



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:02 PM UTC

PDB ID : 8F4C / pdb_00008f4c
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.00 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 : 2.00 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

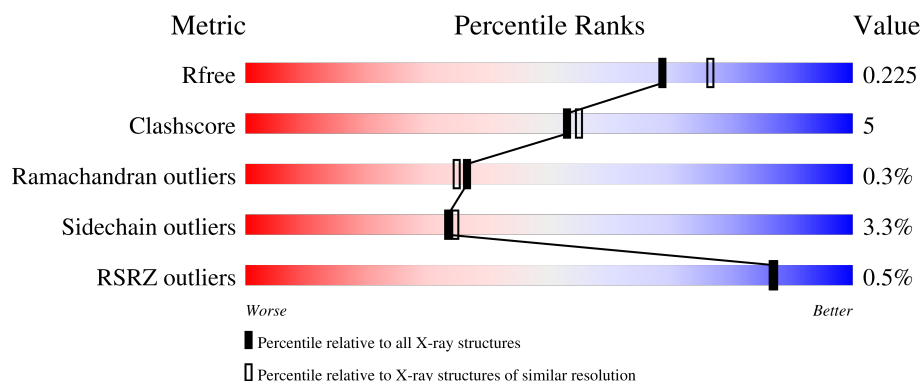
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	 88% 9% .

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

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Mol	Chain	Length	Quality of chain
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	X	-	-	-
25	CLA	A	611	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 53435 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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- 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			
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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
t	1	FME	-	initiating methionine	UNP Q8DIQ0

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

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

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

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

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

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

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

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

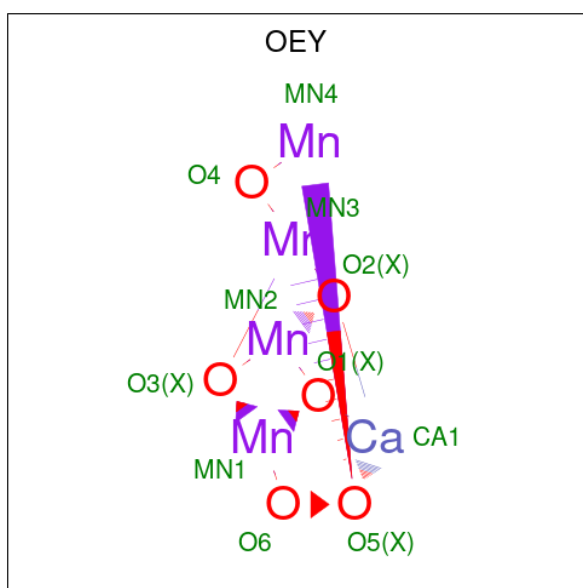
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

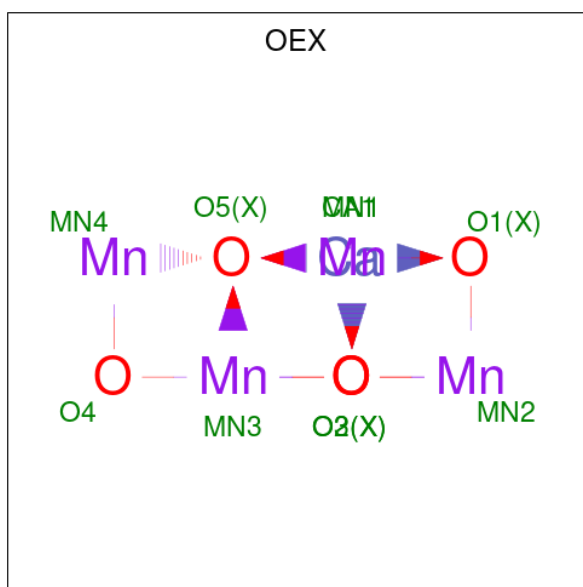
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
20	r	31	Total	C	N	O	0	0	0
			246	166	43	37			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
21	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

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



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

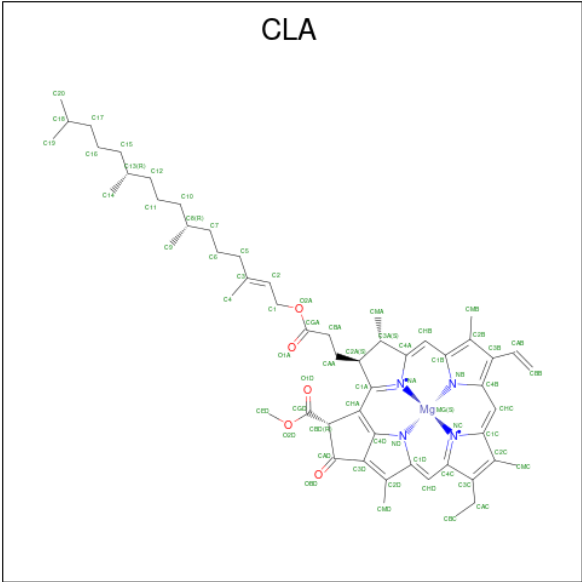
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	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
			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		

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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 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 59	C 49	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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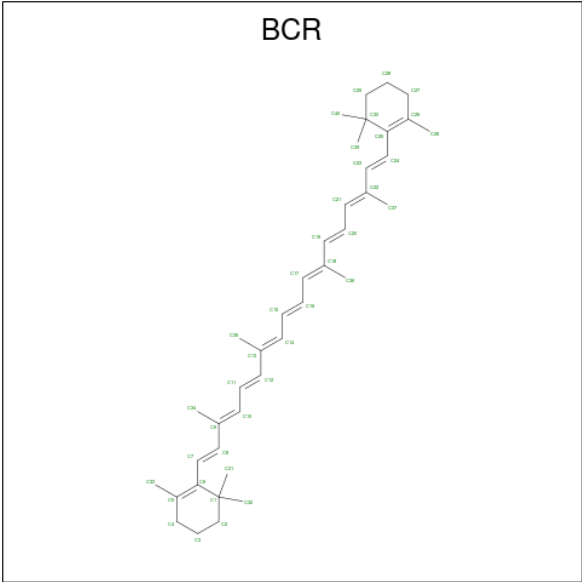
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
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 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	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
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: C₄₀H₅₆).



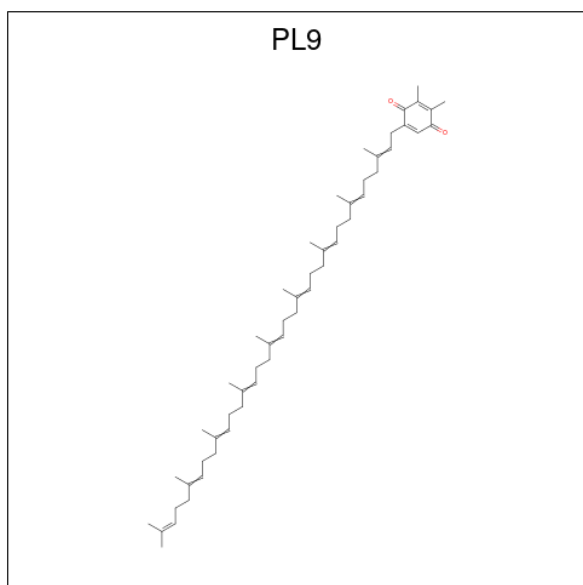
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Z	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	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	x	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).



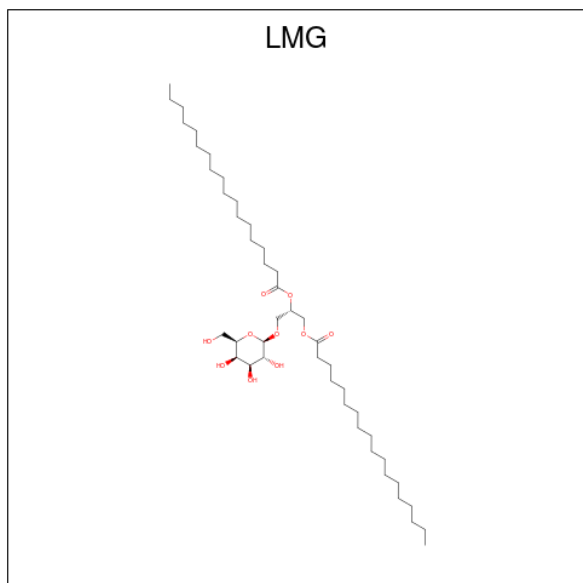
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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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		

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



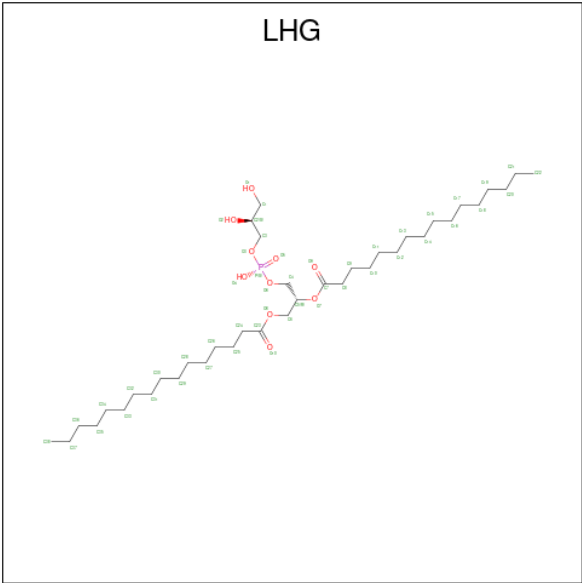
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			48	38	10		
28	B	1	Total	C	O	0	0
			28	24	4		
28	C	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			51	41	10		
28	D	1	Total	C	O	0	0
			33	27	6		
28	M	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



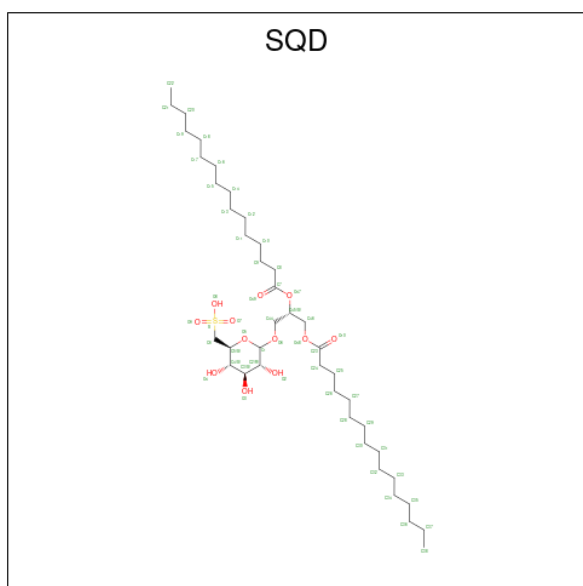
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			47	36	10	1		
29	B	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	E	1	Total	C	O	P	0	0
			49	38	10	1		
29	L	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		

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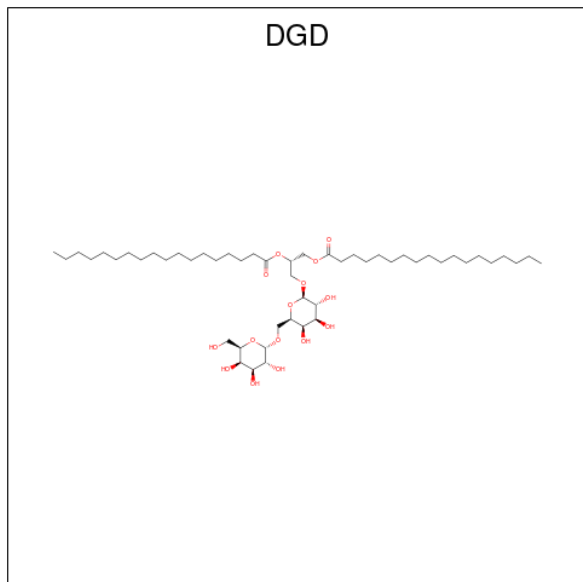
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	d	1	Total	C	O	P	0	0
			39	28	10	1		
29	e	1	Total	C	O	P	0	0
			42	31	10	1		
29	l	1	Total	C	O	P	0	0
			49	38	10	1		

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



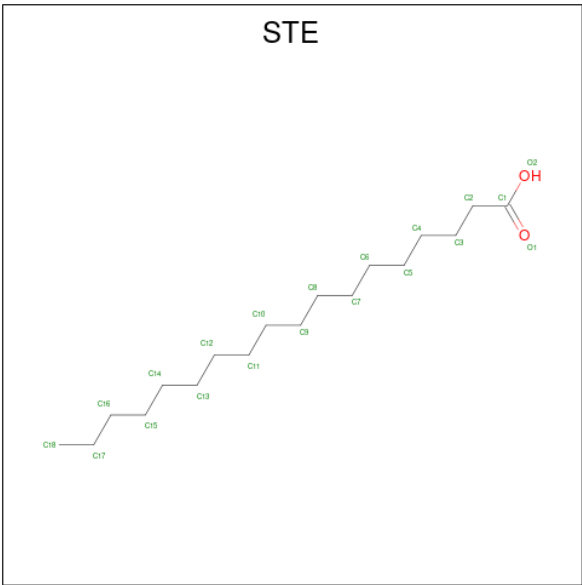
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36	31	5			
30	b	1	Total	C	O	S	0	0
			49	36	12	1		
30	f	1	Total	C	O	S	0	0
			41	28	12	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	C	1	Total	C	O	0	0
			62	47	15		
31	H	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	c	1	Total	C	O	0	0
			62	47	15		
31	h	1	Total	C	O	0	0
			62	47	15		
31	o	1	Total	C	O	0	0
			44	39	5		

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



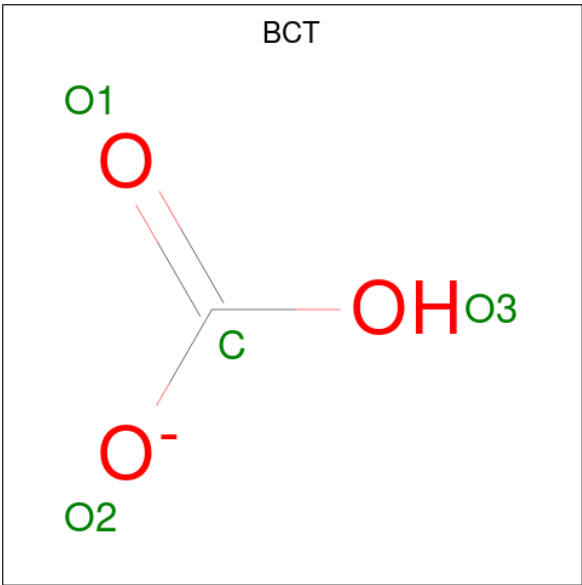
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			17	15	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C	O	0	0
			18	16	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C		0	0
			16	16			
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C		0	0
			16	16			
32	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		
32	M	1	Total	C	O	0	0
			15	13	2		
32	M	1	Total	C		0	0
			10	10			

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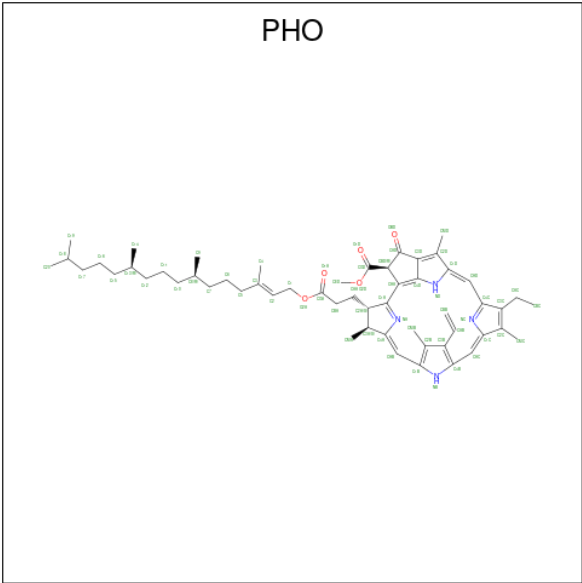
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	T	1	Total C 15 15	0	0
32	T	1	Total C O 20 18 2	0	0
32	X	1	Total C O 20 18 2	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C 16 16	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 2	0	0
32	c	1	Total C O 12 10 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	l	1	Total C 18 18	0	0
32	m	1	Total C O 12 10 2	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 BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



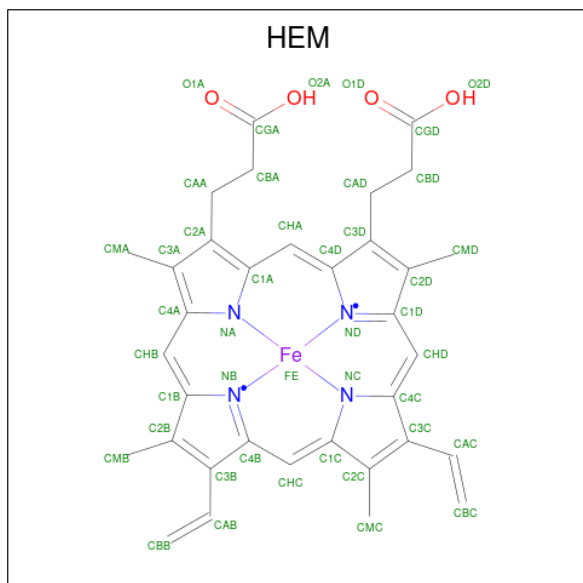
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	N	O	0	0
			64	55	4	5		
34	D	1	Total	C	N	O	0	0
			64	55	4	5		

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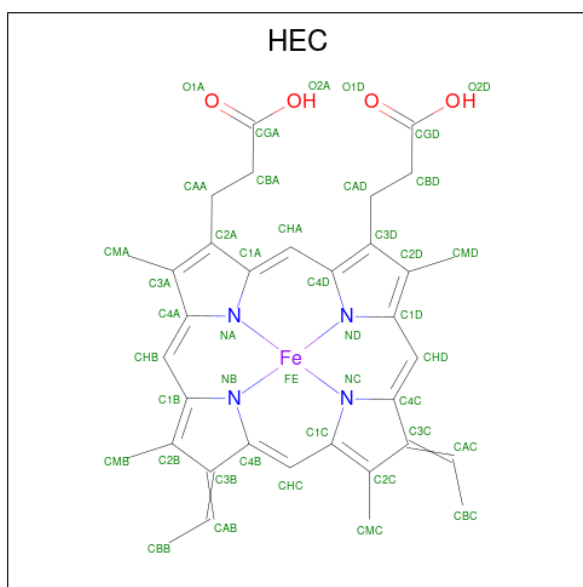
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	d	1	Total 64	C 55	N 4	O 5	0	0
34	d	1	Total 64	C 55	N 4	O 5	0	0

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



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

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	140	Total	O	0	4
			144	144		
37	B	208	Total	O	0	0
			208	208		
37	C	199	Total	O	0	0
			199	199		
37	D	134	Total	O	0	0
			134	134		
37	E	31	Total	O	0	0
			31	31		
37	F	8	Total	O	0	0
			8	8		
37	H	30	Total	O	0	0
			30	30		
37	I	16	Total	O	0	0
			16	16		
37	J	12	Total	O	0	0
			12	12		
37	K	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	L	9	Total O 9 9	0	0
37	M	11	Total O 11 11	0	0
37	O	85	Total O 85 85	0	0
37	T	12	Total O 12 12	0	0
37	U	41	Total O 41 41	0	0
37	V	71	Total O 71 71	0	0
37	Y	5	Total O 5 5	0	0
37	X	9	Total O 9 9	0	0
37	Z	5	Total O 5 5	0	0
37	R	10	Total O 10 10	0	0
37	a	133	Total O 137 137	0	4
37	b	199	Total O 199 199	0	0
37	c	172	Total O 172 172	0	0
37	d	119	Total O 119 119	0	0
37	e	32	Total O 32 32	0	0
37	f	6	Total O 6 6	0	0
37	h	27	Total O 27 27	0	0
37	i	15	Total O 15 15	0	0
37	j	9	Total O 9 9	0	0
37	k	6	Total O 6 6	0	0
37	l	9	Total O 9 9	0	0

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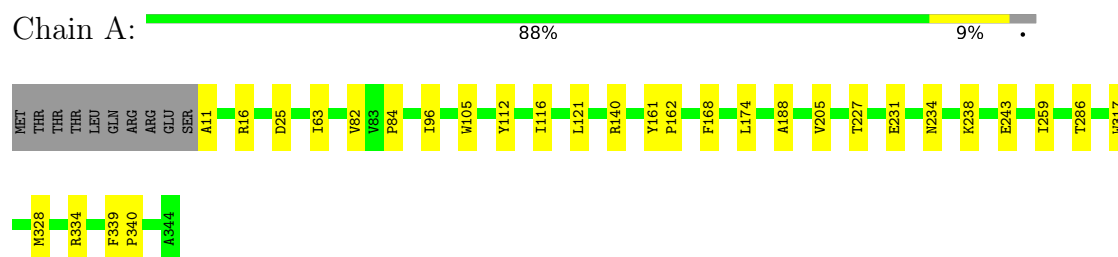
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	10	Total 10	O 10	0	0
37	o	102	Total 102	O 102	0	0
37	t	9	Total 9	O 9	0	0
37	u	53	Total 53	O 53	0	0
37	v	57	Total 57	O 57	0	0
37	y	5	Total 5	O 5	0	0
37	x	9	Total 9	O 9	0	0
37	z	3	Total 3	O 3	0	0
37	r	4	Total 4	O 4	0	0

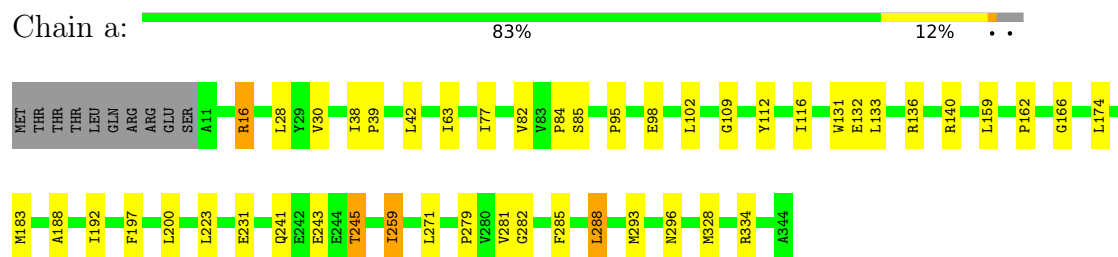
3 Residue-property plots [i](#)

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

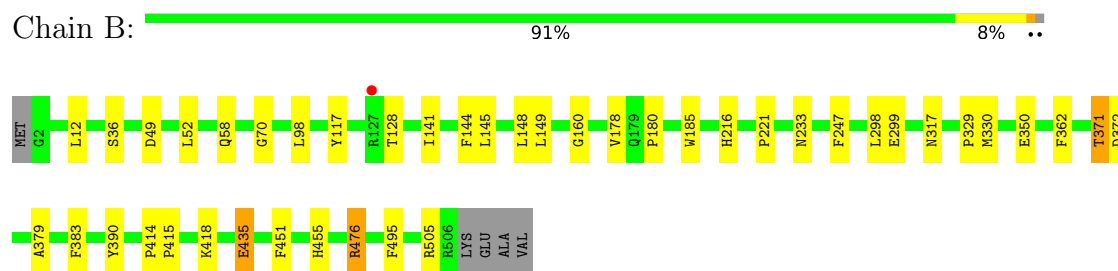
- Molecule 1: Photosystem II protein D1 1



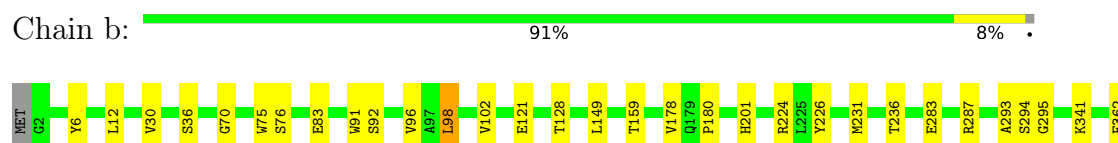
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein

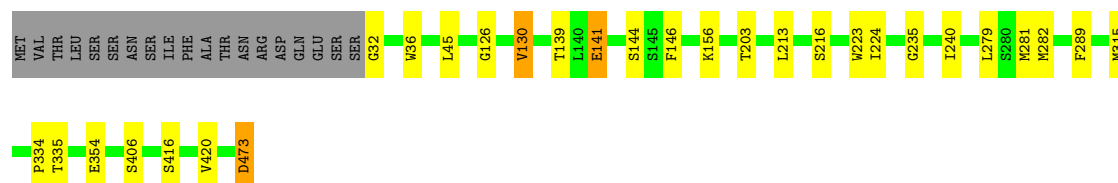
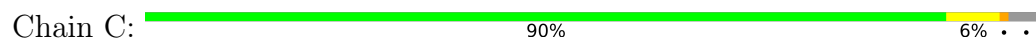


- Molecule 2: Photosystem II CP47 reaction center protein

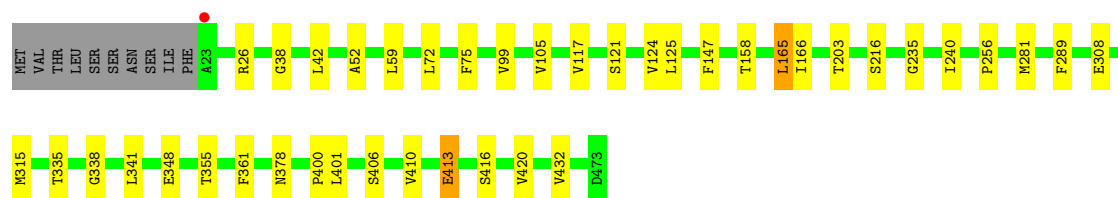
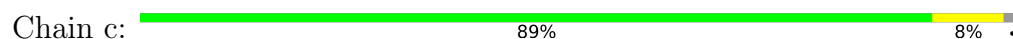




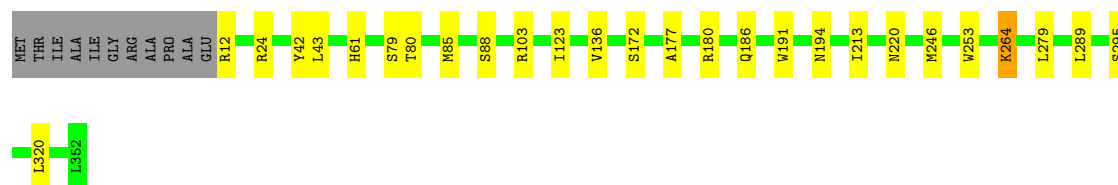
- Molecule 3: Photosystem II CP43 reaction center protein



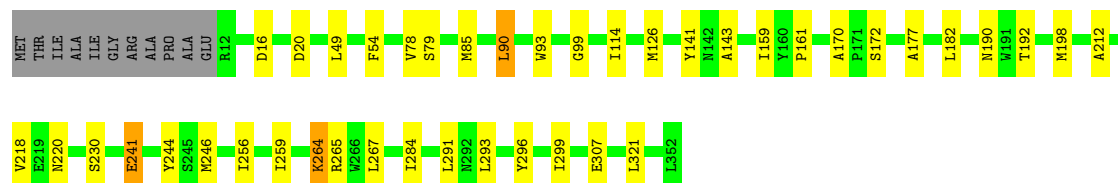
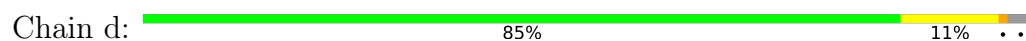
- Molecule 3: Photosystem II CP43 reaction center protein



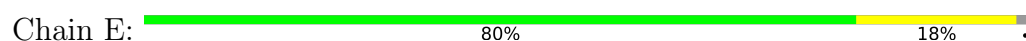
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein

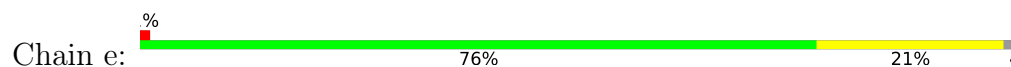


- Molecule 5: Cytochrome b559 subunit alpha





- Molecule 5: Cytochrome b559 subunit alpha



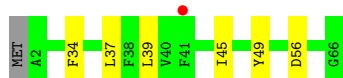
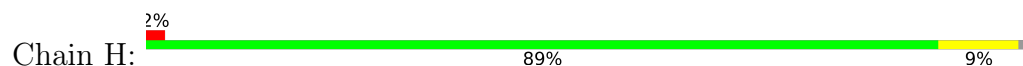
- Molecule 6: Cytochrome b559 subunit beta



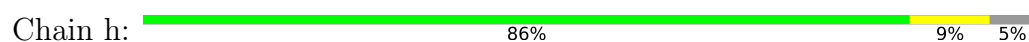
- Molecule 6: Cytochrome b559 subunit beta



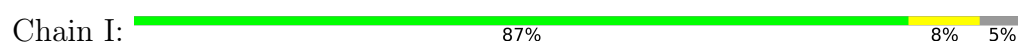
- Molecule 7: Photosystem II reaction center protein H



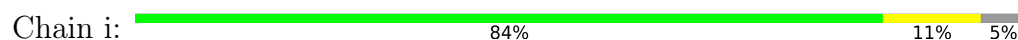
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 72% 18% 10%



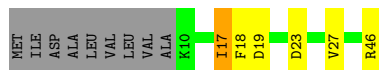
- Molecule 9: Photosystem II reaction center protein J

Chain j: 68% 20% 10%



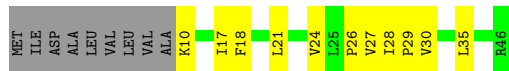
- Molecule 10: Photosystem II reaction center protein K

Chain K: 67% 11% 20%



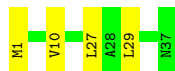
- Molecule 10: Photosystem II reaction center protein K

Chain k: 57% 24% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 89% 11%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 5% 5% 5%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 75% 17% 8%



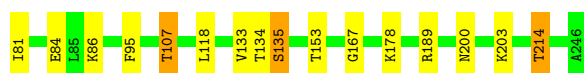
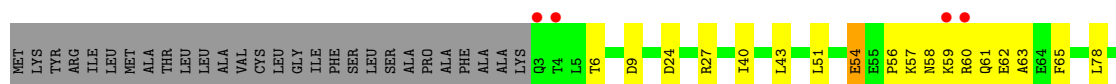
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 8% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 77% 11% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 80% 10% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 81% 12% 6%



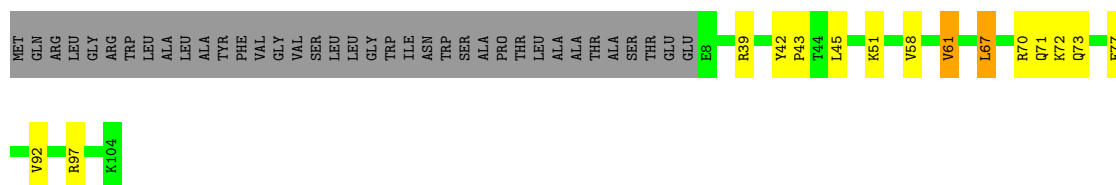
- Molecule 14: Photosystem II reaction center protein T

Chain t: 78% 16% 6%

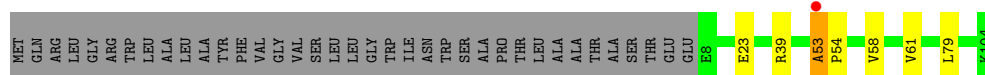


- Molecule 15: Photosystem II 12 kDa extrinsic protein

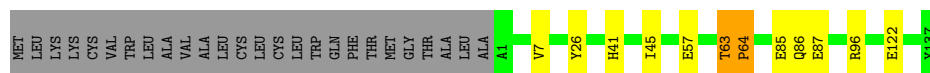
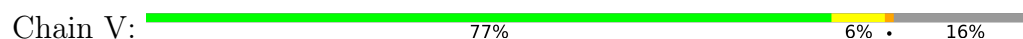
Chain U: 61% 10% 28%



- Molecule 15: Photosystem II 12 kDa extrinsic protein



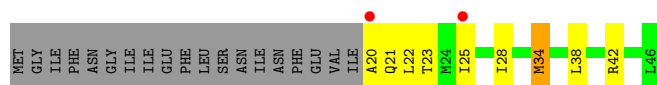
- Molecule 16: Cytochrome c-550



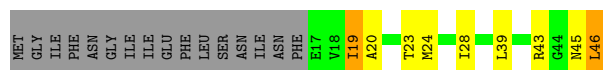
- Molecule 16: Cytochrome c-550



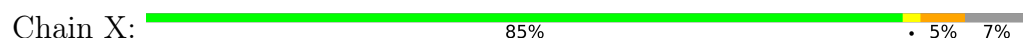
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12

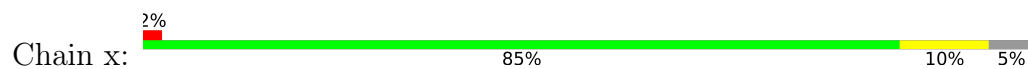


- Molecule 18: Photosystem II reaction center X protein

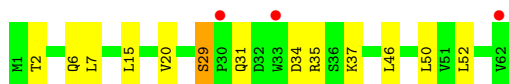
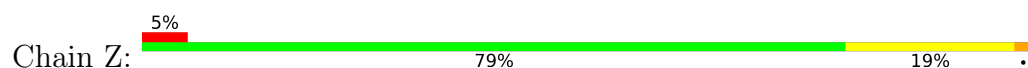




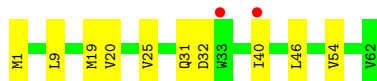
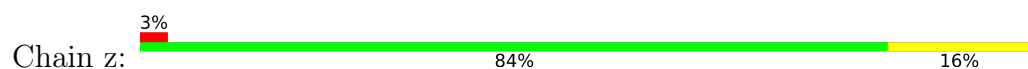
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



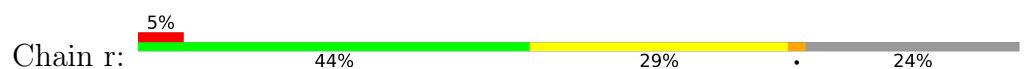
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.33Å 222.79Å 309.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.00 19.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.80-2.00) 85.5 (19.80-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.224 0.180 , 0.225	Depositor DCC
R_{free} test set	4804 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53435	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: OEY, PHO, FME, CLA, BCR, DGD, OEX, PL9, CL, HEC, LHG, LMG, STE, HEM, FE2, BCT, SQD

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	0.31	0/3212	0.49	0/4376
1	a	0.29	0/3209	0.47	0/4372
2	B	0.31	0/4155	0.48	0/5661
2	b	0.30	0/4118	0.45	0/5611
3	C	0.30	0/3625	0.44	0/4935
3	c	0.28	0/3705	0.44	0/5042
4	D	0.33	0/2825	0.49	0/3847
4	d	0.31	0/2834	0.48	0/3859
5	E	0.25	0/688	0.43	0/940
5	e	0.24	0/683	0.43	0/932
6	F	0.26	0/284	0.42	0/387
6	f	0.23	0/284	0.48	0/387
7	H	0.31	0/523	0.46	0/713
7	h	0.26	0/511	0.44	0/697
8	I	0.31	0/293	0.43	0/396
8	i	0.31	0/293	0.41	0/396
9	J	0.25	0/263	0.46	0/356
9	j	0.23	0/263	0.37	0/356
10	K	0.26	0/303	0.41	0/416
10	k	0.26	0/303	0.41	0/416
11	L	0.33	0/311	0.46	0/422
11	l	0.32	0/303	0.47	0/412
12	M	0.30	0/249	0.48	0/341
12	m	0.30	0/244	0.50	0/334
13	O	0.31	0/1904	0.52	0/2585
13	o	0.30	0/1905	0.46	0/2583
14	T	0.34	0/257	0.52	0/349
14	t	0.30	0/255	0.45	0/346
15	U	0.25	0/785	0.47	0/1064
15	u	0.28	0/785	0.48	0/1064
16	V	0.28	0/1085	0.50	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.26	0/1085	0.42	0/1473
17	Y	0.22	0/197	0.35	0/264
17	y	0.20	0/219	0.37	0/294
18	X	0.24	0/284	0.37	0/384
18	x	0.22	0/289	0.28	0/391
19	Z	0.24	0/490	0.44	0/669
19	z	0.30	0/488	0.31	0/666
20	R	0.27	0/277	0.45	0/380
20	r	0.21	0/252	0.37	0/347
All	All	0.30	0/44038	0.46	0/59936

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	2981	21	0
1	a	3110	0	2972	34	0
2	B	4005	0	3871	30	0
2	b	3978	0	3836	34	0
3	C	3509	0	3426	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	24	0
4	D	2731	0	2637	23	0
4	d	2737	0	2643	29	0
5	E	666	0	651	9	0
5	e	664	0	648	17	0
6	F	275	0	282	4	0
6	f	275	0	282	9	0
7	H	510	0	532	6	0
7	h	498	0	518	5	0
8	I	296	0	311	2	0
8	i	296	0	311	2	0
9	J	257	0	268	4	0
9	j	257	0	268	7	0
10	K	293	0	305	4	0
10	k	293	0	305	5	0
11	L	304	0	316	3	0
11	l	296	0	304	2	0
12	M	256	0	269	4	0
12	m	251	0	267	2	0
13	O	1870	0	1830	21	0
13	o	1874	0	1846	15	0
14	T	258	0	261	4	0
14	t	256	0	256	4	0
15	U	774	0	773	8	0
15	u	774	0	773	3	0
16	V	1064	0	1073	5	0
16	v	1064	0	1073	12	0
17	Y	196	0	217	7	0
17	y	218	0	241	7	0
18	X	281	0	312	3	0
18	x	286	0	314	1	0
19	Z	479	0	516	6	0
19	z	477	0	509	3	0
20	R	271	0	298	3	0
20	r	246	0	263	8	0
21	A	11	0	0	1	0
21	a	11	0	0	1	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	6	0
25	B	1035	0	1139	38	0
25	C	839	0	922	16	0
25	D	130	0	144	2	0
25	a	260	0	288	7	0
25	b	1035	0	1139	32	0
25	c	839	0	919	26	0
25	d	130	0	144	3	0
26	A	40	0	56	1	0
26	B	120	0	168	6	0
26	C	40	0	56	3	0
26	D	40	0	56	1	0
26	H	40	0	56	0	0
26	K	80	0	112	3	0
26	T	40	0	56	5	0
26	Z	40	0	56	2	0
26	a	40	0	56	1	0
26	b	120	0	168	5	0
26	c	40	0	56	2	0
26	d	40	0	56	3	0
26	k	120	0	168	6	0
26	t	40	0	56	3	0
26	x	40	0	56	2	0
27	A	55	0	80	5	0
27	D	55	0	80	1	0
27	a	55	0	80	4	0
27	d	55	0	80	1	0
28	A	48	0	66	2	0
28	B	28	0	40	0	0
28	C	48	0	66	0	0
28	D	84	0	117	3	0
28	M	51	0	72	2	0
28	b	106	0	158	2	0
28	c	134	0	181	9	0
28	d	67	0	92	0	0
29	A	47	0	67	5	0
29	B	49	0	74	3	0
29	D	49	0	74	1	0
29	E	49	0	74	4	0
29	L	49	0	74	2	0
29	d	137	0	199	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	e	42	0	57	1	0
29	l	49	0	74	1	0
30	A	91	0	136	4	0
30	B	54	0	78	3	0
30	D	36	0	46	2	0
30	a	90	0	134	4	0
30	b	49	0	65	1	0
30	f	41	0	49	2	0
31	A	66	0	96	7	0
31	C	186	0	246	3	0
31	H	62	0	81	3	0
31	c	186	0	246	3	0
31	h	62	0	82	0	0
31	o	44	0	75	3	0
32	B	75	0	117	2	0
32	C	40	0	63	0	0
32	E	12	0	16	0	0
32	H	18	0	35	1	0
32	I	15	0	26	2	0
32	J	12	0	16	0	0
32	M	25	0	38	0	0
32	T	35	0	64	3	0
32	X	20	0	35	1	0
32	a	12	0	16	0	0
32	b	62	0	106	4	0
32	c	32	0	51	3	0
32	d	37	0	61	4	0
32	j	12	0	16	1	0
32	l	18	0	35	2	0
32	m	12	0	16	0	0
32	t	24	0	36	0	0
33	D	4	0	1	1	0
33	a	4	0	1	0	0
34	D	128	0	148	2	0
34	d	128	0	148	2	0
35	F	43	0	30	2	0
35	f	43	0	30	5	0
36	V	43	0	30	0	0
36	v	43	0	30	1	0
37	A	144	0	0	4	0
37	B	208	0	0	0	0
37	C	199	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	134	0	0	2	0
37	E	31	0	0	0	0
37	F	8	0	0	0	0
37	H	30	0	0	0	0
37	I	16	0	0	0	0
37	J	12	0	0	1	0
37	K	5	0	0	2	0
37	L	9	0	0	0	0
37	M	11	0	0	0	0
37	O	85	0	0	4	0
37	R	10	0	0	0	0
37	T	12	0	0	0	0
37	U	41	0	0	0	0
37	V	71	0	0	0	0
37	X	9	0	0	0	0
37	Y	5	0	0	0	0
37	Z	5	0	0	0	0
37	a	137	0	0	2	0
37	b	199	0	0	3	0
37	c	172	0	0	1	0
37	d	119	0	0	1	0
37	e	32	0	0	2	0
37	f	6	0	0	1	0
37	h	27	0	0	1	0
37	i	15	0	0	0	0
37	j	9	0	0	0	0
37	k	6	0	0	0	0
37	l	9	0	0	1	0
37	m	10	0	0	1	0
37	o	102	0	0	0	0
37	r	4	0	0	2	0
37	t	9	0	0	0	0
37	u	53	0	0	0	0
37	v	57	0	0	0	0
37	x	9	0	0	0	0
37	y	5	0	0	1	0
37	z	3	0	0	0	0
All	All	53435	0	52752	525	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 5.

All (525) 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)
4:d:246:MET:HE3	4:d:264:LYS:HD2	1.53	0.91
27:A:610:PL9:H361	6:F:25:THR:HG21	1.53	0.89
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.57	0.85
5:e:57:ALA:H	5:e:60:GLN:HE21	1.22	0.83
21:a:601[B]:OEY:O6	21:a:601[B]:OEY:O5	1.97	0.81
19:Z:29:SER:HB3	19:Z:31:GLN:HE21	1.44	0.81
27:A:610:PL9:H152	29:E:101:LHG:H372	1.63	0.80
25:B:606:CLA:H72	26:B:619:BCR:H311	1.67	0.76
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.67	0.76
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.04	0.75
25:b:604:CLA:H42	25:b:605:CLA:H2	1.67	0.75
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.53	0.74
25:C:504:CLA:H101	31:C:517:DGD:HBN1	1.70	0.74
2:B:495:PHE:HD2	2:B:505:ARG:HH12	1.36	0.73
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.55	0.70
28:b:622:LMG:O10	12:m:4:ASN:ND2	2.21	0.70
1:A:25:ASP:OD1	37:A:701:HOH:O	2.10	0.70
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.72	0.70
4:D:12:ARG:O	37:D:501:HOH:O	2.10	0.69
25:A:607:CLA:H193	27:A:610:PL9:H221	1.74	0.69
29:A:613:LHG:H151	30:A:614:SQD:H262	1.75	0.69
5:e:61:ARG:NH1	16:v:125:ILE:O	2.26	0.68
29:D:410:LHG:H321	14:T:21:ILE:HD11	1.78	0.66
10:K:19:ASP:OD1	37:K:201:HOH:O	2.13	0.66
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.76	0.66
25:C:502:CLA:H61	25:C:512:CLA:H42	1.78	0.65
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.78	0.65
17:Y:20:ALA:N	17:Y:23:THR:HG1	1.96	0.64
29:A:613:LHG:H141	29:A:613:LHG:H322	1.80	0.64
10:k:21:LEU:HD13	17:y:24:MET:HE2	1.79	0.64
31:A:616:DGD:HB41	32:I:101:STE:H62	1.79	0.64
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.79	0.64
25:c:503:CLA:H203	25:c:510:CLA:HAB	1.80	0.64
26:T:101:BCR:H311	26:T:101:BCR:HC8	1.79	0.63
29:B:622:LHG:H222	12:M:18:PRO:HG3	1.79	0.63
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.80	0.63
1:a:102:LEU:HD12	31:o:301:DGD:HB22	1.79	0.63
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.80	0.63
2:b:91:TRP:HE1	32:b:623:STE:H111	1.64	0.62
4:D:279:LEU:HD22	34:D:403:PHO:HBC3	1.82	0.62
9:J:15:THR:HG22	9:J:19:MET:HE2	1.81	0.62
3:c:281:MET:HG3	28:c:522:LMG:H402	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:615:CLA:H2	25:B:616:CLA:HBB2	1.82	0.62
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.81	0.62
6:f:16:PHE:H	20:r:30:GLN:HE22	1.48	0.62
25:a:609:CLA:H41	25:a:609:CLA:H142	1.81	0.62
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.82	0.61
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.82	0.61
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.81	0.61
2:B:371:THR:HG23	2:B:372:ASP:O	2.01	0.60
3:C:32:GLY:N	37:C:605:HOH:O	2.34	0.60
9:j:26:GLY:HA2	32:j:101:STE:H71	1.83	0.60
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.83	0.60
25:a:608:CLA:HAB	25:d:403:CLA:H72	1.84	0.59
35:F:101:HEM:HBC2	35:F:101:HEM:HHH	1.84	0.59
35:f:101:HEM:HBC2	35:f:101:HEM:HMC2	1.83	0.59
1:A:11:ALA:O	1:A:16:ARG:NH2	2.34	0.59
9:j:15:THR:HG22	9:j:19:MET:HE2	1.85	0.59
13:O:107:THR:HG22	37:O:313:HOH:O	2.03	0.59
2:B:435:GLU:OE1	13:O:178:LYS:NZ	2.35	0.59
25:c:505:CLA:H201	28:c:522:LMG:H121	1.84	0.59
2:b:506:ARG:NH2	37:b:708:HOH:O	2.36	0.59
17:y:43:ARG:NH2	37:y:101:HOH:O	2.35	0.58
4:d:99:GLY:HA3	32:d:413:STE:H142	1.85	0.58
7:h:3:ARG:NE	37:h:202:HOH:O	2.34	0.58
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.86	0.58
2:b:489:GLU:HA	2:b:495:PHE:HD2	1.68	0.58
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.36	0.58
25:a:608:CLA:H203	27:a:611:PL9:H221	1.85	0.58
6:f:24:HIS:O	6:f:28:VAL:HG13	2.03	0.58
29:d:408:LHG:H321	14:t:21:ILE:HD11	1.85	0.57
26:d:405:BCR:H402	9:j:21:VAL:HG21	1.86	0.57
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.19	0.57
31:c:516:DGD:HB22	28:c:518:LMG:H311	1.86	0.57
7:h:4:ARG:NH2	7:h:9:ASP:OD2	2.38	0.56
13:o:56:PRO:HD3	13:o:63:ALA:HB2	1.86	0.56
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.38	0.56
13:O:56:PRO:O	13:O:58:ASN:N	2.37	0.56
15:u:39:ARG:NH2	16:v:60:ALA:O	2.38	0.56
25:b:603:CLA:H202	25:b:609:CLA:H111	1.87	0.56
4:d:126:MET:HE3	4:d:143:ALA:O	2.05	0.56
12:M:8:LEU:HD11	32:T:102:STE:H142	1.88	0.56
31:A:616:DGD:HE4	2:b:76:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:611:CLA:H142	29:L:101:LHG:H371	1.88	0.55
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.36	0.55
25:c:505:CLA:H43	26:c:514:BCR:HC7	1.87	0.55
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.88	0.55
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.88	0.55
1:A:334[B]:ARG:NH2	37:A:703:HOH:O	2.40	0.55
25:B:601:CLA:HBA1	25:B:601:CLA:HBD	1.88	0.55
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.55
5:e:3:GLY:N	37:e:201:HOH:O	2.40	0.55
1:A:286:THR:HG23	25:A:606:CLA:HED3	1.89	0.54
2:b:92:SER:O	2:b:96:VAL:HG23	2.07	0.54
30:a:613:SQD:H291	32:c:521:STE:H71	1.89	0.54
3:c:165:LEU:HD13	25:c:507:CLA:HED1	1.89	0.54
13:O:203:LYS:NZ	37:O:304:HOH:O	2.41	0.54
16:v:7:VAL:O	16:v:124:LYS:NZ	2.38	0.54
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.43	0.54
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.07	0.54
25:B:607:CLA:H192	29:B:622:LHG:H171	1.89	0.53
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.36	0.53
1:a:279:PRO:HG2	4:d:212:ALA:HB2	1.89	0.53
3:c:406:SER:HA	3:c:420:VAL:HG23	1.89	0.53
13:o:57:LYS:HB3	13:o:59:LYS:HE3	1.90	0.53
3:C:146:PHE:O	3:C:156:LYS:NZ	2.42	0.53
29:A:613:LHG:H191	29:A:613:LHG:H371	1.90	0.53
19:z:32:ASP:OD1	19:z:32:ASP:N	2.41	0.53
27:d:406:PL9:H322	29:l:101:LHG:H222	1.90	0.53
20:r:2:ASP:HB3	20:r:5:VAL:HG23	1.90	0.53
5:e:57:ALA:H	5:e:60:GLN:NE2	2.01	0.53
4:d:16:ASP:OD1	37:d:501:HOH:O	2.18	0.53
4:d:192:THR:HG23	25:d:403:CLA:HBC2	1.91	0.52
25:B:607:CLA:H193	11:L:27:LEU:HD11	1.90	0.52
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.89	0.52
27:D:407:PL9:H412	11:L:29:LEU:HD23	1.90	0.52
13:O:133:VAL:C	13:O:135:SER:H	2.17	0.52
3:C:126:GLY:O	3:C:130:VAL:HG13	2.09	0.52
3:C:213:LEU:HG	25:C:506:CLA:H193	1.92	0.52
2:B:149[B]:LEU:HD21	25:B:604:CLA:H171	1.91	0.52
10:K:23:ASP:OD2	37:K:201:HOH:O	2.18	0.52
1:A:334[A]:ARG:NH2	37:A:703:HOH:O	2.43	0.52
28:A:612:LMG:H392	3:C:281:MET:HG3	1.92	0.52
3:C:141:GLU:H	3:C:141:GLU:CD	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:110:MET:HE2	13:o:116:ILE:HD11	1.93	0.51
30:A:614:SQD:H381	9:J:22:ILE:HD11	1.92	0.51
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.91	0.51
2:B:233:ASN:HD21	2:B:476:ARG:NH1	2.08	0.51
25:B:604:CLA:HBD	25:B:605:CLA:H43	1.93	0.51
5:e:26:THR:HA	20:r:15:ALA:HB1	1.93	0.51
4:D:103:ARG:HH21	5:E:77:GLU:CG	2.24	0.51
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.92	0.51
19:Z:34:ASP:O	19:Z:37:LYS:HG2	2.10	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.74	0.51
25:c:504:CLA:H91	25:c:508:CLA:H171	1.93	0.51
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.92	0.51
5:e:30:LEU:HD11	35:f:101:HEM:HBB2	1.93	0.50
13:O:27:ARG:NH1	37:O:303:HOH:O	2.36	0.50
5:E:54:SER:HB2	5:E:83:LEU:HD13	1.93	0.50
31:A:616:DGD:HA62	2:b:98:LEU:HD21	1.93	0.50
26:B:617:BCR:H15C	30:B:623:SQD:H381	1.93	0.50
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.94	0.50
11:l:7:ARG:HH22	32:l:102:STE:C1	2.25	0.50
30:D:409:SQD:H441	20:R:30:GLN:HE21	1.77	0.50
3:c:121:SER:HB3	32:c:519:STE:H183	1.93	0.50
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.46	0.50
25:C:501:CLA:HHC	25:C:501:CLA:HBB1	1.94	0.50
15:U:58:VAL:O	15:U:61:VAL:HG22	2.12	0.50
10:k:28:ILE:HD11	17:y:28:ILE:HD13	1.92	0.49
16:v:69:ILE:HD12	16:v:120:LEU:HD12	1.94	0.49
25:C:511:CLA:H143	19:Z:20:VAL:HG13	1.95	0.49
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.94	0.49
6:f:19:ARG:O	6:f:23:VAL:HG13	2.12	0.49
12:m:5:GLN:O	37:m:201:HOH:O	2.20	0.49
2:B:299[B]:GLU:H	2:B:299[B]:GLU:CD	2.20	0.49
32:d:413:STE:H71	18:x:16:SER:HB3	1.94	0.49
20:r:21:ARG:NH1	37:r:101:HOH:O	2.41	0.49
25:C:505:CLA:HBC2	26:C:514:BCR:H341	1.93	0.49
13:O:84:GLU:OE1	13:O:86:LYS:NZ	2.31	0.49
16:v:41:HIS:CD2	36:v:201:HEC:NB	2.80	0.49
12:M:6:LEU:HD12	28:M:101:LMG:HC92	1.94	0.49
12:M:31:SER:HB3	32:l:102:STE:H22	1.95	0.49
7:H:49:TYR:CE2	31:H:102:DGD:HB41	2.47	0.48
2:b:413:ASP:HB2	37:b:741:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:341:LYS:HD2	2:b:429:ILE:HG22	1.93	0.48
25:b:615:CLA:H2	25:b:616:CLA:CBB	2.43	0.48
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.95	0.48
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.48
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.95	0.48
3:c:166:ILE:HG21	25:c:512:CLA:H202	1.96	0.48
20:r:31:VAL:HG22	20:r:32:GLN:HG3	1.95	0.48
16:V:63:THR:HG22	16:V:64:PRO:CD	2.43	0.48
1:a:334[A]:ARG:NH2	37:a:707:HOH:O	2.46	0.48
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.94	0.48
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.96	0.48
25:B:603:CLA:H91	25:B:603:CLA:H112	1.67	0.48
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.48	0.48
2:b:102:VAL:HG11	25:b:606:CLA:H142	1.96	0.48
10:k:26:PRO:O	10:k:29:PRO:HD2	2.14	0.48
2:b:91:TRP:HD1	32:b:623:STE:H162	1.78	0.48
25:b:602:CLA:HBB1	25:b:602:CLA:HMB3	1.96	0.47
29:d:409:LHG:H272	29:d:409:LHG:H242	1.43	0.47
25:C:504:CLA:H143	25:C:508:CLA:H141	1.96	0.47
5:E:26:THR:HA	20:R:15:ALA:HB1	1.97	0.47
9:J:20:GLY:O	9:J:24:ILE:HG13	2.15	0.47
1:a:133:LEU:HD23	4:d:256:ILE:HG12	1.96	0.47
2:B:49:ASP:OD2	13:o:57:LYS:HD2	2.15	0.47
4:D:123:ILE:HD11	31:H:102:DGD:HAH1	1.96	0.47
25:A:606:CLA:H203	25:A:606:CLA:H162	1.66	0.47
25:B:614:CLA:H191	32:B:625:STE:H112	1.96	0.47
6:f:36:ALA:O	6:f:40:MET:HG3	2.15	0.47
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.97	0.47
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.49	0.47
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.47
2:B:317:ASN:HA	2:B:330:MET:HE1	1.97	0.47
16:V:41:HIS:HA	16:V:45:ILE:O	2.15	0.47
2:b:121:GLU:OE2	7:h:12:ARG:NH1	2.40	0.47
34:d:402:PHO:HHD	34:d:402:PHO:HBC2	1.96	0.47
27:A:610:PL9:H422	27:A:610:PL9:H401	1.58	0.47
25:B:603:CLA:H2	25:B:605:CLA:H91	1.95	0.47
25:c:509:CLA:H142	25:c:509:CLA:H111	1.74	0.47
28:c:520:LMG:H382	28:c:520:LMG:H351	1.54	0.47
4:d:49:LEU:HD13	26:d:405:BCR:C15	2.45	0.47
25:B:614:CLA:H112	30:B:623:SQD:H382	1.96	0.47
29:E:101:LHG:H302	29:E:101:LHG:H271	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:501:CLA:C4D	25:c:503:CLA:H2	2.45	0.47
25:c:511:CLA:H141	25:c:511:CLA:H161	1.70	0.47
2:B:12:LEU:HB2	25:B:612:CLA:HMC2	1.96	0.47
19:Z:2:THR:HG22	19:Z:6:GLN:NE2	2.30	0.47
1:a:334[B]:ARG:NH2	37:a:707:HOH:O	2.47	0.47
2:b:226:TYR:OH	37:b:701:HOH:O	2.20	0.47
17:y:20:ALA:O	17:y:24:MET:HG2	2.14	0.47
13:O:27:ARG:HG3	37:O:303:HOH:O	2.14	0.47
25:c:508:CLA:H91	25:c:508:CLA:H112	1.77	0.47
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.50	0.46
4:D:103:ARG:NH2	5:E:77:GLU:HG3	2.26	0.46
4:D:194:ASN:HA	4:D:295:SER:OG	2.15	0.46
2:b:36:SER:OG	26:b:618:BCR:H362	2.15	0.46
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.50	0.46
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.97	0.46
2:B:414:PRO:O	2:B:418:LYS:HG3	2.15	0.46
25:B:601:CLA:H141	25:B:601:CLA:H162	1.72	0.46
25:b:610:CLA:H8	25:b:610:CLA:H51	1.69	0.46
4:d:79:SER:HA	4:d:172:SER:HB3	1.97	0.46
3:c:158:THR:HG21	3:c:256:PRO:HD3	1.98	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
2:B:52:LEU:HD12	13:o:59:LYS:HE2	1.97	0.46
13:O:54:GLU:O	13:O:63:ALA:HB3	2.15	0.46
25:b:611:CLA:H112	25:b:611:CLA:H72	1.71	0.46
5:e:61:ARG:NH1	37:e:204:HOH:O	2.48	0.46
2:B:221:PRO:HA	25:B:609:CLA:HED3	1.97	0.46
4:D:264:LYS:NZ	33:D:401:BCT:O3	2.48	0.46
1:a:82:VAL:HB	1:a:174[A]:LEU:HB2	1.98	0.46
3:c:147:PHE:CD2	25:c:513:CLA:H3A	2.51	0.46
16:v:99:ASP:N	16:v:99:ASP:OD1	2.47	0.46
20:r:2:ASP:N	37:r:102:HOH:O	2.49	0.46
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.97	0.46
32:T:103:STE:H52	32:T:103:STE:H21	1.60	0.46
2:B:247:PHE:HE1	25:B:602:CLA:H102	1.80	0.46
26:B:618:BCR:H15C	26:B:618:BCR:H351	1.81	0.46
25:C:508:CLA:H162	25:C:508:CLA:H192	1.76	0.46
16:V:26:TYR:OH	16:V:122:GLU:OE1	2.26	0.46
25:c:507:CLA:H61	25:c:507:CLA:H92	1.74	0.46
37:A:758:HOH:O	13:O:107:THR:HG21	2.15	0.46
1:a:296:ASN:HB2	3:c:400:PRO:O	2.16	0.46
29:E:101:LHG:H331	29:E:101:LHG:H361	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:614:CLA:H43	30:b:620:SQD:H102	1.98	0.45
1:a:259:ILE:HG21	27:a:611:PL9:H202	1.99	0.45
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.52	0.45
28:c:520:LMG:H442	28:c:520:LMG:H411	1.77	0.45
13:o:53:LYS:HE3	13:o:65:PHE:CZ	2.52	0.45
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.51	0.45
29:E:101:LHG:H342	29:E:101:LHG:H311	1.79	0.45
3:c:203:THR:O	3:c:235:GLY:HA3	2.17	0.45
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.50	0.45
11:l:2:GLU:HB2	37:l:207:HOH:O	2.15	0.45
13:o:53:LYS:HB2	13:o:65:PHE:CE1	2.51	0.45
30:D:409:SQD:H341	18:X:23:LEU:HD22	1.97	0.45
15:U:73:GLN:O	15:U:77:GLU:HG3	2.15	0.45
2:b:283:GLU:O	2:b:287:ARG:HG3	2.16	0.45
25:b:606:CLA:H141	25:b:606:CLA:H161	1.81	0.45
17:y:46:LEU:HD13	17:y:46:LEU:HA	1.75	0.45
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.52	0.45
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.99	0.45
4:d:85:MET:HE1	5:e:72:ALA:HB2	1.99	0.45
25:B:610:CLA:H143	25:B:610:CLA:H161	1.85	0.45
17:Y:42:ARG:HH21	19:Z:31:GLN:CD	2.25	0.45
25:b:613:CLA:H192	29:d:407:LHG:H212	1.99	0.45
25:B:615:CLA:H152	25:B:615:CLA:H102	1.98	0.45
26:T:101:BCR:H311	26:T:101:BCR:C8	2.47	0.45
1:a:281:VAL:HG11	30:a:613:SQD:H182	1.99	0.45
30:a:613:SQD:H381	9:j:22:ILE:HD11	1.99	0.45
2:b:505:ARG:HG3	2:b:506:ARG:N	2.32	0.45
26:k:102:BCR:H24C	26:k:102:BCR:H371	1.85	0.45
25:B:615:CLA:H2	25:B:616:CLA:CBB	2.47	0.45
25:c:510:CLA:H61	25:c:510:CLA:H2	1.62	0.45
25:B:605:CLA:H61	25:B:605:CLA:H41	1.77	0.44
28:M:101:LMG:H401	28:M:101:LMG:H371	1.64	0.44
1:a:282:GLY:HA2	30:a:613:SQD:H223	1.98	0.44
28:c:520:LMG:H402	28:c:520:LMG:H371	1.68	0.44
5:e:14:ILE:O	5:e:20:TRP:NE1	2.50	0.44
25:C:507:CLA:H93	25:C:507:CLA:H112	1.85	0.44
15:U:70:ARG:NH1	16:V:85:GLU:OE1	2.51	0.44
1:a:162[B]:PRO:O	1:a:166[B]:GLY:N	2.48	0.44
3:c:59:LEU:HD21	26:k:103:BCR:H372	1.99	0.44
5:e:10:PHE:N	29:e:101:LHG:O4	2.47	0.44
5:e:30:LEU:HD11	35:f:101:HEM:CBB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:504:CLA:H62	25:C:504:CLA:H41	1.92	0.44
34:D:402:PHO:HBB1	34:D:402:PHO:HMB3	1.99	0.44
2:b:293:ALA:C	2:b:295:GLY:H	2.25	0.44
4:d:141:TYR:OH	29:d:407:LHG:O4	2.29	0.44
14:t:15:ALA:HB2	26:t:101:BCR:H14C	1.98	0.44
2:B:149[A]:LEU:HD21	25:B:606:CLA:HBB2	1.98	0.44
25:C:513:CLA:H143	25:C:513:CLA:H111	1.77	0.44
26:K:101:BCR:H20C	26:K:101:BCR:H361	1.82	0.44
13:O:6:THR:HG22	13:O:9:ASP:CG	2.42	0.44
1:a:77:ILE:HD11	14:t:6:TYR:HB3	2.00	0.44
25:a:609:CLA:H102	8:i:13:THR:HG23	1.99	0.44
25:b:614:CLA:H61	25:b:614:CLA:H93	1.56	0.44
3:c:378:ASN:HD21	13:o:82:GLN:HE22	1.64	0.44
6:f:12:SER:N	37:f:201:HOH:O	2.50	0.44
26:x:101:BCR:H20C	26:x:101:BCR:H361	1.84	0.44
31:A:616:DGD:HD5	2:b:75:TRP:HB3	2.00	0.44
9:J:36:LEU:O	37:J:201:HOH:O	2.21	0.44
3:c:26:ARG:HA	25:c:511:CLA:OBD	2.18	0.44
6:f:23:VAL:HG21	35:f:101:HEM:HBD2	2.00	0.44
26:k:101:BCR:H24C	26:k:101:BCR:H371	1.85	0.44
1:A:227:THR:HB	1:A:231:GLU:HG3	1.98	0.44
2:b:91:TRP:HE1	32:b:623:STE:H141	1.83	0.44
26:b:618:BCR:H24C	26:b:618:BCR:H371	1.87	0.44
25:c:513:CLA:H102	25:c:513:CLA:H62	1.73	0.44
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.83	0.44
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.00	0.44
27:A:610:PL9:H201	27:A:610:PL9:H222	1.63	0.44
31:A:616:DGD:HBF1	8:I:7:THR:HG21	1.99	0.44
25:B:614:CLA:H62	25:B:614:CLA:H41	1.86	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
4:D:79:SER:HA	4:D:172:SER:HB3	1.99	0.44
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	1.99	0.44
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.77	0.44
25:B:612:CLA:H61	25:B:612:CLA:H102	1.81	0.44
4:D:42:TYR:CE1	6:F:25:THR:HG23	2.53	0.44
6:F:15:ILE:HD13	20:R:23:ILE:HD11	2.00	0.44
13:o:62:GLU:OE2	13:o:63:ALA:N	2.51	0.44
2:B:117:TYR:HA	11:L:1:MET:HE1	2.00	0.43
2:B:350:GLU:H	2:B:350:GLU:HG2	1.59	0.43
7:H:49:TYR:CD2	31:H:102:DGD:HB41	2.53	0.43
16:V:87:GLU:OE1	16:V:96:ARG:NH1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:63[B]:ILE:HB	3:c:335:THR:HG21	1.99	0.43
31:c:517:DGD:HAE2	31:c:517:DGD:HA82	1.92	0.43
13:o:178:LYS:HA	13:o:178:LYS:HD3	1.82	0.43
25:C:512:CLA:H93	25:C:512:CLA:H61	1.62	0.43
15:U:67:LEU:HB3	15:U:72:LYS:HG3	2.00	0.43
25:c:512:CLA:H142	25:c:513:CLA:H151	2.00	0.43
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.54	0.43
29:A:613:LHG:H182	29:A:613:LHG:H152	1.74	0.43
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.43
2:b:498:LYS:HE3	4:d:20:ASP:HA	2.00	0.43
6:F:36:ALA:O	6:F:40:MET:HG3	2.18	0.43
25:b:601:CLA:H111	25:b:601:CLA:H91	1.68	0.43
25:A:607:CLA:H91	28:D:408:LMG:H242	1.99	0.43
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.19	0.43
8:I:7:THR:O	8:I:11:VAL:HG23	2.19	0.43
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.89	0.43
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.99	0.43
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.43
17:Y:34:MET:HB3	17:Y:34:MET:HE3	1.79	0.43
1:a:102:LEU:H	31:o:301:DGD:HA22	1.82	0.43
26:k:102:BCR:H361	26:k:102:BCR:H20C	1.80	0.43
28:A:612:LMG:HC72	3:C:216:SER:HB2	2.01	0.43
25:B:613:CLA:H141	25:B:613:CLA:H162	1.75	0.43
25:C:513:CLA:H61	25:C:513:CLA:H41	1.88	0.43
26:a:610:BCR:H24C	26:a:610:BCR:H371	1.84	0.43
16:v:41:HIS:HA	16:v:45:ILE:O	2.19	0.43
25:B:610:CLA:H152	25:B:612:CLA:O1A	2.18	0.42
26:B:617:BCR:H20C	26:B:617:BCR:H361	1.80	0.42
1:a:183[A]:MET:HA	25:a:607:CLA:HMD1	1.99	0.42
25:b:614:CLA:H62	25:b:614:CLA:H41	1.38	0.42
4:d:267:LEU:C	4:d:267:LEU:HD23	2.43	0.42
29:d:408:LHG:H382	29:d:408:LHG:H352	1.87	0.42
10:k:17:ILE:HG13	10:k:18:PHE:CD1	2.54	0.42
26:k:103:BCR:H20C	26:k:103:BCR:H361	1.86	0.42
31:A:616:DGD:HG31	2:b:75:TRP:CD2	2.53	0.42
31:A:616:DGD:HB61	32:I:101:STE:H31	2.00	0.42
3:C:139:THR:HB	3:C:141:GLU:OE2	2.19	0.42
31:C:515:DGD:HA91	31:C:515:DGD:HAW2	1.85	0.42
25:B:606:CLA:H112	25:B:606:CLA:H91	1.63	0.42
25:B:611:CLA:H71	29:L:101:LHG:H321	2.01	0.42
15:U:70:ARG:HE	15:U:70:ARG:HB3	1.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.99	0.42
5:e:20:TRP:CD1	9:j:8:ILE:HD12	2.55	0.42
2:B:141:ILE:O	2:B:145:LEU:HG	2.19	0.42
2:B:247:PHE:CE1	25:B:602:CLA:H102	2.54	0.42
25:b:605:CLA:H202	25:b:605:CLA:H161	1.82	0.42
25:c:512:CLA:H142	25:c:512:CLA:H112	1.88	0.42
4:d:241:GLU:CD	4:d:241:GLU:H	2.28	0.42
8:i:4:LEU:HD22	31:o:301:DGD:HA92	2.01	0.42
1:A:339[B]:PHE:HB3	1:A:340[B]:PRO:HD2	2.02	0.42
2:B:414:PRO:N	2:B:415:PRO:HD2	2.34	0.42
19:Z:34:ASP:HA	19:Z:37:LYS:HD3	2.01	0.42
26:c:514:BCR:H24C	26:c:514:BCR:H371	1.90	0.42
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.54	0.42
25:C:513:CLA:H162	25:C:513:CLA:H121	1.54	0.42
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.55	0.42
4:D:61:HIS:HE1	4:D:80:THR:O	2.02	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.49	0.42
18:X:16:SER:HB3	32:X:101:STE:H81	2.00	0.42
1:a:16:ARG:HB3	1:a:16:ARG:NH1	2.35	0.42
25:d:404:CLA:C1D	32:d:413:STE:H61	2.50	0.42
5:e:33:ALA:HB2	20:r:11:PRO:HG2	2.00	0.42
10:k:24:VAL:O	10:k:27:VAL:HG22	2.19	0.42
3:C:45:LEU:HA	3:C:139:THR:HG22	2.01	0.42
26:C:514:BCR:H20C	26:C:514:BCR:H361	1.84	0.42
26:K:102:BCR:H10C	17:Y:28:ILE:HG23	2.02	0.42
2:b:159:THR:O	2:b:180:PRO:HB3	2.20	0.42
7:h:4:ARG:HE	7:h:4:ARG:HB3	1.61	0.42
26:k:103:BCR:H24C	26:k:103:BCR:H371	1.83	0.42
25:A:608:CLA:H61	25:A:608:CLA:H41	1.72	0.42
25:C:506:CLA:H91	25:C:506:CLA:H111	1.88	0.42
26:Z:101:BCR:H20C	26:Z:101:BCR:H361	1.88	0.42
25:b:605:CLA:HMA1	25:b:606:CLA:H3A	2.02	0.42
25:b:608:CLA:H161	25:b:608:CLA:H141	1.70	0.42
28:c:520:LMG:H112	28:c:520:LMG:H292	2.01	0.42
26:t:101:BCR:H20C	26:t:101:BCR:H361	1.93	0.42
17:y:19:ILE:O	17:y:23:THR:HG22	2.20	0.42
1:A:82:VAL:HB	1:A:174[B]:LEU:HB2	2.02	0.42
29:A:613:LHG:HC32	3:C:36:TRP:CH2	2.55	0.42
25:B:616:CLA:HMB1	25:B:616:CLA:HBB1	2.01	0.42
26:C:514:BCR:H24C	26:C:514:BCR:H371	1.89	0.42
1:a:112:TYR:O	1:a:116:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:616:CLA:H92	25:b:616:CLA:H62	1.80	0.42
26:d:405:BCR:H15C	26:d:405:BCR:H351	1.91	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.20	0.42
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.02	0.41
28:D:411:LMG:O4	37:D:502:HOH:O	2.21	0.41
25:a:607:CLA:CBD	25:a:612:CLA:HAC2	2.50	0.41
2:b:6:TYR:OH	29:d:407:LHG:HC2	2.20	0.41
25:b:602:CLA:H193	25:b:602:CLA:H161	1.75	0.41
25:B:602:CLA:H43	7:H:45:ILE:HG22	2.01	0.41
25:B:613:CLA:HBB1	25:B:613:CLA:HMB1	2.01	0.41
26:B:617:BCR:H24C	26:B:617:BCR:H371	1.86	0.41
13:O:24:ASP:HA	13:O:203:LYS:HE2	2.02	0.41
13:O:200:ASN:OD1	13:O:214:THR:HG22	2.20	0.41
26:T:101:BCR:H20C	26:T:101:BCR:H361	1.91	0.41
1:a:288:LEU:HG	3:c:432:VAL:HG22	2.03	0.41
27:a:611:PL9:H472	30:f:102:SQD:H302	2.01	0.41
28:c:520:LMG:H292	28:c:520:LMG:HC91	1.71	0.41
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.02	0.41
1:a:197:PHE:HB3	1:a:285:PHE:O	2.20	0.41
26:b:617:BCR:H20C	26:b:617:BCR:H361	1.92	0.41
26:b:619:BCR:H15C	26:b:619:BCR:H351	1.96	0.41
1:A:334[A]:ARG:HD3	4:D:320:LEU:HD13	2.02	0.41
30:A:615:SQD:H341	25:b:616:CLA:C9	2.51	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.21	0.41
14:T:2:GLU:OE1	14:T:2:GLU:N	2.43	0.41
16:v:104:MET:HA	16:v:107:LEU:HD22	2.03	0.41
30:A:615:SQD:H341	25:b:616:CLA:H92	2.03	0.41
3:c:38:GLY:HA3	25:c:511:CLA:HMD2	2.03	0.41
25:B:603:CLA:C2D	25:B:605:CLA:H2	2.50	0.41
25:B:614:CLA:H151	30:B:623:SQD:H383	2.02	0.41
1:a:296:ASN:HB3	3:c:401:LEU:HA	2.02	0.41
25:b:603:CLA:H161	25:b:603:CLA:H141	1.70	0.41
3:c:117:VAL:HG12	32:c:519:STE:H142	2.02	0.41
7:H:34:PHE:HZ	32:H:103:STE:H51	1.86	0.41
14:T:14:ILE:HG22	26:T:101:BCR:H10C	2.02	0.41
2:b:30:VAL:HG12	25:b:605:CLA:HHD	2.03	0.41
25:b:614:CLA:H111	25:b:614:CLA:H152	1.78	0.41
3:c:338:GLY:HA3	3:c:341:LEU:O	2.21	0.41
3:c:348:GLU:OE2	13:o:11:VAL:HA	2.20	0.41
16:v:120:LEU:HD23	16:v:120:LEU:HA	1.88	0.41
31:C:517:DGD:HAW1	31:C:517:DGD:HA91	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:101:BCR:H331	26:T:101:BCR:HC7	1.67	0.41
32:T:102:STE:H151	25:b:614:CLA:H201	2.02	0.41
1:a:132:GLU:O	1:a:136:ARG:HG2	2.20	0.41
1:a:245:THR:HB	4:d:265:ARG:HE	1.86	0.41
1:a:271:LEU:HD21	27:a:611:PL9:HC71	2.01	0.41
2:b:91:TRP:CD1	32:b:623:STE:H162	2.56	0.41
2:b:201:HIS:HB2	25:b:602:CLA:CHB	2.51	0.41
31:c:517:DGD:HE4	9:j:40:LEU:HD21	2.02	0.41
1:A:162[B]:PRO:HB3	1:A:168[B]:PHE:HA	2.03	0.41
26:A:609:BCR:H15C	26:A:609:BCR:H351	1.85	0.41
2:B:36:SER:OG	26:B:618:BCR:H362	2.21	0.41
25:C:510:CLA:H111	25:C:510:CLA:H142	1.87	0.41
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.83	0.41
2:b:149:LEU:HD11	25:b:604:CLA:H111	2.03	0.41
2:b:231:MET:HE2	25:b:610:CLA:HMC2	2.03	0.41
25:b:612:CLA:H171	25:b:612:CLA:H13	1.90	0.41
3:c:52:ALA:HB2	25:c:511:CLA:HMA2	2.02	0.41
25:c:505:CLA:H203	25:c:505:CLA:H162	1.85	0.41
9:j:9:PRO:HG2	9:j:12:ILE:HD12	2.02	0.41
20:r:20:VAL:O	20:r:24:LEU:HB2	2.21	0.41
25:B:610:CLA:HHC	25:B:610:CLA:HBB1	2.03	0.41
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.55	0.41
13:O:57:LYS:HE2	13:O:57:LYS:HB3	1.89	0.41
1:a:85:SER:HA	1:a:109:GLY:HA3	2.03	0.41
25:b:611:CLA:H162	25:b:611:CLA:H143	1.70	0.41
28:b:624:LMG:H352	28:b:624:LMG:H192	2.03	0.41
6:f:16:PHE:HB2	30:f:102:SQD:H82	2.02	0.41
14:t:1:FME:HE2	14:t:1:FME:HB2	1.82	0.41
26:x:101:BCR:H15C	26:x:101:BCR:H351	1.95	0.41
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.09	0.40
32:B:625:STE:H52	32:B:625:STE:H21	1.91	0.40
4:D:246:MET:HE3	4:D:264:LYS:HE2	2.02	0.40
10:K:17:ILE:HG23	10:K:18:PHE:CD2	2.56	0.40
2:b:12:LEU:HB2	25:b:612:CLA:HMC2	2.03	0.40
25:c:503:CLA:H193	25:c:503:CLA:H161	1.99	0.40
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.03	0.40
17:y:39:LEU:HD21	19:z:25:VAL:HA	2.03	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
1:A:234:ASN:HD21	29:B:622:LHG:HC11	1.85	0.40
2:B:216:HIS:HE1	25:B:609:CLA:C1A	2.35	0.40
25:B:613:CLA:H62	25:B:613:CLA:H41	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:246:MET:HE3	4:D:264:LYS:HG3	2.03	0.40
26:D:406:BCR:H361	26:D:406:BCR:H20C	1.84	0.40
17:Y:34:MET:O	17:Y:38:LEU:HG	2.21	0.40
25:a:612:CLA:HED2	4:d:198:MET:SD	2.62	0.40
25:c:505:CLA:H2	25:c:505:CLA:H61	1.82	0.40
28:c:522:LMG:HC5	37:c:635:HOH:O	2.21	0.40
34:d:402:PHO:HMB1	34:d:402:PHO:HBB1	2.03	0.40
1:A:161[B]:TYR:HB3	1:A:162[B]:PRO:HD3	2.03	0.40
2:B:185:TRP:HB3	25:B:601:CLA:HMA3	2.04	0.40
5:E:57:ALA:HB3	5:E:60:GLN:HB2	2.03	0.40
7:H:37:LEU:HD23	7:H:37:LEU:HA	1.91	0.40
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.03	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.78	0.40
1:a:288:LEU:HD12	1:a:288:LEU:HA	1.94	0.40
25:b:602:CLA:H202	4:d:159:ILE:HG12	2.03	0.40
26:b:617:BCR:H11C	26:b:617:BCR:H341	1.96	0.40
4:d:90:LEU:HA	4:d:90:LEU:HD12	1.76	0.40
25:A:607:CLA:H151	25:A:607:CLA:H18	1.87	0.40
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.40
4:D:186:GLN:HB2	25:D:404:CLA:HBC1	2.04	0.40
25:D:405:CLA:H111	25:D:405:CLA:H72	1.89	0.40
28:D:408:LMG:H222	28:D:408:LMG:H191	1.84	0.40
15:U:92:VAL:HG12	15:U:97:ARG:HD2	2.04	0.40
5:e:68:ASP:O	5:e:72:ALA:HB2	2.22	0.40
1:A:84:PRO:HA	1:A:112:TYR:CG	2.57	0.40
25:B:609:CLA:H203	7:H:39:LEU:HD12	2.04	0.40
26:Z:101:BCR:H371	26:Z:101:BCR:H24C	1.90	0.40
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.04	0.40
2:b:442:ILE:HD12	4:d:299:ILE:HG12	2.04	0.40
4:d:93:TRP:HZ3	32:d:413:STE:H62	1.86	0.40
4:d:293:LEU:HD23	4:d:293:LEU:HA	1.95	0.40
6:f:21:VAL:O	6:f:25:THR:HG23	2.21	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%)	389 (98%)	5 (1%)	1 (0%)	36	35
1	a	395/344 (115%)	388 (98%)	5 (1%)	2 (0%)	24	21
2	B	507/510 (99%)	498 (98%)	9 (2%)	0	100	100
2	b	503/510 (99%)	494 (98%)	8 (2%)	1 (0%)	43	42
3	C	451/461 (98%)	443 (98%)	7 (2%)	1 (0%)	43	42
3	c	461/461 (100%)	453 (98%)	7 (2%)	1 (0%)	43	42
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	8 (3%)	4 (2%)	7	3
13	o	242/272 (89%)	236 (98%)	5 (2%)	1 (0%)	30	27
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	14
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5386/5700 (94%)	5265 (98%)	107 (2%)	14 (0%)	36	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
9	J	7	ARG
13	O	60	ARG
15	u	53	ALA
13	O	62	GLU
13	o	61	GLN
13	O	59	LYS
13	O	134	THR
2	b	294	SER
1	a	259	ILE
1	A	259	ILE
1	a	30	VAL

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	78
1	a	321/280 (115%)	310 (97%)	11 (3%)	32	33
2	B	407/407 (100%)	401 (98%)	6 (2%)	57	64
2	b	402/407 (99%)	395 (98%)	7 (2%)	53	60
3	C	353/362 (98%)	344 (98%)	9 (2%)	42	45
3	c	362/362 (100%)	349 (96%)	13 (4%)	31	31
4	D	277/283 (98%)	274 (99%)	3 (1%)	65	73
4	d	278/283 (98%)	269 (97%)	9 (3%)	34	35
5	E	72/73 (99%)	66 (92%)	6 (8%)	10	7
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	25
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	31
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	10
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	56
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	56
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	13
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	25
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	40
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	10
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	31
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	33
13	o	207/228 (91%)	201 (97%)	6 (3%)	37	40
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	27
15	U	84/112 (75%)	80 (95%)	4 (5%)	23	21
15	u	84/112 (75%)	82 (98%)	2 (2%)	43	47
16	V	117/138 (85%)	114 (97%)	3 (3%)	40	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/138 (85%)	114 (97%)	3 (3%)	40	44
17	Y	19/37 (51%)	18 (95%)	1 (5%)	20	18
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	12
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	5
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	3
20	R	28/33 (85%)	26 (93%)	2 (7%)	13	10
20	r	25/33 (76%)	21 (84%)	4 (16%)	2	1
All	All	4450/4654 (96%)	4303 (97%)	147 (3%)	33	34

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
1	A	238	LYS
1	A	243	GLU
2	B	98	LEU
2	B	128	THR
2	B	362	PHE
2	B	371	THR
2	B	435	GLU
2	B	476	ARG
3	C	130	VAL
3	C	141	GLU
3	C	144	SER
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	354[A]	GLU
3	C	354[B]	GLU
3	C	473	ASP
4	D	43	LEU
4	D	136	VAL
4	D	264	LYS
5	E	4	THR
5	E	5	THR
5	E	12	ASP
5	E	22[A]	ILE

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Mol	Chain	Res	Type
5	E	22[B]	ILE
5	E	59	GLU
6	F	25	THR
7	H	56	ASP
8	I	4	LEU
10	K	17	ILE
10	K	27	VAL
10	K	46	ARG
11	L	10	VAL
12	M	9	ILE
12	M	25	LEU
13	O	54	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	189	ARG
13	O	214	THR
15	U	39	ARG
15	U	51	LYS
15	U	61	VAL
15	U	67	LEU
16	V	7	VAL
16	V	57	GLU
16	V	86	GLN
17	Y	34	MET
18	X	23	LEU
18	X	37	VAL
19	Z	7	LEU
19	Z	15	LEU
19	Z	29	SER
19	Z	35	ARG
19	Z	46	LEU
19	Z	50	LEU
19	Z	52	LEU
20	R	21	ARG
20	R	33	LYS
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU

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Mol	Chain	Res	Type
1	a	200	LEU
1	a	223	LEU
1	a	231	GLU
1	a	243	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	236	THR
2	b	362	PHE
2	b	492	GLU
2	b	506	ARG
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	216	SER
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	355[A]	THR
3	c	355[B]	THR
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	182	LEU
4	d	230	SER
4	d	241	GLU
4	d	259	ILE
4	d	264	LYS
4	d	291	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	54	SER
5	e	83	LEU
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
8	i	2	GLU

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Mol	Chain	Res	Type
8	i	34	ARG
9	j	21	VAL
10	k	10	LYS
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	49	THR
13	o	60	ARG
13	o	64	GLU
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
14	t	25	GLU
15	u	23	GLU
15	u	61	VAL
16	v	19	ILE
16	v	52	LEU
16	v	107	LEU
17	y	19	ILE
17	y	45	ASN
17	y	46	LEU
18	x	2	THR
18	x	15	LEU
18	x	34	ILE
19	z	1	MET
19	z	19	MET
19	z	20	VAL
19	z	31	GLN
19	z	40	ILE
19	z	46	LEU
20	r	9	LEU
20	r	10	LEU
20	r	14	LEU
20	r	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	233	ASN
2	B	490	GLN
4	D	336	HIS
13	O	82	GLN
13	O	130	GLN
13	O	155	ASN
13	O	231	HIS
15	U	78	ASN
16	V	86	GLN
17	Y	45	ASN
18	X	38	GLN
19	Z	6	GLN
19	Z	31	GLN
19	Z	38	GLN
1	a	19	ASN
1	a	234	ASN
2	b	338	GLN
2	b	394	GLN
2	b	409	GLN
3	c	28	GLN
3	c	311	GLN
3	c	378	ASN
3	c	382	ASN
5	e	60	GLN
5	e	82	GLN
7	h	59	ASN
13	o	36	GLN
13	o	155	ASN
18	x	33	GLN
19	z	31	GLN
20	r	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.95	0	8,9,11	0.94	0
14	FME	t	1	14	8,9,10	1.09	0	8,9,11	1.01	0
12	FME	M	1	12	8,9,10	1.01	0	8,9,11	0.82	0
14	FME	T	1	14	8,9,10	1.07	0	8,9,11	0.77	0
12	FME	m	1	12	8,9,10	0.95	0	8,9,11	0.85	0
8	FME	I	1	8	8,9,10	0.99	0	8,9,11	0.89	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
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	615	-	69,73,73	1.41	9 (13%)	82,113,113	1.23	7 (8%)
26	BCR	k	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.06	2 (3%)
25	CLA	b	613	-	69,73,73	1.29	7 (10%)	82,113,113	1.54	14 (17%)
29	LHG	d	407	-	48,48,48	0.76	2 (4%)	51,54,54	1.34	6 (11%)
25	CLA	B	603	-	69,73,73	1.21	7 (10%)	82,113,113	1.39	9 (10%)
25	CLA	C	504	37	63,67,73	1.20	8 (12%)	74,105,113	1.28	9 (12%)
25	CLA	c	507	37	69,73,73	1.25	8 (11%)	82,113,113	1.42	8 (9%)
25	CLA	B	616	-	64,68,73	1.29	6 (9%)	76,107,113	1.32	5 (6%)
25	CLA	C	506	-	69,73,73	1.24	8 (11%)	82,113,113	1.16	6 (7%)
25	CLA	a	608	37	69,73,73	1.17	6 (8%)	82,113,113	1.23	7 (8%)
28	LMG	d	411	-	44,44,55	0.81	1 (2%)	52,52,63	1.33	6 (11%)
36	HEC	v	201	16	46,50,50	1.90	6 (13%)	58,82,82	1.75	6 (10%)
32	STE	E	102	-	11,11,19	0.74	0	11,11,19	1.16	1 (9%)
26	BCR	B	618	-	41,41,41	1.01	2 (4%)	56,56,56	1.20	6 (10%)
34	PHO	D	403	-	58,69,69	2.14	9 (15%)	55,99,99	1.39	8 (14%)
29	LHG	A	613	-	46,46,48	0.86	2 (4%)	49,52,54	1.24	4 (8%)
25	CLA	a	607	-	69,73,73	1.50	11 (15%)	82,113,113	1.37	6 (7%)
26	BCR	B	619	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	4 (7%)
32	STE	I	101	-	14,14,19	0.35	0	13,13,19	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	604	-	69,73,73	1.24	7 (10%)	82,113,113	1.45	7 (8%)
25	CLA	B	612	-	69,73,73	1.07	6 (8%)	82,113,113	1.41	12 (14%)
27	PL9	d	406	-	55,55,55	1.20	4 (7%)	68,69,69	1.63	14 (20%)
25	CLA	C	505	-	69,73,73	1.31	6 (8%)	82,113,113	1.35	9 (10%)
26	BCR	a	610	-	41,41,41	0.91	1 (2%)	56,56,56	1.28	6 (10%)
31	DGD	o	301	-	43,43,67	0.80	3 (6%)	45,45,81	1.43	6 (13%)
36	HEC	V	201	16	46,50,50	1.81	5 (10%)	58,82,82	1.82	6 (10%)
25	CLA	c	502	-	69,73,73	1.30	7 (10%)	82,113,113	1.26	9 (10%)
32	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.20	1 (7%)
28	LMG	C	518	-	48,48,55	0.80	1 (2%)	56,56,63	1.33	8 (14%)
25	CLA	b	616	-	64,68,73	1.21	7 (10%)	76,107,113	1.42	10 (13%)
30	SQD	a	613	-	52,54,54	1.57	7 (13%)	62,65,65	1.83	12 (19%)
32	STE	C	520	-	11,11,19	0.72	0	11,11,19	1.19	1 (9%)
32	STE	T	102	-	14,14,19	0.31	0	13,13,19	0.99	0
26	BCR	b	619	-	41,41,41	0.99	2 (4%)	56,56,56	1.12	3 (5%)
32	STE	b	625	-	15,15,19	0.73	0	15,15,19	0.93	0
25	CLA	B	608	-	69,73,73	1.20	7 (10%)	82,113,113	1.36	10 (12%)
26	BCR	t	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	6 (10%)
25	CLA	C	503	-	69,73,73	1.33	10 (14%)	82,113,113	1.61	9 (10%)
29	LHG	d	409	-	38,38,48	0.82	1 (2%)	41,44,54	1.09	2 (4%)
32	STE	B	627	-	15,15,19	0.37	0	14,14,19	0.78	0
26	BCR	C	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	6 (10%)
31	DGD	C	515	-	63,63,67	1.00	4 (6%)	77,77,81	1.36	8 (10%)
25	CLA	a	609	-	69,73,73	1.23	7 (10%)	82,113,113	1.24	6 (7%)
26	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
25	CLA	D	405	-	69,73,73	1.33	8 (11%)	82,113,113	1.21	7 (8%)
25	CLA	c	505	-	69,73,73	1.27	9 (13%)	82,113,113	1.21	8 (9%)
25	CLA	c	508	-	68,72,73	1.24	8 (11%)	80,111,113	1.36	8 (10%)
25	CLA	C	512	-	69,73,73	1.41	10 (14%)	82,113,113	1.29	7 (8%)
25	CLA	b	607	37	69,73,73	1.19	6 (8%)	82,113,113	1.24	5 (6%)
33	BCT	D	401	23	3,3,3	1.00	0	2,3,3	3.32	1 (50%)
27	PL9	D	407	-	55,55,55	0.93	3 (5%)	68,69,69	1.66	14 (20%)
31	DGD	c	515	-	63,63,67	1.00	4 (6%)	77,77,81	1.40	12 (15%)
29	LHG	E	101	-	48,48,48	0.77	2 (4%)	51,54,54	1.26	6 (11%)
25	CLA	b	611	-	69,73,73	1.24	5 (7%)	82,113,113	1.31	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	T	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.25	7 (12%)
28	LMG	b	622	-	51,51,55	0.87	1 (1%)	59,59,63	1.42	7 (11%)
25	CLA	c	504	37	64,68,73	1.13	5 (7%)	76,107,113	1.30	9 (11%)
25	CLA	b	608	-	69,73,73	1.33	9 (13%)	82,113,113	1.36	14 (17%)
25	CLA	A	607	37	69,73,73	1.31	7 (10%)	82,113,113	1.38	9 (10%)
26	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.14	5 (8%)
30	SQD	D	409	-	34,36,54	1.51	5 (14%)	42,45,65	3.17	12 (28%)
32	STE	t	103	-	9,9,19	0.36	0	8,8,19	0.78	0
25	CLA	B	610	37	69,73,73	1.34	11 (15%)	82,113,113	1.28	9 (10%)
25	CLA	B	601	37	69,73,73	1.37	9 (13%)	82,113,113	1.42	8 (9%)
32	STE	m	101	-	11,11,19	0.71	0	11,11,19	1.19	1 (9%)
25	CLA	c	506	-	69,73,73	1.35	9 (13%)	82,113,113	1.27	7 (8%)
26	BCR	D	406	-	41,41,41	1.03	2 (4%)	56,56,56	1.08	3 (5%)
32	STE	M	103	-	9,9,19	0.36	0	8,8,19	0.76	0
25	CLA	A	608	-	58,62,73	1.21	6 (10%)	68,99,113	1.32	5 (7%)
29	LHG	l	101	-	48,48,48	0.70	1 (2%)	51,54,54	1.22	4 (7%)
35	HEM	f	101	5,6	50,50,50	1.59	8 (16%)	67,82,82	1.29	8 (11%)
32	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.07	0
26	BCR	K	102	-	41,41,41	1.01	2 (4%)	56,56,56	1.06	3 (5%)
25	CLA	b	603	-	69,73,73	1.24	9 (13%)	82,113,113	1.35	10 (12%)
25	CLA	B	602	-	69,73,73	1.22	8 (11%)	82,113,113	1.30	10 (12%)
25	CLA	c	513	-	69,73,73	1.23	7 (10%)	82,113,113	1.22	7 (8%)
28	LMG	D	408	-	51,51,55	0.85	2 (3%)	59,59,63	1.32	5 (8%)
32	STE	T	103	-	19,19,19	0.59	0	19,19,19	1.07	1 (5%)
26	BCR	d	405	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	5 (8%)
25	CLA	b	615	-	69,73,73	1.44	9 (13%)	82,113,113	1.41	6 (7%)
30	SQD	B	623	-	52,54,54	1.59	9 (17%)	62,65,65	1.65	11 (17%)
25	CLA	B	613	-	69,73,73	1.18	8 (11%)	82,113,113	1.40	9 (10%)
25	CLA	a	612	37	69,73,73	1.50	9 (13%)	82,113,113	1.36	9 (10%)
25	CLA	d	403	-	69,73,73	1.21	6 (8%)	82,113,113	1.22	5 (6%)
35	HEM	F	101	5,6	50,50,50	1.46	7 (14%)	67,82,82	1.15	3 (4%)
25	CLA	b	609	-	69,73,73	1.29	9 (13%)	82,113,113	1.32	6 (7%)
32	STE	c	521	-	11,11,19	0.73	0	11,11,19	1.15	1 (9%)
25	CLA	b	610	37	69,73,73	1.27	7 (10%)	82,113,113	1.37	11 (13%)
25	CLA	c	501	-	69,73,73	1.13	4 (5%)	82,113,113	1.33	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	b	617	-	41,41,41	1.02	3 (7%)	56,56,56	1.27	4 (7%)
25	CLA	B	607	37	69,73,73	1.15	6 (8%)	82,113,113	1.34	8 (9%)
32	STE	B	624	-	11,11,19	0.76	0	11,11,19	1.27	0
26	BCR	K	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.16	5 (8%)
31	DGD	C	517	-	63,63,67	0.92	2 (3%)	77,77,81	1.38	10 (12%)
29	LHG	D	410	-	48,48,48	0.82	2 (4%)	51,54,54	1.24	7 (13%)
25	CLA	b	601	37	69,73,73	1.25	7 (10%)	82,113,113	1.37	5 (6%)
30	SQD	b	620	-	47,49,54	1.63	9 (19%)	57,60,65	1.75	10 (17%)
25	CLA	c	510	-	69,73,73	1.35	8 (11%)	82,113,113	1.31	8 (9%)
32	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.88	0
25	CLA	B	609	-	69,73,73	1.21	6 (8%)	82,113,113	1.34	8 (9%)
33	BCT	a	606	23	3,3,3	1.12	0	2,3,3	3.07	1 (50%)
25	CLA	c	503	-	69,73,73	1.26	10 (14%)	82,113,113	1.44	7 (8%)
21	OEY	A	601[B]	3,37,1	0,16,16	-	-	-	-	-
32	STE	b	621	-	15,15,19	0.35	0	14,14,19	0.82	0
29	LHG	d	408	-	48,48,48	0.70	1 (2%)	51,54,54	1.24	6 (11%)
22	OEX	A	602[A]	3,37,1	0,15,15	-	-	-	-	-
25	CLA	b	602	-	69,73,73	1.09	6 (8%)	82,113,113	1.33	10 (12%)
30	SQD	f	102	-	39,41,54	1.69	8 (20%)	49,52,65	1.69	11 (22%)
28	LMG	B	621	-	26,26,55	0.68	1 (3%)	26,26,63	1.23	2 (7%)
25	CLA	B	605	-	69,73,73	1.13	6 (8%)	82,113,113	1.28	7 (8%)
25	CLA	d	404	-	69,73,73	1.26	10 (14%)	82,113,113	1.18	4 (4%)
31	DGD	h	101	-	63,63,67	0.97	3 (4%)	77,77,81	1.40	11 (14%)
32	STE	B	625	-	17,17,19	0.61	0	17,17,19	1.16	0
28	LMG	b	624	-	55,55,55	0.78	3 (5%)	63,63,63	1.41	10 (15%)
25	CLA	C	511	3	69,73,73	1.31	6 (8%)	82,113,113	1.40	8 (9%)
32	STE	J	101	-	11,11,19	0.73	0	11,11,19	1.08	0
25	CLA	b	604	-	69,73,73	1.13	7 (10%)	82,113,113	1.46	10 (12%)
25	CLA	C	509	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	8 (9%)
32	STE	c	519	-	19,19,19	0.60	0	19,19,19	1.01	0
25	CLA	C	501	-	69,73,73	1.46	10 (14%)	82,113,113	1.34	5 (6%)
29	LHG	L	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.19	4 (7%)
32	STE	d	413	-	19,19,19	0.65	0	19,19,19	1.03	1 (5%)
32	STE	b	623	-	19,19,19	0.65	0	19,19,19	0.99	0
34	PHO	d	401	-	58,69,69	2.07	10 (17%)	55,99,99	1.31	5 (9%)
31	DGD	C	516	-	63,63,67	1.06	6 (9%)	77,77,81	1.36	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	509	-	69,73,73	1.14	6 (8%)	82,113,113	1.40	8 (9%)
26	BCR	H	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.20	5 (8%)
26	BCR	c	514	-	41,41,41	1.15	3 (7%)	56,56,56	1.22	6 (10%)
28	LMG	M	101	-	51,51,55	0.86	3 (5%)	59,59,63	1.36	5 (8%)
32	STE	d	412	-	16,16,19	0.58	0	16,16,19	1.23	1 (6%)
30	SQD	A	614	-	50,52,54	1.57	8 (16%)	60,63,65	1.91	11 (18%)
28	LMG	c	520	-	48,48,55	0.98	5 (10%)	56,56,63	1.29	7 (12%)
31	DGD	c	516	-	63,63,67	1.01	2 (3%)	77,77,81	1.37	10 (12%)
25	CLA	c	511	3	69,73,73	1.50	7 (10%)	82,113,113	1.42	6 (7%)
25	CLA	b	605	-	69,73,73	1.34	7 (10%)	82,113,113	1.41	9 (10%)
29	LHG	B	622	-	48,48,48	0.80	1 (2%)	51,54,54	1.32	7 (13%)
32	STE	X	101	-	19,19,19	0.59	0	19,19,19	1.17	0
26	BCR	x	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.23	5 (8%)
32	STE	l	102	-	17,17,19	0.31	0	16,16,19	0.95	0
26	BCR	Z	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	4 (7%)
26	BCR	A	609	-	41,41,41	0.94	2 (4%)	56,56,56	1.29	6 (10%)
25	CLA	B	611	-	69,73,73	1.29	7 (10%)	82,113,113	1.33	5 (6%)
25	CLA	b	614	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	8 (9%)
34	PHO	D	402	-	58,69,69	1.94	11 (18%)	55,99,99	1.38	6 (10%)
25	CLA	C	513	-	69,73,73	1.14	7 (10%)	82,113,113	1.41	7 (8%)
25	CLA	b	606	-	69,73,73	1.45	5 (7%)	82,113,113	1.42	7 (8%)
31	DGD	H	102	-	63,63,67	1.20	7 (11%)	77,77,81	1.37	10 (12%)
32	STE	B	626	-	11,11,19	0.69	0	11,11,19	1.34	1 (9%)
30	SQD	A	615	-	38,38,54	1.75	5 (13%)	40,40,65	1.24	3 (7%)
22	OEX	a	602[A]	3,37,1	0,15,15	-	-	-	-	-
25	CLA	B	614	-	69,73,73	1.13	6 (8%)	82,113,113	1.43	9 (10%)
28	LMG	c	518	-	37,37,55	0.99	3 (8%)	45,45,63	1.34	5 (11%)
25	CLA	A	606	-	69,73,73	1.36	9 (13%)	82,113,113	1.19	6 (7%)
25	CLA	C	510	-	69,73,73	1.15	7 (10%)	82,113,113	1.35	8 (9%)
32	STE	a	615	-	11,11,19	0.80	0	11,11,19	1.16	1 (9%)
31	DGD	c	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.34	7 (9%)
34	PHO	d	402	-	58,69,69	2.16	9 (15%)	55,99,99	1.51	8 (14%)
30	SQD	a	614	-	35,35,54	1.69	5 (14%)	37,37,65	1.51	6 (16%)
27	PL9	a	611	-	55,55,55	0.68	1 (1%)	68,69,69	1.53	10 (14%)
25	CLA	C	508	-	69,73,73	1.21	8 (11%)	82,113,113	1.40	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	d	410	-	21,21,55	0.52	0	20,20,63	1.28	3 (15%)
28	LMG	c	522	-	49,49,55	0.89	4 (8%)	57,57,63	1.27	3 (5%)
25	CLA	b	612	-	69,73,73	1.32	10 (14%)	82,113,113	1.40	10 (12%)
32	STE	B	620	-	16,16,19	0.69	0	16,16,19	1.09	0
32	STE	C	519	-	11,11,19	0.69	0	11,11,19	1.44	1 (9%)
25	CLA	D	404	-	69,73,73	1.18	6 (8%)	82,113,113	1.35	9 (10%)
26	BCR	k	103	-	41,41,41	1.05	2 (4%)	56,56,56	1.17	4 (7%)
26	BCR	B	617	-	41,41,41	1.02	3 (7%)	56,56,56	1.20	5 (8%)
25	CLA	C	507	37	69,73,73	1.21	6 (8%)	82,113,113	1.37	10 (12%)
21	OEY	a	601[B]	3,37,1	0,16,16	-	-	-	-	-
27	PL9	A	610	-	55,55,55	0.85	1 (1%)	68,69,69	1.47	12 (17%)
25	CLA	B	606	-	69,73,73	1.47	8 (11%)	82,113,113	1.40	6 (7%)
25	CLA	A	611	37	69,73,73	1.43	10 (14%)	82,113,113	1.35	6 (7%)
31	DGD	A	616	-	67,67,67	1.10	7 (10%)	81,81,81	1.31	8 (9%)
32	STE	b	626	-	9,9,19	0.35	0	8,8,19	0.72	0
32	STE	C	521	-	15,15,19	0.31	0	14,14,19	0.93	0
29	LHG	e	101	-	41,41,48	0.76	1 (2%)	44,47,54	1.35	6 (13%)
32	STE	M	102	-	14,14,19	0.76	0	14,14,19	1.05	0
28	LMG	A	612	-	48,48,55	0.95	4 (8%)	56,56,63	1.23	3 (5%)
28	LMG	D	411	-	31,31,55	0.71	1 (3%)	33,33,63	1.25	3 (9%)
25	CLA	C	502	-	69,73,73	1.16	7 (10%)	82,113,113	1.25	5 (6%)
25	CLA	c	512	-	69,73,73	1.21	7 (10%)	82,113,113	1.31	7 (8%)

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	615	-	1/1/15/20	11/39/115/115	-
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
25	CLA	b	613	-	1/1/15/20	14/39/115/115	-
29	LHG	d	407	-	-	18/53/53/53	-
25	CLA	B	603	-	1/1/15/20	5/39/115/115	-
25	CLA	C	504	37	1/1/13/20	6/32/108/115	-
25	CLA	c	507	37	1/1/15/20	8/39/115/115	-
25	CLA	B	616	-	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	506	-	1/1/15/20	11/39/115/115	-
25	CLA	a	608	37	-	10/39/115/115	-
28	LMG	d	411	-	-	13/39/59/70	0/1/1/1
36	HEC	v	201	16	-	6/14/54/54	-
32	STE	E	102	-	-	6/9/9/17	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
34	PHO	D	403	-	-	1/37/103/103	0/5/6/6
29	LHG	A	613	-	-	18/51/51/53	-
25	CLA	a	607	-	1/1/15/20	3/39/115/115	-
26	BCR	B	619	-	-	6/29/63/63	0/2/2/2
32	STE	I	101	-	-	3/12/12/17	-
25	CLA	B	604	-	1/1/15/20	11/39/115/115	-
25	CLA	B	612	-	1/1/15/20	9/39/115/115	-
27	PL9	d	406	-	-	13/53/73/73	0/1/1/1
25	CLA	C	505	-	1/1/15/20	10/39/115/115	-
26	BCR	a	610	-	-	1/29/63/63	0/2/2/2
31	DGD	o	301	-	-	19/45/45/95	-
36	HEC	V	201	16	-	6/14/54/54	-
25	CLA	c	502	-	1/1/15/20	2/39/115/115	-
32	STE	t	102	-	-	3/11/11/17	-
28	LMG	C	518	-	-	20/43/63/70	0/1/1/1
25	CLA	b	616	-	1/1/14/20	5/33/109/115	-
30	SQD	a	613	-	-	24/49/69/69	0/1/1/1
32	STE	C	520	-	-	4/9/9/17	-
32	STE	T	102	-	-	9/12/12/17	-
26	BCR	b	619	-	-	1/29/63/63	0/2/2/2
32	STE	b	625	-	-	6/13/13/17	-
25	CLA	B	608	-	1/1/15/20	6/39/115/115	-
26	BCR	t	101	-	-	8/29/63/63	0/2/2/2
25	CLA	C	503	-	1/1/15/20	3/39/115/115	-
29	LHG	d	409	-	-	9/43/43/53	-
32	STE	B	627	-	-	7/13/13/17	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
31	DGD	C	515	-	-	24/51/91/95	0/2/2/2
25	CLA	a	609	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	k	101	-	-	8/29/63/63	0/2/2/2
25	CLA	c	505	-	1/1/15/20	8/39/115/115	-
25	CLA	D	405	-	-	6/39/115/115	-
25	CLA	c	508	-	-	3/38/114/115	-
25	CLA	C	512	-	1/1/15/20	17/39/115/115	-
25	CLA	b	607	37	1/1/15/20	13/39/115/115	-
27	PL9	D	407	-	-	13/53/73/73	0/1/1/1
31	DGD	c	515	-	-	26/51/91/95	0/2/2/2
29	LHG	E	101	-	-	23/53/53/53	-
25	CLA	b	611	-	1/1/15/20	4/39/115/115	-
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
28	LMG	b	622	-	-	17/46/66/70	0/1/1/1
25	CLA	c	504	37	1/1/14/20	7/33/109/115	-
25	CLA	b	608	-	1/1/15/20	6/39/115/115	-
25	CLA	A	607	37	1/1/15/20	12/39/115/115	-
26	BCR	b	618	-	-	1/29/63/63	0/2/2/2
30	SQD	D	409	-	-	13/28/48/69	0/1/1/1
32	STE	t	103	-	-	3/7/7/17	-
25	CLA	B	610	37	1/1/15/20	5/39/115/115	-
25	CLA	B	601	37	1/1/15/20	20/39/115/115	-
32	STE	m	101	-	-	4/9/9/17	-
25	CLA	c	506	-	1/1/15/20	15/39/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
32	STE	M	103	-	-	5/7/7/17	-
25	CLA	A	608	-	1/1/12/20	3/26/102/115	-
29	LHG	l	101	-	-	15/53/53/53	-
35	HEM	f	101	5,6	-	4/14/54/54	-
32	STE	j	101	-	-	5/9/9/17	-
26	BCR	K	102	-	-	7/29/63/63	0/2/2/2
25	CLA	b	603	-	1/1/15/20	15/39/115/115	-
25	CLA	B	602	-	1/1/15/20	8/39/115/115	-
25	CLA	c	513	-	1/1/15/20	5/39/115/115	-
28	LMG	D	408	-	-	18/46/66/70	0/1/1/1
32	STE	T	103	-	-	8/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
25	CLA	b	615	-	1/1/15/20	9/39/115/115	-
30	SQD	B	623	-	-	21/49/69/69	0/1/1/1
25	CLA	B	613	-	1/1/15/20	11/39/115/115	-
25	CLA	d	403	-	1/1/15/20	8/39/115/115	-
25	CLA	a	612	37	-	2/39/115/115	-
35	HEM	F	101	5,6	-	2/14/54/54	-
25	CLA	b	609	-	-	6/39/115/115	-
32	STE	c	521	-	-	4/9/9/17	-
25	CLA	b	610	37	1/1/15/20	6/39/115/115	-
25	CLA	c	501	-	1/1/15/20	5/39/115/115	-
26	BCR	b	617	-	-	4/29/63/63	0/2/2/2
25	CLA	B	607	37	1/1/15/20	5/39/115/115	-
32	STE	B	624	-	-	5/9/9/17	-
26	BCR	K	101	-	-	3/29/63/63	0/2/2/2
31	DGD	C	517	-	-	16/51/91/95	0/2/2/2
29	LHG	D	410	-	-	20/53/53/53	-
25	CLA	b	601	37	1/1/15/20	15/39/115/115	-
30	SQD	b	620	-	-	20/44/64/69	0/1/1/1
25	CLA	c	510	-	1/1/15/20	9/39/115/115	-
32	STE	H	103	-	-	10/15/15/17	-
25	CLA	B	609	-	-	2/39/115/115	-
25	CLA	c	503	-	1/1/15/20	7/39/115/115	-
32	STE	b	621	-	-	10/13/13/17	-
29	LHG	d	408	-	-	21/53/53/53	-
25	CLA	b	602	-	1/1/15/20	9/39/115/115	-
30	SQD	f	102	-	-	17/36/56/69	0/1/1/1
28	LMG	B	621	-	-	5/22/22/70	-
25	CLA	B	605	-	1/1/15/20	10/39/115/115	-
25	CLA	d	404	-	1/1/15/20	7/39/115/115	-
31	DGD	h	101	-	-	14/51/91/95	0/2/2/2
32	STE	B	625	-	-	9/15/15/17	-
28	LMG	b	624	-	-	24/50/70/70	0/1/1/1
25	CLA	C	511	3	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	J	101	-	-	7/9/9/17	-
25	CLA	b	604	-	1/1/15/20	7/39/115/115	-
25	CLA	C	509	-	1/1/15/20	14/39/115/115	-
32	STE	c	519	-	-	10/17/17/17	-
25	CLA	C	501	-	1/1/15/20	4/39/115/115	-
29	LHG	L	101	-	-	18/53/53/53	-
32	STE	d	413	-	-	10/17/17/17	-
32	STE	b	623	-	-	12/17/17/17	-
34	PHO	d	401	-	-	0/37/103/103	0/5/6/6
31	DGD	C	516	-	-	21/51/91/95	0/2/2/2
25	CLA	c	509	-	1/1/15/20	12/39/115/115	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
26	BCR	c	514	-	-	5/29/63/63	0/2/2/2
28	LMG	M	101	-	-	23/46/66/70	0/1/1/1
32	STE	d	412	-	-	10/14/14/17	-
30	SQD	A	614	-	-	22/47/67/69	0/1/1/1
28	LMG	c	520	-	-	21/43/63/70	0/1/1/1
31	DGD	c	516	-	-	18/51/91/95	0/2/2/2
25	CLA	c	511	3	1/1/15/20	7/39/115/115	-
25	CLA	b	605	-	1/1/15/20	12/39/115/115	-
29	LHG	B	622	-	-	18/53/53/53	-
32	STE	X	101	-	-	10/17/17/17	-
26	BCR	x	101	-	-	3/29/63/63	0/2/2/2
32	STE	l	102	-	-	9/15/15/17	-
26	BCR	Z	101	-	-	3/29/63/63	0/2/2/2
26	BCR	A	609	-	-	1/29/63/63	0/2/2/2
25	CLA	B	611	-	1/1/15/20	5/39/115/115	-
25	CLA	b	614	-	1/1/15/20	20/39/115/115	-
34	PHO	D	402	-	-	2/37/103/103	0/5/6/6
25	CLA	C	513	-	1/1/15/20	11/39/115/115	-
25	CLA	b	606	-	1/1/15/20	5/39/115/115	-
31	DGD	H	102	-	-	17/51/91/95	0/2/2/2
32	STE	B	626	-	-	6/9/9/17	-
30	SQD	A	615	-	-	12/39/39/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	614	-	1/1/15/20	7/39/115/115	-
28	LMG	c	518	-	-	12/31/51/70	0/1/1/1
25	CLA	A	606	-	1/1/15/20	4/39/115/115	-
25	CLA	C	510	-	1/1/15/20	3/39/115/115	-
32	STE	a	615	-	-	6/9/9/17	-
31	DGD	c	517	-	-	23/51/91/95	0/2/2/2
34	PHO	d	402	-	-	4/37/103/103	0/5/6/6
30	SQD	a	614	-	-	18/37/37/69	-
27	PL9	a	611	-	-	15/53/73/73	0/1/1/1
25	CLA	C	508	-	-	6/39/115/115	-
28	LMG	d	410	-	-	13/17/17/70	-
28	LMG	c	522	-	-	24/44/64/70	0/1/1/1
25	CLA	b	612	-	1/1/15/20	3/39/115/115	-
32	STE	B	620	-	-	8/14/14/17	-
32	STE	C	519	-	-	1/9/9/17	-
25	CLA	D	404	-	1/1/15/20	3/39/115/115	-
26	BCR	k	103	-	-	2/29/63/63	0/2/2/2
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
25	CLA	C	507	37	1/1/15/20	10/39/115/115	-
27	PL9	A	610	-	-	26/53/73/73	0/1/1/1
25	CLA	B	606	-	1/1/15/20	15/39/115/115	-
25	CLA	A	611	37	1/1/15/20	5/39/115/115	-
31	DGD	A	616	-	-	28/55/95/95	0/2/2/2
32	STE	b	626	-	-	5/7/7/17	-
32	STE	C	521	-	-	5/13/13/17	-
29	LHG	e	101	-	-	26/46/46/53	-
32	STE	M	102	-	-	6/12/12/17	-
28	LMG	A	612	-	-	17/43/63/70	0/1/1/1
28	LMG	D	411	-	-	14/33/33/70	-
25	CLA	C	502	-	-	7/39/115/115	-
25	CLA	c	512	-	1/1/15/20	22/39/115/115	-

