



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 04:18 AM UTC

PDB ID : 8F4D / pdb_00008f4d
Title : RT XFEL structure of Photosystem II 50 microseconds after the third illumination at 2.15 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 : 2.15 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

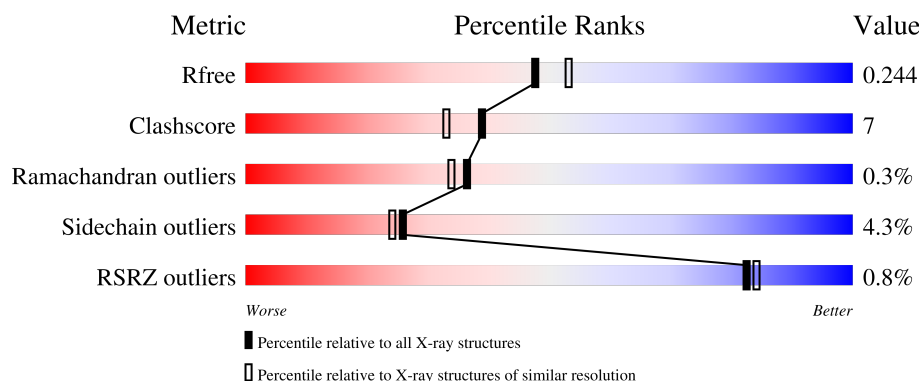
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

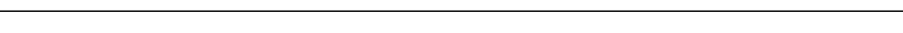
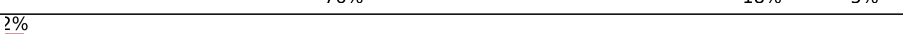
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 52853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	64	0
			3113	2030	513	551	19			
1	a	334	Total	C	N	O	S	0	64	0
			3110	2027	513	551	19			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

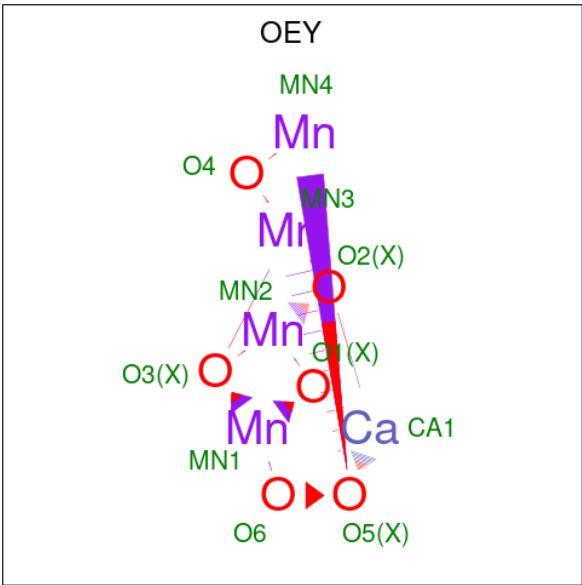
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

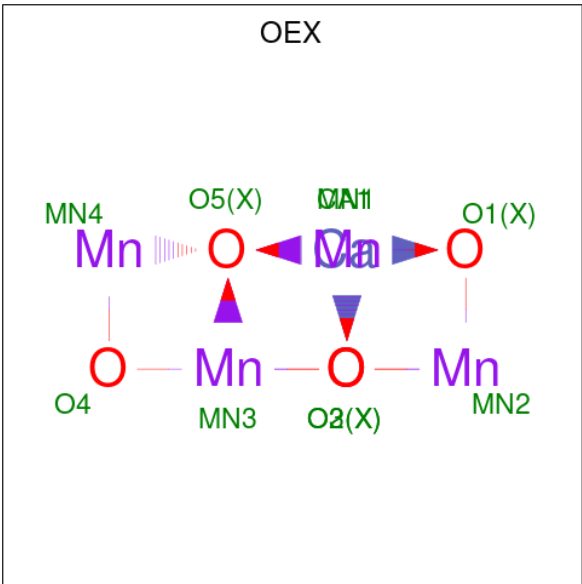
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

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



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

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



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

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

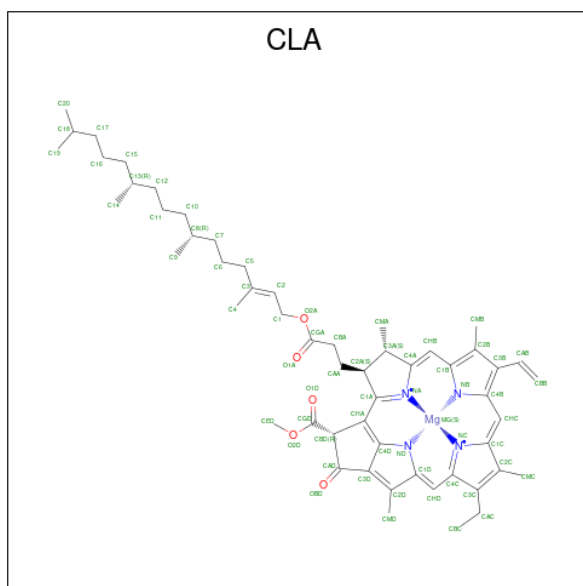
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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

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

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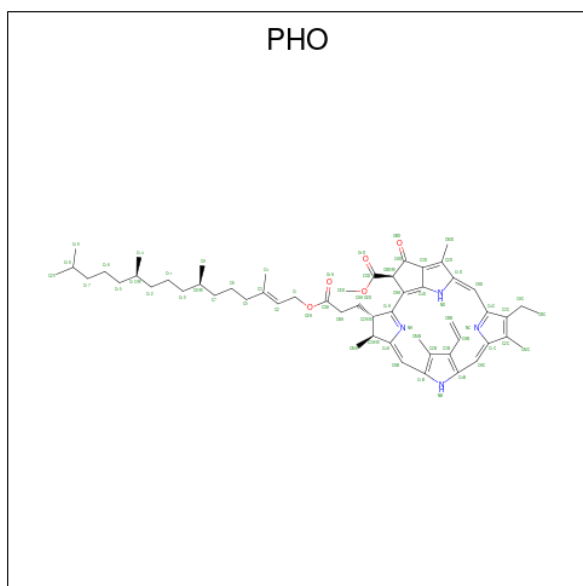
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total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

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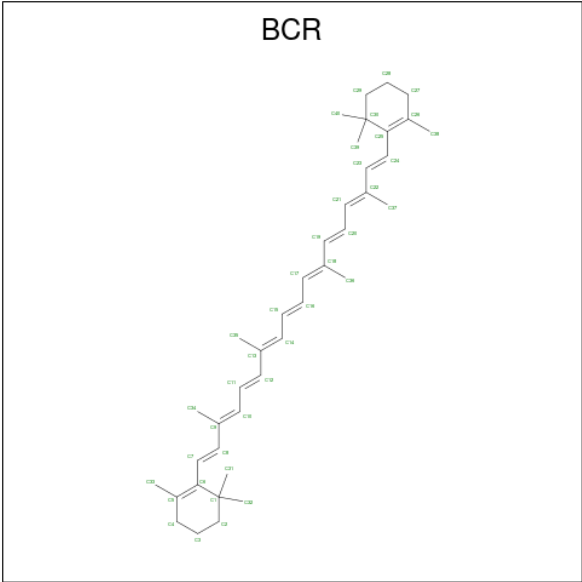
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



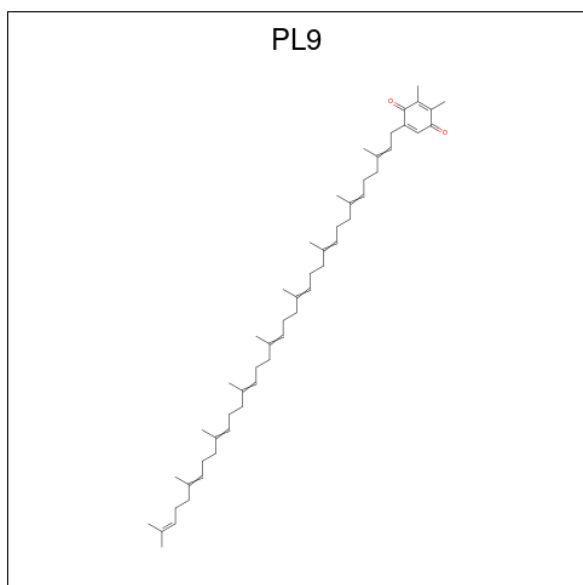
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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

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



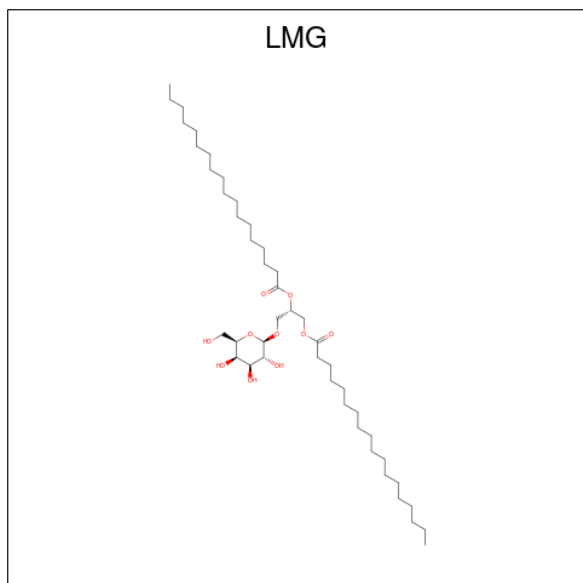
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



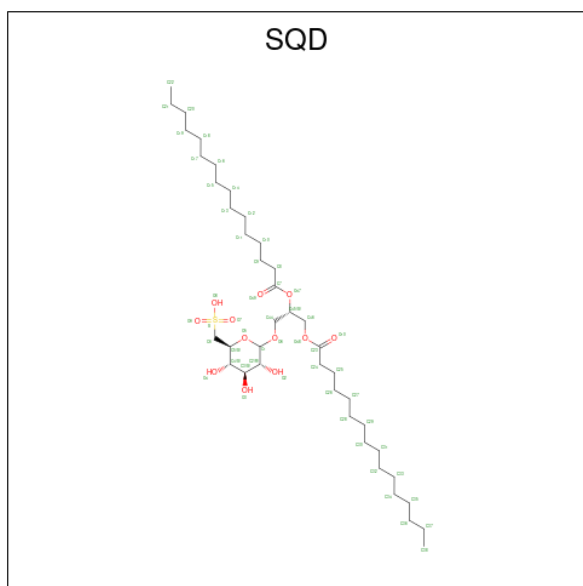
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C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

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

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



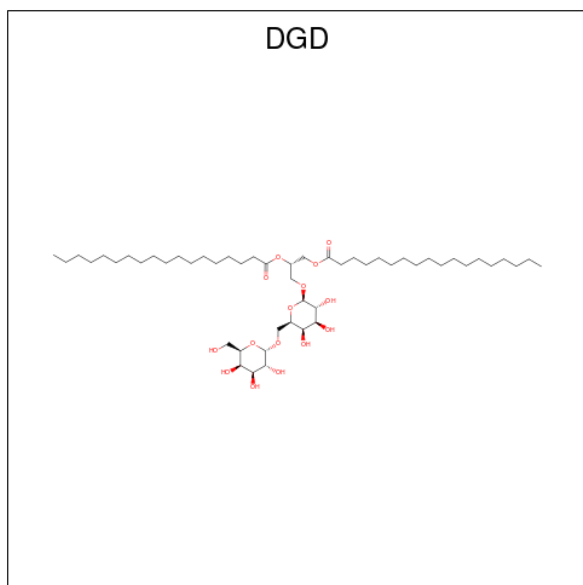
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	L	1	Total	C	O	S	0	0
			49	36	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	f	1	Total	C	O	S	0	0
		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

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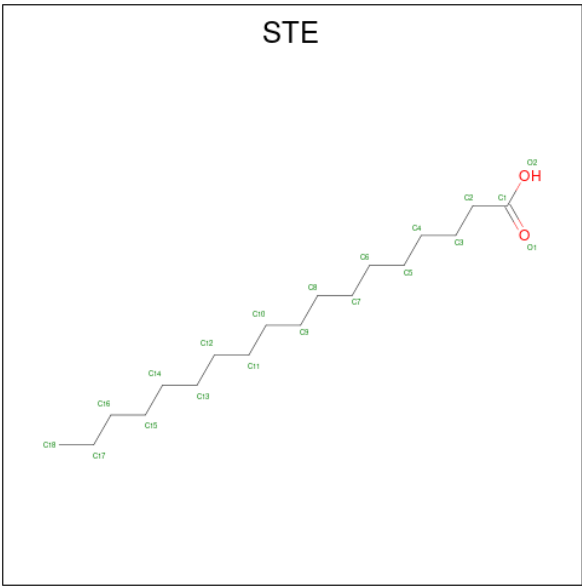
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	t	1	Total	C	O	0	0
			36	31	5		

- 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	a	1	Total	C	O	0	0
			44	39	5		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



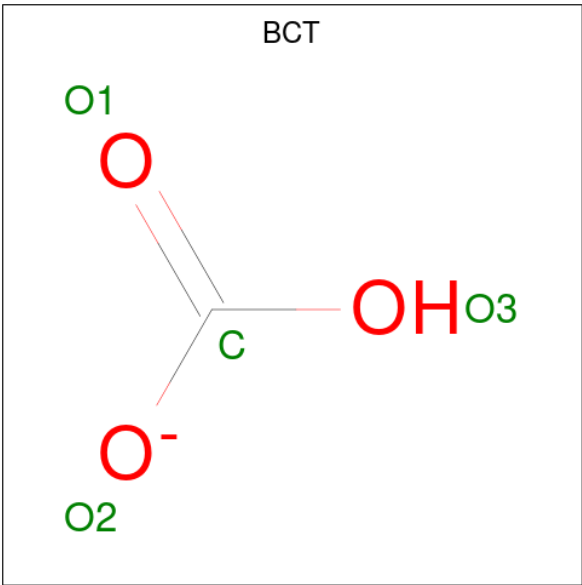
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			17	15	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C		0	0
			16	16			
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C		0	0
			16	16			
32	H	1	Total	C		0	0
			18	18			
32	I	1	Total	C		0	0
			15	15			
32	J	1	Total	C	O	0	0
			12	10	2		
32	L	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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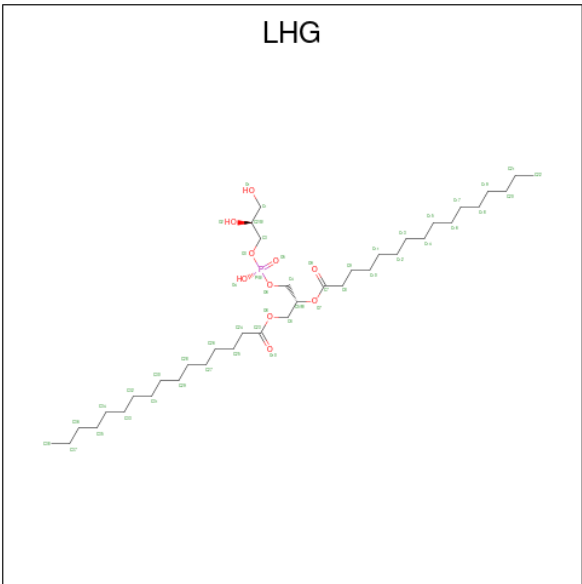
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 20 18 2	0	0
32	R	1	Total C O 12 10 2	0	0
32	a	1	Total C 10 10	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C 16 16	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 15 15	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total 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	t	1	Total C O 14 12 2	0	0
32	t	1	Total C O 18 16 2	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	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



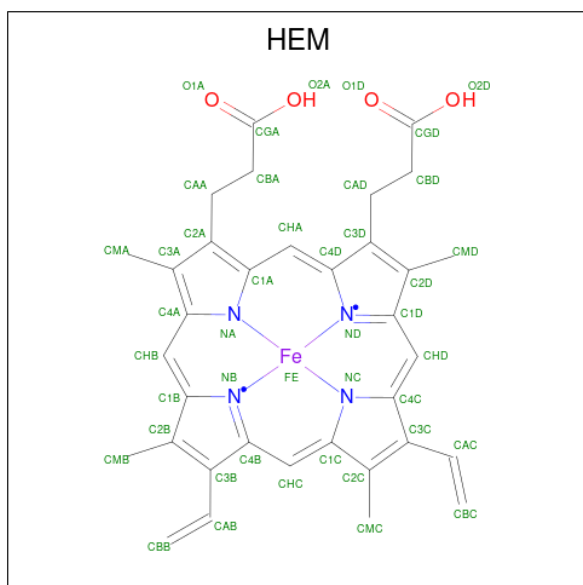
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	O	P	0	0
			49	38	10	1		

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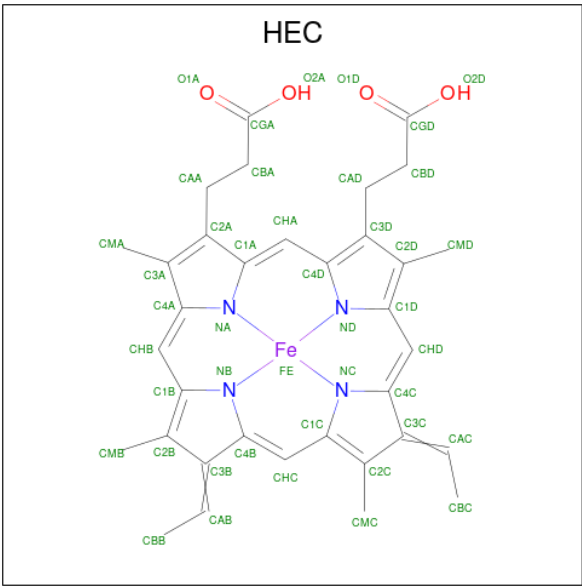
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	O	P	0	0
			47	36	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	E	1	Total	C	O	P	0	0
			49	38	10	1		
34	L	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0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

- 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	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	120	Total	O	0	4
			124	124		
37	B	165	Total	O	0	0
			165	165		
37	C	112	Total	O	0	0
			112	112		
37	D	94	Total	O	0	0
			94	94		
37	E	22	Total	O	0	0
			22	22		
37	F	5	Total	O	0	0
			5	5		
37	H	24	Total	O	0	0
			24	24		
37	I	18	Total	O	0	0
			18	18		
37	J	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	K	2	Total 2	O 2	0	0
37	L	8	Total 8	O 8	0	0
37	M	7	Total 7	O 7	0	0
37	O	66	Total 66	O 66	0	0
37	T	6	Total 6	O 6	0	0
37	U	30	Total 30	O 30	0	0
37	V	45	Total 45	O 45	0	0
37	Y	6	Total 6	O 6	0	0
37	X	10	Total 10	O 10	0	0
37	Z	5	Total 5	O 5	0	0
37	R	9	Total 9	O 9	0	0
37	a	103	Total 107	O 107	0	4
37	b	132	Total 132	O 132	0	0
37	c	128	Total 128	O 128	0	0
37	d	77	Total 77	O 77	0	0
37	e	14	Total 14	O 14	0	0
37	f	2	Total 2	O 2	0	0
37	h	20	Total 20	O 20	0	0
37	i	10	Total 10	O 10	0	0
37	j	7	Total 7	O 7	0	0
37	k	5	Total 5	O 5	0	0

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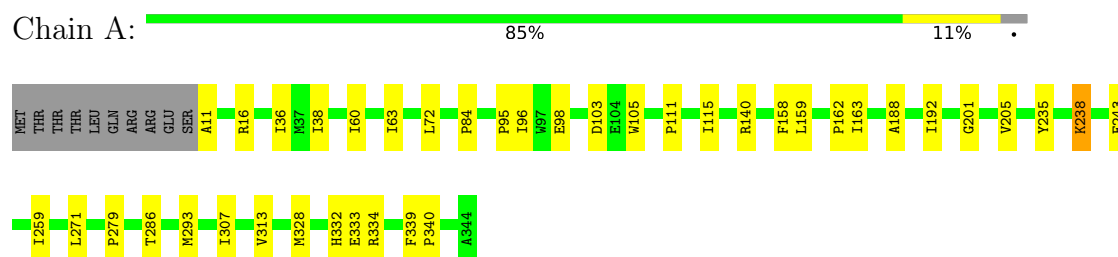
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	l	7	Total 7	O 7	0	0
37	m	3	Total 3	O 3	0	0
37	o	76	Total 76	O 76	0	0
37	t	7	Total 7	O 7	0	0
37	u	34	Total 34	O 34	0	0
37	v	39	Total 39	O 39	0	0
37	y	2	Total 2	O 2	0	0
37	x	4	Total 4	O 4	0	0
37	z	1	Total 1	O 1	0	0
37	r	5	Total 5	O 5	0	0

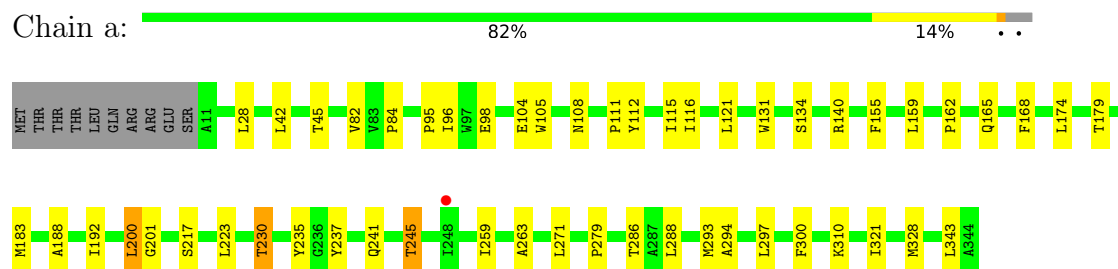
3 Residue-property plots

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

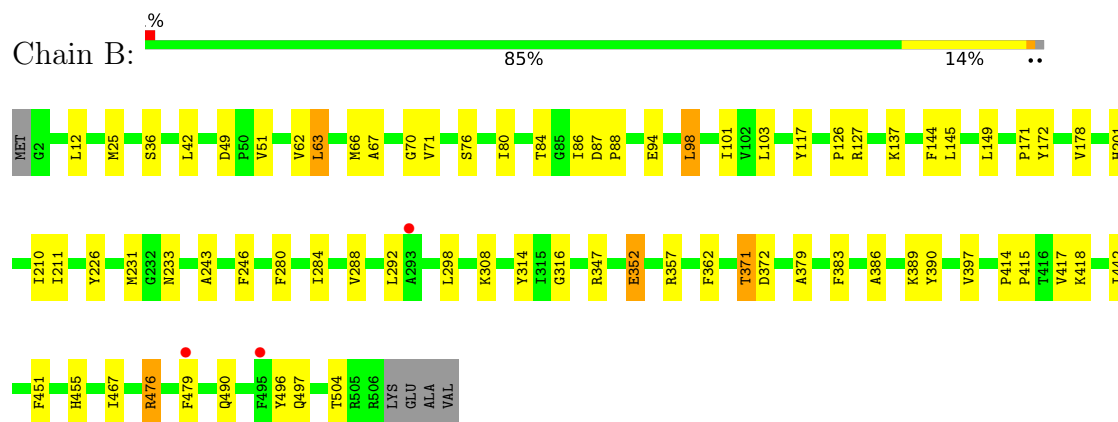
- Molecule 1: Photosystem II protein D1 1



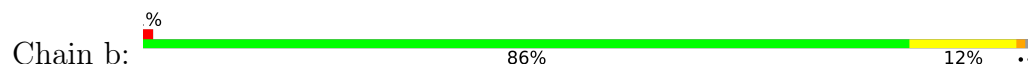
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



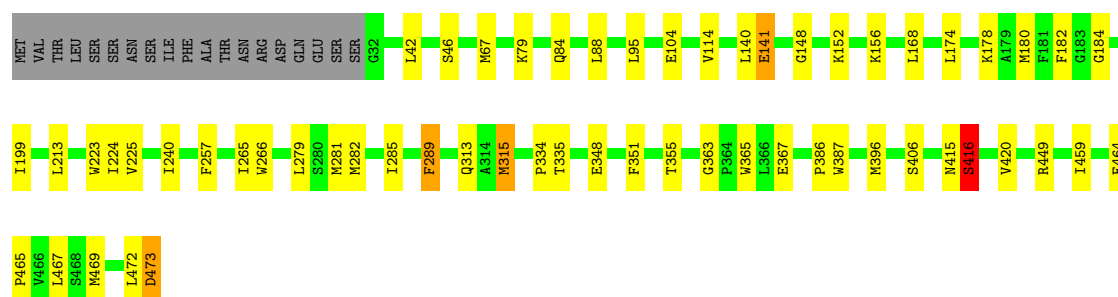
- Molecule 2: Photosystem II CP47 reaction center protein





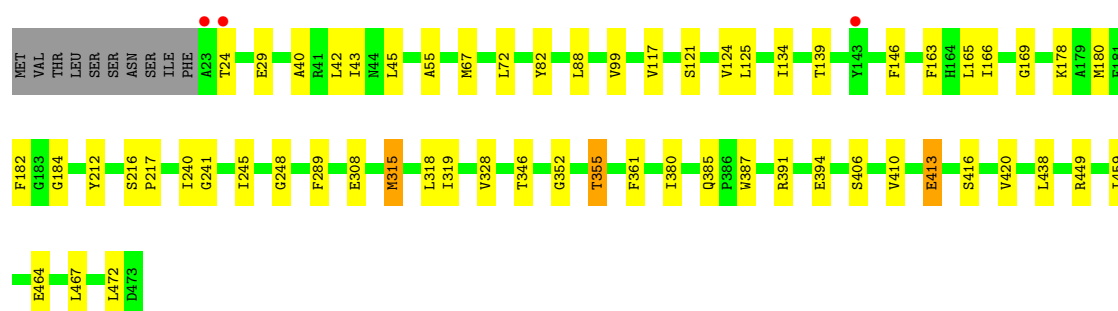
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 83% 12% ..



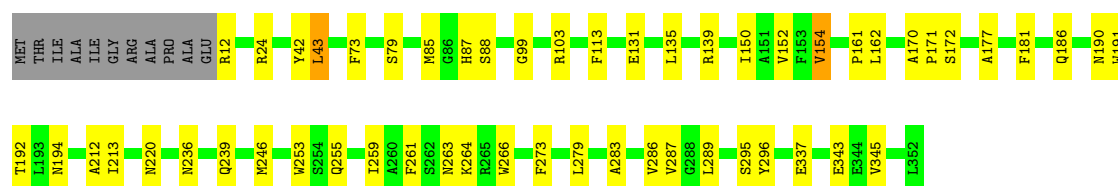
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 85% 12% ..



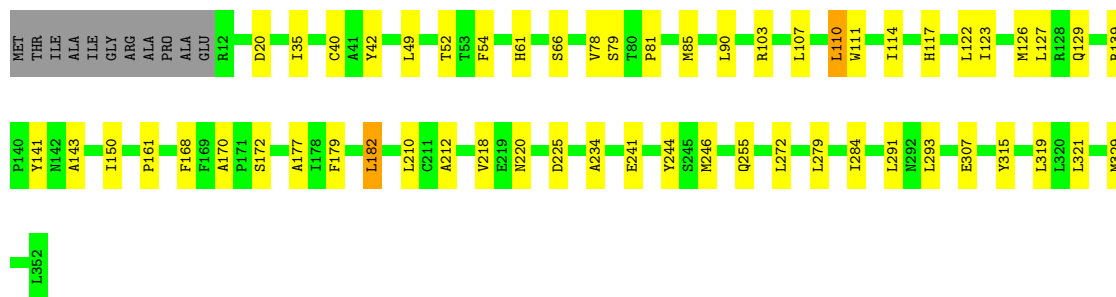
• Molecule 4: Photosystem II D2 protein

Chain D: 82% 15% ..



• Molecule 4: Photosystem II D2 protein

Chain d:  81% 15% ..



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  4% 73% 23% ..



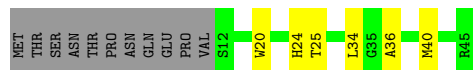
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  4% 74% 21% ..



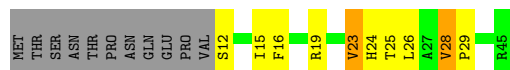
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  62% 13% 24%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  53% 18% 24%

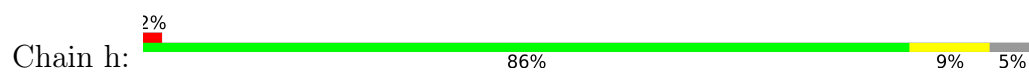


- Molecule 7: Photosystem II reaction center protein H

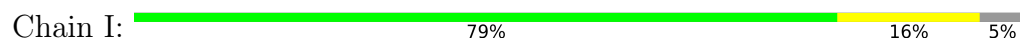
Chain H:  3% 86% 12% .



