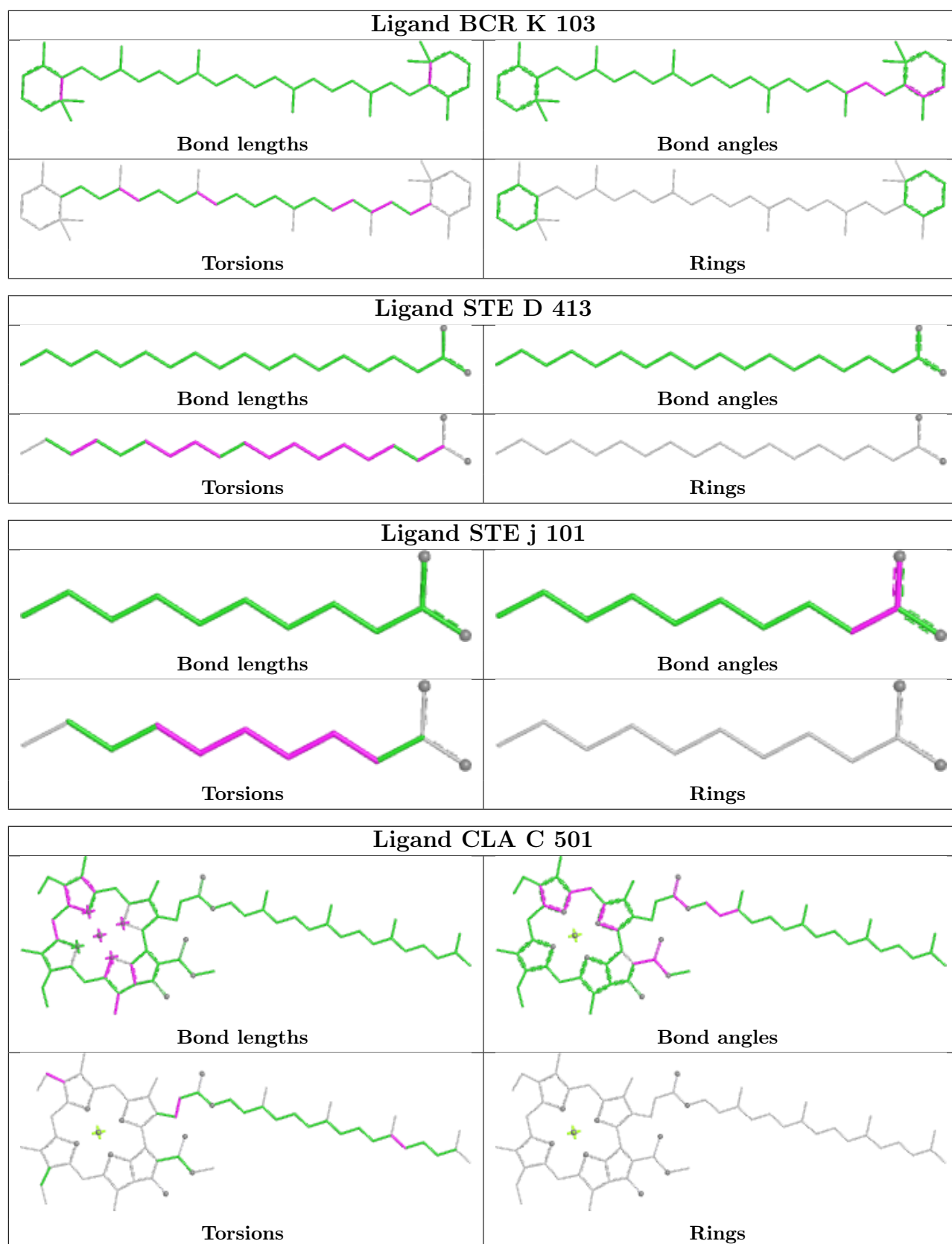


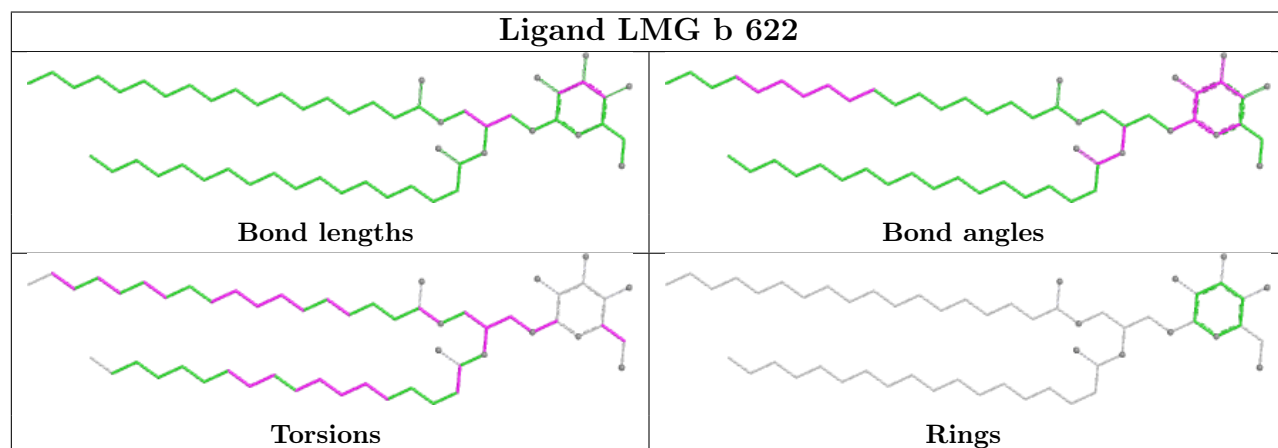
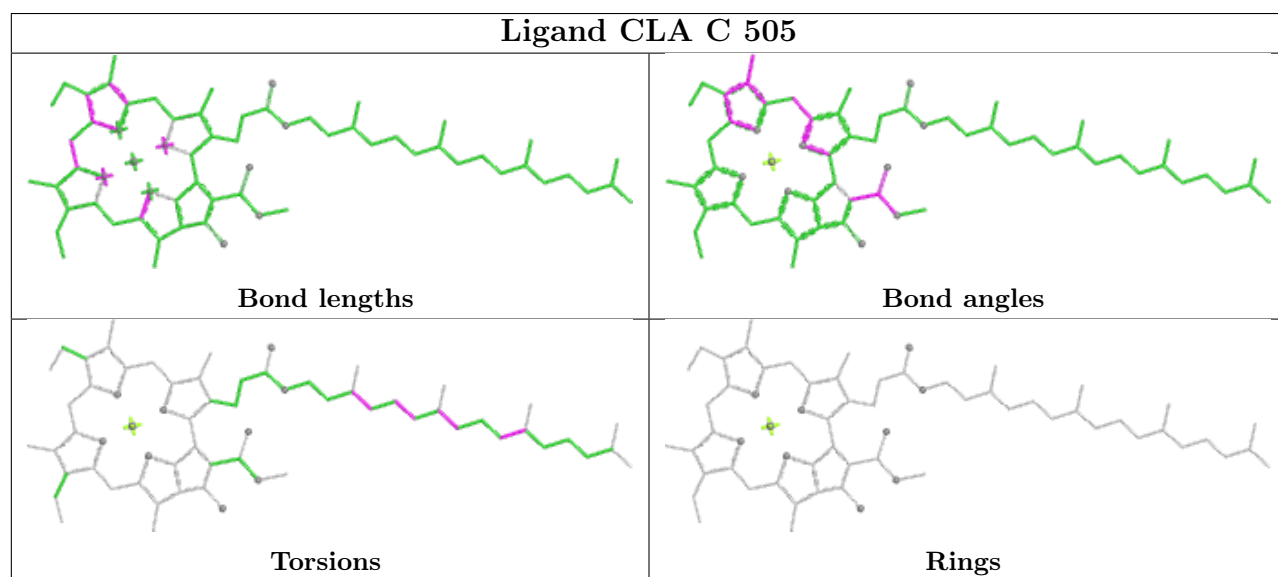
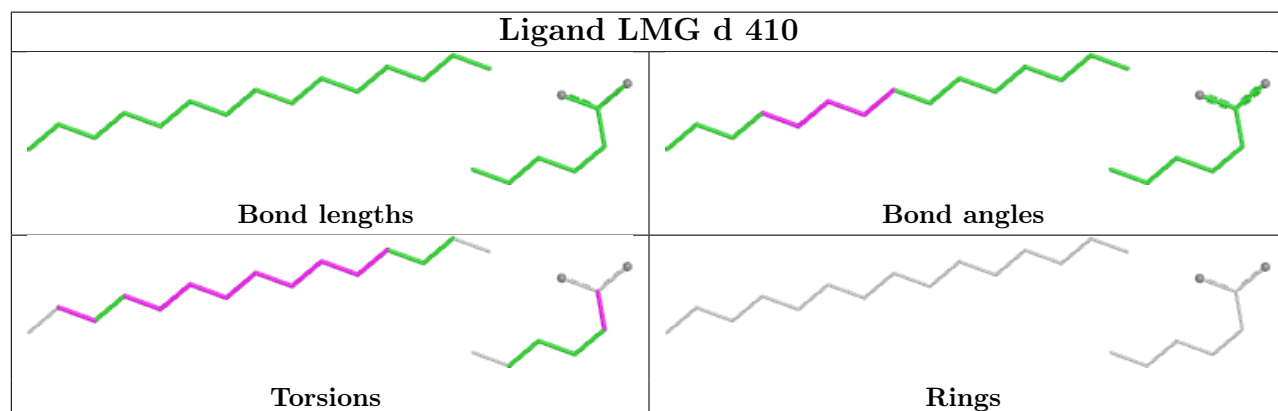
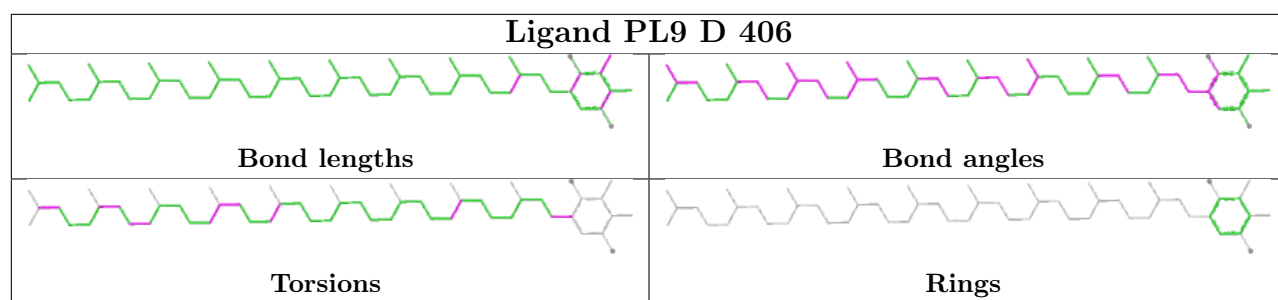
Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

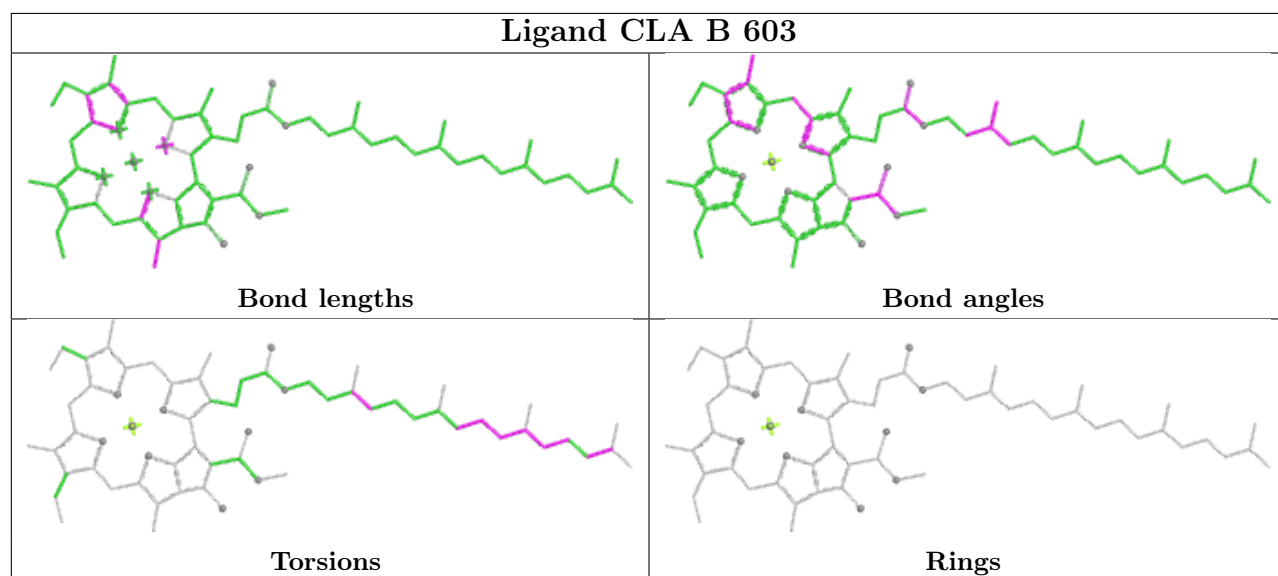
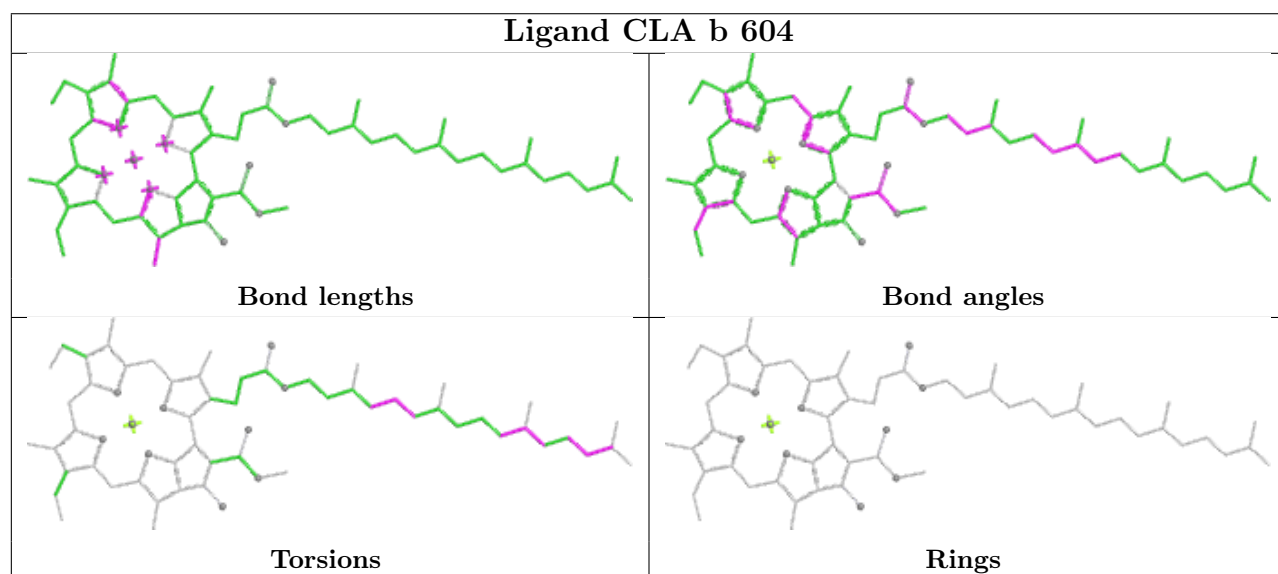
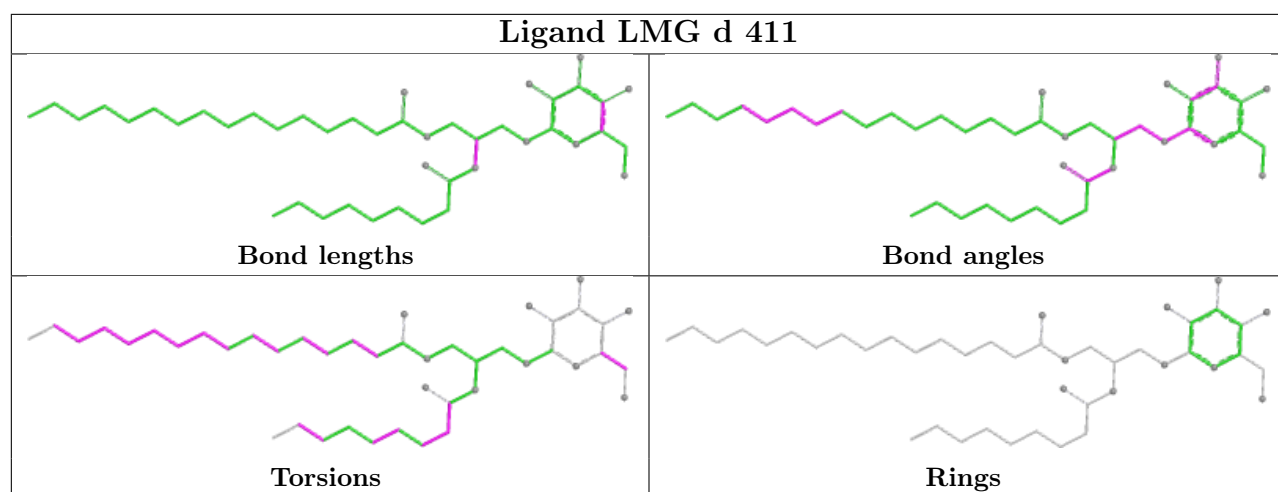
Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

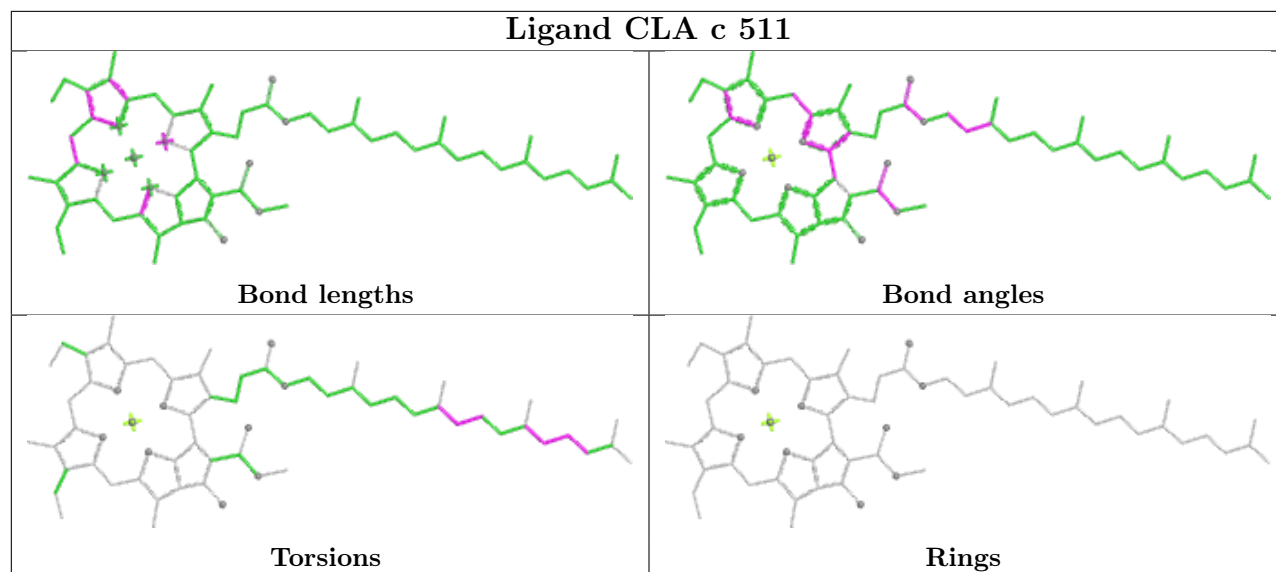
Ligand LHG d 409	
 Bond lengths	 Bond angles
 Torsions	 Rings



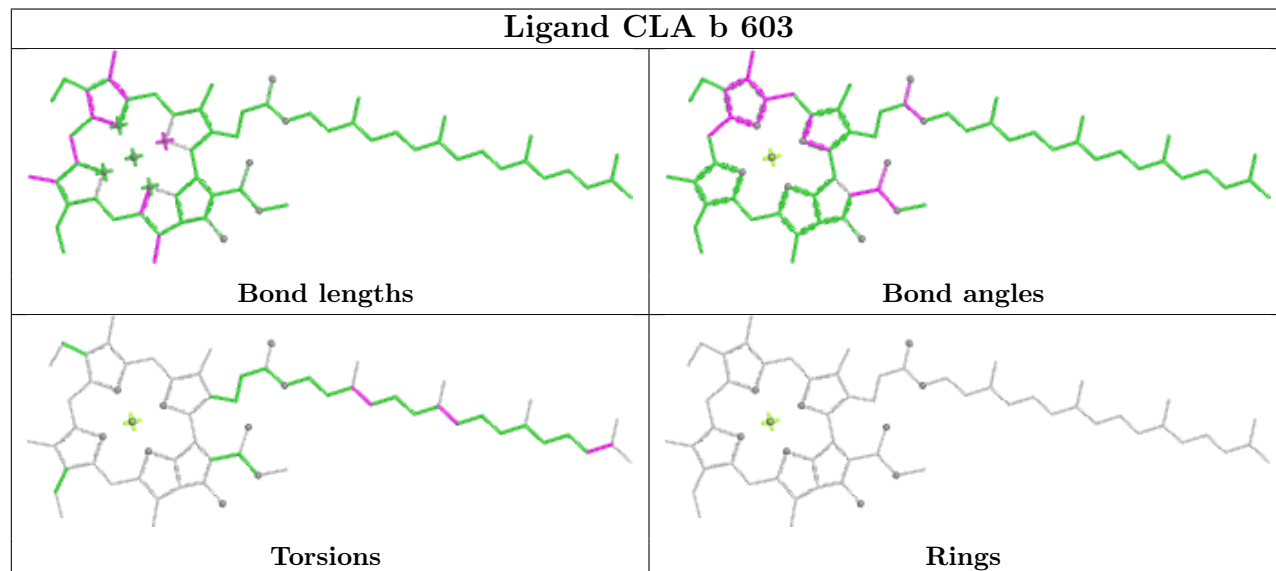




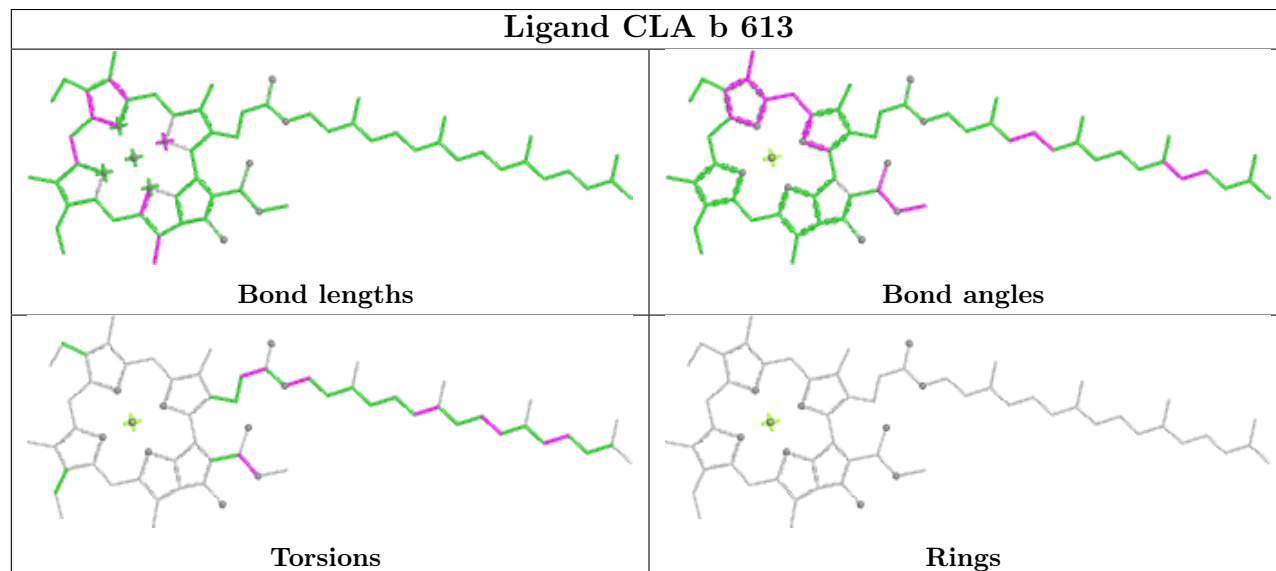
Ligand CLA c 511

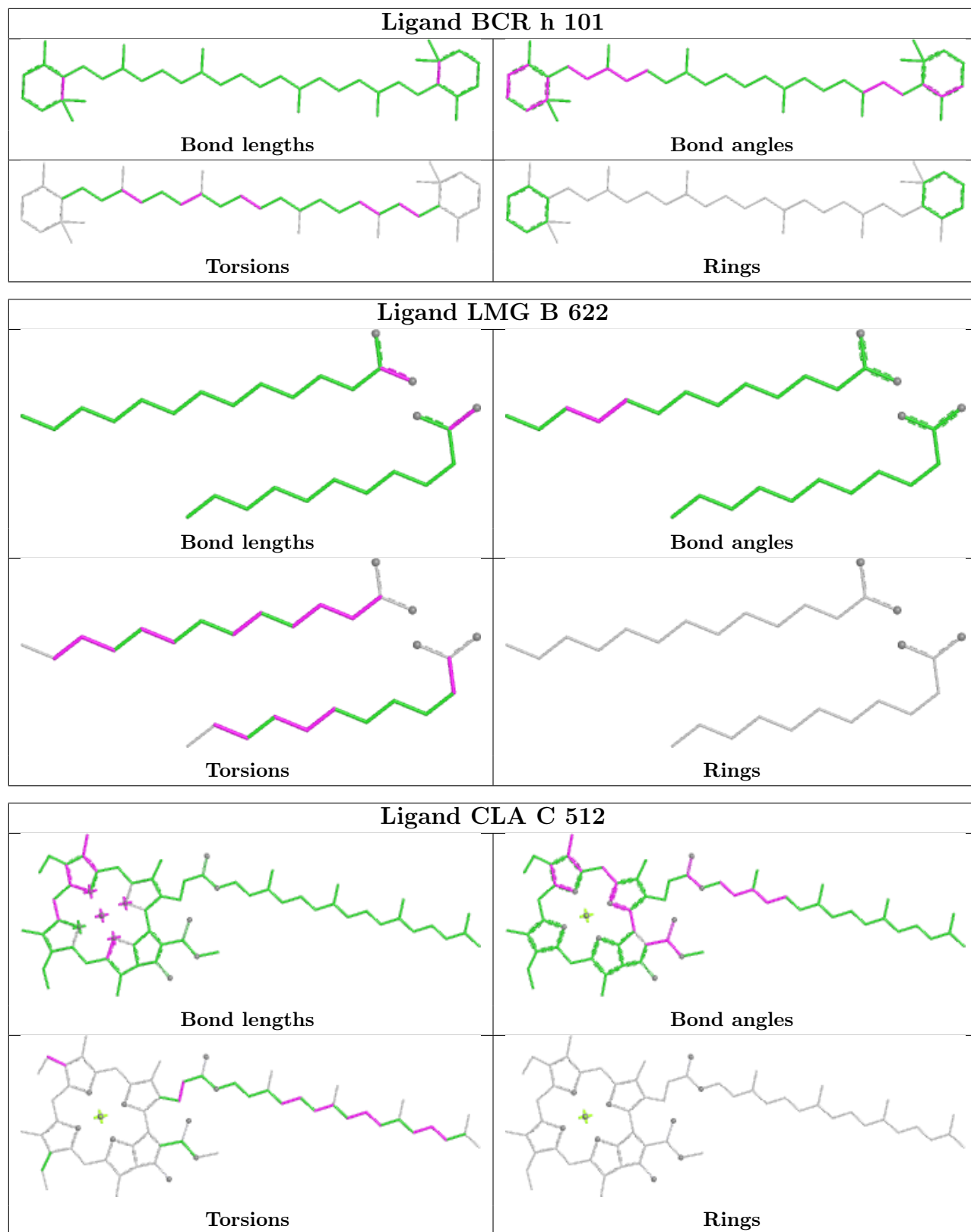


Ligand CLA b 603

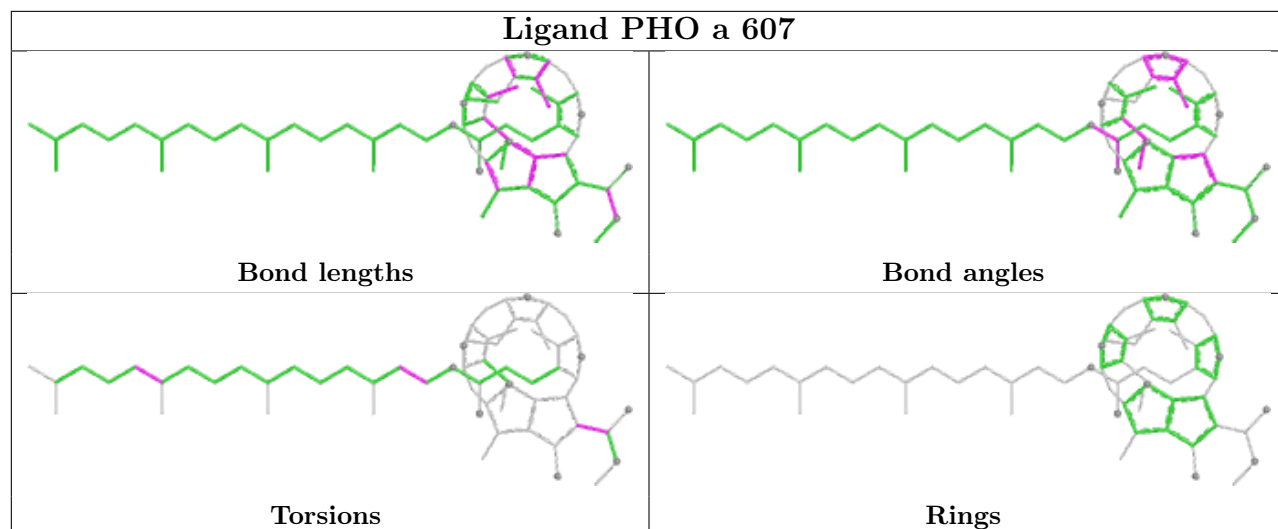


Ligand CLA b 613

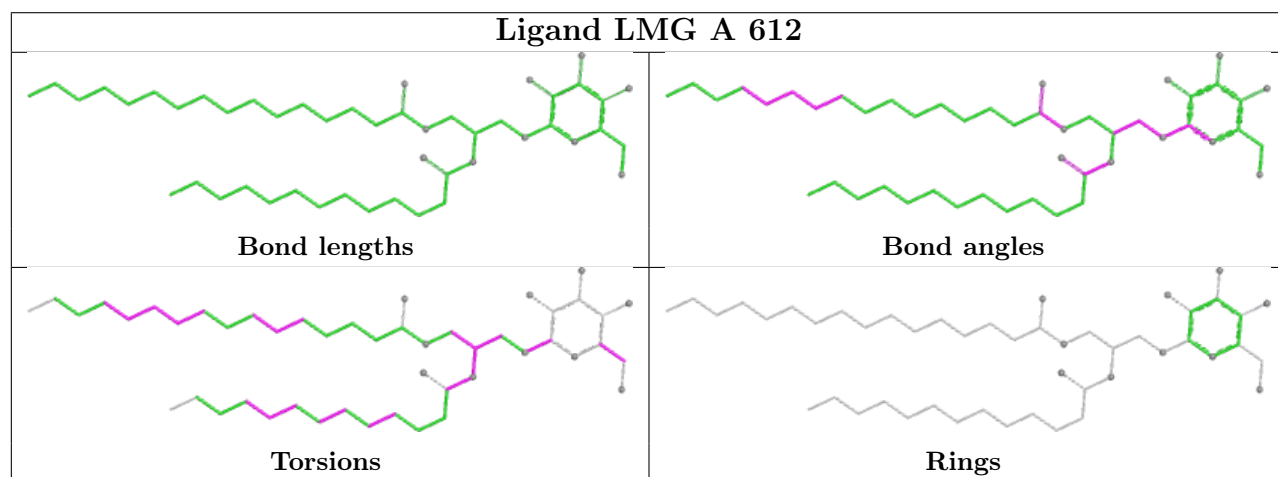




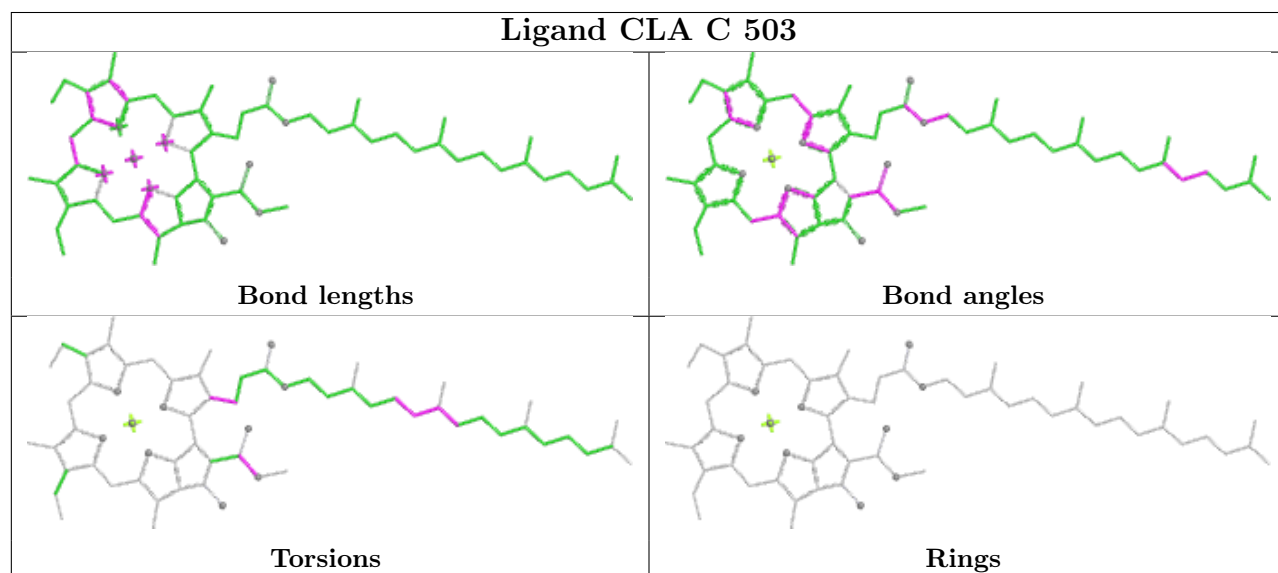
Ligand PHO a 607



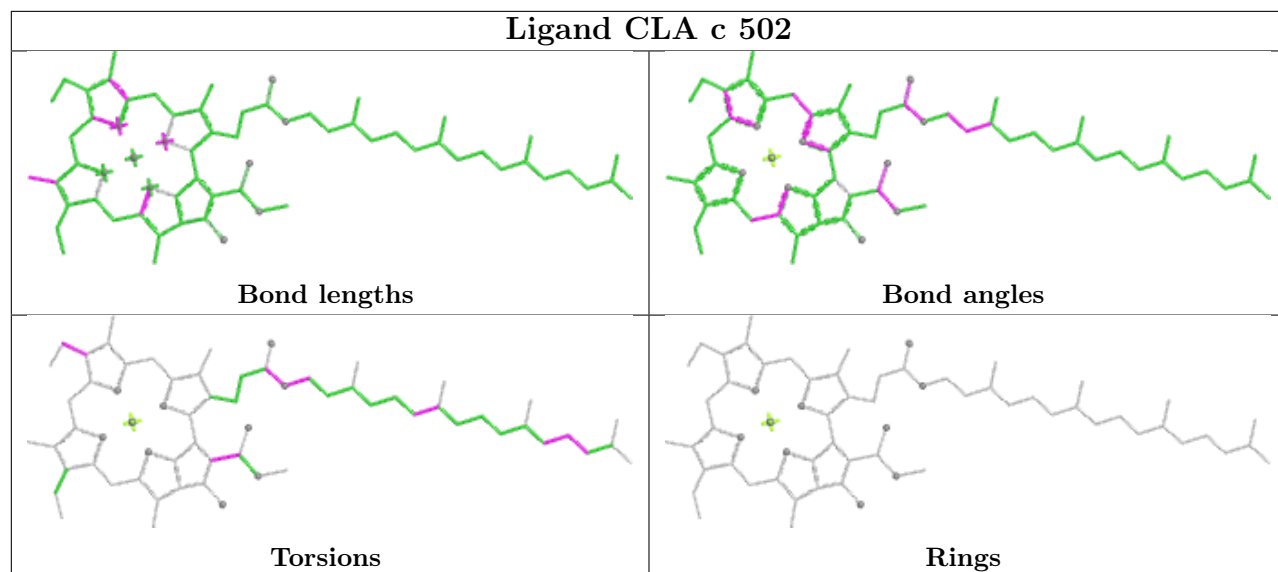
Ligand LMG A 612



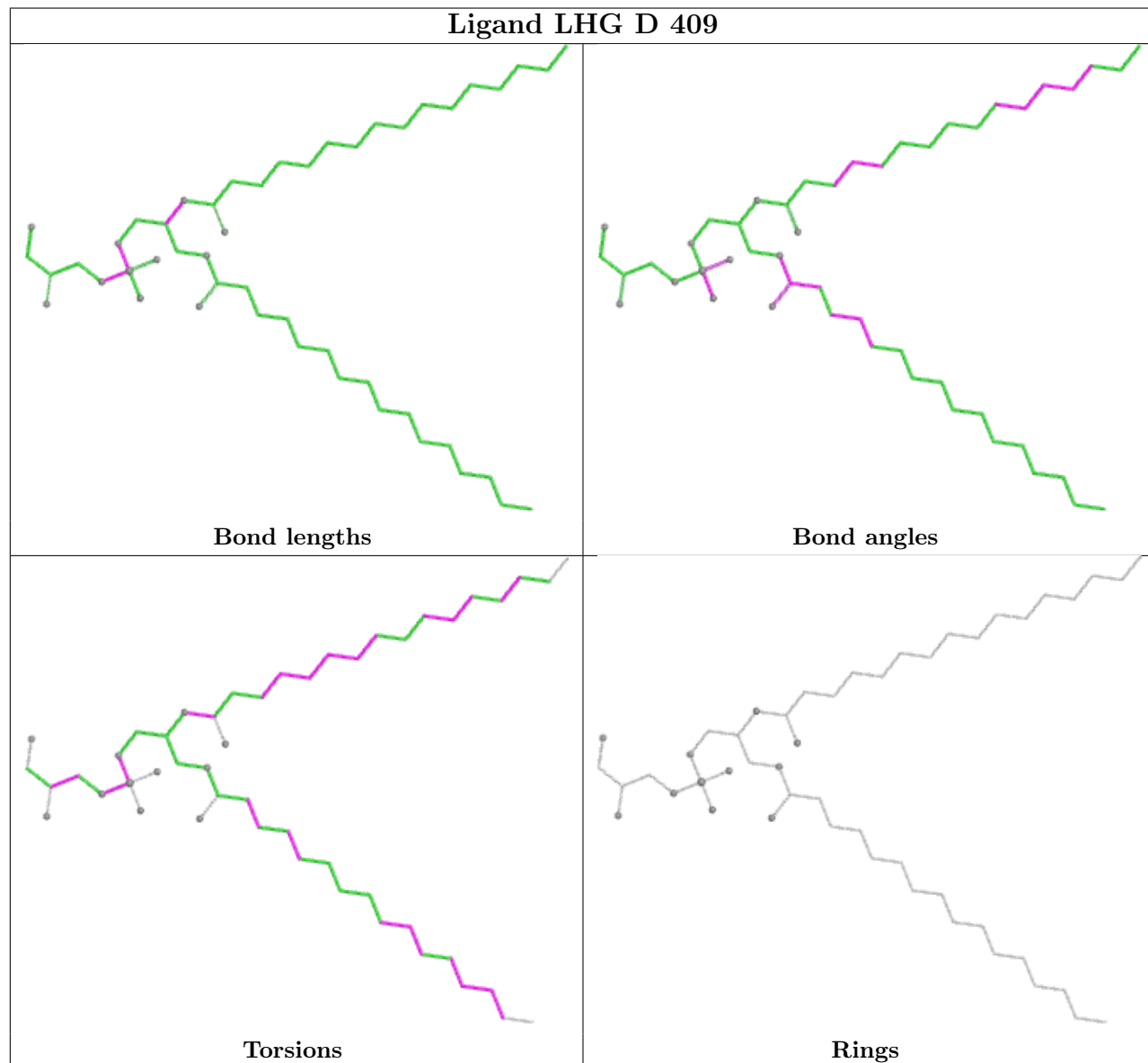
Ligand CLA C 503

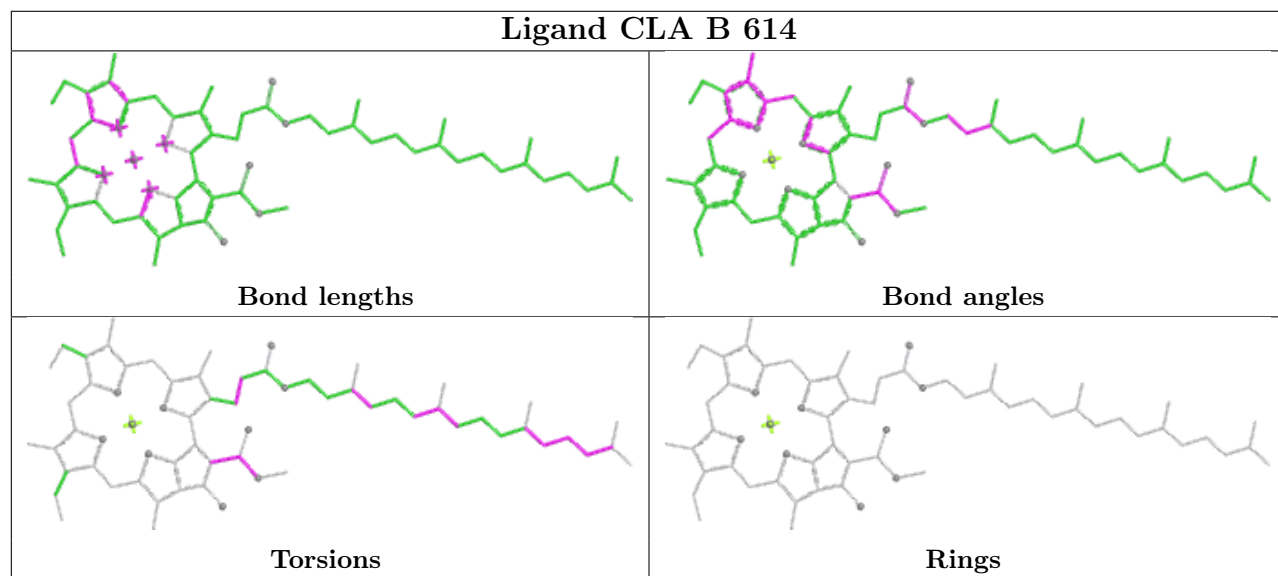
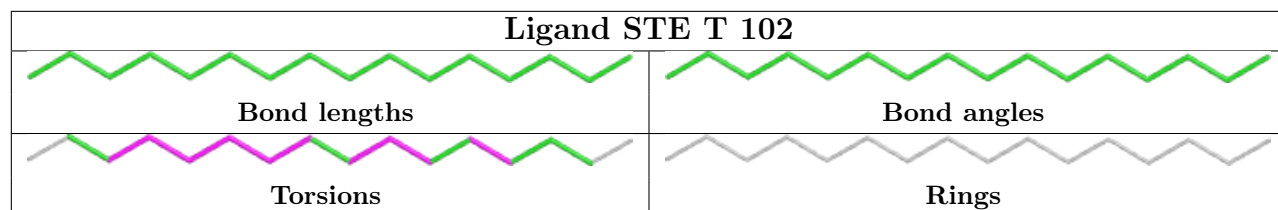


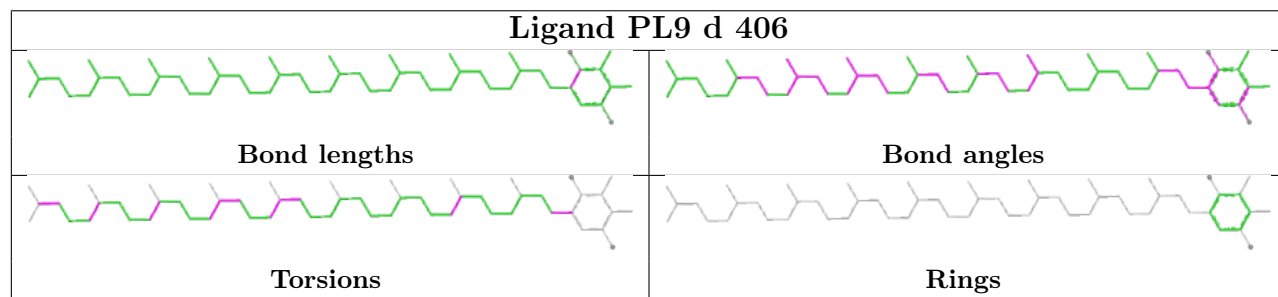
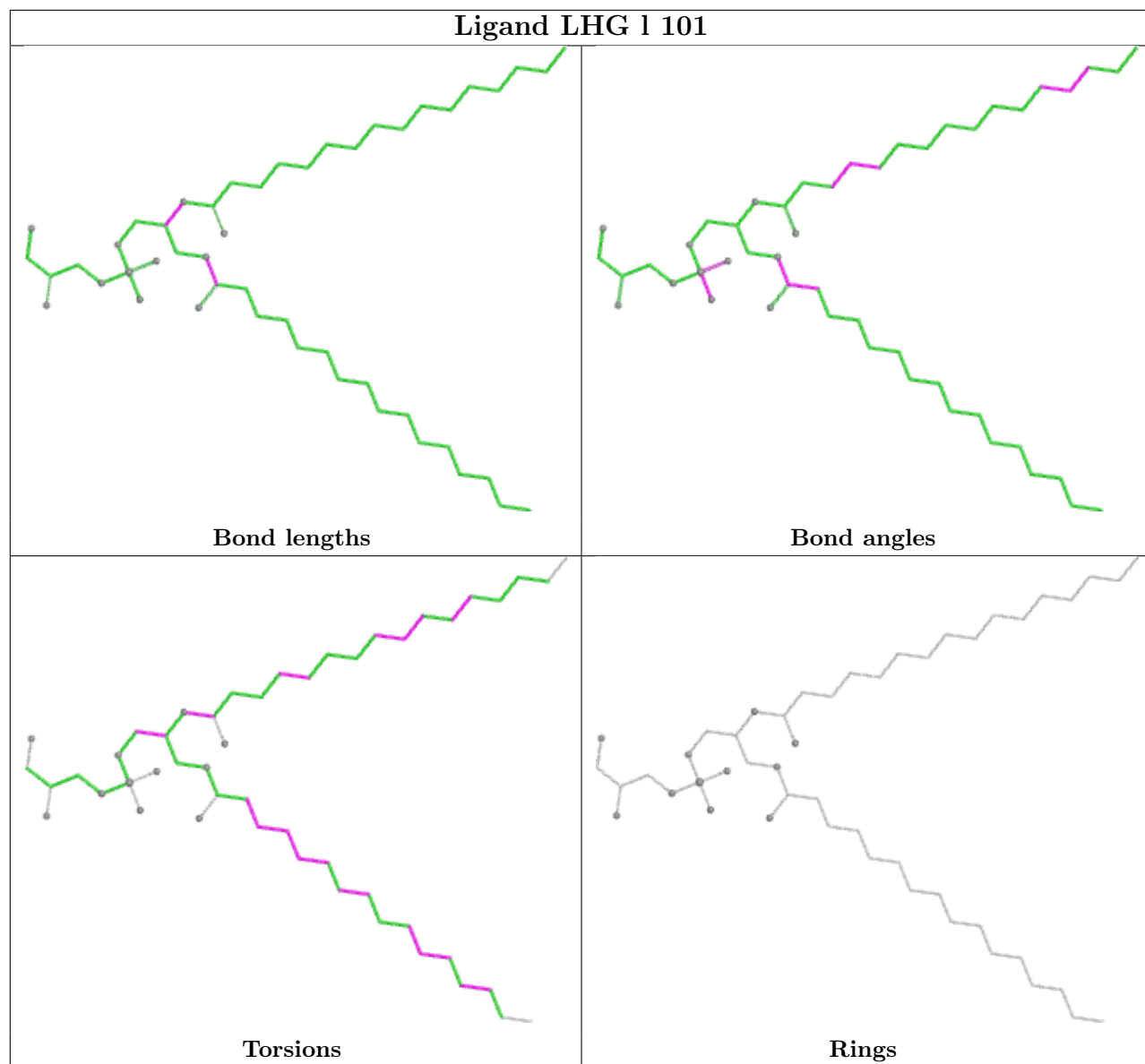
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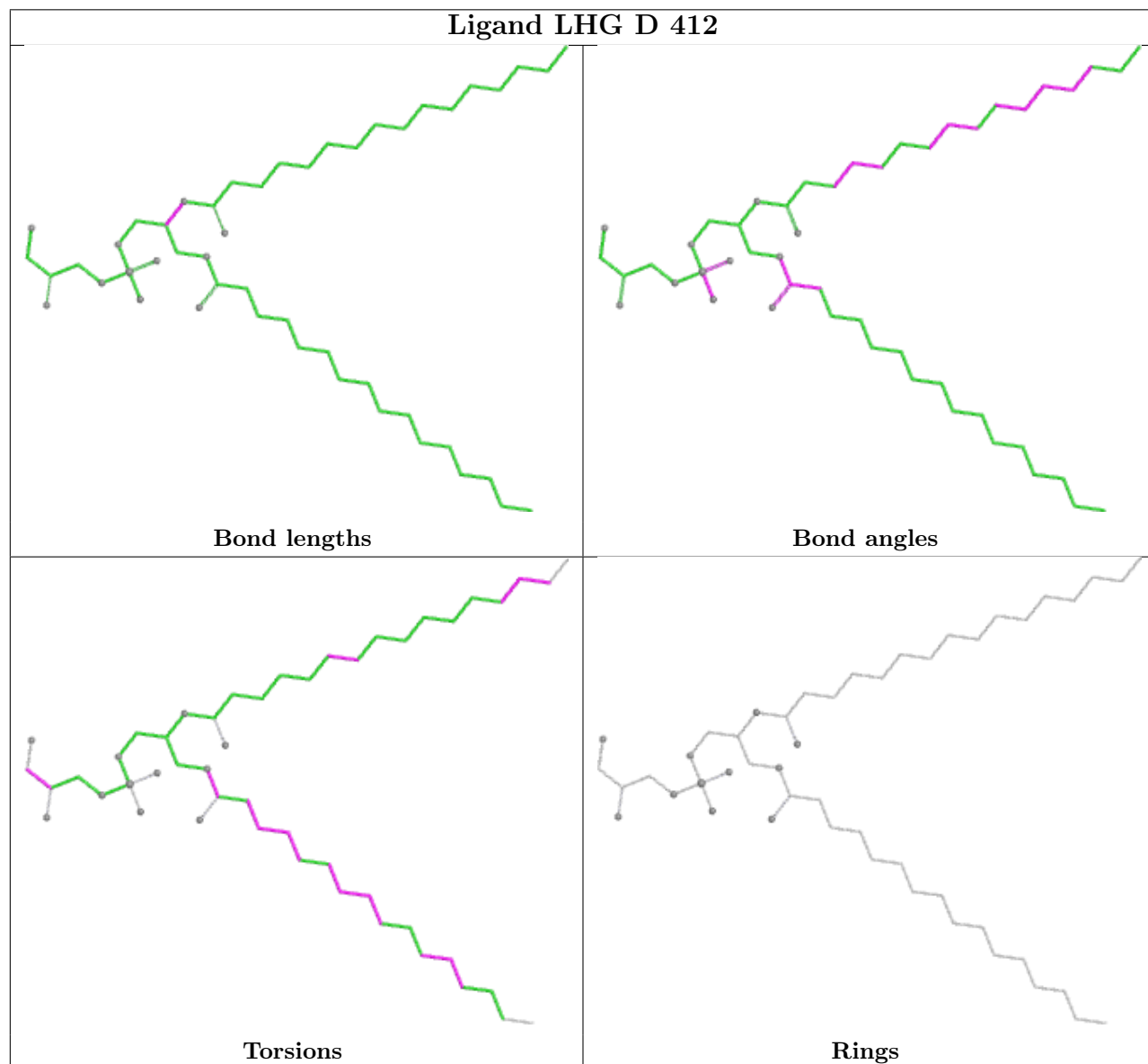
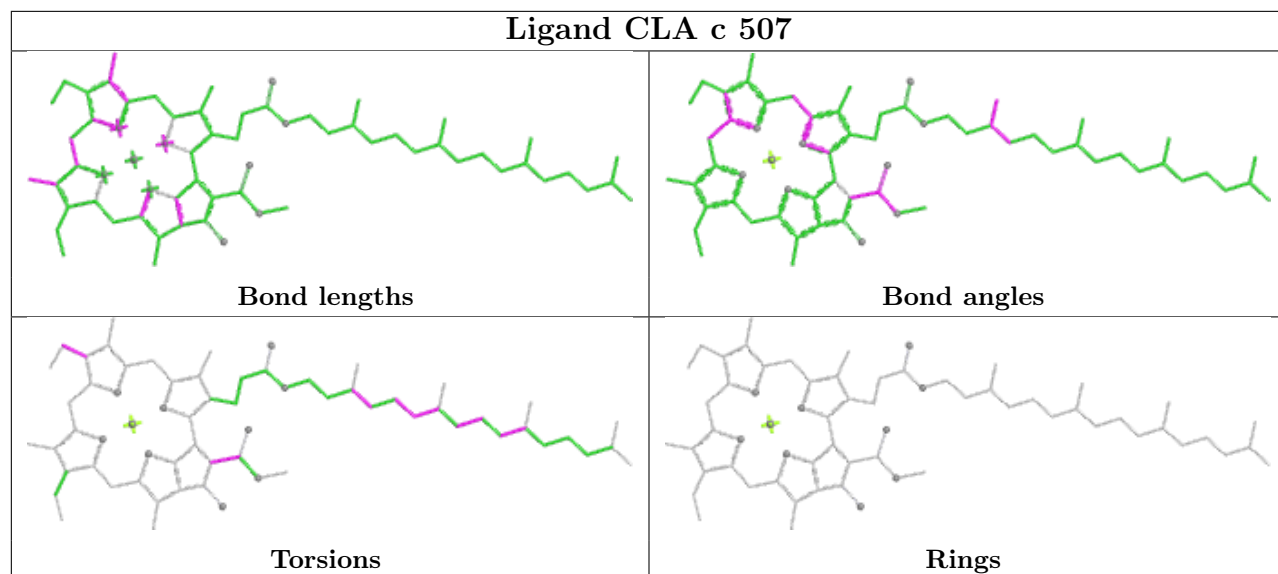