All (782) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	401	PHO	C1B-C2B	9.75	1.50	1.39
34	d	402	PHO	C1B-C2B	9.70	1.50	1.39
34	D	403	PHO	C3B-C4B	9.56	1.51	1.41
34	d	402	PHO	C3B-C4B	9.03	1.50	1.41
34	D	403	PHO	C1B-C2B	8.96	1.49	1.39
34	D	402	PHO	C1B-C2B	8.19	1.48	1.39
25	c	511	CLA	MG-NA	7.77	2.24	2.06
34	d	401	PHO	C3B-C4B	7.66	1.49	1.41
25	B	606	CLA	MG-NA	7.54	2.24	2.06
25	b	606	CLA	MG-NA	7.51	2.24	2.06
25	a	612	CLA	MG-NA	7.26	2.23	2.06
34	D	402	PHO	C3B-C4B	6.85	1.48	1.41
36	V	201	HEC	CAC-C3C	6.66	1.56	1.35
36	v	201	HEC	CAC-C3C	6.60	1.56	1.35
36	v	201	HEC	CAB-C3B	6.27	1.55	1.35
25	b	615	CLA	MG-NA	6.11	2.20	2.06
36	V	201	HEC	CAB-C3B	5.94	1.54	1.35
25	C	505	CLA	MG-NA	5.77	2.20	2.06
35	f	101	HEM	FE-NA	5.73	2.14	1.95
25	C	511	CLA	MG-NA	5.71	2.19	2.06
25	B	615	CLA	MG-NA	5.69	2.19	2.06
25	c	510	CLA	MG-NA	5.57	2.19	2.06
25	B	601	CLA	MG-NA	5.45	2.19	2.06
30	A	615	SQD	O47-C45	-5.44	1.37	1.47
25	b	608	CLA	MG-NA	5.44	2.19	2.06
36	v	201	HEC	C3D-C2D	5.42	1.53	1.38
25	A	606	CLA	MG-NA	5.37	2.19	2.06
25	a	607	CLA	MG-NB	5.34	2.16	2.05
25	C	512	CLA	MG-NB	5.29	2.16	2.05
36	V	201	HEC	C3D-C2D	5.23	1.52	1.38
25	D	404	CLA	MG-NC	5.20	2.18	2.06
25	c	502	CLA	MG-NB	-5.14	1.95	2.05
30	b	620	SQD	O48-C23	5.10	1.48	1.33
25	c	506	CLA	MG-ND	-5.07	1.95	2.05
25	B	603	CLA	MG-NA	5.05	2.18	2.06
30	a	613	SQD	O48-C23	5.00	1.47	1.33
25	B	611	CLA	MG-NA	4.99	2.18	2.06
30	D	409	SQD	O48-C23	4.93	1.47	1.33
25	b	612	CLA	MG-ND	-4.89	1.96	2.05
25	b	611	CLA	MG-NA	4.86	2.17	2.06
30	f	102	SQD	O48-C23	4.80	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	615	SQD	O48-C23	4.78	1.47	1.33
34	d	402	PHO	C1D-C2D	4.75	1.44	1.39
30	B	623	SQD	O48-C23	4.73	1.47	1.33
25	a	607	CLA	MG-NC	4.72	2.17	2.06
25	B	616	CLA	MG-NA	4.71	2.17	2.06
30	a	614	SQD	O48-C23	4.67	1.47	1.33
35	F	101	HEM	FE-NA	4.67	2.10	1.95
25	A	607	CLA	MG-NA	4.64	2.17	2.06
25	A	611	CLA	MG-NB	4.64	2.15	2.05
25	b	615	CLA	MG-NB	4.63	2.15	2.05
25	C	501	CLA	MG-NA	4.63	2.17	2.06
30	A	614	SQD	O48-C23	4.62	1.46	1.33
35	f	101	HEM	FE-NB	4.62	2.09	1.94
25	A	611	CLA	MG-NA	4.61	2.17	2.06
25	D	405	CLA	MG-NB	-4.57	1.96	2.05
27	d	406	PL9	C6-C1	-4.55	1.40	1.48
25	C	501	CLA	MG-ND	-4.38	1.97	2.05
25	C	501	CLA	C1D-ND	4.33	1.43	1.37
25	b	613	CLA	MG-NA	4.28	2.16	2.06
34	D	403	PHO	C1D-C2D	4.28	1.44	1.39
25	B	604	CLA	MG-NA	4.20	2.16	2.06
25	a	609	CLA	C1D-ND	4.20	1.43	1.37
25	b	605	CLA	MG-NB	4.13	2.14	2.05
25	b	610	CLA	C1D-ND	4.11	1.43	1.37
25	D	405	CLA	C1D-ND	4.10	1.43	1.37
25	C	503	CLA	MG-NA	4.04	2.15	2.06
25	c	508	CLA	MG-NC	4.01	2.15	2.06
25	B	602	CLA	MG-NA	3.98	2.15	2.06
25	B	601	CLA	C1D-ND	3.97	1.43	1.37
25	B	613	CLA	MG-NC	3.94	2.15	2.06
25	A	611	CLA	C1D-ND	3.93	1.43	1.37
25	A	606	CLA	MG-ND	-3.88	1.98	2.05
34	D	402	PHO	C1D-C2D	3.85	1.43	1.39
27	d	406	PL9	C3-C4	-3.84	1.43	1.49
25	d	403	CLA	MG-NC	3.84	2.15	2.06
25	c	502	CLA	C1D-ND	3.81	1.42	1.37
25	C	509	CLA	C1D-ND	3.81	1.42	1.37
25	B	609	CLA	MG-NA	3.81	2.15	2.06
34	d	401	PHO	C1D-C2D	3.80	1.43	1.39
25	b	613	CLA	C4B-NB	3.80	1.42	1.37
30	a	614	SQD	O47-C7	3.78	1.45	1.34
25	c	513	CLA	MG-NA	3.78	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	MG-NA	3.77	2.15	2.06
25	B	610	CLA	MG-NA	3.76	2.15	2.06
25	B	608	CLA	MG-NA	3.75	2.15	2.06
25	c	512	CLA	C1D-ND	3.75	1.42	1.37
25	A	608	CLA	C1D-ND	3.74	1.42	1.37
25	B	616	CLA	C1D-ND	3.74	1.42	1.37
25	a	607	CLA	C1D-ND	3.74	1.42	1.37
25	B	615	CLA	C4B-NB	3.72	1.42	1.37
25	B	604	CLA	C1D-ND	3.70	1.42	1.37
25	b	612	CLA	C1D-ND	3.68	1.42	1.37
26	b	618	BCR	C1-C6	-3.67	1.49	1.53
25	C	506	CLA	C1D-ND	3.66	1.42	1.37
25	a	612	CLA	C1D-ND	3.65	1.42	1.37
25	b	601	CLA	MG-NA	3.65	2.14	2.06
30	B	623	SQD	O47-C45	-3.65	1.38	1.46
25	b	610	CLA	MG-NB	-3.64	1.98	2.05
26	c	514	BCR	C1-C6	-3.64	1.49	1.53
25	b	605	CLA	MG-NA	3.63	2.14	2.06
30	A	614	SQD	O47-C45	-3.61	1.38	1.46
25	C	511	CLA	C1D-ND	3.60	1.42	1.37
35	F	101	HEM	FE-NB	3.59	2.06	1.94
30	B	623	SQD	O47-C7	3.59	1.44	1.34
25	b	603	CLA	C1D-ND	3.55	1.42	1.37
30	a	613	SQD	O47-C45	-3.55	1.38	1.46
30	f	102	SQD	O47-C7	3.55	1.44	1.34
25	b	604	CLA	MG-NA	3.54	2.14	2.06
25	B	611	CLA	C1D-ND	3.53	1.42	1.37
26	B	617	BCR	C1-C6	-3.52	1.49	1.53
25	c	509	CLA	C1D-ND	3.52	1.42	1.37
25	c	503	CLA	C1D-ND	3.52	1.42	1.37
25	b	605	CLA	C4B-NB	3.52	1.42	1.37
26	c	514	BCR	C30-C25	-3.50	1.49	1.53
25	C	507	CLA	MG-NA	3.50	2.14	2.06
25	a	608	CLA	C1D-ND	3.50	1.42	1.37
25	C	513	CLA	C1D-ND	3.49	1.42	1.37
26	Z	101	BCR	C30-C25	-3.48	1.49	1.53
26	K	102	BCR	C1-C6	-3.48	1.49	1.53
25	b	601	CLA	C1D-ND	3.48	1.42	1.37
25	a	612	CLA	MG-ND	-3.48	1.98	2.05
26	d	405	BCR	C30-C25	-3.47	1.49	1.53
25	b	602	CLA	C1D-ND	3.47	1.42	1.37
26	b	618	BCR	C30-C25	-3.45	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	C1D-ND	3.45	1.42	1.37
25	b	607	CLA	MG-NC	3.45	2.14	2.06
25	b	613	CLA	C1D-ND	3.45	1.42	1.37
30	b	620	SQD	O47-C7	3.45	1.44	1.34
26	k	101	BCR	C1-C6	-3.44	1.49	1.53
25	c	505	CLA	MG-ND	-3.43	1.99	2.05
25	C	501	CLA	C4B-NB	3.43	1.42	1.37
31	A	616	DGD	C4D-C3D	3.42	1.61	1.52
25	b	609	CLA	MG-NA	3.42	2.14	2.06
25	c	510	CLA	C1D-ND	3.42	1.42	1.37
30	D	409	SQD	C24-C23	3.41	1.60	1.50
25	c	513	CLA	C1D-ND	3.40	1.42	1.37
25	C	512	CLA	MG-NC	3.38	2.14	2.06
25	a	607	CLA	MG-NA	3.38	2.14	2.06
25	d	403	CLA	C1D-ND	3.38	1.42	1.37
25	B	605	CLA	C1B-C2B	3.37	1.51	1.43
30	f	102	SQD	O47-C45	-3.35	1.38	1.46
25	B	605	CLA	C1D-ND	3.34	1.42	1.37
31	H	102	DGD	O5D-C1E	3.34	1.45	1.40
25	B	603	CLA	C4B-NB	3.33	1.42	1.37
25	B	614	CLA	MG-NA	3.33	2.14	2.06
25	c	507	CLA	C1D-ND	3.33	1.42	1.37
25	c	506	CLA	MG-NA	3.33	2.14	2.06
25	b	605	CLA	C1D-ND	3.33	1.42	1.37
25	b	601	CLA	C4B-NB	3.32	1.42	1.37
25	b	616	CLA	C1D-ND	3.31	1.42	1.37
25	b	609	CLA	C4B-NB	3.31	1.42	1.37
25	c	506	CLA	C1D-ND	3.31	1.42	1.37
30	a	614	SQD	C24-C23	3.31	1.60	1.50
25	C	507	CLA	C4B-NB	3.30	1.42	1.37
30	A	615	SQD	O47-C7	3.30	1.43	1.34
25	c	501	CLA	C1D-ND	3.30	1.42	1.37
25	b	607	CLA	C1D-ND	3.30	1.42	1.37
25	C	512	CLA	MG-ND	-3.29	1.99	2.05
25	a	609	CLA	MG-ND	-3.29	1.99	2.05
30	a	613	SQD	O47-C7	3.29	1.43	1.34
30	B	623	SQD	O5-C1	3.28	1.50	1.41
25	B	615	CLA	MG-NB	3.28	2.12	2.05
25	B	601	CLA	C4B-NB	3.28	1.42	1.37
30	b	620	SQD	O5-C1	3.28	1.50	1.41
25	b	611	CLA	C1D-ND	3.28	1.42	1.37
25	B	610	CLA	MG-NC	-3.28	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	402	PHO	C3D-C4D	3.27	1.45	1.41
25	b	603	CLA	C4B-NB	3.26	1.42	1.37
25	b	609	CLA	MG-NC	3.26	2.14	2.06
25	b	615	CLA	C1D-ND	3.26	1.42	1.37
25	B	609	CLA	C1D-ND	3.25	1.42	1.37
26	B	618	BCR	C30-C25	-3.25	1.49	1.53
25	d	404	CLA	C1D-ND	3.25	1.42	1.37
25	B	602	CLA	C1D-ND	3.25	1.42	1.37
25	C	509	CLA	MG-NB	-3.24	1.99	2.05
34	D	402	PHO	C4D-CHA	3.24	1.44	1.39
25	A	607	CLA	C1D-ND	3.23	1.42	1.37
25	b	616	CLA	MG-NA	3.23	2.13	2.06
25	C	504	CLA	C1D-ND	3.22	1.42	1.37
29	D	410	LHG	O7-C5	-3.22	1.39	1.46
26	H	101	BCR	C30-C25	-3.22	1.49	1.53
25	d	404	CLA	C4B-NB	3.21	1.42	1.37
26	k	101	BCR	C30-C25	-3.21	1.49	1.53
25	B	607	CLA	C1D-ND	3.21	1.42	1.37
25	b	611	CLA	C1B-C2B	3.20	1.50	1.43
25	B	606	CLA	C1D-ND	3.20	1.42	1.37
25	C	503	CLA	C1D-ND	3.20	1.42	1.37
25	B	614	CLA	C1D-ND	3.19	1.42	1.37
25	C	505	CLA	C4B-NB	3.19	1.42	1.37
26	C	514	BCR	C1-C6	-3.18	1.49	1.53
29	L	101	LHG	O7-C5	-3.18	1.39	1.46
26	d	405	BCR	C1-C6	-3.18	1.49	1.53
30	f	102	SQD	C24-C23	3.18	1.59	1.50
34	D	402	PHO	CMC-C2C	-3.17	1.45	1.50
25	C	504	CLA	C4B-NB	3.17	1.42	1.37
26	k	103	BCR	C1-C6	-3.17	1.49	1.53
30	A	615	SQD	C24-C23	3.17	1.59	1.50
25	b	605	CLA	C1B-C2B	3.17	1.50	1.43
25	D	404	CLA	C1D-ND	3.17	1.42	1.37
25	c	511	CLA	C1D-ND	3.15	1.42	1.37
25	b	604	CLA	C1D-ND	3.15	1.42	1.37
25	b	614	CLA	C1D-ND	3.14	1.42	1.37
25	c	513	CLA	C4B-NB	3.14	1.42	1.37
25	B	609	CLA	C1B-C2B	3.14	1.50	1.43
25	C	512	CLA	C1D-ND	3.14	1.42	1.37
25	c	505	CLA	C3B-C4B	3.13	1.51	1.42
25	A	606	CLA	C1D-ND	3.13	1.42	1.37
25	a	609	CLA	C4B-NB	3.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	516	DGD	C4D-C3D	3.12	1.60	1.52
25	A	606	CLA	C1B-C2B	3.12	1.50	1.43
25	B	604	CLA	MG-NC	3.12	2.13	2.06
25	b	610	CLA	MG-NA	3.11	2.13	2.06
30	A	614	SQD	O5-C1	3.11	1.49	1.41
25	B	608	CLA	C1D-ND	3.11	1.41	1.37
25	b	604	CLA	C4B-NB	3.10	1.41	1.37
25	b	603	CLA	MG-NA	3.10	2.13	2.06
25	a	609	CLA	C1B-C2B	3.10	1.50	1.43
25	c	508	CLA	C1D-ND	3.10	1.41	1.37
30	b	620	SQD	O47-C45	-3.10	1.39	1.46
26	C	514	BCR	C30-C25	-3.10	1.49	1.53
25	c	505	CLA	MG-NA	3.10	2.13	2.06
25	c	507	CLA	C1B-C2B	3.09	1.50	1.43
26	D	406	BCR	C30-C25	-3.09	1.49	1.53
25	B	616	CLA	C1B-C2B	3.09	1.50	1.43
25	c	503	CLA	MG-NC	3.09	2.13	2.06
25	C	506	CLA	MG-ND	-3.09	1.99	2.05
25	a	607	CLA	C1B-C2B	3.09	1.50	1.43
25	C	513	CLA	C4B-NB	3.09	1.41	1.37
25	B	606	CLA	C1B-C2B	3.09	1.50	1.43
25	B	610	CLA	C1D-ND	3.08	1.41	1.37
25	B	609	CLA	C4B-NB	3.08	1.41	1.37
35	f	101	HEM	CAC-C3C	3.08	1.55	1.47
25	C	510	CLA	C1D-ND	3.08	1.41	1.37
25	B	613	CLA	C1D-ND	3.07	1.41	1.37
25	C	511	CLA	C1B-C2B	3.07	1.50	1.43
25	b	609	CLA	C1D-ND	3.07	1.41	1.37
25	B	602	CLA	C4B-NB	3.06	1.41	1.37
25	c	505	CLA	C1D-ND	3.06	1.41	1.37
26	B	619	BCR	C1-C6	-3.05	1.49	1.53
25	b	614	CLA	C4B-NB	3.05	1.41	1.37
25	C	505	CLA	CHC-C1C	3.05	1.44	1.38
26	K	101	BCR	C1-C6	-3.05	1.49	1.53
25	c	509	CLA	C1B-C2B	3.05	1.50	1.43
30	a	613	SQD	C24-C23	3.04	1.59	1.50
25	C	502	CLA	C1B-C2B	3.04	1.50	1.43
34	d	401	PHO	C4D-CHA	3.04	1.44	1.39
30	A	614	SQD	C24-C23	3.04	1.59	1.50
25	A	607	CLA	C4B-NB	3.04	1.41	1.37
25	c	504	CLA	C4B-NB	3.04	1.41	1.37
26	b	619	BCR	C1-C6	-3.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	608	CLA	C4B-NB	3.03	1.41	1.37
35	F	101	HEM	CAB-C3B	3.02	1.55	1.47
25	d	403	CLA	C1B-C2B	3.02	1.50	1.43
26	k	102	BCR	C30-C25	-3.01	1.49	1.53
25	C	505	CLA	C1D-ND	3.01	1.41	1.37
25	C	503	CLA	C1B-C2B	3.01	1.50	1.43
25	B	606	CLA	C4B-NB	3.01	1.41	1.37
25	A	611	CLA	MG-ND	-3.00	1.99	2.05
25	A	606	CLA	MG-NB	3.00	2.11	2.05
25	b	608	CLA	C1D-ND	3.00	1.41	1.37
26	K	101	BCR	C30-C25	-3.00	1.49	1.53
25	B	608	CLA	C4B-NB	3.00	1.41	1.37
25	a	608	CLA	C4B-NB	3.00	1.41	1.37
25	C	501	CLA	C1B-C2B	3.00	1.50	1.43
25	a	612	CLA	C1B-C2B	2.99	1.50	1.43
25	b	615	CLA	C4B-NB	2.98	1.41	1.37
30	b	620	SQD	C24-C23	2.97	1.59	1.50
26	k	102	BCR	C1-C6	-2.97	1.50	1.53
25	b	606	CLA	C4B-NB	2.97	1.41	1.37
25	C	510	CLA	MG-NA	2.97	2.13	2.06
26	b	617	BCR	C30-C25	-2.97	1.50	1.53
25	B	610	CLA	MG-ND	-2.97	1.99	2.05
25	c	505	CLA	C4B-NB	2.97	1.41	1.37
25	B	602	CLA	C1B-C2B	2.96	1.50	1.43
25	c	511	CLA	C1B-C2B	2.96	1.50	1.43
26	Z	101	BCR	C1-C6	-2.95	1.50	1.53
25	d	403	CLA	MG-ND	-2.94	2.00	2.05
34	d	402	PHO	C4D-CHA	2.94	1.43	1.39
28	c	520	LMG	C3-C2	2.94	1.60	1.52
25	b	608	CLA	CHC-C1C	2.94	1.44	1.38
31	o	301	DGD	O1G-C1A	2.94	1.41	1.33
25	b	606	CLA	C1D-ND	2.92	1.41	1.37
25	c	503	CLA	C4B-NB	2.92	1.41	1.37
25	b	606	CLA	C1B-C2B	2.92	1.50	1.43
25	C	505	CLA	C1B-C2B	2.91	1.50	1.43
25	b	615	CLA	C1B-C2B	2.91	1.50	1.43
29	B	622	LHG	O7-C5	-2.91	1.39	1.46
30	a	614	SQD	O47-C45	-2.91	1.39	1.46
25	b	601	CLA	C1B-C2B	2.90	1.49	1.43
25	c	509	CLA	C4B-NB	2.89	1.41	1.37
29	d	407	LHG	O7-C5	-2.89	1.39	1.46
26	A	609	BCR	C1-C6	-2.89	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	614	SQD	O47-C7	2.89	1.42	1.34
25	b	612	CLA	MG-NB	2.89	2.11	2.05
25	c	507	CLA	MG-NA	2.88	2.13	2.06
25	c	501	CLA	C1B-C2B	2.88	1.49	1.43
25	C	502	CLA	C1D-ND	2.88	1.41	1.37
26	b	617	BCR	C1-C6	-2.88	1.50	1.53
25	b	616	CLA	C4B-NB	2.87	1.41	1.37
30	f	102	SQD	O5-C1	2.87	1.49	1.41
25	C	502	CLA	C4B-NB	2.87	1.41	1.37
25	c	508	CLA	MG-ND	2.86	2.11	2.05
31	A	616	DGD	C4D-C5D	2.86	1.59	1.53
25	B	615	CLA	C1D-ND	2.86	1.41	1.37
25	b	614	CLA	CHC-C1C	2.86	1.44	1.38
25	C	507	CLA	C1B-C2B	2.86	1.49	1.43
25	d	404	CLA	C1B-C2B	2.86	1.49	1.43
27	d	406	PL9	C31-C29	-2.86	1.45	1.51
31	H	102	DGD	C4E-C5E	2.85	1.59	1.53
25	b	616	CLA	C1B-C2B	2.85	1.49	1.43
25	D	405	CLA	MG-NA	2.85	2.13	2.06
25	C	508	CLA	C1D-ND	2.85	1.41	1.37
25	b	614	CLA	MG-NC	2.85	2.13	2.06
26	D	406	BCR	C1-C6	-2.84	1.50	1.53
31	h	101	DGD	C6D-C5D	2.83	1.60	1.51
25	C	513	CLA	C1B-C2B	2.83	1.49	1.43
25	B	614	CLA	C4B-NB	2.82	1.41	1.37
25	B	601	CLA	C1B-C2B	2.82	1.49	1.43
26	x	101	BCR	C30-C25	-2.80	1.50	1.53
30	B	623	SQD	C24-C23	2.80	1.58	1.50
25	b	607	CLA	C1B-C2B	2.80	1.49	1.43
25	c	512	CLA	C1B-C2B	2.79	1.49	1.43
25	b	610	CLA	C1B-C2B	2.79	1.49	1.43
31	C	516	DGD	O2G-C2G	-2.78	1.40	1.46
25	B	615	CLA	CHC-C1C	2.78	1.44	1.38
25	B	607	CLA	MG-NC	2.78	2.12	2.06
25	C	511	CLA	C4B-NB	2.78	1.41	1.37
25	b	605	CLA	CHC-C1C	2.78	1.44	1.38
25	A	608	CLA	C1B-C2B	2.78	1.49	1.43
25	A	606	CLA	C4B-NB	2.78	1.41	1.37
25	A	607	CLA	C1B-C2B	2.78	1.49	1.43
35	F	101	HEM	CAC-C3C	2.77	1.54	1.47
26	T	101	BCR	C30-C25	-2.77	1.50	1.53
28	D	408	LMG	C7-C8	2.77	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	505	CLA	MG-NB	2.77	2.11	2.05
29	A	613	LHG	P-O6	2.77	1.70	1.59
31	C	515	DGD	C4E-C3E	2.77	1.59	1.52
25	d	404	CLA	CHC-C1C	2.77	1.44	1.38
29	A	613	LHG	O3-C3	-2.77	1.34	1.44
31	H	102	DGD	C1E-C2E	2.76	1.60	1.52
25	C	509	CLA	C4B-NB	2.76	1.41	1.37
25	c	507	CLA	MG-ND	2.76	2.11	2.05
25	c	510	CLA	C4B-NB	2.75	1.41	1.37
25	c	510	CLA	C1B-C2B	2.75	1.49	1.43
25	c	511	CLA	C4B-NB	2.74	1.41	1.37
31	h	101	DGD	C4D-C3D	2.74	1.59	1.52
25	b	602	CLA	C1B-C2B	2.74	1.49	1.43
25	C	512	CLA	C3B-C4B	2.74	1.50	1.42
30	a	613	SQD	O5-C1	2.74	1.48	1.41
25	c	506	CLA	C4B-NB	2.74	1.41	1.37
25	C	503	CLA	C4B-NB	2.74	1.41	1.37
25	c	506	CLA	C1B-C2B	2.73	1.49	1.43
27	A	610	PL9	C7-C3	-2.73	1.47	1.51
25	C	508	CLA	C3B-C4B	2.73	1.50	1.42
25	B	610	CLA	C4B-NB	2.73	1.41	1.37
25	C	506	CLA	C4B-NB	2.72	1.41	1.37
25	c	502	CLA	C4B-NB	2.72	1.41	1.37
25	c	508	CLA	C4B-NB	2.72	1.41	1.37
29	d	409	LHG	P-O6	2.71	1.70	1.59
25	c	507	CLA	MG-NB	-2.71	2.00	2.05
25	b	607	CLA	C4B-NB	2.71	1.41	1.37
25	C	508	CLA	C1B-C2B	2.71	1.49	1.43
25	b	606	CLA	MG-NB	-2.71	2.00	2.05
34	D	403	PHO	CMB-C2B	-2.70	1.46	1.51
25	A	611	CLA	C1B-C2B	2.70	1.49	1.43
25	D	405	CLA	MG-NC	2.69	2.12	2.06
25	c	508	CLA	CHC-C1C	2.69	1.43	1.38
25	B	607	CLA	C1B-C2B	2.69	1.49	1.43
25	B	613	CLA	C4B-NB	2.69	1.41	1.37
25	c	503	CLA	C1B-C2B	2.68	1.49	1.43
34	D	403	PHO	C4D-CHA	2.68	1.43	1.39
25	c	503	CLA	MG-NB	2.68	2.11	2.05
26	k	103	BCR	C30-C25	-2.68	1.50	1.53
25	a	608	CLA	C1B-C2B	2.68	1.49	1.43
25	b	609	CLA	C1B-C2B	2.68	1.49	1.43
25	b	608	CLA	C4B-NB	2.67	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	404	CLA	C1B-C2B	2.67	1.49	1.43
26	t	101	BCR	C30-C25	-2.67	1.50	1.53
25	c	510	CLA	CHC-C1C	2.67	1.43	1.38
25	B	610	CLA	CHC-C1C	2.67	1.43	1.38
31	c	516	DGD	C3E-C2E	2.66	1.59	1.52
25	c	502	CLA	MG-NA	2.66	2.12	2.06
25	B	611	CLA	C1B-C2B	2.66	1.49	1.43
25	B	612	CLA	C1D-ND	2.66	1.41	1.37
27	D	407	PL9	C6-C1	-2.66	1.44	1.48
25	B	610	CLA	C3B-C4B	2.65	1.50	1.42
25	C	503	CLA	MG-ND	2.65	2.11	2.05
25	B	612	CLA	C1B-C2B	2.65	1.49	1.43
25	B	604	CLA	C3B-C4B	2.64	1.50	1.42
25	d	404	CLA	MG-NA	2.64	2.12	2.06
29	E	101	LHG	O7-C5	-2.64	1.40	1.46
25	C	502	CLA	MG-NA	2.64	2.12	2.06
35	f	101	HEM	CAB-C3B	2.64	1.54	1.47
25	A	611	CLA	MG-NC	2.63	2.12	2.06
25	C	512	CLA	C1B-C2B	2.63	1.49	1.43
26	t	101	BCR	C1-C6	-2.63	1.50	1.53
25	b	612	CLA	C4B-NB	2.63	1.41	1.37
26	B	619	BCR	C30-C25	-2.63	1.50	1.53
25	c	504	CLA	C1B-C2B	2.63	1.49	1.43
25	B	615	CLA	C1B-C2B	2.62	1.49	1.43
25	c	508	CLA	C1B-C2B	2.62	1.49	1.43
25	B	612	CLA	CHC-C1C	2.62	1.43	1.38
25	c	509	CLA	MG-NC	2.62	2.12	2.06
25	c	503	CLA	CHC-C1C	2.61	1.43	1.38
25	B	612	CLA	C4B-NB	2.61	1.41	1.37
26	b	619	BCR	C30-C25	-2.61	1.50	1.53
25	A	607	CLA	MG-NB	-2.61	2.00	2.05
31	h	101	DGD	C1E-C2E	2.61	1.60	1.52
25	c	512	CLA	C4B-NB	2.61	1.41	1.37
25	C	511	CLA	C3B-C4B	2.61	1.50	1.42
28	b	622	LMG	O7-C8	-2.61	1.40	1.46
35	f	101	HEM	FE-ND	2.60	2.02	1.94
25	A	611	CLA	CHC-C1C	2.60	1.43	1.38
25	C	504	CLA	C3B-C4B	2.59	1.50	1.42
25	D	405	CLA	C1B-C2B	2.59	1.49	1.43
25	c	505	CLA	CHC-C1C	2.59	1.43	1.38
25	A	607	CLA	C3B-C4B	2.59	1.50	1.42
25	c	513	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	C1B-C2B	2.58	1.49	1.43
25	A	608	CLA	CHC-C1C	2.58	1.43	1.38
25	C	506	CLA	C1B-C2B	2.58	1.49	1.43
25	b	615	CLA	C3B-C4B	2.58	1.50	1.42
25	B	610	CLA	C1B-C2B	2.57	1.49	1.43
31	H	102	DGD	C4D-C5D	2.57	1.58	1.53
26	K	102	BCR	C30-C25	-2.57	1.50	1.53
25	B	603	CLA	C1B-C2B	2.57	1.49	1.43
31	C	517	DGD	O3G-C3G	-2.57	1.39	1.43
25	C	509	CLA	C1B-C2B	2.56	1.49	1.43
25	b	614	CLA	C3B-C4B	2.56	1.50	1.42
25	b	601	CLA	CHC-C1C	2.56	1.43	1.38
25	d	404	CLA	MG-ND	-2.55	2.00	2.05
25	b	608	CLA	C1B-C2B	2.55	1.49	1.43
25	b	603	CLA	MG-NC	2.54	2.12	2.06
25	c	507	CLA	C4B-NB	2.54	1.41	1.37
25	b	613	CLA	MG-ND	-2.54	2.00	2.05
25	c	504	CLA	CHC-C1C	2.54	1.43	1.38
31	o	301	DGD	C1G-C2G	2.54	1.58	1.50
31	c	515	DGD	O2G-C2G	-2.54	1.40	1.46
25	B	603	CLA	C1D-ND	2.54	1.41	1.37
25	c	513	CLA	C3B-C4B	2.54	1.50	1.42
29	E	101	LHG	P-O6	2.53	1.69	1.59
25	B	616	CLA	C4B-NB	2.53	1.41	1.37
25	c	502	CLA	C1B-C2B	2.53	1.49	1.43
31	H	102	DGD	O2D-C2D	-2.53	1.36	1.43
25	b	608	CLA	C3B-C4B	2.53	1.50	1.42
25	C	510	CLA	C3B-C4B	2.53	1.50	1.42
25	b	605	CLA	C3B-C4B	2.52	1.50	1.42
25	D	405	CLA	C4B-NB	2.52	1.41	1.37
25	c	508	CLA	C3B-C4B	2.52	1.50	1.42
25	b	608	CLA	MG-NC	-2.52	2.00	2.06
25	c	503	CLA	MG-NA	2.52	2.12	2.06
25	B	606	CLA	MG-NB	2.52	2.10	2.05
25	C	506	CLA	MG-NC	2.51	2.12	2.06
25	a	612	CLA	MG-NB	2.51	2.10	2.05
25	B	615	CLA	C3B-C4B	2.51	1.50	1.42
25	A	607	CLA	CHC-C1C	2.51	1.43	1.38
25	A	611	CLA	C4B-NB	2.50	1.41	1.37
28	A	612	LMG	C4-C5	2.50	1.58	1.53
25	c	512	CLA	C3B-C4B	2.50	1.50	1.42
25	b	602	CLA	C4B-NB	2.50	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	504	CLA	C1D-ND	2.50	1.41	1.37
25	b	612	CLA	C1B-C2B	2.49	1.49	1.43
25	b	610	CLA	C4B-NB	2.49	1.41	1.37
25	C	501	CLA	CHC-C1C	2.49	1.43	1.38
25	c	511	CLA	CHC-C1C	2.49	1.43	1.38
31	A	616	DGD	C1E-C2E	2.49	1.59	1.52
25	B	605	CLA	MG-NA	2.49	2.12	2.06
25	c	506	CLA	MG-NC	2.49	2.12	2.06
34	d	401	PHO	C3D-C4D	2.49	1.44	1.41
25	B	611	CLA	CHC-C1C	2.48	1.43	1.38
25	b	611	CLA	C4B-NB	2.48	1.41	1.37
25	C	508	CLA	C4B-NB	2.48	1.41	1.37
25	B	610	CLA	MG-NB	2.48	2.10	2.05
25	c	509	CLA	CHC-C1C	2.48	1.43	1.38
30	D	409	SQD	O9-S	2.47	1.52	1.45
25	B	608	CLA	CHC-C1C	2.47	1.43	1.38
31	c	516	DGD	C4D-C3D	2.47	1.58	1.52
27	d	406	PL9	C53-C6	-2.46	1.45	1.50
25	C	508	CLA	CHC-C1C	2.46	1.43	1.38
25	B	602	CLA	MG-ND	-2.46	2.00	2.05
25	b	609	CLA	MG-NB	2.46	2.10	2.05
25	C	503	CLA	C3B-C4B	2.46	1.49	1.42
28	c	520	LMG	C4-C3	2.46	1.58	1.52
25	b	615	CLA	CHC-C1C	2.46	1.43	1.38
25	C	503	CLA	MG-NC	2.45	2.12	2.06
25	B	613	CLA	C1B-C2B	2.45	1.48	1.43
25	a	607	CLA	MG-ND	-2.45	2.00	2.05
25	C	512	CLA	C4B-NB	2.45	1.41	1.37
25	B	612	CLA	MG-NA	2.45	2.12	2.06
28	c	522	LMG	C1-C2	2.45	1.59	1.52
25	B	602	CLA	C3B-C4B	2.45	1.49	1.42
34	D	403	PHO	CMD-C2D	-2.45	1.46	1.51
25	b	602	CLA	C3B-C4B	2.45	1.49	1.42
25	C	501	CLA	C3B-C4B	2.45	1.49	1.42
26	B	618	BCR	C1-C6	-2.45	1.50	1.53
26	x	101	BCR	C1-C6	-2.45	1.50	1.53
25	B	606	CLA	CHC-C1C	2.45	1.43	1.38
31	c	515	DGD	C3G-C2G	2.45	1.58	1.50
25	c	513	CLA	CHC-C1C	2.44	1.43	1.38
25	b	614	CLA	C1B-C2B	2.44	1.48	1.43
25	d	404	CLA	C3B-C4B	2.44	1.49	1.42
25	b	613	CLA	C1B-C2B	2.44	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	611	CLA	C4B-NB	2.43	1.41	1.37
31	C	516	DGD	C1E-C2E	2.43	1.59	1.52
25	B	612	CLA	C3B-C4B	2.43	1.49	1.42
28	A	612	LMG	C7-C8	2.43	1.58	1.50
25	C	503	CLA	CHC-C1C	2.42	1.43	1.38
31	A	616	DGD	C6E-C5E	2.42	1.59	1.51
25	b	603	CLA	CHC-C1C	2.42	1.43	1.38
25	b	612	CLA	CMC-C2C	-2.42	1.45	1.50
25	c	505	CLA	C1B-C2B	2.42	1.48	1.43
26	a	610	BCR	C1-C6	-2.42	1.50	1.53
28	D	411	LMG	C7-C8	2.41	1.56	1.51
25	C	504	CLA	MG-NA	2.41	2.12	2.06
31	C	516	DGD	C1G-C2G	2.41	1.58	1.50
25	b	607	CLA	MG-ND	-2.41	2.01	2.05
25	a	608	CLA	C3B-C4B	2.41	1.49	1.42
36	v	201	HEC	CMA-C3A	2.40	1.55	1.50
26	B	617	BCR	C30-C25	-2.40	1.50	1.53
25	b	604	CLA	CHC-C1C	2.40	1.43	1.38
34	D	402	PHO	CMB-C2B	-2.40	1.46	1.51
25	d	403	CLA	C3B-C4B	2.40	1.49	1.42
25	b	614	CLA	CMC-C2C	-2.39	1.45	1.50
28	c	520	LMG	C1-C2	2.39	1.59	1.52
28	c	518	LMG	C4-C5	2.39	1.58	1.53
25	B	608	CLA	C1B-C2B	2.39	1.48	1.43
25	C	509	CLA	MG-NA	2.39	2.12	2.06
25	B	614	CLA	C1B-C2B	2.39	1.48	1.43
25	c	506	CLA	CHC-C1C	2.39	1.43	1.38
25	C	505	CLA	C3B-C4B	2.39	1.49	1.42
25	a	608	CLA	CHC-C1C	2.39	1.43	1.38
25	b	601	CLA	C3B-C4B	2.39	1.49	1.42
34	d	401	PHO	O2D-CGD	2.38	1.39	1.33
25	c	511	CLA	MG-ND	-2.38	2.01	2.05
25	b	612	CLA	MG-NC	2.38	2.11	2.06
25	c	510	CLA	C3B-C4B	2.38	1.49	1.42
25	B	611	CLA	C1D-C2D	2.38	1.50	1.45
28	b	624	LMG	C3-C2	2.38	1.58	1.52
34	D	402	PHO	CMD-C2D	-2.38	1.46	1.51
28	C	518	LMG	O7-C8	-2.38	1.41	1.46
25	C	510	CLA	C4B-NB	2.37	1.41	1.37
36	V	201	HEC	CMB-C2B	2.37	1.55	1.50
25	B	602	CLA	CHC-C1C	2.37	1.43	1.38
25	b	603	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	401	PHO	CMB-C2B	-2.37	1.46	1.51
25	b	612	CLA	C3B-C4B	2.37	1.49	1.42
34	d	401	PHO	C4D-ND	-2.37	1.35	1.38
28	c	522	LMG	C3-C2	2.36	1.58	1.52
25	a	609	CLA	MG-NA	2.36	2.11	2.06
25	d	404	CLA	MG-NC	2.36	2.11	2.06
25	D	404	CLA	C3B-C4B	2.36	1.49	1.42
25	b	604	CLA	C1B-C2B	2.36	1.48	1.43
25	C	510	CLA	CHC-C1C	2.36	1.43	1.38
25	b	602	CLA	CHC-C1C	2.36	1.43	1.38
34	D	402	PHO	O2D-CGD	2.36	1.39	1.33
25	C	508	CLA	MG-ND	2.35	2.10	2.05
25	B	606	CLA	C3B-C4B	2.35	1.49	1.42
30	B	623	SQD	O9-S	2.35	1.51	1.45
25	B	604	CLA	C1B-C2B	2.35	1.48	1.43
25	c	512	CLA	CHC-C1C	2.35	1.43	1.38
31	c	515	DGD	O1G-C1G	-2.35	1.39	1.45
28	D	408	LMG	O6-C5	-2.35	1.38	1.44
25	b	603	CLA	CMD-C2D	-2.35	1.46	1.50
25	b	602	CLA	MG-NC	2.35	2.11	2.06
25	C	506	CLA	CHC-C1C	2.34	1.43	1.38
25	C	506	CLA	C3B-C4B	2.34	1.49	1.42
25	C	512	CLA	CHC-C1C	2.34	1.43	1.38
25	a	612	CLA	C4B-NB	2.34	1.40	1.37
25	B	605	CLA	C3B-C4B	2.34	1.49	1.42
28	b	624	LMG	C4-C3	2.34	1.58	1.52
25	C	513	CLA	MG-NC	2.33	2.11	2.06
25	c	511	CLA	C3B-C4B	2.33	1.49	1.42
30	A	614	SQD	O9-S	2.33	1.51	1.45
28	b	624	LMG	O1-C7	-2.33	1.39	1.43
30	B	623	SQD	O7-S	2.33	1.51	1.45
28	c	520	LMG	O1-C1	2.33	1.44	1.40
25	C	508	CLA	C1D-C2D	2.33	1.49	1.45
25	a	609	CLA	CMC-C2C	-2.32	1.46	1.50
31	C	516	DGD	O3E-C3E	-2.32	1.37	1.43
30	D	409	SQD	O5-C1	2.32	1.47	1.41
25	B	604	CLA	CHC-C1C	2.32	1.43	1.38
30	A	615	SQD	C46-C45	2.32	1.55	1.50
28	A	612	LMG	C4-C3	2.32	1.58	1.52
25	B	616	CLA	CMC-C2C	-2.32	1.46	1.50
25	C	507	CLA	CHC-C1C	2.32	1.43	1.38
25	a	607	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	MG-NB	2.31	2.10	2.05
25	d	404	CLA	CMD-C2D	-2.31	1.46	1.50
25	b	603	CLA	C1B-C2B	2.30	1.48	1.43
25	B	601	CLA	C3B-C4B	2.30	1.49	1.42
30	f	102	SQD	O7-S	2.30	1.51	1.45
25	A	606	CLA	CMD-C2D	-2.30	1.46	1.50
31	C	515	DGD	C3G-C2G	2.30	1.58	1.50
29	l	101	LHG	O7-C5	-2.30	1.41	1.46
35	F	101	HEM	CMD-C2D	2.30	1.55	1.50
25	B	613	CLA	CHC-C1C	2.30	1.43	1.38
25	B	605	CLA	CHC-C1C	2.29	1.43	1.38
25	A	611	CLA	C3B-C4B	2.29	1.49	1.42
25	B	616	CLA	C3B-C4B	2.29	1.49	1.42
25	C	502	CLA	C3B-C4B	2.29	1.49	1.42
30	b	620	SQD	O9-S	2.29	1.51	1.45
35	f	101	HEM	CMA-C3A	2.29	1.55	1.50
34	d	402	PHO	CAC-C3C	-2.28	1.47	1.51
29	d	408	LHG	O7-C5	-2.28	1.41	1.46
30	f	102	SQD	O9-S	2.28	1.51	1.45
28	B	621	LMG	O8-C28	2.28	1.38	1.30
25	c	501	CLA	C4B-NB	2.28	1.40	1.37
25	a	609	CLA	C3B-C4B	2.27	1.49	1.42
25	C	503	CLA	C1D-C2D	2.27	1.49	1.45
25	b	604	CLA	C3B-C4B	2.27	1.49	1.42
35	f	101	HEM	CMC-C2C	2.27	1.55	1.50
25	C	511	CLA	CHC-C1C	2.27	1.43	1.38
31	C	515	DGD	O2G-C2G	-2.26	1.41	1.46
34	d	401	PHO	CAC-C3C	-2.26	1.47	1.51
25	A	606	CLA	C3B-C4B	2.26	1.49	1.42
25	C	502	CLA	CHC-C1C	2.26	1.43	1.38
28	d	411	LMG	C4-C5	2.26	1.57	1.53
25	B	608	CLA	CMB-C2B	-2.26	1.46	1.50
25	B	606	CLA	CMD-C2D	-2.25	1.46	1.50
25	B	613	CLA	C3B-C4B	2.25	1.49	1.42
25	b	612	CLA	CHC-C1C	2.25	1.43	1.38
25	C	504	CLA	C1B-C2B	2.25	1.48	1.43
25	a	607	CLA	C4B-NB	2.25	1.40	1.37
25	D	404	CLA	C4B-NB	2.24	1.40	1.37
31	o	301	DGD	O2G-C1B	2.24	1.40	1.34
25	B	603	CLA	CHC-C1C	2.24	1.43	1.38
31	A	616	DGD	O1G-C1G	-2.24	1.40	1.45
25	c	503	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e	101	LHG	P-O6	2.23	1.68	1.59
25	C	504	CLA	CHC-C1C	2.23	1.43	1.38
25	b	609	CLA	C3B-C4B	2.23	1.49	1.42
25	b	610	CLA	CMB-C2B	-2.22	1.46	1.50
25	b	607	CLA	C3B-C4B	2.22	1.49	1.42
34	D	403	PHO	C3D-C4D	2.22	1.44	1.41
34	d	401	PHO	CMC-C2C	-2.22	1.47	1.50
25	D	405	CLA	CMD-C2D	-2.22	1.46	1.50
25	C	507	CLA	C3B-C4B	2.22	1.49	1.42
29	d	407	LHG	C24-C23	2.22	1.57	1.50
36	v	201	HEC	CMB-C2B	2.21	1.55	1.50
25	b	610	CLA	C3B-C4B	2.21	1.49	1.42
25	C	502	CLA	CMC-C2C	-2.21	1.46	1.50
25	B	607	CLA	C4B-NB	2.21	1.40	1.37
25	c	509	CLA	C3B-C4B	2.20	1.49	1.42
25	D	405	CLA	C3B-C4B	2.20	1.49	1.42
25	A	611	CLA	C3C-C2C	2.20	1.41	1.36
25	B	608	CLA	C3B-C4B	2.20	1.49	1.42
25	A	606	CLA	CHC-C1C	2.20	1.42	1.38
25	B	601	CLA	CHC-C1C	2.20	1.42	1.38
25	a	607	CLA	C3D-C4D	2.20	1.49	1.44
28	c	518	LMG	C3-C2	2.20	1.58	1.52
25	b	616	CLA	CHC-C1C	2.20	1.42	1.38
25	B	603	CLA	C3B-C4B	2.20	1.49	1.42
26	A	609	BCR	C33-C5	-2.20	1.47	1.50
25	B	601	CLA	CMB-C2B	-2.19	1.46	1.50
25	C	513	CLA	C3B-C4B	2.19	1.49	1.42
25	C	513	CLA	CMC-C2C	-2.19	1.46	1.50
34	D	403	PHO	CMC-C2C	-2.19	1.47	1.50
25	b	601	CLA	CMC-C2C	-2.19	1.46	1.50
25	c	506	CLA	MG-NB	2.19	2.10	2.05
30	b	620	SQD	C46-C45	2.18	1.57	1.50
25	C	501	CLA	MG-NC	2.18	2.11	2.06
27	a	611	PL9	C53-C6	-2.18	1.46	1.50
27	D	407	PL9	C3-C4	-2.17	1.46	1.49
27	D	407	PL9	C11-C9	-2.17	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.17	1.46	1.50
25	B	603	CLA	CMD-C2D	-2.17	1.46	1.50
26	b	617	BCR	C33-C5	-2.17	1.47	1.50
36	v	201	HEC	C3B-C2B	-2.17	1.33	1.41
31	c	515	DGD	C6D-C5D	2.17	1.58	1.51
25	a	608	CLA	MG-NA	2.16	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	C3B-C4B	2.16	1.49	1.42
34	D	402	PHO	CAC-C3C	-2.16	1.47	1.51
34	d	402	PHO	C3D-C4D	2.16	1.44	1.41
25	c	502	CLA	C3B-C4B	2.15	1.49	1.42
34	d	402	PHO	C4D-ND	-2.15	1.35	1.38
25	B	613	CLA	CMD-C2D	-2.15	1.46	1.50
25	C	512	CLA	CMD-C2D	-2.15	1.46	1.50
25	b	613	CLA	MG-NC	2.15	2.11	2.06
25	c	507	CLA	C3D-C4D	2.15	1.49	1.44
25	a	612	CLA	C3B-C4B	2.15	1.49	1.42
25	b	612	CLA	CMB-C2B	-2.15	1.46	1.50
25	A	608	CLA	CMD-C2D	-2.14	1.46	1.50
25	d	404	CLA	CMC-C2C	-2.14	1.46	1.50
31	H	102	DGD	C1G-C2G	2.14	1.57	1.50
25	D	404	CLA	CHC-C1C	2.13	1.42	1.38
29	D	410	LHG	P-O6	2.13	1.67	1.59
25	C	504	CLA	CMD-C2D	-2.13	1.46	1.50
25	b	603	CLA	MG-ND	-2.13	2.01	2.05
25	B	610	CLA	C3D-C4D	2.13	1.49	1.44
25	B	607	CLA	C3B-C4B	2.13	1.48	1.42
35	F	101	HEM	C2A-C3A	-2.13	1.33	1.38
34	D	403	PHO	C4D-ND	-2.13	1.35	1.38
25	C	501	CLA	CMD-C2D	-2.12	1.46	1.50
25	B	605	CLA	C4B-NB	2.12	1.40	1.37
25	B	614	CLA	CHC-C1C	2.12	1.42	1.38
25	c	501	CLA	MG-NC	2.12	2.11	2.06
28	A	612	LMG	C1-C2	2.12	1.58	1.52
25	B	609	CLA	C3B-C4B	2.12	1.48	1.42
30	D	409	SQD	O7-S	2.12	1.51	1.45
25	C	509	CLA	C3B-C4B	2.12	1.48	1.42
25	C	512	CLA	CMB-C2B	-2.11	1.46	1.50
25	C	513	CLA	CHC-C1C	2.11	1.42	1.38
30	b	620	SQD	O7-S	2.11	1.51	1.45
28	c	520	LMG	C7-C8	2.11	1.57	1.50
26	T	101	BCR	C1-C6	-2.10	1.51	1.53
25	b	615	CLA	CMD-C2D	-2.10	1.46	1.50
25	b	608	CLA	MG-NB	2.10	2.10	2.05
28	c	518	LMG	C1-C2	2.10	1.58	1.52
31	H	102	DGD	C6D-C5D	2.10	1.57	1.51
25	c	503	CLA	CMC-C2C	-2.10	1.46	1.50
34	D	402	PHO	C4D-ND	-2.10	1.35	1.38
25	c	508	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	CMB-C2B	-2.10	1.46	1.50
26	c	514	BCR	C33-C5	-2.10	1.47	1.50
30	b	620	SQD	O5-C5	2.09	1.49	1.44
25	b	609	CLA	O2D-CGD	2.09	1.38	1.33
25	c	504	CLA	C3B-C4B	2.09	1.48	1.42
25	b	615	CLA	CMB-C2B	-2.09	1.46	1.50
25	C	501	CLA	C1D-C2D	2.08	1.49	1.45
25	B	604	CLA	C4B-NB	2.08	1.40	1.37
30	B	623	SQD	C8-C7	2.08	1.56	1.50
25	a	607	CLA	CHC-C1C	2.08	1.42	1.38
31	c	517	DGD	C6D-C5D	2.08	1.57	1.51
30	A	614	SQD	O7-S	2.08	1.51	1.45
25	c	506	CLA	C3B-C4B	2.07	1.48	1.42
31	C	516	DGD	O3D-C3D	-2.07	1.37	1.43
28	c	522	LMG	C4-C5	2.07	1.57	1.53
28	M	101	LMG	C4-C3	2.07	1.57	1.52
36	V	201	HEC	C3B-C2B	-2.07	1.34	1.41
25	B	601	CLA	CMD-C2D	-2.07	1.46	1.50
25	B	615	CLA	CMC-C2C	-2.07	1.46	1.50
25	c	507	CLA	CMB-C2B	-2.06	1.46	1.50
30	a	613	SQD	O9-S	2.06	1.50	1.45
25	b	613	CLA	CHC-C1C	2.06	1.42	1.38
25	C	510	CLA	CMD-C2D	-2.06	1.46	1.50
34	d	402	PHO	CMD-C2D	-2.06	1.47	1.51
25	B	609	CLA	C3D-C4D	2.06	1.48	1.44
25	C	504	CLA	CMB-C2B	-2.05	1.46	1.50
25	d	403	CLA	CMB-C2B	-2.05	1.46	1.50
31	A	616	DGD	C3E-C2E	2.05	1.57	1.52
30	B	623	SQD	O5-C5	2.05	1.49	1.44
30	a	614	SQD	C44-C45	2.05	1.56	1.51
25	B	611	CLA	C3B-C4B	2.05	1.48	1.42
26	B	617	BCR	C33-C5	-2.05	1.47	1.50
25	c	510	CLA	CMB-C2B	-2.04	1.46	1.50
30	f	102	SQD	O5-C5	2.04	1.49	1.44
25	C	503	CLA	C3D-C4D	2.04	1.48	1.44
34	d	402	PHO	CMC-C2C	-2.04	1.47	1.50
25	b	616	CLA	CMB-C2B	-2.04	1.46	1.50
25	B	614	CLA	CMB-C2B	-2.03	1.46	1.50
25	b	616	CLA	C3B-C4B	2.03	1.48	1.42
25	c	513	CLA	CMB-C2B	-2.03	1.46	1.50
28	M	101	LMG	C9-C8	2.03	1.57	1.50
26	H	101	BCR	C1-C6	-2.03	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	608	CLA	C3B-C4B	2.03	1.48	1.42
25	a	607	CLA	C1D-C2D	2.03	1.49	1.45
35	F	101	HEM	FE-NC	2.03	2.01	1.95
35	f	101	HEM	C3B-C2B	-2.02	1.33	1.37
25	c	505	CLA	CMB-C2B	-2.02	1.46	1.50
25	c	503	CLA	CMD-C2D	-2.02	1.46	1.50
25	C	509	CLA	CHC-C1C	2.02	1.42	1.38
25	B	607	CLA	CMB-C2B	-2.02	1.46	1.50
28	c	522	LMG	C4-C3	2.02	1.57	1.52
31	C	515	DGD	O2D-C2D	-2.02	1.38	1.43
30	A	614	SQD	C8-C7	2.02	1.56	1.50
25	c	502	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	506	CLA	MG-NA	2.01	2.11	2.06
30	a	613	SQD	O7-S	2.01	1.50	1.45
25	B	601	CLA	CMC-C2C	-2.01	1.46	1.50
25	B	615	CLA	C1D-C2D	2.01	1.49	1.45
25	a	612	CLA	CHC-C1C	2.01	1.42	1.38
25	c	510	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	512	CLA	C1D-C2D	2.01	1.49	1.45
25	b	604	CLA	CMD-C2D	-2.01	1.46	1.50
25	B	613	CLA	C1B-NB	-2.01	1.35	1.37
31	C	517	DGD	O2G-C2G	-2.01	1.41	1.46
25	B	610	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	608	CLA	C1D-C2D	2.01	1.49	1.45
28	M	101	LMG	O7-C8	-2.00	1.41	1.46
31	A	616	DGD	O2G-C2G	-2.00	1.41	1.46
25	a	612	CLA	CMB-C2B	-2.00	1.46	1.50

All (1061) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O6-C1-C2	12.90	127.87	108.27
25	C	503	CLA	C4A-NA-C1A	9.31	110.92	106.68
25	c	511	CLA	C4A-NA-C1A	8.54	110.58	106.68
36	v	201	HEC	CBB-CAB-C3B	-8.46	110.52	127.43
25	C	511	CLA	C4A-NA-C1A	8.24	110.44	106.68
30	D	409	SQD	C1-O5-C5	-8.23	97.65	113.72
36	V	201	HEC	CBB-CAB-C3B	-8.21	111.03	127.43
25	b	613	CLA	C4A-NA-C1A	7.94	110.30	106.68
25	C	513	CLA	C4A-NA-C1A	7.93	110.30	106.68
25	B	606	CLA	C4A-NA-C1A	7.77	110.22	106.68
25	B	604	CLA	C4A-NA-C1A	7.70	110.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	601	CLA	C4A-NA-C1A	7.70	110.19	106.68
25	b	615	CLA	C4A-NA-C1A	7.63	110.16	106.68
25	c	507	CLA	C4A-NA-C1A	7.60	110.15	106.68
25	c	509	CLA	C4A-NA-C1A	7.59	110.14	106.68
25	B	609	CLA	C4A-NA-C1A	7.59	110.14	106.68
25	c	503	CLA	C4A-NA-C1A	7.56	110.13	106.68
25	a	607	CLA	C4A-NA-C1A	7.49	110.10	106.68
30	a	613	SQD	O6-C1-C2	7.44	119.57	108.27
25	C	501	CLA	C4A-NA-C1A	7.31	110.01	106.68
25	B	614	CLA	C4A-NA-C1A	7.08	109.91	106.68
25	b	606	CLA	C4A-NA-C1A	7.06	109.90	106.68
25	C	507	CLA	C4A-NA-C1A	7.03	109.88	106.68
25	B	607	CLA	C4A-NA-C1A	6.92	109.83	106.68
25	B	601	CLA	C4A-NA-C1A	6.86	109.81	106.68
30	D	409	SQD	C44-O6-C1	6.71	125.14	113.68
25	b	609	CLA	C4A-NA-C1A	6.70	109.74	106.68
25	b	611	CLA	C4A-NA-C1A	6.63	109.70	106.68
25	C	508	CLA	C4A-NA-C1A	6.63	109.70	106.68
30	a	613	SQD	C1-O5-C5	-6.58	100.88	113.72
25	C	510	CLA	C4A-NA-C1A	6.41	109.60	106.68
36	v	201	HEC	CBC-CAC-C3C	-6.35	114.75	127.43
25	a	612	CLA	C4A-NA-C1A	6.33	109.56	106.68
25	B	605	CLA	C4A-NA-C1A	6.32	109.56	106.68
25	A	611	CLA	C4A-NA-C1A	6.22	109.52	106.68
25	C	502	CLA	C4A-NA-C1A	6.21	109.51	106.68
25	B	616	CLA	C4A-NA-C1A	6.17	109.49	106.68
25	b	604	CLA	C4A-NA-C1A	6.15	109.48	106.68
36	V	201	HEC	CBC-CAC-C3C	-6.13	115.18	127.43
30	A	614	SQD	O6-C1-C2	6.07	117.49	108.27
25	b	605	CLA	C4A-NA-C1A	6.05	109.44	106.68
25	b	616	CLA	C4A-NA-C1A	6.04	109.43	106.68
25	B	611	CLA	C4A-NA-C1A	5.99	109.41	106.68
27	a	611	PL9	C7-C3-C4	5.96	121.82	116.91
25	b	607	CLA	C4A-NA-C1A	5.96	109.40	106.68
30	D	409	SQD	C1-C2-C3	-5.93	97.54	110.01
25	c	510	CLA	C4A-NA-C1A	5.86	109.35	106.68
25	c	504	CLA	C4A-NA-C1A	5.85	109.35	106.68
25	B	612	CLA	C4A-NA-C1A	5.74	109.30	106.68
27	D	407	PL9	C7-C3-C4	5.74	121.64	116.91
25	c	501	CLA	C4A-NA-C1A	5.71	109.28	106.68
25	B	608	CLA	C4A-NA-C1A	5.69	109.28	106.68
25	d	403	CLA	C4A-NA-C1A	5.69	109.28	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	505	CLA	C4A-NA-C1A	5.68	109.27	106.68
30	b	620	SQD	O6-C1-C2	5.67	116.89	108.27
25	c	508	CLA	C4A-NA-C1A	5.50	109.19	106.68
25	b	602	CLA	C4A-NA-C1A	5.49	109.18	106.68
25	D	404	CLA	C4A-NA-C1A	5.48	109.18	106.68
25	b	610	CLA	C4A-NA-C1A	5.42	109.15	106.68
25	a	609	CLA	C4A-NA-C1A	5.41	109.14	106.68
30	B	623	SQD	O47-C7-C8	5.39	123.15	111.48
25	C	506	CLA	C4A-NA-C1A	5.39	109.14	106.68
25	B	615	CLA	C4A-NA-C1A	5.38	109.14	106.68
25	B	603	CLA	C4A-NA-C1A	5.32	109.11	106.68
25	C	512	CLA	C4A-NA-C1A	5.25	109.07	106.68
25	c	512	CLA	C4A-NA-C1A	5.19	109.05	106.68
25	B	613	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	c	506	CLA	C4A-NA-C1A	5.17	109.04	106.68
25	C	504	CLA	C4A-NA-C1A	5.09	109.00	106.68
25	A	606	CLA	C4A-NA-C1A	5.06	108.99	106.68
30	a	614	SQD	O47-C7-C8	5.03	122.37	111.48
34	D	402	PHO	C4D-CHA-CBD	-5.02	106.05	108.45
25	b	612	CLA	C4A-NA-C1A	5.02	108.97	106.68
25	a	608	CLA	C4A-NA-C1A	4.99	108.96	106.68
34	d	401	PHO	C4D-CHA-CBD	-4.98	106.06	108.45
25	D	405	CLA	C4A-NA-C1A	4.98	108.95	106.68
30	A	614	SQD	O7-S-C6	4.96	114.16	106.76
25	c	502	CLA	C4A-NA-C1A	4.94	108.93	106.68
25	c	513	CLA	C4A-NA-C1A	4.89	108.91	106.68
25	B	613	CLA	C1-C2-C3	-4.86	118.24	126.20
25	A	607	CLA	C4A-NA-C1A	4.65	108.80	106.68
30	A	614	SQD	O47-C7-C8	4.63	121.50	111.48
25	B	602	CLA	C4A-NA-C1A	4.62	108.79	106.68
25	A	608	CLA	C4A-NA-C1A	4.61	108.78	106.68
25	c	512	CLA	C1-C2-C3	-4.58	118.69	126.20
34	d	402	PHO	C4D-CHA-CBD	-4.58	106.26	108.45
25	d	404	CLA	C4A-NA-C1A	4.57	108.76	106.68
27	a	611	PL9	C7-C3-C2	-4.50	118.08	123.39
25	C	509	CLA	C4A-NA-C1A	4.49	108.73	106.68
31	C	517	DGD	O3G-C3G-C2G	-4.43	100.05	110.82
29	e	101	LHG	O4-P-O5	4.42	133.01	112.44
30	A	614	SQD	C1-O5-C5	-4.42	105.10	113.72
33	D	401	BCT	O2-C-O1	4.40	130.94	119.68
29	L	101	LHG	O4-P-O5	4.31	132.51	112.44
30	A	614	SQD	C1-C2-C3	-4.31	100.94	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	501	CLA	O2D-CGD-O1D	-4.31	115.46	123.85
29	E	101	LHG	O4-P-O5	4.30	132.44	112.44
34	d	402	PHO	C1-C2-C3	-4.30	119.16	126.20
29	d	408	LHG	O4-P-O5	4.29	132.41	112.44
29	A	613	LHG	O4-P-O5	4.28	132.38	112.44
27	d	406	PL9	C7-C3-C4	4.28	120.43	116.91
25	b	603	CLA	C4A-NA-C1A	4.28	108.63	106.68
30	f	102	SQD	O9-S-O7	-4.26	99.98	113.82
30	B	623	SQD	O6-C1-C2	4.24	114.72	108.27
25	b	606	CLA	O2D-CGD-O1D	-4.23	115.61	123.85
31	o	301	DGD	O3G-C3G-C2G	-4.23	100.90	111.77
29	B	622	LHG	O4-P-O5	4.23	132.10	112.44
29	D	410	LHG	O4-P-O5	4.22	132.08	112.44
25	B	610	CLA	C4A-NA-C1A	4.22	108.60	106.68
27	A	610	PL9	C7-C3-C4	4.21	120.38	116.91
29	d	409	LHG	O4-P-O5	4.20	131.99	112.44
25	A	607	CLA	C3B-C4B-NB	-4.20	106.78	110.53
29	l	101	LHG	O4-P-O5	4.18	131.89	112.44
28	b	624	LMG	C1-O6-C5	-4.17	105.58	113.72
25	c	505	CLA	C4A-NA-C1A	4.12	108.56	106.68
29	d	407	LHG	O4-P-O5	4.12	131.59	112.44
25	B	612	CLA	O2D-CGD-O1D	-4.10	115.87	123.85
33	a	606	BCT	O2-C-O1	4.10	130.15	119.68
25	B	603	CLA	C3B-C4B-NB	-4.05	106.91	110.53
30	A	614	SQD	O9-S-O7	-4.05	100.66	113.82
30	D	409	SQD	O9-S-C6	4.01	112.75	106.76
25	b	603	CLA	O2D-CGD-O1D	-4.01	116.04	123.85
25	b	605	CLA	C3B-C4B-NB	-3.99	106.97	110.53
30	f	102	SQD	O6-C1-C2	3.99	114.33	108.27
25	A	611	CLA	C3B-C4B-NB	-3.98	106.97	110.53
25	b	610	CLA	O2D-CGD-O1D	-3.98	116.11	123.85
27	d	406	PL9	C7-C8-C9	-3.96	120.01	126.83
25	B	614	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
25	c	503	CLA	C3B-C4B-NB	-3.94	107.01	110.53
26	B	617	BCR	C2-C1-C6	3.93	116.15	110.44
25	b	606	CLA	O2D-CGD-CBD	3.93	118.11	111.23
25	c	509	CLA	O2A-CGA-O1A	-3.93	113.81	123.63
25	C	505	CLA	C3B-C4B-NB	-3.91	107.04	110.53
25	A	608	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
25	B	615	CLA	C3B-C4B-NB	-3.89	107.05	110.53
25	b	616	CLA	O2D-CGD-O1D	-3.87	116.31	123.85
26	b	617	BCR	C2-C1-C6	3.86	116.04	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	C1-C2-C3	-3.85	119.88	126.20
25	b	612	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
25	b	608	CLA	C3B-C4B-NB	-3.81	107.13	110.53
25	b	613	CLA	C1-C2-C3	-3.80	119.97	126.20
35	F	101	HEM	CBD-CAD-C3D	-3.77	102.12	112.53
25	B	601	CLA	O2D-CGD-O1D	-3.77	116.52	123.85
31	H	102	DGD	O3G-C3G-C2G	-3.76	101.67	110.82
25	c	505	CLA	C3B-C4B-NB	-3.74	107.19	110.53
25	b	605	CLA	O2D-CGD-O1D	-3.74	116.57	123.85
36	V	201	HEC	CBD-CAD-C3D	-3.74	102.20	112.53
30	b	620	SQD	O9-S-O7	-3.72	101.72	113.82
25	C	513	CLA	O2D-CGD-O1D	-3.71	116.63	123.85
25	B	612	CLA	C3B-C4B-NB	-3.71	107.22	110.53
25	b	603	CLA	C3B-C4B-NB	-3.70	107.22	110.53
25	b	601	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
31	C	515	DGD	O3G-C3G-C2G	-3.69	101.84	110.82
25	b	612	CLA	C1-C2-C3	-3.69	120.16	126.20
25	D	404	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
25	B	606	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
30	f	102	SQD	O5-C5-C4	3.64	116.25	109.70
25	c	505	CLA	O2D-CGD-O1D	-3.62	116.81	123.85
26	B	619	BCR	C2-C1-C6	3.61	115.68	110.44
25	B	603	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
25	A	607	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
27	D	407	PL9	C7-C3-C2	-3.58	119.17	123.39
25	B	602	CLA	O2D-CGD-CBD	3.58	117.48	111.23
25	c	508	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
27	d	406	PL9	C22-C23-C24	-3.57	119.45	127.62
30	a	614	SQD	O48-C23-C24	3.57	122.72	111.83
30	A	615	SQD	O47-C7-C8	3.56	119.19	111.48
30	f	102	SQD	O7-S-C6	3.55	112.05	106.76
25	C	512	CLA	C1-C2-C3	-3.54	120.39	126.20
31	C	516	DGD	O3G-C3G-C2G	-3.54	102.20	110.82
34	D	402	PHO	CMB-C2B-C3B	3.53	131.74	124.68
30	a	613	SQD	O9-S-O7	-3.52	102.38	113.82
30	D	409	SQD	O8-S-C6	3.52	112.76	105.97
35	f	101	HEM	CBD-CAD-C3D	-3.51	102.83	112.53
25	b	604	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
30	D	409	SQD	O48-C23-C24	3.50	122.50	111.83
25	b	615	CLA	C3B-C4B-NB	-3.49	107.42	110.53
34	d	402	PHO	O1D-CGD-CBD	3.49	130.01	124.72
25	c	502	CLA	O2D-CGD-O1D	-3.49	117.06	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
27	d	406	PL9	C7-C3-C2	-3.47	119.30	123.39
25	C	508	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
25	B	611	CLA	C3B-C4B-NB	-3.44	107.46	110.53
27	D	407	PL9	C7-C8-C9	-3.43	120.92	126.83
30	a	613	SQD	O47-C7-C8	3.43	118.89	111.48
25	c	501	CLA	O2D-CGD-CBD	3.42	117.21	111.23
34	D	403	PHO	C1-C2-C3	-3.42	120.60	126.20
25	B	604	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
25	B	604	CLA	C3B-C4B-NB	-3.41	107.49	110.53
25	B	612	CLA	C1-C2-C3	-3.40	120.62	126.20
25	C	505	CLA	C1-C2-C3	-3.40	120.63	126.20
25	C	503	CLA	C3B-C4B-NB	-3.40	107.50	110.53
25	B	610	CLA	CHB-C4A-NA	3.40	129.30	124.40
25	C	512	CLA	C3B-C4B-NB	-3.39	107.50	110.53
25	b	608	CLA	C4A-NA-C1A	3.39	108.22	106.68
30	b	620	SQD	O5-C5-C4	3.38	115.79	109.70
25	B	606	CLA	C3B-C4B-NB	-3.38	107.52	110.53
36	V	201	HEC	C4D-ND-C1D	3.37	111.31	105.82
25	b	613	CLA	CMB-C2B-C1B	-3.37	120.29	125.42
27	A	610	PL9	C7-C3-C2	-3.36	119.43	123.39
25	B	610	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
25	b	614	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	d	404	CLA	C3B-C4B-NB	-3.36	107.53	110.53
31	c	516	DGD	O3G-C3G-C2G	-3.35	102.67	110.82
25	C	508	CLA	C3B-C4B-NB	-3.35	107.54	110.53
31	c	517	DGD	O3G-C3G-C2G	-3.33	102.71	110.82
25	b	614	CLA	C4A-NA-C1A	3.33	108.20	106.68
31	C	517	DGD	O6D-C1D-O3G	-3.32	102.19	110.04
25	b	604	CLA	C1-C2-C3	-3.32	120.75	126.20
30	D	409	SQD	O9-S-O7	-3.32	103.03	113.82
25	b	611	CLA	O2D-CGD-CBD	3.31	117.01	111.23
25	b	601	CLA	C3B-C4B-NB	-3.30	107.58	110.53
25	B	608	CLA	CMB-C2B-C1B	-3.29	120.40	125.42
25	A	608	CLA	CHB-C4A-NA	3.28	129.14	124.40
25	C	506	CLA	C3B-C4B-NB	-3.27	107.61	110.53
25	B	608	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
30	b	620	SQD	O7-S-C6	3.27	111.64	106.76
34	d	402	PHO	CMB-C2B-C3B	3.27	131.21	124.68
25	b	602	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
25	B	602	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
26	x	101	BCR	C2-C1-C6	3.25	115.16	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
25	c	507	CLA	CHB-C4A-NA	3.25	129.09	124.40
25	C	504	CLA	C3B-C4B-NB	-3.24	107.64	110.53
31	A	616	DGD	C3G-C2G-C1G	-3.24	104.23	111.78
25	a	609	CLA	O2D-CGD-CBD	3.24	116.89	111.23
25	C	508	CLA	CHD-C1D-ND	-3.23	120.26	124.80
25	A	607	CLA	C1-C2-C3	-3.23	120.91	126.20
25	c	507	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
25	C	501	CLA	C3B-C4B-NB	-3.22	107.65	110.53
25	c	508	CLA	C3B-C4B-NB	-3.22	107.66	110.53
25	b	602	CLA	CHB-C4A-NA	3.21	129.03	124.40
34	D	403	PHO	C4D-CHA-CBD	-3.20	106.92	108.45
34	D	403	PHO	CMB-C2B-C3B	3.20	131.08	124.68
25	B	603	CLA	O2A-CGA-O1A	-3.20	115.63	123.63
25	b	609	CLA	C3B-C4B-NB	-3.19	107.68	110.53
27	A	610	PL9	C22-C23-C24	-3.17	120.37	127.62
26	c	514	BCR	C27-C26-C25	3.16	126.98	122.70
31	c	516	DGD	O6D-C1D-O3G	-3.16	102.57	110.04
34	D	403	PHO	O2D-CGD-O1D	-3.16	117.69	123.85
30	a	613	SQD	O48-C23-C24	3.16	121.46	111.83
27	d	406	PL9	C42-C43-C44	-3.16	120.40	127.62
30	b	620	SQD	O48-C23-C24	3.15	121.44	111.83
36	v	201	HEC	C4D-ND-C1D	3.15	110.95	105.82
25	b	608	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
26	d	405	BCR	C27-C26-C25	3.14	126.95	122.70
27	d	406	PL9	C37-C38-C39	-3.14	120.43	127.62
25	C	510	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
25	D	404	CLA	C3B-C4B-NB	-3.14	107.73	110.53
25	a	609	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
31	C	515	DGD	CDB-CCB-CBB	-3.13	98.52	114.37
25	B	605	CLA	C3B-C4B-NB	-3.13	107.73	110.53
25	b	612	CLA	C3B-C4B-NB	-3.13	107.73	110.53
25	b	613	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
27	D	407	PL9	C22-C23-C24	-3.13	120.46	127.62
29	d	407	LHG	O8-C23-C24	3.13	121.37	111.83
29	D	410	LHG	O8-C23-C24	3.12	121.36	111.83
25	B	613	CLA	C3B-C4B-NB	-3.12	107.75	110.53
25	C	509	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	C	507	CLA	CHB-C4A-NA	3.11	128.89	124.40
26	b	617	BCR	C27-C26-C25	3.11	126.91	122.70
30	b	620	SQD	C3-C4-C5	3.11	115.86	110.23
30	A	614	SQD	O5-C1-C2	-3.11	103.99	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	620	SQD	C1-C2-C3	-3.10	103.48	110.01
26	A	609	BCR	C27-C26-C25	3.10	126.90	122.70
25	B	614	CLA	C3B-C4B-NB	-3.10	107.76	110.53
30	a	613	SQD	C1-C2-C3	-3.09	103.51	110.01
25	b	602	CLA	C1-C2-C3	-3.09	121.14	126.20
25	b	612	CLA	CMB-C2B-C1B	-3.08	120.72	125.42
25	d	403	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
26	H	101	BCR	C2-C1-C6	3.08	114.92	110.44
25	b	604	CLA	C3B-C4B-NB	-3.08	107.78	110.53
29	B	622	LHG	O8-C23-C24	3.08	121.22	111.83
25	B	610	CLA	O2A-CGA-O1A	-3.08	115.93	123.63
25	A	607	CLA	O2D-CGD-CBD	3.07	116.60	111.23
31	h	101	DGD	O3G-C3G-C2G	-3.07	103.35	110.82
25	b	611	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
25	c	513	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
30	b	620	SQD	O8-S-C6	3.06	111.89	105.97
25	B	611	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
27	D	407	PL9	C40-C39-C41	3.06	120.54	115.23
25	c	502	CLA	C1-C2-C3	-3.06	121.19	126.20
30	B	623	SQD	O48-C23-C24	3.05	121.14	111.83
29	d	408	LHG	O8-C23-C24	3.05	121.12	111.83
25	B	610	CLA	C3B-C4B-NB	-3.05	107.81	110.53
34	d	401	PHO	C2B-C1B-NB	-3.04	107.23	109.43
25	c	512	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
34	D	403	PHO	O1D-CGD-CBD	3.04	129.33	124.72
29	e	101	LHG	O8-C23-C24	3.03	121.08	111.83
27	D	407	PL9	C27-C28-C29	-3.03	120.70	127.62
31	c	515	DGD	O3G-C3G-C2G	-3.02	103.46	110.82
25	b	603	CLA	C1-C2-C3	-3.02	121.26	126.20
30	B	623	SQD	O5-C5-C4	3.01	115.12	109.70
25	b	616	CLA	C1-C2-C3	-3.01	121.27	126.20
25	B	616	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
25	c	508	CLA	O2D-CGD-CBD	3.00	116.47	111.23
25	D	404	CLA	O2D-CGD-CBD	3.00	116.47	111.23
31	c	515	DGD	CDB-CCB-CBB	-2.99	99.24	114.37
25	b	601	CLA	CHB-C4A-NA	2.99	128.72	124.40
25	B	608	CLA	O2D-CGD-CBD	2.99	116.45	111.23
25	b	605	CLA	O1D-CGD-CBD	2.99	130.41	124.52
27	A	610	PL9	C36-C34-C33	-2.98	114.48	121.17
29	d	407	LHG	C11-C10-C9	-2.98	99.32	114.37
28	c	518	LMG	O6-C1-O1	-2.97	103.02	110.04
35	f	101	HEM	C3B-C4B-NB	-2.97	107.33	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	C3B-C4B-NB	-2.97	107.88	110.53
30	B	623	SQD	C1-O5-C5	-2.96	107.94	113.72
30	b	620	SQD	O47-C7-C8	2.96	117.88	111.48
25	D	405	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
32	d	413	STE	C3-C2-C1	-2.96	106.79	114.51
25	C	513	CLA	C3B-C4B-NB	-2.95	107.90	110.53
25	C	506	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
25	C	502	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
28	b	622	LMG	O1-C1-C2	-2.94	103.80	108.27
25	d	403	CLA	C3B-C4B-NB	-2.94	107.91	110.53
25	A	611	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
26	T	101	BCR	C27-C26-C25	2.93	126.66	122.70
26	k	103	BCR	C27-C26-C25	2.92	126.66	122.70
28	d	411	LMG	O6-C1-O1	-2.92	103.15	110.04
25	c	510	CLA	C1-C2-C3	-2.92	121.42	126.20
25	b	614	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
26	C	514	BCR	C2-C1-C6	2.91	114.66	110.44
28	b	622	LMG	O1-C7-C8	-2.90	103.76	110.82
26	B	618	BCR	C15-C14-C13	-2.89	123.22	127.28
25	c	511	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	C	507	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
30	B	623	SQD	C3-C4-C5	2.89	115.47	110.23
25	c	512	CLA	CHB-C4A-NA	2.89	128.57	124.40
34	D	403	PHO	C2B-C1B-NB	-2.88	107.35	109.43
26	k	101	BCR	C15-C14-C13	-2.88	123.24	127.28
25	c	512	CLA	C3B-C4B-NB	-2.88	107.96	110.53
25	c	513	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
34	d	402	PHO	C2B-C1B-NB	-2.88	107.35	109.43
31	h	101	DGD	C4E-C3E-C2E	-2.87	105.79	110.83
28	D	408	LMG	O6-C1-O1	-2.87	103.26	110.04
27	D	407	PL9	C37-C38-C39	-2.87	121.05	127.62
32	C	519	STE	C3-C2-C1	-2.87	107.03	114.51
25	C	501	CLA	O2D-CGD-CBD	2.86	116.23	111.23
25	c	508	CLA	CHB-C4A-NA	2.86	128.53	124.40
29	d	407	LHG	O8-C23-O10	-2.86	116.48	123.63
25	a	608	CLA	C3B-C4B-NB	-2.86	107.98	110.53
27	d	406	PL9	C40-C39-C41	2.85	120.18	115.23
25	c	513	CLA	C3B-C4B-NB	-2.85	107.98	110.53
25	C	503	CLA	C7-C6-C5	-2.84	105.68	113.26
26	k	101	BCR	C33-C5-C6	-2.84	121.38	124.48
25	a	608	CLA	O2A-CGA-O1A	-2.84	116.52	123.63
27	D	407	PL9	C36-C34-C33	-2.84	114.79	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	102	SQD	O48-C23-C24	2.84	120.49	111.83
26	B	618	BCR	C2-C1-C6	2.83	114.55	110.44
28	M	101	LMG	C38-C37-C36	-2.83	100.06	114.37
25	C	510	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
25	b	602	CLA	C3B-C4B-NB	-2.82	108.01	110.53
25	C	511	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
25	c	506	CLA	C3B-C4B-NB	-2.82	108.02	110.53
25	C	505	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
25	D	404	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	b	612	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
29	l	101	LHG	O8-C23-C24	2.81	120.40	111.83
26	T	101	BCR	C33-C5-C6	-2.81	121.42	124.48
34	D	402	PHO	O2D-CGD-CBD	2.81	114.03	110.95
25	b	614	CLA	C1-C2-C3	-2.81	121.60	126.20
26	d	405	BCR	C38-C26-C25	-2.80	121.42	124.48
27	a	611	PL9	C22-C23-C24	-2.80	121.21	127.62
25	a	608	CLA	CHB-C4A-NA	2.80	128.44	124.40
25	b	604	CLA	O2D-CGD-CBD	2.80	116.12	111.23
25	C	510	CLA	C3B-C4B-NB	-2.79	108.03	110.53
26	d	405	BCR	C33-C5-C6	-2.79	121.44	124.48
26	D	406	BCR	C27-C26-C25	2.79	126.47	122.70
25	B	615	CLA	CHB-C4A-NA	2.79	128.42	124.40
35	f	101	HEM	C3B-C2B-C1B	2.78	108.50	106.41
31	o	301	DGD	CDB-CCB-CBB	-2.78	100.31	114.37
25	A	606	CLA	CHB-C4A-NA	2.78	128.41	124.40
25	C	512	CLA	CHB-C4A-NA	2.77	128.40	124.40
25	b	607	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
25	B	601	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	a	612	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
26	k	101	BCR	C27-C26-C25	2.77	126.45	122.70
25	c	501	CLA	CHB-C4A-NA	2.77	128.40	124.40
28	C	518	LMG	O1-C7-C8	-2.77	104.09	110.82
26	x	101	BCR	C27-C26-C25	2.77	126.44	122.70
25	B	614	CLA	C1-C2-C3	-2.77	121.67	126.20
34	d	402	PHO	O2D-CGD-O1D	-2.77	118.47	123.85
36	v	201	HEC	CBD-CAD-C3D	-2.76	104.89	112.53
25	C	504	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
28	b	622	LMG	O3-C3-C2	-2.76	103.88	110.38
25	B	604	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
27	D	407	PL9	C12-C13-C14	-2.75	121.33	127.62
25	b	611	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	c	507	CLA	O2A-CGA-O1A	-2.75	116.75	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	609	BCR	C15-C14-C13	-2.75	123.42	127.28
34	D	402	PHO	O2D-CGD-O1D	-2.74	118.50	123.85
25	C	509	CLA	CHB-C4A-NA	2.74	128.36	124.40
25	C	503	CLA	CHB-C4A-NA	2.74	128.36	124.40
25	b	607	CLA	CHB-C4A-NA	2.74	128.35	124.40
25	B	613	CLA	C16-C15-C13	-2.74	106.86	115.97
25	B	604	CLA	CHB-C4A-NA	2.74	128.35	124.40
25	b	608	CLA	CHB-C4A-NA	2.74	128.35	124.40
31	C	515	DGD	C3D-C4D-C5D	-2.73	105.28	110.23
26	d	405	BCR	C7-C8-C9	-2.73	122.20	126.23
31	h	101	DGD	C1E-O6E-C5E	2.73	119.05	113.72
26	H	101	BCR	C27-C26-C25	2.72	126.38	122.70
25	a	607	CLA	CHB-C4A-NA	2.72	128.33	124.40
25	b	601	CLA	O2D-CGD-CBD	2.72	115.98	111.23
25	B	608	CLA	C3B-C4B-NB	-2.72	108.11	110.53
25	B	603	CLA	O2D-CGD-CBD	2.71	115.97	111.23
25	b	612	CLA	CMB-C2B-C3B	2.71	132.93	126.55
31	h	101	DGD	O6E-C5E-C4E	2.71	114.58	109.70
25	B	602	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
25	A	607	CLA	C1D-ND-C4D	2.71	108.21	106.31
26	a	610	BCR	C11-C10-C9	-2.71	123.48	127.28
26	k	102	BCR	C27-C26-C25	2.71	126.36	122.70
26	k	102	BCR	C33-C5-C6	-2.71	121.53	124.48
25	B	609	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	d	404	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
30	f	102	SQD	O9-S-C6	2.70	110.78	106.76
31	C	516	DGD	O6D-C1D-O3G	-2.70	103.67	110.04
26	c	514	BCR	C33-C5-C6	-2.69	121.55	124.48
25	b	608	CLA	O2D-CGD-CBD	2.69	115.93	111.23
26	d	405	BCR	C30-C25-C26	-2.69	118.96	122.64
29	E	101	LHG	O8-C23-C24	2.68	120.02	111.83
25	b	616	CLA	C3B-C4B-NB	-2.68	108.13	110.53
25	C	502	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	c	509	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	b	602	CLA	O2D-CGD-CBD	2.68	115.92	111.23
25	b	614	CLA	CHB-C4A-NA	2.68	128.27	124.40
26	b	618	BCR	C27-C26-C25	2.68	126.32	122.70
27	a	611	PL9	C37-C38-C39	-2.68	121.50	127.62
31	c	516	DGD	CDB-CCB-CBB	-2.67	100.87	114.37
26	a	610	BCR	C2-C1-C6	2.67	114.31	110.44
31	C	515	DGD	O6D-C1D-O3G	-2.67	103.74	110.04
29	B	622	LHG	C20-C19-C18	-2.67	100.89	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	102	SQD	O47-C7-C8	2.66	120.71	110.93
26	K	102	BCR	C27-C26-C25	2.66	126.30	122.70
25	C	503	CLA	C1-O2A-CGA	2.66	123.09	116.65
25	b	603	CLA	O2D-CGD-CBD	2.66	115.88	111.23
35	F	101	HEM	CHC-C4B-NB	2.66	127.28	124.42
25	C	512	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
25	c	510	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
30	B	623	SQD	O9-S-O7	-2.65	105.19	113.82
25	C	503	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
25	D	404	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
26	Z	101	BCR	C2-C1-C6	2.64	114.28	110.44
25	b	612	CLA	C11-C12-C13	-2.64	107.17	115.97
29	A	613	LHG	O8-C6-C5	-2.64	100.78	108.40
25	c	510	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
26	K	101	BCR	C27-C26-C25	2.64	126.27	122.70
25	c	510	CLA	C3B-C4B-NB	-2.64	108.18	110.53
31	C	517	DGD	CDB-CCB-CBB	-2.63	101.05	114.37
25	b	616	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
31	A	616	DGD	CDB-CCB-CBB	-2.63	101.07	114.37
25	B	612	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
25	a	607	CLA	C3B-C4B-NB	-2.63	108.18	110.53
34	D	402	PHO	C2B-C1B-NB	-2.63	107.53	109.43
25	B	602	CLA	CHB-C4A-NA	2.62	128.19	124.40
25	b	615	CLA	CHB-C4A-NA	2.62	128.19	124.40
25	B	608	CLA	C6-C7-C8	-2.62	107.25	115.97
25	A	608	CLA	O2D-CGD-CBD	2.62	115.81	111.23
27	a	611	PL9	O2-C1-C6	2.62	124.65	120.48
27	D	407	PL9	C20-C19-C21	2.62	119.78	115.23
31	c	515	DGD	C3G-C2G-C1G	-2.62	105.68	111.78
25	c	504	CLA	C1-C2-C3	-2.62	121.91	126.20
25	b	604	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
25	b	613	CLA	CHB-C1B-NB	2.61	127.97	124.05
31	h	101	DGD	CDB-CCB-CBB	-2.61	101.16	114.37
25	C	503	CLA	CHD-C1D-ND	-2.61	121.13	124.80
26	K	101	BCR	C2-C1-C6	2.61	114.23	110.44
30	A	614	SQD	O47-C7-O49	-2.61	117.60	123.70
31	c	517	DGD	CDB-CCB-CBB	-2.61	101.18	114.37
25	c	507	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	b	604	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
25	c	513	CLA	C1-C2-C3	-2.60	121.94	126.20
25	b	616	CLA	O2D-CGD-CBD	2.60	115.77	111.23
34	d	402	PHO	CMA-C3A-C4A	-2.59	109.02	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	101	DGD	C1D-C2D-C3D	-2.59	104.56	110.01
26	b	617	BCR	C15-C14-C13	-2.59	123.64	127.28
25	B	612	CLA	CHB-C4A-NA	2.59	128.14	124.40
25	c	504	CLA	C3B-C4B-NB	-2.59	108.22	110.53
28	c	518	LMG	O8-C28-O10	-2.59	117.16	123.63
27	d	406	PL9	C20-C19-C21	2.59	119.72	115.23
25	a	609	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
26	t	101	BCR	C33-C5-C6	-2.59	121.66	124.48
26	H	101	BCR	C16-C15-C14	-2.58	118.23	123.52
26	b	617	BCR	C33-C5-C6	-2.58	121.66	124.48
25	b	614	CLA	O2A-CGA-O1A	-2.58	117.16	123.63
30	f	102	SQD	C1-O5-C5	-2.58	108.68	113.72
31	A	616	DGD	O6D-C1D-O3G	-2.58	103.94	110.04
27	d	406	PL9	C12-C13-C14	-2.58	121.72	127.62
30	f	102	SQD	O5-C1-C2	-2.58	105.07	110.37
25	C	509	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
25	b	610	CLA	CAA-CBA-CGA	-2.57	105.90	113.21
30	D	409	SQD	O5-C5-C4	2.57	114.33	109.70
34	d	401	PHO	CMB-C2B-C3B	2.57	129.82	124.68
28	b	624	LMG	O2-C2-C1	-2.57	103.95	110.08
25	b	615	CLA	O2A-CGA-O1A	-2.56	117.21	123.63
25	a	609	CLA	CHB-C4A-NA	2.56	128.10	124.40
30	a	613	SQD	O9-S-C6	2.56	110.58	106.76
25	B	610	CLA	C1-C2-C3	-2.56	122.00	126.20
25	c	504	CLA	O2D-CGD-CBD	2.56	115.71	111.23
28	b	622	LMG	O6-C1-O1	-2.56	104.00	110.04
25	a	608	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
25	C	506	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
27	A	610	PL9	C20-C19-C21	2.56	119.67	115.23
25	C	511	CLA	CHB-C4A-NA	2.56	128.09	124.40
31	C	516	DGD	CDB-CCB-CBB	-2.56	101.45	114.37
27	A	610	PL9	C7-C8-C9	-2.55	122.43	126.83
31	C	516	DGD	O2D-C2D-C1D	-2.55	103.99	110.08
25	C	513	CLA	CHB-C4A-NA	2.55	128.08	124.40
31	c	515	DGD	CBB-CAB-C9B	-2.55	101.48	114.37
27	A	610	PL9	C27-C28-C29	-2.55	121.79	127.62
25	B	601	CLA	O2D-CGD-CBD	2.55	115.68	111.23
29	E	101	LHG	C11-C10-C9	-2.54	101.50	114.37
25	c	502	CLA	O1D-CGD-CBD	2.54	129.54	124.52
26	B	617	BCR	C29-C30-C25	2.54	114.13	110.44
28	d	411	LMG	O1-C7-C8	-2.54	104.63	110.82
25	c	508	CLA	O2A-CGA-O1A	-2.54	117.27	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	516	DGD	O2D-C2D-C1D	-2.54	104.02	110.08
25	C	502	CLA	C1-C2-C3	-2.54	122.03	126.20
25	b	612	CLA	CHB-C4A-NA	2.54	128.07	124.40
31	C	517	DGD	C3G-C2G-C1G	-2.54	105.87	111.78
26	k	103	BCR	C11-C10-C9	-2.54	123.72	127.28
25	B	615	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
25	c	509	CLA	CHB-C4A-NA	2.54	128.06	124.40
27	a	611	PL9	C27-C28-C29	-2.53	121.82	127.62
25	c	506	CLA	C4-C3-C5	2.53	119.62	115.23
26	T	101	BCR	C2-C1-C6	2.53	114.11	110.44
25	A	606	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
26	t	101	BCR	C11-C10-C9	-2.53	123.73	127.28
25	B	602	CLA	C1-C2-C3	-2.53	122.06	126.20
34	D	402	PHO	C1-C2-C3	-2.53	122.06	126.20
25	B	606	CLA	O2D-CGD-CBD	2.53	115.65	111.23
25	C	508	CLA	O2D-CGD-CBD	2.53	115.65	111.23
29	l	101	LHG	C11-C10-C9	-2.52	101.61	114.37
28	A	612	LMG	C38-C37-C36	-2.52	101.62	114.37
29	B	622	LHG	C11-C10-C9	-2.52	101.63	114.37
32	d	412	STE	O2-C1-C2	2.52	121.96	114.00
25	b	610	CLA	CHB-C4A-NA	2.52	128.03	124.40
25	B	601	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
31	o	301	DGD	C1G-C2G-C3G	-2.52	105.99	111.80
26	a	610	BCR	C16-C15-C14	-2.51	118.37	123.52
25	c	504	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
25	c	505	CLA	C1-C2-C3	-2.51	122.08	126.20
26	t	101	BCR	C27-C26-C25	2.51	126.10	122.70
25	C	504	CLA	CHB-C4A-NA	2.51	128.03	124.40
25	C	502	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
26	k	103	BCR	C33-C5-C6	-2.51	121.75	124.48
25	C	509	CLA	O2D-CGD-CBD	2.51	115.62	111.23
26	k	101	BCR	C2-C1-C6	2.51	114.08	110.44
29	e	101	LHG	C11-C10-C9	-2.51	101.69	114.37
25	b	608	CLA	C1D-ND-C4D	2.51	108.07	106.31
25	b	603	CLA	CHC-C4B-NB	2.51	127.81	124.05
25	a	607	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
25	C	512	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
25	c	504	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	C	503	CLA	O1D-CGD-CBD	2.50	129.46	124.52
26	C	514	BCR	C27-C26-C25	2.50	126.08	122.70
30	a	613	SQD	O8-S-C6	2.50	110.80	105.97
25	c	512	CLA	O2A-CGA-O1A	-2.50	117.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	606	CLA	CHC-C4B-NB	2.50	127.80	124.05
25	b	616	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
25	a	612	CLA	O2D-CGD-CBD	2.50	115.60	111.23
35	f	101	HEM	CBA-CAA-C2A	-2.50	105.63	112.53
26	B	619	BCR	C29-C30-C25	2.50	114.06	110.44
25	B	614	CLA	CHB-C4A-NA	2.49	128.00	124.40
31	H	102	DGD	O5D-C1E-C2E	2.49	112.06	108.27
28	c	522	LMG	O6-C1-O1	-2.49	104.16	110.04
25	B	613	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
25	C	509	CLA	C1-C2-C3	-2.49	122.12	126.20
25	A	611	CLA	O2D-CGD-CBD	2.49	115.58	111.23
29	d	408	LHG	C18-C17-C16	-2.49	101.79	114.37
25	c	506	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
31	C	515	DGD	O5D-C6D-C5D	-2.49	103.81	109.42
25	b	605	CLA	CHD-C1D-ND	-2.49	121.30	124.80
25	a	612	CLA	CHB-C4A-NA	2.49	127.99	124.40
31	A	616	DGD	O3G-C3G-C2G	-2.49	104.77	110.82
25	B	612	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
31	H	102	DGD	O6D-C1D-O3G	-2.49	104.17	110.04
25	b	604	CLA	CHB-C4A-NA	2.49	127.99	124.40
25	C	507	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
28	M	101	LMG	C40-C39-C38	-2.48	101.84	114.37
26	a	610	BCR	C7-C8-C9	-2.48	122.57	126.23
26	T	101	BCR	C3-C4-C5	-2.48	109.64	114.06
25	c	503	CLA	CHB-C4A-NA	2.47	127.97	124.40
25	C	509	CLA	C3B-C4B-NB	-2.47	108.32	110.53
26	t	101	BCR	C15-C16-C17	-2.47	118.46	123.52
25	b	608	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
31	H	102	DGD	C1D-C2D-C3D	-2.47	104.82	110.01
30	A	615	SQD	O48-C23-C24	2.47	119.36	111.83
25	C	509	CLA	CMB-C2B-C3B	2.47	132.35	126.55
29	d	408	LHG	C20-C19-C18	-2.47	101.90	114.37
25	B	607	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	b	610	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
25	b	606	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
25	b	605	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	B	603	CLA	CHB-C1B-NB	2.46	127.73	124.05
25	b	606	CLA	CHB-C1B-NB	2.46	127.73	124.05
25	C	505	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
25	B	609	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
25	b	603	CLA	CHB-C1B-NB	2.45	127.73	124.05
25	B	601	CLA	C4-C3-C5	2.45	119.49	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	502	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	c	513	CLA	CMB-C2B-C3B	2.45	132.31	126.55
25	B	603	CLA	CHC-C4B-NB	2.45	127.72	124.05
25	b	613	CLA	C2A-C1A-CHA	2.45	128.12	123.87
25	c	507	CLA	CHC-C4B-NB	2.45	127.72	124.05
26	K	101	BCR	C15-C16-C17	-2.44	118.52	123.52
27	A	610	PL9	O2-C1-C6	2.44	124.36	120.48
25	D	404	CLA	C4-C3-C5	2.44	119.47	115.23
25	c	507	CLA	O2D-CGD-CBD	2.44	115.50	111.23
31	H	102	DGD	O6E-C5E-C4E	2.44	114.09	109.70
28	c	522	LMG	C38-C37-C36	-2.44	102.04	114.37
25	B	614	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
26	A	609	BCR	C2-C1-C6	2.44	113.98	110.44
25	B	601	CLA	O2A-C1-C2	-2.44	98.73	108.11
25	C	510	CLA	CMB-C2B-C3B	2.43	132.27	126.55
25	c	509	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
25	b	613	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
26	K	102	BCR	C33-C5-C6	-2.43	121.83	124.48
31	C	515	DGD	CBB-CAB-C9B	-2.43	102.10	114.37
26	Z	101	BCR	C27-C26-C25	2.43	125.98	122.70
31	h	101	DGD	C6D-C5D-C4D	2.42	117.16	112.07
25	C	511	CLA	C1-C2-C3	-2.42	122.22	126.20
25	B	605	CLA	C16-C15-C13	-2.42	107.91	115.97
26	a	610	BCR	C29-C30-C25	2.42	113.95	110.44
28	b	622	LMG	C38-C37-C36	-2.42	102.14	114.37
27	a	611	PL9	O2-C1-C2	-2.42	116.33	121.83
25	B	606	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	B	612	CLA	CMB-C2B-C3B	2.42	132.24	126.55
31	h	101	DGD	O6D-C1D-O3G	-2.42	104.33	110.04
25	c	510	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	b	605	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
26	a	610	BCR	C27-C26-C25	2.42	125.97	122.70
31	C	516	DGD	C1D-C2D-C3D	-2.41	104.94	110.01
29	d	407	LHG	C18-C17-C16	-2.41	102.18	114.37
26	b	619	BCR	C2-C1-C6	2.41	113.94	110.44
27	a	611	PL9	C32-C33-C34	-2.41	122.11	127.62
25	C	506	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	D	408	LMG	C38-C37-C36	-2.41	102.19	114.37
25	b	616	CLA	CHB-C4A-NA	2.41	127.87	124.40
25	b	602	CLA	CAC-C3C-C4C	2.41	127.92	124.79
31	A	616	DGD	O2D-C2D-C1D	-2.41	104.34	110.08
28	C	518	LMG	C40-C39-C38	-2.40	102.21	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	o	301	DGD	CFB-CEB-CDB	-2.40	102.22	114.37
25	B	608	CLA	CMB-C2B-C3B	2.40	132.20	126.55
25	B	602	CLA	CMB-C2B-C3B	2.40	132.20	126.55
25	B	605	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
25	b	608	CLA	CMB-C2B-C3B	2.40	132.19	126.55
25	A	611	CLA	CHB-C4A-NA	2.40	127.86	124.40
36	V	201	HEC	CMC-C2C-C1C	-2.40	121.77	125.42
25	B	602	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
25	B	610	CLA	O2D-CGD-CBD	2.40	115.42	111.23
31	C	515	DGD	O2D-C2D-C1D	-2.40	104.37	110.08
25	b	613	CLA	C3B-C4B-NB	-2.39	108.39	110.53
30	B	623	SQD	O8-S-C6	2.39	110.59	105.97
25	C	511	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
31	c	516	DGD	C1D-C2D-C3D	-2.39	104.98	110.01
25	C	501	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
25	C	508	CLA	CHD-C1D-C2D	2.39	130.45	125.49
30	a	614	SQD	C46-C45-C44	-2.38	106.30	111.80
25	b	604	CLA	CHB-C1B-NB	2.38	127.62	124.05
25	B	608	CLA	CHD-C1D-ND	-2.38	121.45	124.80
26	b	618	BCR	C11-C10-C9	-2.38	123.94	127.28
26	T	101	BCR	C7-C8-C9	-2.38	122.72	126.23
25	d	403	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
35	f	101	HEM	C1B-NB-C4B	2.37	108.02	105.21
32	B	626	STE	O2-C1-C2	2.37	121.49	114.00
25	C	511	CLA	C3B-C4B-NB	-2.36	108.42	110.53
28	b	622	LMG	O8-C28-O10	-2.36	117.71	123.63
25	C	504	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
25	b	603	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
28	C	518	LMG	O6-C1-O1	-2.36	104.47	110.04
25	b	607	CLA	C1-O2A-CGA	2.36	122.36	116.65
25	C	510	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
26	k	101	BCR	C15-C16-C17	-2.36	118.69	123.52
27	d	406	PL9	C36-C34-C33	-2.36	115.88	121.17
25	b	609	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
29	A	613	LHG	C11-C10-C9	-2.35	102.47	114.37
28	b	624	LMG	O7-C10-O9	-2.35	118.20	123.70
26	K	101	BCR	C33-C5-C6	-2.35	121.92	124.48
25	B	607	CLA	C3B-C4B-NB	-2.35	108.43	110.53
25	B	607	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
25	c	503	CLA	C7-C6-C5	-2.35	107.00	113.26
26	H	101	BCR	C24-C23-C22	-2.35	122.76	126.23
25	B	608	CLA	CHB-C1B-NB	2.35	127.57	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	518	LMG	O2-C2-C1	-2.35	104.49	110.08
25	B	611	CLA	C1-C2-C3	-2.34	122.36	126.20
28	A	612	LMG	C40-C39-C38	-2.34	102.52	114.37
30	f	102	SQD	C3-C4-C5	2.34	114.48	110.23
27	a	611	PL9	C7-C8-C9	-2.34	122.79	126.83
25	c	502	CLA	CHB-C1B-NB	2.34	127.56	124.05
31	C	515	DGD	C3G-C2G-C1G	-2.34	106.33	111.78
25	D	405	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
28	D	408	LMG	C40-C39-C38	-2.34	102.55	114.37
31	C	516	DGD	C5B-C4B-C3B	-2.34	102.56	114.37
25	c	511	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
26	t	101	BCR	C1-C6-C5	-2.33	119.44	122.64
31	A	616	DGD	CBB-CAB-C9B	-2.33	102.57	114.37
26	b	619	BCR	C27-C26-C25	2.33	125.86	122.70
29	B	622	LHG	C18-C17-C16	-2.33	102.58	114.37
25	b	615	CLA	CHC-C1C-NC	2.33	127.82	124.31
27	d	406	PL9	C8-C7-C3	2.33	118.06	112.03
29	D	410	LHG	C18-C17-C16	-2.33	102.59	114.37
29	E	101	LHG	C20-C19-C18	-2.33	102.59	114.37
31	C	517	DGD	CAB-C9B-C8B	-2.33	102.59	114.37
25	b	611	CLA	C7-C6-C5	-2.33	107.05	113.26
25	a	607	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
25	B	607	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
27	a	611	PL9	C40-C39-C41	2.33	119.27	115.23
32	t	102	STE	O2-C1-C2	2.32	121.34	114.00
27	A	610	PL9	O2-C1-C2	-2.32	116.55	121.83
31	c	515	DGD	O2D-C2D-C1D	-2.32	104.55	110.08
26	C	514	BCR	C15-C16-C17	-2.32	118.77	123.52
25	C	504	CLA	CHD-C1D-ND	-2.32	121.54	124.80
28	M	101	LMG	O6-C1-O1	-2.32	104.57	110.04
29	L	101	LHG	C20-C19-C18	-2.32	102.66	114.37
25	C	510	CLA	CHB-C4A-NA	2.32	127.74	124.40
25	B	612	CLA	C11-C12-C13	-2.32	108.27	115.97
25	B	603	CLA	C4-C3-C5	2.31	119.25	115.23
31	c	516	DGD	CBB-CAB-C9B	-2.31	102.67	114.37
31	c	516	DGD	C3E-C4E-C5E	-2.31	106.04	110.23
25	b	614	CLA	CHD-C1D-ND	-2.31	121.55	124.80
35	f	101	HEM	CAB-C3B-C2B	-2.31	120.92	128.43
25	c	502	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
25	C	508	CLA	CHD-C4C-NC	2.31	127.81	124.23
28	c	518	LMG	C40-C39-C38	-2.31	102.71	114.37
31	H	102	DGD	O2D-C2D-C1D	-2.31	104.58	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	610	CLA	CHD-C1D-ND	-2.31	121.56	124.80
28	b	624	LMG	C3-C4-C5	-2.31	106.05	110.23
25	b	616	CLA	CMB-C2B-C3B	2.30	131.97	126.55
30	f	102	SQD	C1-C2-C3	-2.30	105.17	110.01
31	C	517	DGD	C1D-C2D-C3D	-2.30	105.17	110.01
30	A	614	SQD	O9-S-C6	2.30	110.19	106.76
30	D	409	SQD	O6-C44-C45	-2.30	101.56	109.37
25	C	508	CLA	CHB-C4A-NA	2.30	127.72	124.40
28	D	408	LMG	O3-C3-C2	-2.30	104.95	110.38
25	b	608	CLA	CHD-C1D-C2D	2.30	130.27	125.49
30	a	614	SQD	C9-C8-C7	-2.30	105.27	113.69
25	C	504	CLA	C1-C2-C3	-2.30	122.43	126.20
25	c	503	CLA	CHD-C4C-NC	2.30	127.79	124.23
28	c	520	LMG	O2-C2-C1	-2.29	104.61	110.08
26	B	618	BCR	C35-C13-C14	-2.29	119.10	122.82
25	C	513	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
29	d	407	LHG	C20-C19-C18	-2.29	102.80	114.37
30	A	614	SQD	O48-C23-C24	2.29	118.81	111.83
26	B	619	BCR	C3-C4-C5	-2.29	109.98	114.06
25	b	608	CLA	CHD-C1D-ND	-2.29	121.59	124.80
25	B	616	CLA	C3B-C4B-NB	-2.29	108.49	110.53
25	C	513	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
25	D	404	CLA	C1-C2-C3	-2.28	122.46	126.20
26	D	406	BCR	C38-C26-C25	-2.28	121.99	124.48
25	C	508	CLA	C7-C6-C5	-2.28	107.18	113.26
25	b	613	CLA	CMB-C2B-C3B	2.28	131.91	126.55
29	D	410	LHG	O8-C23-O10	-2.28	117.93	123.63
28	C	518	LMG	O2-C2-C1	-2.28	104.64	110.08
27	A	610	PL9	O1-C4-C3	-2.28	118.33	120.73
25	C	506	CLA	O1D-CGD-CBD	2.28	129.01	124.52
25	a	612	CLA	C3B-C4B-NB	-2.28	108.50	110.53
31	c	517	DGD	O2D-C2D-C1D	-2.27	104.66	110.08
25	b	610	CLA	C3B-C4B-NB	-2.27	108.50	110.53
25	a	612	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
28	C	518	LMG	C38-C37-C36	-2.27	102.88	114.37
30	b	620	SQD	O9-S-C6	2.27	110.15	106.76
25	c	503	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
28	c	520	LMG	C40-C39-C38	-2.27	102.90	114.37
25	B	616	CLA	O2D-CGD-CBD	2.27	115.19	111.23
25	C	512	CLA	O2D-CGD-CBD	2.27	115.19	111.23
28	C	518	LMG	O8-C28-O10	-2.27	117.96	123.63
25	C	504	CLA	CHD-C4C-NC	2.27	127.74	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	503	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
25	B	613	CLA	CMB-C2B-C3B	2.26	131.88	126.55
31	o	301	DGD	C5B-C4B-C3B	-2.26	102.93	114.37
25	b	609	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	B	612	CLA	O2D-CGD-CBD	2.26	115.18	111.23
25	b	611	CLA	C3B-C4B-NB	-2.26	108.51	110.53
26	B	617	BCR	C3-C4-C5	-2.26	110.03	114.06
28	c	518	LMG	C38-C37-C36	-2.26	102.95	114.37
25	b	608	CLA	CHB-C1B-NB	2.26	127.44	124.05
25	B	607	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
25	a	608	CLA	CHA-C1A-NA	-2.25	121.28	126.39
29	e	101	LHG	C20-C19-C18	-2.25	102.98	114.37
28	d	411	LMG	O2-C2-C1	-2.25	104.71	110.08
31	C	516	DGD	C3D-C4D-C5D	-2.25	106.15	110.23
31	C	516	DGD	O5D-C6D-C5D	-2.25	104.35	109.42
29	D	410	LHG	C20-C19-C18	-2.25	102.99	114.37
25	B	613	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
31	A	616	DGD	C1D-C2D-C3D	-2.25	105.28	110.01
25	b	603	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
31	C	516	DGD	O3G-C1D-C2D	-2.25	104.86	108.27
25	B	612	CLA	O1D-CGD-CBD	2.25	128.95	124.52
31	c	517	DGD	O6D-C1D-O3G	-2.25	104.74	110.04
28	D	411	LMG	O1-C7-C8	-2.25	106.00	111.77
32	C	520	STE	O2-C1-C2	2.24	121.09	114.00
25	B	611	CLA	O2D-CGD-CBD	2.24	115.15	111.23
31	H	102	DGD	C8B-C7B-C6B	-2.24	103.03	114.37
25	B	605	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
29	D	410	LHG	C11-C10-C9	-2.24	103.05	114.37
25	b	612	CLA	O2D-CGD-CBD	2.24	115.14	111.23
25	C	507	CLA	C3B-C4B-NB	-2.24	108.53	110.53
35	f	101	HEM	CHD-C4C-NC	2.24	126.89	124.45
28	b	624	LMG	C40-C39-C38	-2.24	103.06	114.37
27	A	610	PL9	C40-C39-C41	2.24	119.11	115.23
25	c	504	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
31	c	515	DGD	O6D-C1D-O3G	-2.23	104.77	110.04
25	C	513	CLA	O2D-CGD-CBD	2.23	115.13	111.23
31	C	517	DGD	O3E-C3E-C2E	-2.23	105.12	110.38
30	a	614	SQD	O48-C23-O10	-2.23	118.06	123.63
25	C	510	CLA	CHD-C1D-ND	-2.23	121.67	124.80
25	b	608	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
25	B	608	CLA	CHB-C4A-NA	2.22	127.61	124.40
31	H	102	DGD	O3E-C3E-C2E	-2.22	105.14	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	d	401	PHO	C1-C2-C3	-2.22	122.56	126.20
29	l	101	LHG	C20-C19-C18	-2.22	103.15	114.37
25	D	405	CLA	CHB-C4A-NA	2.22	127.60	124.40
25	d	403	CLA	CHB-C4A-NA	2.22	127.60	124.40
28	C	518	LMG	C1-O6-C5	-2.22	109.39	113.72
25	C	503	CLA	CHD-C1D-C2D	2.22	130.10	125.49
25	A	608	CLA	C3B-C4B-NB	-2.22	108.55	110.53
31	c	515	DGD	C7B-C6B-C5B	-2.22	103.16	114.37
29	E	101	LHG	C18-C17-C16	-2.22	103.17	114.37
26	C	514	BCR	C33-C5-C6	-2.22	122.07	124.48
25	B	606	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
28	b	624	LMG	O5-C6-C5	-2.21	103.80	111.33
27	A	610	PL9	C12-C13-C14	-2.21	122.56	127.62
25	b	605	CLA	CHD-C1D-C2D	2.21	130.09	125.49
25	D	405	CLA	C1-C2-C3	-2.21	122.58	126.20
25	A	607	CLA	C2D-C1D-ND	-2.21	107.94	110.13
25	c	506	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	B	614	CLA	O2D-CGD-CBD	2.21	115.09	111.23
25	b	613	CLA	CHC-C4B-NB	2.21	127.36	124.05
26	C	514	BCR	C7-C8-C9	-2.21	122.97	126.23
26	x	101	BCR	C3-C4-C5	-2.21	110.12	114.06
25	B	604	CLA	C1-O2A-CGA	-2.21	111.31	116.65
25	b	610	CLA	O2D-CGD-CBD	2.21	115.08	111.23
25	a	612	CLA	CHC-C4B-NB	2.21	127.36	124.05
26	b	619	BCR	C24-C23-C22	-2.20	122.97	126.23
29	E	101	LHG	C27-C26-C25	-2.20	103.24	114.37
28	d	410	LMG	O7-C10-O9	-2.20	117.67	123.33
28	b	622	LMG	C40-C39-C38	-2.20	103.24	114.37
25	B	609	CLA	CHB-C4A-NA	2.20	127.58	124.40
25	a	612	CLA	CMB-C2B-C3B	2.20	131.72	126.55
30	B	623	SQD	O7-S-C6	2.20	110.04	106.76
30	B	623	SQD	C46-C45-C44	-2.20	106.66	111.78
30	A	614	SQD	C45-O47-C7	-2.20	112.54	117.80
25	b	614	CLA	O1D-CGD-CBD	2.20	128.85	124.52
28	d	411	LMG	C38-C37-C36	-2.19	103.27	114.37
28	D	408	LMG	O2-C2-C1	-2.19	104.85	110.08
27	d	406	PL9	C35-C34-C36	2.19	119.04	115.23
25	c	509	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
31	H	102	DGD	C1D-O6D-C5D	-2.19	109.44	113.72
28	b	624	LMG	O1-C7-C8	-2.19	105.49	110.82
25	c	510	CLA	CMB-C2B-C3B	2.19	131.70	126.55
25	B	604	CLA	O2D-CGD-CBD	2.19	115.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	615	CLA	CHB-C1B-NB	2.19	127.33	124.05
28	B	621	LMG	C38-C37-C36	-2.19	103.32	114.37
29	d	408	LHG	C11-C10-C9	-2.19	103.32	114.37
25	c	508	CLA	C1-C2-C3	-2.19	122.62	126.20
26	A	609	BCR	C16-C17-C18	-2.19	124.21	127.28
25	b	611	CLA	CHD-C1D-ND	-2.19	121.73	124.80
25	b	605	CLA	C1-C2-C3	-2.18	122.62	126.20
28	D	411	LMG	O7-C10-O9	-2.18	118.61	123.70
29	e	101	LHG	C18-C17-C16	-2.18	103.36	114.37
25	c	505	CLA	CHB-C1B-NB	2.18	127.32	124.05
29	D	410	LHG	C27-C26-C25	-2.18	103.36	114.37
25	b	613	CLA	CHB-C4A-NA	2.18	127.54	124.40
28	c	520	LMG	O6-C1-O1	-2.18	104.90	110.04
25	A	606	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
25	c	501	CLA	CHD-C1D-ND	-2.17	121.74	124.80
25	C	508	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
25	b	610	CLA	O1D-CGD-CBD	2.17	128.80	124.52
26	b	618	BCR	C30-C25-C26	-2.17	119.67	122.64
25	B	601	CLA	C1-C2-C3	-2.17	122.64	126.20
25	b	604	CLA	CMB-C2B-C3B	2.17	131.65	126.55
28	c	522	LMG	C40-C39-C38	-2.17	103.41	114.37
31	c	515	DGD	O3E-C3E-C2E	-2.17	105.27	110.38
25	c	511	CLA	C2A-C1A-CHA	2.17	127.63	123.87
28	b	624	LMG	C38-C37-C36	-2.17	103.42	114.37
25	c	509	CLA	O2A-CGA-CBA	2.17	118.44	111.83
28	A	612	LMG	O3-C3-C2	-2.16	105.27	110.38
32	a	615	STE	C3-C2-C1	-2.16	108.86	114.51
28	d	411	LMG	C40-C39-C38	-2.16	103.43	114.37
26	B	617	BCR	C33-C5-C6	-2.16	122.12	124.48
25	C	507	CLA	C2A-C1A-CHA	2.16	127.62	123.87
31	c	516	DGD	O5D-C6D-C5D	-2.16	104.55	109.42
25	C	505	CLA	CMB-C2B-C3B	2.16	131.63	126.55
25	C	508	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
29	d	409	LHG	O8-C23-C24	2.16	118.42	111.83
26	A	609	BCR	C16-C15-C14	-2.16	119.10	123.52
25	a	609	CLA	CGD-CBD-CAD	-2.16	103.87	110.85
27	d	406	PL9	C27-C28-C29	-2.16	122.69	127.62
26	c	514	BCR	C15-C16-C17	-2.15	119.11	123.52
26	c	514	BCR	C11-C10-C9	-2.15	124.26	127.28
35	f	101	HEM	CHB-C1B-NB	2.15	127.03	124.37
25	C	507	CLA	C1-C2-C3	-2.15	122.67	126.20
25	B	609	CLA	CHC-C4B-NB	2.15	127.28	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	615	SQD	C45-O47-C7	-2.15	114.68	117.78
32	m	101	STE	O2-C1-C2	2.15	120.79	114.00
28	B	621	LMG	O7-C10-O9	-2.15	117.81	123.33
25	c	510	CLA	C7-C6-C5	-2.15	107.54	113.26
26	C	514	BCR	C11-C10-C9	-2.14	124.27	127.28
25	c	511	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	C	505	CLA	O2D-CGD-CBD	2.14	114.97	111.23
25	A	607	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
25	d	404	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	b	609	CLA	CHC-C4B-NB	2.14	127.26	124.05
25	C	504	CLA	O2D-CGD-CBD	2.14	114.97	111.23
25	B	614	CLA	O1D-CGD-CBD	2.14	128.74	124.52
25	b	613	CLA	C7-C6-C5	-2.14	107.56	113.26
25	b	602	CLA	CMB-C2B-C3B	2.14	131.58	126.55
36	v	201	HEC	CHB-C1B-NB	2.14	127.73	123.86
26	D	406	BCR	C7-C8-C9	-2.14	123.08	126.23
25	B	615	CLA	O2D-CGD-CBD	2.14	114.96	111.23
31	h	101	DGD	CBB-CAB-C9B	-2.13	103.58	114.37
26	B	618	BCR	C28-C27-C26	-2.13	110.25	114.06
25	c	501	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
26	b	618	BCR	C8-C7-C6	-2.13	121.30	127.00
31	C	516	DGD	O6E-C1E-O5D	-2.13	105.01	110.04
25	b	615	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
25	C	507	CLA	O2D-CGD-CBD	2.13	114.95	111.23
25	A	607	CLA	C4D-CHA-C1A	2.13	123.78	121.24
25	c	507	CLA	C7-C6-C5	-2.13	107.60	113.26
25	C	505	CLA	CHB-C4A-NA	2.12	127.47	124.40
26	b	618	BCR	C15-C14-C13	-2.12	124.30	127.28
32	E	102	STE	O2-C1-C2	2.12	120.70	114.00
25	A	611	CLA	C1-C2-C3	-2.12	122.72	126.20
29	A	613	LHG	C18-C17-C16	-2.12	103.67	114.37
27	D	407	PL9	C42-C43-C44	-2.11	122.78	127.62
25	b	603	CLA	CMB-C2B-C3B	2.11	131.52	126.55
31	H	102	DGD	CDB-CCB-CBB	-2.11	103.68	114.37
25	B	609	CLA	C7-C6-C5	-2.11	107.63	113.26
25	b	606	CLA	C3B-C4B-NB	-2.11	108.64	110.53
26	T	101	BCR	C31-C1-C6	2.11	113.56	110.24
31	c	517	DGD	CAB-C9B-C8B	-2.11	103.69	114.37
25	b	610	CLA	CHA-C1A-NA	-2.11	121.61	126.39
25	c	506	CLA	C1-C2-C3	-2.11	122.75	126.20
27	D	407	PL9	C32-C33-C34	-2.10	122.81	127.62
25	B	607	CLA	CED-O2D-CGD	2.10	120.69	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	613	SQD	C44-O6-C1	-2.10	109.29	113.80
31	A	616	DGD	CAB-C9B-C8B	-2.10	103.75	114.37
25	c	502	CLA	CMB-C2B-C3B	2.10	131.49	126.55
30	a	613	SQD	O5-C1-C2	-2.10	106.06	110.37
31	c	517	DGD	C1D-C2D-C3D	-2.10	105.60	110.01
25	A	606	CLA	C3B-C4B-NB	-2.10	108.66	110.53
31	h	101	DGD	O5E-C6E-C5E	-2.10	104.19	111.33
31	c	515	DGD	C1D-C2D-C3D	-2.10	105.60	110.01
26	B	617	BCR	C8-C7-C6	-2.10	121.40	127.00
34	D	403	PHO	OBD-CAD-CBD	-2.10	122.75	125.82
25	D	405	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
28	c	520	LMG	C38-C37-C36	-2.09	103.78	114.37
28	c	520	LMG	C42-C41-C40	-2.09	103.78	114.37
26	B	618	BCR	C27-C26-C25	2.09	125.53	122.70
25	B	603	CLA	CHB-C4A-NA	2.09	127.41	124.40
25	B	605	CLA	CAA-CBA-CGA	-2.09	107.28	113.21
31	C	517	DGD	O6E-C1E-O5D	-2.09	105.11	110.04
28	b	624	LMG	O8-C28-O10	-2.09	118.41	123.63
25	D	405	CLA	CMB-C2B-C3B	2.08	131.45	126.55
34	D	403	PHO	C3D-C4D-ND	2.08	110.38	107.71
31	c	515	DGD	O5D-C6D-C5D	-2.08	104.73	109.42
28	C	518	LMG	O7-C10-O9	-2.08	118.85	123.70
29	e	101	LHG	C27-C26-C25	-2.08	103.88	114.37
26	K	101	BCR	C11-C10-C9	-2.07	124.37	127.28
25	b	609	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
25	B	615	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	c	505	CLA	O2D-CGD-CBD	2.07	114.85	111.23
25	B	613	CLA	C6-C5-C3	-2.07	108.43	113.47
26	k	103	BCR	C24-C23-C22	-2.06	123.18	126.23
25	C	511	CLA	C3A-C2A-C1A	2.06	104.43	101.34
25	b	608	CLA	CHC-C1C-NC	2.06	127.42	124.31
28	d	411	LMG	O3-C3-C2	-2.06	105.52	110.38
29	B	622	LHG	O8-C23-O10	-2.06	118.47	123.63
26	t	101	BCR	C7-C8-C9	-2.06	123.19	126.23
25	B	616	CLA	CHD-C1D-ND	-2.06	121.90	124.80
26	x	101	BCR	C7-C8-C9	-2.06	123.19	126.23
25	C	508	CLA	CMB-C2B-C3B	2.06	131.40	126.55
30	D	409	SQD	O4-C4-C3	-2.06	105.52	110.38
25	a	608	CLA	C2A-C1A-CHA	2.06	127.44	123.87
30	a	613	SQD	C3-C4-C5	2.06	113.96	110.23
28	c	520	LMG	O1-C1-C2	-2.06	105.15	108.27
25	c	502	CLA	CMB-C2B-C1B	-2.05	122.29	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	CMD-C2D-C3D	2.05	132.40	127.69
28	D	411	LMG	C38-C37-C36	-2.05	104.00	114.37
25	b	607	CLA	CHD-C1D-ND	-2.05	121.92	124.80
36	V	201	HEC	CHB-C4A-NA	2.05	126.68	124.45
26	T	101	BCR	C1-C6-C7	2.05	121.21	115.65
31	C	516	DGD	C3E-C4E-C5E	-2.05	106.52	110.23
29	L	101	LHG	C18-C17-C16	-2.05	104.02	114.37
35	F	101	HEM	C4D-ND-C1D	2.05	107.63	105.21
28	d	410	LMG	C38-C37-C36	-2.05	104.03	114.37
31	c	515	DGD	C5B-C4B-C3B	-2.05	104.03	114.37
29	d	408	LHG	O8-C23-O10	-2.05	118.51	123.63
25	c	508	CLA	CHD-C4C-NC	2.04	127.40	124.23
31	c	515	DGD	O3D-C3D-C4D	-2.04	105.56	110.38
25	a	607	CLA	C7-C6-C5	-2.04	107.81	113.26
26	c	514	BCR	C7-C8-C9	-2.04	123.21	126.23
27	D	407	PL9	O2-C1-C2	-2.04	117.19	121.83
30	a	614	SQD	O49-C7-C8	-2.04	115.80	123.78
31	h	101	DGD	C7B-C6B-C5B	-2.04	104.06	114.37
25	b	608	CLA	C2D-C1D-ND	-2.04	108.11	110.13
31	C	517	DGD	CBB-CAB-C9B	-2.04	104.06	114.37
25	B	609	CLA	CHA-C1A-NA	-2.04	121.78	126.39
26	A	609	BCR	C37-C22-C21	-2.04	119.51	122.82
25	a	612	CLA	C1-C2-C3	-2.04	122.86	126.20
28	M	101	LMG	C6-C5-C4	-2.04	108.02	113.02
28	b	624	LMG	C42-C41-C40	-2.04	104.08	114.37
25	c	513	CLA	CHB-C4A-NA	2.04	127.34	124.40
25	C	508	CLA	C1-C2-C3	-2.03	122.86	126.20
28	d	410	LMG	C40-C39-C38	-2.03	104.08	114.37
25	c	511	CLA	C1-C2-C3	-2.03	122.86	126.20
25	c	505	CLA	CHB-C4A-NA	2.03	127.33	124.40
25	B	612	CLA	C16-C15-C13	-2.03	109.21	115.97
25	c	506	CLA	CHA-C1A-NA	-2.03	121.79	126.39
32	c	521	STE	O2-C1-C2	2.03	120.42	114.00
26	B	619	BCR	C15-C16-C17	-2.03	119.37	123.52
25	C	507	CLA	CHA-C1A-NA	-2.03	121.80	126.39
27	D	407	PL9	C8-C7-C3	2.03	117.28	112.03
25	C	511	CLA	O1D-CGD-CBD	2.03	128.52	124.52
31	C	516	DGD	C7B-C6B-C5B	-2.03	104.11	114.37
26	B	618	BCR	C33-C5-C6	-2.03	122.27	124.48
26	Z	101	BCR	C15-C14-C13	-2.03	124.44	127.28
26	Z	101	BCR	C33-C5-C6	-2.03	122.27	124.48
26	c	514	BCR	C35-C13-C14	-2.03	119.53	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	C1-O2A-CGA	-2.03	111.75	116.65
25	b	616	CLA	CHC-C4B-NB	2.03	127.09	124.05
32	T	103	STE	C3-C2-C1	-2.02	109.22	114.51
30	B	623	SQD	O47-C7-O49	-2.02	118.97	123.70
31	o	301	DGD	CBB-CAB-C9B	-2.02	104.14	114.37
25	b	602	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
31	C	516	DGD	CAB-C9B-C8B	-2.02	104.14	114.37
25	B	613	CLA	CHB-C4A-NA	2.02	127.31	124.40
29	L	101	LHG	C11-C10-C9	-2.02	104.16	114.37
25	b	613	CLA	C3A-C2A-C1A	2.02	104.36	101.34
25	b	610	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
25	b	602	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
25	B	605	CLA	CHB-C4A-NA	2.02	127.31	124.40
25	c	512	CLA	C4-C3-C5	2.02	118.73	115.23
25	B	614	CLA	CHB-C1B-NB	2.02	127.07	124.05
30	a	613	SQD	O7-S-C6	2.01	109.76	106.76
29	B	622	LHG	O8-C6-C5	-2.01	102.60	108.40
28	c	520	LMG	C9-C8-C7	-2.01	107.10	111.78
31	c	516	DGD	C7B-C6B-C5B	-2.01	104.20	114.37
31	c	517	DGD	CBB-CAB-C9B	-2.01	104.20	114.37
25	c	505	CLA	CHA-C1A-NA	-2.01	121.84	126.39
25	B	609	CLA	CAC-C3C-C4C	2.01	127.41	124.79
25	B	607	CLA	CMB-C2B-C3B	2.01	131.28	126.55
26	x	101	BCR	C11-C10-C9	-2.01	124.46	127.28
25	B	610	CLA	CHA-C1A-NA	-2.01	121.84	126.39
25	C	507	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
28	M	101	LMG	O2-C2-C1	-2.01	105.29	110.08
26	K	102	BCR	C8-C7-C6	-2.01	121.63	127.00
36	v	201	HEC	CHD-C1D-ND	2.01	127.50	123.86
25	b	613	CLA	CHA-C1A-NA	-2.01	121.85	126.39
34	d	401	PHO	CBC-CAC-C3C	-2.01	110.00	112.87
34	d	402	PHO	O2A-CGA-O1A	-2.01	118.61	123.63
31	C	517	DGD	C5B-C4B-C3B	-2.01	104.23	114.37
27	d	406	PL9	O1-C4-C3	-2.00	118.62	120.73
25	B	602	CLA	C11-C12-C13	-2.00	109.30	115.97
25	C	505	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
31	c	516	DGD	C5B-C4B-C3B	-2.00	104.24	114.37
30	D	409	SQD	O3-C3-C2	2.00	115.10	110.38
25	A	606	CLA	CAA-CBA-CGA	-2.00	107.53	113.21
31	C	516	DGD	CBB-CAB-C9B	-2.00	104.25	114.37
25	c	504	CLA	O1A-CGA-CBA	2.00	131.61	123.78
26	H	101	BCR	C1-C6-C5	-2.00	119.90	122.64