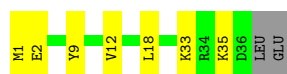
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

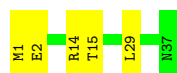


- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  84% 11% . .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 17% 8%



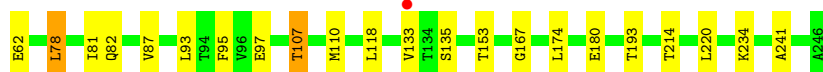
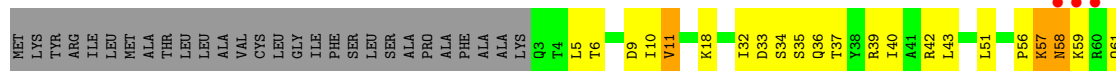
- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 17% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  74% 14% . 10%

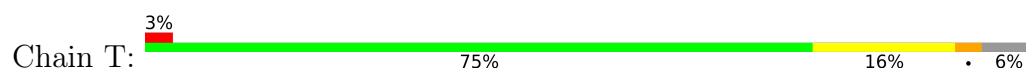


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

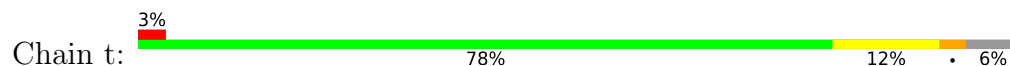
Chain o:  75% 14% . 10%



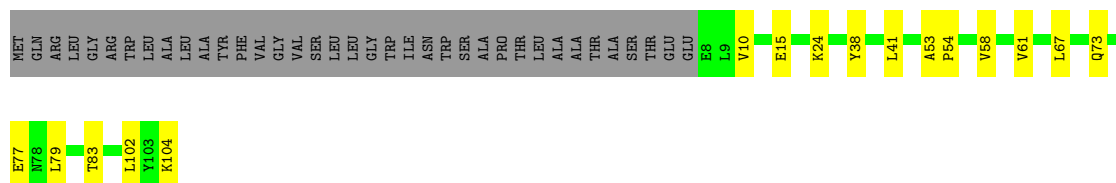
- Molecule 14: Photosystem II reaction center protein T



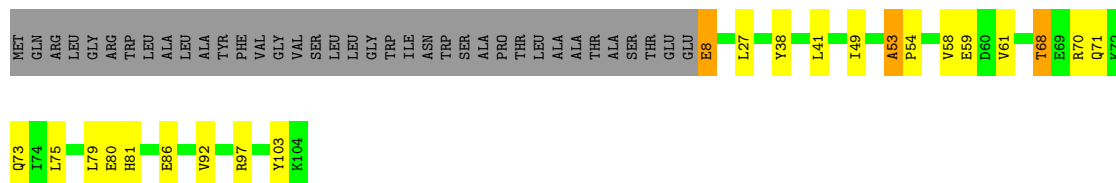
- Molecule 14: Photosystem II reaction center protein T



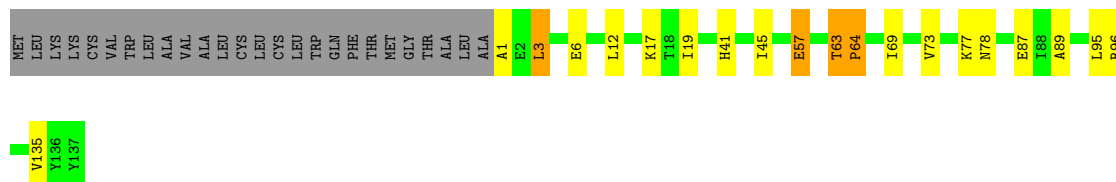
- Molecule 15: Photosystem II 12 kDa extrinsic protein



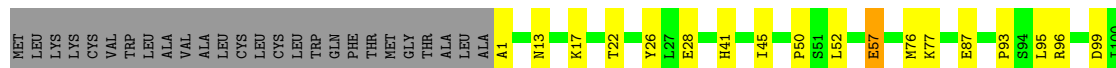
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

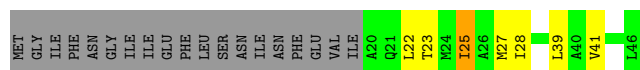


- Molecule 16: Cytochrome c-550

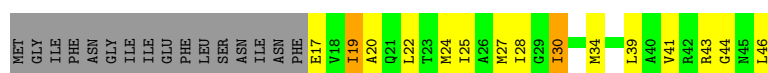
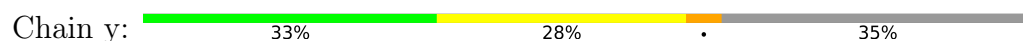




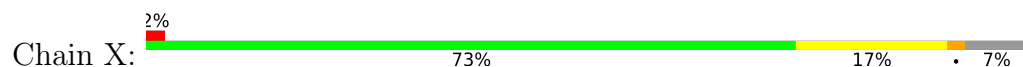
- Molecule 17: Photosystem II reaction center protein Ycf12



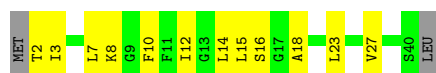
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



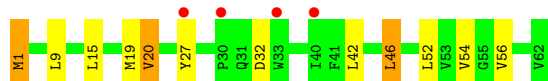
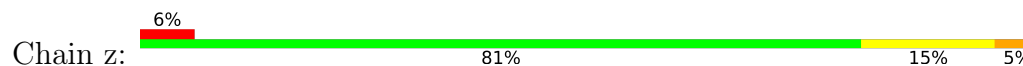
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z

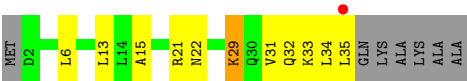


- Molecule 19: Photosystem II reaction center protein Z

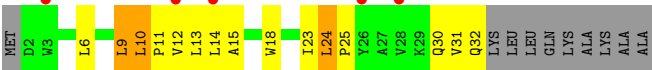


- Molecule 20: Photosystem II protein Y





● 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	117.10Å 222.20Å 308.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.74 – 2.15 33.74 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.74-2.15) 85.0 (33.74-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.42 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.243 0.188 , 0.244	Depositor DCC
R_{free} test set	3853 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52853	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/3212	0.51	0/4376
1	a	0.30	0/3209	0.48	0/4372
2	B	0.34	0/4155	0.50	0/5661
2	b	0.31	0/4118	0.47	0/5611
3	C	0.32	0/3625	0.47	0/4935
3	c	0.30	0/3705	0.46	0/5042
4	D	0.35	0/2825	0.50	0/3847
4	d	0.34	0/2834	0.51	0/3859
5	E	0.27	0/688	0.45	0/940
5	e	0.24	0/683	0.44	0/932
6	F	0.30	0/284	0.48	0/387
6	f	0.26	0/284	0.49	0/387
7	H	0.33	0/523	0.50	0/713
7	h	0.31	0/511	0.49	0/697
8	I	0.33	0/293	0.47	0/396
8	i	0.34	0/293	0.46	0/396
9	J	0.28	0/263	0.46	0/356
9	j	0.26	0/263	0.39	0/356
10	K	0.28	0/303	0.44	0/416
10	k	0.26	0/303	0.51	0/416
11	L	0.37	0/311	0.45	0/422
11	l	0.32	0/303	0.43	0/412
12	M	0.33	0/249	0.54	0/341
12	m	0.35	0/244	0.52	0/334
13	O	0.32	0/1904	0.50	0/2585
13	o	0.32	0/1905	0.51	0/2583
14	T	0.36	0/257	0.54	0/349
14	t	0.32	0/255	0.48	0/346
15	U	0.29	0/785	0.46	0/1064
15	u	0.31	0/785	0.51	0/1064
16	V	0.30	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.29	0/1085	0.47	0/1473
17	Y	0.23	0/197	0.36	0/264
17	y	0.20	0/219	0.43	0/294
18	X	0.26	0/284	0.40	0/384
18	x	0.23	0/289	0.35	0/391
19	Z	0.22	0/490	0.43	0/669
19	z	0.19	0/488	0.33	0/666
20	R	0.27	0/277	0.53	0/380
20	r	0.23	0/252	0.40	0/347
All	All	0.31	0/44038	0.48	0/59936

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	2981	28	0
1	a	3110	0	2972	36	0
2	B	4005	0	3871	48	0
2	b	3978	0	3836	46	0
3	C	3509	0	3426	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	35	0
4	D	2731	0	2637	41	0
4	d	2737	0	2643	41	0
5	E	666	0	651	13	0
5	e	664	0	648	15	0
6	F	275	0	282	5	0
6	f	275	0	282	9	0
7	H	510	0	532	6	0
7	h	498	0	518	3	0
8	I	296	0	311	2	0
8	i	296	0	311	4	0
9	J	257	0	268	5	0
9	j	257	0	268	5	0
10	K	293	0	305	3	0
10	k	293	0	305	8	0
11	L	304	0	316	4	0
11	l	296	0	304	2	0
12	M	256	0	269	5	0
12	m	251	0	267	4	0
13	O	1870	0	1830	27	0
13	o	1874	0	1846	20	0
14	T	258	0	261	4	0
14	t	256	0	256	3	0
15	U	774	0	773	8	0
15	u	774	0	773	14	0
16	V	1064	0	1073	15	0
16	v	1064	0	1073	15	0
17	Y	196	0	217	4	0
17	y	218	0	241	11	0
18	X	281	0	312	7	0
18	x	286	0	314	8	0
19	Z	479	0	516	13	0
19	z	477	0	509	6	0
20	R	271	0	298	3	0
20	r	246	0	263	10	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	184	0	192	5	0
25	B	1035	0	1139	42	0
25	C	839	0	922	31	0
25	D	195	0	216	6	0
25	a	260	0	288	6	0
25	b	1035	0	1139	42	0
25	c	839	0	919	23	0
25	d	130	0	144	5	0
26	A	64	0	74	1	0
26	D	64	0	74	1	0
26	a	64	0	74	1	0
26	d	64	0	74	4	0
27	A	40	0	56	0	0
27	B	120	0	168	6	0
27	C	80	0	112	6	0
27	D	40	0	56	0	0
27	H	40	0	56	0	0
27	K	80	0	112	1	0
27	T	40	0	56	5	0
27	a	40	0	56	2	0
27	b	120	0	168	7	0
27	c	80	0	112	5	0
27	d	40	0	56	2	0
27	h	40	0	56	2	0
27	k	80	0	112	5	0
27	t	40	0	56	3	0
28	A	55	0	80	8	0
28	D	55	0	80	1	0
28	a	55	0	80	7	0
28	d	55	0	80	2	0
29	A	48	0	66	0	0
29	B	28	0	40	1	0
29	C	48	0	66	2	0
29	D	84	0	117	4	0
29	M	51	0	72	1	0
29	b	55	0	86	3	0
29	c	134	0	181	11	0
29	d	67	0	92	1	0
29	m	51	0	72	3	0
30	A	91	0	136	7	0
30	B	54	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D	36	0	46	0	0
30	L	49	0	65	4	0
30	a	54	0	78	3	0
30	f	41	0	49	0	0
30	t	36	0	56	3	0
31	A	66	0	96	6	0
31	C	186	0	246	8	0
31	H	62	0	82	3	0
31	a	44	0	75	1	0
31	c	186	0	245	9	0
31	h	62	0	82	1	0
32	B	57	0	89	2	0
32	C	40	0	63	3	0
32	H	18	0	35	3	0
32	I	15	0	26	3	0
32	J	12	0	16	1	0
32	L	12	0	16	1	0
32	M	25	0	38	0	0
32	R	12	0	16	0	0
32	X	20	0	35	4	0
32	a	22	0	32	0	0
32	b	97	0	170	5	0
32	c	32	0	51	2	0
32	d	37	0	61	3	0
32	j	12	0	16	0	0
32	l	18	0	35	2	0
32	t	32	0	48	1	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	D	145	0	215	10	0
34	E	49	0	74	4	0
34	L	49	0	74	3	0
34	d	137	0	199	7	0
34	e	42	0	57	4	0
34	l	49	0	74	2	0
35	F	43	0	30	4	0
35	e	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	0	0
37	A	124	0	0	2	0
37	B	165	0	0	0	0
37	C	112	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	94	0	0	0	0
37	E	22	0	0	1	0
37	F	5	0	0	0	0
37	H	24	0	0	0	0
37	I	18	0	0	0	0
37	J	8	0	0	1	0
37	K	2	0	0	0	0
37	L	8	0	0	0	0
37	M	7	0	0	0	0
37	O	66	0	0	2	0
37	R	9	0	0	0	0
37	T	6	0	0	0	0
37	U	30	0	0	1	0
37	V	45	0	0	2	0
37	X	10	0	0	0	0
37	Y	6	0	0	0	0
37	Z	5	0	0	1	0
37	a	107	0	0	1	0
37	b	132	0	0	1	0
37	c	128	0	0	1	0
37	d	77	0	0	0	0
37	e	14	0	0	0	0
37	f	2	0	0	1	0
37	h	20	0	0	0	0
37	i	10	0	0	0	0
37	j	7	0	0	0	0
37	k	5	0	0	1	0
37	l	7	0	0	0	0
37	m	3	0	0	0	0
37	o	76	0	0	1	0
37	r	5	0	0	0	0
37	t	7	0	0	1	0
37	u	34	0	0	3	0
37	v	39	0	0	0	0
37	x	4	0	0	0	0
37	y	2	0	0	0	0
37	z	1	0	0	0	0
All	All	52853	0	52752	707	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 7.