Ligand LHG D 409

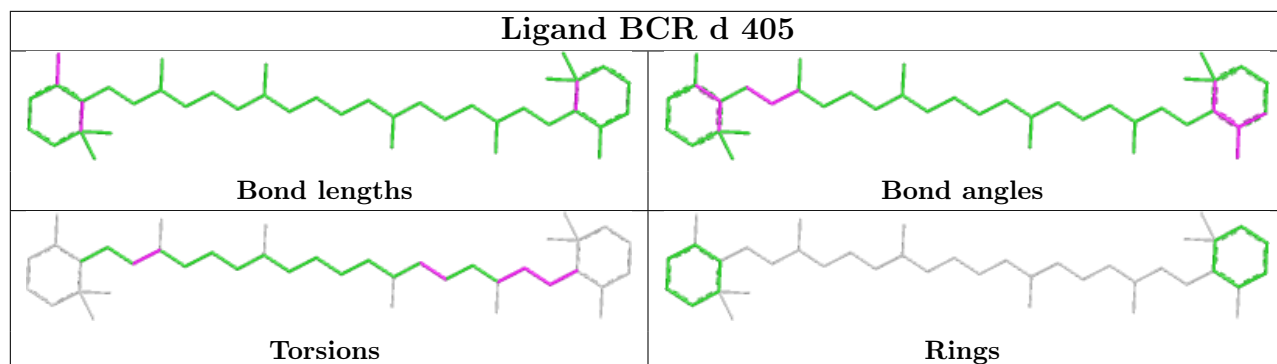




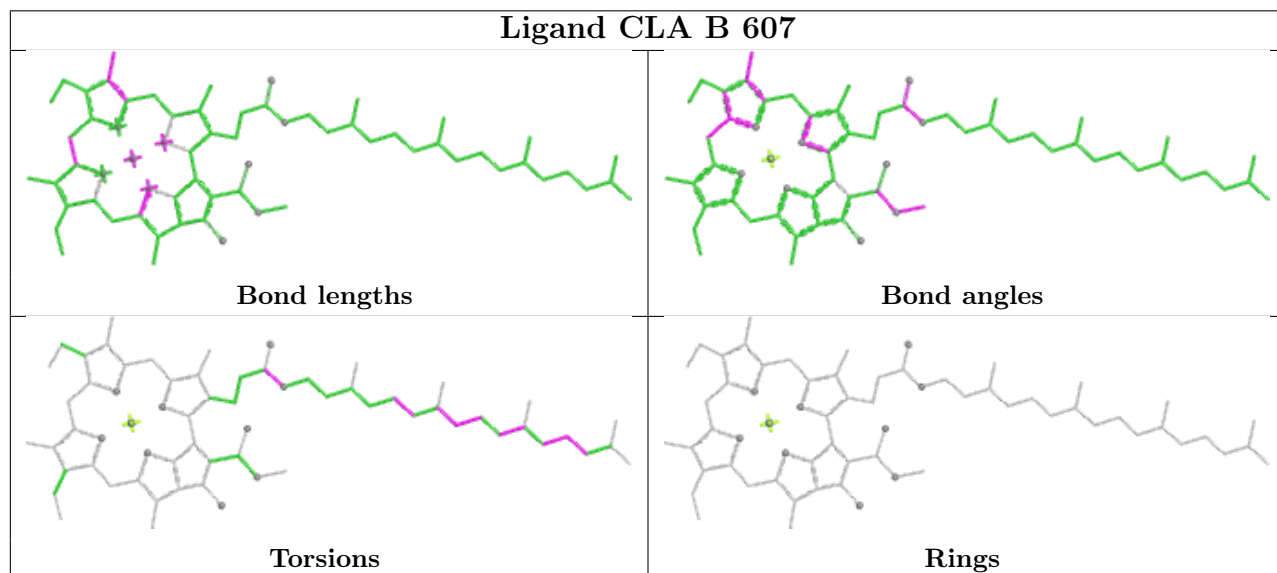




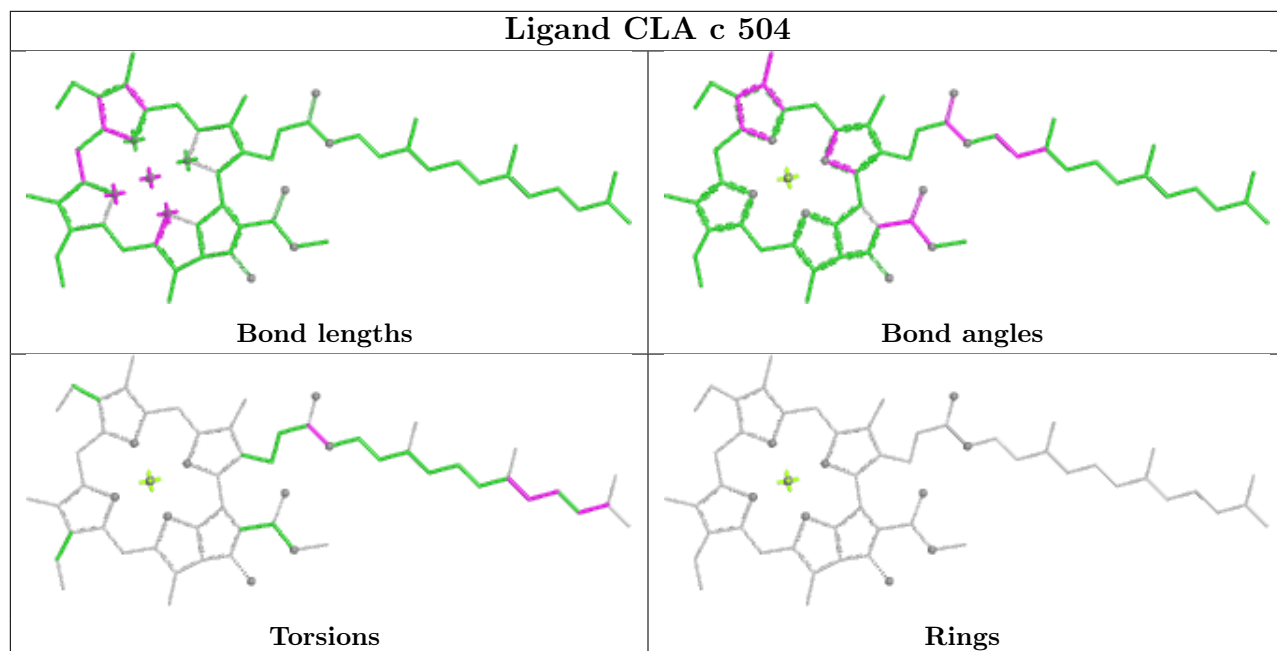
Ligand BCR d 405

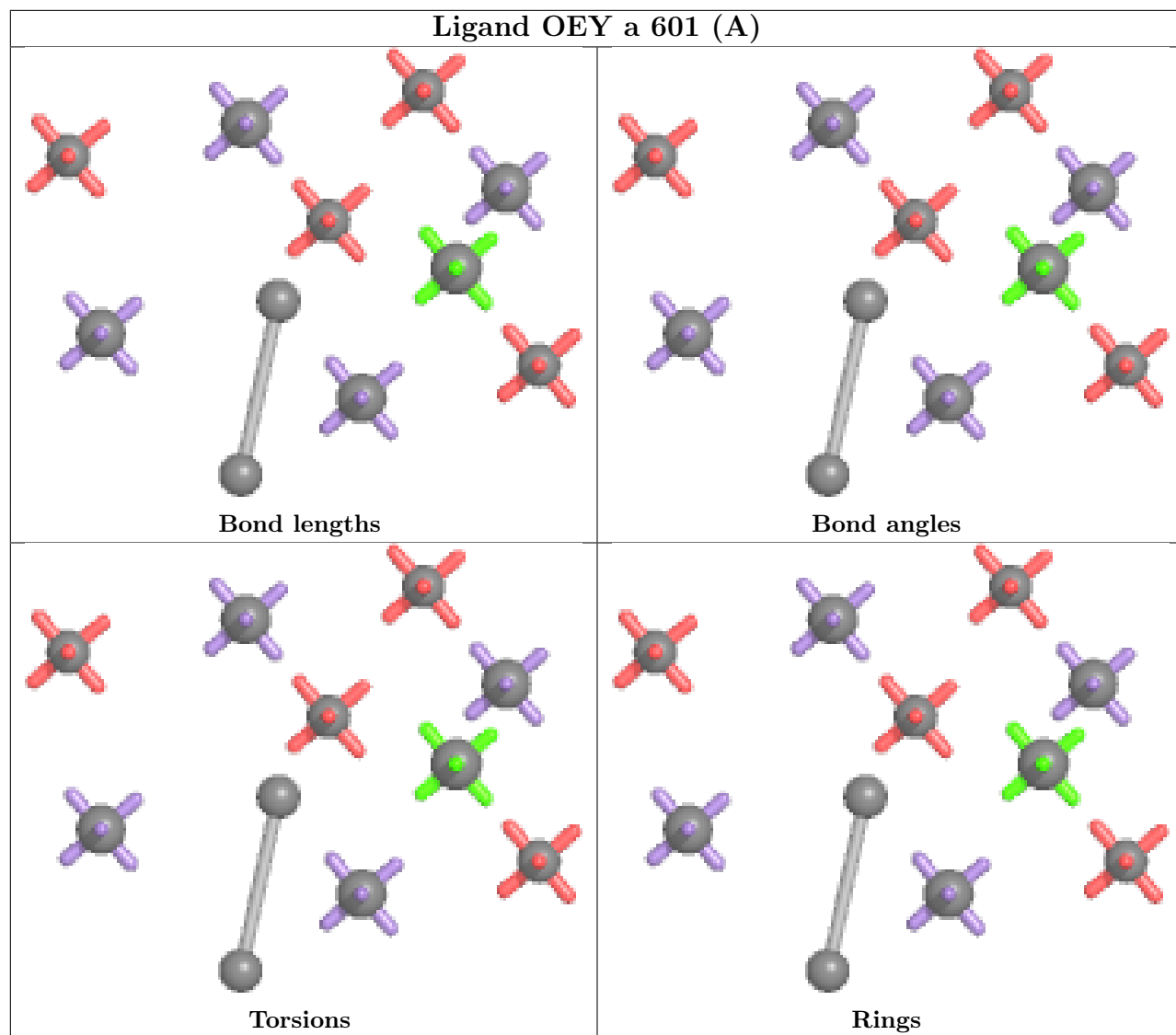


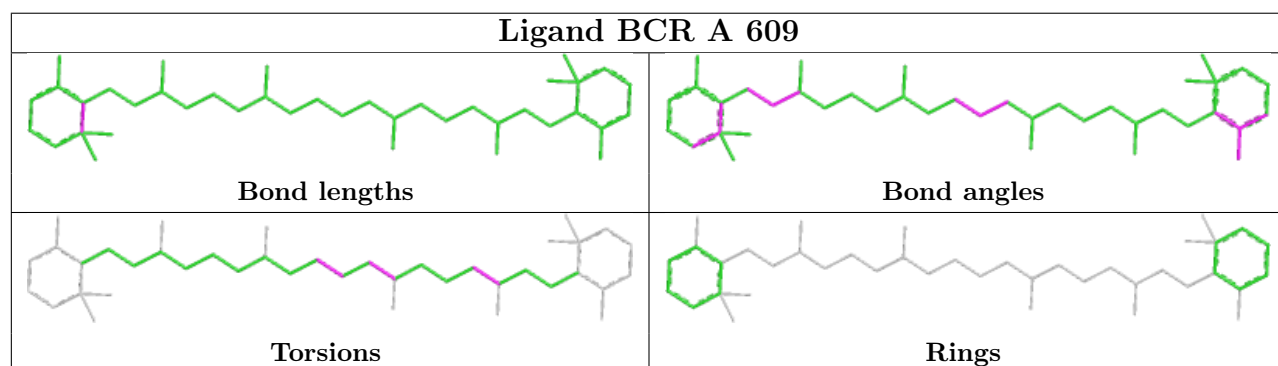
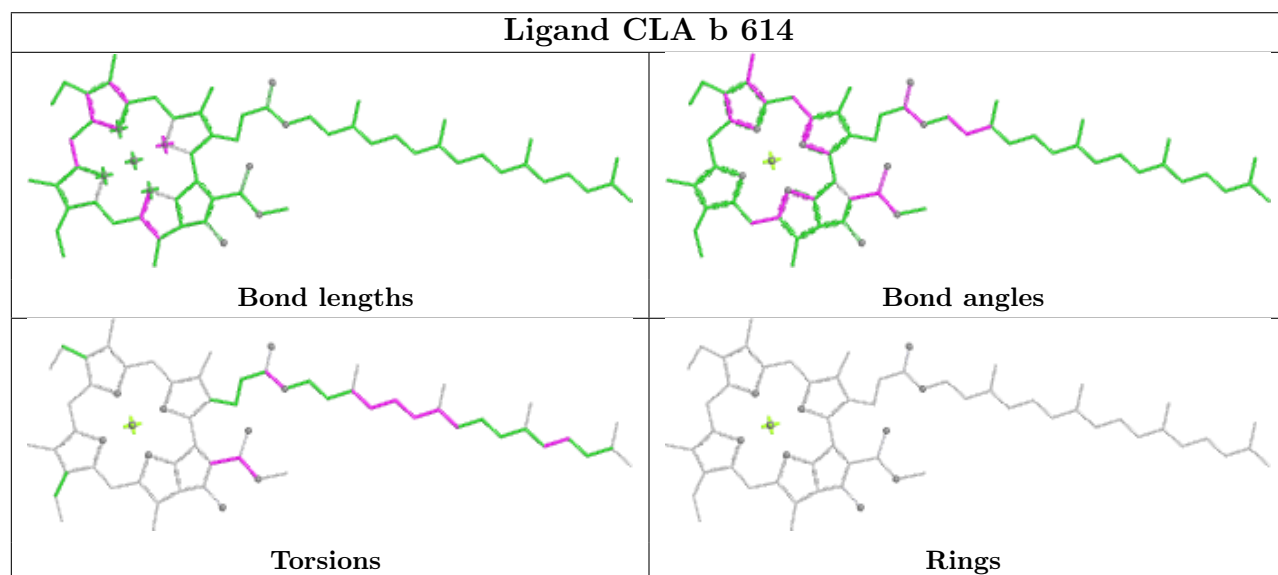
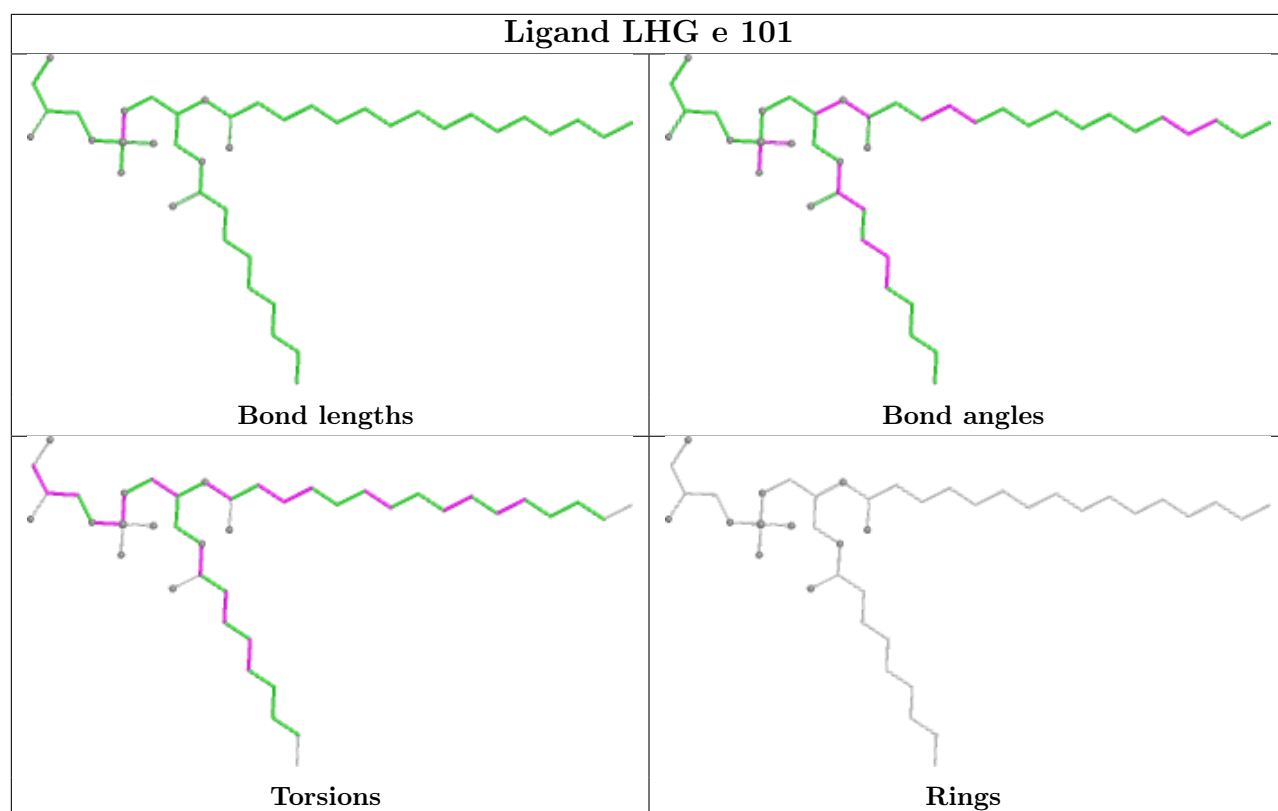
Ligand CLA B 607

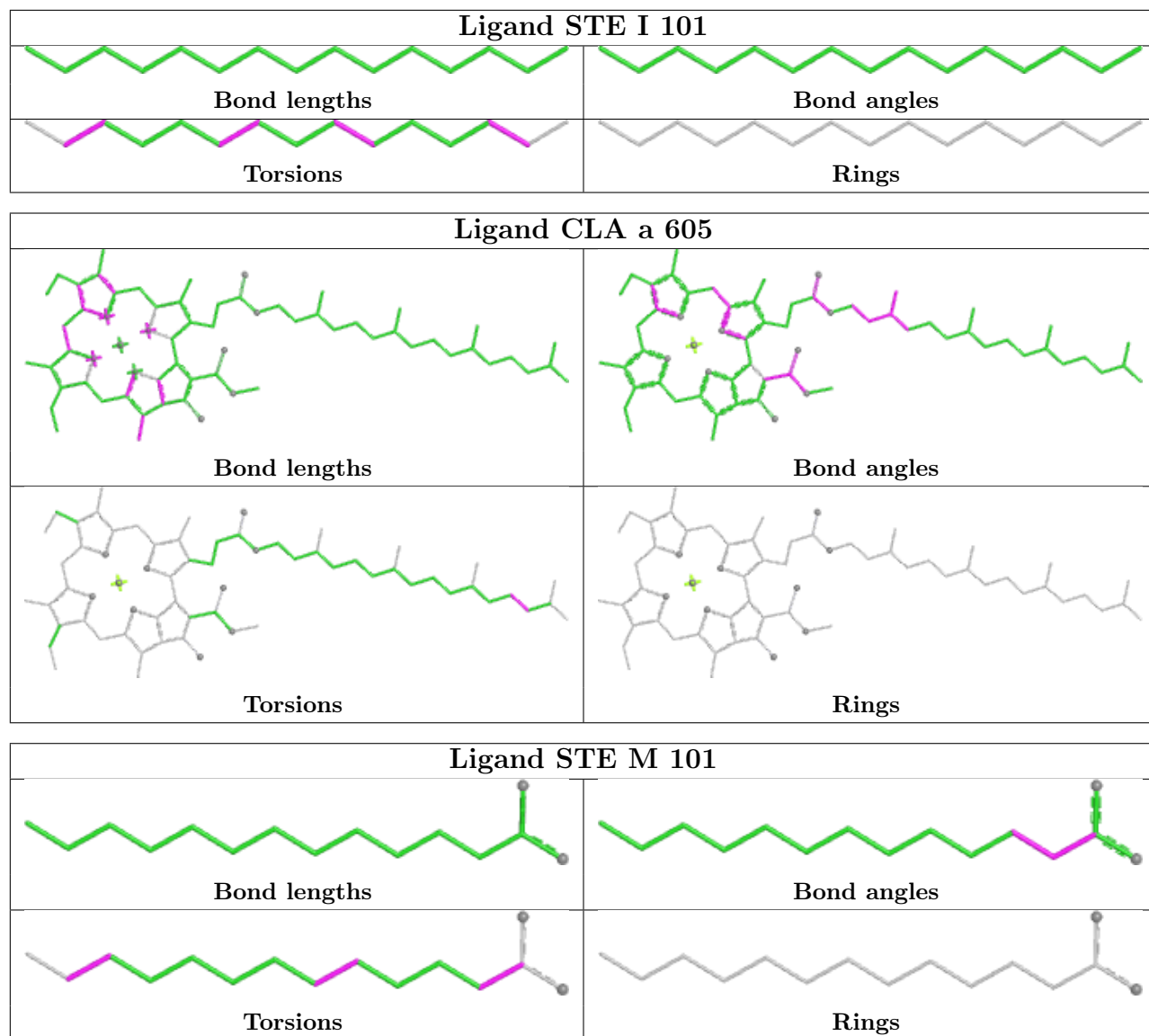


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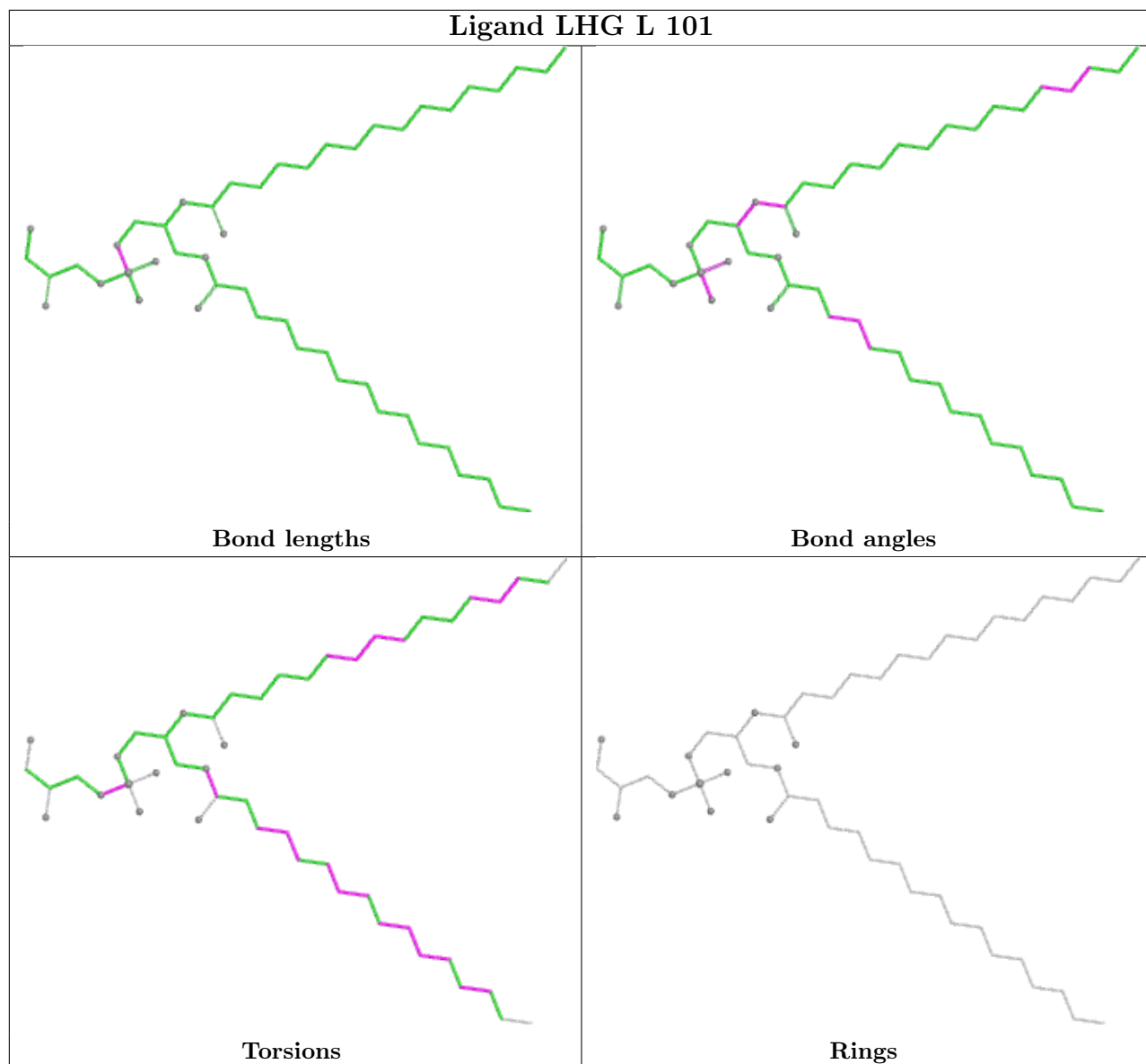




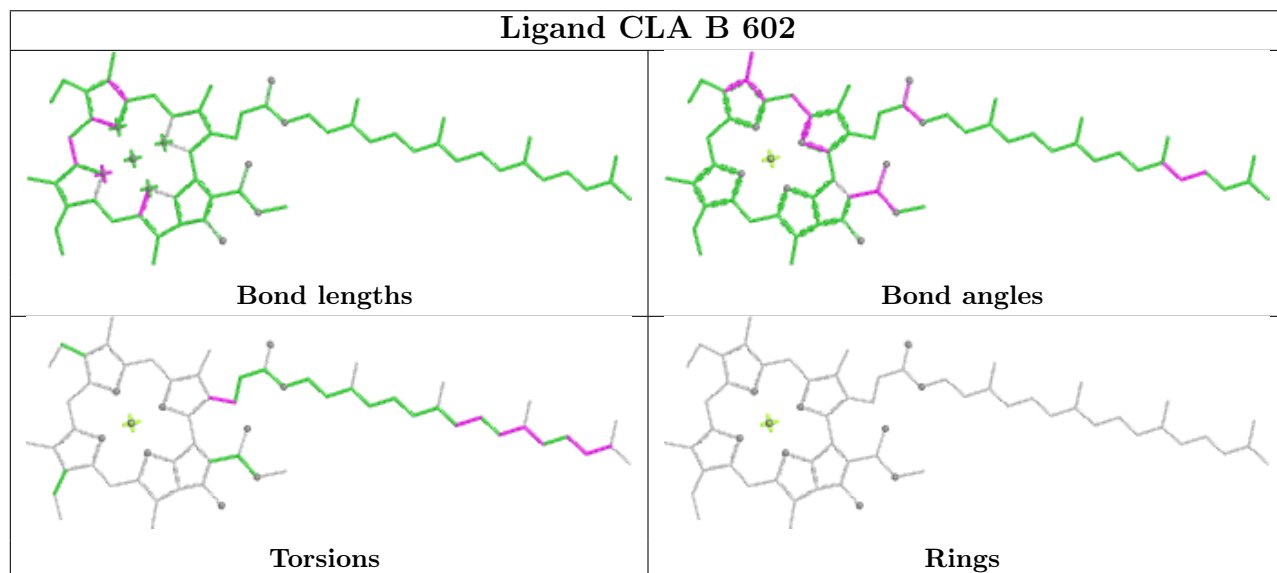




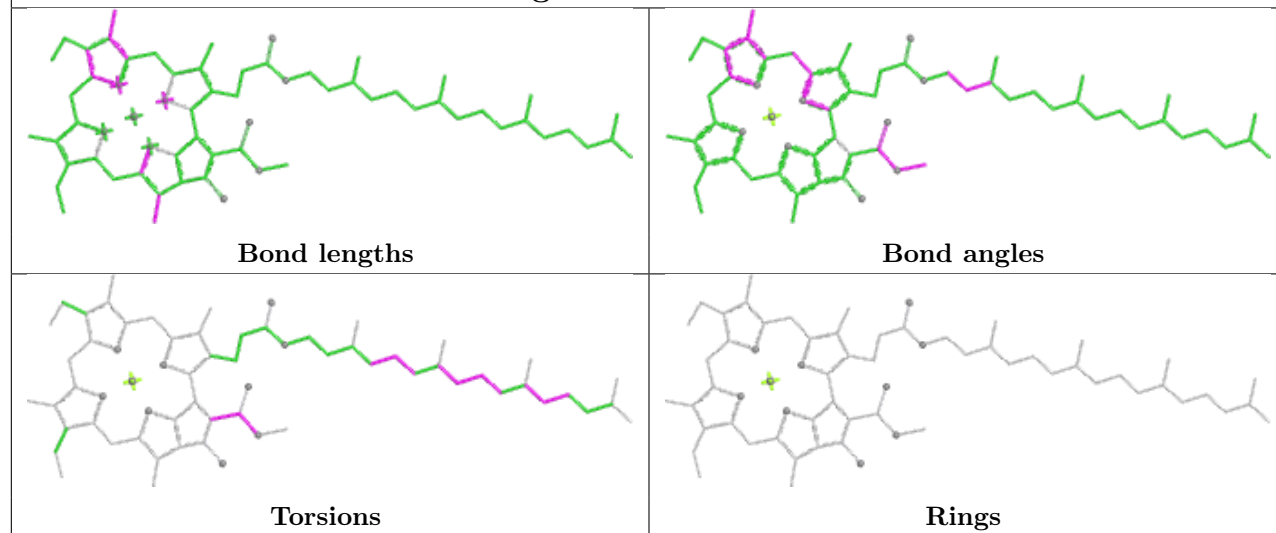
Ligand LHG L 101



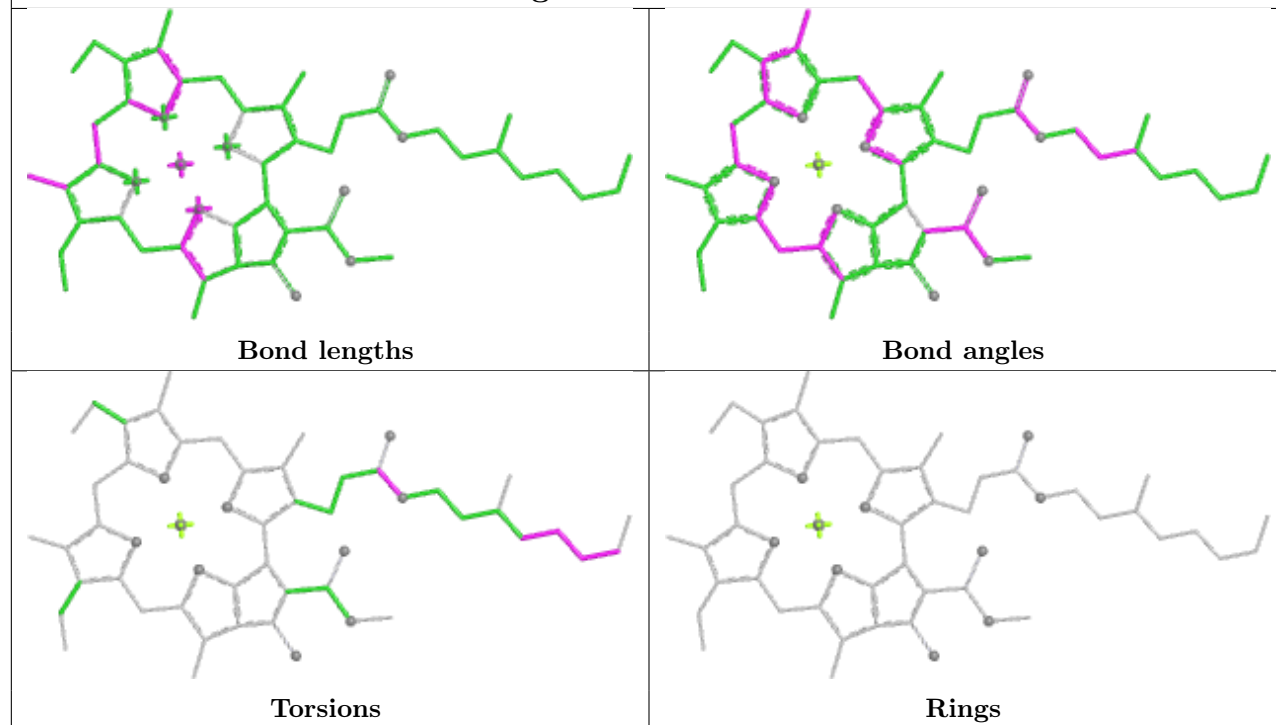
Ligand CLA B 602

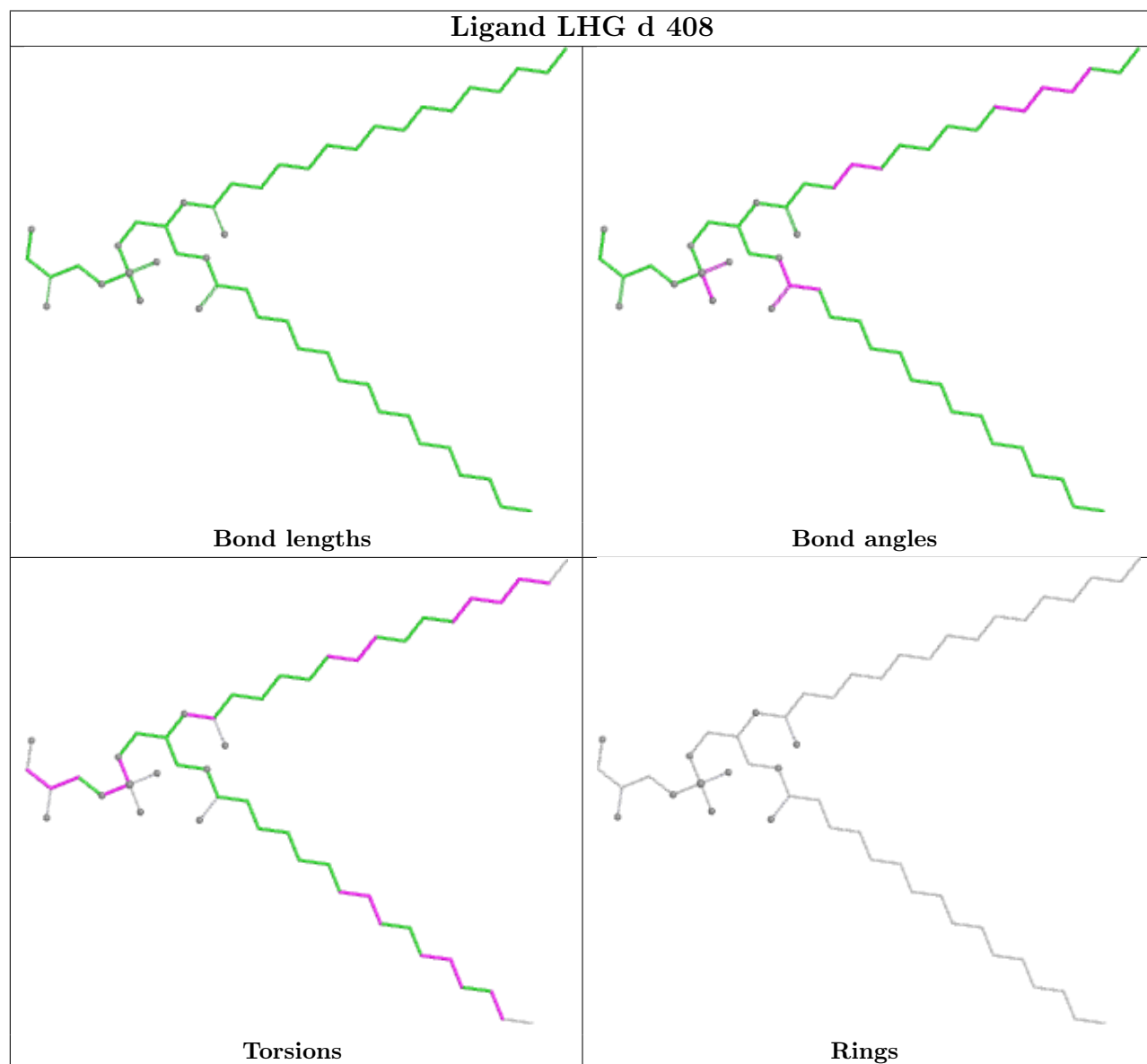
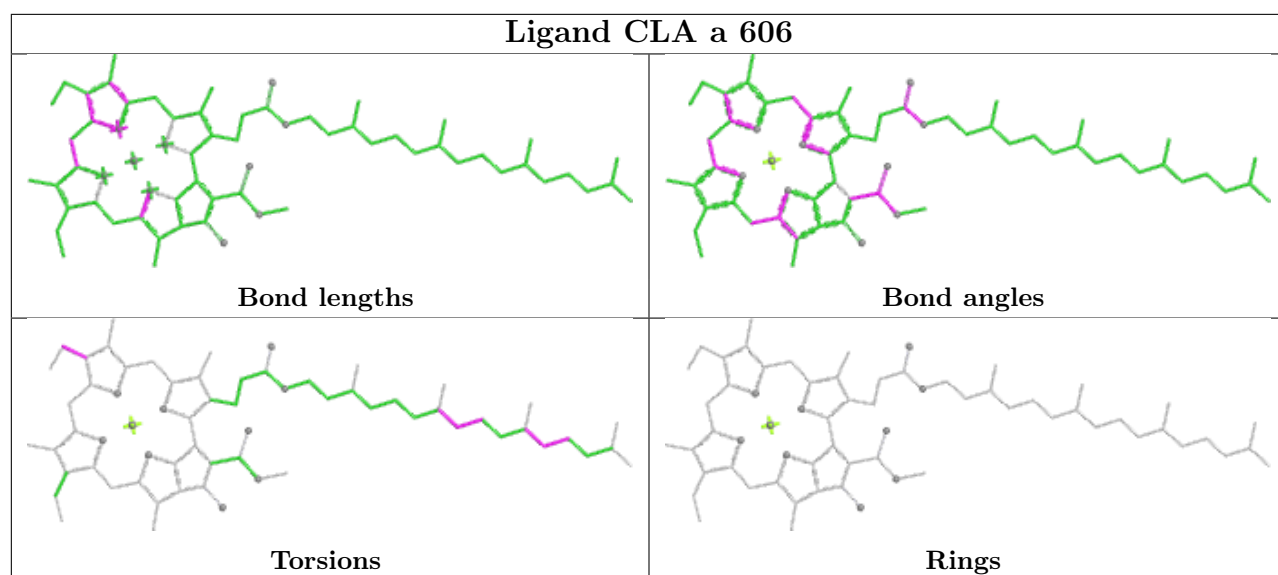


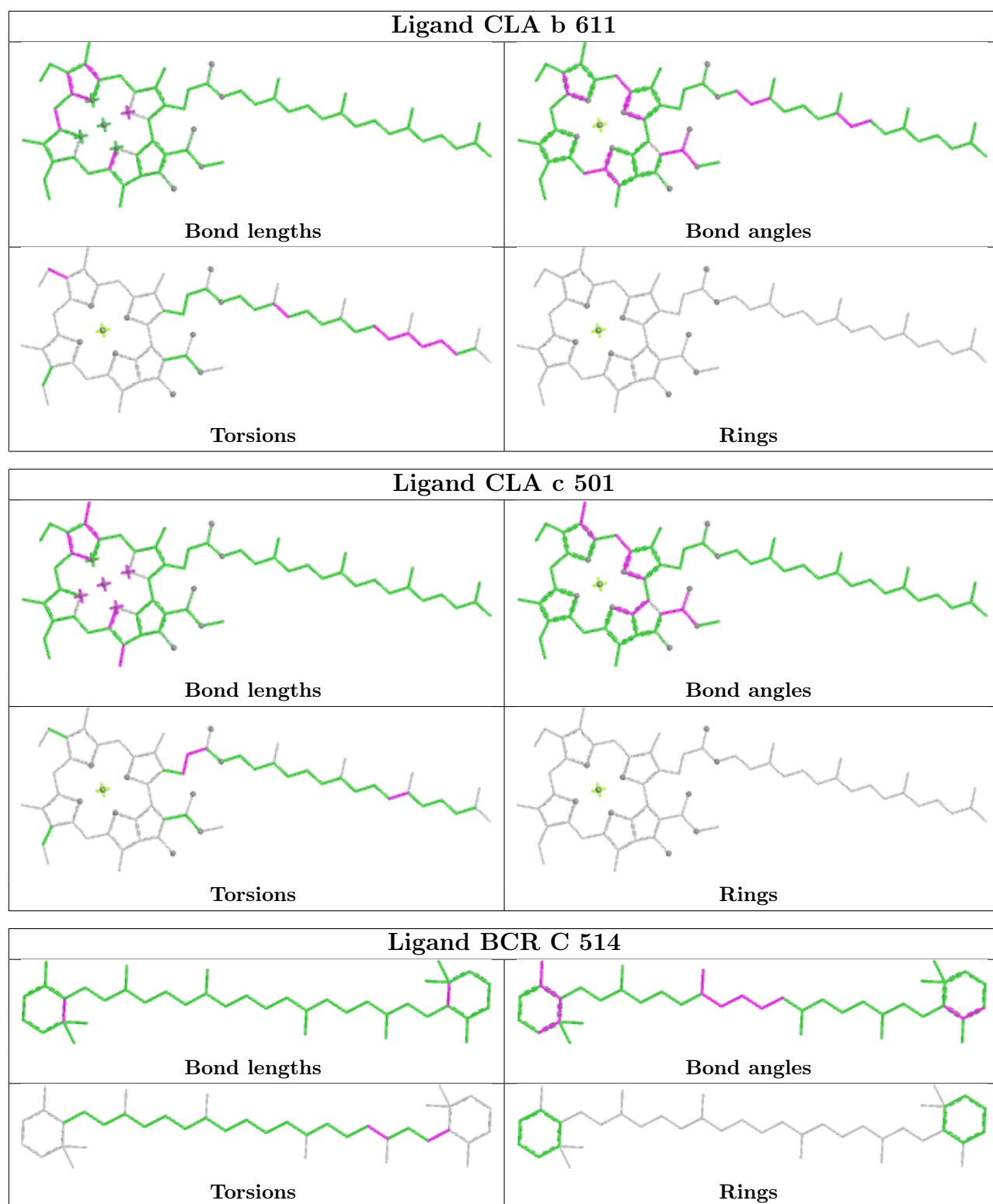
Ligand CLA C 509

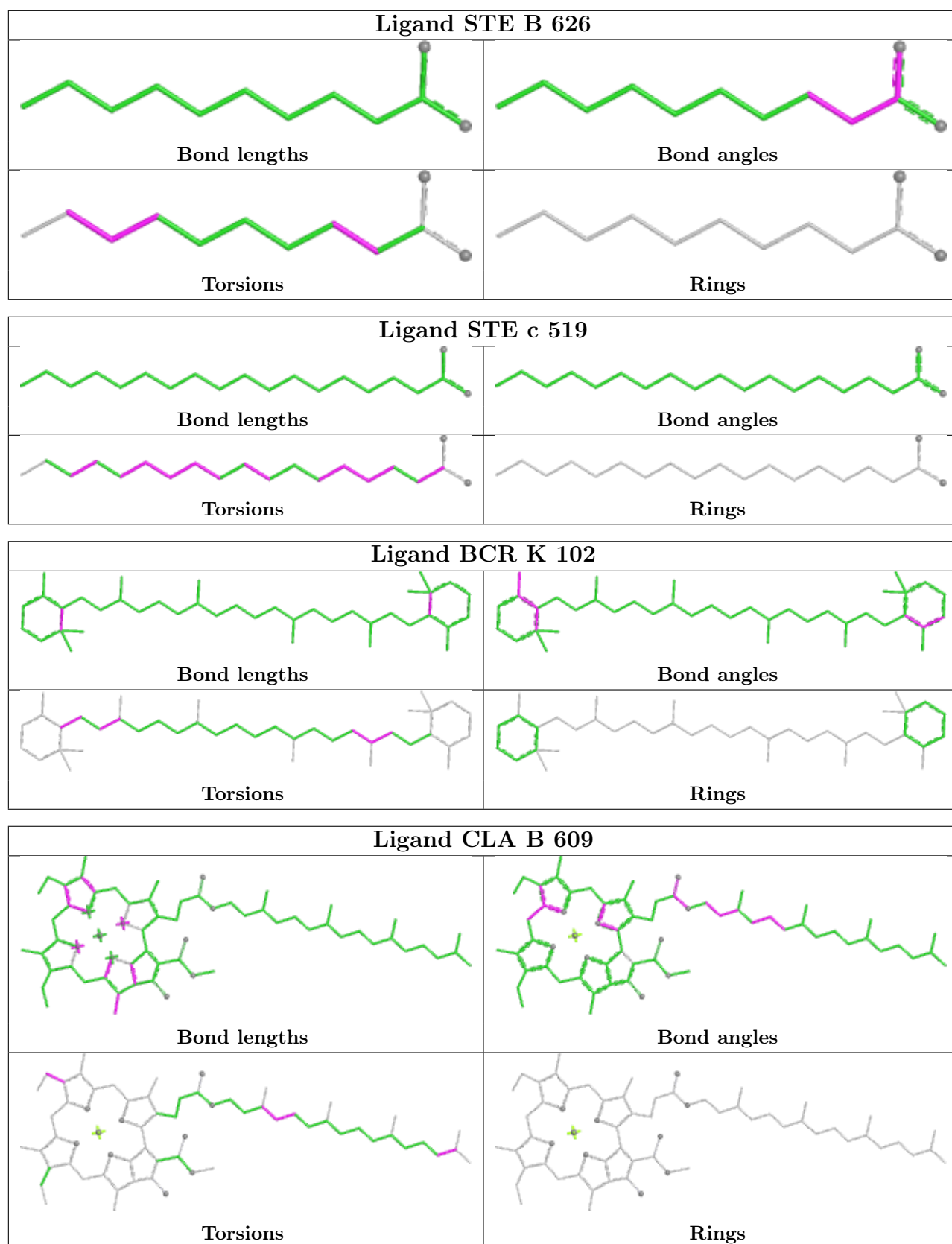


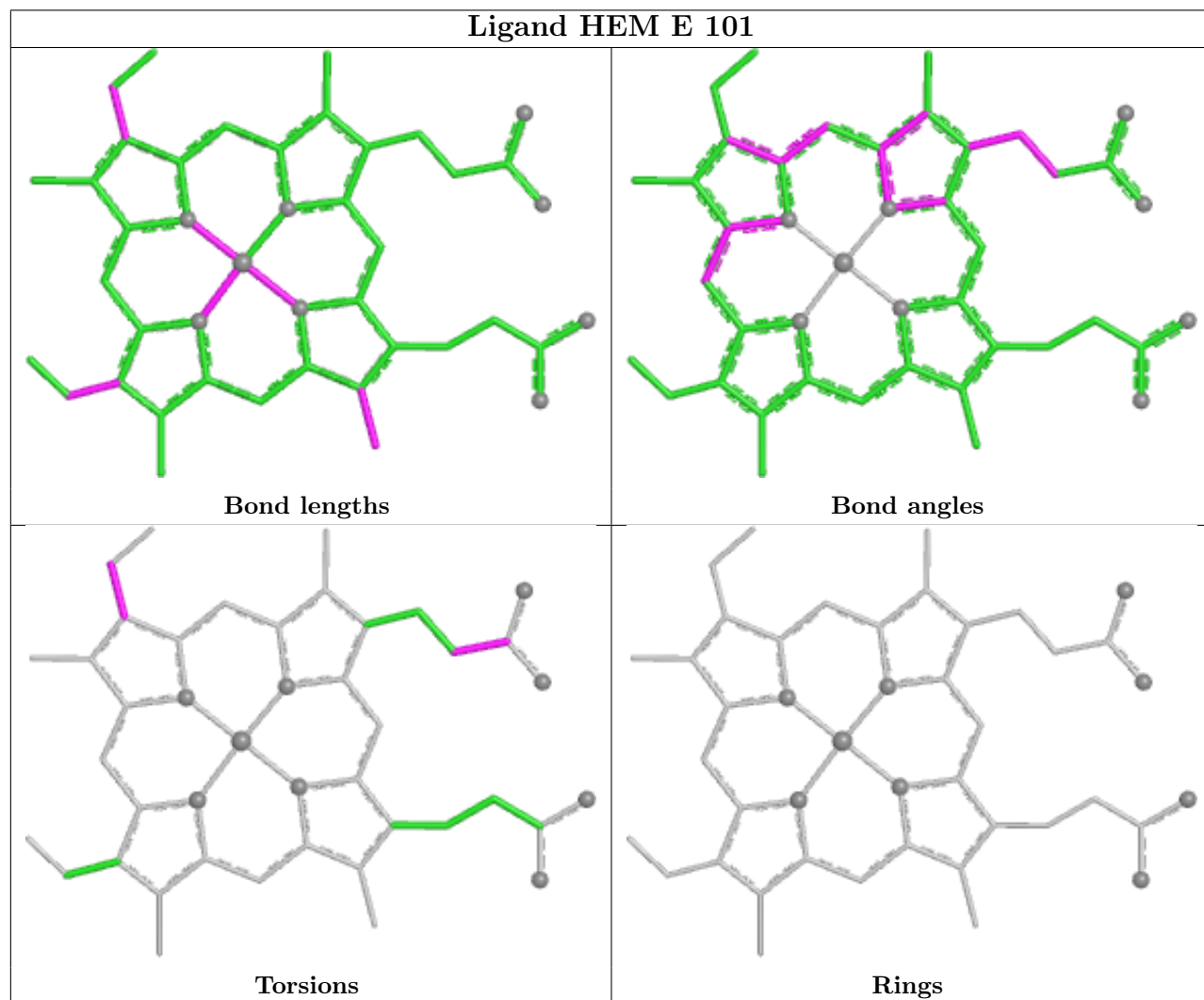
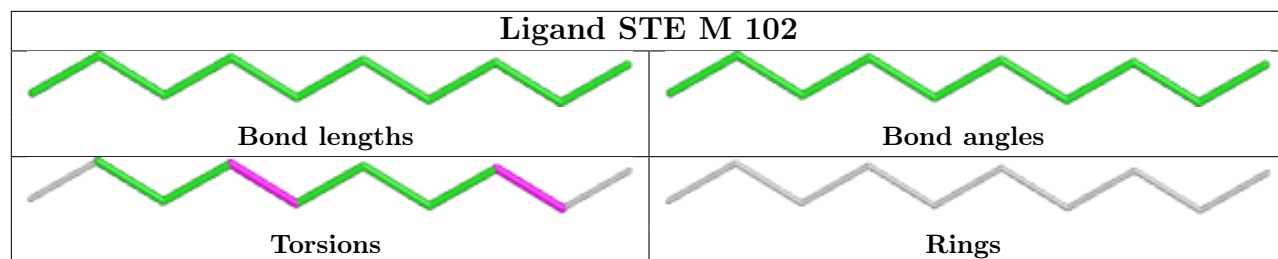
Ligand CLA A 608

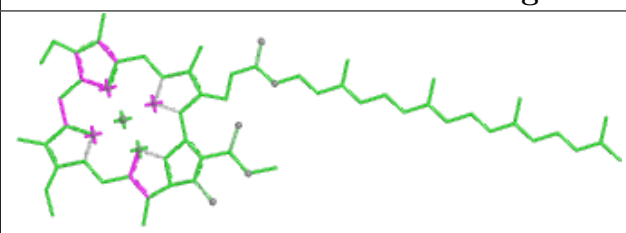
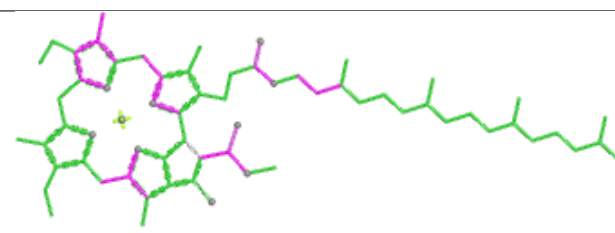
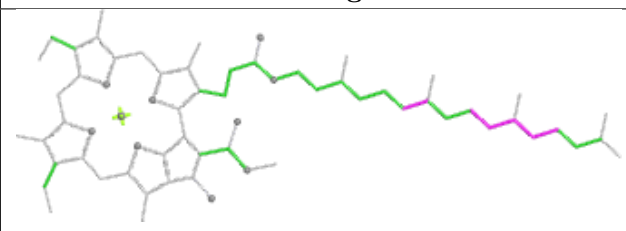
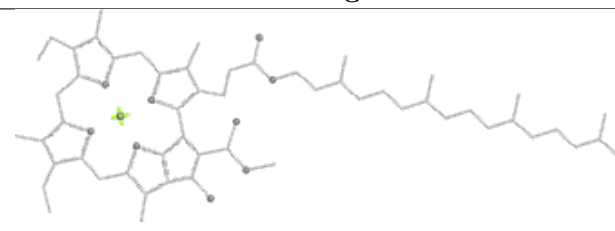


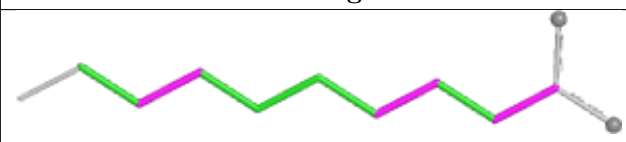
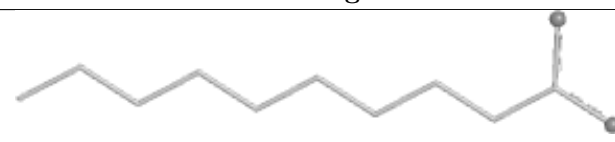


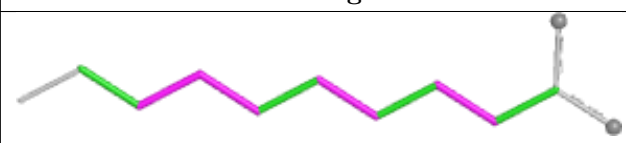
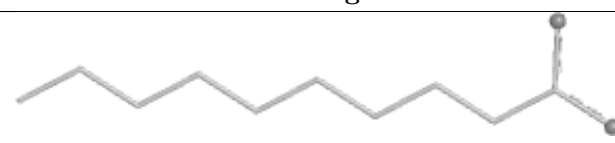


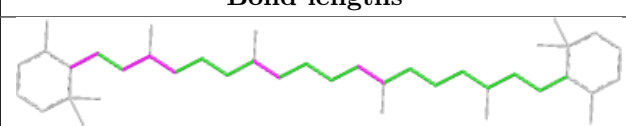
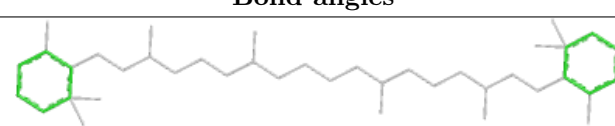




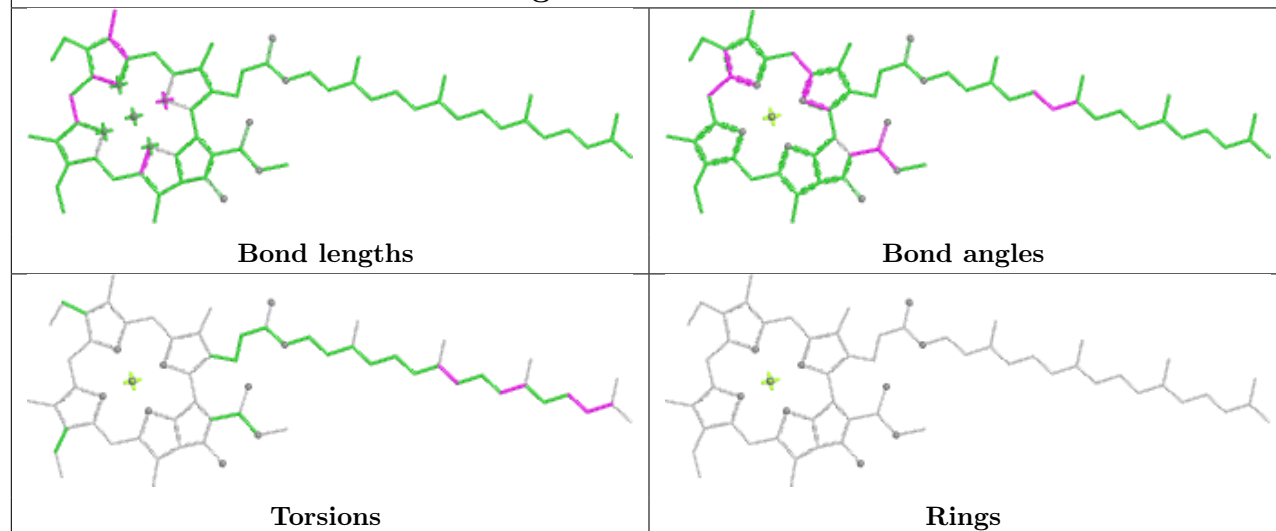
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE k 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

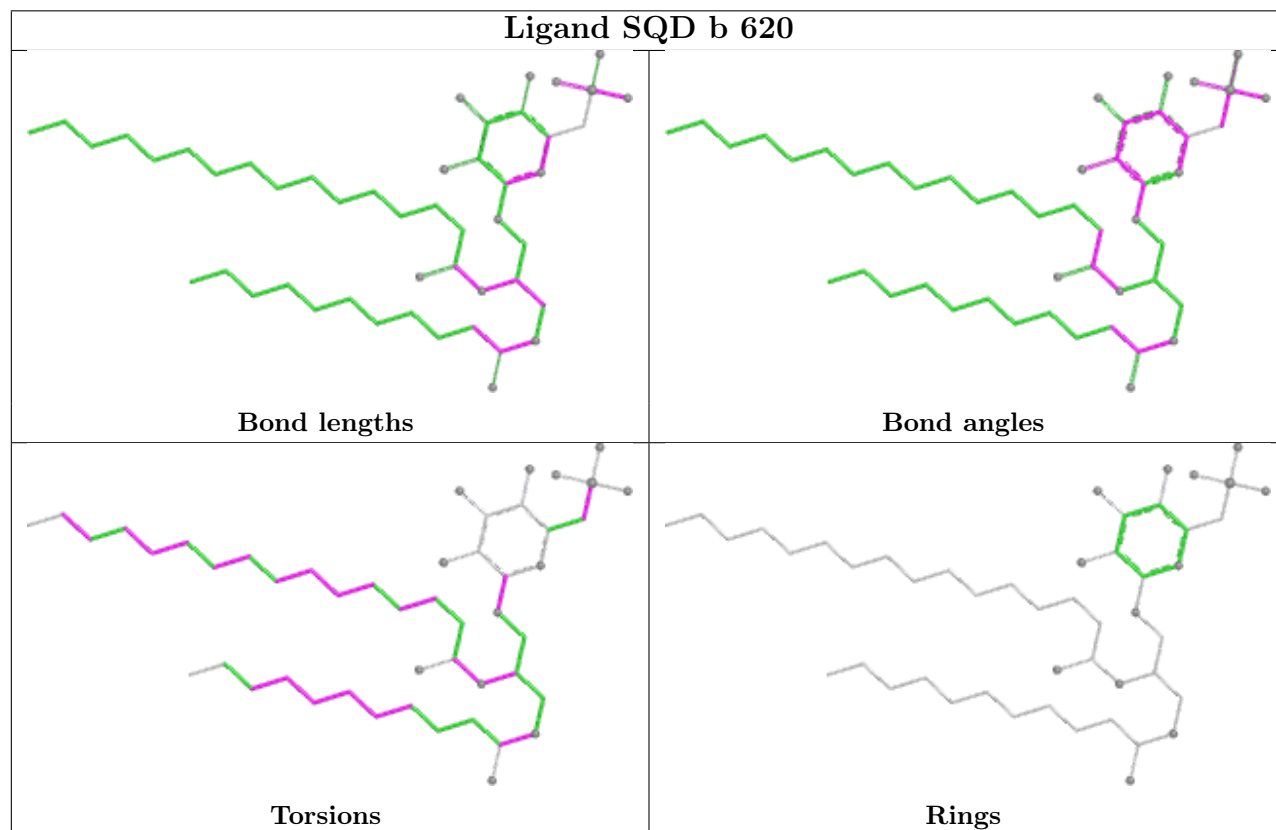
Ligand STE L 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

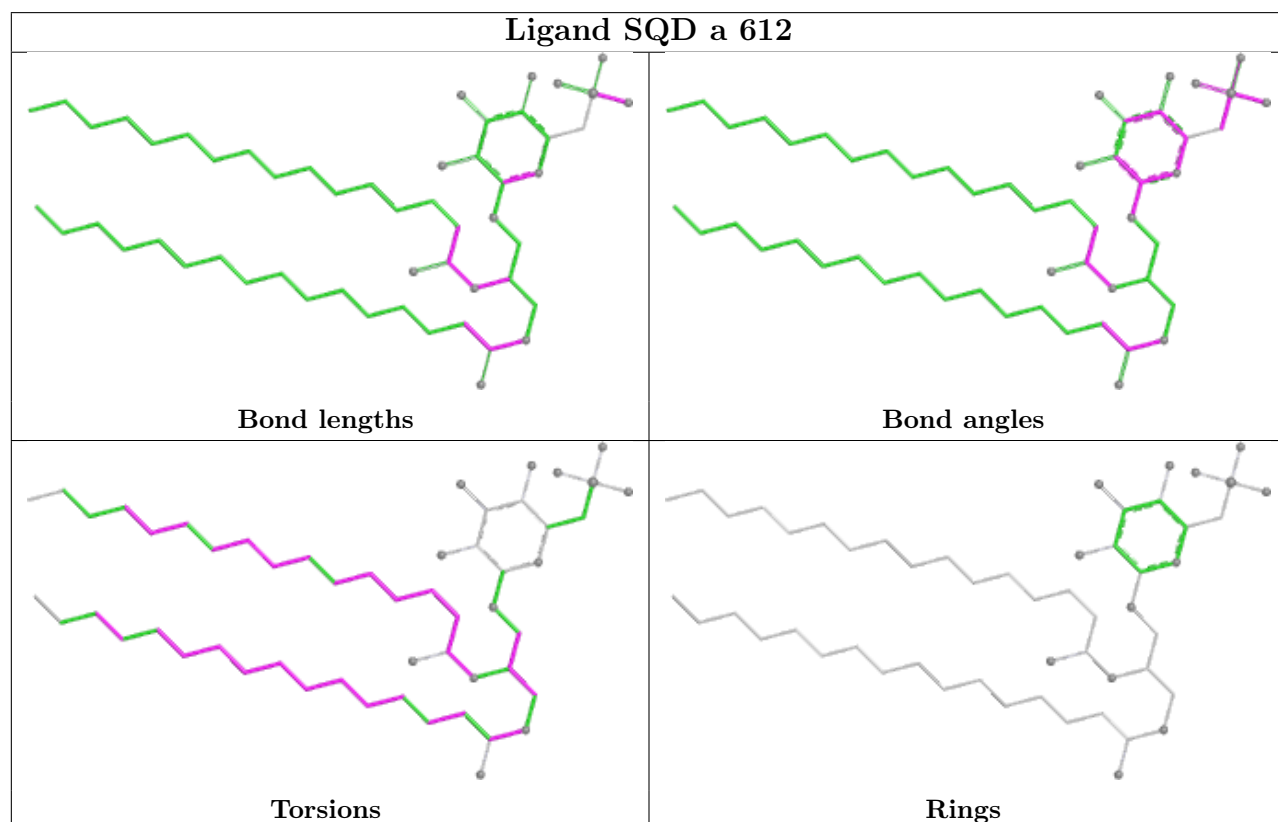
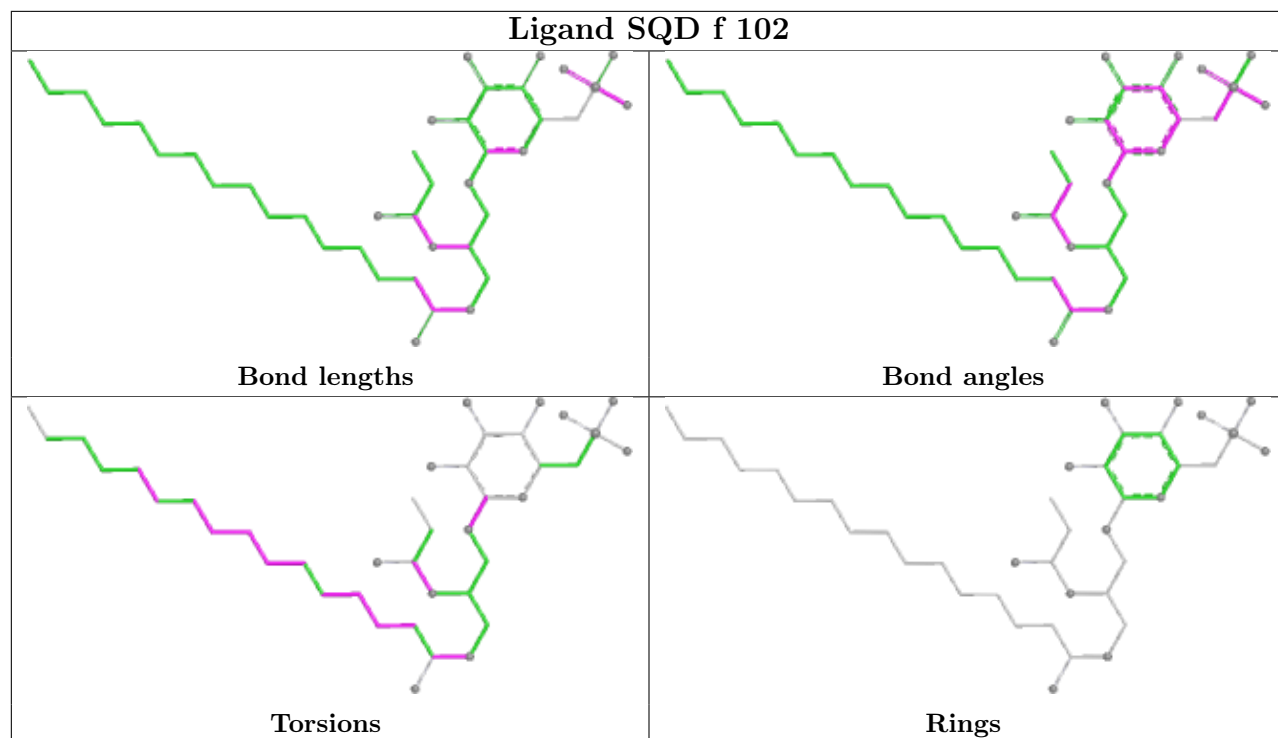
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 615