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	608	CLA	ND
25	A	611	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	501	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	404	CLA	ND
25	a	607	CLA	ND
25	a	609	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	610	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND

All (1717) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	602	CLA	C14-C13-C15-C16
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	C4-C3-C5-C6
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C4B-C3B-CAB-CBB
25	D	405	CLA	C2-C3-C5-C6
25	D	405	CLA	C4-C3-C5-C6
25	a	608	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	a	608	CLA	C4B-C3B-CAB-CBB
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	C6-C7-C8-C9
25	b	616	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	C2-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	c	509	CLA	C6-C7-C8-C9
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
26	D	406	BCR	C37-C22-C23-C24
26	K	102	BCR	C5-C6-C7-C8
26	K	102	BCR	C16-C17-C18-C36
26	K	102	BCR	C37-C22-C23-C24
26	T	101	BCR	C16-C17-C18-C36
26	b	617	BCR	C21-C22-C23-C24
26	c	514	BCR	C7-C8-C9-C10
26	k	102	BCR	C5-C6-C7-C8
26	t	101	BCR	C7-C8-C9-C34
27	A	610	PL9	C22-C23-C24-C26
27	A	610	PL9	C37-C38-C39-C40
27	D	407	PL9	C32-C33-C34-C36
27	a	611	PL9	C22-C23-C24-C25
27	a	611	PL9	C28-C29-C31-C32
27	a	611	PL9	C47-C48-C49-C50
27	d	406	PL9	C32-C33-C34-C36
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	518	LMG	C11-C10-O7-C8
28	D	411	LMG	O1-C7-C8-C9
28	D	411	LMG	O1-C7-C8-O7
28	D	411	LMG	C11-C10-O7-C8
28	b	624	LMG	C9-C8-O7-C10
28	c	520	LMG	C11-C10-O7-C8
28	c	522	LMG	C2-C1-O1-C7
28	c	522	LMG	O6-C1-O1-C7
29	A	613	LHG	O1-C1-C2-C3
29	A	613	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
29	B	622	LHG	O1-C1-C2-C3
29	B	622	LHG	C3-O3-P-O4
29	D	410	LHG	O2-C2-C3-O3
29	D	410	LHG	C3-O3-P-O4
29	D	410	LHG	C3-O3-P-O5
29	D	410	LHG	C3-O3-P-O6
29	D	410	LHG	C4-O6-P-O3
29	D	410	LHG	C4-O6-P-O4
29	E	101	LHG	C4-O6-P-O4
29	L	101	LHG	C3-O3-P-O4
29	L	101	LHG	C4-O6-P-O4
29	d	407	LHG	C3-O3-P-O5
29	d	407	LHG	C3-O3-P-O6
29	d	408	LHG	O1-C1-C2-C3
29	d	408	LHG	C3-O3-P-O4
29	d	408	LHG	C3-O3-P-O6
29	d	408	LHG	C4-O6-P-O3
29	d	408	LHG	C4-O6-P-O4
29	d	409	LHG	C4-O6-P-O4
29	e	101	LHG	O1-C1-C2-O2
29	e	101	LHG	O1-C1-C2-C3
29	e	101	LHG	C1-C2-C3-O3
29	e	101	LHG	C3-O3-P-O4
29	e	101	LHG	C3-O3-P-O6
29	l	101	LHG	C4-O6-P-O3
30	B	623	SQD	C2-C1-O6-C44
30	B	623	SQD	O5-C1-O6-C44
30	B	623	SQD	O6-C44-C45-O47
30	B	623	SQD	O49-C7-O47-C45
30	B	623	SQD	C8-C7-O47-C45
30	a	613	SQD	O6-C44-C45-O47
30	a	614	SQD	O49-C7-O47-C45
30	a	614	SQD	C8-C7-O47-C45
30	b	620	SQD	C8-C7-O47-C45
30	b	620	SQD	O10-C23-O48-C46
30	f	102	SQD	C2-C1-O6-C44
30	f	102	SQD	O5-C1-O6-C44
31	A	616	DGD	C2B-C1B-O2G-C2G
31	A	616	DGD	O1B-C1B-O2G-C2G
31	A	616	DGD	O2G-C2G-C3G-O3G
31	o	301	DGD	O1B-C1B-O2G-C2G
36	V	201	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	V	201	HEC	C4B-C3B-CAB-CBB
36	V	201	HEC	C2C-C3C-CAC-CBC
36	V	201	HEC	C4C-C3C-CAC-CBC
36	v	201	HEC	C2B-C3B-CAB-CBB
36	v	201	HEC	C2C-C3C-CAC-CBC
36	v	201	HEC	C4C-C3C-CAC-CBC
25	C	509	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	CBD-CGD-O2D-CED
28	c	520	LMG	O10-C28-O8-C9
29	e	101	LHG	O10-C23-O8-C6
27	D	407	PL9	C47-C48-C49-C51
27	a	611	PL9	C47-C48-C49-C51
25	C	509	CLA	O1D-CGD-O2D-CED
28	c	520	LMG	C29-C28-O8-C9
29	e	101	LHG	C24-C23-O8-C6
28	M	101	LMG	O10-C28-O8-C9
28	c	522	LMG	O10-C28-O8-C9
29	E	101	LHG	O10-C23-O8-C6
30	f	102	SQD	O10-C23-O48-C46
25	b	601	CLA	O1D-CGD-O2D-CED
28	D	411	LMG	O9-C10-O7-C8
28	b	624	LMG	O9-C10-O7-C8
28	c	520	LMG	O9-C10-O7-C8
30	b	620	SQD	O49-C7-O47-C45
27	D	407	PL9	C47-C48-C49-C50
25	B	616	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
28	c	522	LMG	C29-C28-O8-C9
29	E	101	LHG	C24-C23-O8-C6
30	b	620	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
25	A	608	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	C	513	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
27	A	610	PL9	C40-C39-C41-C42
27	A	610	PL9	C45-C44-C46-C47
27	a	611	PL9	C25-C24-C26-C27
25	A	608	CLA	C2-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	C2-C3-C5-C6
27	A	610	PL9	C23-C24-C26-C27
27	A	610	PL9	C43-C44-C46-C47
27	a	611	PL9	C23-C24-C26-C27
28	M	101	LMG	C29-C28-O8-C9
30	D	409	SQD	C24-C23-O48-C46
27	A	610	PL9	C22-C23-C24-C25
27	d	406	PL9	C32-C33-C34-C35
27	A	610	PL9	C37-C38-C39-C41
27	a	611	PL9	C22-C23-C24-C26
31	o	301	DGD	O1A-C1A-O1G-C1G
25	b	605	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	B	601	CLA	CBA-CGA-O2A-C1
28	c	520	LMG	C4-C5-C6-O5
28	c	522	LMG	C4-C5-C6-O5
25	C	513	CLA	CBD-CGD-O2D-CED
28	b	624	LMG	C11-C10-O7-C8
31	o	301	DGD	C2B-C1B-O2G-C2G
28	b	624	LMG	O6-C5-C6-O5
27	A	610	PL9	C47-C48-C49-C51
25	B	614	CLA	C2-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	B	601	CLA	O1A-CGA-O2A-C1
30	D	409	SQD	O10-C23-O48-C46
27	D	407	PL9	C44-C46-C47-C48
27	a	611	PL9	C24-C26-C27-C28
25	B	601	CLA	CBD-CGD-O2D-CED
25	C	501	CLA	CBD-CGD-O2D-CED
30	a	614	SQD	C24-C23-O48-C46
25	c	512	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
28	c	522	LMG	O6-C5-C6-O5
28	c	520	LMG	O6-C5-C6-O5
27	A	610	PL9	C12-C13-C14-C16
27	a	611	PL9	C27-C28-C29-C31
32	m	101	STE	C6-C7-C8-C9
30	a	614	SQD	O10-C23-O48-C46
31	o	301	DGD	C2A-C1A-O1G-C1G
27	A	610	PL9	C20-C19-C21-C22
27	A	610	PL9	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	C11-C10-C8-C9
25	B	611	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C10-C8-C9
25	C	502	CLA	C14-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	C	513	CLA	C11-C12-C13-C14
25	b	601	CLA	C14-C13-C15-C16
25	b	605	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C9
25	c	511	CLA	C14-C13-C15-C16
25	c	512	CLA	C6-C7-C8-C9
30	D	409	SQD	C2-C1-O6-C44
29	l	101	LHG	C7-C8-C9-C10
30	A	614	SQD	C23-C24-C25-C26
29	e	101	LHG	O2-C2-C3-O3
31	C	515	DGD	O6E-C5E-C6E-O5E
26	B	618	BCR	C7-C8-C9-C34
26	B	619	BCR	C37-C22-C23-C24
26	T	101	BCR	C11-C12-C13-C35
26	b	619	BCR	C37-C22-C23-C24
26	c	514	BCR	C7-C8-C9-C34
26	d	405	BCR	C37-C22-C23-C24
26	k	101	BCR	C11-C12-C13-C35
26	k	102	BCR	C7-C8-C9-C34
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
30	D	409	SQD	C45-C46-O48-C23
28	c	522	LMG	C10-C11-C12-C13
30	A	614	SQD	C7-C8-C9-C10
25	B	613	CLA	C8-C10-C11-C12
25	C	506	CLA	C8-C10-C11-C12
25	C	513	CLA	C15-C16-C17-C18
25	b	611	CLA	C13-C15-C16-C17
25	b	611	CLA	C15-C16-C17-C18
29	B	622	LHG	O1-C1-C2-O2
25	A	607	CLA	C15-C16-C17-C18
25	B	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	513	CLA	C6-C7-C8-C10
29	d	409	LHG	C24-C25-C26-C27
29	e	101	LHG	C23-C24-C25-C26
27	A	610	PL9	C34-C36-C37-C38
27	A	610	PL9	C39-C41-C42-C43
27	A	610	PL9	C44-C46-C47-C48
27	a	611	PL9	C39-C41-C42-C43
25	C	512	CLA	C5-C6-C7-C8
25	b	601	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17
28	D	411	LMG	C10-C11-C12-C13
29	d	407	LHG	C23-C24-C25-C26
29	d	409	LHG	C23-C24-C25-C26
31	c	515	DGD	C1B-C2B-C3B-C4B
31	c	517	DGD	O1A-C1A-O1G-C1G
25	c	506	CLA	CBA-CGA-O2A-C1
25	C	503	CLA	C5-C6-C7-C8
25	a	609	CLA	C5-C6-C7-C8
25	b	607	CLA	C10-C11-C12-C13
25	b	613	CLA	C10-C11-C12-C13
25	b	614	CLA	C5-C6-C7-C8
25	c	503	CLA	C8-C10-C11-C12
25	c	509	CLA	C13-C15-C16-C17
25	c	510	CLA	C10-C11-C12-C13
25	c	512	CLA	C2A-CAA-CBA-CGA
25	A	607	CLA	C10-C11-C12-C13
25	B	613	CLA	C5-C6-C7-C8
25	C	508	CLA	C15-C16-C17-C18
25	c	507	CLA	C5-C6-C7-C8
25	c	511	CLA	C13-C15-C16-C17
28	b	624	LMG	C10-C11-C12-C13
28	c	520	LMG	C10-C11-C12-C13
28	d	411	LMG	C28-C29-C30-C31
29	E	101	LHG	C23-C24-C25-C26
30	f	102	SQD	C23-C24-C25-C26
32	X	101	STE	C1-C2-C3-C4
28	b	624	LMG	O6-C1-O1-C7
29	E	101	LHG	C27-C28-C29-C30
30	a	613	SQD	C17-C18-C19-C20
25	B	607	CLA	C13-C15-C16-C17
25	C	506	CLA	C15-C16-C17-C18
25	C	509	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C10-C11-C12-C13
25	b	615	CLA	C10-C11-C12-C13
25	c	503	CLA	C5-C6-C7-C8
25	c	511	CLA	C15-C16-C17-C18
25	d	404	CLA	C10-C11-C12-C13
25	b	613	CLA	CBD-CGD-O2D-CED
28	b	622	LMG	C10-C11-C12-C13
28	c	522	LMG	C28-C29-C30-C31
25	D	405	CLA	C13-C15-C16-C17
25	b	615	CLA	C13-C15-C16-C17
25	c	512	CLA	C13-C15-C16-C17
28	b	624	LMG	C4-C5-C6-O5
25	B	608	CLA	C3-C5-C6-C7
25	C	509	CLA	C13-C15-C16-C17
25	C	510	CLA	C10-C11-C12-C13
25	C	512	CLA	CBD-CGD-O2D-CED
27	D	407	PL9	C33-C34-C36-C37
31	H	102	DGD	C1B-C2B-C3B-C4B
32	C	519	STE	C4-C5-C6-C7
25	B	601	CLA	C5-C6-C7-C8
25	B	602	CLA	C8-C10-C11-C12
25	B	604	CLA	C15-C16-C17-C18
25	a	608	CLA	C8-C10-C11-C12
25	b	603	CLA	C5-C6-C7-C8
25	B	616	CLA	C5-C6-C7-C8
25	c	510	CLA	C5-C6-C7-C8
25	c	506	CLA	O1A-CGA-O2A-C1
28	C	518	LMG	O9-C10-O7-C8
29	D	410	LHG	C1-C2-C3-O3
25	a	609	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	B	601	CLA	C13-C15-C16-C17
25	B	606	CLA	C8-C10-C11-C12
25	B	607	CLA	C5-C6-C7-C8
25	b	609	CLA	C15-C16-C17-C18
25	c	509	CLA	C10-C11-C12-C13
31	c	515	DGD	O6E-C5E-C6E-O5E
25	B	601	CLA	C15-C16-C17-C18
25	c	506	CLA	C8-C10-C11-C12
25	B	615	CLA	C13-C15-C16-C17
25	b	607	CLA	C8-C10-C11-C12
25	b	613	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	C	518	LMG	C29-C28-O8-C9
30	a	613	SQD	C7-C8-C9-C10
25	B	613	CLA	C4-C3-C5-C6
27	A	610	PL9	C38-C39-C41-C42
25	b	605	CLA	C10-C11-C12-C13
25	D	405	CLA	C11-C12-C13-C14
28	b	624	LMG	C2-C1-O1-C7
31	C	516	DGD	C2E-C1E-O5D-C6D
31	c	516	DGD	C2E-C1E-O5D-C6D
25	C	505	CLA	C10-C11-C12-C13
27	A	610	PL9	C9-C11-C12-C13
29	d	407	LHG	O2-C2-C3-O3
30	B	623	SQD	C11-C10-C9-C8
26	A	609	BCR	C11-C10-C9-C34
26	D	406	BCR	C20-C21-C22-C37
26	H	101	BCR	C16-C17-C18-C36
26	b	617	BCR	C20-C21-C22-C37
26	k	101	BCR	C11-C10-C9-C34
26	k	102	BCR	C20-C21-C22-C37
26	k	103	BCR	C20-C21-C22-C37
25	C	513	CLA	O1D-CGD-O2D-CED
26	B	619	BCR	C11-C12-C13-C35
26	Z	101	BCR	C37-C22-C23-C24
26	c	514	BCR	C11-C12-C13-C35
25	B	606	CLA	C15-C16-C17-C18
29	d	407	LHG	O1-C1-C2-C3
29	d	409	LHG	O1-C1-C2-C3
29	l	101	LHG	C23-C24-C25-C26
30	D	409	SQD	C23-C24-C25-C26
28	D	411	LMG	C9-C8-O7-C10
30	b	620	SQD	C46-C45-O47-C7
25	A	607	CLA	C16-C17-C18-C20
25	B	603	CLA	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
26	B	619	BCR	C12-C13-C14-C15
26	K	102	BCR	C16-C17-C18-C19
26	T	101	BCR	C12-C13-C14-C15
26	k	101	BCR	C12-C13-C14-C15
26	k	102	BCR	C20-C21-C22-C23
26	t	101	BCR	C12-C13-C14-C15
26	x	101	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	C	516	DGD	O6E-C1E-O5D-C6D
31	c	516	DGD	O6E-C1E-O5D-C6D
25	B	601	CLA	C8-C10-C11-C12
25	B	601	CLA	O1D-CGD-O2D-CED
31	A	616	DGD	C1B-C2B-C3B-C4B
32	b	625	STE	C1-C2-C3-C4
25	c	506	CLA	C2-C1-O2A-CGA
25	B	601	CLA	C16-C17-C18-C20
25	B	603	CLA	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C20
25	B	611	CLA	C16-C17-C18-C20
25	C	502	CLA	C16-C17-C18-C19
25	C	509	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C20
25	C	511	CLA	C8-C10-C11-C12
25	c	512	CLA	O1D-CGD-O2D-CED
29	A	613	LHG	C25-C26-C27-C28
29	B	622	LHG	C9-C10-C11-C12
29	L	101	LHG	C18-C19-C20-C21
30	f	102	SQD	C28-C29-C30-C31
31	h	101	DGD	C2B-C3B-C4B-C5B
32	b	625	STE	C3-C4-C5-C6
28	C	518	LMG	C12-C13-C14-C15
28	M	101	LMG	C29-C30-C31-C32
28	b	624	LMG	C31-C32-C33-C34
28	c	518	LMG	C31-C32-C33-C34
29	d	408	LHG	C26-C27-C28-C29
30	B	623	SQD	C13-C14-C15-C16
30	f	102	SQD	C29-C30-C31-C32
31	C	515	DGD	C5A-C6A-C7A-C8A
31	C	516	DGD	C4A-C5A-C6A-C7A
29	E	101	LHG	C28-C29-C30-C31
29	d	409	LHG	C26-C27-C28-C29
30	A	615	SQD	C11-C12-C13-C14
30	a	614	SQD	C10-C11-C12-C13
31	C	515	DGD	CAB-CBB-CCB-CDB
31	h	101	DGD	C5B-C6B-C7B-C8B
32	T	103	STE	C7-C8-C9-C10
32	a	615	STE	C4-C5-C6-C7
28	D	408	LMG	C16-C17-C18-C19
28	D	408	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
28	D	411	LMG	C12-C13-C14-C15
29	B	622	LHG	C29-C30-C31-C32
29	d	408	LHG	C28-C29-C30-C31
30	A	614	SQD	C30-C31-C32-C33
30	a	614	SQD	C11-C12-C13-C14
30	f	102	SQD	C25-C26-C27-C28
31	A	616	DGD	C7A-C8A-C9A-CAA
31	C	517	DGD	C7B-C8B-C9B-CAB
31	C	517	DGD	CBB-CCB-CDB-CEB
31	c	516	DGD	C7A-C8A-C9A-CAA
31	o	301	DGD	C4A-C5A-C6A-C7A
31	o	301	DGD	C2B-C3B-C4B-C5B
32	X	101	STE	C11-C12-C13-C14
32	b	621	STE	C11-C10-C9-C8
32	c	519	STE	C2-C3-C4-C5
32	t	102	STE	C6-C7-C8-C9
29	A	613	LHG	O1-C1-C2-O2
29	d	408	LHG	O1-C1-C2-O2
29	E	101	LHG	C18-C19-C20-C21
29	e	101	LHG	C14-C15-C16-C17
31	A	616	DGD	CCA-CDA-CEA-CFA
31	H	102	DGD	CCA-CDA-CEA-CFA
31	h	101	DGD	C6B-C7B-C8B-C9B
32	B	626	STE	C2-C3-C4-C5
32	c	519	STE	C11-C12-C13-C14
25	b	610	CLA	C4B-C3B-CAB-CBB
28	b	622	LMG	C11-C12-C13-C14
32	B	624	STE	C2-C3-C4-C5
32	H	103	STE	C5-C6-C7-C8
32	b	626	STE	C3-C4-C5-C6
25	C	502	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C19
25	b	607	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
30	a	614	SQD	C12-C13-C14-C15
32	j	101	STE	C4-C5-C6-C7
25	C	505	CLA	C5-C6-C7-C8
25	b	614	CLA	C10-C11-C12-C13
29	e	101	LHG	C8-C7-O7-C5
28	D	411	LMG	C11-C12-C13-C14
29	A	613	LHG	C9-C10-C11-C12
29	L	101	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	a	613	SQD	C30-C31-C32-C33
31	A	616	DGD	C4A-C5A-C6A-C7A
25	C	513	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C15
29	e	101	LHG	C16-C17-C18-C19
30	D	409	SQD	C30-C31-C32-C33
31	A	616	DGD	C6B-C7B-C8B-C9B
31	C	517	DGD	C6A-C7A-C8A-C9A
32	B	620	STE	C3-C4-C5-C6
32	B	627	STE	C11-C12-C13-C14
28	c	518	LMG	C28-C29-C30-C31
25	B	606	CLA	C13-C15-C16-C17
28	b	622	LMG	C38-C39-C40-C41
28	c	522	LMG	C12-C13-C14-C15
29	E	101	LHG	C24-C25-C26-C27
29	L	101	LHG	C27-C28-C29-C30
29	d	408	LHG	C32-C33-C34-C35
30	B	623	SQD	C33-C34-C35-C36
31	o	301	DGD	C5A-C6A-C7A-C8A
32	T	102	STE	C11-C12-C13-C14
25	a	609	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	C3A-C2A-CAA-CBA
28	b	624	LMG	C16-C17-C18-C19
28	c	522	LMG	C38-C39-C40-C41
30	A	615	SQD	C15-C16-C17-C18
30	D	409	SQD	C27-C28-C29-C30
30	f	102	SQD	C26-C27-C28-C29
28	c	518	LMG	C36-C37-C38-C39
29	A	613	LHG	C33-C34-C35-C36
31	c	516	DGD	CBA-CCA-CDA-CEA
32	I	101	STE	C11-C10-C9-C8
25	C	501	CLA	O1D-CGD-O2D-CED
29	e	101	LHG	C7-C8-C9-C10
32	c	519	STE	C12-C13-C14-C15
28	A	612	LMG	C16-C17-C18-C19
28	D	408	LMG	C17-C18-C19-C20
29	d	408	LHG	C33-C34-C35-C36
30	a	613	SQD	C11-C12-C13-C14
31	c	517	DGD	CBA-CCA-CDA-CEA
31	h	101	DGD	C8A-C9A-CAA-CBA
32	B	625	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	f	102	SQD	C32-C33-C34-C35
32	b	623	STE	C13-C14-C15-C16
28	b	622	LMG	C29-C28-O8-C9
28	c	520	LMG	O1-C7-C8-C9
28	M	101	LMG	C39-C40-C41-C42
28	d	410	LMG	C39-C40-C41-C42
29	D	410	LHG	C14-C15-C16-C17
31	C	516	DGD	CBB-CCB-CDB-CEB
32	C	521	STE	C4-C5-C6-C7
32	T	102	STE	C11-C10-C9-C8
32	b	623	STE	C14-C15-C16-C17
32	b	625	STE	C11-C10-C9-C8
28	A	612	LMG	C37-C38-C39-C40
28	D	408	LMG	C36-C37-C38-C39
28	M	101	LMG	C14-C15-C16-C17
28	b	624	LMG	C13-C14-C15-C16
28	d	410	LMG	C31-C32-C33-C34
28	d	411	LMG	C13-C14-C15-C16
29	A	613	LHG	C11-C12-C13-C14
29	A	613	LHG	C34-C35-C36-C37
29	D	410	LHG	C11-C12-C13-C14
31	A	616	DGD	C5B-C6B-C7B-C8B
32	E	102	STE	C3-C4-C5-C6
32	E	102	STE	C4-C5-C6-C7
28	c	522	LMG	C14-C15-C16-C17
29	E	101	LHG	C33-C34-C35-C36
31	c	517	DGD	C6A-C7A-C8A-C9A
32	b	623	STE	C5-C6-C7-C8
32	C	520	STE	C5-C6-C7-C8
25	B	615	CLA	C5-C6-C7-C8
28	D	408	LMG	C31-C32-C33-C34
28	c	520	LMG	C31-C32-C33-C34
28	c	522	LMG	C33-C34-C35-C36
29	A	613	LHG	C29-C30-C31-C32
30	A	614	SQD	C11-C12-C13-C14
31	C	517	DGD	C5A-C6A-C7A-C8A
31	c	515	DGD	C5A-C6A-C7A-C8A
25	A	607	CLA	C16-C17-C18-C19
25	C	509	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C20
31	c	516	DGD	C1A-C2A-C3A-C4A
25	A	607	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	D	406	BCR	C23-C24-C25-C26
26	D	406	BCR	C23-C24-C25-C30
26	K	102	BCR	C1-C6-C7-C8
26	k	102	BCR	C1-C6-C7-C8
26	t	101	BCR	C1-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
28	b	622	LMG	C30-C31-C32-C33
28	c	518	LMG	C33-C34-C35-C36
28	c	520	LMG	C30-C31-C32-C33
29	d	408	LHG	C12-C13-C14-C15
31	c	515	DGD	C7A-C8A-C9A-CAA
25	B	603	CLA	C13-C15-C16-C17
25	c	503	CLA	C15-C16-C17-C18
31	C	517	DGD	CAB-CBB-CCB-CDB
25	c	513	CLA	O1D-CGD-O2D-CED
28	d	411	LMG	C36-C37-C38-C39
29	A	613	LHG	C10-C11-C12-C13
31	A	616	DGD	C4B-C5B-C6B-C7B
31	c	517	DGD	C2A-C3A-C4A-C5A
32	M	102	STE	C11-C10-C9-C8
32	c	519	STE	C6-C7-C8-C9
32	d	413	STE	C14-C15-C16-C17
32	d	413	STE	C1-C2-C3-C4
25	a	607	CLA	C15-C16-C17-C18
25	C	504	CLA	C11-C12-C13-C14
29	D	410	LHG	C10-C11-C12-C13
27	d	406	PL9	C4-C3-C7-C8
29	d	407	LHG	C17-C18-C19-C20
31	c	515	DGD	C4B-C5B-C6B-C7B
32	a	615	STE	C5-C6-C7-C8
25	c	504	CLA	C4-C3-C5-C6
28	c	518	LMG	C38-C39-C40-C41
31	A	616	DGD	C9A-CAA-CBA-CCA
31	A	616	DGD	C2B-C3B-C4B-C5B
31	o	301	DGD	C3B-C4B-C5B-C6B
31	o	301	DGD	C6B-C7B-C8B-C9B
32	B	620	STE	C9-C10-C11-C12
32	B	625	STE	C6-C7-C8-C9
25	c	512	CLA	C5-C6-C7-C8
25	c	504	CLA	C2-C3-C5-C6
27	A	610	PL9	C33-C34-C36-C37
28	C	518	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	M	101	LMG	C13-C14-C15-C16
29	d	408	LHG	C14-C15-C16-C17
29	e	101	LHG	C24-C25-C26-C27
30	A	615	SQD	C29-C30-C31-C32
31	c	515	DGD	C6A-C7A-C8A-C9A
31	c	517	DGD	C4A-C5A-C6A-C7A
32	B	627	STE	C11-C10-C9-C8
32	l	102	STE	C3-C4-C5-C6
30	a	613	SQD	C23-C24-C25-C26
30	B	623	SQD	C24-C23-O48-C46
25	d	404	CLA	C6-C7-C8-C9
28	C	518	LMG	C17-C18-C19-C20
29	e	101	LHG	C27-C28-C29-C30
30	b	620	SQD	C29-C30-C31-C32
31	H	102	DGD	C7B-C8B-C9B-CAB
32	d	413	STE	C12-C13-C14-C15
29	E	101	LHG	C11-C10-C9-C8
29	L	101	LHG	C10-C11-C12-C13
30	b	620	SQD	C26-C27-C28-C29
32	a	615	STE	C2-C3-C4-C5
28	C	518	LMG	O6-C1-O1-C7
28	M	101	LMG	C31-C32-C33-C34
31	c	517	DGD	C5B-C6B-C7B-C8B
32	C	520	STE	C3-C4-C5-C6
28	d	410	LMG	C37-C38-C39-C40
32	X	101	STE	C5-C6-C7-C8
32	b	621	STE	C14-C15-C16-C17
29	B	622	LHG	C23-C24-C25-C26
28	C	518	LMG	C32-C33-C34-C35
31	C	515	DGD	C2A-C3A-C4A-C5A
28	d	410	LMG	C33-C34-C35-C36
30	A	614	SQD	C26-C27-C28-C29
30	a	613	SQD	C12-C13-C14-C15
31	A	616	DGD	CEB-CFB-CGB-CHB
31	C	516	DGD	CAA-CBA-CCA-CDA
31	H	102	DGD	C6B-C7B-C8B-C9B
30	f	102	SQD	C8-C7-O47-C45
30	A	615	SQD	C19-C20-C21-C22
32	H	103	STE	C3-C4-C5-C6
32	l	102	STE	C14-C15-C16-C17
30	f	102	SQD	O49-C7-O47-C45
29	E	101	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	T	102	STE	C12-C13-C14-C15
29	d	408	LHG	C29-C30-C31-C32
31	h	101	DGD	C3B-C4B-C5B-C6B
25	b	605	CLA	C15-C16-C17-C18
26	x	101	BCR	C7-C8-C9-C34
29	D	410	LHG	C9-C10-C11-C12
28	b	622	LMG	C12-C13-C14-C15
28	b	622	LMG	C36-C37-C38-C39
30	D	409	SQD	C29-C30-C31-C32
25	B	616	CLA	CBA-CGA-O2A-C1
28	b	624	LMG	C32-C33-C34-C35
29	D	410	LHG	C33-C34-C35-C36
31	c	515	DGD	C6B-C7B-C8B-C9B
31	o	301	DGD	C6A-C7A-C8A-C9A
25	B	601	CLA	C16-C17-C18-C19
25	B	612	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C19
29	l	101	LHG	C24-C25-C26-C27
29	l	101	LHG	C28-C29-C30-C31
25	B	613	CLA	C2-C3-C5-C6
28	d	410	LMG	C32-C33-C34-C35
31	c	517	DGD	C4B-C5B-C6B-C7B
32	d	413	STE	C10-C11-C12-C13
25	b	603	CLA	C10-C11-C12-C13
29	d	407	LHG	C25-C26-C27-C28
32	b	623	STE	C4-C5-C6-C7
28	M	101	LMG	O6-C5-C6-O5
25	c	509	CLA	C5-C6-C7-C8
30	a	613	SQD	C32-C33-C34-C35
28	C	518	LMG	C28-C29-C30-C31
28	D	411	LMG	C28-C29-C30-C31
30	A	615	SQD	C7-C8-C9-C10
31	c	516	DGD	C1B-C2B-C3B-C4B
28	C	518	LMG	C30-C31-C32-C33
29	E	101	LHG	C29-C30-C31-C32
30	A	614	SQD	C11-C10-C9-C8
28	A	612	LMG	C39-C40-C41-C42
28	c	522	LMG	C32-C33-C34-C35
29	d	407	LHG	C12-C13-C14-C15
25	A	611	CLA	C13-C15-C16-C17
25	B	607	CLA	C15-C16-C17-C18
28	A	612	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	d	407	LHG	C16-C17-C18-C19
32	T	103	STE	C9-C10-C11-C12
30	A	614	SQD	C24-C25-C26-C27
32	X	101	STE	C11-C10-C9-C8
28	A	612	LMG	C36-C37-C38-C39
28	c	518	LMG	O6-C5-C6-O5
28	A	612	LMG	O1-C7-C8-O7
30	a	614	SQD	O47-C45-C46-O48
31	A	616	DGD	O1G-C1G-C2G-O2G
28	C	518	LMG	C31-C32-C33-C34
32	E	102	STE	C6-C7-C8-C9
32	d	412	STE	C11-C12-C13-C14
28	D	408	LMG	C14-C15-C16-C17
31	C	516	DGD	C4B-C5B-C6B-C7B
31	c	517	DGD	C5A-C6A-C7A-C8A
25	B	601	CLA	C10-C11-C12-C13
25	c	511	CLA	C8-C10-C11-C12
28	c	520	LMG	C11-C12-C13-C14
28	c	522	LMG	C19-C20-C21-C22
32	M	102	STE	C7-C8-C9-C10
32	X	101	STE	C10-C11-C12-C13
31	h	101	DGD	CBA-CCA-CDA-CEA
29	B	622	LHG	C28-C29-C30-C31
31	c	517	DGD	C3A-C4A-C5A-C6A
32	T	102	STE	C5-C6-C7-C8
32	X	101	STE	C12-C13-C14-C15
32	b	621	STE	C5-C6-C7-C8
25	C	505	CLA	C4-C3-C5-C6
25	C	506	CLA	C4-C3-C5-C6
29	d	407	LHG	C1-C2-C3-O3
28	d	410	LMG	C35-C36-C37-C38
29	d	409	LHG	C29-C30-C31-C32
30	A	614	SQD	C16-C17-C18-C19
32	b	621	STE	C13-C14-C15-C16
32	d	412	STE	C3-C4-C5-C6
25	C	508	CLA	CBD-CGD-O2D-CED
28	b	624	LMG	C18-C19-C20-C21
28	d	410	LMG	C34-C35-C36-C37
29	D	410	LHG	C15-C16-C17-C18
30	A	615	SQD	C32-C33-C34-C35
31	c	516	DGD	C8A-C9A-CAA-CBA
32	J	101	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	B	623	SQD	C34-C35-C36-C37
32	B	625	STE	C11-C12-C13-C14
32	c	521	STE	C5-C6-C7-C8
28	D	408	LMG	C37-C38-C39-C40
28	d	411	LMG	C38-C39-C40-C41
29	d	407	LHG	C28-C29-C30-C31
25	A	611	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C19
29	d	407	LHG	O1-C1-C2-O2
25	B	616	CLA	O1A-CGA-O2A-C1
30	B	623	SQD	O10-C23-O48-C46
25	b	602	CLA	C3-C5-C6-C7
28	c	522	LMG	C17-C18-C19-C20
25	b	601	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	B	607	CLA	C8-C10-C11-C12
28	B	621	LMG	C33-C34-C35-C36
30	a	613	SQD	C28-C29-C30-C31
31	C	516	DGD	C9B-CAB-CBB-CCB
32	B	620	STE	C11-C12-C13-C14
25	C	512	CLA	O1D-CGD-O2D-CED
31	C	515	DGD	C4B-C5B-C6B-C7B
32	T	102	STE	C13-C14-C15-C16
32	d	413	STE	C3-C4-C5-C6
28	d	410	LMG	C36-C37-C38-C39
28	d	410	LMG	C38-C39-C40-C41
29	B	622	LHG	C27-C28-C29-C30
31	H	102	DGD	C3A-C4A-C5A-C6A
32	C	521	STE	C11-C10-C9-C8
25	C	507	CLA	C10-C11-C12-C13
29	e	101	LHG	O9-C7-O7-C5
28	b	624	LMG	C39-C40-C41-C42
32	b	625	STE	C6-C7-C8-C9
25	B	602	CLA	C12-C13-C15-C16
25	B	604	CLA	C11-C12-C13-C15
25	B	611	CLA	C11-C12-C13-C15
25	C	505	CLA	C12-C13-C15-C16
25	C	506	CLA	C11-C12-C13-C15
25	C	506	CLA	C12-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C7
25	C	512	CLA	C6-C7-C8-C10
25	C	513	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	a	609	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C12-C13-C15
25	b	606	CLA	C12-C13-C15-C16
25	b	614	CLA	C12-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	510	CLA	C11-C12-C13-C15
25	d	403	CLA	C11-C12-C13-C15
30	B	623	SQD	C30-C31-C32-C33
32	b	626	STE	C5-C6-C7-C8
28	d	411	LMG	O6-C5-C6-O5
32	c	519	STE	C1-C2-C3-C4
31	C	516	DGD	C2B-C3B-C4B-C5B
32	d	412	STE	C5-C6-C7-C8
27	d	406	PL9	C28-C29-C31-C32
31	C	516	DGD	C3B-C4B-C5B-C6B
31	o	301	DGD	C7A-C8A-C9A-CAA
25	C	513	CLA	C8-C10-C11-C12
25	B	604	CLA	C11-C12-C13-C14
25	C	506	CLA	C14-C13-C15-C16
25	b	603	CLA	C11-C10-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	605	CLA	C6-C7-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	b	608	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	d	404	CLA	C11-C12-C13-C14
29	d	408	LHG	C30-C31-C32-C33
30	b	620	SQD	C28-C29-C30-C31
25	b	615	CLA	C16-C17-C18-C20
30	a	613	SQD	C24-C23-O48-C46
25	c	505	CLA	C5-C6-C7-C8
29	E	101	LHG	C32-C33-C34-C35
30	f	102	SQD	C24-C25-C26-C27
28	D	411	LMG	C7-C8-C9-O8
29	E	101	LHG	C4-C5-C6-O8
29	e	101	LHG	C4-C5-C6-O8
30	a	613	SQD	O6-C44-C45-C46
31	A	616	DGD	C1G-C2G-C3G-O3G
29	d	407	LHG	C11-C12-C13-C14
30	B	623	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	D	409	SQD	C25-C26-C27-C28
30	a	614	SQD	C16-C17-C18-C19
31	C	517	DGD	C3A-C4A-C5A-C6A
31	c	517	DGD	CCA-CDA-CEA-CFA
31	c	515	DGD	C3B-C4B-C5B-C6B
30	a	614	SQD	C18-C19-C20-C21
31	C	515	DGD	C9B-CAB-CBB-CCB
32	B	620	STE	C6-C7-C8-C9
28	D	408	LMG	O6-C5-C6-O5
28	b	622	LMG	C15-C16-C17-C18
27	A	610	PL9	C47-C48-C49-C50
26	B	617	BCR	C35-C13-C14-C15
25	B	605	CLA	C15-C16-C17-C18
25	B	611	CLA	C8-C10-C11-C12
25	C	506	CLA	C10-C11-C12-C13
25	C	512	CLA	C3-C5-C6-C7
28	M	101	LMG	C28-C29-C30-C31
30	B	623	SQD	C26-C27-C28-C29
32	C	521	STE	C7-C8-C9-C10
32	X	101	STE	C7-C8-C9-C10
25	C	505	CLA	C2-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
29	l	101	LHG	C32-C33-C34-C35
26	C	514	BCR	C7-C8-C9-C34
31	c	515	DGD	C5B-C6B-C7B-C8B
30	D	409	SQD	C28-C29-C30-C31
31	A	616	DGD	C7B-C8B-C9B-CAB
25	b	611	CLA	C8-C10-C11-C12
25	c	509	CLA	C8-C10-C11-C12
31	C	516	DGD	C6B-C7B-C8B-C9B
32	T	102	STE	C9-C10-C11-C12
28	C	518	LMG	C37-C38-C39-C40
29	L	101	LHG	C30-C31-C32-C33
30	a	613	SQD	C9-C10-C11-C12
30	a	614	SQD	C29-C30-C31-C32
31	c	517	DGD	C7B-C8B-C9B-CAB
28	c	520	LMG	C41-C42-C43-C44
30	A	615	SQD	C17-C18-C19-C20
30	a	613	SQD	C24-C25-C26-C27
30	b	620	SQD	C25-C26-C27-C28
31	c	517	DGD	C6B-C7B-C8B-C9B
26	B	619	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	k	101	BCR	C10-C11-C12-C13
25	A	606	CLA	C15-C16-C17-C18
25	B	608	CLA	C13-C15-C16-C17
25	C	502	CLA	C15-C16-C17-C18
30	A	614	SQD	C13-C14-C15-C16
31	H	102	DGD	C9A-CAA-CBA-CCA
26	k	101	BCR	C13-C14-C15-C16
32	B	625	STE	C12-C13-C14-C15
30	A	614	SQD	C27-C28-C29-C30
32	t	102	STE	C3-C4-C5-C6
26	T	101	BCR	C16-C17-C18-C19
28	D	408	LMG	C12-C13-C14-C15
30	a	614	SQD	C11-C10-C9-C8
30	A	615	SQD	C14-C15-C16-C17
32	B	625	STE	C13-C14-C15-C16
28	M	101	LMG	C38-C39-C40-C41
31	A	616	DGD	C5A-C6A-C7A-C8A
31	C	516	DGD	C6A-C7A-C8A-C9A
31	c	515	DGD	CCB-CDB-CEB-CFB
32	H	103	STE	C11-C10-C9-C8
25	b	609	CLA	C2-C3-C5-C6
29	A	613	LHG	C35-C36-C37-C38
29	L	101	LHG	C19-C20-C21-C22
32	m	101	STE	C5-C6-C7-C8
29	e	101	LHG	C13-C14-C15-C16
29	l	101	LHG	C26-C27-C28-C29
30	a	613	SQD	C25-C26-C27-C28
31	h	101	DGD	C7A-C8A-C9A-CAA
32	T	102	STE	C10-C11-C12-C13
31	c	515	DGD	O6D-C5D-C6D-O5D
31	c	516	DGD	C3A-C4A-C5A-C6A
32	J	101	STE	C3-C4-C5-C6
28	c	520	LMG	O1-C7-C8-O7
32	b	626	STE	C7-C8-C9-C10
29	A	613	LHG	C30-C31-C32-C33
28	D	411	LMG	C31-C32-C33-C34
28	b	624	LMG	C17-C18-C19-C20
30	a	613	SQD	C10-C11-C12-C13
31	C	516	DGD	C8A-C9A-CAA-CBA
32	c	521	STE	C2-C3-C4-C5
31	h	101	DGD	O2G-C1B-C2B-C3B
29	A	613	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	d	412	STE	C10-C11-C12-C13
31	o	301	DGD	CBA-CCA-CDA-CEA
25	c	506	CLA	C16-C17-C18-C20
31	o	301	DGD	CFA-CGA-CHA-CIA
25	B	604	CLA	O1D-CGD-O2D-CED
28	D	408	LMG	C34-C35-C36-C37
27	D	407	PL9	C22-C23-C24-C25
27	d	406	PL9	C42-C43-C44-C45
29	D	410	LHG	C25-C26-C27-C28
29	d	409	LHG	C27-C28-C29-C30
32	H	103	STE	C10-C11-C12-C13
25	a	609	CLA	C10-C11-C12-C13
28	d	411	LMG	C35-C36-C37-C38
29	d	409	LHG	C30-C31-C32-C33
31	c	515	DGD	C4A-C5A-C6A-C7A
25	b	613	CLA	O1D-CGD-O2D-CED
25	B	602	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C20
31	C	516	DGD	C8B-C9B-CAB-CBB
25	b	609	CLA	C4-C3-C5-C6
30	a	613	SQD	C29-C30-C31-C32
31	c	517	DGD	C2A-C1A-O1G-C1G
34	d	402	PHO	C2C-C3C-CAC-CBC
28	A	612	LMG	C35-C36-C37-C38
32	b	623	STE	C10-C11-C12-C13
28	c	522	LMG	C13-C14-C15-C16
32	H	103	STE	C11-C12-C13-C14
32	M	102	STE	C6-C7-C8-C9
32	t	103	STE	C4-C5-C6-C7
25	B	604	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	C	506	CLA	C11-C12-C13-C14
25	a	608	CLA	C14-C13-C15-C16
25	a	609	CLA	C14-C13-C15-C16
25	b	602	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C10-C8-C9
25	b	614	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
25	c	509	CLA	C11-C12-C13-C14
25	d	403	CLA	C11-C12-C13-C14
30	f	102	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	M	103	STE	C5-C6-C7-C8
25	c	510	CLA	C15-C16-C17-C18
25	b	601	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
28	b	622	LMG	C17-C18-C19-C20
29	E	101	LHG	C12-C13-C14-C15
31	c	516	DGD	CCB-CDB-CEB-CFB
28	b	624	LMG	C15-C16-C17-C18
30	a	613	SQD	C26-C27-C28-C29
25	c	505	CLA	C10-C11-C12-C13
25	B	609	CLA	C16-C17-C18-C19
30	A	614	SQD	C17-C18-C19-C20
25	C	501	CLA	C2A-CAA-CBA-CGA
28	d	411	LMG	C30-C31-C32-C33
31	H	102	DGD	C6A-C7A-C8A-C9A
32	a	615	STE	C3-C4-C5-C6
30	A	614	SQD	C10-C11-C12-C13
31	C	515	DGD	CBB-CCB-CDB-CEB
31	H	102	DGD	C4B-C5B-C6B-C7B
29	l	101	LHG	O6-C4-C5-C6
28	D	408	LMG	C35-C36-C37-C38
30	A	615	SQD	C16-C17-C18-C19
30	B	623	SQD	C28-C29-C30-C31
30	a	613	SQD	C11-C10-C9-C8
32	B	625	STE	C4-C5-C6-C7
32	E	102	STE	C7-C8-C9-C10
32	H	103	STE	C1-C2-C3-C4
25	B	604	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C7
25	B	605	CLA	C12-C13-C15-C16
25	B	608	CLA	C6-C7-C8-C10
25	B	614	CLA	C12-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C10
25	C	509	CLA	C12-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C15
25	a	608	CLA	C11-C10-C8-C7
25	a	608	CLA	C12-C13-C15-C16
25	b	602	CLA	C6-C7-C8-C10
25	b	603	CLA	C11-C10-C8-C7
25	b	605	CLA	C6-C7-C8-C10
25	b	605	CLA	C11-C10-C8-C7
25	b	607	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	b	607	CLA	C11-C12-C13-C15
25	b	608	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C10-C8-C7
25	c	505	CLA	C6-C7-C8-C10
28	c	518	LMG	C11-C10-O7-C8
27	a	611	PL9	C15-C14-C16-C17
25	b	601	CLA	C10-C11-C12-C13
31	C	515	DGD	O6D-C5D-C6D-O5D
32	B	627	STE	C3-C4-C5-C6
29	L	101	LHG	C16-C17-C18-C19
31	c	515	DGD	C2B-C3B-C4B-C5B
28	A	612	LMG	C34-C35-C36-C37
30	a	613	SQD	O10-C23-O48-C46
26	k	103	BCR	C19-C20-C21-C22
32	C	520	STE	C6-C7-C8-C9
32	l	102	STE	C13-C14-C15-C16
31	c	517	DGD	CDA-CEA-CFA-CGA
31	A	616	DGD	CFA-CGA-CHA-CIA
25	b	607	CLA	CBA-CGA-O2A-C1
29	D	410	LHG	C13-C14-C15-C16
28	A	612	LMG	O1-C7-C8-C9
28	C	518	LMG	O1-C7-C8-C9
28	M	101	LMG	C7-C8-C9-O8
28	c	522	LMG	C7-C8-C9-O8
30	a	614	SQD	C44-C45-C46-O48
25	c	501	CLA	CBD-CGD-O2D-CED
32	T	102	STE	C6-C7-C8-C9
28	c	518	LMG	C40-C41-C42-C43
25	B	608	CLA	C16-C17-C18-C19
25	B	612	CLA	C16-C17-C18-C19
25	c	507	CLA	C8-C10-C11-C12
32	l	102	STE	C15-C16-C17-C18
29	B	622	LHG	C18-C19-C20-C21
31	c	515	DGD	CAB-CBB-CCB-CDB
32	M	102	STE	C3-C4-C5-C6
25	B	605	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
31	A	616	DGD	CBB-CCB-CDB-CEB
25	B	602	CLA	C16-C17-C18-C20
25	B	608	CLA	C16-C17-C18-C20
25	b	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	e	101	LHG	O6-C4-C5-O7
29	l	101	LHG	O6-C4-C5-O7
28	c	518	LMG	C35-C36-C37-C38
31	h	101	DGD	CAB-CBB-CCB-CDB
26	b	617	BCR	C1-C6-C7-C8
31	C	515	DGD	O1G-C1A-C2A-C3A
25	a	609	CLA	C13-C15-C16-C17
28	b	622	LMG	C21-C22-C23-C24
31	c	517	DGD	C9B-CAB-CBB-CCB
29	B	622	LHG	C25-C26-C27-C28
29	e	101	LHG	C11-C10-C9-C8
30	a	614	SQD	C9-C10-C11-C12
25	A	611	CLA	C15-C16-C17-C18
25	B	612	CLA	C10-C11-C12-C13
28	c	520	LMG	C33-C34-C35-C36
29	L	101	LHG	C12-C13-C14-C15
31	h	101	DGD	CAA-CBA-CCA-CDA
32	t	102	STE	C11-C10-C9-C8
29	A	613	LHG	C11-C10-C9-C8
25	A	611	CLA	C16-C17-C18-C19
25	c	505	CLA	C15-C16-C17-C18
28	C	518	LMG	O1-C7-C8-O7
28	M	101	LMG	O7-C8-C9-O8
28	b	624	LMG	O1-C7-C8-O7
28	c	522	LMG	O7-C8-C9-O8
29	e	101	LHG	O7-C5-C6-O8
30	A	614	SQD	O6-C44-C45-O47
27	A	610	PL9	C4-C3-C7-C8
27	a	611	PL9	C4-C3-C7-C8
29	L	101	LHG	C32-C33-C34-C35
28	d	410	LMG	C29-C30-C31-C32
28	A	612	LMG	C10-C11-C12-C13
31	C	517	DGD	C7A-C8A-C9A-CAA
28	D	411	LMG	C34-C35-C36-C37
29	A	613	LHG	C32-C33-C34-C35
30	A	615	SQD	C9-C10-C11-C12
25	c	503	CLA	C16-C17-C18-C19
32	l	102	STE	C5-C6-C7-C8
28	c	522	LMG	C40-C41-C42-C43
30	a	614	SQD	C31-C32-C33-C34
28	b	622	LMG	C28-C29-C30-C31
31	c	517	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
25	B	614	CLA	C11-C12-C13-C14
25	B	615	CLA	C6-C7-C8-C9
25	a	608	CLA	C11-C10-C8-C9
25	c	504	CLA	C11-C10-C8-C9
34	D	402	PHO	C14-C13-C15-C16
32	b	621	STE	C10-C11-C12-C13
26	D	406	BCR	C22-C23-C24-C25
26	d	405	BCR	C22-C23-C24-C25
28	D	408	LMG	C10-C11-C12-C13
28	b	624	LMG	C40-C41-C42-C43
25	a	608	CLA	C16-C17-C18-C20
25	c	511	CLA	C16-C17-C18-C19
28	M	101	LMG	C15-C16-C17-C18
28	d	410	LMG	C30-C31-C32-C33
30	a	614	SQD	O6-C44-C45-O47
31	c	517	DGD	C8B-C9B-CAB-CBB
31	H	102	DGD	C7A-C8A-C9A-CAA
32	b	623	STE	C7-C8-C9-C10
25	b	603	CLA	CBA-CGA-O2A-C1
30	A	614	SQD	C32-C33-C34-C35
32	T	102	STE	C14-C15-C16-C17
28	B	621	LMG	C32-C33-C34-C35
31	A	616	DGD	C8B-C9B-CAB-CBB
28	M	101	LMG	C36-C37-C38-C39
30	A	615	SQD	C10-C11-C12-C13
26	b	618	BCR	C16-C17-C18-C36
26	t	101	BCR	C20-C21-C22-C37
29	B	622	LHG	C14-C15-C16-C17
25	C	502	CLA	C13-C15-C16-C17
25	b	607	CLA	C5-C6-C7-C8
25	c	511	CLA	C16-C17-C18-C20
28	A	612	LMG	C17-C18-C19-C20
26	d	405	BCR	C7-C8-C9-C34
28	b	622	LMG	C20-C21-C22-C23
25	A	607	CLA	C11-C12-C13-C15
25	B	606	CLA	C11-C10-C8-C7
25	B	616	CLA	C6-C7-C8-C10
25	C	504	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C10-C8-C7
25	b	601	CLA	C12-C13-C15-C16
25	b	604	CLA	C12-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C11-C10-C8-C7
25	c	512	CLA	C6-C7-C8-C10
25	d	404	CLA	C11-C12-C13-C15
25	d	404	CLA	C12-C13-C15-C16
29	e	101	LHG	C28-C29-C30-C31
32	B	627	STE	C6-C7-C8-C9
26	K	102	BCR	C21-C22-C23-C24
28	B	621	LMG	C31-C32-C33-C34
31	C	516	DGD	C5D-C6D-O5D-C1E
31	c	516	DGD	C5D-C6D-O5D-C1E
25	B	604	CLA	C10-C11-C12-C13
25	C	505	CLA	C15-C16-C17-C18
32	d	412	STE	C12-C13-C14-C15
29	e	101	LHG	C18-C19-C20-C21
30	b	620	SQD	C24-C25-C26-C27
31	c	515	DGD	C3A-C4A-C5A-C6A
32	H	103	STE	C2-C3-C4-C5
25	c	512	CLA	C2-C3-C5-C6
28	M	101	LMG	C35-C36-C37-C38
32	I	101	STE	C12-C13-C14-C15
29	D	410	LHG	C29-C30-C31-C32
32	d	412	STE	C7-C8-C9-C10
25	b	607	CLA	O1A-CGA-O2A-C1
25	b	615	CLA	C5-C6-C7-C8
32	c	519	STE	C7-C8-C9-C10
32	M	102	STE	C10-C11-C12-C13
26	B	618	BCR	C11-C10-C9-C8
26	t	101	BCR	C20-C21-C22-C23
32	b	623	STE	C11-C12-C13-C14
29	d	408	LHG	O9-C7-O7-C5
28	D	411	LMG	C33-C34-C35-C36
30	f	102	SQD	C33-C34-C35-C36
32	T	103	STE	C13-C14-C15-C16
32	t	103	STE	C5-C6-C7-C8
31	C	515	DGD	C4A-C5A-C6A-C7A
28	M	101	LMG	O1-C7-C8-C9
28	b	624	LMG	O1-C7-C8-C9
30	B	623	SQD	O6-C44-C45-C46
31	A	616	DGD	O1G-C1G-C2G-C3G
31	c	515	DGD	O1G-C1G-C2G-C3G
29	d	407	LHG	C19-C20-C21-C22
35	f	101	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C16-C17-C18-C19
28	d	411	LMG	C14-C15-C16-C17
31	c	516	DGD	CCA-CDA-CEA-CFA
29	d	408	LHG	C25-C26-C27-C28
31	H	102	DGD	CAB-CBB-CCB-CDB
27	d	406	PL9	C30-C29-C31-C32
25	B	605	CLA	C2-C3-C5-C6
25	D	405	CLA	C3-C5-C6-C7
32	b	621	STE	C7-C8-C9-C10
32	b	625	STE	C9-C10-C11-C12
31	C	515	DGD	O1G-C1G-C2G-O2G
31	c	515	DGD	O1G-C1G-C2G-O2G
28	c	522	LMG	C20-C21-C22-C23
25	c	512	CLA	C15-C16-C17-C18
25	A	607	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	b	607	CLA	C14-C13-C15-C16
25	b	611	CLA	C14-C13-C15-C16
25	b	616	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C10-C8-C9
25	c	510	CLA	C11-C12-C13-C14
25	c	512	CLA	C16-C17-C18-C19
31	c	515	DGD	CBA-CCA-CDA-CEA
25	b	603	CLA	O1A-CGA-O2A-C1
28	M	101	LMG	C30-C31-C32-C33
32	c	519	STE	C14-C15-C16-C17
29	l	101	LHG	C15-C16-C17-C18
25	B	602	CLA	C13-C15-C16-C17
25	b	613	CLA	C15-C16-C17-C18
31	C	515	DGD	C2B-C3B-C4B-C5B
28	C	518	LMG	C2-C1-O1-C7
25	a	612	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C19
25	B	610	CLA	C13-C15-C16-C17
25	C	512	CLA	C13-C15-C16-C17
25	b	602	CLA	C15-C16-C17-C18
28	c	522	LMG	C16-C17-C18-C19
27	A	610	PL9	C32-C33-C34-C36
25	B	604	CLA	C13-C15-C16-C17
31	c	516	DGD	CAA-CBA-CCA-CDA
28	b	624	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
29	d	407	LHG	C29-C30-C31-C32
30	A	614	SQD	C31-C32-C33-C34
31	C	515	DGD	C6B-C7B-C8B-C9B
25	B	613	CLA	C16-C17-C18-C20
25	a	608	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C20
25	b	613	CLA	C16-C17-C18-C20
25	c	512	CLA	C10-C11-C12-C13
26	T	101	BCR	C14-C15-C16-C17
31	C	516	DGD	CCA-CDA-CEA-CFA
29	d	408	LHG	C11-C12-C13-C14
32	d	413	STE	C9-C10-C11-C12
29	D	410	LHG	C11-C10-C9-C8
25	c	510	CLA	C3-C5-C6-C7
25	c	512	CLA	C8-C10-C11-C12
28	c	518	LMG	C29-C28-O8-C9
28	M	101	LMG	C33-C34-C35-C36
29	d	407	LHG	C30-C31-C32-C33
31	C	515	DGD	C4D-C5D-C6D-O5D
25	B	601	CLA	C4B-C3B-CAB-CBB
25	b	605	CLA	C4B-C3B-CAB-CBB
30	B	623	SQD	C17-C18-C19-C20
30	b	620	SQD	C11-C12-C13-C14
28	c	522	LMG	C31-C32-C33-C34
29	e	101	LHG	C25-C26-C27-C28
31	c	516	DGD	C7B-C8B-C9B-CAB
31	c	515	DGD	C4D-C5D-C6D-O5D
32	T	103	STE	C2-C3-C4-C5
34	d	402	PHO	CBD-CGD-O2D-CED
29	E	101	LHG	C25-C26-C27-C28
31	A	616	DGD	CFB-CGB-CHB-CIB
25	B	606	CLA	C11-C12-C13-C15
25	B	610	CLA	C11-C12-C13-C15
25	b	602	CLA	C12-C13-C15-C16
25	b	608	CLA	C11-C10-C8-C7
25	b	615	CLA	C12-C13-C15-C16
25	c	507	CLA	C11-C10-C8-C7
25	c	511	CLA	C12-C13-C15-C16
25	b	616	CLA	C11-C12-C13-C14
32	B	627	STE	C7-C8-C9-C10
31	A	616	DGD	O6D-C5D-C6D-O5D
30	A	615	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
36	v	201	HEC	C4B-C3B-CAB-CBB
25	c	512	CLA	C16-C17-C18-C20
32	j	101	STE	C7-C8-C9-C10
32	C	521	STE	C12-C13-C14-C15
32	X	101	STE	C13-C14-C15-C16
29	A	613	LHG	C17-C18-C19-C20
32	H	103	STE	C7-C8-C9-C10
25	A	607	CLA	C11-C12-C13-C14
25	B	606	CLA	C14-C13-C15-C16
25	B	608	CLA	C6-C7-C8-C9
25	B	614	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	504	CLA	C11-C10-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C14
25	b	604	CLA	C14-C13-C15-C16
25	b	615	CLA	C14-C13-C15-C16
29	L	101	LHG	O10-C23-O8-C6
32	l	102	STE	C9-C10-C11-C12
25	b	608	CLA	C16-C17-C18-C19
29	L	101	LHG	C15-C16-C17-C18
25	C	512	CLA	C10-C11-C12-C13
25	C	513	CLA	C13-C15-C16-C17
25	b	608	CLA	C13-C15-C16-C17
30	b	620	SQD	O5-C5-C6-S
30	A	614	SQD	C14-C15-C16-C17
32	J	101	STE	C2-C3-C4-C5
29	B	622	LHG	C7-C8-C9-C10
28	A	612	LMG	C12-C13-C14-C15
31	c	515	DGD	CBB-CCB-CDB-CEB
28	D	411	LMG	O7-C8-C9-O8
28	c	520	LMG	O7-C8-C9-O8
30	b	620	SQD	O6-C44-C45-O47
30	b	620	SQD	O47-C45-C46-O48
32	d	412	STE	C2-C3-C4-C5
30	A	614	SQD	O6-C44-C45-C46
28	b	622	LMG	C32-C33-C34-C35
32	T	103	STE	C15-C16-C17-C18
25	C	502	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
31	C	515	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
29	E	101	LHG	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C20
28	A	612	LMG	C14-C15-C16-C17
28	D	408	LMG	C11-C12-C13-C14
30	A	614	SQD	C12-C13-C14-C15
32	T	103	STE	C3-C4-C5-C6
29	B	622	LHG	C19-C20-C21-C22
25	B	612	CLA	CAD-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O1D
26	K	101	BCR	C13-C14-C15-C16
26	a	610	BCR	C19-C20-C21-C22
29	D	410	LHG	C4-O6-P-O5
29	L	101	LHG	C4-O6-P-O3
29	d	408	LHG	C4-O6-P-O5
29	l	101	LHG	C4-O6-P-O5
29	l	101	LHG	C17-C18-C19-C20
27	a	611	PL9	C32-C33-C34-C35
25	B	612	CLA	C8-C10-C11-C12
27	d	406	PL9	C15-C14-C16-C17
25	b	601	CLA	C2B-C3B-CAB-CBB
25	b	610	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
31	c	517	DGD	C1B-C2B-C3B-C4B
32	M	102	STE	C9-C10-C11-C12
29	L	101	LHG	C7-C8-C9-C10
31	C	517	DGD	C2B-C3B-C4B-C5B
32	B	627	STE	C4-C5-C6-C7
28	D	408	LMG	C30-C31-C32-C33
31	c	516	DGD	CAB-CBB-CCB-CDB
32	B	626	STE	C1-C2-C3-C4
28	c	522	LMG	C37-C38-C39-C40
29	L	101	LHG	C11-C12-C13-C14
28	A	612	LMG	C9-C8-O7-C10
31	o	301	DGD	C1G-C2G-O2G-C1B
31	C	517	DGD	C3B-C4B-C5B-C6B
27	A	610	PL9	C19-C21-C22-C23
25	c	513	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	B	620	STE	C10-C11-C12-C13
32	b	623	STE	C12-C13-C14-C15
26	k	102	BCR	C19-C20-C21-C22
25	b	602	CLA	C16-C17-C18-C20
25	B	605	CLA	C8-C10-C11-C12
29	e	101	LHG	O6-C4-C5-C6
28	C	518	LMG	C19-C20-C21-C22
25	B	605	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
25	b	614	CLA	C11-C10-C8-C9
25	b	615	CLA	C11-C10-C8-C9
25	c	505	CLA	C6-C7-C8-C9
25	A	607	CLA	C6-C7-C8-C10
25	C	511	CLA	C6-C7-C8-C10
26	B	619	BCR	C11-C10-C9-C8
26	H	101	BCR	C11-C10-C9-C8
32	E	102	STE	C1-C2-C3-C4
32	a	615	STE	C1-C2-C3-C4
31	C	515	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	CCB-CDB-CEB-CFB
32	X	101	STE	C14-C15-C16-C17
26	K	101	BCR	C14-C15-C16-C17
29	B	622	LHG	C32-C33-C34-C35
29	d	407	LHG	C27-C28-C29-C30
31	A	616	DGD	CDA-CEA-CFA-CGA
25	B	606	CLA	C5-C6-C7-C8
32	b	621	STE	C12-C13-C14-C15
27	d	406	PL9	C38-C39-C41-C42
25	a	612	CLA	C16-C17-C18-C20
25	A	608	CLA	C5-C6-C7-C8
28	d	411	LMG	C32-C33-C34-C35
31	c	515	DGD	C8A-C9A-CAA-CBA
29	l	101	LHG	C16-C17-C18-C19
29	E	101	LHG	O7-C5-C6-O8
29	L	101	LHG	C11-C10-C9-C8
25	c	509	CLA	CAA-CBA-CGA-O2A
30	D	409	SQD	O48-C23-C24-C25
31	H	102	DGD	O2G-C1B-C2B-C3B
32	J	101	STE	C4-C5-C6-C7
28	c	518	LMG	C39-C40-C41-C42
31	C	516	DGD	C7B-C8B-C9B-CAB
25	C	509	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	o	301	DGD	CAB-CBB-CCB-CDB
32	b	625	STE	C7-C8-C9-C10
29	e	101	LHG	C26-C27-C28-C29
27	A	610	PL9	C14-C16-C17-C18
32	B	624	STE	C1-C2-C3-C4
30	D	409	SQD	O6-C44-C45-C46
31	c	515	DGD	O1G-C1A-C2A-C3A
25	d	404	CLA	C16-C17-C18-C19
25	c	509	CLA	C3-C5-C6-C7
32	b	621	STE	C4-C5-C6-C7
32	a	615	STE	C7-C8-C9-C10
29	d	408	LHG	C31-C32-C33-C34
25	c	501	CLA	C2A-CAA-CBA-CGA
26	k	101	BCR	C9-C10-C11-C12
29	B	622	LHG	C31-C32-C33-C34
31	C	517	DGD	C1B-C2B-C3B-C4B
27	a	611	PL9	C30-C29-C31-C32
32	M	103	STE	C7-C8-C9-C10
25	C	508	CLA	C16-C17-C18-C19
25	A	607	CLA	C11-C10-C8-C9
25	b	602	CLA	C14-C13-C15-C16
25	b	608	CLA	C11-C10-C8-C9
25	c	507	CLA	C11-C10-C8-C9
25	C	508	CLA	O1D-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
30	B	623	SQD	C32-C33-C34-C35
32	T	103	STE	O2-C1-C2-C3
34	d	402	PHO	C5-C6-C7-C8
31	c	515	DGD	CDB-CEB-CFB-CGB
29	D	410	LHG	C35-C36-C37-C38
28	c	520	LMG	C35-C36-C37-C38
29	L	101	LHG	C29-C30-C31-C32
32	l	102	STE	C4-C5-C6-C7
31	A	616	DGD	C4D-C5D-C6D-O5D
25	b	613	CLA	C16-C17-C18-C19
32	b	621	STE	C3-C4-C5-C6
31	C	517	DGD	CCB-CDB-CEB-CFB
25	B	601	CLA	C11-C10-C8-C7
25	B	615	CLA	C11-C10-C8-C7
25	c	505	CLA	C12-C13-C15-C16
25	c	512	CLA	C12-C13-C15-C16
32	d	412	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CAA-CBA-CGA-O2A
32	B	627	STE	C10-C11-C12-C13
28	M	101	LMG	O1-C7-C8-O7
32	d	413	STE	C11-C12-C13-C14
25	B	601	CLA	C3A-C2A-CAA-CBA
28	d	411	LMG	C39-C40-C41-C42
31	c	517	DGD	CBB-CCB-CDB-CEB
27	a	611	PL9	C13-C14-C16-C17
32	b	626	STE	C1-C2-C3-C4
30	a	613	SQD	C35-C36-C37-C38
25	b	605	CLA	C16-C17-C18-C20
28	M	101	LMG	C19-C20-C21-C22
26	k	102	BCR	C16-C17-C18-C36
26	t	101	BCR	C35-C13-C14-C15
30	b	620	SQD	O5-C1-O6-C44
29	l	101	LHG	C9-C10-C11-C12
32	d	412	STE	O2-C1-C2-C3
30	a	614	SQD	C17-C18-C19-C20
32	l	102	STE	C11-C12-C13-C14
25	B	604	CLA	C16-C17-C18-C20
25	c	504	CLA	C8-C10-C11-C12
29	E	101	LHG	C2-C3-O3-P
31	A	616	DGD	CCB-CDB-CEB-CFB
34	d	402	PHO	O1D-CGD-O2D-CED
27	d	406	PL9	C45-C44-C46-C47
25	D	404	CLA	C16-C17-C18-C19
31	o	301	DGD	C3A-C4A-C5A-C6A
32	T	103	STE	O1-C1-C2-C3
29	d	408	LHG	C15-C16-C17-C18
25	B	615	CLA	C8-C10-C11-C12
30	D	409	SQD	C31-C32-C33-C34
25	B	603	CLA	C11-C10-C8-C9
25	B	615	CLA	C11-C12-C13-C14
25	C	511	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C12-C13-C14
25	b	610	CLA	C14-C13-C15-C16
25	c	505	CLA	C11-C10-C8-C9
25	c	512	CLA	C14-C13-C15-C16
29	E	101	LHG	C17-C18-C19-C20
30	b	620	SQD	C14-C15-C16-C17
29	d	408	LHG	C11-C10-C9-C8
36	v	201	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C10-C11-C12-C13
25	B	613	CLA	O1D-CGD-O2D-CED
26	K	102	BCR	C13-C14-C15-C16
32	d	412	STE	O1-C1-C2-C3
36	v	201	HEC	CAD-CBD-CGD-O1D
31	C	515	DGD	CAA-CBA-CCA-CDA
31	H	102	DGD	C4A-C5A-C6A-C7A
29	E	101	LHG	C15-C16-C17-C18
30	a	613	SQD	C13-C14-C15-C16
32	j	101	STE	C6-C7-C8-C9
32	J	101	STE	C5-C6-C7-C8
25	B	601	CLA	C2B-C3B-CAB-CBB
25	B	605	CLA	C2B-C3B-CAB-CBB
25	b	603	CLA	C2B-C3B-CAB-CBB
25	b	605	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C1-C6-C7-C8
26	Z	101	BCR	C1-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	c	514	BCR	C1-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C30
26	k	101	BCR	C1-C6-C7-C8
32	B	624	STE	C5-C6-C7-C8
32	H	103	STE	C4-C5-C6-C7
36	V	201	HEC	CAD-CBD-CGD-O2D
31	C	517	DGD	C9A-CAA-CBA-CCA
29	A	613	LHG	C2-C3-O3-P
28	C	518	LMG	C38-C39-C40-C41
28	b	622	LMG	C31-C32-C33-C34
25	C	505	CLA	C16-C17-C18-C19
31	C	516	DGD	CDA-CEA-CFA-CGA
32	t	103	STE	C7-C8-C9-C10
32	b	623	STE	O1-C1-C2-C3
30	B	623	SQD	C9-C10-C11-C12
31	h	101	DGD	CCB-CDB-CEB-CFB
31	c	516	DGD	C4E-C5E-C6E-O5E
31	c	517	DGD	C7A-C8A-C9A-CAA
25	A	607	CLA	C11-C10-C8-C7
25	B	606	CLA	C6-C7-C8-C10
25	B	615	CLA	C11-C12-C13-C15
25	b	603	CLA	C6-C7-C8-C10
25	b	615	CLA	C11-C10-C8-C7
25	c	501	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	c	503	CLA	C11-C10-C8-C7
29	A	613	LHG	C24-C25-C26-C27
30	A	614	SQD	C28-C29-C30-C31
32	b	623	STE	C3-C4-C5-C6
25	b	610	CLA	C2A-CAA-CBA-CGA
35	F	101	HEM	CAD-CBD-CGD-O1D
32	M	103	STE	C6-C7-C8-C9
31	C	515	DGD	CCB-CDB-CEB-CFB
31	A	616	DGD	C9B-CAB-CBB-CCB
31	o	301	DGD	C9B-CAB-CBB-CCB
28	b	624	LMG	O10-C28-O8-C9
28	d	410	LMG	O9-C10-C11-C12
32	b	623	STE	O2-C1-C2-C3
30	b	620	SQD	C12-C13-C14-C15
31	C	515	DGD	O1B-C1B-O2G-C2G
32	B	626	STE	C3-C4-C5-C6
25	b	613	CLA	C5-C6-C7-C8
25	c	506	CLA	C4-C3-C5-C6
27	d	406	PL9	C43-C44-C46-C47
25	B	613	CLA	C2-C1-O2A-CGA
25	b	616	CLA	C3-C5-C6-C7
32	B	620	STE	C4-C5-C6-C7
31	h	101	DGD	CDB-CEB-CFB-CGB
25	B	601	CLA	C4-C3-C5-C6
25	C	512	CLA	C4-C3-C5-C6
25	c	508	CLA	C4-C3-C5-C6
25	b	610	CLA	C15-C16-C17-C18
31	H	102	DGD	CCB-CDB-CEB-CFB
25	b	614	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	CBA-CGA-O2A-C1
32	B	624	STE	O2-C1-C2-C3
32	C	520	STE	C4-C5-C6-C7
31	C	515	DGD	O1G-C1G-C2G-C3G
29	D	410	LHG	C28-C29-C30-C31
28	B	621	LMG	C37-C38-C39-C40
25	b	603	CLA	C2A-CAA-CBA-CGA
35	F	101	HEM	CAD-CBD-CGD-O2D
25	B	613	CLA	C16-C17-C18-C19
25	b	612	CLA	C16-C17-C18-C20
26	B	617	BCR	C11-C10-C9-C34
26	K	101	BCR	C11-C10-C9-C34
26	d	405	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
28	b	622	LMG	C40-C41-C42-C43
27	d	406	PL9	C35-C34-C36-C37
25	C	512	CLA	C15-C16-C17-C18
27	D	407	PL9	C18-C19-C21-C22
27	D	407	PL9	C28-C29-C31-C32
29	d	409	LHG	C2-C3-O3-P
30	B	623	SQD	C24-C25-C26-C27
36	V	201	HEC	CAD-CBD-CGD-O1D
28	d	411	LMG	C37-C38-C39-C40
31	o	301	DGD	C1A-C2A-C3A-C4A
28	d	411	LMG	C29-C30-C31-C32
32	I	101	STE	C6-C7-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	b	603	CLA	C14-C13-C15-C16
31	c	517	DGD	O6D-C5D-C6D-O5D
31	C	517	DGD	C5B-C6B-C7B-C8B
32	c	519	STE	C4-C5-C6-C7
30	b	620	SQD	C45-C44-O6-C1
25	c	504	CLA	C11-C12-C13-C15
28	c	520	LMG	C34-C35-C36-C37
28	b	624	LMG	C30-C31-C32-C33
32	B	620	STE	C5-C6-C7-C8
25	b	609	CLA	C13-C15-C16-C17
32	c	519	STE	O2-C1-C2-C3
28	C	518	LMG	C15-C16-C17-C18
31	C	515	DGD	C6A-C7A-C8A-C9A
34	D	403	PHO	C2C-C3C-CAC-CBC
28	b	622	LMG	C35-C36-C37-C38
31	c	516	DGD	CDA-CEA-CFA-CGA
30	a	614	SQD	C30-C31-C32-C33
32	b	626	STE	C6-C7-C8-C9
28	C	518	LMG	O10-C28-O8-C9
32	J	101	STE	O2-C1-C2-C3
25	D	404	CLA	C16-C17-C18-C20
28	M	101	LMG	C12-C13-C14-C15
32	B	624	STE	O1-C1-C2-C3
32	d	413	STE	C11-C10-C9-C8
32	c	519	STE	O1-C1-C2-C3
35	f	101	HEM	CAD-CBD-CGD-O1D
31	H	102	DGD	C2B-C3B-C4B-C5B
28	c	520	LMG	C7-C8-C9-O8
30	b	620	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
25	B	610	CLA	C8-C10-C11-C12
25	a	608	CLA	C13-C15-C16-C17
32	d	413	STE	C4-C5-C6-C7
32	C	521	STE	C10-C11-C12-C13
25	b	612	CLA	CAA-CBA-CGA-O2A
29	l	101	LHG	O7-C7-C8-C9
26	B	617	BCR	C19-C20-C21-C22
25	A	611	CLA	C4C-C3C-CAC-CBC
25	c	509	CLA	C16-C17-C18-C20
32	c	521	STE	C7-C8-C9-C10
31	C	516	DGD	C5B-C6B-C7B-C8B
28	C	518	LMG	C18-C19-C20-C21
32	H	103	STE	C14-C15-C16-C17
25	A	606	CLA	C13-C15-C16-C17
32	j	101	STE	C5-C6-C7-C8
32	J	101	STE	O1-C1-C2-C3
25	B	612	CLA	CAA-CBA-CGA-O2A
28	d	411	LMG	C34-C35-C36-C37
32	m	101	STE	C3-C4-C5-C6
30	a	613	SQD	O47-C45-C46-O48
31	A	616	DGD	CAA-CBA-CCA-CDA
25	C	506	CLA	C13-C15-C16-C17
25	c	508	CLA	C13-C15-C16-C17
25	B	606	CLA	C11-C12-C13-C14
25	b	601	CLA	C11-C10-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	613	CLA	C14-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C14
25	c	506	CLA	C6-C7-C8-C9
25	B	604	CLA	C16-C17-C18-C19
28	D	408	LMG	O7-C10-C11-C12
28	M	101	LMG	C22-C23-C24-C25
25	C	507	CLA	C8-C10-C11-C12
25	b	602	CLA	C4-C3-C5-C6
25	A	606	CLA	C16-C17-C18-C20
31	C	516	DGD	CDB-CEB-CFB-CGB
25	B	612	CLA	C6-C7-C8-C10
25	C	503	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C10-C8-C7
25	a	607	CLA	C12-C13-C15-C16
25	b	601	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	C6-C7-C8-C10
25	c	505	CLA	C11-C10-C8-C7
25	c	510	CLA	C2B-C3B-CAB-CBB
26	Z	101	BCR	C5-C6-C7-C8
26	c	514	BCR	C5-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
26	k	101	BCR	C5-C6-C7-C8
26	x	101	BCR	C23-C24-C25-C30
29	B	622	LHG	O9-C7-O7-C5
32	X	101	STE	C2-C3-C4-C5
25	D	404	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
32	M	103	STE	C1-C2-C3-C4
28	c	520	LMG	C17-C18-C19-C20
25	b	603	CLA	C16-C17-C18-C19
27	d	406	PL9	C20-C19-C21-C22
31	C	515	DGD	CCA-CDA-CEA-CFA
31	H	102	DGD	C1A-C2A-C3A-C4A
25	b	601	CLA	C2A-CAA-CBA-CGA
30	B	623	SQD	C29-C30-C31-C32
32	c	521	STE	C4-C5-C6-C7
25	d	403	CLA	C10-C11-C12-C13
32	b	623	STE	C15-C16-C17-C18
28	d	410	LMG	O7-C10-C11-C12
31	C	517	DGD	CBA-CCA-CDA-CEA
28	c	522	LMG	C18-C19-C20-C21
31	c	515	DGD	O2G-C1B-C2B-C3B
27	D	407	PL9	C38-C39-C41-C42
32	B	625	STE	O2-C1-C2-C3
32	B	626	STE	O2-C1-C2-C3
32	B	626	STE	C5-C6-C7-C8
31	C	516	DGD	C2A-C3A-C4A-C5A
32	l	102	STE	C1-C2-C3-C4
25	b	613	CLA	CAA-CBA-CGA-O2A
30	A	614	SQD	O47-C7-C8-C9
28	c	520	LMG	C32-C33-C34-C35
25	B	601	CLA	C11-C10-C8-C9
25	B	610	CLA	C11-C12-C13-C14
25	c	513	CLA	C6-C7-C8-C9
30	f	102	SQD	O48-C23-C24-C25
29	E	101	LHG	C11-C12-C13-C14
25	B	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	b	603	CLA	C4B-C3B-CAB-CBB
29	d	407	LHG	C26-C27-C28-C29
25	C	509	CLA	C3-C5-C6-C7
27	A	610	PL9	C12-C11-C9-C10
27	A	610	PL9	C25-C24-C26-C27
26	B	619	BCR	C22-C23-C24-C25
31	C	516	DGD	O6D-C1D-O3G-C3G
27	D	407	PL9	C11-C12-C13-C14
26	D	406	BCR	C21-C22-C23-C24
26	T	101	BCR	C13-C14-C15-C16
25	C	507	CLA	C13-C15-C16-C17
31	c	515	DGD	O1A-C1A-O1G-C1G
31	h	101	DGD	C5A-C6A-C7A-C8A
28	b	624	LMG	O7-C10-C11-C12
25	B	610	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	O1D-CGD-O2D-CED
28	D	408	LMG	C22-C23-C24-C25
28	c	518	LMG	C37-C38-C39-C40
30	a	613	SQD	O47-C7-C8-C9
28	B	621	LMG	O7-C10-C11-C12
31	o	301	DGD	C9A-CAA-CBA-CCA
25	C	504	CLA	C2-C1-O2A-CGA
25	a	607	CLA	C2-C1-O2A-CGA
25	C	505	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C12-C13-C15
25	C	507	CLA	C6-C7-C8-C10
25	D	405	CLA	C12-C13-C15-C16
25	c	509	CLA	C6-C7-C8-C10
25	C	512	CLA	C2-C3-C5-C6
25	B	615	CLA	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C20
30	A	614	SQD	C33-C34-C35-C36
32	m	101	STE	C7-C8-C9-C10
25	B	613	CLA	CAA-CBA-CGA-O2A
31	c	516	DGD	CBB-CCB-CDB-CEB
25	B	606	CLA	O1D-CGD-O2D-CED
35	f	101	HEM	CAD-CBD-CGD-O2D
27	D	407	PL9	C46-C47-C48-C49
29	B	622	LHG	C24-C25-C26-C27
28	D	408	LMG	C15-C16-C17-C18
25	B	602	CLA	C3A-C2A-CAA-CBA
25	b	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	C	517	DGD	CDB-CEB-CFB-CGB
28	D	408	LMG	C28-C29-C30-C31
32	B	620	STE	C11-C10-C9-C8
26	t	101	BCR	C11-C10-C9-C8
25	B	605	CLA	C10-C11-C12-C13
31	c	517	DGD	O6E-C5E-C6E-O5E
30	A	614	SQD	O49-C7-C8-C9
30	f	102	SQD	O10-C23-C24-C25
32	b	621	STE	C11-C12-C13-C14
27	A	610	PL9	C21-C22-C23-C24
32	B	626	STE	O1-C1-C2-C3
25	c	503	CLA	C11-C10-C8-C9
25	d	404	CLA	C14-C13-C15-C16
32	B	625	STE	C7-C8-C9-C10
25	b	604	CLA	C15-C16-C17-C18
31	C	515	DGD	C9A-CAA-CBA-CCA
27	D	407	PL9	C32-C33-C34-C35
28	c	520	LMG	C40-C41-C42-C43
31	H	102	DGD	C9B-CAB-CBB-CCB
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
25	C	507	CLA	C5-C6-C7-C8
28	M	101	LMG	C8-C7-O1-C1
29	B	622	LHG	C1-C2-C3-O3
30	a	613	SQD	O49-C7-C8-C9
31	c	516	DGD	O1B-C1B-C2B-C3B
25	b	606	CLA	C16-C17-C18-C19
25	c	504	CLA	C11-C12-C13-C14
25	B	615	CLA	C10-C11-C12-C13
30	b	620	SQD	O6-C44-C45-C46
31	c	515	DGD	C1G-C2G-C3G-O3G
25	B	613	CLA	CAA-CBA-CGA-O1A
25	c	510	CLA	C4-C3-C5-C6
27	D	407	PL9	C20-C19-C21-C22
34	D	402	PHO	C10-C11-C12-C13
25	C	510	CLA	CAA-CBA-CGA-O2A
32	B	625	STE	O1-C1-C2-C3
35	f	101	HEM	CAA-CBA-CGA-O2A
31	C	515	DGD	O1B-C1B-C2B-C3B
32	j	101	STE	C1-C2-C3-C4
29	E	101	LHG	C35-C36-C37-C38
25	B	601	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	612	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	b	601	CLA	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
25	B	603	CLA	C8-C10-C11-C12
31	H	102	DGD	CDA-CEA-CFA-CGA
31	C	517	DGD	O6D-C5D-C6D-O5D
25	A	606	CLA	C2-C1-O2A-CGA
28	b	624	LMG	O9-C10-C11-C12
25	b	606	CLA	C16-C17-C18-C20
32	M	103	STE	C2-C3-C4-C5
32	E	102	STE	O2-C1-C2-C3
31	h	101	DGD	CDA-CEA-CFA-CGA
32	d	413	STE	O2-C1-C2-C3
25	c	501	CLA	CAA-CBA-CGA-O2A
28	b	622	LMG	O7-C10-C11-C12
27	d	406	PL9	C42-C43-C44-C46
25	b	613	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

142 monomers are involved in 268 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	615	CLA	3	0
26	k	102	BCR	2	0
25	b	613	CLA	1	0
29	d	407	LHG	3	0
25	B	603	CLA	3	0
25	C	504	CLA	3	0
25	c	507	CLA	3	0
25	B	616	CLA	3	0
25	C	506	CLA	2	0
25	a	608	CLA	2	0
36	v	201	HEC	1	0
26	B	618	BCR	2	0
34	D	403	PHO	1	0
29	A	613	LHG	5	0
25	a	607	CLA	2	0
26	B	619	BCR	1	0
32	I	101	STE	2	0
25	B	604	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	612	CLA	3	0
27	d	406	PL9	1	0
25	C	505	CLA	1	0
26	a	610	BCR	1	0
31	o	301	DGD	3	0
25	b	616	CLA	5	0
30	a	613	SQD	4	0
32	T	102	STE	2	0
26	b	619	BCR	1	0
26	t	101	BCR	3	0
29	d	409	LHG	1	0
26	C	514	BCR	3	0
31	C	515	DGD	1	0
25	a	609	CLA	2	0
26	k	101	BCR	1	0
25	D	405	CLA	1	0
25	c	505	CLA	5	0
25	c	508	CLA	2	0
25	C	512	CLA	2	0
33	D	401	BCT	1	0
27	D	407	PL9	1	0
29	E	101	LHG	4	0
25	b	611	CLA	2	0
26	T	101	BCR	5	0
28	b	622	LMG	1	0
25	c	504	CLA	1	0
25	b	608	CLA	1	0
25	A	607	CLA	3	0
26	b	618	BCR	2	0
30	D	409	SQD	2	0
25	B	610	CLA	3	0
25	B	601	CLA	3	0
26	D	406	BCR	1	0
25	A	608	CLA	1	0
29	l	101	LHG	1	0
35	f	101	HEM	5	0
32	j	101	STE	1	0
26	K	102	BCR	1	0
25	b	603	CLA	2	0
25	B	602	CLA	3	0
25	c	513	CLA	3	0
28	D	408	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	T	103	STE	1	0
26	d	405	BCR	3	0
25	b	615	CLA	2	0
30	B	623	SQD	3	0
25	B	613	CLA	3	0
25	a	612	CLA	2	0
25	d	403	CLA	2	0
35	F	101	HEM	2	0
25	b	609	CLA	1	0
32	c	521	STE	1	0
25	b	610	CLA	2	0
25	c	501	CLA	3	0
26	b	617	BCR	2	0
25	B	607	CLA	2	0
26	K	101	BCR	2	0
31	C	517	DGD	2	0
29	D	410	LHG	1	0
25	b	601	CLA	1	0
30	b	620	SQD	1	0
25	c	510	CLA	2	0
32	H	103	STE	1	0
25	B	609	CLA	3	0
25	c	503	CLA	4	0
21	A	601[B]	OEY	1	0
29	d	408	LHG	2	0
25	b	602	CLA	4	0
30	f	102	SQD	2	0
25	B	605	CLA	4	0
25	d	404	CLA	1	0
32	B	625	STE	2	0
28	b	624	LMG	1	0
25	C	511	CLA	1	0
25	b	604	CLA	2	0
32	c	519	STE	2	0
25	C	501	CLA	1	0
29	L	101	LHG	2	0
32	d	413	STE	4	0
32	b	623	STE	4	0
25	c	509	CLA	1	0
26	c	514	BCR	2	0
28	M	101	LMG	2	0
30	A	614	SQD	2	0

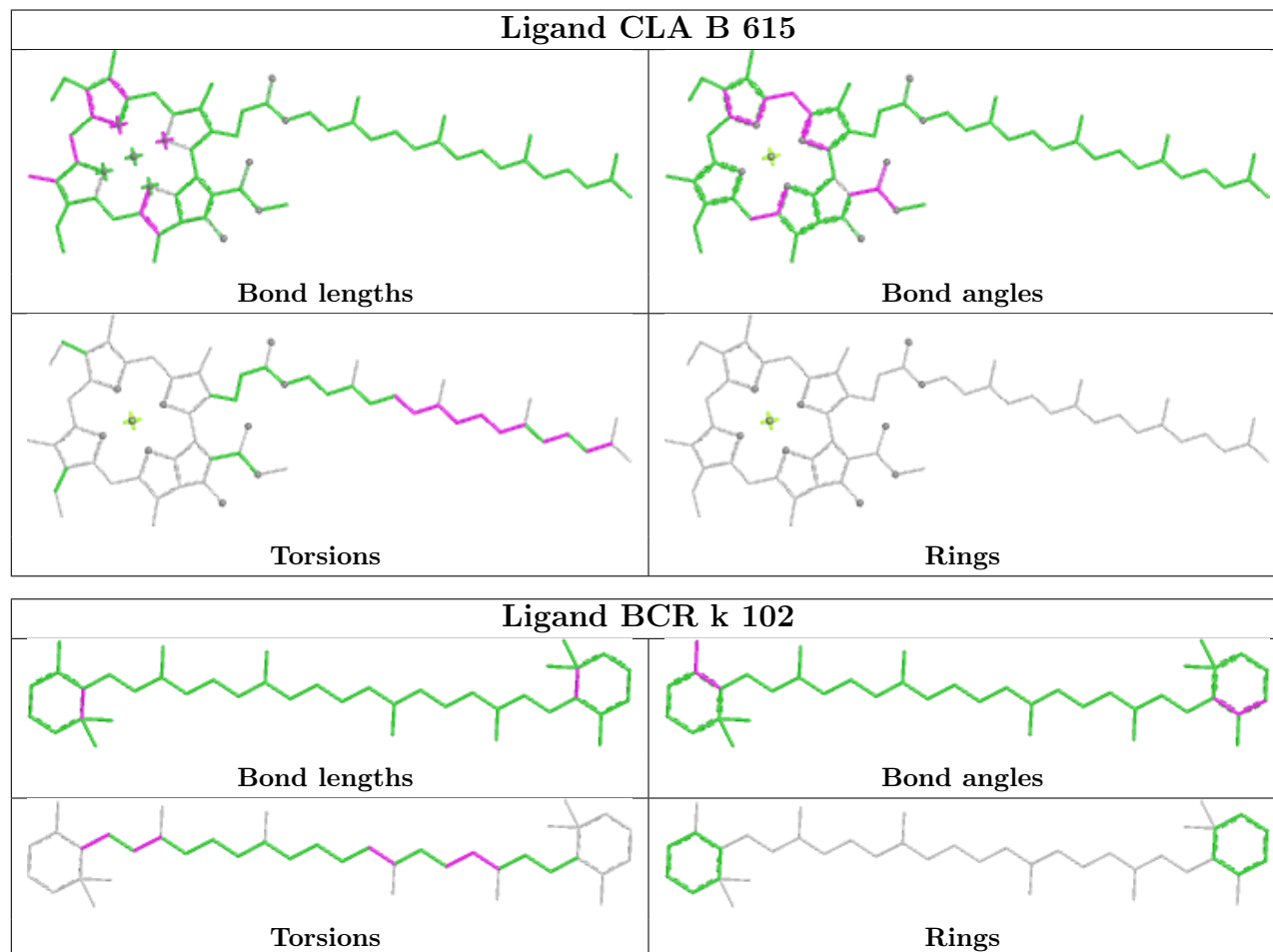
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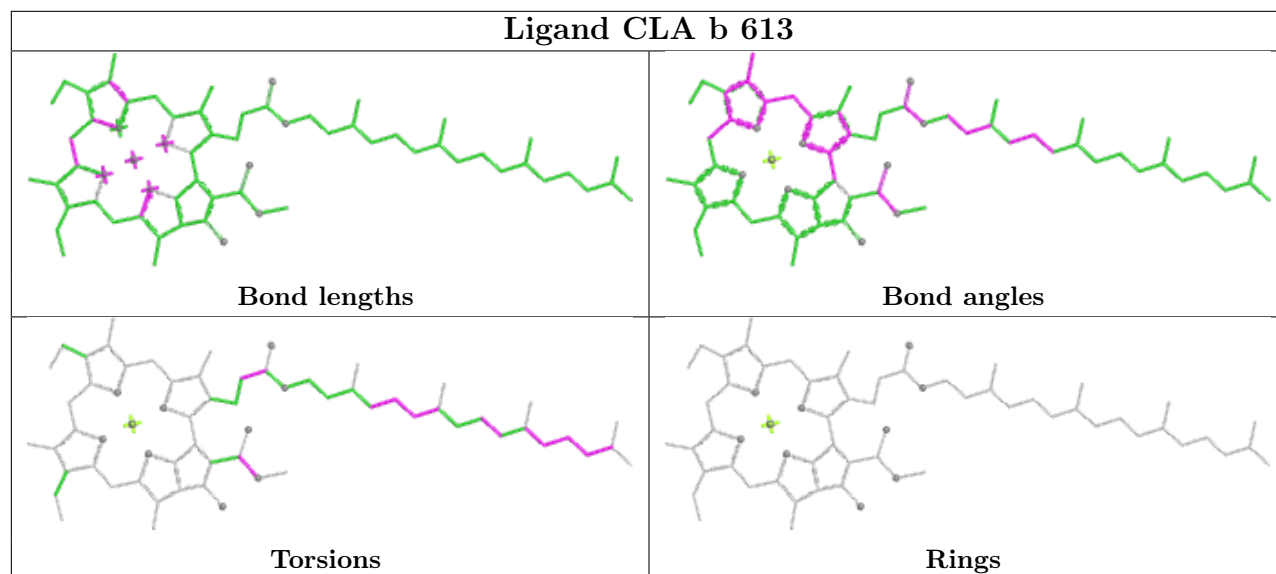
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	c	520	LMG	5	0
31	c	516	DGD	1	0
25	c	511	CLA	5	0
25	b	605	CLA	4	0
29	B	622	LHG	3	0
32	X	101	STE	1	0
26	x	101	BCR	2	0
32	l	102	STE	2	0
26	Z	101	BCR	2	0
26	A	609	BCR	1	0
25	B	611	CLA	2	0
25	b	614	CLA	5	0
34	D	402	PHO	1	0
25	C	513	CLA	3	0
25	b	606	CLA	3	0
31	H	102	DGD	3	0
30	A	615	SQD	2	0
25	B	614	CLA	4	0
28	c	518	LMG	1	0
25	A	606	CLA	2	0
25	C	510	CLA	1	0
31	c	517	DGD	2	0
34	d	402	PHO	2	0
27	a	611	PL9	4	0
25	C	508	CLA	2	0
28	c	522	LMG	3	0
25	b	612	CLA	2	0
25	D	404	CLA	1	0
26	k	103	BCR	3	0
26	B	617	BCR	3	0
25	C	507	CLA	1	0
21	a	601[B]	OEY	1	0
27	A	610	PL9	5	0
25	B	606	CLA	3	0
31	A	616	DGD	7	0
29	e	101	LHG	1	0
28	A	612	LMG	2	0
28	D	411	LMG	1	0
25	C	502	CLA	1	0
25	c	512	CLA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

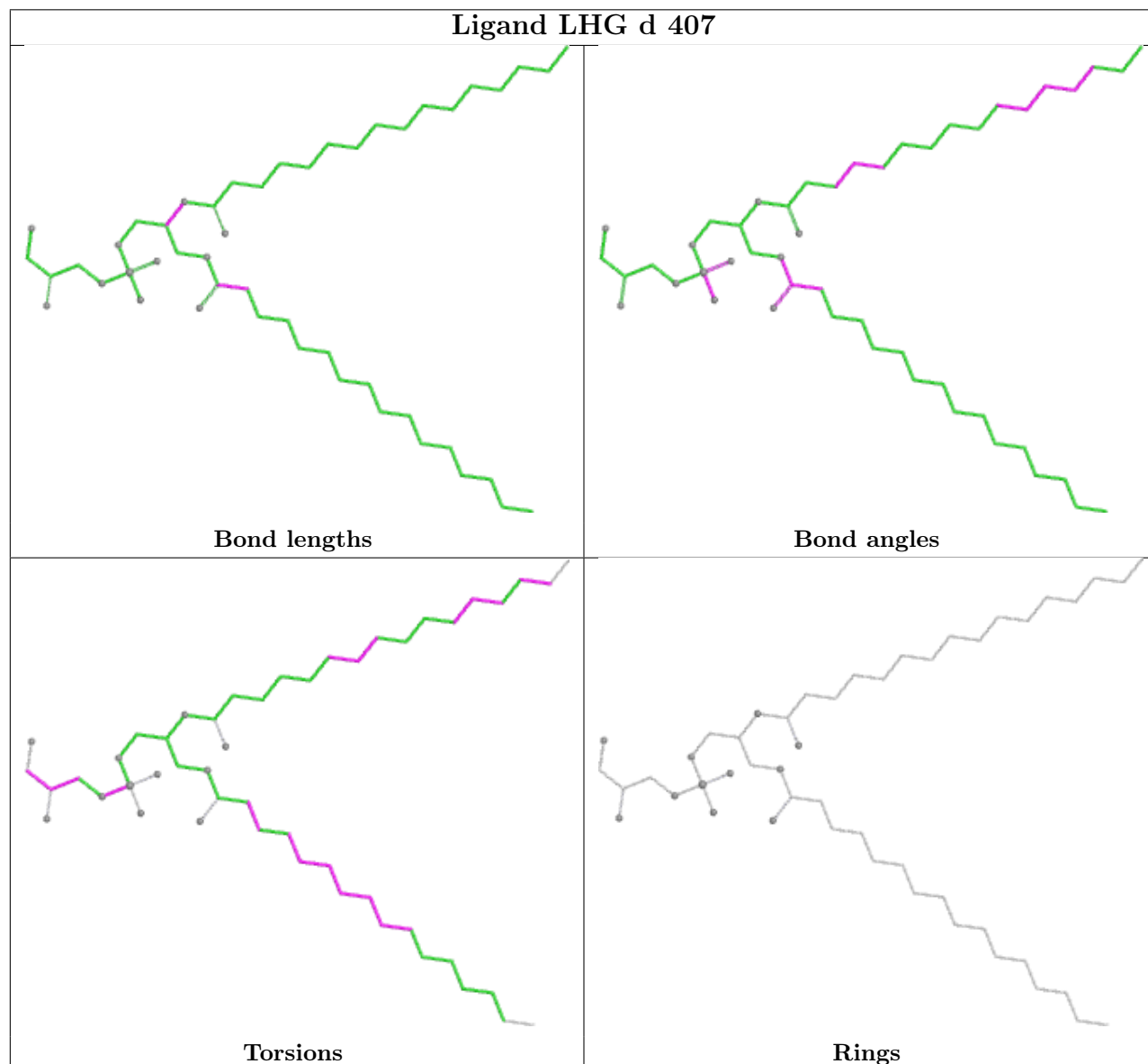
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



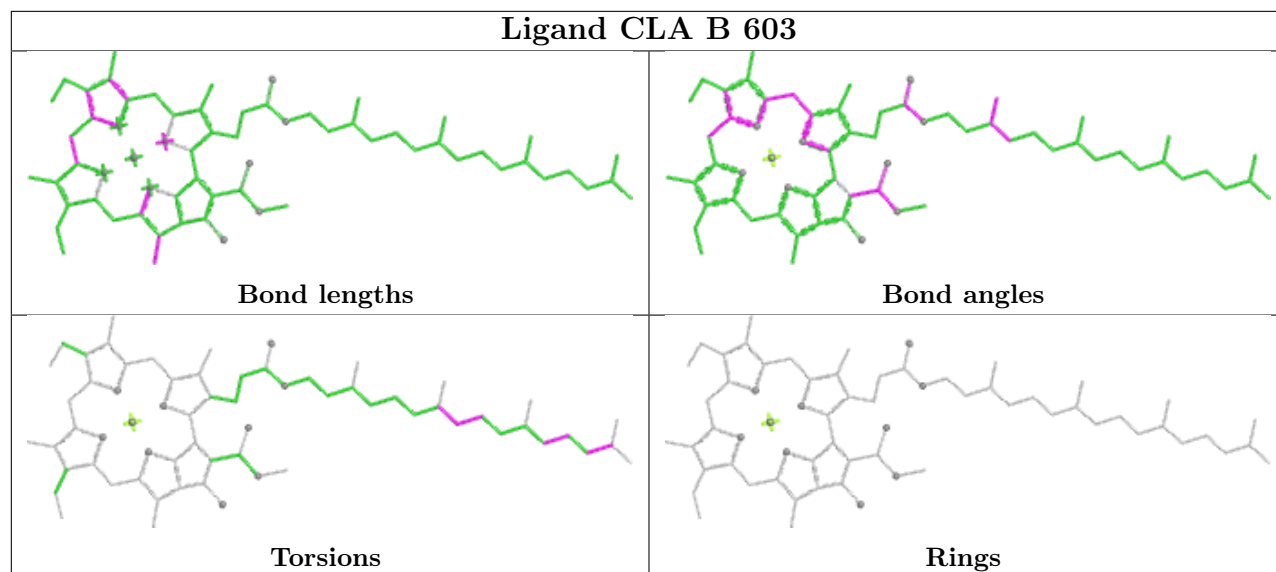
Ligand CLA b 613



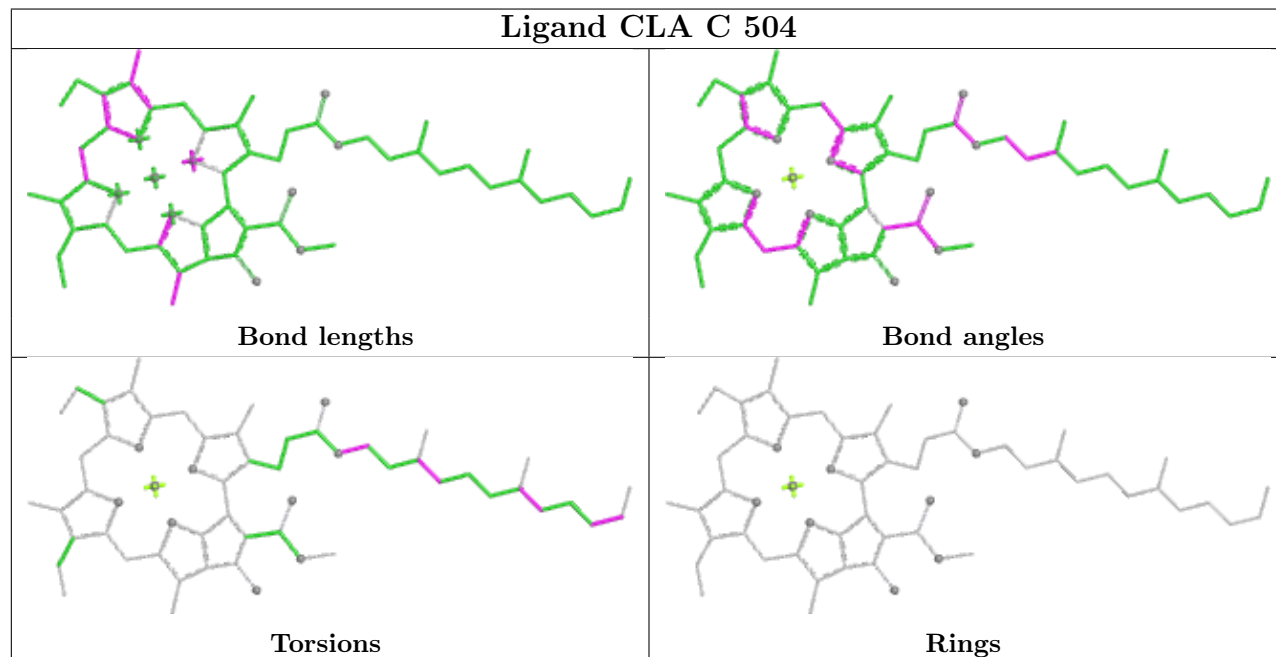
Ligand LHG d 407



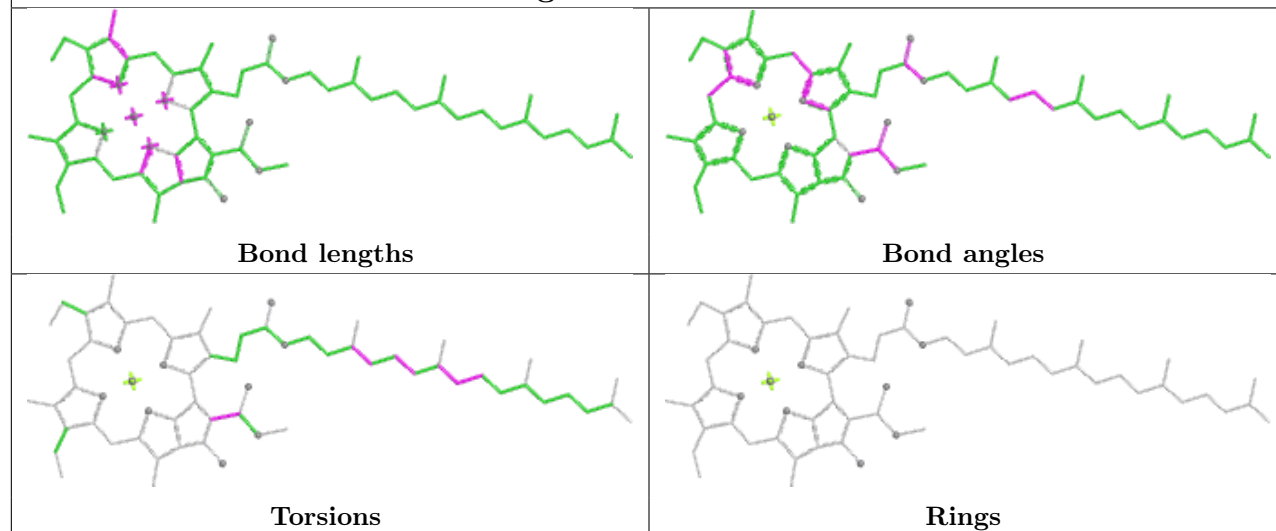
Ligand CLA B 603



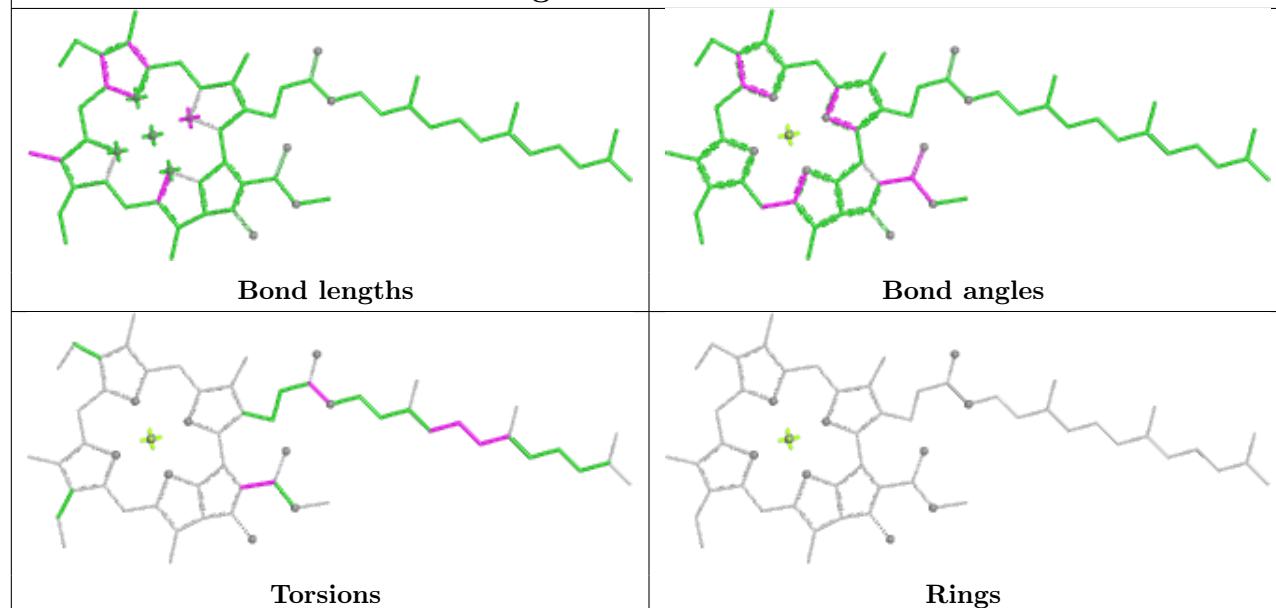
Ligand CLA C 504



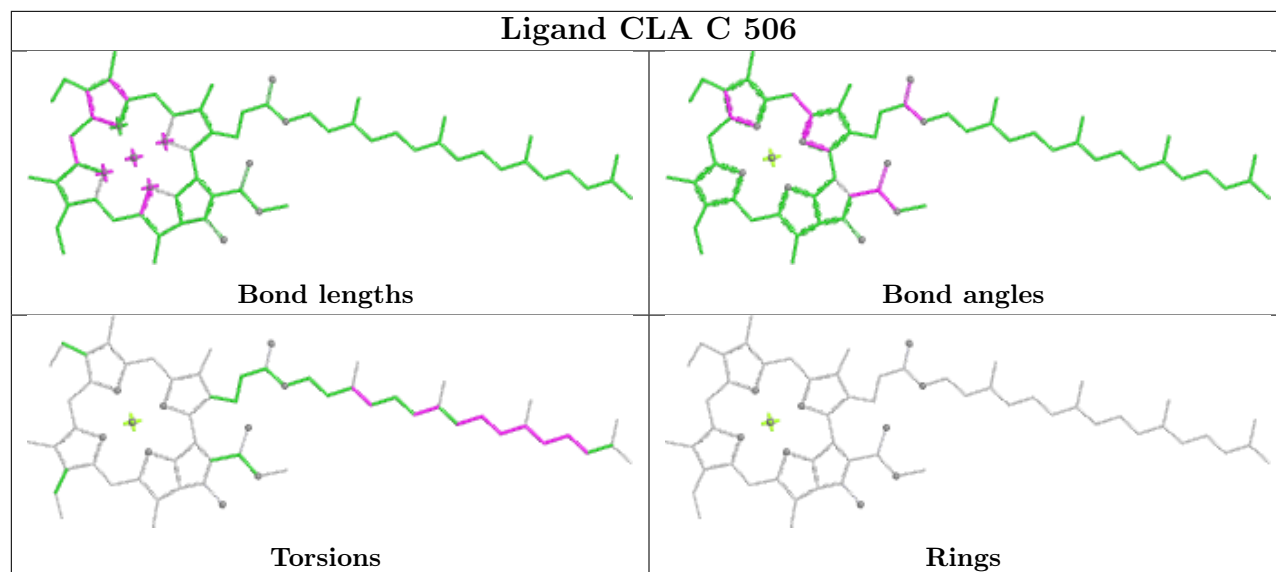
Ligand CLA c 507



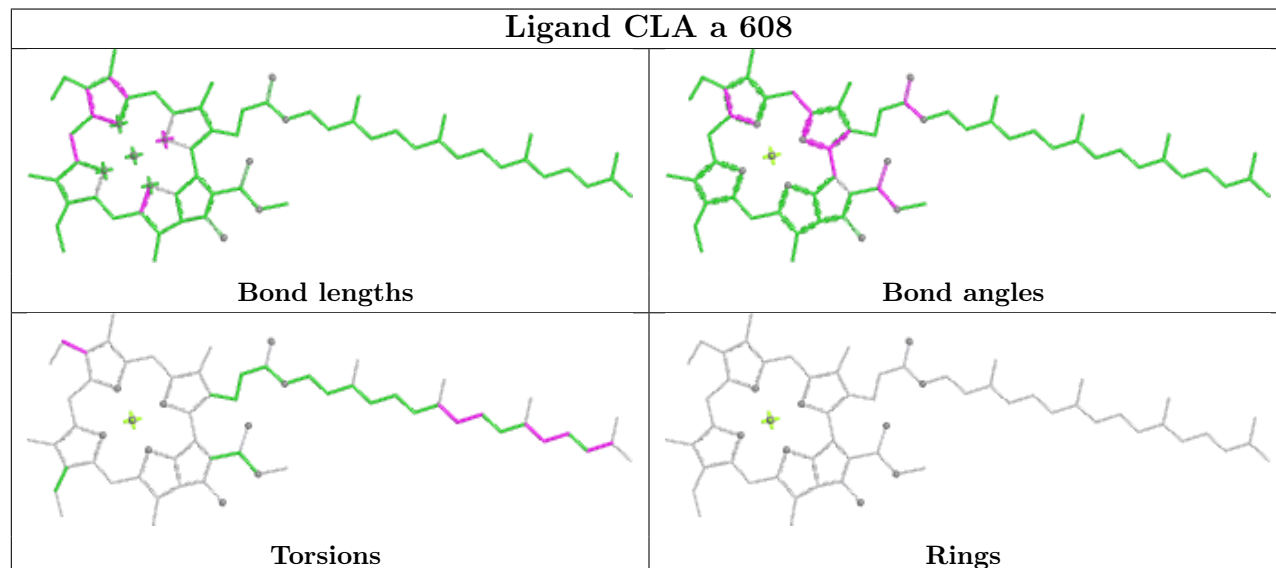
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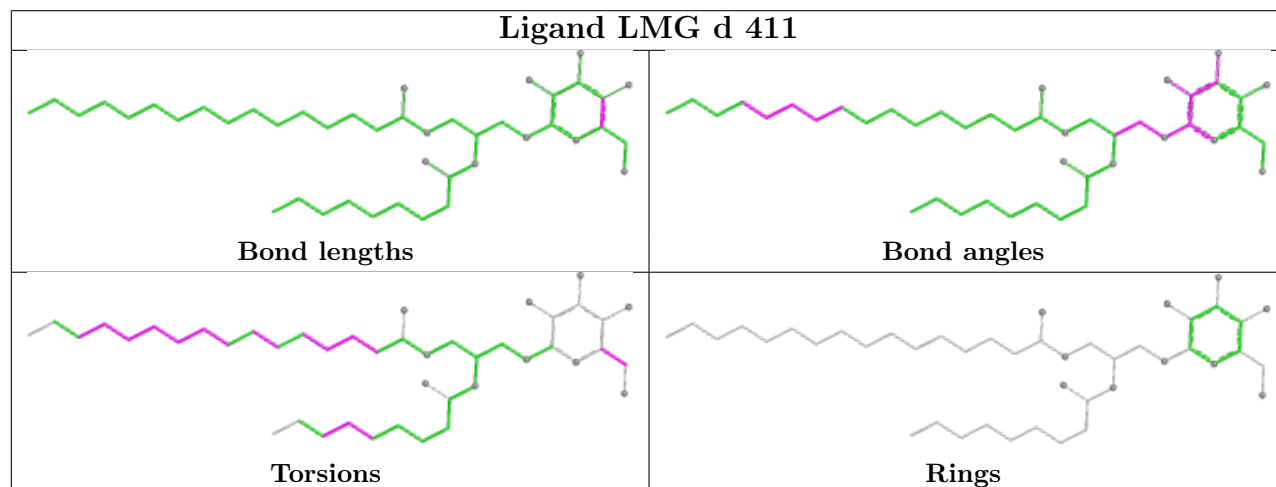
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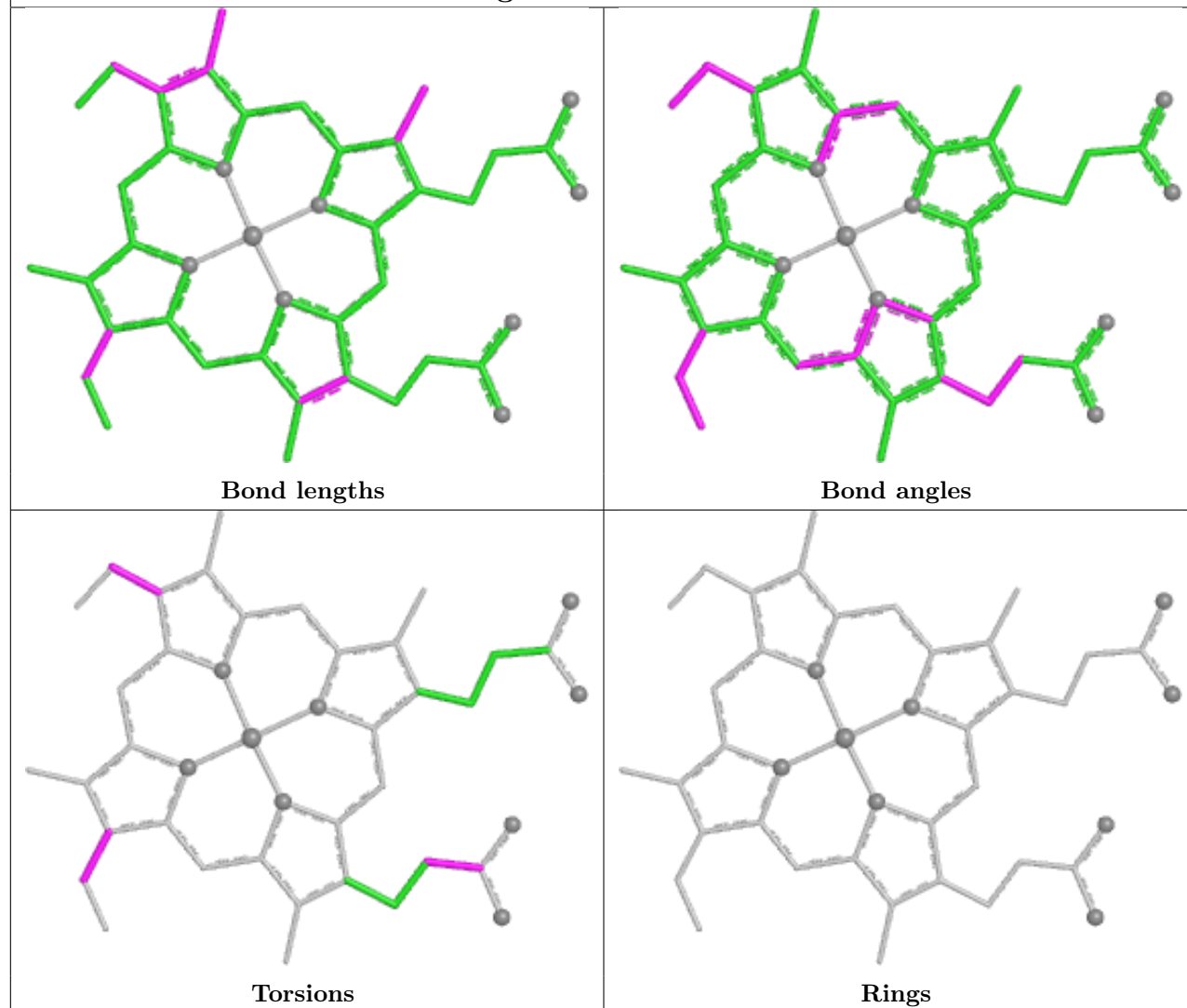
Ligand CLA a 608