All (707) 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)
25:B:601:CLA:H92	32:H:103:STE:H162	1.61	0.82
12:m:4:ASN:ND2	29:m:101:LMG:O10	2.13	0.81
5:E:3:GLY:N	37:E:201:HOH:O	2.14	0.80
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.62	0.80
15:u:53:ALA:O	37:u:201:HOH:O	2.01	0.79
6:f:16:PHE:H	20:r:30:GLN:HE22	1.31	0.78
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.65	0.78
28:A:611:PL9:H361	6:F:25:THR:HG21	1.67	0.76
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.68	0.75
3:C:148:GLY:O	3:C:156:LYS:NZ	2.20	0.75
9:J:15:THR:HG22	9:J:19:MET:HE2	1.68	0.75
16:v:104:MET:HA	16:v:107:LEU:HD22	1.69	0.74
25:C:506:CLA:H91	25:C:506:CLA:H203	1.70	0.74
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.06	0.73
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.71	0.73
25:D:405:CLA:H141	18:X:15:LEU:HD12	1.71	0.73
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.71	0.73
21:a:601[B]:OEY:O5	21:a:601[B]:OEY:O6	2.06	0.73
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.72	0.71
2:b:103:LEU:HD22	25:b:606:CLA:H51	1.73	0.71
19:Z:1:MET:N	37:Z:101:HOH:O	2.24	0.70
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.73	0.70
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.73	0.69
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.74	0.69
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.24	0.69
27:T:101:BCR:H311	27:T:101:BCR:HC8	1.73	0.69
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.75	0.69
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.57	0.68
1:a:300:PHE:HZ	31:c:518:DGD:HB61	1.59	0.67
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.77	0.67
31:A:615:DGD:HA62	2:b:98:LEU:HD21	1.75	0.67
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.29	0.66
3:c:406:SER:HA	3:c:420:VAL:HG23	1.78	0.66
25:B:604:CLA:H93	25:B:605:CLA:HAB	1.77	0.66
10:k:19:ASP:OD2	37:k:201:HOH:O	2.14	0.66
2:B:98:LEU:HD11	31:a:614:DGD:HBW1	1.78	0.66
34:L:102:LHG:H322	12:M:18:PRO:HB3	1.78	0.65
7:H:59:ASN:HD21	7:H:61:SER:HB3	1.61	0.65
5:e:10:PHE:N	34:e:102:LHG:O4	2.30	0.65
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.26	0.65
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.78	0.64
27:B:619:BCR:H382	30:t:102:SQD:H82	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:102:VAL:HG11	25:b:606:CLA:H142	1.79	0.64
2:B:12:LEU:HB2	25:B:612:CLA:HMC2	1.80	0.64
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.31	0.64
25:B:611:CLA:H203	25:B:613:CLA:H8	1.80	0.63
25:B:606:CLA:H72	27:B:619:BCR:H311	1.79	0.63
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.80	0.63
6:F:36:ALA:O	6:F:40:MET:HG3	1.99	0.63
25:b:613:CLA:H172	34:d:407:LHG:H212	1.80	0.63
25:b:613:CLA:H192	34:d:407:LHG:H221	1.81	0.62
5:e:56:TYR:O	16:v:1:ALA:N	2.30	0.62
3:C:281:MET:HE2	25:C:501:CLA:H112	1.80	0.62
25:B:601:CLA:H61	32:H:103:STE:H183	1.82	0.62
25:B:614:CLA:H42	32:L:103:STE:H22	1.82	0.61
28:D:407:PL9:H412	11:L:29:LEU:HD23	1.80	0.61
4:D:42:TYR:CE1	6:F:25:THR:HG22	2.36	0.61
25:b:608:CLA:HAB	4:d:123:ILE:HG12	1.82	0.61
32:I:101:STE:H131	25:b:606:CLA:H192	1.82	0.61
16:V:12:LEU:HB2	16:V:19:ILE:HG12	1.82	0.61
4:D:279:LEU:HD22	26:D:402:PHO:HBC3	1.82	0.61
19:Z:23:VAL:HG22	19:Z:40:ILE:HD12	1.83	0.61
2:B:371:THR:HG23	2:B:372:ASP:O	2.01	0.61
28:A:611:PL9:H262	34:E:101:LHG:H222	1.83	0.61
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.83	0.61
25:B:601:CLA:HAB	32:H:103:STE:H131	1.82	0.61
3:C:114:VAL:HG22	32:C:522:STE:H102	1.81	0.60
2:B:490:GLN:HG3	2:B:496:TYR:HE2	1.67	0.60
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.67	0.60
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.84	0.60
10:k:21:LEU:HD13	17:y:24:MET:HE2	1.83	0.60
16:v:77:LYS:HG2	16:v:95:LEU:HD12	1.84	0.60
3:c:178:LYS:NZ	3:c:184:GLY:O	2.33	0.60
4:d:141:TYR:OH	34:d:407:LHG:O4	2.12	0.60
28:d:406:PL9:H201	34:l:101:LHG:H202	1.83	0.60
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.83	0.59
2:b:155:ALA:HB1	29:b:622:LMG:H122	1.84	0.59
19:Z:29:SER:HB3	19:Z:31:GLN:HE21	1.68	0.59
25:c:511:CLA:H93	27:k:102:BCR:H272	1.83	0.59
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.85	0.59
25:d:404:CLA:H92	18:x:18:ALA:HB2	1.85	0.59
5:E:26:THR:HA	20:R:15:ALA:HB1	1.85	0.59
4:D:99:GLY:HA3	32:X:101:STE:H21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:59:ASN:ND2	7:H:61:SER:HB3	2.18	0.58
25:c:503:CLA:H203	25:c:510:CLA:HAB	1.85	0.58
31:c:518:DGD:HB72	31:c:518:DGD:HA61	1.86	0.58
4:d:279:LEU:HD22	26:d:402:PHO:HBC3	1.85	0.58
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.85	0.57
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.85	0.57
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.86	0.57
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.85	0.57
2:B:479[A]:PHE:O	4:D:139:ARG:NH2	2.25	0.57
3:c:121:SER:HB3	32:c:520:STE:H182	1.86	0.57
1:a:84:PRO:HA	1:a:112:TYR:CG	2.40	0.57
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.86	0.57
30:L:101:SQD:H222	2:b:29:LEU:HD23	1.86	0.57
37:C:693:HOH:O	8:I:33:LYS:HE3	2.05	0.57
3:C:415:ASN:O	3:C:416:SER:HB2	2.04	0.57
16:V:87:GLU:CD	16:V:96:ARG:HH12	2.13	0.57
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.87	0.56
3:C:178:LYS:NZ	3:C:184:GLY:O	2.35	0.56
13:O:36:GLN:HE21	13:O:37:THR:H	1.53	0.56
4:d:241:GLU:CD	4:d:241:GLU:H	2.12	0.56
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.87	0.56
31:A:615:DGD:HB41	32:I:101:STE:H62	1.87	0.56
34:D:410:LHG:HC62	11:L:15:THR:HG23	1.87	0.56
25:b:609:CLA:H42	32:b:623:STE:H91	1.88	0.56
34:d:407:LHG:H351	34:d:407:LHG:H101	1.85	0.56
1:A:103:ASP:OD1	31:A:615:DGD:O2E	2.24	0.56
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.21	0.56
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.88	0.56
1:a:45:THR:HG23	25:a:612:CLA:H201	1.88	0.56
4:d:126:MET:HE3	4:d:143:ALA:O	2.06	0.56
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.40	0.56
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.87	0.56
25:b:602:CLA:H193	31:h:102:DGD:HA72	1.87	0.55
3:c:315:MET:HE3	3:c:319:ILE:HD11	1.88	0.55
27:B:617:BCR:H322	29:M:101:LMG:H111	1.88	0.55
2:b:92:SER:O	2:b:96:VAL:HG23	2.06	0.55
27:t:101:BCR:H321	27:t:101:BCR:HC8	1.87	0.55
30:A:613:SQD:H381	9:J:22:ILE:HD11	1.88	0.55
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.87	0.55
1:a:165[B]:GLN:NE2	1:a:294:ALA:O	2.39	0.55
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:24:HIS:O	6:f:28:VAL:HG13	2.07	0.55
25:B:603:CLA:C3D	25:B:605:CLA:H2	2.37	0.55
19:z:15:LEU:HD22	19:z:46:LEU:HD12	1.87	0.55
31:A:615:DGD:HB61	32:I:101:STE:H51	1.89	0.55
35:e:101:HEM:HHC	35:e:101:HEM:HBB2	1.89	0.55
3:c:55:ALA:HB1	27:k:102:BCR:H373	1.88	0.55
25:c:508:CLA:H91	34:d:409:LHG:H361	1.89	0.55
4:D:286:VAL:HG21	25:D:404:CLA:HED2	1.88	0.54
25:b:615:CLA:H2	25:b:616:CLA:HBB2	1.89	0.54
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.42	0.54
34:E:101:LHG:H251	34:E:101:LHG:H302	1.89	0.54
25:C:513:CLA:H201	32:C:522:STE:H171	1.89	0.54
2:b:489:GLU:HA	2:b:495:PHE:HD2	1.72	0.54
2:B:171:PRO:HA	7:H:65:LEU:HD12	1.90	0.54
25:A:607:CLA:H162	28:A:611:PL9:H252	1.90	0.54
4:D:103:ARG:HH21	5:E:77:GLU:CG	2.21	0.54
4:D:43:LEU:HG	4:D:113:PHE:HZ	1.73	0.54
15:U:58:VAL:O	15:U:61:VAL:HG22	2.08	0.54
15:u:86:GLU:H	15:u:86:GLU:CD	2.16	0.53
25:B:605:CLA:HBB1	25:B:606:CLA:H52	1.90	0.53
31:A:615:DGD:HD5	2:b:75:TRP:HB3	1.90	0.53
1:A:38:ILE:HD13	30:A:614:SQD:H121	1.91	0.53
30:A:614:SQD:H383	27:b:619:BCR:HC8	1.91	0.53
4:d:127:LEU:HD13	32:d:412:STE:H71	1.89	0.53
30:A:614:SQD:H301	27:b:619:BCR:H363	1.91	0.53
4:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.90	0.53
25:c:511:CLA:H203	19:z:20:VAL:HA	1.89	0.53
13:O:56:PRO:O	13:O:58:ASN:N	2.38	0.53
25:B:604:CLA:H143	25:B:615:CLA:H92	1.91	0.53
29:C:519:LMG:H191	10:K:27:VAL:HG11	1.91	0.53
13:O:107:THR:HG22	37:O:317:HOH:O	2.08	0.53
2:B:36:SER:OG	27:B:618:BCR:H362	2.08	0.53
2:B:172:TYR:OH	7:H:63:LYS:NZ	2.42	0.53
3:c:245:ILE:HD13	29:c:521:LMG:H382	1.90	0.53
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.91	0.53
3:C:406:SER:HA	3:C:420:VAL:HG23	1.90	0.53
29:b:622:LMG:H371	29:b:622:LMG:H192	1.91	0.52
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.91	0.52
25:C:505:CLA:H43	27:C:514:BCR:HC7	1.91	0.52
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.91	0.52
20:r:31:VAL:HG12	20:r:32:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.44	0.52
3:c:134:ILE:HD12	25:c:511:CLA:H43	1.90	0.52
4:D:150:ILE:O	4:D:154:VAL:HG13	2.10	0.52
2:b:44:THR:HG22	32:b:620:STE:H61	1.92	0.52
28:d:406:PL9:H322	34:l:101:LHG:H222	1.90	0.52
1:a:235:TYR:OH	11:l:11:GLU:OE2	2.22	0.52
2:b:359:MET:HB2	2:b:425:ILE:HD12	1.90	0.52
2:B:49:ASP:OD2	13:o:57:LYS:HD2	2.10	0.52
1:A:271:LEU:HD11	28:A:611:PL9:HC71	1.90	0.52
3:c:391[B]:ARG:NE	3:c:391[B]:ARG:HA	2.24	0.52
1:A:332[A]:HIS:O	1:A:333[A]:GLU:C	2.52	0.52
25:c:501:CLA:C2D	25:c:503:CLA:H2	2.39	0.52
25:C:503:CLA:HAB	25:C:513:CLA:H201	1.92	0.51
16:v:57:GLU:CD	16:v:57:GLU:H	2.17	0.51
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.46	0.51
3:C:152:LYS:HD3	3:C:266:TRP:O	2.11	0.51
34:D:411:LHG:H141	34:D:411:LHG:H322	1.92	0.51
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.92	0.51
17:y:39:LEU:O	17:y:44:GLY:N	2.34	0.51
10:k:39:TRP:CD1	17:y:46:LEU:HD12	2.45	0.51
3:C:213:LEU:HG	25:C:506:CLA:H193	1.92	0.51
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.91	0.51
31:A:615:DGD:HB91	31:A:615:DGD:HB42	1.92	0.51
18:x:3:ILE:HA	18:x:7:LEU:HD23	1.93	0.51
13:O:51:LEU:HB2	13:O:234:LYS:HB3	1.93	0.50
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.93	0.50
1:A:286:THR:HG23	25:A:606:CLA:HED3	1.92	0.50
2:B:145:LEU:HD22	25:B:604:CLA:H193	1.93	0.50
30:t:102:SQD:O6	37:t:201:HOH:O	2.18	0.50
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.47	0.50
25:C:504:CLA:H143	25:C:508:CLA:H141	1.92	0.50
4:D:263:ASN:HB3	34:D:410:LHG:HC32	1.94	0.50
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.11	0.50
19:Z:31:GLN:CD	19:Z:32:ASP:H	2.19	0.50
19:Z:34:ASP:O	19:Z:37:LYS:HG2	2.12	0.50
2:b:159:THR:O	2:b:180:PRO:HB3	2.11	0.50
5:e:25:ILE:HD13	20:r:18:TRP:NE1	2.27	0.50
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.46	0.50
16:V:41:HIS:HA	16:V:45:ILE:O	2.12	0.50
2:b:231:MET:HG2	25:b:610:CLA:HBC3	1.93	0.50
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.93	0.50
2:b:65:PHE:HE1	25:b:604:CLA:HED2	1.77	0.50
5:e:17:VAL:HG23	9:j:7:ARG:HB2	1.93	0.50
13:o:147:ASN:HB3	13:o:192:LEU:HD11	1.94	0.50
13:o:127:ALA:HB1	13:o:142:PHE:HB3	1.93	0.50
25:C:502:CLA:H102	25:C:503:CLA:CHB	2.42	0.50
10:K:26:PRO:O	10:K:29:PRO:HD2	2.11	0.50
2:b:16:PRO:HB3	2:b:133:LEU:HD21	1.94	0.50
25:B:614:CLA:H112	30:B:622:SQD:H382	1.94	0.50
1:a:279:PRO:HG2	4:d:212:ALA:HB2	1.94	0.50
25:b:604:CLA:HMB1	25:b:604:CLA:HBB1	1.93	0.49
34:d:409:LHG:HC81	34:d:409:LHG:HC31	1.94	0.49
9:j:18:GLY:O	9:j:22:ILE:HD13	2.12	0.49
15:u:80:GLU:HG3	15:u:81:HIS:CD2	2.47	0.49
34:D:413:LHG:H222	12:M:18:PRO:HG3	1.94	0.49
3:c:352:GLY:O	3:c:355[A]:THR:HG22	2.12	0.49
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.77	0.49
3:C:363:GLY:O	3:C:367:GLU:HG2	2.11	0.49
4:D:236:ASN:HB3	4:D:239:GLN:HB3	1.94	0.49
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.95	0.49
17:y:20:ALA:O	17:y:24:MET:HG2	2.12	0.49
16:v:26:TYR:OH	16:v:122:GLU:OE1	2.17	0.49
2:B:117:TYR:HA	11:L:1:MET:HE1	1.95	0.49
2:B:442:ILE:HD11	13:O:174:LEU:HD23	1.94	0.49
26:a:608:PHO:HBB1	26:a:608:PHO:HMB3	1.94	0.49
25:b:601:CLA:CHA	25:b:601:CLA:HBA2	2.43	0.49
18:X:12:ILE:HD13	32:X:101:STE:O2	2.12	0.49
1:a:321:ILE:HD11	4:d:179:PHE:HB2	1.94	0.49
10:k:39:TRP:HD1	17:y:46:LEU:HD12	1.77	0.49
13:O:58:ASN:HD22	13:O:58:ASN:H	1.61	0.49
31:c:518:DGD:HG12	9:j:32:ALA:HB1	1.94	0.48
3:C:313:GLN:HB2	3:C:396:MET:HG3	1.95	0.48
13:O:56:PRO:O	13:O:58:ASN:ND2	2.37	0.48
2:b:383:PHE:O	13:o:166:SER:HA	2.13	0.48
3:c:45:LEU:HA	3:c:139:THR:HG22	1.94	0.48
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.94	0.48
25:b:614:CLA:H92	27:b:617:BCR:H362	1.94	0.48
25:c:510:CLA:H102	25:c:510:CLA:H61	1.46	0.48
3:c:117:VAL:HG12	32:c:520:STE:H141	1.94	0.48
3:c:180:MET:HE1	29:c:521:LMG:HC72	1.95	0.48
4:d:79:SER:HA	4:d:172:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:41:HIS:HA	16:v:45:ILE:O	2.13	0.48
1:A:201:GLY:HA3	1:A:286:THR:HB	1.96	0.48
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.46	0.48
25:b:604:CLA:H42	25:b:605:CLA:H2	1.96	0.48
25:c:512:CLA:H112	25:c:513:CLA:H151	1.95	0.48
2:B:386:ALA:HB3	15:U:102:LEU:HD22	1.95	0.48
1:A:163[B]:ILE:HD11	31:C:516:DGD:HA32	1.94	0.48
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.96	0.48
2:B:497:GLN:HB2	2:B:504:THR:HB	1.95	0.48
8:I:7:THR:O	8:I:11:VAL:HG23	2.14	0.48
15:U:24:LYS:HB2	15:U:83:THR:HG22	1.96	0.48
2:b:505:ARG:HG3	2:b:506:ARG:N	2.28	0.48
14:t:18:PHE:HD1	27:t:101:BCR:HC7	1.79	0.48
2:b:62:VAL:HB	25:b:605:CLA:HED3	1.95	0.48
15:u:70:ARG:NH1	15:u:73:GLN:OE1	2.47	0.48
2:B:103:LEU:HD21	25:B:605:CLA:HMC3	1.96	0.47
3:C:315:MET:HE3	3:C:351:PHE:HZ	1.78	0.47
12:M:8:LEU:HD22	14:T:1:FME:HE3	1.95	0.47
2:b:481:GLY:HA2	4:d:139:ARG:HD2	1.96	0.47
2:b:496:TYR:HE1	2:b:505:ARG:HD3	1.78	0.47
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.44	0.47
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.50	0.47
19:Z:12:LEU:HD13	19:Z:50:LEU:HB3	1.96	0.47
25:B:602:CLA:H202	31:H:102:DGD:HA72	1.96	0.47
3:c:163:PHE:CG	25:c:512:CLA:HAB	2.49	0.47
18:X:16:SER:HB3	32:X:101:STE:H112	1.95	0.47
8:i:33:LYS:O	8:i:35:LYS:NZ	2.41	0.47
5:E:72:ALA:O	5:E:76:VAL:HG23	2.14	0.47
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.94	0.47
25:b:601:CLA:H92	27:h:101:BCR:H402	1.95	0.47
32:b:620:STE:H41	32:b:624:STE:H82	1.95	0.47
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.96	0.47
17:y:41:VAL:C	17:y:43:ARG:H	2.22	0.47
3:C:79:LYS:HB2	3:C:84:GLN:NE2	2.28	0.47
16:V:69:ILE:O	16:V:73:VAL:HG23	2.14	0.47
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.49	0.47
4:D:79:SER:HA	4:D:172:SER:HB3	1.96	0.47
29:D:408:LMG:H222	29:D:408:LMG:H191	1.65	0.47
2:b:150:CYS:HB2	25:b:603:CLA:CMC	2.44	0.47
3:C:141:GLU:H	3:C:141:GLU:CD	2.22	0.47
4:d:81:PRO:HD3	4:d:111:TRP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334[B]:ARG:HD3	37:A:766:HOH:O	2.13	0.47
28:a:611:PL9:H261	34:e:102:LHG:H201	1.96	0.47
25:b:607:CLA:H18	34:d:407:LHG:H161	1.97	0.47
25:B:610:CLA:H122	25:B:615:CLA:HAA1	1.97	0.47
1:a:179[B]:THR:O	1:a:183[B]:MET:HG3	2.14	0.47
3:c:217:PRO:HG3	31:c:516:DGD:HA81	1.97	0.47
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.97	0.47
19:z:32:ASP:OD1	19:z:32:ASP:N	2.47	0.47
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.50	0.46
2:b:148:LEU:HD23	2:b:148:LEU:HA	1.78	0.46
20:r:9:LEU:O	20:r:13:LEU:HG	2.15	0.46
2:B:42:LEU:HD13	2:B:94:GLU:HG3	1.97	0.46
1:a:201:GLY:HA3	1:a:286:THR:HB	1.97	0.46
9:j:18:GLY:O	9:j:21:VAL:HG13	2.16	0.46
25:B:606:CLA:H91	30:t:102:SQD:H211	1.96	0.46
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.97	0.46
2:B:25:MET:HE3	27:B:617:BCR:H23C	1.96	0.46
30:B:622:SQD:H442	14:t:23:PHE:CD1	2.51	0.46
3:C:42:LEU:HD21	25:C:511:CLA:H2A	1.97	0.46
13:o:153:THR:HB	37:u:224:HOH:O	2.15	0.46
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.97	0.46
25:C:512:CLA:H93	25:C:512:CLA:H61	1.65	0.46
9:J:36:LEU:O	37:J:201:HOH:O	2.21	0.46
5:e:56:TYR:HA	5:e:60:GLN:HE21	1.81	0.46
32:t:104:STE:H52	32:t:104:STE:H21	1.76	0.46
2:B:62:VAL:HB	25:B:605:CLA:HED3	1.97	0.46
2:B:149[B]:LEU:HD11	25:B:604:CLA:H162	1.98	0.46
29:D:408:LMG:H202	29:D:408:LMG:H172	1.46	0.46
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.96	0.46
25:B:615:CLA:H52	25:B:615:CLA:H8	1.57	0.46
25:C:508:CLA:H203	31:C:517:DGD:HAE1	1.98	0.46
13:O:6:THR:HG22	13:O:9:ASP:CG	2.41	0.46
15:U:104:LYS:O	37:U:201:HOH:O	2.20	0.46
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.98	0.46
3:C:467:LEU:HD23	3:C:467:LEU:HA	1.74	0.46
25:C:501:CLA:H112	25:C:501:CLA:H142	1.75	0.46
5:E:53:ASP:O	16:V:1:ALA:N	2.48	0.46
13:o:42:ARG:O	13:o:241:ALA:HA	2.16	0.46
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.97	0.46
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.98	0.46
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:l:102:STE:H22	32:l:102:STE:H52	1.73	0.46
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	1.97	0.46
25:C:502:CLA:H61	25:C:512:CLA:H42	1.97	0.46
31:C:517:DGD:HA32	32:J:101:STE:H61	1.98	0.46
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.98	0.46
1:a:155:PHE:HE1	29:c:523:LMG:H201	1.81	0.46
3:c:385:GLN:HB2	3:c:387:TRP:CD1	2.51	0.46
29:m:101:LMG:H381	29:m:101:LMG:H412	1.66	0.46
2:B:347:ARG:HA	2:B:352:GLU:O	2.16	0.45
25:C:503:CLA:H101	25:C:503:CLA:H61	1.44	0.45
28:a:611:PL9:H251	28:a:611:PL9:H272	1.44	0.45
2:b:149:LEU:HD11	25:b:604:CLA:H111	1.98	0.45
13:o:164:LEU:HD13	13:o:188:LYS:O	2.15	0.45
1:A:111:PRO:O	1:A:115:ILE:HG13	2.17	0.45
25:B:601:CLA:HBA1	25:B:601:CLA:HBD	1.97	0.45
25:C:512:CLA:H162	25:C:512:CLA:H141	1.72	0.45
5:E:17:VAL:HG23	9:J:7:ARG:HG3	1.98	0.45
27:B:618:BCR:H15C	27:B:618:BCR:H351	1.78	0.45
3:C:472:LEU:HD11	4:D:255:GLN:HG3	1.98	0.45
32:C:520:STE:H41	32:C:520:STE:H71	1.82	0.45
11:L:14:ARG:HH22	30:L:101:SQD:H3	1.80	0.45
25:c:510:CLA:H2A	25:c:510:CLA:O2A	2.16	0.45
4:d:40:CYS:HB3	4:d:117:HIS:O	2.16	0.45
6:f:19:ARG:O	6:f:23:VAL:HG13	2.17	0.45
6:f:26:LEU:O	6:f:29:PRO:HD2	2.16	0.45
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.97	0.45
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.51	0.45
3:c:459:ILE:HG21	3:c:464:GLU:HG3	1.98	0.45
25:c:505:CLA:H122	25:c:505:CLA:H161	1.76	0.45
29:c:521:LMG:H292	29:c:521:LMG:H112	1.97	0.45
15:u:8:GLU:N	37:u:207:HOH:O	2.49	0.45
19:z:52:LEU:O	19:z:56:VAL:HG22	2.16	0.45
3:C:223:TRP:HZ3	3:C:285:ILE:HG12	1.82	0.45
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.99	0.45
25:b:614:CLA:H93	25:b:614:CLA:H61	1.74	0.45
3:c:146:PHE:HZ	25:c:512:CLA:HBB2	1.80	0.45
2:B:389:LYS:HD3	2:B:389:LYS:HA	1.69	0.45
25:B:606:CLA:H91	25:B:606:CLA:H112	1.54	0.45
25:b:605:CLA:H8	25:b:612:CLA:H201	1.99	0.45
16:v:87:GLU:OE1	16:v:96:ARG:NH2	2.49	0.45
28:A:611:PL9:H28	34:E:101:LHG:H202	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:HIS:HB2	25:B:602:CLA:CHB	2.47	0.45
25:B:605:CLA:H61	25:B:605:CLA:H41	1.69	0.45
30:a:613:SQD:H291	10:k:37:PHE:CZ	2.51	0.45
2:b:12:LEU:HD13	2:b:19:LEU:HA	1.99	0.45
18:x:23:LEU:O	18:x:27:VAL:HG23	2.17	0.45
3:C:257:PHE:CE2	25:C:506:CLA:HED3	2.52	0.45
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.98	0.45
25:c:501:CLA:C19	25:c:507:CLA:HBB1	2.42	0.45
28:A:611:PL9:H471	28:A:611:PL9:H451	1.42	0.45
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.45
1:a:82:VAL:HB	1:a:174[B]:LEU:HB2	1.99	0.45
2:b:222:PRO:HB3	7:h:26:GLY:HA3	1.99	0.45
13:O:57:LYS:HE2	13:O:57:LYS:HB3	1.69	0.45
20:R:29:LYS:O	20:R:32:GLN:HB3	2.17	0.45
27:a:610:BCR:H15C	27:a:610:BCR:H351	1.82	0.45
4:d:225:ASP:HB2	4:d:234:ALA:HB1	1.98	0.45
27:k:101:BCR:HC7	27:k:102:BCR:H353	1.98	0.45
2:B:145:LEU:HD11	25:B:615:CLA:HMB1	1.99	0.44
32:B:624:STE:H62	32:B:625:STE:H102	1.99	0.44
25:c:509:CLA:H141	25:c:509:CLA:H161	1.74	0.44
27:c:515:BCR:H11C	27:c:515:BCR:H341	1.84	0.44
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.98	0.44
25:C:505:CLA:H193	25:C:505:CLA:H162	1.74	0.44
13:O:36:GLN:NE2	13:O:37:THR:H	2.15	0.44
25:a:612:CLA:H43	25:a:612:CLA:O1A	2.17	0.44
3:c:67:MET:HB3	3:c:88:LEU:HD12	1.99	0.44
31:C:518:DGD:HBH1	31:C:518:DGD:HBT2	1.64	0.44
15:U:73:GLN:O	15:U:77:GLU:HG3	2.17	0.44
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.81	0.44
25:b:608:CLA:H141	25:b:608:CLA:H161	1.64	0.44
15:u:38:TYR:HB2	15:u:41:LEU:HD12	1.99	0.44
19:z:1:MET:SD	19:z:1:MET:N	2.89	0.44
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.99	0.44
2:B:357:ARG:NH2	4:D:337:GLU:O	2.37	0.44
34:e:102:LHG:HC61	34:e:102:LHG:H241	1.63	0.44
11:l:7:ARG:HH11	32:l:102:STE:H21	1.83	0.44
25:b:608:CLA:HHD	25:b:608:CLA:HAC2	1.88	0.44
32:d:413:STE:H71	18:x:16:SER:HB3	2.00	0.44
9:j:15:THR:HG22	9:j:19:MET:HE2	2.00	0.44
13:o:154:ALA:HB1	13:o:165:ALA:HB2	1.99	0.44
13:O:133:VAL:C	13:O:135:SER:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:230:THR:O	2:b:3:LEU:HD23	2.17	0.44
30:a:613:SQD:H361	10:k:34:ALA:HB2	2.00	0.44
2:b:266:GLU:HB2	37:b:747:HOH:O	2.18	0.44
2:b:292:LEU:HD21	2:b:298:LEU:HD23	2.00	0.44
3:c:464:GLU:HB3	3:c:467:LEU:HD12	2.00	0.44
26:d:402:PHO:H3A	25:d:403:CLA:H142	1.99	0.44
5:e:33:ALA:HB2	20:r:11:PRO:HG2	1.99	0.44
16:v:99:ASP:OD1	16:v:99:ASP:N	2.49	0.44
30:A:614:SQD:H242	27:b:619:BCR:H382	1.98	0.44
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.53	0.44
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.05	0.44
2:b:67:ALA:HA	2:b:71:VAL:O	2.17	0.44
25:b:602:CLA:H43	7:h:45:ILE:HG22	1.98	0.44
32:b:624:STE:H101	32:b:624:STE:H72	1.70	0.44
26:d:402:PHO:H152	25:d:403:CLA:H171	2.00	0.44
15:u:59:GLU:H	15:u:59:GLU:CD	2.25	0.44
2:B:211:ILE:HG23	32:B:624:STE:H61	1.98	0.44
31:C:517:DGD:HBN2	31:C:517:DGD:HBW1	1.74	0.44
16:V:89:ALA:HB2	37:V:320:HOH:O	2.17	0.44
25:b:615:CLA:H152	25:b:615:CLA:H112	1.47	0.44
25:A:606:CLA:H201	34:D:410:LHG:H181	1.99	0.44
25:B:604:CLA:H62	25:B:604:CLA:H41	1.55	0.44
27:C:514:BCR:H20C	27:C:514:BCR:H361	1.84	0.44
16:V:17:LYS:NZ	37:V:305:HOH:O	2.51	0.44
1:a:263:ALA:O	28:a:611:PL9:H152	2.17	0.44
25:b:612:CLA:H171	25:b:612:CLA:H13	1.66	0.44
5:e:61:ARG:HH22	16:v:125:ILE:C	2.25	0.44
15:u:27:LEU:HD22	15:u:49:ILE:HG21	2.00	0.44
15:u:68:THR:OG1	15:u:71:GLN:HG3	2.18	0.44
28:A:611:PL9:H201	28:A:611:PL9:H222	1.63	0.43
5:E:14:ILE:HG22	5:E:19:TYR:CE2	2.53	0.43
34:E:101:LHG:H223	34:E:101:LHG:H191	1.81	0.43
25:b:614:CLA:H62	25:b:614:CLA:H41	1.73	0.43
25:B:609:CLA:H203	25:B:609:CLA:H161	1.87	0.43
30:L:101:SQD:H202	27:T:101:BCR:H15C	2.00	0.43
1:a:200:LEU:HD13	31:c:518:DGD:HAW2	2.00	0.43
25:a:609:CLA:H2	8:i:12:VAL:HG11	2.00	0.43
2:b:12:LEU:HB2	25:b:612:CLA:HMC2	2.00	0.43
2:B:467:ILE:HD13	2:B:467:ILE:HA	1.87	0.43
25:B:603:CLA:H141	25:B:603:CLA:H161	1.64	0.43
3:C:223:TRP:CG	3:C:224:ILE:H	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:33:ASP:CG	13:O:35:SER:HG	2.26	0.43
1:a:310:LYS:HD2	16:v:1:ALA:HB1	2.00	0.43
25:b:601:CLA:H91	27:h:101:BCR:H23C	2.00	0.43
25:b:614:CLA:H91	25:b:614:CLA:H112	1.76	0.43
1:A:60[A]:ILE:HD12	1:A:84:PRO:HD2	2.01	0.43
4:D:152:VAL:HG21	4:D:279:LEU:HG	2.01	0.43
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.54	0.43
2:b:247:PHE:CE1	25:b:602:CLA:H102	2.53	0.43
5:e:83:LEU:HD12	5:e:83:LEU:HA	1.88	0.43
13:o:160:LYS:HA	13:o:160:LYS:HD2	1.76	0.43
1:A:36:ILE:HG23	25:A:609:CLA:HBB1	2.01	0.43
1:A:339[A]:PHE:HB3	1:A:340[A]:PRO:HD2	2.00	0.43
4:D:73:PHE:CE2	29:D:408:LMG:H181	2.53	0.43
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.01	0.43
37:a:715:HOH:O	3:c:410:VAL:HB	2.17	0.43
2:b:79:SER:OG	2:b:83:GLU:HG2	2.19	0.43
2:b:498:LYS:HE3	4:d:20:ASP:HA	2.01	0.43
25:A:607:CLA:H111	25:A:607:CLA:H91	1.81	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.19	0.43
3:C:180:MET:HG2	3:C:199:ILE:O	2.18	0.43
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	2.00	0.43
2:b:216:HIS:HE1	25:b:609:CLA:C1A	2.32	0.43
25:b:608:CLA:H162	25:d:404:CLA:H3A	2.01	0.43
4:d:61:HIS:CE1	4:d:168:PHE:CE1	3.06	0.43
16:V:12:LEU:HD13	16:V:19:ILE:HG13	2.01	0.43
16:V:77:LYS:HG2	16:V:95:LEU:HD12	2.01	0.43
28:a:611:PL9:H221	28:a:611:PL9:H201	1.62	0.43
2:b:220:ARG:HA	2:b:220:ARG:HD2	1.81	0.43
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.72	0.43
4:d:122:LEU:HB3	4:d:150:ILE:CD1	2.49	0.43
25:B:611:CLA:H72	25:B:611:CLA:H112	1.59	0.43
25:B:611:CLA:H121	25:B:611:CLA:H162	1.83	0.43
4:D:43:LEU:HG	4:D:113:PHE:CZ	2.53	0.43
4:D:283:ALA:O	4:D:287:VAL:HG23	2.19	0.43
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.43
28:a:611:PL9:H28	34:e:102:LHG:H222	2.00	0.43
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.54	0.43
25:B:601:CLA:H71	25:B:601:CLA:H111	1.51	0.43
25:B:603:CLA:C2D	25:B:605:CLA:H2	2.49	0.43
25:B:608:CLA:H141	25:B:609:CLA:H192	2.01	0.43
25:C:505:CLA:HBC2	27:C:514:BCR:H341	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:509:CLA:H62	25:C:509:CLA:H92	1.79	0.43
9:J:20:GLY:O	9:J:24:ILE:HG13	2.19	0.43
27:K:101:BCR:H24C	27:K:101:BCR:H371	1.81	0.43
13:O:110:MET:HB3	13:O:110:MET:HE2	1.74	0.43
1:a:112:TYR:O	1:a:116:ILE:HG12	2.19	0.43
10:k:26:PRO:O	10:k:29:PRO:HD2	2.18	0.43
1:A:11:ALA:O	1:A:16:ARG:NH2	2.52	0.43
25:C:504:CLA:H41	25:C:504:CLA:H62	1.78	0.43
4:d:103:ARG:NH1	5:e:77:GLU:HG3	2.34	0.43
15:u:103:TYR:CD1	16:v:50:PRO:HG2	2.54	0.43
2:B:397:VAL:HG12	2:B:417:VAL:HG11	2.00	0.42
3:C:67:MET:HB3	3:C:88:LEU:HD12	2.01	0.42
16:V:57:GLU:CD	16:V:57:GLU:H	2.27	0.42
8:i:18:LEU:HD23	8:i:18:LEU:HA	1.79	0.42
27:k:102:BCR:H24C	27:k:102:BCR:H371	1.79	0.42
2:B:63:LEU:HA	2:B:66:MET:HE3	2.01	0.42
25:C:513:CLA:H121	25:C:513:CLA:H162	1.92	0.42
31:C:517:DGD:HA82	31:C:517:DGD:HAE2	1.56	0.42
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.01	0.42
5:E:36:LEU:HA	5:E:39:SER:OG	2.18	0.42
1:a:95:PRO:HD2	1:a:98:GLU:HG3	2.00	0.42
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.54	0.42
25:B:612:CLA:HBB1	25:B:612:CLA:HMB1	2.01	0.42
25:C:507:CLA:H161	25:C:507:CLA:H141	1.77	0.42
4:D:131:GLU:O	4:D:135:LEU:HG	2.19	0.42
4:D:261:PHE:CZ	34:D:410:LHG:HC81	2.55	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.84	0.42
19:Z:6:GLN:HE21	19:Z:6:GLN:HB3	1.51	0.42
1:a:343[B]:LEU:HA	1:a:343[B]:LEU:HD23	1.80	0.42
2:b:201:HIS:HB2	25:b:602:CLA:CHB	2.50	0.42
25:b:604:CLA:H12	25:b:605:CLA:C1D	2.50	0.42
3:c:318:LEU:HD21	3:c:380:ILE:HG23	2.01	0.42
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.19	0.42
1:A:158:PHE:O	1:A:162[B]:PRO:HG2	2.19	0.42
2:B:288:VAL:O	2:B:292:LEU:HG	2.20	0.42
25:B:614:CLA:H61	25:B:614:CLA:H41	1.32	0.42
25:D:403:CLA:H141	25:D:403:CLA:H161	1.62	0.42
31:H:102:DGD:HBT1	31:H:102:DGD:HBH2	1.92	0.42
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.01	0.42
3:c:40:ALA:O	3:c:43:ILE:HD12	2.20	0.42
25:c:505:CLA:H142	25:c:505:CLA:H111	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:608:PHO:HBC2	26:A:608:PHO:HHD	2.02	0.42
30:A:613:SQD:H122	34:D:411:LHG:H172	2.02	0.42
13:O:32:ILE:HG21	13:O:93:LEU:HD21	2.02	0.42
19:Z:35:ARG:O	19:Z:35:ARG:HD3	2.19	0.42
1:a:111:PRO:O	1:a:115:ILE:HG13	2.19	0.42
4:d:54:PHE:O	5:e:49:THR:OG1	2.32	0.42
12:m:8:LEU:HD22	14:t:1:FME:HE3	2.01	0.42
17:y:30:ILE:O	17:y:30:ILE:HG12	2.19	0.42
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.07	0.42
25:C:503:CLA:H111	25:C:503:CLA:H142	1.83	0.42
27:C:514:BCR:H24C	27:C:514:BCR:H371	1.86	0.42
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.42
13:O:34:SER:HB3	13:O:87:VAL:HG11	2.02	0.42
3:c:328[B]:VAL:HG22	37:c:652:HOH:O	2.20	0.42
3:c:352:GLY:O	3:c:355[B]:THR:HG22	2.18	0.42
29:c:523:LMG:HC2	8:i:9:TYR:OH	2.19	0.42
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.85	0.42
5:e:26:THR:HA	20:r:15:ALA:HB1	2.02	0.42
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.55	0.42
25:C:509:CLA:H93	25:C:509:CLA:H112	1.82	0.42
13:O:5:LEU:HD13	13:O:10:ILE:HD11	2.01	0.42
25:a:609:CLA:HMA2	29:c:523:LMG:H142	2.01	0.42
28:a:611:PL9:H253	26:d:402:PHO:HBA2	2.01	0.42
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.01	0.42
25:c:507:CLA:H92	25:c:507:CLA:H61	1.63	0.42
27:c:515:BCR:H24C	27:c:515:BCR:H371	1.92	0.42
1:A:159[B]:LEU:C	1:A:162[B]:PRO:HD2	2.45	0.42
3:c:438:LEU:HD11	25:c:505:CLA:HBB1	2.02	0.42
4:d:35:ILE:O	25:d:404:CLA:HBB2	2.20	0.42
25:B:602:CLA:H152	25:B:602:CLA:H18	1.57	0.42
25:B:614:CLA:H18	25:B:614:CLA:H152	1.81	0.42
3:C:168:LEU:HD21	25:C:509:CLA:H61	2.01	0.42
16:V:3:LEU:HD23	16:V:3:LEU:HA	1.72	0.42
16:V:6:GLU:CD	16:V:6:GLU:H	2.27	0.42
1:a:131:TRP:HZ2	3:c:449:ARG:HD2	1.85	0.42
4:d:126:MET:HA	4:d:129:GLN:OE1	2.18	0.42
32:d:413:STE:H172	18:x:12:ILE:HD12	2.02	0.42
20:r:6:LEU:HD12	20:r:10:LEU:HD23	2.01	0.42
2:B:414:PRO:N	2:B:415:PRO:HD2	2.33	0.41
4:D:266:TRP:CD1	34:D:410:LHG:HC31	2.55	0.41
10:K:28:ILE:HD11	17:Y:28:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:L:101:SQD:H102	25:b:614:CLA:H43	2.01	0.41
12:M:31:SER:HB2	12:m:32:GLN:OE1	2.20	0.41
27:T:101:BCR:H15C	27:T:101:BCR:H351	1.88	0.41
18:X:17:GLY:HA2	32:X:101:STE:H152	2.02	0.41
3:c:166:ILE:HG13	3:c:248:GLY:HA3	2.02	0.41
25:c:509:CLA:H142	25:c:509:CLA:H112	1.90	0.41
1:A:334[B]:ARG:NH2	37:A:723:HOH:O	2.53	0.41
3:C:95:LEU:HD21	25:C:501:CLA:OBD	2.20	0.41
35:F:101:HEM:HBB2	35:F:101:HEM:CMB	2.50	0.41
25:C:508:CLA:H203	29:C:519:LMG:H351	2.02	0.41
19:Z:50:LEU:HD13	19:Z:50:LEU:HA	1.91	0.41
2:b:91:TRP:HE1	32:b:621:STE:H111	1.84	0.41
3:c:472:LEU:HD11	4:d:255:GLN:HG3	2.01	0.41
30:A:614:SQD:H223	25:D:403:CLA:H201	2.02	0.41
2:B:233:ASN:HD21	2:B:476:ARG:NH1	2.19	0.41
13:O:42:ARG:O	13:O:241:ALA:HA	2.20	0.41
18:X:34:ILE:HG22	20:R:34:LEU:HD22	2.03	0.41
1:a:104:GLU:O	1:a:108:ASN:ND2	2.47	0.41
1:a:271:LEU:HD21	28:a:611:PL9:C3	2.50	0.41
29:b:622:LMG:H152	29:b:622:LMG:H182	1.88	0.41
19:Z:46:LEU:HD23	19:Z:46:LEU:HA	1.91	0.41
1:a:297:LEU:HD12	1:a:297:LEU:HA	1.87	0.41
3:c:212:TYR:CD2	27:c:515:BCR:H401	2.56	0.41
31:c:517:DGD:HB22	29:c:519:LMG:H311	2.03	0.41
17:y:17:GLU:N	17:y:19:ILE:HD13	2.35	0.41
18:x:8:LYS:HA	18:x:8:LYS:HD2	1.68	0.41
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.02	0.41
2:B:86:ILE:HD12	2:B:88:PRO:HD3	2.02	0.41
2:B:347:ARG:O	2:B:397:VAL:HA	2.21	0.41
4:D:24:ARG:HH22	18:X:35:ASP:CG	2.29	0.41
4:D:286:VAL:CG2	25:D:404:CLA:HED2	2.51	0.41
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.55	0.41
29:c:521:LMG:H351	29:c:521:LMG:H381	1.86	0.41
4:d:85:MET:HE3	4:d:107:LEU:HB3	2.01	0.41
27:k:101:BCR:H24C	27:k:101:BCR:H371	1.86	0.41
28:A:611:PL9:H422	28:A:611:PL9:H401	1.79	0.41
3:C:46:SER:HG	3:C:140:LEU:H	1.68	0.41
4:D:12:ARG:NE	4:D:12:ARG:HA	2.36	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
19:Z:57:LEU:HD23	19:Z:57:LEU:HA	1.83	0.41
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:405:BCR:H381	29:d:411:LMG:H142	2.03	0.41
13:o:49:THR:HG23	13:o:236:GLN:HB2	2.02	0.41
13:o:130:GLN:HB2	37:o:310:HOH:O	2.20	0.41
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.46	0.41
2:B:149[B]:LEU:HG	25:B:604:CLA:H18	2.02	0.41
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.94	0.41
34:D:410:LHG:H182	14:T:17:PHE:HZ	1.85	0.41
34:D:413:LHG:H161	34:L:102:LHG:H292	2.03	0.41
6:F:34:LEU:HD23	6:F:34:LEU:HA	1.88	0.41
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.02	0.41
16:V:63:THR:HG22	16:V:64:PRO:CD	2.50	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.55	0.41
31:c:516:DGD:HA91	29:c:523:LMG:H151	2.02	0.41
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.03	0.41
4:d:246:MET:HE2	4:d:246:MET:HA	2.03	0.41
17:y:17:GLU:O	17:y:20:ALA:HB3	2.21	0.41
3:C:174:LEU:HB3	25:C:502:CLA:H152	2.02	0.41
3:C:213:LEU:HD12	3:C:213:LEU:HA	1.85	0.41
35:F:101:HEM:HBC2	35:F:101:HEM:CHD	2.42	0.41
31:H:102:DGD:HB21	31:H:102:DGD:HB51	1.69	0.41
1:a:217:SER:HA	4:d:272:LEU:HD12	2.03	0.41
25:a:606:CLA:HBD	25:a:612:CLA:HAC2	2.03	0.41
25:b:610:CLA:H143	25:b:610:CLA:H161	1.82	0.41
3:c:82:TYR:OH	3:c:394:GLU:OE2	2.37	0.41
4:d:315:TYR:CZ	4:d:319:LEU:HD11	2.55	0.41
29:m:101:LMG:H322	29:m:101:LMG:H291	1.65	0.41
27:t:101:BCR:H24C	27:t:101:BCR:H371	1.96	0.41
18:x:23:LEU:HA	18:x:23:LEU:HD23	1.79	0.41
3:C:365:TRP:HA	3:C:387:TRP:CH2	2.56	0.41
25:C:508:CLA:C20	31:C:517:DGD:HAE1	2.51	0.41
25:C:511:CLA:H143	19:Z:20:VAL:HG13	2.03	0.41
31:C:518:DGD:HAE2	31:C:518:DGD:HA82	1.57	0.41
4:D:273:PHE:CE1	34:L:102:LHG:H121	2.55	0.41
1:a:237:TYR:OH	4:d:246:MET:HG2	2.21	0.41
25:c:513:CLA:H61	25:c:513:CLA:H41	1.74	0.41
6:f:16:PHE:H	20:r:30:GLN:NE2	2.07	0.41
13:o:10:ILE:O	13:o:11:VAL:C	2.64	0.41
25:B:612:CLA:H61	25:B:612:CLA:H102	1.95	0.40
29:B:621:LMG:H182	29:D:412:LMG:H182	2.03	0.40
25:C:503:CLA:H202	25:C:503:CLA:H161	1.85	0.40
13:O:180:GLU:OE1	37:O:301:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:609:CLA:H91	25:b:609:CLA:H112	1.78	0.40
25:b:615:CLA:H2	25:b:616:CLA:CBB	2.50	0.40
27:c:515:BCR:H20C	27:c:515:BCR:H361	1.94	0.40
4:d:139:ARG:H	4:d:139:ARG:HG3	1.73	0.40
4:d:225:ASP:CB	4:d:234:ALA:HB1	2.51	0.40
5:e:68:ASP:OD2	5:e:71:GLU:HG2	2.20	0.40
13:o:30:TYR:O	13:o:135:SER:HB2	2.20	0.40
25:B:615:CLA:H201	25:B:615:CLA:C1B	2.51	0.40
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.22	0.40
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.57	0.40
5:E:9:PRO:O	5:E:13:ILE:HG13	2.21	0.40
5:E:81:GLU:C	5:E:83:LEU:H	2.30	0.40
27:a:610:BCR:H20C	27:a:610:BCR:H361	1.82	0.40
2:b:36:SER:OG	27:b:618:BCR:H362	2.21	0.40
4:d:52:THR:O	4:d:66:SER:HA	2.21	0.40
5:e:23:HIS:HA	5:e:26:THR:OG1	2.21	0.40
2:B:67:ALA:HA	2:B:71:VAL:O	2.22	0.40
2:B:144:PHE:HE1	2:B:210:ILE:HG23	1.86	0.40
2:b:25:MET:HG2	27:b:617:BCR:H23C	2.04	0.40
31:c:517:DGD:HA91	31:c:518:DGD:HB71	2.04	0.40
35:e:101:HEM:HBA2	20:r:23:ILE:HD13	2.03	0.40
15:u:75:LEU:HD23	15:u:75:LEU:HA	1.92	0.40
1:A:235:TYR:O	1:A:238:LYS:HE3	2.22	0.40
2:B:126:PRO:HG3	7:H:12:ARG:CZ	2.51	0.40
2:B:414:PRO:O	2:B:418:LYS:HG3	2.22	0.40
25:B:607:CLA:H142	25:B:613:CLA:H203	2.02	0.40
25:B:613:CLA:H62	25:B:613:CLA:H41	1.62	0.40
3:C:168:LEU:HD23	3:C:168:LEU:HA	1.92	0.40
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.03	0.40
3:C:465:PRO:O	3:C:469:MET:HG3	2.22	0.40
27:C:514:BCR:H15C	27:C:514:BCR:H351	1.92	0.40
14:T:15:ALA:HB2	27:T:101:BCR:H14C	2.03	0.40
1:a:162[B]:PRO:HB3	1:a:168[B]:PHE:HA	2.03	0.40
25:b:613:CLA:H93	25:b:613:CLA:H62	1.80	0.40
10:k:28:ILE:HD11	17:y:28:ILE:HD13	2.03	0.40
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.57	0.40
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	2.03	0.40
4:D:194:ASN:HA	4:D:295:SER:OG	2.20	0.40
27:T:101:BCR:H361	27:T:101:BCR:H20C	1.84	0.40
1:a:155:PHE:CE1	29:c:523:LMG:H201	2.56	0.40
25:a:606:CLA:CBD	25:a:612:CLA:HAC2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:613:SQD:H382	30:a:613:SQD:H351	1.93	0.40
25:b:611:CLA:H143	25:b:611:CLA:H162	1.82	0.40
27:b:618:BCR:H24C	27:b:618:BCR:H371	1.85	0.40
3:c:169:GLY:HA2	3:c:241:GLY:HA2	2.03	0.40
31:c:517:DGD:HB72	29:c:519:LMG:H402	2.02	0.40
4:d:49:LEU:HD13	27:d:405:BCR:C15	2.52	0.40
4:d:210:LEU:HD23	4:d:210:LEU:HA	1.94	0.40
6:f:12:SER:N	37:f:201:HOH:O	2.53	0.40
20:r:24:LEU:N	20:r:25:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/344 (115%)	389 (98%)	5 (1%)	1 (0%)	36	34
1	a	395/344 (115%)	388 (98%)	6 (2%)	1 (0%)	36	34
2	B	507/510 (99%)	502 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	495 (98%)	7 (1%)	1 (0%)	43	44
3	C	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	43	44
3	c	461/461 (100%)	447 (97%)	13 (3%)	1 (0%)	43	44
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	78 (96%)	2 (2%)	1 (1%)	10	5
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	30 (88%)	4 (12%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	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%)	34 (97%)	1 (3%)	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%)	9 (4%)	3 (1%)	10	5
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	30	26
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	7
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	13
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	2
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5386/5700 (94%)	5242 (97%)	130 (2%)	14 (0%)	36	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER