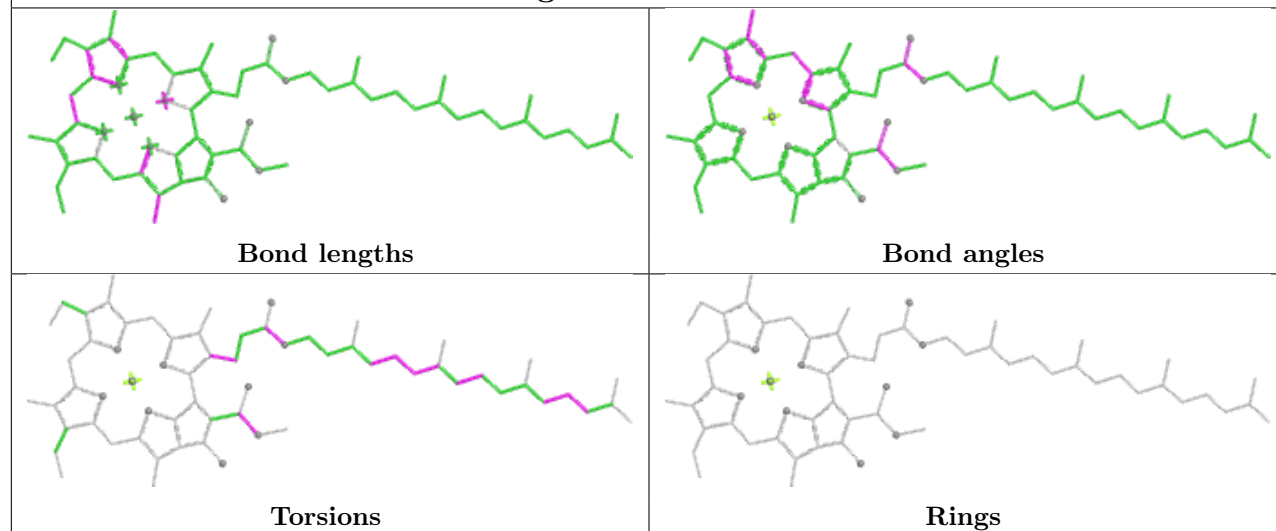


Ligand SQD b 620

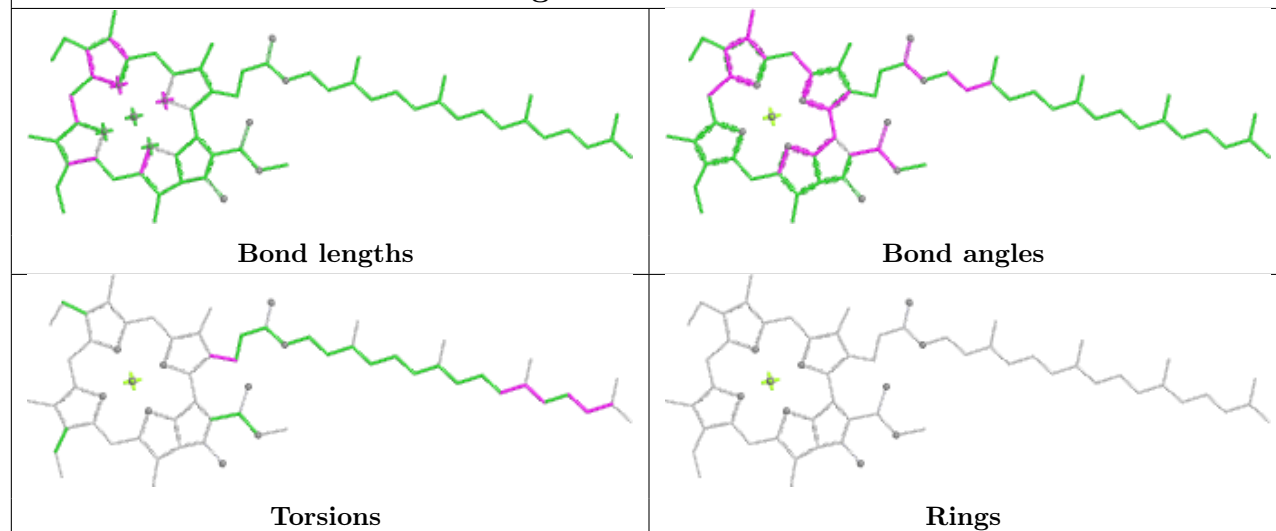




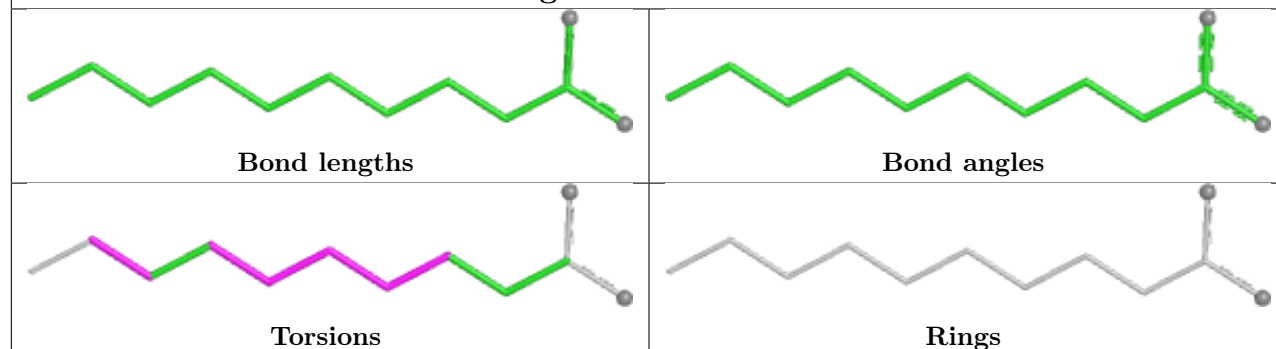
Ligand CLA c 513



Ligand CLA A 607

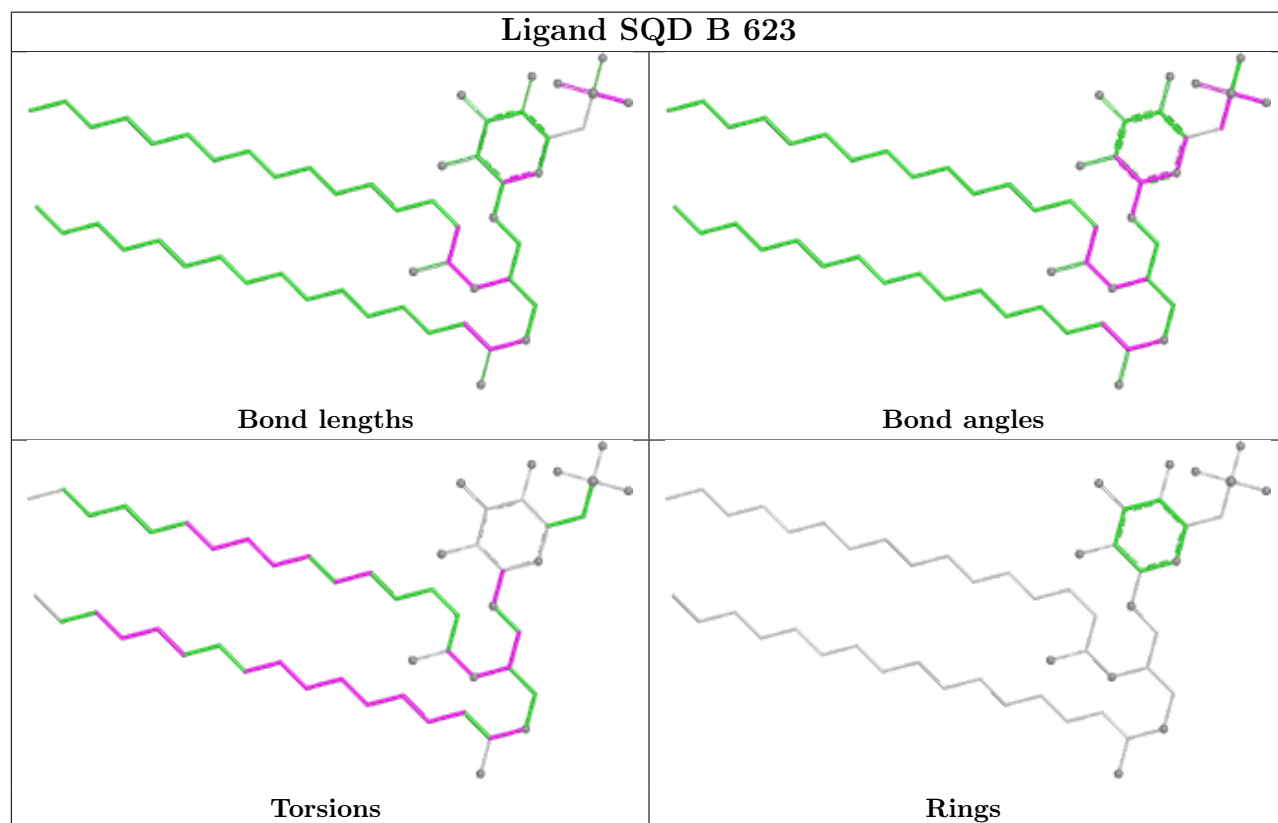
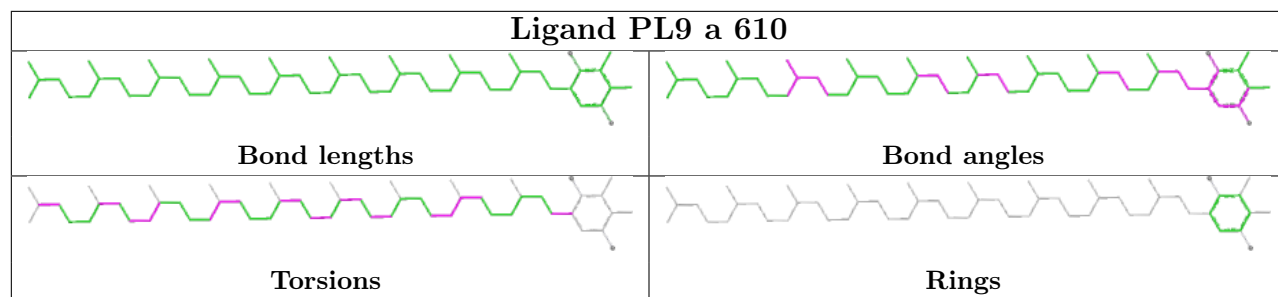


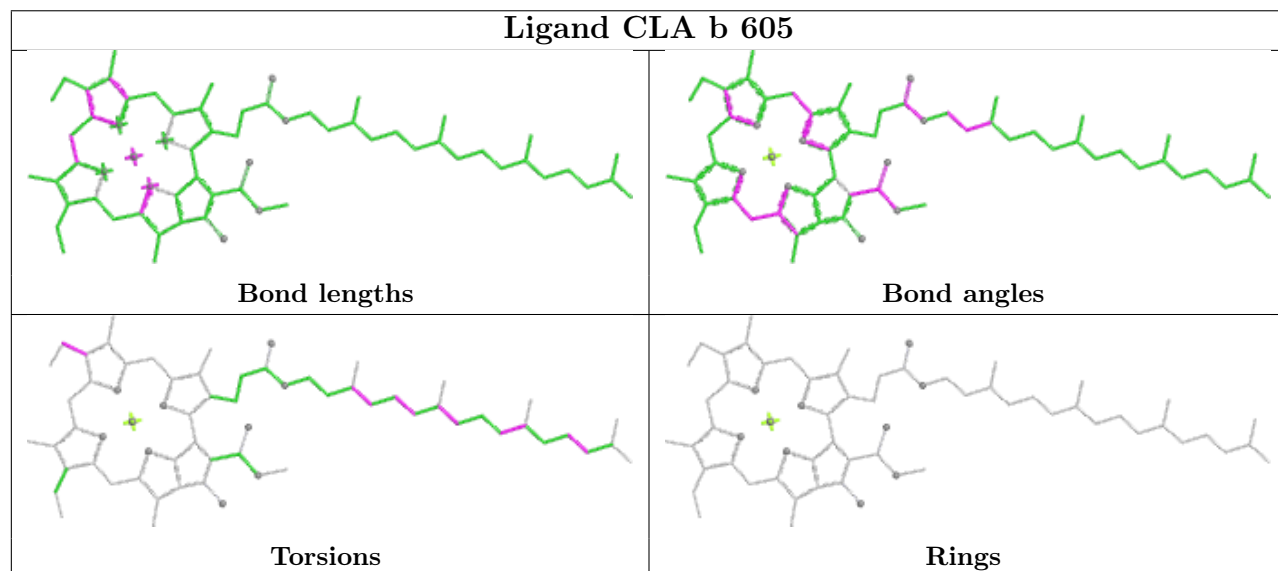
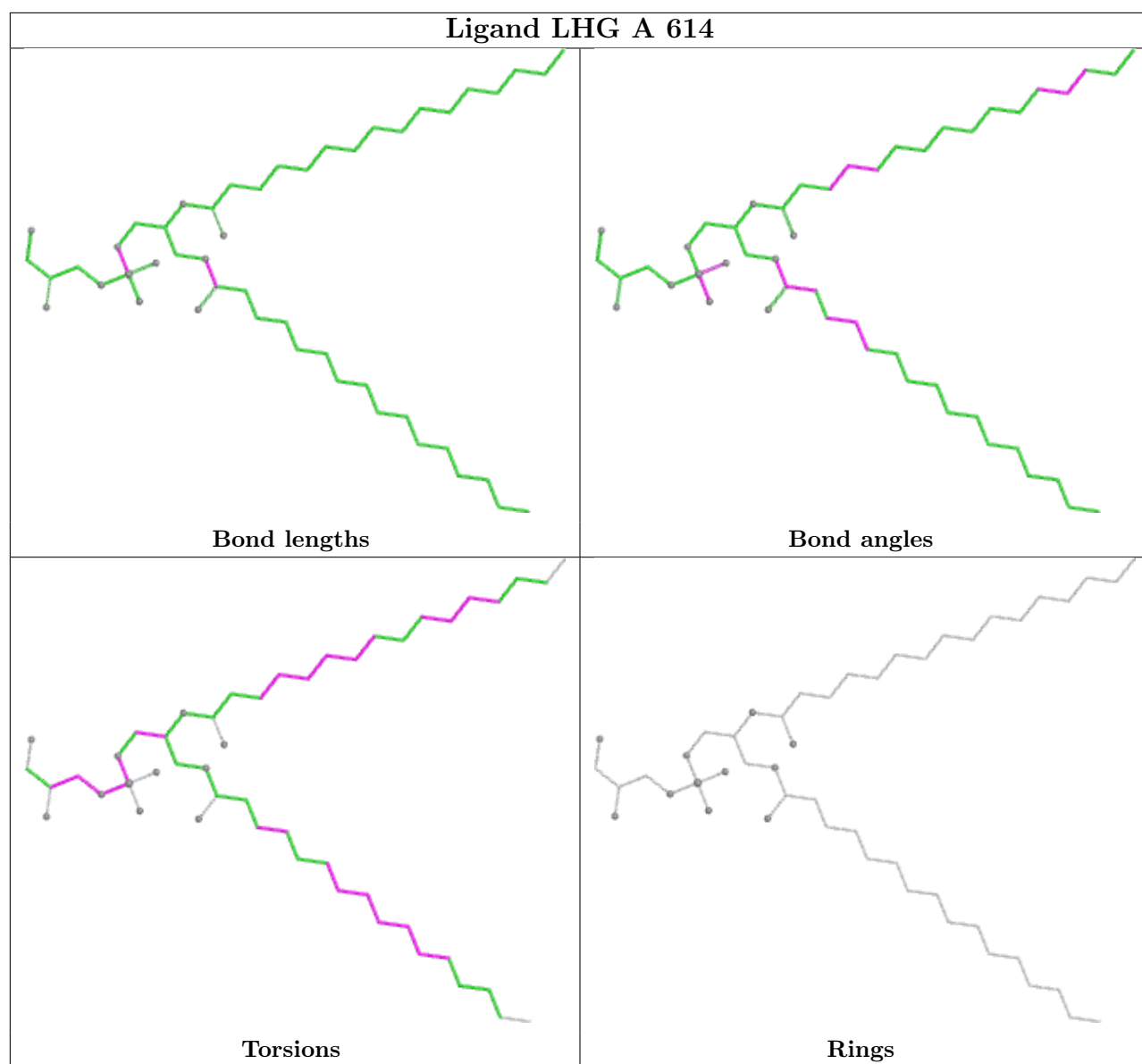
Ligand STE a 615



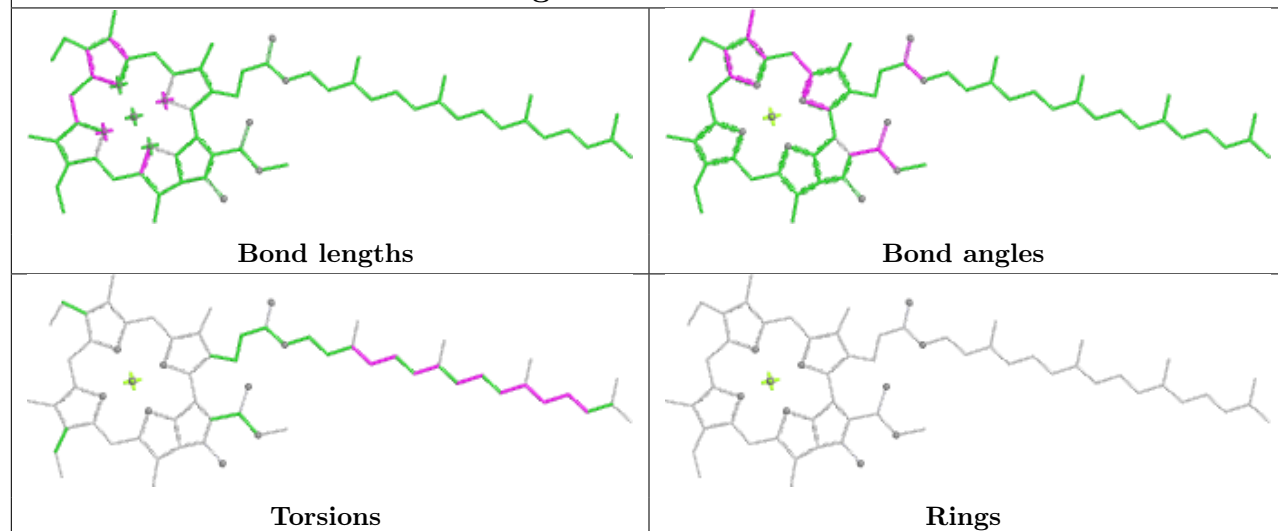
Ligand STE m 102



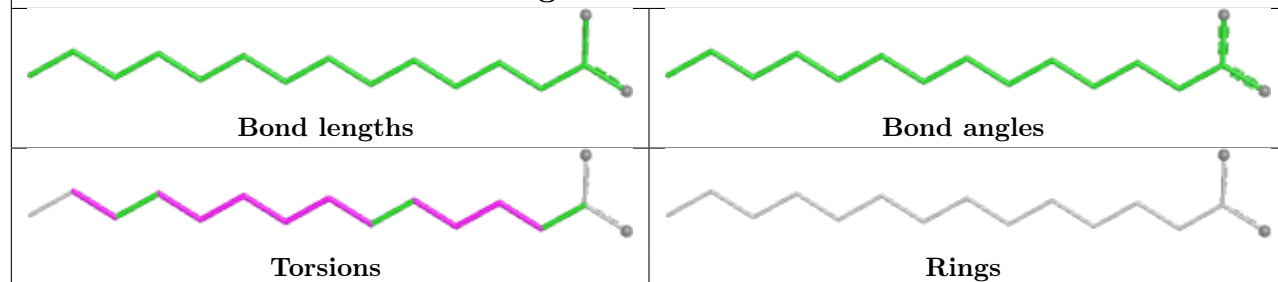




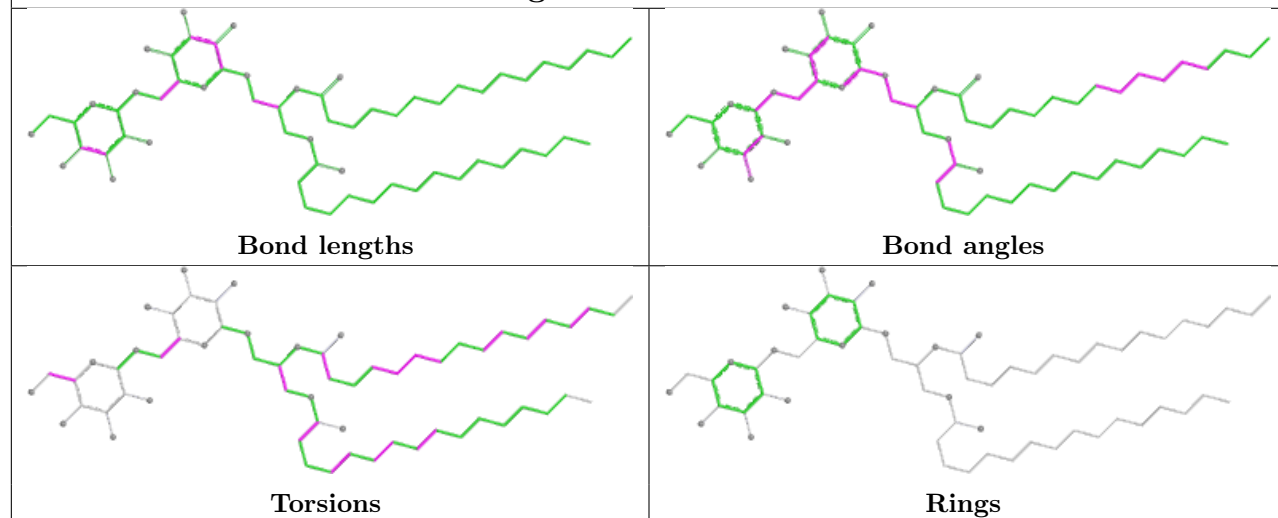
Ligand CLA C 506



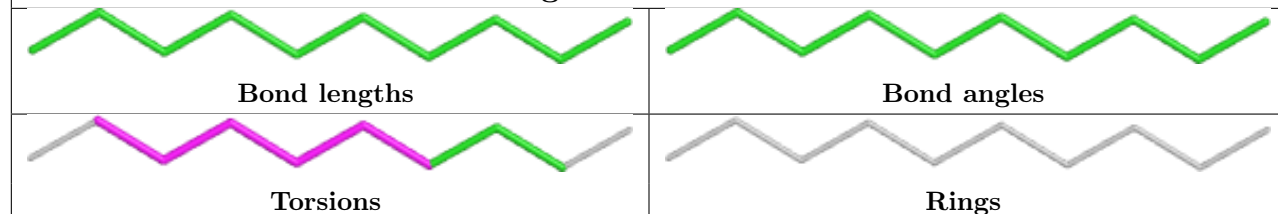
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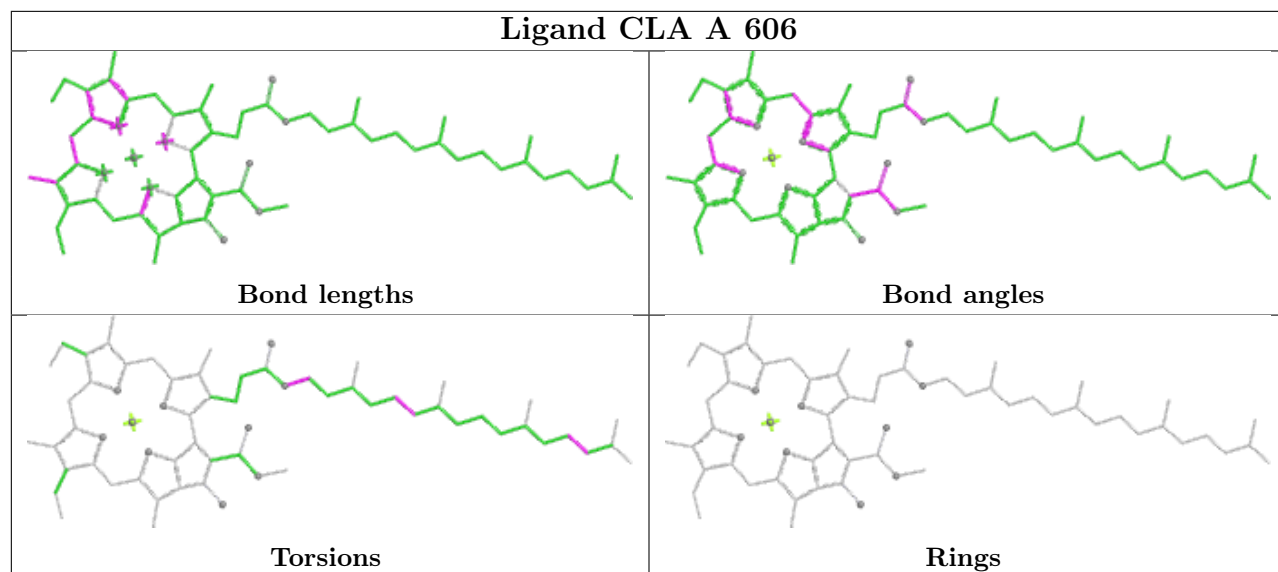
Ligand DGD C 515



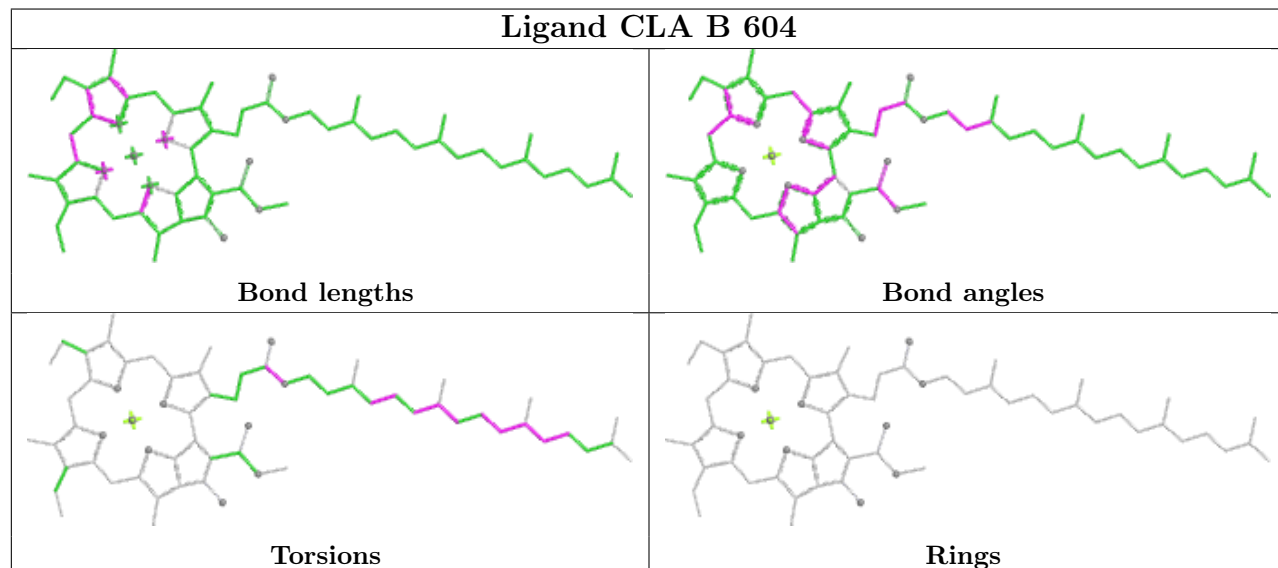
Ligand STE t 103



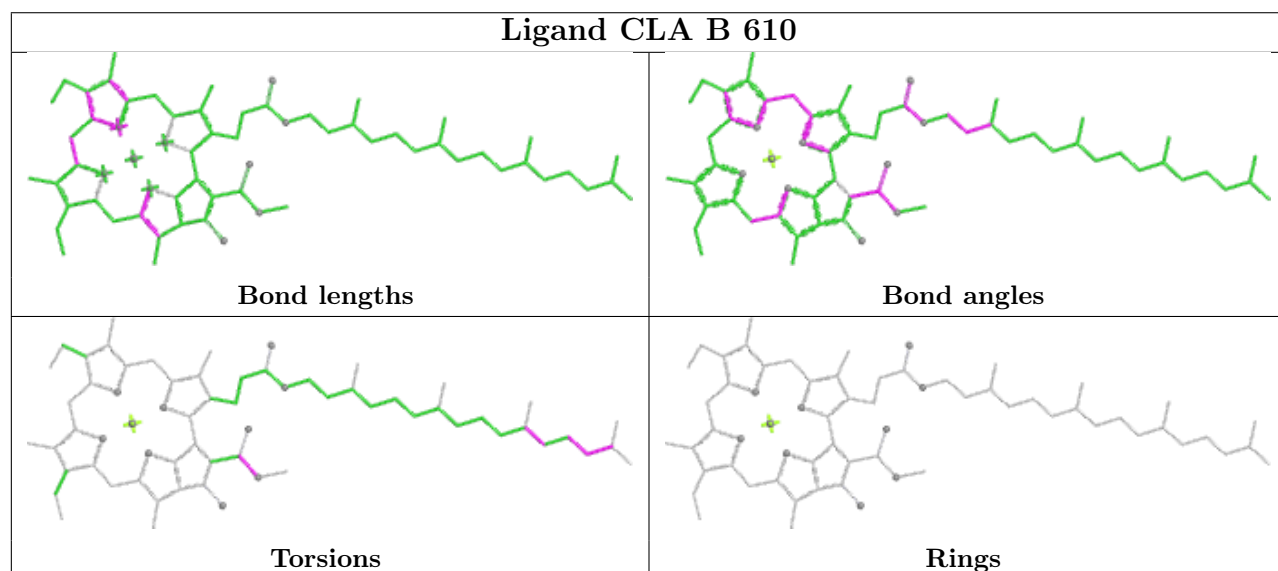
Ligand CLA A 606

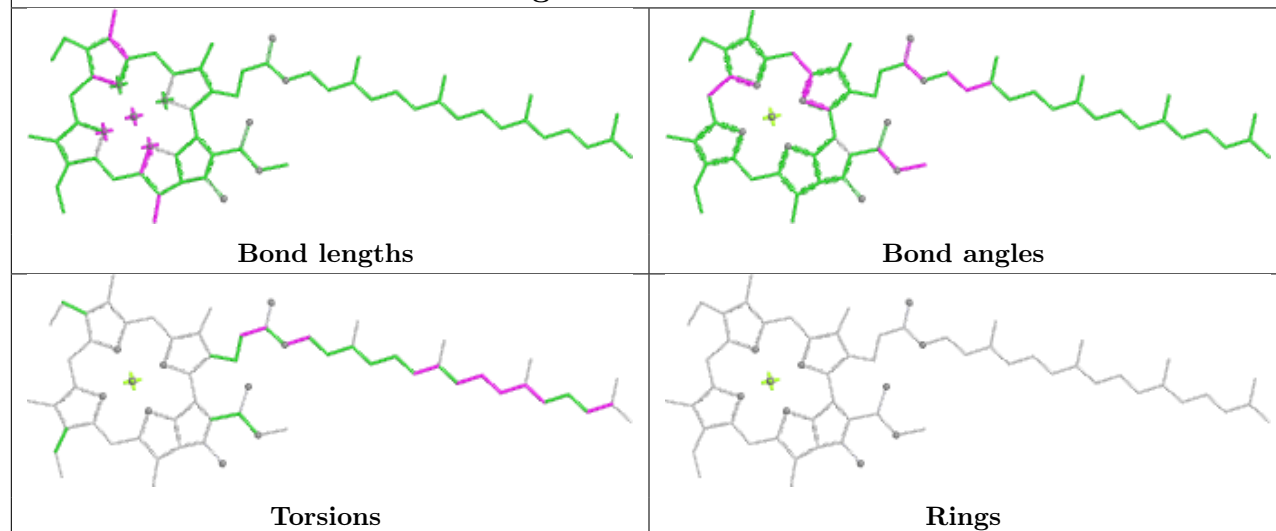
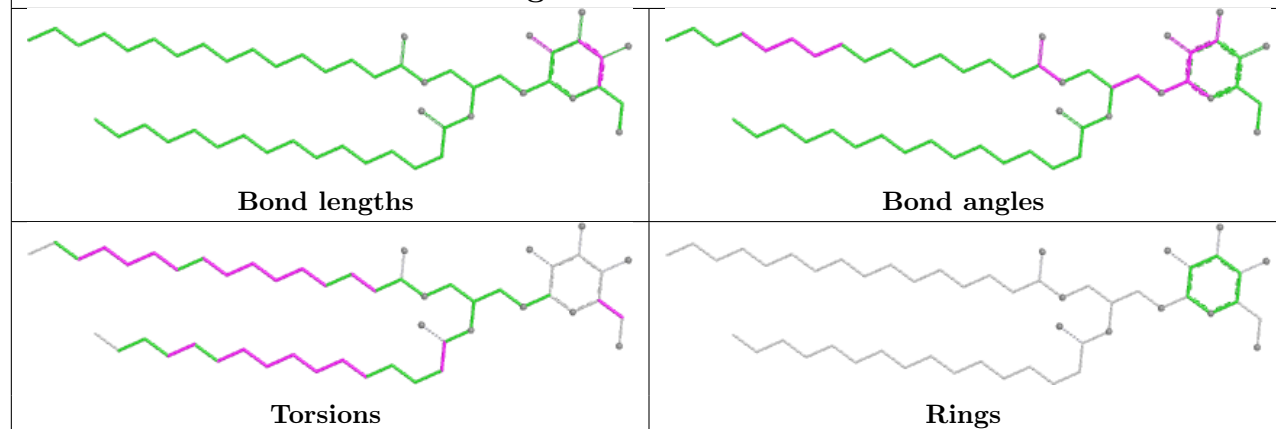


Ligand CLA B 604

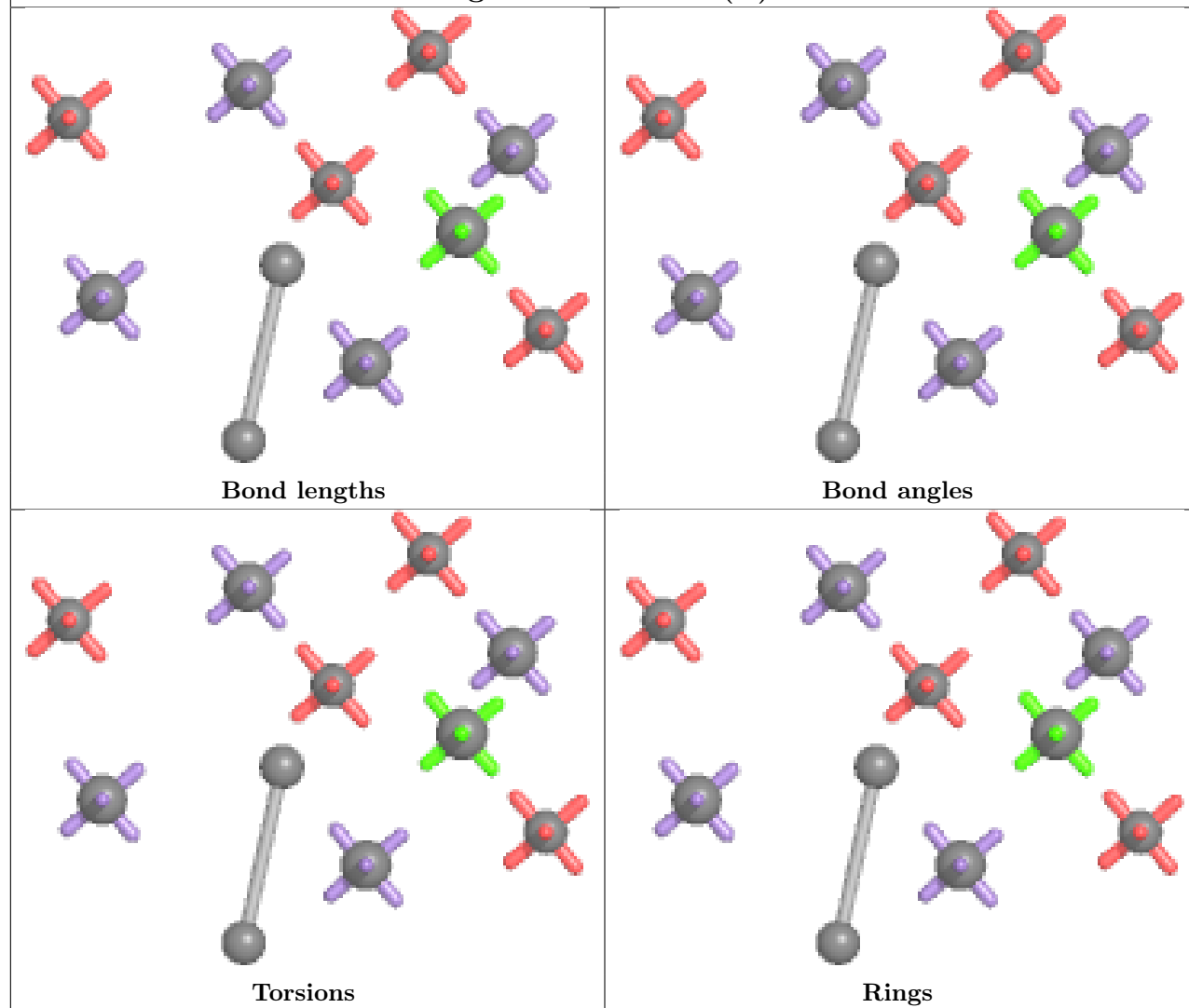


Ligand CLA B 610

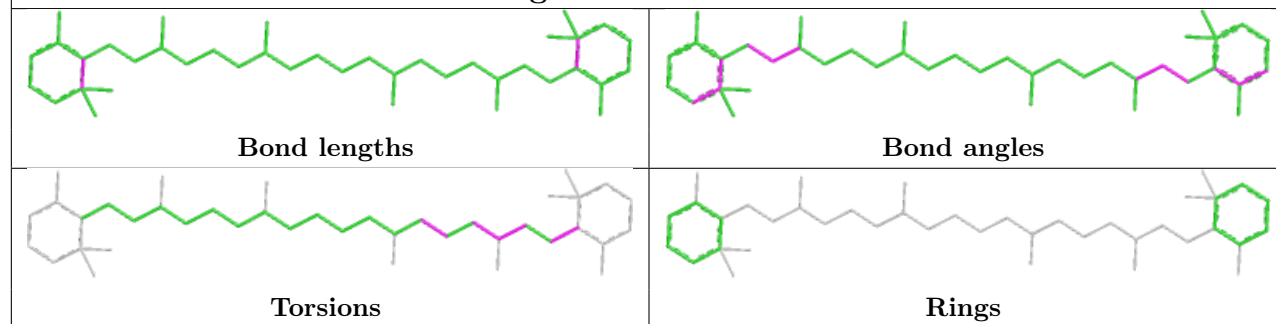


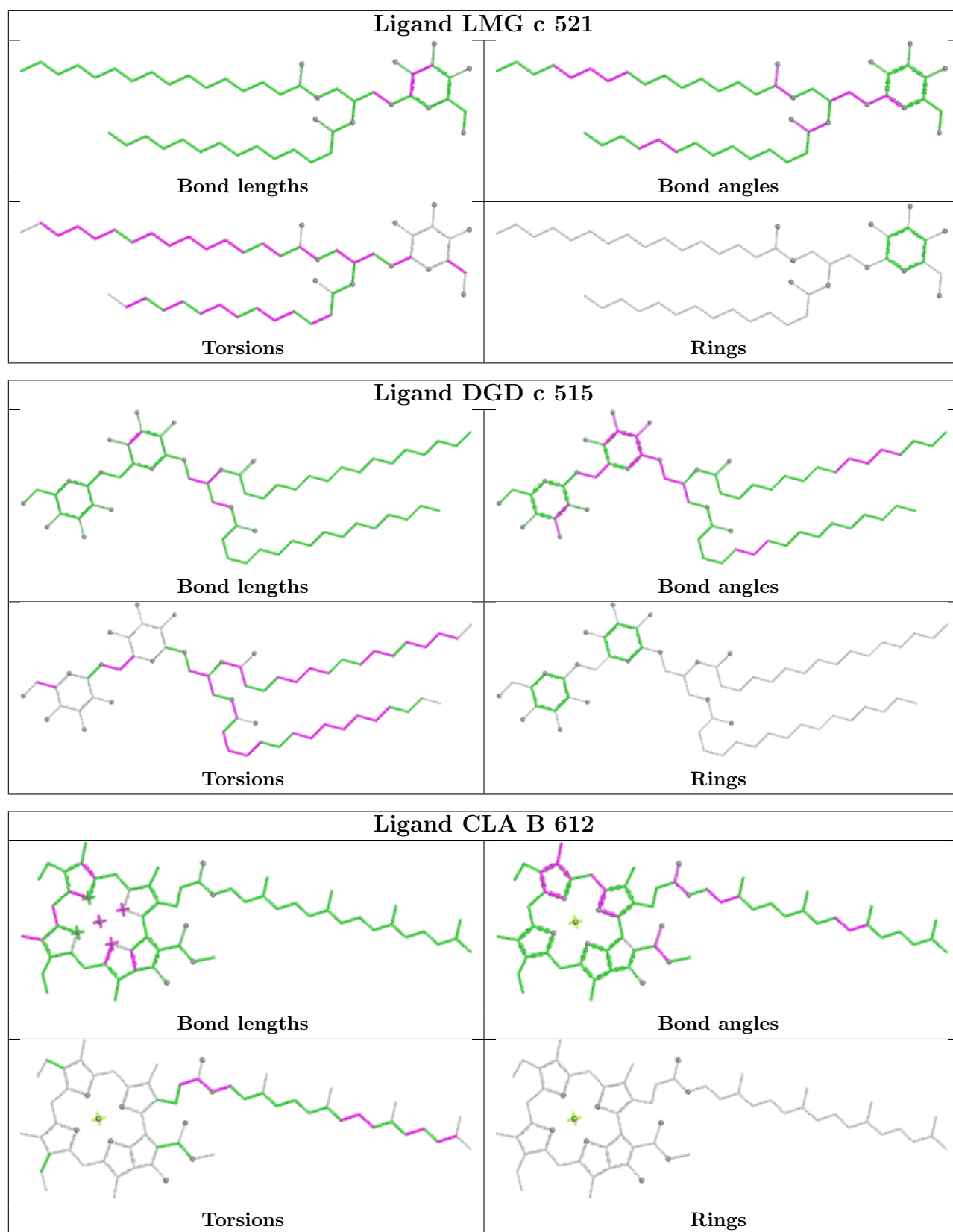
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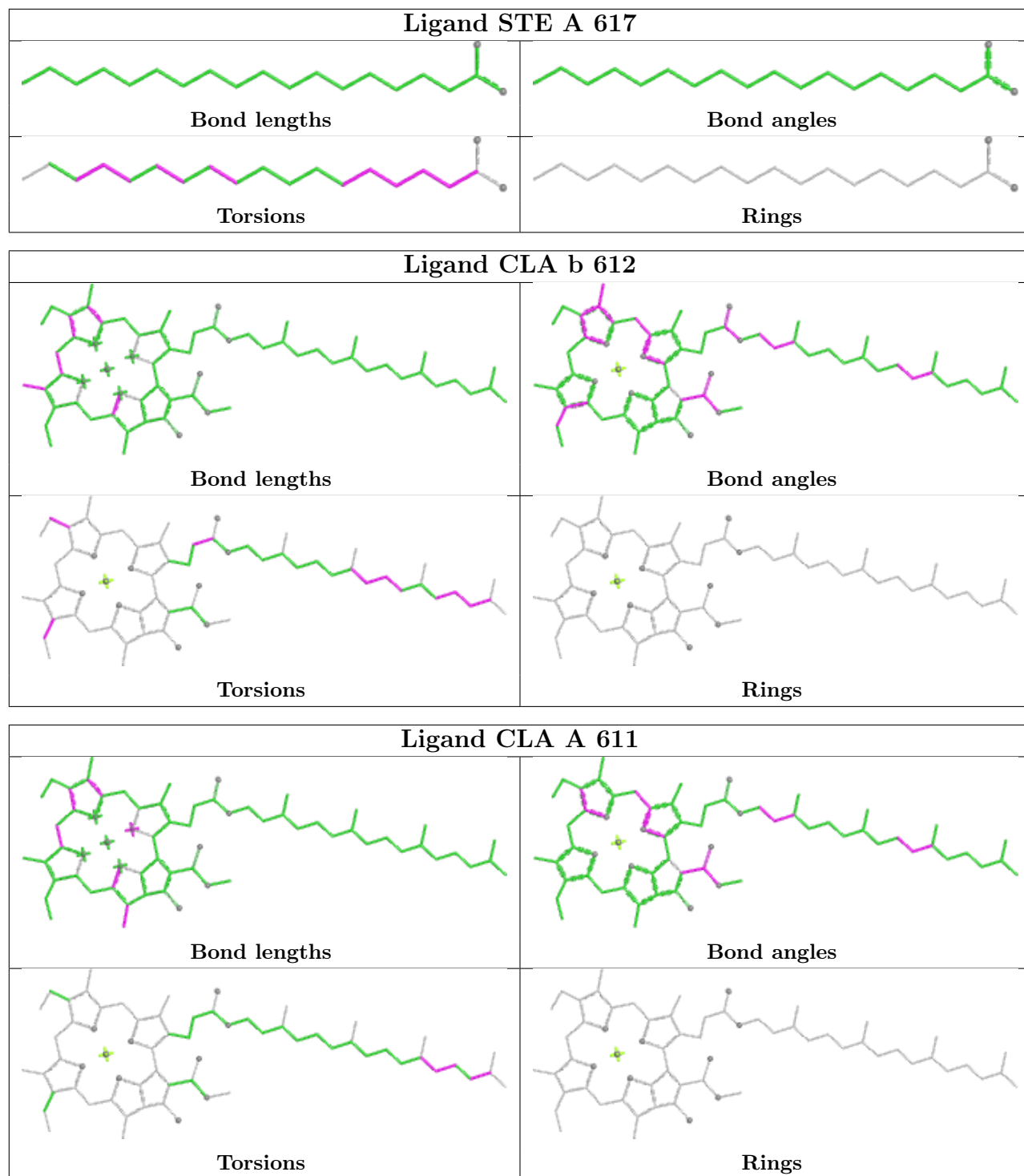
Ligand OEY a 601 (B)

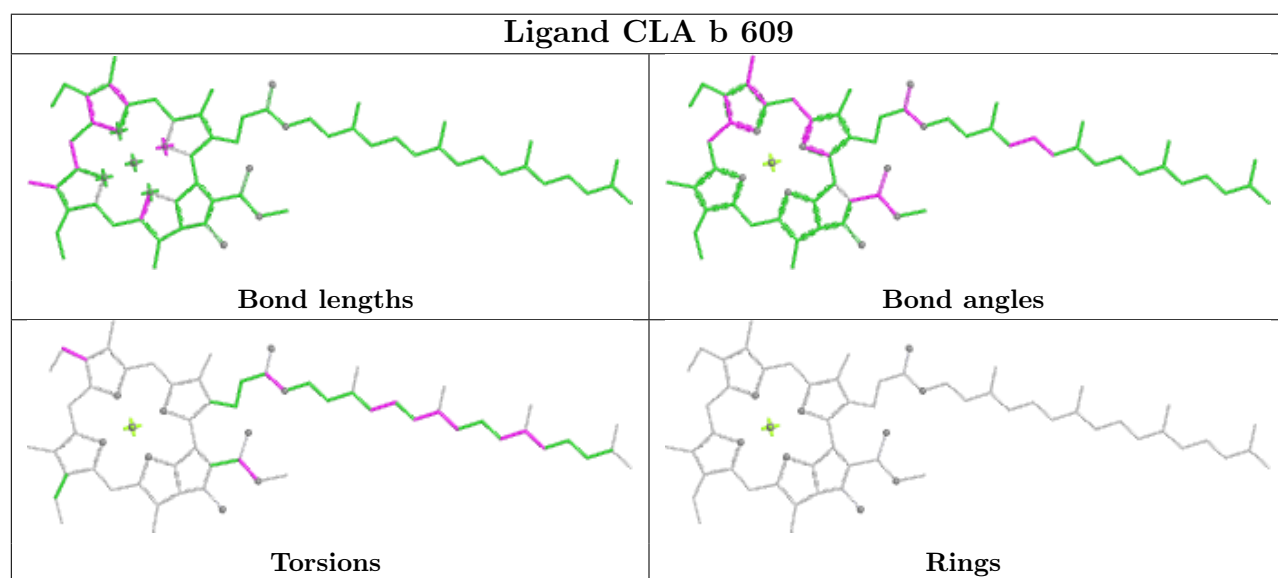
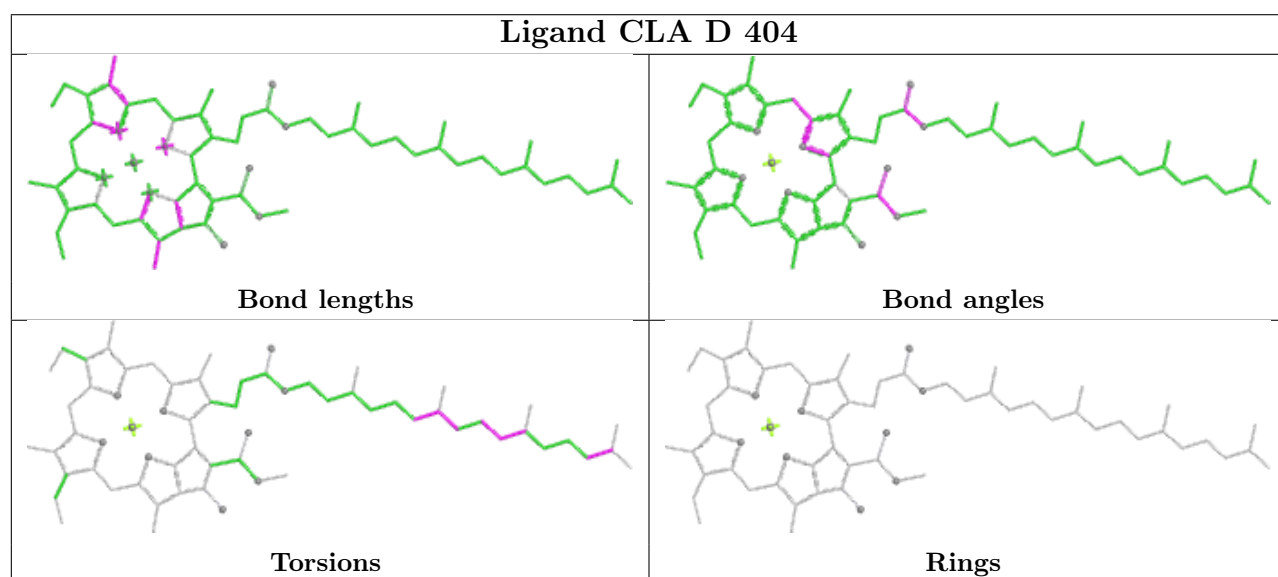
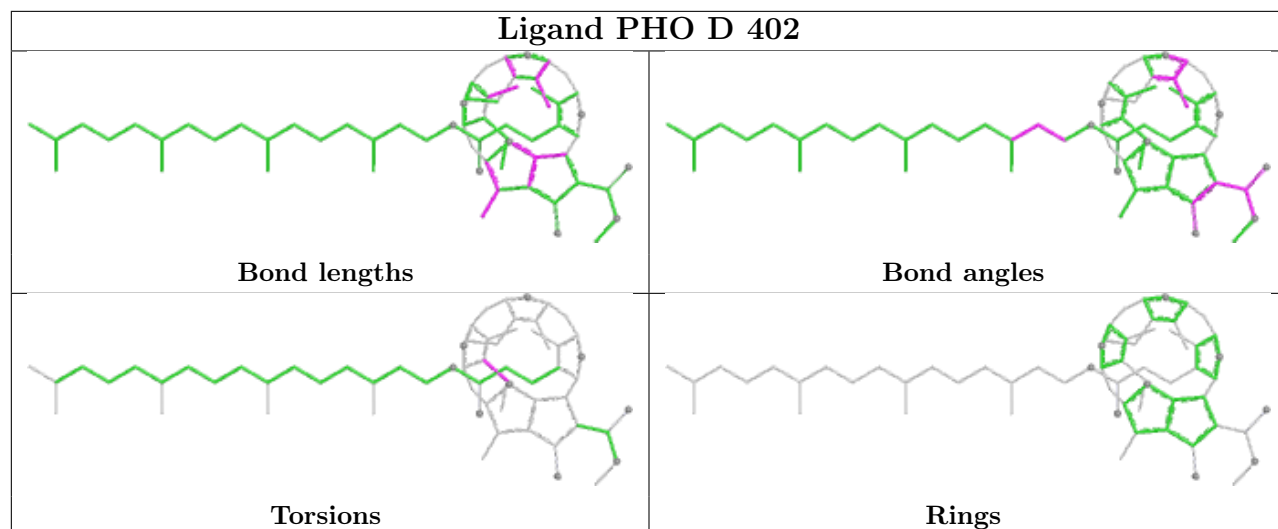


Ligand BCR D 405

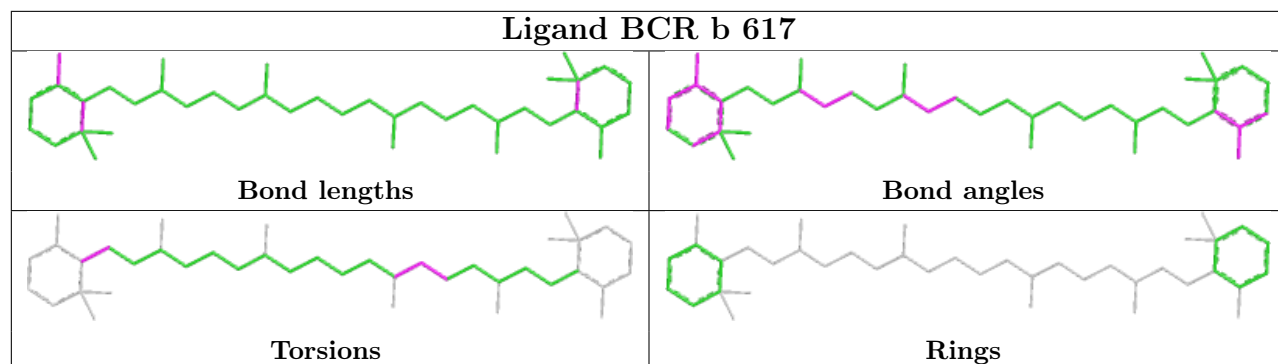




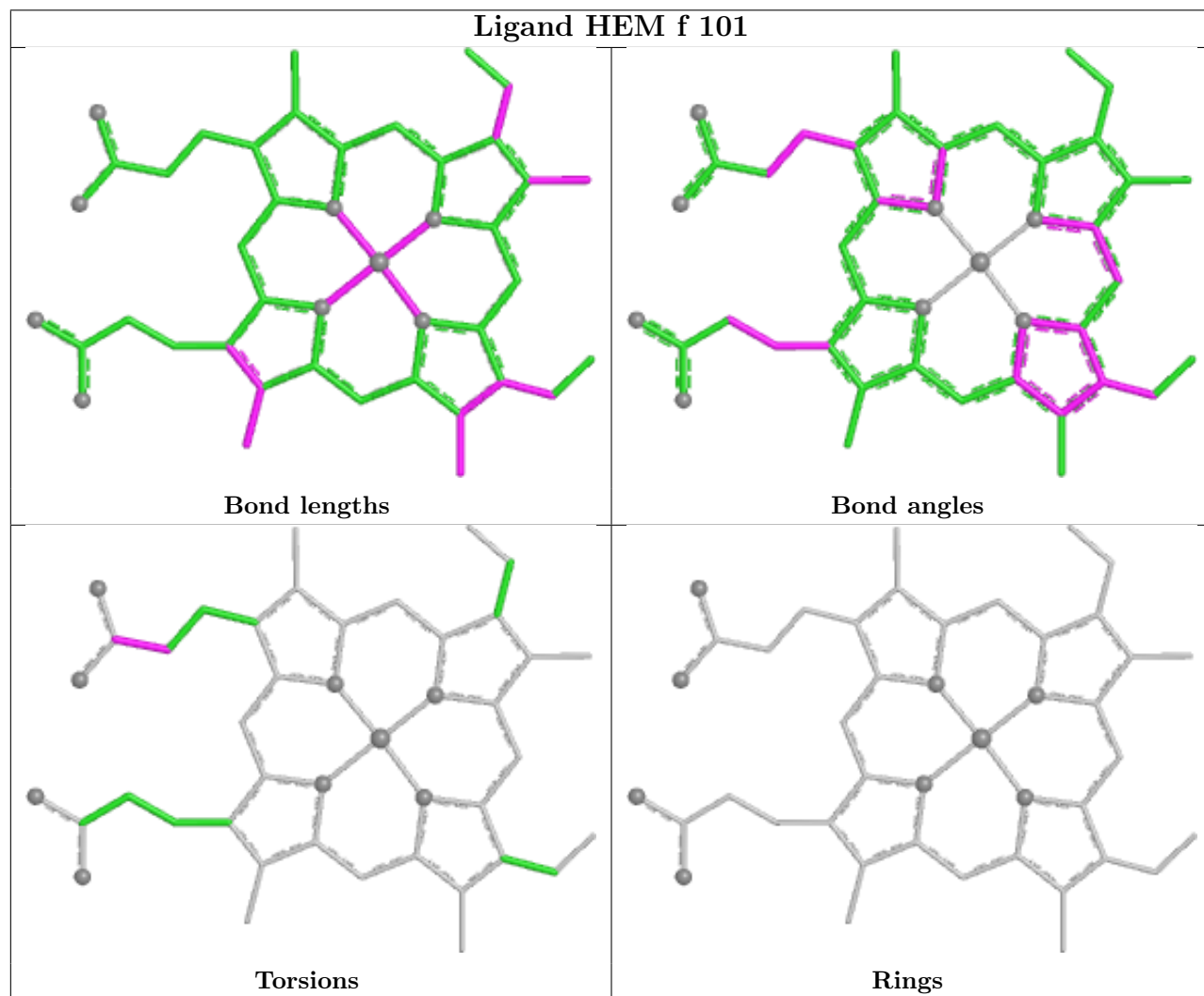


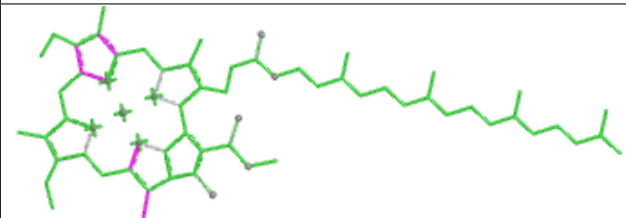
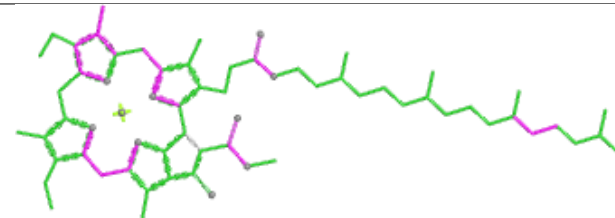
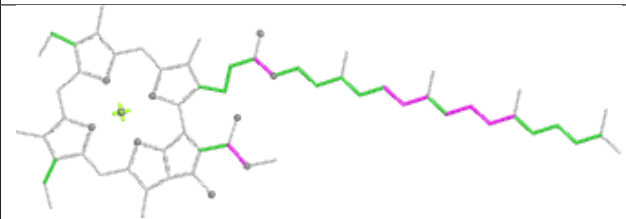
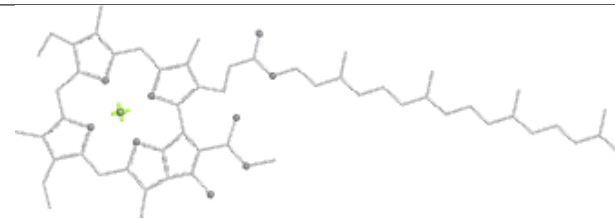