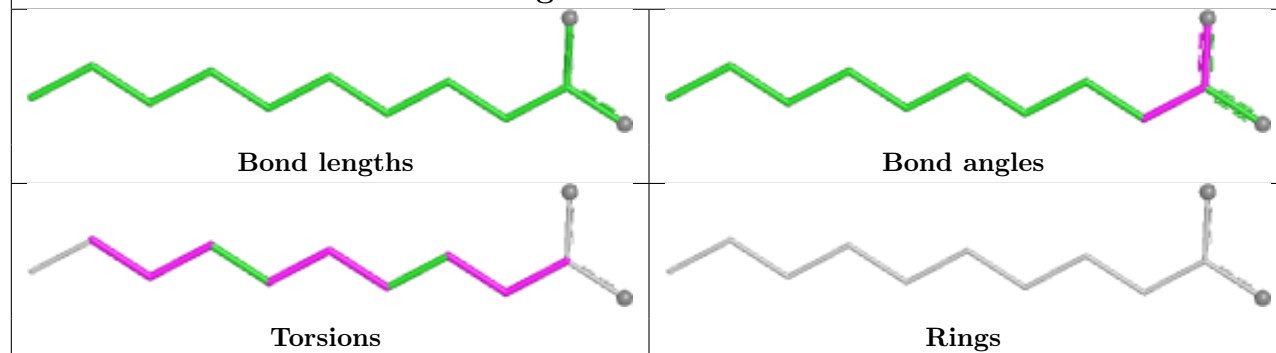
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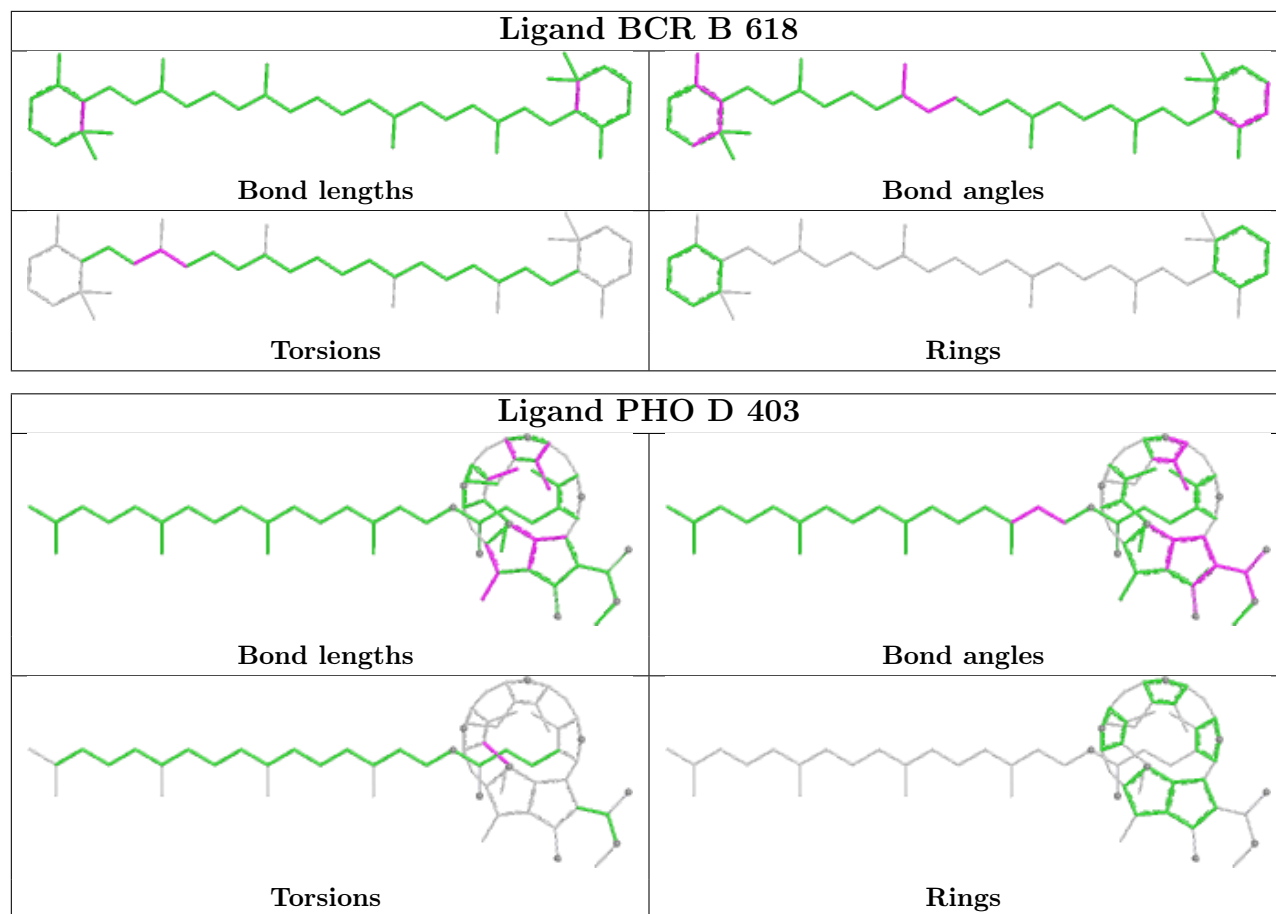


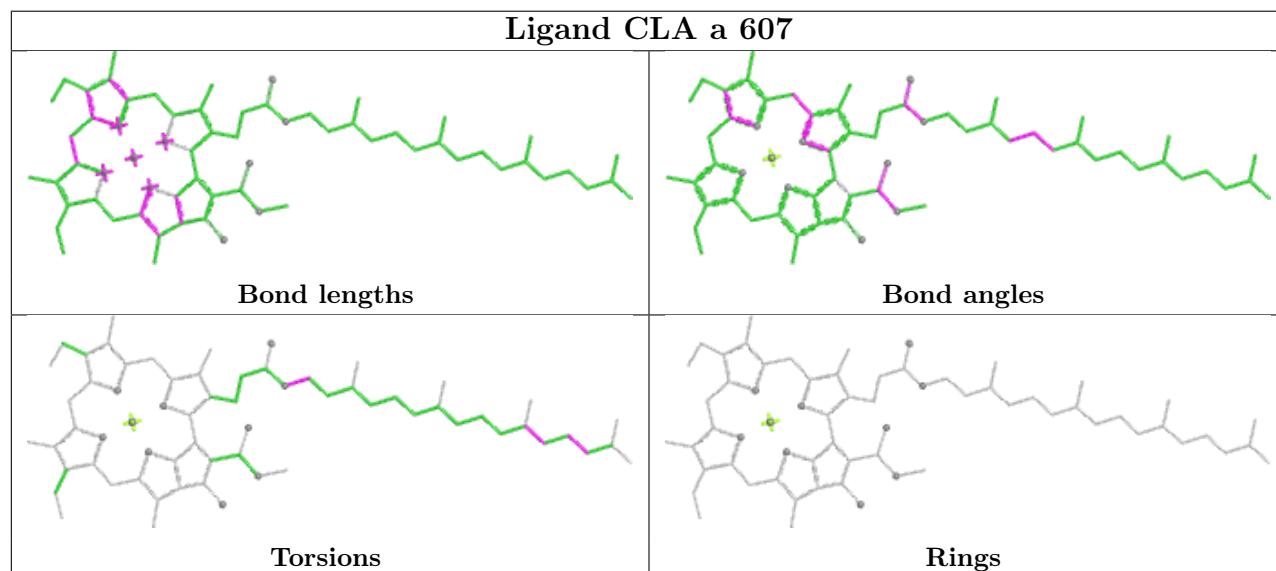
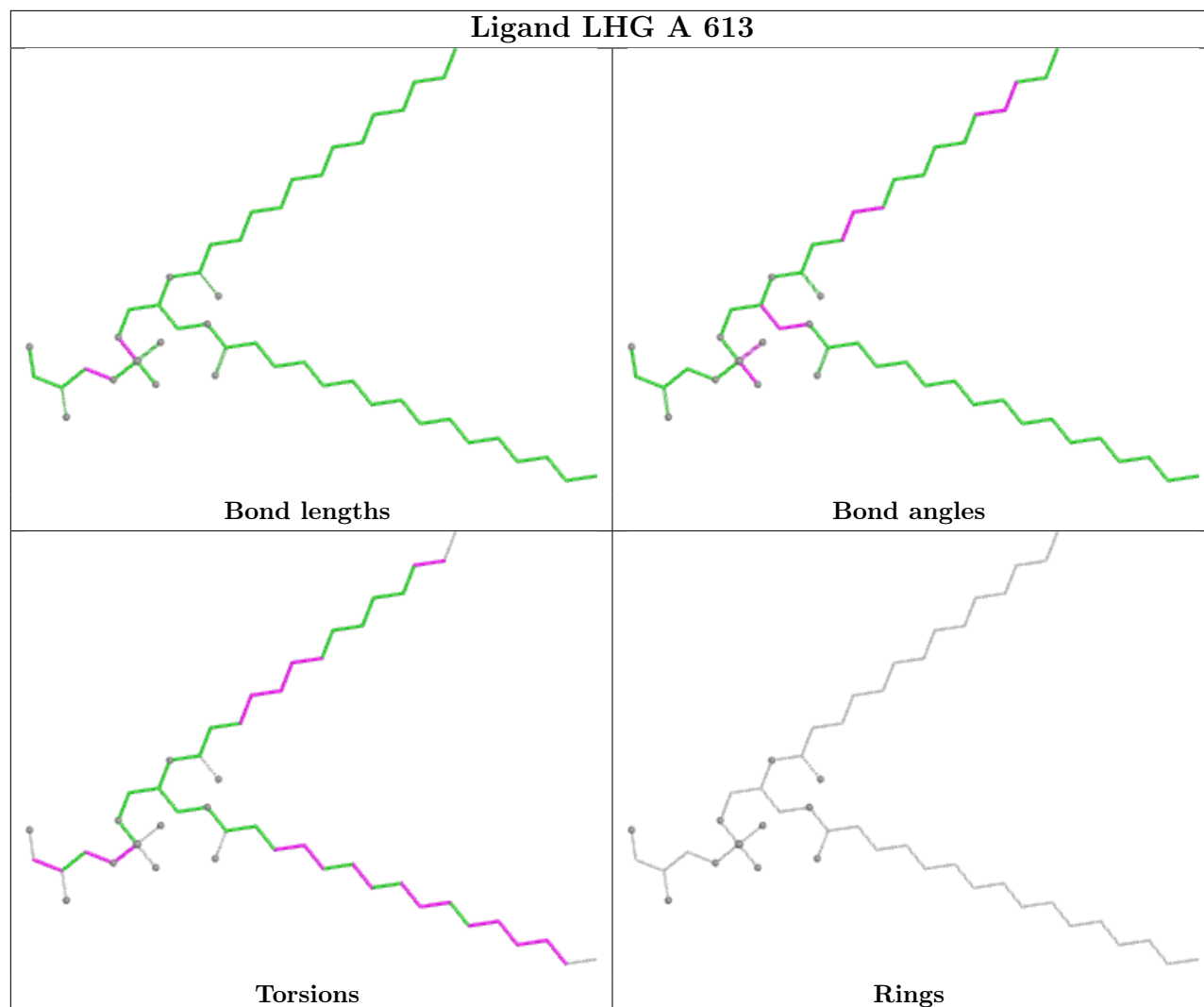
Ligand HEC v 201

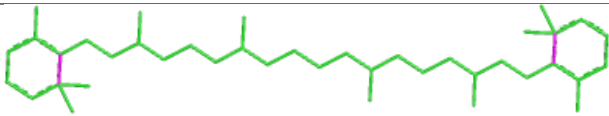
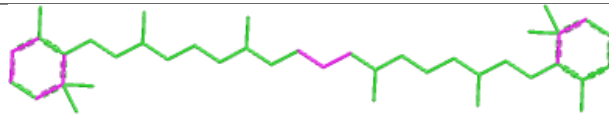
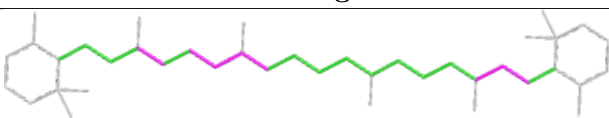
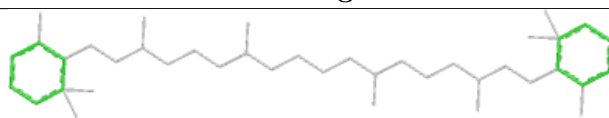


Ligand STE E 102

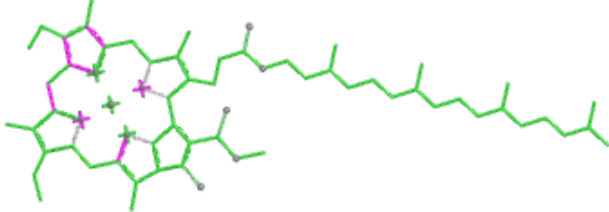
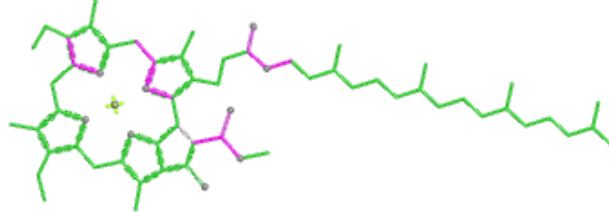
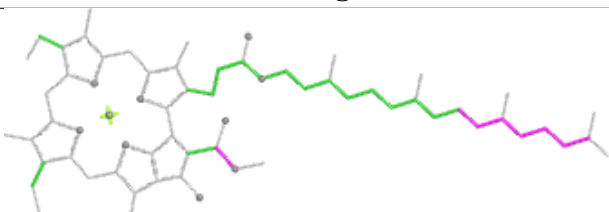
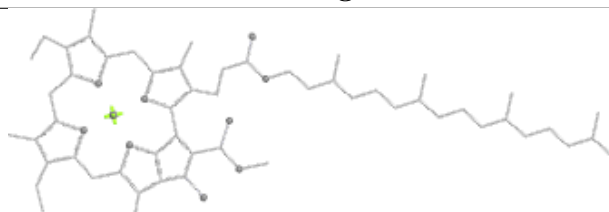


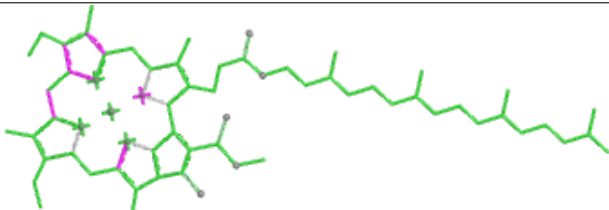
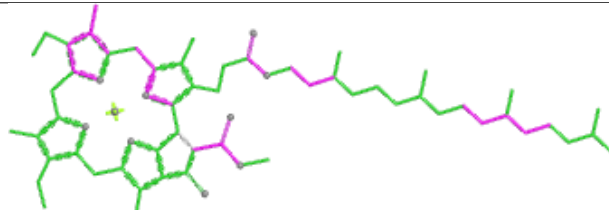
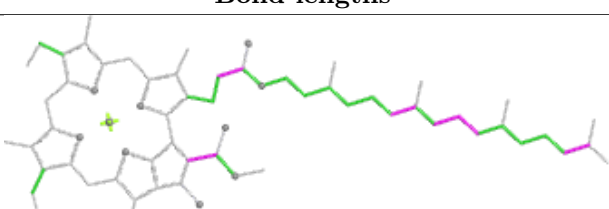
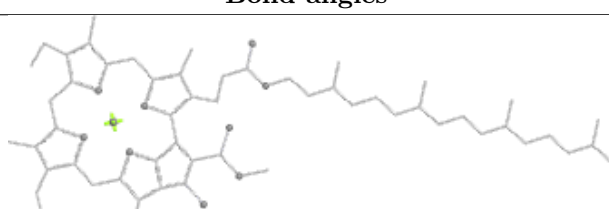


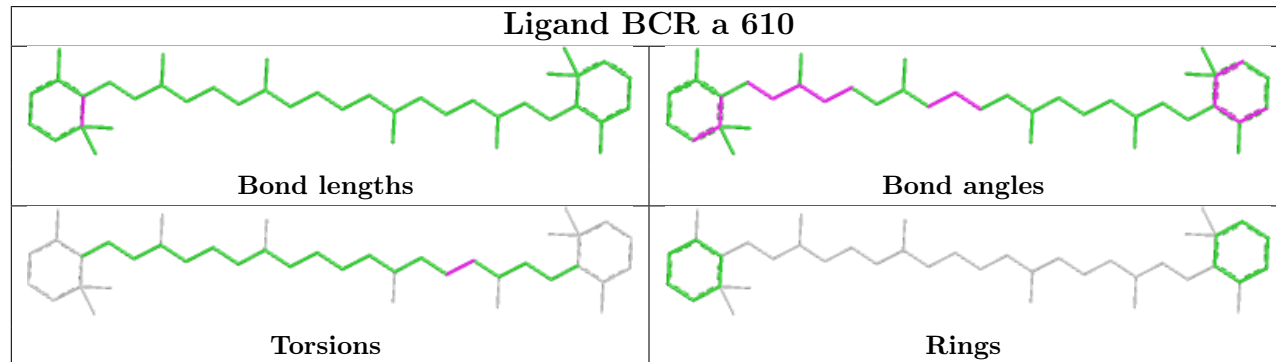
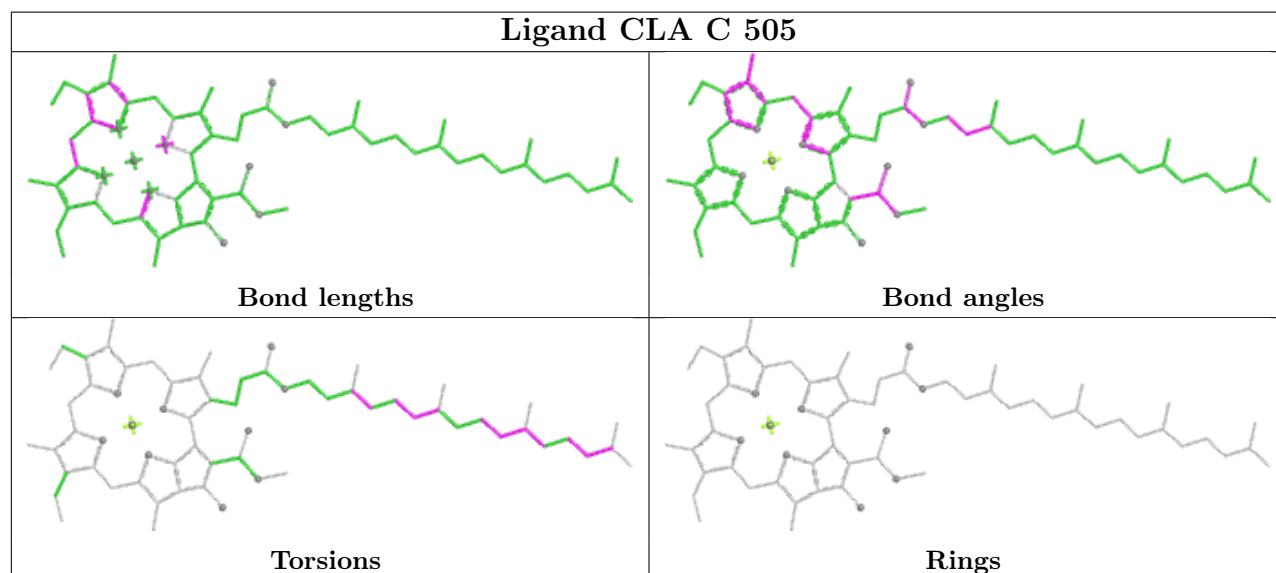
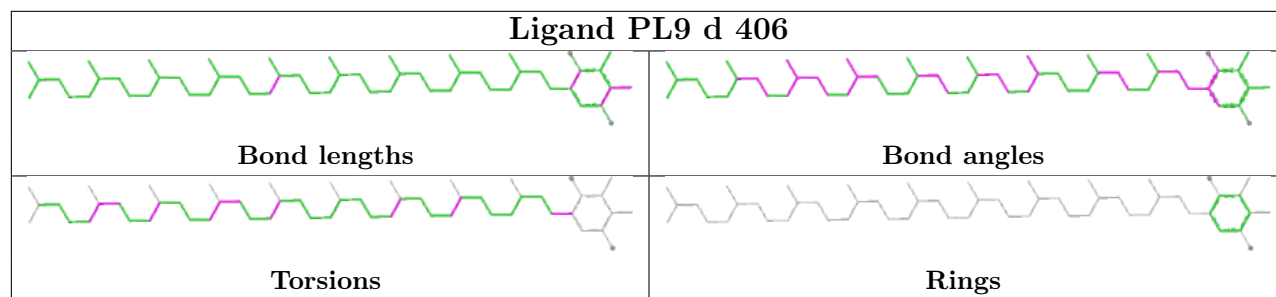


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

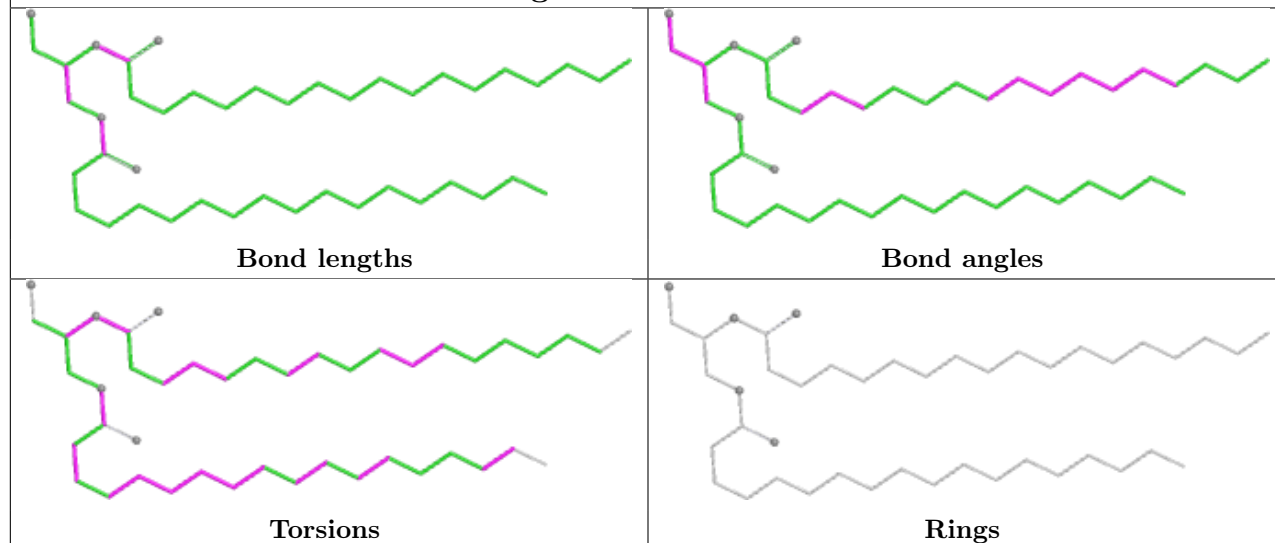
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

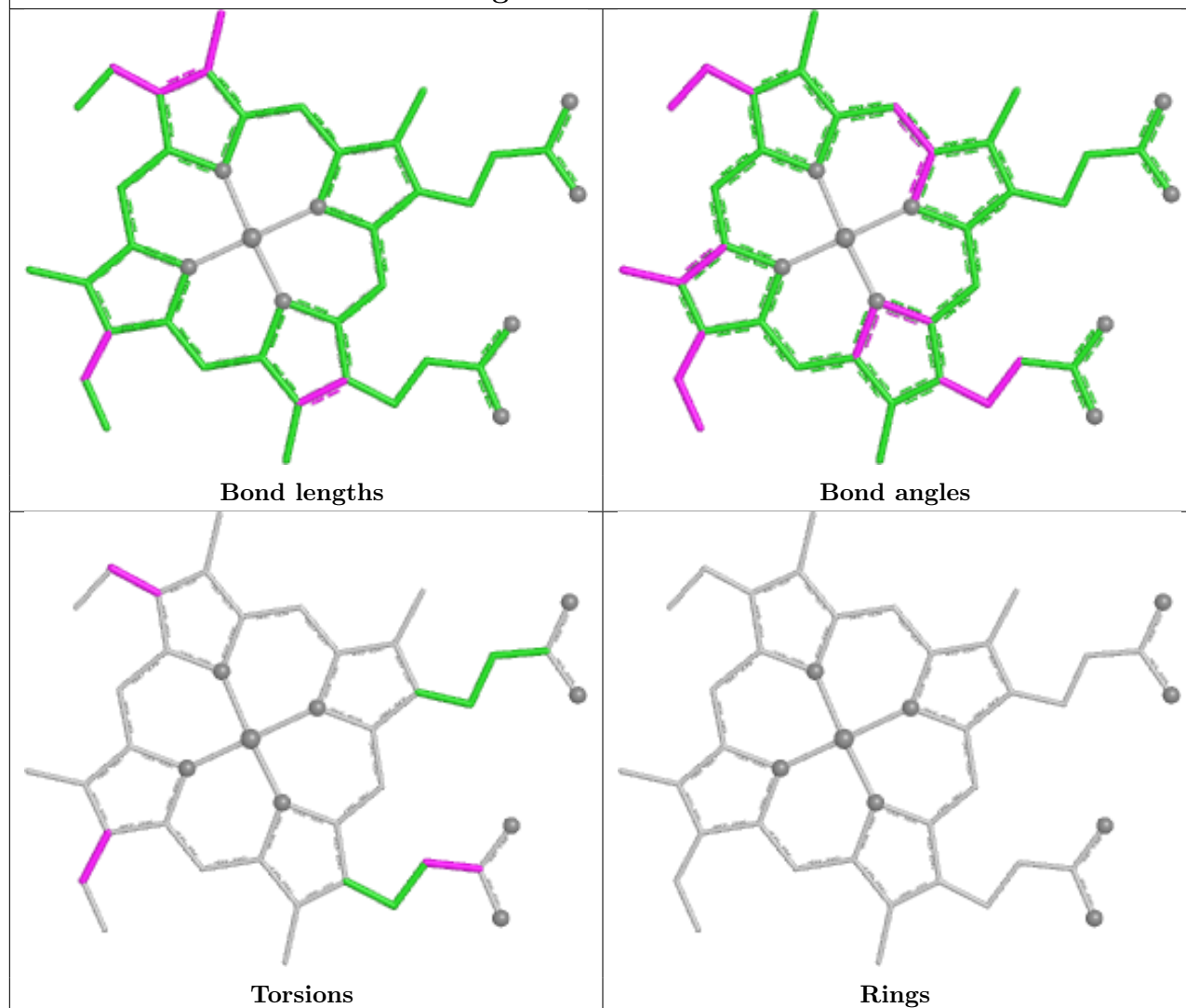
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

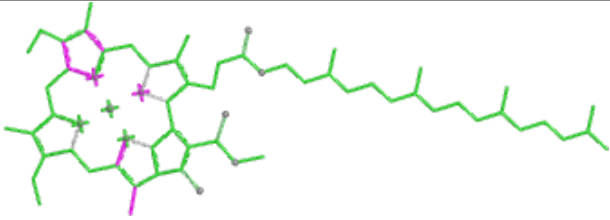
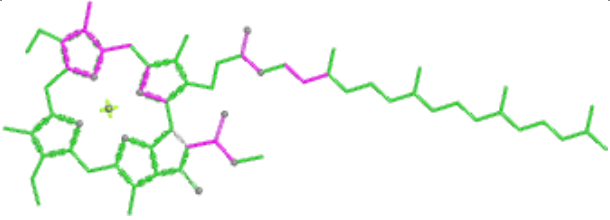
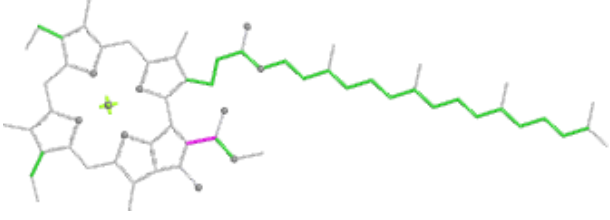
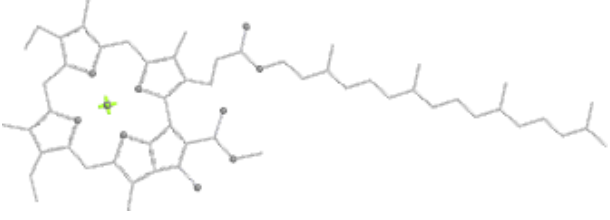
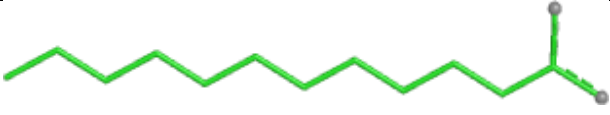
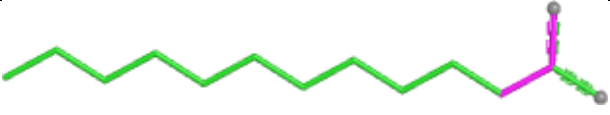
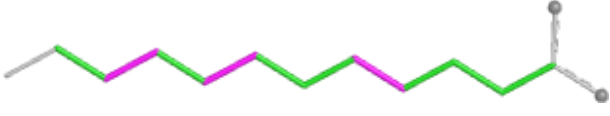
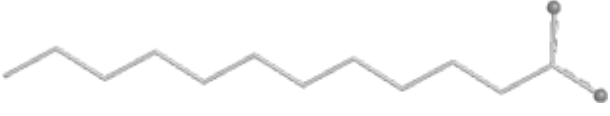
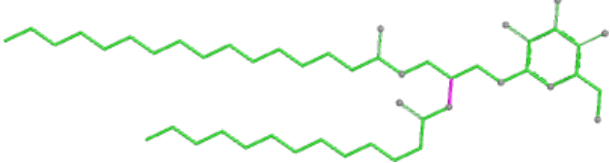
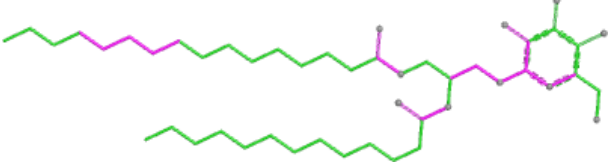
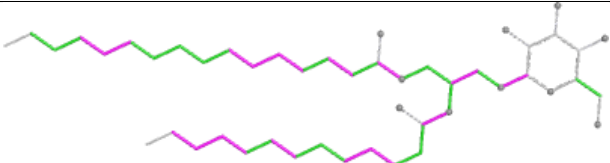
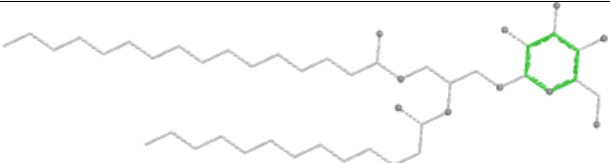


Ligand DGD o 301

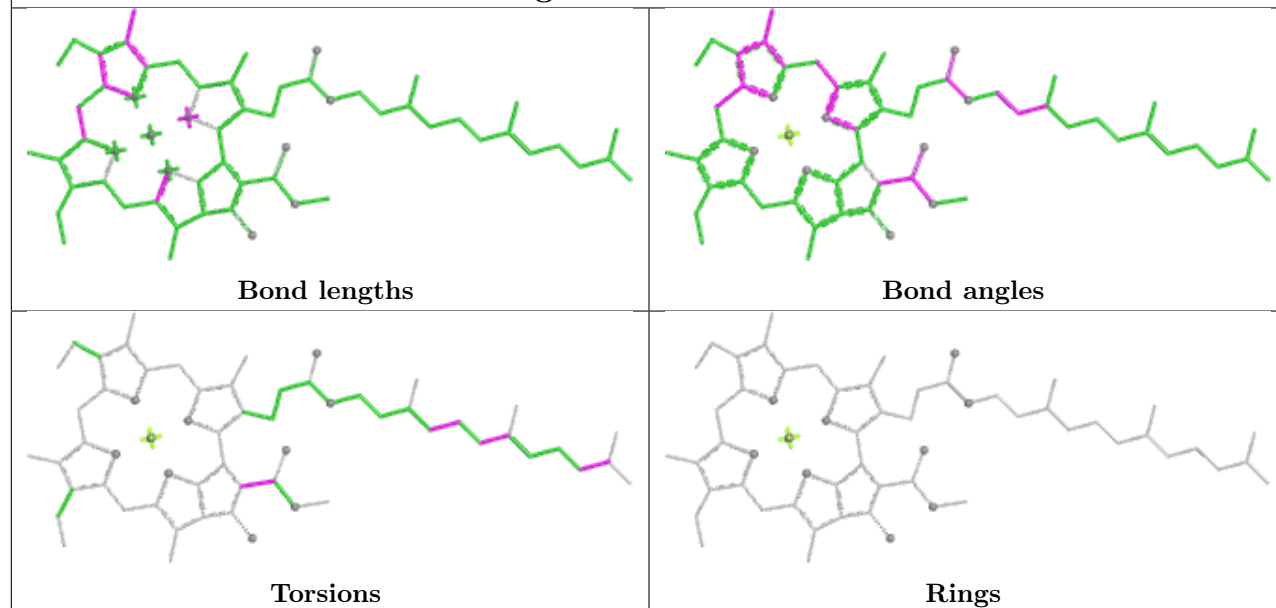


Ligand HEC V 201

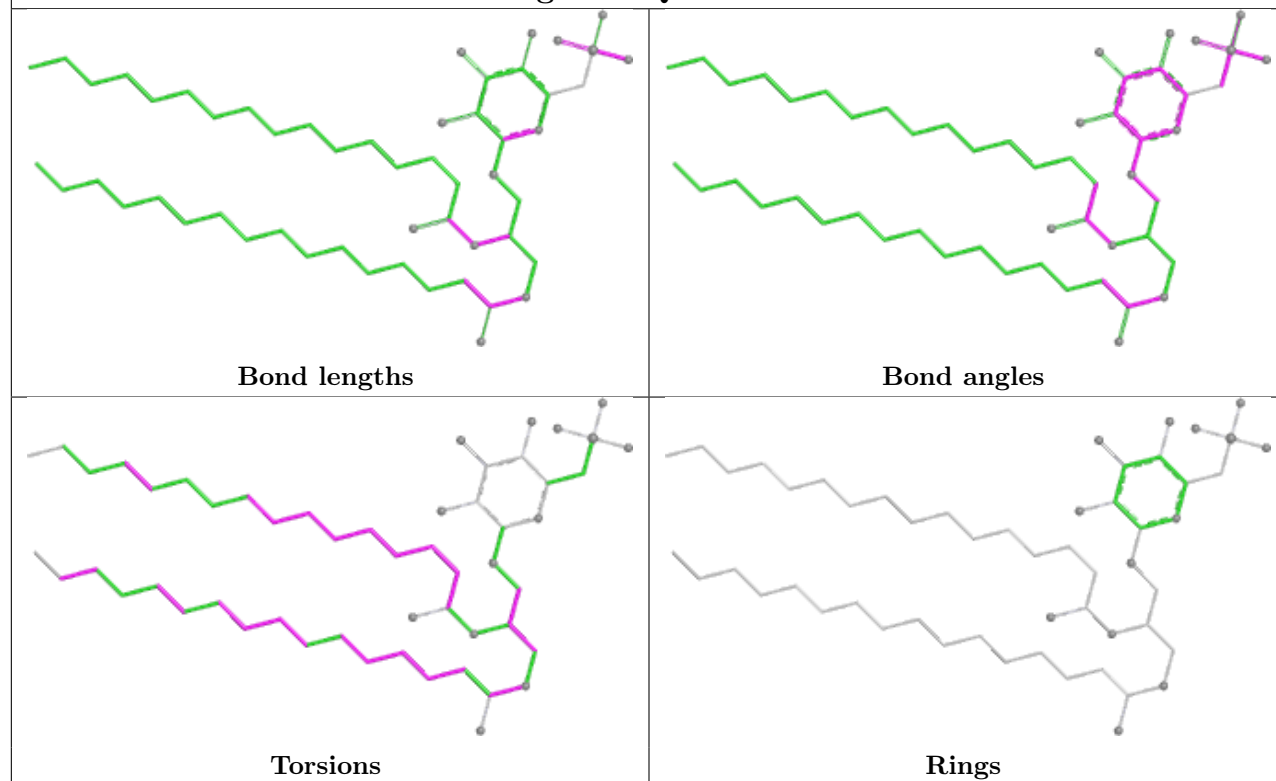


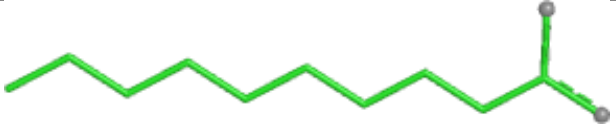
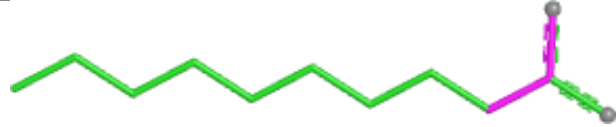
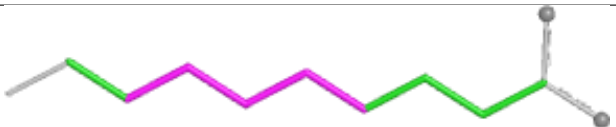
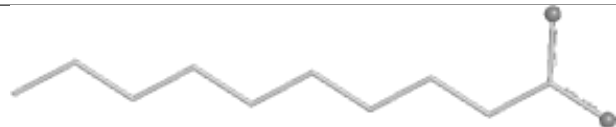
Ligand CLA c 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE t 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

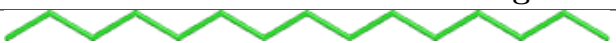
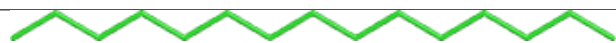
Ligand CLA b 616

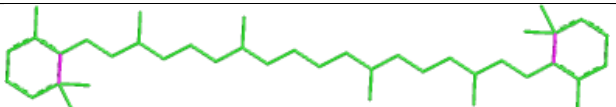
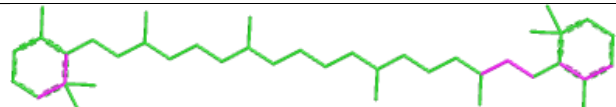
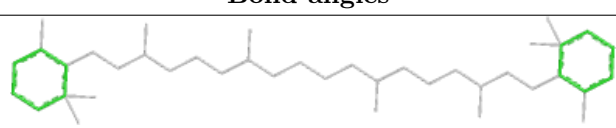


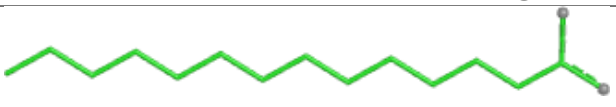
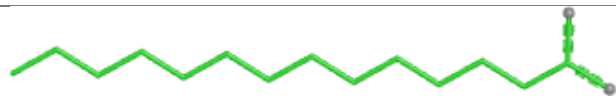
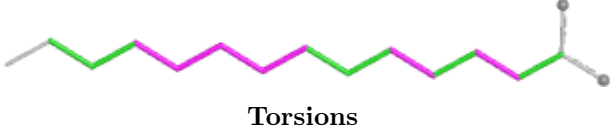
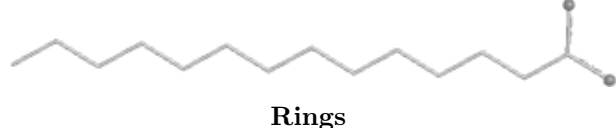
Ligand SQD a 613



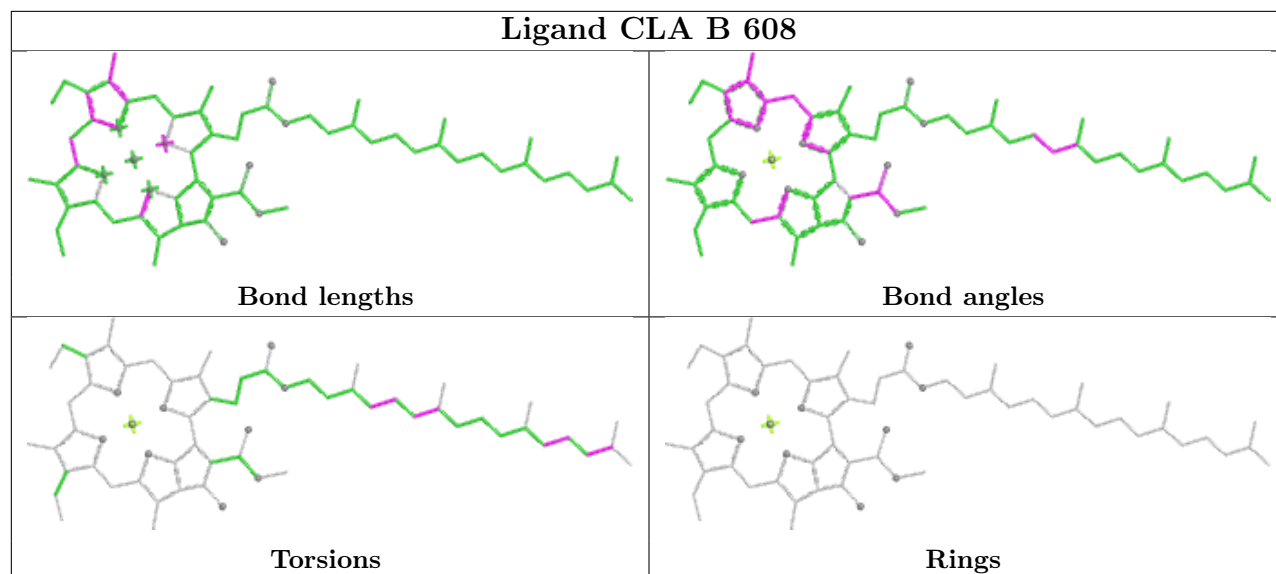
Ligand STE C 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

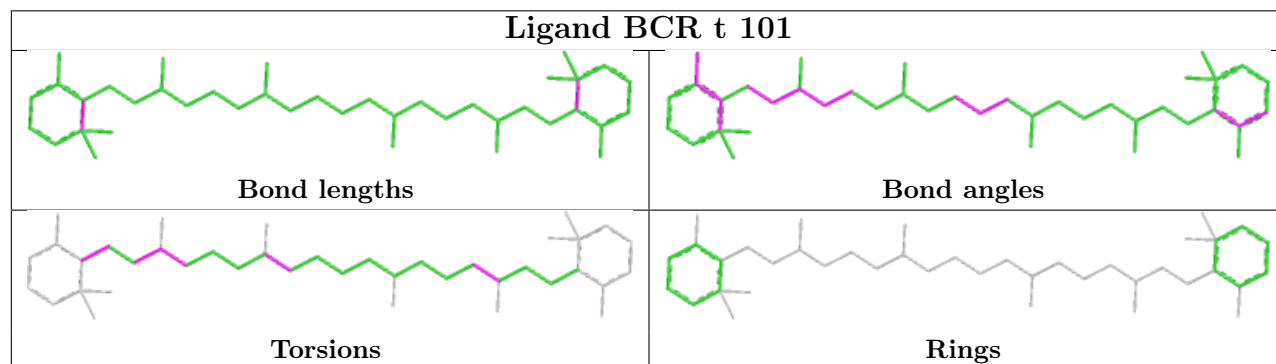
Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

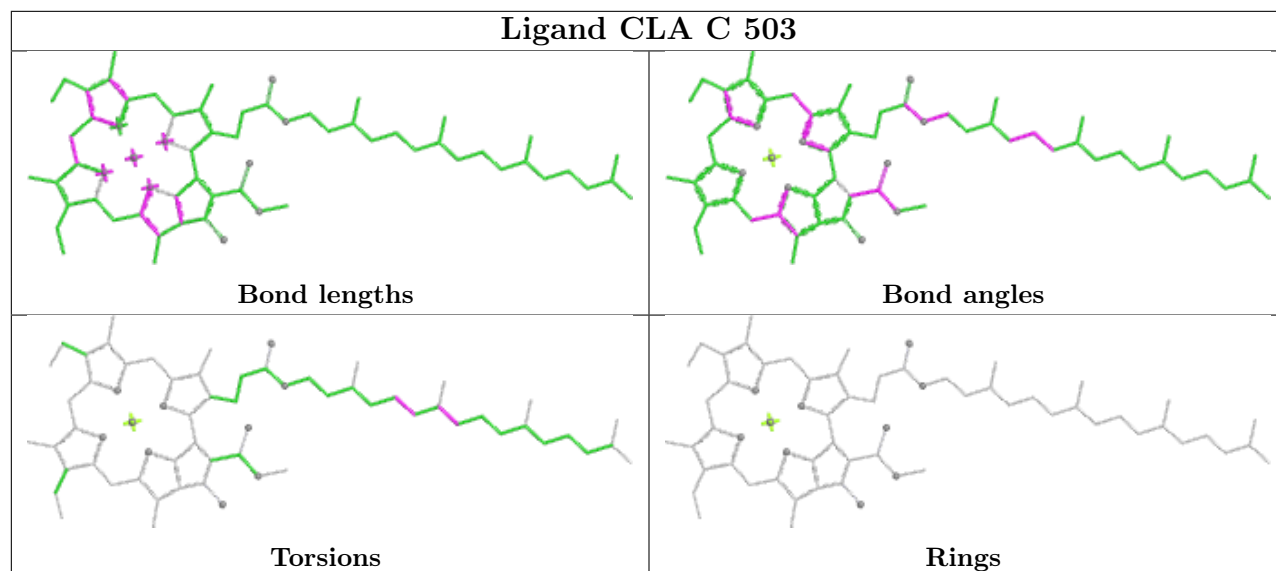
Ligand CLA B 608

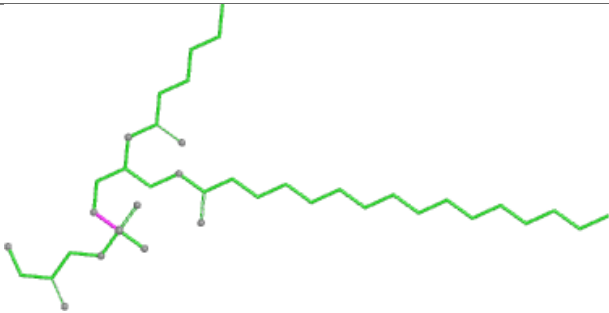
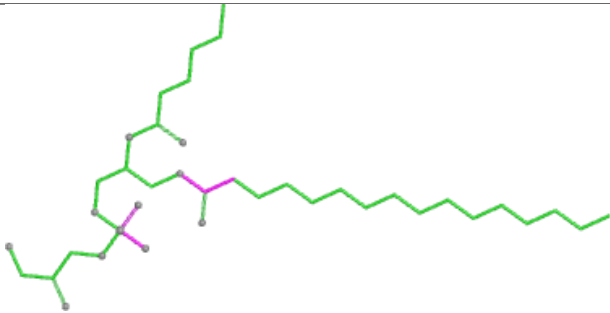
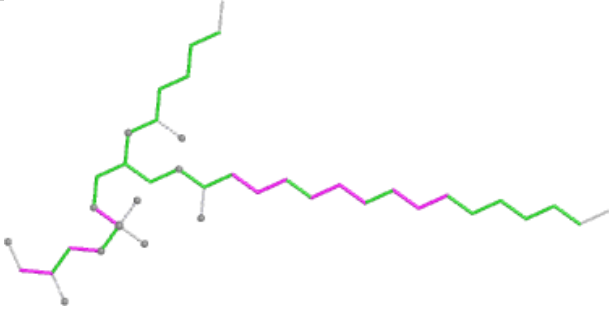
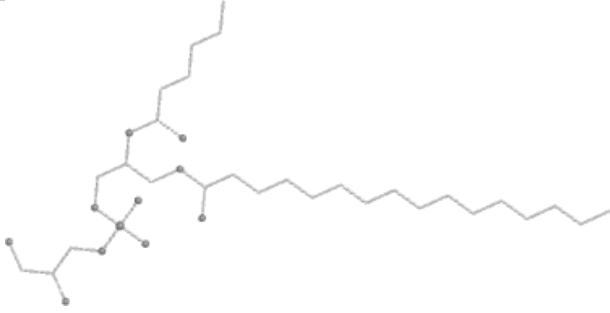


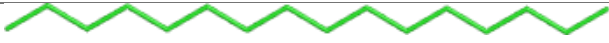
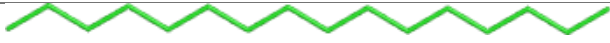
Ligand BCR t 101

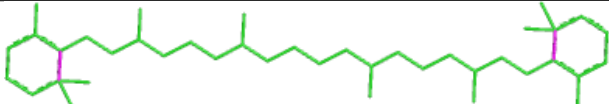
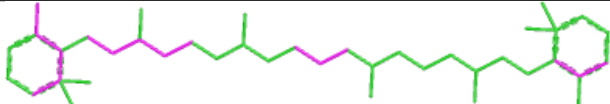
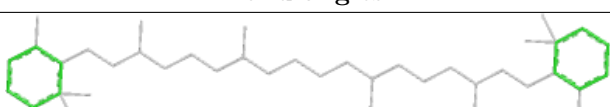


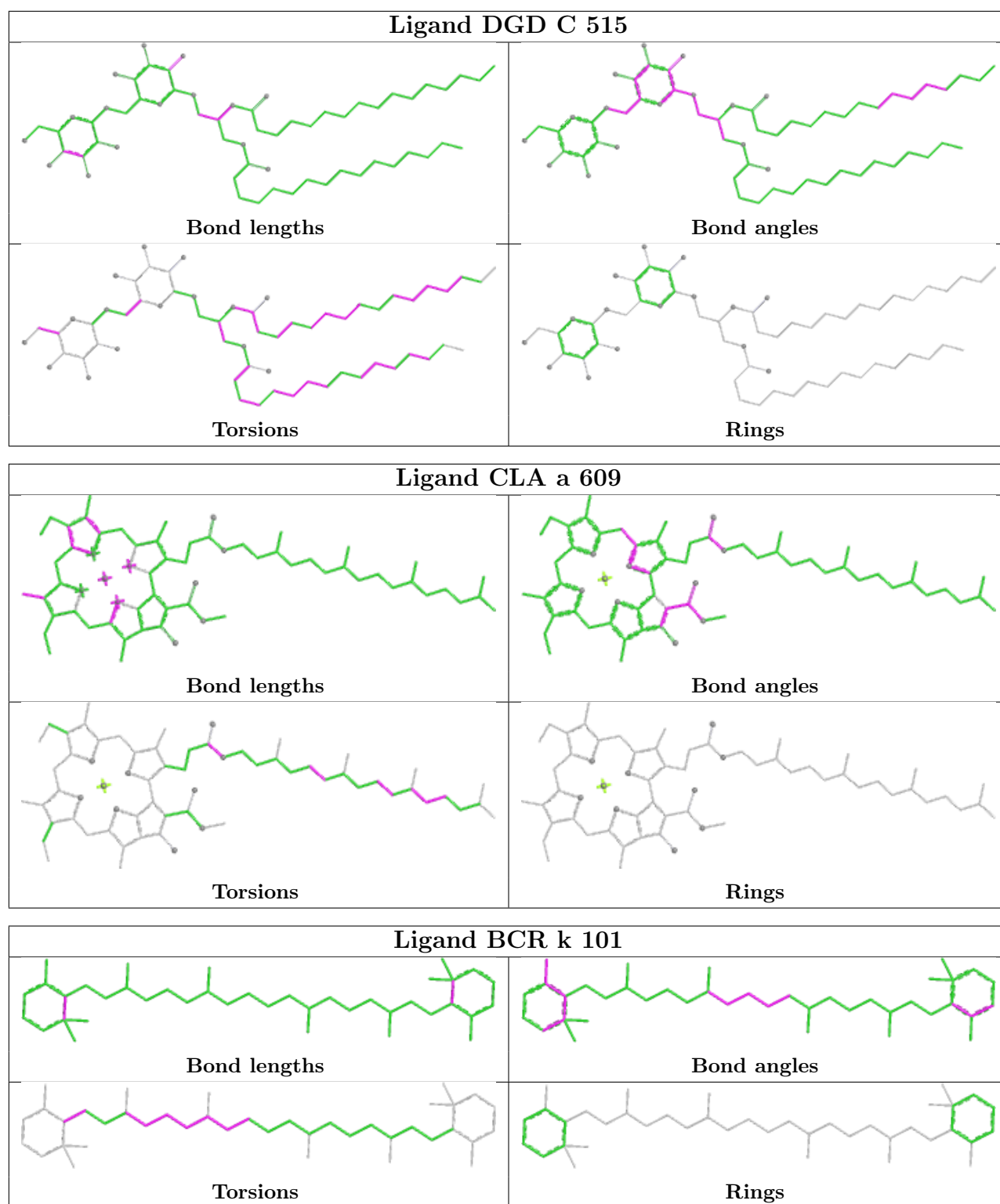
Ligand CLA C 503



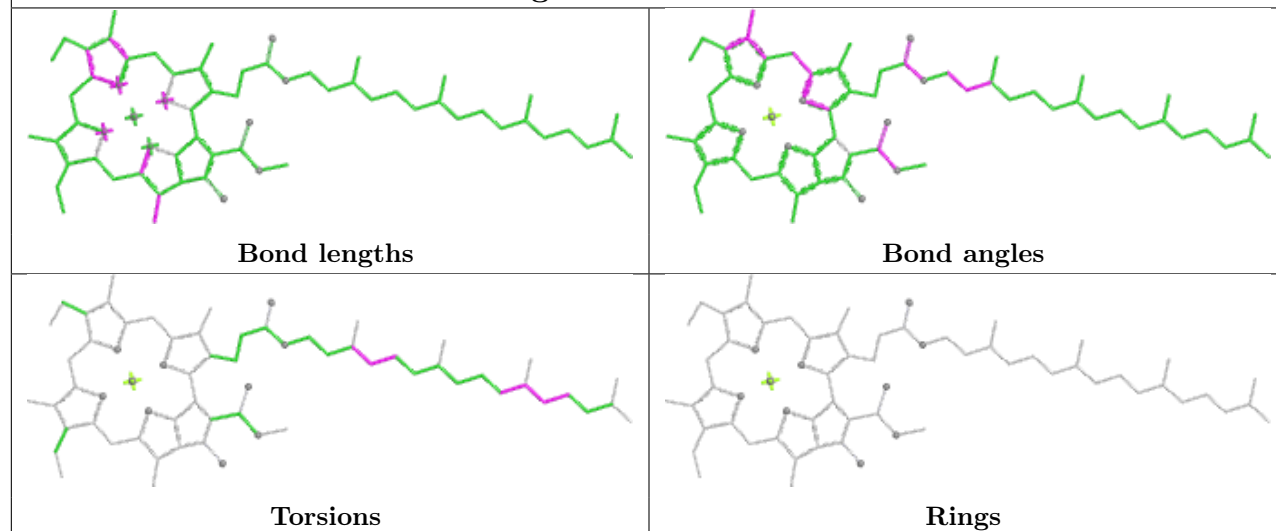
Ligand LHG d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

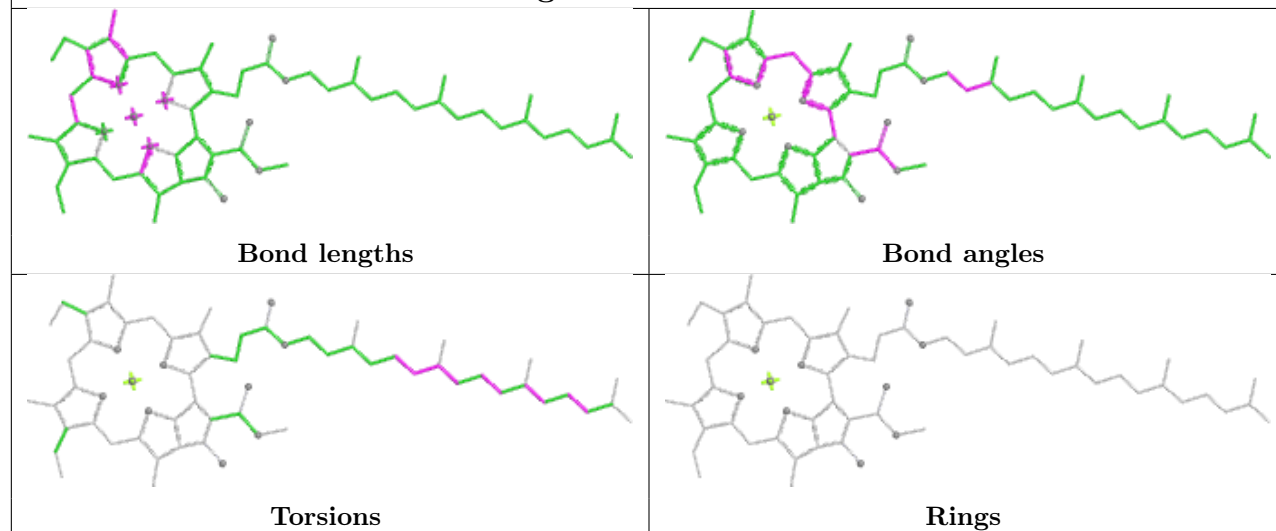
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings



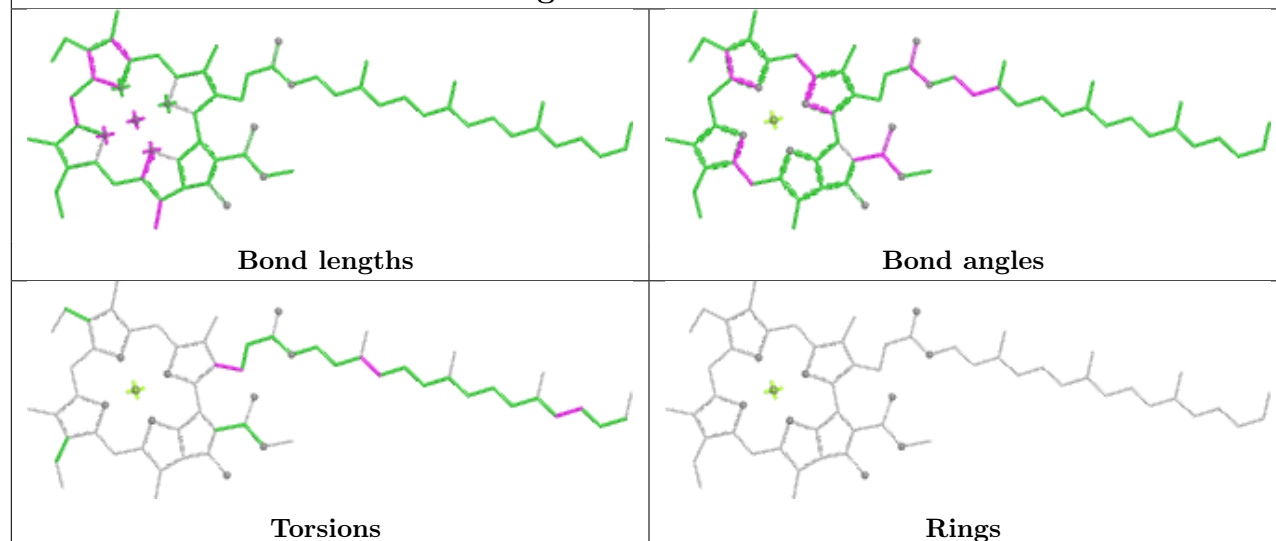
Ligand CLA D 405

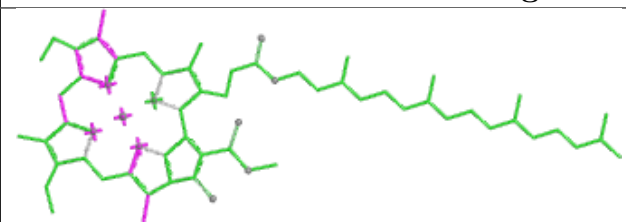
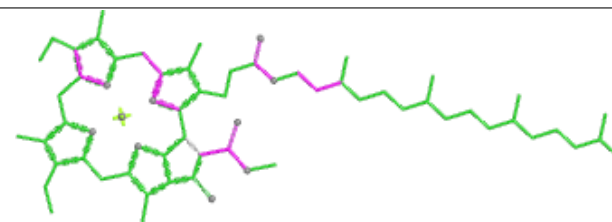
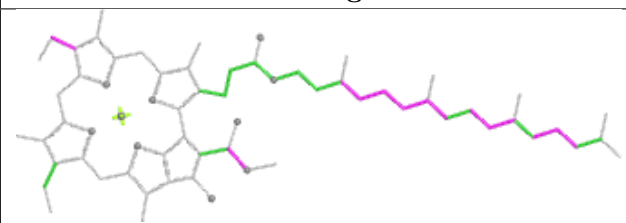
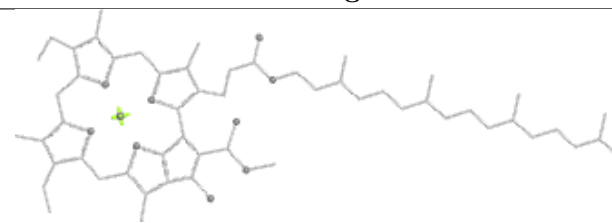
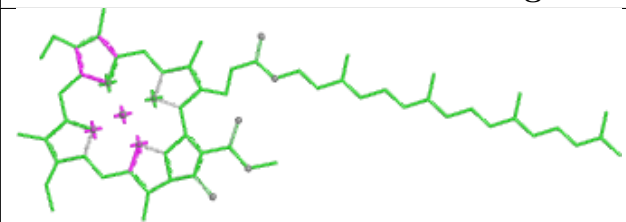
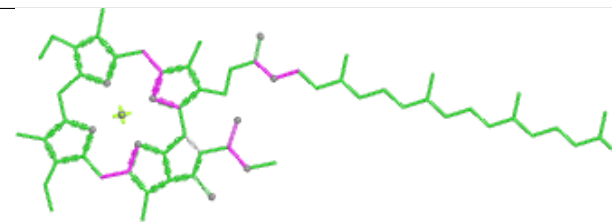
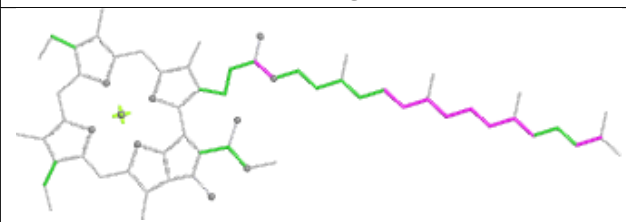
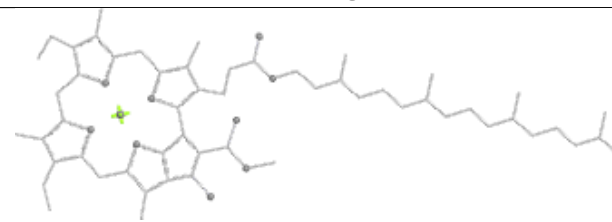
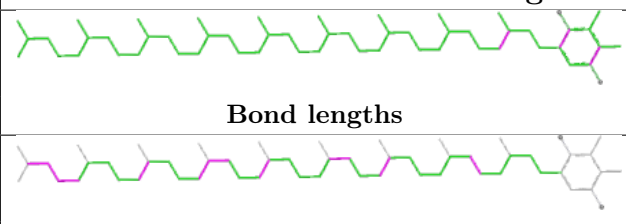
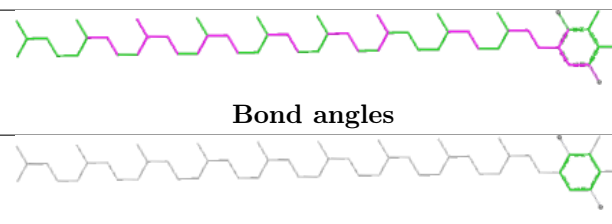
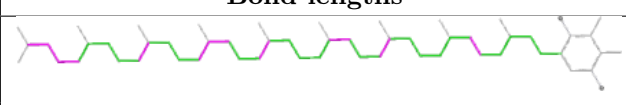
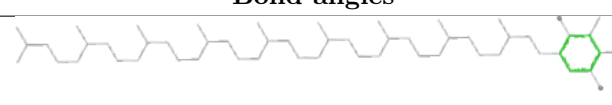


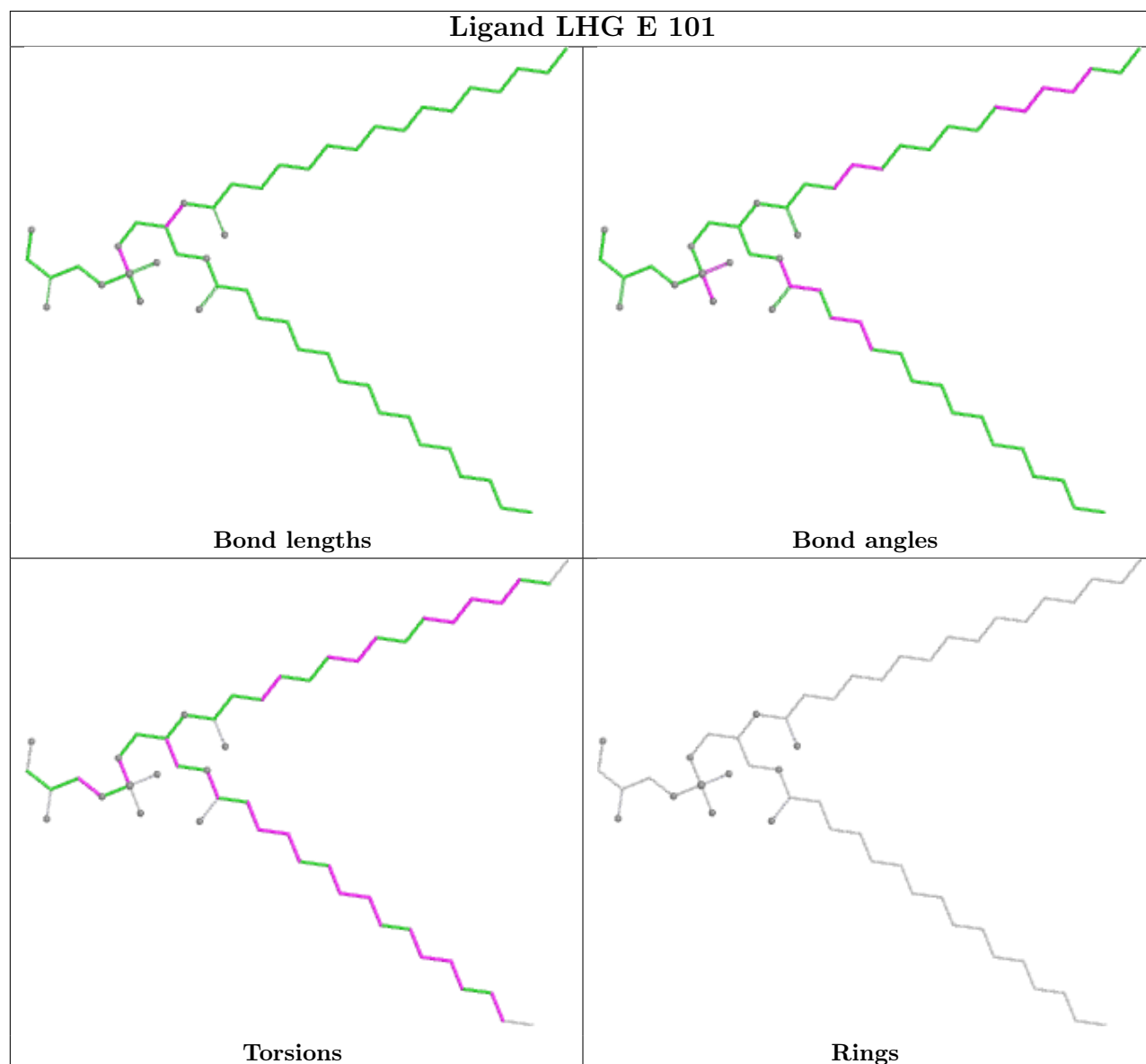
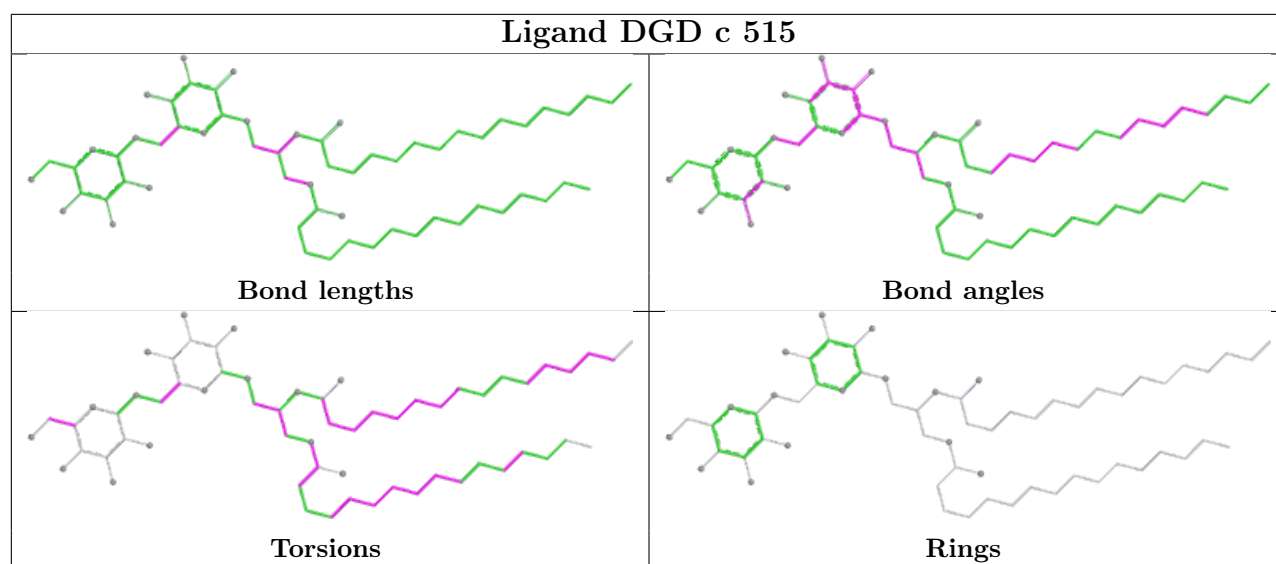
Ligand CLA c 505

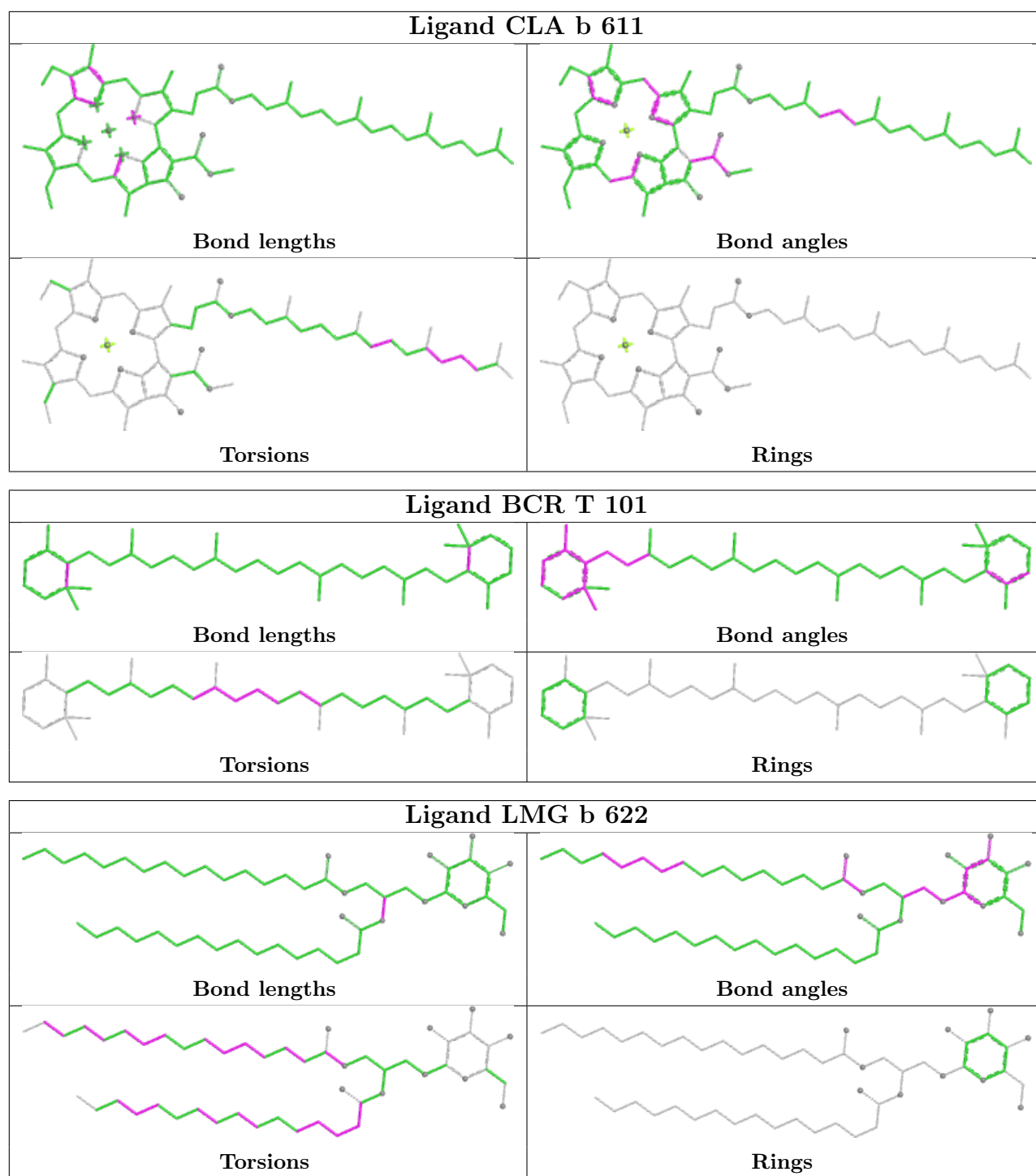


Ligand CLA c 508

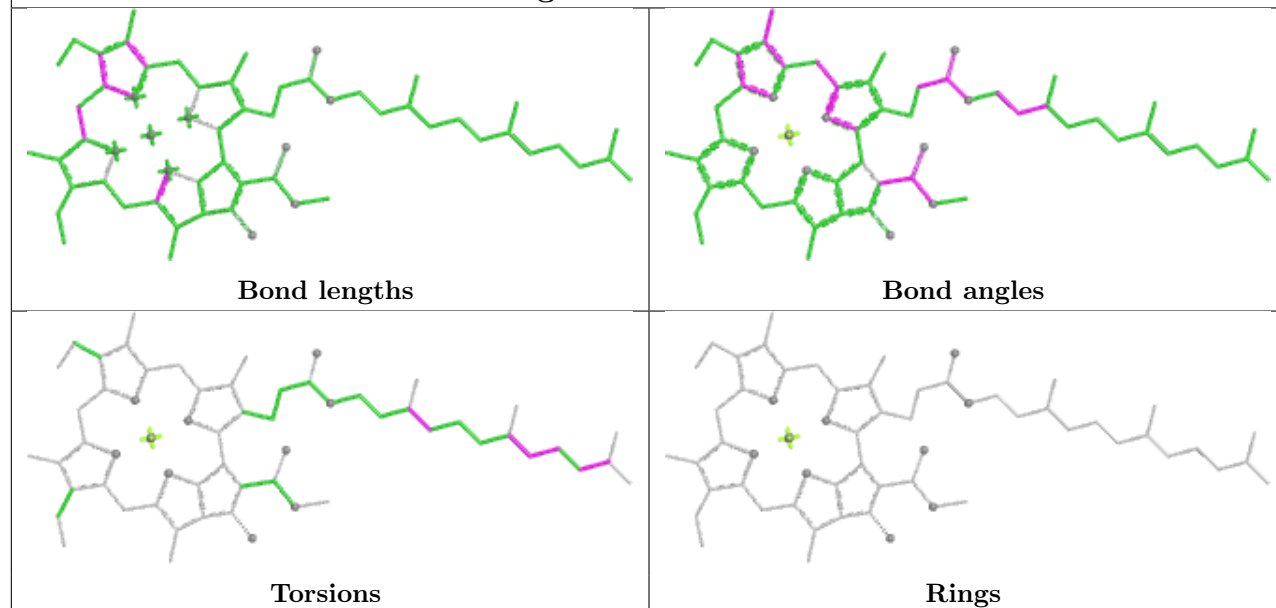


Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

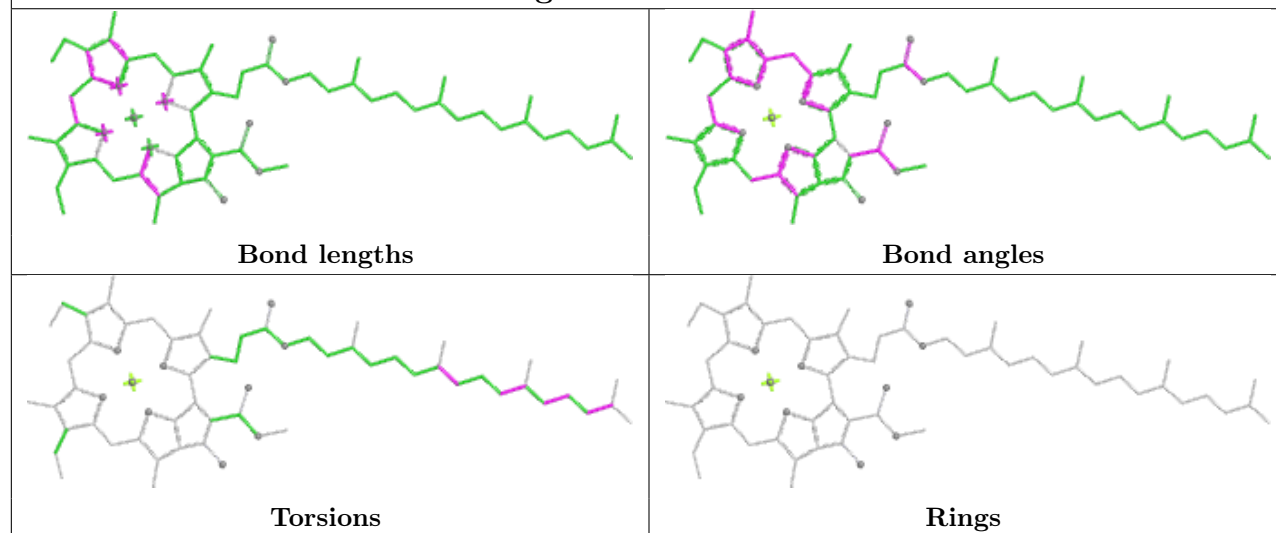


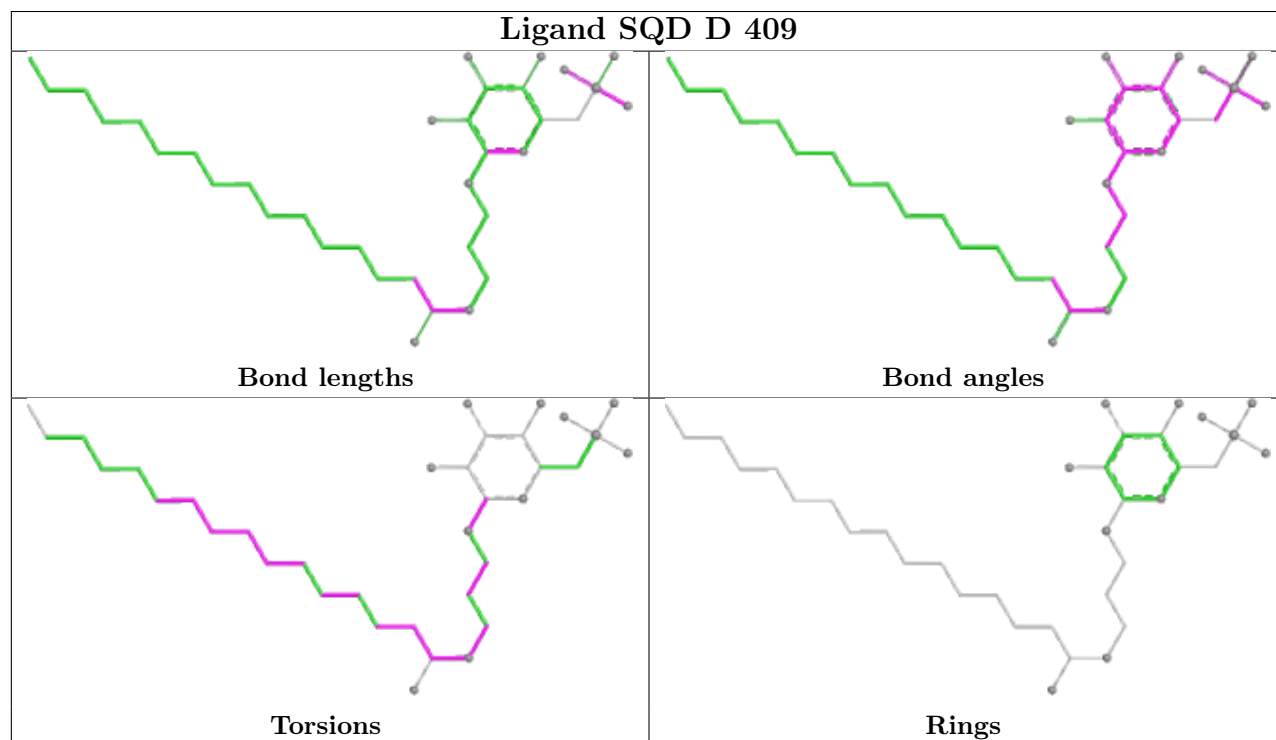
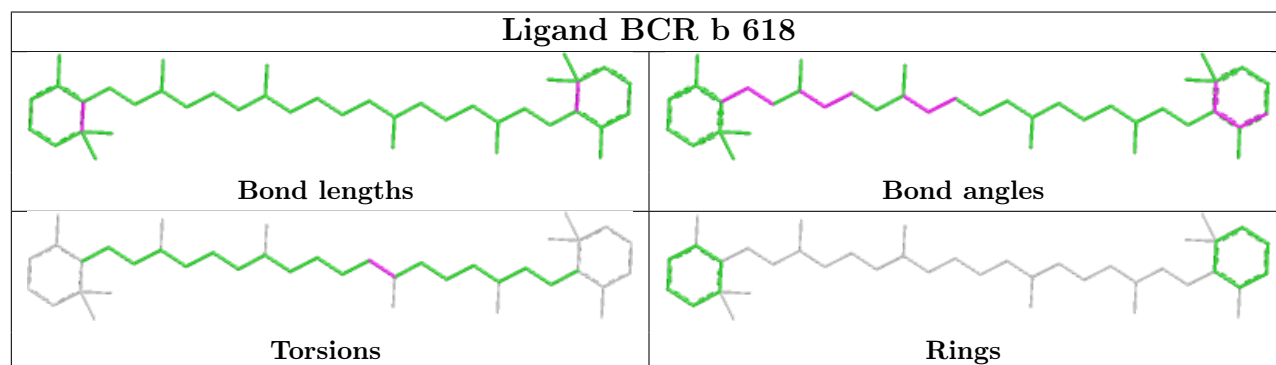
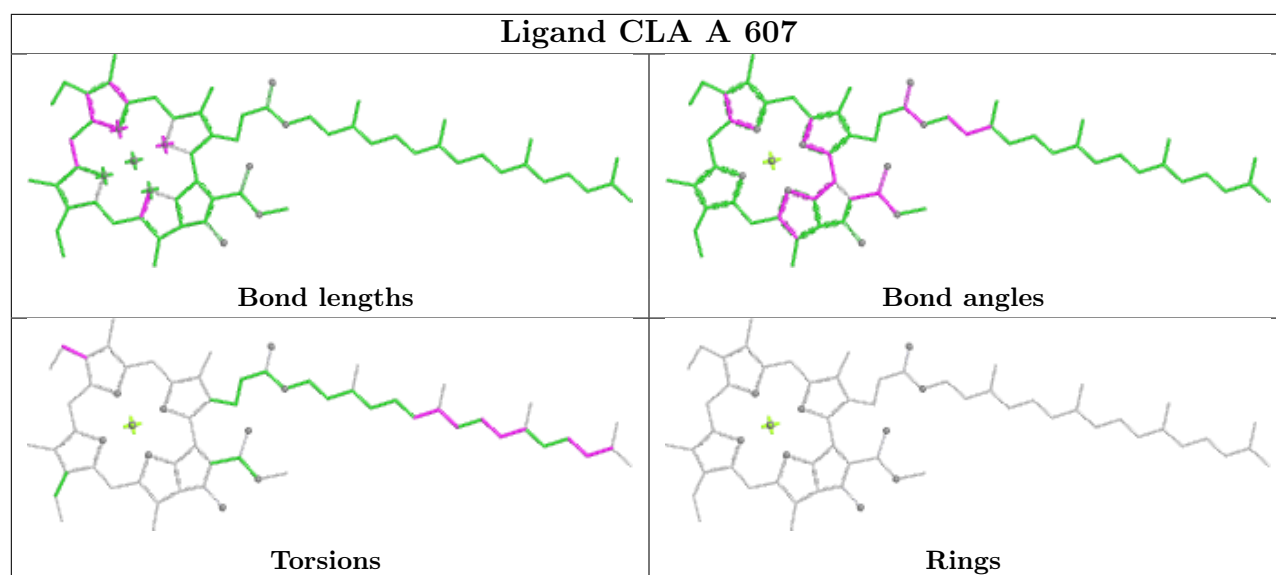


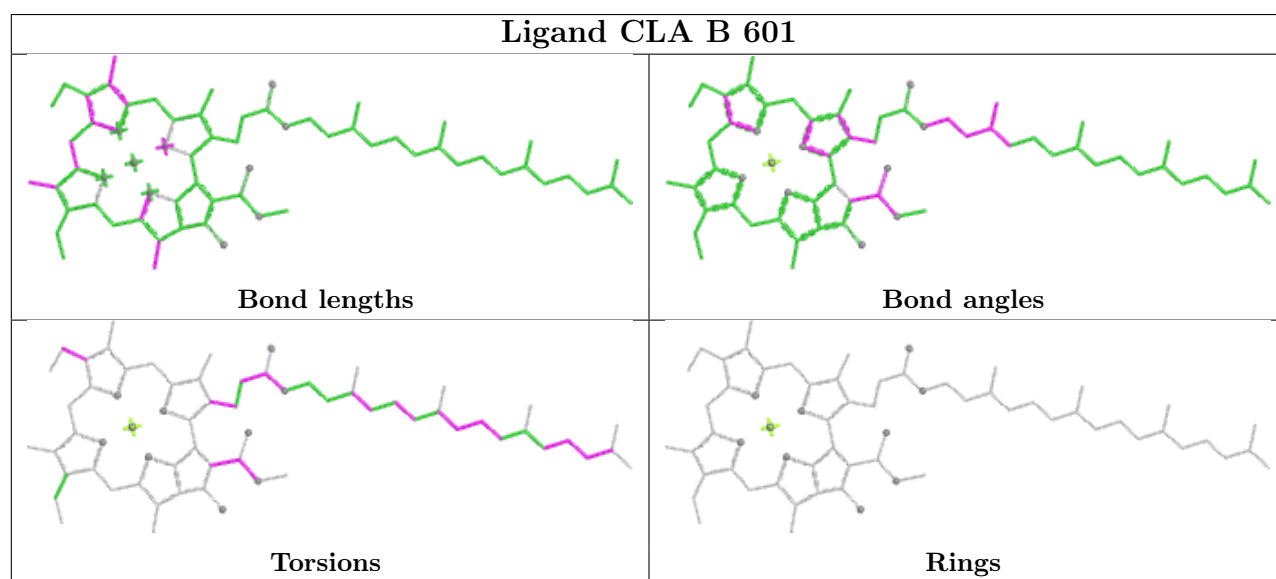
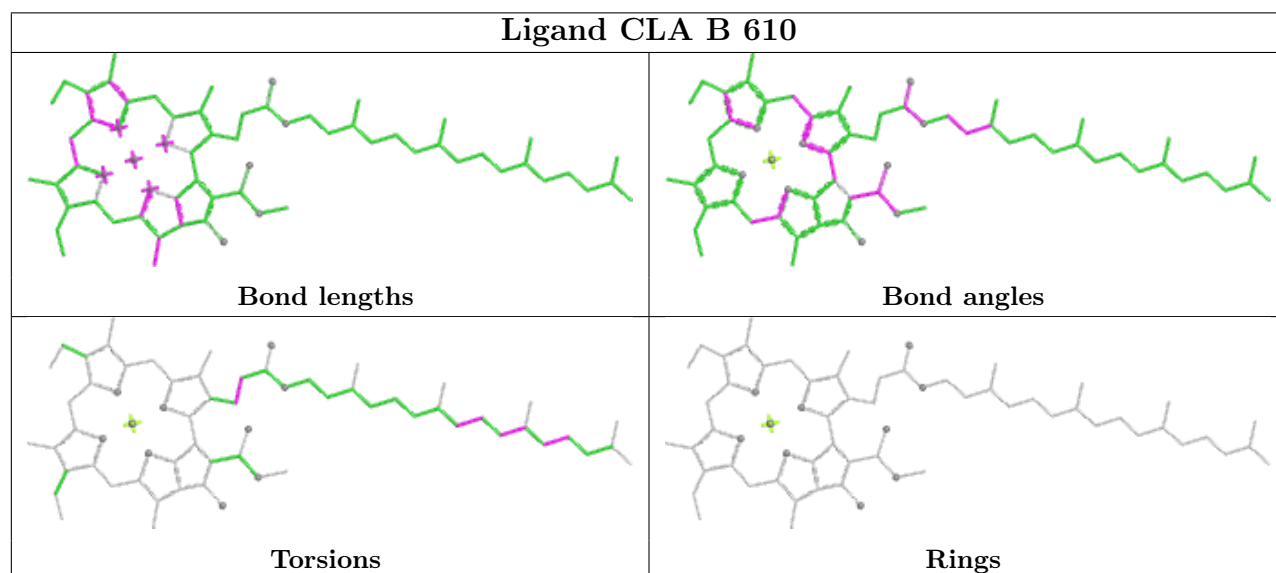
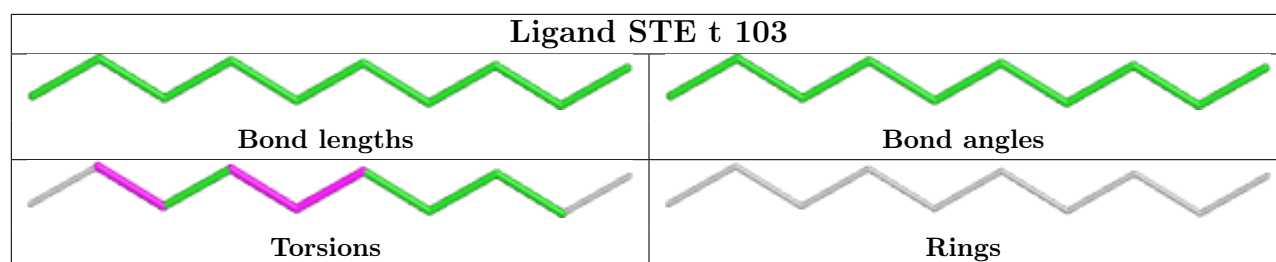
Ligand CLA c 504

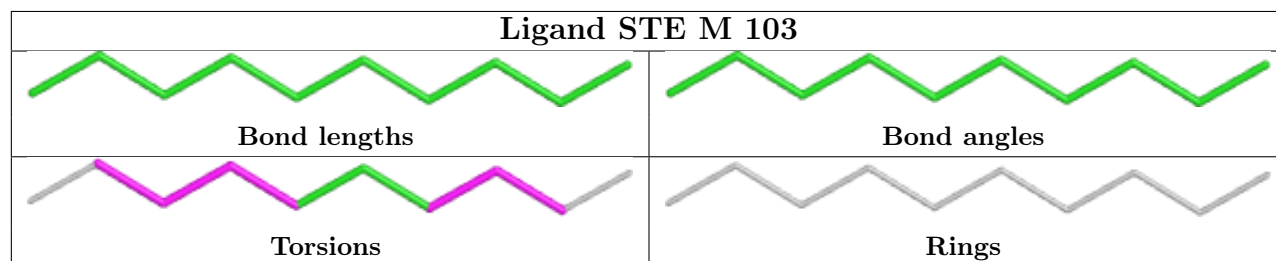
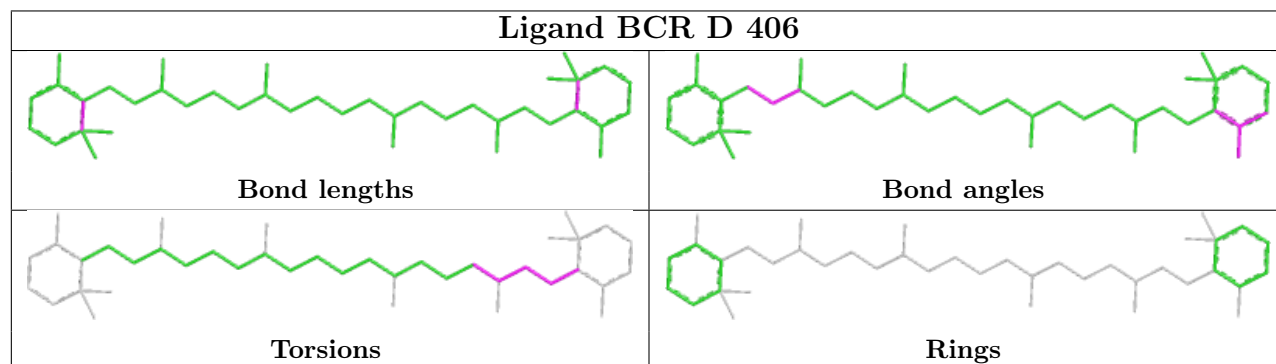
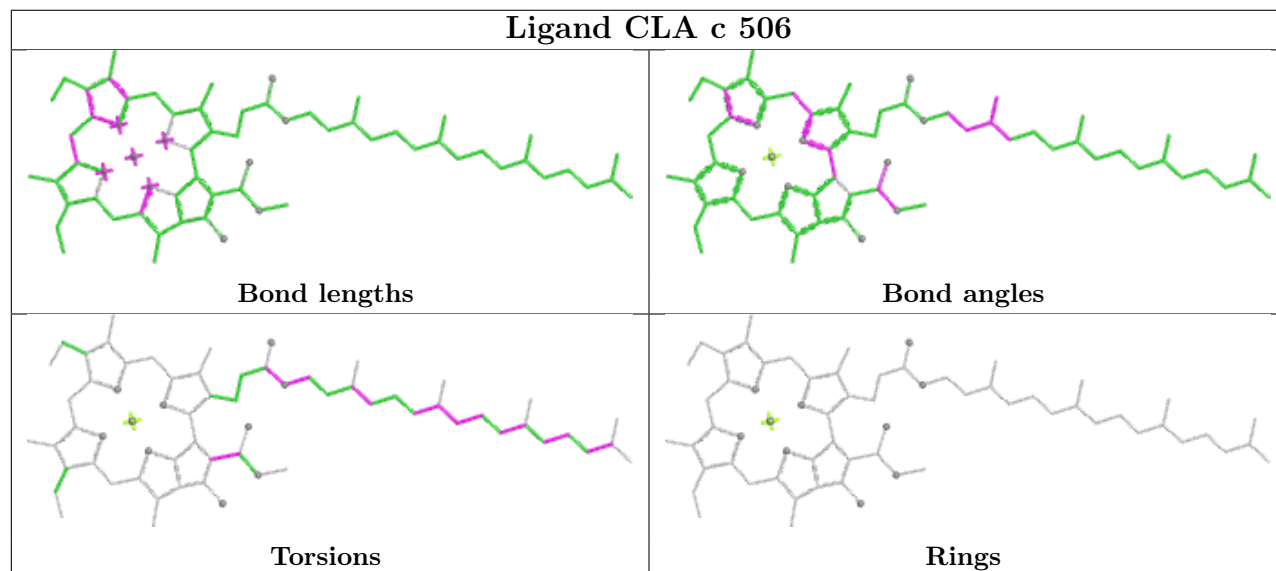
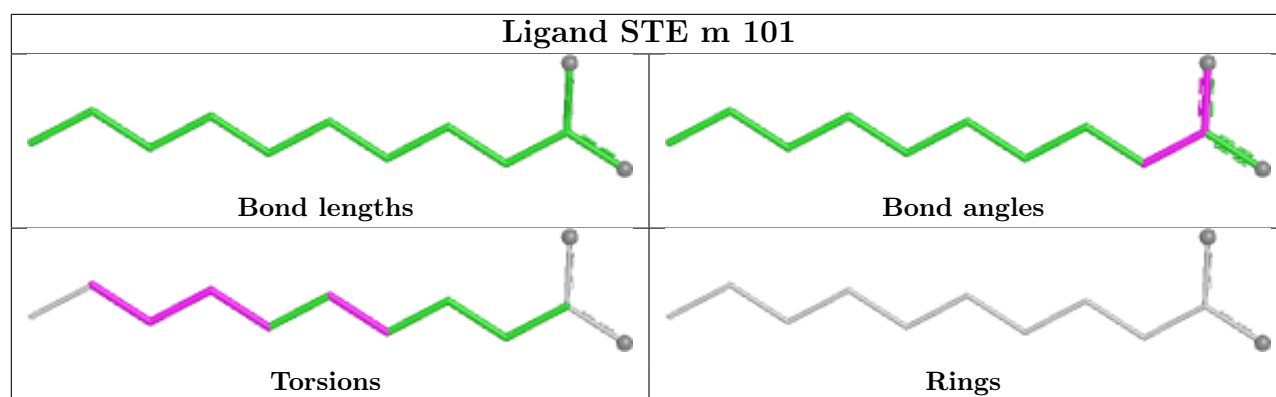


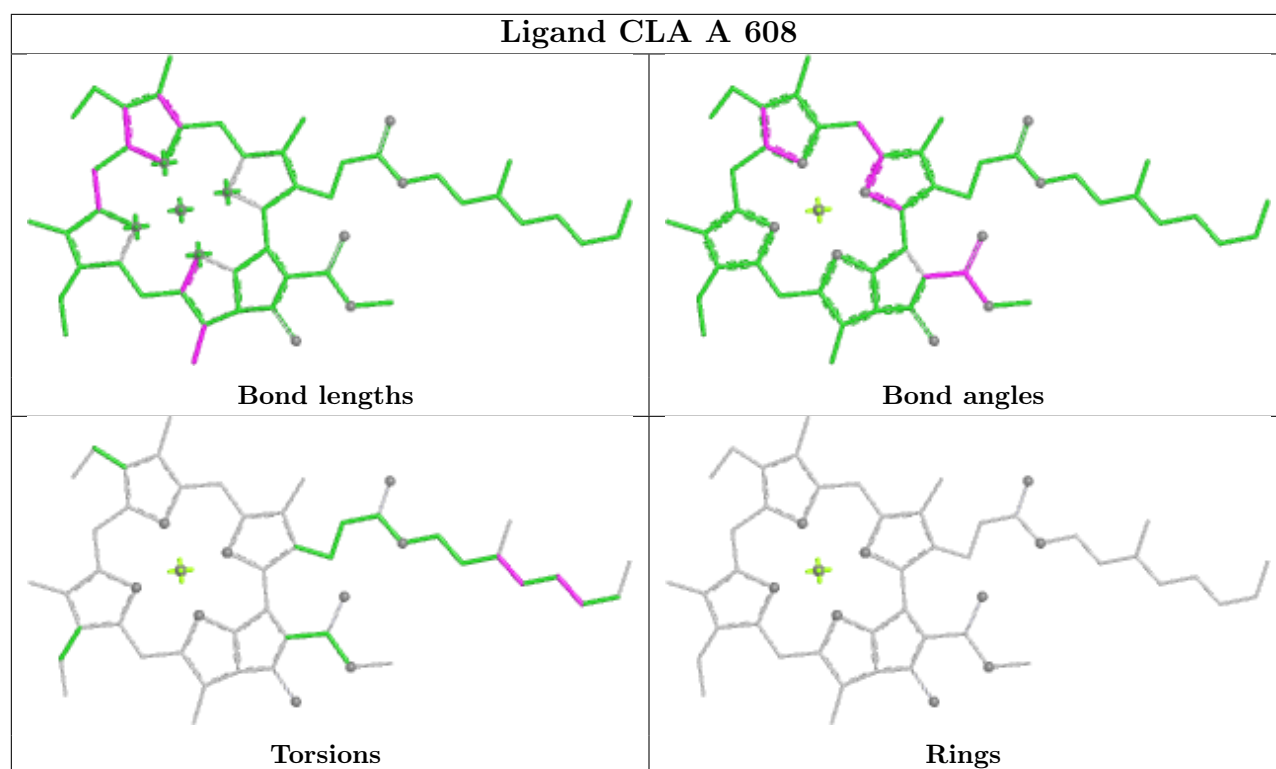
Ligand CLA b 608

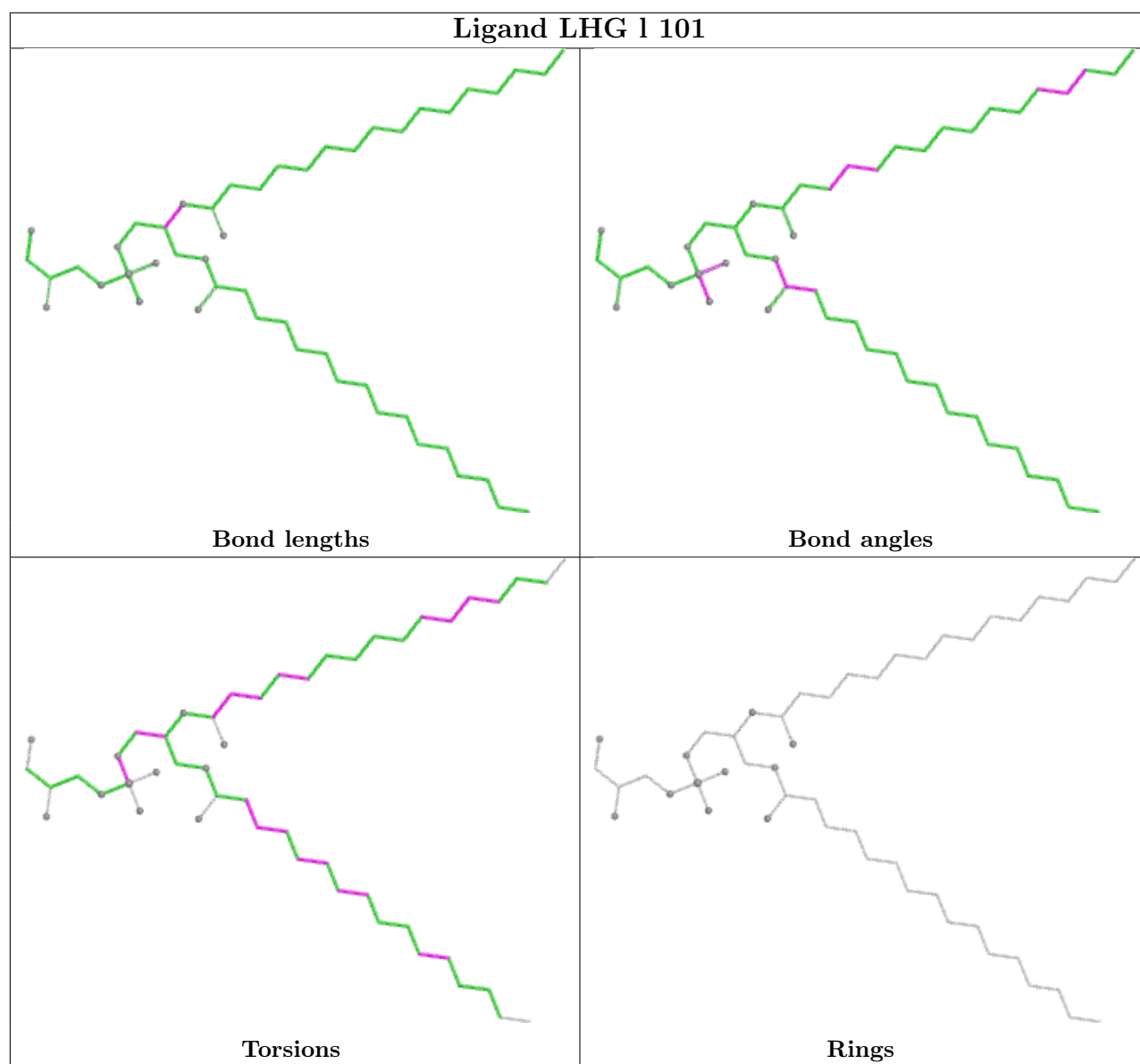




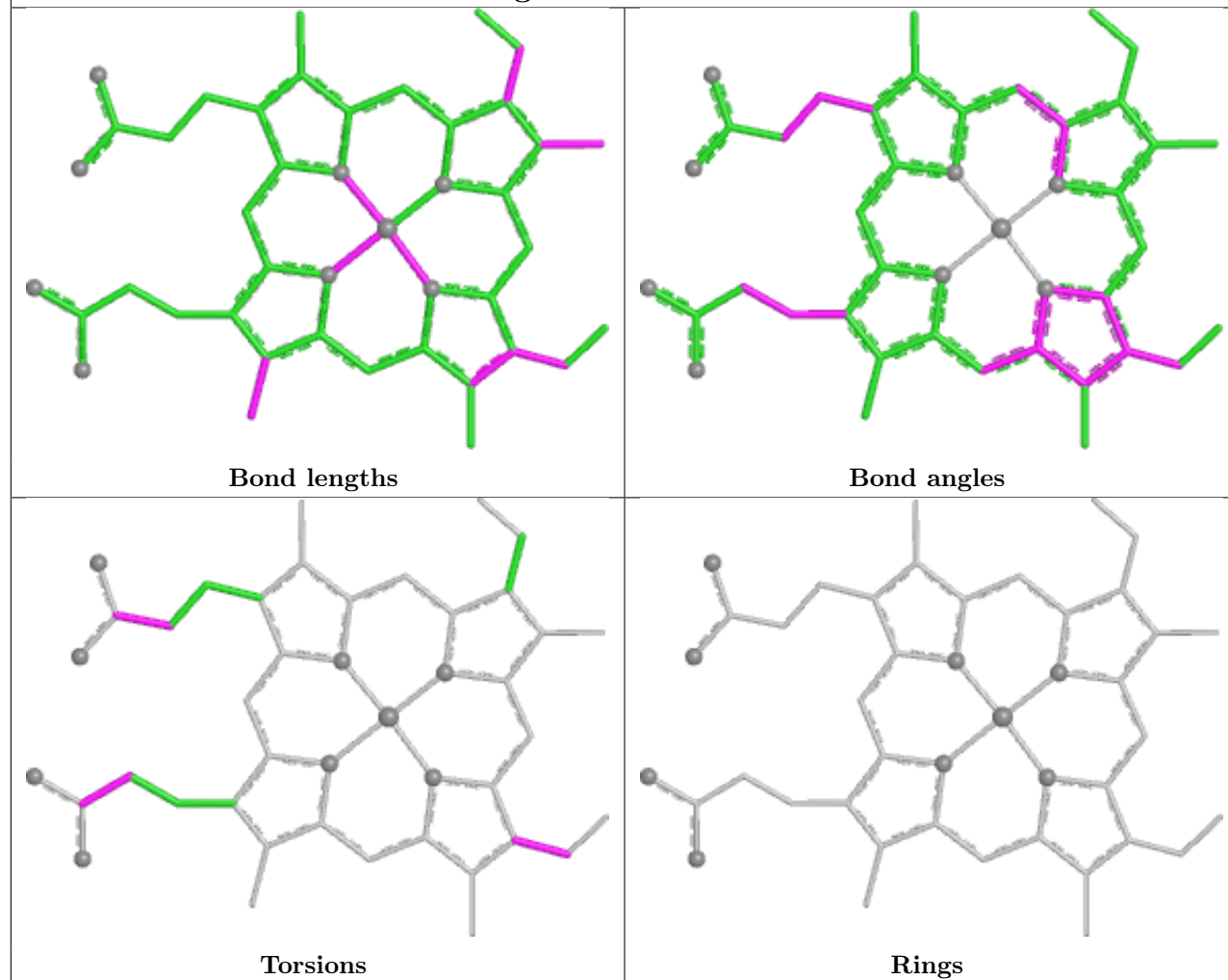




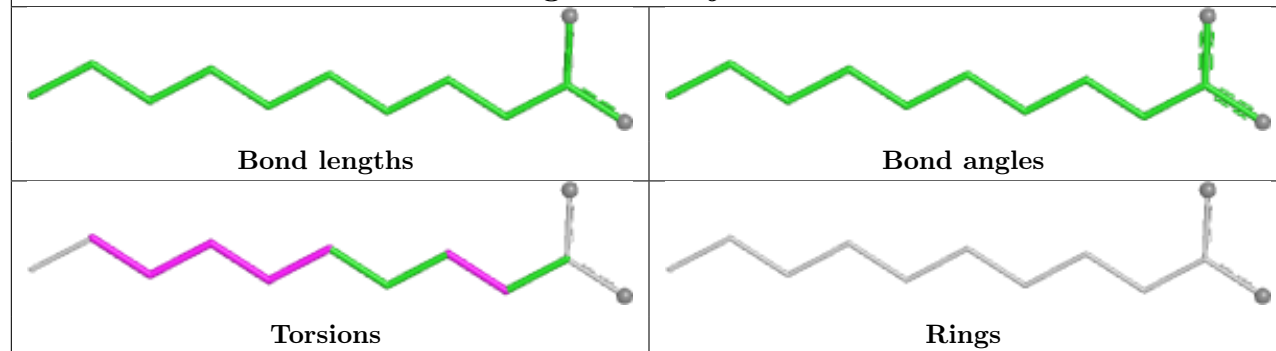


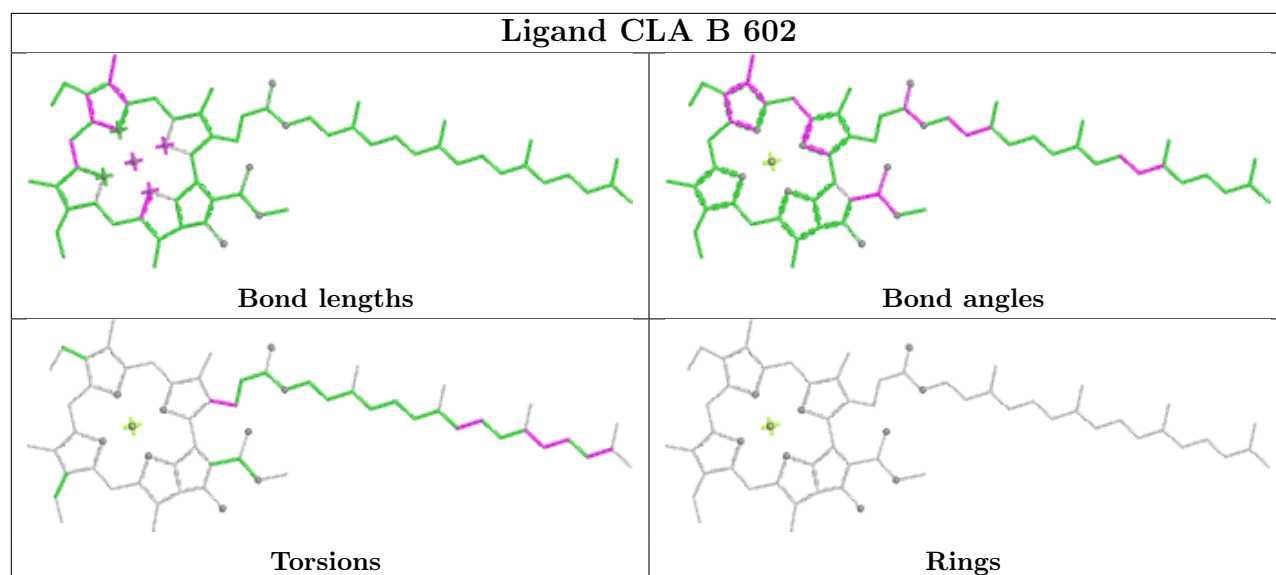
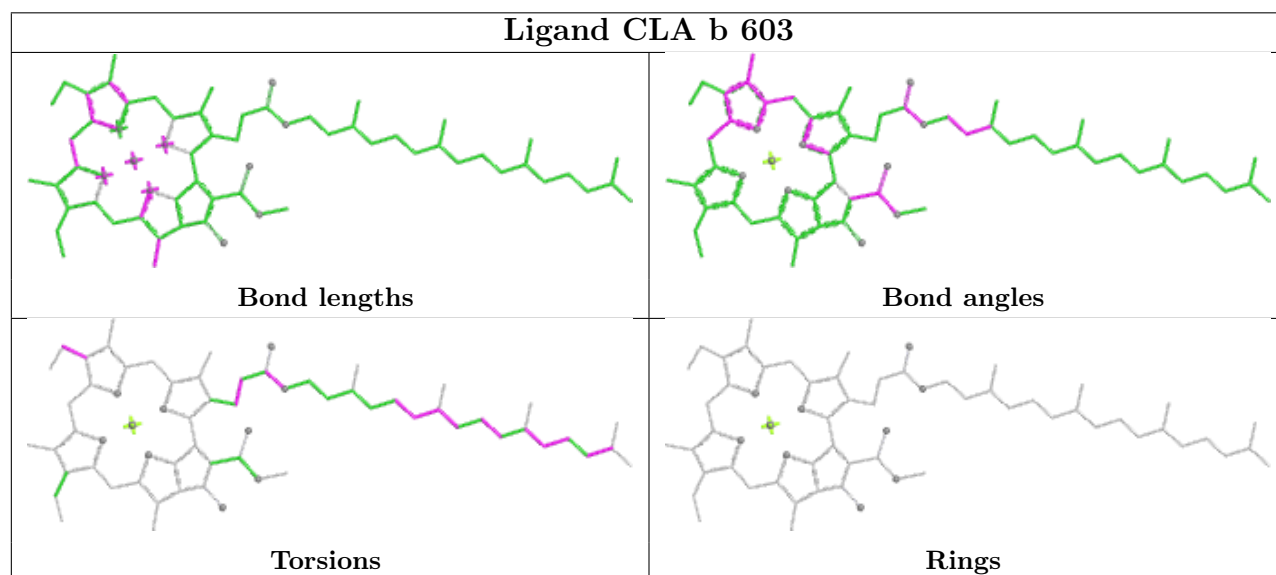
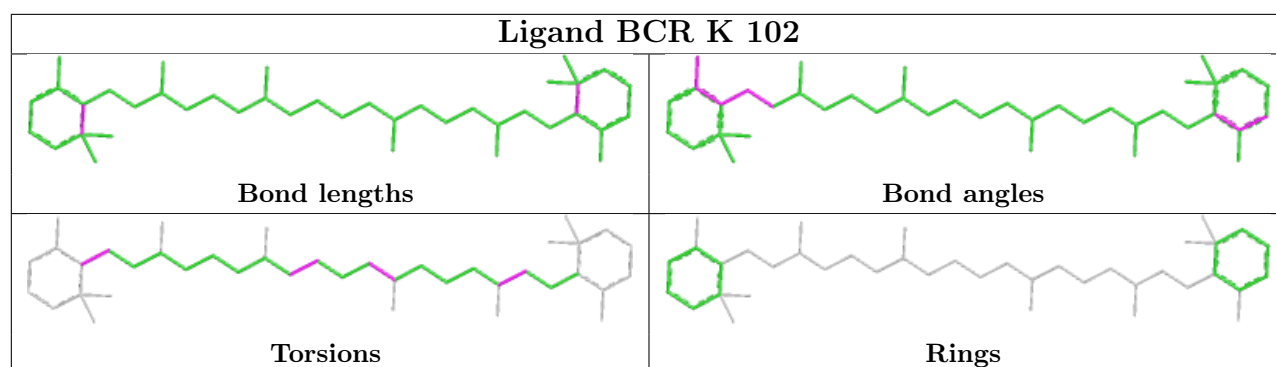