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Mol	Chain	Res	Type
16	V	64	PRO
3	c	416	SER
13	O	59	LYS
13	O	62	GLU
15	u	53	ALA
9	J	6	GLY
19	Z	31	GLN
5	E	82	GLN
13	O	57	LYS
2	b	127	ARG
13	o	73	ARG
1	A	259	ILE
1	a	259	ILE

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	77
1	a	321/280 (115%)	310 (97%)	11 (3%)	32	33
2	B	407/407 (100%)	393 (97%)	14 (3%)	32	33
2	b	402/407 (99%)	389 (97%)	13 (3%)	34	36
3	C	353/362 (98%)	343 (97%)	10 (3%)	38	40
3	c	362/362 (100%)	346 (96%)	16 (4%)	25	23
4	D	277/283 (98%)	272 (98%)	5 (2%)	51	58
4	d	278/283 (98%)	270 (97%)	8 (3%)	37	39
5	E	72/73 (99%)	65 (90%)	7 (10%)	8	4
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	9
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	56
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	11
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	37
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	6
10	K	30/37 (81%)	26 (87%)	4 (13%)	4	1
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	39
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	31
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	19
13	o	207/228 (91%)	198 (96%)	9 (4%)	26	24
14	T	26/28 (93%)	24 (92%)	2 (8%)	12	7
14	t	25/28 (89%)	23 (92%)	2 (8%)	11	7
15	U	84/112 (75%)	81 (96%)	3 (4%)	31	31
15	u	84/112 (75%)	81 (96%)	3 (4%)	31	31
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	60
16	v	117/138 (85%)	112 (96%)	5 (4%)	26	24
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6	3
17	y	22/37 (60%)	18 (82%)	4 (18%)	2	0
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	11
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	11
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
20	R	28/33 (85%)	20 (71%)	8 (29%)	0	0
20	r	25/33 (76%)	20 (80%)	5 (20%)	1	0
All	All	4450/4654 (96%)	4258 (96%)	192 (4%)	26	24

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
1	A	238	LYS

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Mol	Chain	Res	Type
1	A	243	GLU
2	B	63	LEU
2	B	76	SER
2	B	80	ILE
2	B	84	THR
2	B	87	ASP
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	137	LYS
2	B	298	LEU
2	B	352	GLU
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	104	GLU
3	C	141	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	355[A]	THR
3	C	355[B]	THR
3	C	386	PRO
3	C	416	SER
3	C	473	ASP
4	D	43	LEU
4	D	154	VAL
4	D	192	THR
4	D	259	ILE
4	D	345	VAL
5	E	4	THR
5	E	14	ILE
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	54	SER
5	E	62	SER
5	E	81	GLU
7	H	56	ASP
8	I	3	THR
8	I	4	LEU
10	K	10	LYS
10	K	13	GLU

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Mol	Chain	Res	Type
10	K	19	ASP
10	K	24	VAL
11	L	2	GLU
12	M	25	LEU
13	O	11	VAL
13	O	18	LYS
13	O	39	ARG
13	O	58	ASN
13	O	78	LEU
13	O	82	GLN
13	O	97	GLU
13	O	107	THR
13	O	118	LEU
13	O	214	THR
14	T	25	GLU
14	T	29	ILE
15	U	10	VAL
15	U	15	GLU
15	U	67	LEU
16	V	3	LEU
16	V	57	GLU
17	Y	25	ILE
17	Y	41	VAL
18	X	12	ILE
18	X	29	ILE
19	Z	6	GLN
19	Z	15	LEU
19	Z	17	PHE
19	Z	32	ASP
19	Z	35	ARG
19	Z	46	LEU
19	Z	50	LEU
20	R	6	LEU
20	R	13	LEU
20	R	21	ARG
20	R	22	ASN
20	R	29	LYS
20	R	31	VAL
20	R	33	LYS
20	R	35	LEU
1	a	28	LEU
1	a	42	LEU

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Mol	Chain	Res	Type
1	a	121	LEU
1	a	134	SER
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	230	THR
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	86	ILE
2	b	128	THR
2	b	148	LEU
2	b	161	LEU
2	b	179	GLN
2	b	236	THR
2	b	299	GLU
2	b	362	PHE
2	b	405	GLU
2	b	485	GLU
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	216	SER
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	346	THR
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	110	LEU
4	d	182	LEU
4	d	291	LEU

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Mol	Chain	Res	Type
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	4	THR
5	e	60	GLN
5	e	65	LEU
5	e	66	VAL
5	e	83	LEU
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
7	h	27	THR
7	h	37	LEU
8	i	2	GLU
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	17	ILE
10	k	27	VAL
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	10	ILE
13	o	49	THR
13	o	53	LYS
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	143	LYS
14	t	25	GLU
14	t	29	ILE
15	u	8	GLU
15	u	61	VAL
15	u	68	THR

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Mol	Chain	Res	Type
16	v	22	THR
16	v	28	GLU
16	v	52	LEU
16	v	57	GLU
16	v	107	LEU
17	y	19	ILE
17	y	27	MET
17	y	30	ILE
17	y	34	MET
18	x	2	THR
18	x	15	LEU
19	z	1	MET
19	z	19	MET
19	z	20	VAL
19	z	27	TYR
19	z	42	LEU
19	z	46	LEU
20	r	9	LEU
20	r	10	LEU
20	r	12	VAL
20	r	14	LEU
20	r	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	233	ASN
2	B	409	GLN
3	C	201	ASN
3	C	385	GLN
3	C	415	ASN
7	H	59	ASN
13	O	36	GLN
13	O	88	ASN
13	O	130	GLN
13	O	219	GLN
13	O	231	HIS
15	U	37	GLN
18	X	38	GLN
19	Z	31	GLN
20	R	22	ASN
1	a	19	ASN

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Mol	Chain	Res	Type
1	a	234	ASN
2	b	281	GLN
2	b	338	GLN
2	b	409	GLN
3	c	378	ASN
3	c	382	ASN
4	d	301	GLN
4	d	350	ASN
5	e	60	GLN
7	h	59	ASN
8	i	31	ASN
13	o	61	GLN
13	o	80	GLN
13	o	155	ASN
15	u	37	GLN
15	u	81	HIS
17	y	45	ASN
18	x	33	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	$\# Z > 2$
14	FME	T	1	14	8,9,10	1.06	1 (12%)	8,9,11	1.03	0
14	FME	t	1	14	8,9,10	1.18	1 (12%)	8,9,11	0.89	0
8	FME	I	1	8	8,9,10	1.04	0	8,9,11	1.44	1 (12%)
12	FME	m	1	12	8,9,10	1.04	1 (12%)	8,9,11	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	1.08	1 (12%)	8,9,11	0.83	0
12	FME	M	1	12	8,9,10	1.04	1 (12%)	8,9,11	1.10	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
14	FME	T	1	14	-	1/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.36	1.43	1.46
12	M	1	FME	CA-N	-2.15	1.43	1.46
14	T	1	FME	CA-N	-2.09	1.43	1.46
12	m	1	FME	CA-N	-2.08	1.43	1.46
8	i	1	FME	CA-N	-2.01	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-3.18	117.93	122.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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$
32	STE	c	522	-	11,11,19	0.74	0	11,11,19	1.22	1 (9%)
27	BCR	C	514	-	41,41,41	1.15	3 (7%)	56,56,56	1.27	8 (14%)
34	LHG	D	413	-	48,48,48	0.92	2 (4%)	51,54,54	1.40	6 (11%)
32	STE	C	520	-	11,11,19	0.68	0	11,11,19	1.52	1 (9%)
32	STE	R	101	-	11,11,19	0.71	0	11,11,19	1.15	1 (9%)
27	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	3 (5%)
25	CLA	B	607	37	69,73,73	1.34	7 (10%)	82,113,113	1.43	10 (12%)
27	BCR	d	405	-	41,41,41	1.08	3 (7%)	56,56,56	1.12	3 (5%)
25	CLA	C	513	-	69,73,73	1.30	6 (8%)	82,113,113	1.28	6 (7%)
25	CLA	b	606	-	69,73,73	1.38	7 (10%)	82,113,113	1.48	9 (10%)
32	STE	C	522	-	15,15,19	0.41	0	14,14,19	0.69	0
32	STE	b	625	-	19,19,19	0.61	0	19,19,19	1.01	1 (5%)
25	CLA	a	612	37	69,73,73	1.42	10 (14%)	82,113,113	1.23	7 (8%)
25	CLA	B	606	-	69,73,73	1.27	5 (7%)	82,113,113	1.39	9 (10%)
25	CLA	B	615	-	69,73,73	1.27	8 (11%)	82,113,113	1.25	6 (7%)
25	CLA	c	501	-	69,73,73	1.20	5 (7%)	82,113,113	1.39	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	a	610	-	41,41,41	0.96	3 (7%)	56,56,56	1.26	4 (7%)
28	PL9	d	406	-	55,55,55	1.04	3 (5%)	68,69,69	1.68	16 (23%)
25	CLA	c	507	37	69,73,73	1.26	7 (10%)	82,113,113	1.26	7 (8%)
25	CLA	B	601	37	69,73,73	1.39	9 (13%)	82,113,113	1.32	11 (13%)
26	PHO	A	608	-	58,69,69	1.92	10 (17%)	55,99,99	1.57	7 (12%)
29	LMG	c	521	-	48,48,55	0.96	4 (8%)	56,56,63	1.31	7 (12%)
32	STE	B	625	-	15,15,19	0.36	0	14,14,19	0.84	0
32	STE	t	103	-	13,13,19	0.67	0	13,13,19	1.25	2 (15%)
25	CLA	B	616	-	64,68,73	1.25	7 (10%)	76,107,113	1.29	4 (5%)
27	BCR	c	514	-	41,41,41	1.07	3 (7%)	56,56,56	1.28	8 (14%)
30	SQD	t	102	-	35,35,54	1.71	5 (14%)	37,37,65	1.50	5 (13%)
32	STE	M	102	-	14,14,19	0.73	0	14,14,19	1.09	1 (7%)
32	STE	X	101	-	19,19,19	0.65	0	19,19,19	1.06	0
32	STE	b	621	-	19,19,19	0.61	0	19,19,19	1.09	1 (5%)
34	LHG	E	101	-	48,48,48	0.78	2 (4%)	51,54,54	1.23	6 (11%)
25	CLA	A	609	-	58,62,73	1.22	5 (8%)	68,99,113	1.32	8 (11%)
25	CLA	a	606	-	69,73,73	1.30	9 (13%)	82,113,113	1.30	7 (8%)
27	BCR	b	618	-	41,41,41	1.13	3 (7%)	56,56,56	1.26	6 (10%)
25	CLA	B	611	-	69,73,73	1.17	6 (8%)	82,113,113	1.49	7 (8%)
25	CLA	c	510	-	69,73,73	1.22	8 (11%)	82,113,113	1.41	9 (10%)
36	HEC	v	201	16	46,50,50	1.84	6 (13%)	58,82,82	2.00	8 (13%)
25	CLA	D	405	-	69,73,73	1.32	7 (10%)	82,113,113	1.28	6 (7%)
25	CLA	d	403	-	69,73,73	1.11	7 (10%)	82,113,113	1.19	6 (7%)
26	PHO	d	402	-	58,69,69	2.13	9 (15%)	55,99,99	1.66	8 (14%)
27	BCR	D	406	-	41,41,41	1.16	3 (7%)	56,56,56	1.29	6 (10%)
29	LMG	B	621	-	26,26,55	0.77	2 (7%)	26,26,63	1.19	1 (3%)
32	STE	d	413	-	19,19,19	0.71	0	19,19,19	0.85	1 (5%)
32	STE	B	623	-	11,11,19	0.77	0	11,11,19	1.13	1 (9%)
21	OEY	a	601[B]	1,37,3	0,16,16	-	-	-	-	-
29	LMG	c	519	-	37,37,55	1.02	4 (10%)	45,45,63	1.33	6 (13%)
32	STE	B	624	-	11,11,19	0.68	0	11,11,19	1.22	2 (18%)
30	SQD	D	409	-	34,36,54	1.52	5 (14%)	42,45,65	3.01	11 (26%)
34	LHG	D	411	-	46,46,48	0.92	2 (4%)	49,52,54	1.27	4 (8%)
34	LHG	d	407	-	48,48,48	0.81	2 (4%)	51,54,54	1.35	7 (13%)
22	OEX	a	602[A]	1,37,3	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	513	-	69,73,73	1.27	9 (13%)	82,113,113	1.08	5 (6%)
25	CLA	B	604	-	69,73,73	1.30	7 (10%)	82,113,113	1.64	9 (10%)
25	CLA	C	507	37	69,73,73	1.19	8 (11%)	82,113,113	1.41	8 (9%)
32	STE	d	412	-	16,16,19	0.66	0	16,16,19	1.11	1 (6%)
25	CLA	c	506	-	69,73,73	1.27	8 (11%)	82,113,113	1.32	4 (4%)
30	SQD	B	622	-	52,54,54	1.58	8 (15%)	62,65,65	1.76	11 (17%)
25	CLA	b	605	-	69,73,73	1.11	5 (7%)	82,113,113	1.38	8 (9%)
31	DGD	C	516	-	63,63,67	1.05	3 (4%)	77,77,81	1.35	10 (12%)
25	CLA	B	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.37	8 (9%)
32	STE	j	101	-	11,11,19	0.80	0	11,11,19	1.16	0
29	LMG	b	622	-	55,55,55	0.81	1 (1%)	63,63,63	1.38	6 (9%)
25	CLA	B	610	37	69,73,73	1.19	10 (14%)	82,113,113	1.41	10 (12%)
25	CLA	c	512	-	69,73,73	1.28	9 (13%)	82,113,113	1.35	8 (9%)
27	BCR	B	617	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	7 (12%)
31	DGD	c	518	-	63,63,67	0.92	3 (4%)	77,77,81	1.46	14 (18%)
25	CLA	b	613	-	69,73,73	1.40	9 (13%)	82,113,113	1.47	13 (15%)
25	CLA	a	607	37	69,73,73	1.16	7 (10%)	82,113,113	1.29	8 (9%)
26	PHO	D	402	-	58,69,69	2.10	11 (18%)	55,99,99	1.65	11 (20%)
25	CLA	B	605	-	69,73,73	1.26	9 (13%)	82,113,113	1.23	7 (8%)
25	CLA	B	609	-	69,73,73	1.12	7 (10%)	82,113,113	1.24	8 (9%)
25	CLA	b	608	-	69,73,73	1.36	9 (13%)	82,113,113	1.50	11 (13%)
25	CLA	C	502	-	69,73,73	1.39	8 (11%)	82,113,113	1.10	8 (9%)
25	CLA	b	611	-	69,73,73	1.27	9 (13%)	82,113,113	1.39	5 (6%)
36	HEC	V	201	16	46,50,50	1.77	6 (13%)	58,82,82	2.00	9 (15%)
31	DGD	h	102	-	63,63,67	0.91	2 (3%)	77,77,81	1.50	14 (18%)
32	STE	t	104	-	17,17,19	0.57	0	17,17,19	1.20	1 (5%)
25	CLA	B	613	-	69,73,73	1.20	7 (10%)	82,113,113	1.36	10 (12%)
26	PHO	a	608	-	58,69,69	2.03	10 (17%)	55,99,99	1.54	8 (14%)
27	BCR	K	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.39	9 (16%)
30	SQD	A	613	-	50,52,54	1.58	8 (16%)	60,63,65	2.01	13 (21%)
32	STE	b	626	-	9,9,19	0.35	0	8,8,19	0.74	0
27	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.35	6 (10%)
32	STE	a	616	-	11,11,19	0.84	0	11,11,19	0.86	0
34	LHG	D	410	-	48,48,48	0.79	1 (2%)	51,54,54	1.34	7 (13%)
27	BCR	T	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.22	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	506	-	69,73,73	1.21	8 (11%)	82,113,113	1.31	6 (7%)
29	LMG	D	412	-	31,31,55	0.67	1 (3%)	33,33,63	1.20	2 (6%)
25	CLA	C	501	-	69,73,73	1.32	10 (14%)	82,113,113	1.42	8 (9%)
34	LHG	d	409	-	38,38,48	0.72	1 (2%)	41,44,54	1.17	3 (7%)
25	CLA	C	512	-	69,73,73	1.45	10 (14%)	82,113,113	1.38	9 (10%)
28	PL9	a	611	-	55,55,55	0.76	1 (1%)	68,69,69	1.52	11 (16%)
29	LMG	d	410	-	21,21,55	0.61	0	20,20,63	1.15	0
25	CLA	b	609	-	69,73,73	1.24	9 (13%)	82,113,113	1.36	8 (9%)
25	CLA	b	604	-	69,73,73	1.24	8 (11%)	82,113,113	1.55	12 (14%)
25	CLA	c	502	-	69,73,73	1.26	10 (14%)	82,113,113	1.41	7 (8%)
29	LMG	c	523	-	49,49,55	0.84	2 (4%)	57,57,63	1.30	4 (7%)
31	DGD	C	517	-	63,63,67	0.96	6 (9%)	77,77,81	1.42	9 (11%)
25	CLA	B	614	-	69,73,73	1.39	7 (10%)	82,113,113	1.24	9 (10%)
27	BCR	c	515	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	4 (7%)
25	CLA	b	603	-	69,73,73	1.36	10 (14%)	82,113,113	1.44	12 (14%)
25	CLA	c	504	37	64,68,73	1.21	6 (9%)	76,107,113	1.21	5 (6%)
29	LMG	A	612	-	48,48,55	0.97	3 (6%)	56,56,63	1.31	8 (14%)
35	HEM	F	101	6,5	50,50,50	1.37	8 (16%)	67,82,82	1.17	1 (1%)
25	CLA	C	509	-	69,73,73	1.37	10 (14%)	82,113,113	1.34	9 (10%)
27	BCR	k	101	-	41,41,41	1.07	4 (9%)	56,56,56	1.13	3 (5%)
29	LMG	m	101	-	51,51,55	0.90	3 (5%)	59,59,63	1.47	9 (15%)
31	DGD	c	517	-	63,63,67	1.00	5 (7%)	77,77,81	1.46	12 (15%)
27	BCR	t	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
25	CLA	c	508	-	68,72,73	1.28	9 (13%)	80,111,113	1.29	9 (11%)
25	CLA	C	508	-	69,73,73	1.26	7 (10%)	82,113,113	1.46	11 (13%)
25	CLA	A	606	-	69,73,73	1.22	7 (10%)	82,113,113	1.34	5 (6%)
31	DGD	a	614	-	43,43,67	0.73	2 (4%)	45,45,81	1.46	6 (13%)
25	CLA	a	609	-	69,73,73	1.24	7 (10%)	82,113,113	1.20	8 (9%)
27	BCR	H	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	4 (7%)
25	CLA	B	612	-	69,73,73	1.17	9 (13%)	82,113,113	1.38	11 (13%)
25	CLA	b	602	-	69,73,73	1.39	10 (14%)	82,113,113	1.45	8 (9%)
32	STE	l	102	-	17,17,19	0.33	0	16,16,19	0.95	0
29	LMG	C	519	-	48,48,55	0.86	2 (4%)	56,56,63	1.34	6 (10%)
25	CLA	b	615	-	69,73,73	1.26	8 (11%)	82,113,113	1.42	4 (4%)
31	DGD	c	516	-	63,63,67	1.07	8 (12%)	77,77,81	1.39	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	a	615	-	9,9,19	0.43	0	8,8,19	0.60	0
25	CLA	c	511	3	69,73,73	1.33	6 (8%)	82,113,113	1.33	6 (7%)
29	LMG	d	411	-	44,44,55	0.83	2 (4%)	52,52,63	1.33	6 (11%)
27	BCR	b	617	-	41,41,41	0.99	3 (7%)	56,56,56	1.26	5 (8%)
25	CLA	B	608	-	69,73,73	1.18	7 (10%)	82,113,113	1.32	7 (8%)
34	LHG	d	408	-	48,48,48	0.63	0	51,54,54	1.34	7 (13%)
25	CLA	c	503	-	69,73,73	1.32	8 (11%)	82,113,113	1.44	8 (9%)
27	BCR	B	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	7 (12%)
29	LMG	D	408	-	51,51,55	0.78	1 (1%)	59,59,63	1.24	6 (10%)
25	CLA	C	511	3	69,73,73	1.41	7 (10%)	82,113,113	1.28	3 (3%)
25	CLA	c	505	-	69,73,73	1.28	7 (10%)	82,113,113	1.33	9 (10%)
33	BCT	d	401	23	3,3,3	1.16	0	2,3,3	2.97	1 (50%)
22	OEX	A	602[A]	1,37,3	0,15,15	-	-	-		
31	DGD	C	518	-	63,63,67	0.83	3 (4%)	77,77,81	1.45	12 (15%)
32	STE	J	101	-	11,11,19	0.74	0	11,11,19	1.35	2 (18%)
25	CLA	C	505	-	69,73,73	1.43	7 (10%)	82,113,113	1.33	11 (13%)
29	LMG	M	101	-	51,51,55	0.84	4 (7%)	59,59,63	1.38	7 (11%)
25	CLA	b	616	-	64,68,73	1.14	6 (9%)	76,107,113	1.47	6 (7%)
32	STE	H	103	-	17,17,19	0.37	0	16,16,19	0.80	0
27	BCR	A	610	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	6 (10%)
27	BCR	b	619	-	41,41,41	1.02	2 (4%)	56,56,56	1.20	3 (5%)
32	STE	L	103	-	11,11,19	0.66	0	11,11,19	1.38	1 (9%)
34	LHG	L	102	-	48,48,48	0.72	0	51,54,54	1.25	5 (9%)
25	CLA	d	404	-	69,73,73	1.21	8 (11%)	82,113,113	1.17	9 (10%)
32	STE	C	521	-	11,11,19	0.74	0	11,11,19	1.17	1 (9%)
25	CLA	c	509	-	69,73,73	1.06	4 (5%)	82,113,113	1.51	8 (9%)
25	CLA	b	601	37	69,73,73	1.32	7 (10%)	82,113,113	1.34	6 (7%)
35	HEM	e	101	6,5	50,50,50	1.62	8 (16%)	67,82,82	1.32	9 (13%)
34	LHG	e	102	-	41,41,48	0.79	1 (2%)	44,47,54	1.33	6 (13%)
27	BCR	K	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
25	CLA	C	510	-	69,73,73	1.20	8 (11%)	82,113,113	1.31	7 (8%)
30	SQD	A	614	-	38,38,54	1.78	5 (13%)	40,40,65	1.27	3 (7%)
25	CLA	C	504	37	63,67,73	1.40	12 (19%)	74,105,113	1.32	11 (14%)
25	CLA	B	603	-	69,73,73	1.47	9 (13%)	82,113,113	1.35	8 (9%)
25	CLA	A	607	37	69,73,73	1.18	9 (13%)	82,113,113	1.34	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	I	101	-	14,14,19	0.40	0	13,13,19	0.66	0
32	STE	b	620	-	15,15,19	0.39	0	14,14,19	0.88	0
30	SQD	L	101	-	47,49,54	1.63	10 (21%)	57,60,65	1.93	13 (22%)
25	CLA	D	404	-	69,73,73	1.21	6 (8%)	82,113,113	1.35	7 (8%)
28	PL9	A	611	-	55,55,55	0.91	2 (3%)	68,69,69	1.47	10 (14%)
25	CLA	C	503	-	69,73,73	1.48	12 (17%)	82,113,113	1.36	7 (8%)
28	PL9	D	407	-	55,55,55	0.99	3 (5%)	68,69,69	1.48	14 (20%)
30	SQD	f	101	-	39,41,54	1.70	8 (20%)	49,52,65	1.77	11 (22%)
21	OEY	A	601[B]	1,37,3	0,16,16	-	-	-	-	-
25	CLA	b	614	-	69,73,73	1.26	9 (13%)	82,113,113	1.23	9 (10%)
32	STE	b	623	-	15,15,19	0.80	0	15,15,19	0.89	0
32	STE	M	103	-	9,9,19	0.39	0	8,8,19	0.67	0
34	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.28	8 (15%)
27	BCR	h	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	8 (14%)
27	BCR	k	102	-	41,41,41	1.07	4 (9%)	56,56,56	1.22	6 (10%)
31	DGD	H	102	-	63,63,67	1.16	4 (6%)	77,77,81	1.43	11 (14%)
31	DGD	A	615	-	67,67,67	1.04	7 (10%)	81,81,81	1.41	16 (19%)
25	CLA	b	612	-	69,73,73	1.23	8 (11%)	82,113,113	1.39	12 (14%)
25	CLA	b	610	37	69,73,73	1.31	6 (8%)	82,113,113	1.26	8 (9%)
32	STE	b	624	-	14,14,19	0.29	0	13,13,19	0.98	0
33	BCT	D	401	23	3,3,3	1.13	0	2,3,3	2.86	1 (50%)
32	STE	c	520	-	19,19,19	0.64	0	19,19,19	0.98	0
30	SQD	a	613	-	52,54,54	1.55	6 (11%)	62,65,65	1.98	12 (19%)
25	CLA	D	403	37	69,73,73	1.23	7 (10%)	82,113,113	1.27	7 (8%)
25	CLA	b	607	37	69,73,73	1.32	9 (13%)	82,113,113	1.22	10 (12%)
32	STE	B	620	-	16,16,19	0.69	0	16,16,19	1.11	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
32	STE	c	522	-	-	5/9/9/17	-
27	BCR	C	514	-	-	7/29/63/63	0/2/2/2
34	LHG	D	413	-	-	23/53/53/53	-
32	STE	C	520	-	-	3/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	R	101	-	-	4/9/9/17	-
27	BCR	C	515	-	-	6/29/63/63	0/2/2/2
25	CLA	B	607	37	1/1/15/20	16/39/115/115	-
27	BCR	d	405	-	-	9/29/63/63	0/2/2/2
25	CLA	C	513	-	1/1/15/20	13/39/115/115	-
25	CLA	b	606	-	1/1/15/20	7/39/115/115	-
32	STE	C	522	-	-	5/13/13/17	-
32	STE	b	625	-	-	11/17/17/17	-
25	CLA	a	612	37	1/1/15/20	2/39/115/115	-
25	CLA	B	606	-	1/1/15/20	12/39/115/115	-
25	CLA	B	615	-	1/1/15/20	10/39/115/115	-
25	CLA	c	501	-	1/1/15/20	4/39/115/115	-
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2
28	PL9	d	406	-	-	16/53/73/73	0/1/1/1
25	CLA	c	507	37	1/1/15/20	13/39/115/115	-
25	CLA	B	601	37	1/1/15/20	23/39/115/115	-
26	PHO	A	608	-	-	9/37/103/103	0/5/6/6
29	LMG	c	521	-	-	25/43/63/70	0/1/1/1
32	STE	B	625	-	-	2/13/13/17	-
32	STE	t	103	-	-	3/11/11/17	-
25	CLA	B	616	-	1/1/14/20	8/33/109/115	-
27	BCR	c	514	-	-	7/29/63/63	0/2/2/2
30	SQD	t	102	-	-	19/37/37/69	-
32	STE	M	102	-	-	8/12/12/17	-
32	STE	X	101	-	-	11/17/17/17	-
32	STE	b	621	-	-	10/17/17/17	-
34	LHG	E	101	-	-	29/53/53/53	-
25	CLA	A	609	-	1/1/12/20	5/26/102/115	-
25	CLA	a	606	-	1/1/15/20	3/39/115/115	-
27	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	CLA	B	611	-	1/1/15/20	8/39/115/115	-
25	CLA	c	510	-	1/1/15/20	13/39/115/115	-
36	HEC	v	201	16	-	6/14/54/54	-
25	CLA	D	405	-	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	403	-	1/1/15/20	8/39/115/115	-
26	PHO	d	402	-	-	5/37/103/103	0/5/6/6
27	BCR	D	406	-	-	7/29/63/63	0/2/2/2
29	LMG	B	621	-	-	14/22/22/70	-
32	STE	d	413	-	-	11/17/17/17	-
32	STE	B	623	-	-	5/9/9/17	-
29	LMG	c	519	-	-	10/31/51/70	0/1/1/1
32	STE	B	624	-	-	4/9/9/17	-
30	SQD	D	409	-	-	14/28/48/69	0/1/1/1
34	LHG	D	411	-	-	19/51/51/53	-
34	LHG	d	407	-	-	18/53/53/53	-
25	CLA	c	513	-	1/1/15/20	11/39/115/115	-
25	CLA	B	604	-	1/1/15/20	16/39/115/115	-
25	CLA	C	507	37	1/1/15/20	11/39/115/115	-
32	STE	d	412	-	-	7/14/14/17	-
25	CLA	c	506	-	1/1/15/20	12/39/115/115	-
30	SQD	B	622	-	-	24/49/69/69	0/1/1/1
25	CLA	b	605	-	1/1/15/20	9/39/115/115	-
31	DGD	C	516	-	-	23/51/91/95	0/2/2/2
25	CLA	B	602	-	1/1/15/20	9/39/115/115	-
32	STE	j	101	-	-	5/9/9/17	-
29	LMG	b	622	-	-	24/50/70/70	0/1/1/1
25	CLA	B	610	37	1/1/15/20	5/39/115/115	-
25	CLA	c	512	-	1/1/15/20	20/39/115/115	-
27	BCR	B	617	-	-	4/29/63/63	0/2/2/2
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
25	CLA	b	613	-	1/1/15/20	11/39/115/115	-
25	CLA	a	607	37	1/1/15/20	16/39/115/115	-
26	PHO	D	402	-	-	2/37/103/103	0/5/6/6
25	CLA	B	605	-	1/1/15/20	11/39/115/115	-
25	CLA	B	609	-	-	7/39/115/115	-
25	CLA	b	608	-	1/1/15/20	7/39/115/115	-
25	CLA	C	502	-	1/1/15/20	11/39/115/115	-
25	CLA	b	611	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HEC	V	201	16	-	6/14/54/54	-
31	DGD	h	102	-	-	14/51/91/95	0/2/2/2
32	STE	t	104	-	-	9/15/15/17	-
25	CLA	B	613	-	1/1/15/20	15/39/115/115	-
26	PHO	a	608	-	-	4/37/103/103	0/5/6/6
27	BCR	K	101	-	-	7/29/63/63	0/2/2/2
30	SQD	A	613	-	-	19/47/67/69	0/1/1/1
32	STE	b	626	-	-	2/7/7/17	-
27	BCR	B	619	-	-	8/29/63/63	0/2/2/2
32	STE	a	616	-	-	4/9/9/17	-
34	LHG	D	410	-	-	19/53/53/53	-
27	BCR	T	101	-	-	7/29/63/63	0/2/2/2
25	CLA	C	506	-	1/1/15/20	13/39/115/115	-
29	LMG	D	412	-	-	19/33/33/70	-
25	CLA	C	501	-	1/1/15/20	7/39/115/115	-
34	LHG	d	409	-	-	12/43/43/53	-
25	CLA	C	512	-	1/1/15/20	10/39/115/115	-
28	PL9	a	611	-	-	23/53/73/73	0/1/1/1
29	LMG	d	410	-	-	13/17/17/70	-
25	CLA	b	609	-	1/1/15/20	8/39/115/115	-
25	CLA	b	604	-	1/1/15/20	7/39/115/115	-
25	CLA	c	502	-	-	6/39/115/115	-
29	LMG	c	523	-	-	28/44/64/70	0/1/1/1
31	DGD	C	517	-	-	21/51/91/95	0/2/2/2
25	CLA	B	614	-	1/1/15/20	18/39/115/115	-
27	BCR	c	515	-	-	3/29/63/63	0/2/2/2
25	CLA	b	603	-	1/1/15/20	7/39/115/115	-
25	CLA	c	504	37	1/1/14/20	8/33/109/115	-
29	LMG	A	612	-	-	19/43/63/70	0/1/1/1
35	HEM	F	101	6,5	-	2/14/54/54	-
25	CLA	C	509	-	1/1/15/20	13/39/115/115	-
27	BCR	k	101	-	-	8/29/63/63	0/2/2/2
29	LMG	m	101	-	-	20/46/66/70	0/1/1/1
31	DGD	c	517	-	-	19/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	t	101	-	-	7/29/63/63	0/2/2/2
25	CLA	c	508	-	-	6/38/114/115	-
25	CLA	C	508	-	-	5/39/115/115	-
25	CLA	A	606	-	1/1/15/20	3/39/115/115	-
31	DGD	a	614	-	-	26/45/45/95	-
25	CLA	a	609	-	1/1/15/20	6/39/115/115	-
27	BCR	H	101	-	-	4/29/63/63	0/2/2/2
25	CLA	B	612	-	1/1/15/20	12/39/115/115	-
25	CLA	b	602	-	1/1/15/20	8/39/115/115	-
32	STE	l	102	-	-	7/15/15/17	-
29	LMG	C	519	-	-	18/43/63/70	0/1/1/1
25	CLA	b	615	-	1/1/15/20	17/39/115/115	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
32	STE	a	615	-	-	5/7/7/17	-
25	CLA	c	511	3	1/1/15/20	16/39/115/115	-
29	LMG	d	411	-	-	10/39/59/70	0/1/1/1
27	BCR	b	617	-	-	6/29/63/63	0/2/2/2
25	CLA	B	608	-	1/1/15/20	5/39/115/115	-
34	LHG	d	408	-	-	20/53/53/53	-
25	CLA	c	503	-	-	15/39/115/115	-
27	BCR	B	618	-	-	8/29/63/63	0/2/2/2
29	LMG	D	408	-	-	21/46/66/70	0/1/1/1
25	CLA	C	511	3	1/1/15/20	6/39/115/115	-
25	CLA	c	505	-	1/1/15/20	11/39/115/115	-
31	DGD	C	518	-	-	14/51/91/95	0/2/2/2
32	STE	J	101	-	-	3/9/9/17	-
25	CLA	C	505	-	1/1/15/20	12/39/115/115	-
29	LMG	M	101	-	-	20/46/66/70	0/1/1/1
25	CLA	b	616	-	1/1/14/20	13/33/109/115	-
32	STE	H	103	-	-	10/15/15/17	-
27	BCR	A	610	-	-	2/29/63/63	0/2/2/2
27	BCR	b	619	-	-	6/29/63/63	0/2/2/2
32	STE	L	103	-	-	6/9/9/17	-
34	LHG	L	102	-	-	20/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	404	-	1/1/15/20	7/39/115/115	-
32	STE	C	521	-	-	5/9/9/17	-
25	CLA	c	509	-	1/1/15/20	5/39/115/115	-
25	CLA	b	601	37	1/1/15/20	21/39/115/115	-
35	HEM	e	101	6,5	-	3/14/54/54	-
34	LHG	e	102	-	-	22/46/46/53	-
27	BCR	K	102	-	-	6/29/63/63	0/2/2/2
25	CLA	C	510	-	1/1/15/20	9/39/115/115	-
30	SQD	A	614	-	-	14/39/39/69	-
25	CLA	C	504	37	1/1/13/20	7/32/108/115	-
25	CLA	B	603	-	1/1/15/20	9/39/115/115	-
25	CLA	A	607	37	-	7/39/115/115	-
32	STE	I	101	-	-	5/12/12/17	-
32	STE	b	620	-	-	5/13/13/17	-
30	SQD	L	101	-	-	25/44/64/69	0/1/1/1
25	CLA	D	404	-	-	17/39/115/115	-
28	PL9	A	611	-	-	21/53/73/73	0/1/1/1
25	CLA	C	503	-	1/1/15/20	11/39/115/115	-
28	PL9	D	407	-	-	15/53/73/73	0/1/1/1
30	SQD	f	101	-	-	15/36/56/69	0/1/1/1
25	CLA	b	614	-	1/1/15/20	18/39/115/115	-
32	STE	b	623	-	-	8/13/13/17	-
32	STE	M	103	-	-	3/7/7/17	-
34	LHG	l	101	-	-	20/53/53/53	-
27	BCR	h	101	-	-	4/29/63/63	0/2/2/2
27	BCR	k	102	-	-	5/29/63/63	0/2/2/2
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
31	DGD	A	615	-	-	22/55/95/95	0/2/2/2
25	CLA	b	612	-	1/1/15/20	10/39/115/115	-
25	CLA	b	610	37	1/1/15/20	9/39/115/115	-
32	STE	b	624	-	-	9/12/12/17	-
32	STE	c	520	-	-	14/17/17/17	-
30	SQD	a	613	-	-	23/49/69/69	0/1/1/1
25	CLA	D	403	37	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	607	37	1/1/15/20	14/39/115/115	-
32	STE	B	620	-	-	10/14/14/17	-