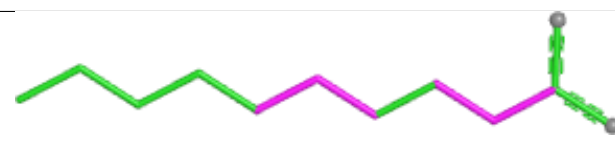
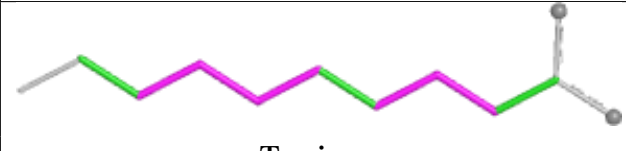
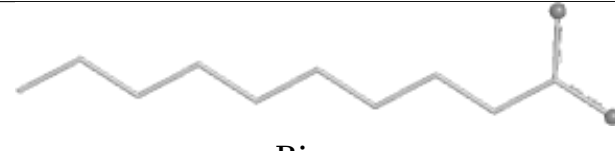
Ligand BCR b 617

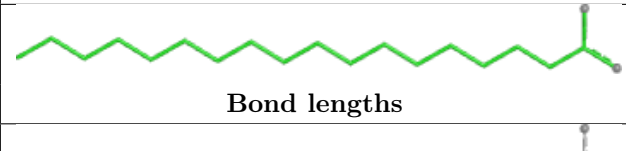
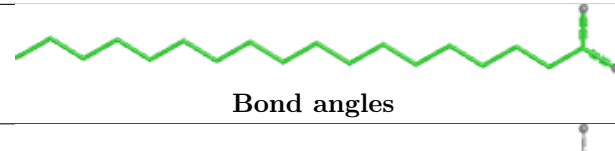
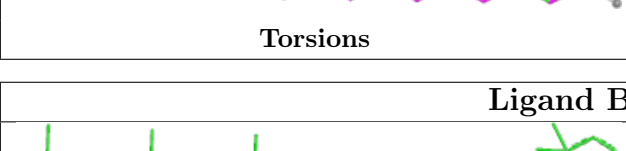


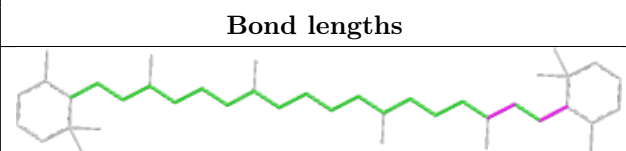
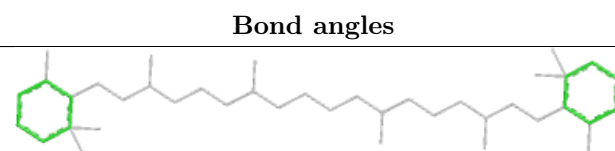
Ligand HEM f 101



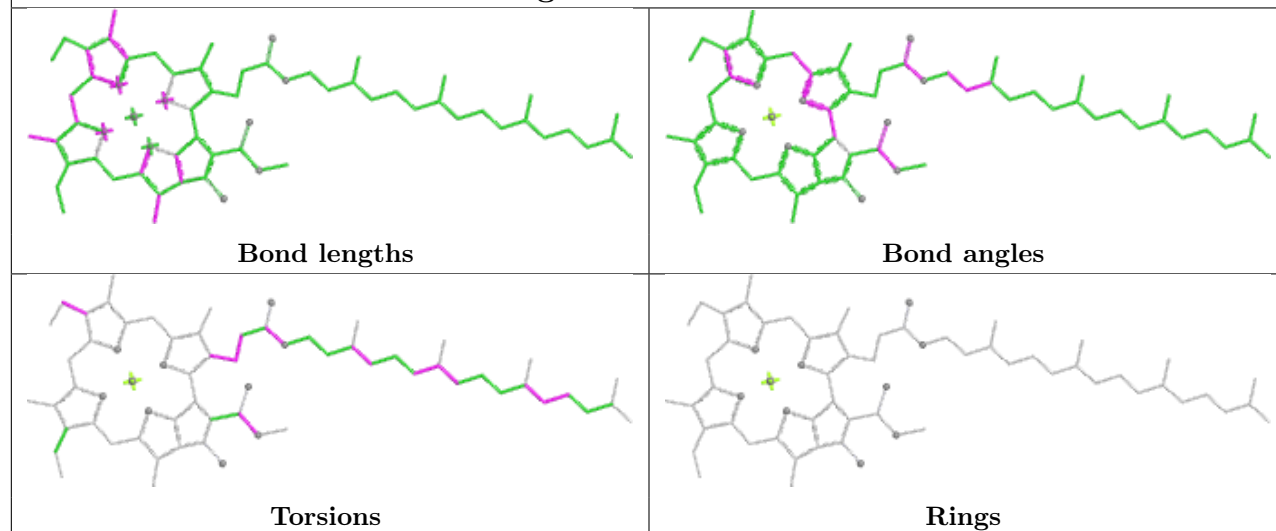
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

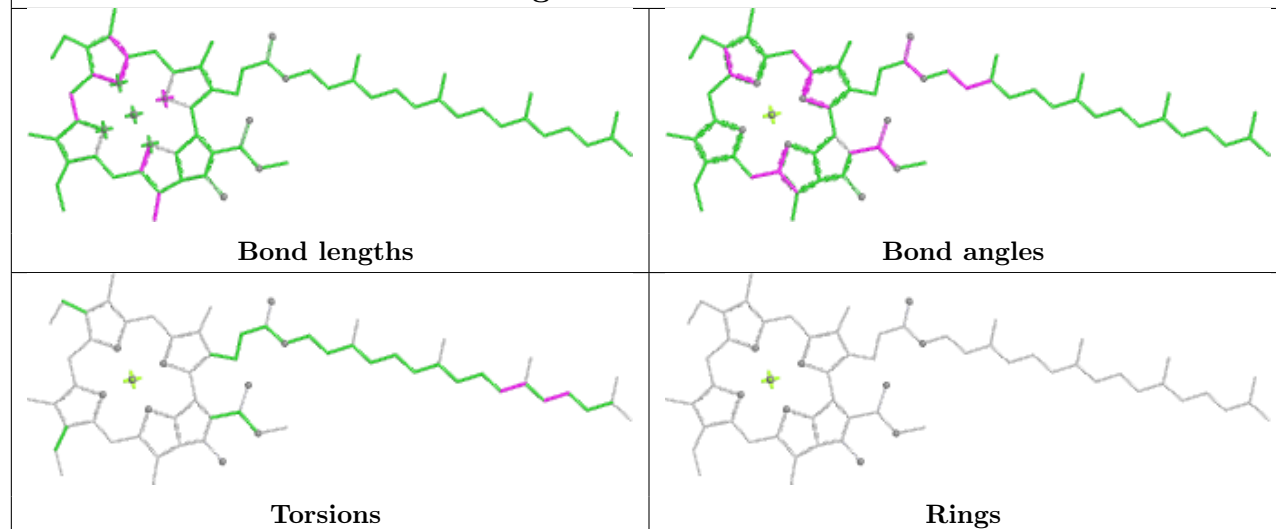
Ligand STE b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

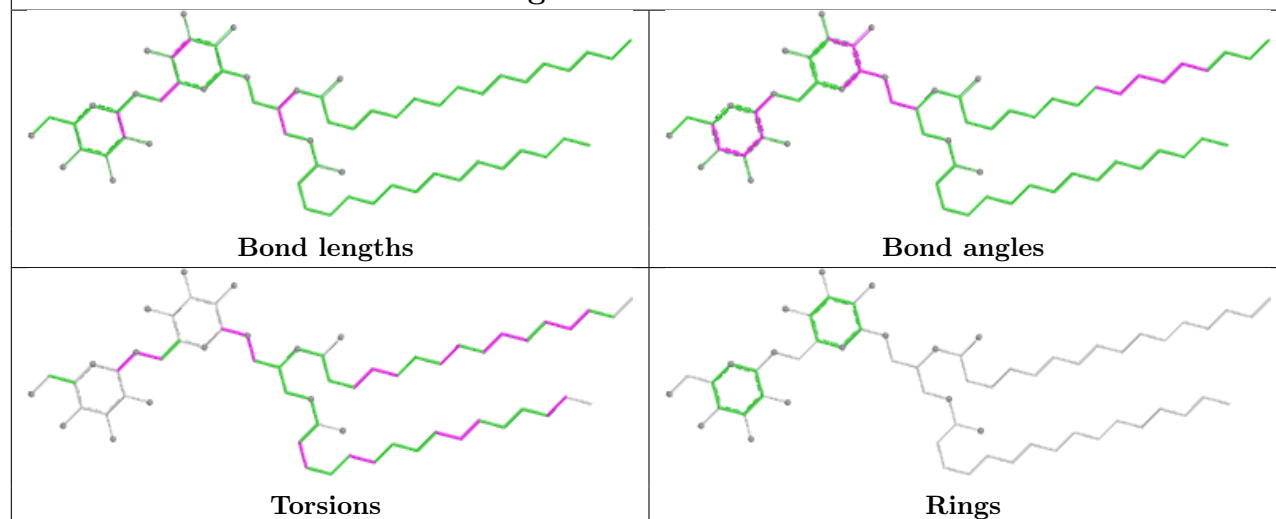
Ligand CLA c 512



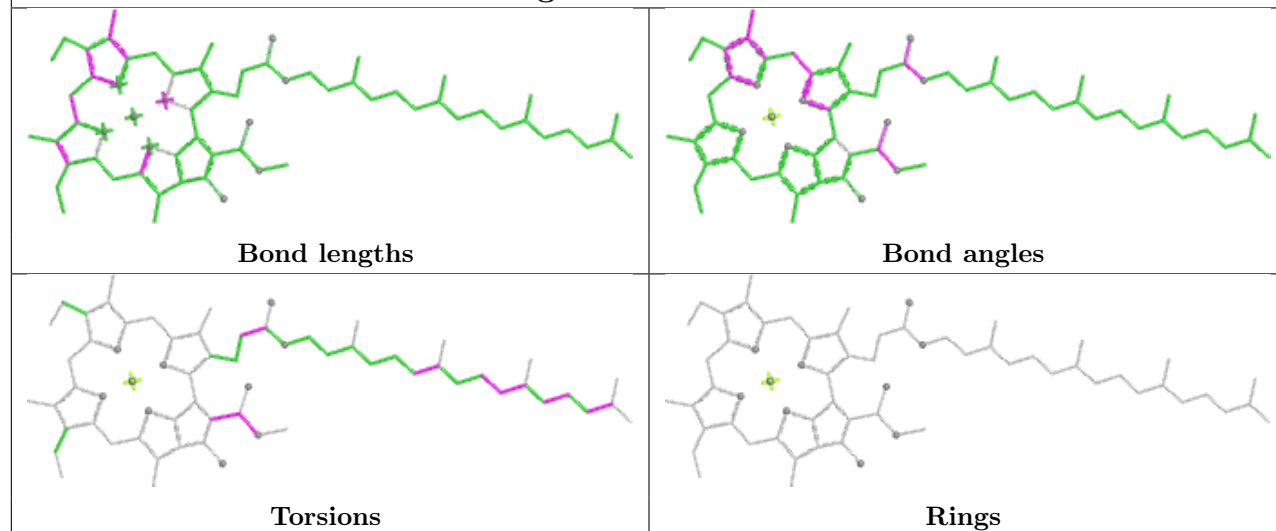
Ligand CLA B 611



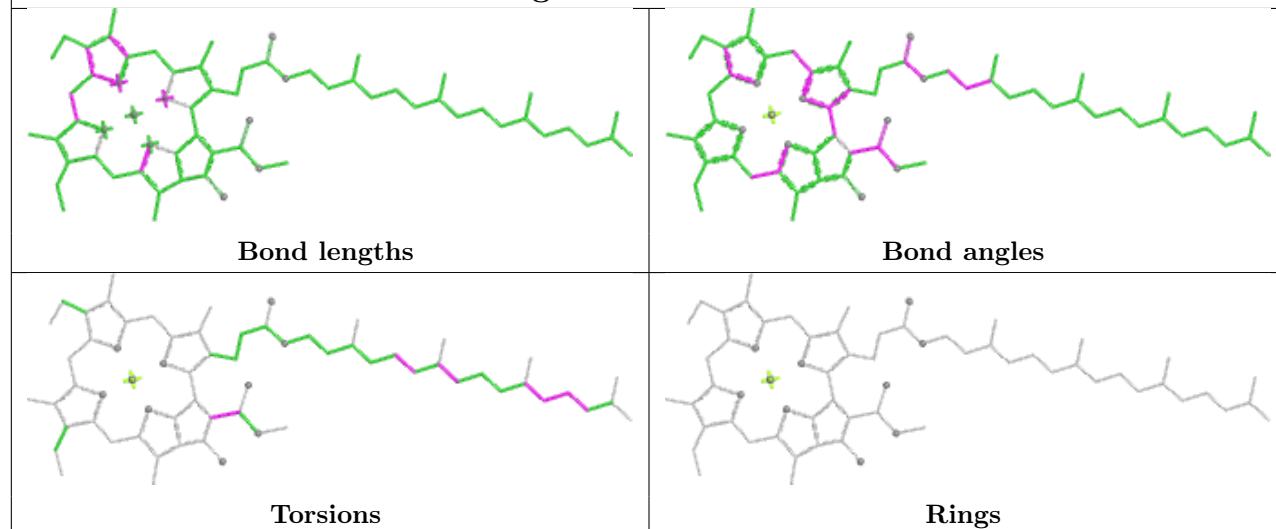
Ligand DGD C 516



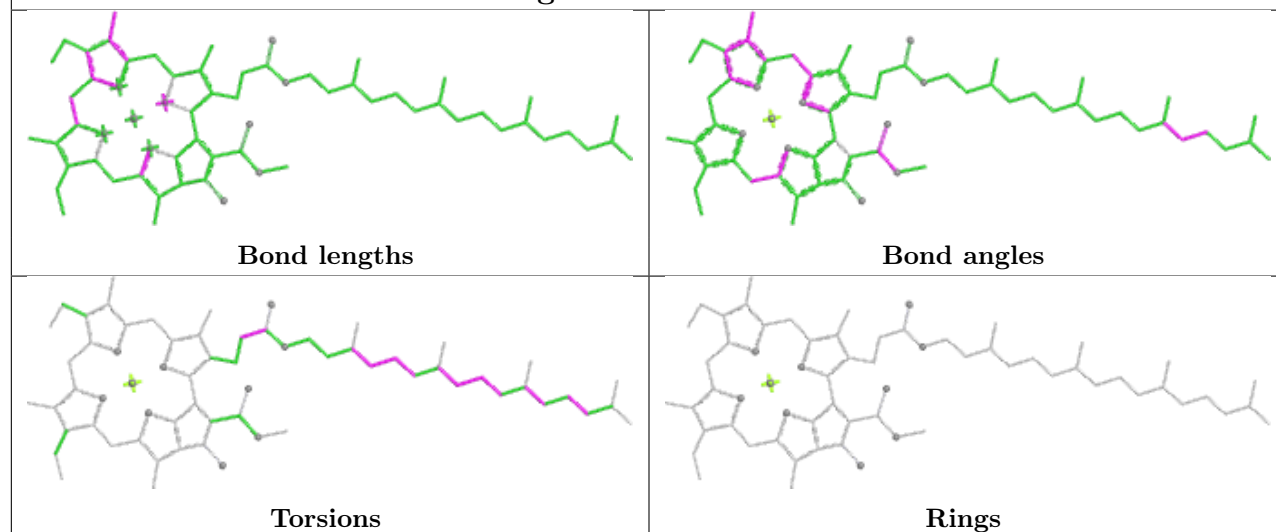
Ligand CLA c 509



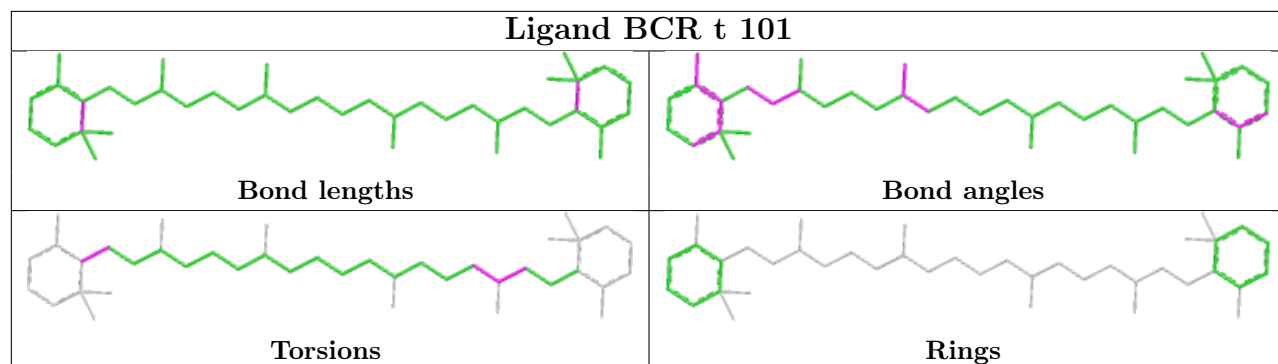
Ligand CLA C 507



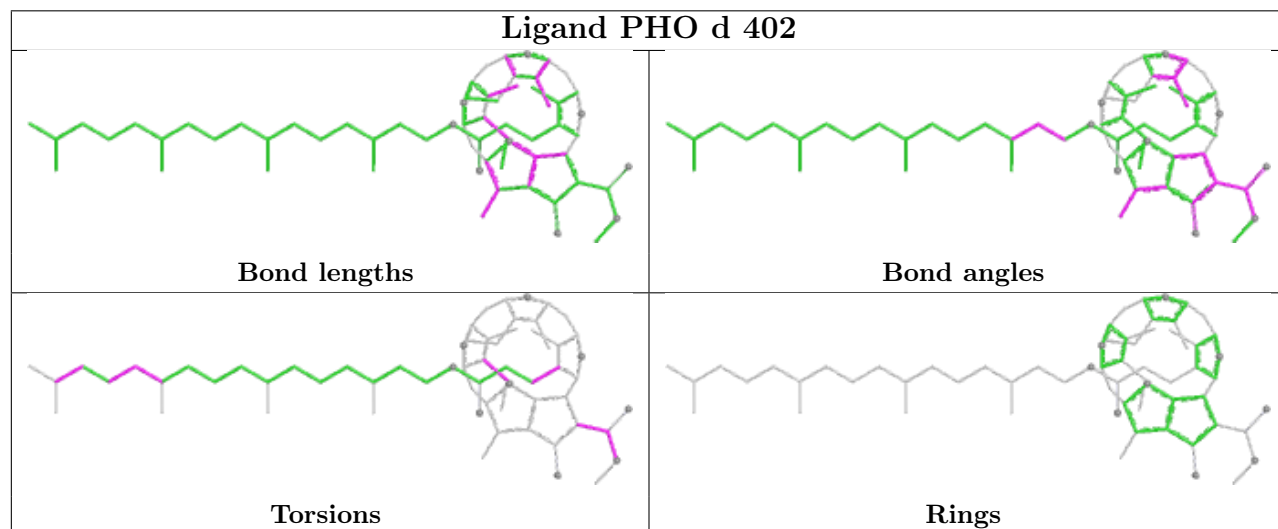
Ligand CLA c 510



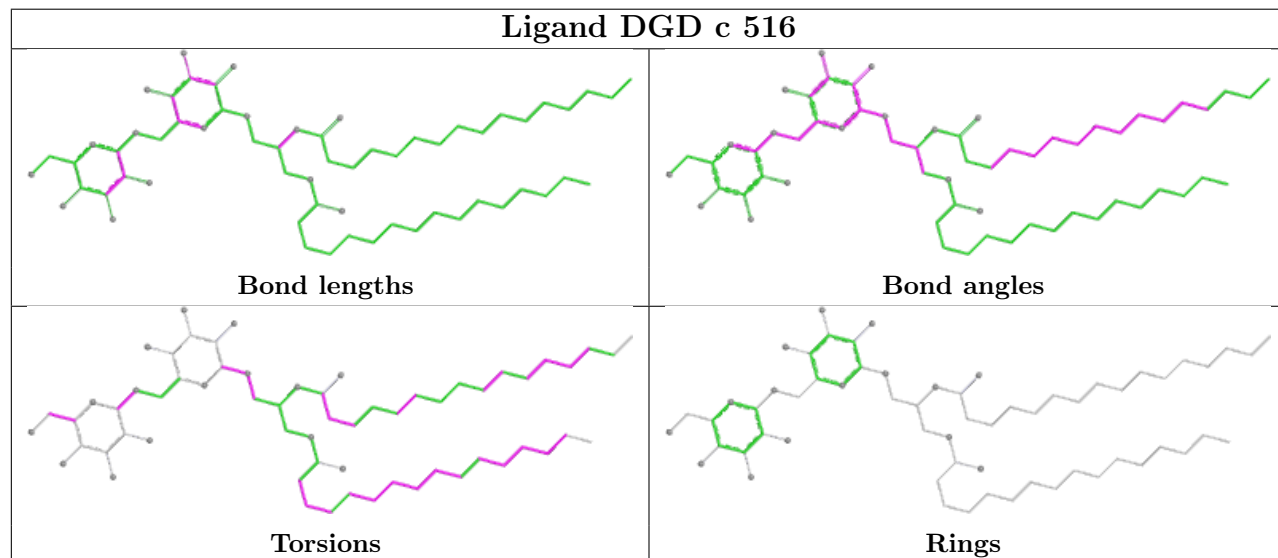
Ligand BCR t 101

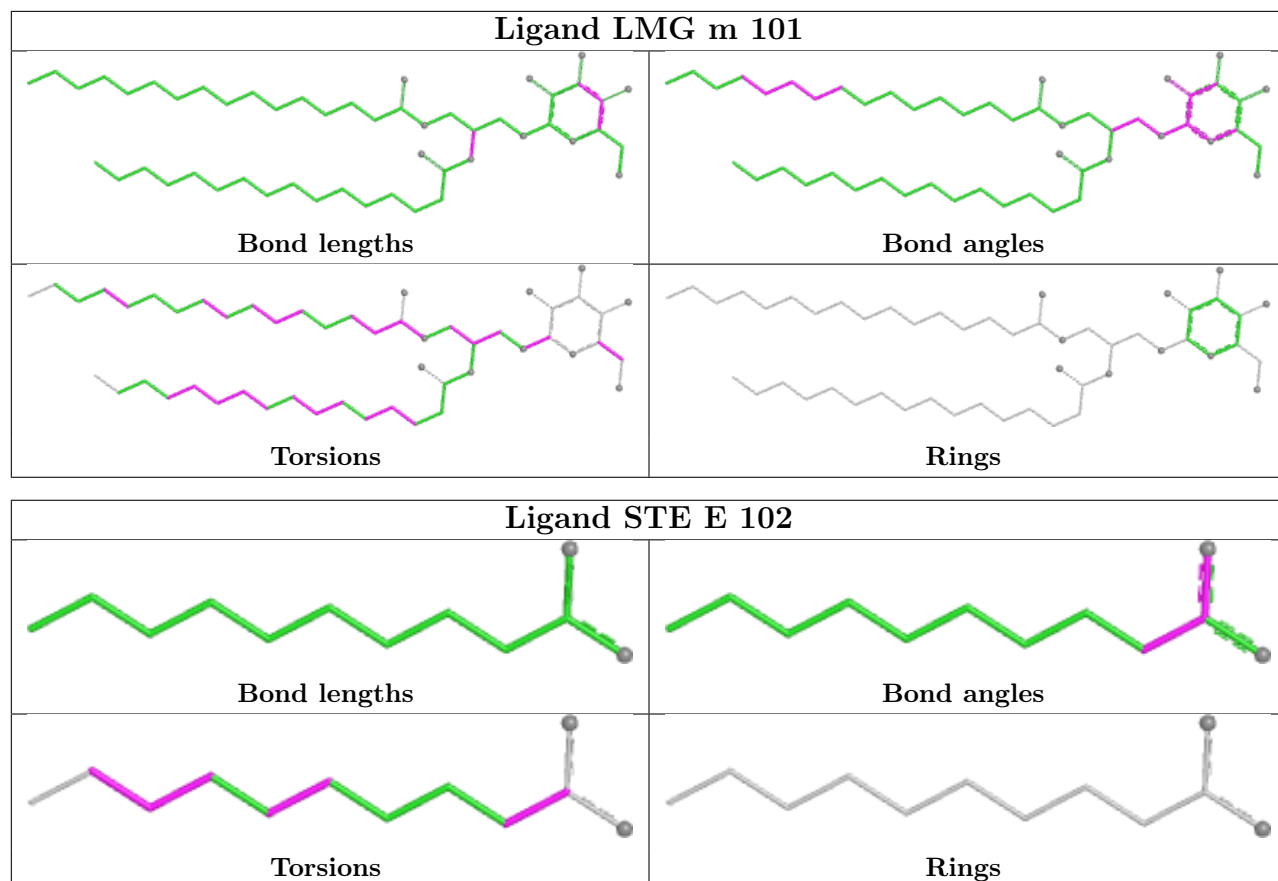


Ligand PHO d 402



Ligand DGD c 516





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%)	-0.33	2 (0%) 85 86	11, 28, 49, 77	64 (19%)
1	a	334/344 (97%)	-0.22	2 (0%) 85 86	11, 31, 57, 73	64 (19%)
2	B	505/510 (99%)	-0.21	4 (0%) 82 83	18, 32, 60, 86	4 (0%)
2	b	505/510 (99%)	-0.11	5 (0%) 79 80	26, 36, 69, 98	0
3	C	442/461 (95%)	-0.18	1 (0%) 91 91	13, 35, 50, 72	11 (2%)
3	c	451/461 (97%)	-0.03	1 (0%) 91 91	13, 40, 61, 86	12 (2%)
4	D	341/352 (96%)	-0.36	1 (0%) 90 90	14, 30, 47, 77	2 (0%)
4	d	341/352 (96%)	-0.21	1 (0%) 90 90	15, 34, 58, 75	3 (0%)
5	E	82/84 (97%)	0.43	1 (1%) 76 76	32, 50, 68, 82	1 (1%)
5	e	82/84 (97%)	0.70	2 (2%) 59 60	42, 61, 76, 84	0
6	F	34/45 (75%)	0.06	0 100 100	35, 42, 61, 80	0
6	f	34/45 (75%)	0.48	2 (5%) 28 27	43, 50, 77, 96	0
7	H	65/66 (98%)	0.05	1 (1%) 72 72	32, 41, 53, 68	0
7	h	63/66 (95%)	0.34	1 (1%) 70 70	40, 52, 60, 65	0
8	I	35/38 (92%)	-0.01	0 100 100	31, 38, 60, 73	0
8	i	35/38 (92%)	-0.02	0 100 100	30, 40, 64, 78	0
9	J	36/40 (90%)	0.38	1 (2%) 55 54	34, 49, 72, 83	0
9	j	36/40 (90%)	0.54	3 (8%) 17 16	39, 55, 88, 88	0
10	K	37/46 (80%)	0.20	0 100 100	41, 51, 65, 70	0
10	k	37/46 (80%)	0.43	0 100 100	49, 57, 75, 84	0
11	L	37/37 (100%)	-0.33	0 100 100	25, 29, 58, 66	0
11	l	36/37 (97%)	-0.41	0 100 100	27, 30, 58, 73	0
12	M	32/36 (88%)	-0.25	0 100 100	26, 33, 56, 69	0
12	m	31/36 (86%)	-0.28	0 100 100	29, 33, 52, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.03	2 (0%) 82 83	26, 41, 74, 127	1 (0%)
13	o	244/272 (89%)	0.03	3 (1%) 76 76	26, 40, 73, 103	0
14	T	29/32 (90%)	-0.40	1 (3%) 48 47	26, 31, 52, 67	0
14	t	29/32 (90%)	-0.31	0 100 100	26, 32, 65, 78	0
15	U	97/134 (72%)	0.02	0 100 100	33, 42, 69, 83	0
15	u	97/134 (72%)	-0.02	1 (1%) 79 80	30, 40, 54, 78	0
16	V	137/163 (84%)	-0.11	1 (0%) 84 84	29, 40, 53, 69	0
16	v	137/163 (84%)	0.13	0 100 100	34, 47, 69, 90	0
17	Y	27/46 (58%)	1.00	3 (11%) 10 9	51, 72, 91, 99	0
17	y	30/46 (65%)	0.91	0 100 100	64, 74, 87, 93	0
18	X	38/41 (92%)	0.31	2 (5%) 32 31	41, 51, 74, 75	0
18	x	39/41 (95%)	0.56	1 (2%) 57 57	50, 60, 82, 95	0
19	Z	62/62 (100%)	0.87	5 (8%) 18 17	51, 64, 102, 110	0
19	z	62/62 (100%)	1.04	6 (9%) 13 12	62, 74, 108, 118	0
20	R	34/41 (82%)	0.90	2 (5%) 28 27	56, 67, 76, 80	0
20	r	31/41 (75%)	1.20	4 (12%) 7 6	65, 78, 95, 98	0
All	All	5302/5700 (93%)	-0.04	59 (1%) 78 78	11, 38, 72, 127	162 (3%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	4.1
19	Z	33	TRP	4.0
20	R	35	LEU	3.7
13	o	58	ASN	3.4
2	B	488	PRO	3.3
4	D	237	PRO	3.1
2	b	496	TYR	3.0
19	z	33	TRP	3.0
13	O	59	LYS	2.9
13	O	60	ARG	2.8
5	e	79	PHE	2.8
7	h	64	ALA	2.6
20	r	20	VAL	2.6
1	a	248	ILE	2.6
2	B	490	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
17	Y	40	ALA	2.5
20	r	31	VAL	2.5
1	A	11	ALA	2.5
2	B	491	VAL	2.4
19	z	40	ILE	2.5
6	f	13	TYR	2.4
19	z	29	SER	2.4
16	V	64	PRO	2.4
9	j	5	GLY	2.4
5	E	79	PHE	2.4
3	c	134	ILE	2.4
2	B	487	SER	2.4
17	Y	25	ILE	2.3
18	X	3	ILE	2.3
19	Z	3	ILE	2.3
18	x	37	VAL	2.3
6	f	15	ILE	2.3
13	o	63	ALA	2.3
20	r	23	ILE	2.3
15	u	40	GLY	2.3
2	b	495	PHE	2.2
4	d	28	VAL	2.2
18	X	2	THR	2.2
20	r	15	ALA	2.2
19	z	39	LEU	2.2
19	z	62	VAL	2.2
3	C	184	GLY	2.2
9	j	8	ILE	2.2
9	j	6	GLY	2.2
20	R	28	VAL	2.1
1	a	11	ALA	2.1
9	J	5	GLY	2.1
2	b	261	ALA	2.1
5	e	5	THR	2.1
14	T	30	THR	2.1
19	Z	30	PRO	2.1
7	H	41	PHE	2.1
19	z	26	ALA	2.1
17	Y	46	LEU	2.0
2	b	488	PRO	2.0
13	o	56	PRO	2.0
2	b	494	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	13	LEU	2.0
19	Z	27	TYR	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	0.89	0.10	32,34,49,55	0
12	FME	M	1	10/11	0.92	0.09	39,45,59,60	0
14	FME	T	1	10/11	0.95	0.09	28,32,52,66	0
8	FME	i	1	10/11	0.95	0.07	36,44,49,52	0
12	FME	m	1	10/11	0.95	0.08	34,47,55,64	0
8	FME	I	1	10/11	0.95	0.08	38,43,50,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	LHG	A	614	49/49	0.72	0.17	50,74,90,93	0
32	STE	H	103	18/20	0.72	0.17	48,62,67,71	0
32	STE	k	104	12/20	0.74	0.14	61,66,72,82	0
32	STE	L	102	12/20	0.76	0.19	50,55,63,64	0
27	PL9	A	610	55/55	0.77	0.16	35,58,68,70	0
28	LMG	c	520	48/55	0.77	0.15	45,66,74,78	0
32	STE	a	615	12/20	0.78	0.14	52,57,68,69	0
28	LMG	d	410	23/55	0.79	0.18	48,57,66,67	0
28	LMG	b	622	55/55	0.79	0.16	46,59,69,72	0
32	STE	d	412	17/20	0.79	0.15	46,51,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	601	65/65	0.79	0.14	47,66,83,86	0
32	STE	b	621	20/20	0.80	0.13	40,48,67,73	0
32	STE	b	625	10/20	0.80	0.18	44,53,65,68	0
31	DGD	a	614	44/66	0.80	0.14	37,49,60,70	0
29	SQD	a	613	36/54	0.80	0.14	41,53,65,70	0
32	STE	b	624	15/20	0.81	0.16	45,48,60,69	0
28	LMG	D	411	33/55	0.81	0.14	37,53,72,74	0
32	STE	B	625	18/20	0.82	0.16	39,52,69,76	0
32	STE	b	623	16/20	0.82	0.15	48,59,75,76	0
28	LMG	c	518	37/55	0.82	0.12	49,62,78,80	0
32	STE	B	621	17/20	0.83	0.13	36,47,63,65	0
32	STE	B	624	12/20	0.83	0.15	40,51,59,60	0
31	DGD	A	616	66/66	0.83	0.12	42,54,64,66	0
32	STE	B	626	12/20	0.83	0.14	47,54,63,63	0
32	STE	D	413	20/20	0.83	0.13	37,45,67,73	0
32	STE	c	519	20/20	0.83	0.14	41,49,76,82	0
27	PL9	a	610	55/55	0.83	0.15	42,61,72,74	0
32	STE	A	617	20/20	0.83	0.12	41,50,64,64	0
32	STE	B	627	16/20	0.84	0.14	42,49,60,61	0
32	STE	d	413	20/20	0.84	0.12	42,50,63,64	0
28	LMG	A	612	48/55	0.84	0.11	37,50,62,73	0
32	STE	C	518	12/20	0.85	0.13	36,44,54,57	0
32	STE	C	519	12/20	0.85	0.12	46,54,59,62	0
28	LMG	B	622	28/55	0.85	0.13	38,45,55,60	0
32	STE	E	102	12/20	0.85	0.13	51,63,72,74	0
32	STE	j	101	12/20	0.85	0.12	47,53,58,58	0
30	LHG	e	101	42/49	0.85	0.12	58,74,88,99	0
29	SQD	b	620	49/54	0.86	0.11	38,50,70,73	0
29	SQD	f	102	41/54	0.86	0.13	55,72,85,88	0
28	LMG	c	521	49/55	0.86	0.11	37,50,74,82	0
26	BCR	d	405	40/40	0.86	0.11	39,49,75,79	0
28	LMG	m	101	51/55	0.86	0.11	33,47,59,61	0
29	SQD	A	615	39/54	0.86	0.13	36,51,71,75	0
28	LMG	C	517	48/55	0.86	0.12	44,61,67,69	0
32	STE	t	102	14/20	0.86	0.11	37,43,50,53	0
32	STE	t	103	10/20	0.86	0.11	46,54,55,57	0
28	LMG	B	620	51/55	0.87	0.11	31,46,58,63	0
26	BCR	k	102	40/40	0.87	0.12	51,61,68,73	0
26	BCR	h	101	40/40	0.87	0.12	40,53,63,65	0
32	STE	T	102	16/20	0.87	0.13	39,47,55,57	0
26	BCR	k	101	40/40	0.88	0.11	45,56,63,66	0
32	STE	I	101	15/20	0.89	0.13	46,50,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	J	102	12/20	0.89	0.11	48,53,60,61	0
25	CLA	B	601	65/65	0.89	0.10	41,53,69,75	0
26	BCR	D	405	40/40	0.89	0.10	34,42,66,71	0
32	STE	C	520	16/20	0.89	0.10	39,46,51,52	0
31	DGD	H	102	62/66	0.89	0.11	34,42,51,57	0
32	STE	m	102	18/20	0.89	0.14	32,42,61,63	0
29	SQD	B	623	54/54	0.89	0.10	39,52,71,82	0
29	SQD	D	408	36/54	0.89	0.12	44,60,68,70	0
29	SQD	a	612	54/54	0.90	0.10	38,57,66,72	0
26	BCR	K	101	40/40	0.90	0.11	44,50,59,62	0
31	DGD	c	516	62/66	0.90	0.10	36,45,70,78	0
26	BCR	k	103	40/40	0.90	0.13	45,51,62,64	0
26	BCR	K	102	40/40	0.90	0.10	41,47,59,62	0
25	CLA	c	512	65/65	0.90	0.11	47,53,65,72	0
26	BCR	B	618	40/40	0.90	0.09	24,37,45,45	0
25	CLA	C	513	65/65	0.90	0.10	41,52,73,76	0
28	LMG	D	407	51/55	0.91	0.11	32,44,66,69	0
26	BCR	b	619	40/40	0.91	0.09	29,43,57,60	0
25	CLA	c	513	65/65	0.91	0.10	43,60,78,84	0
26	BCR	H	101	40/40	0.91	0.09	31,40,52,53	0
31	DGD	C	516	62/66	0.91	0.10	30,43,72,87	0
26	BCR	B	619	40/40	0.91	0.08	28,37,51,56	0
32	STE	M	101	15/20	0.91	0.10	38,45,56,65	0
32	STE	M	102	10/20	0.91	0.12	41,44,53,54	0
26	BCR	C	514	40/40	0.91	0.09	26,35,47,48	0
26	BCR	T	101	40/40	0.91	0.08	29,36,47,50	0
31	DGD	h	102	62/66	0.91	0.10	35,44,54,56	0
29	SQD	A	613	52/54	0.92	0.10	34,50,68,75	0
30	LHG	d	407	49/49	0.92	0.10	34,43,59,64	0
26	BCR	t	101	40/40	0.92	0.08	29,35,45,49	0
25	CLA	C	512	65/65	0.92	0.09	35,46,70,72	0
26	BCR	b	618	40/40	0.92	0.07	26,35,44,49	0
25	CLA	c	511	65/65	0.93	0.10	42,52,60,67	0
25	CLA	C	508	65/65	0.93	0.09	25,35,67,76	0
30	LHG	d	409	39/49	0.93	0.10	35,40,54,55	0
26	BCR	K	103	40/40	0.93	0.11	37,47,58,59	0
24	BCT	d	401	4/4	0.93	0.08	33,34,43,43	0
26	BCR	b	617	40/40	0.93	0.08	28,40,45,48	0
26	BCR	A	609	40/40	0.93	0.07	22,31,36,37	0
25	CLA	B	606	65/65	0.93	0.09	25,33,54,60	0
26	BCR	c	514	40/40	0.93	0.09	31,44,51,55	0
31	DGD	c	517	62/66	0.93	0.09	32,45,62,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	503	65/65	0.93	0.08	29,36,42,53	0
25	CLA	b	614	65/65	0.93	0.09	28,35,59,64	0
25	CLA	c	503	65/65	0.93	0.09	34,41,47,52	0
25	CLA	c	510	65/65	0.93	0.08	33,42,51,55	0
25	CLA	C	501	65/65	0.94	0.07	24,32,43,44	0
30	LHG	D	410	47/49	0.94	0.09	28,39,59,63	0
30	LHG	D	412	49/49	0.94	0.09	28,38,53,55	0
24	BCT	A	605	4/4	0.94	0.07	28,32,34,34	0
25	CLA	C	506	65/65	0.94	0.09	29,37,64,72	0
25	CLA	b	606	65/65	0.94	0.08	26,37,56,69	0
30	LHG	l	101	49/49	0.94	0.09	33,40,48,54	0
26	BCR	B	617	40/40	0.94	0.08	28,37,45,46	0
31	DGD	C	515	62/66	0.94	0.09	23,33,60,66	0
25	CLA	b	609	65/65	0.94	0.09	34,42,56,64	0
25	CLA	B	616	60/65	0.94	0.10	26,34,63,70	0
31	DGD	J	101	62/66	0.94	0.09	28,39,66,75	0
25	CLA	b	616	60/65	0.94	0.09	31,39,71,75	0
31	DGD	c	515	62/66	0.94	0.09	24,37,60,72	0
28	LMG	d	411	44/55	0.94	0.09	37,47,70,72	0
25	CLA	C	510	65/65	0.94	0.08	28,37,47,57	0
25	CLA	c	504	60/65	0.94	0.09	31,40,63,68	0
25	CLA	c	505	65/65	0.94	0.08	27,36,50,52	0
27	PL9	D	406	55/55	0.94	0.07	20,29,37,39	0
25	CLA	c	508	64/65	0.94	0.09	32,40,73,83	0
27	PL9	d	406	55/55	0.94	0.07	25,32,39,40	0
25	CLA	c	509	65/65	0.94	0.09	33,43,54,58	0
25	CLA	C	511	65/65	0.94	0.10	34,45,57,63	0
26	BCR	a	609	40/40	0.94	0.07	22,30,39,44	0
33	PHO	d	402	64/64	0.94	0.07	28,37,43,45	0
25	CLA	a	606	65/65	0.95	0.08	25,35,74,77	0
25	CLA	a	608	65/65	0.95	0.09	22,30,63,67	0
25	CLA	d	403	65/65	0.95	0.07	22,28,48,53	0
25	CLA	d	404	65/65	0.95	0.09	28,38,73,79	0
25	CLA	B	610	65/65	0.95	0.07	22,28,37,39	0
25	CLA	b	602	65/65	0.95	0.08	29,38,49,55	0
25	CLA	C	504	59/65	0.95	0.07	28,37,67,70	0
25	CLA	b	608	65/65	0.95	0.07	29,39,54,57	0
25	CLA	C	505	65/65	0.95	0.07	26,34,53,59	0
25	CLA	b	610	65/65	0.95	0.08	29,35,43,46	0
25	CLA	b	613	65/65	0.95	0.08	23,30,58,67	0
25	CLA	B	611	65/65	0.95	0.06	23,28,38,44	0
25	CLA	b	615	65/65	0.95	0.07	29,37,49,52	0

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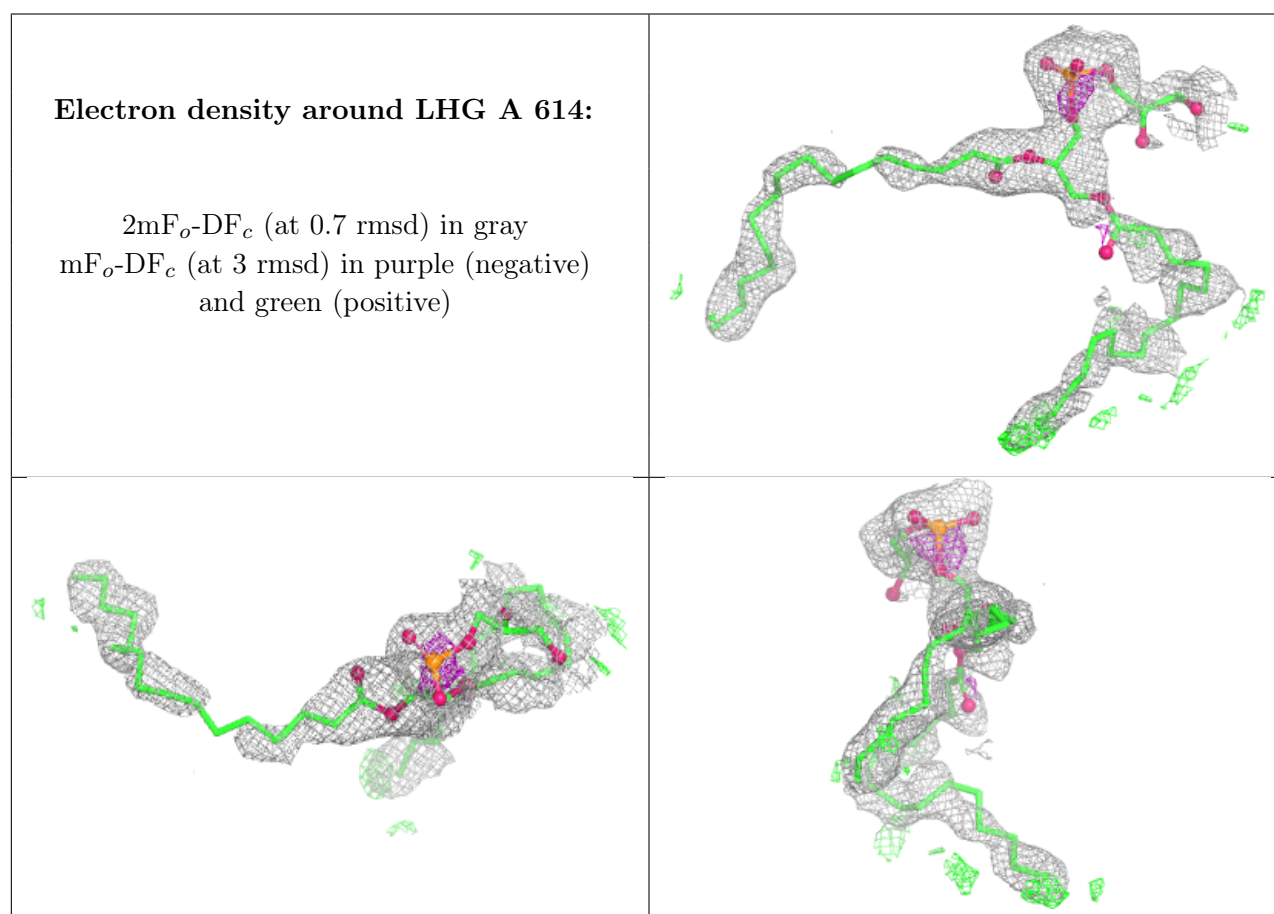
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	507	65/65	0.95	0.08	26,34,46,52	0
25	CLA	c	501	65/65	0.95	0.07	29,36,47,53	0
25	CLA	c	502	65/65	0.95	0.07	31,36,48,52	0
25	CLA	B	614	65/65	0.95	0.08	23,34,58,63	0
25	CLA	C	509	65/65	0.95	0.09	27,35,52,54	0
25	CLA	B	615	65/65	0.95	0.08	27,33,50,55	0
25	CLA	c	506	65/65	0.95	0.08	35,42,67,73	0
25	CLA	c	507	65/65	0.95	0.08	32,39,48,51	0
25	CLA	B	602	65/65	0.95	0.07	23,32,51,55	0
25	CLA	B	607	65/65	0.95	0.08	20,27,51,56	0
25	CLA	C	502	65/65	0.95	0.07	25,33,46,55	0
33	PHO	a	607	64/64	0.95	0.07	21,28,34,37	0
25	CLA	a	605	65/65	0.95	0.07	22,28,36,43	0
25	CLA	B	604	65/65	0.96	0.07	21,27,59,65	0
25	CLA	a	611	65/65	0.96	0.06	19,28,39,46	0
25	CLA	B	605	65/65	0.96	0.07	20,28,40,44	0
25	CLA	A	611	65/65	0.96	0.06	17,25,34,37	0
25	CLA	b	603	65/65	0.96	0.07	21,31,53,59	0
25	CLA	b	604	65/65	0.96	0.07	22,30,56,61	0
25	CLA	b	605	65/65	0.96	0.07	23,31,39,43	0
25	CLA	A	606	65/65	0.96	0.06	19,26,36,44	0
25	CLA	b	607	65/65	0.96	0.07	22,30,52,58	0
25	CLA	B	608	65/65	0.96	0.07	25,31,49,59	0
25	CLA	B	609	65/65	0.96	0.07	23,34,52,58	0
30	LHG	L	101	49/49	0.96	0.07	28,36,43,55	0
25	CLA	A	607	65/65	0.96	0.09	22,29,77,81	0
30	LHG	d	408	49/49	0.96	0.08	27,37,44,50	0
25	CLA	b	611	65/65	0.96	0.07	24,30,42,49	0
25	CLA	b	612	65/65	0.96	0.07	24,32,40,46	0
25	CLA	D	403	65/65	0.96	0.07	19,25,41,56	0
25	CLA	D	404	65/65	0.96	0.08	27,33,73,82	0
33	PHO	D	401	64/64	0.96	0.06	19,26,33,38	0
33	PHO	D	402	64/64	0.96	0.06	24,31,35,37	0
25	CLA	B	603	65/65	0.96	0.07	20,27,49,55	0
25	CLA	B	612	65/65	0.96	0.06	21,27,38,41	0
34	HEM	E	101	43/43	0.96	0.09	38,45,55,63	0
34	HEM	f	101	43/43	0.96	0.09	47,56,67,76	0
25	CLA	A	608	54/65	0.97	0.06	19,26,50,54	0
30	LHG	D	409	49/49	0.97	0.07	24,35,44,49	0
25	CLA	B	613	65/65	0.97	0.06	20,26,54,58	0
35	HEC	V	201	43/43	0.98	0.06	24,30,38,43	0
35	HEC	v	201	43/43	0.98	0.06	29,35,42,46	0

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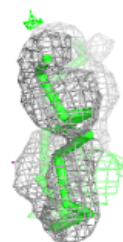
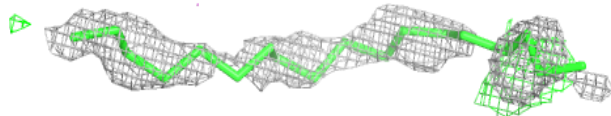
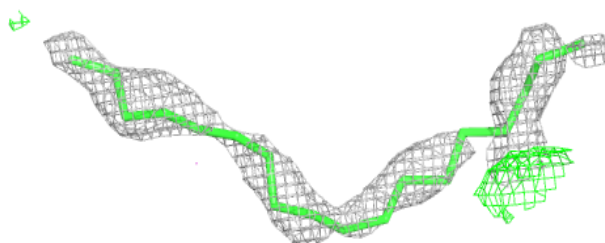
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CL	a	603	1/1	0.99	0.03	31,31,31,31	0
23	CL	a	604	1/1	0.99	0.09	32,32,32,32	0
21	OEY	A	601[A]	11/11	0.99	0.03	29,32,36,36	11
21	OEY	A	601[B]	11/11	0.99	0.03	23,28,31,31	11
21	OEY	a	601[A]	11/11	0.99	0.03	28,31,33,35	11
21	OEY	a	601[B]	11/11	0.99	0.03	24,29,29,31	11
22	FE2	A	602	1/1	0.99	0.01	29,29,29,29	0
22	FE2	a	602	1/1	0.99	0.02	32,32,32,32	0
23	CL	A	603	1/1	0.99	0.04	27,27,27,27	0
23	CL	A	604	1/1	0.99	0.02	29,29,29,29	0

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

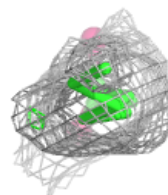
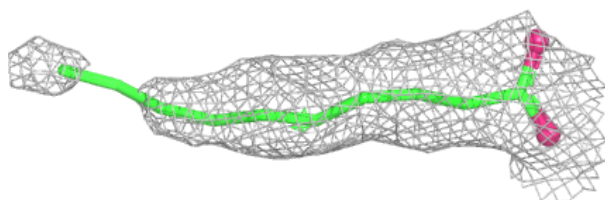


Electron density around STE H 103:

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

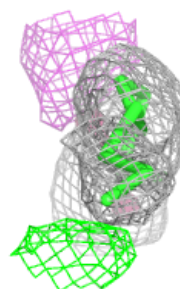
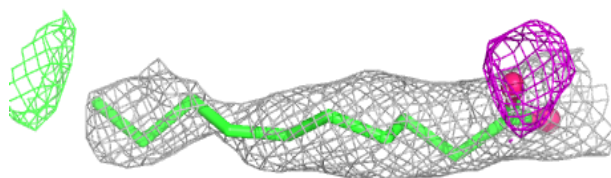
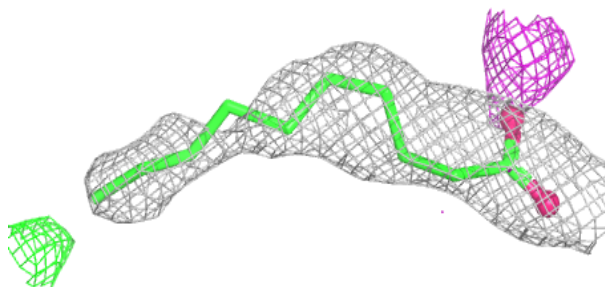
**Electron density around STE k 104:**

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

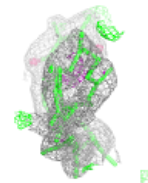
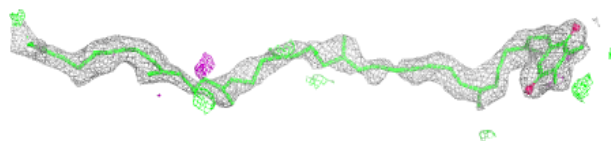
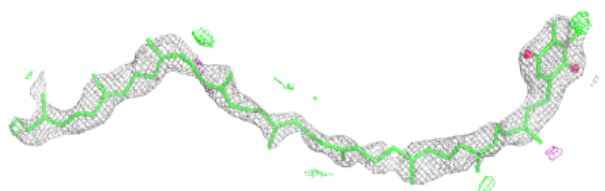


Electron density around STE L 102:

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

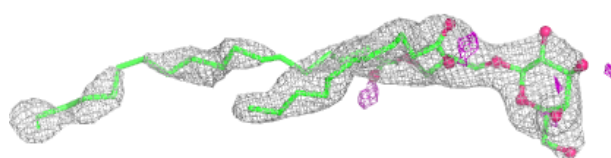
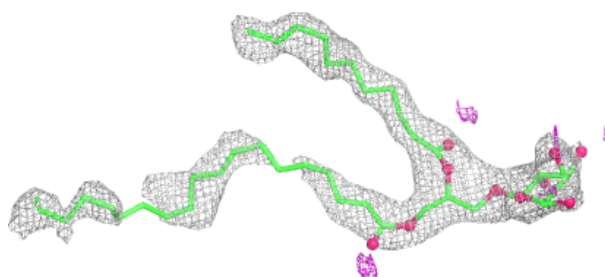
**Electron density around PL9 A 610:**

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

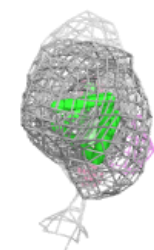
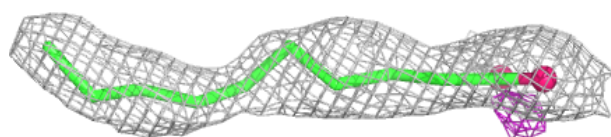
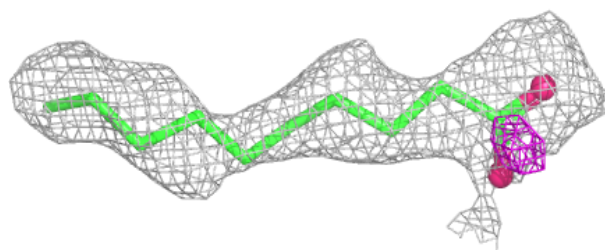


Electron density around LMG c 520:

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

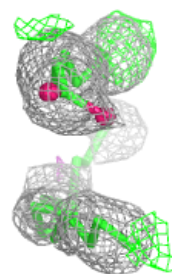
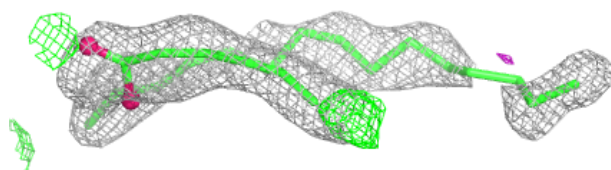
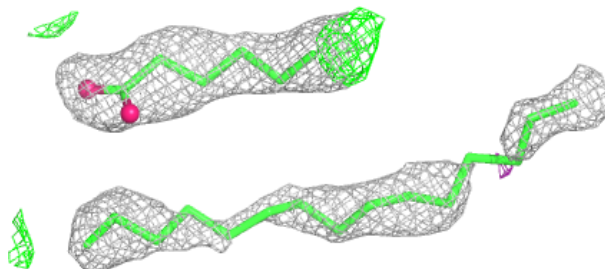
**Electron density around STE a 615:**

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

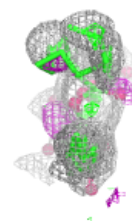
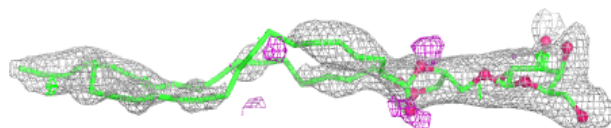
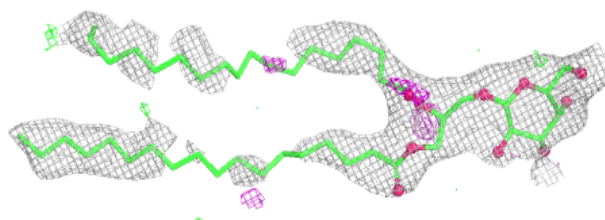


Electron density around LMG d 410:

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

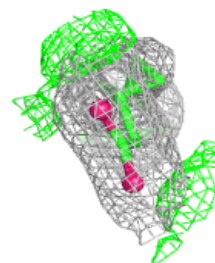
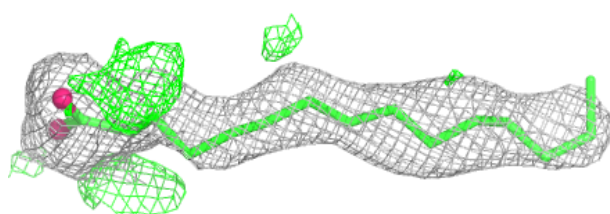
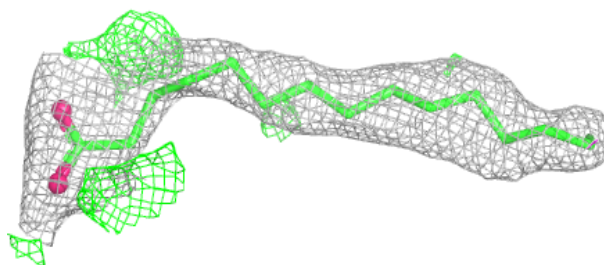
**Electron density around LMG b 622:**

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

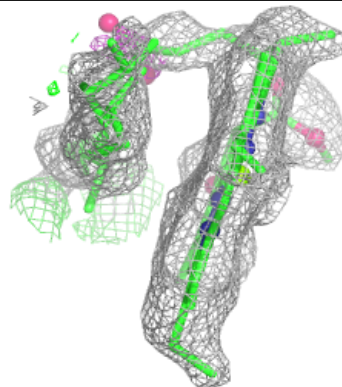
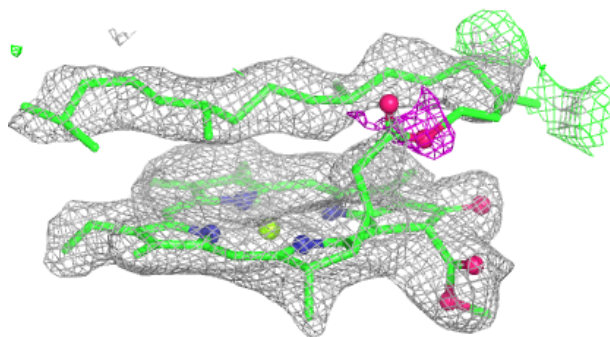
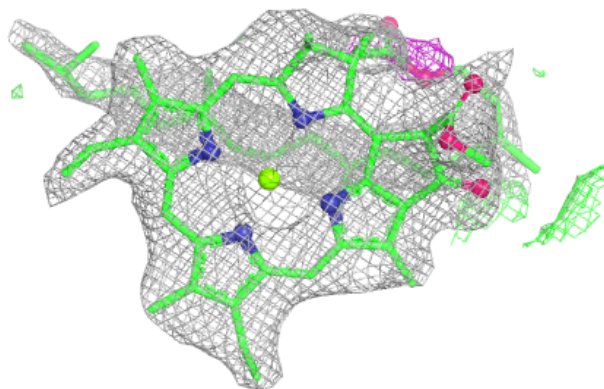


Electron density around STE d 412:

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

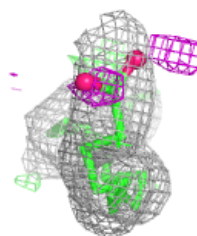
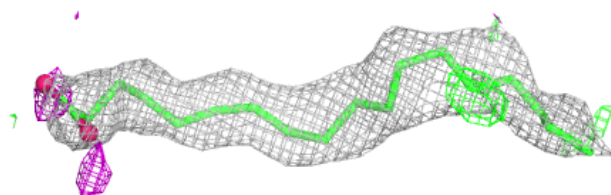
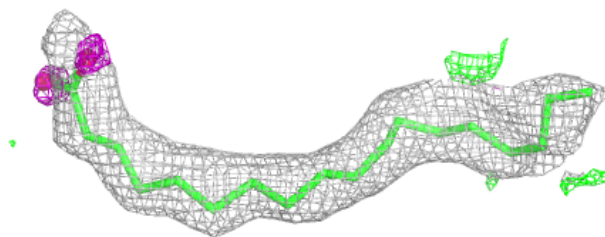
**Electron density around CLA b 601:**

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

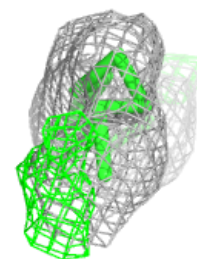
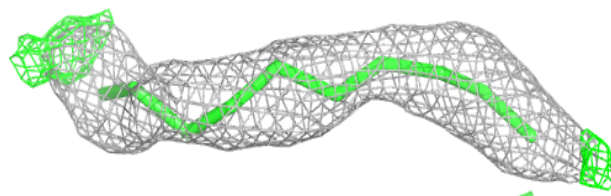
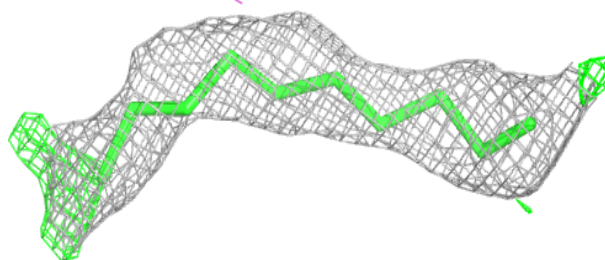


Electron density around STE b 621:

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

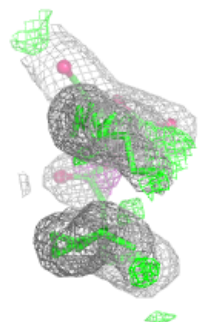
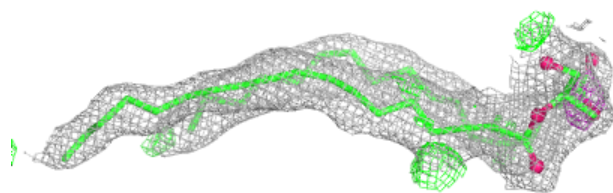
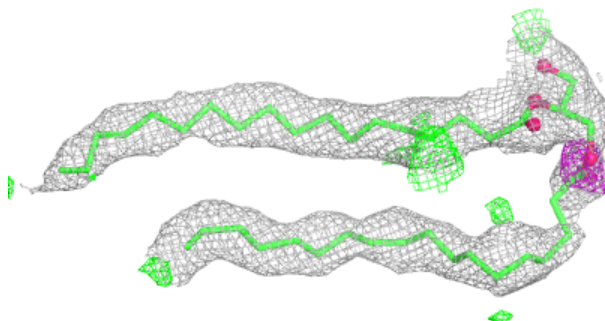
**Electron density around STE b 625:**

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



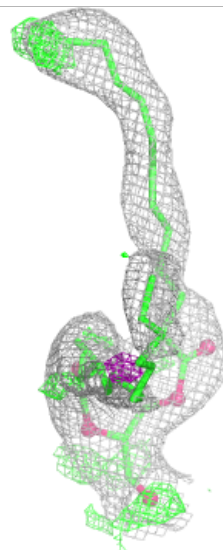
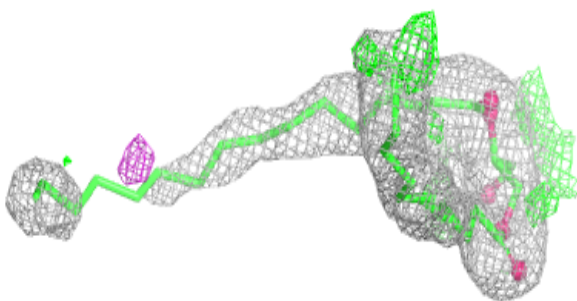
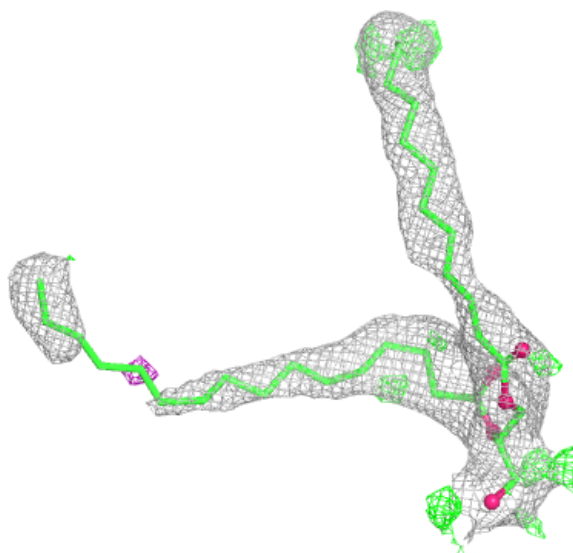
Electron density around DGD a 614:

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



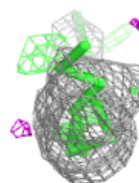
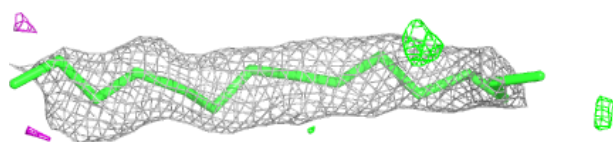
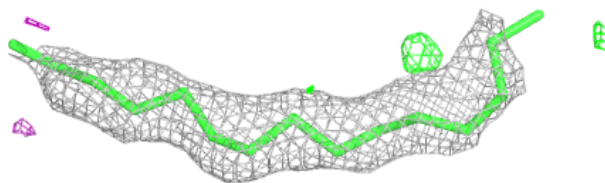
Electron density around SQD a 613:

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

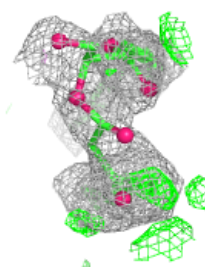
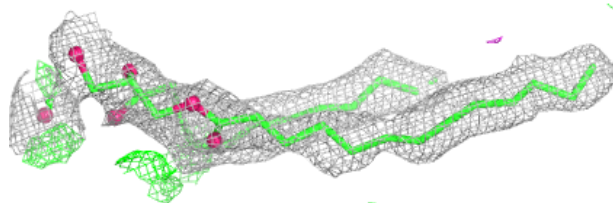
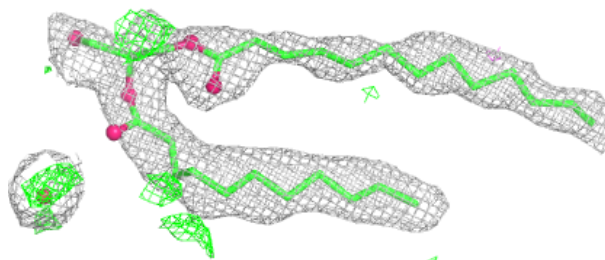


Electron density around STE b 624:

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

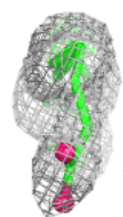
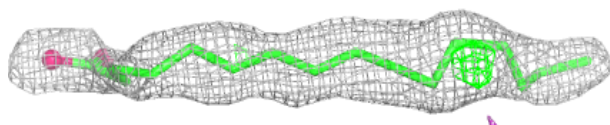
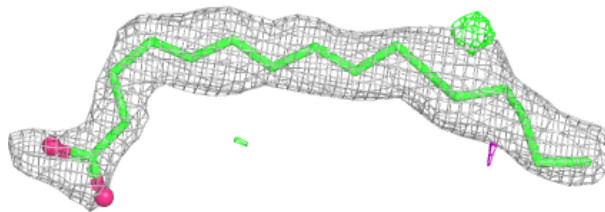
**Electron density around LMG D 411:**

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

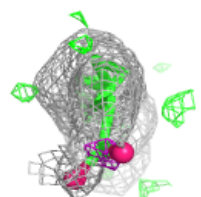
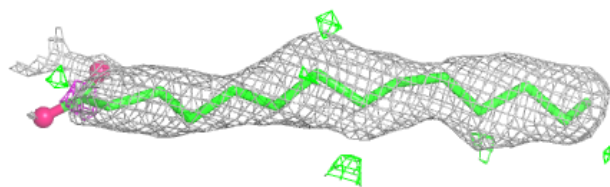
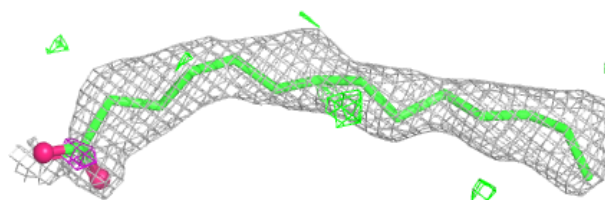


Electron density around STE B 625:

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

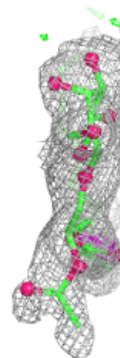
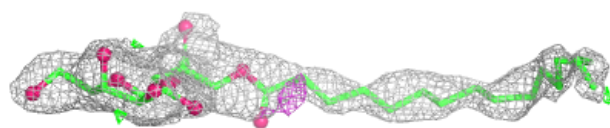
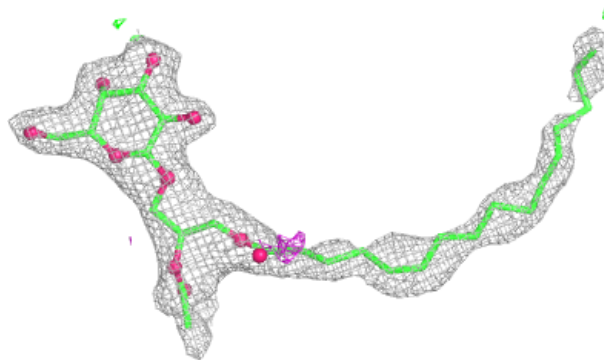
**Electron density around STE b 623:**

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

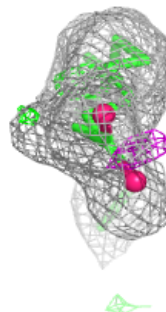
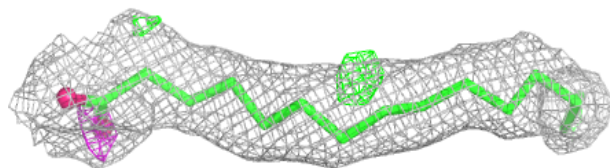
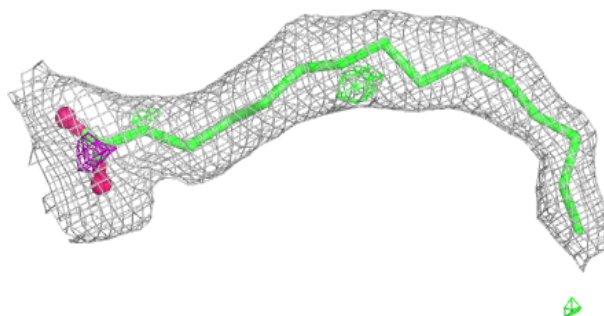


Electron density around LMG c 518:

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

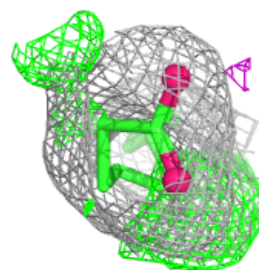
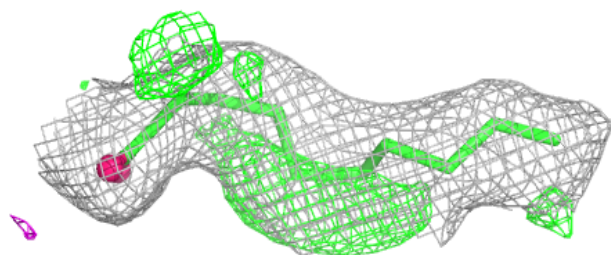
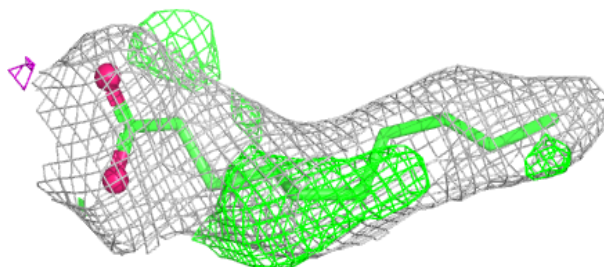
**Electron density around STE B 621:**

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

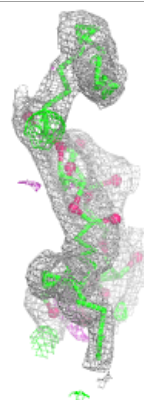
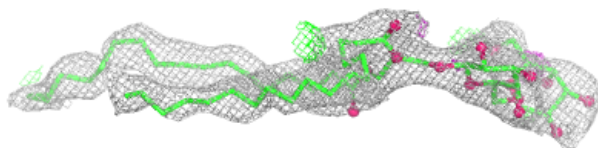
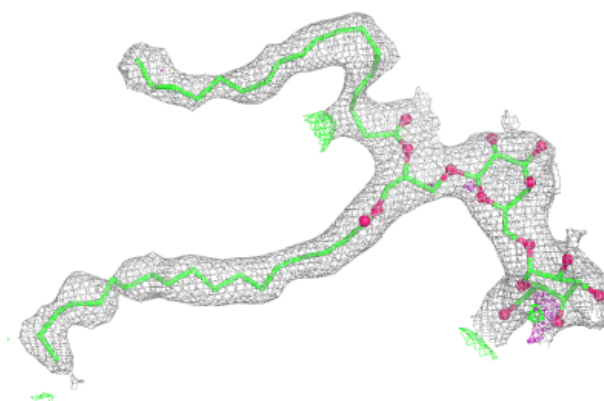


Electron density around STE B 624:

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

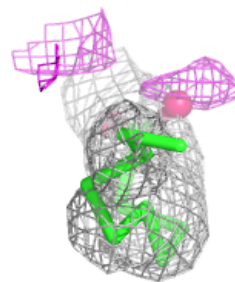
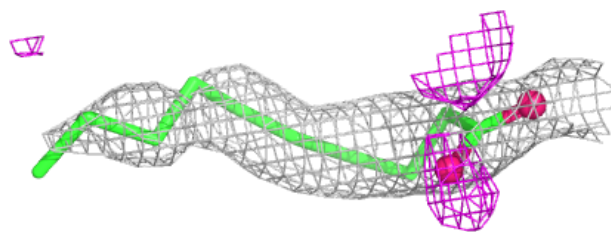
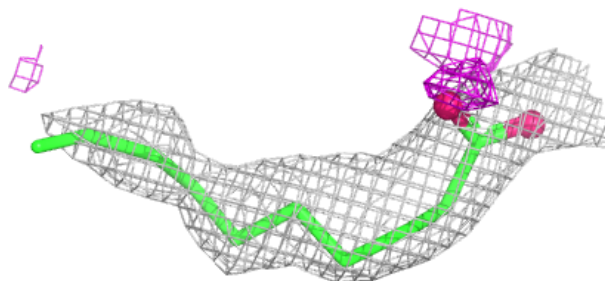
**Electron density around DGD A 616:**

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

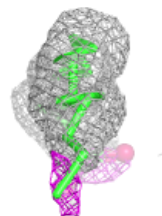
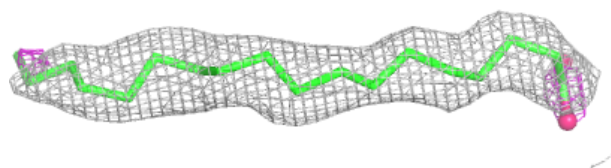
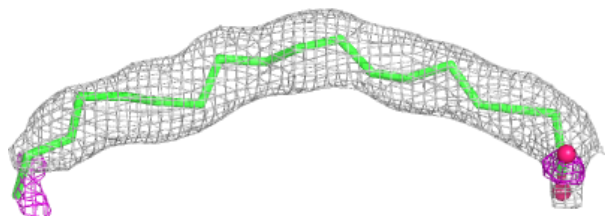


Electron density around STE B 626:

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

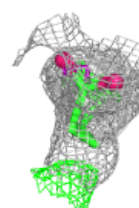
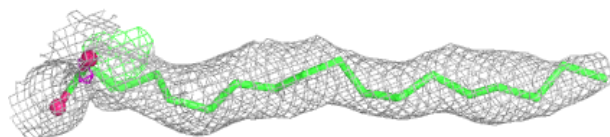
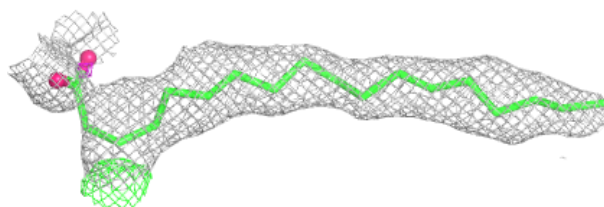
**Electron density around STE D 413:**

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

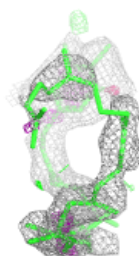
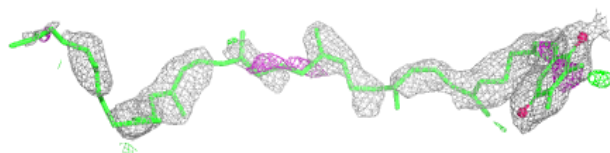
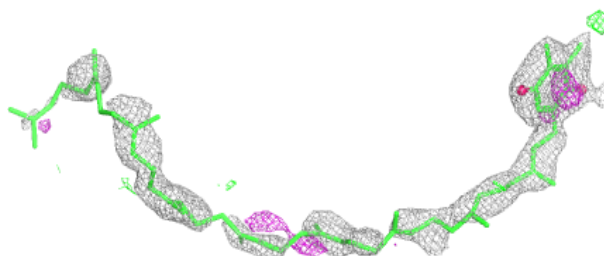


Electron density around STE c 519:

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

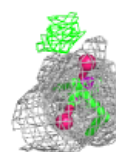
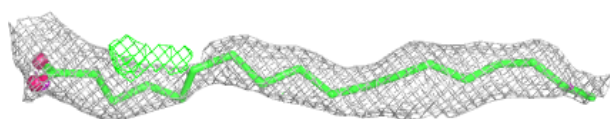
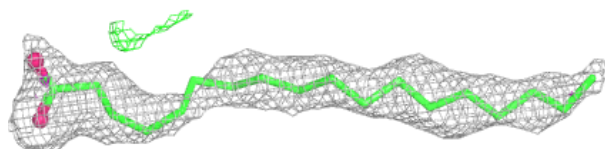
**Electron density around PL9 a 610:**

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

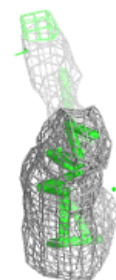
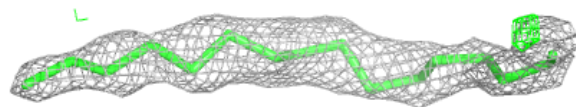
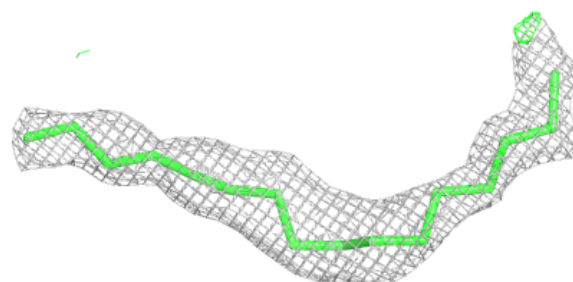


Electron density around STE A 617:

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

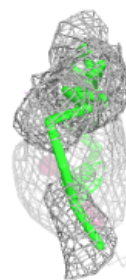
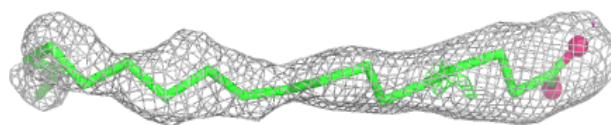
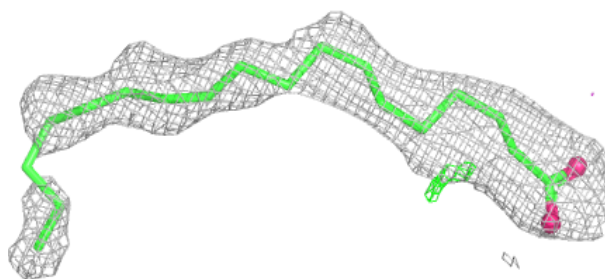
**Electron density around STE B 627:**

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

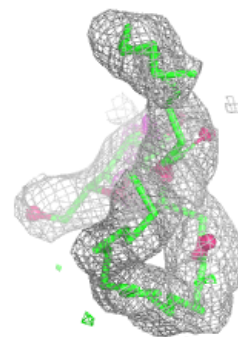
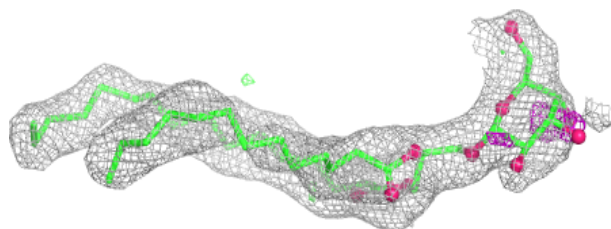
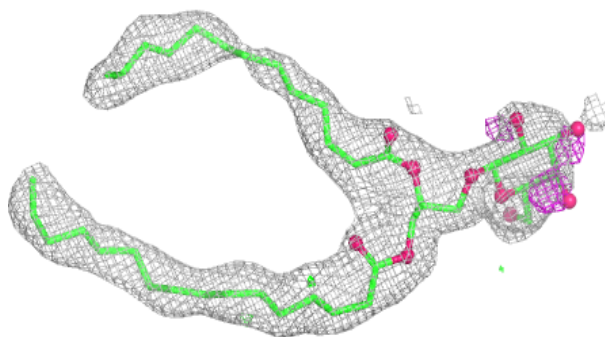


Electron density around STE d 413:

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

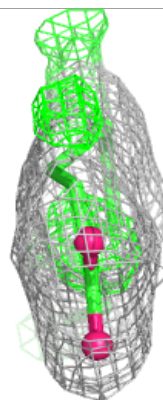
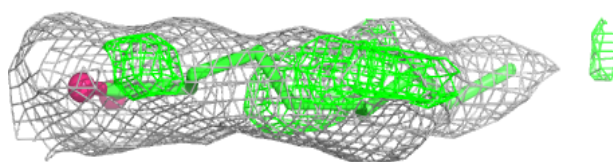
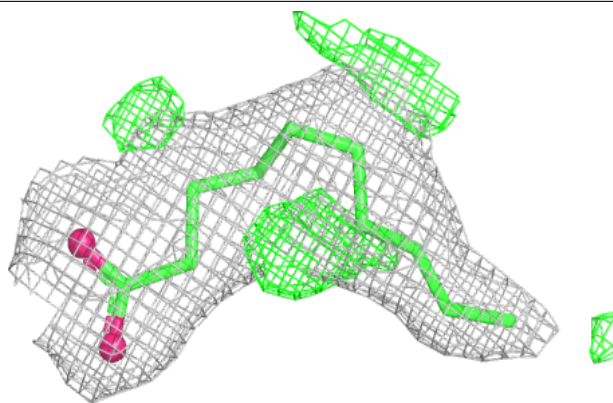
**Electron density around LMG A 612:**

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

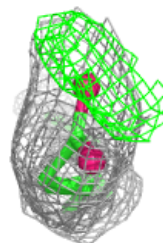
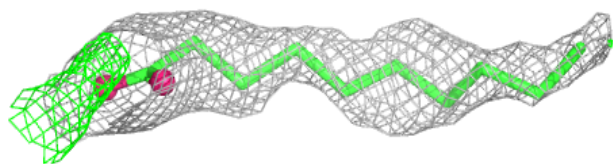
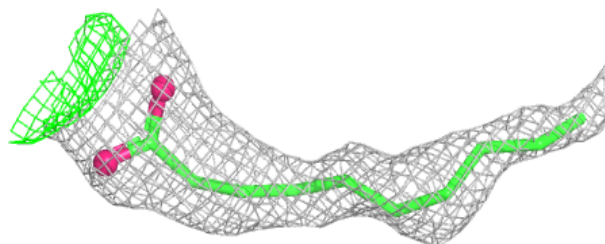


Electron density around STE C 518:

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

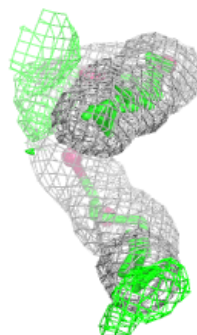
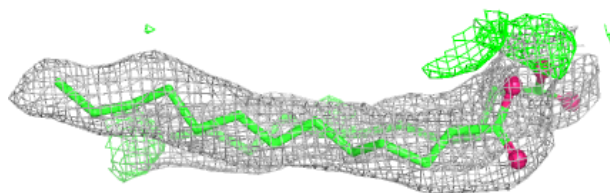
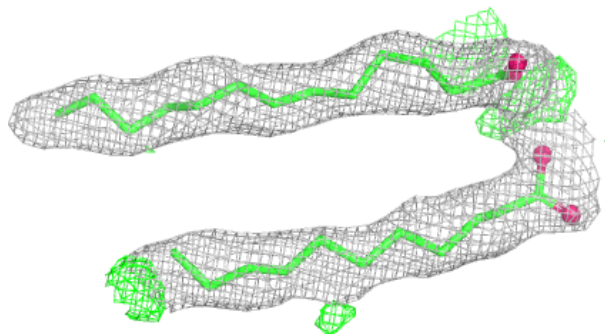
**Electron density around STE C 519:**

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

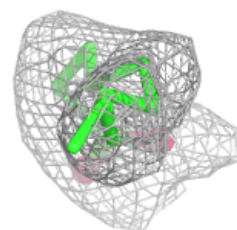
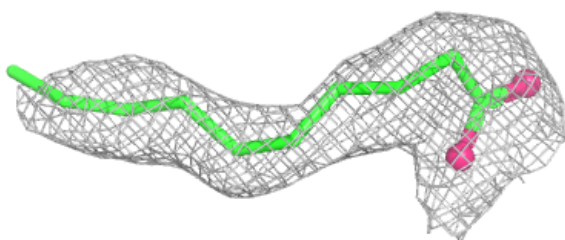
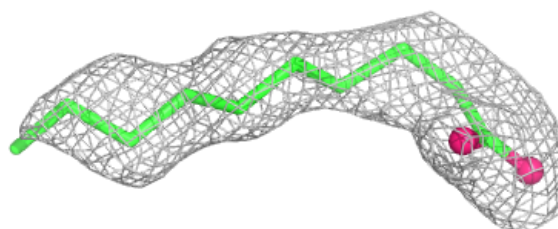


Electron density around LMG B 622:

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

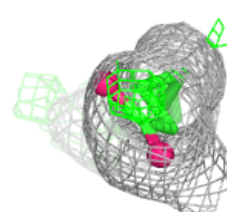
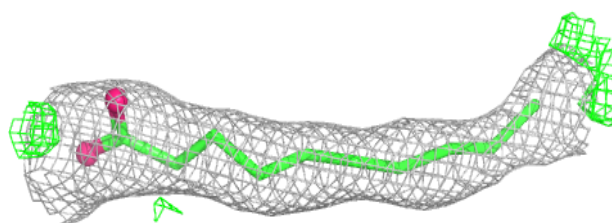
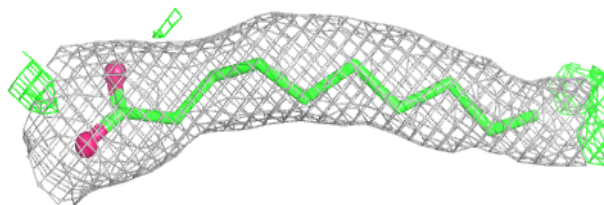
**Electron density around STE E 102:**

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

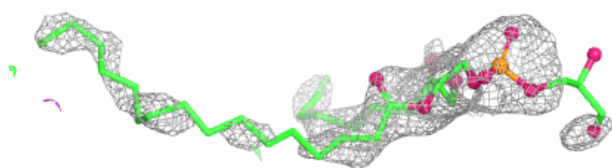
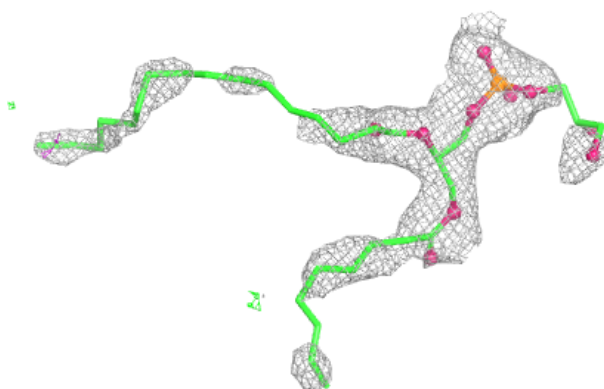


Electron density around STE j 101:

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

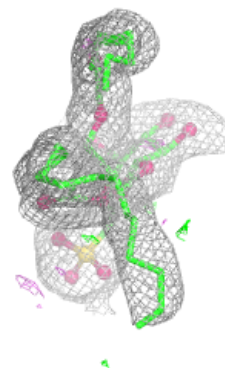
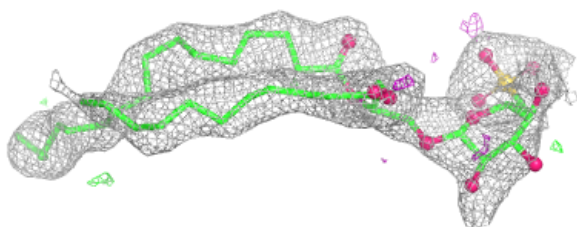
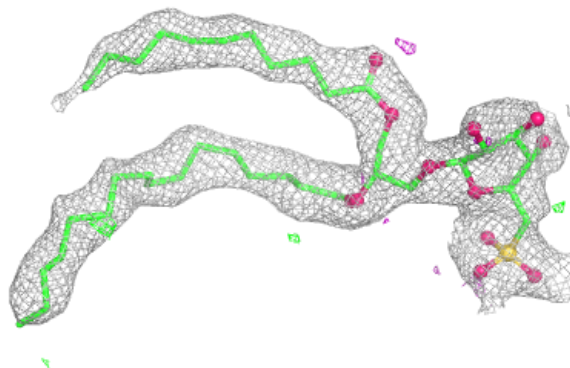
**Electron density around LHG e 101:**

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

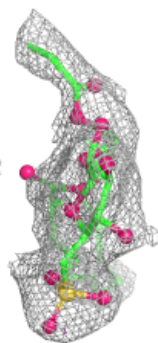
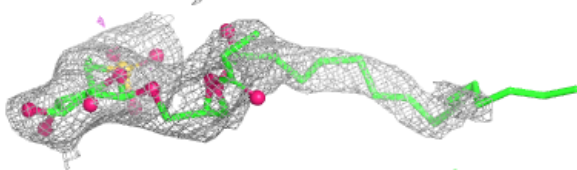
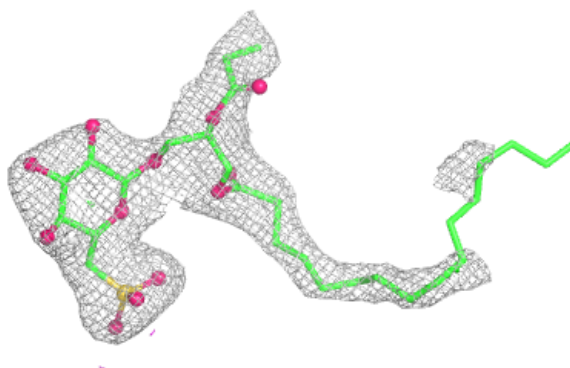


Electron density around SQD b 620:

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

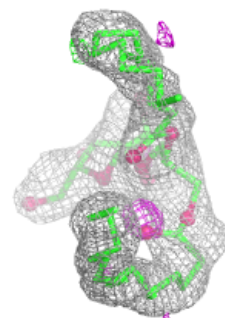
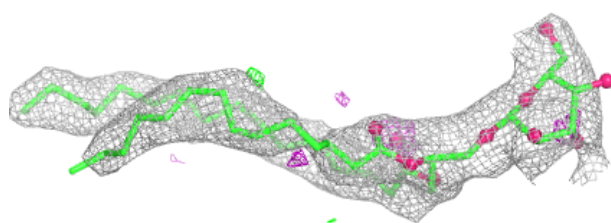
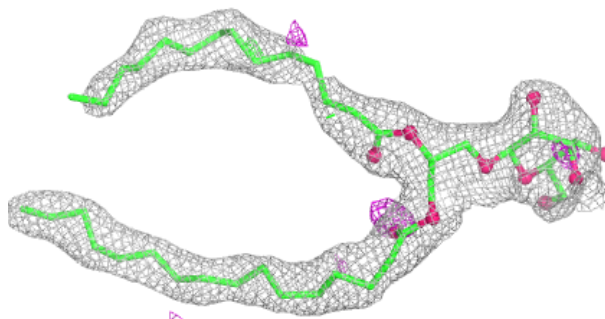
**Electron density around SQD f 102:**

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

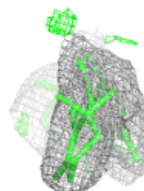
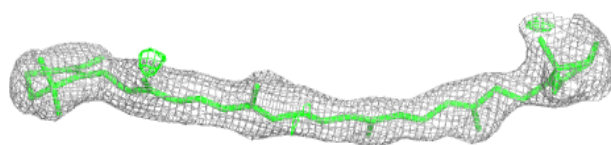
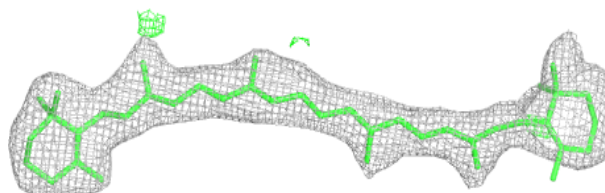


Electron density around LMG c 521:

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

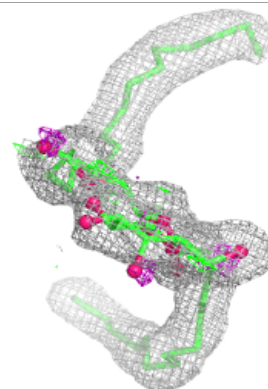
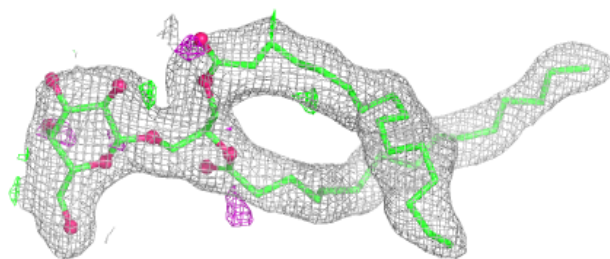
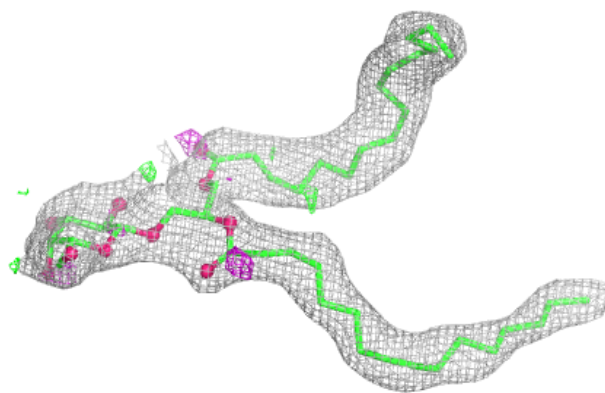
**Electron density around BCR d 405:**

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



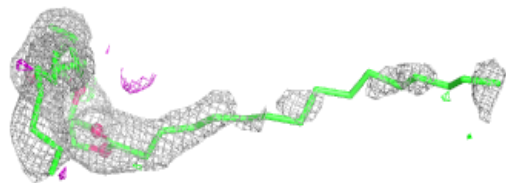
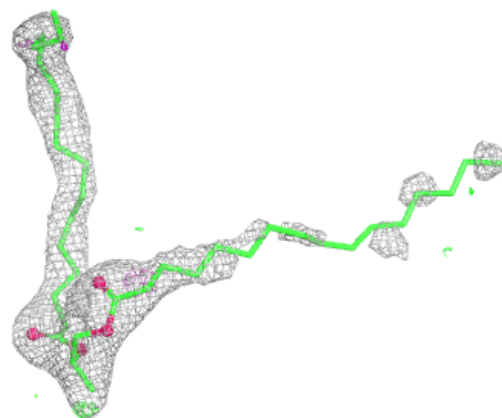
Electron density around LMG m 101:

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



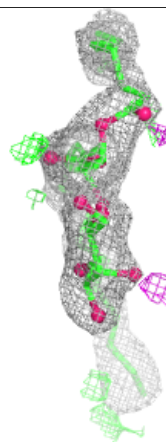
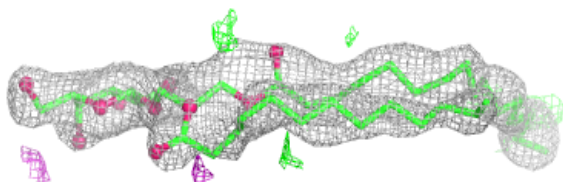
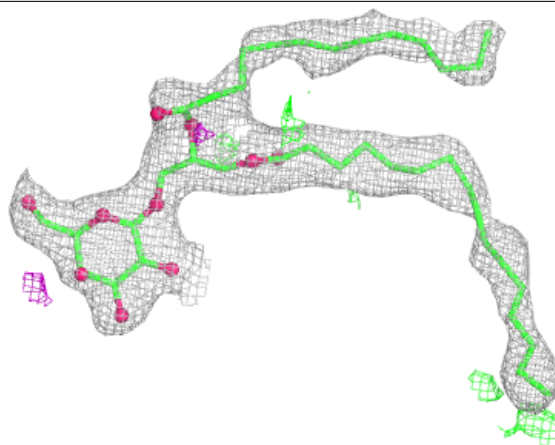
Electron density around SQD A 615:

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

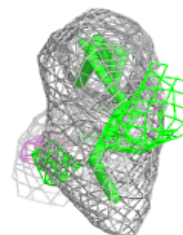
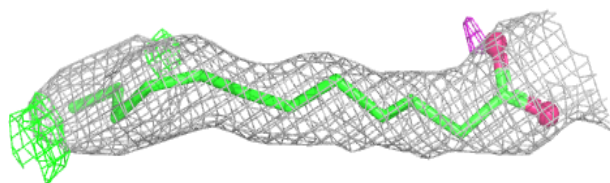
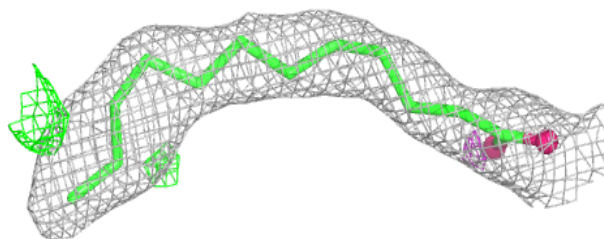


Electron density around LMG C 517:

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

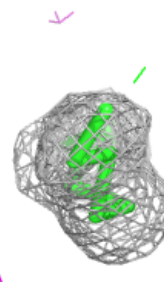
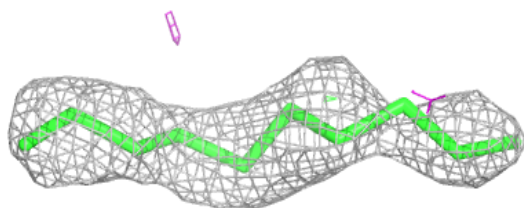
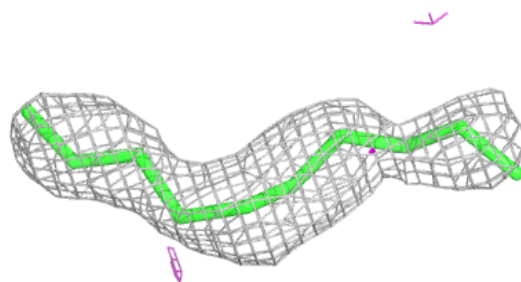
**Electron density around STE t 102:**

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

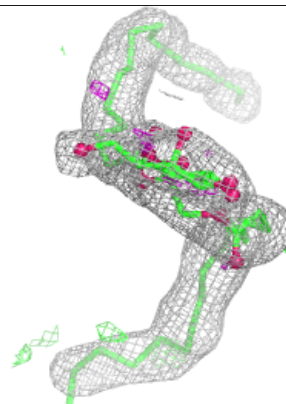
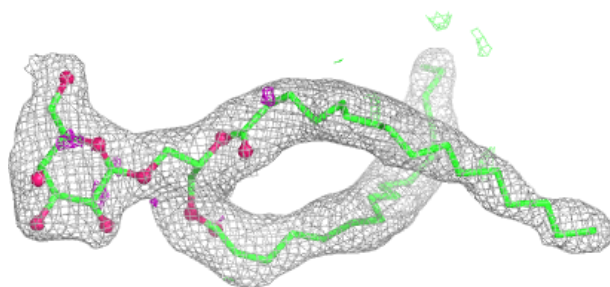
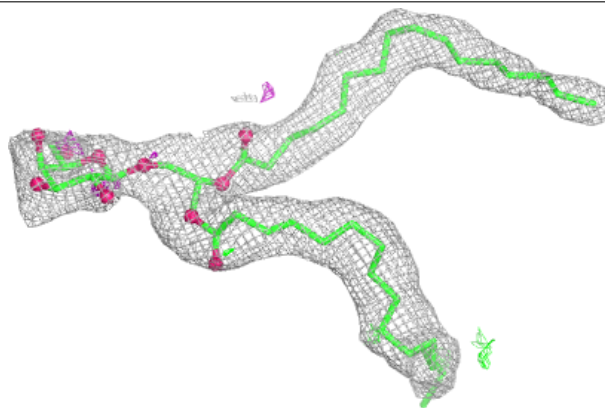


Electron density around STE t 103:

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

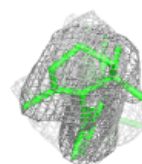
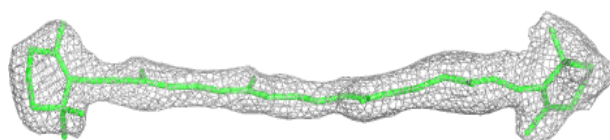
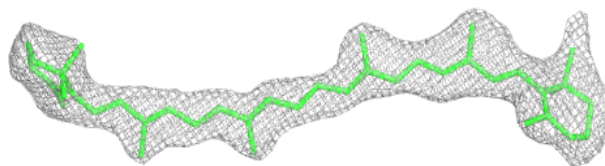
**Electron density around LMG B 620:**

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

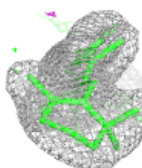
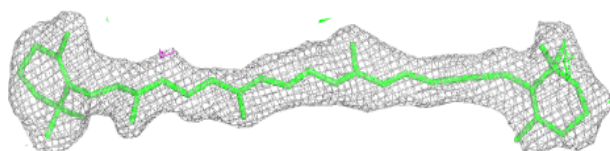
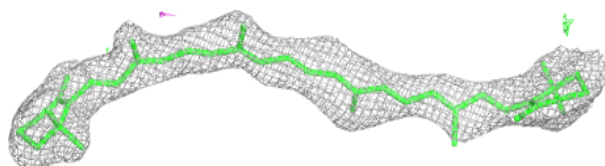


Electron density around BCR k 102:

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

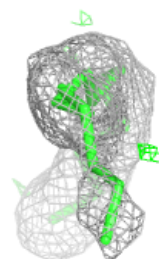
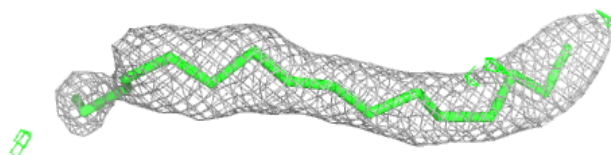
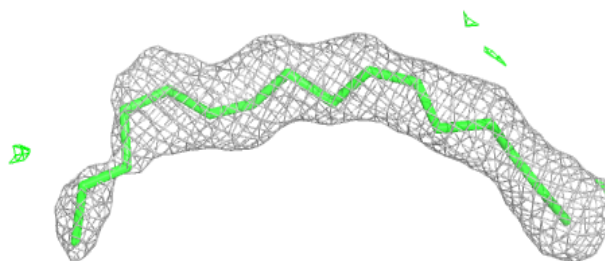
**Electron density around BCR h 101:**

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

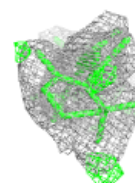
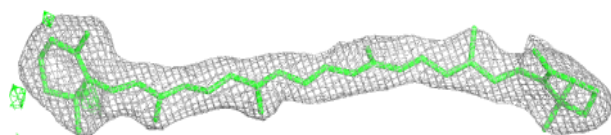
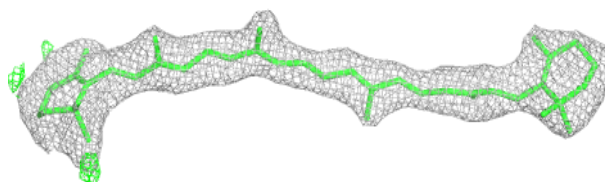


Electron density around STE T 102:

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

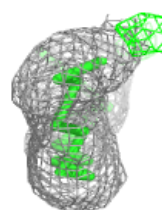
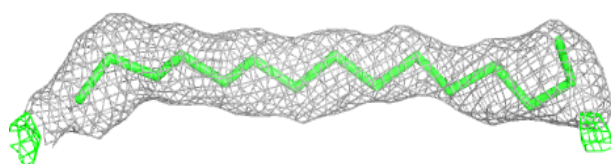
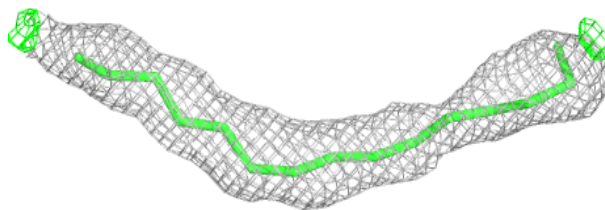
**Electron density around BCR k 101:**

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

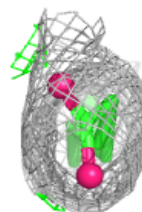
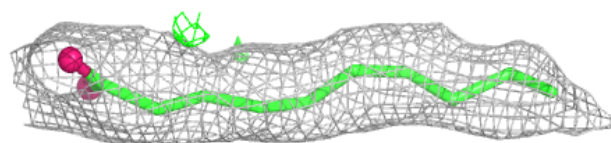
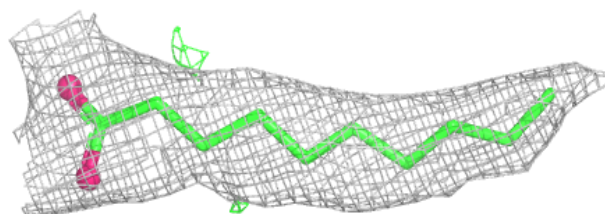


Electron density around STE I 101:

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

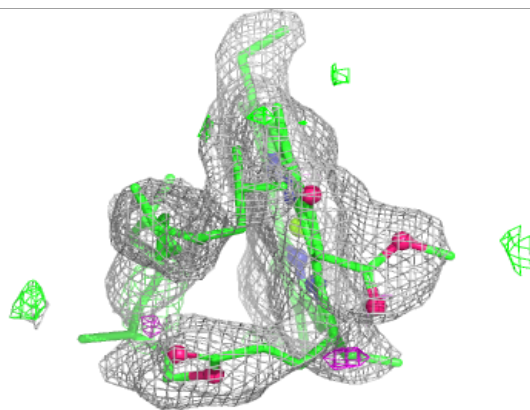
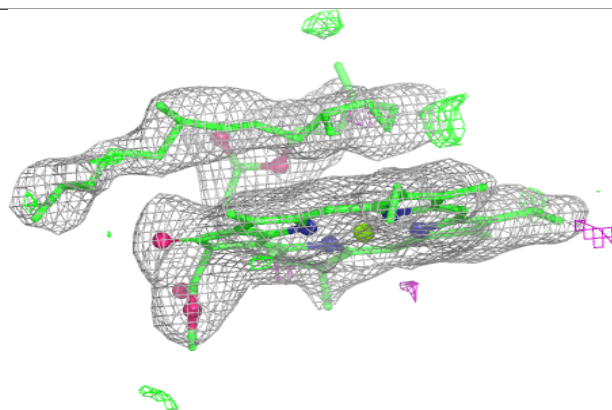
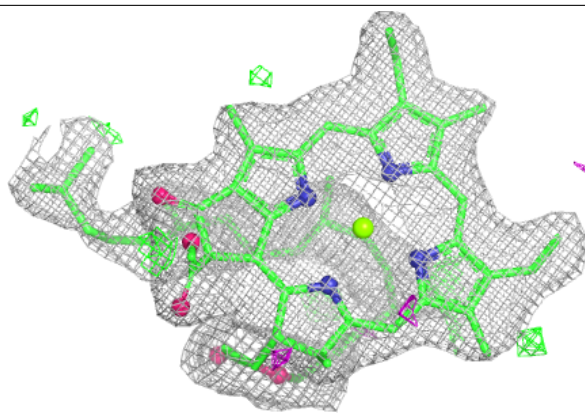
**Electron density around STE J 102:**

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

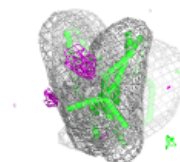
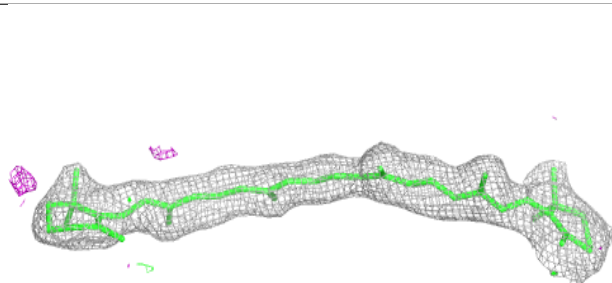
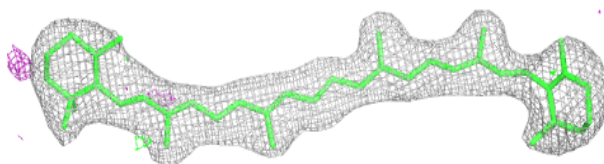


Electron density around CLA B 601:

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

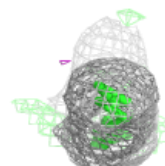
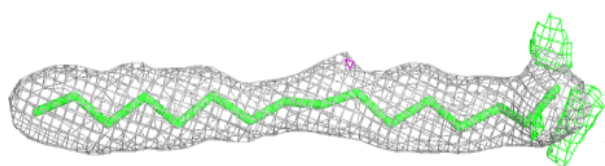
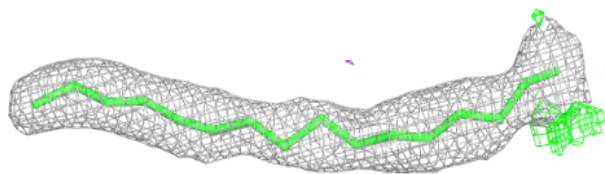
**Electron density around BCR D 405:**

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

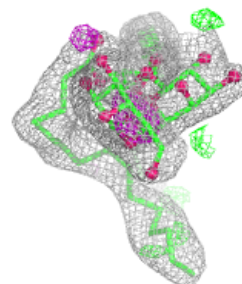
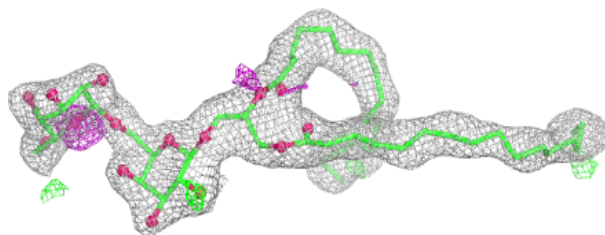
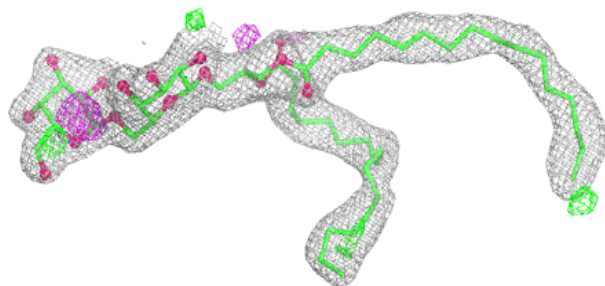


Electron density around STE C 520:

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

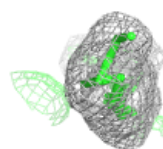
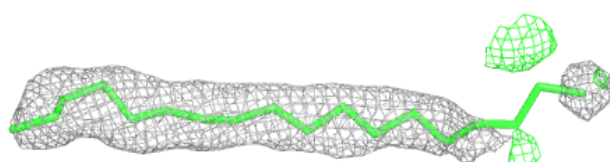
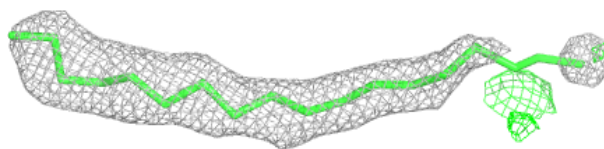
**Electron density around DGD H 102:**

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

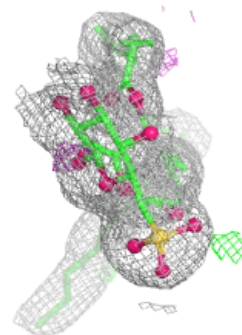
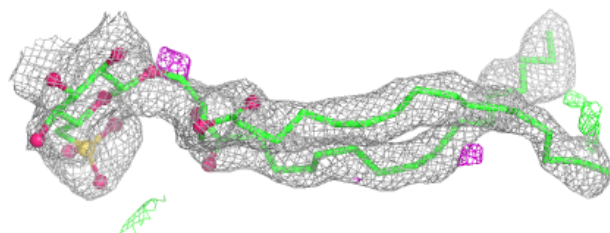
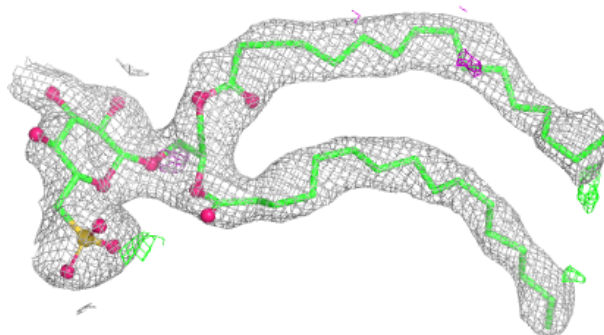


Electron density around STE m 102:

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

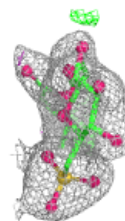
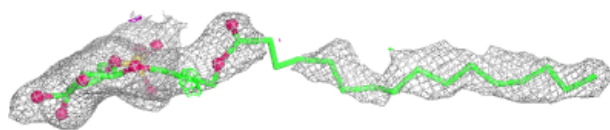
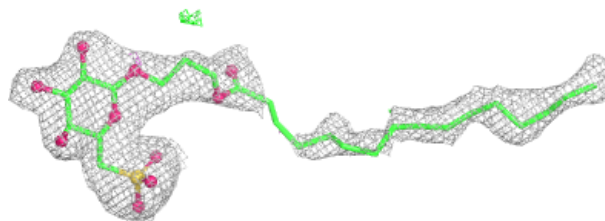
**Electron density around SQD B 623:**

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



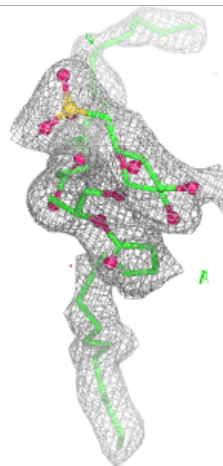
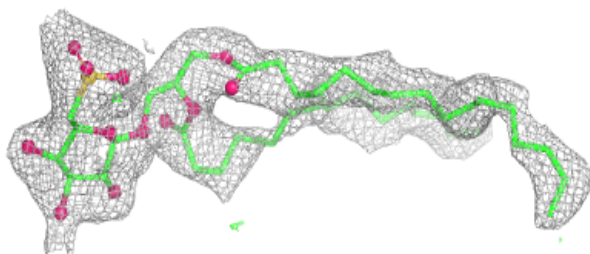
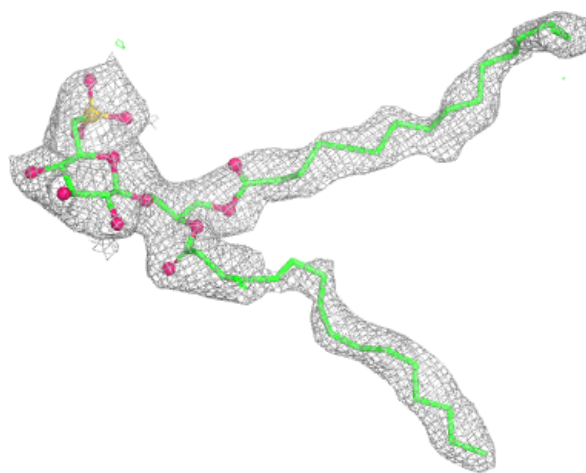
Electron density around SQD D 408:

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



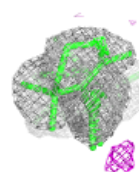
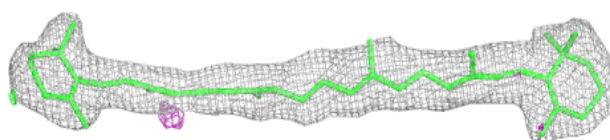
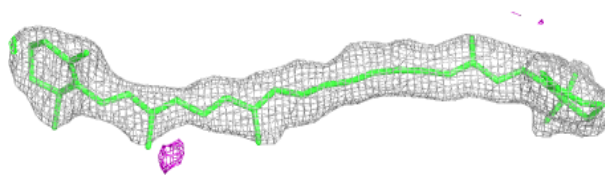
Electron density around SQD a 612:

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

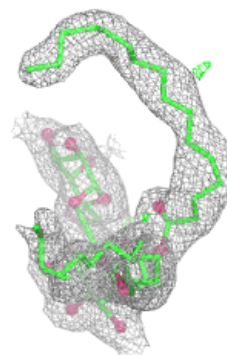
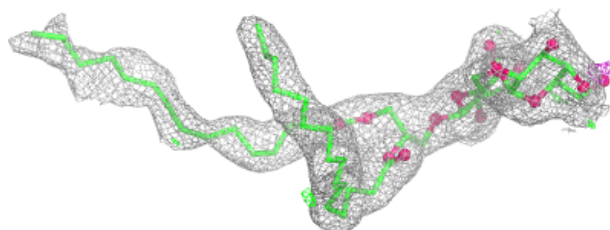
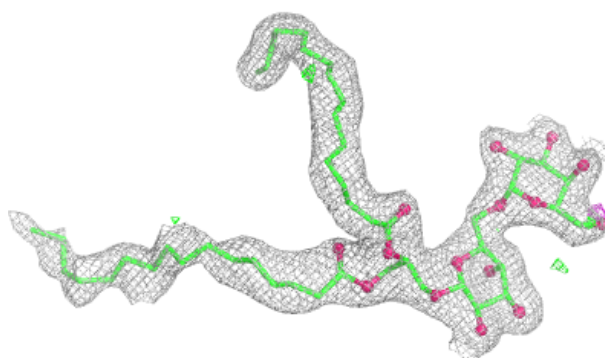


Electron density around BCR K 101:

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

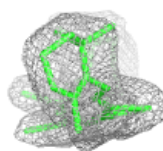
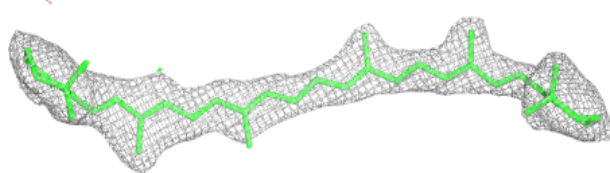
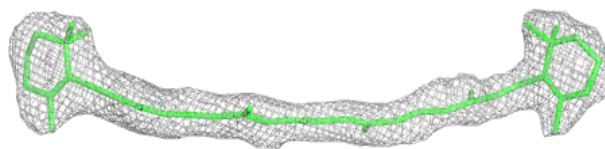
**Electron density around DGD c 516:**

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

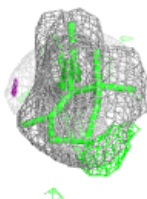
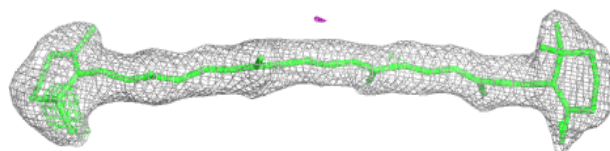
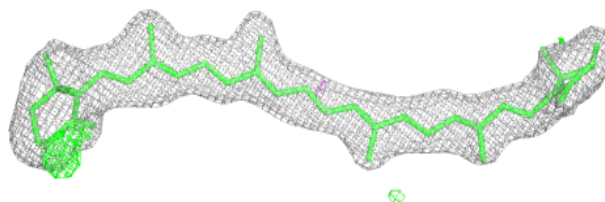


Electron density around BCR k 103:

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

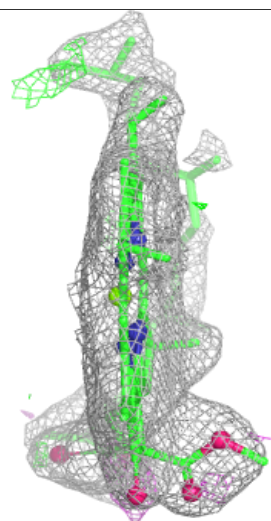
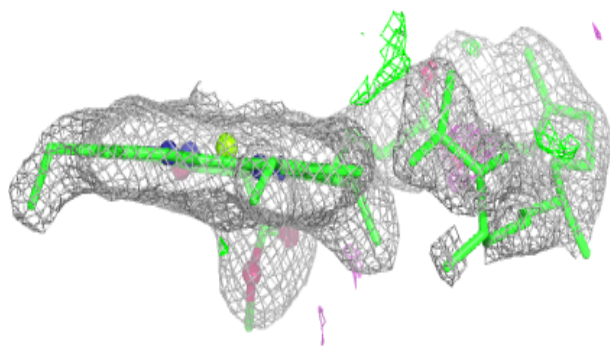
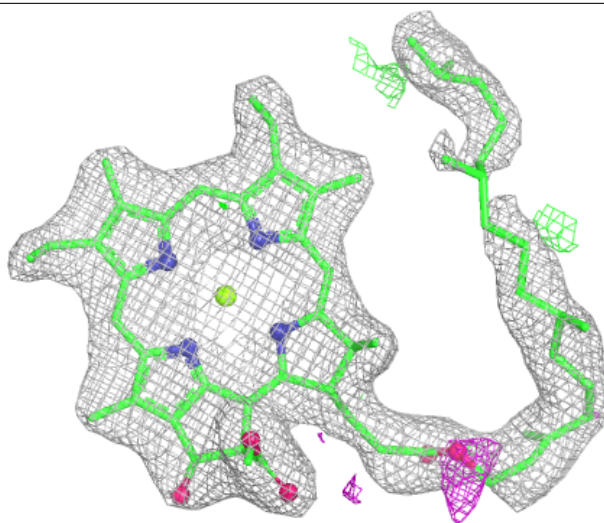
**Electron density around BCR K 102:**

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



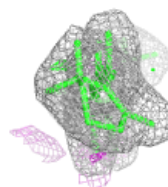
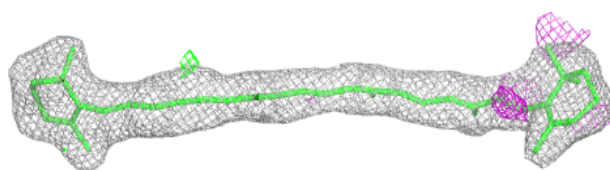
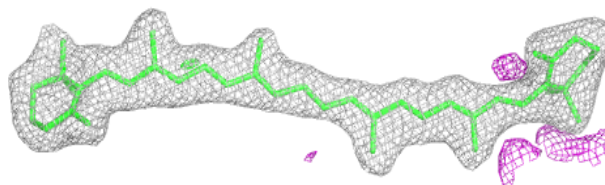
Electron density around CLA c 512:

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

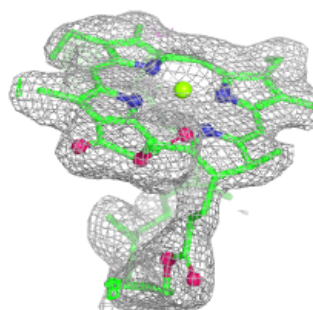
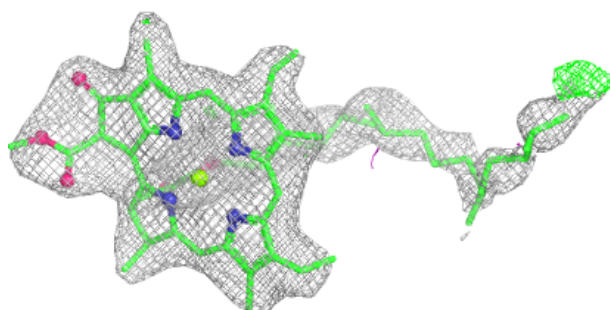
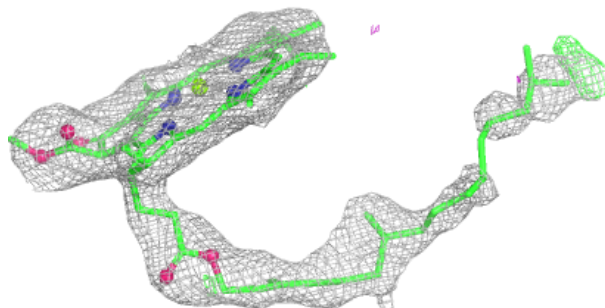


Electron density around BCR B 618:

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

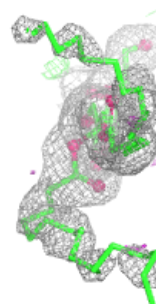
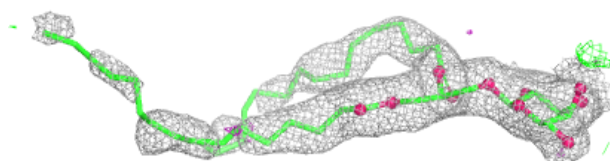
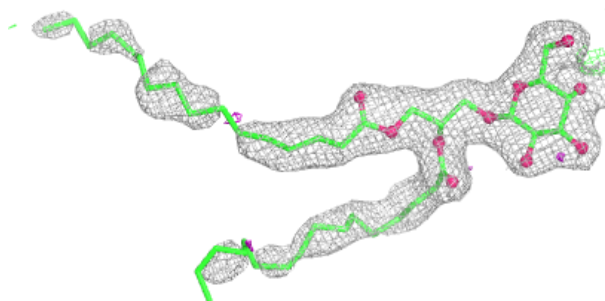
**Electron density around CLA C 513:**

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

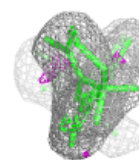
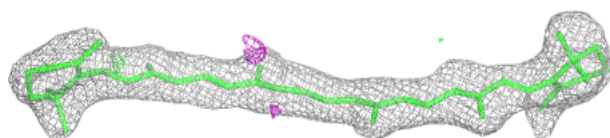
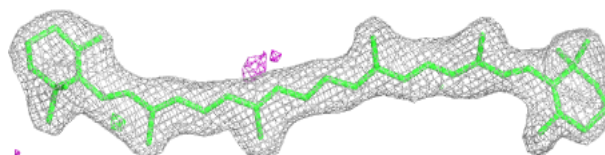


Electron density around LMG D 407:

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

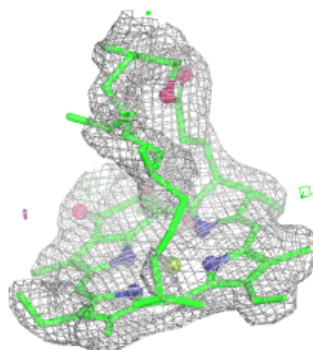
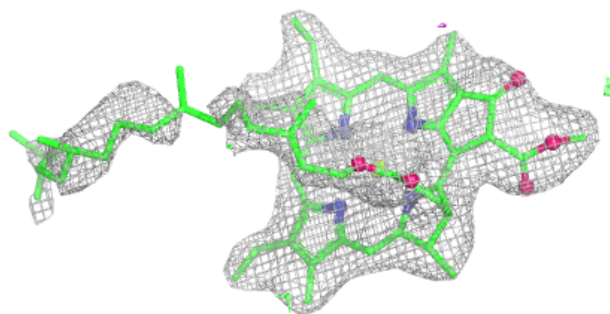
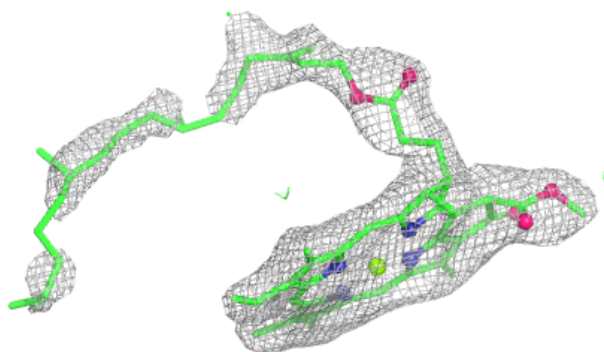
**Electron density around BCR b 619:**

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

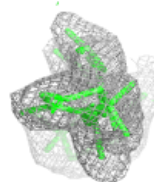
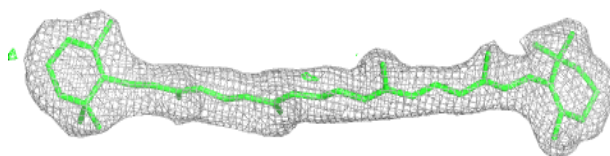
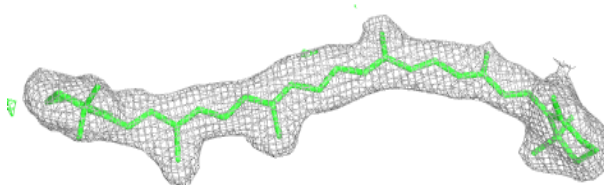


Electron density around CLA c 513:

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

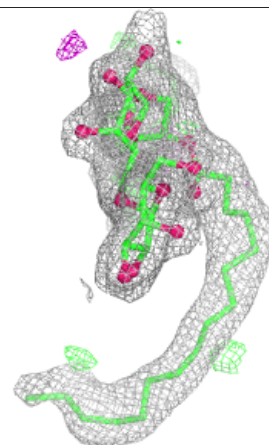
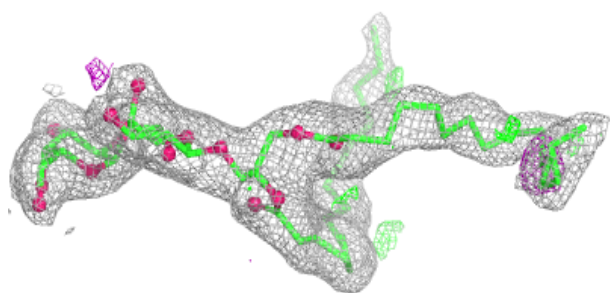
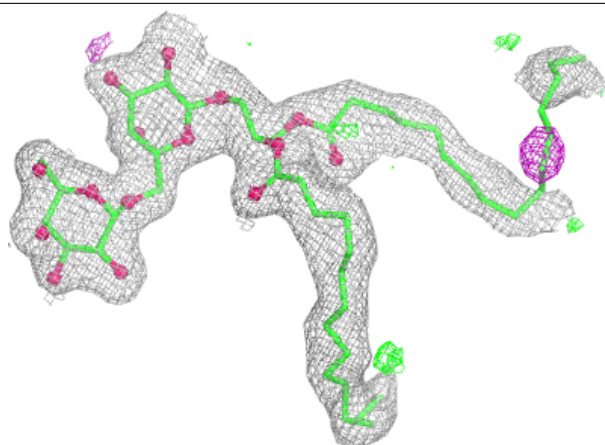
**Electron density around BCR H 101:**

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

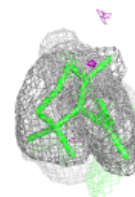
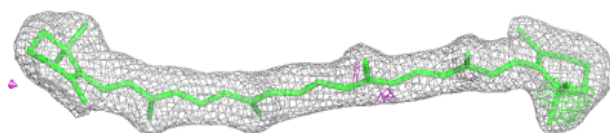
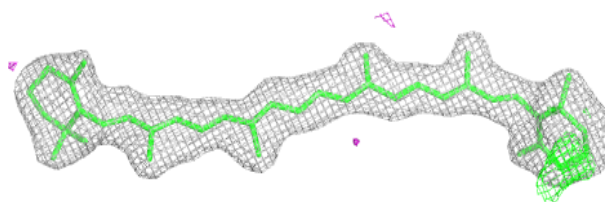


Electron density around DGD C 516:

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

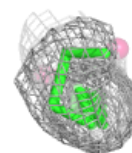
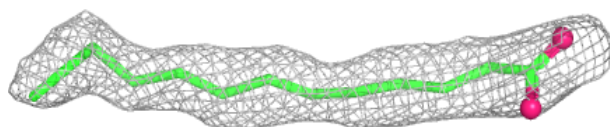
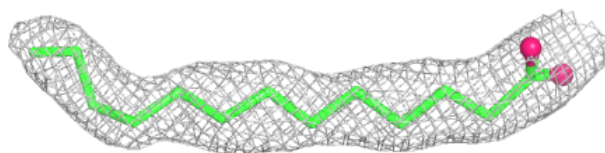
**Electron density around BCR B 619:**

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

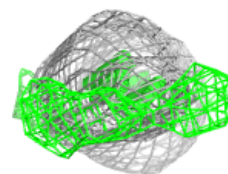
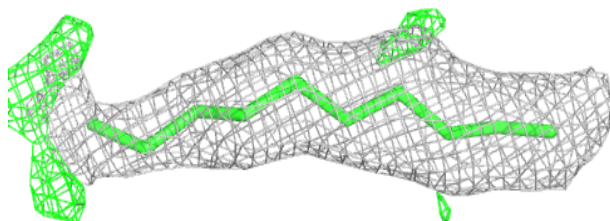
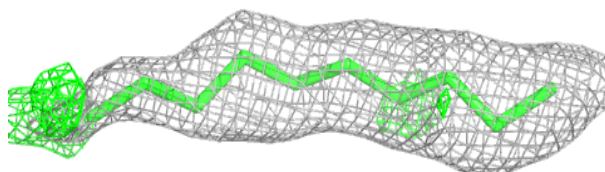


Electron density around STE M 101:

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

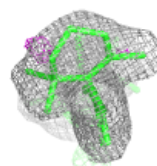
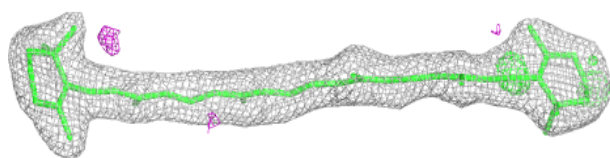
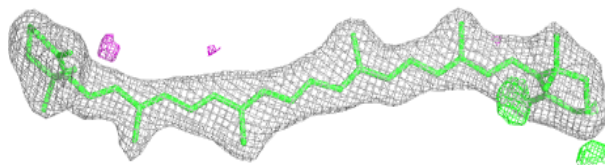
**Electron density around STE M 102:**

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

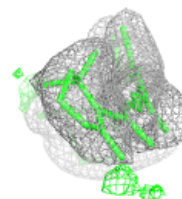
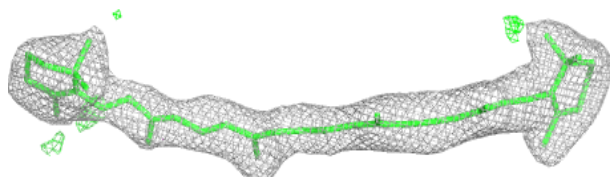
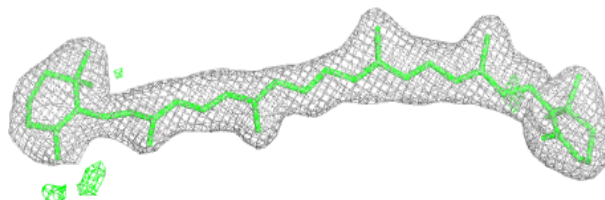


Electron density around BCR C 514:

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

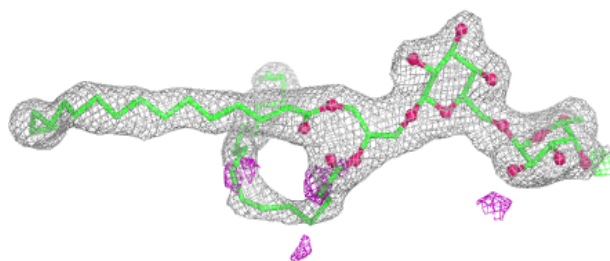
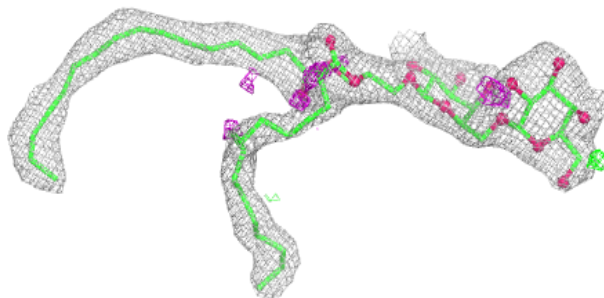
**Electron density around BCR T 101:**

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



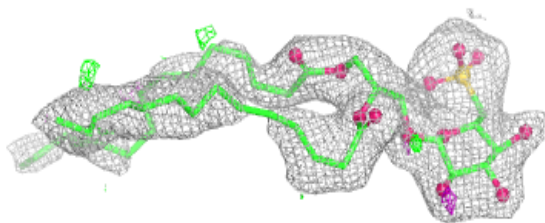
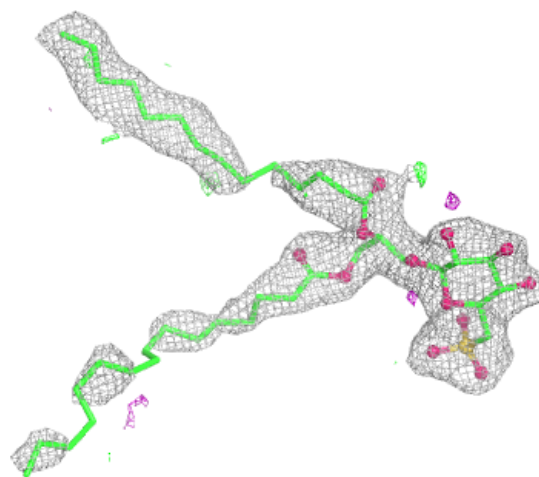
Electron density around DGD h 102:

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



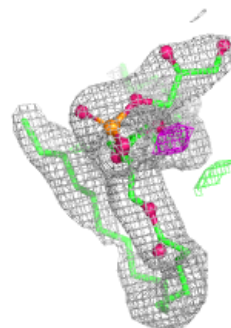
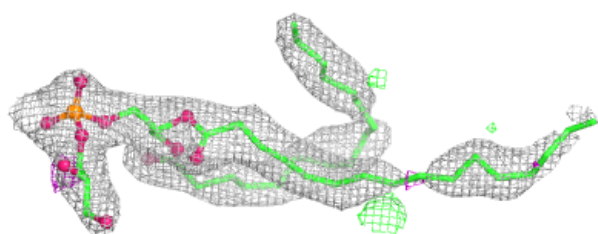
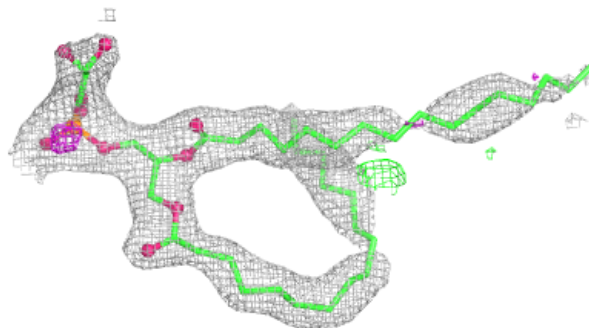
Electron density around SQD A 613:

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

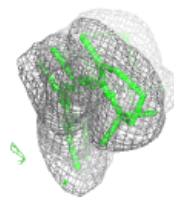
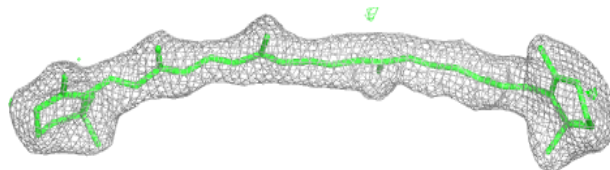
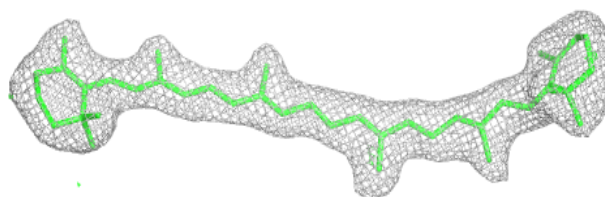


Electron density around LHG d 407:

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

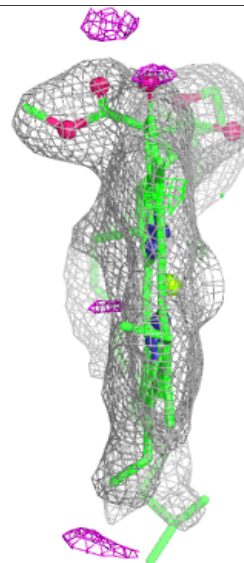
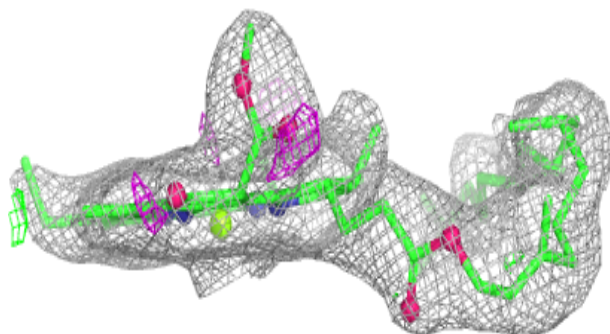
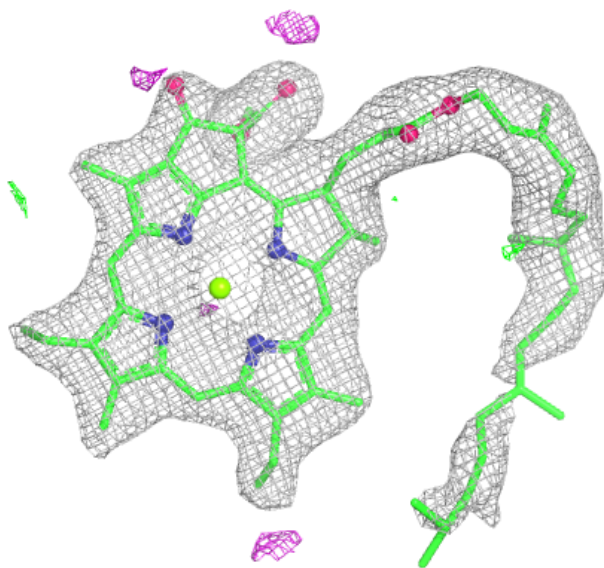
**Electron density around BCR t 101:**

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



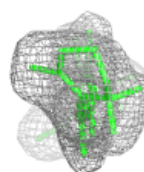
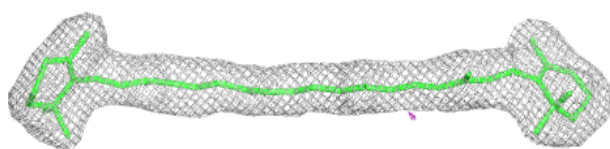
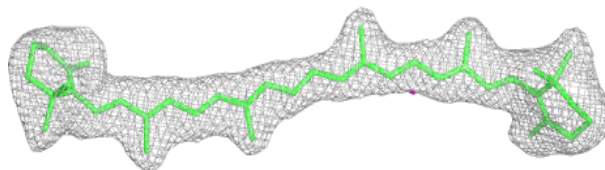
Electron density around CLA C 512:

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

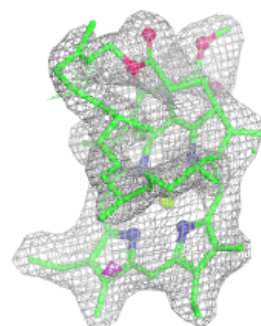
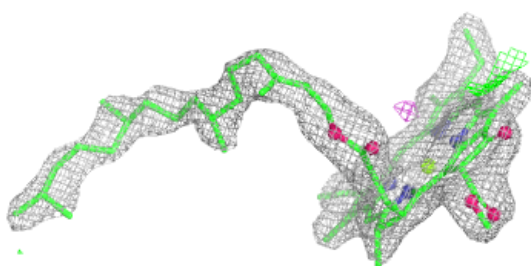
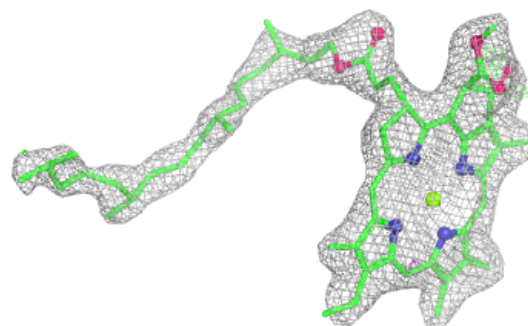


Electron density around BCR b 618:

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

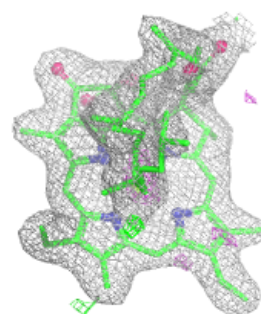
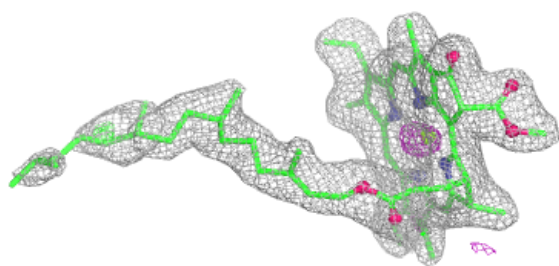
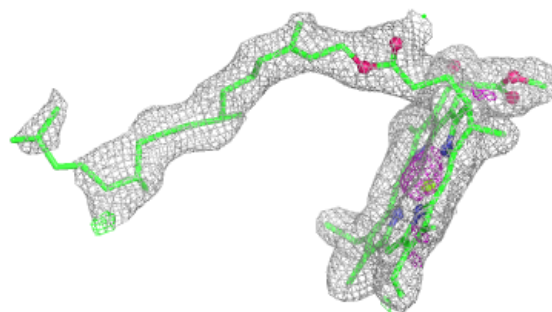
**Electron density around CLA c 511:**

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

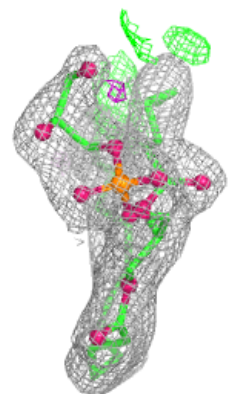
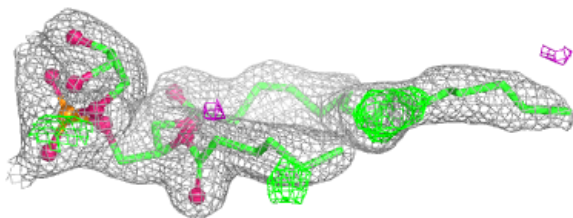
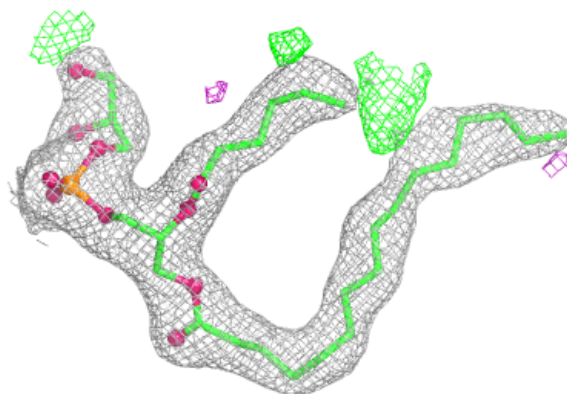


Electron density around CLA C 508:

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

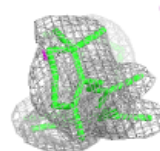
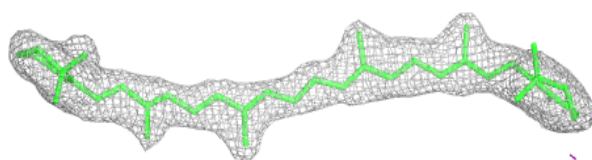
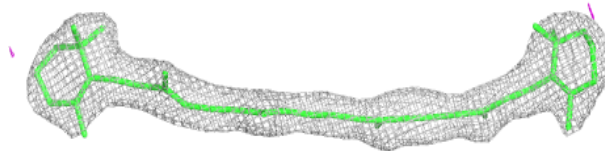
**Electron density around LHG d 409:**

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

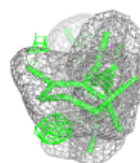
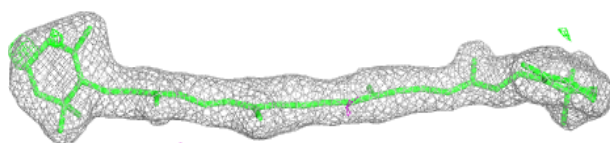
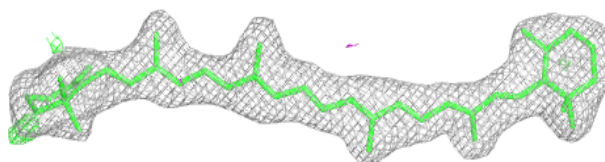


Electron density around BCR K 103:

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

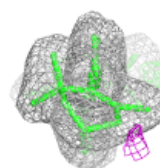
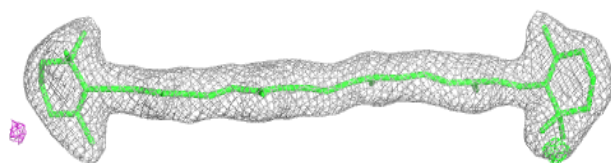
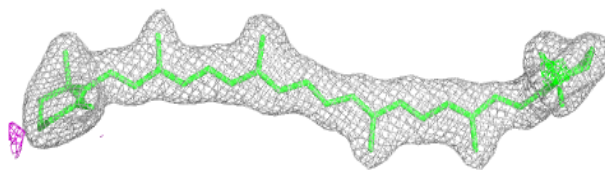
**Electron density around BCR b 617:**

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



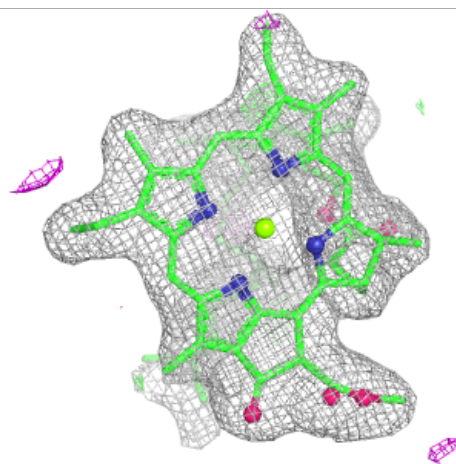
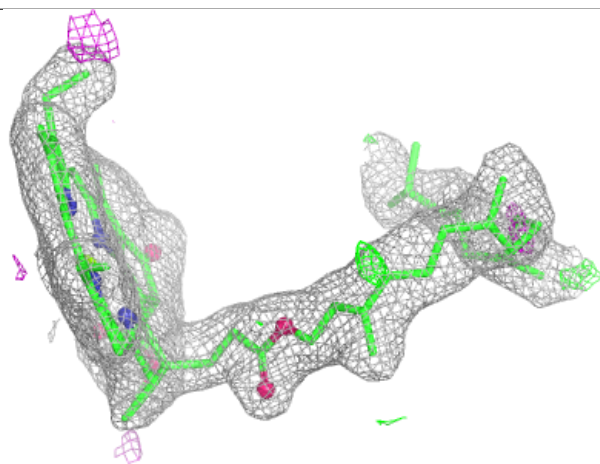
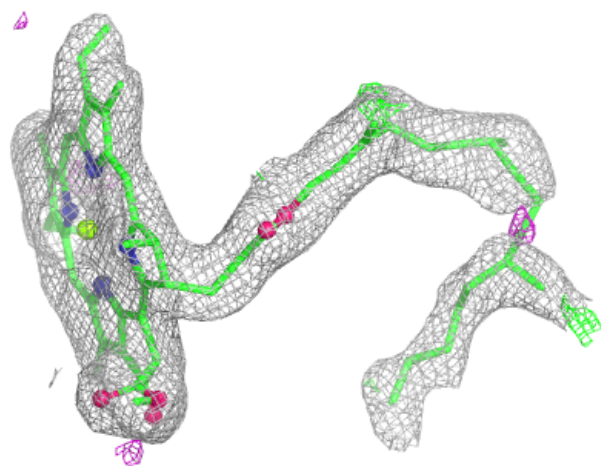
Electron density around BCR A 609:

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



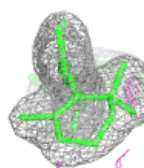
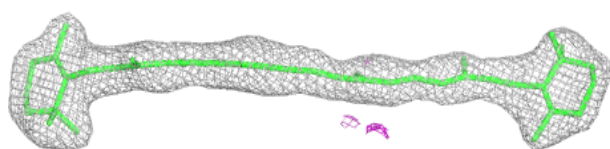
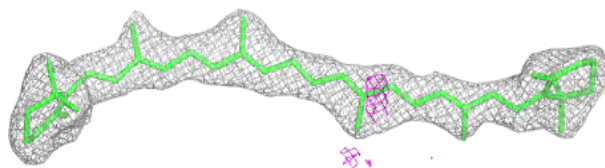
Electron density around CLA B 606:

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

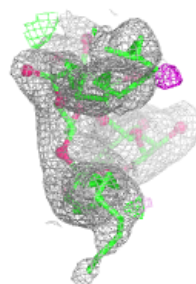
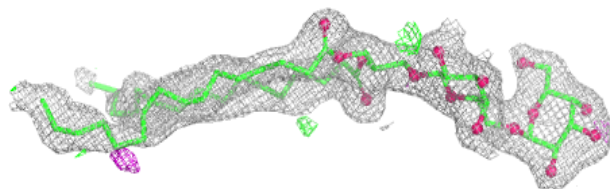
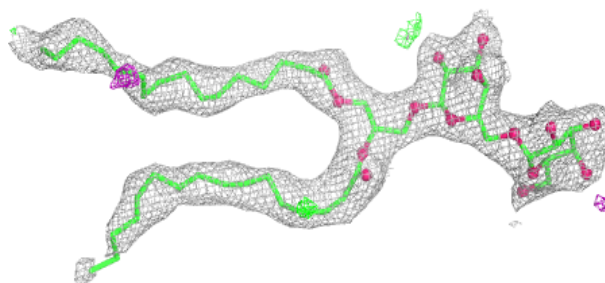


Electron density around BCR c 514:

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

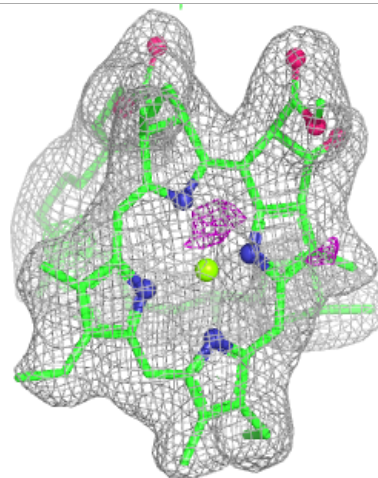
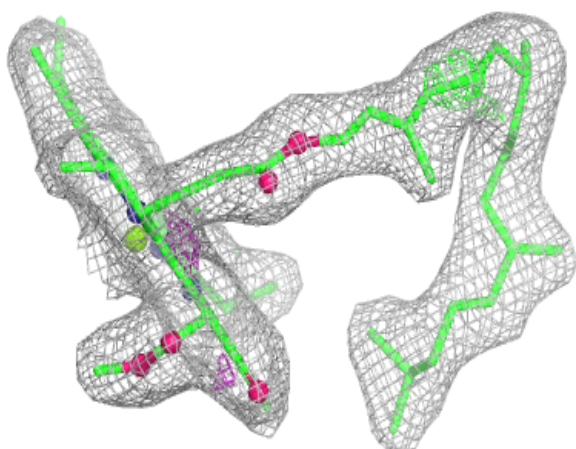
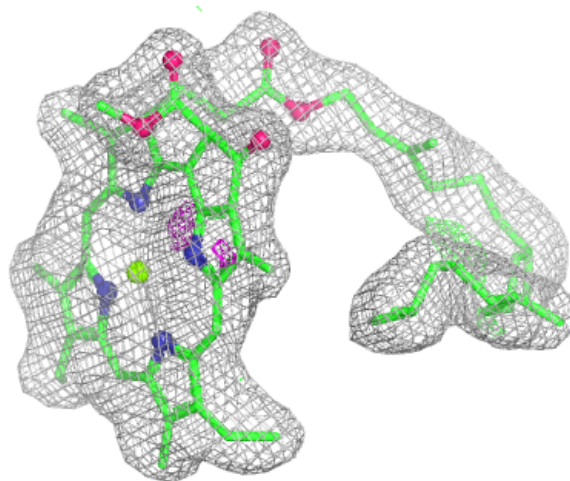
**Electron density around DGD c 517:**

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



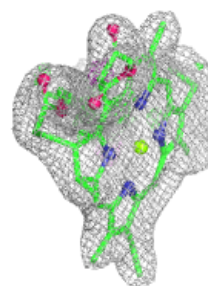
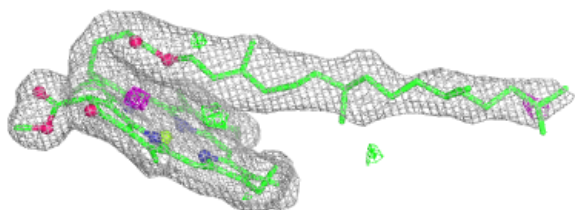
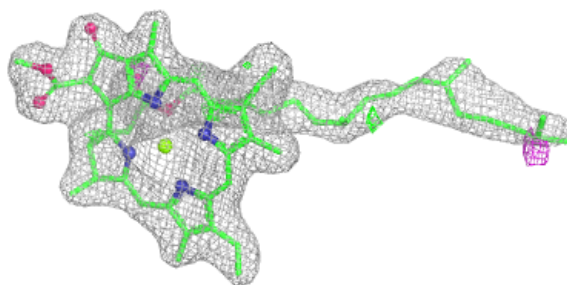
Electron density around CLA C 503:

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



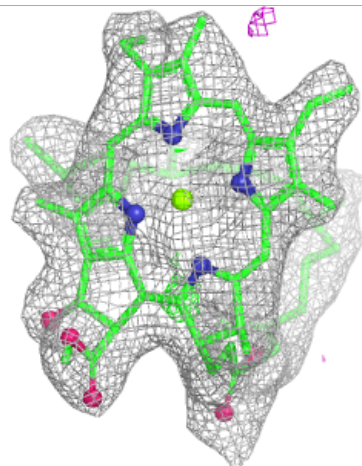
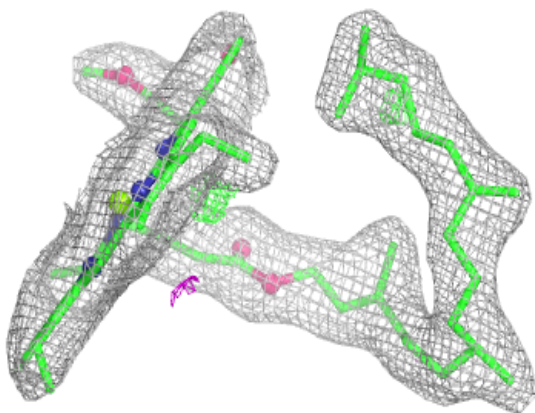
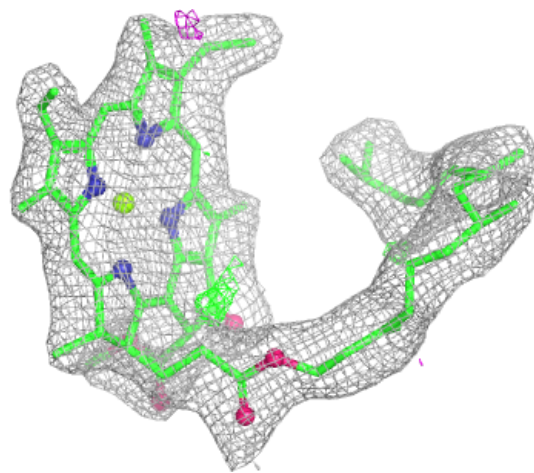
Electron density around CLA b 614:

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



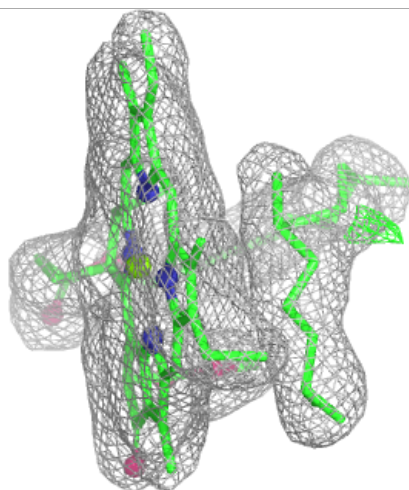
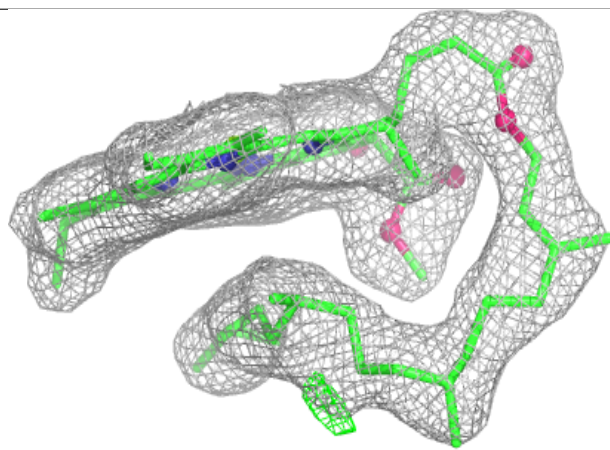
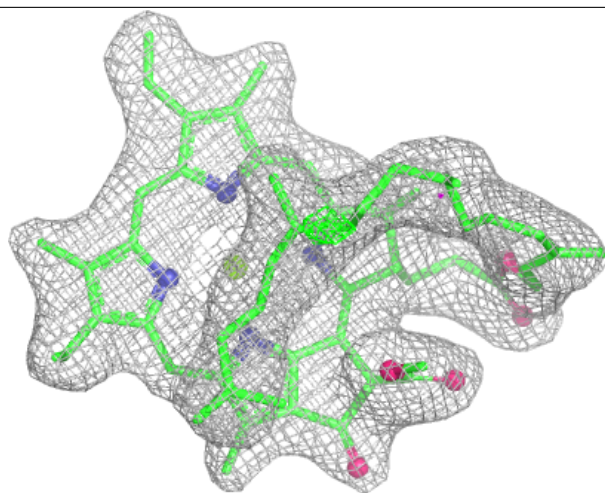
Electron density around CLA c 503:

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



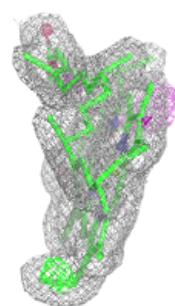
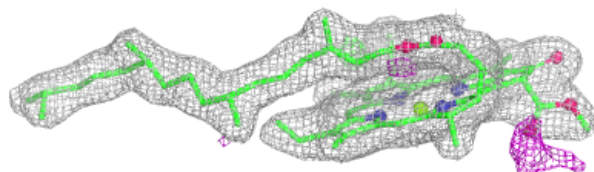
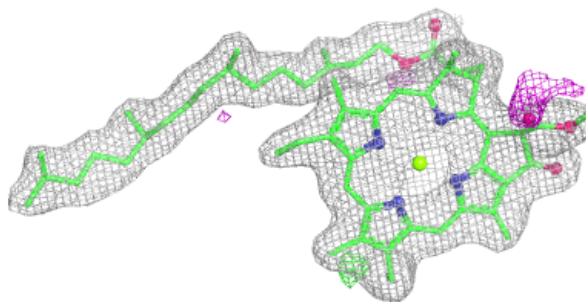
Electron density around CLA c 510:

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

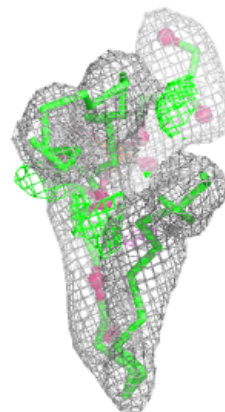
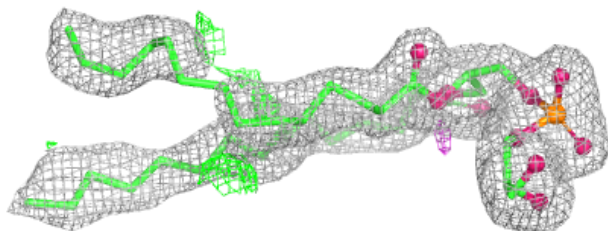
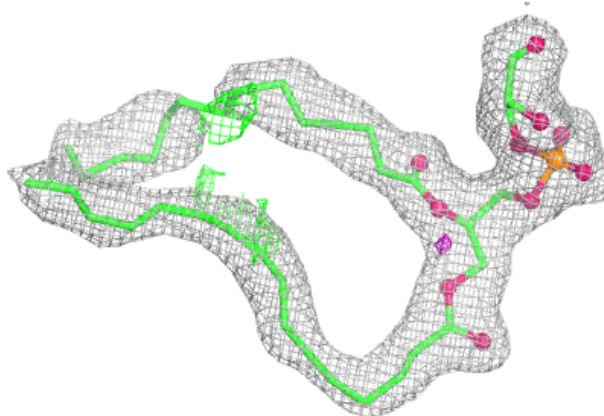


Electron density around CLA C 501:

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

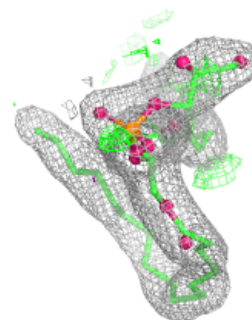
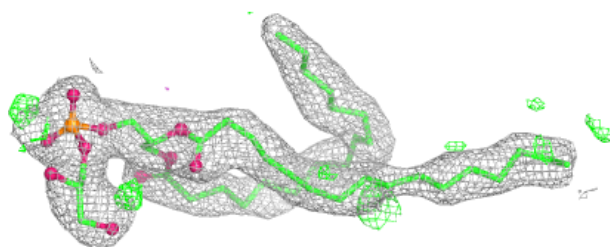
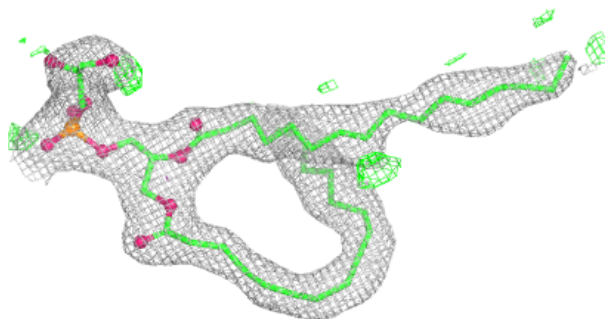
**Electron density around LHG D 410:**

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

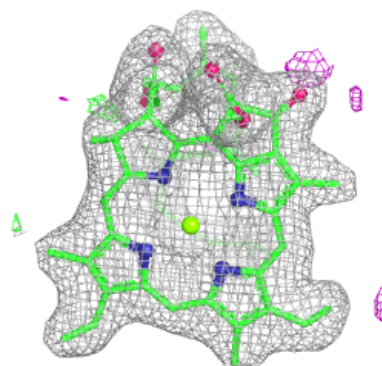
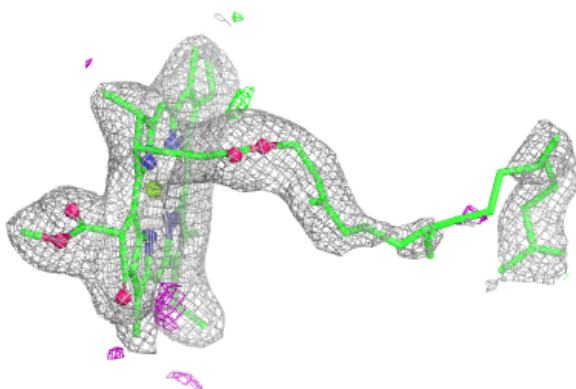
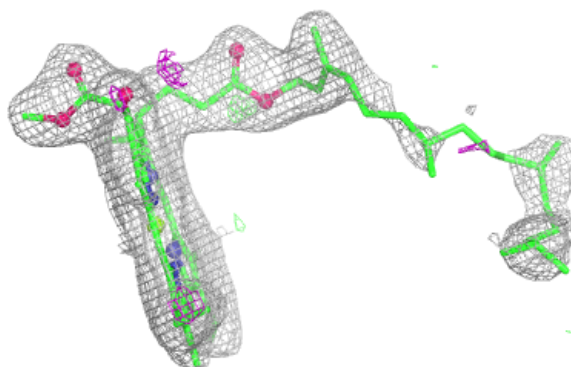


Electron density around LHG D 412:

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

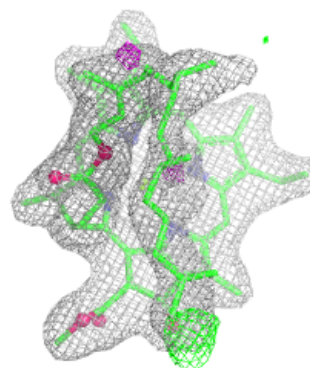
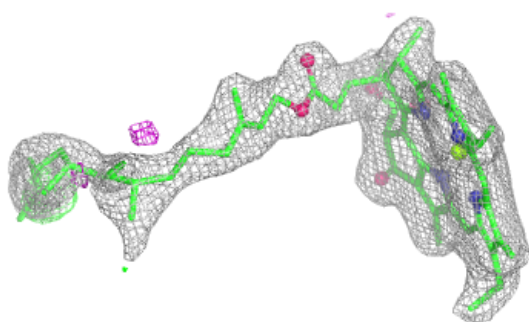
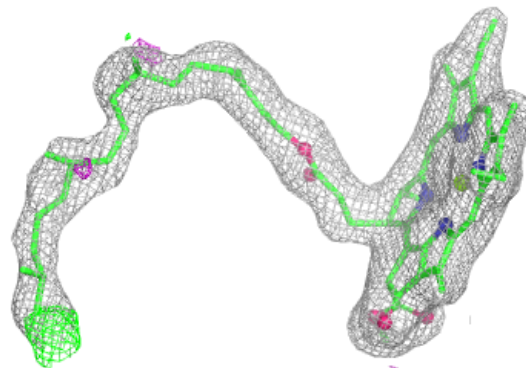
**Electron density around CLA C 506:**

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



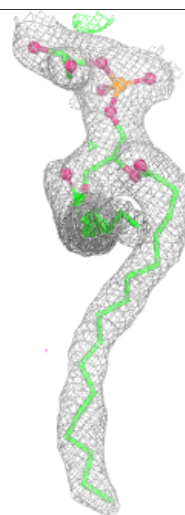
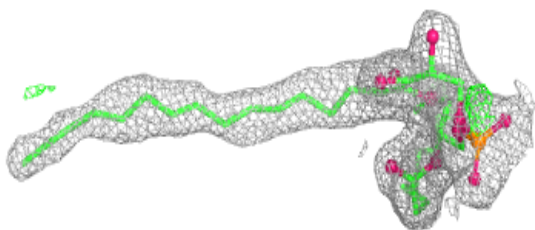
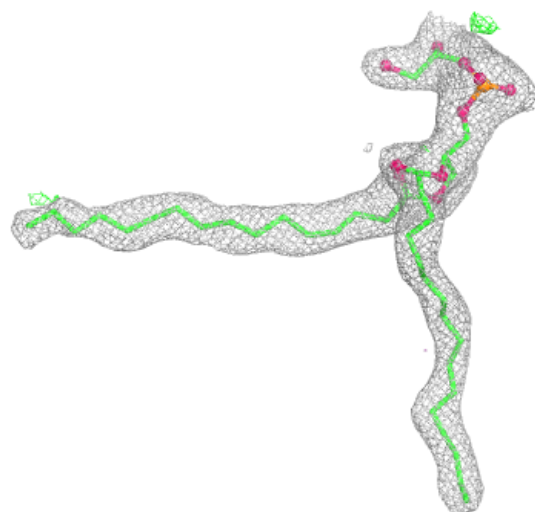
Electron density around CLA b 606:

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



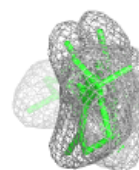
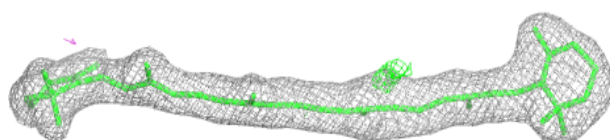
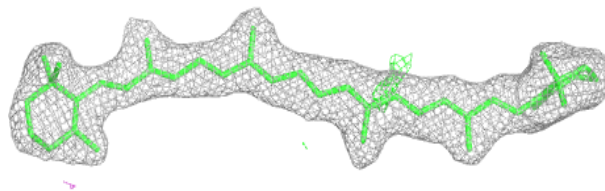
Electron density around LHG 1 101:

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

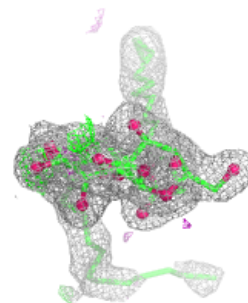
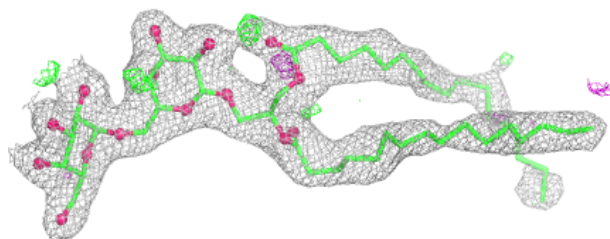
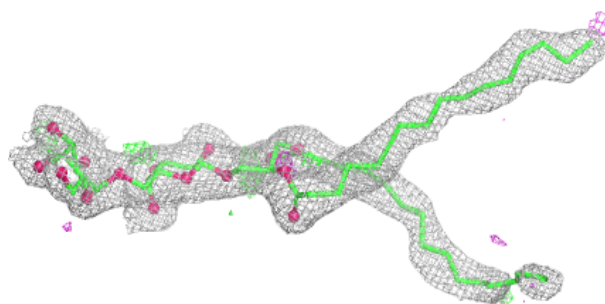


Electron density around BCR B 617:

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

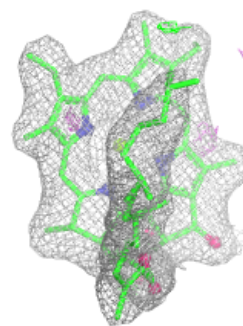
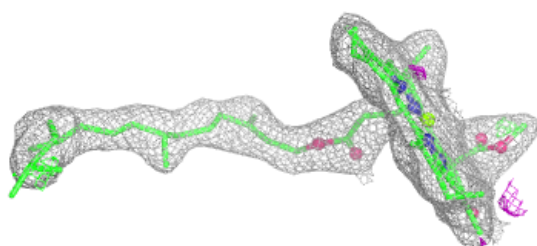
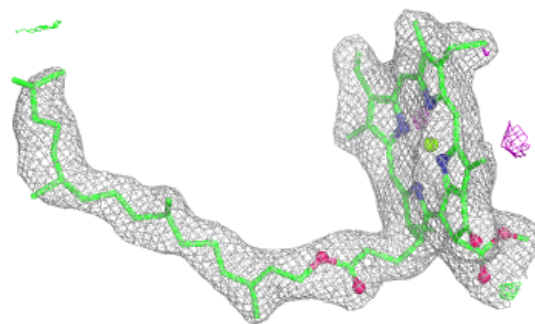
**Electron density around DGD C 515:**

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



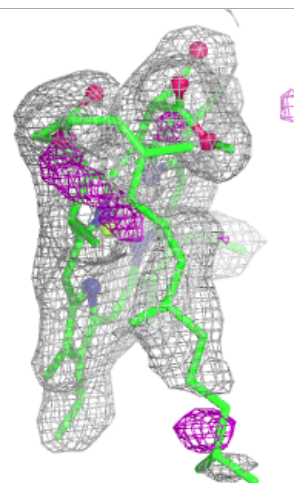
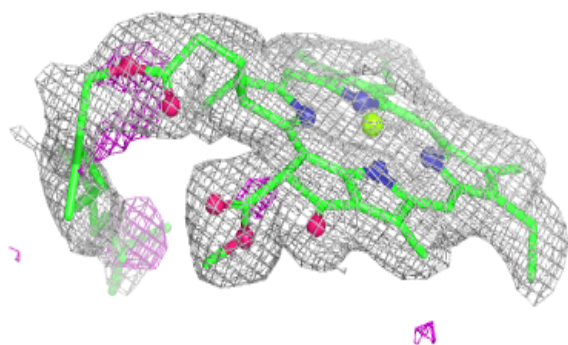
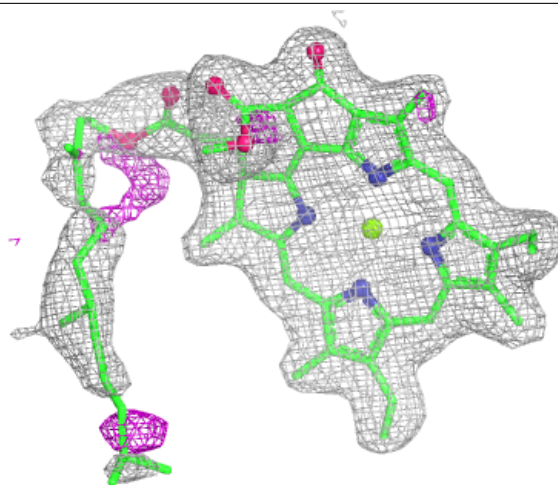
Electron density around CLA b 609:

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



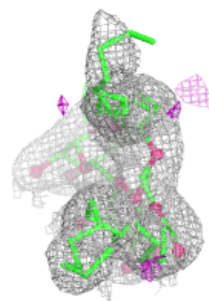
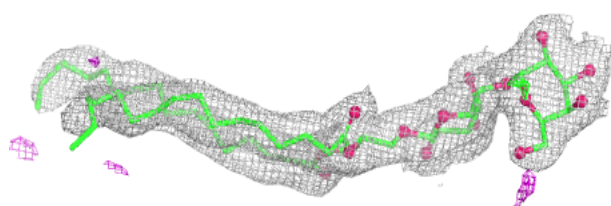
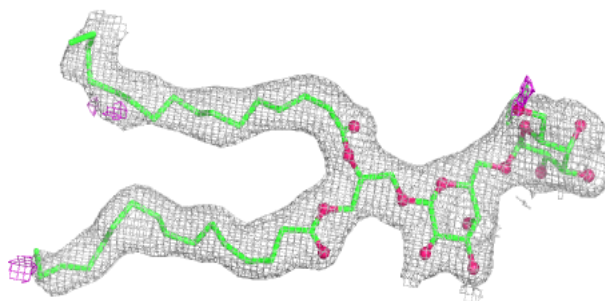
Electron density around CLA B 616:

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



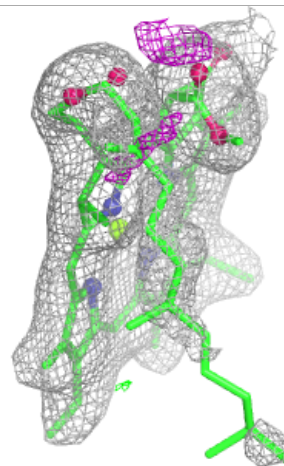
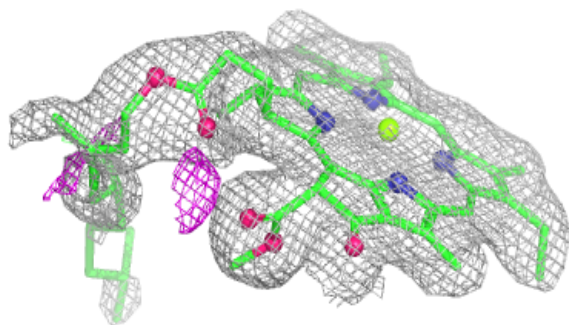
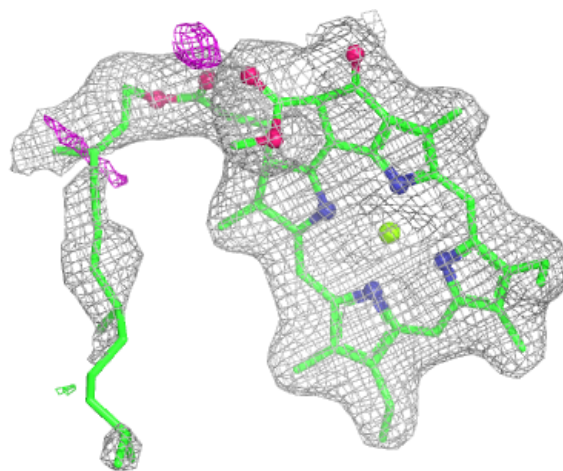
Electron density around DGD J 101:

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



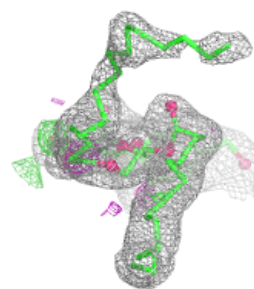
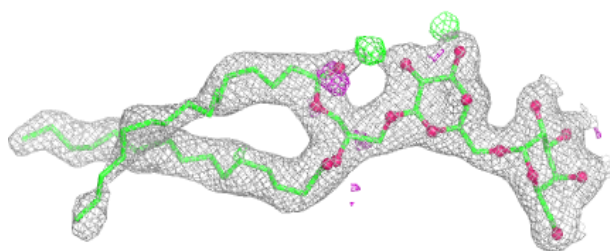
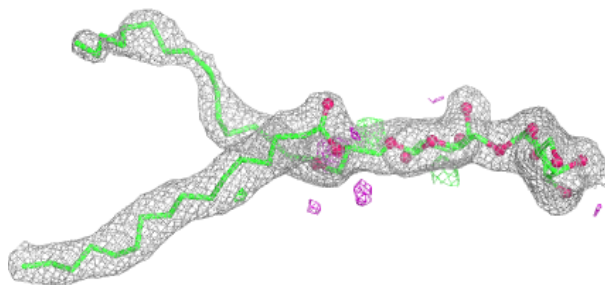
Electron density around CLA b 616:

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

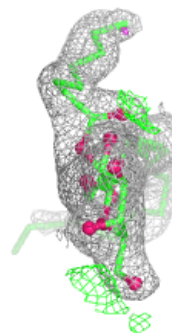
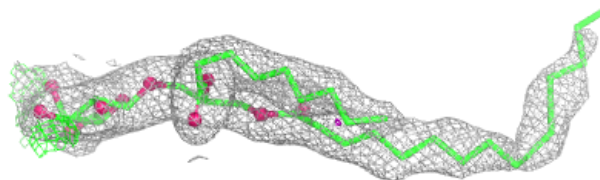
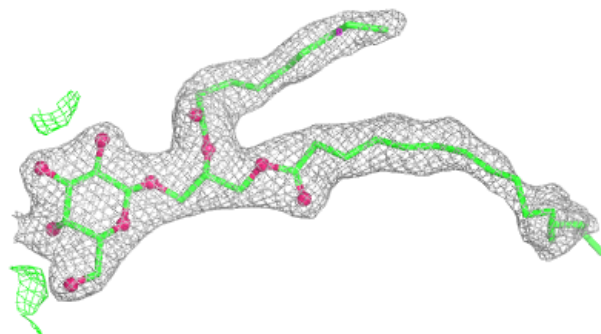


Electron density around DGD c 515:

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

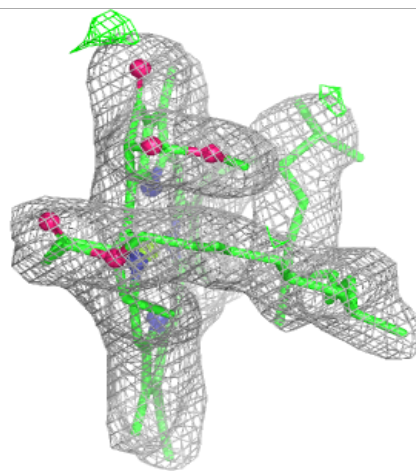
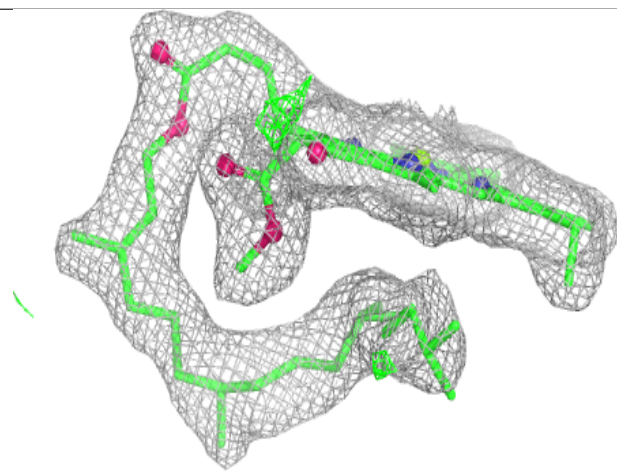
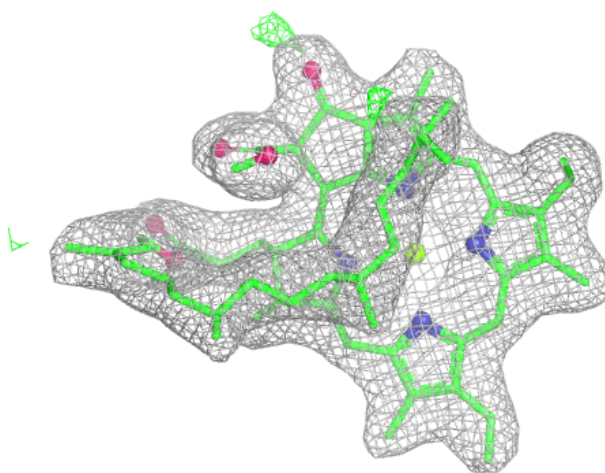
**Electron density around LMG d 411:**

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



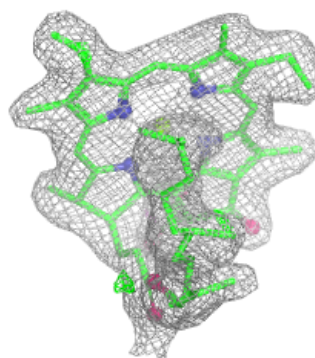
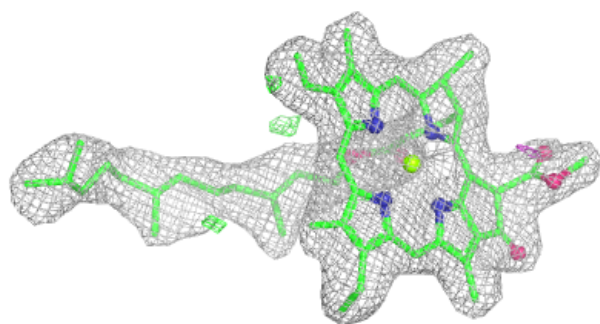
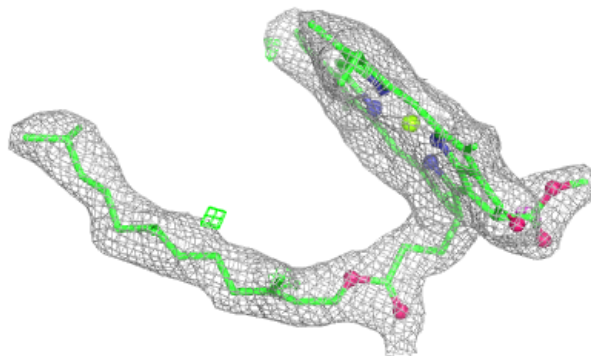
Electron density around CLA C 510:

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

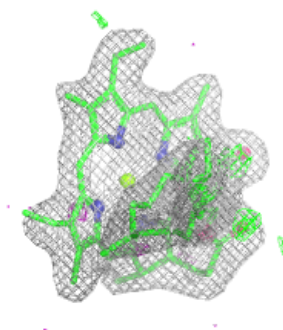
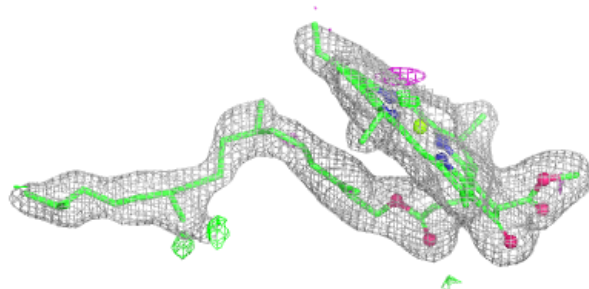
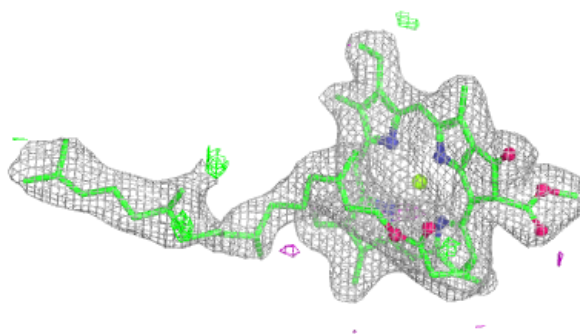


Electron density around CLA c 504:

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

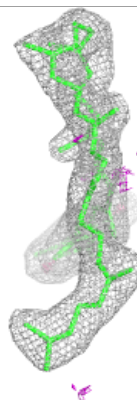
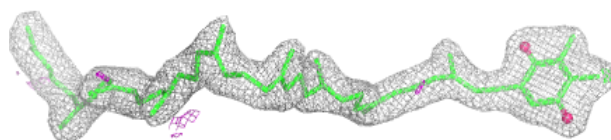
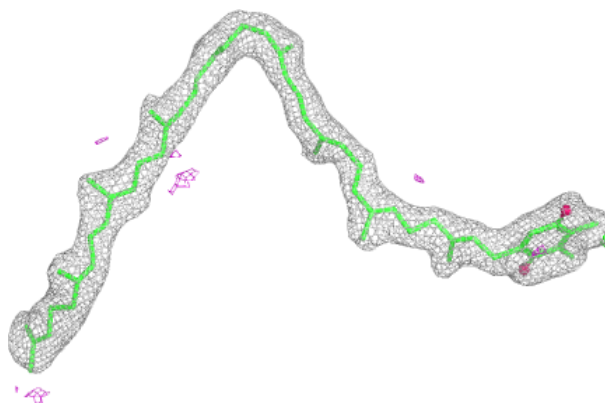
**Electron density around CLA c 505:**

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

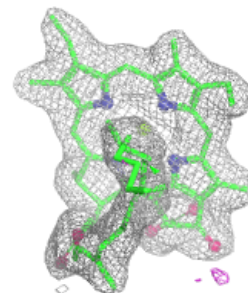
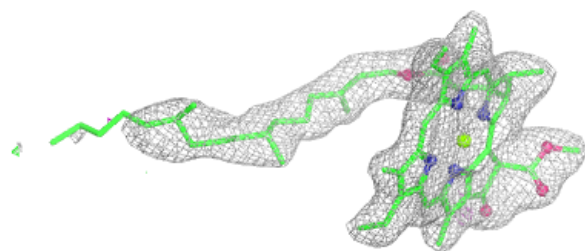
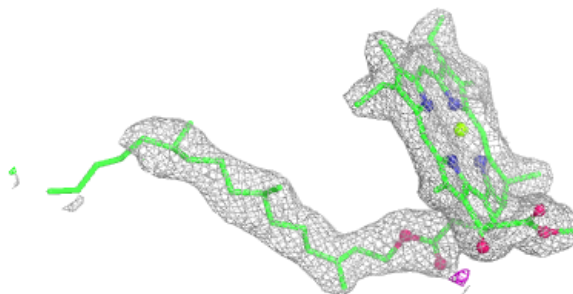


Electron density around PL9 D 406:

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

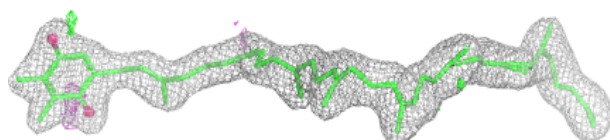
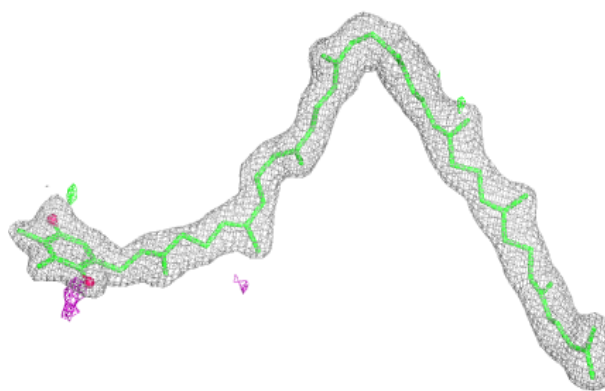
**Electron density around CLA c 508:**

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

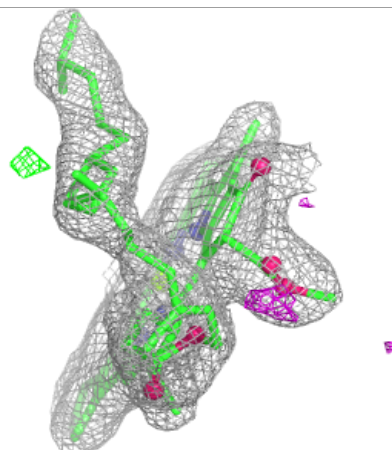
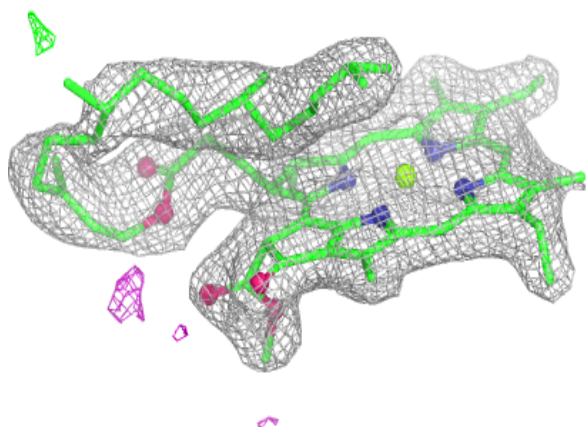
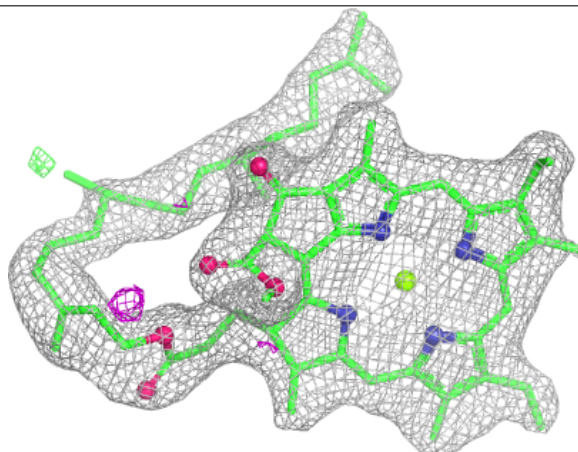


Electron density around PL9 d 406:

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

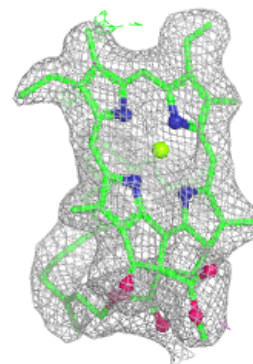
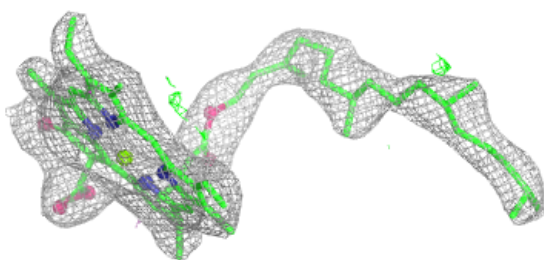
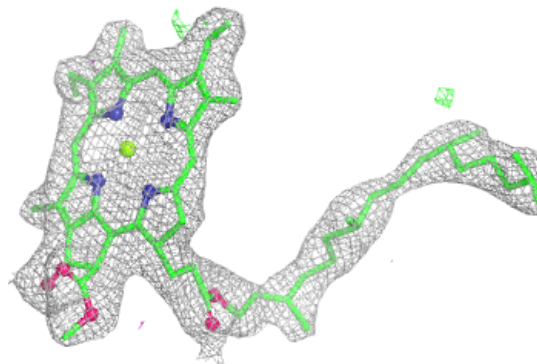
**Electron density around CLA c 509:**

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

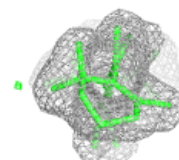
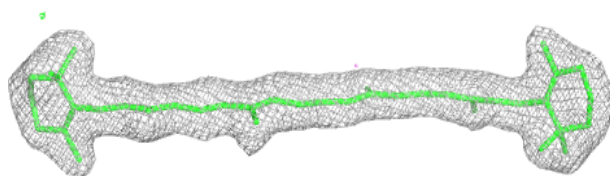
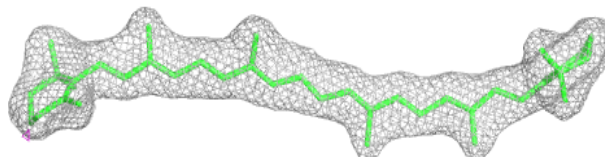


Electron density around CLA C 511:

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

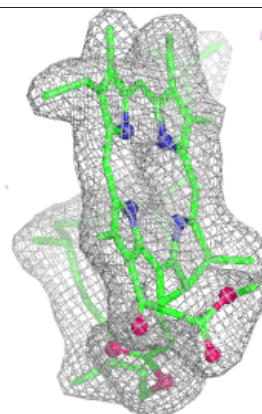
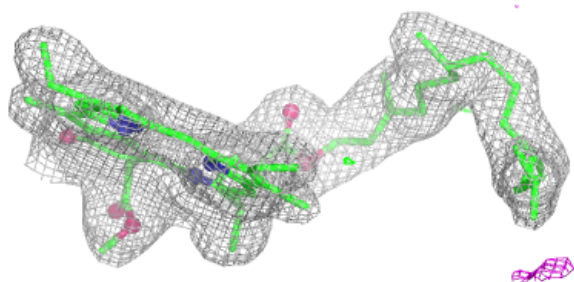
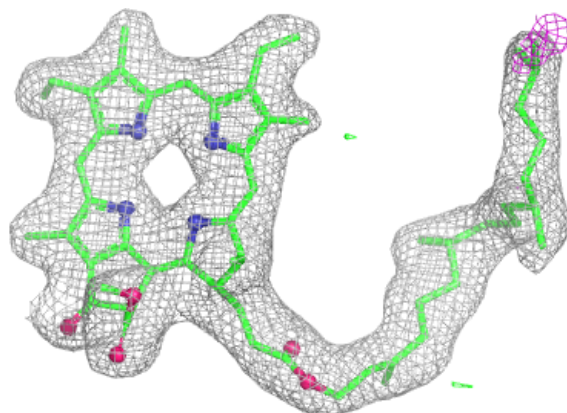
**Electron density around BCR a 609:**

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

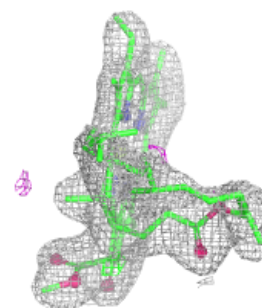
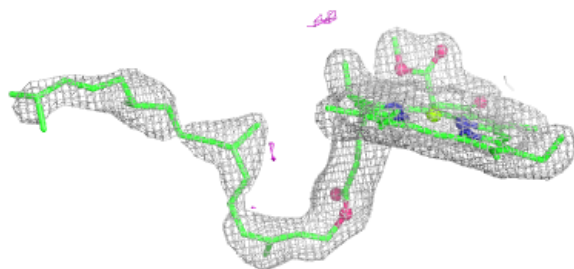
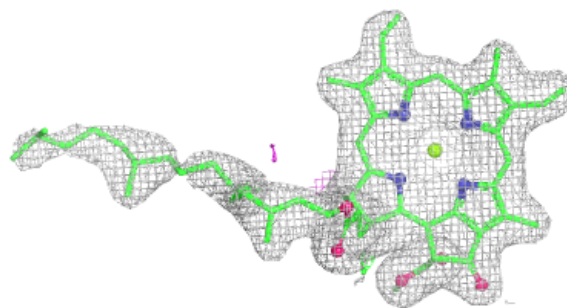


Electron density around PHO d 402:

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

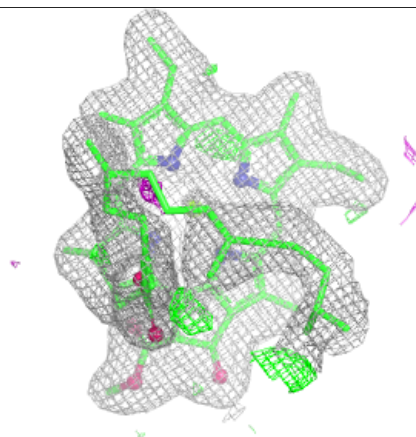
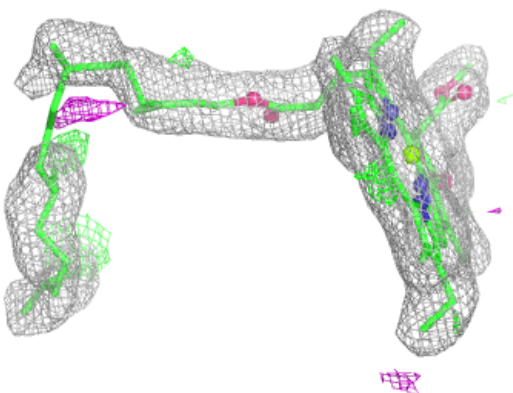
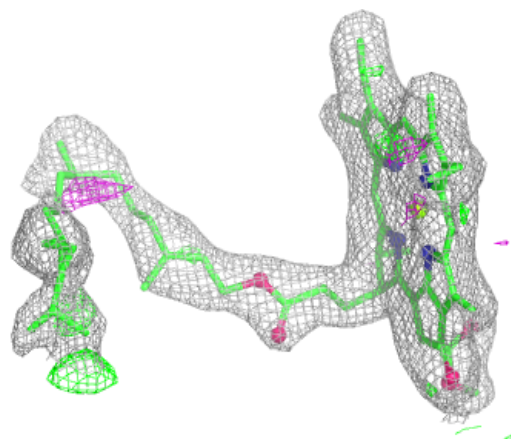
**Electron density around CLA a 606:**

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



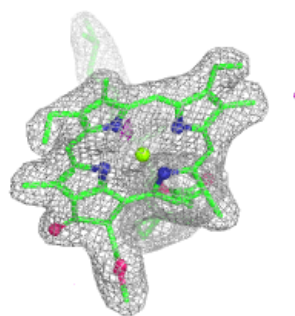
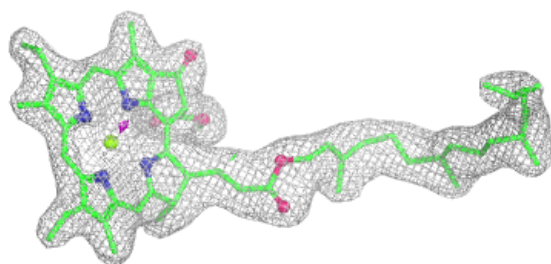
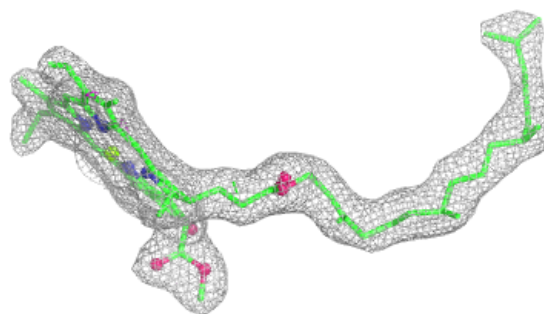
Electron density around CLA a 608:

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

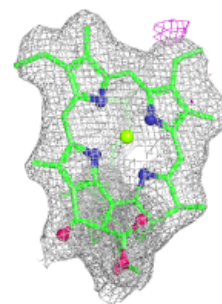
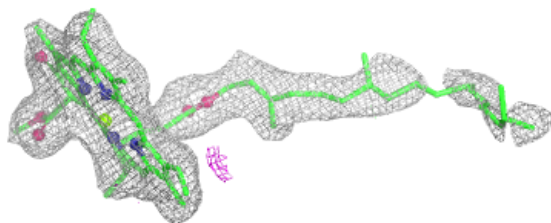
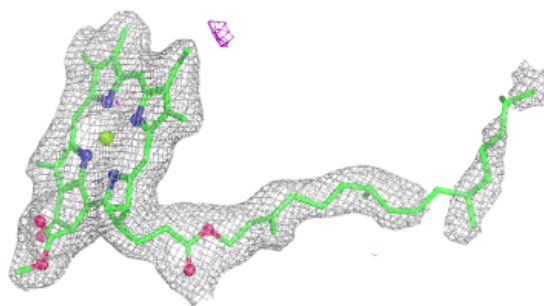


Electron density around CLA d 403:

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

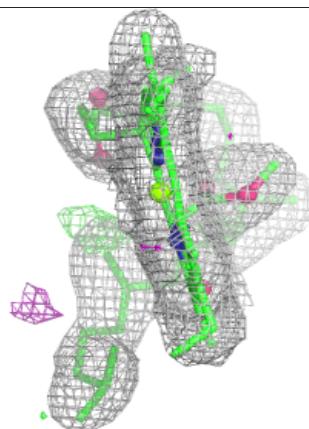
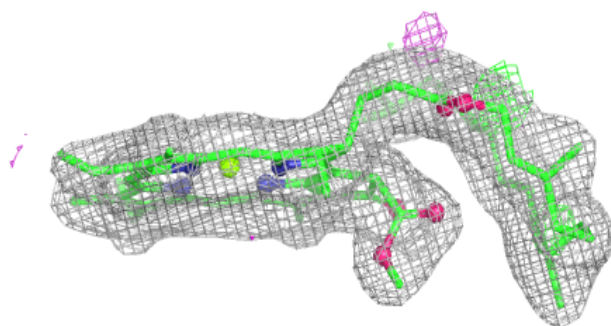
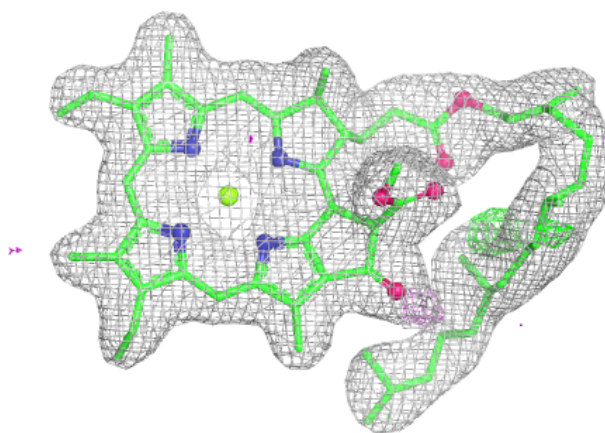
**Electron density around CLA d 404:**

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

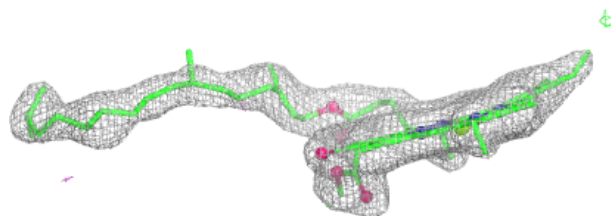
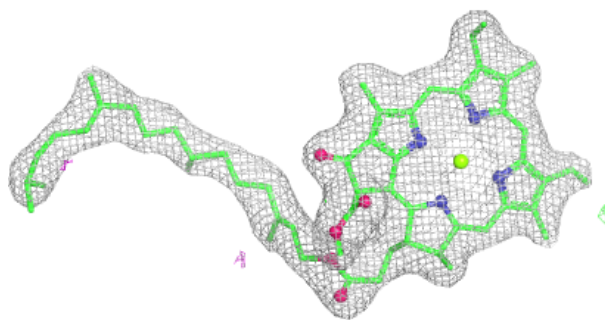


Electron density around CLA B 610:

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

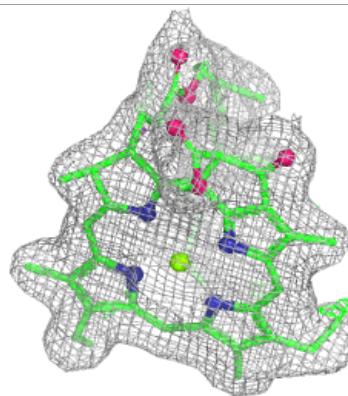
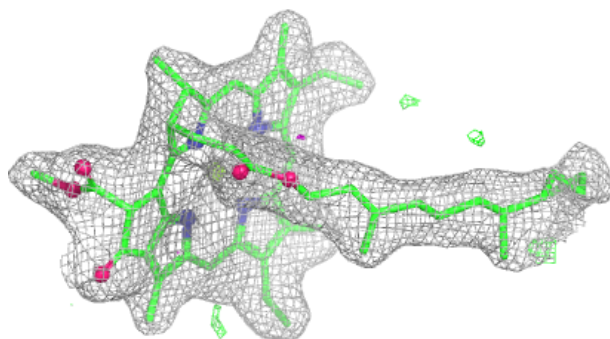
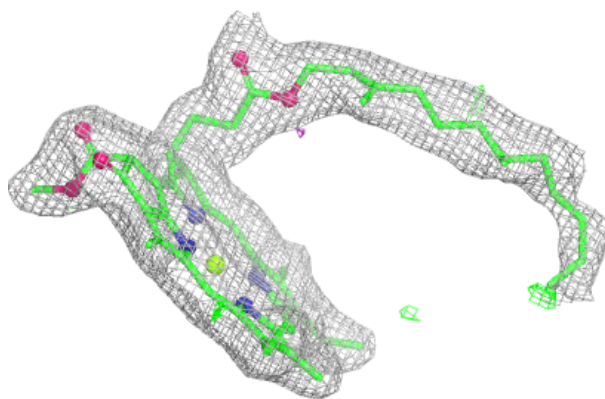
**Electron density around CLA b 602:**

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

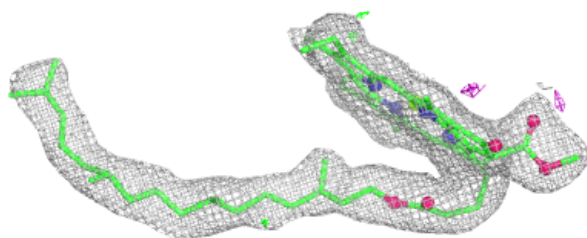
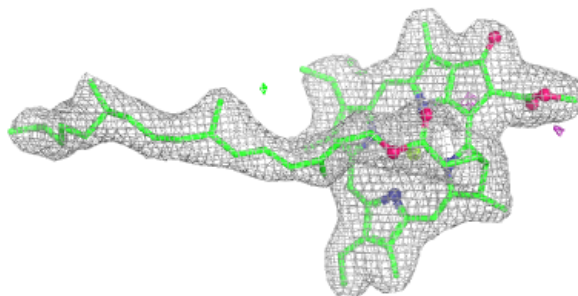


Electron density around CLA C 504:

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

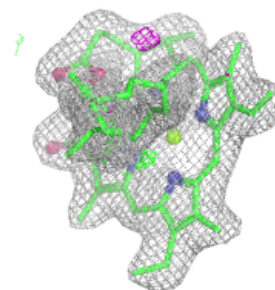
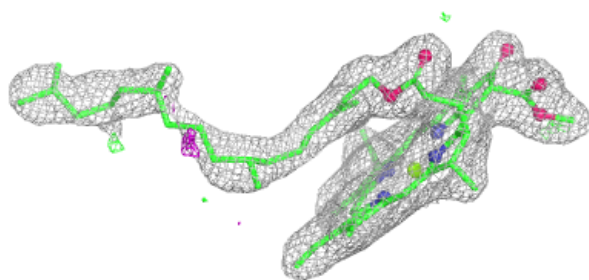
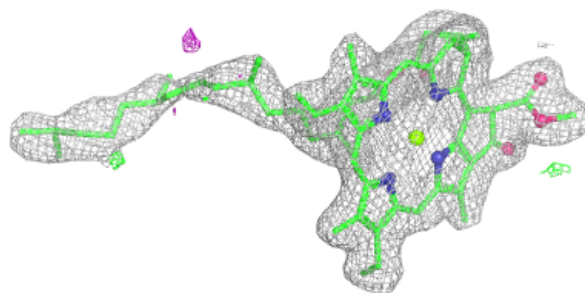
**Electron density around CLA b 608:**

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



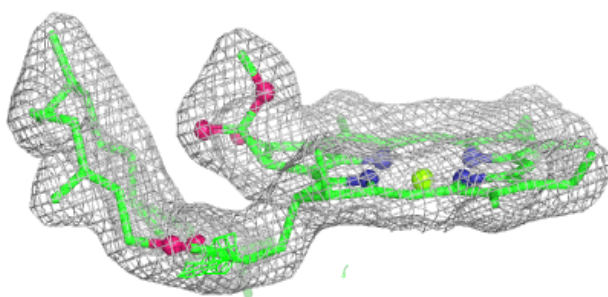
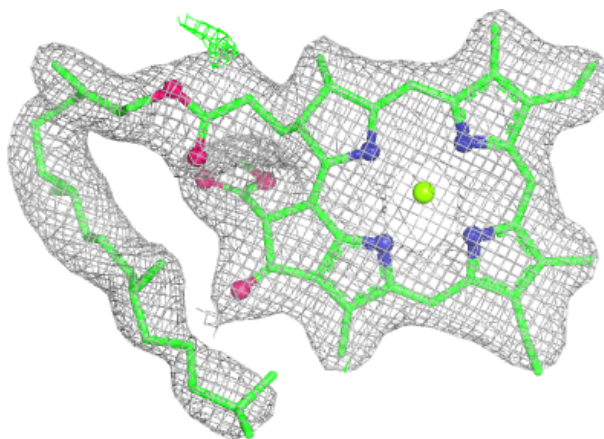
Electron density around CLA C 505:

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



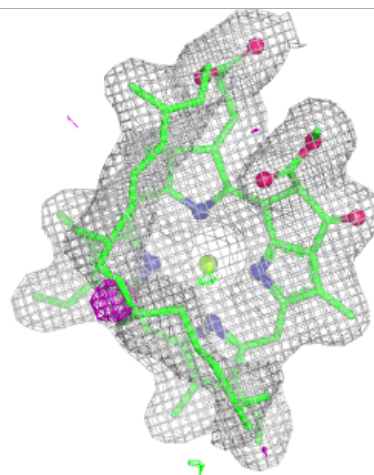
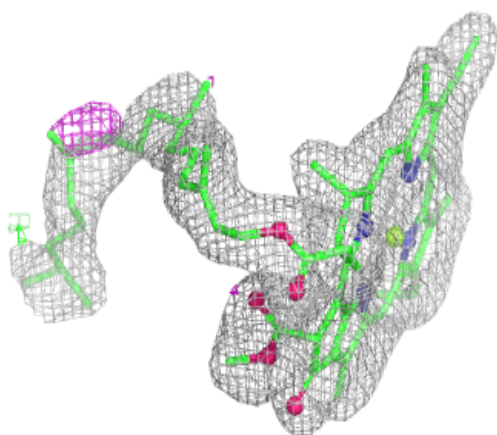
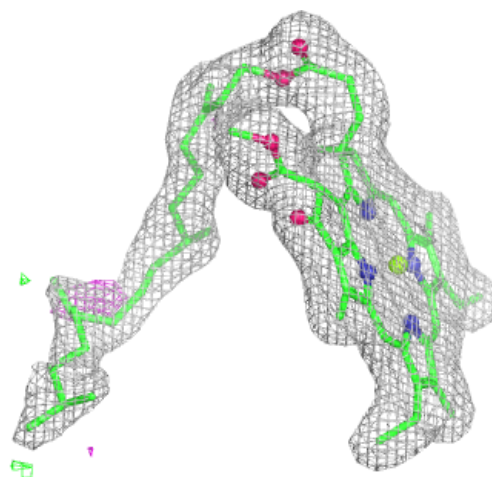
Electron density around CLA b 610:

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



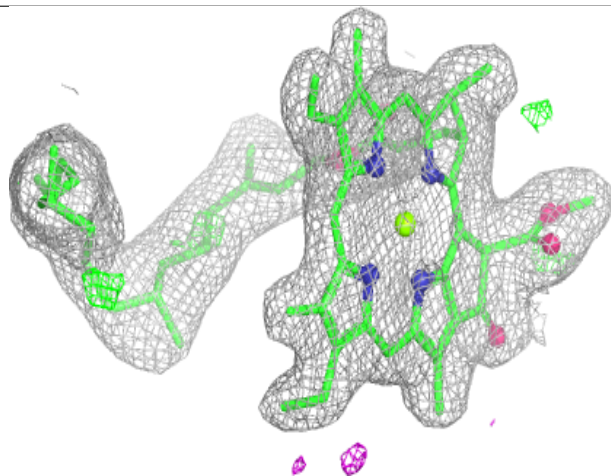
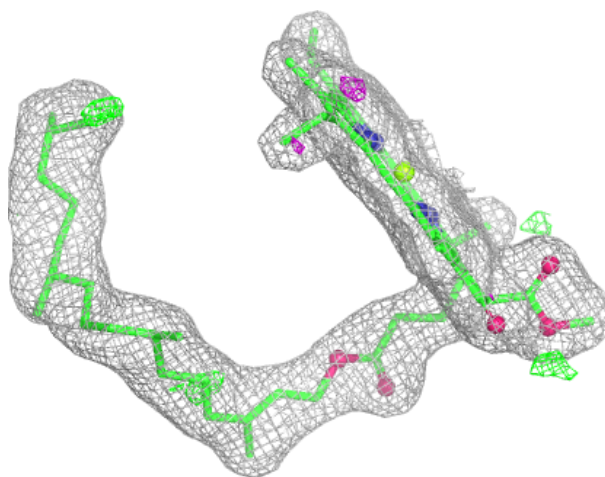
Electron density around CLA b 613:

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



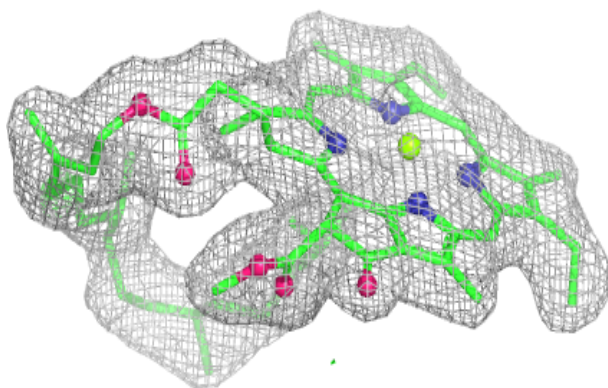
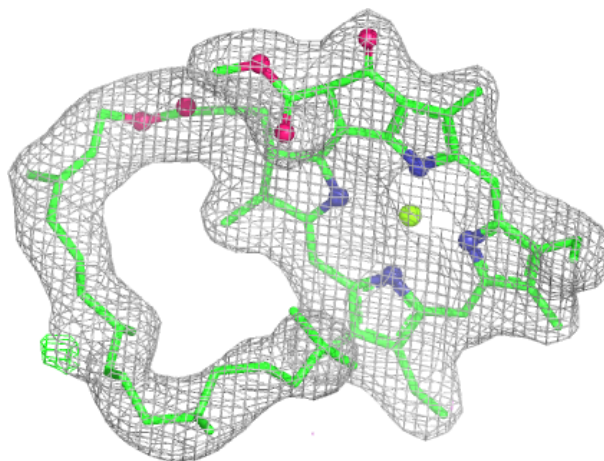
Electron density around CLA B 611:

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



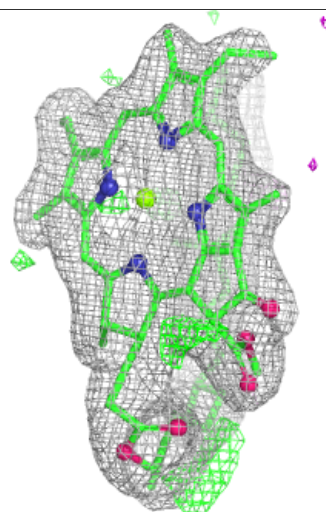
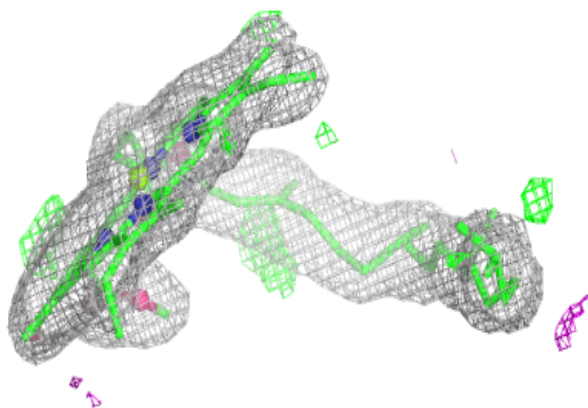
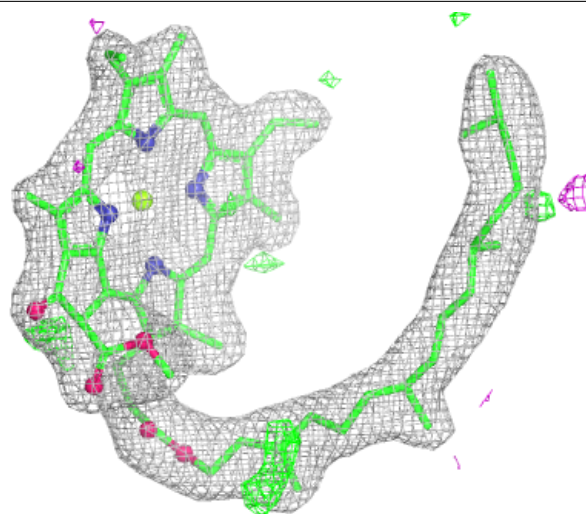
Electron density around CLA b 615:

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



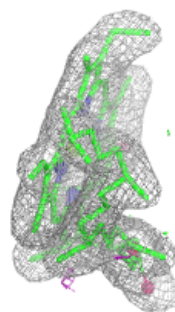
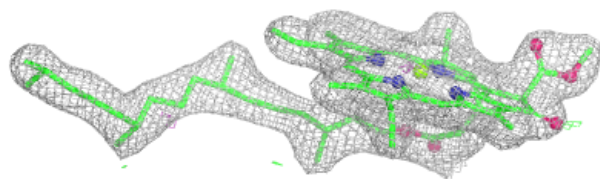
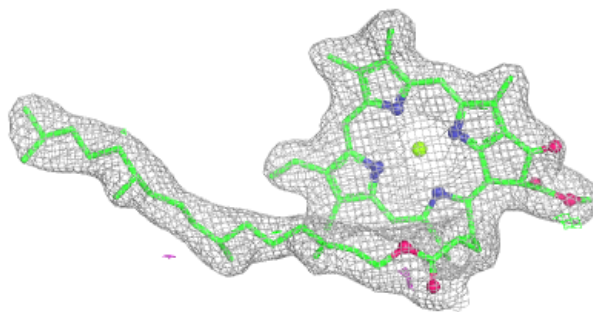
Electron density around CLA C 507:

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

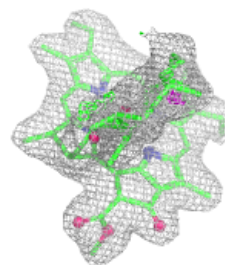
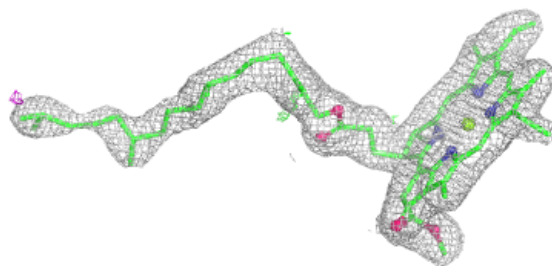


Electron density around CLA c 501:

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

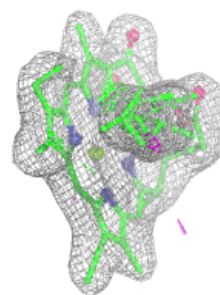
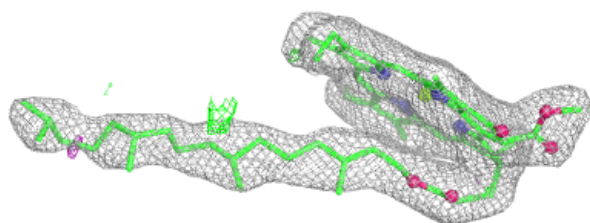
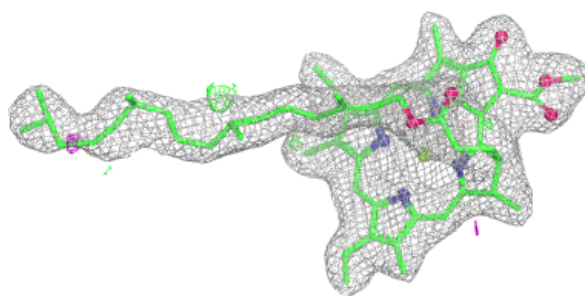
**Electron density around CLA c 502:**

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



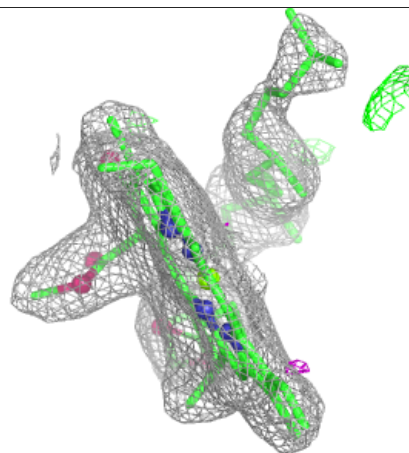
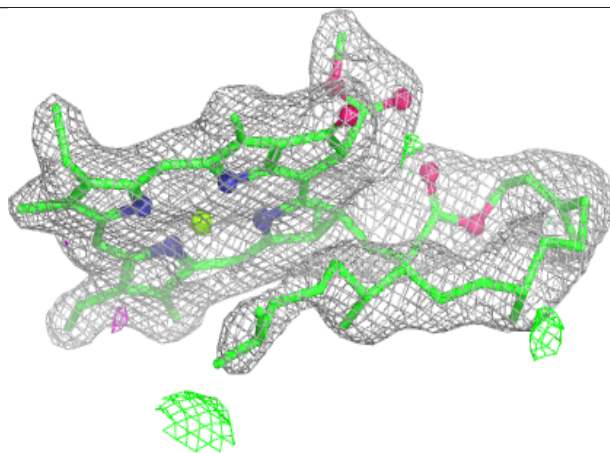
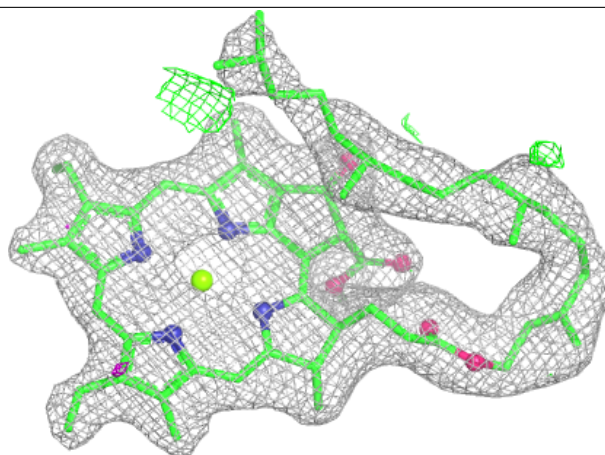
Electron density around CLA B 614:

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



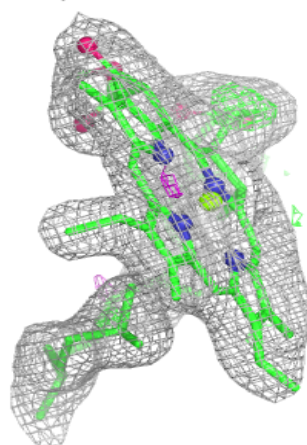
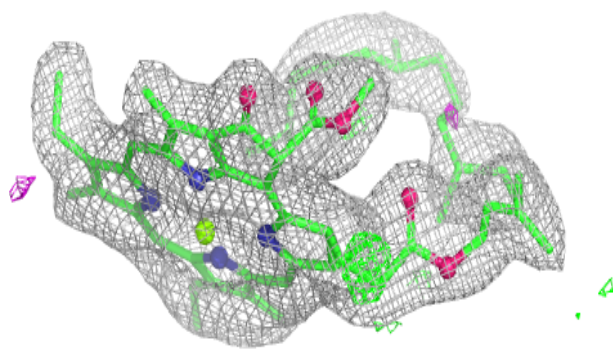
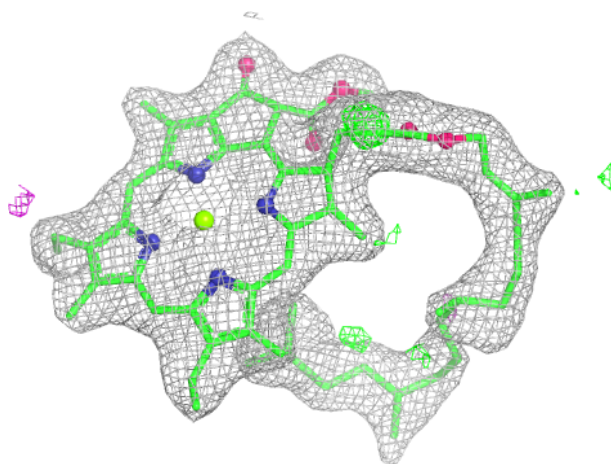
Electron density around CLA C 509:

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



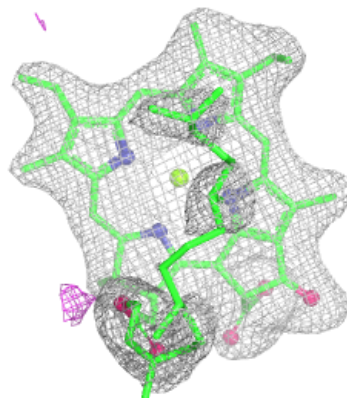
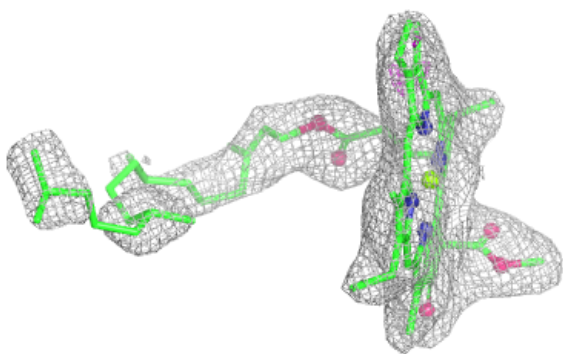
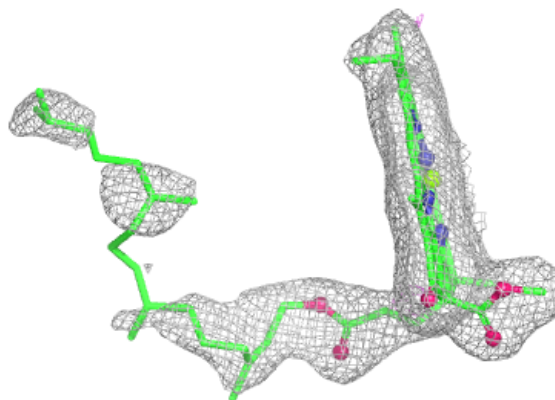
Electron density around CLA B 615:

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



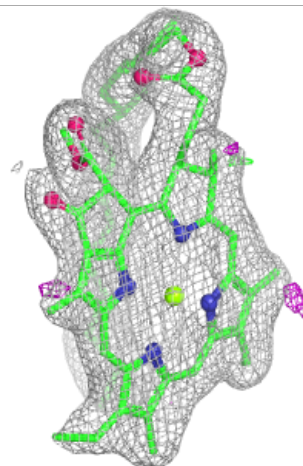
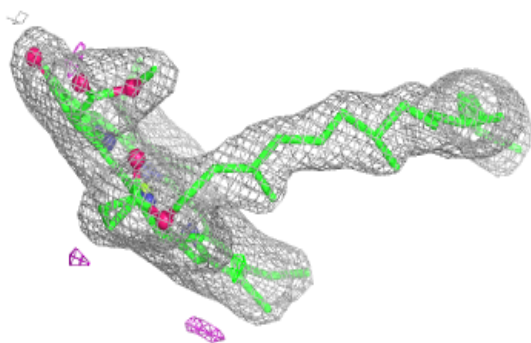
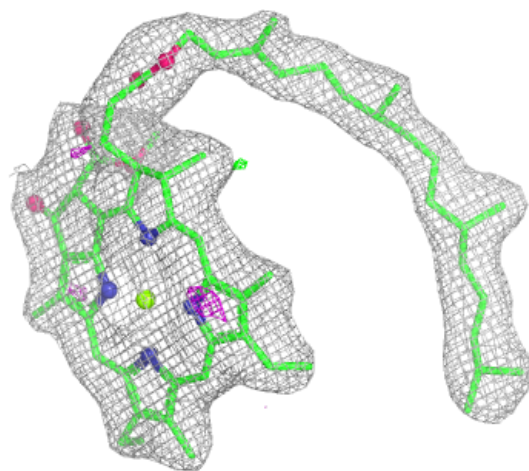
Electron density around CLA c 506:

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



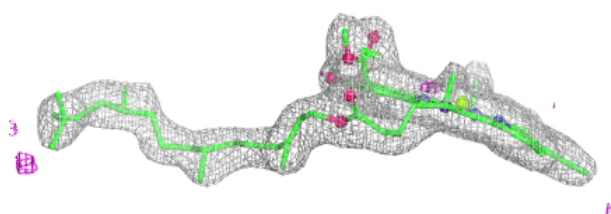
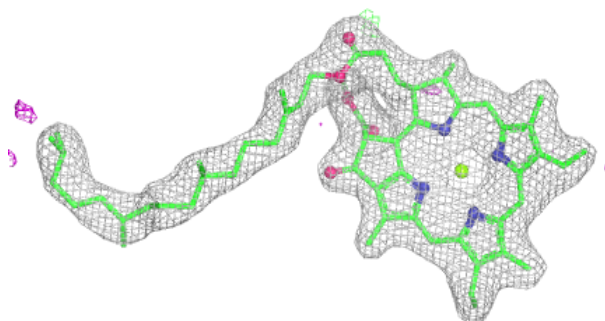
Electron density around CLA c 507:

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

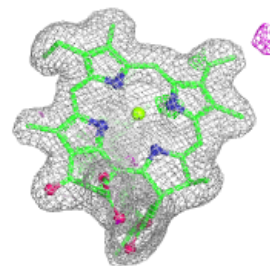
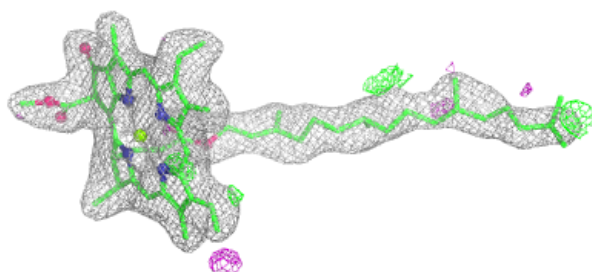
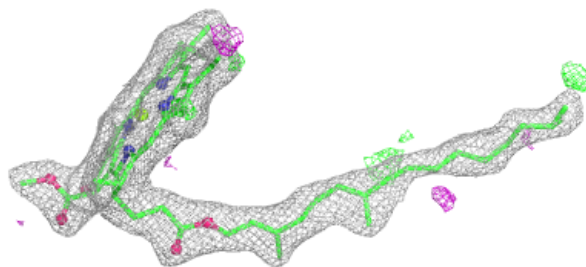


Electron density around CLA B 602:

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

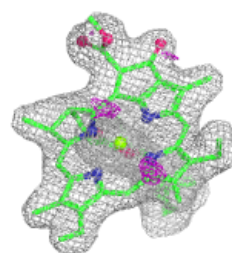
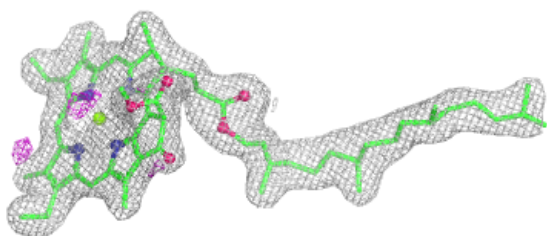
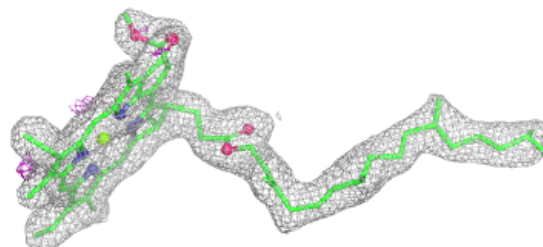
**Electron density around CLA B 607:**

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



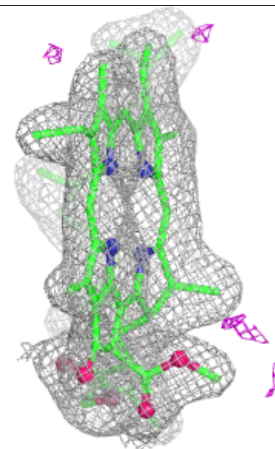
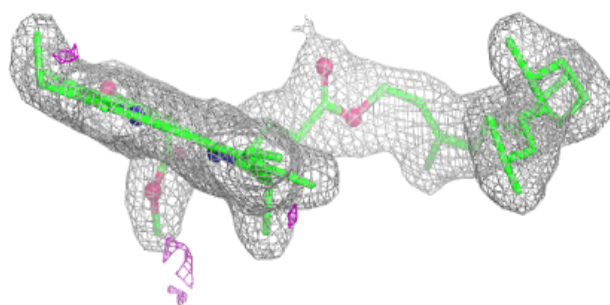
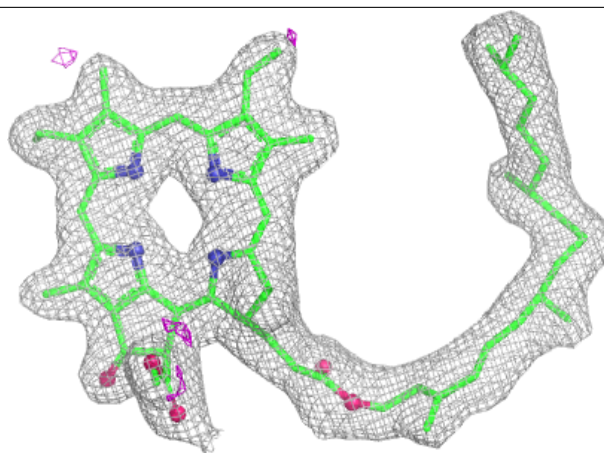
Electron density around CLA C 502:

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



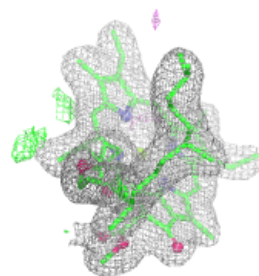
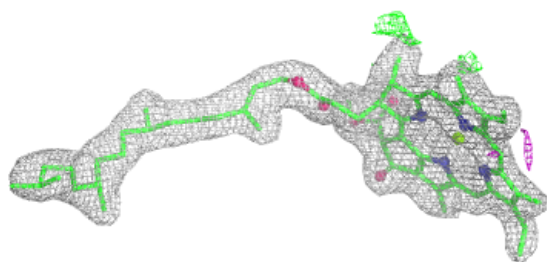
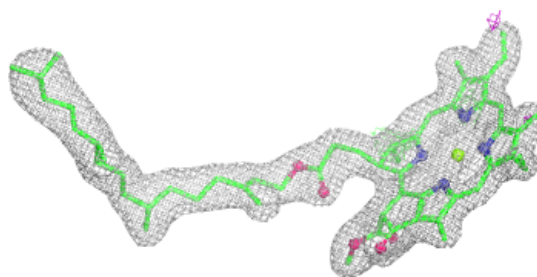
Electron density around PHO a 607:

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

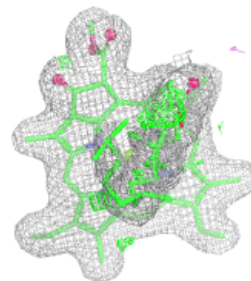
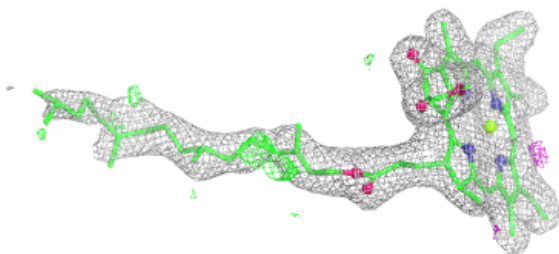
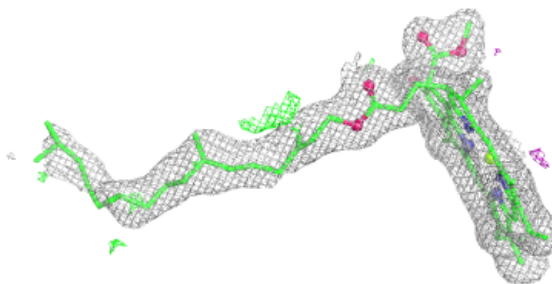


Electron density around CLA a 605:

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

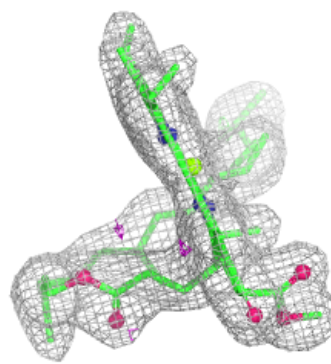
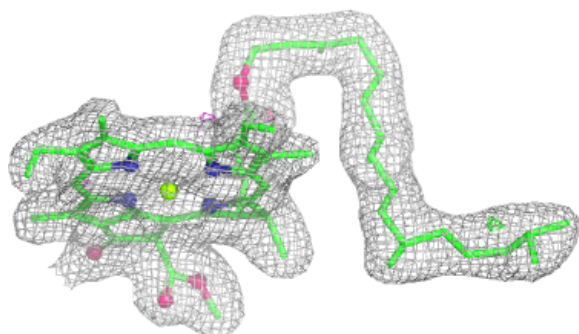
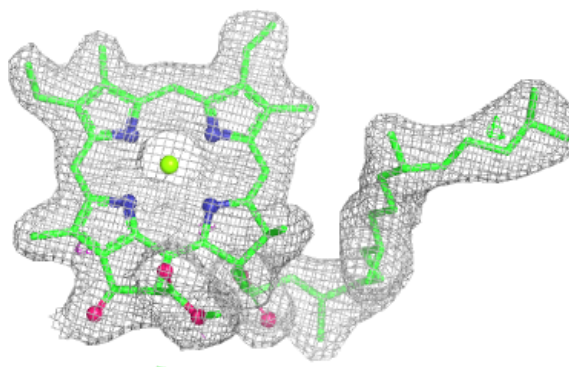
**Electron density around CLA B 604:**

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

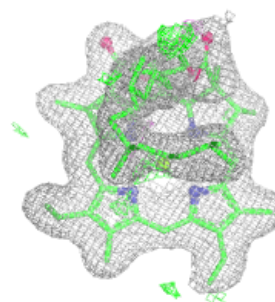
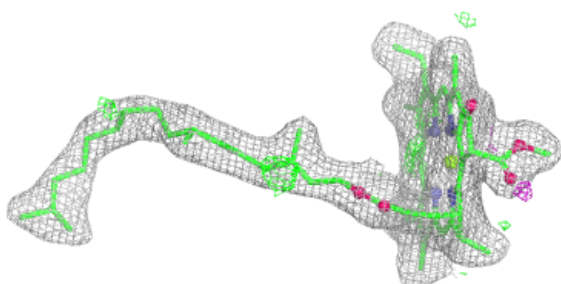
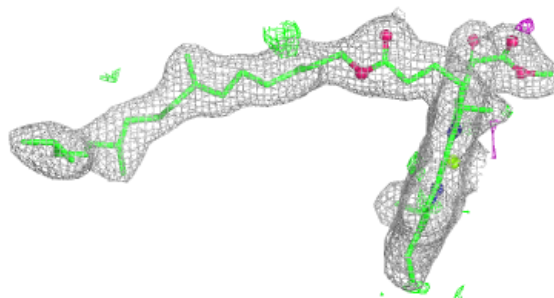


Electron density around CLA a 611:

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

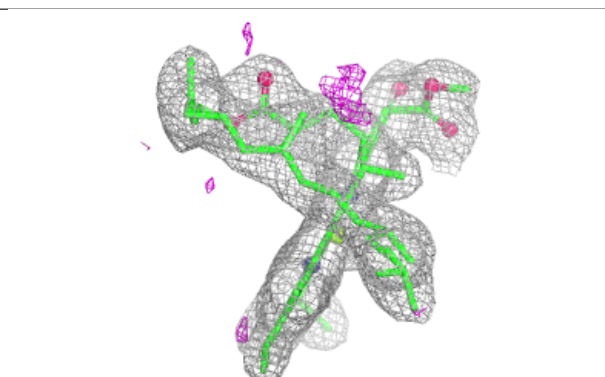
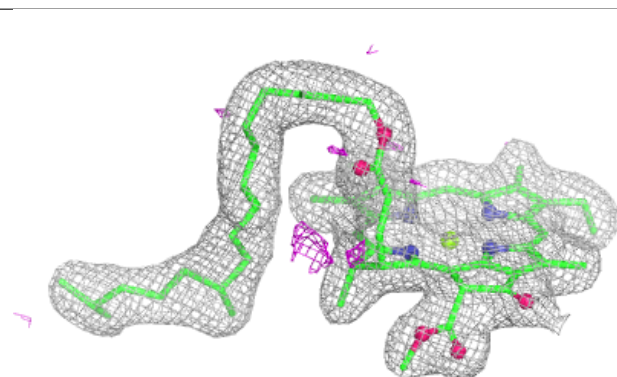
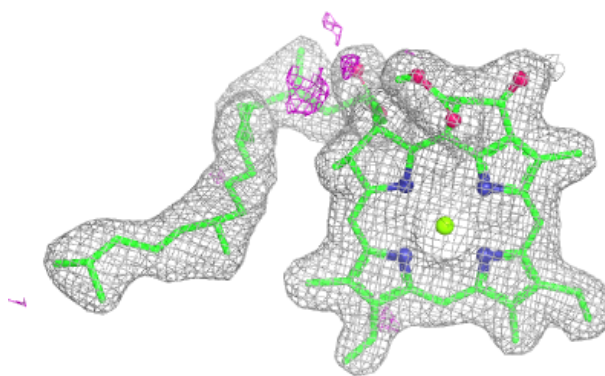
**Electron density around CLA B 605:**

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

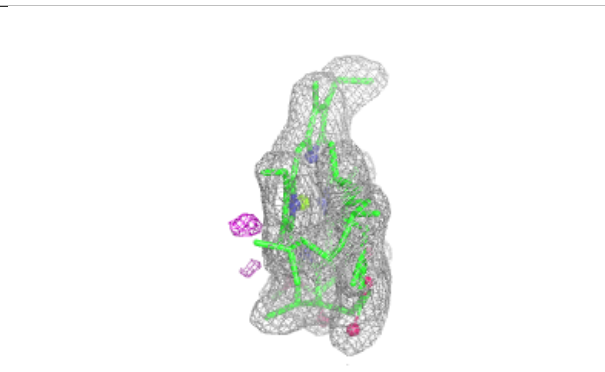
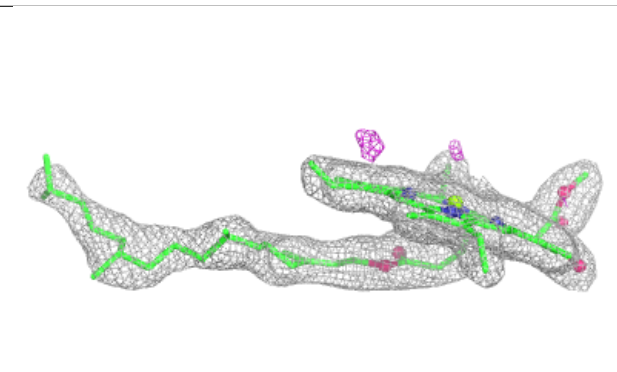
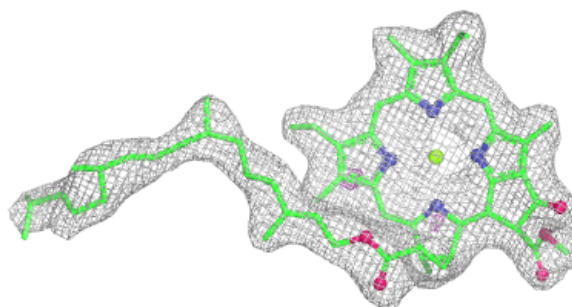


Electron density around CLA A 611:

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

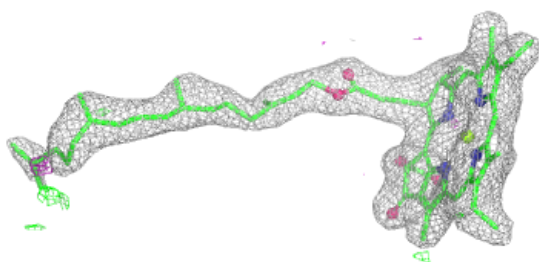
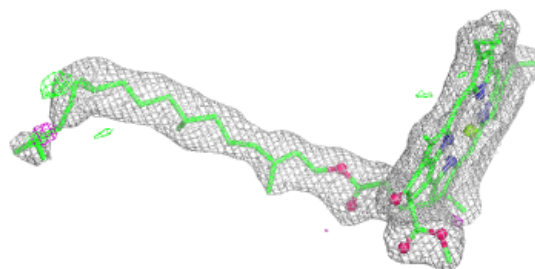
**Electron density around CLA b 603:**

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

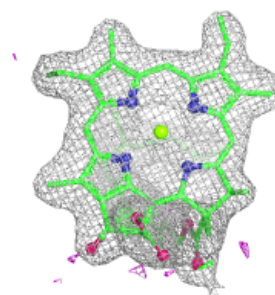
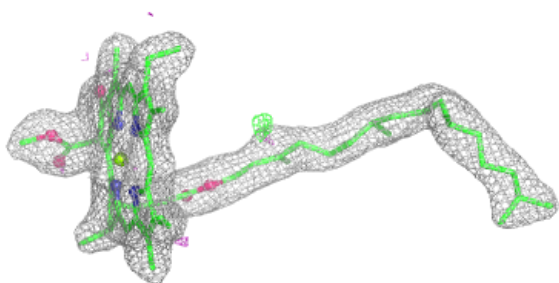
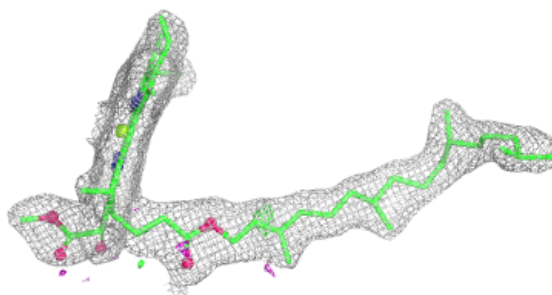


Electron density around CLA b 604:

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

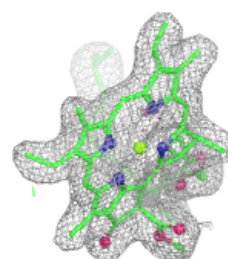
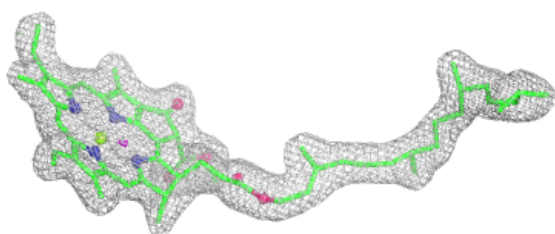
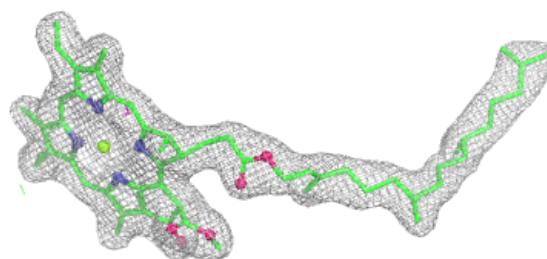
**Electron density around CLA b 605:**

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

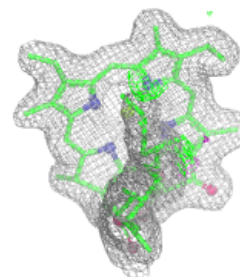
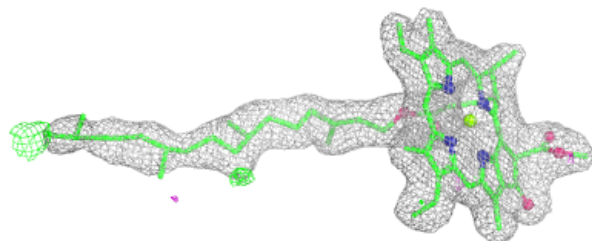
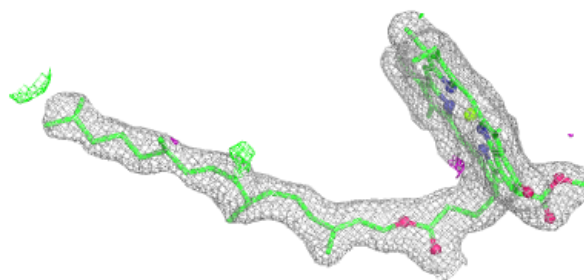


Electron density around CLA A 606:

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

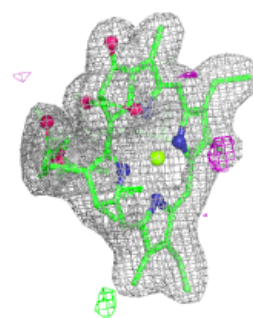
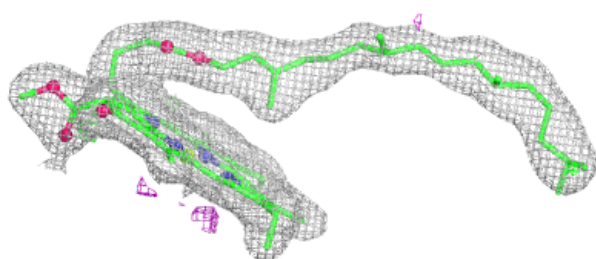
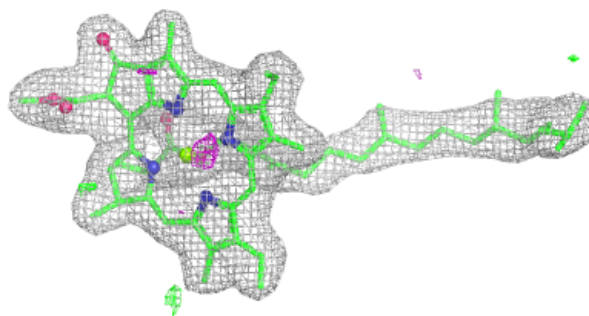
**Electron density around CLA b 607:**

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

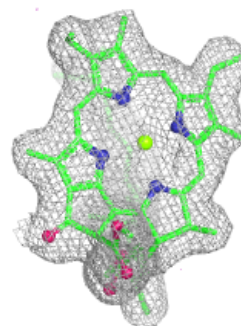
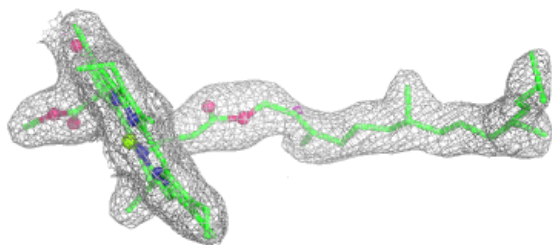
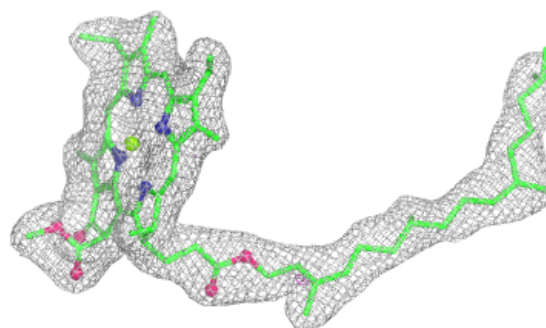


Electron density around CLA B 608:

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

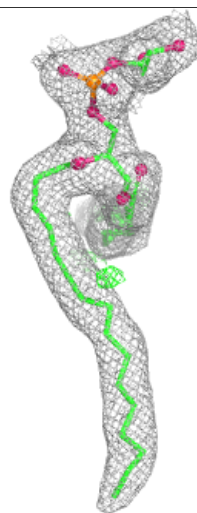
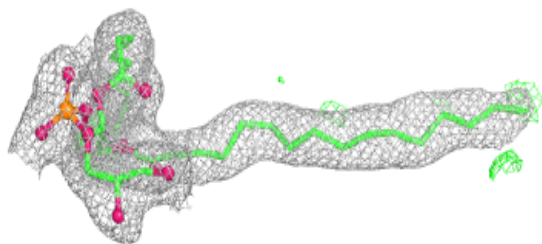
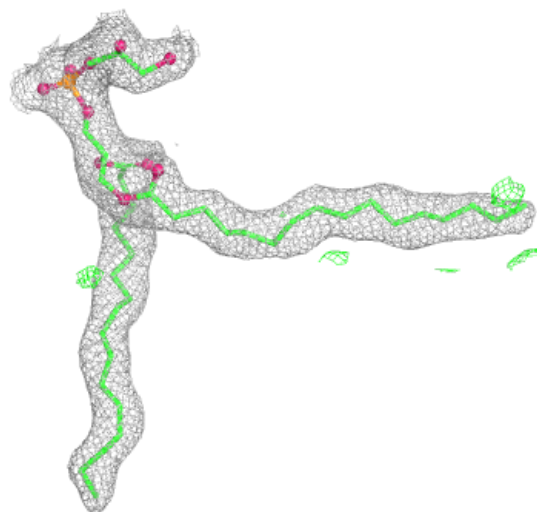
**Electron density around CLA B 609:**

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



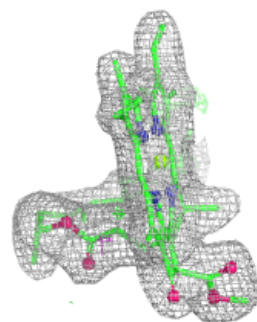
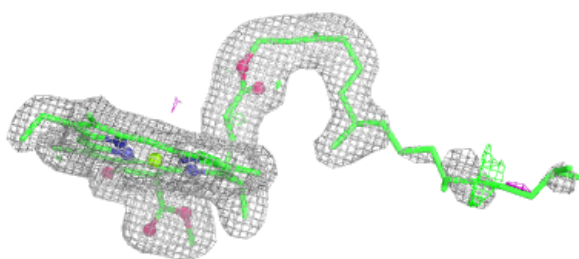
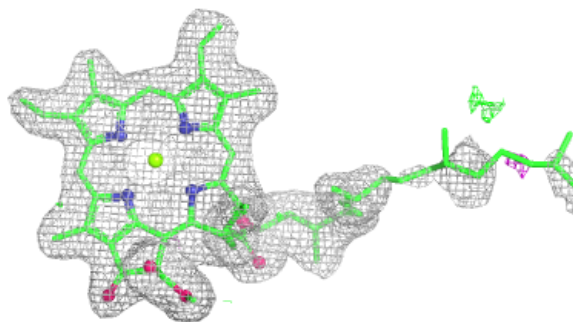
Electron density around LHG L 101:

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

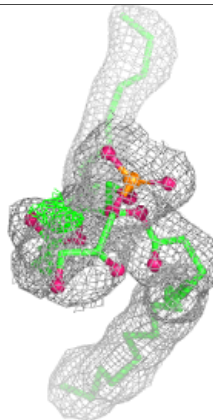
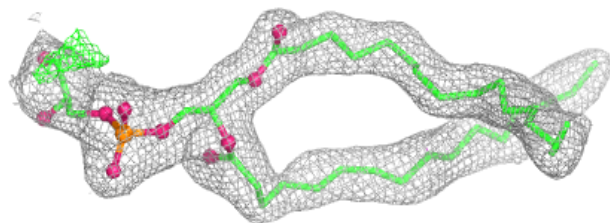
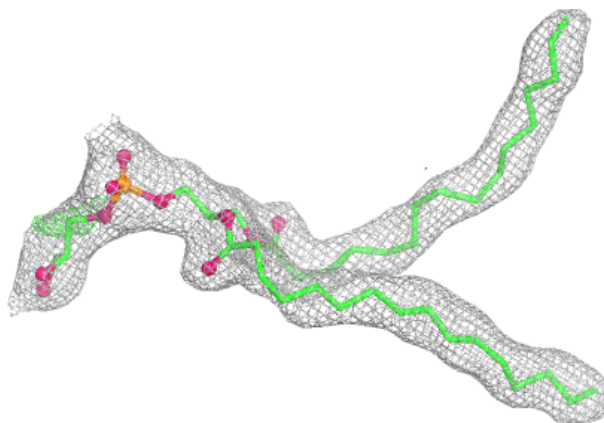


Electron density around CLA A 607:

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

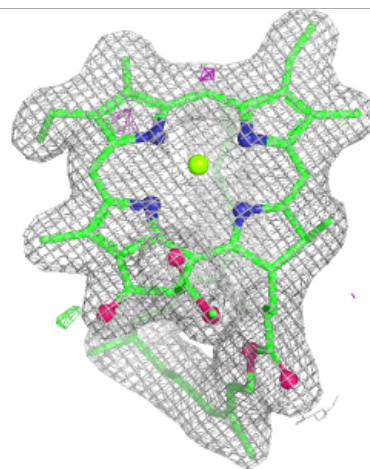
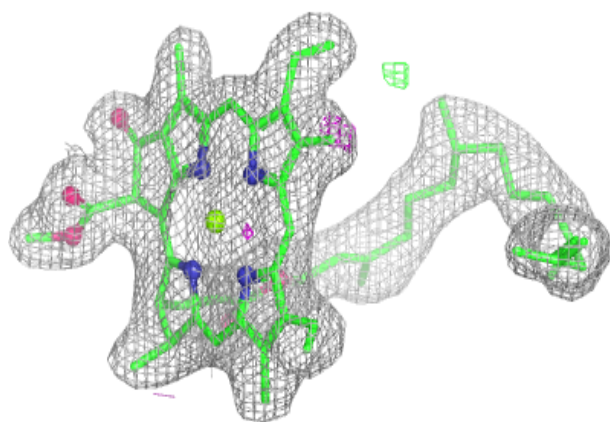
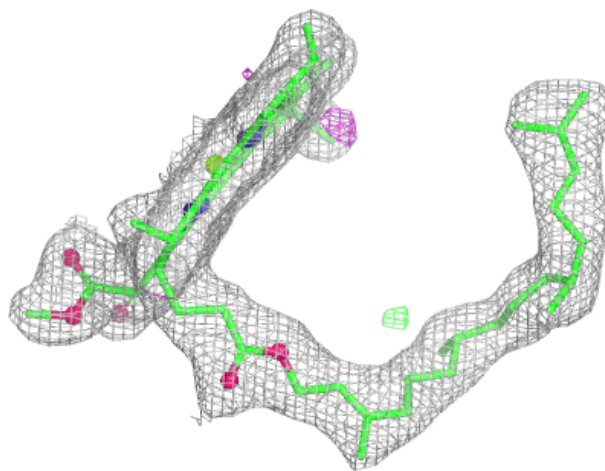
**Electron density around LHG d 408:**

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



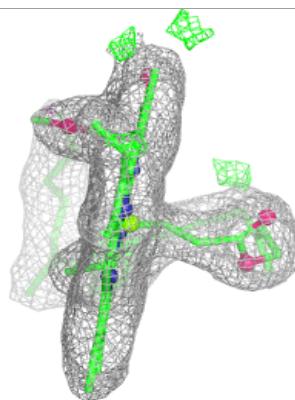
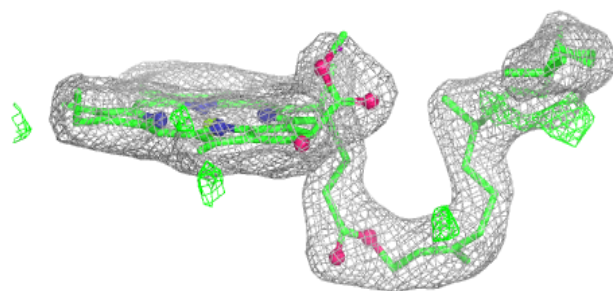
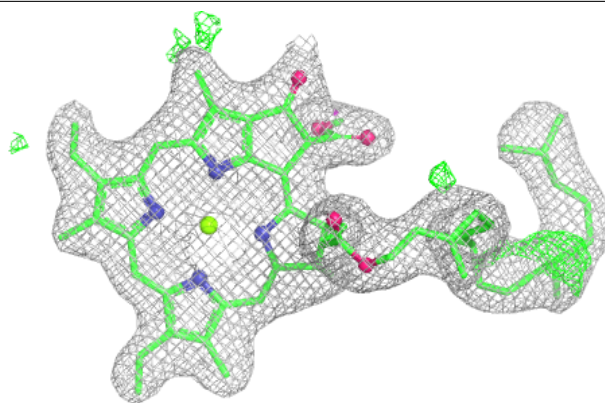
Electron density around CLA b 611:

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

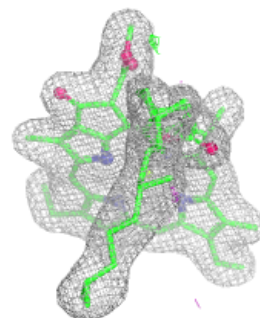
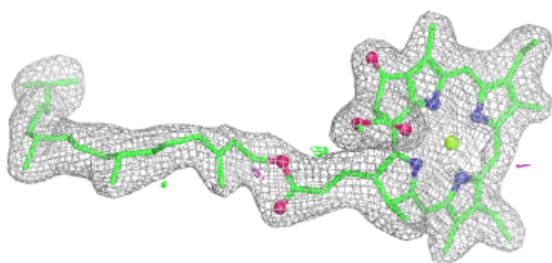
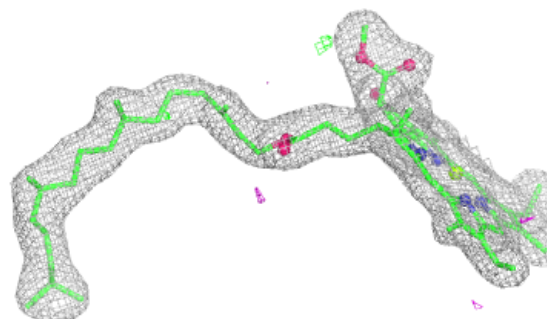


Electron density around CLA b 612:

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

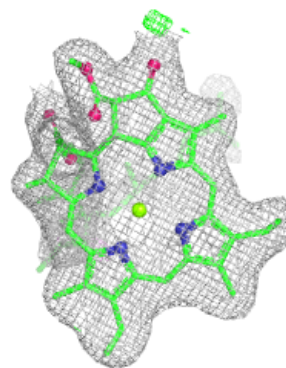
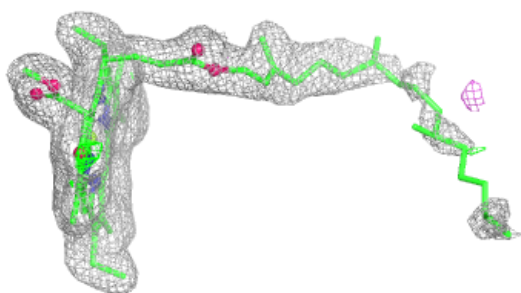
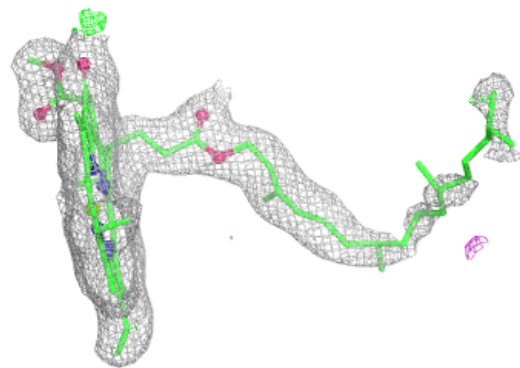
**Electron density around CLA D 403:**

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

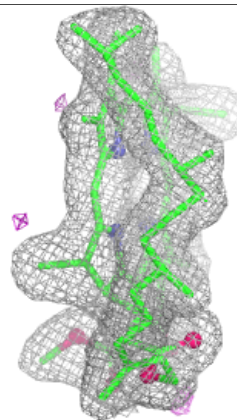
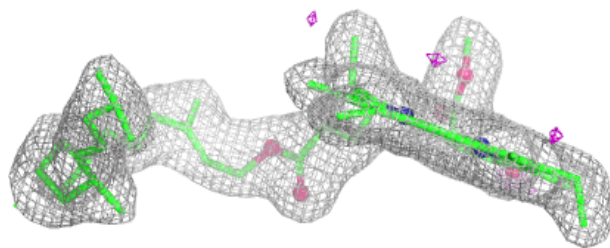
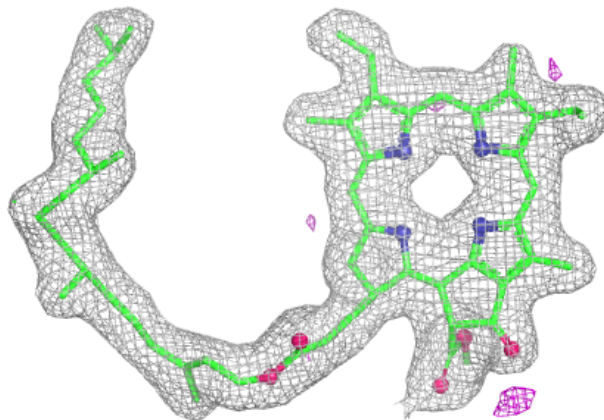


Electron density around CLA D 404:

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

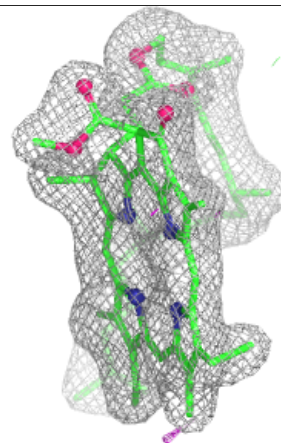
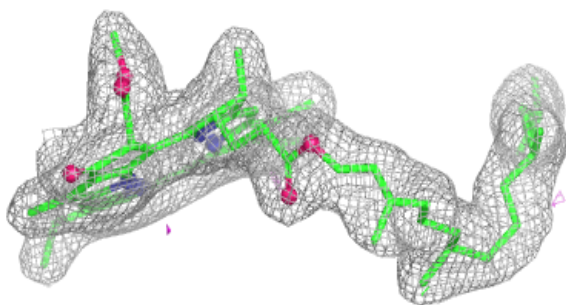
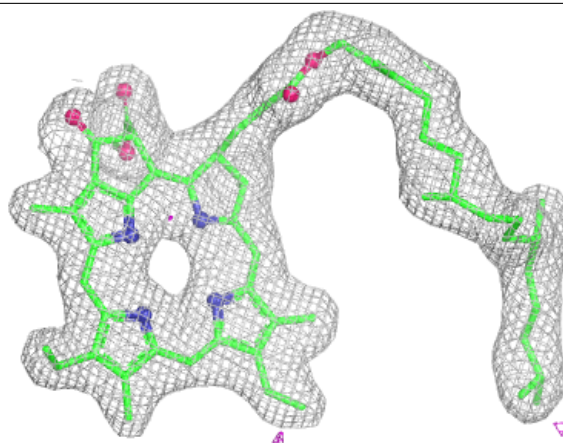
**Electron density around PHO D 401:**

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



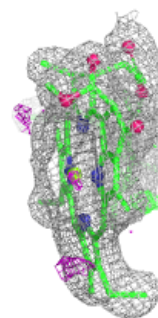
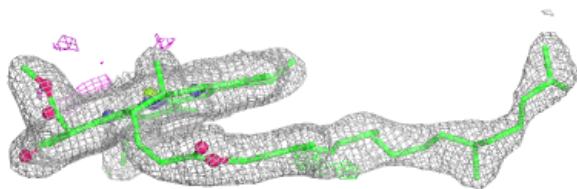
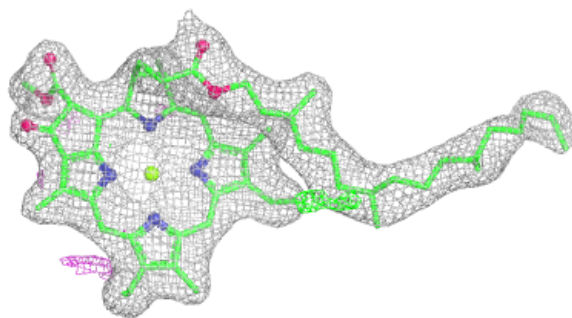
Electron density around PHO D 402:

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

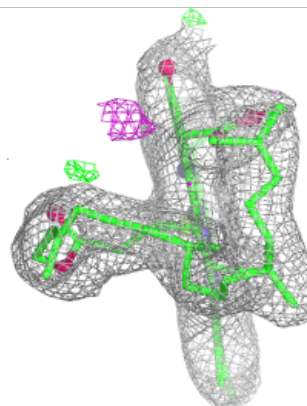
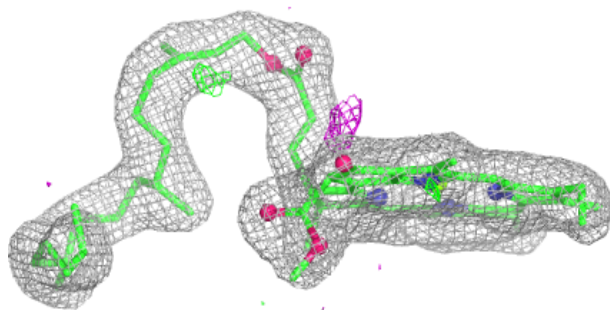
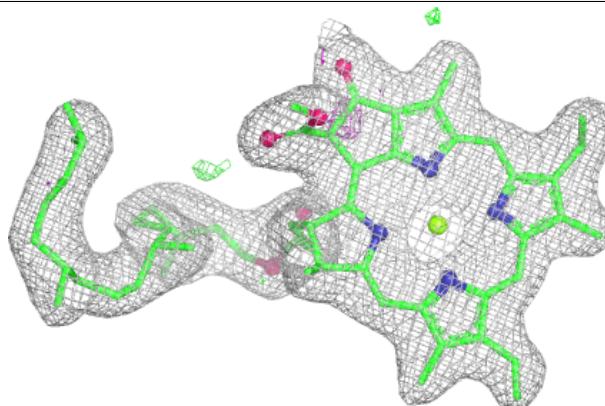


Electron density around CLA B 603:

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

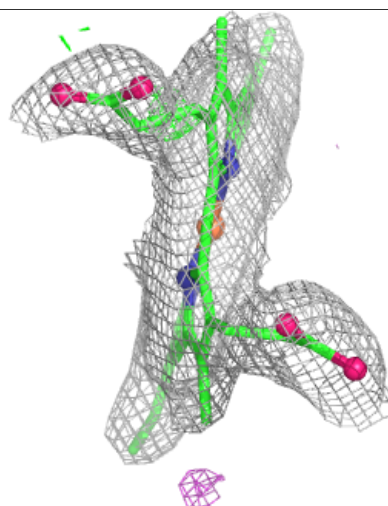
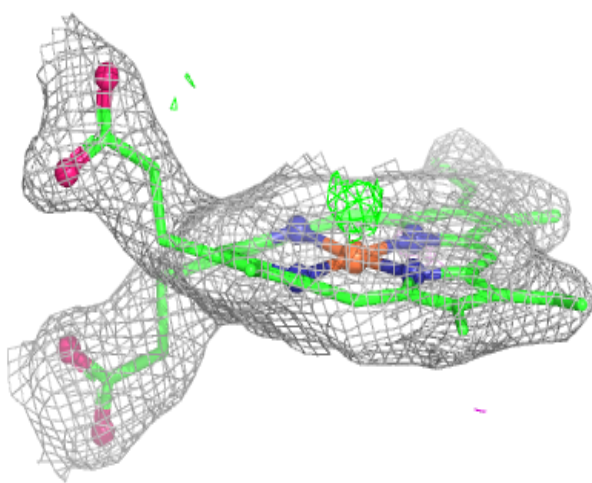
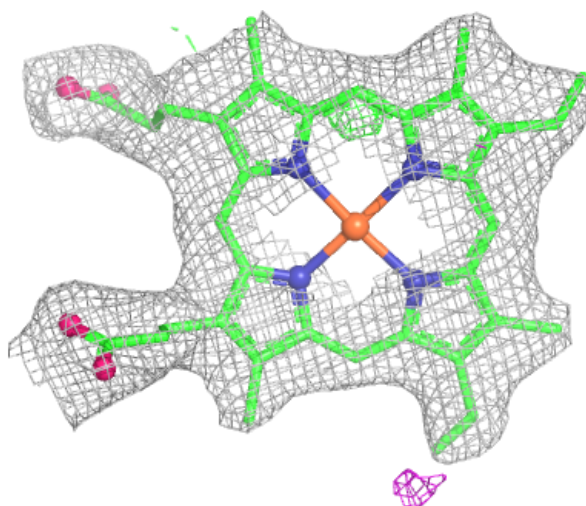
**Electron density around CLA B 612:**

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



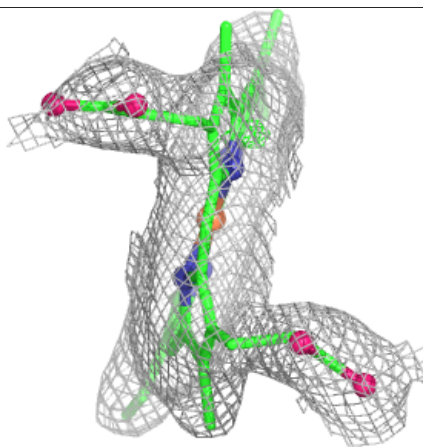
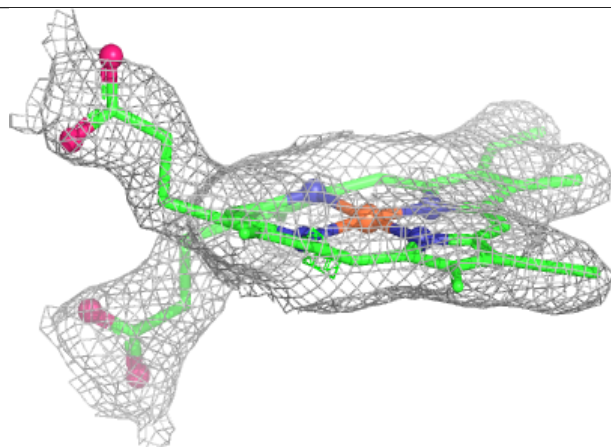
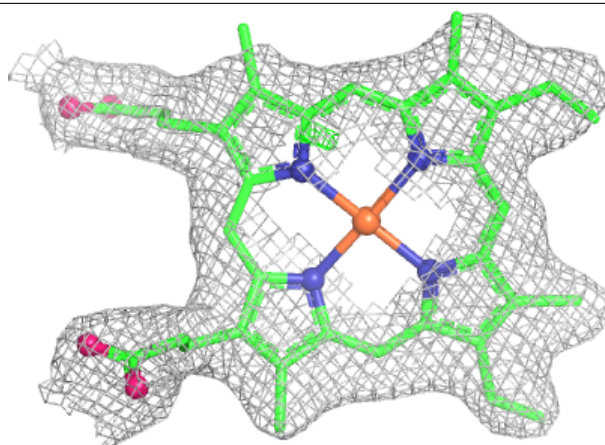
Electron density around HEM E 101:

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



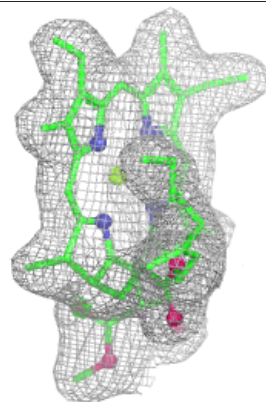
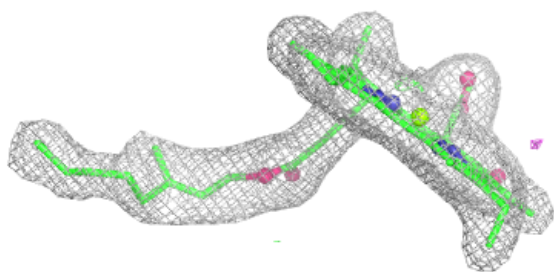
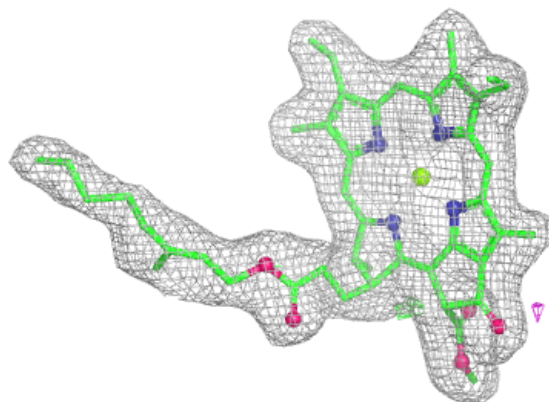
Electron density around HEM f 101:

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

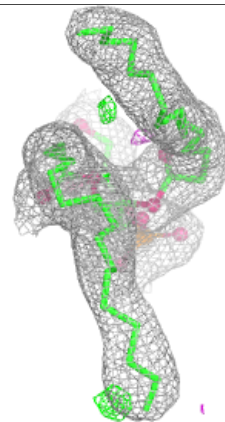
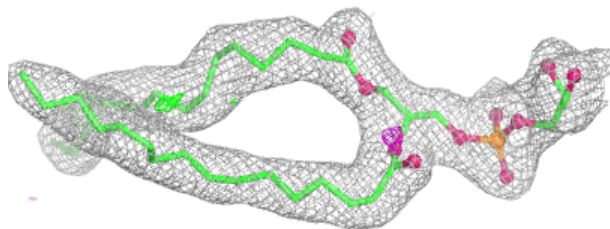
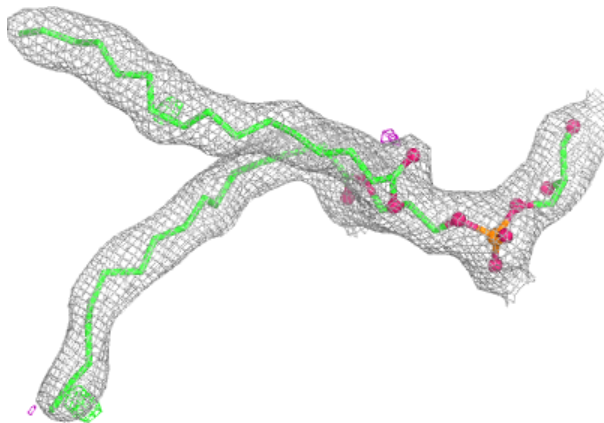


Electron density around CLA A 608:

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

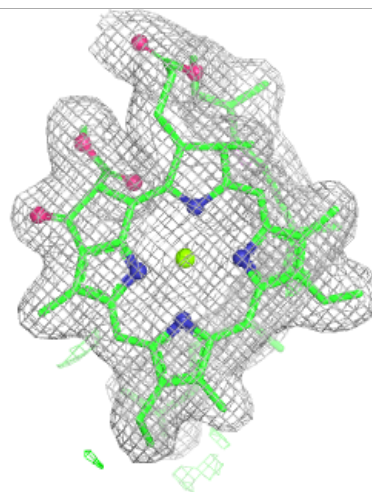
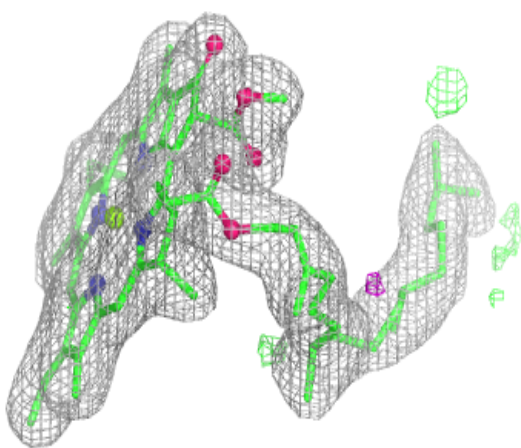
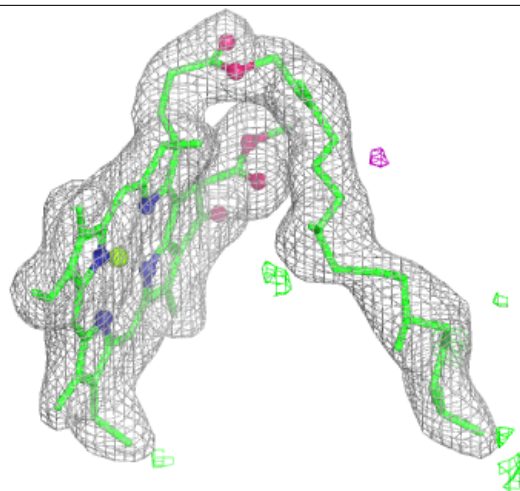
**Electron density around LHG D 409:**

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



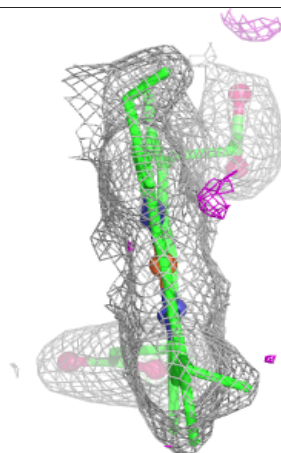
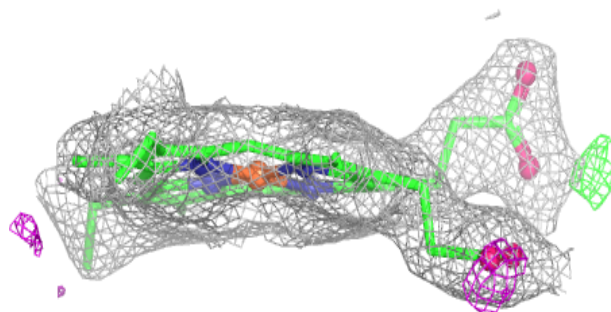
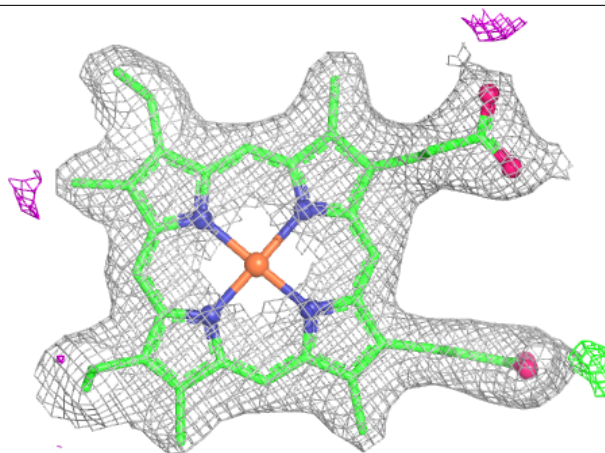
Electron density around CLA B 613:

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



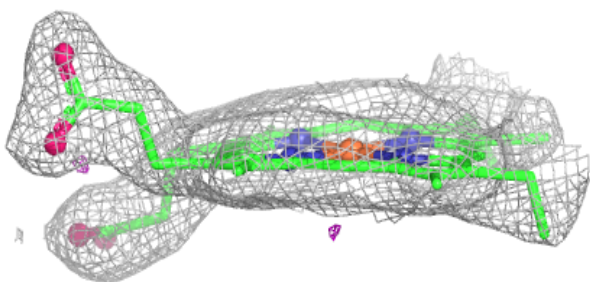
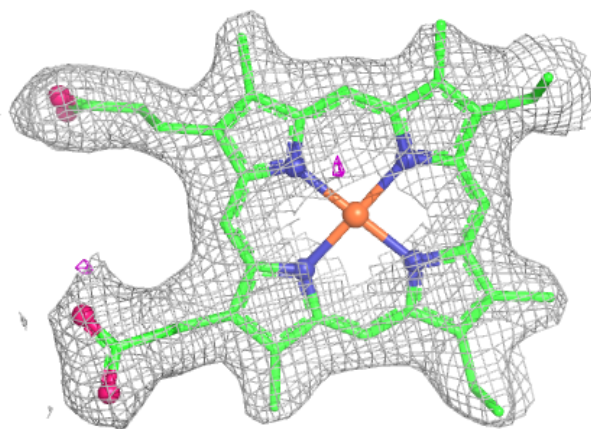
Electron density around HEC V 201:

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



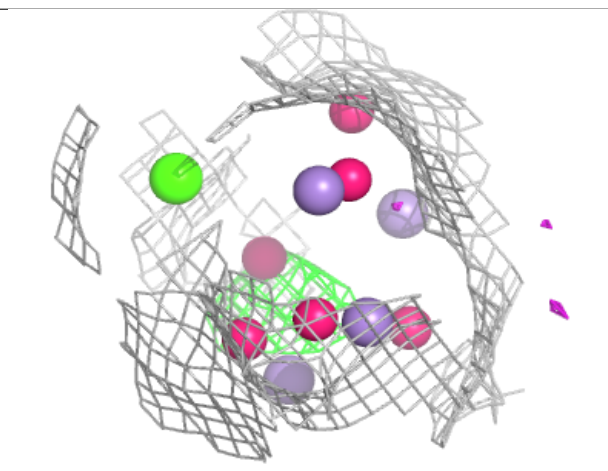
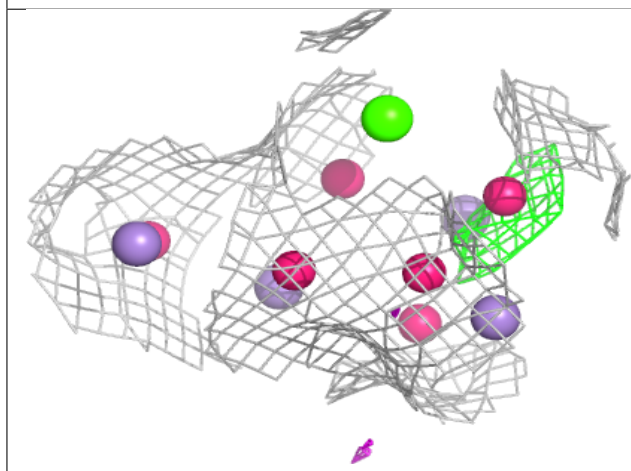
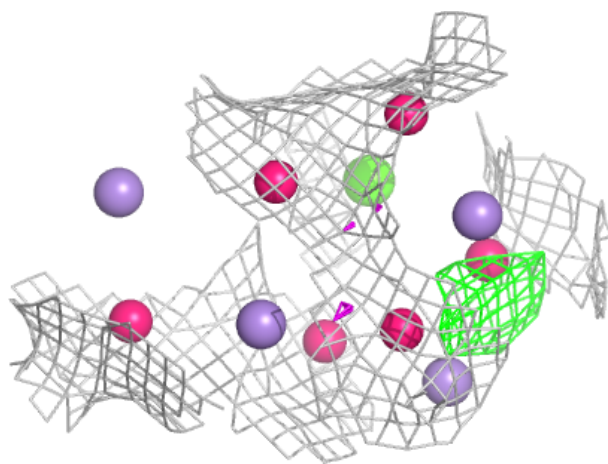
Electron density around HEC v 201:

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



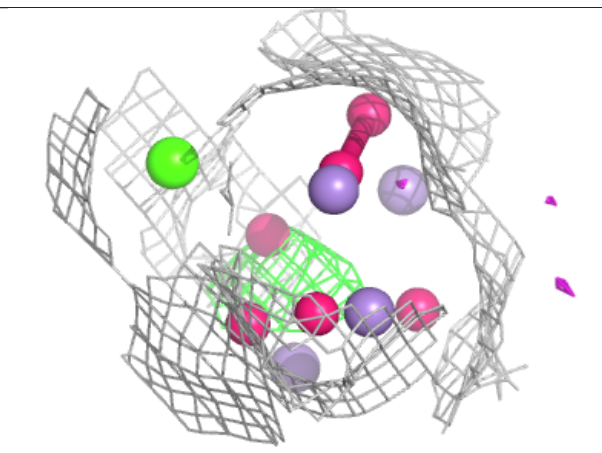
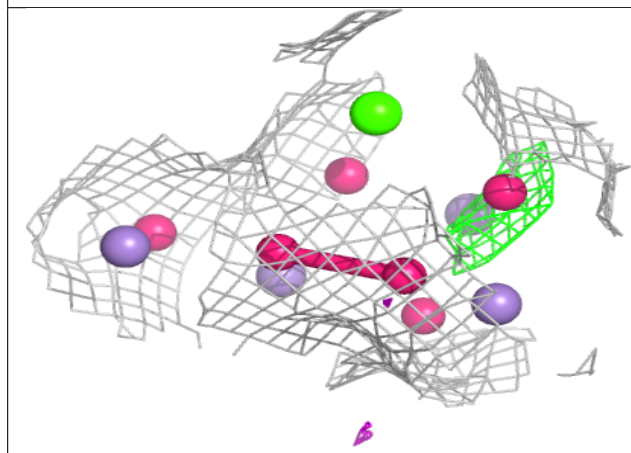
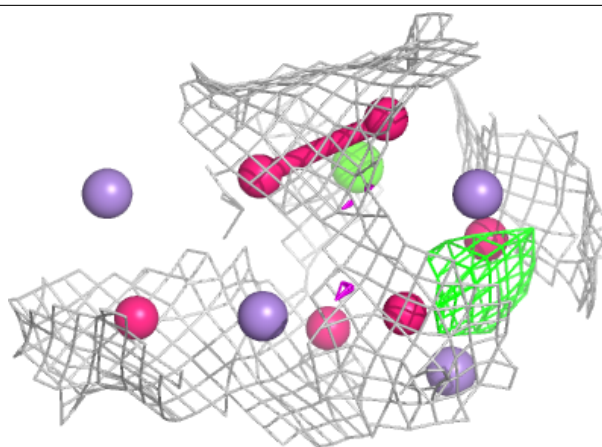
Electron density around OEY A 601 (A):

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



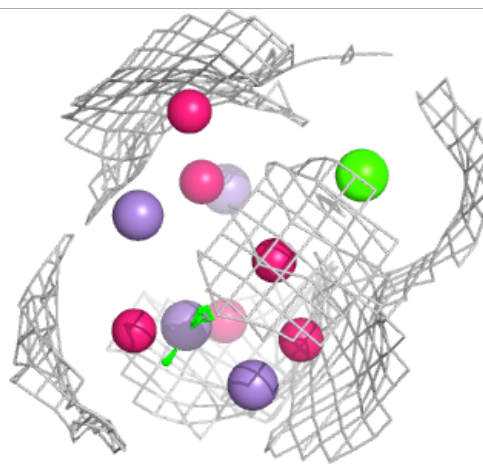
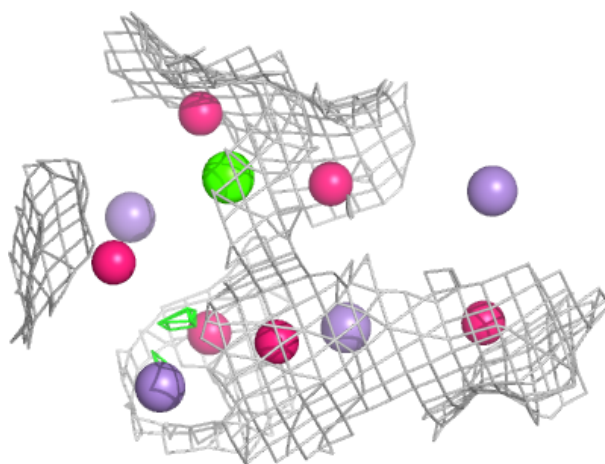
Electron density around OEY A 601 (B):

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



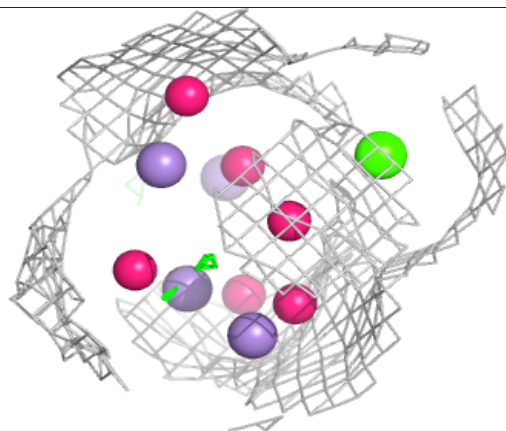
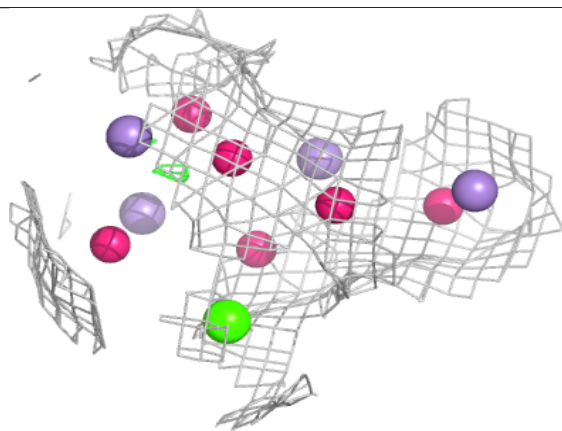
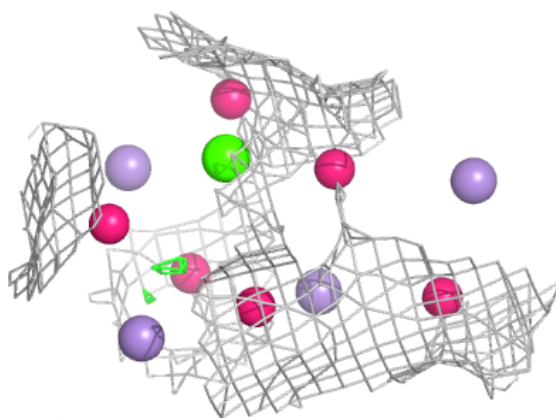
Electron density around OEY a 601 (Å):

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.