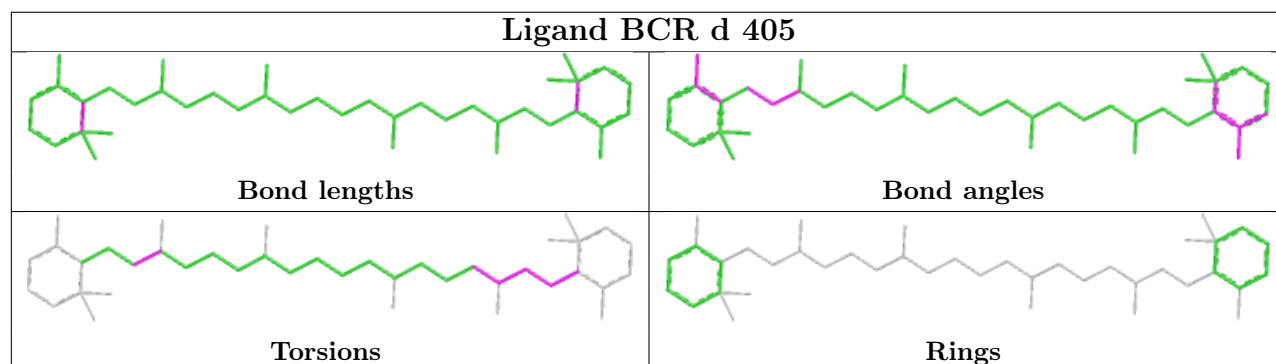
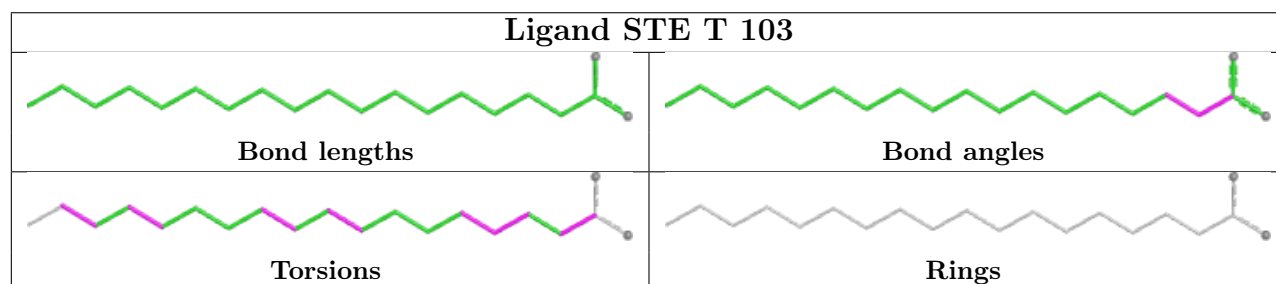
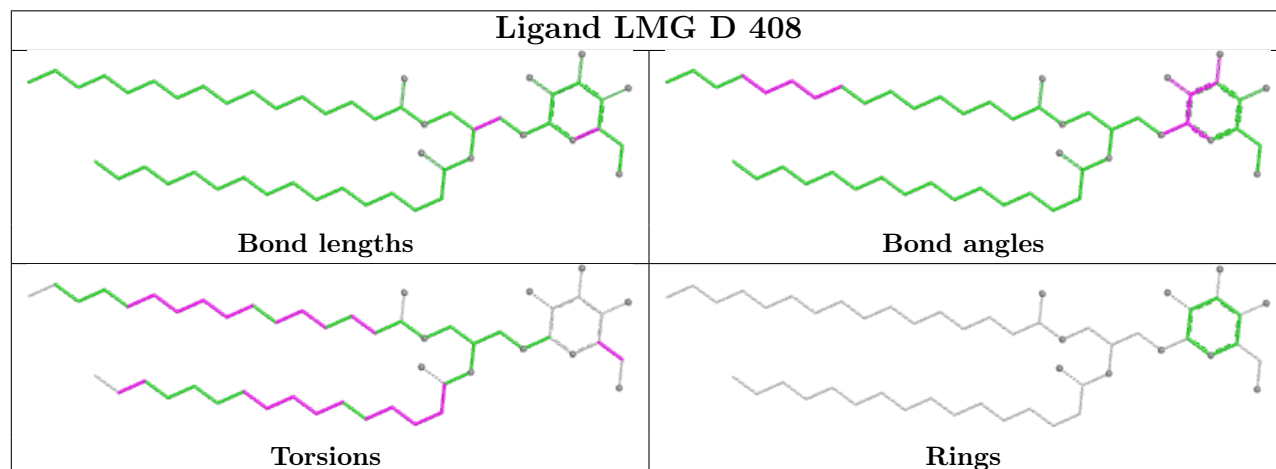
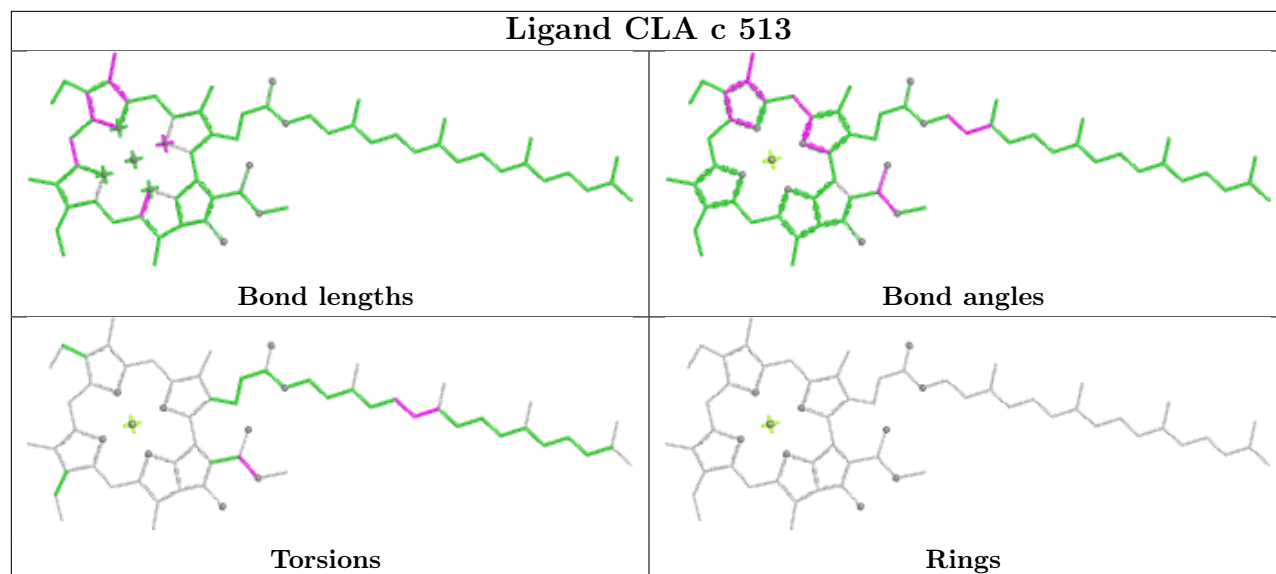
Ligand HEM f 101



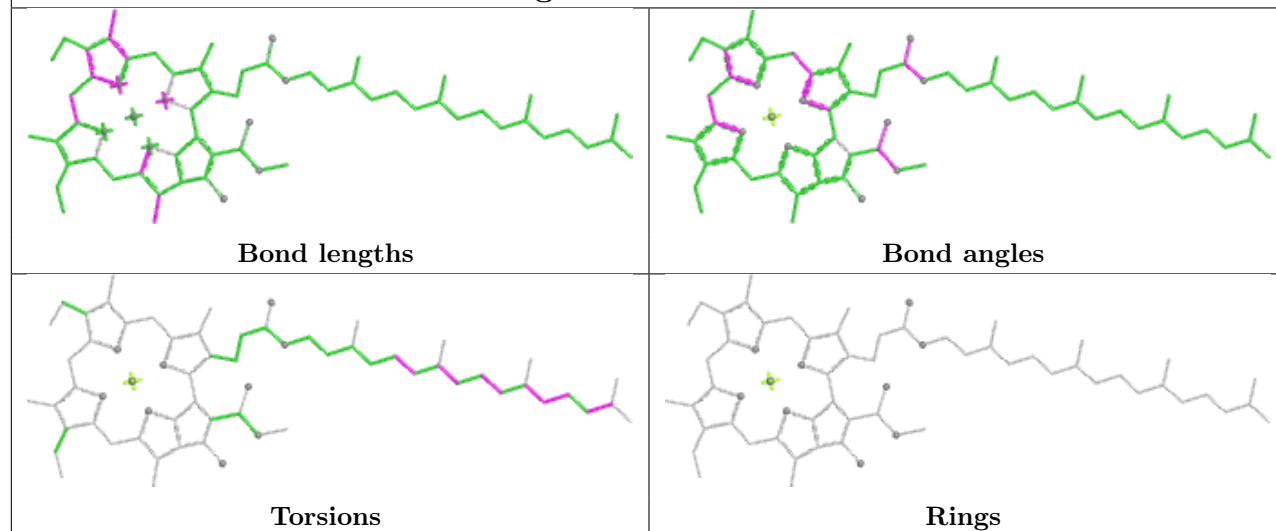
Ligand STE j 101



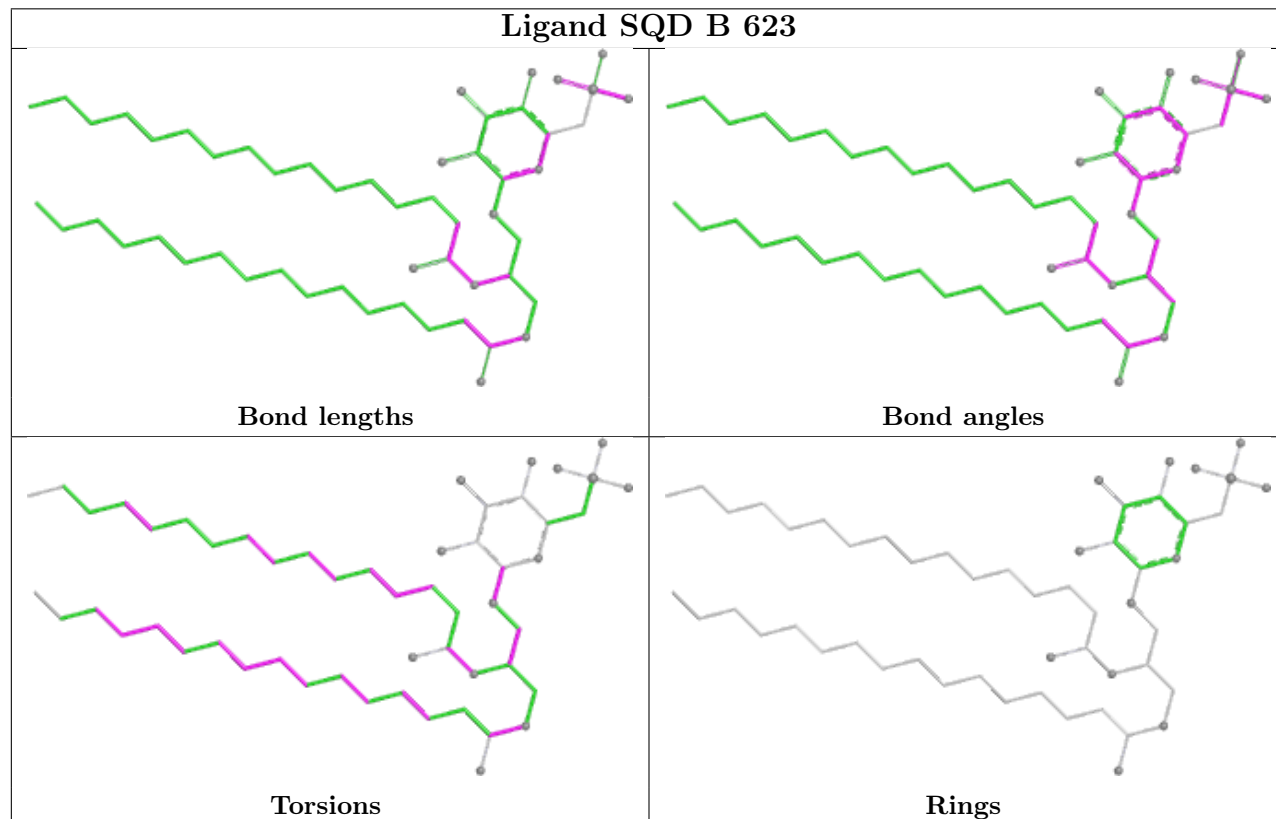




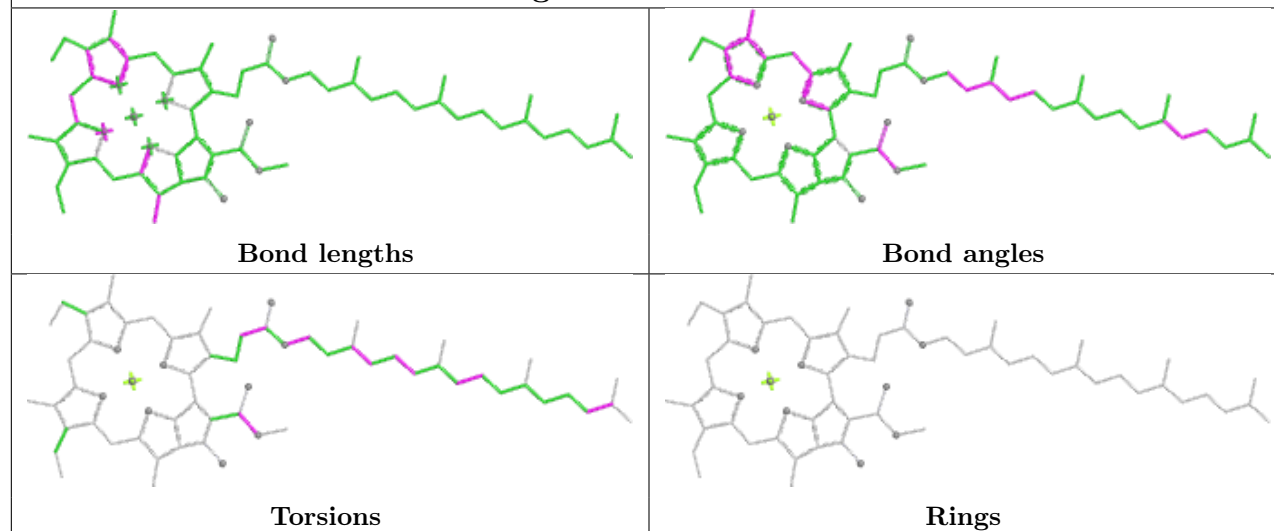
Ligand CLA b 615



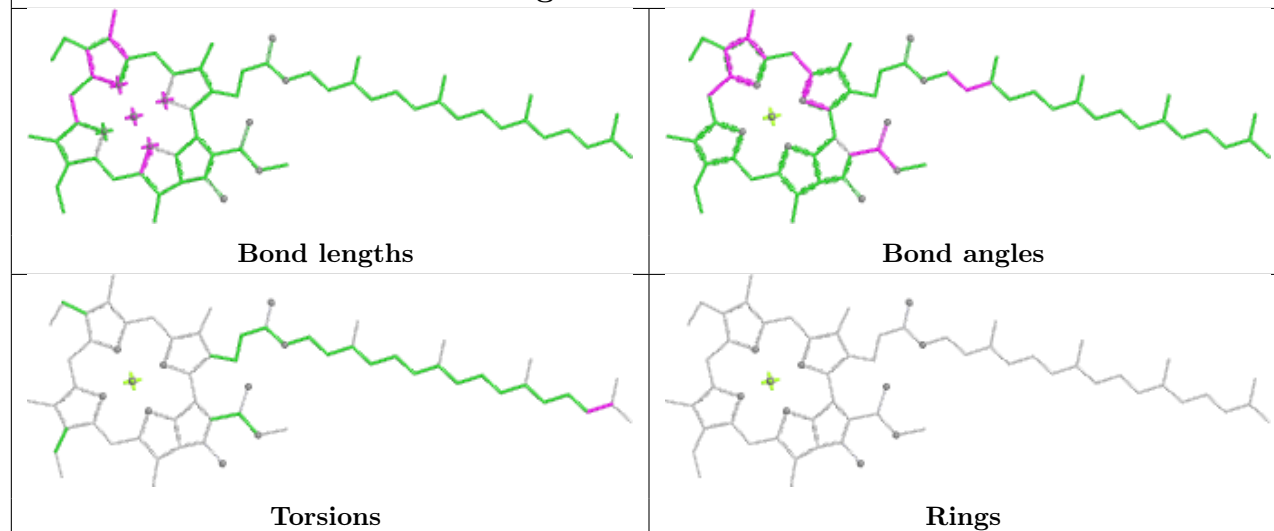
Ligand SQD B 623



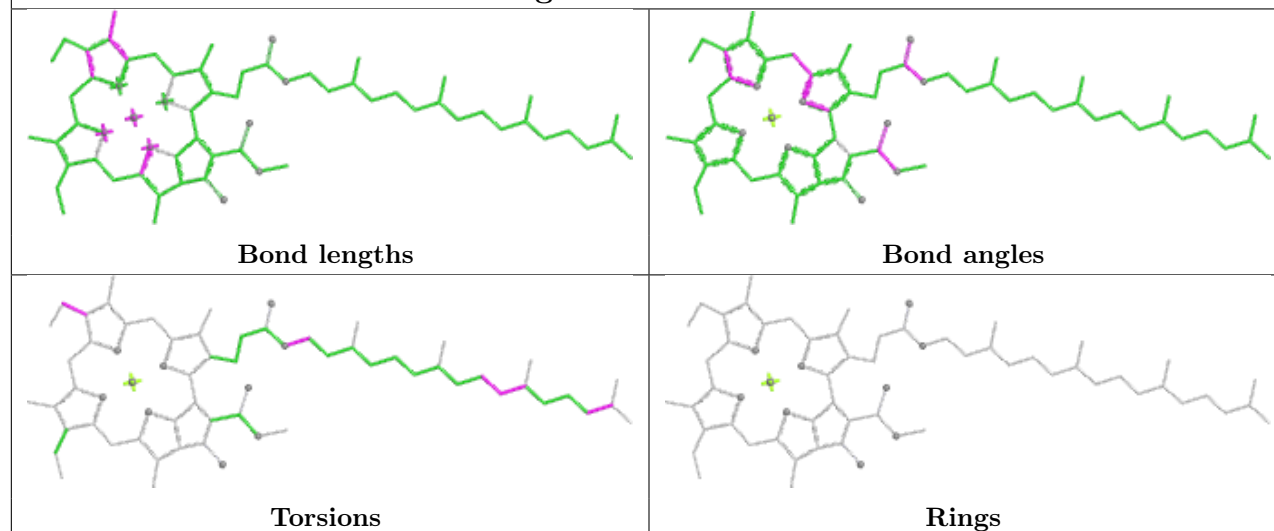
Ligand CLA B 613

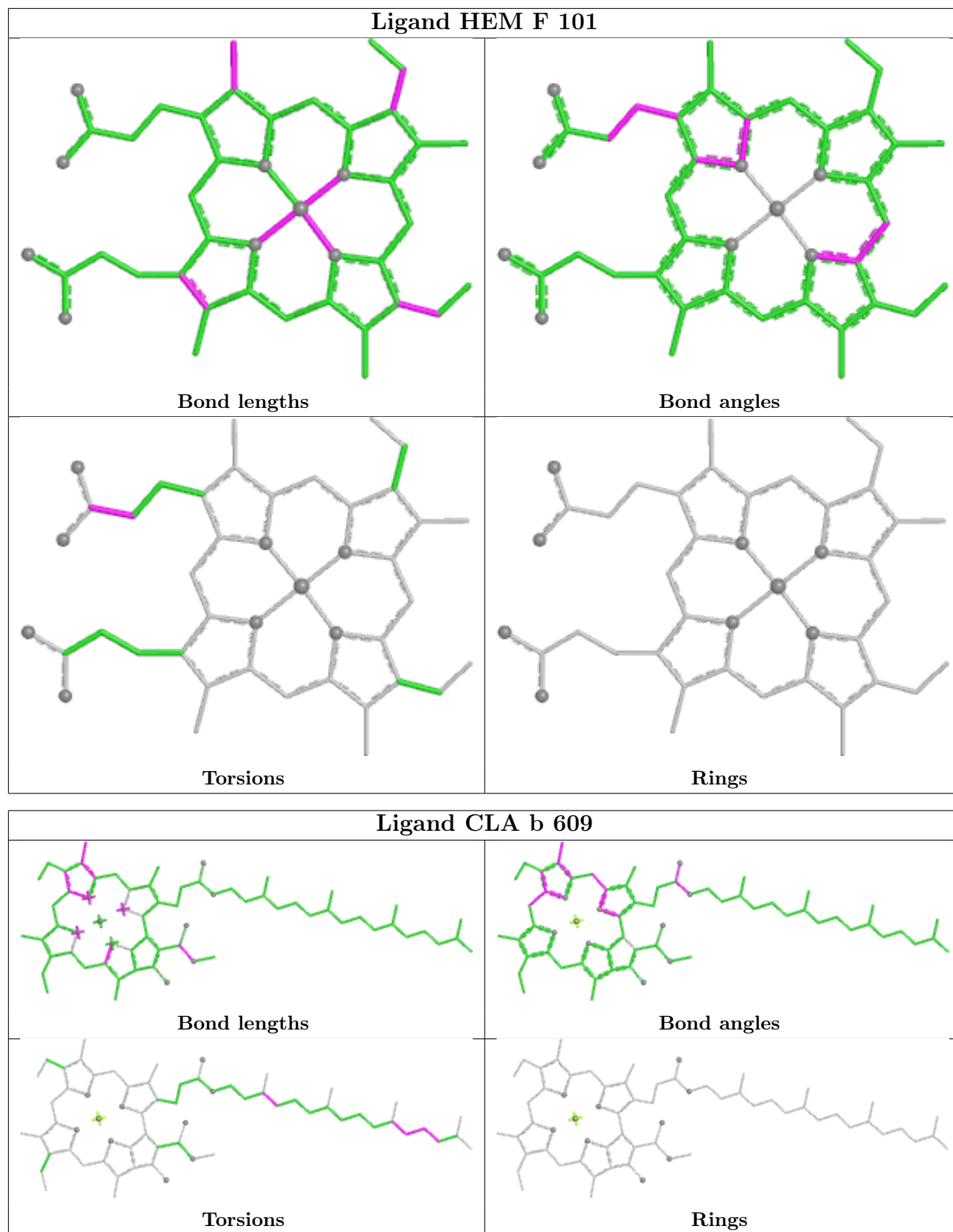


Ligand CLA a 612

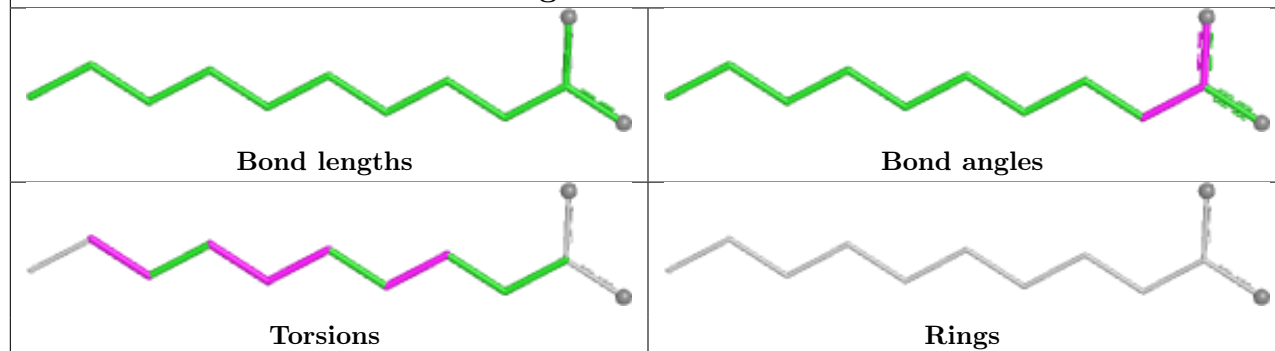


Ligand CLA d 403

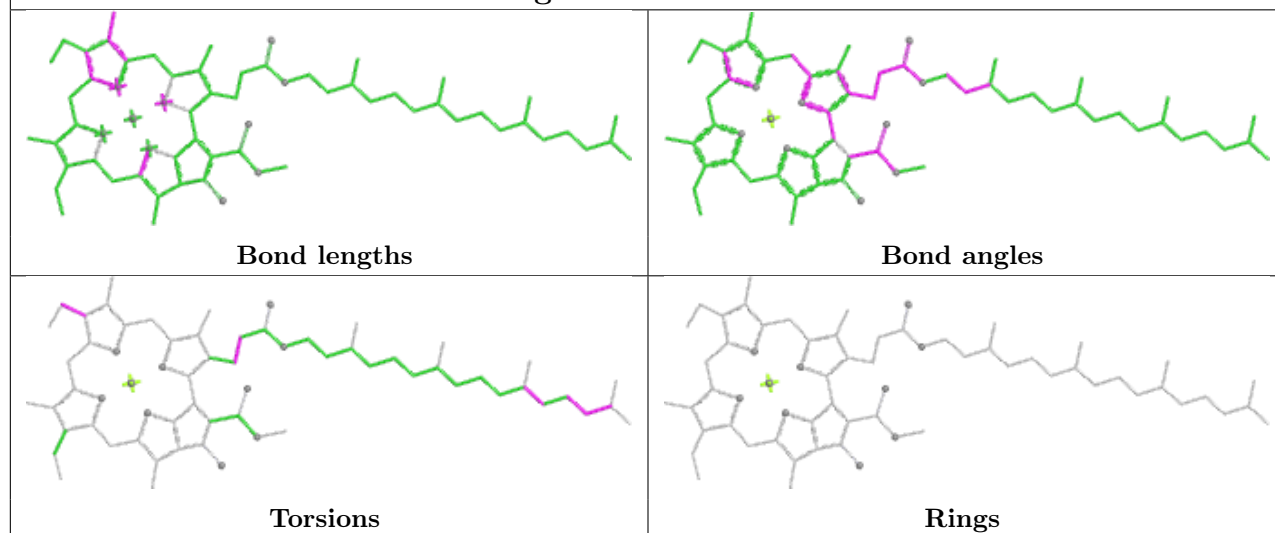




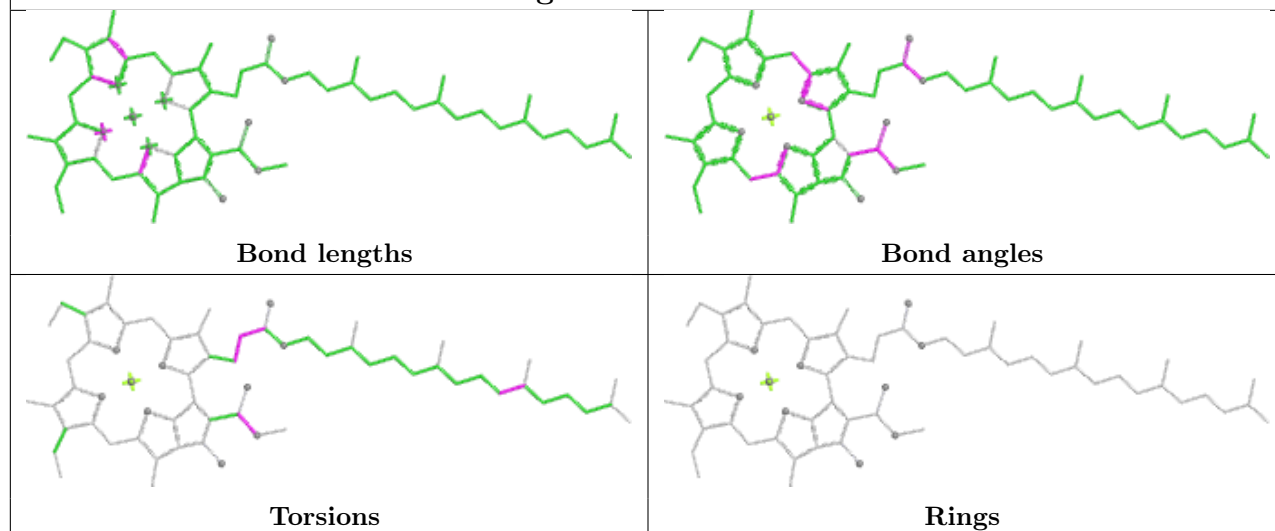
Ligand STE c 521



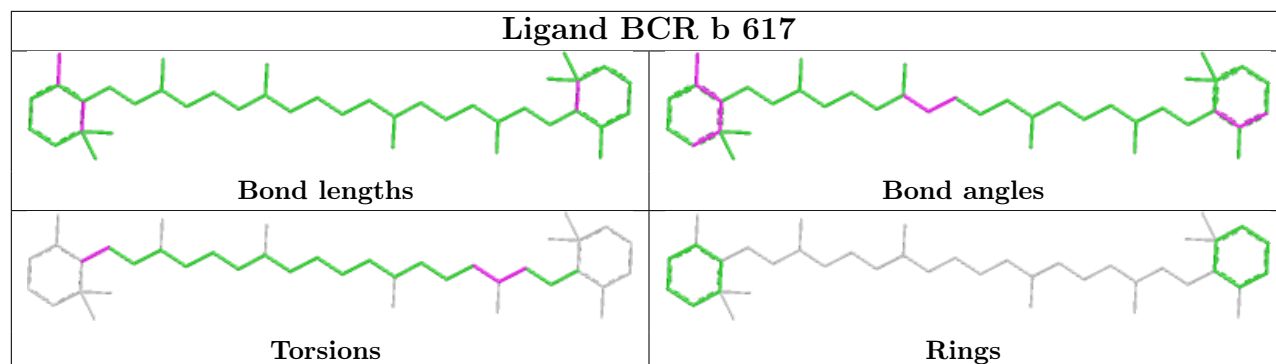
Ligand CLA b 610



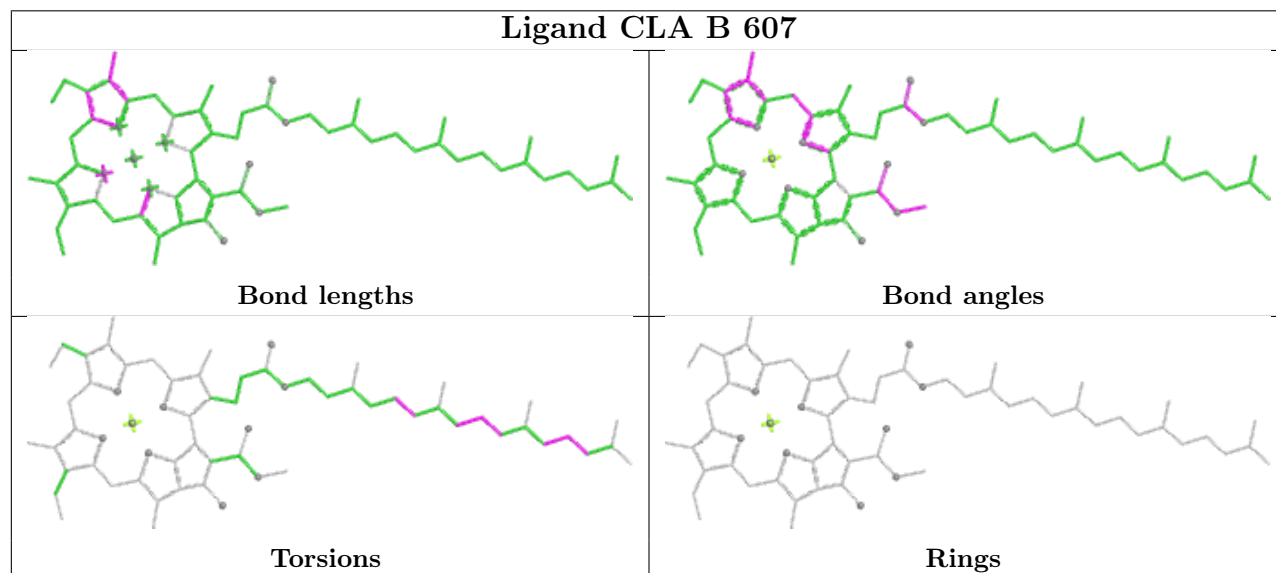
Ligand CLA c 501



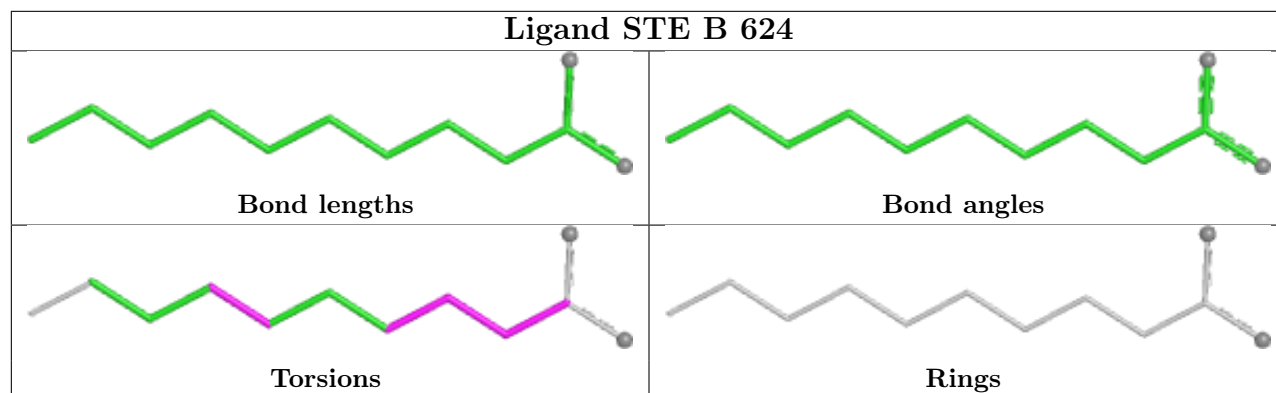
Ligand BCR b 617



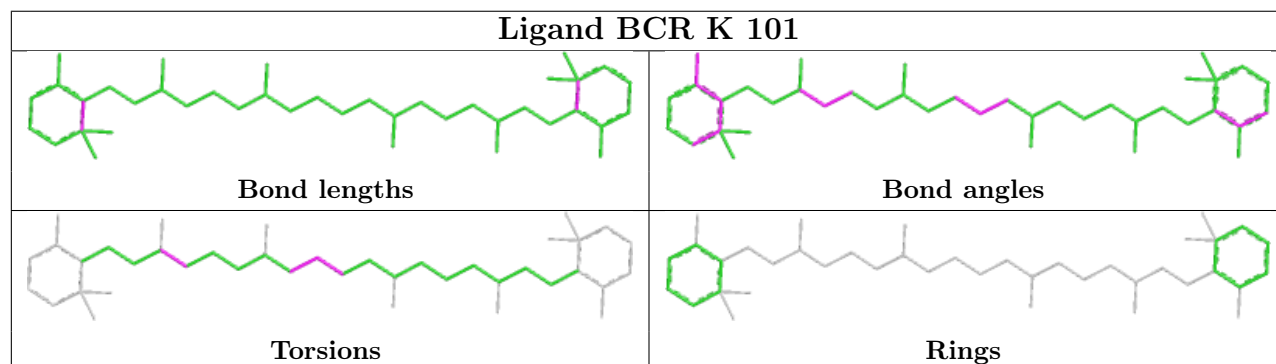
Ligand CLA B 607

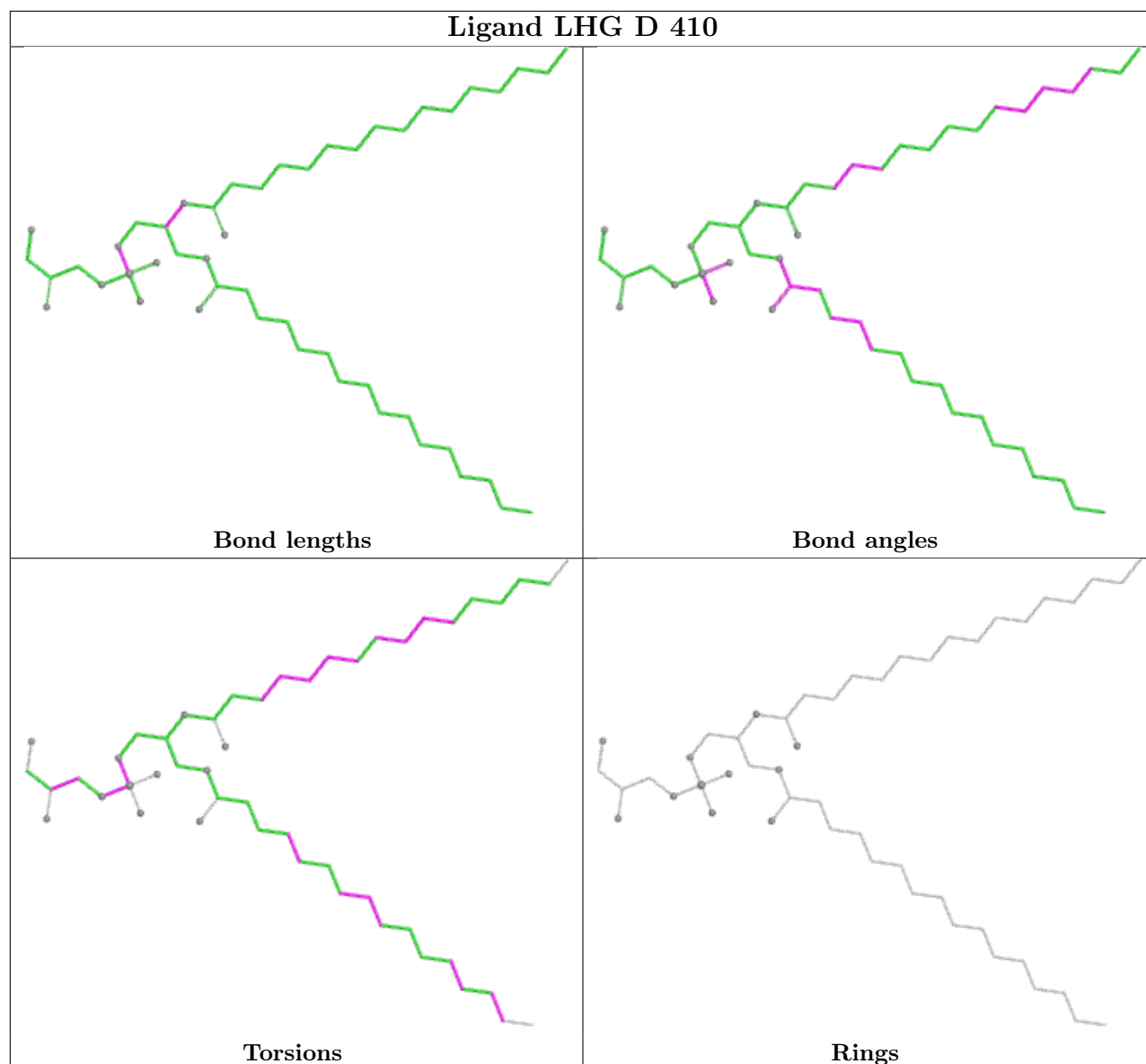
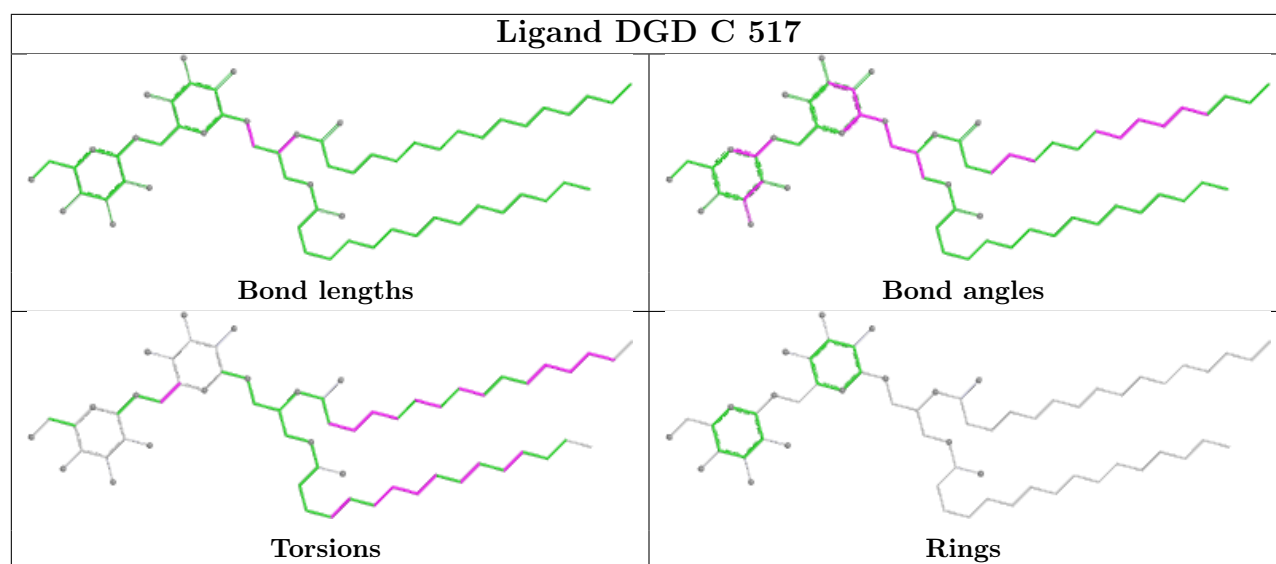


Ligand STE B 624

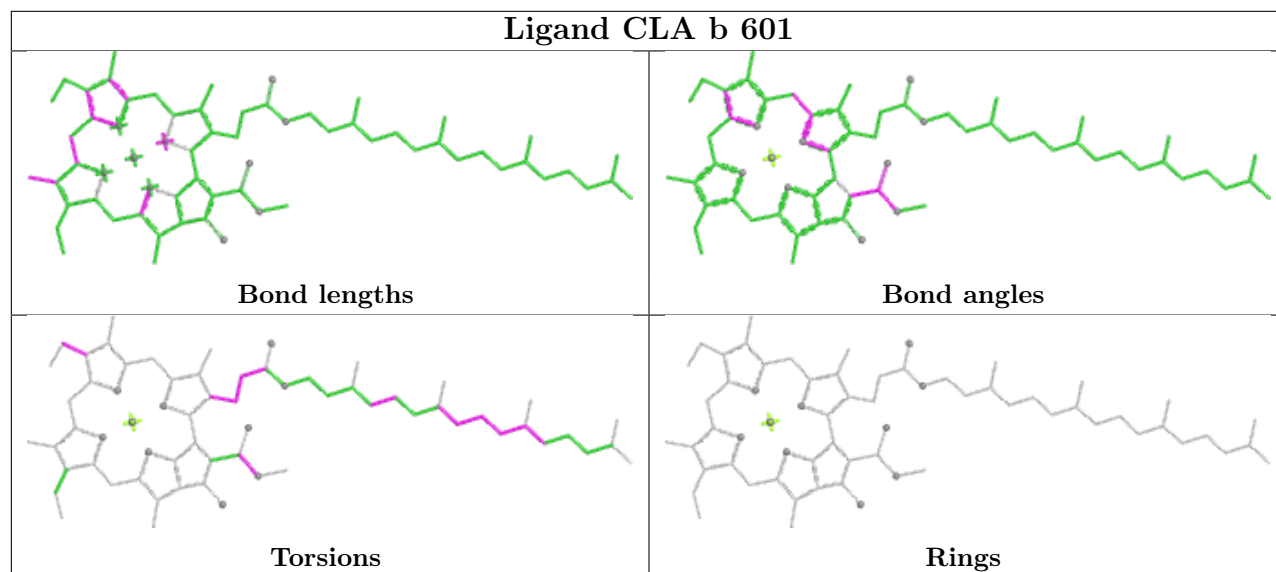


Ligand BCR K 101

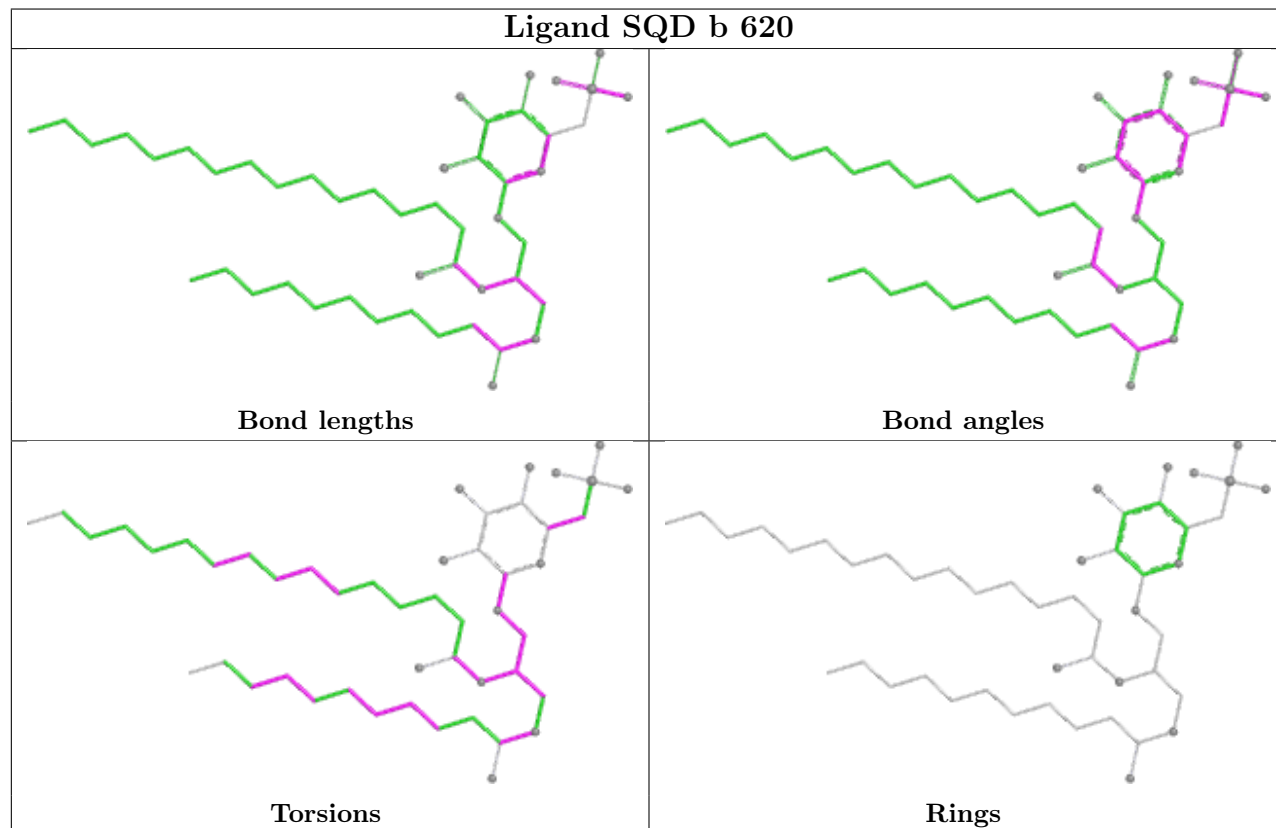


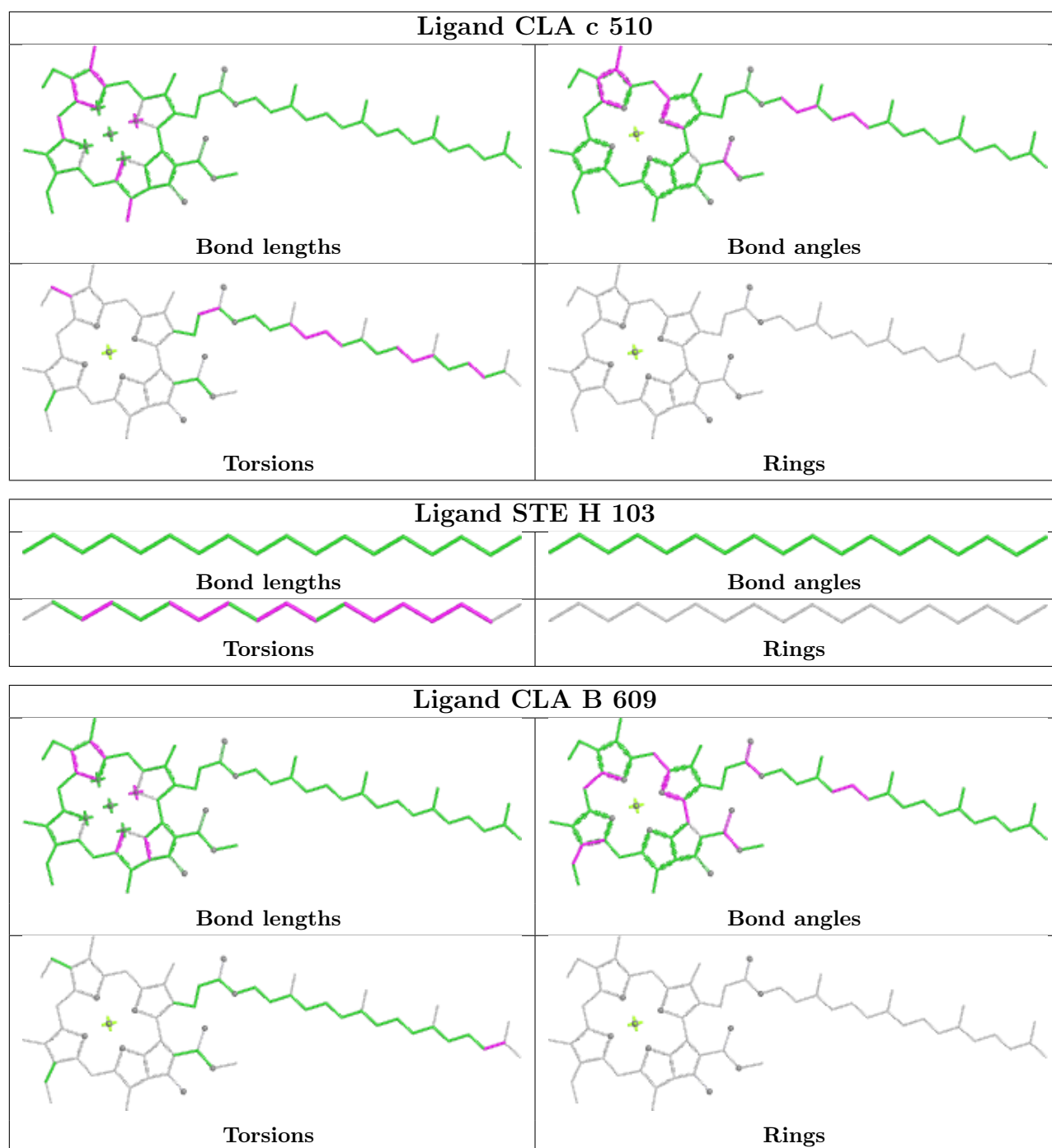


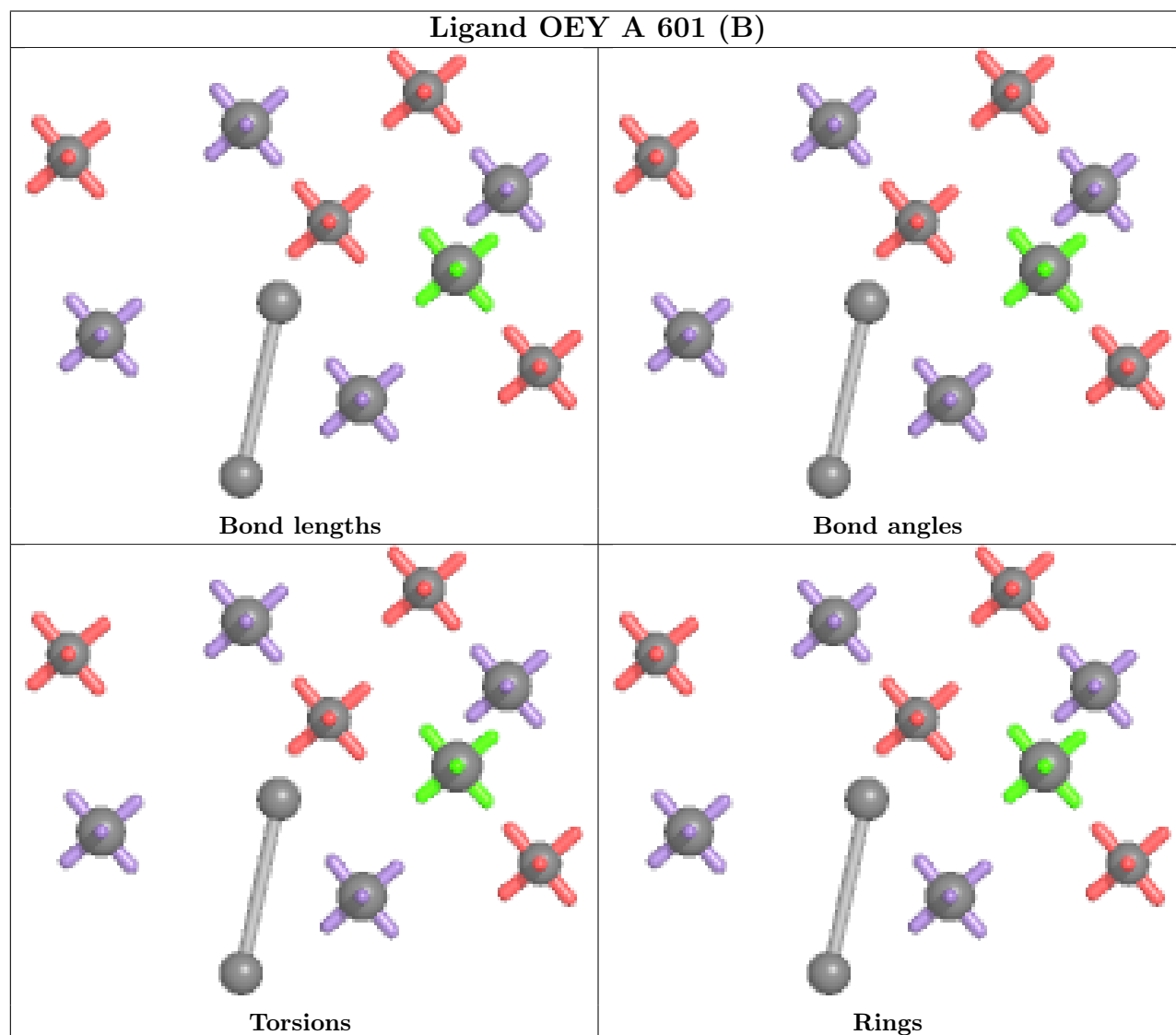
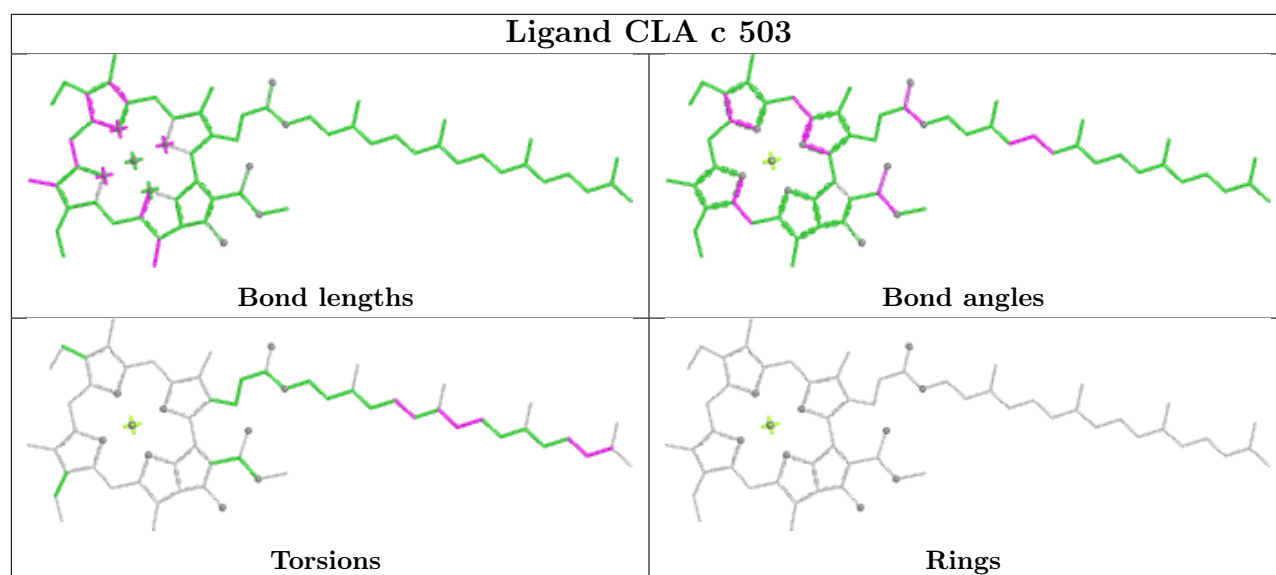
Ligand CLA b 601

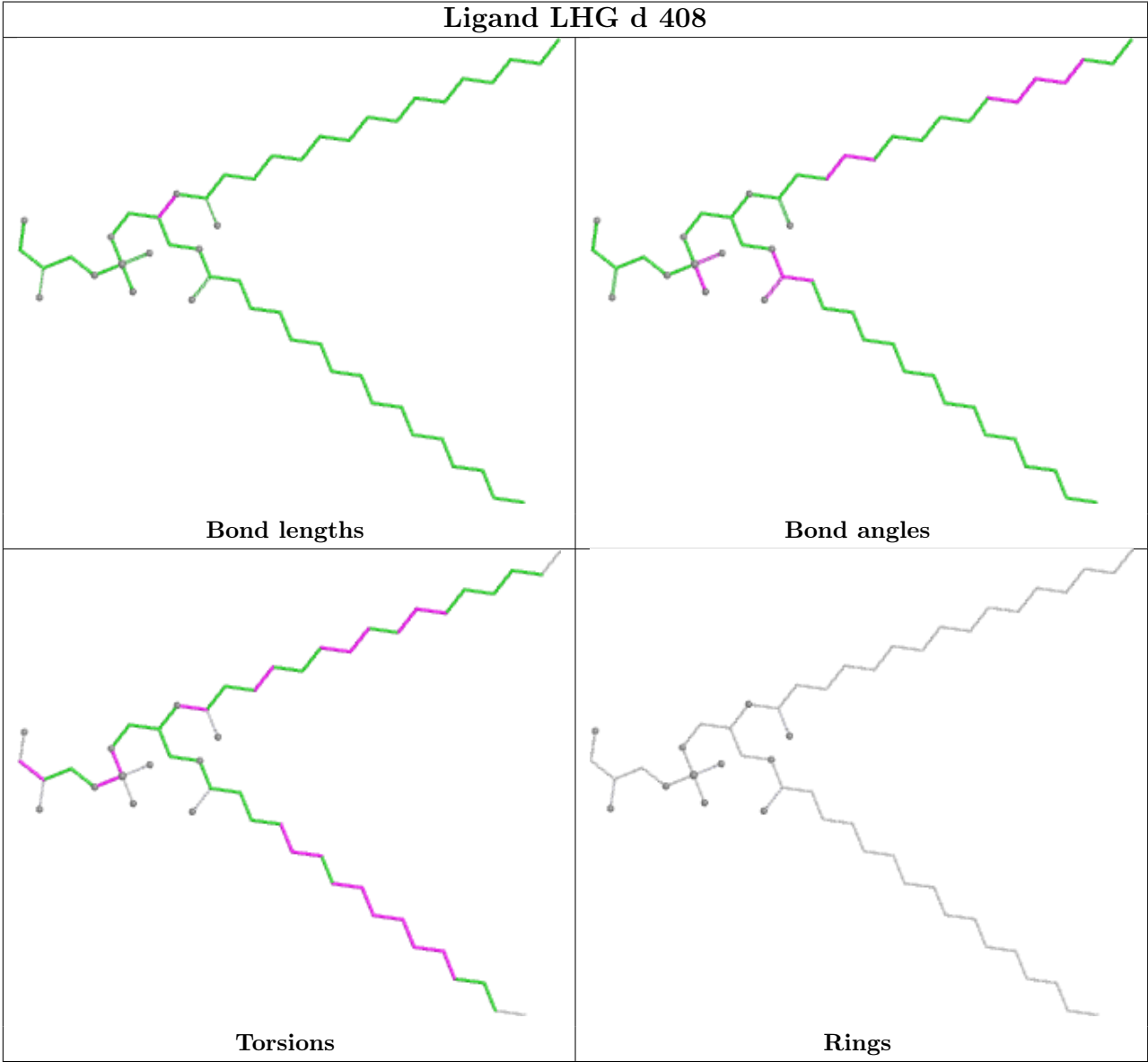
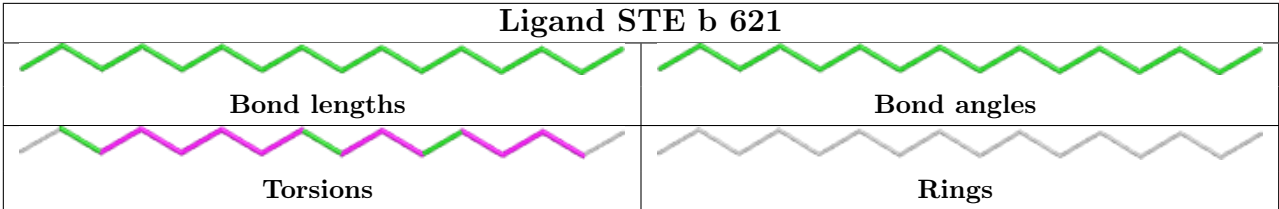


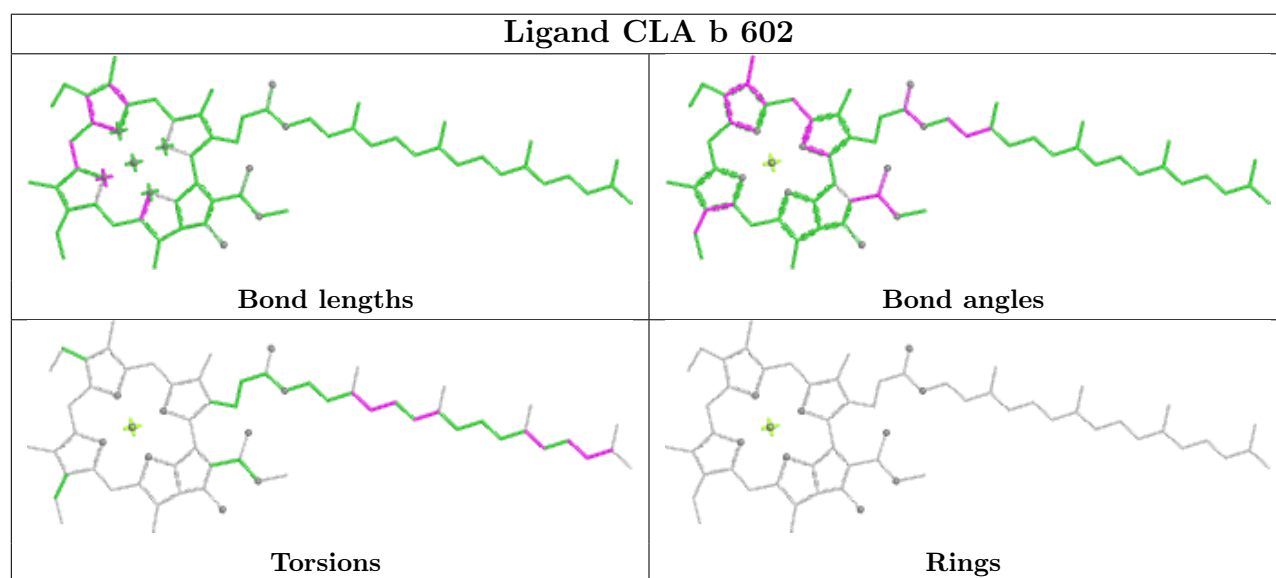
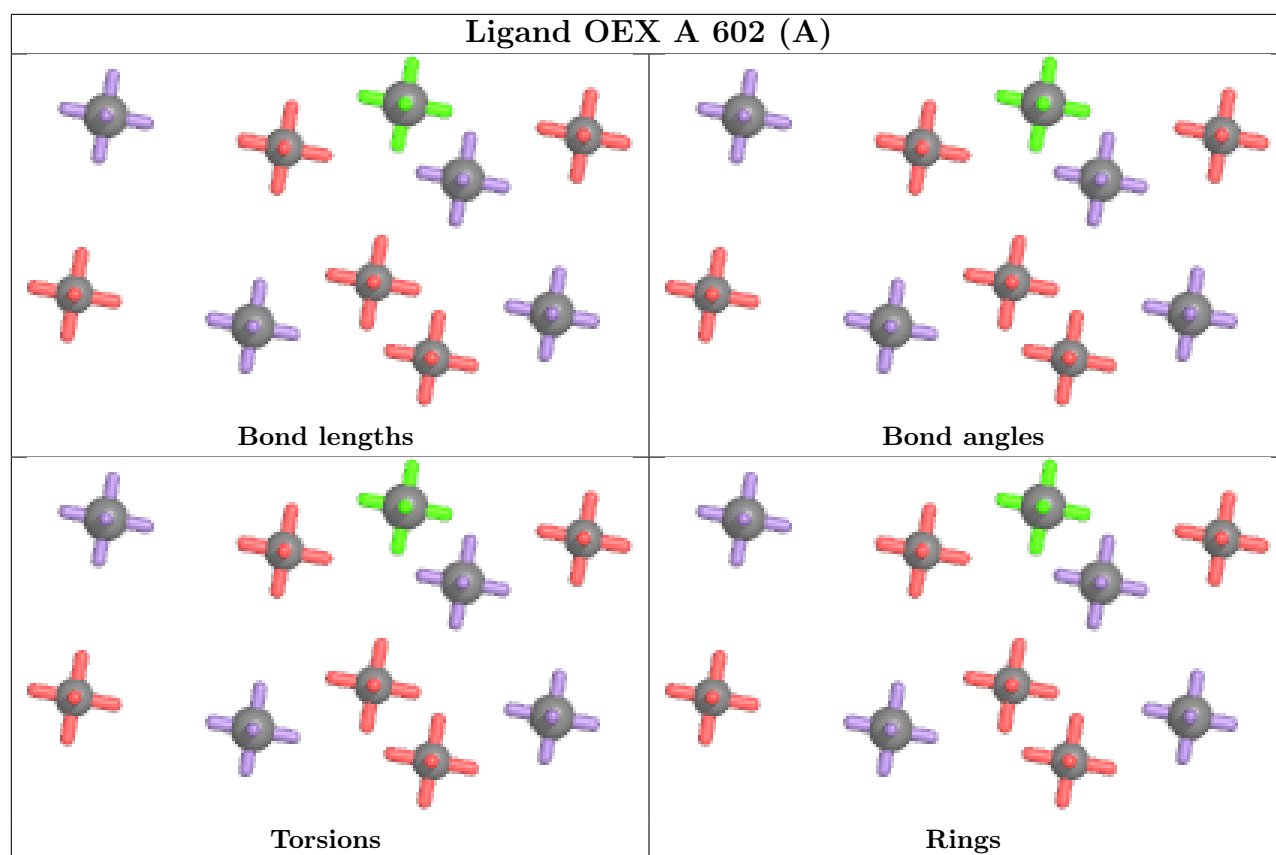
Ligand SQD b 620

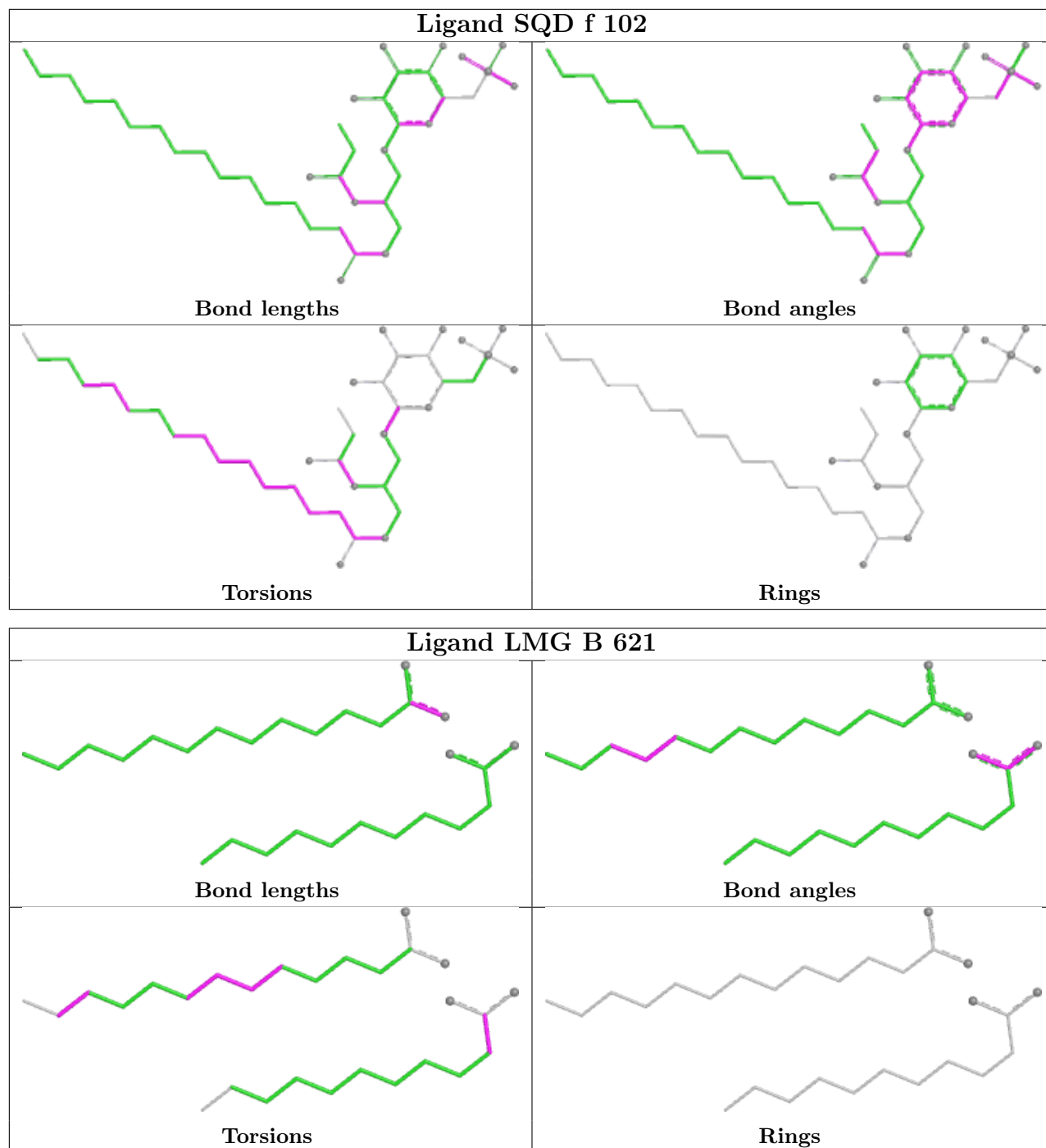


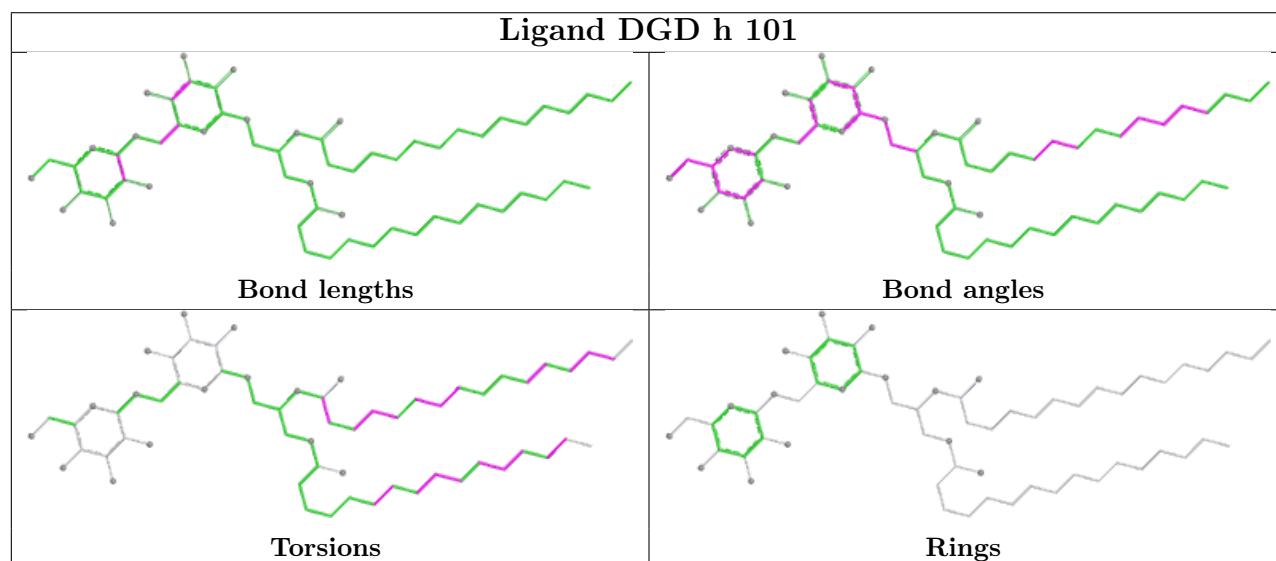
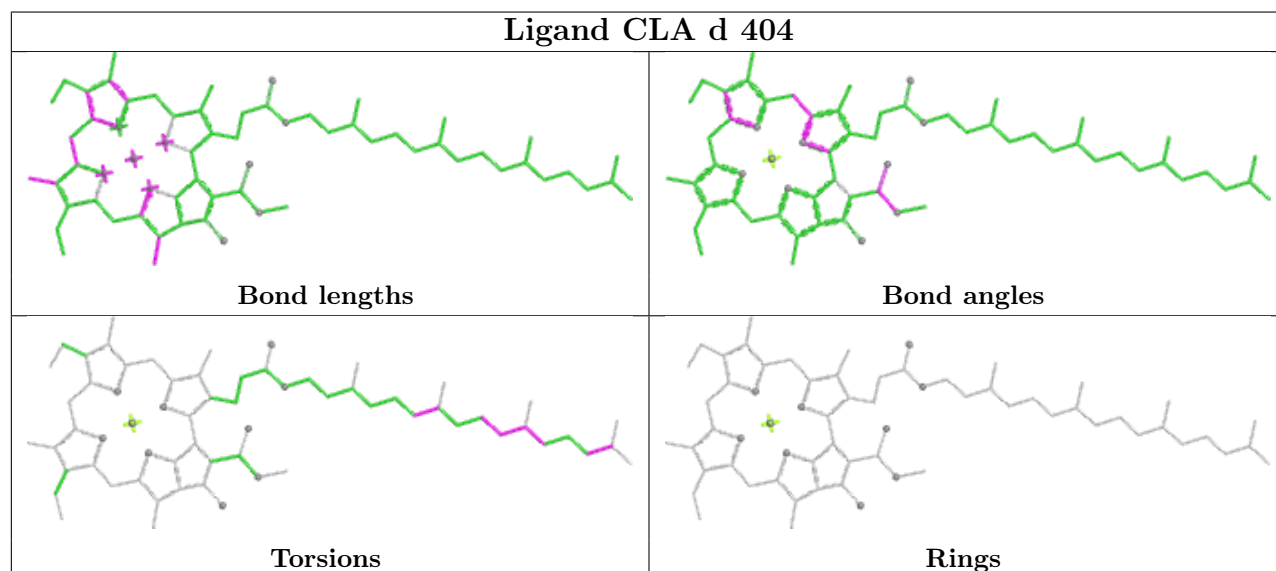
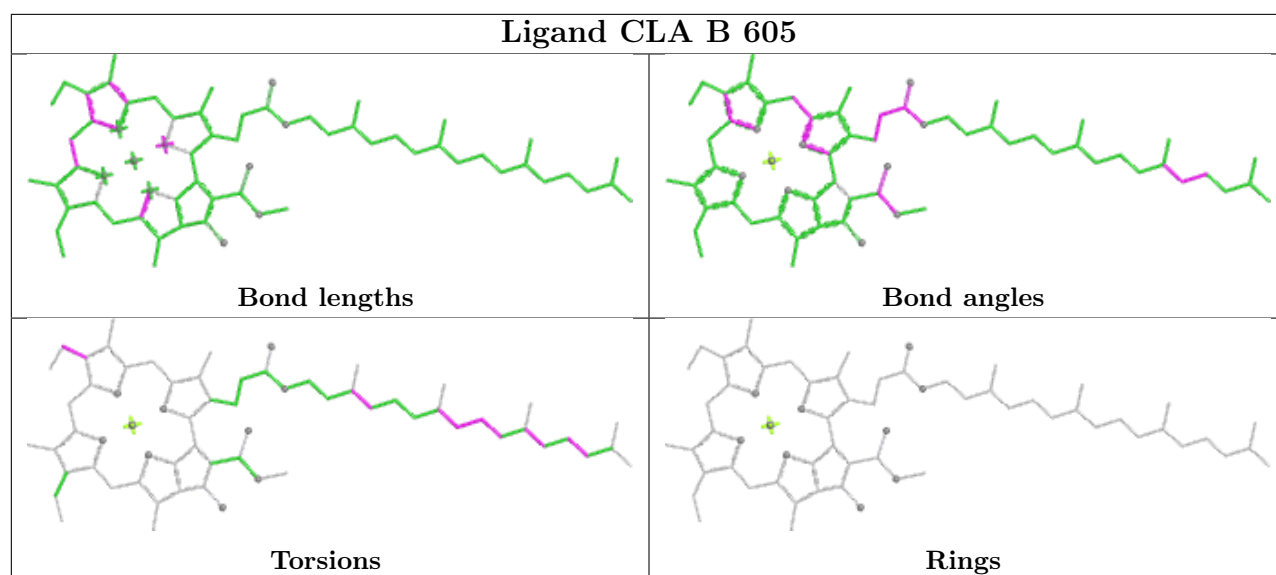


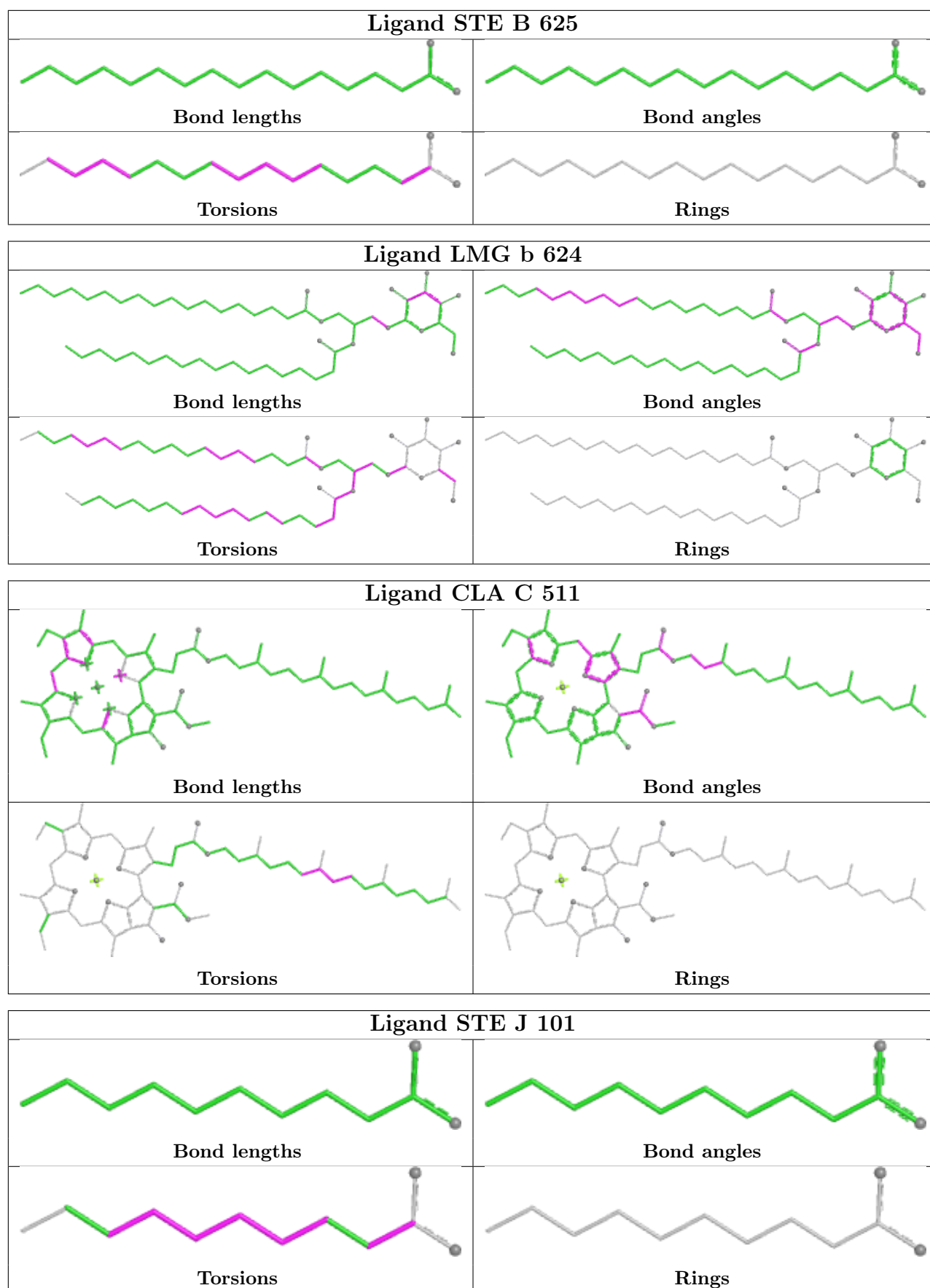




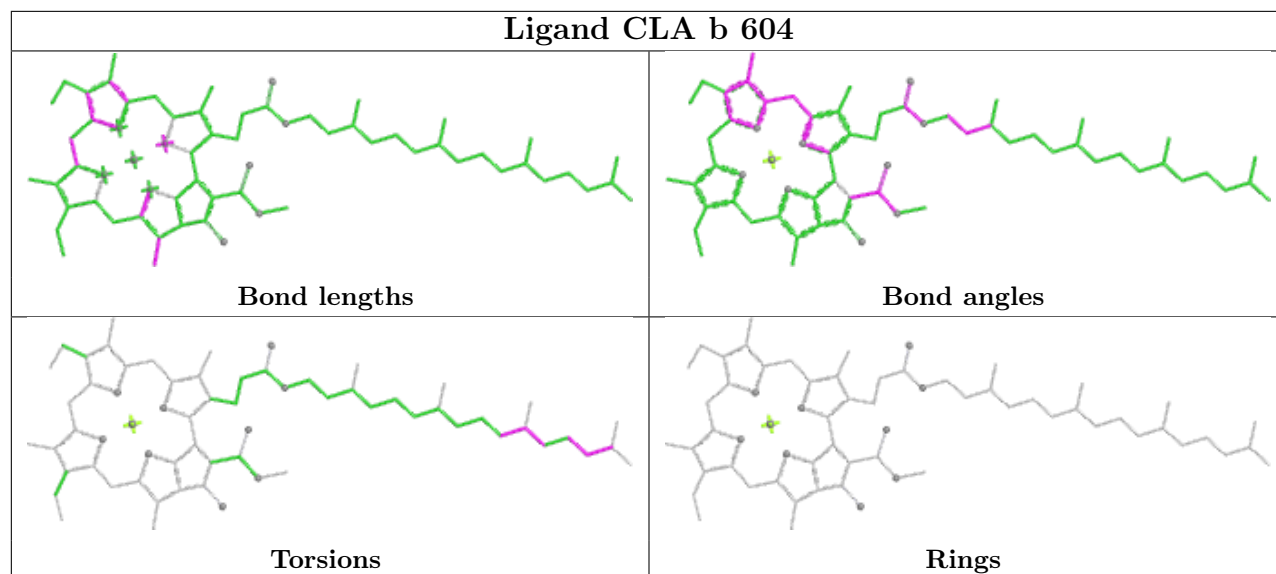




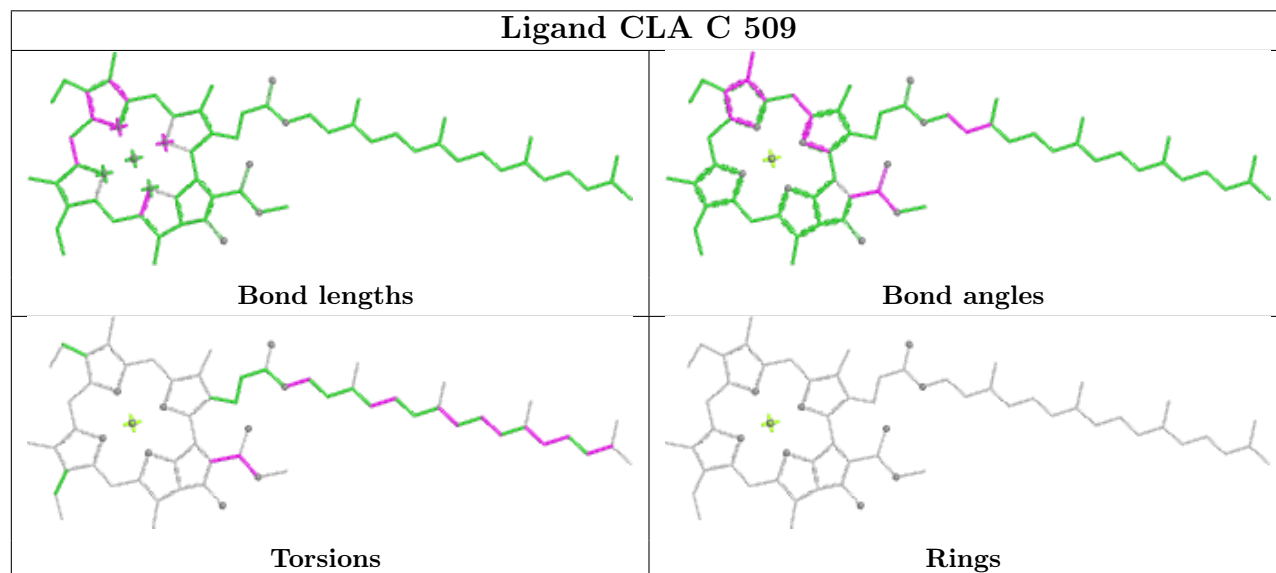




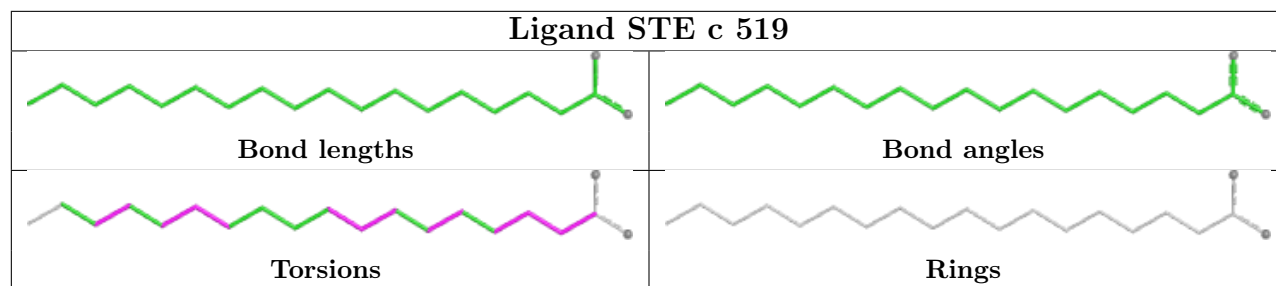
Ligand CLA b 604

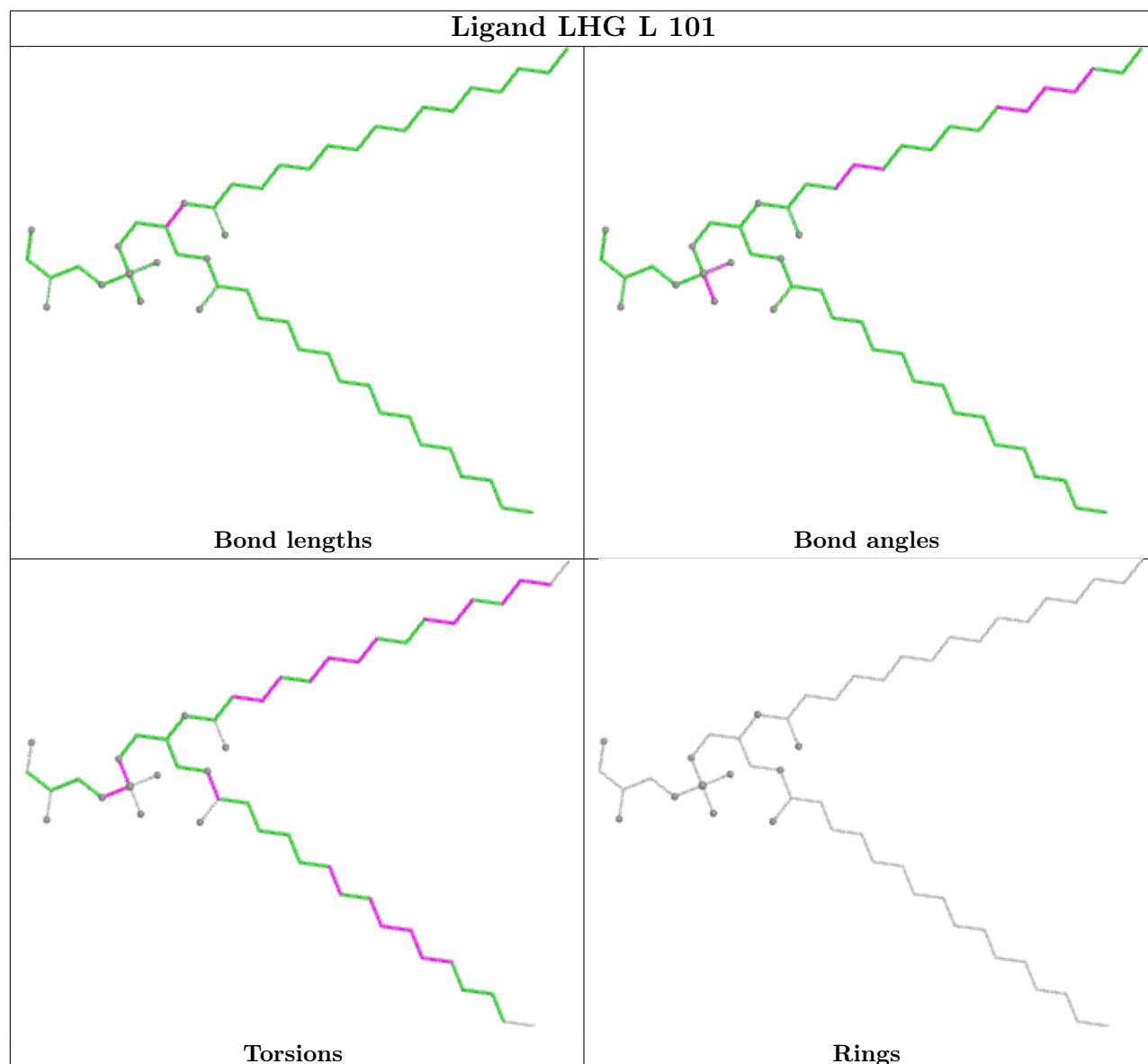
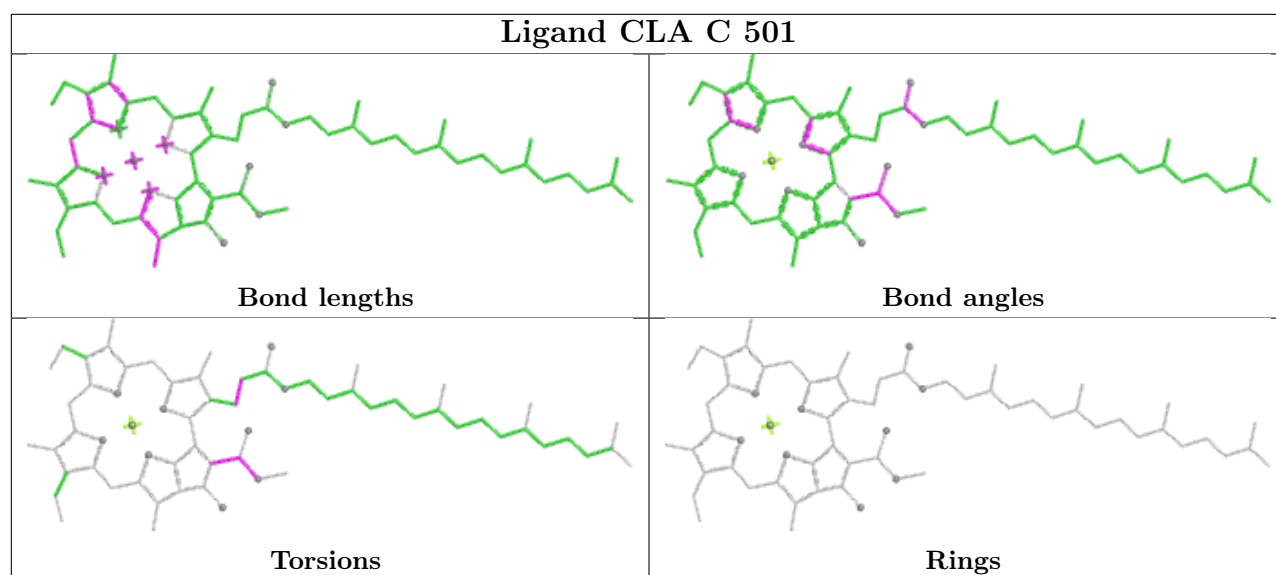


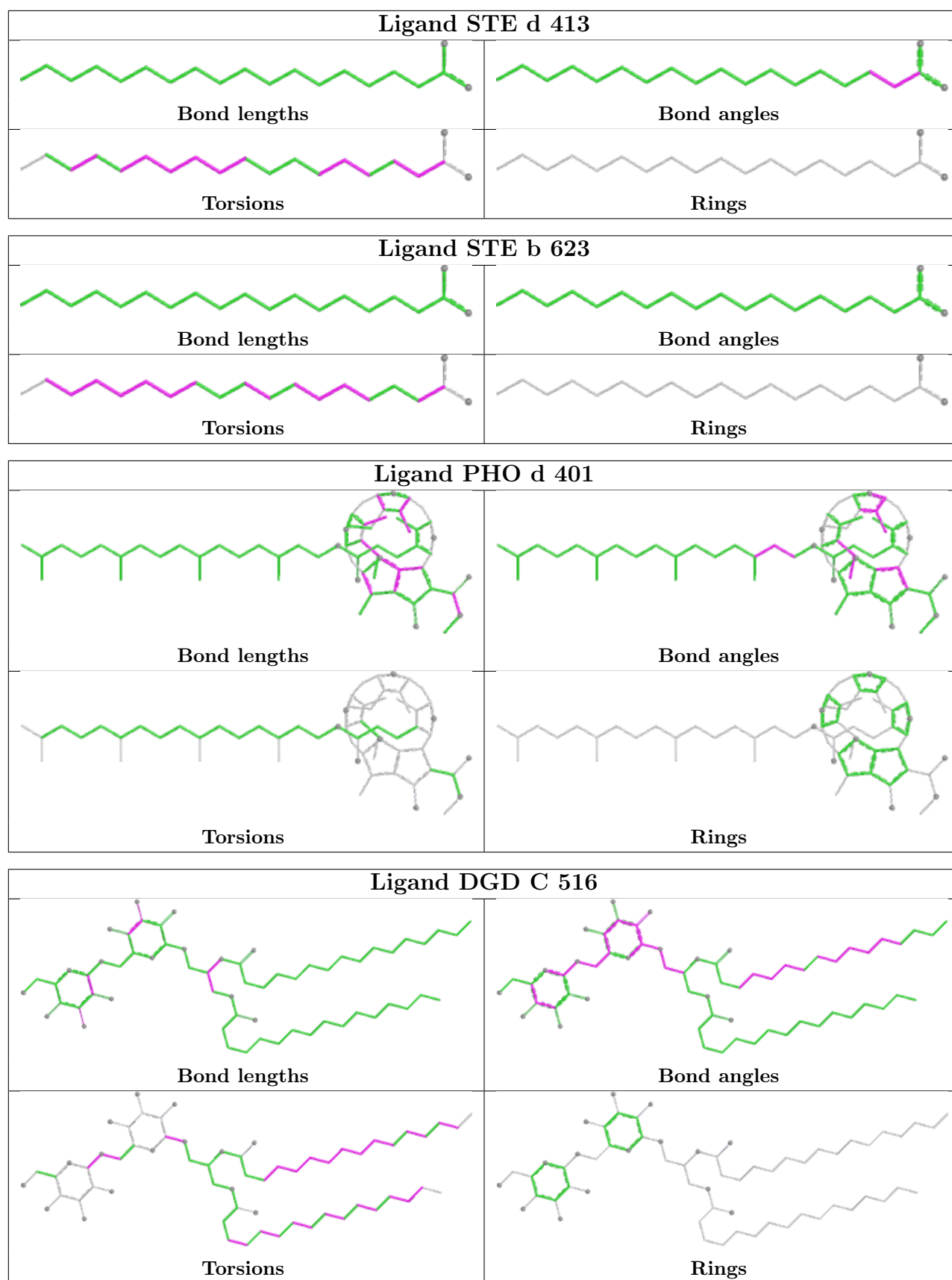
Ligand CLA C 509

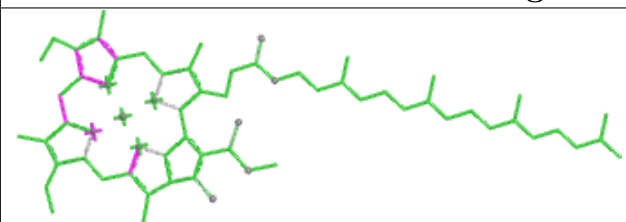
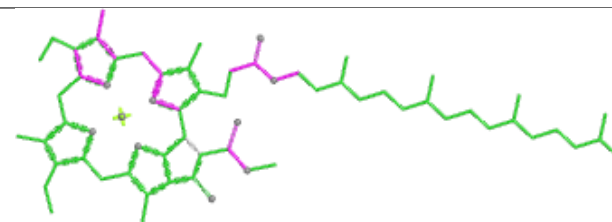
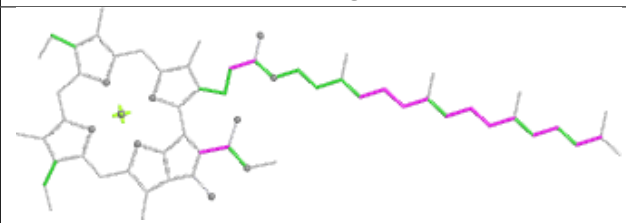
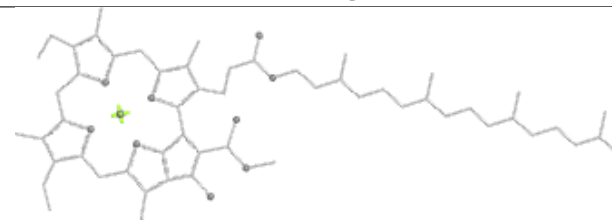


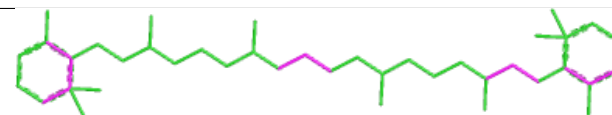
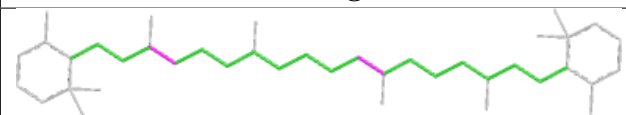
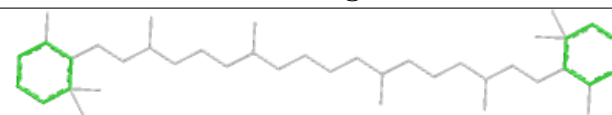
Ligand STE c 519

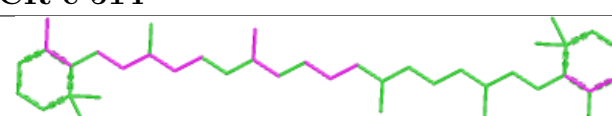
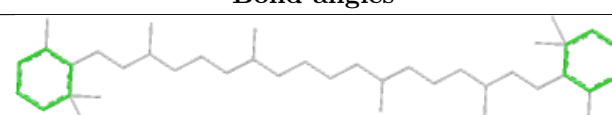


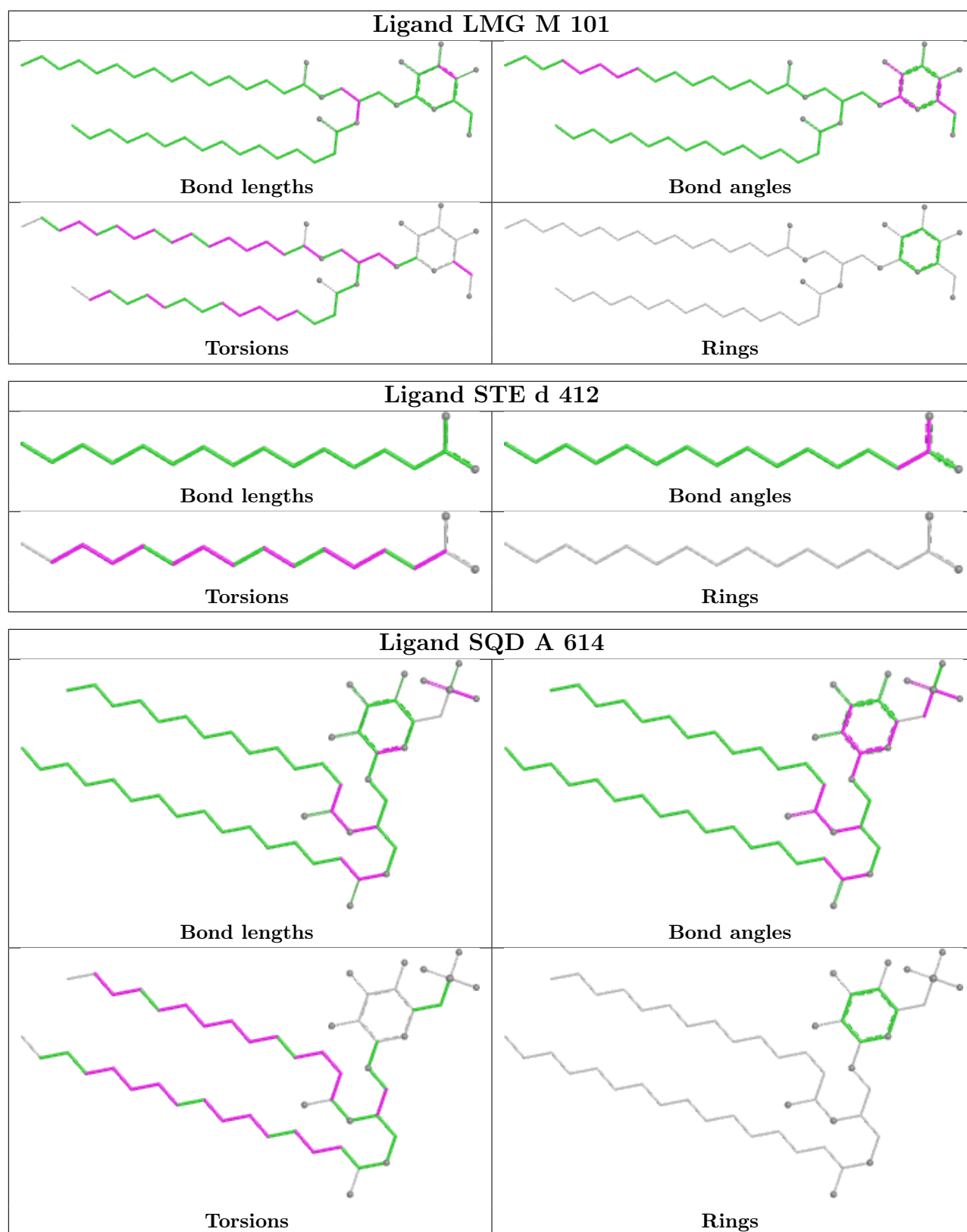




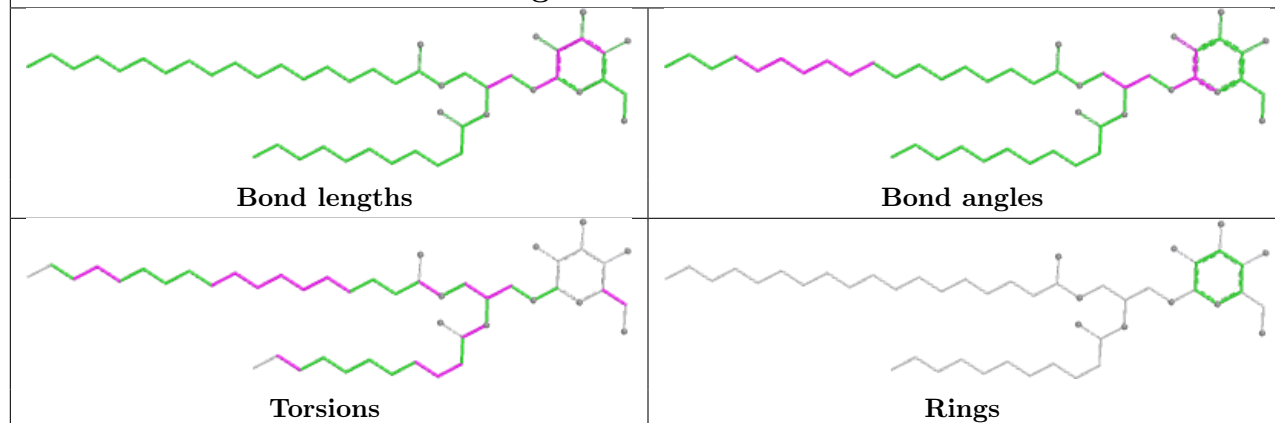
Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

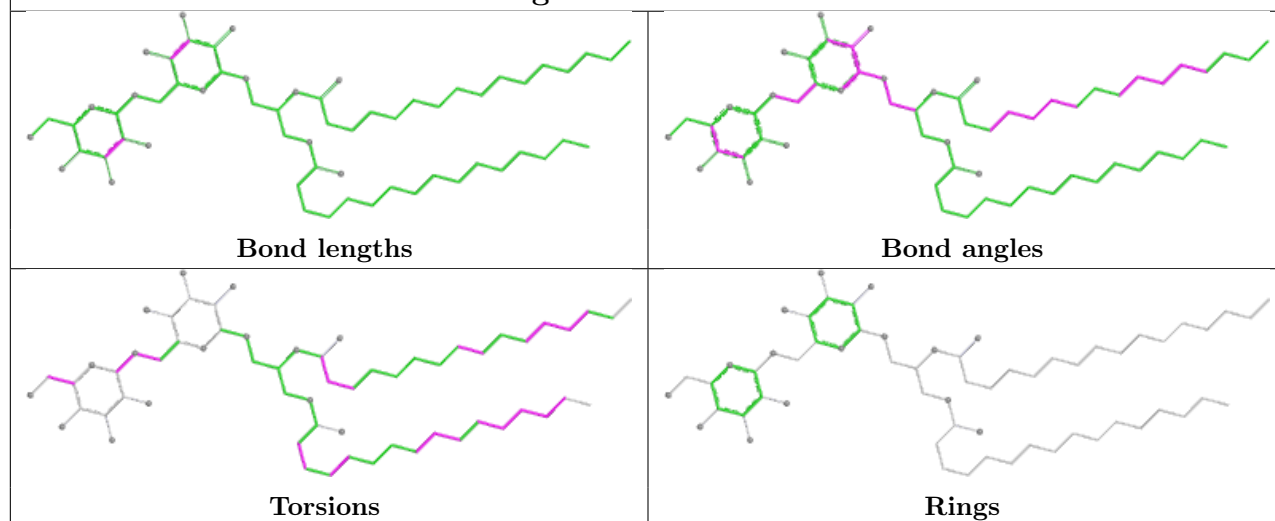
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings



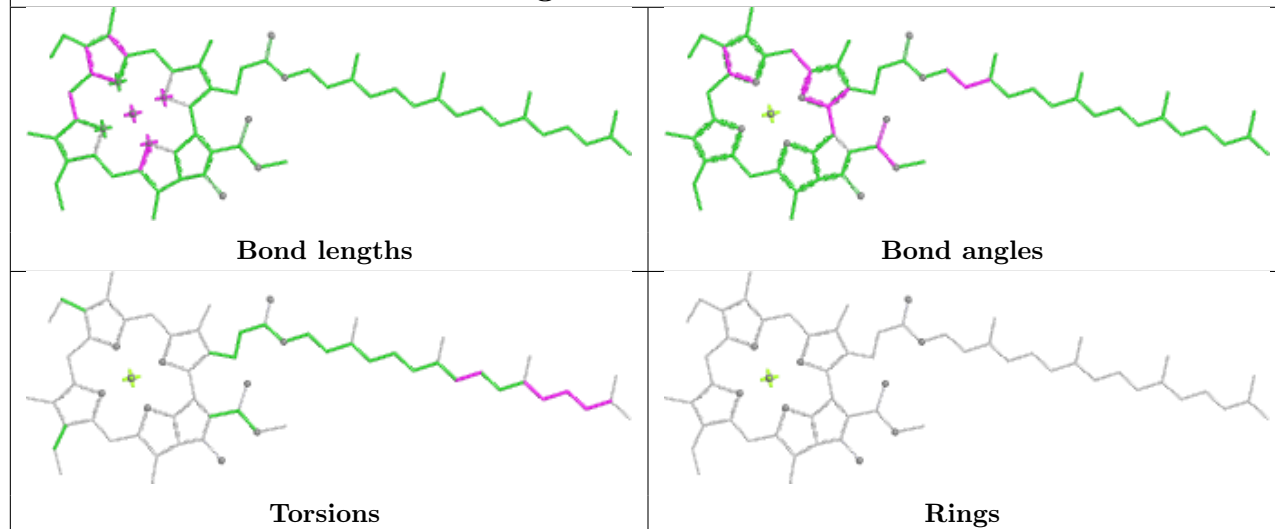
Ligand LMG c 520

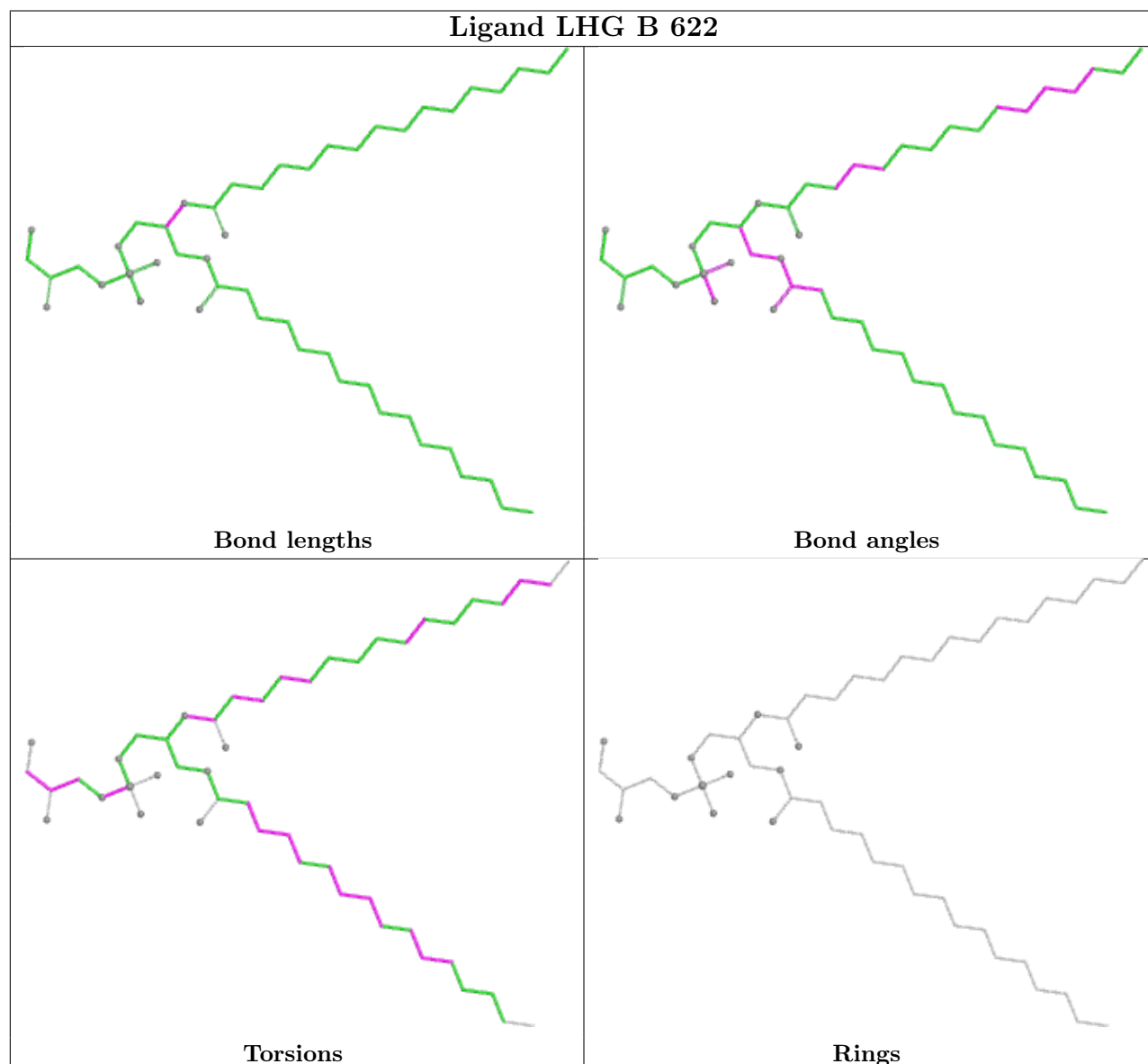
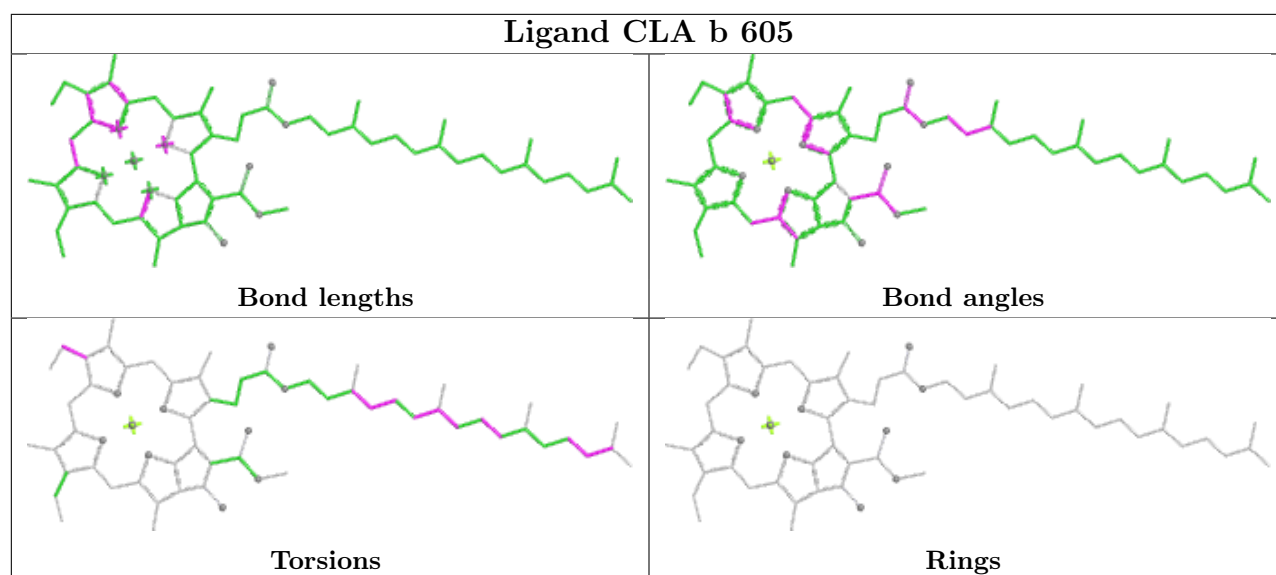


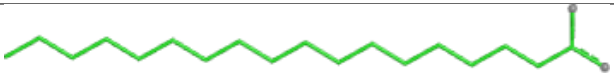
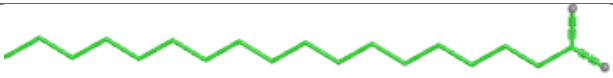
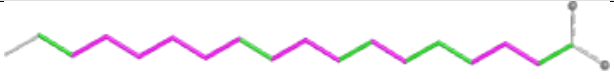
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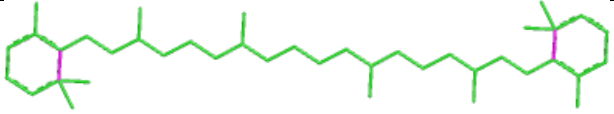
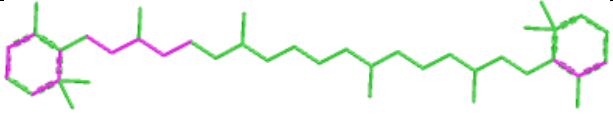
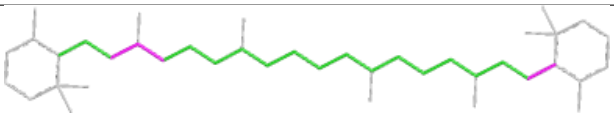
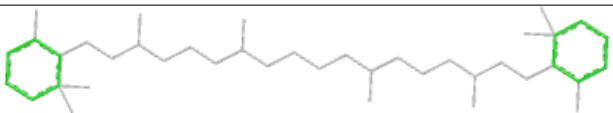