All (821) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	402	PHO	C1B-C2B	9.20	1.49	1.39
26	d	402	PHO	C3B-C4B	9.00	1.50	1.41
26	a	608	PHO	C1B-C2B	8.90	1.49	1.39
26	D	402	PHO	C1B-C2B	8.81	1.49	1.39
26	D	402	PHO	C3B-C4B	8.52	1.50	1.41
25	B	603	CLA	MG-NA	8.19	2.25	2.06
26	A	608	PHO	C1B-C2B	8.03	1.48	1.39
26	a	608	PHO	C3B-C4B	7.65	1.49	1.41
26	A	608	PHO	C3B-C4B	7.02	1.48	1.41
25	b	606	CLA	MG-NA	6.91	2.22	2.06
25	C	511	CLA	MG-NA	6.65	2.22	2.06
36	V	201	HEC	CAC-C3C	6.45	1.56	1.35
36	v	201	HEC	CAB-C3B	6.33	1.55	1.35
36	v	201	HEC	CAC-C3C	6.22	1.55	1.35
35	e	101	HEM	FE-NA	6.19	2.15	1.95
36	V	201	HEC	CAB-C3B	5.76	1.53	1.35
25	B	607	CLA	MG-NA	5.72	2.19	2.06
25	b	610	CLA	MG-NB	-5.61	1.94	2.05
30	A	614	SQD	O47-C45	-5.53	1.37	1.47
25	b	603	CLA	MG-NA	5.47	2.19	2.06
36	v	201	HEC	C3D-C2D	5.44	1.53	1.38
25	C	505	CLA	MG-NA	5.37	2.19	2.06
25	c	511	CLA	MG-NA	5.35	2.19	2.06
25	B	606	CLA	MG-NA	5.31	2.18	2.06
25	b	608	CLA	MG-NA	5.30	2.18	2.06
25	a	612	CLA	MG-NA	5.21	2.18	2.06
25	b	602	CLA	MG-NA	5.20	2.18	2.06
25	C	512	CLA	MG-NA	5.18	2.18	2.06
25	D	404	CLA	MG-NC	5.16	2.18	2.06
25	C	505	CLA	MG-ND	-5.14	1.95	2.05
25	C	503	CLA	MG-ND	5.11	2.15	2.05
25	b	613	CLA	MG-NA	5.09	2.18	2.06
30	D	409	SQD	O48-C23	5.07	1.48	1.33
25	B	614	CLA	MG-ND	-5.06	1.95	2.05
25	D	405	CLA	MG-NB	-5.03	1.95	2.05
30	L	101	SQD	O48-C23	4.99	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	V	201	HEC	C3D-C2D	4.97	1.51	1.38
25	c	505	CLA	MG-NA	4.89	2.17	2.06
25	b	607	CLA	MG-NB	-4.88	1.96	2.05
35	e	101	HEM	FE-NB	4.87	2.09	1.94
25	B	601	CLA	MG-NA	4.86	2.17	2.06
30	A	613	SQD	O48-C23	4.75	1.47	1.33
25	C	501	CLA	MG-NA	4.72	2.17	2.06
30	f	101	SQD	O48-C23	4.69	1.47	1.33
25	C	502	CLA	MG-NA	4.66	2.17	2.06
30	a	613	SQD	O48-C23	4.62	1.46	1.33
30	B	622	SQD	O48-C23	4.61	1.46	1.33
25	b	612	CLA	MG-ND	-4.61	1.96	2.05
30	t	102	SQD	O48-C23	4.59	1.46	1.33
25	B	615	CLA	MG-NA	4.57	2.17	2.06
25	C	509	CLA	MG-NA	4.57	2.17	2.06
25	b	601	CLA	MG-NA	4.57	2.17	2.06
25	a	612	CLA	MG-ND	-4.56	1.96	2.05
30	A	614	SQD	O48-C23	4.55	1.46	1.33
25	c	507	CLA	MG-NA	4.55	2.17	2.06
25	b	615	CLA	MG-NA	4.48	2.16	2.06
25	C	504	CLA	MG-NA	4.45	2.16	2.06
25	C	512	CLA	MG-ND	-4.33	1.97	2.05
25	C	513	CLA	MG-NA	4.32	2.16	2.06
25	c	503	CLA	MG-NB	4.30	2.14	2.05
25	c	501	CLA	MG-NC	4.27	2.16	2.06
25	a	606	CLA	MG-NA	4.25	2.16	2.06
25	C	508	CLA	MG-NA	4.17	2.16	2.06
25	D	403	CLA	C1D-ND	4.13	1.43	1.37
25	B	604	CLA	MG-NA	4.11	2.16	2.06
25	c	506	CLA	C1D-ND	4.08	1.43	1.37
25	c	508	CLA	C1D-ND	4.05	1.43	1.37
27	K	102	BCR	C1-C6	-4.03	1.48	1.53
25	B	602	CLA	C1D-ND	4.01	1.43	1.37
26	d	402	PHO	C1D-C2D	4.01	1.44	1.39
27	B	617	BCR	C1-C6	-3.96	1.48	1.53
25	c	513	CLA	MG-ND	-3.96	1.97	2.05
25	b	602	CLA	MG-NB	-3.95	1.98	2.05
25	B	605	CLA	MG-NB	3.94	2.13	2.05
30	a	613	SQD	O47-C45	-3.92	1.37	1.46
25	b	609	CLA	C1D-ND	3.91	1.43	1.37
34	D	413	LHG	O7-C5	-3.87	1.37	1.46
25	a	609	CLA	C1D-ND	3.86	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	C1D-ND	3.86	1.42	1.37
25	b	607	CLA	C1D-ND	3.86	1.42	1.37
27	C	515	BCR	C1-C6	-3.85	1.48	1.53
25	B	616	CLA	C1D-ND	3.85	1.42	1.37
25	c	512	CLA	MG-NB	3.85	2.13	2.05
26	a	608	PHO	C1D-C2D	3.84	1.43	1.39
25	b	613	CLA	MG-ND	-3.84	1.98	2.05
25	C	503	CLA	MG-NA	3.84	2.15	2.06
27	C	514	BCR	C1-C6	-3.83	1.48	1.53
25	a	606	CLA	C1D-ND	3.83	1.42	1.37
27	D	406	BCR	C30-C25	-3.80	1.48	1.53
25	b	614	CLA	C4B-NB	3.79	1.42	1.37
26	D	402	PHO	C1D-C2D	3.79	1.43	1.39
25	D	403	CLA	MG-NA	3.78	2.15	2.06
25	C	513	CLA	C1D-ND	3.76	1.42	1.37
25	C	502	CLA	MG-NB	-3.76	1.98	2.05
25	b	612	CLA	C1D-ND	3.73	1.42	1.37
25	c	503	CLA	C1D-ND	3.73	1.42	1.37
25	C	509	CLA	MG-ND	3.73	2.13	2.05
25	C	506	CLA	MG-NA	3.73	2.15	2.06
30	B	622	SQD	O47-C7	3.73	1.44	1.34
25	B	613	CLA	C1D-ND	3.73	1.42	1.37
25	a	612	CLA	C1D-ND	3.71	1.42	1.37
25	b	608	CLA	MG-NB	3.70	2.13	2.05
30	t	102	SQD	O47-C7	3.69	1.44	1.34
27	c	515	BCR	C1-C6	-3.69	1.49	1.53
25	A	606	CLA	C1D-ND	3.69	1.42	1.37
25	c	503	CLA	MG-NA	3.69	2.15	2.06
31	A	615	DGD	C4D-C5D	3.68	1.60	1.53
25	c	504	CLA	C4B-NB	3.65	1.42	1.37
30	f	101	SQD	O47-C7	3.65	1.44	1.34
30	A	614	SQD	O47-C7	3.65	1.44	1.34
27	H	101	BCR	C30-C25	-3.64	1.49	1.53
27	b	618	BCR	C30-C25	-3.63	1.49	1.53
25	d	403	CLA	C1D-ND	3.63	1.42	1.37
26	A	608	PHO	C4D-CHA	3.61	1.44	1.39
25	B	608	CLA	MG-NA	3.60	2.14	2.06
25	D	405	CLA	C1D-ND	3.60	1.42	1.37
25	b	611	CLA	C1D-ND	3.60	1.42	1.37
27	K	102	BCR	C30-C25	-3.60	1.49	1.53
25	C	506	CLA	C1D-ND	3.60	1.42	1.37
27	B	618	BCR	C30-C25	-3.59	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	CLA	C1D-ND	3.59	1.42	1.37
25	c	510	CLA	MG-NA	3.58	2.14	2.06
25	B	614	CLA	MG-NC	3.58	2.14	2.06
27	h	101	BCR	C30-C25	-3.57	1.49	1.53
25	B	614	CLA	C1D-ND	3.56	1.42	1.37
25	c	501	CLA	C1D-ND	3.55	1.42	1.37
25	B	604	CLA	MG-NC	3.54	2.14	2.06
25	B	607	CLA	C1D-ND	3.54	1.42	1.37
25	C	504	CLA	C4B-NB	3.54	1.42	1.37
25	b	613	CLA	C1D-ND	3.53	1.42	1.37
26	D	402	PHO	C4D-CHA	3.52	1.44	1.39
25	b	616	CLA	C1D-ND	3.51	1.42	1.37
25	B	601	CLA	C4B-NB	3.51	1.42	1.37
28	d	406	PL9	C3-C4	-3.51	1.44	1.49
25	A	606	CLA	C1B-C2B	3.50	1.51	1.43
27	A	610	BCR	C1-C6	-3.50	1.49	1.53
30	A	613	SQD	O47-C7	3.50	1.44	1.34
25	B	601	CLA	C1D-ND	3.50	1.42	1.37
29	A	612	LMG	C4-C3	3.50	1.61	1.52
30	L	101	SQD	O47-C7	3.50	1.44	1.34
25	c	513	CLA	C1D-ND	3.49	1.42	1.37
25	B	604	CLA	C1D-ND	3.49	1.42	1.37
25	b	603	CLA	C1D-ND	3.49	1.42	1.37
25	B	613	CLA	MG-ND	-3.47	1.98	2.05
25	d	404	CLA	MG-ND	-3.46	1.98	2.05
25	C	511	CLA	C1D-ND	3.46	1.42	1.37
25	b	614	CLA	C1D-ND	3.46	1.42	1.37
27	c	514	BCR	C1-C6	-3.45	1.49	1.53
25	B	602	CLA	C4B-NB	3.45	1.42	1.37
25	b	601	CLA	C1D-ND	3.44	1.42	1.37
30	A	613	SQD	O47-C45	-3.43	1.38	1.46
25	c	511	CLA	C1D-ND	3.43	1.42	1.37
25	b	602	CLA	C1D-ND	3.42	1.42	1.37
25	B	612	CLA	MG-ND	-3.42	1.99	2.05
25	c	510	CLA	C1D-ND	3.42	1.42	1.37
30	t	102	SQD	C24-C23	3.40	1.60	1.50
25	B	602	CLA	MG-NA	3.40	2.14	2.06
34	D	411	LHG	P-O6	3.40	1.72	1.59
30	D	409	SQD	C24-C23	3.39	1.60	1.50
27	K	101	BCR	C30-C25	-3.39	1.49	1.53
26	a	608	PHO	C4D-CHA	3.39	1.44	1.39
25	B	601	CLA	MG-NB	-3.38	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	613	CLA	C4B-NB	3.38	1.42	1.37
25	C	507	CLA	C1D-ND	3.38	1.42	1.37
30	B	622	SQD	O47-C45	-3.37	1.38	1.46
25	C	502	CLA	C1D-ND	3.37	1.42	1.37
25	c	507	CLA	C1D-ND	3.37	1.42	1.37
26	a	608	PHO	C3D-C4D	3.37	1.45	1.41
27	k	101	BCR	C1-C6	-3.37	1.49	1.53
25	C	503	CLA	C1D-ND	3.36	1.42	1.37
25	C	501	CLA	C1D-ND	3.36	1.42	1.37
25	C	505	CLA	C4B-NB	3.36	1.42	1.37
25	c	506	CLA	MG-NA	3.36	2.14	2.06
27	C	514	BCR	C30-C25	-3.36	1.49	1.53
25	B	611	CLA	C1D-ND	3.34	1.42	1.37
25	C	503	CLA	MG-NC	3.33	2.14	2.06
25	B	614	CLA	C4B-NB	3.33	1.42	1.37
25	d	404	CLA	C1D-ND	3.33	1.42	1.37
25	b	601	CLA	C4B-NB	3.33	1.42	1.37
25	C	509	CLA	C1D-ND	3.33	1.42	1.37
27	D	406	BCR	C1-C6	-3.32	1.49	1.53
25	b	615	CLA	C1D-ND	3.32	1.42	1.37
25	C	501	CLA	C4B-NB	3.32	1.42	1.37
25	b	605	CLA	C1D-ND	3.31	1.42	1.37
25	C	512	CLA	MG-NB	3.31	2.12	2.05
25	c	512	CLA	C1D-ND	3.29	1.42	1.37
25	B	615	CLA	C4B-NB	3.29	1.42	1.37
25	b	604	CLA	C1D-ND	3.29	1.42	1.37
27	k	102	BCR	C1-C6	-3.29	1.49	1.53
25	b	608	CLA	C1D-ND	3.28	1.42	1.37
34	l	101	LHG	O7-C5	-3.28	1.38	1.46
30	f	101	SQD	O47-C45	-3.28	1.38	1.46
31	C	516	DGD	C4E-C3E	3.28	1.60	1.52
26	d	402	PHO	C4D-CHA	3.27	1.44	1.39
25	D	404	CLA	C1D-ND	3.25	1.42	1.37
25	C	507	CLA	C4B-NB	3.24	1.42	1.37
25	C	503	CLA	MG-NB	-3.24	1.99	2.05
25	c	502	CLA	C1D-ND	3.23	1.42	1.37
28	A	611	PL9	C7-C3	-3.23	1.47	1.51
25	D	405	CLA	C1B-C2B	3.23	1.50	1.43
31	c	516	DGD	O2G-C2G	-3.23	1.39	1.46
25	c	509	CLA	C1D-ND	3.22	1.42	1.37
25	A	606	CLA	C4B-NB	3.22	1.42	1.37
27	d	405	BCR	C1-C6	-3.21	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	605	CLA	C1D-ND	3.21	1.42	1.37
25	B	612	CLA	C1D-ND	3.20	1.42	1.37
25	b	605	CLA	C4B-NB	3.19	1.42	1.37
25	c	502	CLA	MG-NB	-3.19	1.99	2.05
25	b	606	CLA	C1D-ND	3.18	1.42	1.37
28	a	611	PL9	C53-C6	-3.18	1.44	1.50
25	C	512	CLA	C1D-ND	3.18	1.42	1.37
30	f	101	SQD	C24-C23	3.17	1.59	1.50
25	C	511	CLA	C1B-C2B	3.17	1.50	1.43
25	c	509	CLA	C1B-C2B	3.17	1.50	1.43
30	A	614	SQD	C24-C23	3.16	1.59	1.50
25	b	607	CLA	C4B-NB	3.15	1.42	1.37
25	B	614	CLA	MG-NA	3.15	2.13	2.06
28	d	406	PL9	C7-C3	-3.14	1.47	1.51
25	B	602	CLA	MG-NB	3.14	2.12	2.05
35	F	101	HEM	FE-NB	3.13	2.04	1.94
25	C	513	CLA	C4B-NB	3.12	1.42	1.37
25	B	602	CLA	C1B-C2B	3.12	1.50	1.43
25	a	607	CLA	C4B-NB	3.11	1.41	1.37
30	a	613	SQD	O47-C7	3.11	1.43	1.34
30	L	101	SQD	O5-C1	3.10	1.49	1.41
25	c	512	CLA	C1B-C2B	3.10	1.50	1.43
25	B	605	CLA	MG-ND	-3.10	1.99	2.05
27	B	619	BCR	C1-C6	-3.09	1.49	1.53
30	t	102	SQD	O47-C45	-3.09	1.39	1.46
25	B	608	CLA	C4B-NB	3.08	1.41	1.37
25	c	505	CLA	C4B-NB	3.08	1.41	1.37
25	B	616	CLA	C1B-C2B	3.08	1.50	1.43
27	b	619	BCR	C1-C6	-3.08	1.49	1.53
25	C	503	CLA	C4B-NB	3.08	1.41	1.37
25	a	607	CLA	C1D-ND	3.07	1.41	1.37
25	A	607	CLA	MG-ND	3.07	2.11	2.05
25	C	509	CLA	MG-NB	-3.07	1.99	2.05
25	C	505	CLA	CHC-C1C	3.07	1.44	1.38
29	m	101	LMG	C4-C3	3.06	1.60	1.52
35	F	101	HEM	FE-NA	3.06	2.05	1.95
25	b	601	CLA	C1B-C2B	3.04	1.50	1.43
26	D	402	PHO	CMC-C2C	-3.04	1.45	1.50
25	B	613	CLA	C1B-C2B	3.04	1.50	1.43
25	C	510	CLA	MG-NA	3.04	2.13	2.06
27	k	101	BCR	C30-C25	-3.03	1.49	1.53
27	b	618	BCR	C1-C6	-3.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	C1B-C2B	3.03	1.50	1.43
31	H	102	DGD	O5D-C1E	3.02	1.45	1.40
25	c	508	CLA	C4B-NB	3.02	1.41	1.37
30	a	613	SQD	O5-C1	3.02	1.49	1.41
30	A	613	SQD	C24-C23	3.02	1.59	1.50
31	a	614	DGD	O1G-C1A	3.01	1.42	1.33
25	B	615	CLA	C1D-ND	3.01	1.41	1.37
25	c	513	CLA	C4B-NB	3.01	1.41	1.37
25	a	609	CLA	MG-NC	-3.01	1.99	2.06
25	c	508	CLA	C1B-C2B	3.00	1.50	1.43
25	b	602	CLA	C1B-C2B	3.00	1.50	1.43
26	A	608	PHO	CMC-C2C	-3.00	1.45	1.50
25	B	606	CLA	C1B-C2B	3.00	1.50	1.43
25	B	601	CLA	C1B-C2B	3.00	1.50	1.43
27	C	515	BCR	C30-C25	-3.00	1.49	1.53
25	a	612	CLA	C1B-C2B	2.99	1.50	1.43
27	d	405	BCR	C30-C25	-2.99	1.50	1.53
25	c	511	CLA	C1B-C2B	2.99	1.50	1.43
27	t	101	BCR	C1-C6	-2.97	1.50	1.53
25	c	507	CLA	C1B-C2B	2.96	1.50	1.43
25	B	610	CLA	C1D-ND	2.96	1.41	1.37
25	b	604	CLA	MG-NA	2.95	2.13	2.06
25	B	604	CLA	C1B-C2B	2.95	1.50	1.43
30	a	613	SQD	C24-C23	2.94	1.59	1.50
25	c	511	CLA	C4B-NB	2.94	1.41	1.37
25	C	509	CLA	C4B-NB	2.94	1.41	1.37
25	a	609	CLA	C1B-C2B	2.93	1.50	1.43
25	b	605	CLA	C1B-C2B	2.93	1.50	1.43
30	B	622	SQD	C24-C23	2.92	1.59	1.50
25	c	510	CLA	C1B-C2B	2.92	1.50	1.43
25	B	602	CLA	CHC-C1C	2.92	1.44	1.38
25	c	502	CLA	C1B-C2B	2.91	1.50	1.43
25	B	610	CLA	C1B-C2B	2.91	1.49	1.43
26	A	608	PHO	C1D-C2D	2.91	1.42	1.39
25	B	606	CLA	C4B-NB	2.90	1.41	1.37
25	c	508	CLA	MG-NA	2.90	2.13	2.06
25	c	512	CLA	C4B-NB	2.90	1.41	1.37
25	C	512	CLA	C4B-NB	2.90	1.41	1.37
25	b	609	CLA	C1B-C2B	2.90	1.49	1.43
25	b	603	CLA	MG-ND	-2.89	2.00	2.05
25	B	605	CLA	C1B-C2B	2.89	1.49	1.43
30	L	101	SQD	C24-C23	2.89	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	101	SQD	O47-C45	-2.88	1.39	1.46
35	e	101	HEM	CAC-C3C	2.88	1.55	1.47
25	C	508	CLA	C4B-NB	2.88	1.41	1.37
25	b	616	CLA	C1B-C2B	2.88	1.49	1.43
25	c	506	CLA	C4B-NB	2.88	1.41	1.37
25	B	609	CLA	C1D-ND	2.88	1.41	1.37
29	M	101	LMG	C4-C5	2.87	1.59	1.53
34	d	407	LHG	O7-C5	-2.87	1.39	1.46
25	a	606	CLA	CHC-C1C	2.87	1.44	1.38
26	D	402	PHO	CMD-C2D	-2.87	1.45	1.51
25	C	505	CLA	C1D-ND	2.86	1.41	1.37
25	b	610	CLA	C1B-C2B	2.86	1.49	1.43
25	C	502	CLA	C4B-NB	2.86	1.41	1.37
27	K	101	BCR	C1-C6	-2.86	1.50	1.53
25	b	608	CLA	CHC-C1C	2.86	1.44	1.38
25	C	502	CLA	C1B-C2B	2.86	1.49	1.43
25	C	513	CLA	C1B-C2B	2.86	1.49	1.43
25	b	604	CLA	C4B-NB	2.85	1.41	1.37
25	B	603	CLA	C1B-C2B	2.85	1.49	1.43
25	D	404	CLA	C1B-C2B	2.85	1.49	1.43
29	d	411	LMG	O7-C8	-2.84	1.39	1.46
25	B	611	CLA	MG-NA	2.84	2.13	2.06
25	B	608	CLA	C1B-C2B	2.84	1.49	1.43
25	C	504	CLA	C1D-ND	2.84	1.41	1.37
25	b	615	CLA	C1B-C2B	2.83	1.49	1.43
25	b	604	CLA	MG-NC	2.83	2.13	2.06
25	B	610	CLA	C3B-C4B	2.83	1.51	1.42
30	B	622	SQD	O5-C1	2.83	1.49	1.41
29	c	521	LMG	C3-C2	2.82	1.59	1.52
31	H	102	DGD	C6D-C5D	2.82	1.60	1.51
25	c	505	CLA	C3B-C4B	2.81	1.50	1.42
27	k	102	BCR	C30-C25	-2.81	1.50	1.53
25	c	505	CLA	CHC-C1C	2.81	1.44	1.38
25	b	606	CLA	C1B-C2B	2.80	1.49	1.43
25	C	508	CLA	C3B-C4B	2.80	1.50	1.42
25	C	507	CLA	MG-NA	2.80	2.12	2.06
25	C	501	CLA	CHC-C1C	2.80	1.44	1.38
25	B	610	CLA	C4B-NB	2.80	1.41	1.37
25	c	501	CLA	C1B-C2B	2.80	1.49	1.43
25	C	507	CLA	C1B-C2B	2.79	1.49	1.43
29	B	621	LMG	O8-C28	2.79	1.40	1.30
25	d	404	CLA	C4B-NB	2.79	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	615	CLA	C1B-C2B	2.78	1.49	1.43
25	C	508	CLA	C1B-C2B	2.78	1.49	1.43
31	C	516	DGD	O2G-C2G	-2.77	1.40	1.46
27	b	617	BCR	C30-C25	-2.77	1.50	1.53
25	C	510	CLA	C1D-ND	2.77	1.41	1.37
30	f	101	SQD	O5-C1	2.77	1.49	1.41
25	C	501	CLA	C3B-C4B	2.77	1.50	1.42
34	d	407	LHG	C24-C23	2.77	1.58	1.50
25	C	503	CLA	C1B-C2B	2.77	1.49	1.43
25	C	504	CLA	CHC-C1C	2.76	1.44	1.38
26	d	402	PHO	CMC-C2C	-2.76	1.46	1.50
31	C	517	DGD	O6D-C5D	-2.76	1.37	1.44
25	B	607	CLA	MG-NB	-2.76	2.00	2.05
25	c	505	CLA	C1B-C2B	2.76	1.49	1.43
25	b	612	CLA	C4B-NB	2.76	1.41	1.37
27	c	514	BCR	C30-C25	-2.76	1.50	1.53
27	a	610	BCR	C1-C6	-2.75	1.50	1.53
25	b	611	CLA	MG-NA	2.75	2.12	2.06
25	C	510	CLA	C1B-C2B	2.74	1.49	1.43
25	c	504	CLA	C1B-C2B	2.74	1.49	1.43
25	b	613	CLA	MG-NC	2.74	2.12	2.06
25	b	614	CLA	C1B-C2B	2.74	1.49	1.43
25	c	503	CLA	C1B-C2B	2.74	1.49	1.43
25	C	510	CLA	CHC-C1C	2.73	1.44	1.38
25	b	610	CLA	C4B-NB	2.73	1.41	1.37
26	A	608	PHO	C3D-C4D	2.73	1.44	1.41
25	c	513	CLA	C1B-C2B	2.72	1.49	1.43
30	A	614	SQD	C46-C45	2.72	1.56	1.50
27	b	617	BCR	C1-C6	-2.72	1.50	1.53
28	d	406	PL9	C6-C1	-2.72	1.44	1.48
25	B	606	CLA	C1D-ND	2.72	1.41	1.37
25	C	506	CLA	C4B-NB	2.72	1.41	1.37
25	A	606	CLA	CHC-C1C	2.71	1.43	1.38
35	F	101	HEM	CAB-C3B	2.71	1.54	1.47
25	A	609	CLA	C4B-NB	2.71	1.41	1.37
25	D	405	CLA	C4B-NB	2.71	1.41	1.37
25	A	607	CLA	C4B-NB	2.71	1.41	1.37
25	B	609	CLA	MG-NA	2.70	2.12	2.06
25	c	502	CLA	MG-NA	2.70	2.12	2.06
25	B	602	CLA	C3B-C4B	2.70	1.50	1.42
25	b	606	CLA	MG-ND	2.69	2.11	2.05
25	C	512	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	619	BCR	C30-C25	-2.69	1.50	1.53
25	B	608	CLA	C1D-ND	2.69	1.41	1.37
25	B	613	CLA	C4B-NB	2.68	1.41	1.37
26	A	608	PHO	CMD-C2D	-2.68	1.46	1.51
25	b	615	CLA	C4B-NB	2.68	1.41	1.37
25	C	512	CLA	C3B-C4B	2.68	1.50	1.42
25	c	511	CLA	C3B-C4B	2.67	1.50	1.42
27	t	101	BCR	C30-C25	-2.67	1.50	1.53
34	l	101	LHG	O8-C23	2.67	1.41	1.33
25	A	607	CLA	CHC-C1C	2.66	1.43	1.38
25	a	606	CLA	MG-NC	2.66	2.12	2.06
25	c	513	CLA	C3B-C4B	2.66	1.50	1.42
25	b	611	CLA	C4B-NB	2.66	1.41	1.37
25	B	616	CLA	MG-NA	2.66	2.12	2.06
25	B	603	CLA	C3B-C4B	2.65	1.50	1.42
34	E	101	LHG	P-O6	2.65	1.69	1.59
25	b	603	CLA	MG-NB	2.65	2.11	2.05
34	D	410	LHG	O7-C5	-2.65	1.40	1.46
25	c	508	CLA	MG-NB	2.65	2.11	2.05
25	C	504	CLA	C3B-C4B	2.65	1.50	1.42
25	B	611	CLA	C1B-C2B	2.64	1.49	1.43
25	d	404	CLA	C1B-C2B	2.64	1.49	1.43
25	C	505	CLA	C1B-C2B	2.64	1.49	1.43
25	c	502	CLA	C4B-NB	2.63	1.41	1.37
25	b	601	CLA	CHC-C1C	2.63	1.43	1.38
25	B	611	CLA	CHC-C1C	2.63	1.43	1.38
25	a	606	CLA	C1B-C2B	2.63	1.49	1.43
25	B	616	CLA	MG-NC	2.63	2.12	2.06
35	F	101	HEM	FE-NC	2.63	2.03	1.95
31	A	615	DGD	C3D-C2D	2.63	1.59	1.52
25	A	607	CLA	C1D-ND	2.62	1.41	1.37
25	b	605	CLA	MG-NA	2.62	2.12	2.06
25	b	604	CLA	C1B-C2B	2.62	1.49	1.43
25	c	506	CLA	MG-ND	-2.61	2.00	2.05
35	e	101	HEM	CAB-C3B	2.61	1.54	1.47
31	C	517	DGD	O1G-C1G	-2.61	1.39	1.45
35	F	101	HEM	CAC-C3C	2.61	1.54	1.47
25	b	611	CLA	MG-NC	2.61	2.12	2.06
25	B	609	CLA	C4B-NB	2.61	1.41	1.37
25	C	508	CLA	C1D-ND	2.60	1.41	1.37
25	C	510	CLA	C4B-NB	2.60	1.41	1.37
25	A	609	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	504	CLA	C1B-C2B	2.60	1.49	1.43