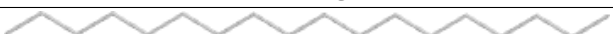
Ligand CLA c 511

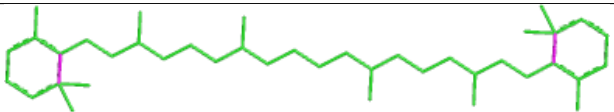
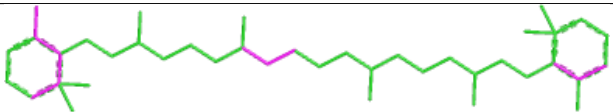
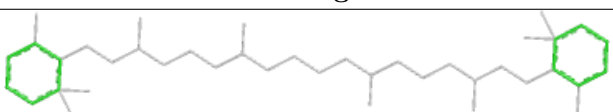


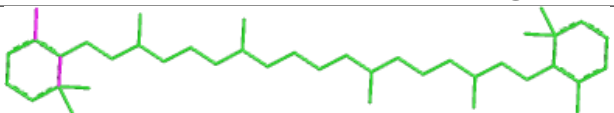
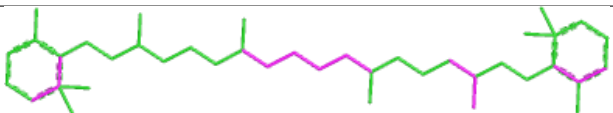
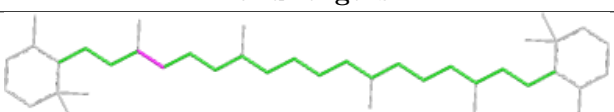
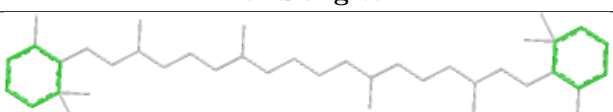


Ligand STE X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

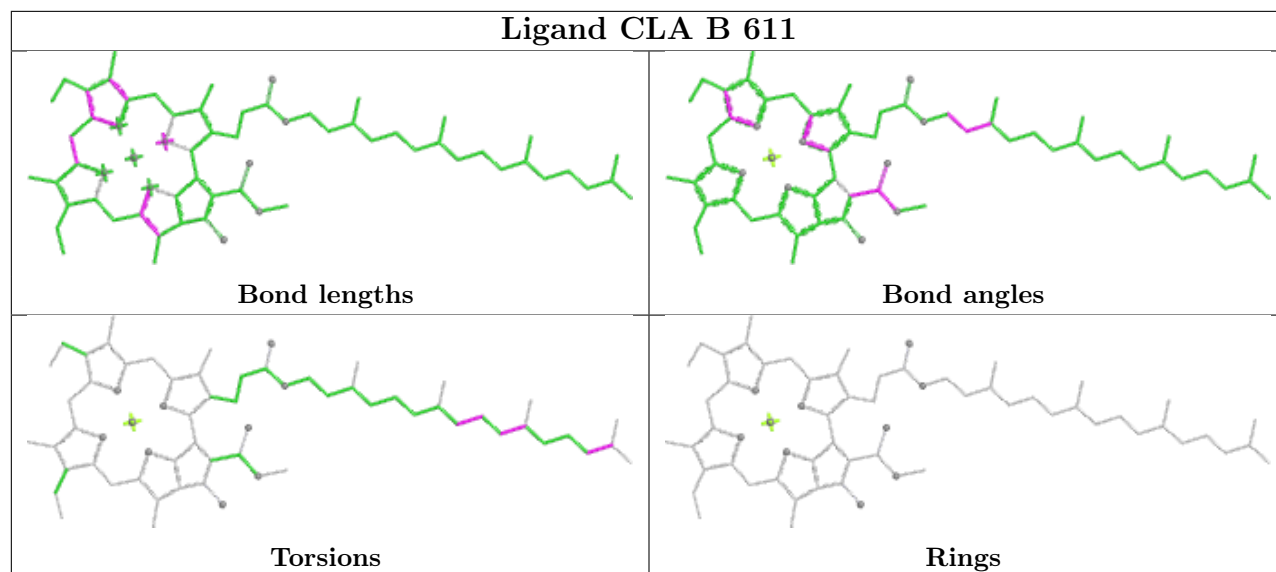
Ligand BCR x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE l 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

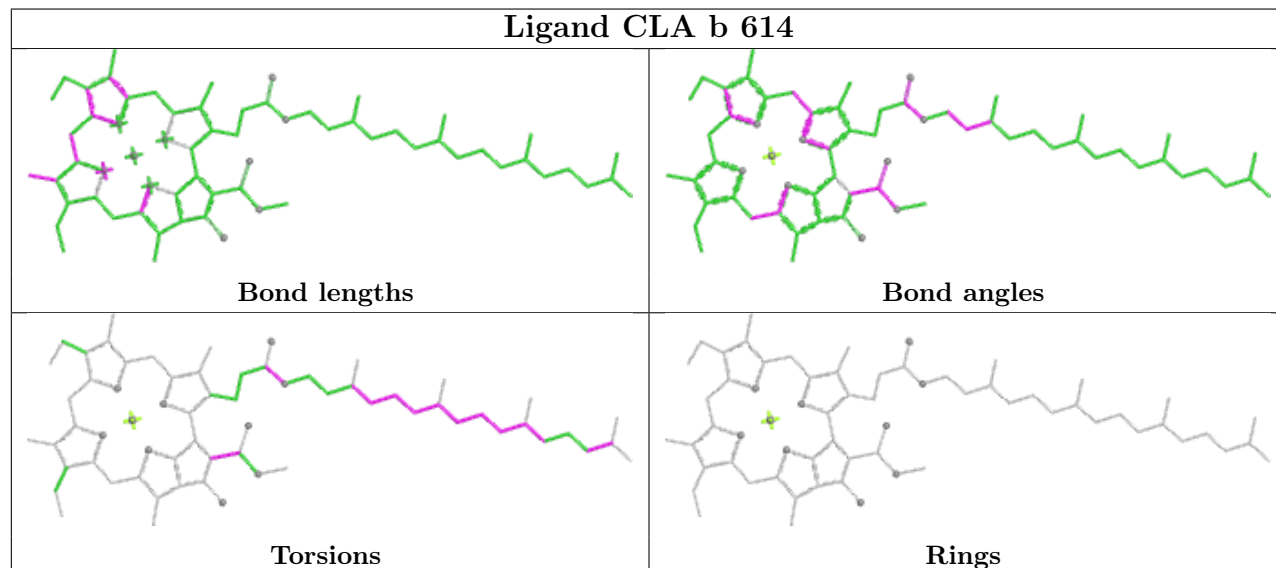
Ligand BCR Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

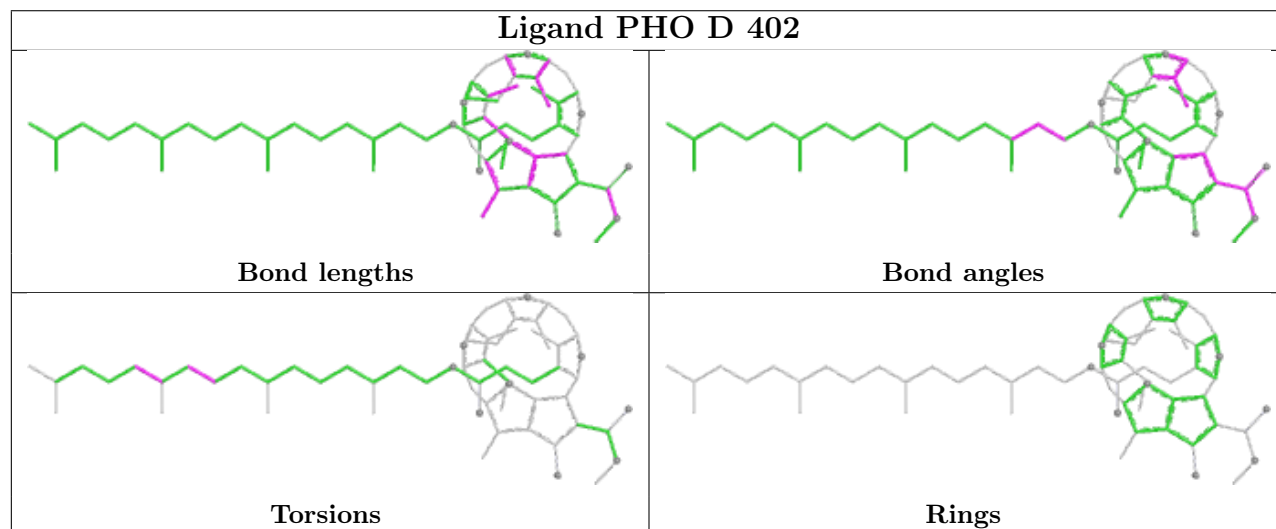
Ligand CLA B 611



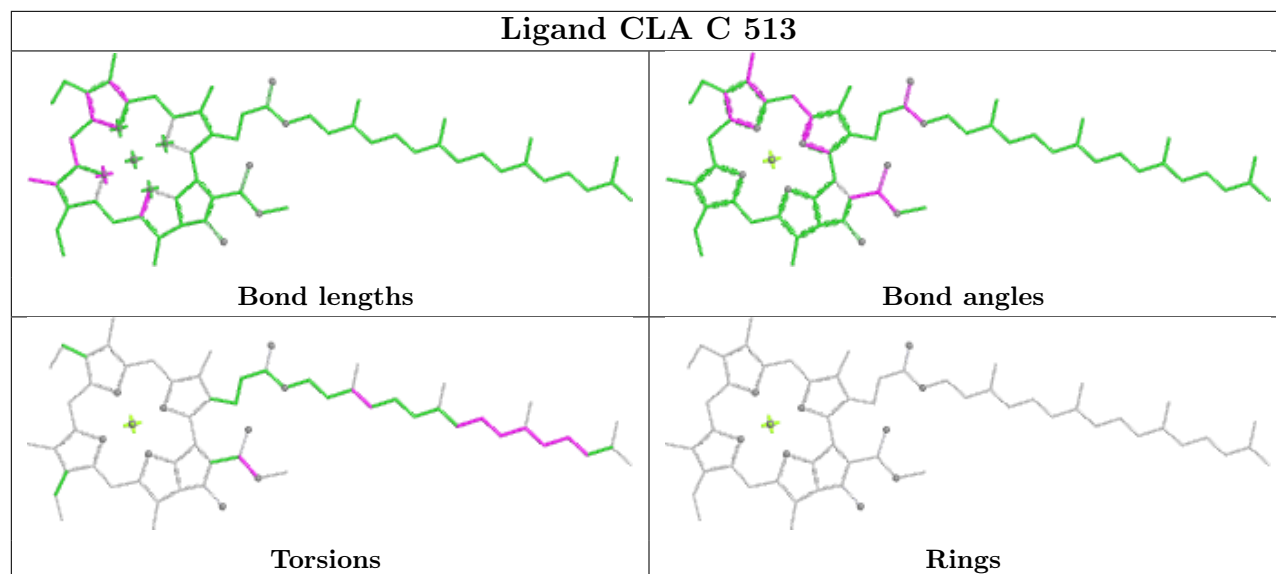
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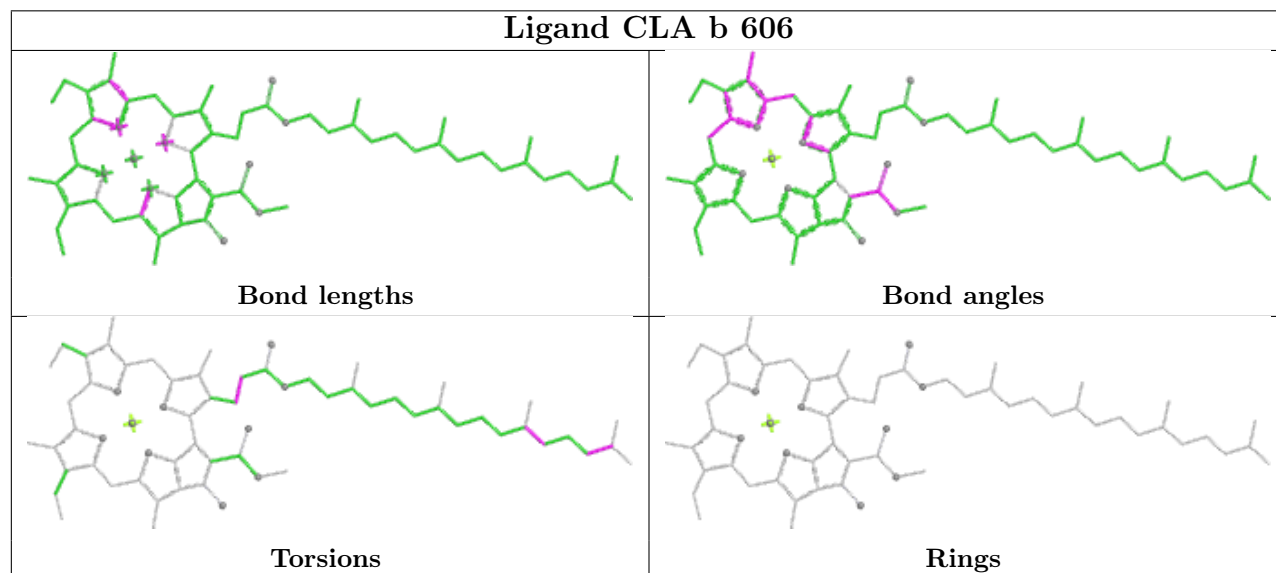
Ligand PHO D 402



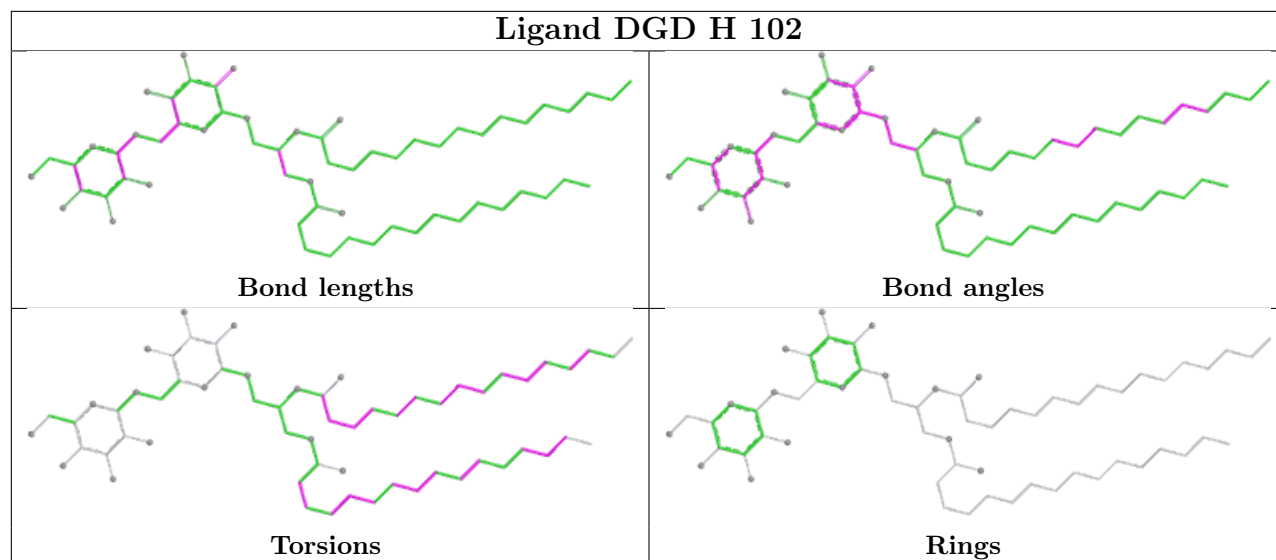
Ligand CLA C 513

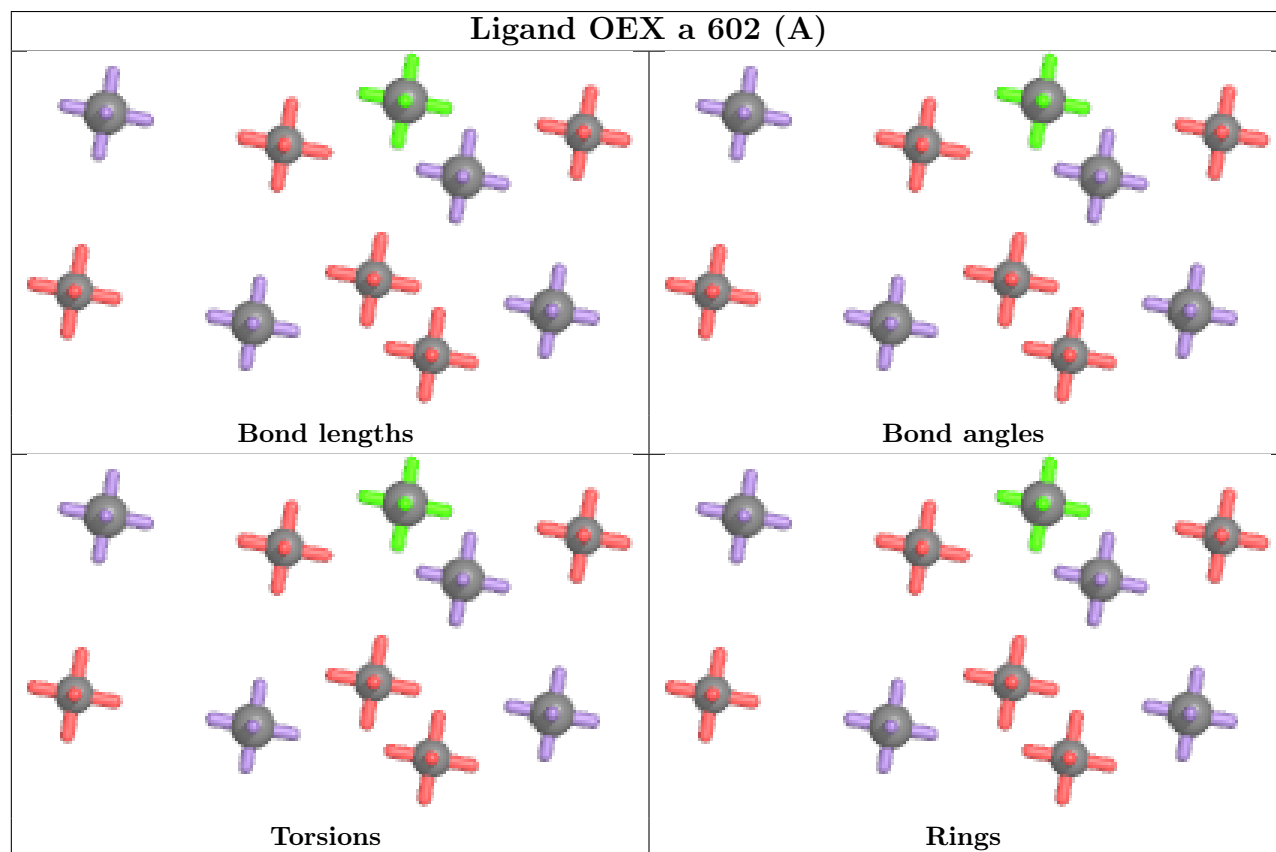
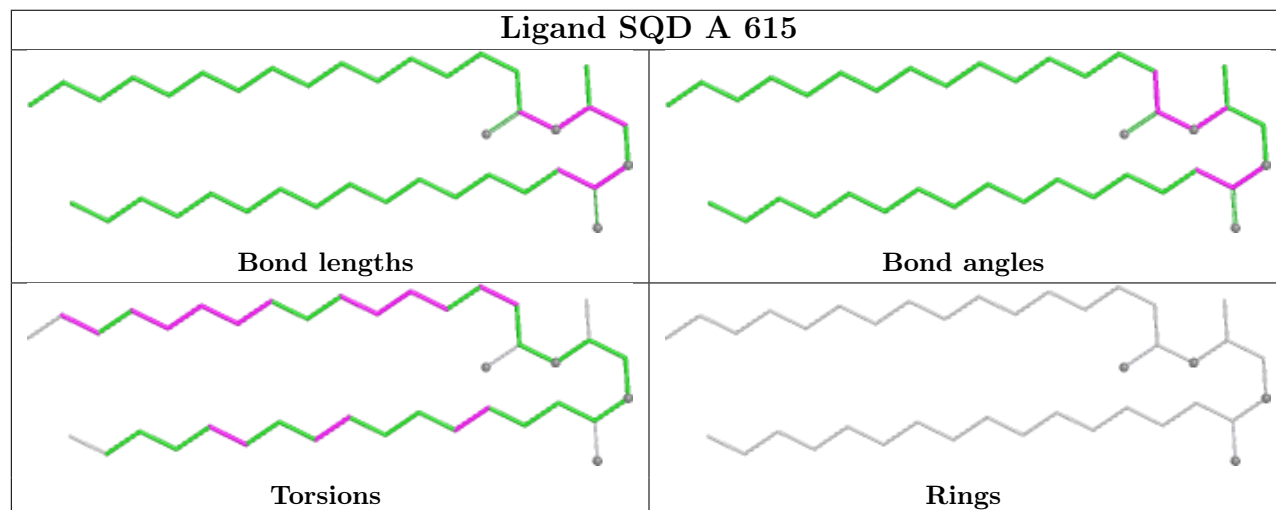
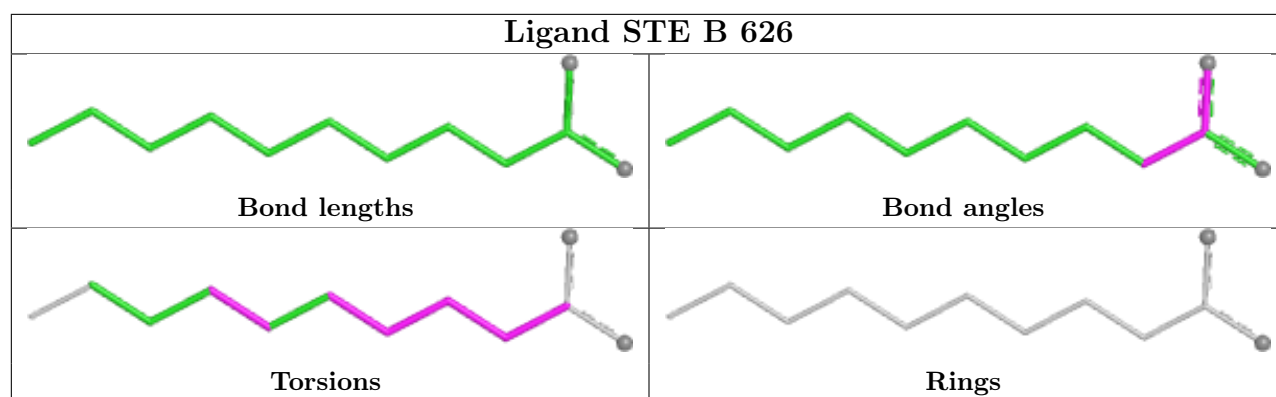


Ligand CLA b 606

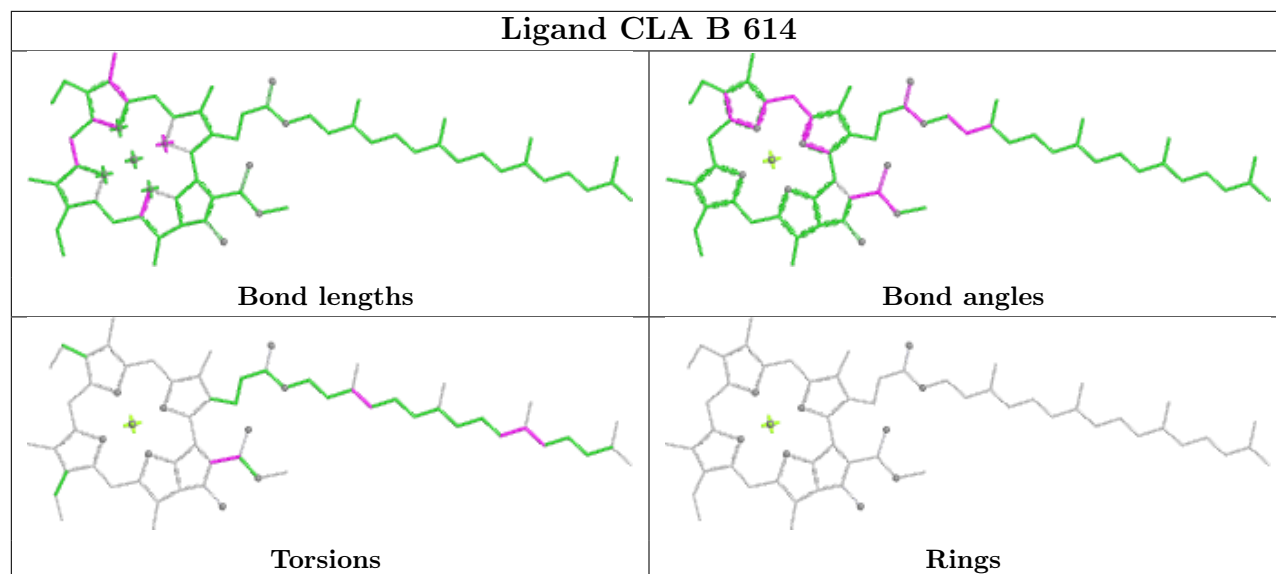


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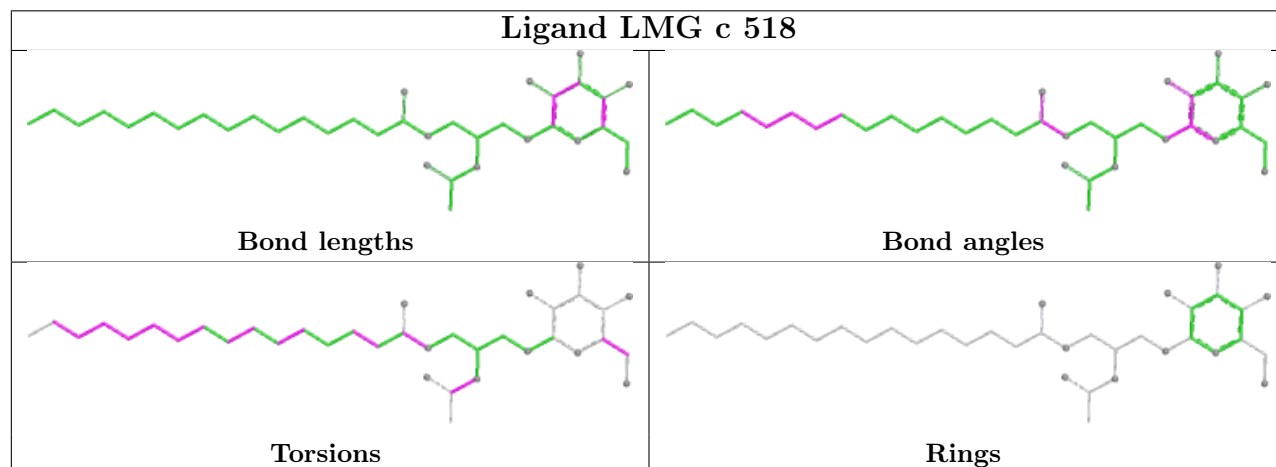




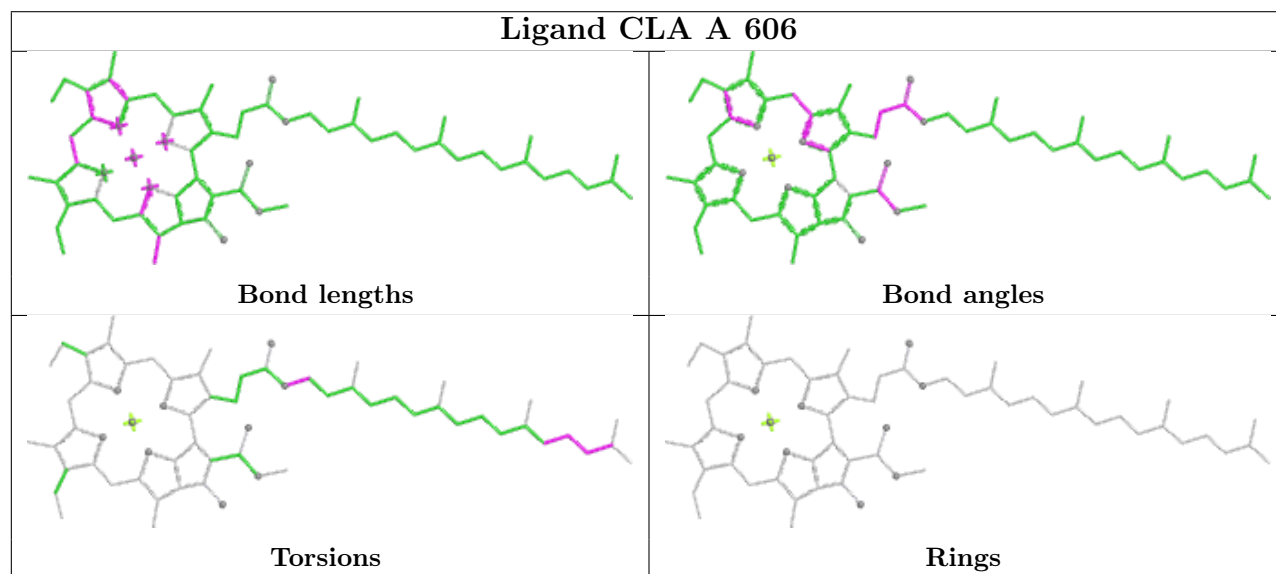
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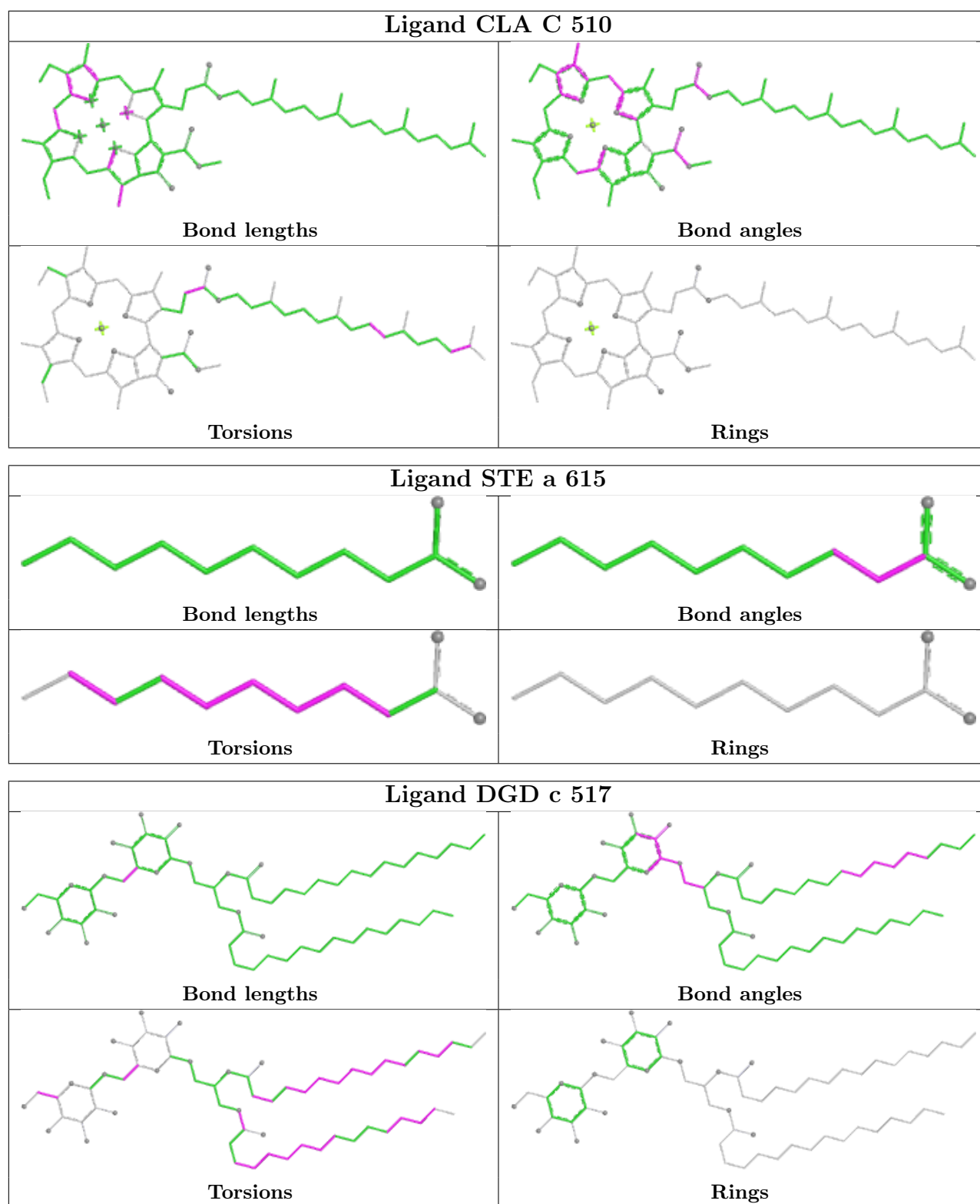


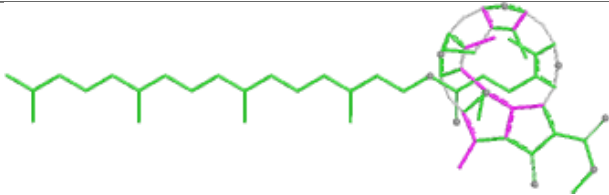
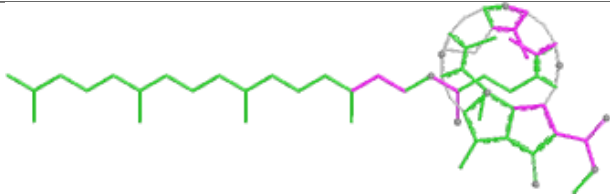
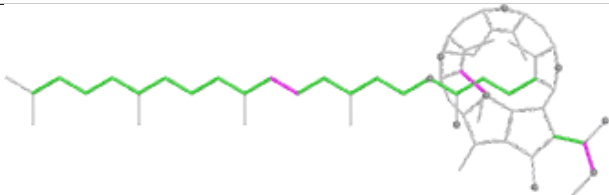
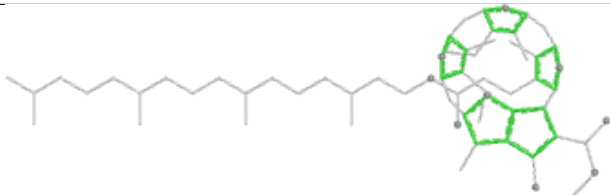
Ligand LMG c 518

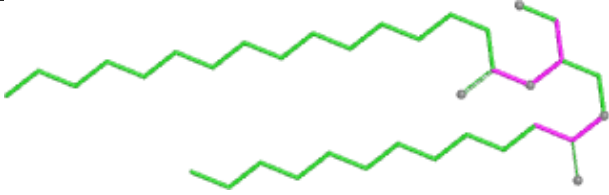
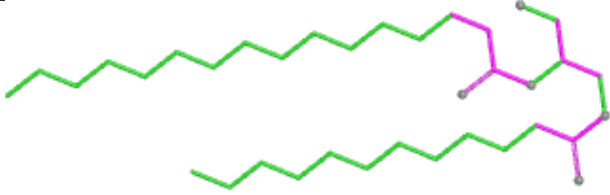
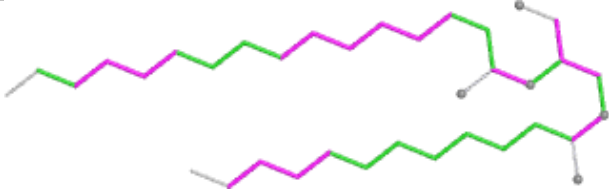


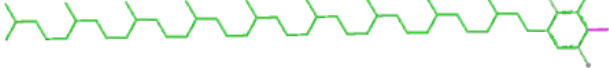
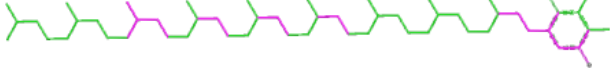
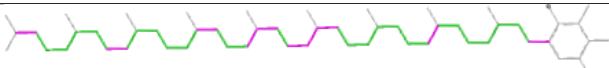
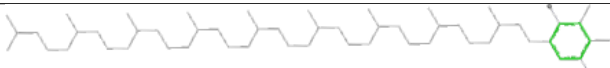
Ligand CLA A 606

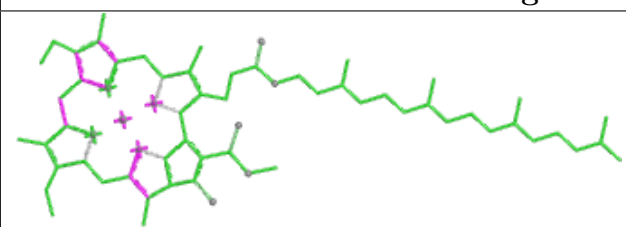
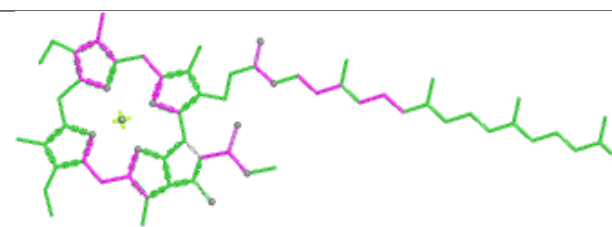
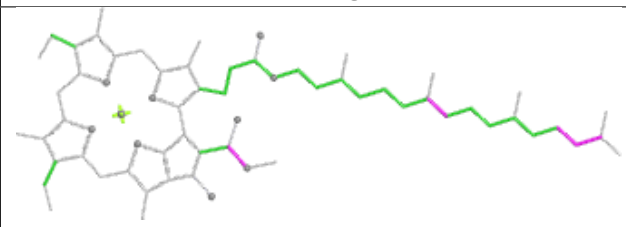
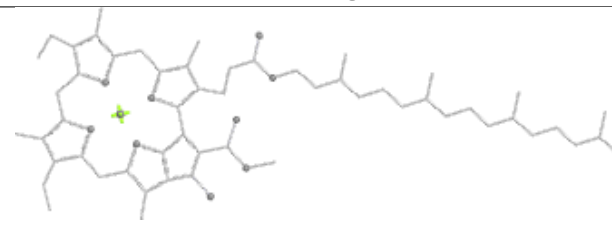


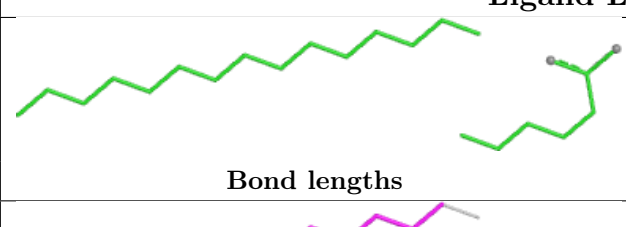
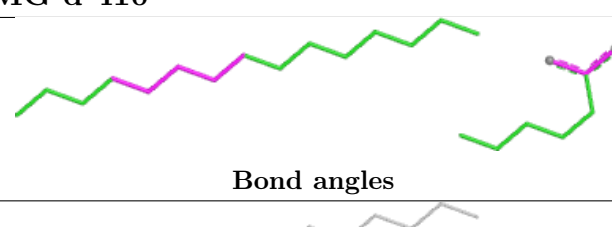
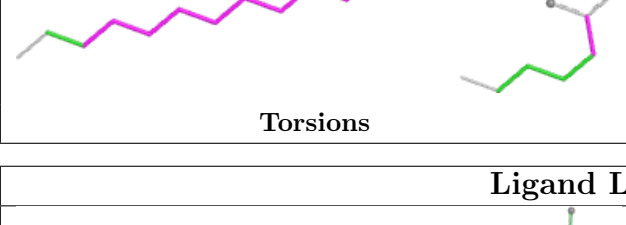


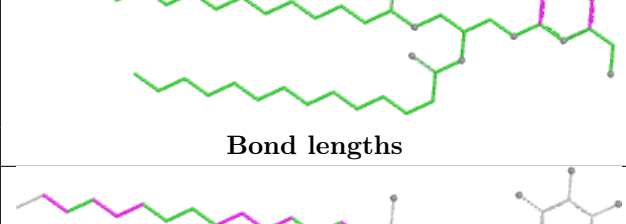
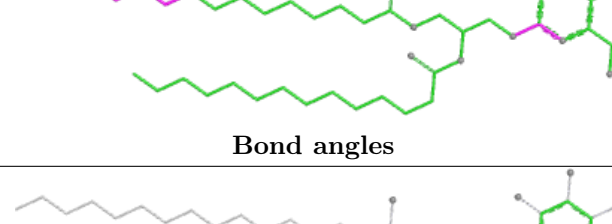
Ligand PHO d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

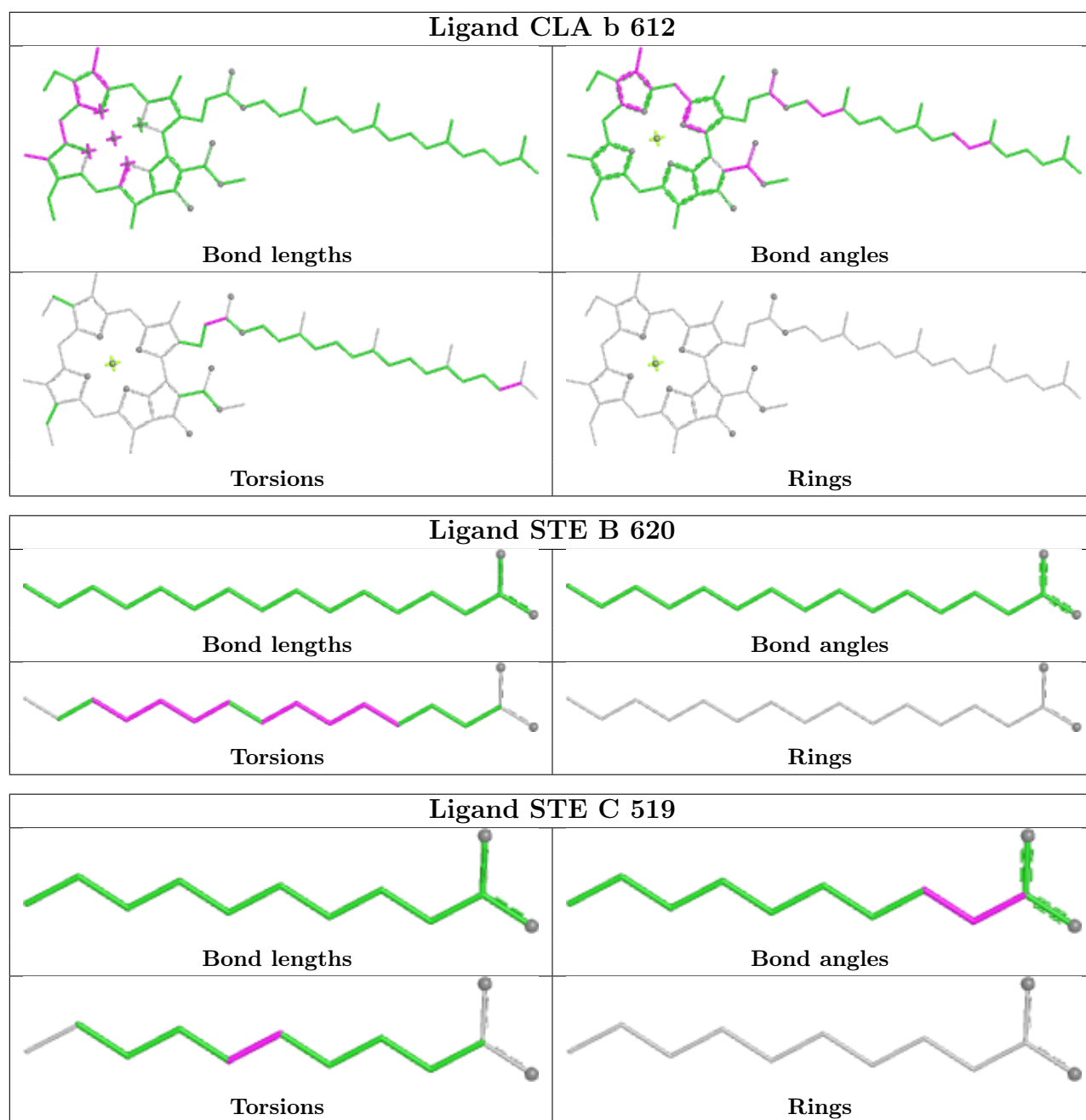
Ligand SQD a 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

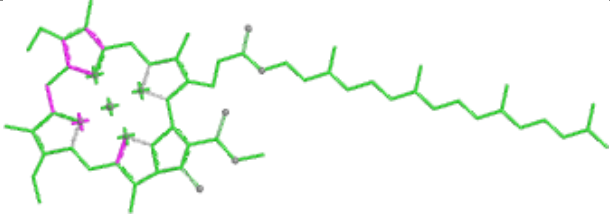
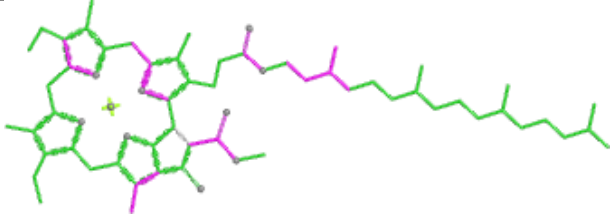
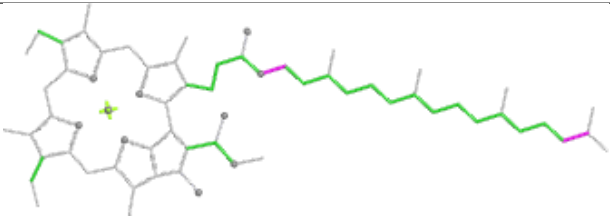
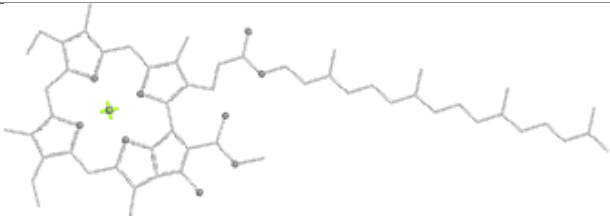
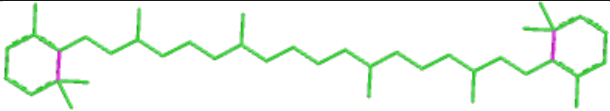
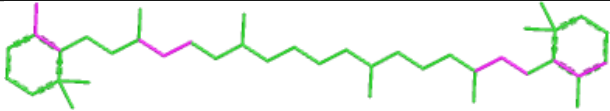
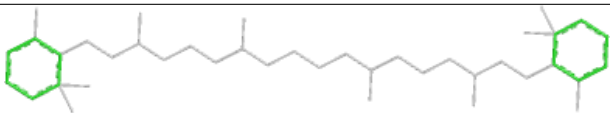
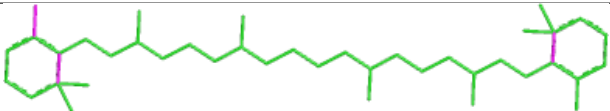
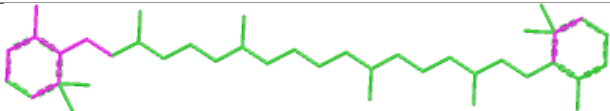
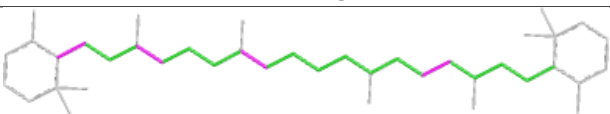
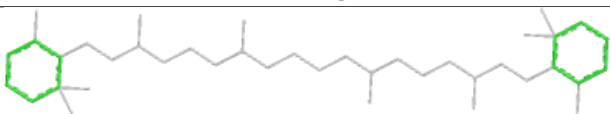
Ligand PL9 a 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

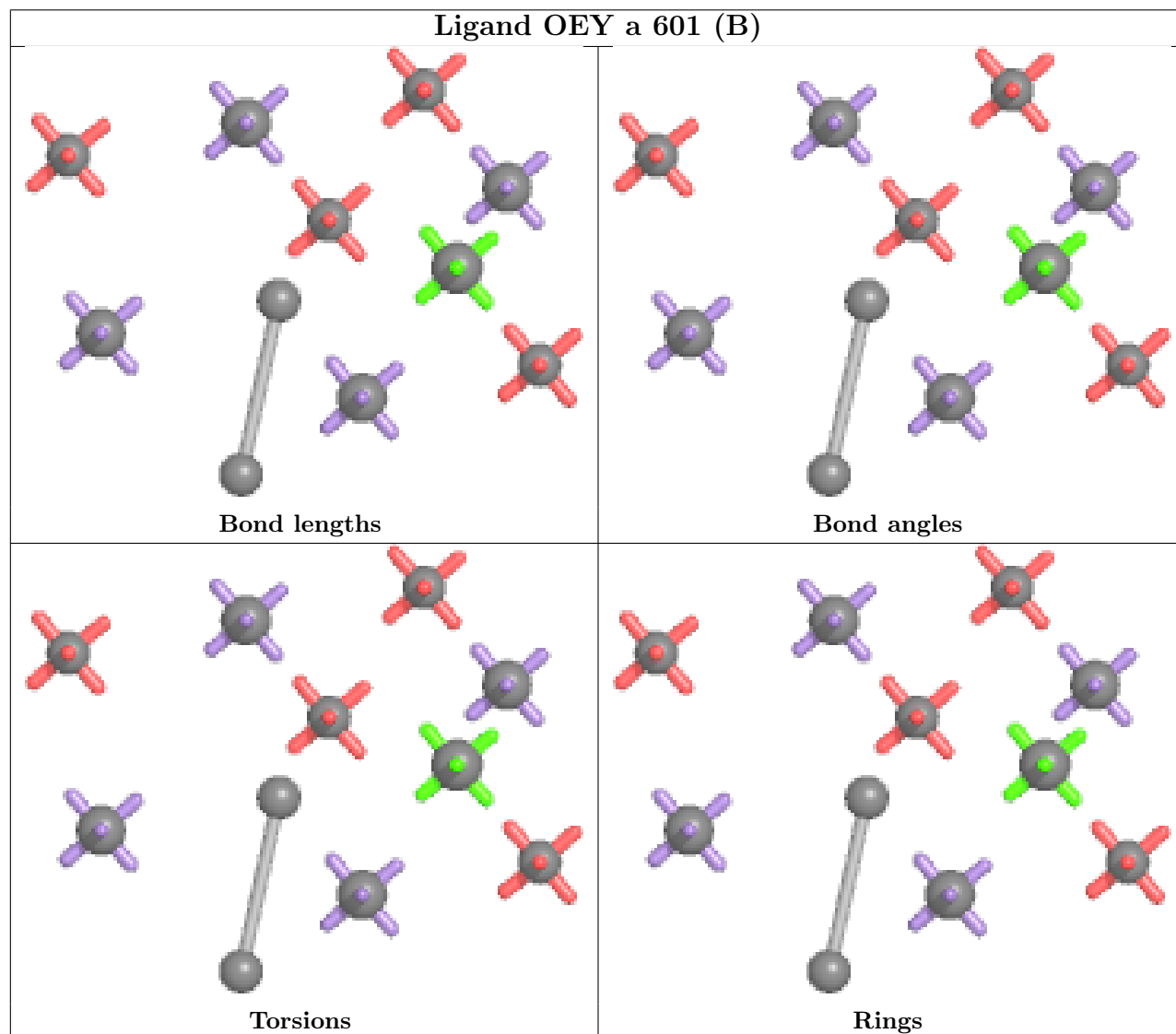
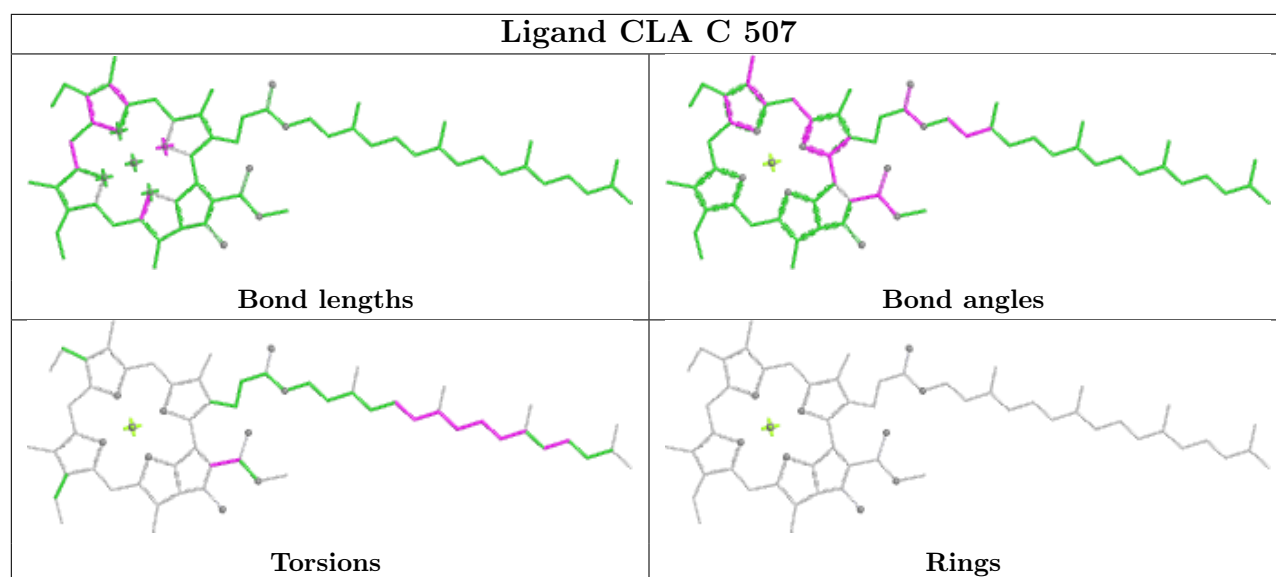
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

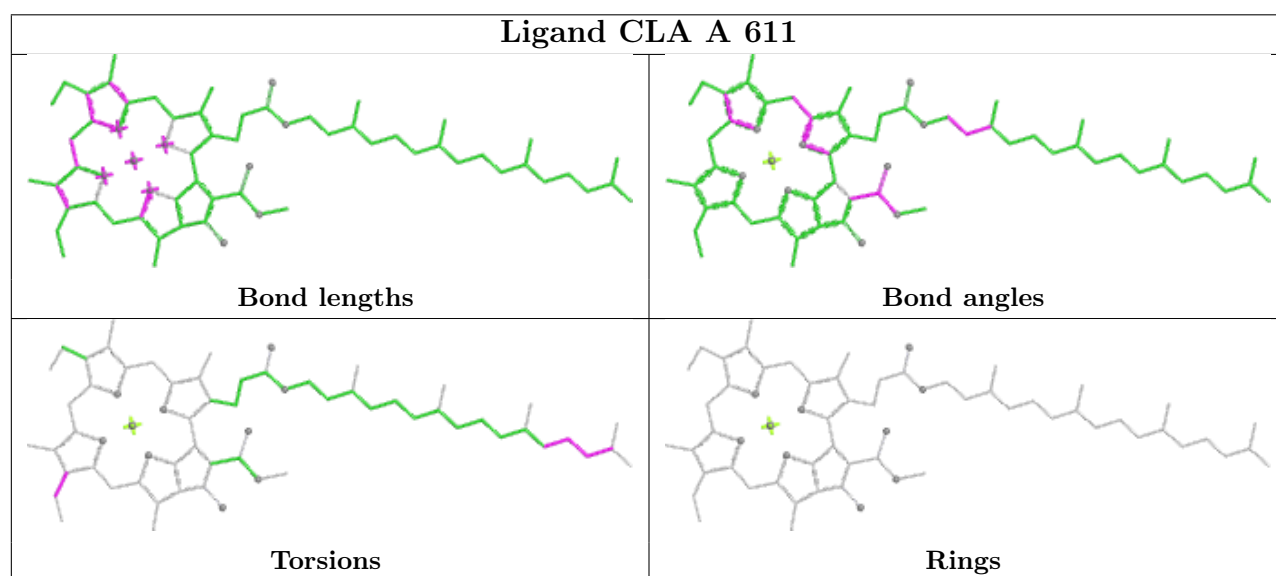
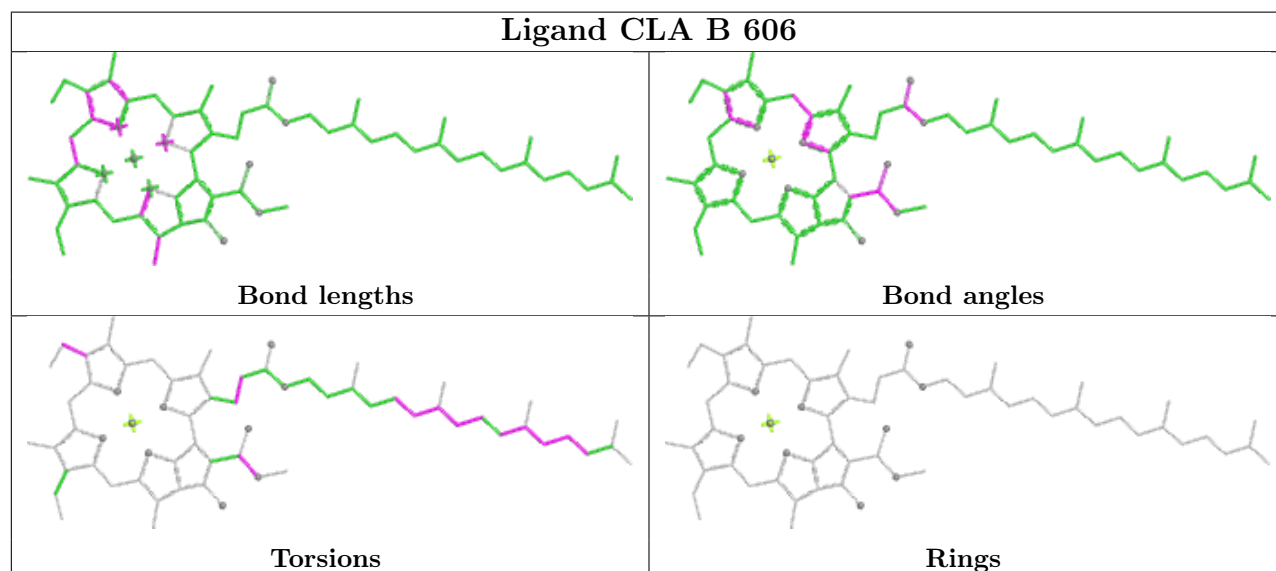
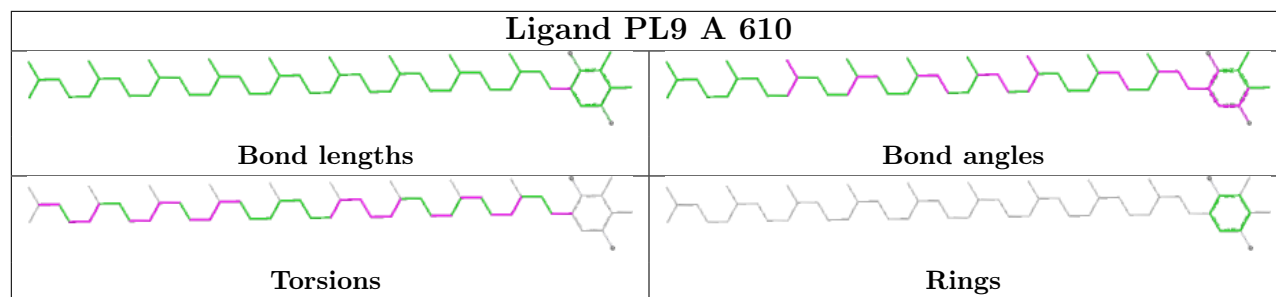
Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

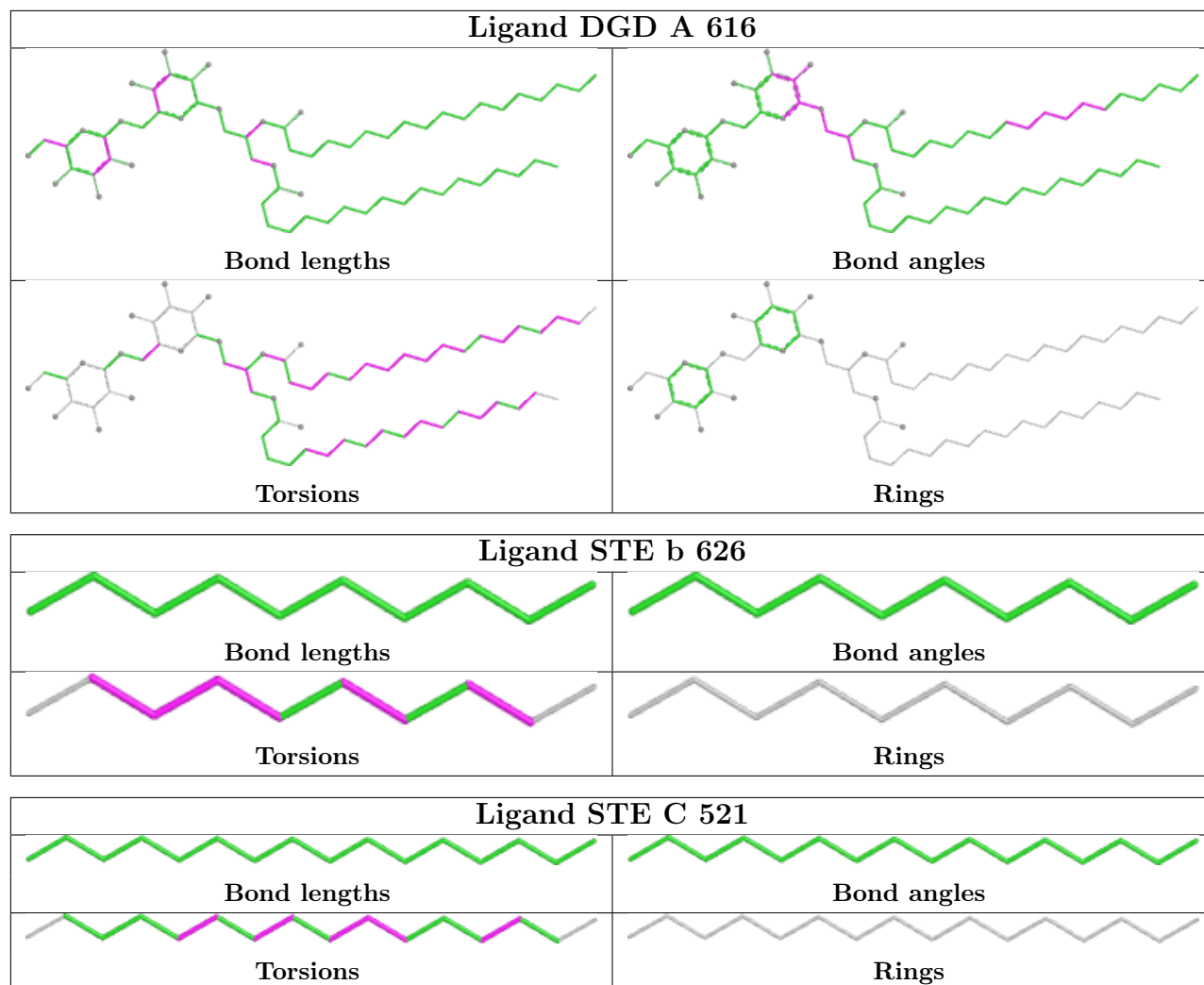
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

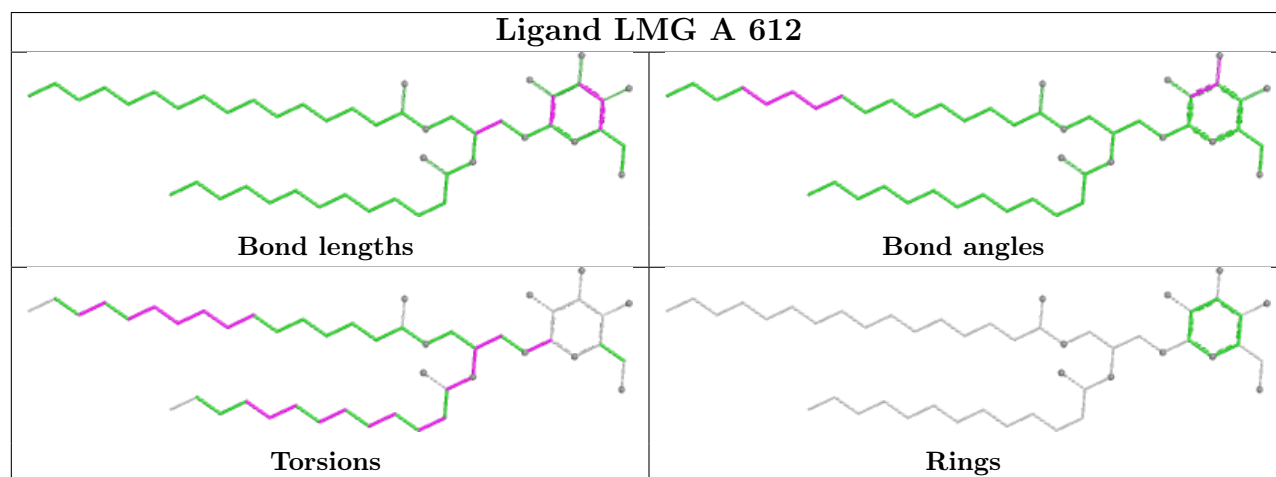
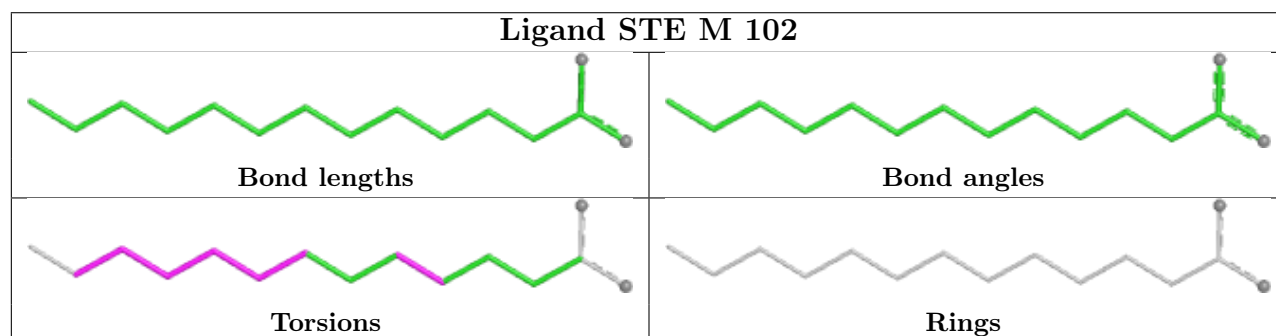
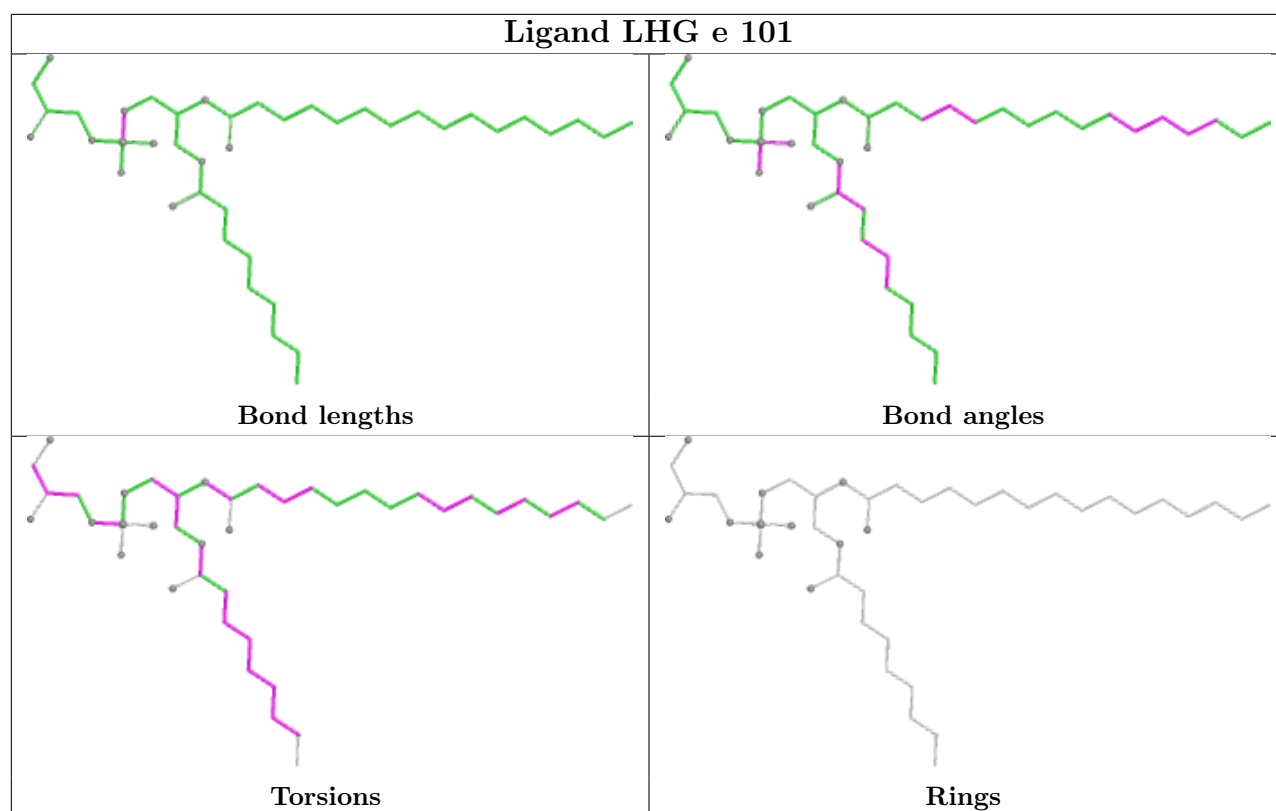


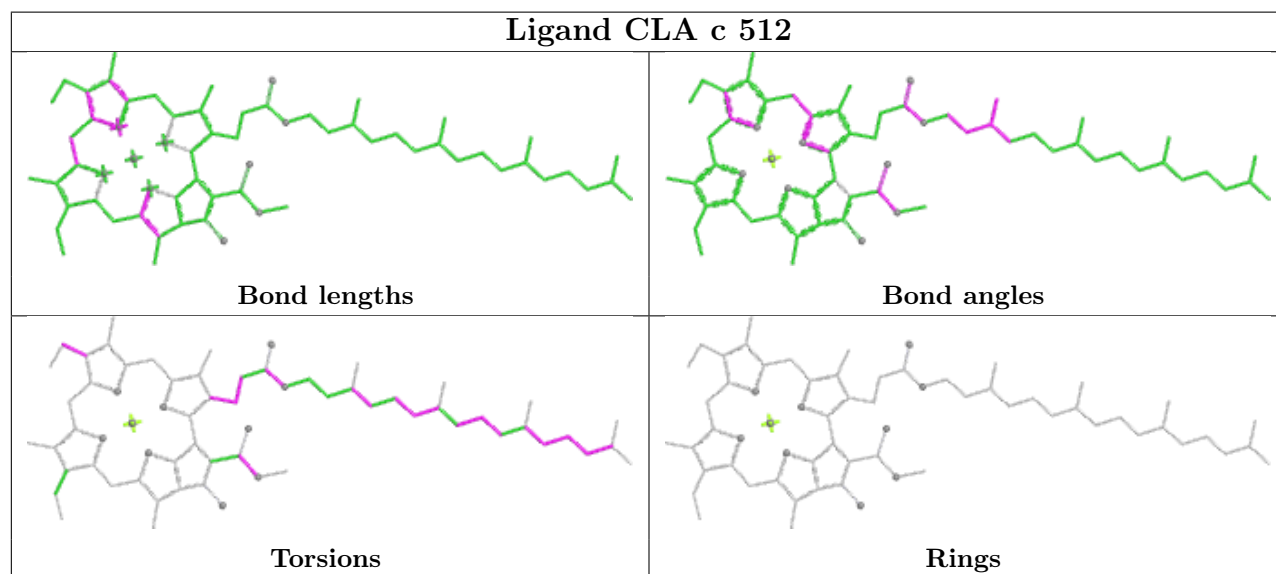
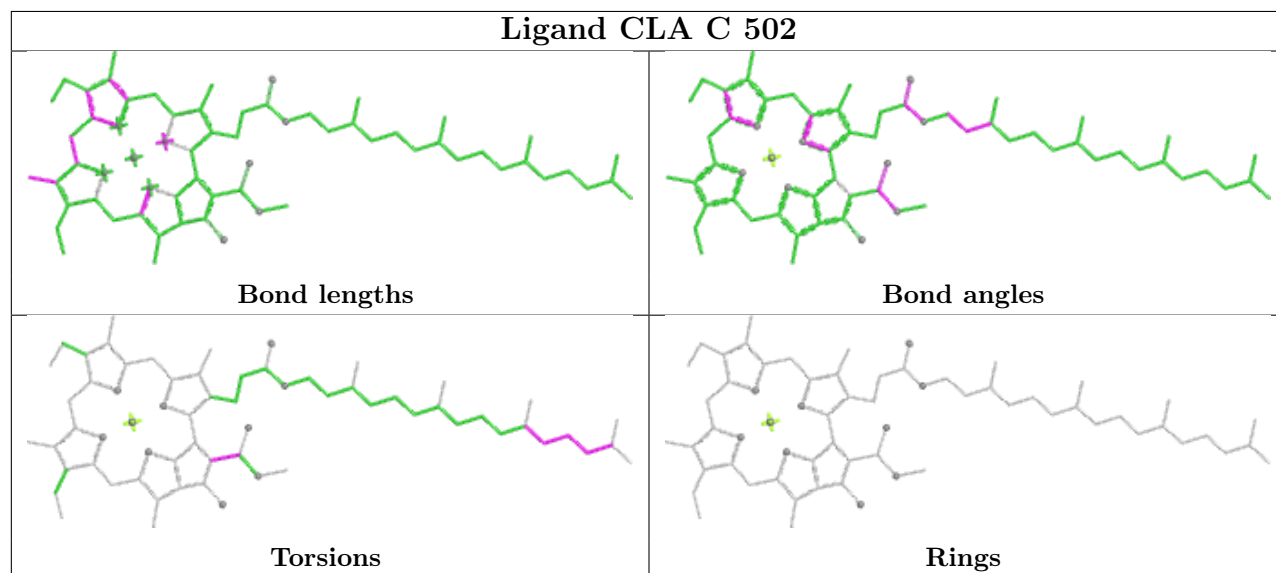
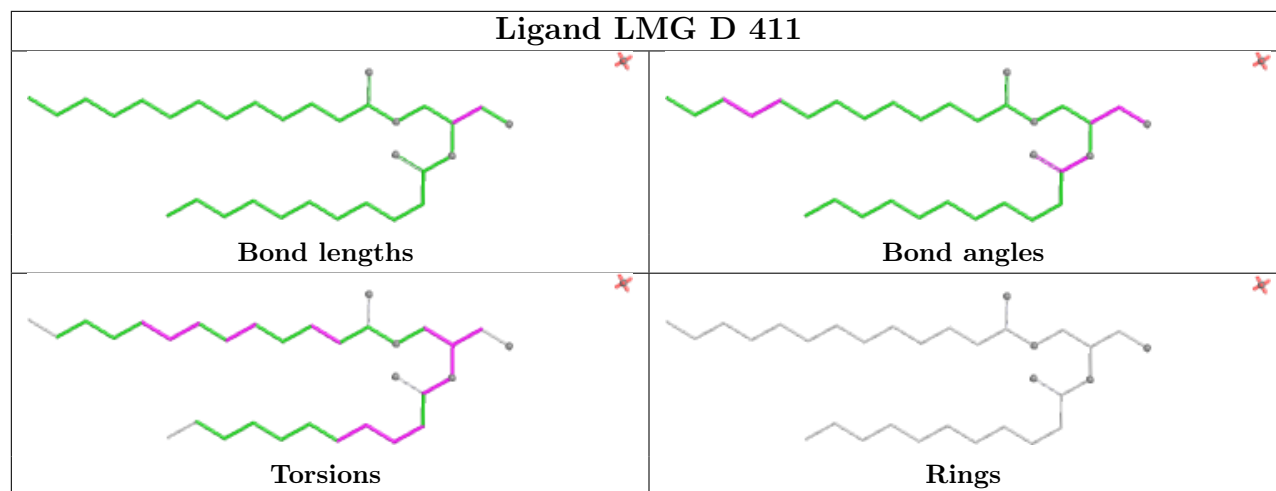
Ligand CLA D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.71	0 100 100	11, 28, 45, 75	64 (19%)
1	a	334/344 (97%)	-0.65	0 100 100	11, 29, 54, 72	64 (19%)
2	B	505/510 (99%)	-0.57	1 (0%) 91 90	17, 32, 57, 88	4 (0%)
2	b	505/510 (99%)	-0.47	1 (0%) 91 90	25, 35, 67, 99	0
3	C	442/461 (95%)	-0.60	0 100 100	13, 34, 50, 69	11 (2%)
3	c	451/461 (97%)	-0.46	1 (0%) 91 90	13, 38, 57, 93	12 (2%)
4	D	341/352 (96%)	-0.74	0 100 100	14, 29, 44, 72	2 (0%)
4	d	341/352 (96%)	-0.62	0 100 100	14, 33, 55, 79	3 (0%)
5	E	82/84 (97%)	-0.05	0 100 100	31, 47, 66, 79	1 (1%)
5	e	82/84 (97%)	0.11	1 (1%) 76 76	39, 54, 73, 84	0
6	F	34/45 (75%)	-0.26	0 100 100	34, 42, 57, 87	0
6	f	34/45 (75%)	-0.11	0 100 100	39, 48, 76, 83	0
7	H	65/66 (98%)	-0.30	1 (1%) 72 71	32, 39, 54, 68	0
7	h	63/66 (95%)	-0.10	0 100 100	38, 49, 58, 61	0
8	I	35/38 (92%)	-0.42	0 100 100	33, 39, 62, 81	0
8	i	35/38 (92%)	-0.38	0 100 100	32, 39, 68, 86	0
9	J	36/40 (90%)	-0.25	0 100 100	32, 46, 70, 78	0
9	j	36/40 (90%)	-0.12	0 100 100	36, 51, 83, 93	0
10	K	37/46 (80%)	-0.34	0 100 100	38, 46, 61, 67	0
10	k	37/46 (80%)	-0.10	0 100 100	44, 52, 66, 74	0
11	L	37/37 (100%)	-0.59	0 100 100	25, 29, 59, 67	0
11	l	36/37 (97%)	-0.60	0 100 100	26, 29, 61, 80	0
12	M	32/36 (88%)	-0.60	0 100 100	27, 32, 57, 67	0
12	m	31/36 (86%)	-0.54	0 100 100	29, 34, 48, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.34	4 (1%) 70 70	26, 40, 75, 127	1 (0%)
13	o	244/272 (89%)	-0.34	2 (0%) 82 82	26, 40, 76, 115	0
14	T	29/32 (90%)	-0.64	1 (3%) 48 47	27, 30, 56, 71	0
14	t	29/32 (90%)	-0.60	0 100 100	26, 32, 68, 81	0
15	U	97/134 (72%)	-0.43	0 100 100	32, 41, 65, 91	0
15	u	97/134 (72%)	-0.43	1 (1%) 79 79	30, 38, 54, 83	0
16	V	137/163 (84%)	-0.49	0 100 100	29, 38, 52, 71	0
16	v	137/163 (84%)	-0.33	0 100 100	34, 45, 63, 79	0
17	Y	27/46 (58%)	0.53	2 (7%) 20 19	49, 64, 79, 87	0
17	y	30/46 (65%)	0.27	0 100 100	56, 66, 76, 90	0
18	X	38/41 (92%)	-0.16	0 100 100	40, 48, 64, 71	0
18	x	39/41 (95%)	0.16	1 (2%) 57 56	47, 59, 79, 91	0
19	Z	62/62 (100%)	0.51	3 (4%) 35 34	48, 62, 100, 113	0
19	z	62/62 (100%)	0.33	2 (3%) 50 49	55, 64, 104, 112	0
20	R	34/41 (82%)	0.57	1 (2%) 53 52	56, 65, 78, 79	0
20	r	31/41 (75%)	1.04	2 (6%) 25 23	67, 81, 97, 101	0
All	All	5302/5700 (93%)	-0.44	24 (0%) 87 87	11, 36, 68, 127	162 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	35	LEU	4.3
18	x	37	VAL	3.4
19	Z	62	VAL	3.3
20	r	31	VAL	3.1
13	o	58	ASN	3.0
13	o	56	PRO	2.8
13	O	59	LYS	2.8
19	Z	33	TRP	2.7
13	O	4	THR	2.6
20	r	12	VAL	2.6
13	O	60	ARG	2.6
17	Y	20	ALA	2.4
19	z	33	TRP	2.4
15	u	53	ALA	2.4
2	b	495	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
13	O	3	GLN	2.2
14	T	30	THR	2.2
17	Y	25	ILE	2.1
5	e	3	GLY	2.1
7	H	41	PHE	2.1
2	B	127	ARG	2.1
19	Z	30	PRO	2.1
19	z	40	ILE	2.1
3	c	23	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.92	0.07	31,38,52,59	0
12	FME	M	1	10/11	0.93	0.09	36,46,59,62	0
14	FME	T	1	10/11	0.94	0.08	30,36,56,60	0
8	FME	I	1	10/11	0.95	0.06	38,44,50,50	0
12	FME	m	1	10/11	0.97	0.06	35,44,61,62	0
8	FME	i	1	10/11	0.98	0.06	37,45,47,48	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
32	STE	H	103	18/20	0.68	0.13	55,64,72,72	0
32	STE	a	615	12/20	0.75	0.10	51,57,70,73	0
32	STE	T	103	20/20	0.76	0.12	42,52,69,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
28	LMG	b	624	55/55	0.76	0.14	50,63,76,77	0
32	STE	b	625	16/20	0.77	0.11	49,56,68,71	0
29	LHG	e	101	42/49	0.78	0.12	56,75,91,95	0
32	STE	m	101	12/20	0.78	0.13	51,58,64,67	0
28	LMG	d	410	23/55	0.79	0.12	47,61,65,68	0
32	STE	c	521	12/20	0.79	0.12	57,66,70,71	0
29	LHG	E	101	49/49	0.79	0.12	40,69,89,97	0
32	STE	B	625	18/20	0.80	0.12	42,52,76,82	0
32	STE	B	627	16/20	0.80	0.12	46,56,68,68	0
28	LMG	c	520	48/55	0.80	0.12	52,68,80,83	0
31	DGD	o	301	44/66	0.80	0.12	36,50,67,70	0
32	STE	b	626	10/20	0.81	0.11	48,53,60,60	0
32	STE	T	102	15/20	0.81	0.13	43,50,65,66	0
32	STE	E	102	12/20	0.81	0.11	57,67,81,82	0
27	PL9	A	610	55/55	0.82	0.12	35,57,67,71	0
32	STE	B	626	12/20	0.82	0.10	50,54,67,69	0
31	DGD	A	616	66/66	0.82	0.10	45,55,63,68	0
28	LMG	D	411	33/55	0.82	0.10	38,51,70,71	0
32	STE	X	101	20/20	0.83	0.14	36,48,61,65	0
30	SQD	a	614	36/54	0.83	0.10	38,54,64,70	0
25	CLA	b	601	65/65	0.83	0.10	45,61,78,84	0
30	SQD	f	102	41/54	0.84	0.11	58,72,82,85	0
32	STE	J	101	12/20	0.84	0.10	46,52,61,63	0
30	SQD	A	615	39/54	0.84	0.10	41,51,74,77	0
27	PL9	a	611	55/55	0.84	0.12	39,60,70,76	0
32	STE	d	413	20/20	0.84	0.12	43,50,57,58	0
32	STE	B	620	17/20	0.84	0.11	36,47,60,64	0
32	STE	t	103	10/20	0.84	0.10	44,53,60,61	0
30	SQD	B	623	54/54	0.85	0.10	36,56,72,80	0
28	LMG	c	518	37/55	0.85	0.10	43,57,68,69	0
32	STE	I	101	15/20	0.85	0.10	42,50,56,56	0
28	LMG	A	612	48/55	0.85	0.09	41,54,62,65	0
32	STE	b	621	16/20	0.85	0.11	34,45,55,61	0
32	STE	t	102	14/20	0.85	0.09	40,44,57,58	0
32	STE	b	623	20/20	0.85	0.11	37,49,67,69	0
28	LMG	c	522	49/55	0.86	0.09	40,50,70,76	0
30	SQD	b	620	49/54	0.86	0.09	41,50,73,78	0
28	LMG	b	622	51/55	0.87	0.09	33,49,60,63	0
32	STE	C	519	12/20	0.87	0.10	39,44,58,59	0
32	STE	C	520	12/20	0.87	0.09	43,49,53,54	0
28	LMG	B	621	28/55	0.87	0.10	38,45,59,69	0
26	BCR	k	102	40/40	0.87	0.10	43,52,58,60	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	0.88	0.10	38,51,72,80	0
32	STE	j	101	12/20	0.88	0.09	46,52,58,58	0
32	STE	c	519	20/20	0.88	0.09	40,49,80,81	0
32	STE	B	624	12/20	0.88	0.11	44,53,58,60	0
32	STE	d	412	17/20	0.88	0.10	42,47,61,64	0
28	LMG	M	101	51/55	0.89	0.08	33,47,59,61	0
32	STE	M	103	10/20	0.89	0.09	40,43,49,51	0
28	LMG	C	518	48/55	0.89	0.09	38,59,70,72	0
26	BCR	x	101	40/40	0.90	0.09	38,50,63,64	0
26	BCR	K	102	40/40	0.90	0.09	38,44,53,55	0
32	STE	C	521	16/20	0.90	0.08	36,44,51,58	0
26	BCR	D	406	40/40	0.91	0.08	32,40,68,75	0
32	STE	l	102	18/20	0.91	0.09	35,45,60,62	0
30	SQD	a	613	54/54	0.91	0.10	37,54,73,77	0
25	CLA	C	513	65/65	0.91	0.08	41,51,72,76	0
26	BCR	d	405	40/40	0.91	0.08	38,44,70,72	0
31	DGD	c	516	62/66	0.92	0.07	34,45,68,72	0
26	BCR	k	101	40/40	0.92	0.08	42,52,57,60	0
32	STE	M	102	15/20	0.92	0.07	36,44,54,63	0
26	BCR	H	101	40/40	0.92	0.07	34,40,53,54	0
30	SQD	D	409	36/54	0.92	0.09	43,60,66,69	0
26	BCR	K	101	40/40	0.92	0.08	41,48,54,56	0
31	DGD	H	102	62/66	0.92	0.08	29,40,46,53	0
31	DGD	C	516	62/66	0.93	0.07	32,42,75,84	0
25	CLA	c	512	65/65	0.93	0.08	39,50,70,74	0
26	BCR	b	618	40/40	0.93	0.06	25,34,45,50	0
31	DGD	h	101	62/66	0.93	0.08	35,45,52,57	0
26	BCR	A	609	40/40	0.93	0.06	26,31,37,41	0
29	LHG	d	407	49/49	0.93	0.07	33,44,58,66	0
28	LMG	D	408	51/55	0.93	0.09	28,42,67,71	0
30	SQD	A	614	52/54	0.93	0.09	33,47,67,69	0
26	BCR	B	619	40/40	0.93	0.07	29,39,48,52	0
33	BCT	a	606	4/4	0.93	0.08	32,35,39,44	0
31	DGD	C	517	62/66	0.94	0.07	26,38,62,70	0
26	BCR	B	618	40/40	0.94	0.06	24,34,44,46	0
26	BCR	k	103	40/40	0.94	0.08	41,47,55,58	0
31	DGD	c	517	62/66	0.94	0.07	29,44,64,76	0
28	LMG	d	411	44/55	0.94	0.07	34,43,71,73	0
25	CLA	C	506	65/65	0.94	0.07	28,37,68,69	0
26	BCR	C	514	40/40	0.94	0.07	29,36,47,47	0
25	CLA	b	616	60/65	0.94	0.08	29,37,77,79	0
25	CLA	c	506	65/65	0.94	0.07	32,40,70,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	c	508	64/65	0.94	0.07	32,38,74,85	0
25	CLA	C	512	65/65	0.94	0.08	35,44,66,69	0
26	BCR	a	610	40/40	0.94	0.06	22,30,38,41	0
26	BCR	b	617	40/40	0.94	0.06	29,36,44,44	0
25	CLA	c	513	65/65	0.94	0.08	38,53,79,85	0
26	BCR	b	619	40/40	0.94	0.06	30,40,53,56	0
26	BCR	c	514	40/40	0.94	0.06	31,40,48,51	0
25	CLA	B	606	65/65	0.94	0.07	25,33,58,63	0
31	DGD	C	515	62/66	0.94	0.07	25,34,63,67	0
26	BCR	B	617	40/40	0.94	0.06	27,33,42,44	0
34	PHO	d	402	64/64	0.94	0.06	23,35,40,43	0
26	BCR	T	101	40/40	0.95	0.05	28,34,45,47	0
26	BCR	Z	101	40/40	0.95	0.07	34,42,53,54	0
25	CLA	C	508	65/65	0.95	0.06	28,34,75,82	0
29	LHG	A	613	47/49	0.95	0.08	27,39,64,68	0
29	LHG	B	622	49/49	0.95	0.07	30,39,53,55	0
25	CLA	c	503	65/65	0.95	0.06	31,39,43,50	0
25	CLA	c	504	60/65	0.95	0.06	29,38,70,72	0
25	CLA	C	510	65/65	0.95	0.06	27,35,46,51	0
29	LHG	l	101	49/49	0.95	0.06	32,39,46,52	0
25	CLA	c	507	65/65	0.95	0.07	29,37,46,49	0
25	CLA	C	511	65/65	0.95	0.07	30,41,54,56	0
25	CLA	c	509	65/65	0.95	0.07	31,38,52,55	0
25	CLA	c	510	65/65	0.95	0.07	32,40,51,53	0
25	CLA	c	511	65/65	0.95	0.07	36,47,58,62	0
26	BCR	t	101	40/40	0.95	0.05	25,36,46,48	0
25	CLA	C	501	65/65	0.95	0.06	26,31,43,47	0
25	CLA	C	503	65/65	0.95	0.06	30,36,40,48	0
25	CLA	d	403	65/65	0.95	0.07	22,29,47,56	0
27	PL9	d	406	55/55	0.95	0.06	25,31,36,38	0
25	CLA	d	404	65/65	0.95	0.08	30,38,76,78	0
25	CLA	a	607	65/65	0.95	0.06	21,27,37,45	0
25	CLA	a	608	65/65	0.95	0.07	27,34,72,79	0
31	DGD	c	515	62/66	0.95	0.07	22,35,58,66	0
25	CLA	B	609	65/65	0.95	0.06	27,34,47,54	0
25	CLA	b	602	65/65	0.95	0.07	29,36,49,55	0
25	CLA	b	606	65/65	0.95	0.07	29,35,61,64	0
25	CLA	b	608	65/65	0.95	0.06	27,36,53,59	0
25	CLA	b	609	65/65	0.95	0.07	29,38,56,66	0
33	BCT	D	401	4/4	0.95	0.06	29,32,34,35	0
25	CLA	b	610	65/65	0.95	0.07	27,34,41,47	0
25	CLA	b	614	65/65	0.95	0.06	26,35,62,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LHG	L	101	49/49	0.96	0.06	28,35,46,55	0
25	CLA	D	405	65/65	0.96	0.07	27,33,74,84	0
29	LHG	d	408	49/49	0.96	0.06	30,37,48,50	0
29	LHG	d	409	39/49	0.96	0.07	33,38,53,55	0
25	CLA	B	616	60/65	0.96	0.07	25,33,69,74	0
25	CLA	B	602	65/65	0.96	0.06	24,32,47,50	0
25	CLA	a	609	65/65	0.96	0.08	22,28,62,68	0
25	CLA	a	612	65/65	0.96	0.05	22,27,38,44	0
25	CLA	C	502	65/65	0.96	0.06	26,32,44,50	0
25	CLA	B	604	65/65	0.96	0.06	22,28,57,59	0
27	PL9	D	407	55/55	0.96	0.05	22,28,37,39	0
25	CLA	b	603	65/65	0.96	0.06	26,31,52,61	0
25	CLA	C	504	59/65	0.96	0.06	28,34,67,70	0
25	CLA	b	607	65/65	0.96	0.06	23,30,54,57	0
25	CLA	C	505	65/65	0.96	0.06	26,35,56,62	0
25	CLA	A	607	65/65	0.96	0.06	22,28,73,79	0
25	CLA	B	607	65/65	0.96	0.06	21,28,49,55	0
25	CLA	b	611	65/65	0.96	0.05	25,30,43,50	0
25	CLA	b	612	65/65	0.96	0.06	23,30,38,45	0
25	CLA	b	613	65/65	0.96	0.06	19,28,60,65	0
25	CLA	C	509	65/65	0.96	0.07	24,33,50,54	0
25	CLA	b	615	65/65	0.96	0.06	28,36,50,57	0
25	CLA	A	606	65/65	0.96	0.05	18,25,38,47	0
25	CLA	c	501	65/65	0.96	0.06	29,35,45,52	0
25	CLA	c	502	65/65	0.96	0.06	25,35,47,51	0
25	CLA	B	610	65/65	0.96	0.06	23,29,36,39	0
25	CLA	B	613	65/65	0.96	0.06	21,26,55,61	0
25	CLA	c	505	65/65	0.96	0.06	29,35,56,65	0
34	PHO	D	402	64/64	0.96	0.05	19,26,33,37	0
34	PHO	D	403	64/64	0.96	0.05	22,30,34,37	0
25	CLA	B	614	65/65	0.96	0.06	20,32,57,62	0
25	CLA	C	507	65/65	0.97	0.06	25,34,47,50	0
25	CLA	B	605	65/65	0.97	0.05	22,27,37,39	0
25	CLA	B	603	65/65	0.97	0.06	21,27,50,56	0
25	CLA	B	611	65/65	0.97	0.05	21,27,41,47	0
25	CLA	B	612	65/65	0.97	0.06	21,27,37,42	0
25	CLA	A	611	65/65	0.97	0.05	21,25,40,46	0
25	CLA	B	608	65/65	0.97	0.05	25,30,46,53	0
25	CLA	b	604	65/65	0.97	0.06	24,29,65,75	0
25	CLA	b	605	65/65	0.97	0.05	23,30,42,45	0
25	CLA	D	404	65/65	0.97	0.05	20,24,43,50	0
29	LHG	D	410	49/49	0.97	0.06	27,34,44,48	0

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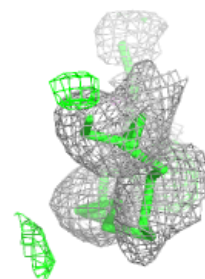
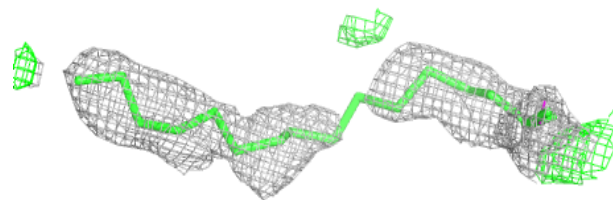
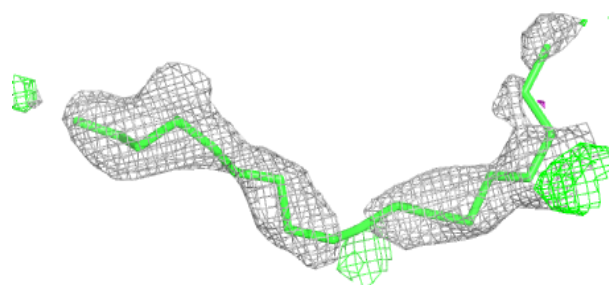
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	PHO	d	401	64/64	0.97	0.05	24,28,33,36	0
25	CLA	B	615	65/65	0.97	0.05	23,32,52,60	0
35	HEM	F	101	43/43	0.97	0.08	39,44,55,61	0
35	HEM	f	101	43/43	0.97	0.08	46,52,65,78	0
25	CLA	A	608	54/65	0.98	0.05	21,26,53,57	0
24	CL	A	604	1/1	0.98	0.03	28,28,28,28	0
36	HEC	V	201	43/43	0.98	0.05	25,29,36,40	0
22	OEX	A	602[A]	10/10	0.99	0.04	21,29,33,33	10
22	OEX	a	602[A]	10/10	0.99	0.03	24,28,31,31	10
23	FE2	a	603	1/1	0.99	0.02	33,33,33,33	0
21	OEY	A	601[B]	11/11	0.99	0.03	24,27,30,30	11
24	CL	A	605	1/1	0.99	0.05	29,29,29,29	0
24	CL	a	604	1/1	0.99	0.04	30,30,30,30	0
24	CL	a	605	1/1	0.99	0.06	30,30,30,30	0
21	OEY	a	601[B]	11/11	0.99	0.03	26,29,32,32	11
36	HEC	v	201	43/43	0.99	0.05	29,33,40,44	0
23	FE2	A	603	1/1	1.00	0.01	27,27,27,27	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.

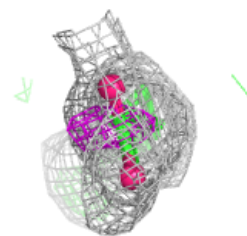
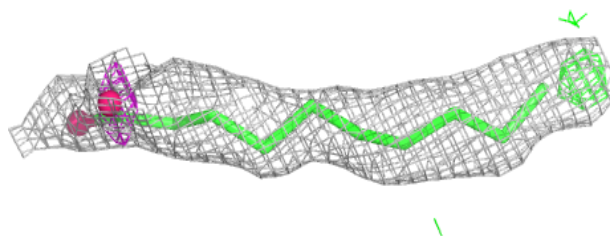
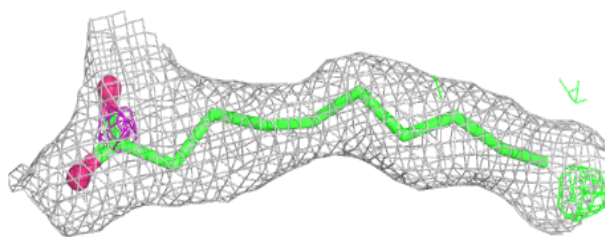
Electron density around STE H 103:

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

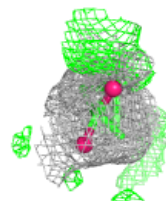
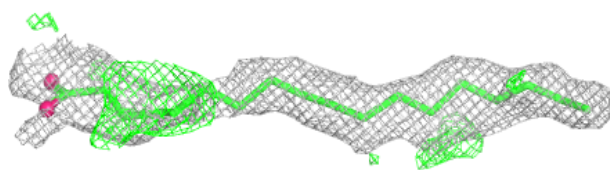
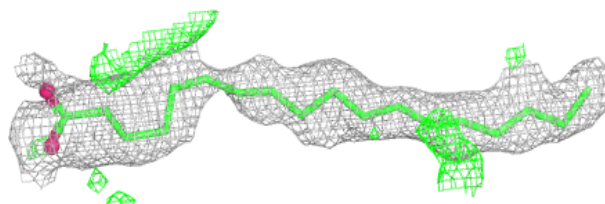


Electron density around STE a 615:

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

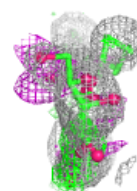
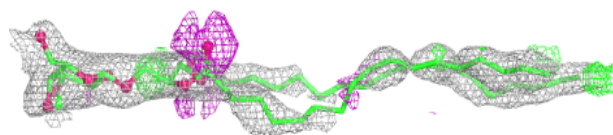
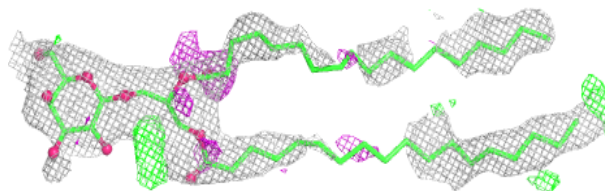
**Electron density around STE T 103:**

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

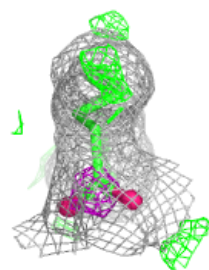
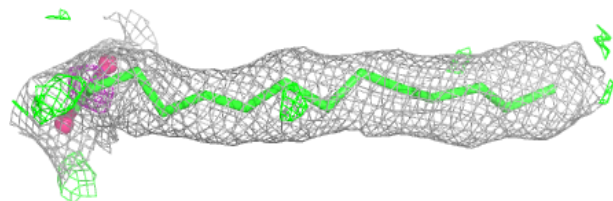
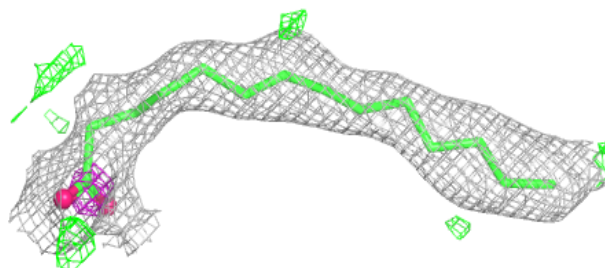


Electron density around LMG b 624:

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

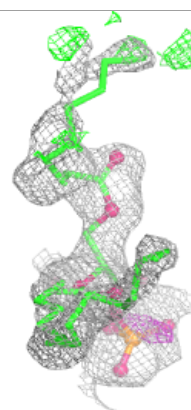
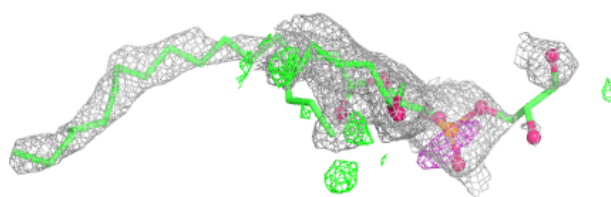
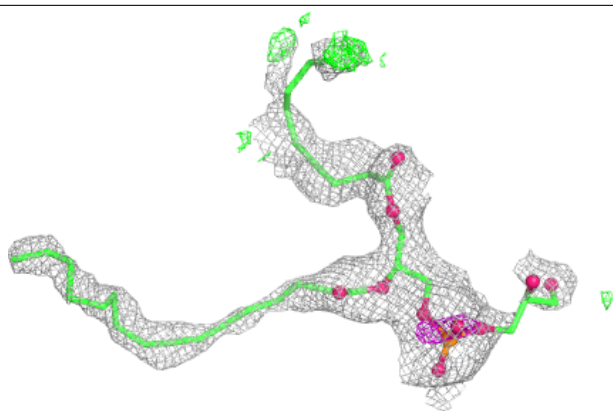
**Electron density around STE b 625:**

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

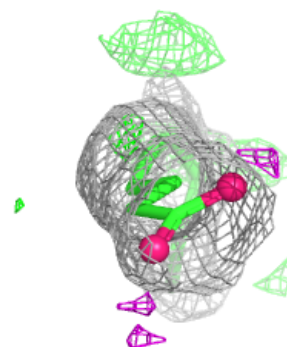
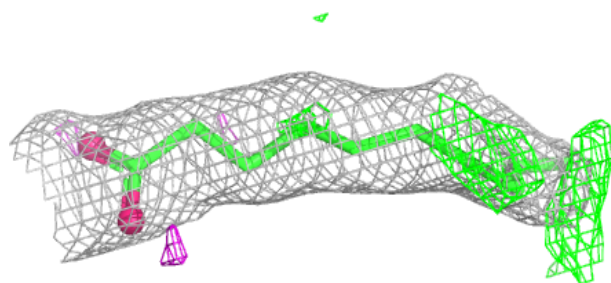
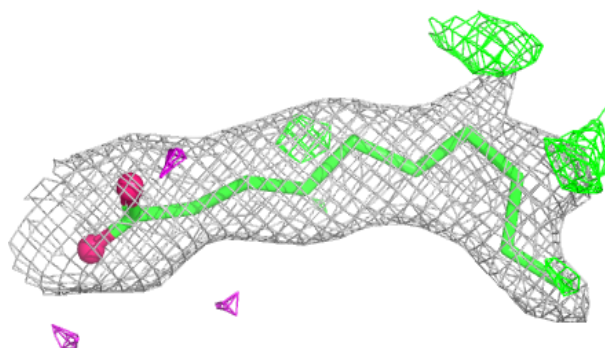


Electron density around LHG e 101:

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

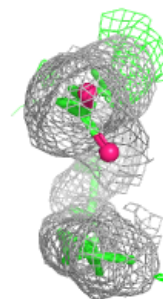
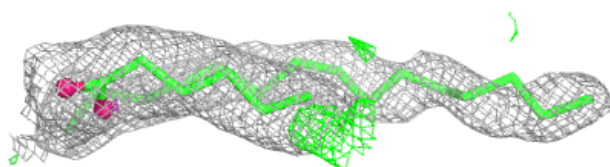
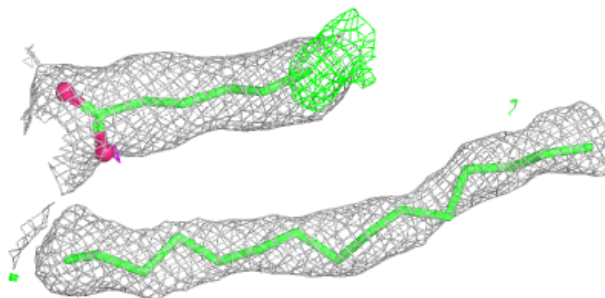
**Electron density around STE m 101:**

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

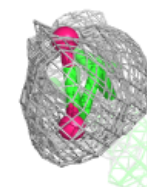
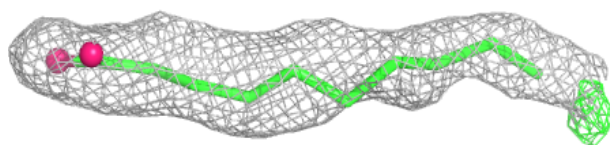
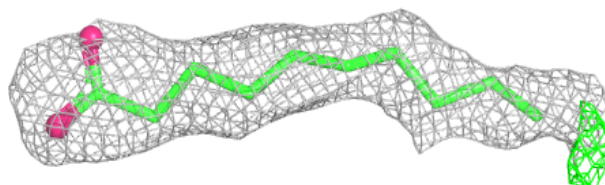


Electron density around LMG d 410:

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

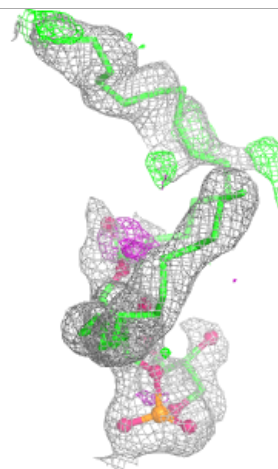
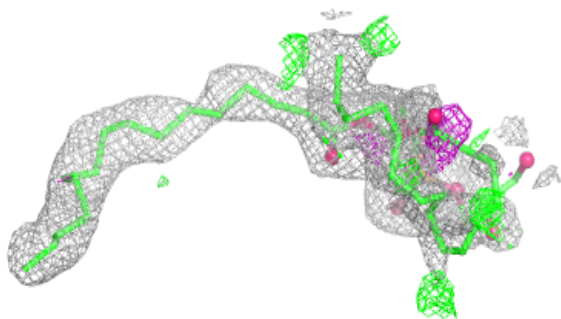
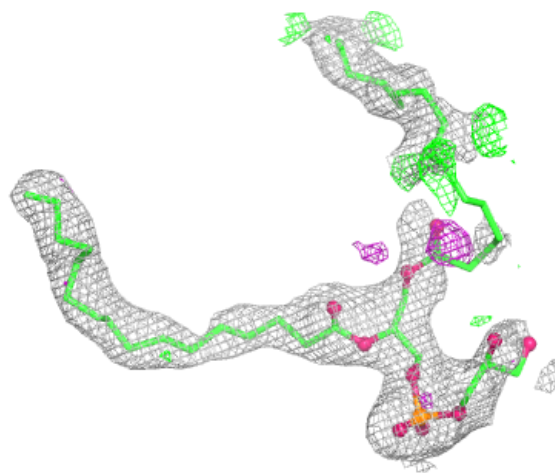
**Electron density around STE c 521:**

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



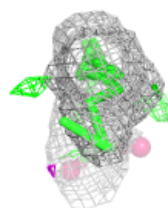
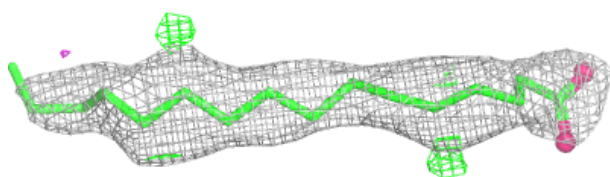
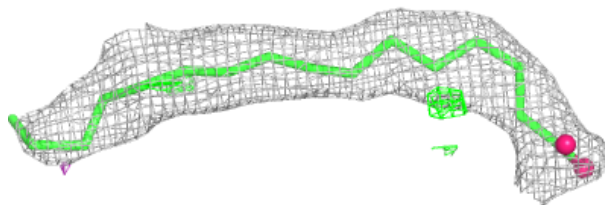
Electron density around LHG E 101:

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

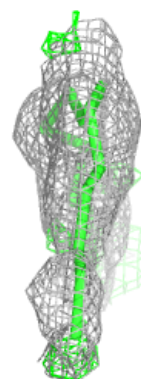
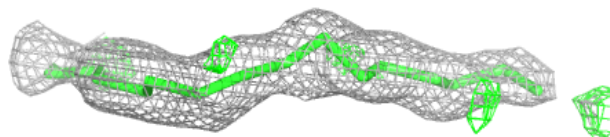


Electron density around STE B 625:

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

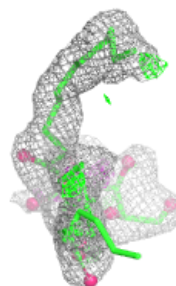
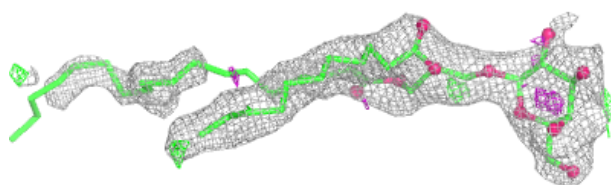
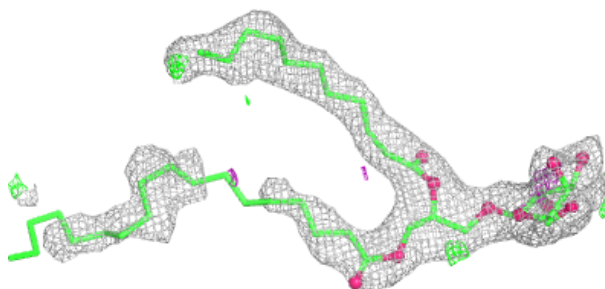
**Electron density around STE B 627:**

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

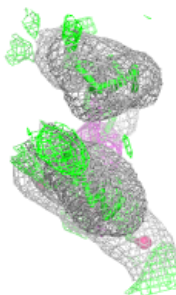
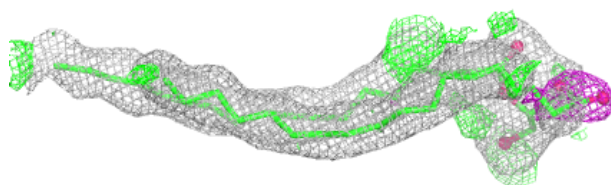
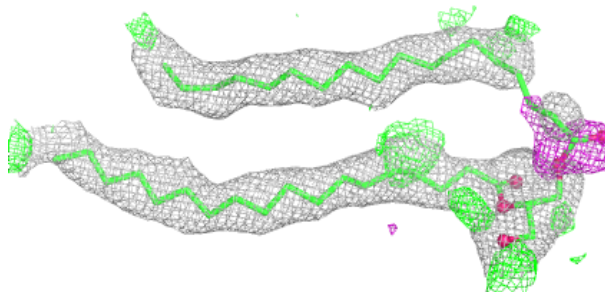


Electron density around LMG c 520:

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

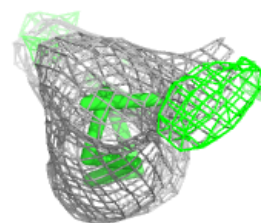
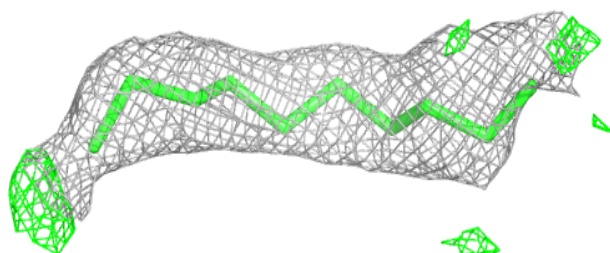
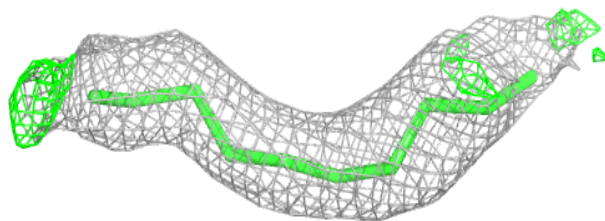
**Electron density around DGD o 301:**

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

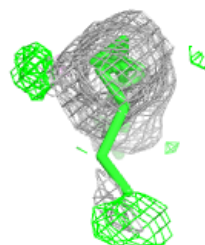
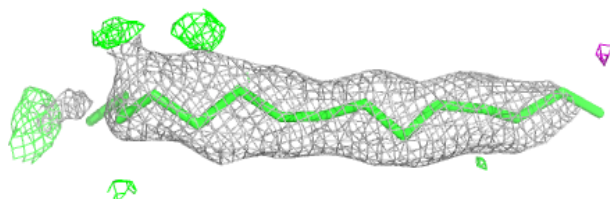
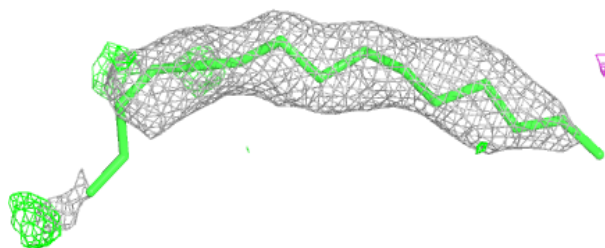


Electron density around STE b 626:

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

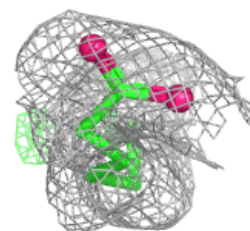
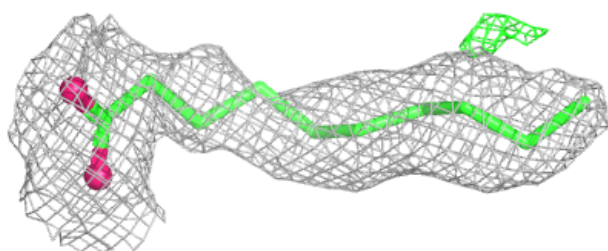
**Electron density around STE T 102:**

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

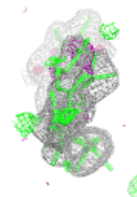
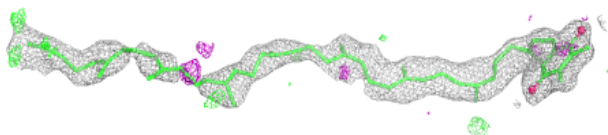
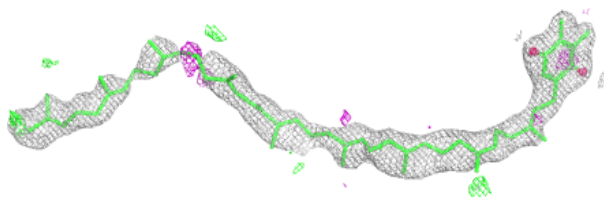


Electron density around STE E 102:

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

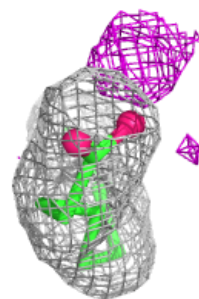
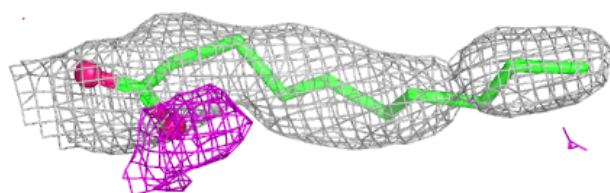
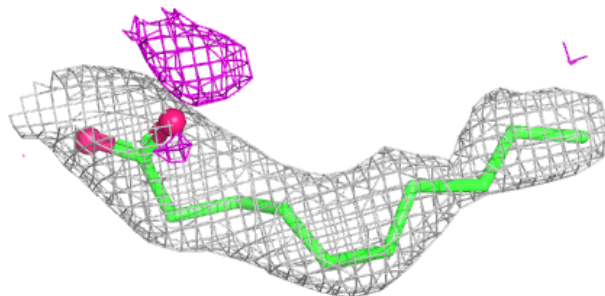
**Electron density around PL9 A 610:**

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

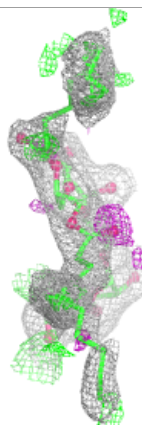
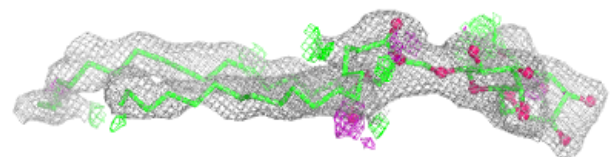
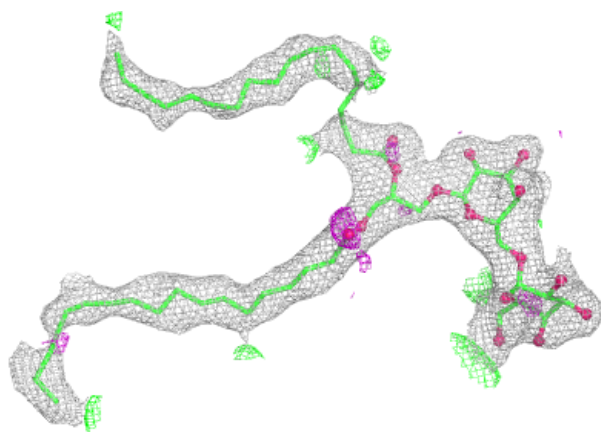


Electron density around STE B 626:

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

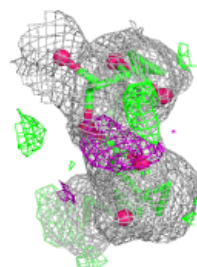
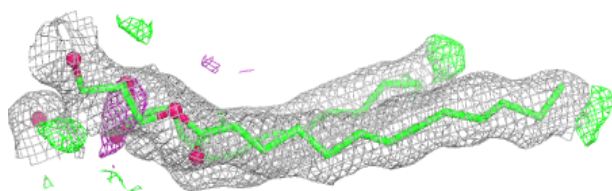
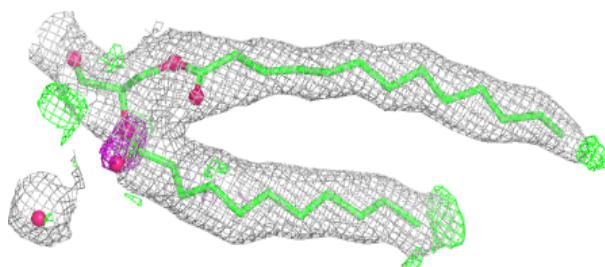
**Electron density around DGD A 616:**

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

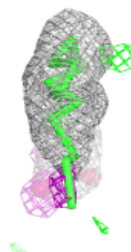
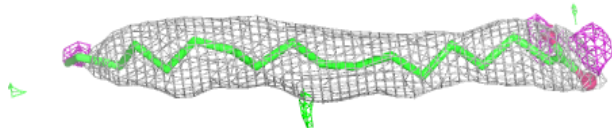
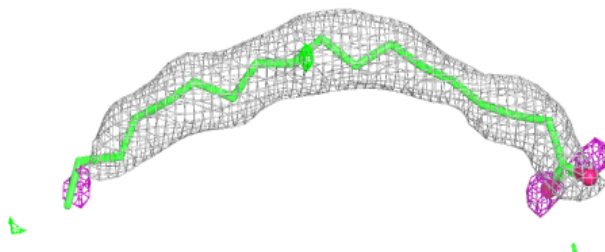


Electron density around LMG D 411:

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

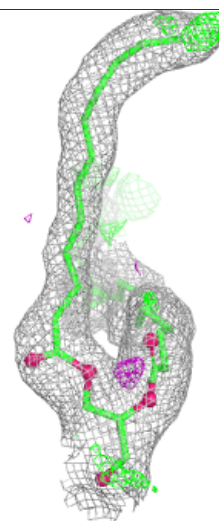
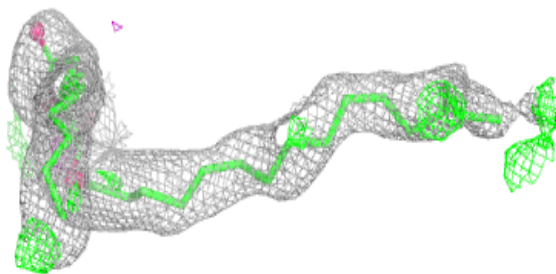
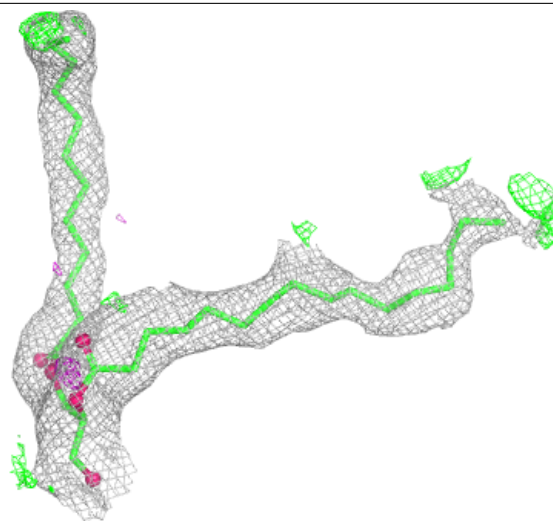
**Electron density around STE X 101:**

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



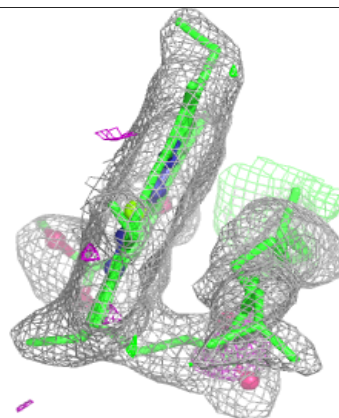
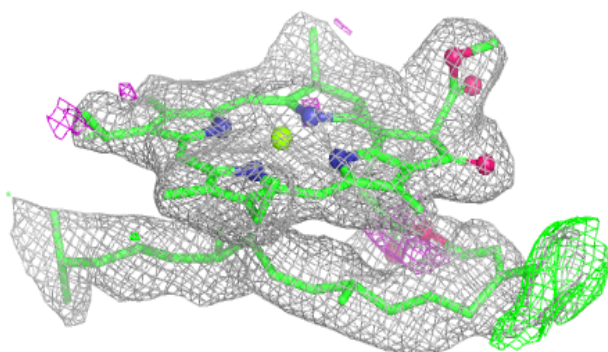
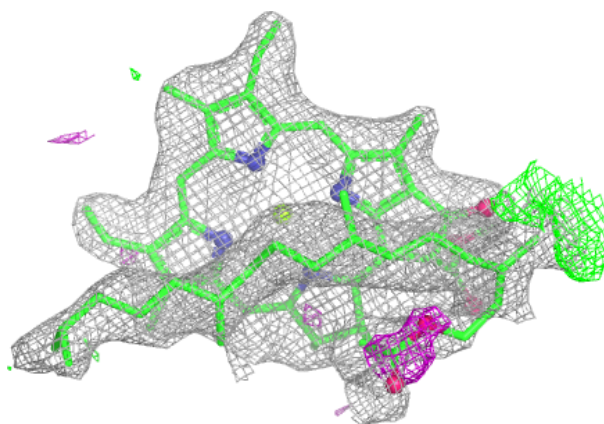
Electron density around SQD a 614:

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

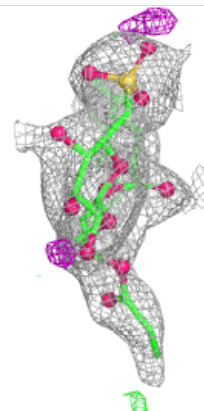
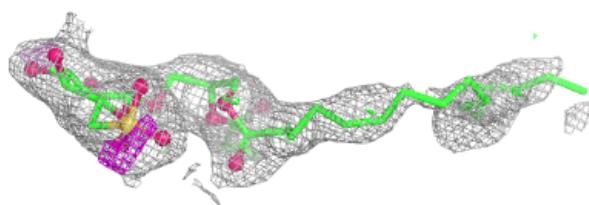
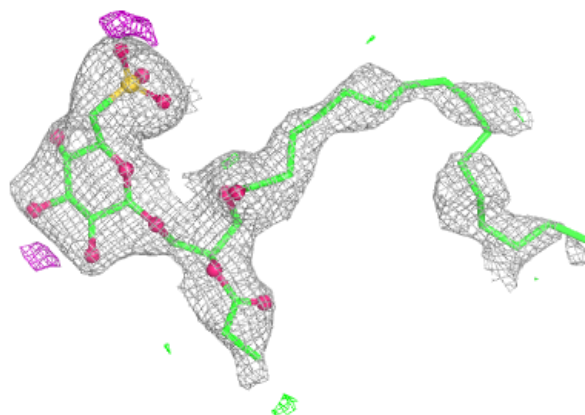


Electron density around CLA b 601:

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

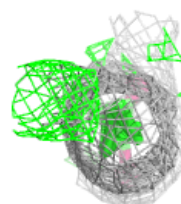
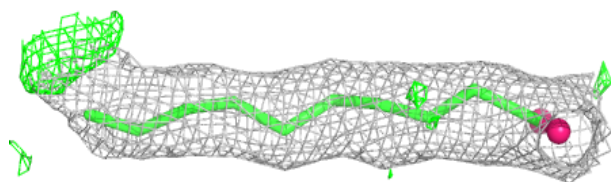
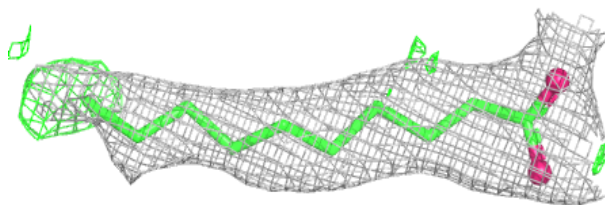
**Electron density around SQD f 102:**

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



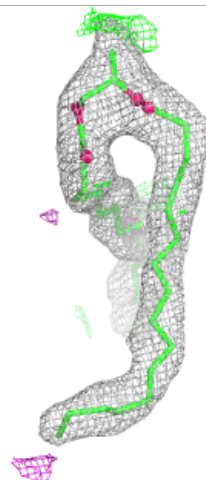
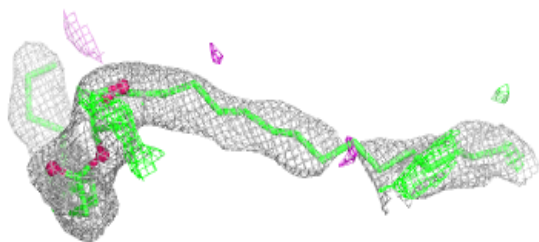
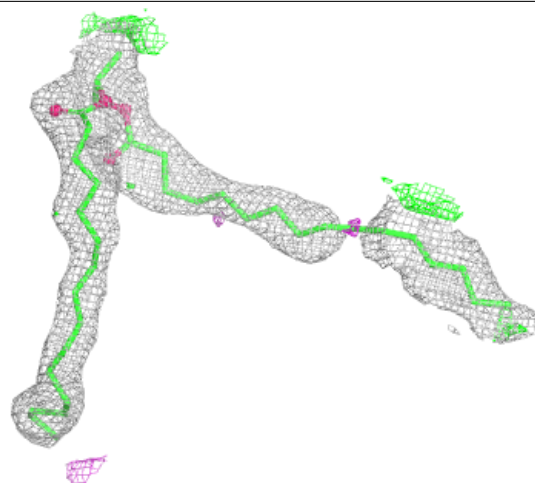
Electron density around STE J 101:

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



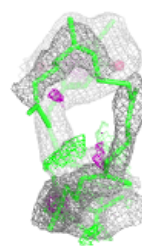
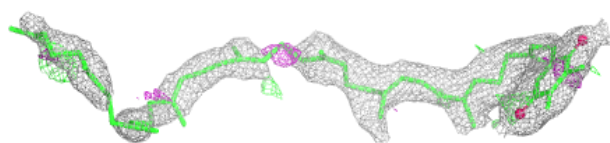
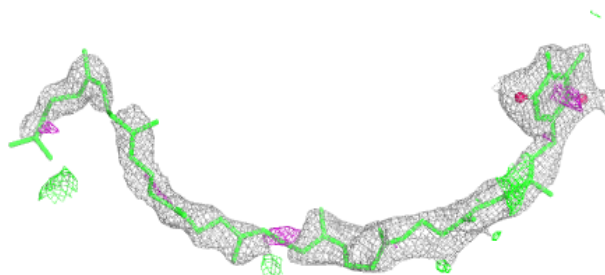
Electron density around SQD A 615:

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

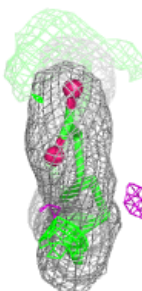
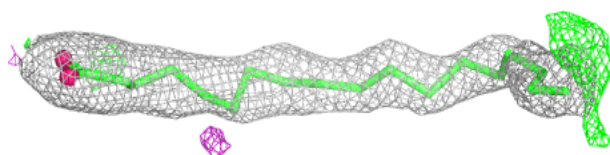
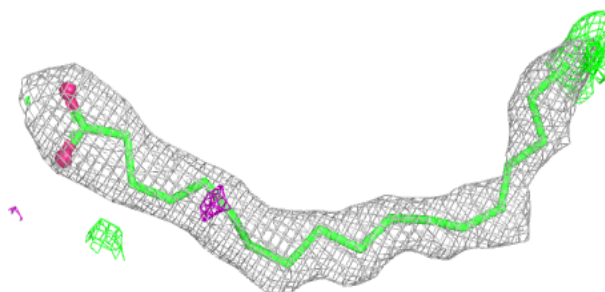


Electron density around PL9 a 611:

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

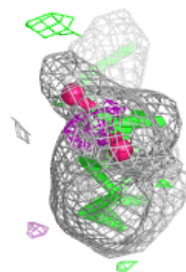
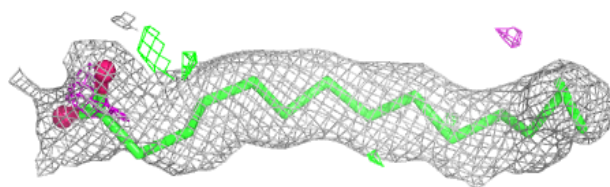
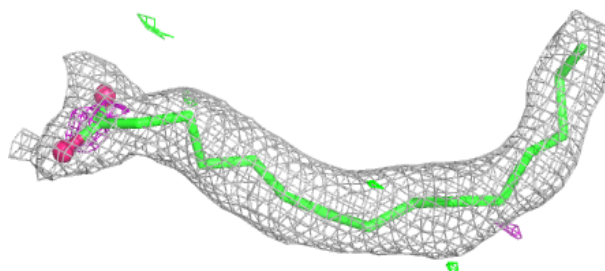
**Electron density around STE d 413:**

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

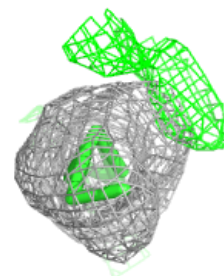
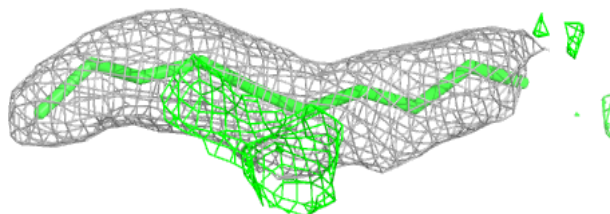
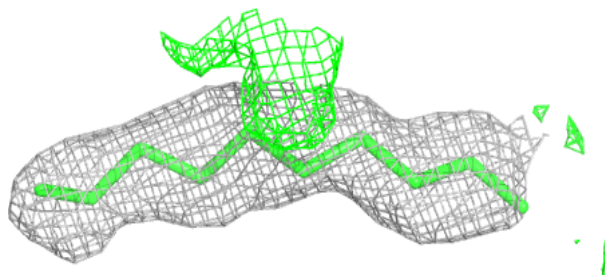


Electron density around STE B 620:

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

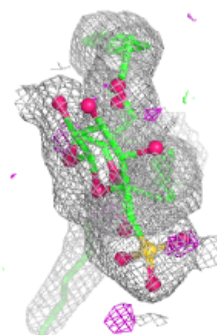
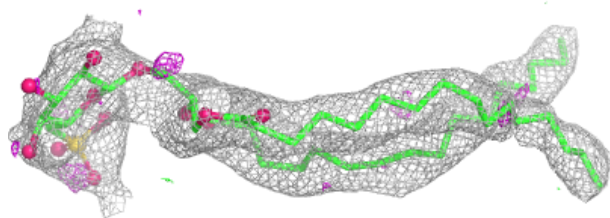
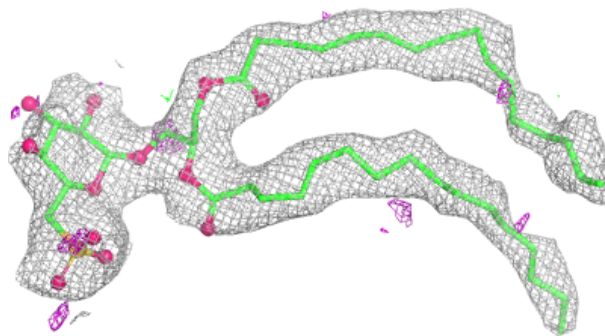
**Electron density around STE t 103:**

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

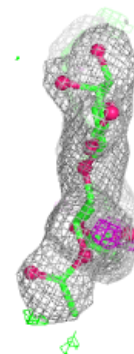
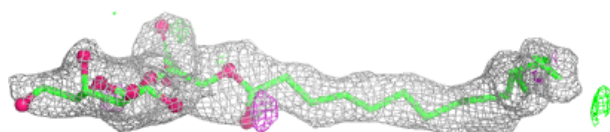
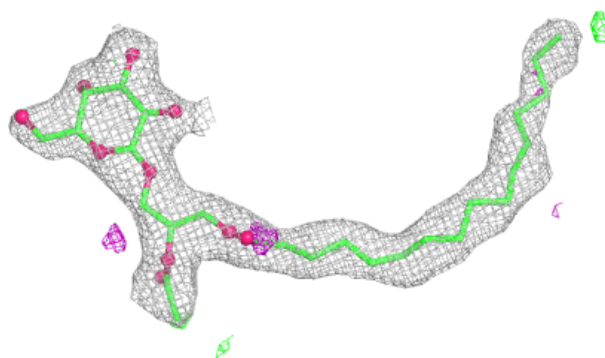


Electron density around SQD B 623:

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

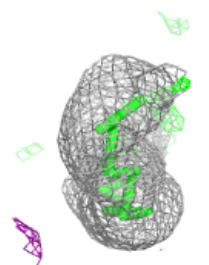
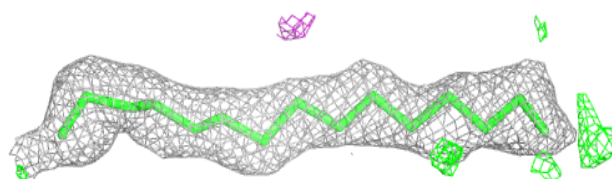
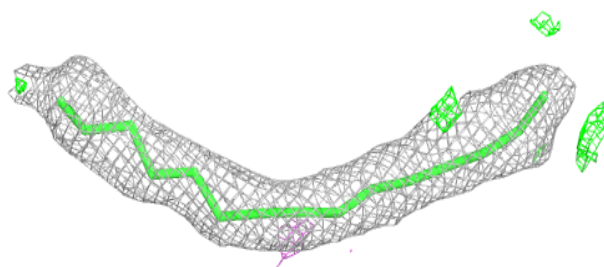
**Electron density around LMG c 518:**

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

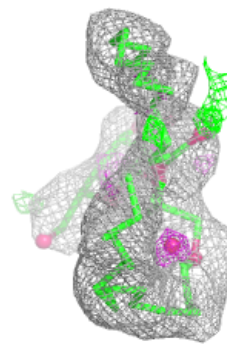
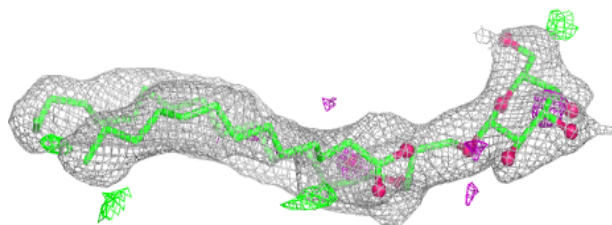
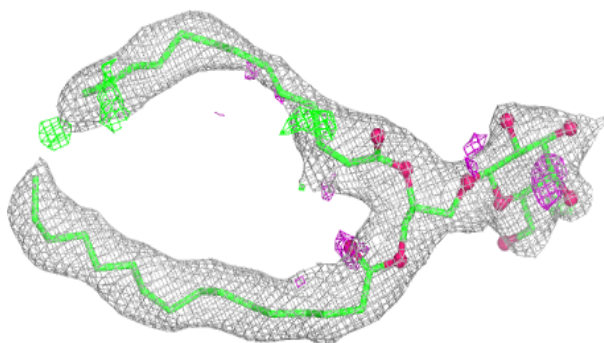


Electron density around STE I 101:

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

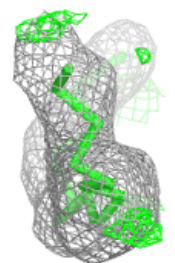
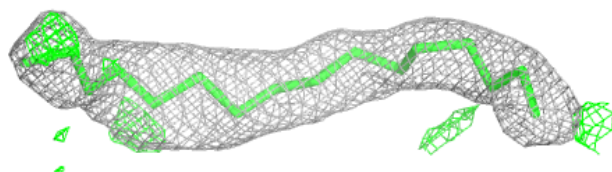
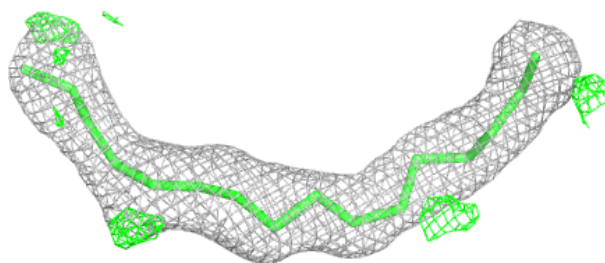
**Electron density around LMG A 612:**

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

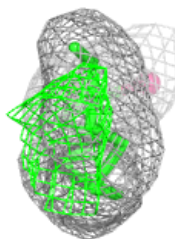
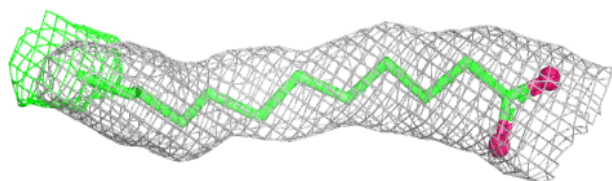
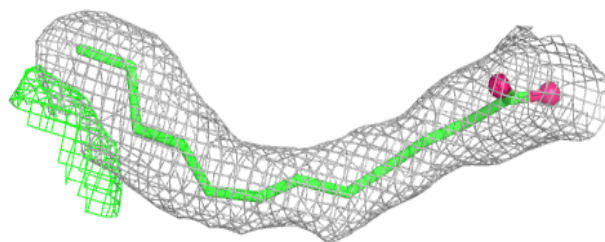


Electron density around STE b 621:

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

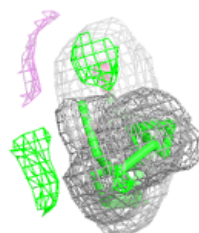
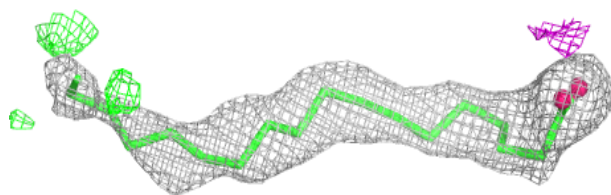
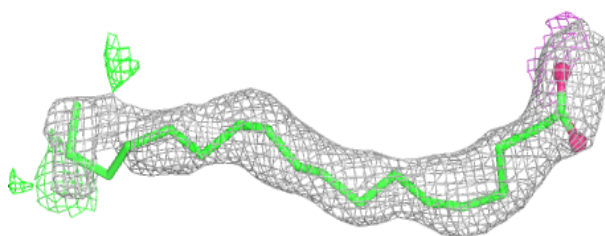
**Electron density around STE t 102:**

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

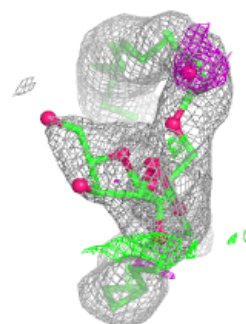
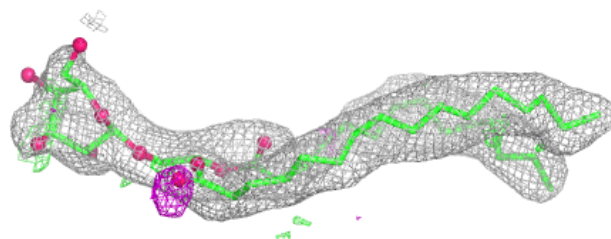
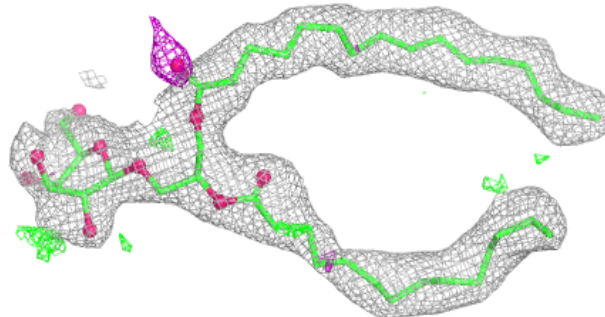


Electron density around STE b 623:

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

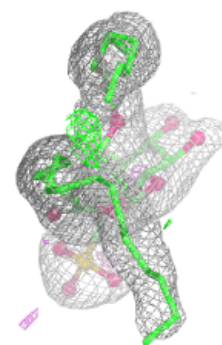
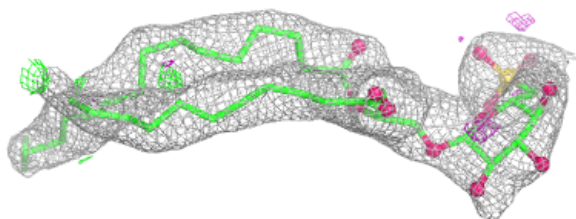
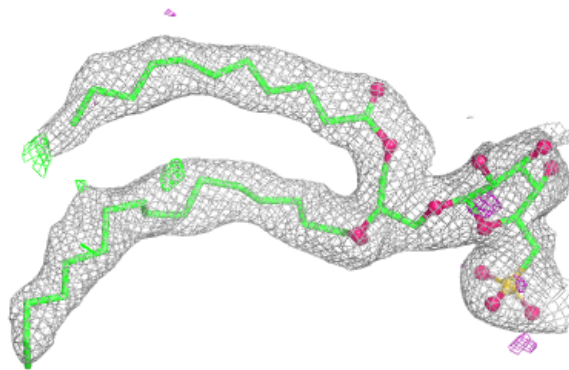
**Electron density around LMG c 522:**

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

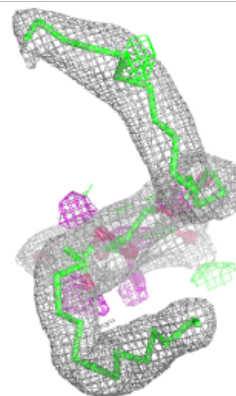
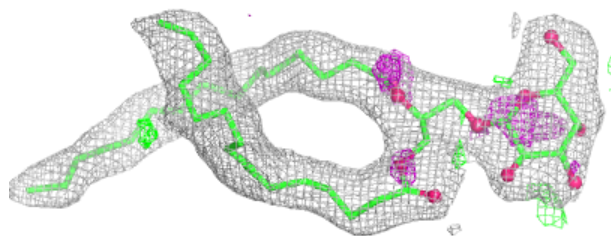
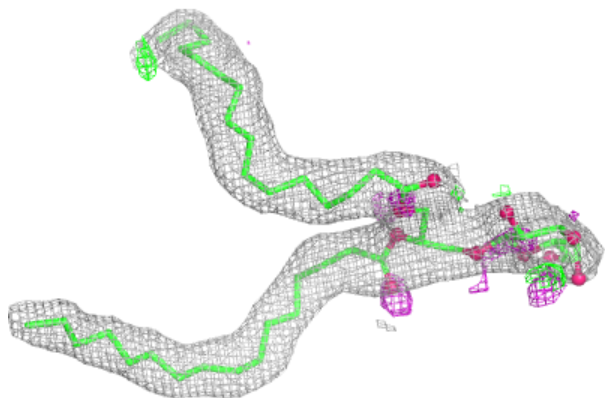


Electron density around SQD b 620:

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

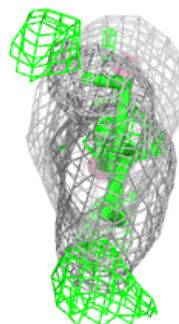
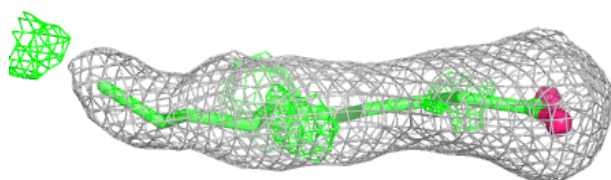
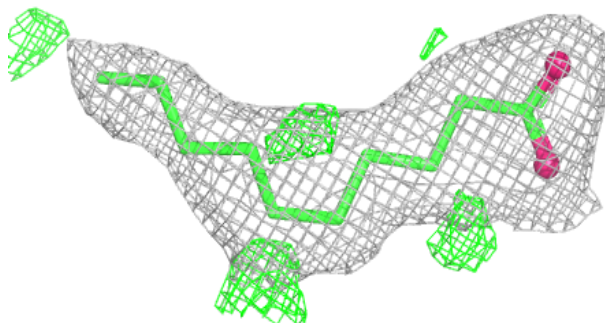
**Electron density around LMG b 622:**

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

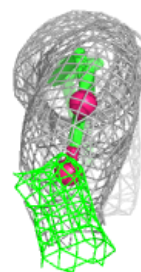
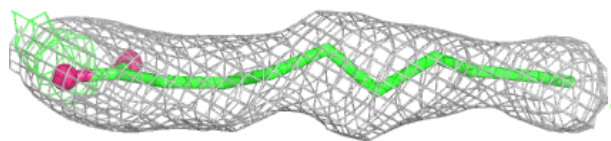
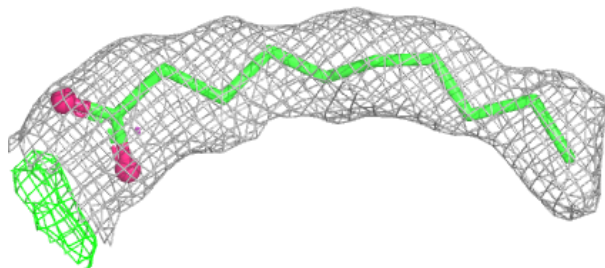


Electron density around STE C 519:

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

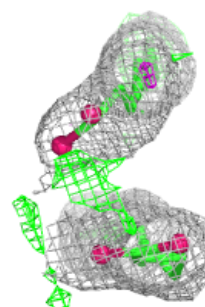
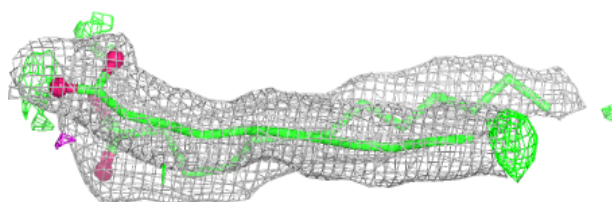
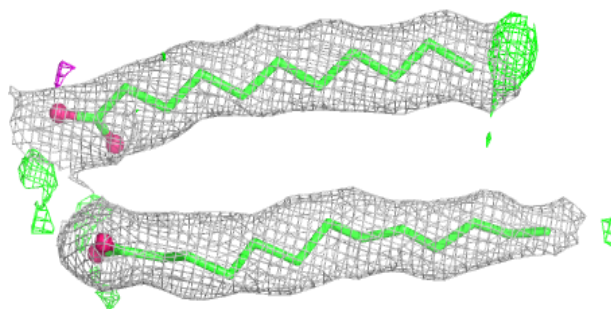
**Electron density around STE C 520:**

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

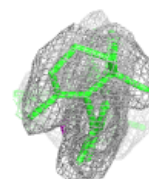
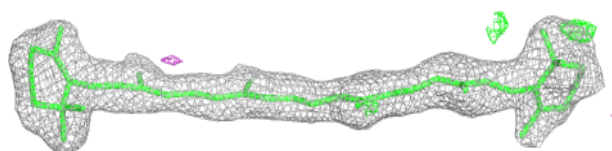
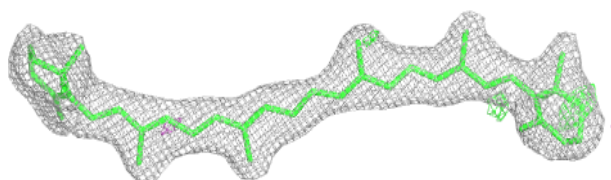


Electron density around LMG B 621:

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

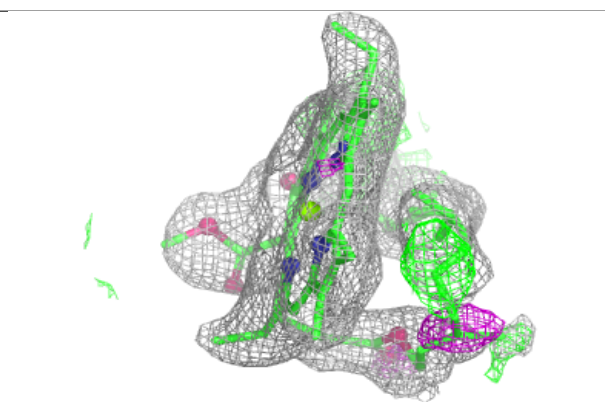
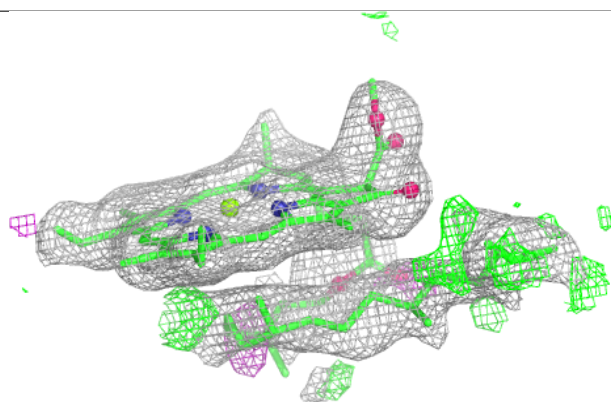
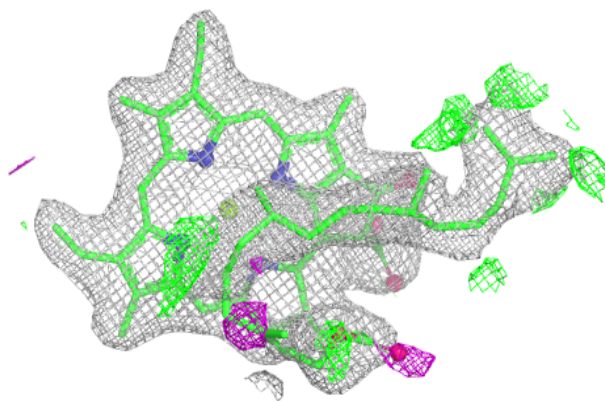
**Electron density around BCR k 102:**

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

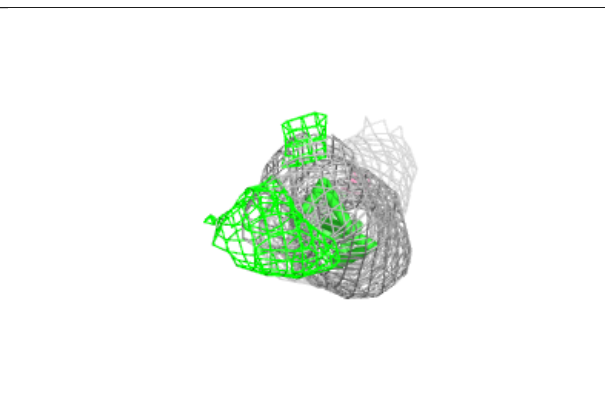
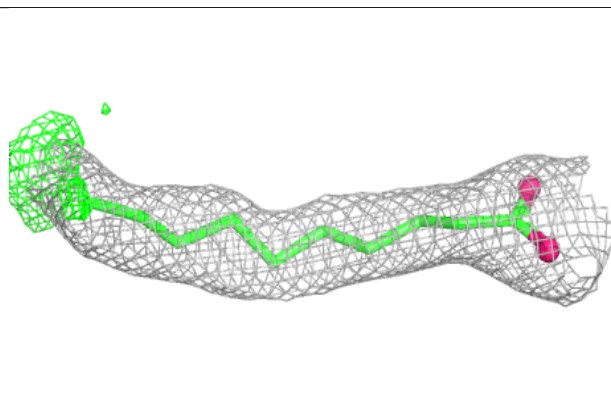
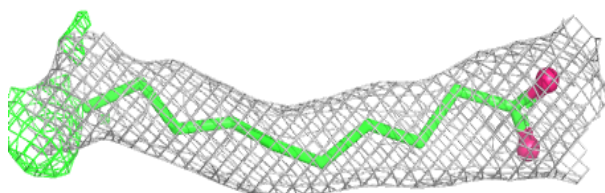


Electron density around CLA B 601:

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

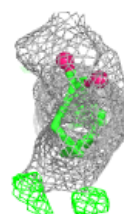
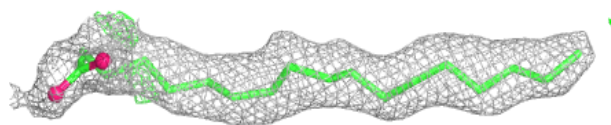
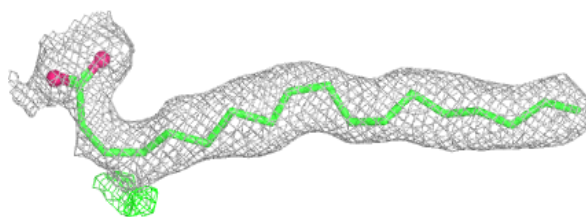
**Electron density around STE j 101:**

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

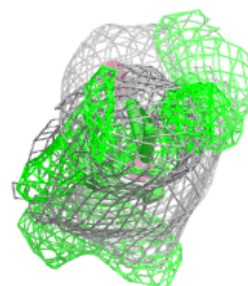
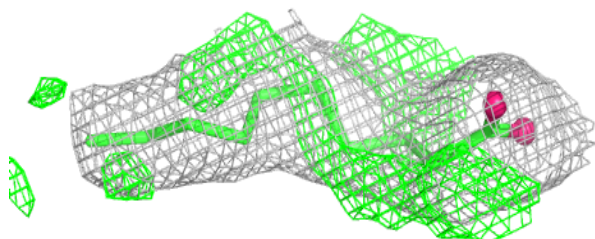
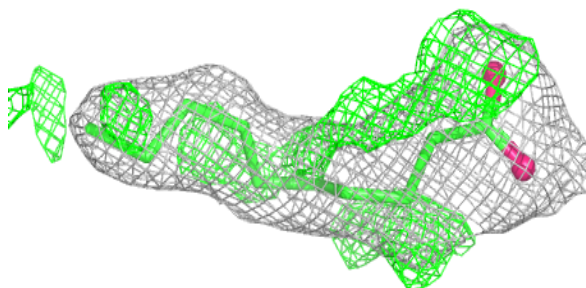


Electron density around STE c 519:

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

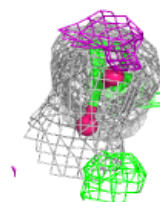
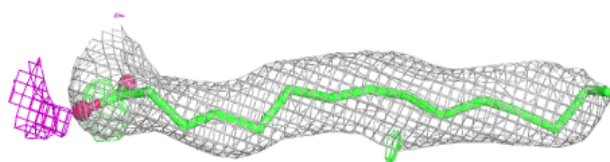
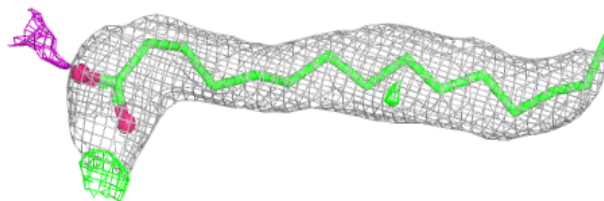
**Electron density around STE B 624:**

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

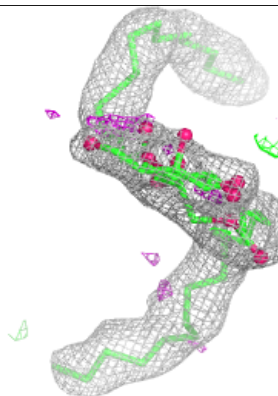
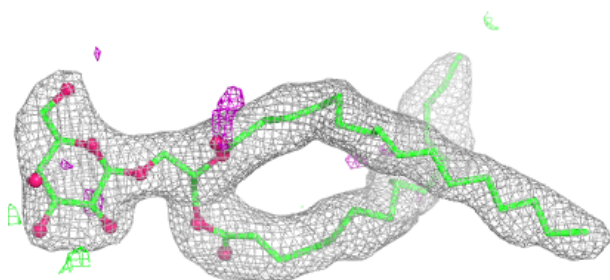
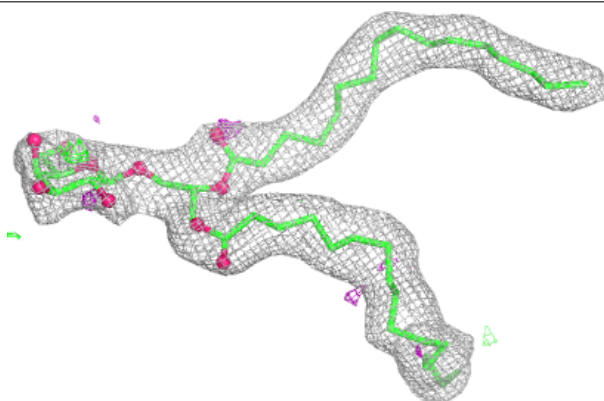


Electron density around STE d 412:

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

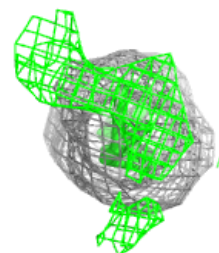
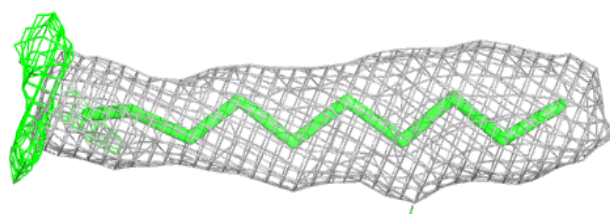
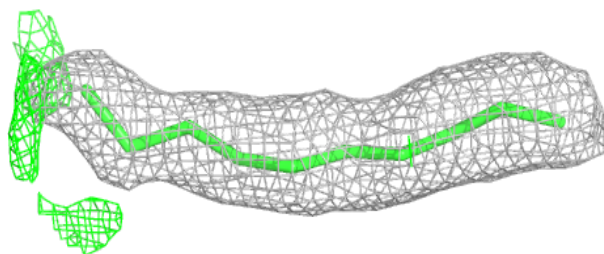
**Electron density around LMG M 101:**

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

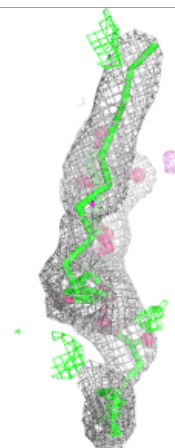
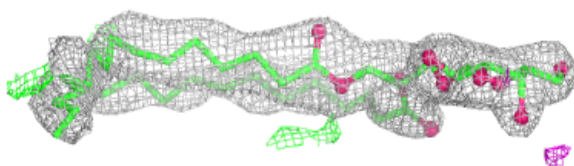
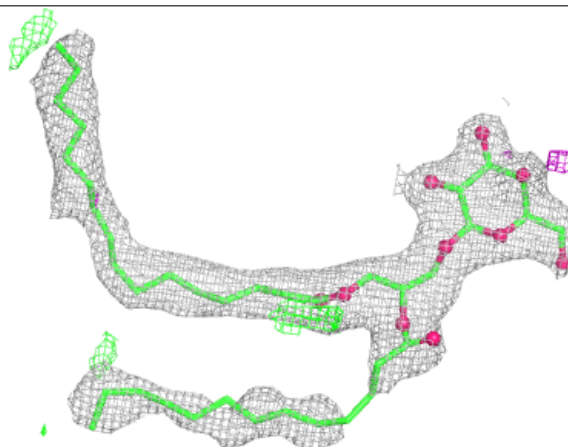


Electron density around STE M 103:

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

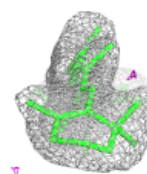
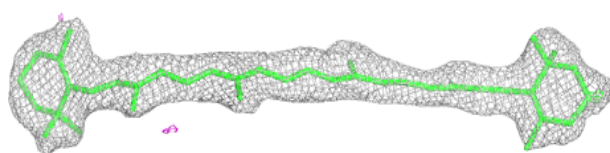
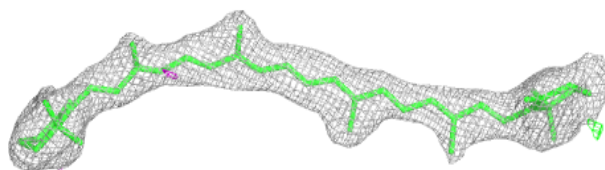
**Electron density around LMG C 518:**

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

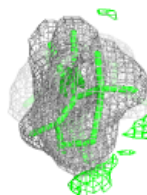
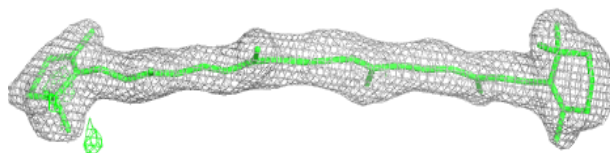
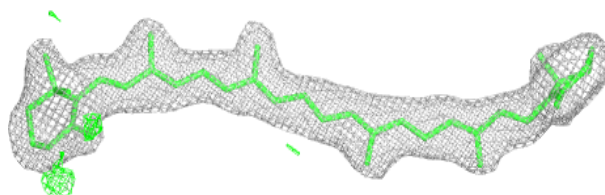


Electron density around BCR x 101:

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

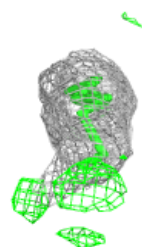
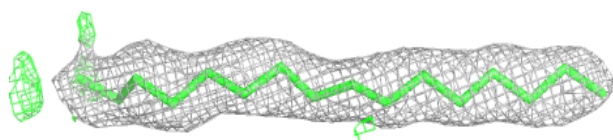
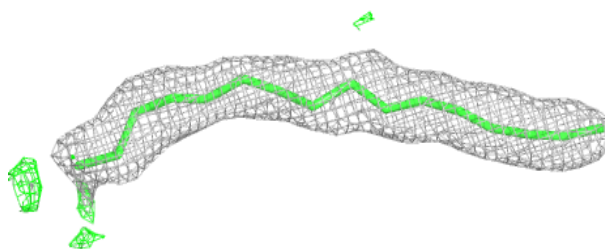
**Electron density around BCR K 102:**

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

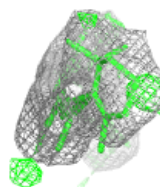
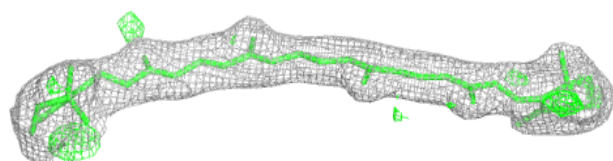
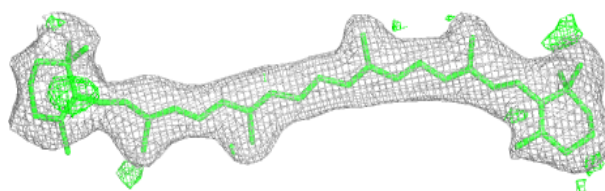


Electron density around STE C 521:

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

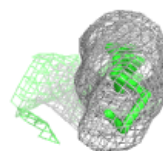
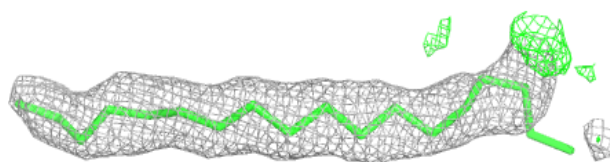
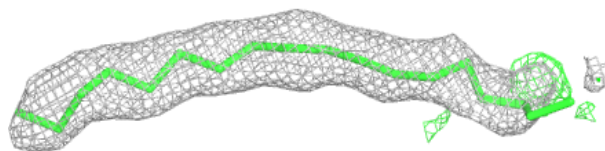
**Electron density around BCR D 406:**

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



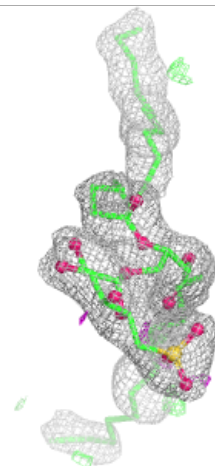
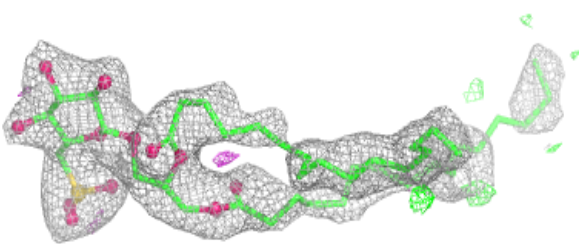
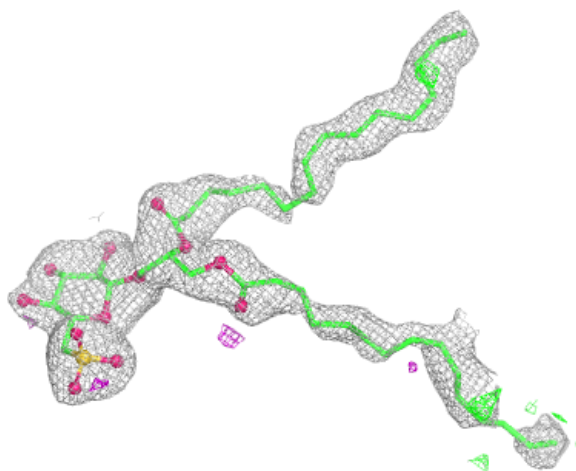
Electron density around STE 1 102:

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



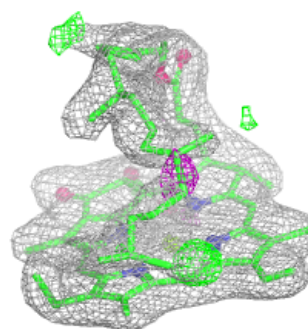
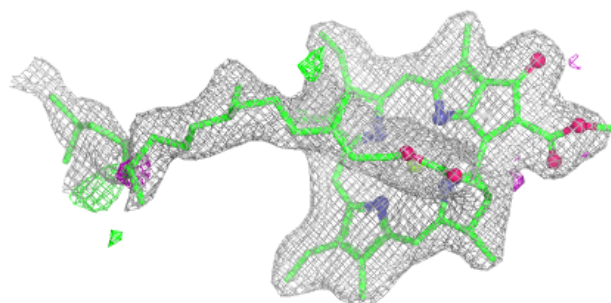
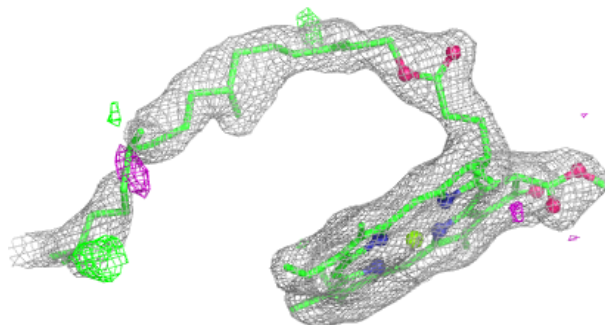
Electron density around SQD a 613:

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

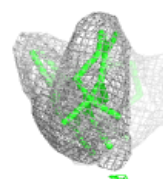
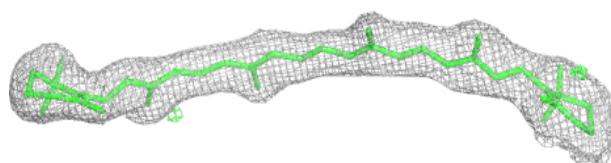
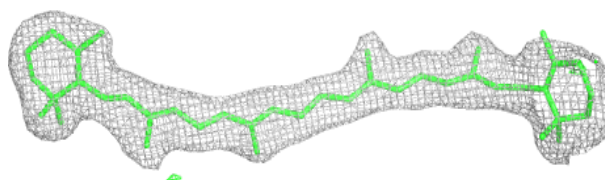


Electron density around CLA C 513:

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

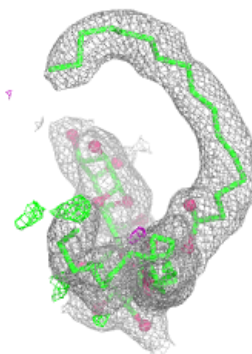
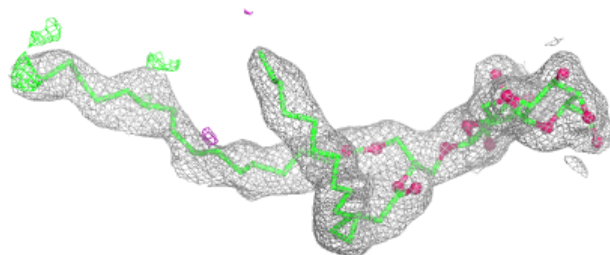
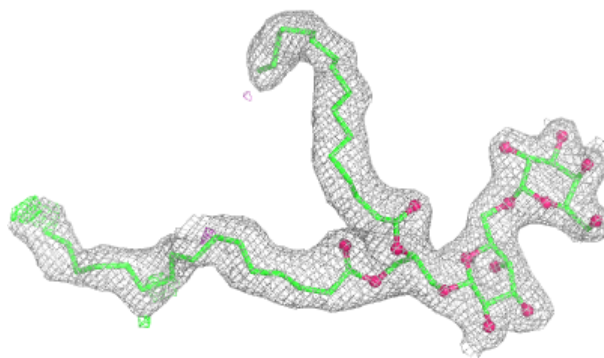
**Electron density around BCR d 405:**

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

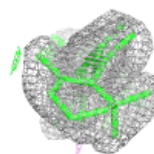
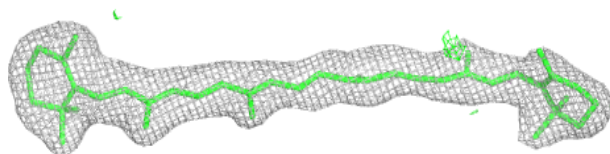
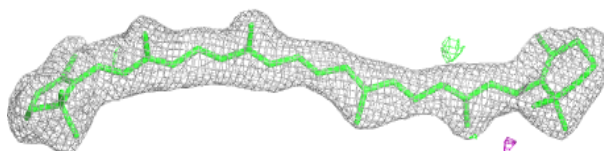


Electron density around DGD c 516:

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

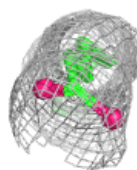
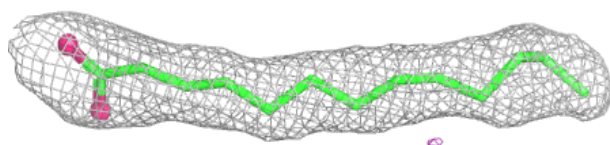
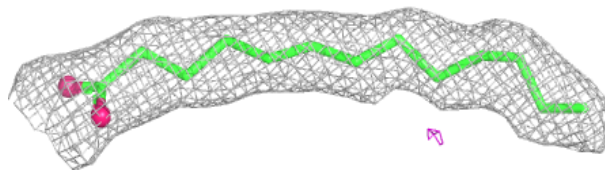
**Electron density around BCR k 101:**

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

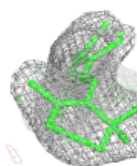
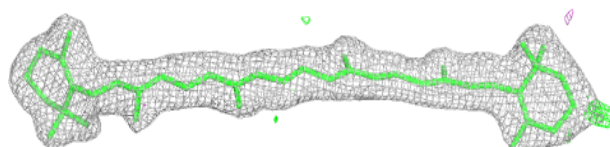
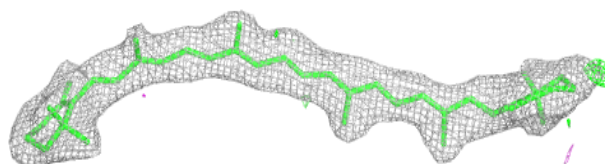


Electron density around STE M 102:

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

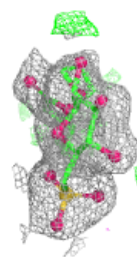
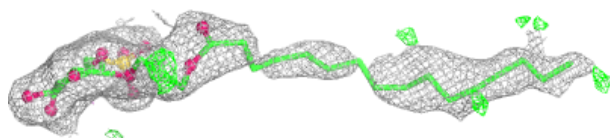
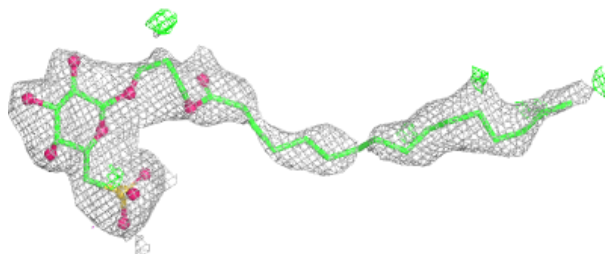
**Electron density around BCR H 101:**

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

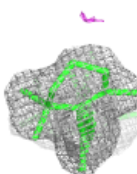
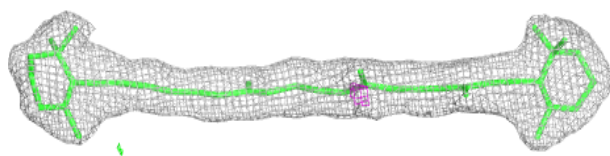
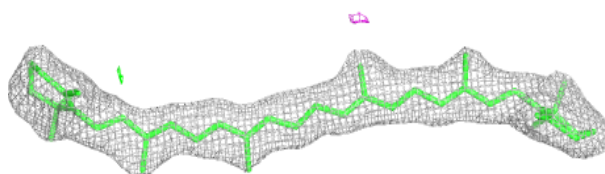


Electron density around SQD D 409:

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

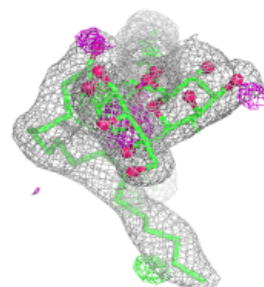
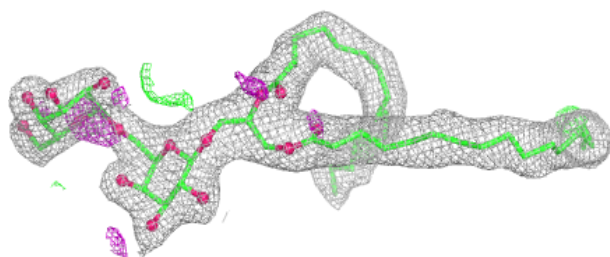
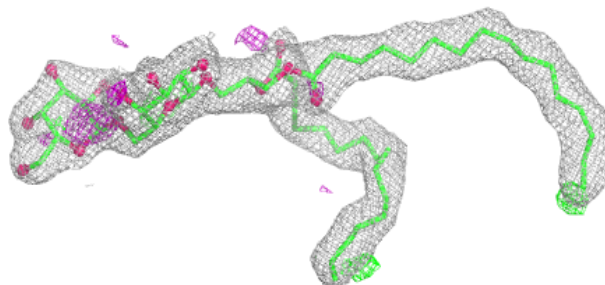
**Electron density around BCR K 101:**

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

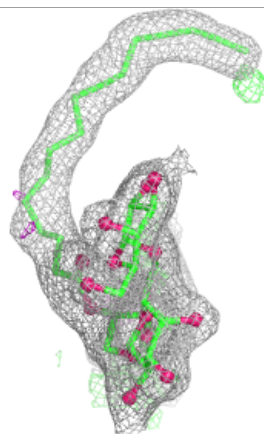
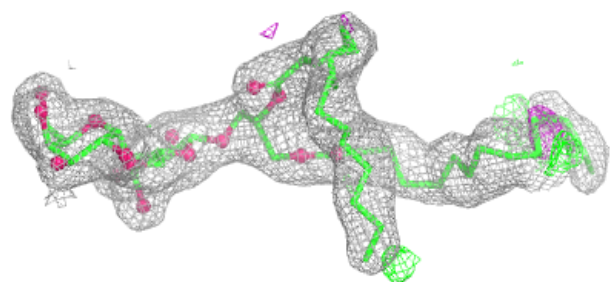
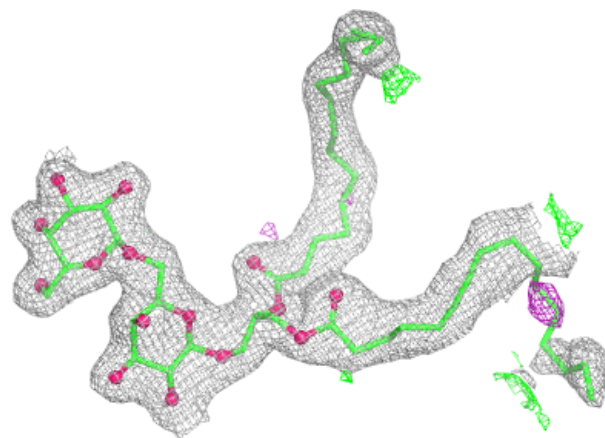


Electron density around DGD H 102:

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

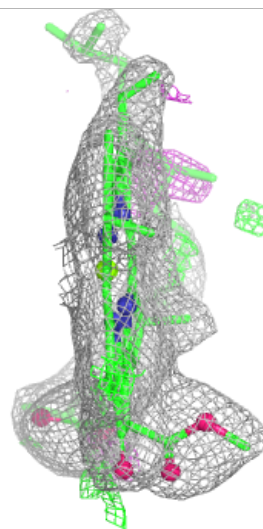
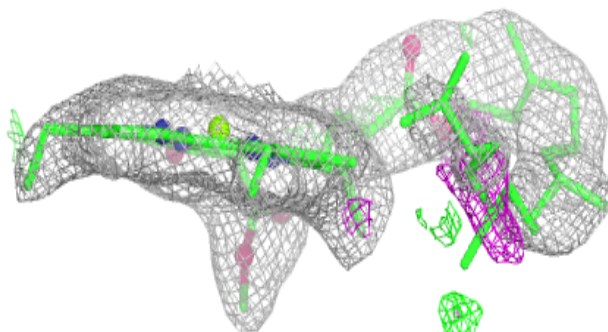
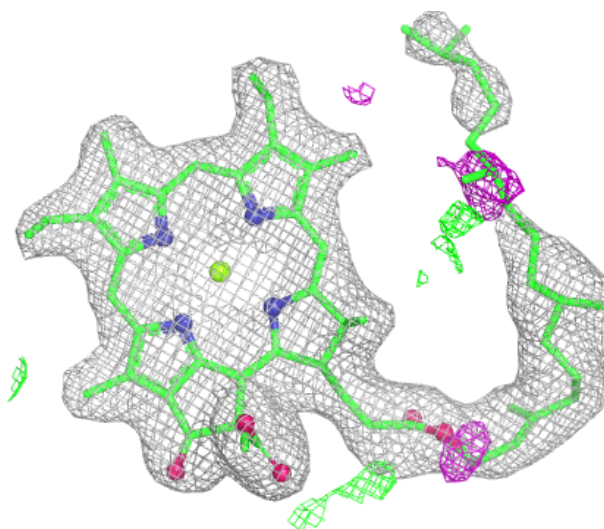
**Electron density around DGD C 516:**

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



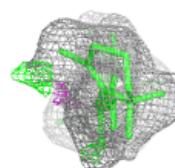
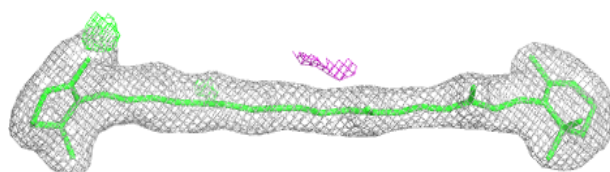
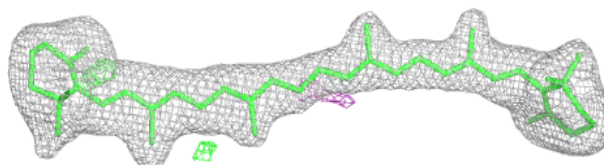
Electron density around CLA c 512:

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

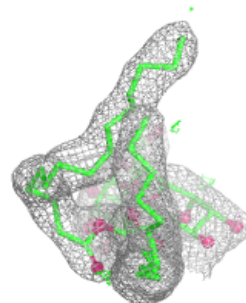
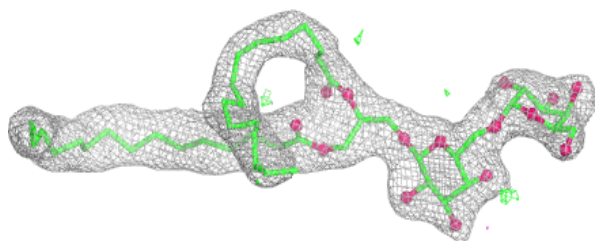
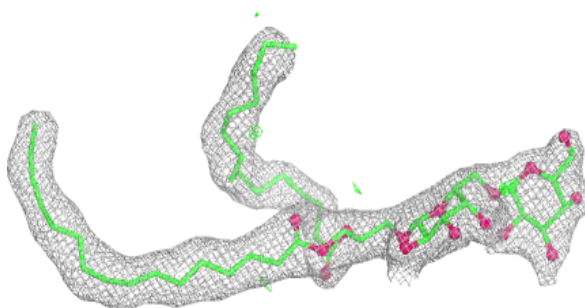


Electron density around BCR b 618:

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

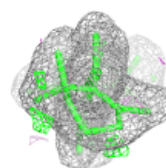
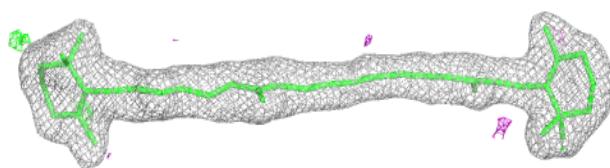
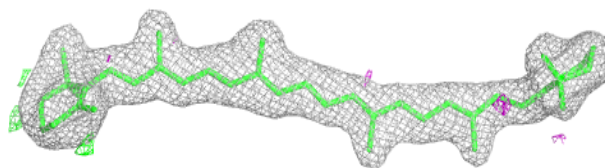
**Electron density around DGD h 101:**

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

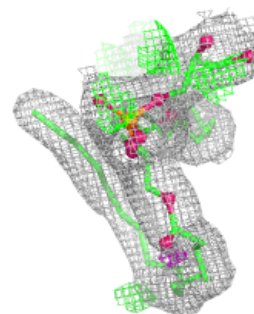
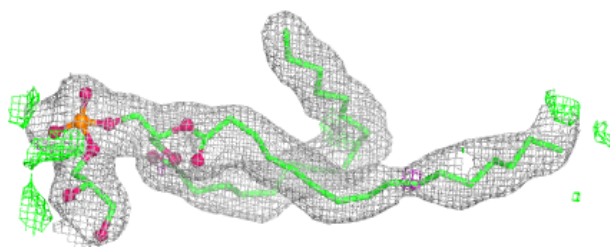
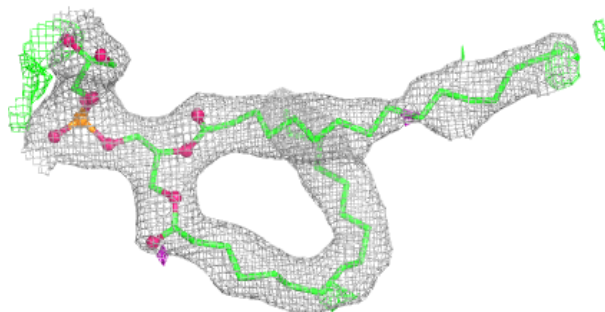


Electron density around BCR A 609:

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

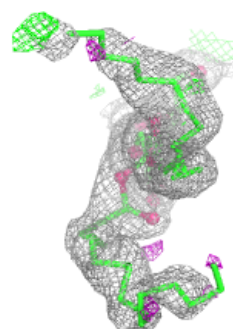
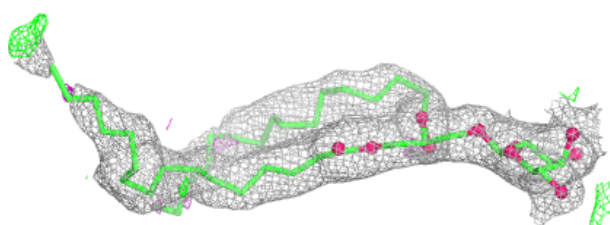
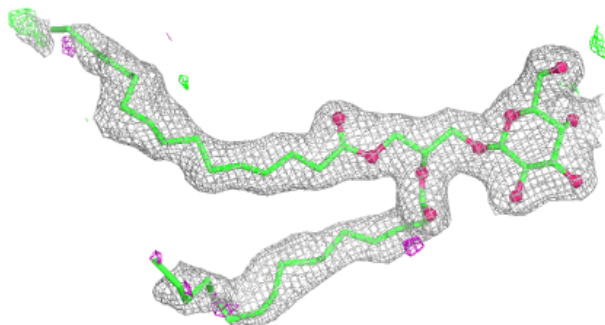
**Electron density around LHG d 407:**

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

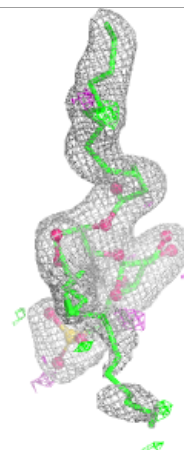
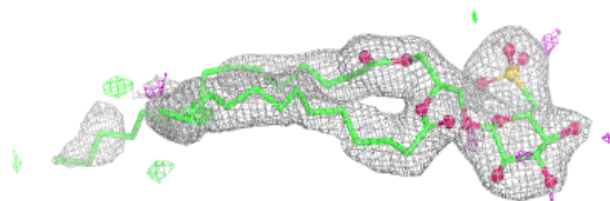
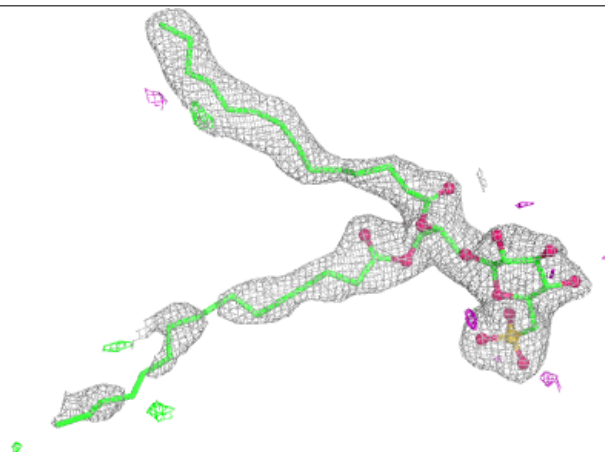


Electron density around LMG D 408:

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

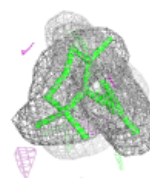
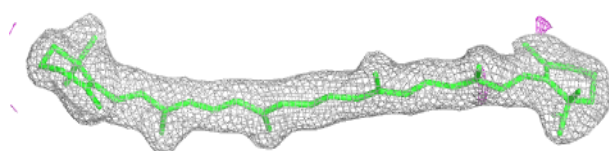
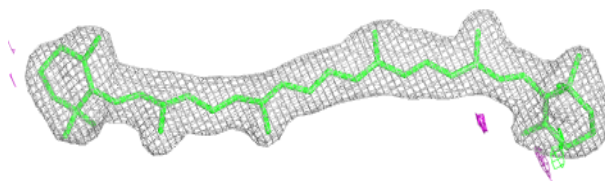
**Electron density around SQD A 614:**

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

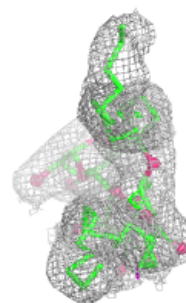
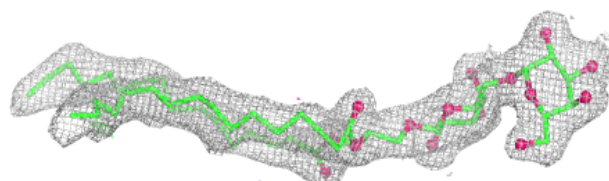
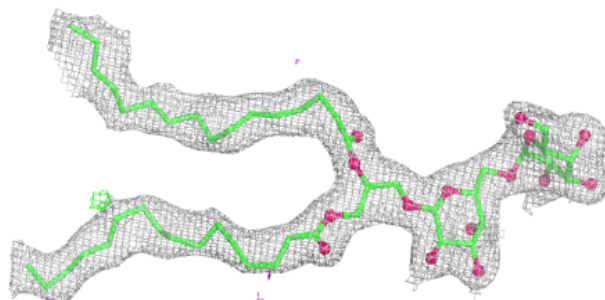


Electron density around BCR B 619:

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

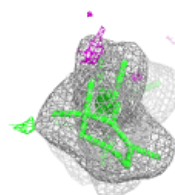
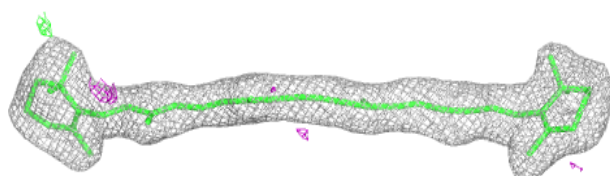
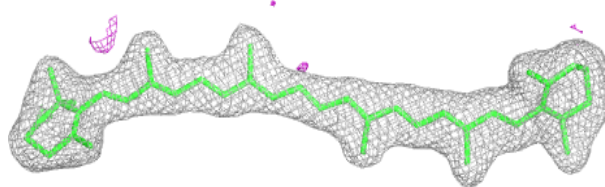
**Electron density around DGD C 517:**

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

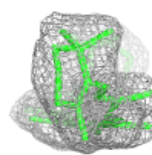
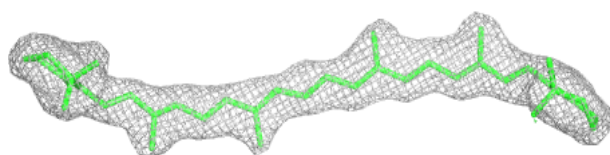
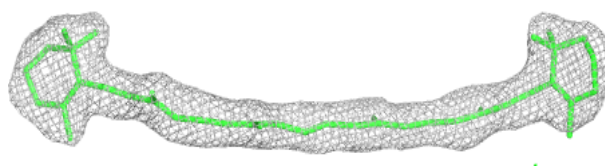


Electron density around BCR B 618:

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

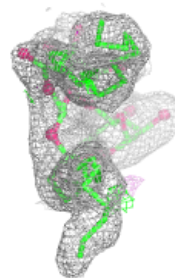
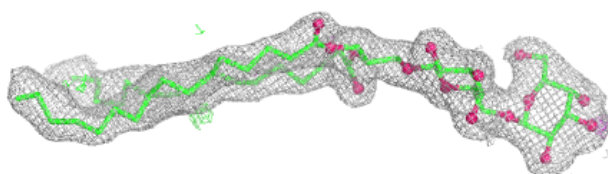
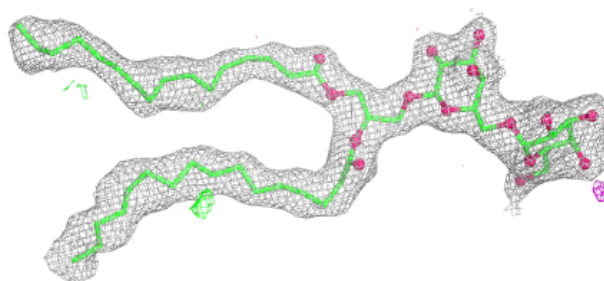
**Electron density around BCR k 103:**

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

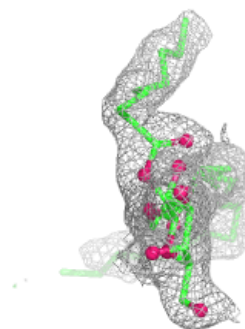
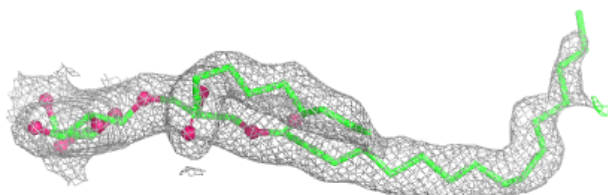
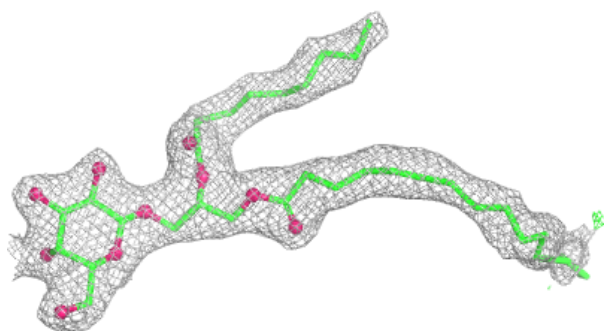


Electron density around DGD c 517:

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

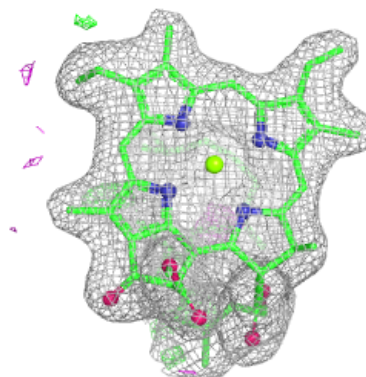
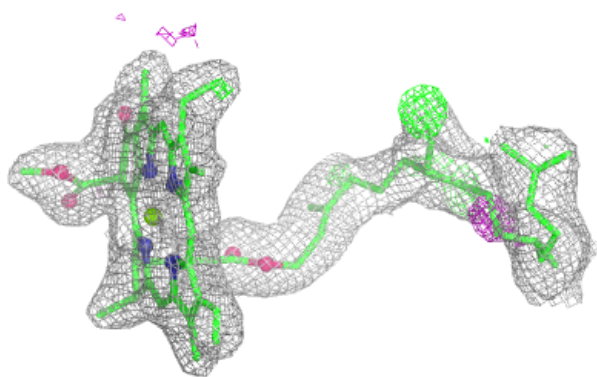
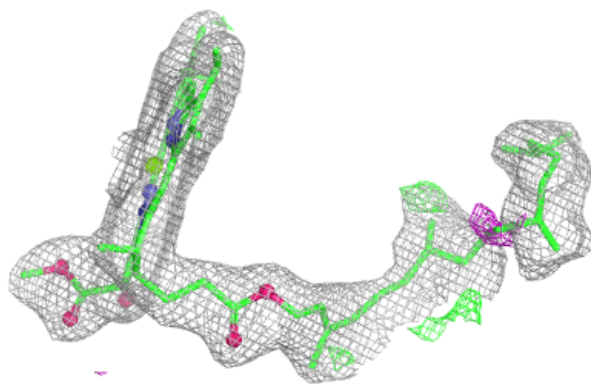
**Electron density around LMG d 411:**

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

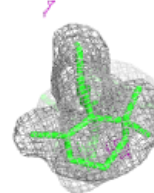
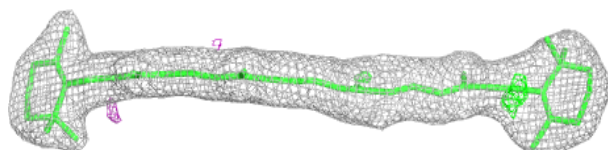
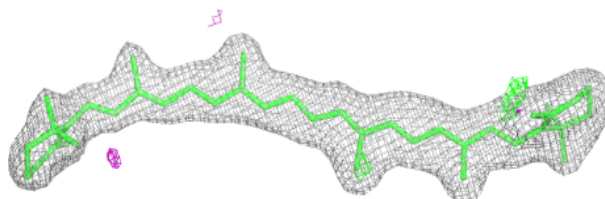


Electron density around CLA C 506:

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

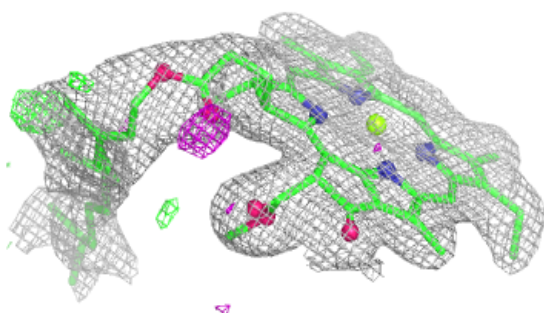
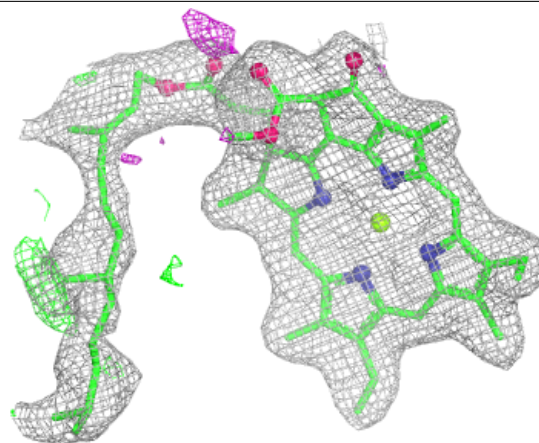
**Electron density around BCR C 514:**

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



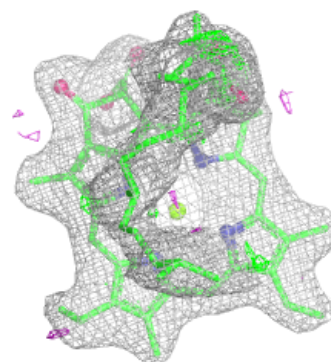
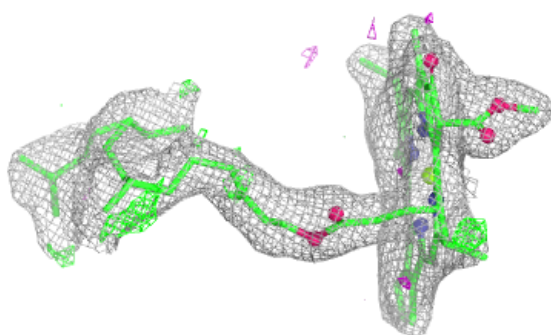
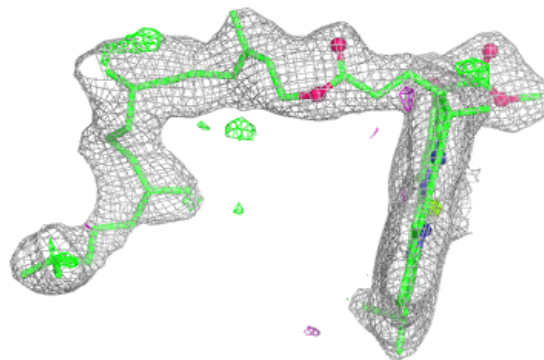
Electron density around CLA b 616:

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

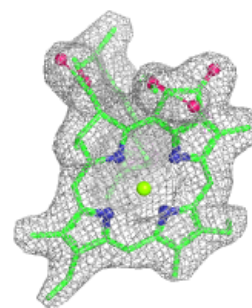
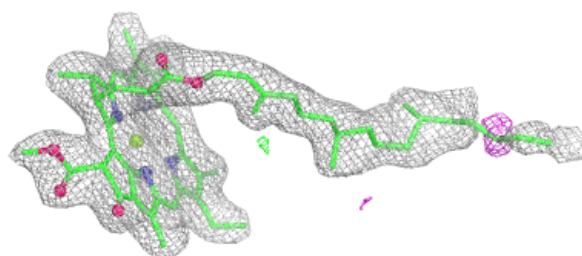
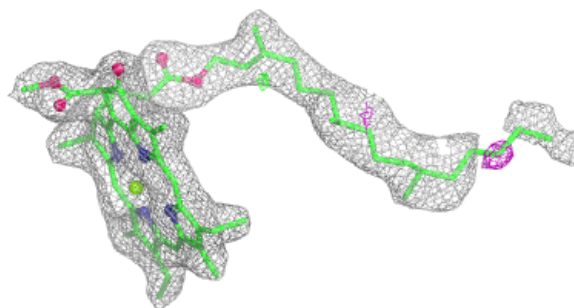


Electron density around CLA c 506:

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

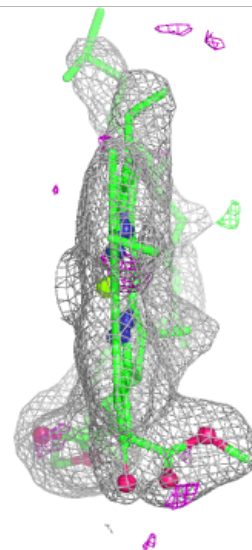
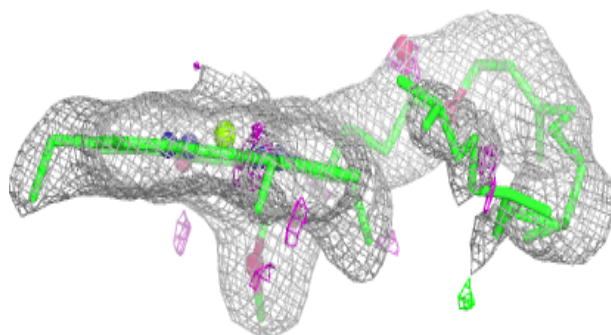
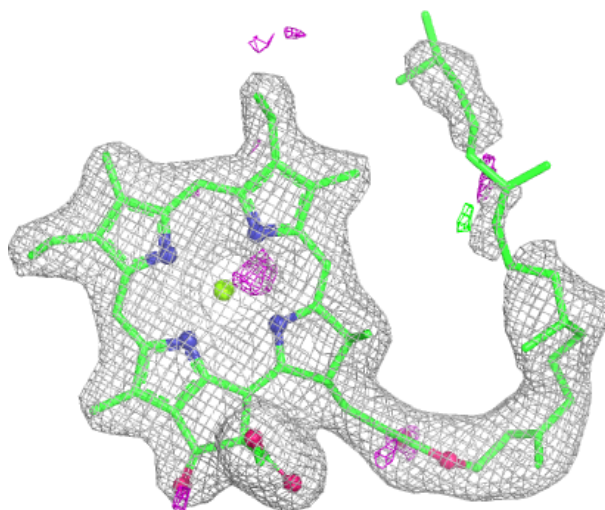
**Electron density around CLA c 508:**

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



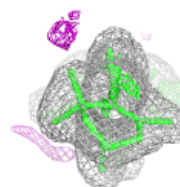
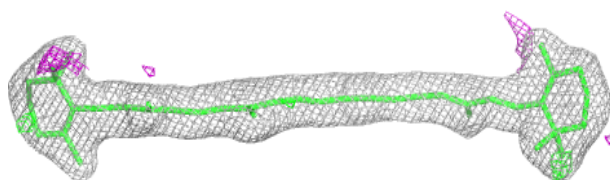
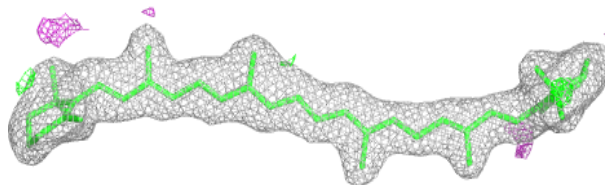
Electron density around CLA C 512:

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

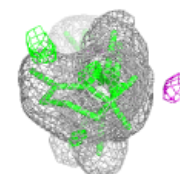
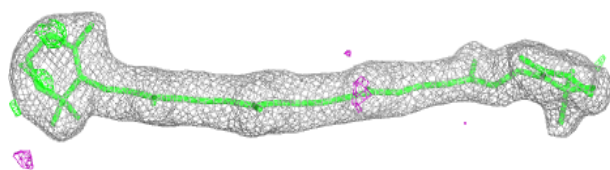
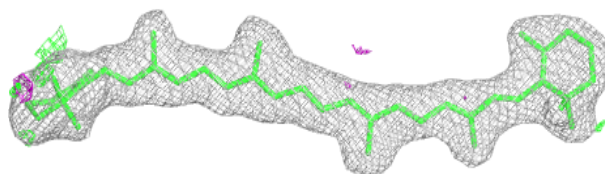


Electron density around BCR a 610:

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

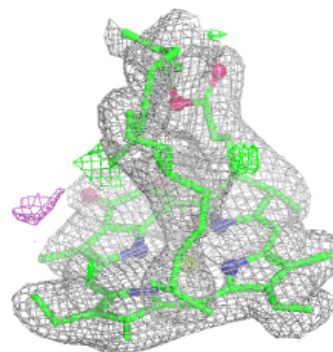
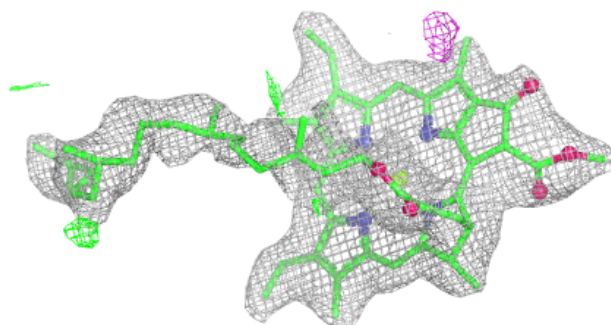
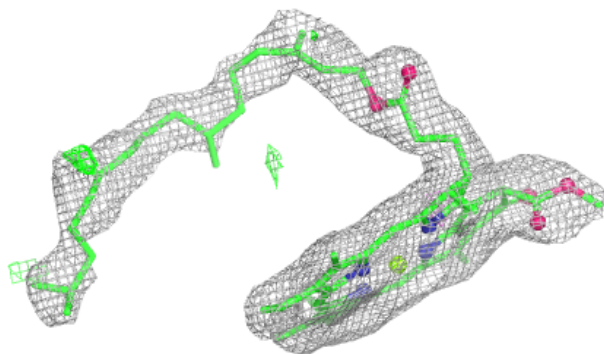
**Electron density around BCR b 617:**

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

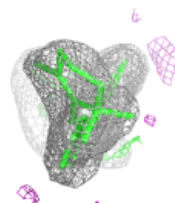
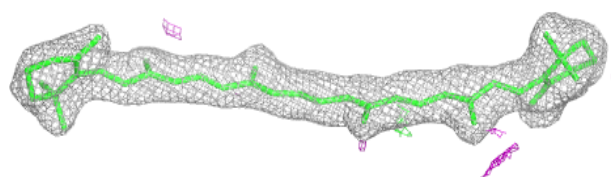
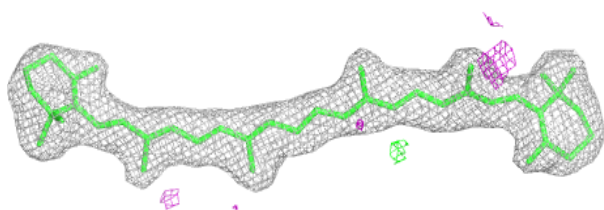


Electron density around CLA c 513:

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

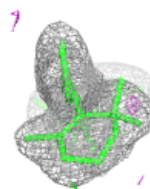
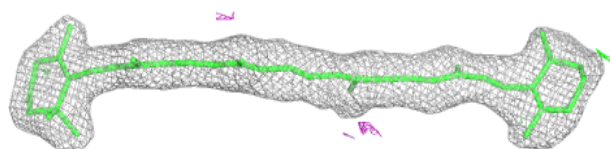
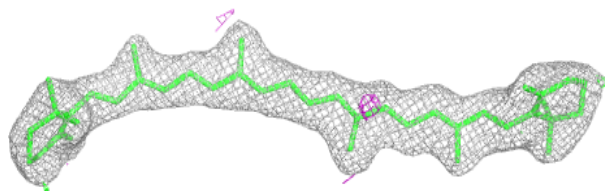
**Electron density around BCR b 619:**

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



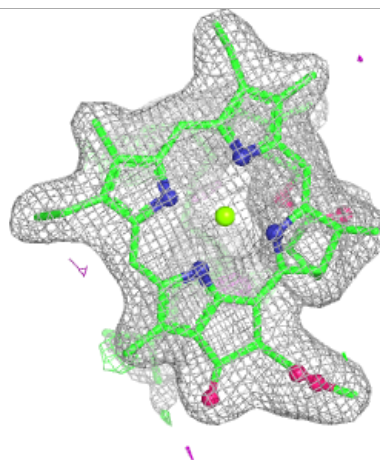
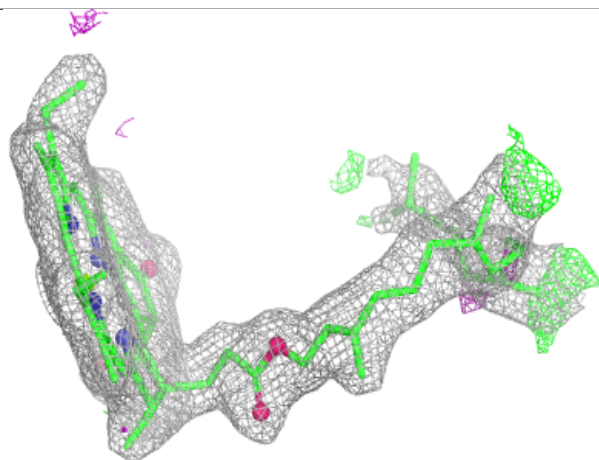
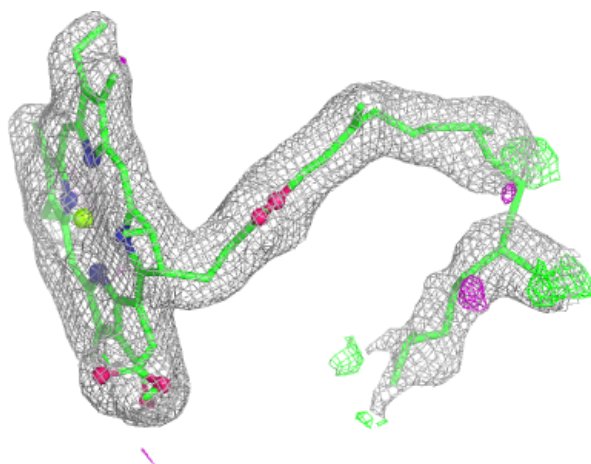
Electron density around BCR c 514:

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



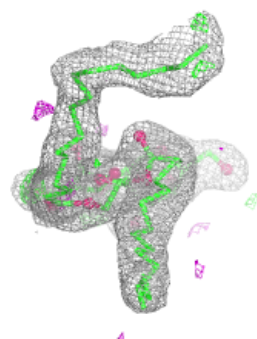
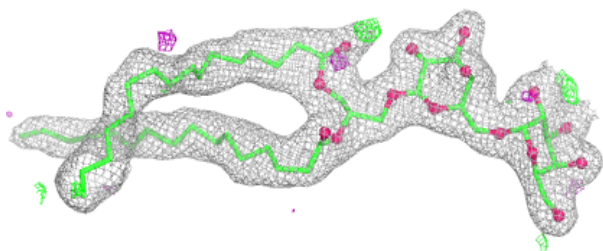
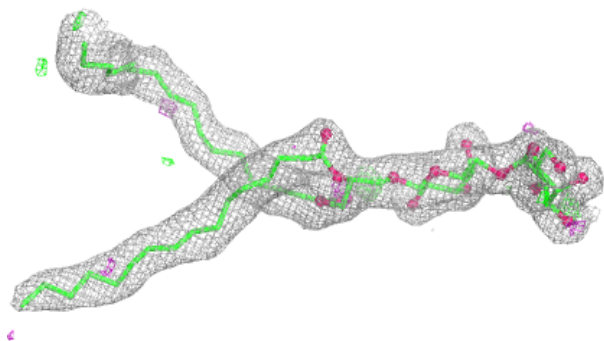
Electron density around CLA B 606:

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

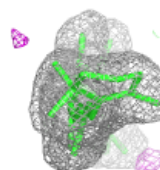
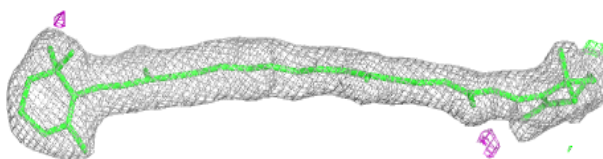
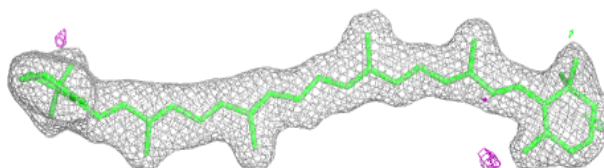


Electron density around DGD C 515:

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

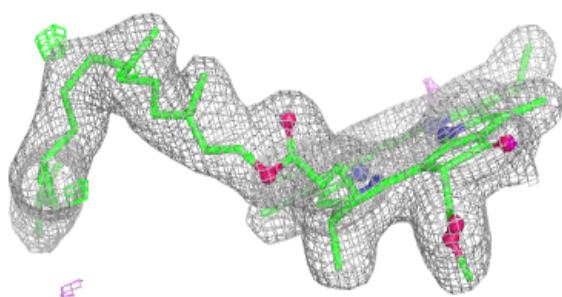
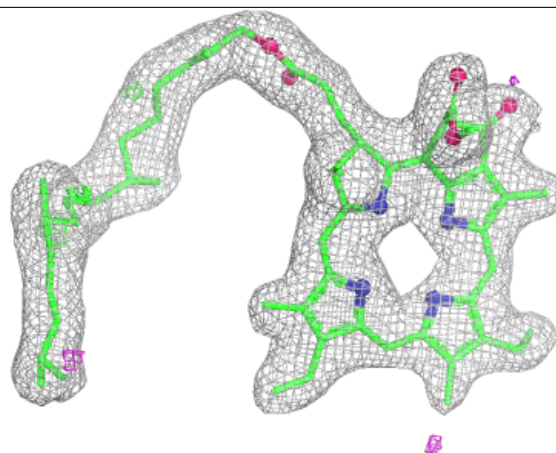
**Electron density around BCR B 617:**

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

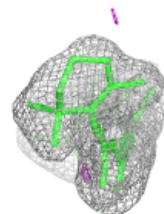
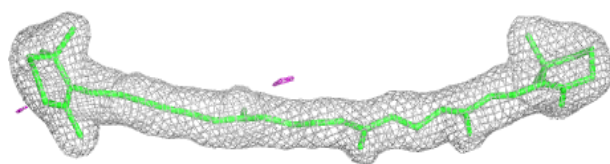
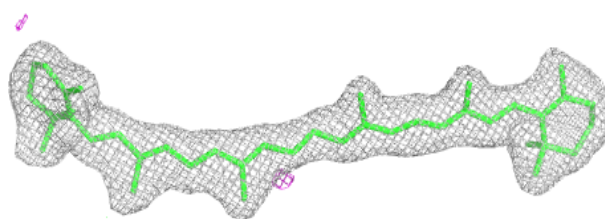


Electron density around PHO d 402:

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

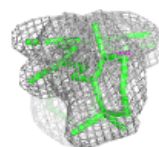
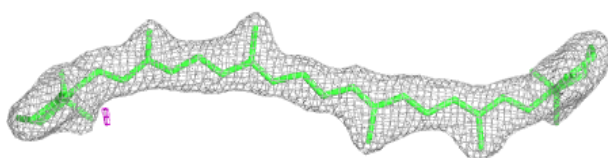
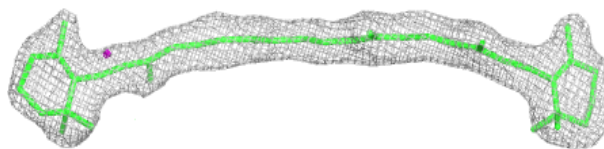
**Electron density around BCR T 101:**

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

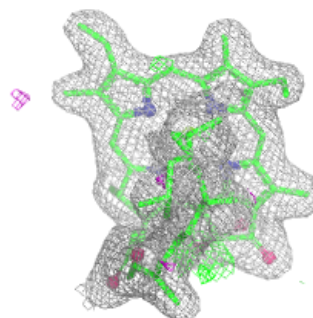
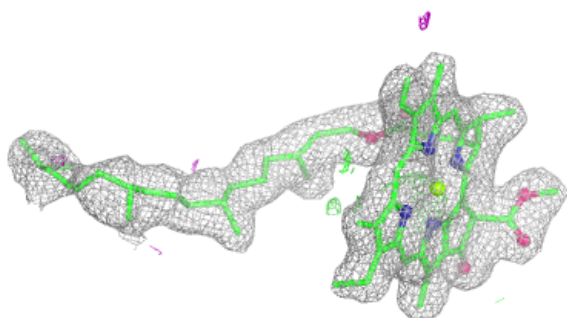
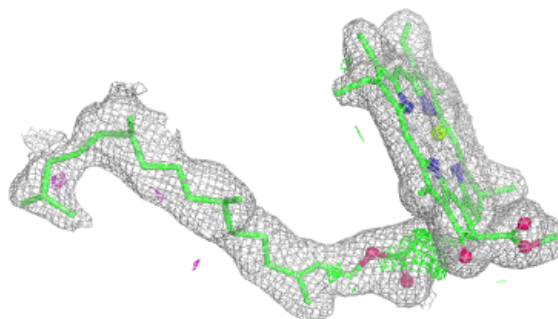


Electron density around BCR Z 101:

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

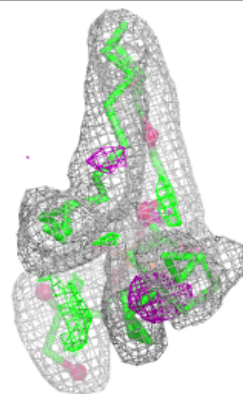
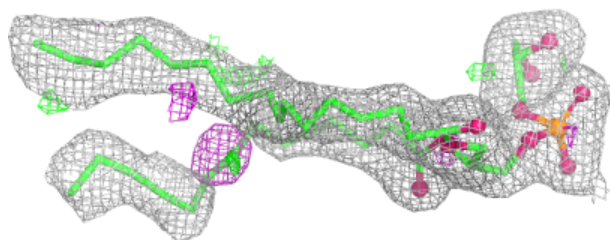
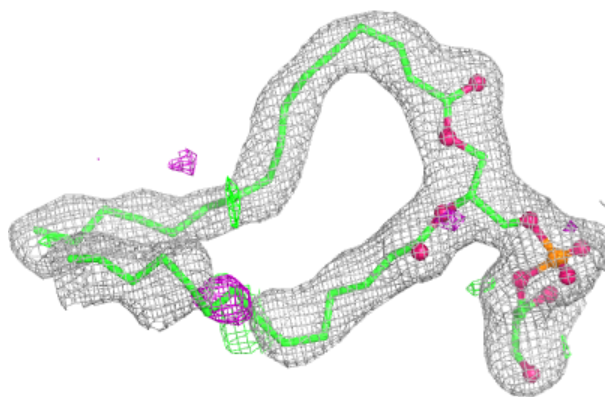
**Electron density around CLA C 508:**

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

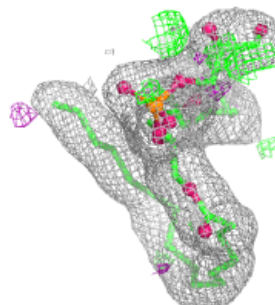
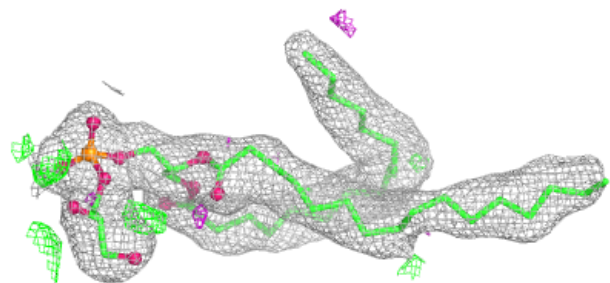
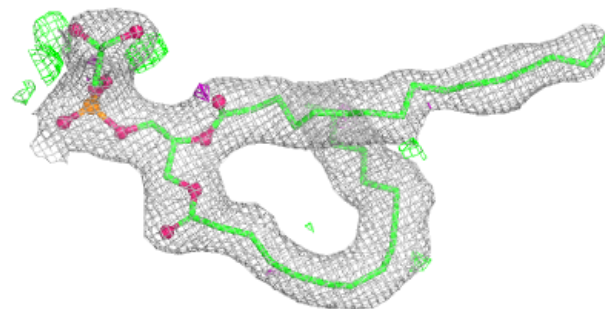


Electron density around LHG A 613:

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

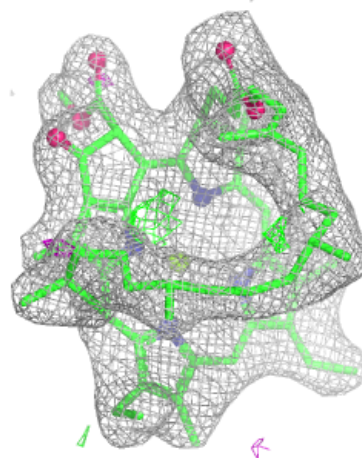
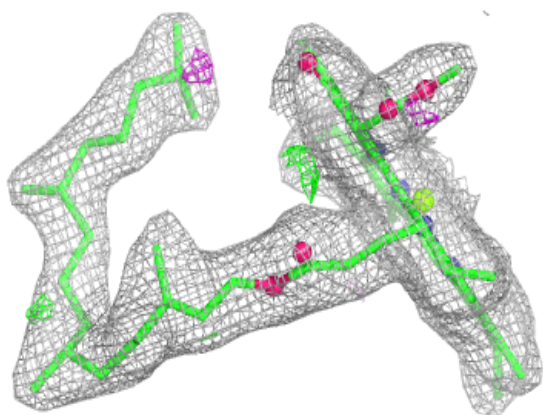
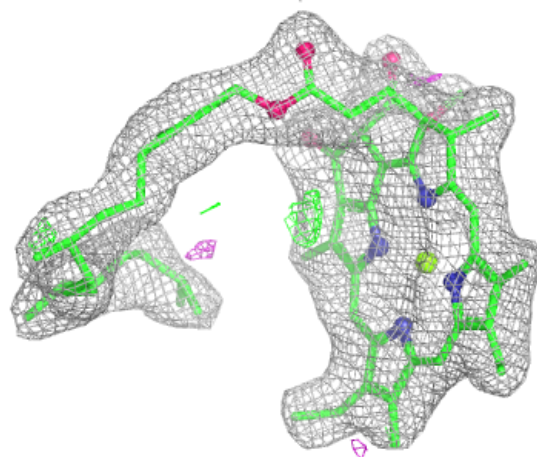
**Electron density around LHG B 622:**

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



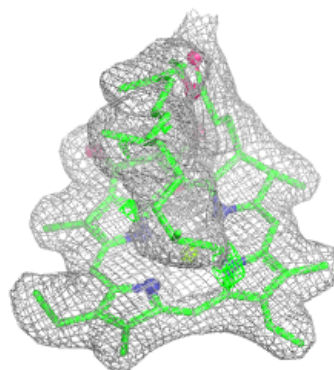
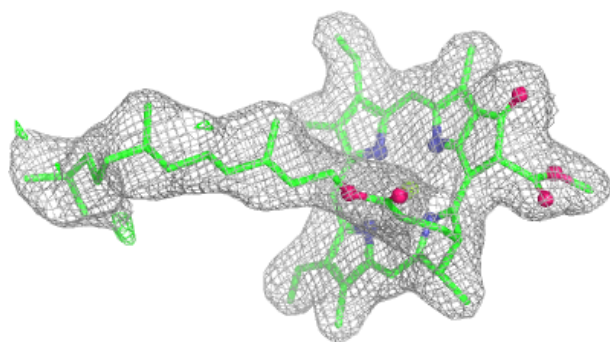
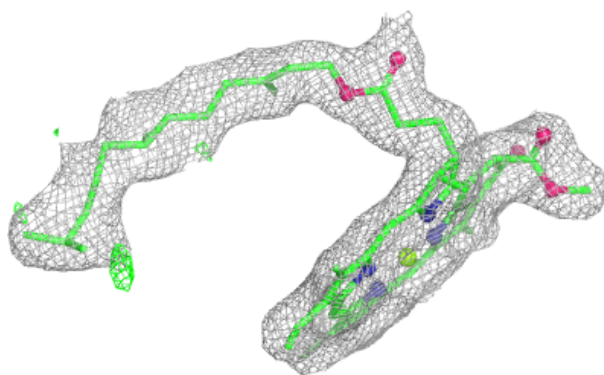
Electron density around CLA c 503:

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

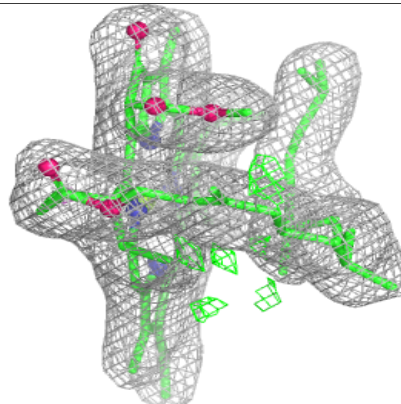
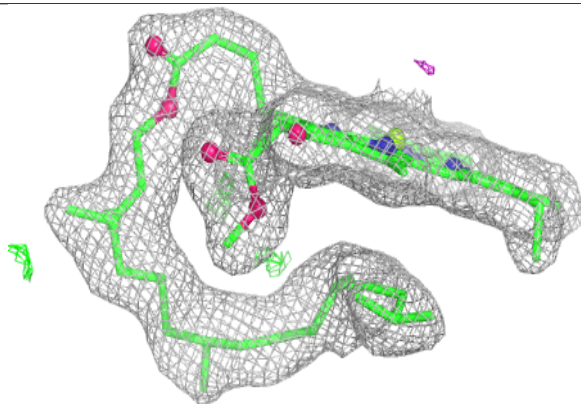
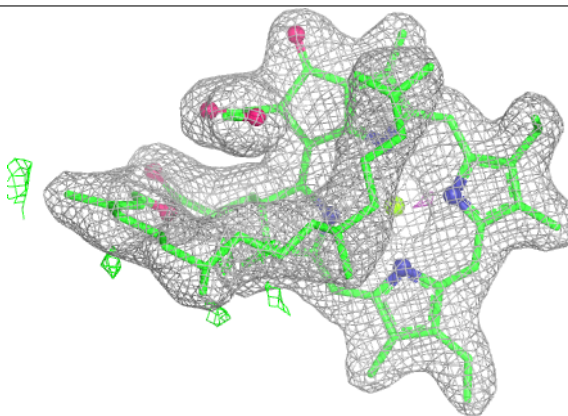


Electron density around CLA c 504:

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

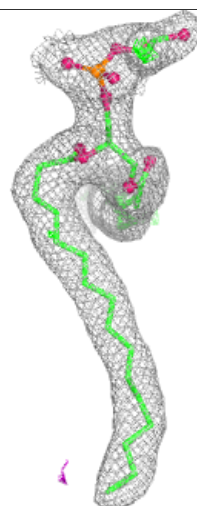
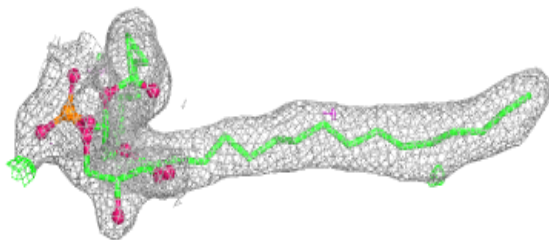
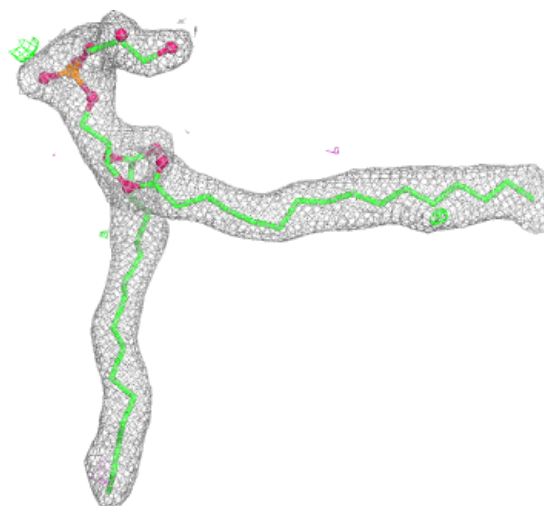
**Electron density around CLA C 510:**

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



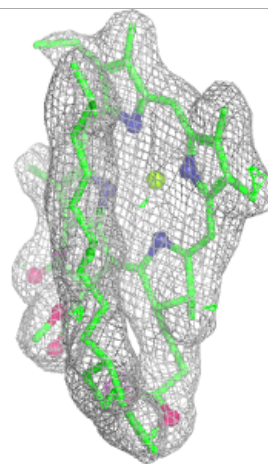
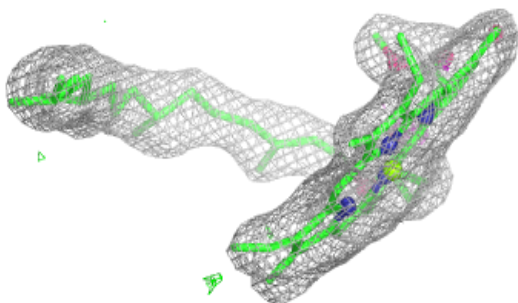
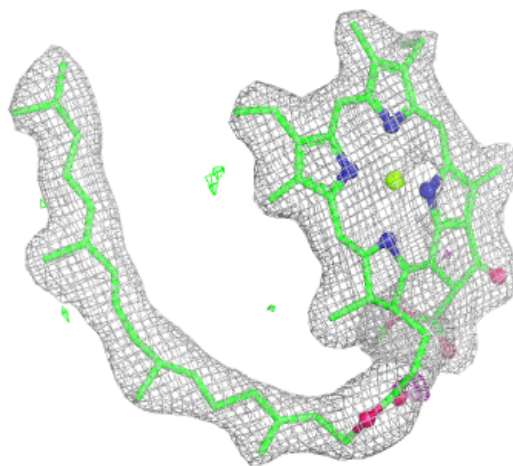
Electron density around LHG 1 101:

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



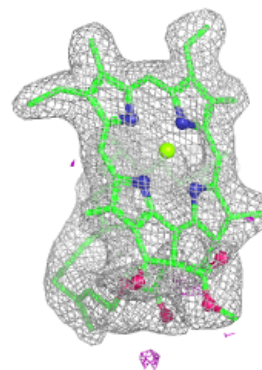
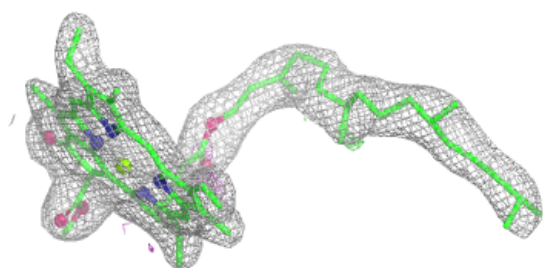
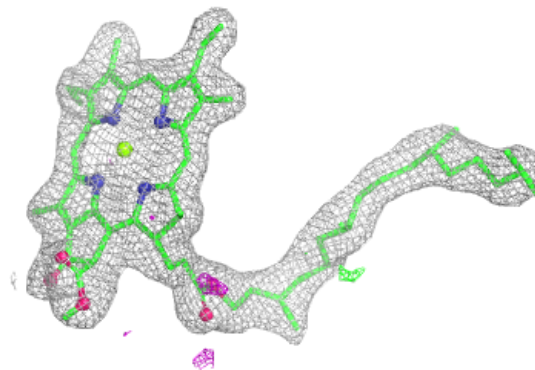
Electron density around CLA c 507:

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



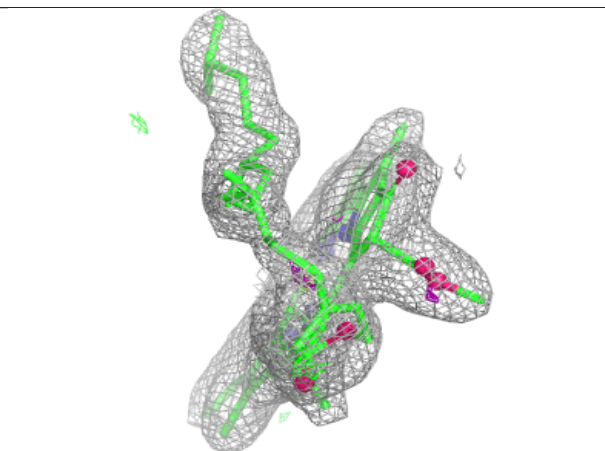
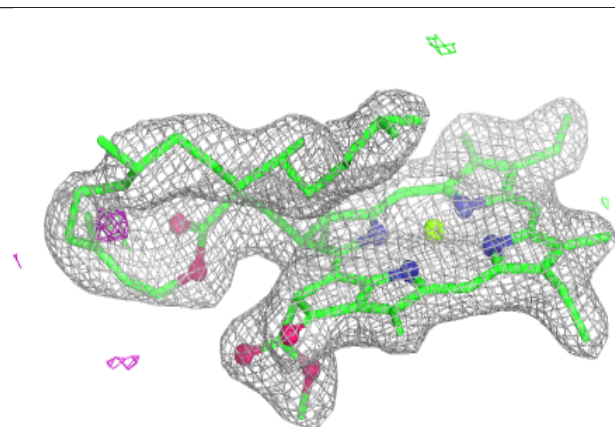
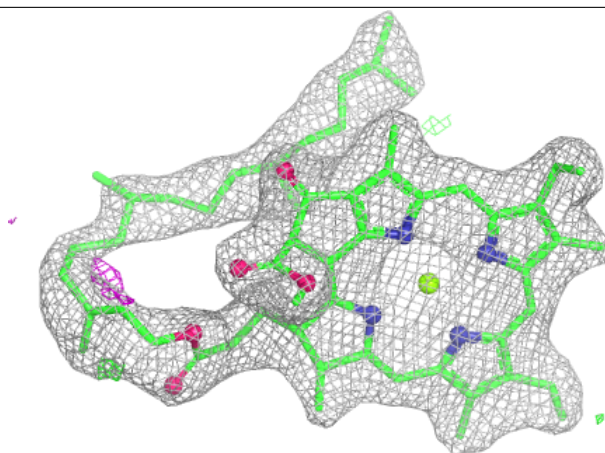
Electron density around CLA C 511:

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



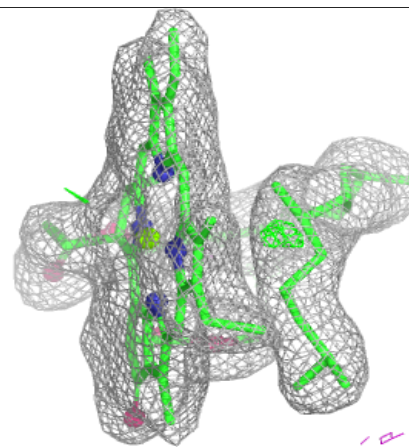
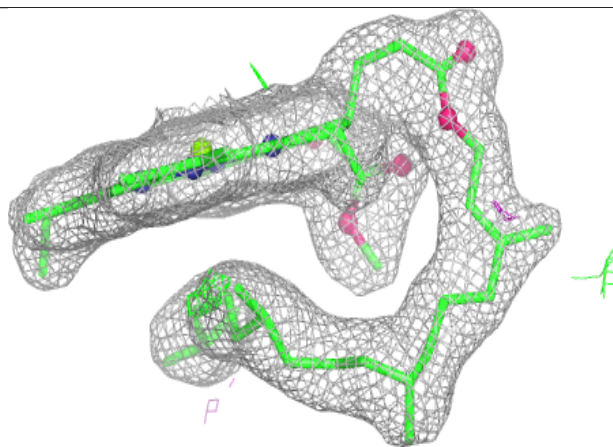
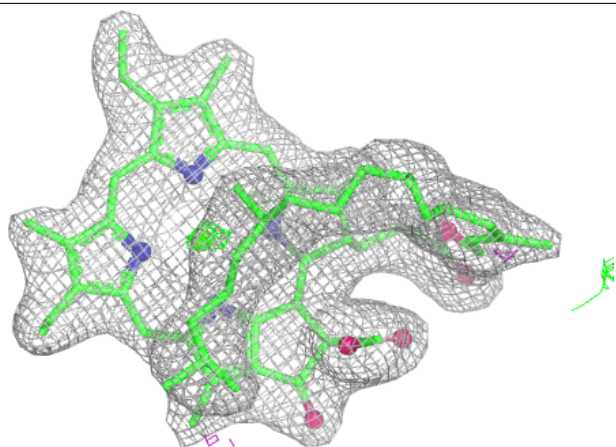
Electron density around CLA c 509:

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



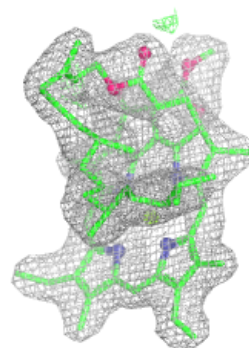
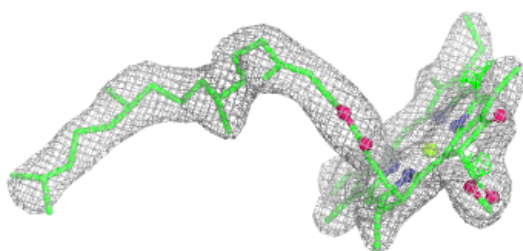
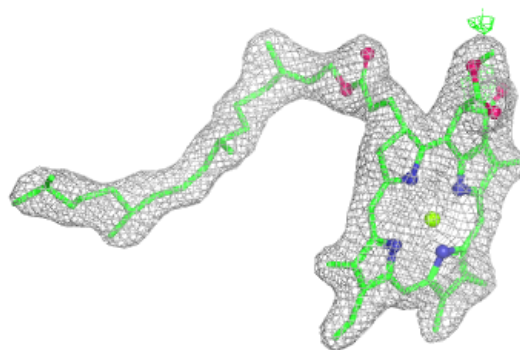
Electron density around CLA c 510:

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

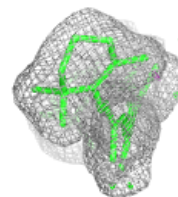
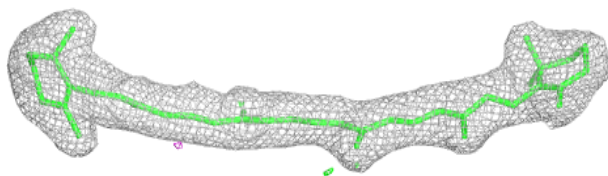
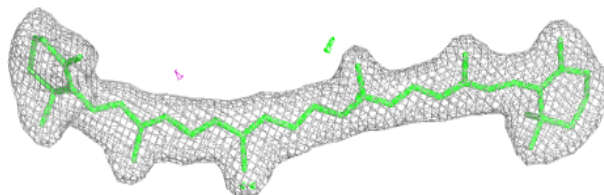


Electron density around CLA c 511:

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

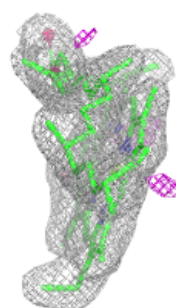
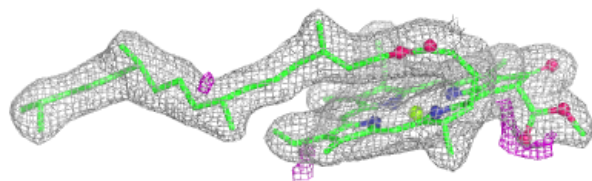
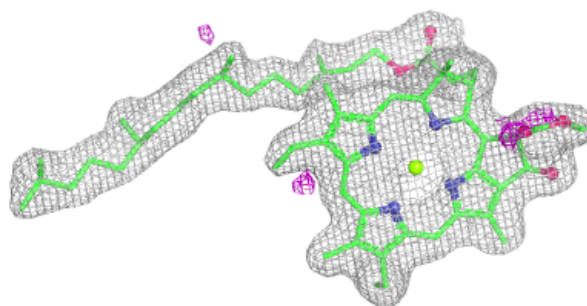
**Electron density around BCR t 101:**

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



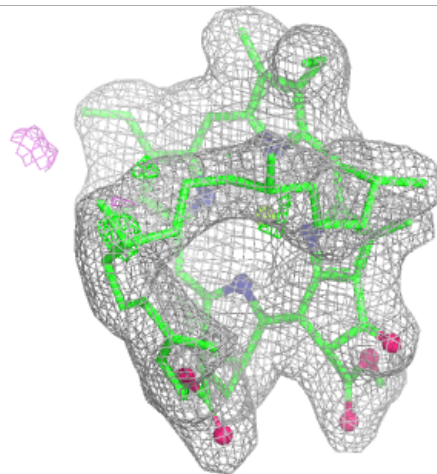
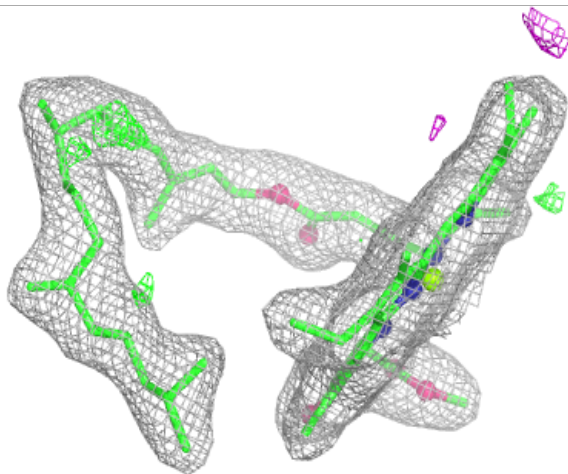
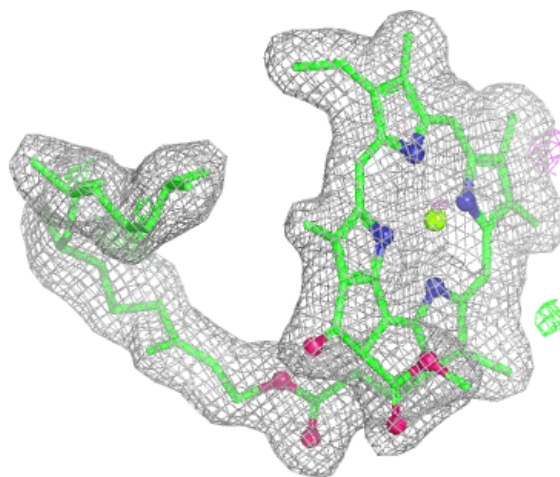
Electron density around CLA C 501:

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



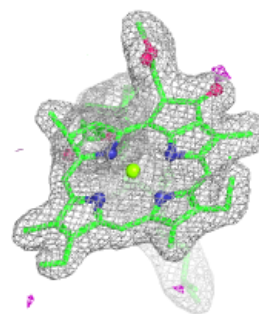
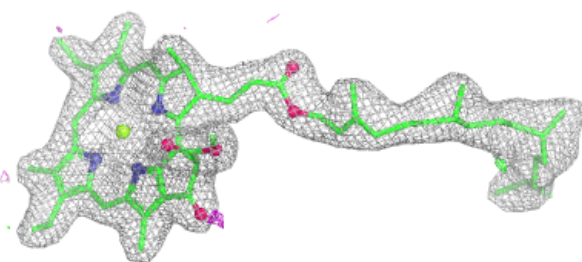
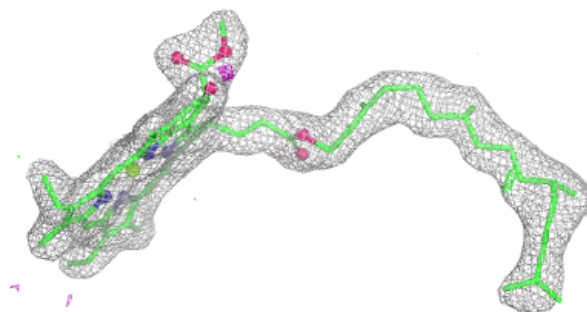
Electron density around CLA C 503:

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

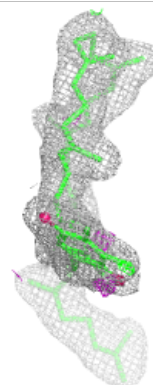
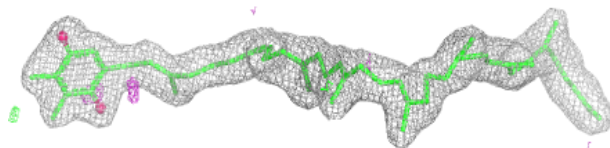
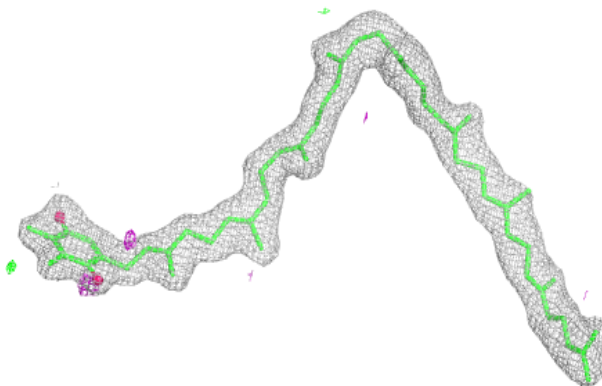


Electron density around CLA d 403:

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

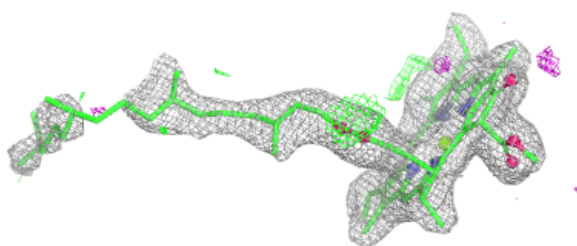
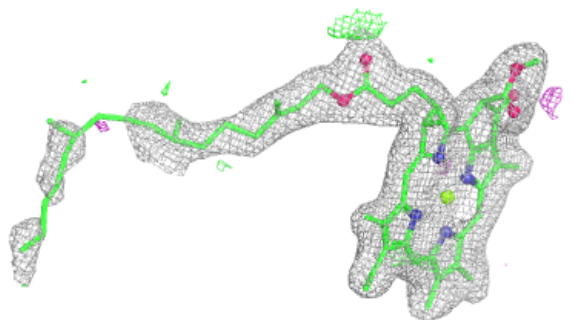
**Electron density around PL9 d 406:**

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

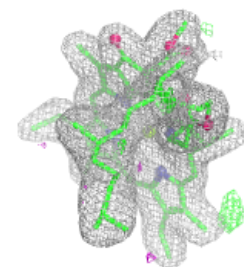
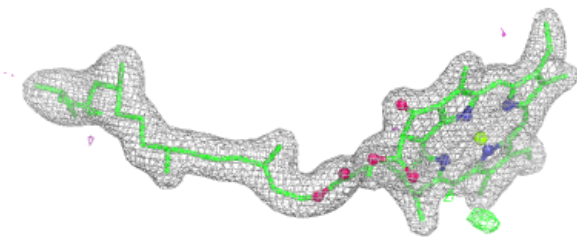
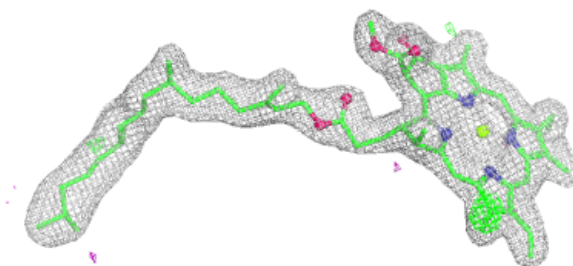


Electron density around CLA d 404:

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

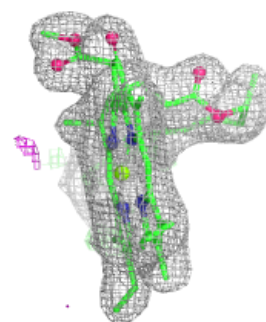
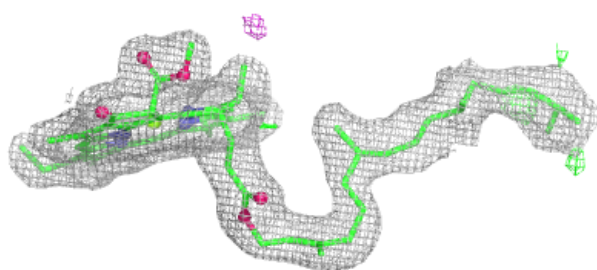
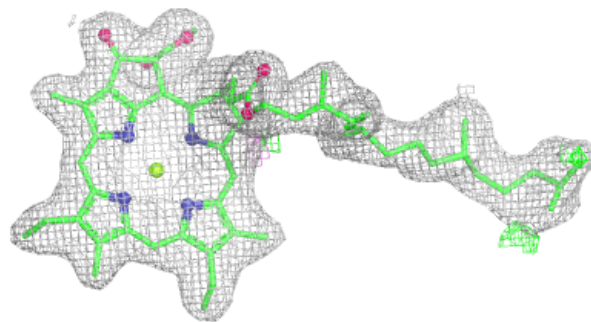
**Electron density around CLA a 607:**

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

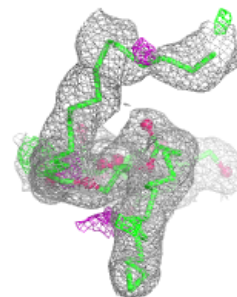
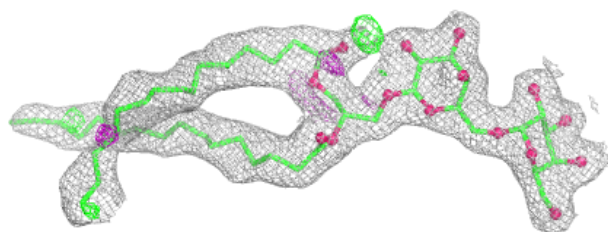
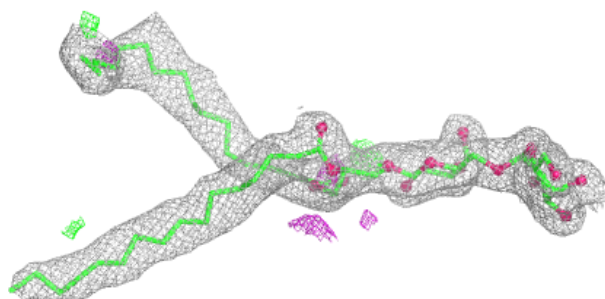


Electron density around CLA a 608:

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

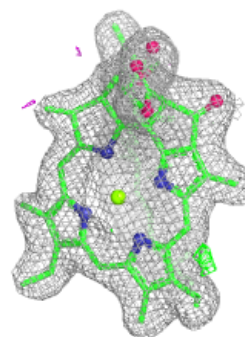
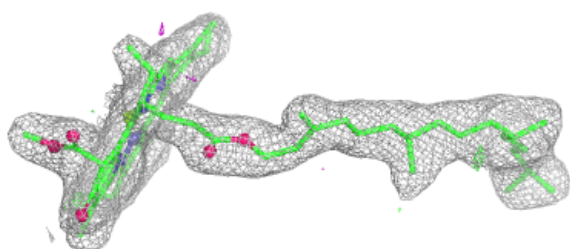
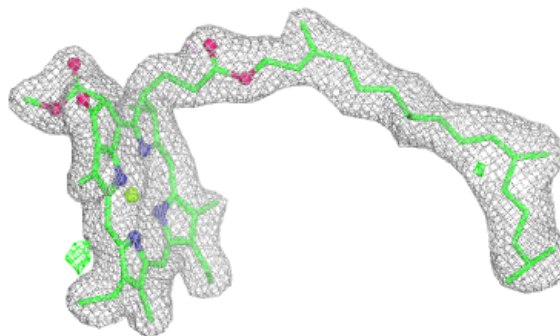
**Electron density around DGD c 515:**

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

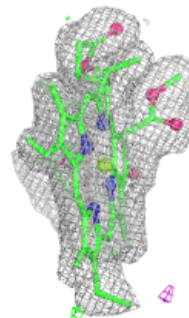
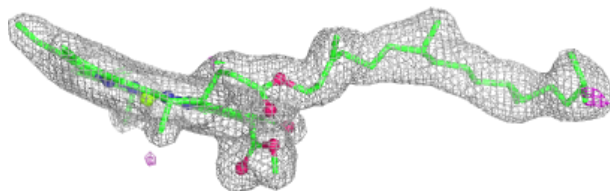
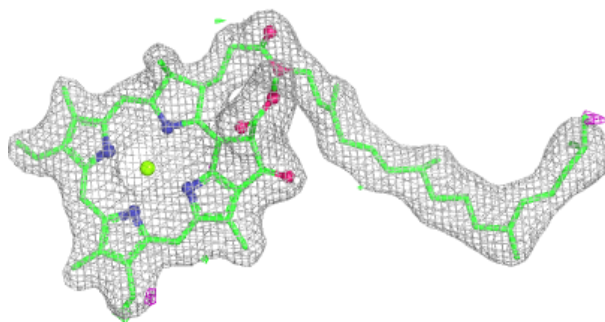


Electron density around CLA B 609:

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

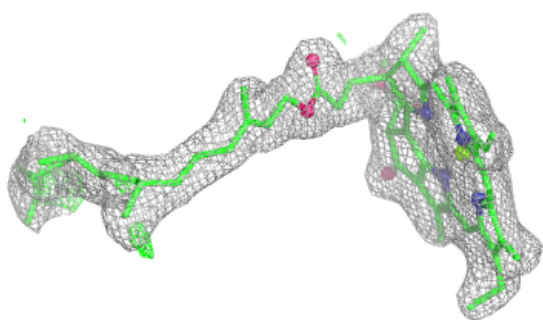
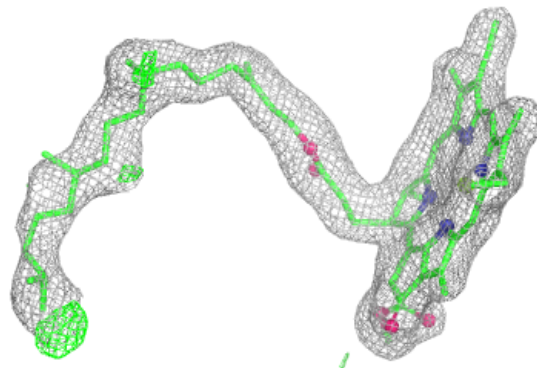
**Electron density around CLA b 602:**

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

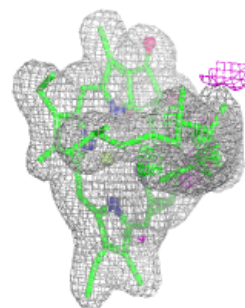
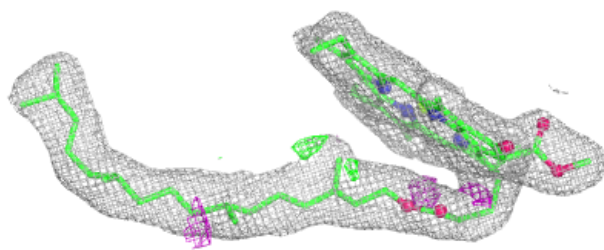
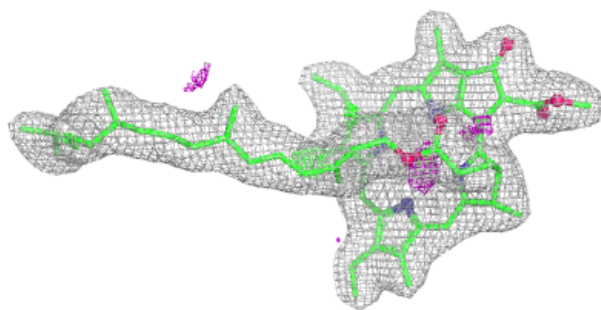


Electron density around CLA b 606:

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

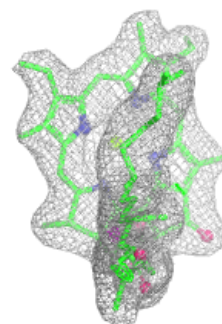
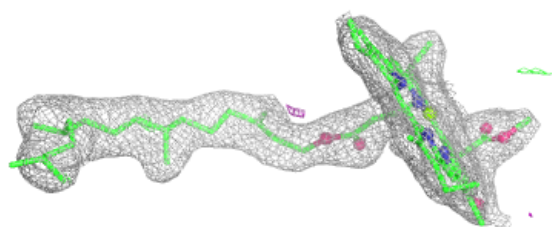
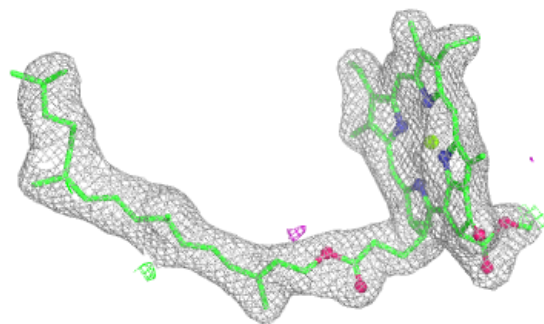
**Electron density around CLA b 608:**

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

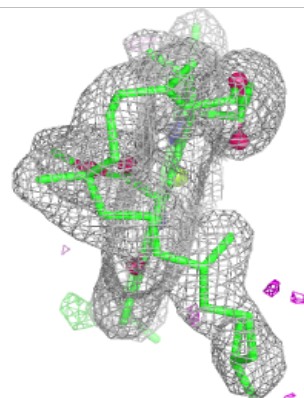
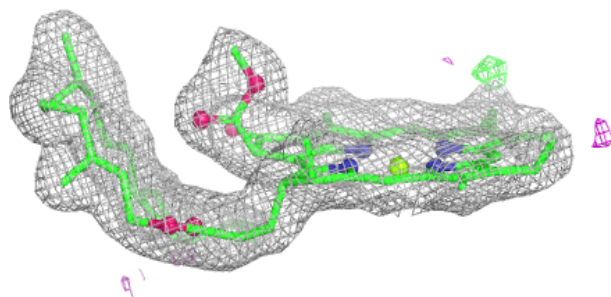
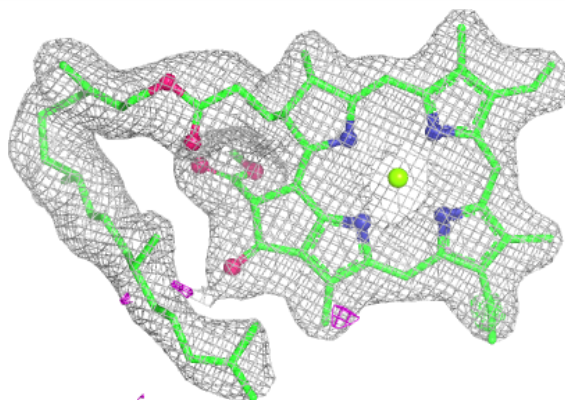


Electron density around CLA b 609:

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

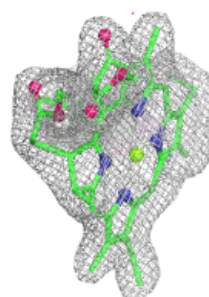
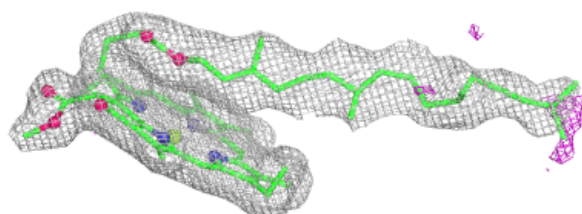
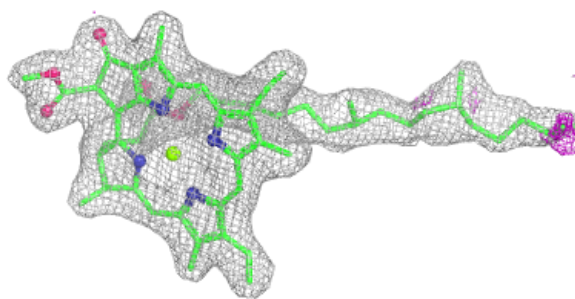
**Electron density around CLA b 610:**

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



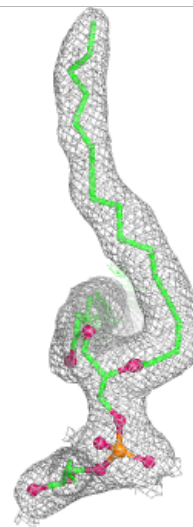
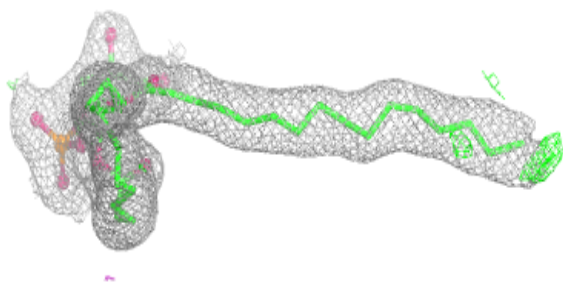
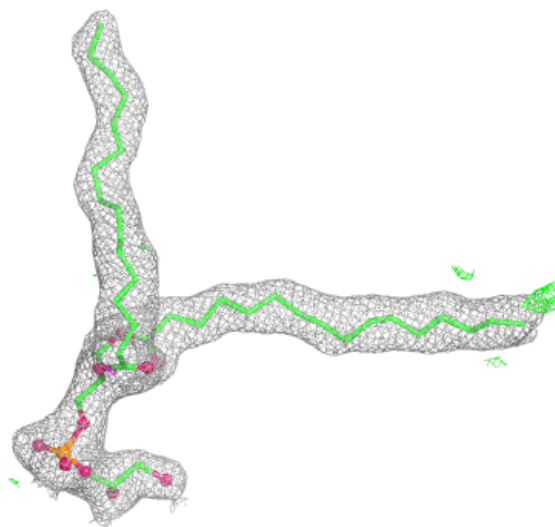
Electron density around CLA b 614:

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



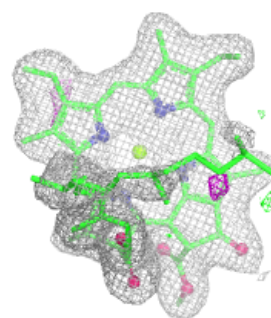
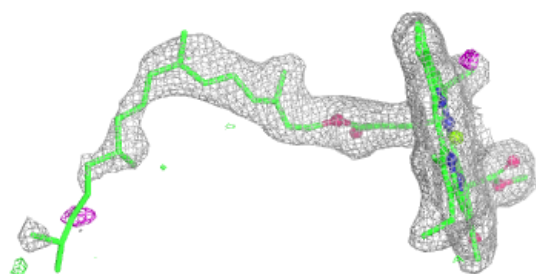
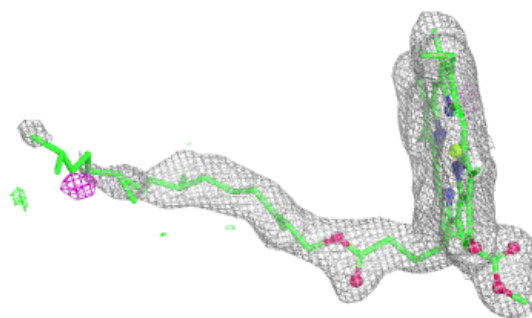
Electron density around LHG L 101:

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

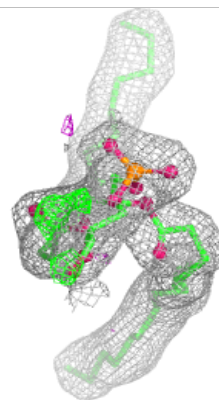
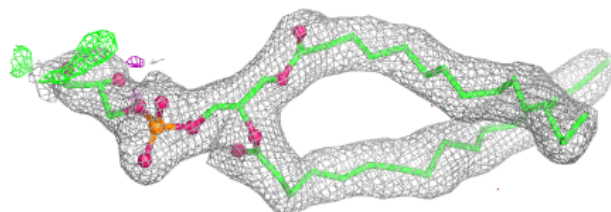
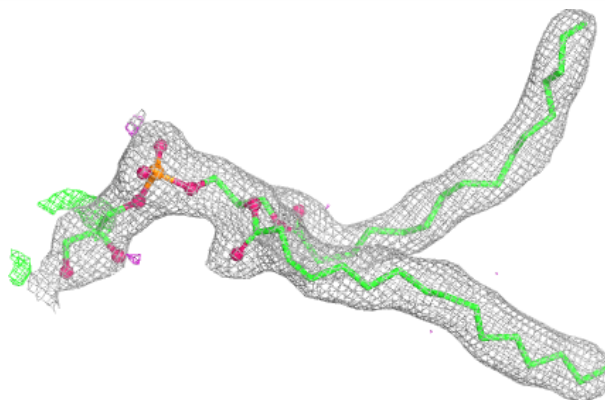


Electron density around CLA D 405:

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

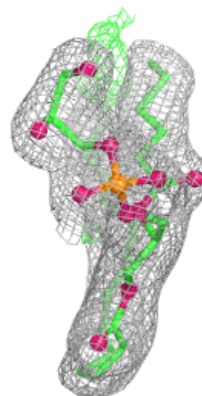
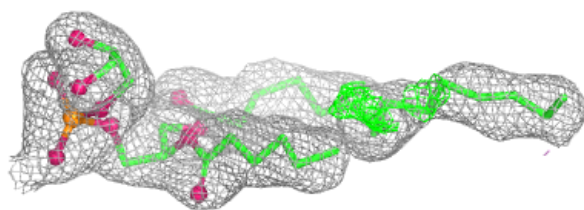
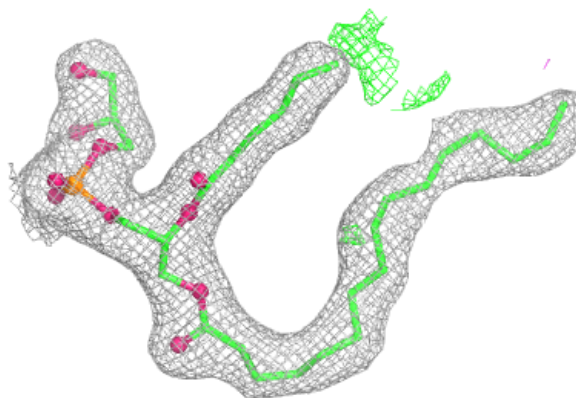
**Electron density around LHG d 408:**

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



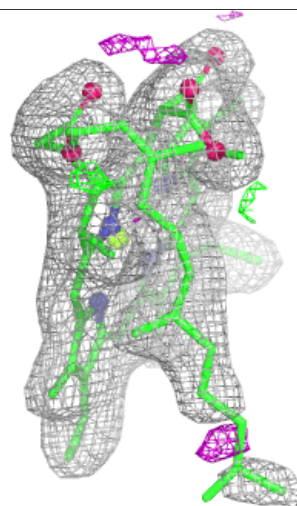
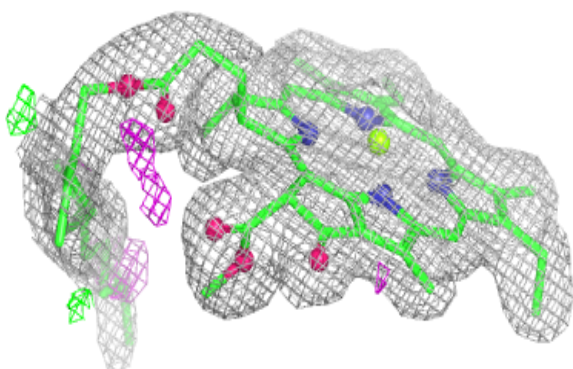
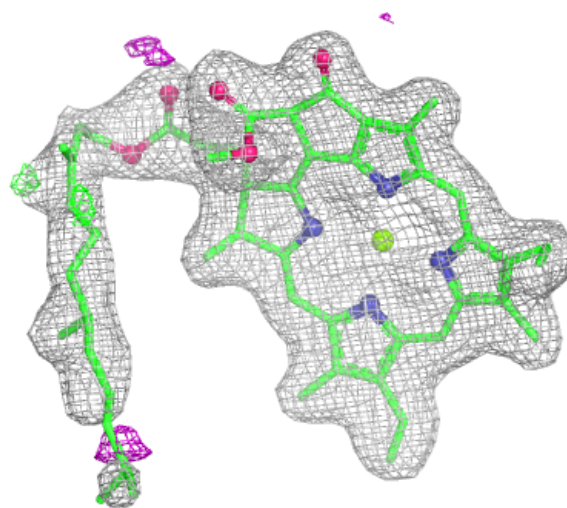
Electron density around LHG d 409:

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



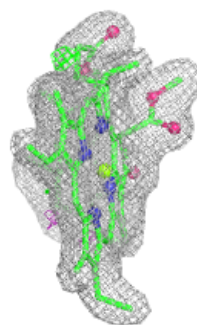
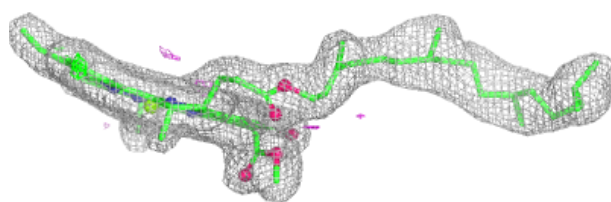
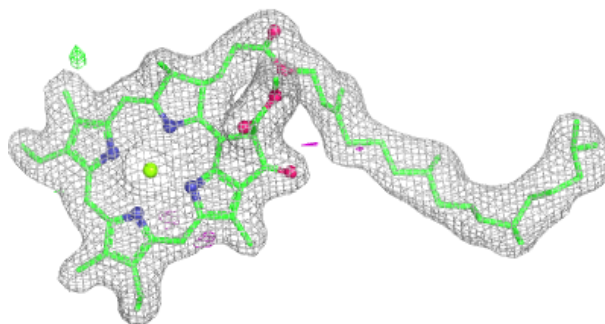
Electron density around CLA B 616:

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

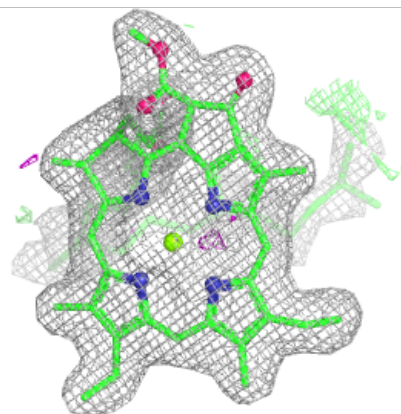
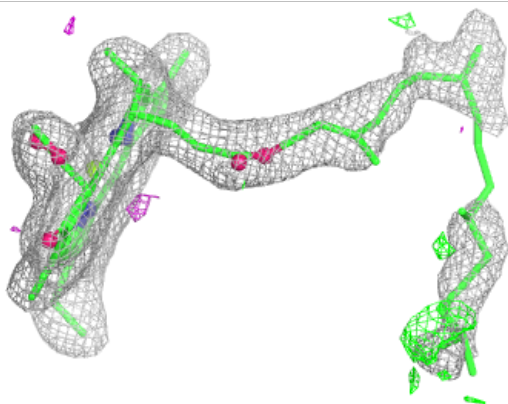
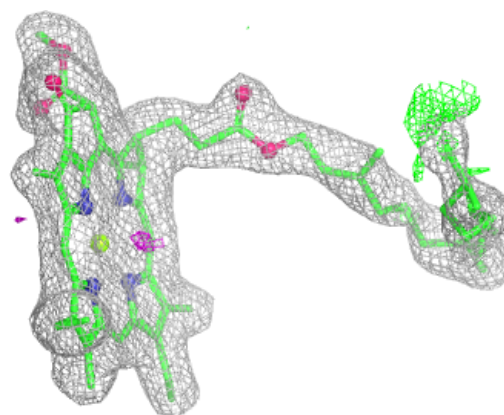


Electron density around CLA B 602:

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

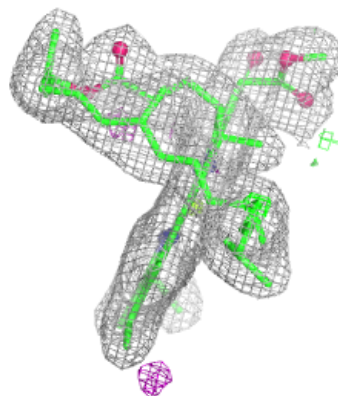
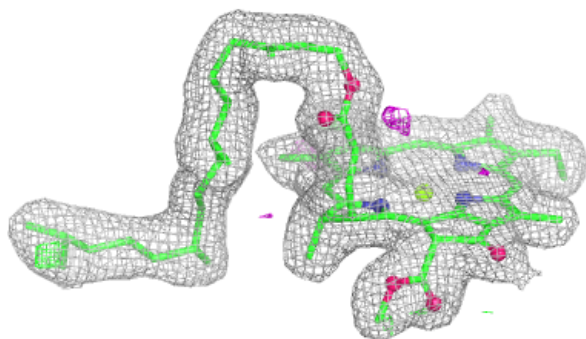
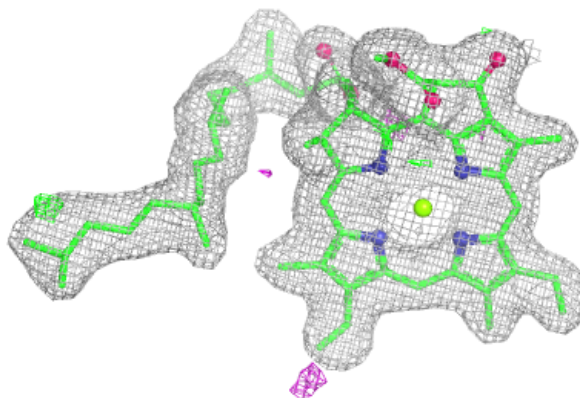
**Electron density around CLA a 609:**

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

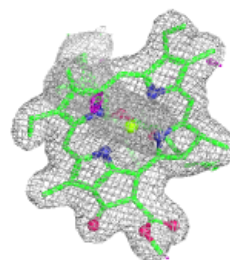
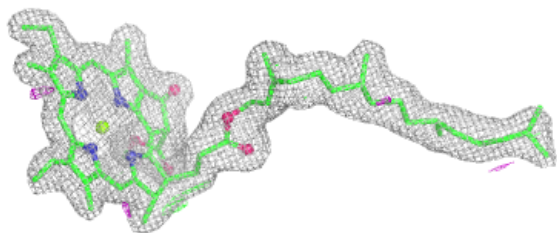
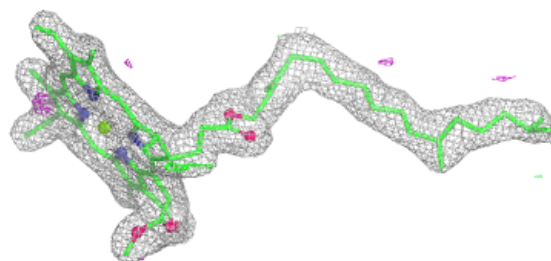


Electron density around CLA a 612:

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

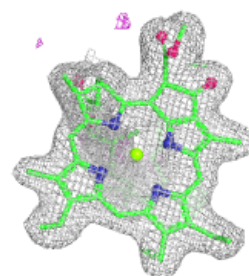
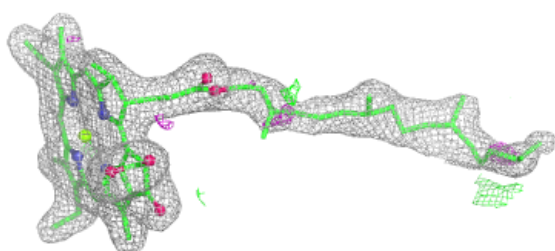
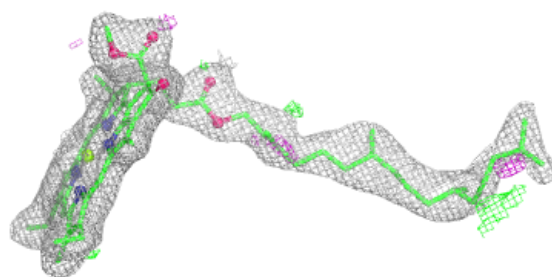
**Electron density around CLA C 502:**

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

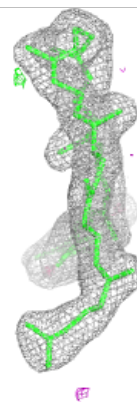
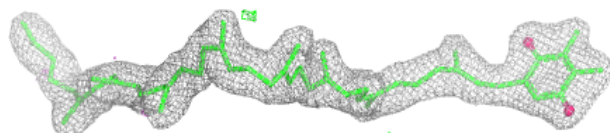
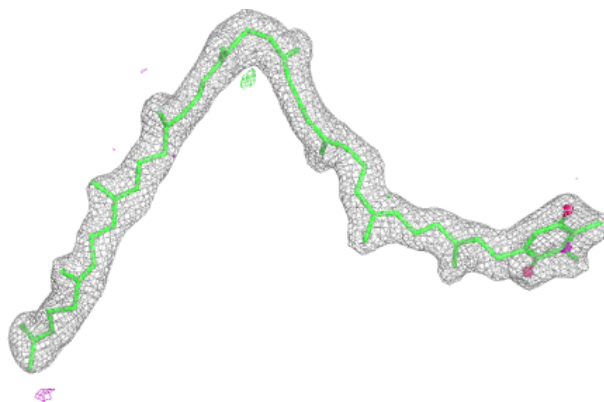


Electron density around CLA B 604:

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

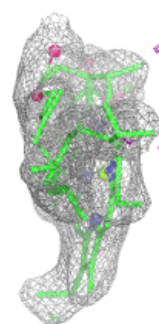
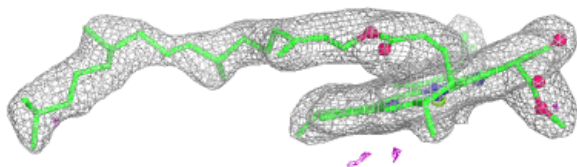
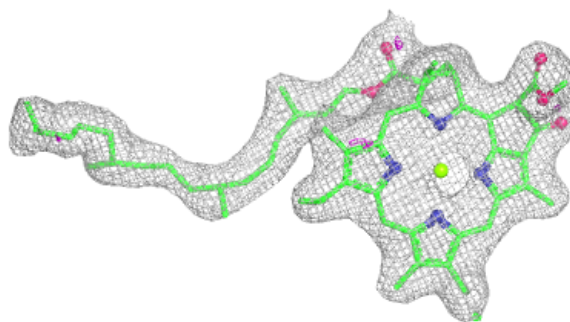
**Electron density around PL9 D 407:**

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

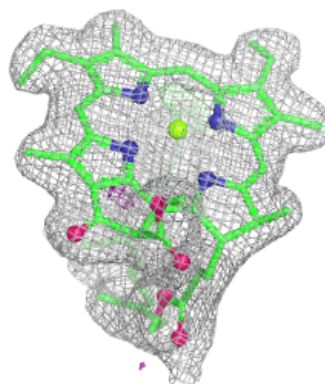
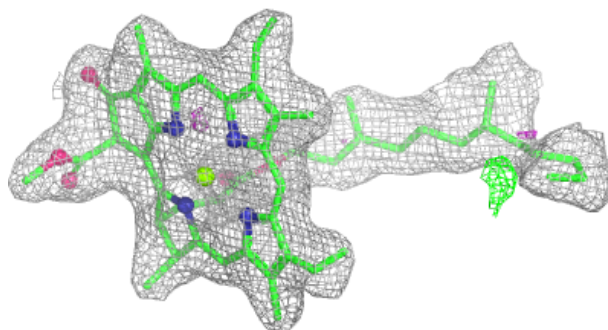
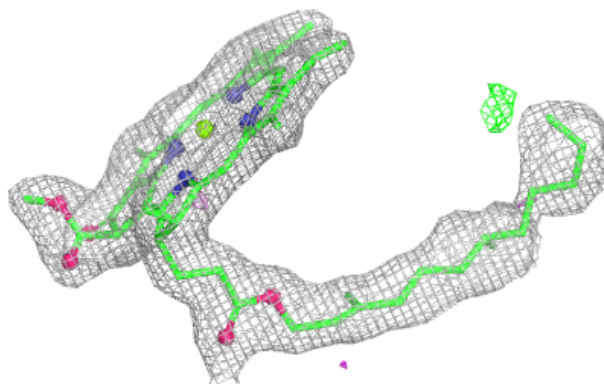


Electron density around CLA b 603:

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

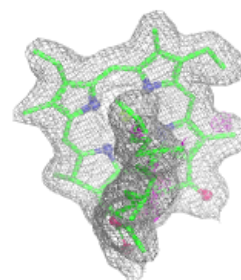
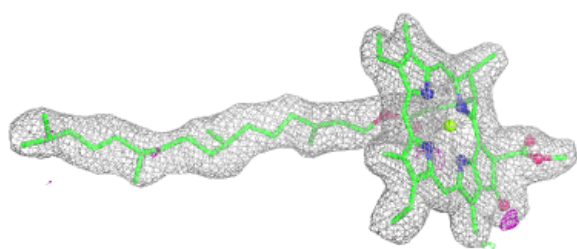
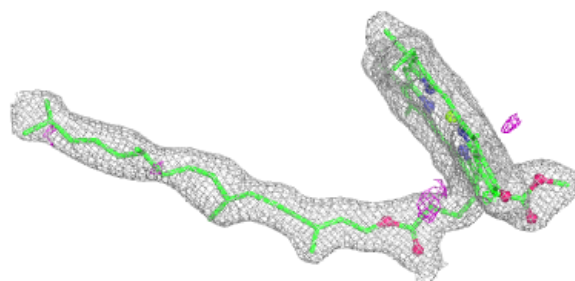
**Electron density around CLA C 504:**

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

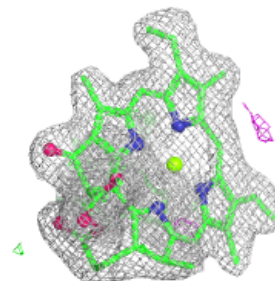
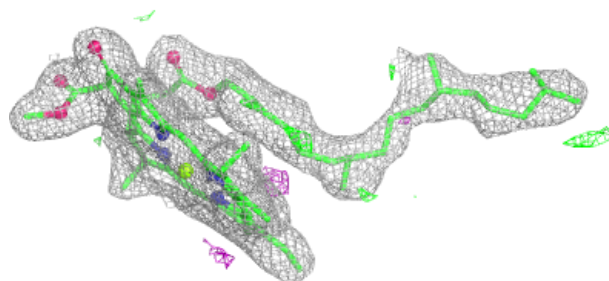
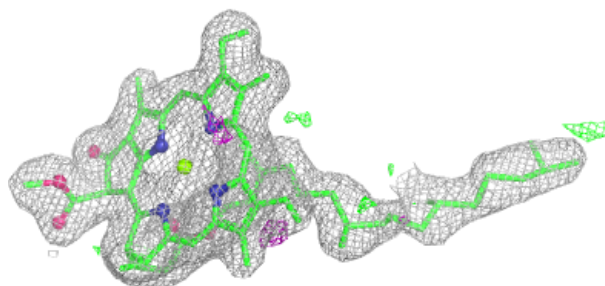


Electron density around CLA b 607:

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

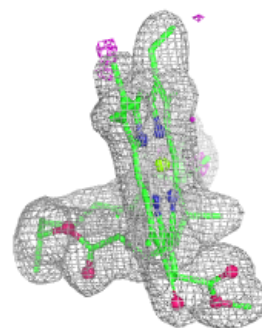
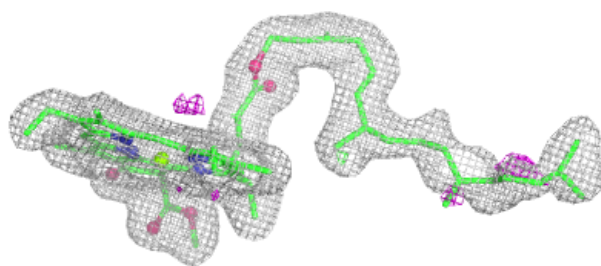
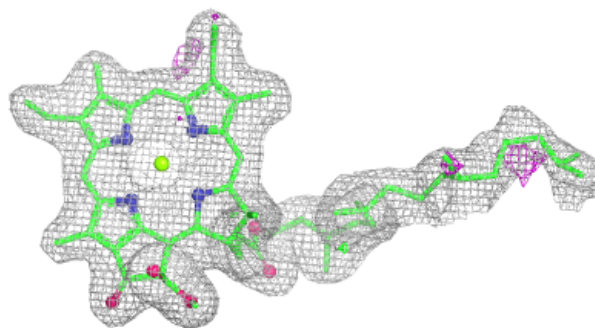
**Electron density around CLA C 505:**

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

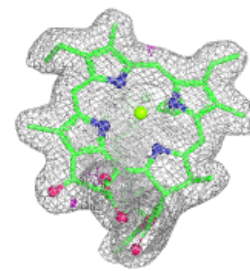
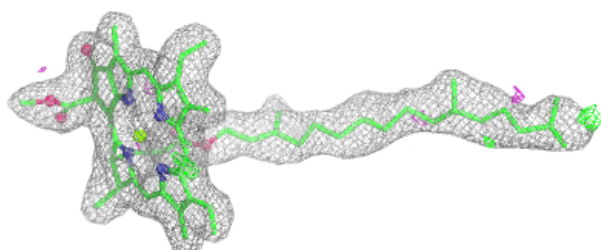
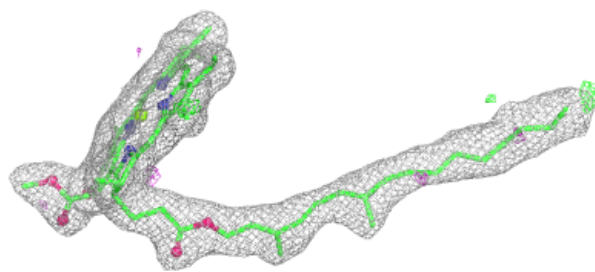


Electron density around CLA A 607:

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

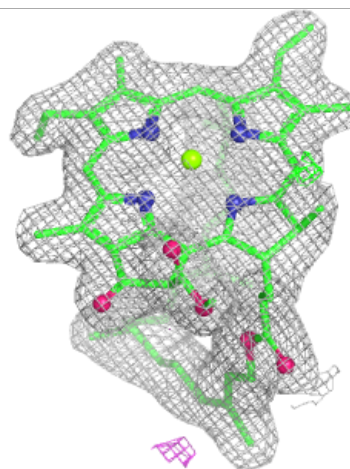
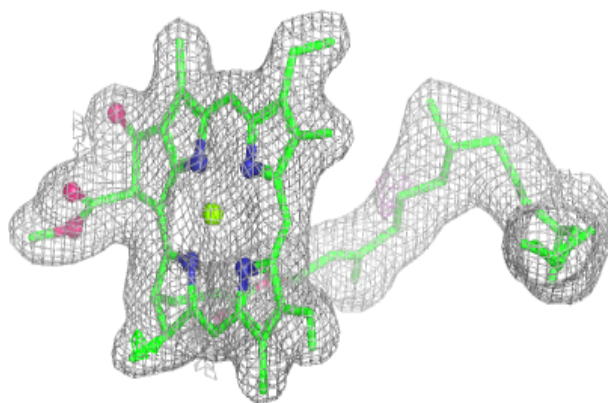
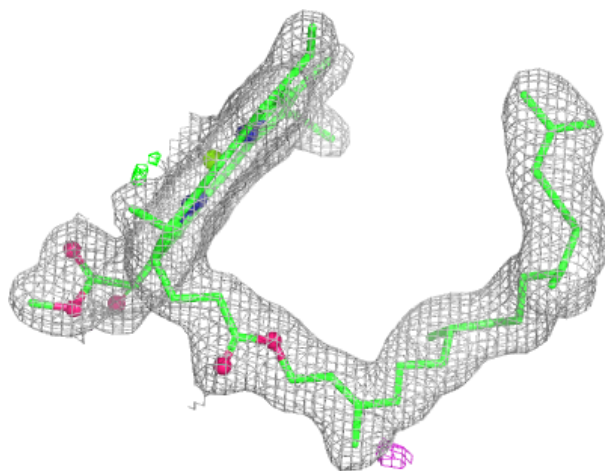
**Electron density around CLA B 607:**

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



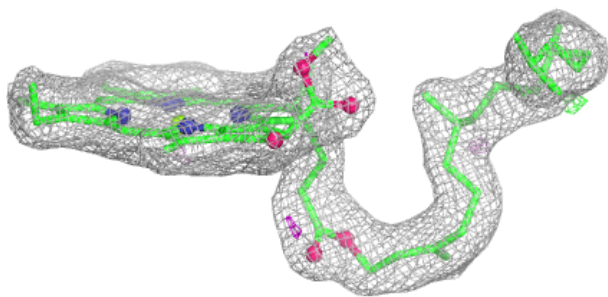
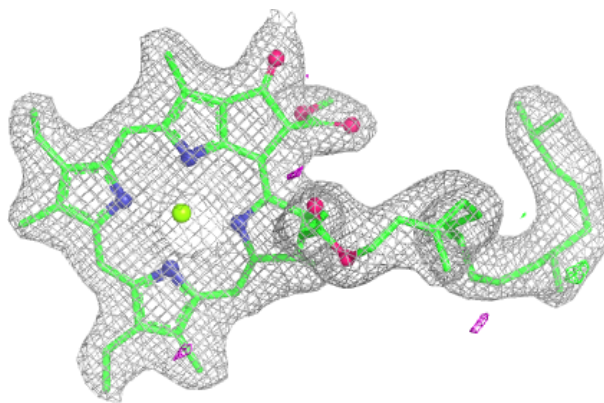
Electron density around CLA b 611:

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

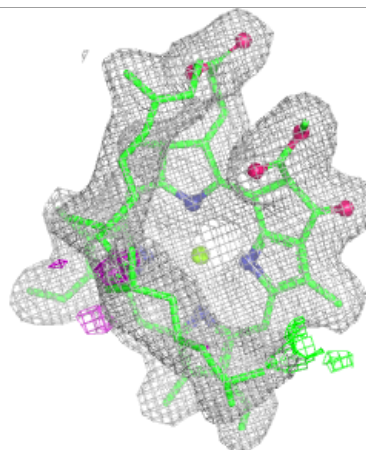
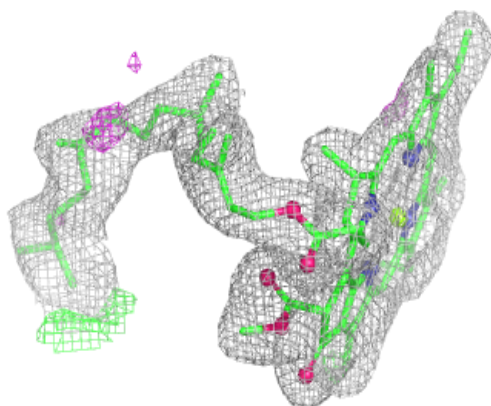
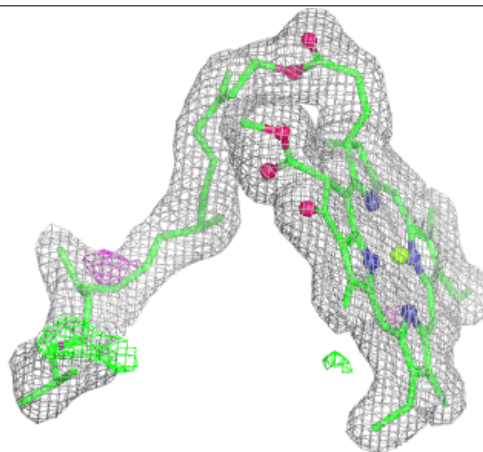


Electron density around CLA b 612:

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

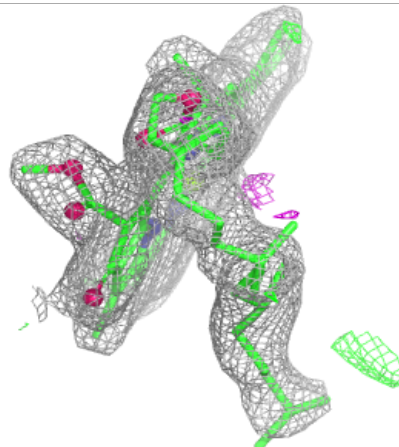
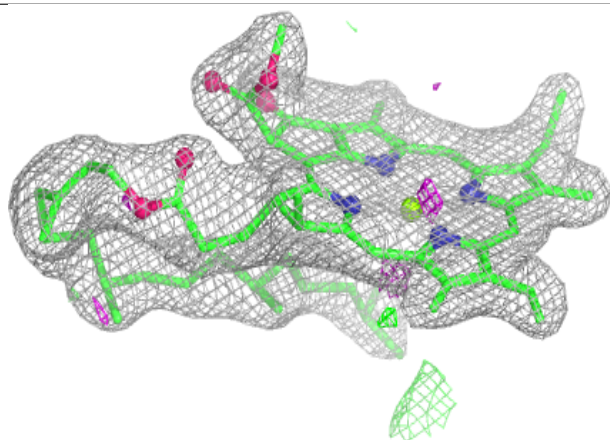
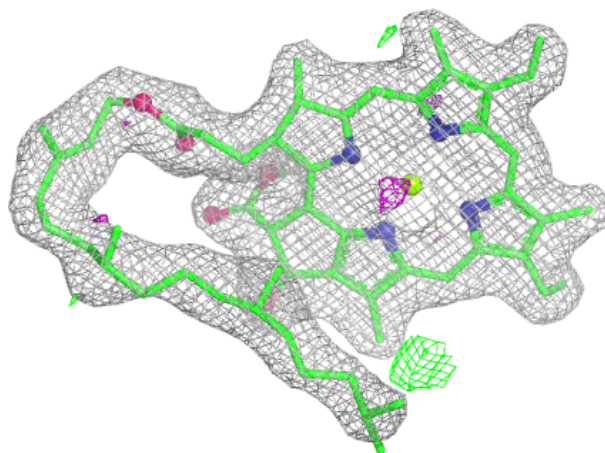
**Electron density around CLA b 613:**

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



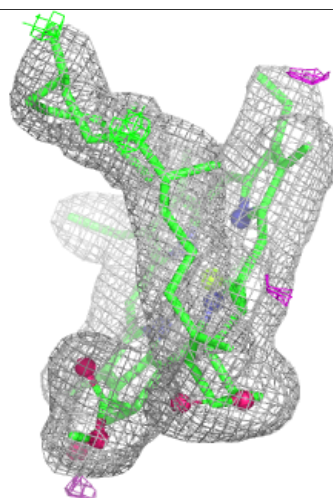
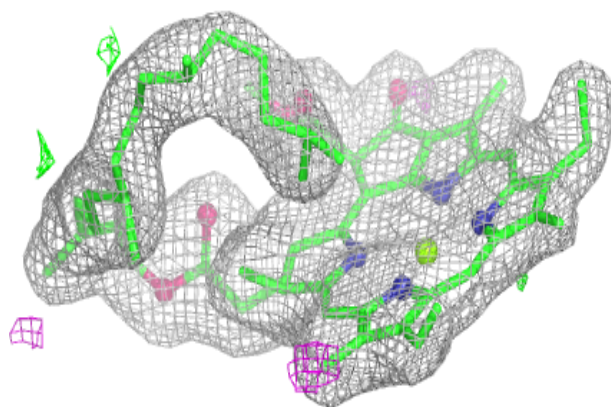
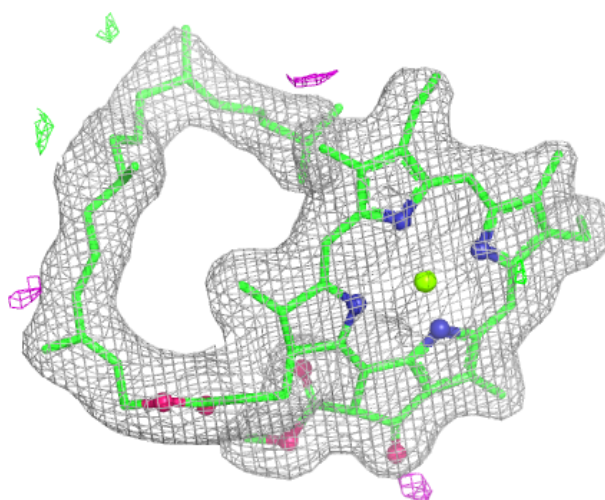
Electron density around CLA C 509:

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



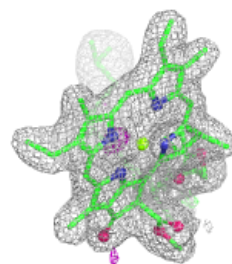
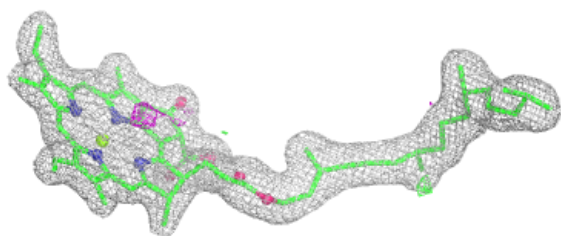
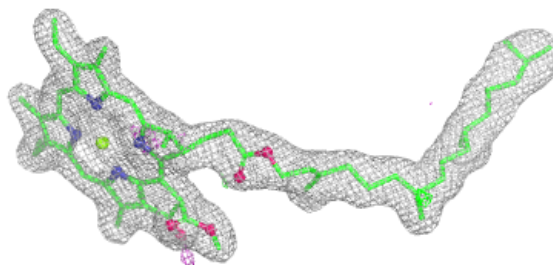
Electron density around CLA b 615:

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

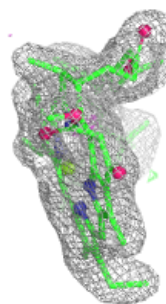
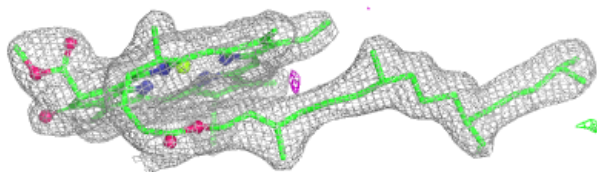
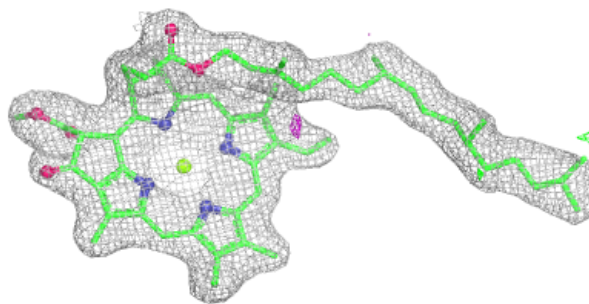


Electron density around CLA A 606:

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

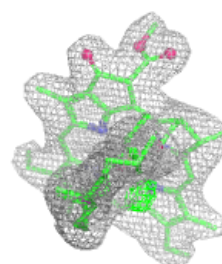
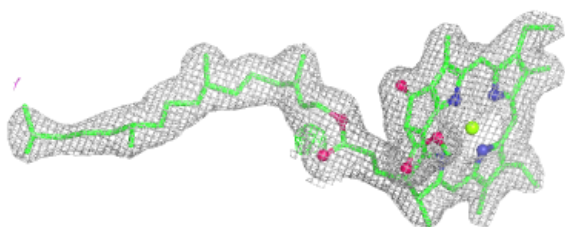
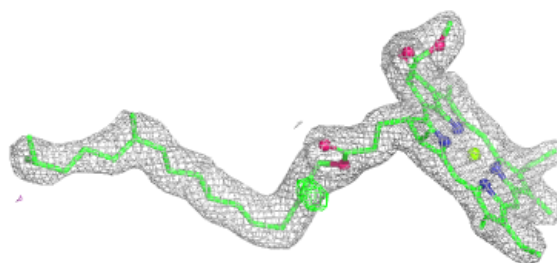
**Electron density around CLA c 501:**

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



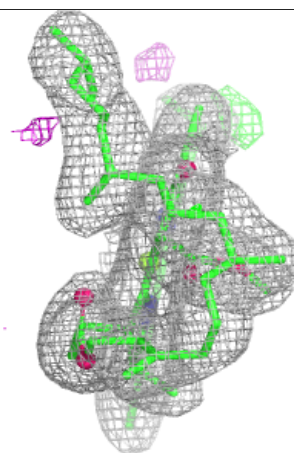
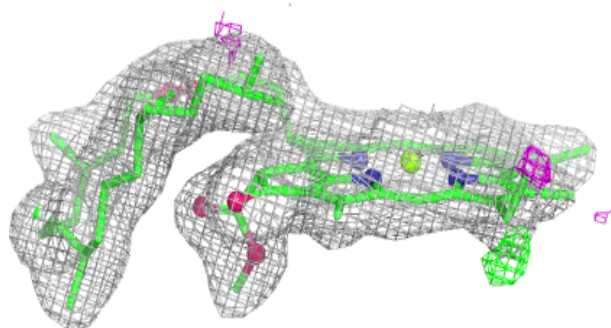
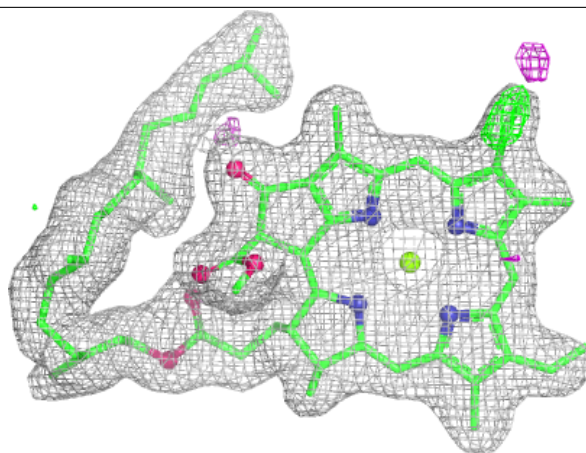
Electron density around CLA c 502:

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



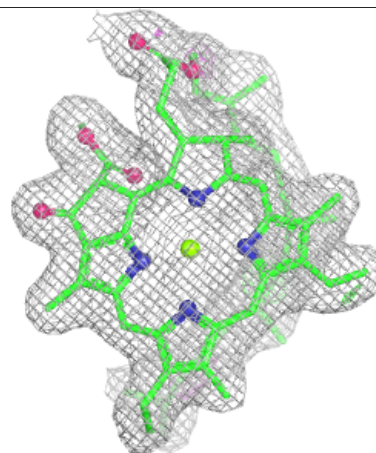
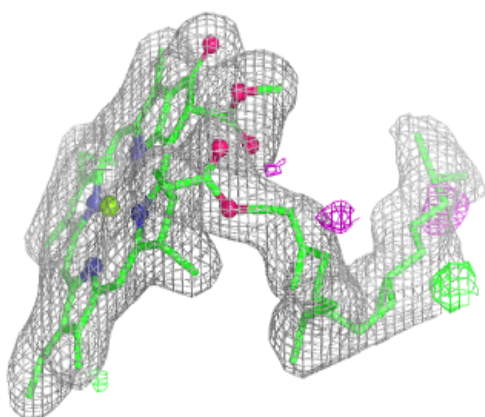
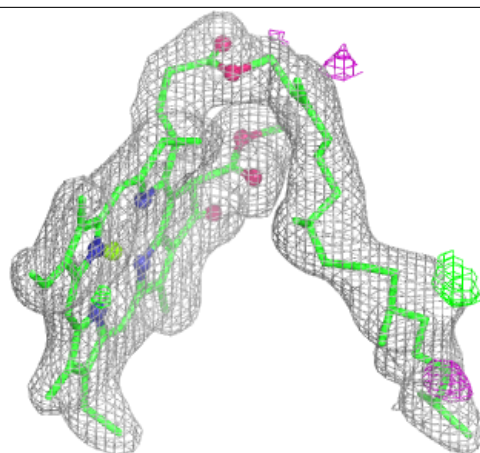
Electron density around CLA B 610:

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

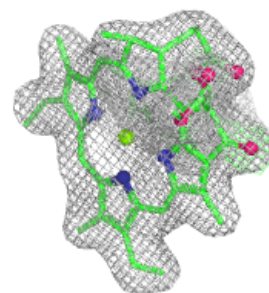
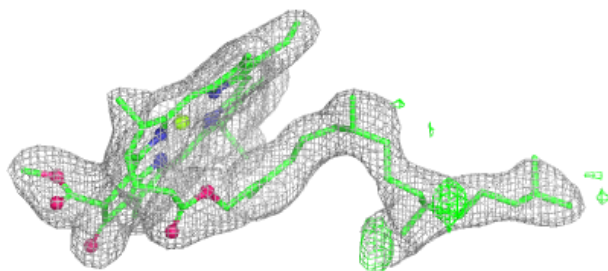
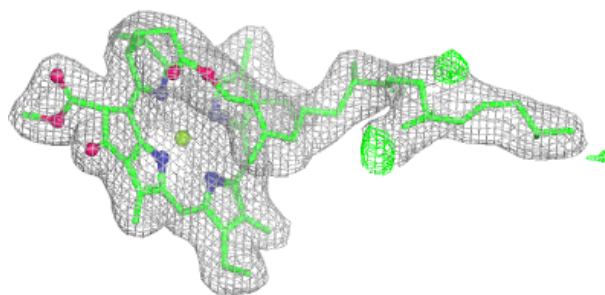


Electron density around CLA B 613:

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

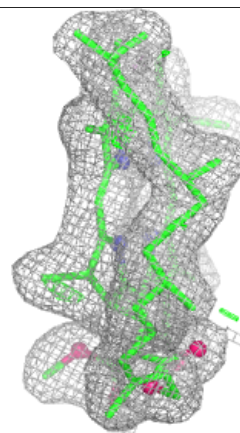
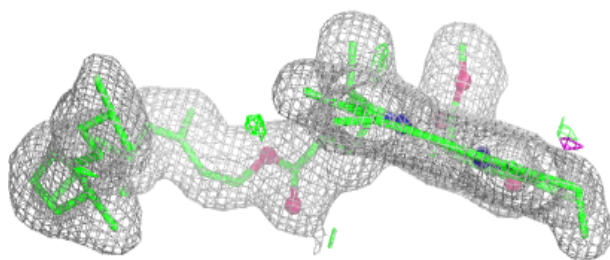
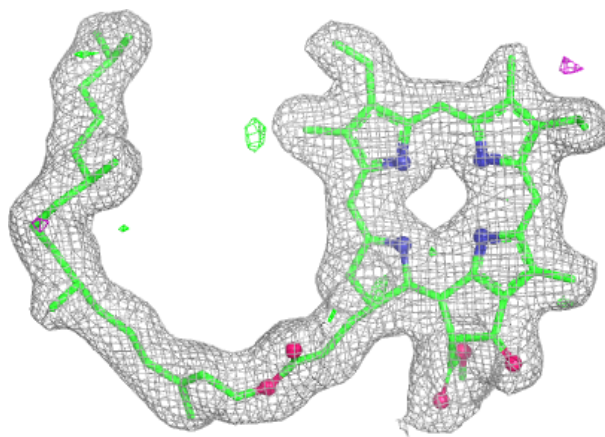
**Electron density around CLA c 505:**

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



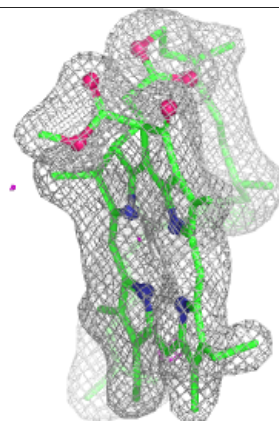
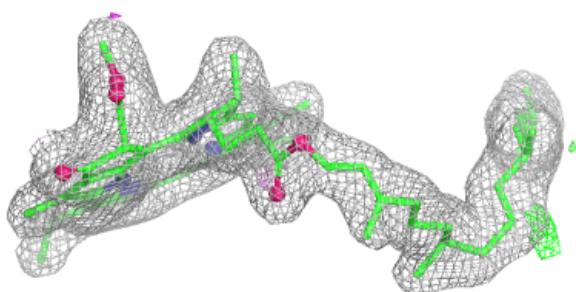
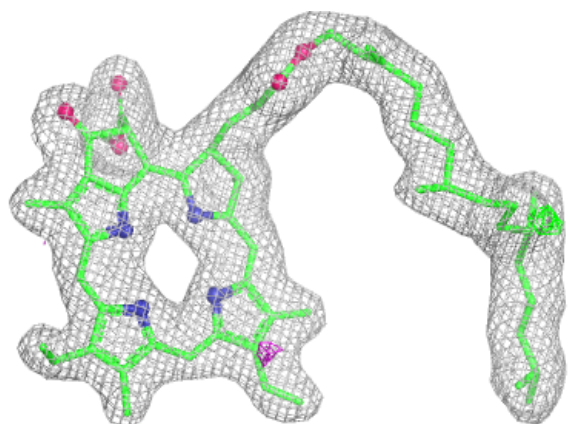
Electron density around PHO D 402:

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

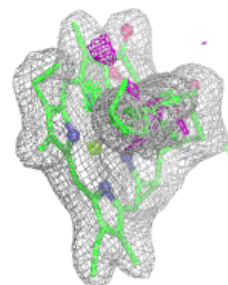
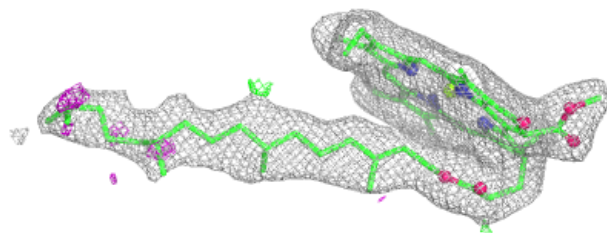
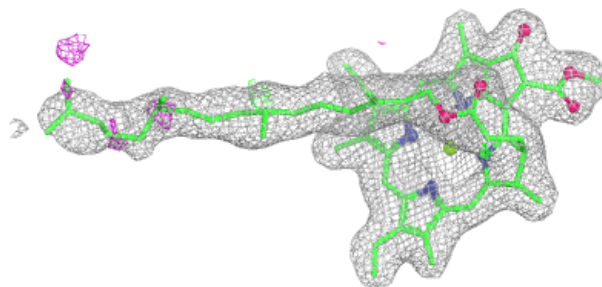


Electron density around PHO D 403:

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

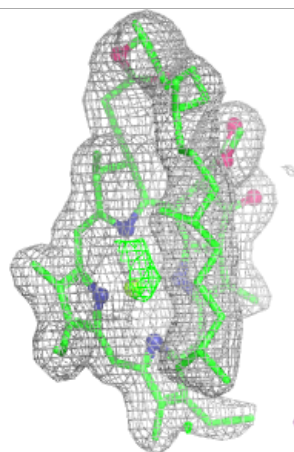
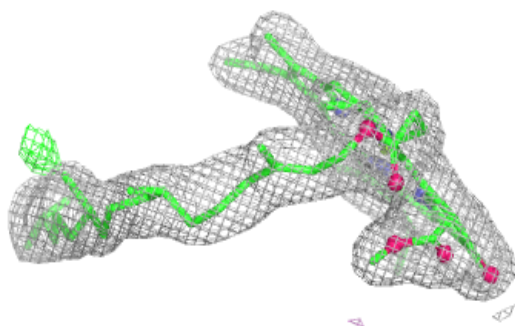
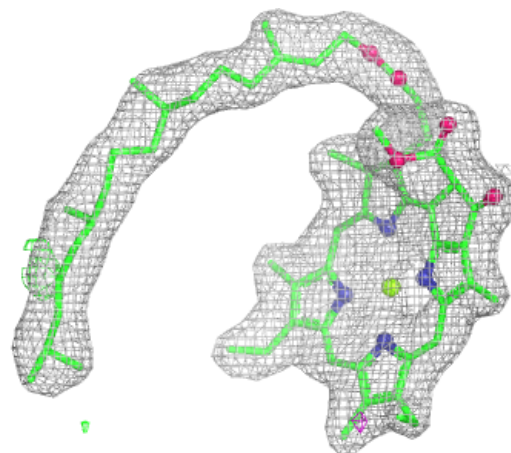
**Electron density around CLA B 614:**

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



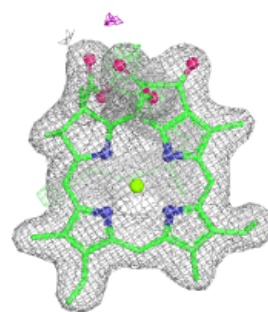
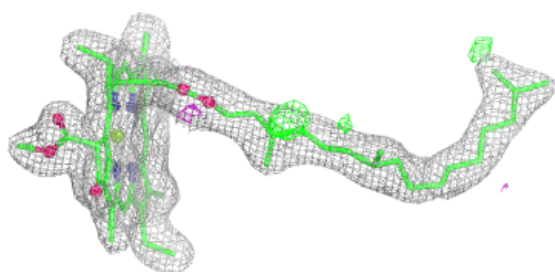
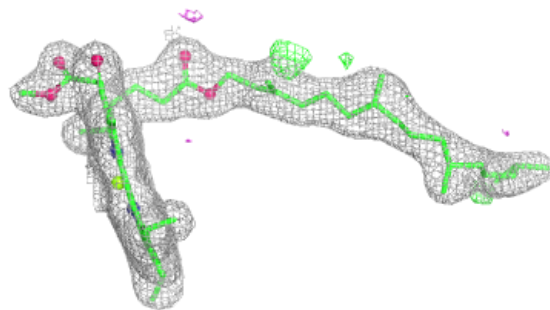
Electron density around CLA C 507:

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

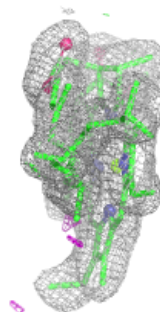
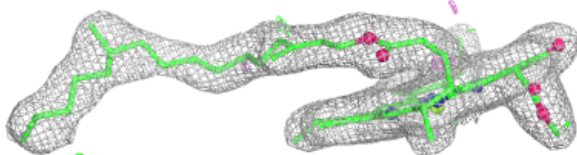
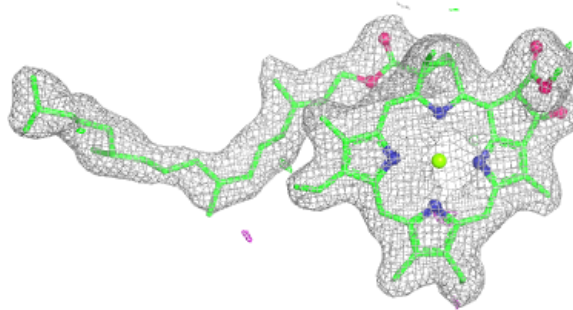


Electron density around CLA B 605:

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

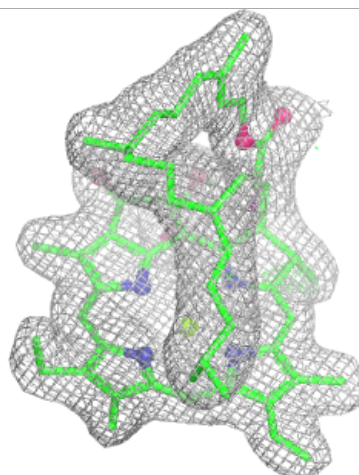
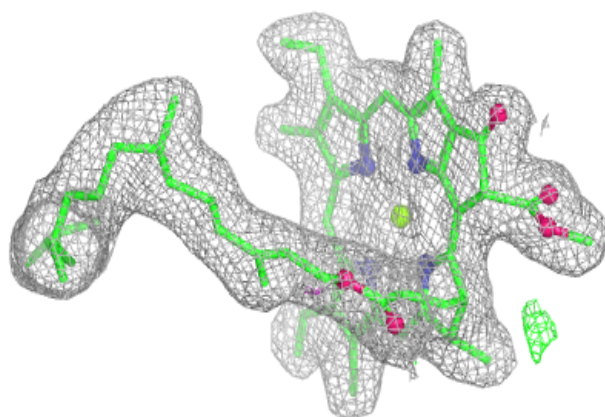
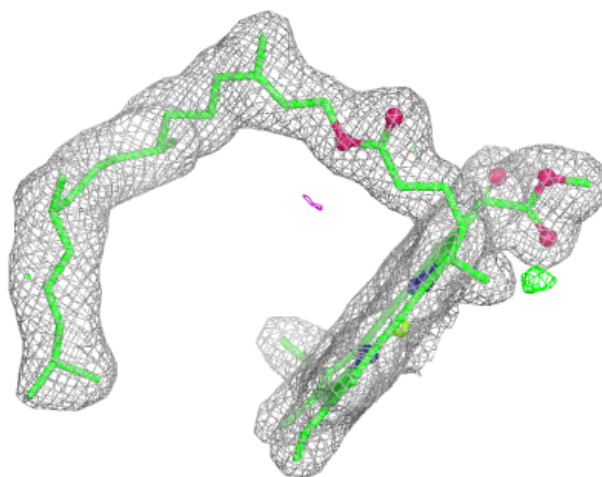
**Electron density around CLA B 603:**

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



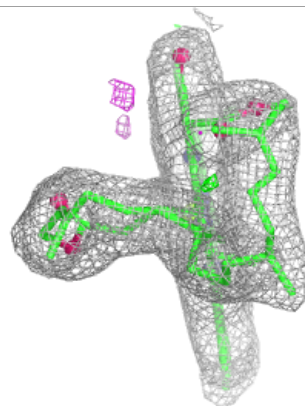
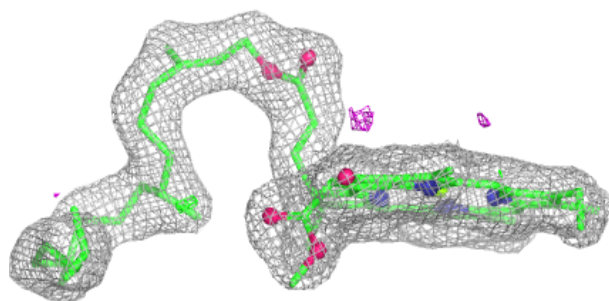
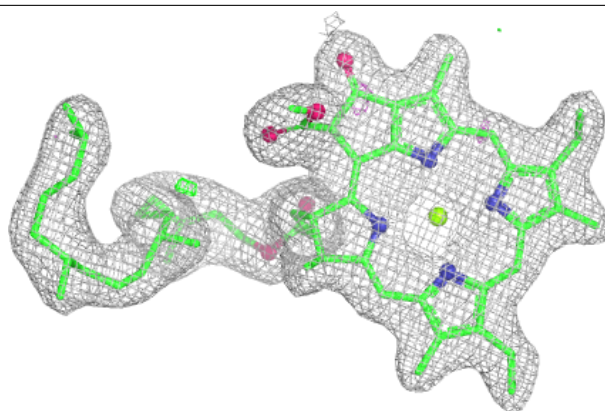
Electron density around CLA B 611:

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

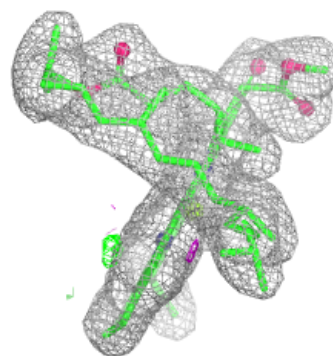
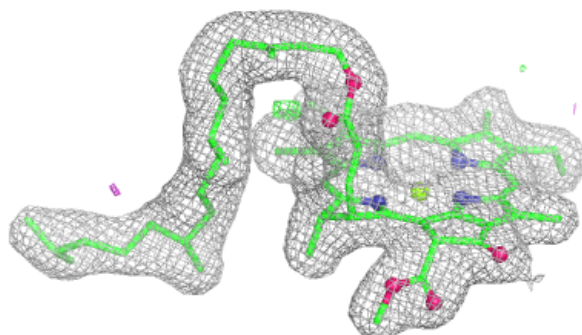
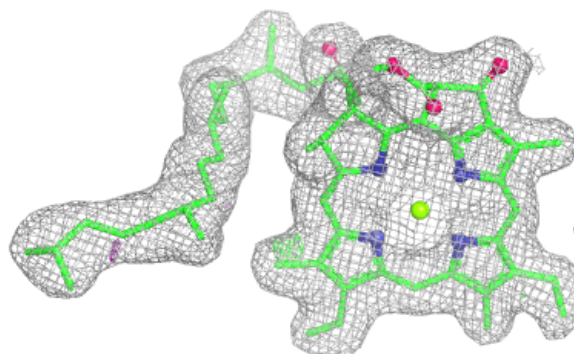


Electron density around CLA B 612:

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

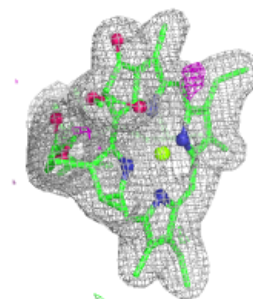
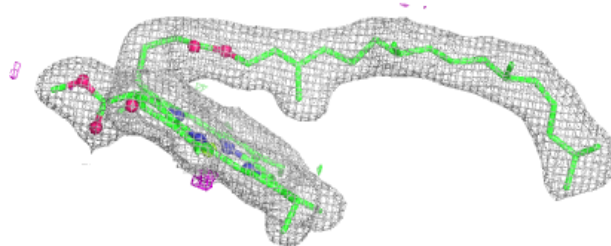
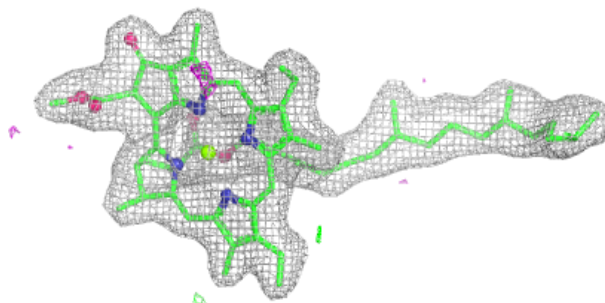
**Electron density around CLA A 611:**

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

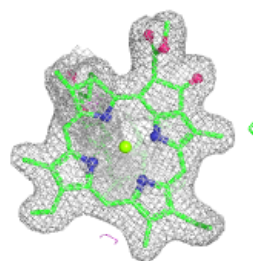
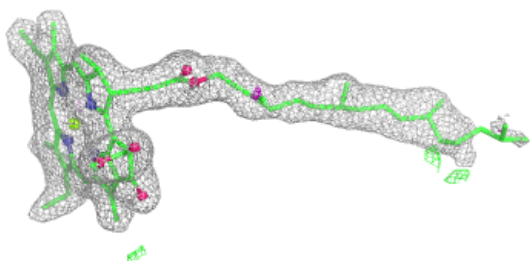
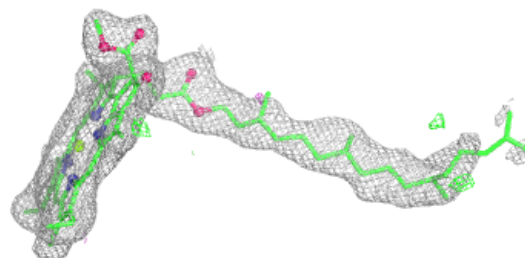


Electron density around CLA B 608:

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

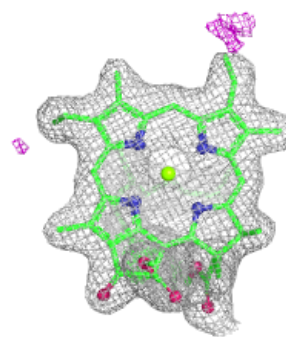
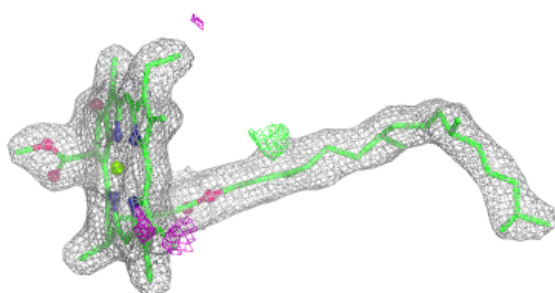
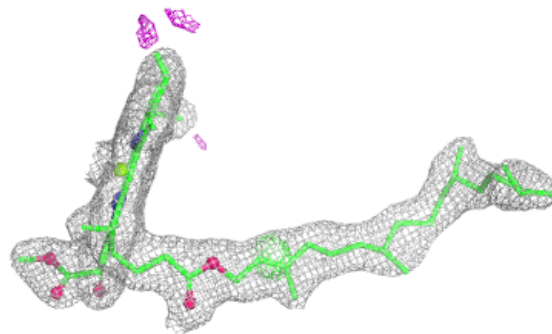
**Electron density around CLA b 604:**

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

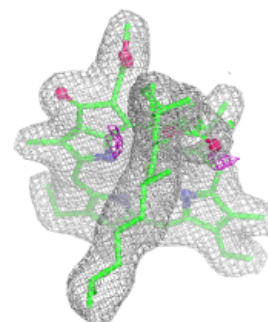
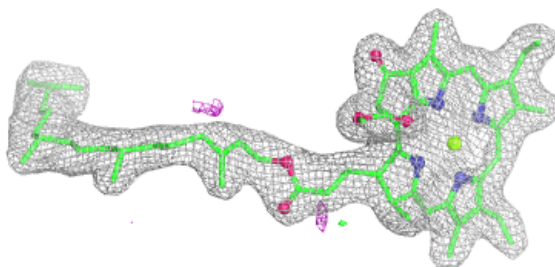
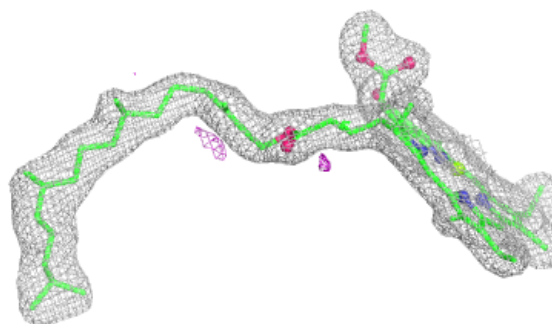


Electron density around CLA b 605:

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

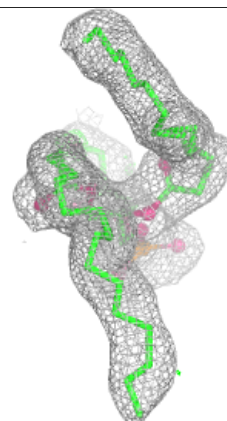
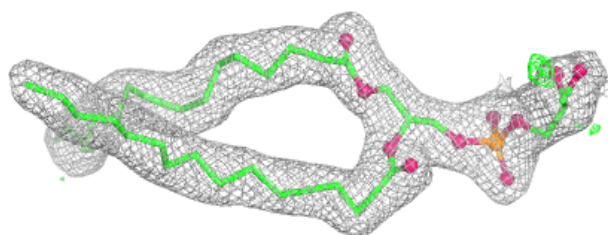
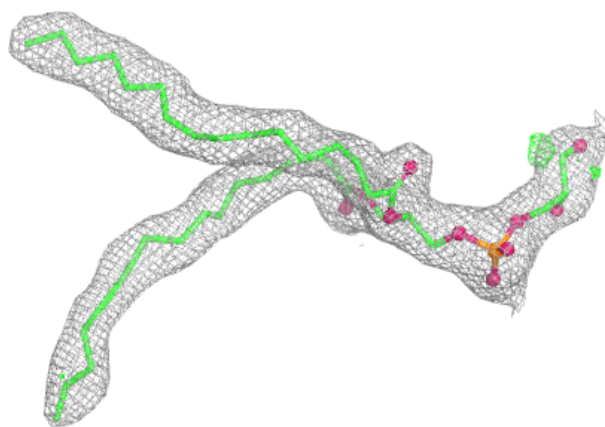
**Electron density around CLA D 404:**

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



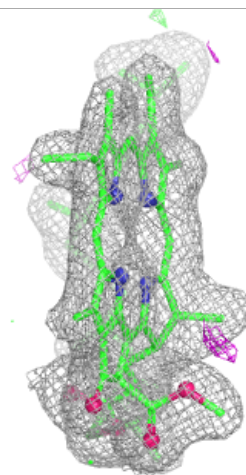
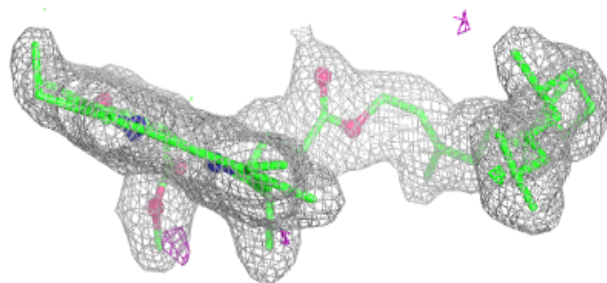
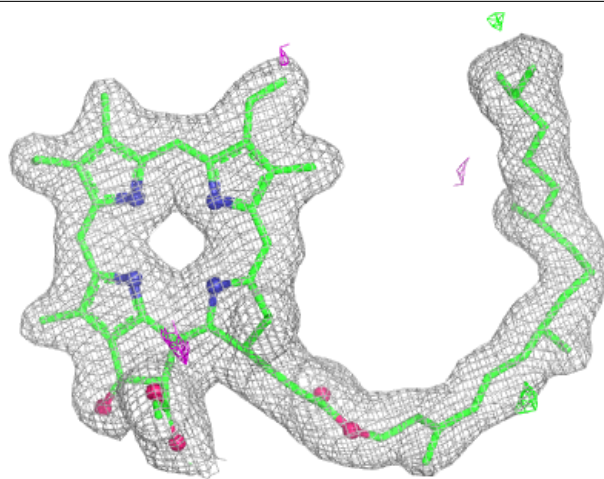
Electron density around LHG D 410:

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



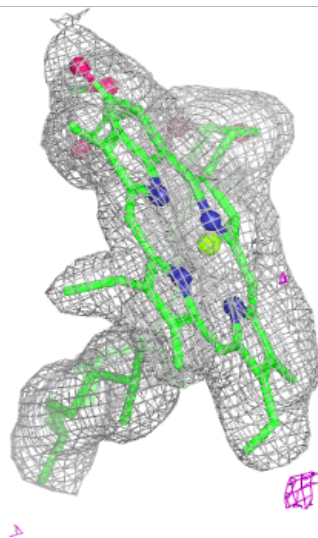
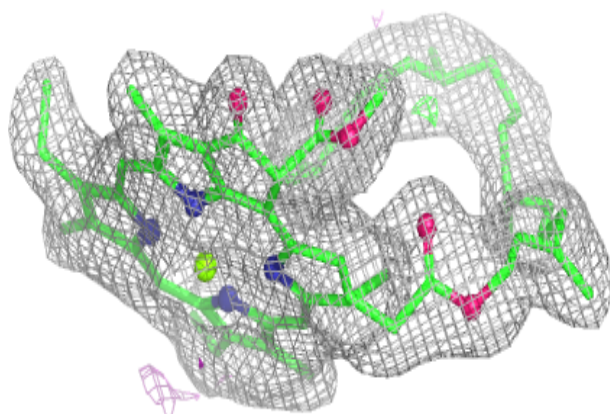
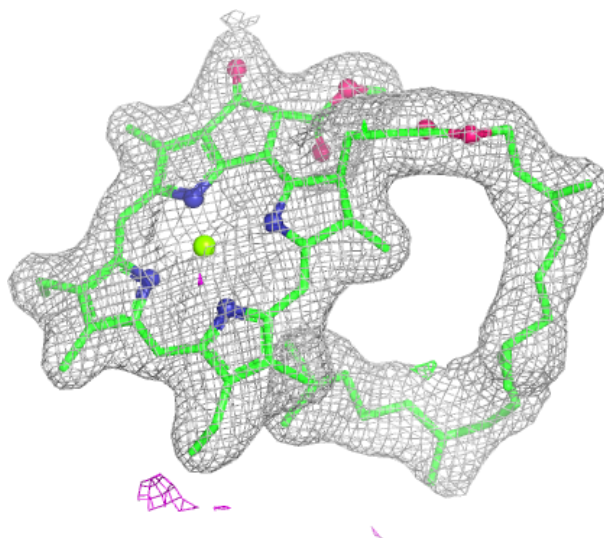
Electron density around PHO d 401:

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



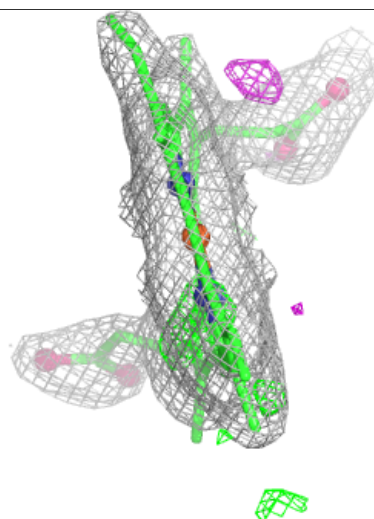
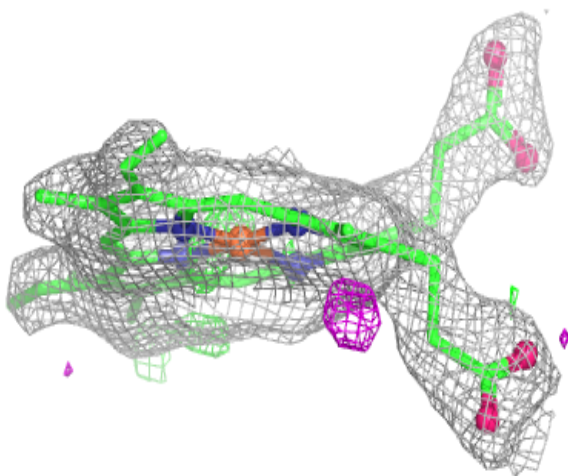
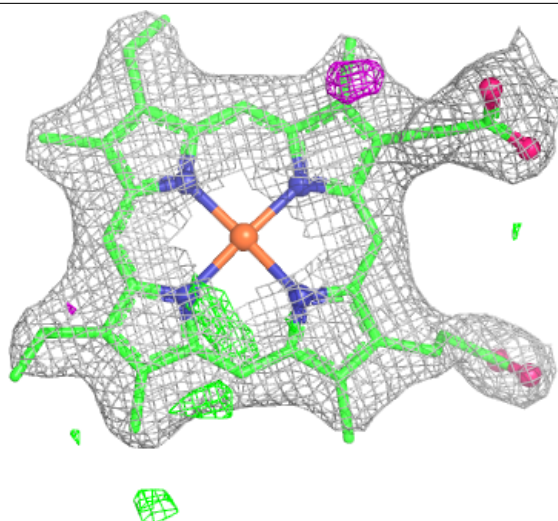
Electron density around CLA B 615:

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



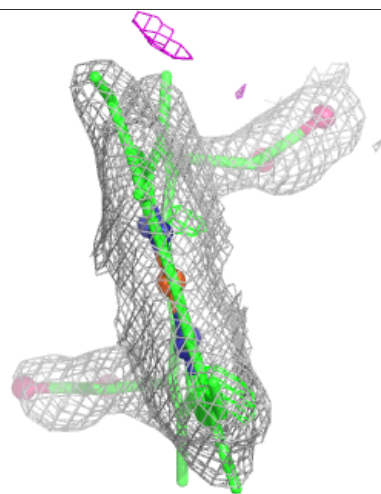
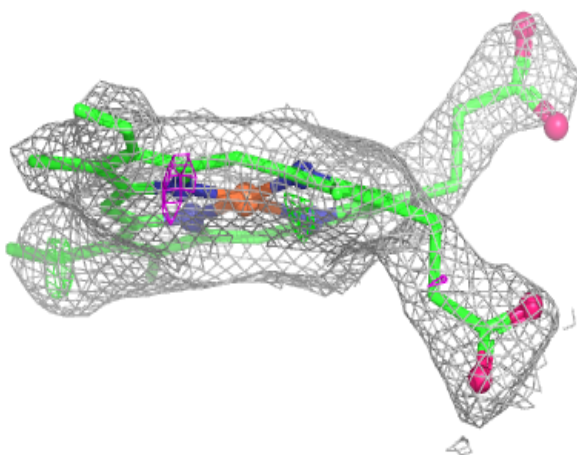
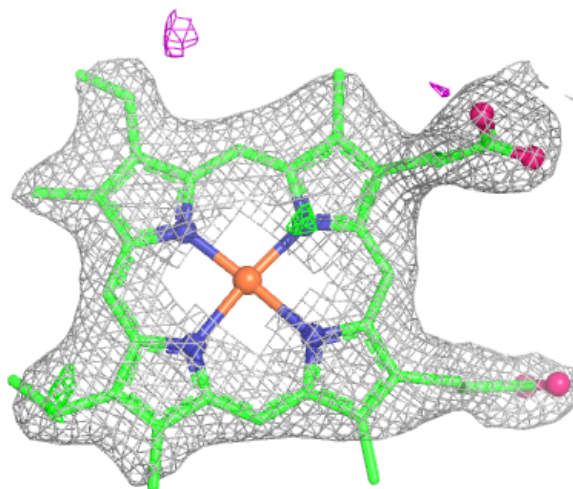
Electron density around HEM F 101:

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



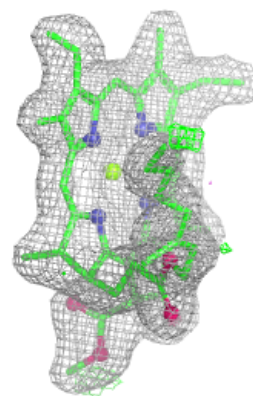
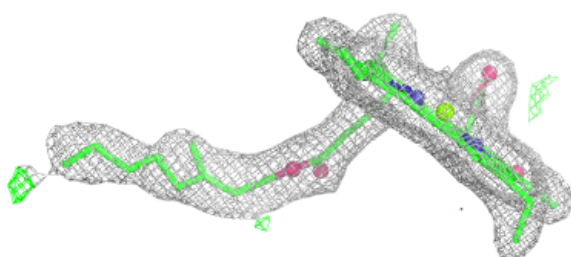
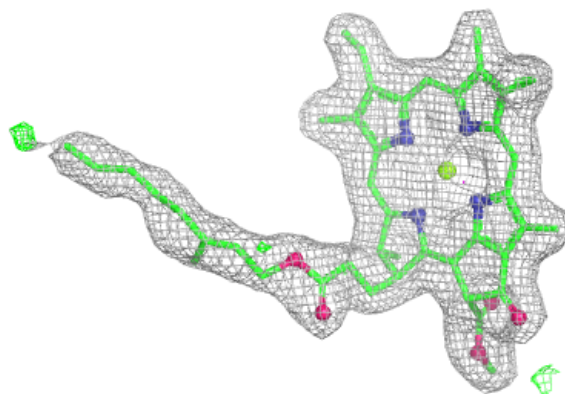
Electron density around HEM f 101:

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



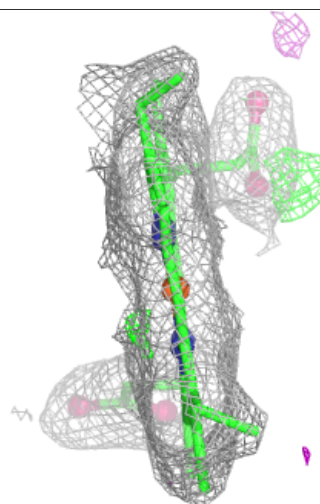
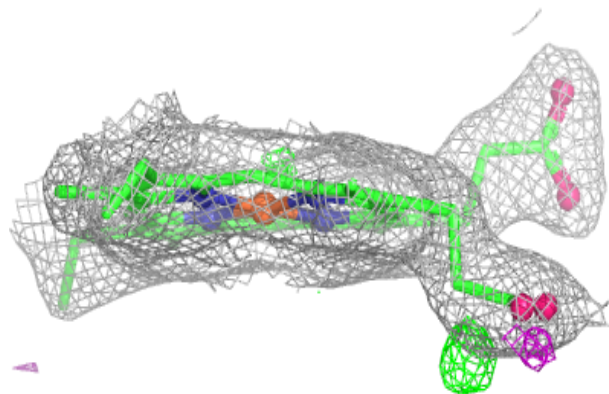
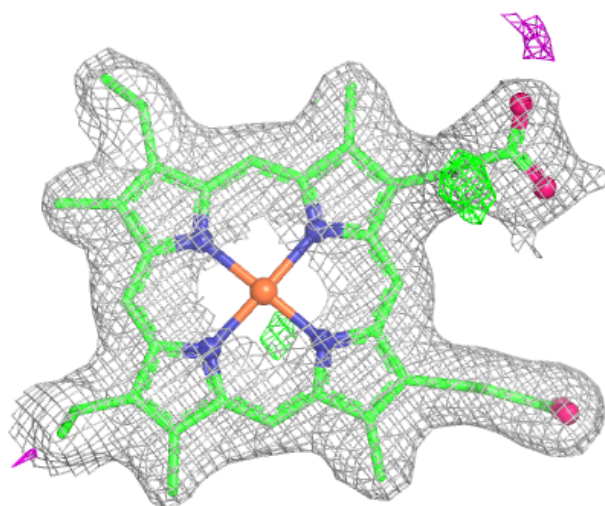
Electron density around CLA A 608:

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



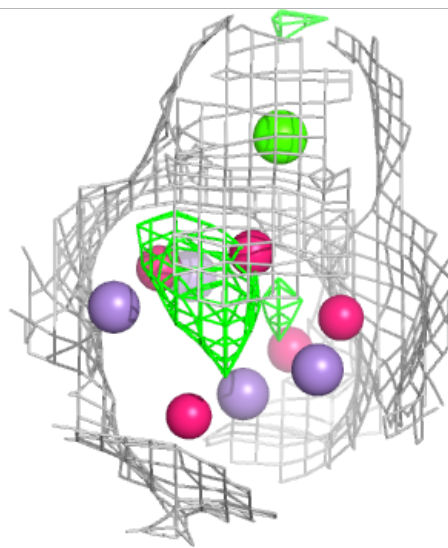
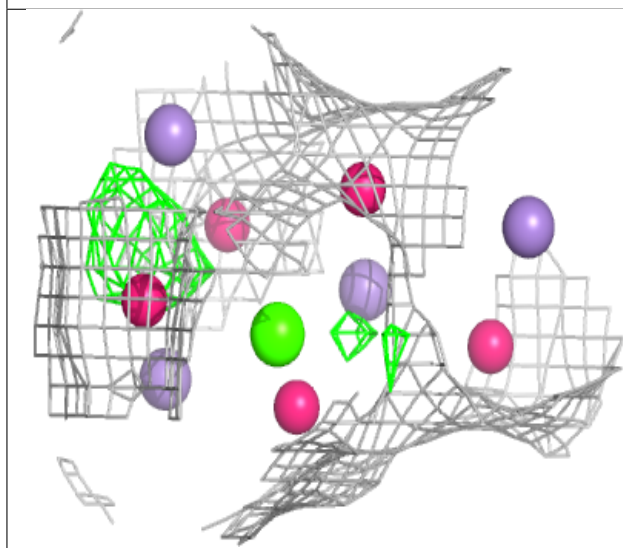
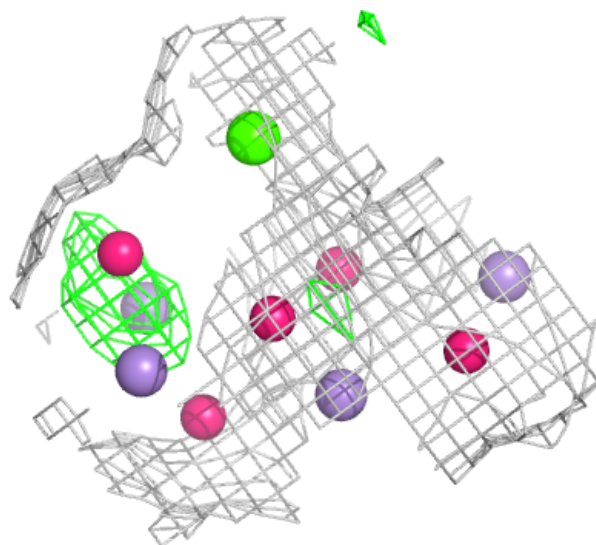
Electron density around HEC V 201:

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



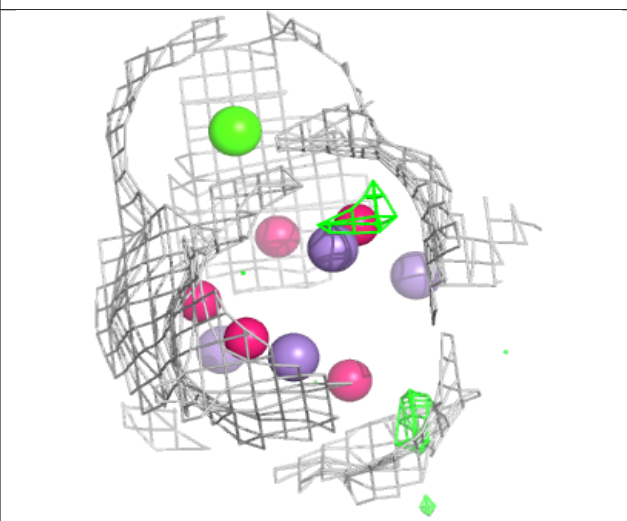
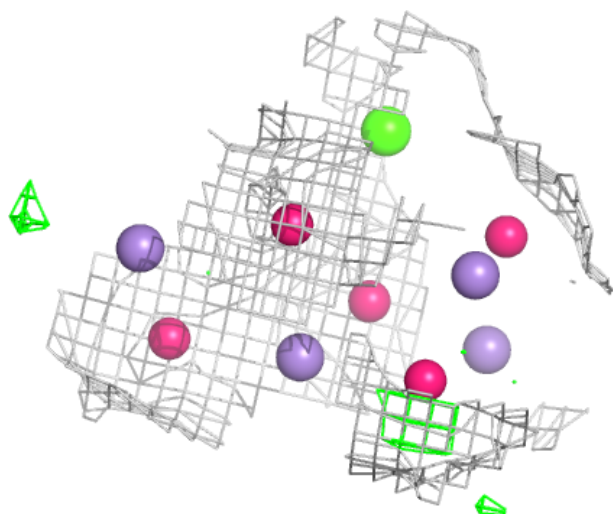
Electron density around OEX A 602 (A):

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



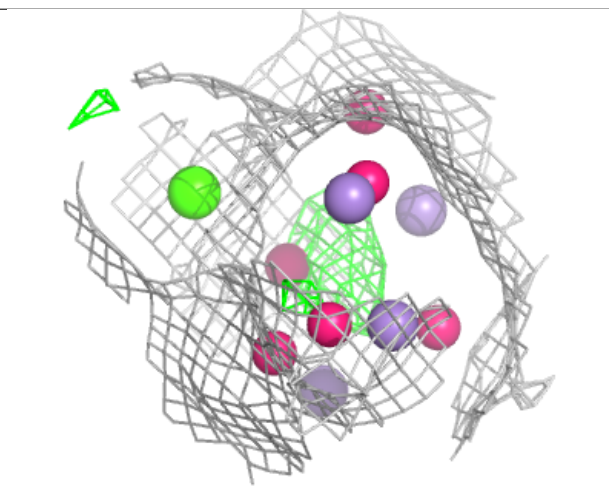
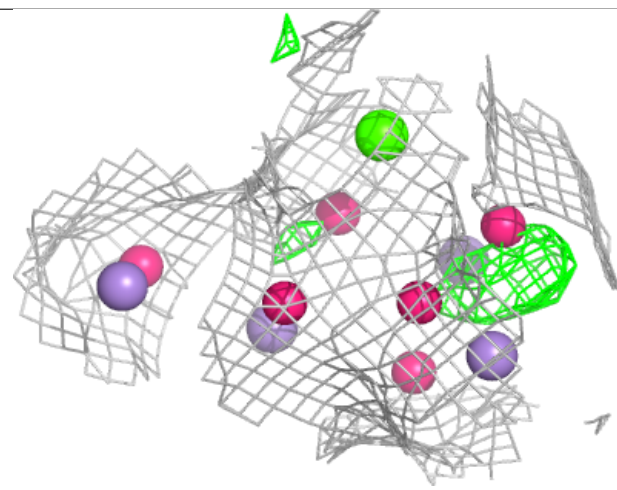
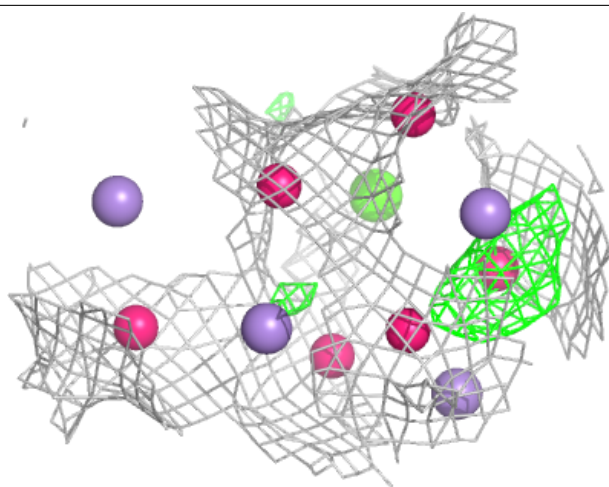
Electron density around OEX a 602 (A):

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



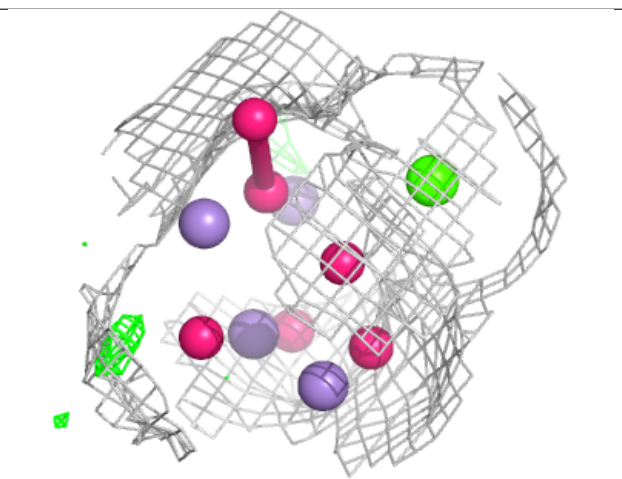
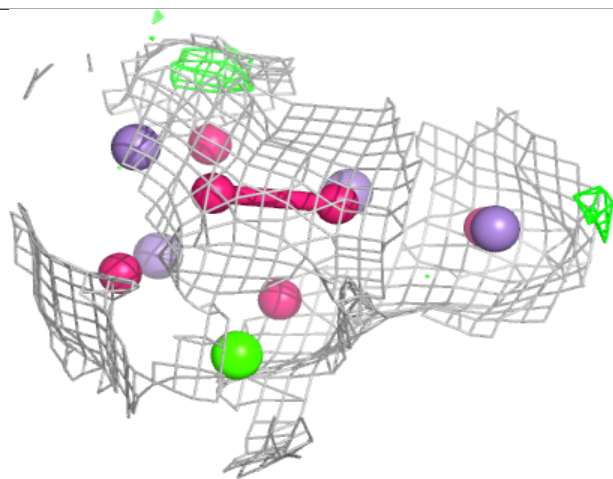
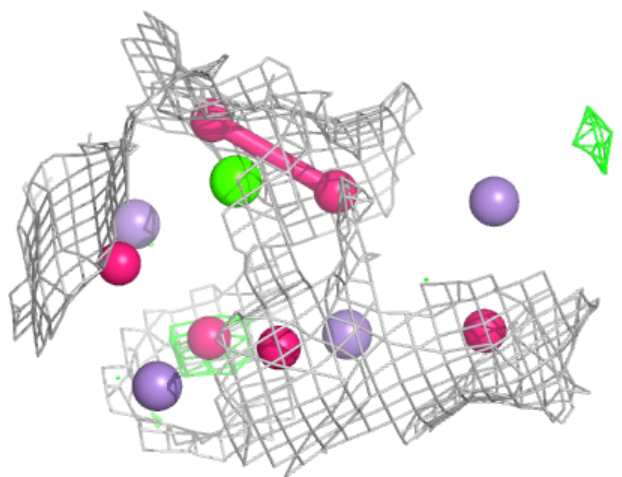
Electron density around OEY A 601 (B):

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



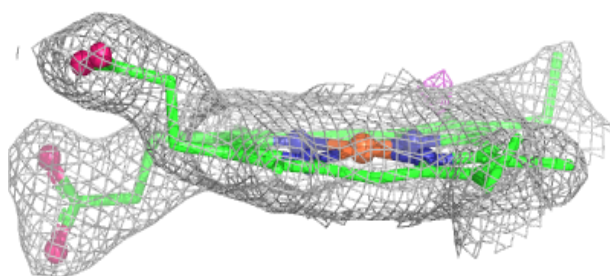
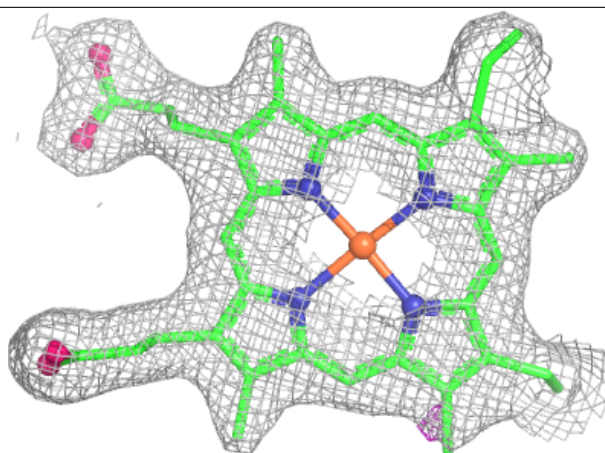
Electron density around OEY a 601 (B):

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.