28	D	407	PL9	C3-C4	-2.59	1.45	1.49
25	B	612	CLA	MG-NA	2.59	2.12	2.06
25	B	603	CLA	C1D-ND	2.59	1.41	1.37
25	b	602	CLA	C4B-NB	2.59	1.41	1.37
25	b	609	CLA	C4B-NB	2.59	1.41	1.37
25	d	403	CLA	C4B-NB	2.59	1.41	1.37
25	B	609	CLA	C1B-C2B	2.58	1.49	1.43
25	b	609	CLA	MG-NA	2.58	2.12	2.06
25	b	607	CLA	C1B-C2B	2.57	1.49	1.43
25	C	512	CLA	CHC-C1C	2.57	1.43	1.38
25	B	607	CLA	MG-ND	-2.57	2.00	2.05
29	c	519	LMG	C1-C2	2.57	1.60	1.52
31	c	517	DGD	O3D-C3D	-2.57	1.36	1.43
25	C	511	CLA	C3B-C4B	2.57	1.50	1.42
25	b	601	CLA	C3B-C4B	2.56	1.50	1.42
25	A	606	CLA	C3B-C4B	2.56	1.50	1.42
25	c	511	CLA	CHC-C1C	2.56	1.43	1.38
26	D	402	PHO	CMB-C2B	-2.56	1.46	1.51
29	m	101	LMG	O1-C7	-2.55	1.39	1.43
25	d	403	CLA	C1B-C2B	2.55	1.49	1.43
25	c	508	CLA	CHC-C1C	2.55	1.43	1.38
25	a	612	CLA	MG-NB	2.55	2.10	2.05
28	D	407	PL9	C52-C5	-2.54	1.45	1.50
25	C	501	CLA	C1B-C2B	2.54	1.49	1.43
25	D	403	CLA	CHC-C1C	2.53	1.43	1.38
25	b	608	CLA	C1B-C2B	2.53	1.49	1.43
25	c	513	CLA	CHC-C1C	2.53	1.43	1.38
25	a	607	CLA	C1B-C2B	2.53	1.49	1.43
25	c	510	CLA	CMB-C2B	-2.53	1.45	1.50
31	A	615	DGD	C4D-C3D	2.53	1.58	1.52
25	B	610	CLA	CHC-C1C	2.53	1.43	1.38
25	c	512	CLA	C3B-C4B	2.52	1.50	1.42
30	A	613	SQD	O5-C1	2.52	1.48	1.41
26	d	402	PHO	CAC-C3C	-2.52	1.47	1.51
25	b	605	CLA	C3B-C4B	2.52	1.50	1.42
25	c	504	CLA	C1D-ND	2.52	1.41	1.37
25	B	612	CLA	C4B-NB	2.52	1.41	1.37
25	B	616	CLA	C4B-NB	2.51	1.41	1.37
25	a	607	CLA	C3B-C4B	2.51	1.50	1.42
34	e	102	LHG	P-O6	2.51	1.69	1.59
25	c	507	CLA	C4B-NB	2.51	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	CHC-C1C	2.51	1.43	1.38
25	A	607	CLA	C3B-C4B	2.51	1.50	1.42
25	B	605	CLA	C3B-C4B	2.51	1.50	1.42
30	D	409	SQD	O9-S	2.50	1.52	1.45
25	b	603	CLA	C1B-C2B	2.50	1.49	1.43
25	B	601	CLA	C3B-C4B	2.50	1.50	1.42
25	a	606	CLA	C4B-NB	2.50	1.41	1.37
25	a	607	CLA	CHC-C1C	2.50	1.43	1.38
29	c	521	LMG	C1-C2	2.50	1.59	1.52
25	C	509	CLA	C3B-C4B	2.49	1.50	1.42
29	A	612	LMG	C4-C5	2.49	1.58	1.53
28	D	407	PL9	C6-C1	-2.49	1.44	1.48
25	C	506	CLA	MG-ND	-2.49	2.00	2.05
25	c	509	CLA	C4B-NB	2.49	1.41	1.37
25	B	612	CLA	C1B-C2B	2.49	1.49	1.43
25	a	609	CLA	C4B-NB	2.49	1.41	1.37
29	c	519	LMG	C4-C5	2.49	1.58	1.53
25	B	615	CLA	CHC-C1C	2.48	1.43	1.38
27	B	618	BCR	C1-C6	-2.48	1.50	1.53
31	a	614	DGD	O2G-C2G	-2.48	1.40	1.46
27	T	101	BCR	C1-C6	-2.48	1.50	1.53
30	B	622	SQD	O9-S	2.48	1.52	1.45
27	H	101	BCR	C1-C6	-2.48	1.50	1.53
25	b	604	CLA	C3B-C4B	2.48	1.49	1.42
25	C	507	CLA	MG-NC	2.48	2.12	2.06
26	a	608	PHO	CAC-C3C	-2.48	1.47	1.51
25	B	605	CLA	MG-NA	2.47	2.12	2.06
25	a	612	CLA	C4B-NB	2.47	1.41	1.37
25	C	511	CLA	C4B-NB	2.47	1.41	1.37
25	c	512	CLA	CHC-C1C	2.47	1.43	1.38
25	D	403	CLA	C1B-C2B	2.47	1.48	1.43
25	C	503	CLA	CHC-C1C	2.47	1.43	1.38
26	d	402	PHO	CMD-C2D	-2.46	1.46	1.51
31	c	516	DGD	O1G-C1G	-2.46	1.39	1.45
25	B	601	CLA	CHC-C1C	2.46	1.43	1.38
25	B	604	CLA	CHC-C1C	2.46	1.43	1.38
25	c	502	CLA	MG-ND	2.45	2.10	2.05
31	c	517	DGD	O2G-C2G	-2.45	1.40	1.46
25	B	611	CLA	C3B-C4B	2.44	1.49	1.42
25	c	505	CLA	CMB-C2B	-2.44	1.45	1.50
25	c	505	CLA	C1D-ND	2.44	1.41	1.37
29	D	412	LMG	C7-C8	2.43	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	MG-NB	2.43	2.10	2.05
25	a	606	CLA	C3B-C4B	2.43	1.49	1.42
26	D	402	PHO	C4D-ND	-2.43	1.34	1.38
29	C	519	LMG	O7-C8	-2.43	1.40	1.46
25	c	510	CLA	C4B-NB	2.43	1.41	1.37
25	b	615	CLA	CMD-C2D	-2.43	1.45	1.50
25	C	509	CLA	C1B-C2B	2.42	1.48	1.43
34	d	409	LHG	P-O6	2.42	1.68	1.59
31	H	102	DGD	O2G-C1B	2.42	1.41	1.34
25	B	615	CLA	MG-NB	2.42	2.10	2.05
25	C	503	CLA	C3B-C4B	2.42	1.49	1.42
25	c	502	CLA	CMC-C2C	-2.41	1.45	1.50
31	C	516	DGD	O2E-C2E	-2.41	1.37	1.43
25	c	502	CLA	CMD-C2D	-2.41	1.45	1.50
25	a	612	CLA	CHC-C1C	2.40	1.43	1.38
31	c	516	DGD	O4D-C4D	-2.40	1.37	1.43
25	C	509	CLA	MG-NC	-2.40	2.00	2.06
25	B	616	CLA	C3B-C4B	2.40	1.49	1.42
29	B	621	LMG	O7-C10	2.39	1.38	1.30
25	b	604	CLA	CHC-C1C	2.39	1.43	1.38
25	b	611	CLA	C3B-C4B	2.39	1.49	1.42
27	a	610	BCR	C30-C25	-2.39	1.50	1.53
26	A	608	PHO	CMB-C2B	-2.39	1.46	1.51
30	D	409	SQD	O5-C1	2.39	1.48	1.41
30	L	101	SQD	O9-S	2.38	1.51	1.45
25	b	612	CLA	C3B-C4B	2.38	1.49	1.42
25	b	613	CLA	C1B-C2B	2.38	1.48	1.43
34	E	101	LHG	O7-C5	-2.38	1.41	1.46
30	f	101	SQD	O7-S	2.37	1.51	1.45
29	M	101	LMG	O7-C8	-2.37	1.41	1.46
34	D	411	LHG	O7-C7	2.36	1.41	1.34
25	B	604	CLA	C3B-C4B	2.36	1.49	1.42
25	b	603	CLA	C4B-NB	2.36	1.41	1.37
25	b	603	CLA	CMD-C2D	-2.36	1.45	1.50
31	c	517	DGD	C3E-C2E	2.36	1.58	1.52
26	D	402	PHO	CAC-C3C	-2.35	1.47	1.51
27	T	101	BCR	C30-C25	-2.35	1.50	1.53
25	c	509	CLA	CHC-C1C	2.35	1.43	1.38
25	b	606	CLA	C4B-NB	2.35	1.40	1.37
29	m	101	LMG	O8-C9	-2.34	1.39	1.45
31	A	615	DGD	C1E-C2E	2.34	1.59	1.52
31	c	518	DGD	O2G-C2G	-2.34	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	CLA	MG-NA	2.34	2.11	2.06
25	b	604	CLA	MG-ND	-2.33	2.01	2.05
31	c	516	DGD	C3G-C2G	2.33	1.58	1.50
31	h	102	DGD	O1G-C1G	-2.33	1.40	1.45
25	c	506	CLA	C1B-C2B	2.33	1.48	1.43
29	c	521	LMG	O7-C8	-2.32	1.41	1.46
25	B	605	CLA	CHC-C1C	2.32	1.43	1.38
31	C	518	DGD	O3G-C3G	-2.32	1.39	1.43
25	B	610	CLA	C1D-C2D	2.32	1.49	1.45
25	d	404	CLA	CHC-C1C	2.32	1.43	1.38
25	b	608	CLA	C3B-C4B	2.31	1.49	1.42
25	d	404	CLA	C3B-C4B	2.31	1.49	1.42
25	B	614	CLA	CHC-C1C	2.31	1.43	1.38
26	d	402	PHO	CMB-C2B	-2.31	1.47	1.51
25	D	405	CLA	CMD-C2D	-2.31	1.46	1.50
31	C	517	DGD	O2G-C2G	-2.31	1.41	1.46
25	a	609	CLA	MG-NB	-2.30	2.01	2.05
25	B	605	CLA	C4B-NB	2.30	1.40	1.37
25	b	608	CLA	C4B-NB	2.30	1.40	1.37
25	c	501	CLA	C4B-NB	2.30	1.40	1.37
25	B	603	CLA	MG-NC	-2.30	2.00	2.06
30	A	613	SQD	C46-C45	2.30	1.58	1.50
25	c	504	CLA	C3B-C4B	2.30	1.49	1.42
26	A	608	PHO	C3B-C2B	-2.30	1.37	1.40
25	C	513	CLA	C3B-C4B	2.29	1.49	1.42
25	A	607	CLA	C1B-C2B	2.29	1.48	1.43
25	B	613	CLA	C3B-C4B	2.29	1.49	1.42
25	B	604	CLA	C4B-NB	2.29	1.40	1.37
25	C	510	CLA	CMD-C2D	-2.28	1.46	1.50
25	B	616	CLA	CMC-C2C	-2.28	1.46	1.50
25	b	612	CLA	CMC-C2C	-2.28	1.46	1.50
25	D	403	CLA	C1D-C2D	2.28	1.49	1.45
25	b	603	CLA	CMB-C2B	-2.28	1.46	1.50
25	b	614	CLA	C3B-C4B	2.28	1.49	1.42
25	c	506	CLA	CHC-C1C	2.27	1.43	1.38
25	C	509	CLA	CMD-C2D	-2.27	1.46	1.50
25	b	611	CLA	CHC-C1C	2.27	1.43	1.38
25	D	404	CLA	CMD-C2D	-2.27	1.46	1.50
26	a	608	PHO	C4D-ND	-2.27	1.35	1.38
25	c	503	CLA	C3B-C4B	2.27	1.49	1.42
25	a	609	CLA	CMC-C2C	-2.27	1.46	1.50
30	a	613	SQD	O7-S	2.27	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	521	LMG	C4-C3	2.26	1.58	1.52
25	b	602	CLA	C3B-C4B	2.26	1.49	1.42
25	b	607	CLA	C3B-C4B	2.26	1.49	1.42
27	c	515	BCR	C30-C25	-2.26	1.50	1.53
25	b	606	CLA	CHC-C1C	2.26	1.43	1.38
25	C	502	CLA	MG-NC	-2.26	2.00	2.06
27	h	101	BCR	C1-C6	-2.26	1.50	1.53
25	C	502	CLA	C3B-C4B	2.26	1.49	1.42
25	A	606	CLA	MG-NB	2.26	2.10	2.05
25	c	508	CLA	C3B-C4B	2.26	1.49	1.42
25	c	503	CLA	C4B-NB	2.25	1.40	1.37
25	B	611	CLA	CMD-C2D	-2.25	1.46	1.50
31	c	516	DGD	C4D-C3D	2.25	1.58	1.52
30	f	101	SQD	O9-S	2.25	1.51	1.45
25	A	606	CLA	CMD-C2D	-2.25	1.46	1.50
25	b	610	CLA	C3B-C4B	2.24	1.49	1.42
30	L	101	SQD	C46-C45	2.24	1.57	1.50
25	b	614	CLA	MG-NC	2.24	2.11	2.06
26	a	608	PHO	CMC-C2C	-2.24	1.47	1.50
25	b	616	CLA	C4B-NB	2.23	1.40	1.37
25	B	602	CLA	CMB-C2B	-2.23	1.46	1.50
25	b	603	CLA	C3B-C4B	2.23	1.49	1.42
25	B	614	CLA	C1B-C2B	2.22	1.48	1.43
25	a	612	CLA	MG-NC	-2.22	2.01	2.06
25	B	606	CLA	C3B-C4B	2.22	1.49	1.42
25	C	504	CLA	CMB-C2B	-2.22	1.46	1.50
25	c	503	CLA	CHC-C1C	2.21	1.42	1.38
25	C	507	CLA	CMB-C2B	-2.21	1.46	1.50
29	A	612	LMG	C1-C2	2.21	1.59	1.52
25	C	511	CLA	CHC-C1C	2.21	1.42	1.38
35	e	101	HEM	CMA-C3A	2.21	1.55	1.50
25	b	607	CLA	CMB-C2B	-2.21	1.46	1.50
25	b	608	CLA	MG-ND	-2.21	2.01	2.05
26	A	608	PHO	C4D-ND	-2.21	1.35	1.38
25	C	501	CLA	MG-ND	2.21	2.10	2.05
25	B	615	CLA	CMB-C2B	-2.20	1.46	1.50
30	B	622	SQD	O7-S	2.20	1.51	1.45
25	b	616	CLA	CMC-C2C	-2.20	1.46	1.50
25	c	510	CLA	C3B-C4B	2.20	1.49	1.42
25	A	609	CLA	CMD-C2D	-2.20	1.46	1.50
36	V	201	HEC	C3B-C2B	-2.20	1.33	1.41
25	b	609	CLA	MG-NC	2.20	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	M	101	LMG	C9-C8	2.20	1.57	1.50
25	B	613	CLA	CMC-C2C	-2.19	1.46	1.50
25	C	508	CLA	CHC-C1C	2.19	1.42	1.38
31	c	517	DGD	C1E-C2E	2.19	1.58	1.52
31	A	615	DGD	C3E-C2E	2.19	1.58	1.52
25	b	610	CLA	CMD-C2D	-2.19	1.46	1.50
25	C	509	CLA	CHC-C1C	2.19	1.42	1.38
25	b	602	CLA	MG-ND	2.19	2.10	2.05
25	B	609	CLA	C3B-C4B	2.18	1.49	1.42
25	b	609	CLA	CMB-C2B	-2.18	1.46	1.50
31	c	517	DGD	O3G-C3G	-2.18	1.40	1.43
25	a	612	CLA	C3B-C4B	2.18	1.49	1.42
35	F	101	HEM	FE-ND	2.18	2.01	1.94
25	b	613	CLA	C3B-C4B	2.18	1.49	1.42
26	d	402	PHO	C4D-ND	-2.18	1.35	1.38
29	C	519	LMG	C1-C2	2.18	1.58	1.52
31	c	516	DGD	C4E-C3E	2.18	1.58	1.52
25	c	504	CLA	CHC-C1C	2.18	1.42	1.38
25	c	513	CLA	MG-NC	2.18	2.11	2.06
25	c	502	CLA	CHC-C1C	2.18	1.42	1.38
29	D	408	LMG	O7-C8	-2.17	1.41	1.46
30	A	613	SQD	O9-S	2.17	1.51	1.45
25	B	603	CLA	CHC-C1C	2.17	1.42	1.38
25	B	609	CLA	CMD-C2D	-2.17	1.46	1.50
25	B	613	CLA	CHC-C1C	2.17	1.42	1.38
25	B	608	CLA	C1B-NB	-2.17	1.35	1.37
25	b	612	CLA	CHC-C1C	2.17	1.42	1.38
25	b	609	CLA	C3B-C4B	2.17	1.49	1.42
31	C	518	DGD	C1G-C2G	2.17	1.57	1.50
25	a	607	CLA	CMC-C2C	-2.17	1.46	1.50
25	d	403	CLA	CMB-C2B	-2.17	1.46	1.50
25	c	507	CLA	CHC-C1C	2.16	1.42	1.38
27	b	618	BCR	C38-C26	-2.16	1.47	1.50
25	C	512	CLA	CMD-C2D	-2.16	1.46	1.50
25	C	504	CLA	CMD-C2D	-2.16	1.46	1.50
25	D	405	CLA	CMC-C2C	-2.16	1.46	1.50
25	a	606	CLA	C3D-C4D	2.16	1.49	1.44
31	h	102	DGD	O2G-C1B	2.16	1.40	1.34
25	b	607	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	616	CLA	CMB-C2B	-2.16	1.46	1.50
25	B	612	CLA	CMD-C2D	-2.15	1.46	1.50
29	d	411	LMG	C4-C5	2.15	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	MG-NB	-2.15	2.01	2.05
25	C	503	CLA	CMD-C2D	-2.15	1.46	1.50
25	c	510	CLA	CMC-C2C	-2.15	1.46	1.50
35	e	101	HEM	C3B-C2B	-2.15	1.32	1.37
27	B	617	BCR	C33-C5	-2.15	1.47	1.50
25	C	501	CLA	CMC-C2C	-2.15	1.46	1.50
25	c	507	CLA	CMB-C2B	-2.15	1.46	1.50
25	b	612	CLA	CMB-C2B	-2.15	1.46	1.50
25	C	507	CLA	C3B-C4B	2.15	1.49	1.42
31	C	517	DGD	C4D-C5D	2.15	1.57	1.53
27	k	102	BCR	C38-C26	-2.15	1.47	1.50
25	B	601	CLA	CMC-C2C	-2.14	1.46	1.50
25	b	616	CLA	C3B-C4B	2.14	1.49	1.42
25	C	512	CLA	CMB-C2B	-2.14	1.46	1.50
25	C	507	CLA	CHC-C1C	2.14	1.42	1.38
25	C	510	CLA	C3B-C4B	2.14	1.49	1.42
30	f	101	SQD	O5-C5	2.14	1.49	1.44
25	C	502	CLA	MG-ND	-2.14	2.01	2.05
25	C	504	CLA	MG-ND	-2.14	2.01	2.05
36	v	201	HEC	C3B-C2B	-2.14	1.34	1.41
25	b	611	CLA	CMB-C2B	-2.14	1.46	1.50
30	t	102	SQD	C44-C45	2.13	1.56	1.51
31	c	518	DGD	O2E-C2E	-2.13	1.37	1.43
26	D	402	PHO	C3D-C4D	2.13	1.44	1.41
29	M	101	LMG	C4-C3	2.13	1.57	1.52
25	C	503	CLA	CMC-C2C	-2.13	1.46	1.50
25	b	614	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	615	CLA	C3B-C4B	2.13	1.48	1.42
31	C	517	DGD	C1G-C2G	2.13	1.57	1.50
25	C	506	CLA	CHC-C1C	2.13	1.42	1.38
25	c	501	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	603	CLA	MG-NB	2.13	2.10	2.05
25	B	612	CLA	C1B-NB	-2.13	1.35	1.37
25	a	609	CLA	C3B-C4B	2.13	1.48	1.42
35	e	101	HEM	CMC-C2C	2.12	1.55	1.50
29	c	523	LMG	C1-C2	2.12	1.58	1.52
25	D	405	CLA	CHC-C4B	-2.12	1.34	1.39
29	c	519	LMG	C7-C8	2.12	1.57	1.50
30	B	622	SQD	C8-C7	2.12	1.56	1.50
27	A	610	BCR	C33-C5	-2.11	1.47	1.50
25	c	510	CLA	CMD-C2D	-2.11	1.46	1.50
27	B	617	BCR	C30-C25	-2.11	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	V	201	HEC	CMB-C2B	2.11	1.55	1.50
25	c	508	CLA	CMC-C2C	-2.11	1.46	1.50
25	D	403	CLA	C3B-C4B	2.10	1.48	1.42
35	e	101	HEM	FE-ND	2.10	2.01	1.94
25	B	608	CLA	CMD-C2D	-2.10	1.46	1.50
25	C	511	CLA	CMB-C2B	-2.10	1.46	1.50
29	c	519	LMG	C4-C3	2.10	1.57	1.52
27	a	610	BCR	C38-C26	-2.10	1.47	1.50
25	b	614	CLA	C1D-C2D	2.10	1.49	1.45
25	b	607	CLA	CHC-C1C	2.10	1.42	1.38
25	B	607	CLA	CMB-C2B	-2.10	1.46	1.50
25	A	607	CLA	CMB-C2B	-2.10	1.46	1.50
25	c	512	CLA	C1D-C2D	2.09	1.49	1.45
25	a	606	CLA	CMB-C2B	-2.09	1.46	1.50
31	C	517	DGD	C4D-C3D	2.09	1.57	1.52
25	D	404	CLA	C4B-NB	2.09	1.40	1.37
25	C	505	CLA	C3B-C4B	2.09	1.48	1.42
25	b	613	CLA	CMD-C2D	-2.09	1.46	1.50
25	c	513	CLA	CMB-C2B	-2.09	1.46	1.50
25	c	507	CLA	C3D-C4D	2.09	1.48	1.44
25	A	607	CLA	CMD-C2D	-2.09	1.46	1.50
25	C	501	CLA	CMD-C2D	-2.09	1.46	1.50
25	a	607	CLA	MG-NC	2.09	2.11	2.06
25	b	607	CLA	CMC-C2C	-2.09	1.46	1.50
35	F	101	HEM	CMD-C2D	2.09	1.55	1.50
25	C	504	CLA	MG-NB	2.08	2.09	2.05
25	c	513	CLA	CMD-C2D	-2.08	1.46	1.50
27	k	102	BCR	C33-C5	-2.08	1.47	1.50
25	c	506	CLA	C3B-C4B	2.08	1.48	1.42
25	C	513	CLA	CHC-C1C	2.08	1.42	1.38
25	b	602	CLA	MG-NC	-2.07	2.01	2.06
25	B	601	CLA	CMB-C2B	-2.07	1.46	1.50
31	H	102	DGD	C1E-C2E	2.07	1.58	1.52
25	C	504	CLA	O2D-CGD	2.07	1.38	1.33
27	D	406	BCR	C38-C26	-2.07	1.47	1.50
36	v	201	HEC	CMC-C2C	2.07	1.55	1.50
25	c	506	CLA	CMD-C2D	-2.07	1.46	1.50
25	c	504	CLA	O2D-CGD	2.07	1.38	1.33
25	C	506	CLA	C1B-C2B	2.07	1.48	1.43
25	A	607	CLA	C3C-C2C	2.07	1.41	1.36
35	F	101	HEM	C2A-C3A	-2.07	1.33	1.38
31	A	615	DGD	O5D-C6D	-2.07	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	CMC-C2C	-2.06	1.46	1.50
25	b	601	CLA	C3D-C4D	2.06	1.48	1.44
25	a	612	CLA	CMB-C2B	-2.06	1.46	1.50
29	b	622	LMG	C3-C2	2.06	1.57	1.52
25	c	502	CLA	C3B-C4B	2.06	1.48	1.42
25	d	403	CLA	CMC-C2C	-2.06	1.46	1.50
25	c	512	CLA	C3D-C4D	2.06	1.48	1.44
25	d	403	CLA	C3B-C4B	2.06	1.48	1.42
31	c	516	DGD	C3D-C2D	2.06	1.57	1.52
31	c	516	DGD	O3G-C3G	-2.05	1.40	1.43
34	D	413	LHG	C24-C23	2.05	1.56	1.50
25	b	609	CLA	CMD-C2D	-2.05	1.46	1.50
25	B	610	CLA	CMC-C2C	-2.05	1.46	1.50
25	c	512	CLA	CMD-C2D	-2.05	1.46	1.50
25	d	404	CLA	CMD-C2D	-2.05	1.46	1.50
25	D	403	CLA	C4B-NB	2.05	1.40	1.37
25	b	615	CLA	C3B-C4B	2.05	1.48	1.42
31	C	518	DGD	O2G-C2G	-2.04	1.41	1.46
26	a	608	PHO	O2D-CGD	2.04	1.38	1.33
25	B	607	CLA	CHC-C1C	2.04	1.42	1.38
25	b	615	CLA	CHC-C1C	2.04	1.42	1.38
25	B	605	CLA	CMD-C2D	-2.04	1.46	1.50
30	L	101	SQD	O5-C5	2.04	1.49	1.44
25	C	510	CLA	O2A-CGA	2.04	1.39	1.33
25	C	501	CLA	C1D-C2D	2.04	1.49	1.45
25	b	614	CLA	MG-NA	2.04	2.11	2.06
26	a	608	PHO	CMB-C2B	-2.04	1.47	1.51
36	V	201	HEC	CMC-C2C	2.04	1.55	1.50
27	b	617	BCR	C33-C5	-2.04	1.47	1.50
25	B	612	CLA	C3B-C4B	2.04	1.48	1.42
29	c	523	LMG	O7-C8	-2.04	1.41	1.46
30	L	101	SQD	O7-S	2.04	1.50	1.45
25	B	608	CLA	CMC-C2C	-2.03	1.46	1.50
25	b	608	CLA	CMB-C2B	-2.03	1.46	1.50
25	B	612	CLA	CHC-C1C	2.03	1.42	1.38
31	A	615	DGD	O1G-C1G	-2.03	1.40	1.45
25	C	503	CLA	CMB-C2B	-2.03	1.46	1.50
31	c	518	DGD	O1G-C1G	-2.03	1.40	1.45
30	D	409	SQD	O7-S	2.03	1.50	1.45
25	b	613	CLA	CMB-C2B	-2.03	1.46	1.50
25	D	404	CLA	C3B-C4B	2.03	1.48	1.42
27	C	514	BCR	C33-C5	-2.02	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	CMB-C2B	-2.02	1.46	1.50
27	k	101	BCR	C38-C26	-2.02	1.47	1.50
25	b	609	CLA	C3D-C4D	2.02	1.48	1.44
25	B	610	CLA	C3D-C4D	2.02	1.48	1.44
25	C	508	CLA	C1D-C2D	2.02	1.49	1.45
28	A	611	PL9	C3-C4	-2.02	1.46	1.49
27	k	101	BCR	C33-C5	-2.02	1.47	1.50
36	v	201	HEC	CMD-C2D	2.02	1.54	1.50
30	L	101	SQD	C44-C45	2.02	1.57	1.50
26	D	402	PHO	C3D-C2D	2.02	1.43	1.39
25	b	606	CLA	C3B-C4B	2.02	1.48	1.42
25	A	609	CLA	CHC-C1C	2.02	1.42	1.38
25	B	609	CLA	O2D-CGD	2.02	1.38	1.33
25	b	602	CLA	CHC-C4B	-2.01	1.34	1.39
25	b	612	CLA	CMD-C2D	-2.01	1.46	1.50
27	d	405	BCR	C38-C26	-2.01	1.47	1.50
25	b	603	CLA	CHC-C1C	2.01	1.42	1.38
25	B	610	CLA	CMB-C2B	-2.01	1.46	1.50
25	b	602	CLA	CMD-C2D	-2.01	1.46	1.50
25	B	607	CLA	C1B-C2B	2.01	1.47	1.43
25	d	403	CLA	CHC-C1C	2.01	1.42	1.38
30	A	613	SQD	C8-C7	2.01	1.56	1.50
25	B	603	CLA	CMC-C2C	-2.01	1.46	1.50
27	c	514	BCR	C38-C26	-2.00	1.47	1.50
25	C	506	CLA	C1B-NB	-2.00	1.35	1.37
25	C	504	CLA	CMC-C2C	-2.00	1.46	1.50
25	C	506	CLA	CMD-C2D	-2.00	1.46	1.50
25	c	508	CLA	CMB-C2B	-2.00	1.46	1.50
25	b	615	CLA	CMB-C2B	-2.00	1.46	1.50

All (1134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O6-C1-C2	13.59	128.91	108.27
36	V	201	HEC	CBB-CAB-C3B	-9.67	108.12	127.43
25	B	604	CLA	C4A-NA-C1A	9.23	110.89	106.68
36	v	201	HEC	CBB-CAB-C3B	-8.93	109.59	127.43
25	c	509	CLA	C4A-NA-C1A	8.52	110.57	106.68
25	C	507	CLA	C4A-NA-C1A	7.94	110.30	106.68
36	v	201	HEC	CBC-CAC-C3C	-7.88	111.68	127.43
25	b	615	CLA	C4A-NA-C1A	7.84	110.25	106.68
25	A	606	CLA	C4A-NA-C1A	7.47	110.09	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	616	CLA	C4A-NA-C1A	7.44	110.07	106.68
25	B	606	CLA	C4A-NA-C1A	7.42	110.06	106.68
25	c	511	CLA	C4A-NA-C1A	7.40	110.06	106.68
25	C	511	CLA	C4A-NA-C1A	7.38	110.05	106.68
25	c	501	CLA	C4A-NA-C1A	7.35	110.03	106.68
25	c	503	CLA	C4A-NA-C1A	7.31	110.01	106.68
25	C	508	CLA	C4A-NA-C1A	7.29	110.00	106.68
25	C	503	CLA	C4A-NA-C1A	7.28	110.00	106.68
25	b	606	CLA	C4A-NA-C1A	7.28	110.00	106.68
25	B	607	CLA	C4A-NA-C1A	7.27	110.00	106.68
25	c	502	CLA	C4A-NA-C1A	7.23	109.98	106.68
30	a	613	SQD	O6-C1-C2	7.15	119.13	108.27
25	b	604	CLA	C4A-NA-C1A	7.09	109.92	106.68
25	c	510	CLA	C4A-NA-C1A	6.98	109.86	106.68
25	B	611	CLA	C4A-NA-C1A	6.96	109.86	106.68
25	b	611	CLA	C4A-NA-C1A	6.83	109.80	106.68
25	b	601	CLA	C4A-NA-C1A	6.81	109.79	106.68
36	V	201	HEC	CBC-CAC-C3C	-6.81	113.83	127.43
30	L	101	SQD	O6-C1-C2	6.80	118.60	108.27
25	C	501	CLA	C4A-NA-C1A	6.63	109.71	106.68
30	a	613	SQD	C1-O5-C5	-6.62	100.79	113.72
25	C	513	CLA	C4A-NA-C1A	6.55	109.67	106.68
25	c	507	CLA	C4A-NA-C1A	6.53	109.66	106.68
25	c	506	CLA	C4A-NA-C1A	6.47	109.63	106.68
25	b	602	CLA	C4A-NA-C1A	6.42	109.61	106.68
30	D	409	SQD	C1-O5-C5	-6.35	101.33	113.72
30	A	613	SQD	O6-C1-C2	6.23	117.74	108.27
25	C	510	CLA	C4A-NA-C1A	6.21	109.51	106.68
25	b	608	CLA	C4A-NA-C1A	6.12	109.47	106.68
25	c	508	CLA	C4A-NA-C1A	6.11	109.47	106.68
25	C	506	CLA	C4A-NA-C1A	6.09	109.46	106.68
25	B	602	CLA	C4A-NA-C1A	6.08	109.45	106.68
26	A	608	PHO	C4D-CHA-CBD	-6.01	105.57	108.45
26	a	608	PHO	C4D-CHA-CBD	-5.99	105.58	108.45
25	D	404	CLA	C4A-NA-C1A	5.92	109.38	106.68
25	b	609	CLA	C4A-NA-C1A	5.91	109.37	106.68
25	B	601	CLA	C4A-NA-C1A	5.78	109.32	106.68
25	B	608	CLA	C4A-NA-C1A	5.76	109.31	106.68
25	B	616	CLA	C4A-NA-C1A	5.74	109.30	106.68
26	d	402	PHO	C1-C2-C3	-5.73	116.80	126.20
25	B	603	CLA	C4A-NA-C1A	5.69	109.28	106.68
25	B	605	CLA	C4A-NA-C1A	5.69	109.28	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	606	CLA	C4A-NA-C1A	5.67	109.26	106.68
25	B	615	CLA	C4A-NA-C1A	5.61	109.24	106.68
25	c	512	CLA	C4A-NA-C1A	5.58	109.22	106.68
25	B	613	CLA	C1-C2-C3	-5.53	117.13	126.20
25	b	603	CLA	C4A-NA-C1A	5.49	109.19	106.68
25	b	613	CLA	C4A-NA-C1A	5.42	109.15	106.68
30	A	613	SQD	C1-O5-C5	-5.39	103.19	113.72
25	c	505	CLA	C4A-NA-C1A	5.39	109.14	106.68
28	a	611	PL9	C7-C3-C4	5.32	121.30	116.91
30	t	102	SQD	O47-C7-C8	5.23	122.80	111.48
25	D	405	CLA	C4A-NA-C1A	5.23	109.06	106.68
30	D	409	SQD	C44-O6-C1	5.22	122.59	113.68
25	C	509	CLA	C4A-NA-C1A	5.20	109.05	106.68
25	A	609	CLA	C4A-NA-C1A	5.17	109.04	106.68
25	d	403	CLA	C4A-NA-C1A	5.17	109.04	106.68
25	C	504	CLA	C4A-NA-C1A	5.12	109.02	106.68
25	D	403	CLA	C4A-NA-C1A	5.10	109.01	106.68
30	B	622	SQD	O47-C7-C8	5.07	122.46	111.48
25	b	605	CLA	C4A-NA-C1A	5.02	108.97	106.68
30	B	622	SQD	O6-C1-C2	4.97	115.81	108.27
25	C	512	CLA	C4A-NA-C1A	4.92	108.92	106.68
25	B	609	CLA	C4A-NA-C1A	4.90	108.92	106.68
25	b	603	CLA	O2D-CGD-O1D	-4.87	114.36	123.85
25	B	612	CLA	C4A-NA-C1A	4.84	108.89	106.68
28	A	611	PL9	C7-C3-C4	4.81	120.87	116.91
25	B	612	CLA	O2D-CGD-O1D	-4.81	114.50	123.85
25	b	610	CLA	C4A-NA-C1A	4.77	108.86	106.68
34	d	408	LHG	O4-P-O5	4.74	134.49	112.44
26	D	402	PHO	C4D-CHA-CBD	-4.73	106.19	108.45
25	b	616	CLA	O2D-CGD-O1D	-4.72	114.67	123.85
31	c	517	DGD	O3G-C3G-C2G	-4.71	99.37	110.82
26	D	402	PHO	C1-C2-C3	-4.62	118.63	126.20
31	a	614	DGD	O3G-C3G-C2G	-4.60	99.96	111.77
30	L	101	SQD	O47-C7-C8	4.59	121.42	111.48
25	B	610	CLA	O2D-CGD-O1D	-4.58	114.94	123.85
30	A	613	SQD	O7-S-C6	4.48	113.45	106.76
25	A	607	CLA	C4A-NA-C1A	4.46	108.72	106.68
25	b	606	CLA	O2D-CGD-O1D	-4.44	115.20	123.85
30	A	613	SQD	O9-S-O7	-4.44	99.39	113.82
25	b	608	CLA	C3B-C4B-NB	-4.40	106.60	110.53
25	b	604	CLA	C1-C2-C3	-4.39	119.01	126.20
30	D	409	SQD	O8-S-C6	4.39	114.44	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	e	102	LHG	O4-P-O5	4.38	132.80	112.44
30	A	613	SQD	O47-C7-C8	4.36	120.91	111.48
25	a	607	CLA	C4A-NA-C1A	4.36	108.67	106.68
25	B	601	CLA	O2D-CGD-O1D	-4.34	115.40	123.85
34	D	410	LHG	O4-P-O5	4.34	132.63	112.44
25	B	604	CLA	C1-C2-C3	-4.33	119.10	126.20
34	D	411	LHG	O4-P-O5	4.33	132.59	112.44
25	c	513	CLA	C4A-NA-C1A	4.32	108.65	106.68
34	E	101	LHG	O4-P-O5	4.31	132.47	112.44
28	d	406	PL9	C7-C8-C9	-4.28	119.47	126.83
34	d	409	LHG	O4-P-O5	4.26	132.24	112.44
30	D	409	SQD	C1-C2-C3	-4.25	101.06	110.01
25	A	607	CLA	O2D-CGD-O1D	-4.25	115.58	123.85
30	a	613	SQD	C1-C2-C3	-4.24	101.08	110.01
28	D	407	PL9	C7-C3-C4	4.24	120.40	116.91
34	D	413	LHG	O4-P-O5	4.24	132.17	112.44
30	f	101	SQD	O9-S-O7	-4.23	100.06	113.82
25	B	610	CLA	C4A-NA-C1A	4.22	108.60	106.68
30	B	622	SQD	O7-S-C6	4.20	113.03	106.76
25	C	505	CLA	C4A-NA-C1A	4.19	108.59	106.68
28	d	406	PL9	C7-C3-C4	4.18	120.35	116.91
25	a	612	CLA	C4A-NA-C1A	4.17	108.58	106.68
25	c	504	CLA	C4A-NA-C1A	4.17	108.58	106.68
30	B	622	SQD	C1-O5-C5	-4.16	105.60	113.72
25	b	611	CLA	O2D-CGD-O1D	-4.13	115.80	123.85
31	C	518	DGD	O3G-C3G-C2G	-4.13	100.78	110.82
34	L	102	LHG	O4-P-O5	4.13	131.65	112.44
30	f	101	SQD	O5-C5-C4	4.10	117.09	109.70
25	a	607	CLA	O2D-CGD-O1D	-4.07	115.93	123.85
31	H	102	DGD	O3G-C3G-C2G	-4.06	100.95	110.82
34	l	101	LHG	O4-P-O5	4.06	131.31	112.44
30	f	101	SQD	O6-C1-C2	4.06	114.43	108.27
28	a	611	PL9	C7-C3-C2	-4.05	118.62	123.39
33	d	401	BCT	O2-C-O1	4.04	130.01	119.68
34	d	407	LHG	O4-P-O5	4.04	131.23	112.44
25	B	611	CLA	C3B-C4B-NB	-4.03	106.93	110.53
25	c	509	CLA	O2A-CGA-O1A	-4.01	113.61	123.63
25	b	605	CLA	O2D-CGD-O1D	-4.00	116.06	123.85
25	B	614	CLA	C3B-C4B-NB	-4.00	106.96	110.53
26	D	402	PHO	C2B-C1B-NB	-3.99	106.54	109.43
25	b	612	CLA	C1-C2-C3	-3.99	119.66	126.20
30	A	613	SQD	C1-C2-C3	-3.98	101.63	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	611	CLA	O2D-CGD-O1D	-3.98	116.10	123.85
26	d	402	PHO	O1D-CGD-CBD	3.97	130.75	124.72
25	B	614	CLA	C4A-NA-C1A	3.96	108.49	106.68
25	b	613	CLA	C1-C2-C3	-3.94	119.74	126.20
25	c	510	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
29	m	101	LMG	O1-C7-C8	-3.93	101.27	110.82
25	D	404	CLA	C1-C2-C3	-3.92	119.78	126.20
28	A	611	PL9	C7-C3-C2	-3.90	118.79	123.39
26	A	608	PHO	O2D-CGD-CBD	3.90	115.23	110.95
29	b	622	LMG	O1-C1-C2	-3.90	102.35	108.27
30	a	613	SQD	O9-S-C6	3.89	112.56	106.76
31	c	516	DGD	O3G-C3G-C2G	-3.85	101.45	110.82
25	c	512	CLA	C1-C2-C3	-3.84	119.90	126.20
33	D	401	BCT	O2-C-O1	3.84	129.50	119.68
30	f	101	SQD	O9-S-C6	3.83	112.48	106.76
25	d	404	CLA	C4A-NA-C1A	3.82	108.42	106.68
30	D	409	SQD	O5-C1-C2	-3.81	102.54	110.37
25	c	502	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
25	B	613	CLA	C4A-NA-C1A	3.77	108.40	106.68
35	F	101	HEM	CBD-CAD-C3D	-3.76	102.13	112.53
25	B	603	CLA	O2D-CGD-O1D	-3.76	116.54	123.85
30	A	614	SQD	O47-C7-C8	3.75	119.59	111.48
30	B	622	SQD	O9-S-O7	-3.74	101.65	113.82
25	c	505	CLA	C3B-C4B-NB	-3.74	107.19	110.53
30	L	101	SQD	O5-C5-C4	3.73	116.43	109.70
25	C	510	CLA	C3B-C4B-NB	-3.73	107.20	110.53
25	B	614	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
30	L	101	SQD	O9-S-O7	-3.71	101.77	113.82
25	b	607	CLA	C4A-NA-C1A	3.70	108.37	106.68
30	D	409	SQD	O9-S-O7	-3.69	101.82	113.82
27	B	617	BCR	C2-C1-C6	3.68	115.78	110.44
25	C	507	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
25	A	606	CLA	CHB-C4A-NA	3.67	129.69	124.40
25	b	606	CLA	O2D-CGD-CBD	3.66	117.63	111.23
28	d	406	PL9	C37-C38-C39	-3.63	119.31	127.62
25	b	616	CLA	O2D-CGD-CBD	3.63	117.57	111.23
25	C	505	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
25	c	512	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
25	C	503	CLA	C3B-C4B-NB	-3.62	107.30	110.53
25	a	606	CLA	C3B-C4B-NB	-3.61	107.31	110.53
26	d	402	PHO	O2D-CGD-O1D	-3.61	116.82	123.85
25	B	604	CLA	O2D-CGD-O1D	-3.61	116.82	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	O2D-CGD-CBD	3.60	117.52	111.23
26	a	608	PHO	C1-C2-C3	-3.60	120.31	126.20
25	B	611	CLA	O2D-CGD-CBD	3.58	117.50	111.23
25	C	513	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
25	C	501	CLA	C3B-C4B-NB	-3.58	107.34	110.53
25	A	607	CLA	C3B-C4B-NB	-3.57	107.34	110.53
30	A	613	SQD	O5-C1-C2	-3.57	103.03	110.37
25	c	501	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
31	C	516	DGD	O6D-C1D-O3G	-3.57	101.62	110.04
31	c	518	DGD	O3G-C3G-C2G	-3.56	102.17	110.82
30	a	613	SQD	O9-S-O7	-3.55	102.27	113.82
26	A	608	PHO	C2B-C1B-NB	-3.55	106.86	109.43
25	b	612	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
31	h	102	DGD	C1E-O6E-C5E	3.52	120.60	113.72
25	B	608	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
25	C	512	CLA	C1-C2-C3	-3.51	120.45	126.20
31	c	518	DGD	O6D-C1D-O3G	-3.51	101.76	110.04
25	a	607	CLA	CHB-C4A-NA	3.50	129.45	124.40
25	b	610	CLA	C1-C2-C3	-3.50	120.47	126.20
25	b	613	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
25	B	610	CLA	O2D-CGD-CBD	3.48	117.32	111.23
34	D	413	LHG	O8-C23-C24	3.48	122.44	111.83
25	b	615	CLA	C3B-C4B-NB	-3.47	107.44	110.53
28	A	611	PL9	C7-C8-C9	-3.46	120.87	126.83
31	h	102	DGD	O3G-C3G-C2G	-3.46	102.41	110.82
26	d	402	PHO	CMB-C2B-C3B	3.46	131.59	124.68
28	d	406	PL9	C40-C39-C41	3.45	121.22	115.23
27	A	610	BCR	C27-C26-C25	3.45	127.37	122.70
27	b	617	BCR	C2-C1-C6	3.45	115.45	110.44
28	d	406	PL9	C7-C3-C2	-3.44	119.33	123.39
36	v	201	HEC	C4D-ND-C1D	3.44	111.44	105.82
25	D	404	CLA	C3B-C4B-NB	-3.44	107.46	110.53
30	t	102	SQD	O48-C23-C24	3.43	122.28	111.83
31	C	517	DGD	O3G-C3G-C2G	-3.42	102.49	110.82
25	C	512	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
27	K	101	BCR	C15-C16-C17	-3.41	116.53	123.52
25	b	602	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
27	c	514	BCR	C24-C23-C22	-3.40	121.21	126.23
25	D	403	CLA	C3B-C4B-NB	-3.40	107.50	110.53
25	b	605	CLA	C1-C2-C3	-3.38	120.66	126.20
30	L	101	SQD	C1-C2-C3	-3.37	102.91	110.01
25	c	505	CLA	O2D-CGD-O1D	-3.37	117.29	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	510	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
35	e	101	HEM	CBD-CAD-C3D	-3.37	103.22	112.53
25	C	504	CLA	C3B-C4B-NB	-3.37	107.53	110.53
25	C	506	CLA	C3B-C4B-NB	-3.36	107.53	110.53
25	b	608	CLA	O2D-CGD-CBD	3.36	117.11	111.23
25	a	612	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
25	b	608	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
25	B	615	CLA	C3B-C4B-NB	-3.35	107.54	110.53
31	C	518	DGD	O6D-C1D-O3G	-3.35	102.14	110.04
30	L	101	SQD	O7-S-C6	3.34	111.74	106.76
30	L	101	SQD	O48-C23-C24	3.33	121.98	111.83
25	c	509	CLA	CHB-C4A-NA	3.33	129.20	124.40
25	B	616	CLA	O2D-CGD-O1D	-3.33	117.38	123.85
25	B	605	CLA	C3B-C4B-NB	-3.32	107.56	110.53
25	B	603	CLA	C3B-C4B-NB	-3.32	107.56	110.53
25	b	611	CLA	O2D-CGD-CBD	3.32	117.03	111.23
27	D	406	BCR	C2-C1-C6	3.31	115.25	110.44
31	C	516	DGD	O3G-C3G-C2G	-3.30	102.79	110.82
27	B	618	BCR	C15-C14-C13	-3.30	122.65	127.28
25	B	610	CLA	C3B-C4B-NB	-3.30	107.59	110.53
34	d	407	LHG	O8-C23-O10	-3.29	115.40	123.63
27	H	101	BCR	C16-C15-C14	-3.29	116.79	123.52
26	d	402	PHO	C4D-CHA-CBD	-3.29	106.88	108.45
25	B	602	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
25	d	403	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
25	c	502	CLA	C1-C2-C3	-3.26	120.85	126.20
25	b	614	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
25	c	505	CLA	O2D-CGD-CBD	3.25	116.91	111.23
30	a	613	SQD	O7-S-C6	3.25	111.60	106.76
30	a	613	SQD	O48-C23-C24	3.23	121.69	111.83
25	C	502	CLA	C4A-NA-C1A	3.23	108.15	106.68
25	b	608	CLA	CHB-C4A-NA	3.23	129.06	124.40
27	T	101	BCR	C3-C4-C5	-3.23	108.30	114.06
27	C	514	BCR	C15-C16-C17	-3.21	116.94	123.52
25	b	612	CLA	O2A-CGA-O1A	-3.21	115.60	123.63
25	B	610	CLA	O2A-CGA-O1A	-3.20	115.63	123.63
25	B	603	CLA	O2D-CGD-CBD	3.19	116.81	111.23
26	a	608	PHO	C2B-C1B-NB	-3.19	107.12	109.43
25	c	512	CLA	C3B-C4B-NB	-3.19	107.68	110.53
27	h	101	BCR	C27-C26-C25	3.19	127.01	122.70
34	D	413	LHG	O8-C23-O10	-3.18	115.67	123.63
30	D	409	SQD	O9-S-C6	3.18	111.50	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	601	CLA	C3B-C4B-NB	-3.17	107.70	110.53
25	b	603	CLA	O2D-CGD-CBD	3.17	116.78	111.23
25	b	601	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
30	L	101	SQD	C3-C4-C5	3.17	115.97	110.23
31	H	102	DGD	O2D-C2D-C1D	-3.16	102.55	110.08
25	b	614	CLA	C3B-C4B-NB	-3.16	107.71	110.53
27	c	515	BCR	C11-C10-C9	-3.15	122.86	127.28
27	h	101	BCR	C3-C4-C5	-3.15	108.44	114.06
25	D	405	CLA	CHB-C4A-NA	3.15	128.94	124.40
27	C	514	BCR	C2-C1-C6	3.15	115.01	110.44
25	D	404	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
27	b	618	BCR	C15-C14-C13	-3.13	122.88	127.28
25	c	503	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
31	h	102	DGD	C1D-C2D-C3D	-3.12	103.44	110.01
25	b	603	CLA	C3B-C4B-NB	-3.12	107.74	110.53
25	B	604	CLA	C3B-C4B-NB	-3.12	107.75	110.53
25	B	610	CLA	C1-C2-C3	-3.12	121.09	126.20
25	C	512	CLA	C3B-C4B-NB	-3.11	107.75	110.53
27	B	617	BCR	C3-C4-C5	-3.11	108.50	114.06
25	b	614	CLA	C4A-NA-C1A	3.11	108.10	106.68
25	C	509	CLA	C3B-C4B-NB	-3.11	107.75	110.53
30	D	409	SQD	O48-C23-C24	3.11	121.31	111.83
25	c	512	CLA	CHB-C4A-NA	3.10	128.88	124.40
26	D	402	PHO	OBD-CAD-CBD	-3.10	121.27	125.82
27	B	618	BCR	C2-C1-C6	3.09	114.93	110.44
25	C	505	CLA	C3B-C4B-NB	-3.09	107.78	110.53
25	b	616	CLA	CHB-C4A-NA	3.08	128.85	124.40
25	b	612	CLA	C4A-NA-C1A	3.08	108.08	106.68
36	V	201	HEC	C4D-ND-C1D	3.08	110.84	105.82
25	B	610	CLA	CHB-C4A-NA	3.08	128.84	124.40
31	c	517	DGD	O3G-C1D-C2D	-3.08	103.60	108.27
25	b	602	CLA	CHB-C4A-NA	3.08	128.84	124.40
31	c	517	DGD	O6D-C1D-O3G	-3.07	102.78	110.04
25	C	509	CLA	CHD-C1D-ND	-3.07	120.48	124.80
25	D	405	CLA	C1-C2-C3	-3.07	121.17	126.20
32	C	520	STE	C3-C2-C1	-3.07	106.51	114.51
25	c	513	CLA	C3B-C4B-NB	-3.06	107.79	110.53
25	a	606	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
25	c	503	CLA	CHB-C4A-NA	3.06	128.82	124.40
27	b	617	BCR	C11-C10-C9	-3.06	122.99	127.28
27	T	101	BCR	C2-C1-C6	3.05	114.87	110.44
30	B	622	SQD	O48-C23-C24	3.05	121.13	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
35	e	101	HEM	C3B-C2B-C1B	3.05	108.70	106.41
25	B	612	CLA	O2D-CGD-CBD	3.04	116.55	111.23
25	a	609	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
26	A	608	PHO	O2D-CGD-O1D	-3.04	117.93	123.85
30	a	613	SQD	O47-C7-C8	3.04	118.05	111.48
29	c	523	LMG	O6-C1-O1	-3.04	102.87	110.04
34	d	407	LHG	O8-C23-C24	3.03	121.08	111.83
25	b	614	CLA	C1-C2-C3	-3.03	121.23	126.20
25	a	609	CLA	C4A-NA-C1A	3.03	108.06	106.68
25	B	614	CLA	CHC-C4B-NB	3.03	128.59	124.05
25	b	611	CLA	C3B-C4B-NB	-3.03	107.83	110.53
25	C	506	CLA	O2A-CGA-O1A	-3.03	116.06	123.63
27	c	514	BCR	C2-C1-C6	3.03	114.84	110.44
30	A	613	SQD	O48-C23-C24	3.02	121.04	111.83
25	b	605	CLA	O1D-CGD-CBD	3.02	130.47	124.52
25	c	503	CLA	C3B-C4B-NB	-3.01	107.84	110.53
27	B	618	BCR	C27-C26-C25	3.01	126.77	122.70
25	B	607	CLA	O2A-CGA-O1A	-3.01	116.10	123.63
28	d	406	PL9	C27-C28-C29	-3.01	120.74	127.62
25	b	606	CLA	C1-C2-C3	-3.01	121.27	126.20
29	b	622	LMG	O2-C2-C1	-3.01	102.91	110.08
34	D	411	LHG	O8-C23-C24	3.00	120.97	111.83
25	B	601	CLA	CAA-C2A-C3A	-3.00	104.90	113.00
36	v	201	HEC	CBD-CAD-C3D	-2.99	104.26	112.53
25	c	502	CLA	C3B-C4B-NB	-2.99	107.86	110.53
25	B	609	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
25	c	501	CLA	O2D-CGD-CBD	2.98	116.45	111.23
30	a	613	SQD	C3-C4-C5	2.98	115.64	110.23
25	B	601	CLA	C3B-C4B-NB	-2.98	107.87	110.53
27	t	101	BCR	C11-C10-C9	-2.98	123.10	127.28
25	C	508	CLA	C3B-C4B-NB	-2.98	107.87	110.53
29	c	519	LMG	O6-C1-O1	-2.97	103.02	110.04
25	b	601	CLA	CHB-C4A-NA	2.96	128.68	124.40
27	k	102	BCR	C24-C23-C22	-2.96	121.86	126.23
27	D	406	BCR	C27-C26-C25	2.96	126.70	122.70
34	e	102	LHG	O8-C23-C24	2.95	120.83	111.83
26	A	608	PHO	CMB-C2B-C3B	2.95	130.57	124.68
31	C	517	DGD	O6D-C1D-O3G	-2.94	103.09	110.04
25	c	511	CLA	C3B-C4B-NB	-2.94	107.91	110.53
25	C	508	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
29	C	519	LMG	O6-C1-O1	-2.94	103.11	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	BCR	C27-C26-C25	2.93	126.67	122.70
30	B	622	SQD	C3-C4-C5	2.93	115.55	110.23
25	C	509	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
25	c	506	CLA	C3B-C4B-NB	-2.93	107.92	110.53
25	C	509	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	b	610	CLA	CAA-CBA-CGA	-2.92	104.91	113.21
25	b	610	CLA	CHB-C4A-NA	2.92	128.62	124.40
31	C	518	DGD	O3G-C1D-C2D	-2.92	103.84	108.27
28	d	406	PL9	C42-C43-C44	-2.92	120.94	127.62
25	B	602	CLA	CHB-C4A-NA	2.92	128.61	124.40
25	B	602	CLA	C3B-C4B-NB	-2.91	107.93	110.53
27	c	515	BCR	C27-C26-C25	2.91	126.64	122.70
27	k	101	BCR	C33-C5-C6	-2.91	121.31	124.48
27	t	101	BCR	C33-C5-C6	-2.91	121.31	124.48
27	a	610	BCR	C15-C14-C13	-2.91	123.20	127.28
26	d	402	PHO	C2B-C1B-NB	-2.91	107.33	109.43
27	h	101	BCR	C2-C1-C6	2.91	114.66	110.44
27	a	610	BCR	C2-C1-C6	2.90	114.66	110.44
25	a	612	CLA	C1-C2-C3	-2.90	121.44	126.20
27	d	405	BCR	C27-C26-C25	2.90	126.62	122.70
25	C	513	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	m	101	LMG	C1-O6-C5	-2.90	108.06	113.72
25	b	604	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	c	508	CLA	C1-C2-C3	-2.89	121.46	126.20
27	t	101	BCR	C7-C8-C9	-2.89	121.96	126.23
26	D	402	PHO	CMB-C2B-C3B	2.89	130.45	124.68
29	d	411	LMG	O6-C1-O1	-2.88	103.24	110.04
25	a	609	CLA	O2D-CGD-CBD	2.88	116.26	111.23
32	L	103	STE	O2-C1-C2	2.88	123.09	114.00
25	a	609	CLA	CHB-C4A-NA	2.87	128.55	124.40
27	T	101	BCR	C27-C26-C25	2.87	126.58	122.70
28	a	611	PL9	C37-C38-C39	-2.87	121.06	127.62
30	L	101	SQD	O8-S-C6	2.87	111.51	105.97
27	D	406	BCR	C3-C4-C5	-2.87	108.94	114.06
25	c	513	CLA	CHB-C4A-NA	2.86	128.53	124.40
25	B	607	CLA	C3B-C4B-NB	-2.86	107.98	110.53
30	a	613	SQD	C44-O6-C1	-2.85	107.68	113.80
25	a	612	CLA	O2D-CGD-CBD	2.85	116.22	111.23
25	B	608	CLA	O2D-CGD-CBD	2.85	116.21	111.23
25	B	611	CLA	C1-C2-C3	-2.85	121.53	126.20
25	B	609	CLA	O2A-CGA-O1A	-2.85	116.51	123.63
34	L	102	LHG	O8-C23-C24	2.85	120.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	101	SQD	O2-C2-C1	2.84	116.85	110.08
25	D	403	CLA	CHB-C4A-NA	2.84	128.49	124.40
27	K	102	BCR	C33-C5-C6	-2.83	121.39	124.48
28	D	407	PL9	C12-C13-C14	-2.82	121.16	127.62
27	b	619	BCR	C11-C10-C9	-2.82	123.32	127.28
25	D	403	CLA	O2D-CGD-CBD	2.82	116.16	111.23
27	a	610	BCR	C27-C26-C25	2.82	126.51	122.70
25	B	615	CLA	CHB-C4A-NA	2.82	128.47	124.40
25	B	606	CLA	C3B-C4B-NB	-2.82	108.02	110.53
29	D	408	LMG	O6-C1-O1	-2.81	103.39	110.04
25	B	615	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
25	b	606	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	a	607	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
31	c	516	DGD	O3E-C3E-C2E	-2.81	103.76	110.38
34	D	410	LHG	O8-C23-C24	2.80	120.39	111.83
25	B	607	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
27	D	406	BCR	C7-C8-C9	-2.80	122.10	126.23
27	K	101	BCR	C33-C5-C6	-2.80	121.43	124.48
28	d	406	PL9	C20-C19-C21	2.79	120.08	115.23
25	D	405	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
31	H	102	DGD	C1D-C2D-C3D	-2.79	104.14	110.01
34	d	408	LHG	O8-C23-C24	2.79	120.33	111.83
28	d	406	PL9	C8-C7-C3	2.79	119.24	112.03
25	C	501	CLA	C4D-CHA-C1A	2.79	124.57	121.24
31	c	516	DGD	O6D-C1D-O3G	-2.78	103.47	110.04
29	b	622	LMG	C1-O6-C5	-2.78	108.29	113.72
25	A	609	CLA	CHB-C4A-NA	2.78	128.41	124.40
27	b	618	BCR	C11-C10-C9	-2.78	123.38	127.28
25	b	612	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	a	608	PHO	CMB-C2B-C3B	2.78	130.23	124.68
25	b	607	CLA	CMB-C2B-C1B	-2.76	121.21	125.42
25	b	610	CLA	C3B-C4B-NB	-2.76	108.06	110.53
25	b	609	CLA	CHB-C4A-NA	2.76	128.38	124.40
34	d	409	LHG	O8-C23-C24	2.76	120.25	111.83
25	B	615	CLA	C6-C7-C8	-2.75	106.81	115.97
34	D	413	LHG	C11-C10-C9	-2.75	100.46	114.37
25	b	613	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
29	C	519	LMG	O1-C7-C8	-2.75	104.14	110.82
27	H	101	BCR	C27-C26-C25	2.75	126.41	122.70
25	b	603	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
25	c	505	CLA	C1-C2-C3	-2.74	121.71	126.20
25	C	504	CLA	CED-O2D-CGD	2.74	122.13	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	402	PHO	C3B-C4B-NB	-2.74	105.68	107.46
25	B	613	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
27	c	515	BCR	C2-C1-C6	2.74	114.41	110.44
27	C	515	BCR	C27-C26-C25	2.73	126.40	122.70
25	b	611	CLA	CHB-C4A-NA	2.73	128.34	124.40
30	f	101	SQD	C3-C4-C5	2.73	115.19	110.23
27	b	619	BCR	C27-C26-C25	2.73	126.39	122.70
29	m	101	LMG	O8-C28-O10	-2.73	116.81	123.63
25	B	609	CLA	C1-C2-C3	-2.73	121.73	126.20
25	c	504	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
30	B	622	SQD	C46-C45-C44	-2.72	105.44	111.78
27	b	618	BCR	C2-C1-C6	2.72	114.39	110.44
25	d	403	CLA	CHB-C4A-NA	2.71	128.31	124.40
29	b	622	LMG	O7-C10-O9	-2.71	117.37	123.70
28	D	407	PL9	C27-C28-C29	-2.71	121.42	127.62
27	K	101	BCR	C24-C23-C22	-2.71	122.23	126.23
30	f	101	SQD	O7-S-C6	2.71	110.80	106.76
25	B	612	CLA	C1-C2-C3	-2.71	121.76	126.20
27	k	102	BCR	C33-C5-C6	-2.71	121.53	124.48
25	d	403	CLA	C3B-C4B-NB	-2.70	108.12	110.53
28	a	611	PL9	C20-C19-C21	2.70	119.92	115.23
30	t	102	SQD	C9-C8-C7	-2.70	103.79	113.69
28	A	611	PL9	C22-C23-C24	-2.70	121.44	127.62
25	C	509	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
31	h	102	DGD	C3D-C4D-C5D	-2.70	105.34	110.23
27	K	101	BCR	C7-C8-C9	-2.70	122.25	126.23
25	C	507	CLA	C3B-C4B-NB	-2.70	108.12	110.53
31	h	102	DGD	O6D-C1D-O3G	-2.70	103.67	110.04
28	D	407	PL9	C22-C23-C24	-2.69	121.46	127.62
25	B	607	CLA	CHB-C1B-NB	2.69	128.09	124.05
25	B	604	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	B	602	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
25	b	613	CLA	O2D-CGD-CBD	2.69	115.93	111.23
30	f	101	SQD	O5-C1-C2	-2.69	104.84	110.37
27	B	619	BCR	C11-C10-C9	-2.69	123.51	127.28
25	b	610	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
25	C	508	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
30	f	101	SQD	C1-C2-C3	-2.68	104.37	110.01
31	C	517	DGD	O2D-C2D-C1D	-2.68	103.69	110.08
30	A	613	SQD	C44-O6-C1	-2.68	108.05	113.80
25	c	513	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
25	C	501	CLA	O2A-CGA-O1A	-2.67	116.95	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	518	DGD	O6E-C5E-C4E	2.67	114.51	109.70
28	a	611	PL9	C22-C23-C24	-2.67	121.52	127.62
27	C	514	BCR	C15-C14-C13	-2.66	123.54	127.28
31	h	102	DGD	C4E-C3E-C2E	-2.66	106.15	110.83
25	B	612	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	C	509	CLA	CHD-C4C-NC	2.66	128.36	124.23
28	D	407	PL9	C36-C34-C33	-2.66	115.19	121.17
27	B	619	BCR	C2-C1-C6	2.66	114.30	110.44
26	D	402	PHO	O2D-CGD-O1D	-2.66	118.67	123.85
25	a	606	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
27	A	610	BCR	C11-C10-C9	-2.66	123.55	127.28
31	A	615	DGD	C3G-C2G-C1G	-2.65	105.60	111.78
25	b	602	CLA	O2D-CGD-CBD	2.65	115.86	111.23
25	B	611	CLA	CHB-C4A-NA	2.65	128.23	124.40
36	v	201	HEC	CHA-C4D-ND	2.65	128.66	123.86
28	D	407	PL9	C8-C7-C3	2.65	118.87	112.03
25	B	610	CLA	CAC-C3C-C4C	2.64	128.23	124.79
25	A	609	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
25	d	403	CLA	O2D-CGD-CBD	2.64	115.85	111.23
25	c	509	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
25	D	403	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
31	c	518	DGD	CDB-CCB-CBB	-2.64	101.05	114.37
25	C	509	CLA	CMB-C2B-C3B	2.64	132.75	126.55
31	C	516	DGD	O5D-C6D-C5D	-2.63	103.48	109.42
31	h	102	DGD	CDB-CCB-CBB	-2.63	101.06	114.37
28	A	611	PL9	O2-C1-C6	2.63	124.67	120.48
32	J	101	STE	C3-C2-C1	-2.63	107.64	114.51
34	d	408	LHG	C20-C19-C18	-2.63	101.07	114.37
28	A	611	PL9	O1-C4-C3	-2.63	117.96	120.73
25	B	605	CLA	CHB-C4A-NA	2.63	128.19	124.40
28	A	611	PL9	C20-C19-C21	2.62	119.78	115.23
25	b	613	CLA	CHB-C1B-NB	2.62	127.98	124.05
31	h	102	DGD	O6E-C5E-C6E	-2.62	99.95	106.44
25	b	612	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
25	B	606	CLA	CGD-CBD-CAD	-2.62	102.37	110.85
25	C	501	CLA	CHD-C1D-ND	-2.62	121.12	124.80
25	A	607	CLA	CHB-C4A-NA	2.62	128.18	124.40
31	C	516	DGD	CDB-CCB-CBB	-2.62	101.14	114.37
28	D	407	PL9	C7-C3-C2	-2.62	120.30	123.39
34	D	410	LHG	O8-C23-O10	-2.62	117.09	123.63
31	c	516	DGD	CDB-CCB-CBB	-2.61	101.16	114.37
25	b	612	CLA	CHB-C4A-NA	2.61	128.17	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	405	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
25	B	603	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
25	B	612	CLA	C3B-C4B-NB	-2.61	108.20	110.53
34	E	101	LHG	O8-C23-C24	2.61	119.79	111.83
25	b	602	CLA	C1-C2-C3	-2.61	121.92	126.20
32	d	413	STE	C3-C2-C1	-2.61	107.70	114.51
31	A	615	DGD	O6D-C1D-O3G	-2.61	103.88	110.04
25	b	605	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
28	a	611	PL9	C7-C8-C9	-2.60	122.34	126.83
30	A	614	SQD	O48-C23-C24	2.60	119.77	111.83
25	b	604	CLA	CHB-C4A-NA	2.60	128.16	124.40
34	d	408	LHG	C18-C17-C16	-2.60	101.22	114.37
27	D	406	BCR	C30-C25-C26	-2.60	119.08	122.64
31	c	517	DGD	O2D-C2D-C1D	-2.60	103.88	110.08
27	B	619	BCR	C29-C30-C25	2.60	114.22	110.44
27	H	101	BCR	C2-C1-C6	2.60	114.21	110.44
36	V	201	HEC	CMC-C2C-C1C	-2.60	121.46	125.42
25	c	508	CLA	C3B-C4B-NB	-2.60	108.21	110.53
25	c	510	CLA	CHB-C4A-NA	2.59	128.14	124.40
25	c	501	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
25	a	606	CLA	CHB-C4A-NA	2.59	128.14	124.40
26	D	402	PHO	O1D-CGD-CBD	2.59	128.65	124.72
25	c	507	CLA	CHB-C4A-NA	2.59	128.14	124.40
28	A	611	PL9	C12-C13-C14	-2.59	121.70	127.62
31	A	615	DGD	O2D-C2D-C1D	-2.59	103.91	110.08
27	C	514	BCR	C27-C26-C25	2.59	126.20	122.70
31	h	102	DGD	C3G-C2G-C1G	-2.58	105.76	111.78
31	C	518	DGD	CDB-CCB-CBB	-2.58	101.30	114.37
25	C	506	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
27	c	514	BCR	C27-C26-C25	2.58	126.19	122.70
25	b	613	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
25	c	508	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
25	c	511	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
25	c	504	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
28	D	407	PL9	C7-C8-C9	-2.58	122.39	126.83
25	C	508	CLA	CHD-C1D-ND	-2.58	121.17	124.80
25	d	404	CLA	C3B-C4B-NB	-2.58	108.23	110.53
25	B	612	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
34	D	410	LHG	C20-C19-C18	-2.58	101.35	114.37
26	a	608	PHO	O2D-CGD-O1D	-2.57	118.84	123.85
25	B	606	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
27	b	618	BCR	C27-C26-C25	2.56	126.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	615	DGD	O5D-C6D-C5D	-2.56	103.64	109.42
25	B	605	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
31	c	517	DGD	O3D-C3D-C4D	-2.56	104.35	110.38
25	c	504	CLA	C1-C2-C3	-2.55	122.01	126.20
30	f	101	SQD	O47-C7-C8	2.55	120.30	110.93
29	A	612	LMG	C38-C37-C36	-2.55	101.48	114.37
31	c	518	DGD	C1D-C2D-C3D	-2.55	104.65	110.01
29	M	101	LMG	O6-C1-O1	-2.54	104.03	110.04
31	C	517	DGD	C1D-C2D-C3D	-2.54	104.66	110.01
27	B	617	BCR	C11-C10-C9	-2.54	123.71	127.28
25	C	510	CLA	CHB-C4A-NA	2.54	128.07	124.40
31	c	517	DGD	CBB-CAB-C9B	-2.54	101.53	114.37
25	d	404	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
25	b	606	CLA	CHB-C4A-NA	2.54	128.06	124.40
30	D	409	SQD	O2-C2-C1	2.54	116.12	110.08
25	B	607	CLA	CMB-C2B-C3B	2.54	132.52	126.55
29	m	101	LMG	O3-C3-C2	-2.53	104.40	110.38
25	b	608	CLA	CHD-C4C-NC	2.53	128.16	124.23
27	d	405	BCR	C38-C26-C25	-2.53	121.72	124.48
31	A	615	DGD	CDB-CCB-CBB	-2.53	101.58	114.37
28	d	406	PL9	C22-C23-C24	-2.53	121.83	127.62
25	C	505	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
28	A	611	PL9	O2-C1-C2	-2.53	116.08	121.83
27	C	514	BCR	C7-C8-C9	-2.53	122.50	126.23
25	B	602	CLA	C1-C2-C3	-2.53	122.06	126.20
29	M	101	LMG	O3-C3-C2	-2.52	104.42	110.38
27	H	101	BCR	C24-C23-C22	-2.52	122.50	126.23
27	B	617	BCR	C15-C16-C17	-2.52	118.35	123.52
25	C	502	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
25	A	607	CLA	CHD-C1D-ND	-2.52	121.25	124.80
27	t	101	BCR	C15-C16-C17	-2.52	118.36	123.52
27	K	101	BCR	C2-C1-C6	2.52	114.10	110.44
25	b	613	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	a	612	CLA	CHB-C4A-NA	2.52	128.04	124.40
25	c	509	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	c	507	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
30	f	101	SQD	O48-C23-C24	2.52	119.52	111.83
25	B	606	CLA	CHB-C4A-NA	2.52	128.04	124.40
25	b	604	CLA	O2D-CGD-CBD	2.52	115.64	111.23
35	e	101	HEM	C3B-C4B-NB	-2.52	107.66	109.47
29	D	412	LMG	O1-C7-C8	-2.52	105.30	111.77
30	B	622	SQD	O5-C5-C4	2.52	114.23	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	607	CLA	C3B-C4B-NB	-2.52	108.28	110.53
31	c	518	DGD	C3G-C2G-C1G	-2.52	105.92	111.78
25	A	609	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
27	b	619	BCR	C15-C16-C17	-2.51	118.37	123.52
25	b	614	CLA	CHD-C1D-ND	-2.51	121.27	124.80
25	A	609	CLA	CHD-C1D-ND	-2.51	121.27	124.80
27	C	515	BCR	C15-C16-C17	-2.51	118.39	123.52
25	b	610	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
25	A	606	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	c	512	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
27	b	617	BCR	C3-C4-C5	-2.51	109.59	114.06
34	L	102	LHG	C5-O7-C7	-2.50	111.80	117.80
27	t	101	BCR	C27-C26-C25	2.50	126.09	122.70
25	B	606	CLA	C1-C2-C3	-2.50	122.10	126.20
25	C	507	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	C	501	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
27	b	617	BCR	C27-C26-C25	2.50	126.08	122.70
29	c	521	LMG	C40-C39-C38	-2.50	101.75	114.37
31	c	517	DGD	CDB-CCB-CBB	-2.50	101.76	114.37
29	D	408	LMG	O2-C2-C1	-2.49	104.13	110.08
29	A	612	LMG	C40-C39-C38	-2.49	101.77	114.37
31	c	518	DGD	O6E-C1E-O5D	-2.49	104.16	110.04
29	m	101	LMG	O6-C1-O1	-2.49	104.17	110.04
28	d	406	PL9	C50-C49-C48	-2.49	115.19	122.66
25	B	613	CLA	CMB-C2B-C3B	2.48	132.39	126.55
28	a	611	PL9	O1-C4-C3	-2.48	118.11	120.73
25	b	616	CLA	C3B-C4B-NB	-2.48	108.32	110.53
25	C	502	CLA	CHA-C1A-NA	-2.48	120.78	126.39
25	c	503	CLA	C1-C2-C3	-2.48	122.14	126.20
36	V	201	HEC	CMD-C2D-C1D	2.47	129.19	125.42
34	l	101	LHG	O8-C23-C24	2.47	119.38	111.83
27	K	101	BCR	C11-C10-C9	-2.47	123.81	127.28
25	D	403	CLA	CHD-C1D-ND	-2.47	121.32	124.80
25	C	501	CLA	CHD-C1D-C2D	2.47	130.63	125.49
29	c	523	LMG	C40-C39-C38	-2.47	101.87	114.37
25	A	607	CLA	C1-C2-C3	-2.47	122.15	126.20
27	K	101	BCR	C15-C14-C13	-2.47	123.82	127.28
27	A	610	BCR	C2-C1-C6	2.47	114.02	110.44
36	V	201	HEC	CHB-C4A-NA	2.47	127.14	124.45
25	C	505	CLA	CHB-C1B-NB	2.47	127.75	124.05
29	m	101	LMG	C40-C39-C38	-2.46	101.92	114.37
25	C	512	CLA	O2A-CGA-O1A	-2.46	117.47	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	605	CLA	CHB-C4A-NA	2.46	127.95	124.40
27	h	101	BCR	C15-C16-C17	-2.46	118.49	123.52
25	b	612	CLA	CMB-C2B-C3B	2.46	132.33	126.55
29	c	521	LMG	O6-C1-O1	-2.46	104.24	110.04
25	a	609	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
27	B	618	BCR	C33-C5-C6	-2.45	121.81	124.48
31	A	615	DGD	C4E-C3E-C2E	-2.45	106.54	110.83
29	M	101	LMG	C38-C37-C36	-2.44	102.01	114.37
27	K	101	BCR	C27-C26-C25	2.44	126.01	122.70
25	a	607	CLA	C3B-C4B-NB	-2.44	108.35	110.53
27	h	101	BCR	C11-C10-C9	-2.44	123.85	127.28
34	l	101	LHG	C5-O7-C7	-2.44	111.95	117.80
25	C	505	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
30	f	101	SQD	C1-O5-C5	-2.44	108.95	113.72
25	B	601	CLA	O1D-CGD-CBD	2.44	129.33	124.52
29	d	411	LMG	C40-C39-C38	-2.44	102.05	114.37
34	D	410	LHG	C27-C26-C25	-2.44	102.05	114.37
25	b	604	CLA	CAA-CBA-CGA	-2.44	106.29	113.21
27	c	514	BCR	C33-C5-C6	-2.43	121.83	124.48
25	A	607	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
25	c	510	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
25	b	602	CLA	C16-C15-C13	-2.43	107.90	115.97
25	C	503	CLA	C1-O2A-CGA	2.43	122.53	116.65
25	A	606	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
25	b	615	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
25	c	507	CLA	C3B-C4B-NB	-2.43	108.36	110.53
27	C	514	BCR	C33-C5-C6	-2.42	121.84	124.48
32	M	102	STE	C3-C2-C1	-2.42	108.18	114.51
31	H	102	DGD	O3D-C3D-C4D	-2.42	104.67	110.38
29	c	519	LMG	C38-C37-C36	-2.42	102.14	114.37
30	L	101	SQD	O9-S-C6	2.42	110.36	106.76
34	e	102	LHG	C11-C10-C9	-2.42	102.16	114.37
25	a	609	CLA	C1-C2-C3	-2.42	122.24	126.20
30	A	613	SQD	O9-S-C6	2.41	110.36	106.76
25	b	607	CLA	CMB-C2B-C3B	2.41	132.22	126.55
27	C	514	BCR	C11-C10-C9	-2.41	123.90	127.28
27	B	617	BCR	C27-C26-C25	2.41	125.96	122.70
25	d	404	CLA	CMB-C2B-C3B	2.41	132.22	126.55
31	C	518	DGD	O3E-C3E-C2E	-2.41	104.70	110.38
26	A	608	PHO	O2A-CGA-O1A	-2.41	117.60	123.63
31	C	517	DGD	CDB-CCB-CBB	-2.41	102.19	114.37
28	D	407	PL9	C20-C19-C21	2.41	119.41	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	613	CLA	CHA-C1A-NA	-2.41	120.94	126.39
35	e	101	HEM	CHB-C1B-NB	2.41	127.34	124.37
34	d	407	LHG	C20-C19-C18	-2.40	102.21	114.37
34	d	408	LHG	C27-C26-C25	-2.40	102.21	114.37
25	b	612	CLA	O1D-CGD-CBD	2.40	129.26	124.52
28	D	407	PL9	O1-C4-C3	-2.40	118.20	120.73
25	B	607	CLA	C1-C2-C3	-2.40	122.26	126.20
25	A	607	CLA	O1D-CGD-CBD	2.40	129.26	124.52
27	C	515	BCR	C2-C1-C6	2.40	113.93	110.44
25	D	404	CLA	C4-C3-C5	2.40	119.39	115.23
30	A	614	SQD	C45-O47-C7	-2.40	114.32	117.78
25	C	508	CLA	CHD-C1D-C2D	2.40	130.47	125.49
25	B	607	CLA	C2A-C1A-CHA	2.39	128.02	123.87
25	b	607	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
34	D	411	LHG	O8-C23-O10	-2.39	117.65	123.63
25	B	601	CLA	C2A-C1A-CHA	2.39	128.01	123.87
25	B	614	CLA	O2D-CGD-CBD	2.39	115.41	111.23
36	V	201	HEC	CAD-CBD-CGD	-2.39	107.33	113.67
25	B	616	CLA	CHB-C4A-NA	2.39	127.84	124.40
25	C	501	CLA	O2D-CGD-CBD	2.38	115.40	111.23
25	b	603	CLA	CHD-C1D-ND	-2.38	121.45	124.80
28	A	611	PL9	C40-C39-C41	2.38	119.36	115.23
31	A	615	DGD	O3G-C3G-C2G	-2.38	105.03	110.82
34	D	410	LHG	C18-C17-C16	-2.38	102.33	114.37
25	b	604	CLA	C11-C12-C13	-2.38	108.06	115.97
31	c	516	DGD	C5B-C4B-C3B	-2.38	102.35	114.37
25	C	512	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	B	605	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
31	H	102	DGD	CDB-CCB-CBB	-2.37	102.36	114.37
30	t	102	SQD	O48-C23-O10	-2.37	117.69	123.63
26	a	608	PHO	O2D-CGD-CBD	2.37	113.55	110.95
31	c	516	DGD	O2D-C2D-C1D	-2.37	104.43	110.08
25	c	502	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
28	D	407	PL9	C40-C39-C41	2.36	119.33	115.23
25	b	601	CLA	CHD-C1D-ND	-2.36	121.48	124.80
27	A	610	BCR	C33-C5-C6	-2.36	121.91	124.48
27	k	102	BCR	C27-C26-C25	2.36	125.89	122.70
31	c	518	DGD	O3E-C3E-C2E	-2.36	104.82	110.38
25	C	513	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
25	A	609	CLA	O2D-CGD-CBD	2.35	115.34	111.23
28	a	611	PL9	O2-C1-C2	-2.35	116.48	121.83
25	b	612	CLA	CAC-C3C-C4C	2.35	127.85	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	CLA	C1-C2-C3	-2.35	122.35	126.20
27	k	101	BCR	C27-C26-C25	2.35	125.88	122.70
25	b	609	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
30	A	613	SQD	O5-C5-C4	2.35	113.93	109.70
25	b	605	CLA	C3B-C4B-NB	-2.35	108.44	110.53
35	e	101	HEM	CAB-C3B-C2B	-2.35	120.81	128.43
31	a	614	DGD	CAB-C9B-C8B	-2.35	102.51	114.37
25	C	504	CLA	CHD-C4C-NC	2.34	127.87	124.23
31	a	614	DGD	C6B-C5B-C4B	-2.34	102.52	114.37
25	c	506	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
29	C	519	LMG	C40-C39-C38	-2.34	102.52	114.37
25	c	510	CLA	O2D-CGD-CBD	2.34	115.33	111.23
25	c	508	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	b	610	CLA	O1D-CGD-CBD	2.34	129.14	124.52
36	V	201	HEC	CBD-CAD-C3D	-2.34	106.06	112.53
29	m	101	LMG	O7-C10-O9	-2.34	118.23	123.70
27	k	101	BCR	C7-C8-C9	-2.34	122.77	126.23
34	D	413	LHG	C20-C19-C18	-2.34	102.54	114.37
25	d	404	CLA	CHB-C4A-NA	2.34	127.77	124.40
25	c	503	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
25	c	512	CLA	O1D-CGD-CBD	2.34	129.13	124.52
31	A	615	DGD	C1E-O6E-C5E	2.34	118.28	113.72
31	H	102	DGD	C3E-C4E-C5E	-2.34	106.00	110.23
25	c	503	CLA	C4-C3-C5	2.33	119.28	115.23
34	e	102	LHG	C20-C19-C18	-2.33	102.57	114.37
25	C	508	CLA	O2D-CGD-CBD	2.33	115.31	111.23
25	C	511	CLA	CHB-C4A-NA	2.33	127.77	124.40
32	t	103	STE	O2-C1-C2	2.33	121.37	114.00
30	A	613	SQD	O8-S-C6	2.33	110.47	105.97
31	H	102	DGD	C7B-C6B-C5B	-2.33	102.59	114.37
28	d	406	PL9	C36-C34-C33	-2.33	115.94	121.17
27	a	610	BCR	C3-C4-C5	-2.33	109.91	114.06
34	E	101	LHG	C11-C10-C9	-2.32	102.62	114.37
29	c	523	LMG	C38-C37-C36	-2.32	102.62	114.37
25	B	608	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
25	B	615	CLA	C16-C15-C13	-2.32	108.25	115.97
31	H	102	DGD	CAB-C9B-C8B	-2.32	102.64	114.37
25	b	601	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
29	M	101	LMG	O7-C10-O9	-2.32	118.29	123.70
34	E	101	LHG	C20-C19-C18	-2.32	102.67	114.37
25	C	505	CLA	C11-C10-C8	-2.31	108.27	115.97
25	d	404	CLA	O2D-CGD-O1D	-2.31	119.34	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	101	HEM	C4D-ND-C1D	2.31	107.94	105.21
25	c	509	CLA	CHD-C1D-ND	-2.31	121.55	124.80
29	d	411	LMG	O3-C3-C2	-2.31	104.93	110.38
34	D	413	LHG	C18-C17-C16	-2.31	102.71	114.37
29	c	521	LMG	O8-C28-O10	-2.31	117.86	123.63
25	B	601	CLA	O2D-CGD-CBD	2.31	115.26	111.23
29	A	612	LMG	O8-C28-O10	-2.31	117.86	123.63
31	C	516	DGD	CAB-C9B-C8B	-2.31	102.71	114.37
34	D	410	LHG	C11-C10-C9	-2.30	102.72	114.37
25	b	614	CLA	CHD-C1D-C2D	2.30	130.28	125.49
34	d	407	LHG	C11-C10-C9	-2.30	102.73	114.37
25	C	510	CLA	O2D-CGD-CBD	2.30	115.25	111.23
25	b	604	CLA	CHB-C1B-NB	2.30	127.49	124.05
28	D	407	PL9	C37-C38-C39	-2.30	122.37	127.62
34	L	102	LHG	C20-C19-C18	-2.30	102.76	114.37
25	B	614	CLA	CHB-C4A-NA	2.29	127.71	124.40
25	b	614	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
25	C	502	CLA	C3B-C4B-NB	-2.29	108.48	110.53
25	C	507	CLA	C1-C2-C3	-2.29	122.44	126.20
25	b	609	CLA	O1D-CGD-CBD	2.29	129.04	124.52
28	D	407	PL9	C30-C29-C31	-2.29	111.25	115.23
29	m	101	LMG	C9-C8-C7	-2.29	106.45	111.78
29	c	521	LMG	C38-C37-C36	-2.29	102.81	114.37
31	a	614	DGD	CDB-CCB-CBB	-2.29	102.81	114.37
25	C	507	CLA	CHC-C4B-NB	2.29	127.48	124.05
25	D	404	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
25	C	508	CLA	C1D-ND-C4D	2.28	107.91	106.31
25	C	510	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
29	M	101	LMG	O8-C28-O10	-2.28	117.93	123.63
31	h	102	DGD	O3E-C3E-C2E	-2.28	105.00	110.38
27	D	406	BCR	C24-C23-C22	-2.28	122.87	126.23
25	b	613	CLA	CHB-C4A-NA	2.28	127.68	124.40
25	a	607	CLA	O1D-CGD-CBD	2.28	129.01	124.52
31	c	517	DGD	O5D-C6D-C5D	-2.27	104.29	109.42
34	L	102	LHG	C11-C10-C9	-2.27	102.87	114.37
29	c	521	LMG	O7-C10-O9	-2.27	118.39	123.70
25	C	504	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
31	c	518	DGD	CAB-C9B-C8B	-2.27	102.89	114.37
25	C	504	CLA	CHB-C1B-NB	2.27	127.45	124.05
25	C	503	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
25	B	610	CLA	CHD-C1D-ND	-2.27	121.61	124.80
32	t	103	STE	C3-C2-C1	-2.27	108.59	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	411	LMG	O1-C7-C8	-2.27	105.31	110.82
27	B	619	BCR	C1-C6-C5	-2.27	119.54	122.64
32	C	521	STE	C3-C2-C1	-2.26	108.60	114.51
31	h	102	DGD	CBB-CAB-C9B	-2.26	102.92	114.37
25	b	606	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
27	c	515	BCR	C15-C16-C17	-2.26	118.89	123.52
29	d	411	LMG	O2-C2-C1	-2.26	104.69	110.08
25	B	613	CLA	C3B-C4B-NB	-2.26	108.51	110.53
32	d	412	STE	O2-C1-C2	2.26	121.14	114.00
25	C	506	CLA	CHB-C4A-NA	2.26	127.66	124.40
28	a	611	PL9	C40-C39-C41	2.26	119.15	115.23
25	b	606	CLA	CHD-C4C-NC	2.26	127.73	124.23
29	B	621	LMG	C38-C37-C36	-2.26	102.95	114.37
25	b	607	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	C	502	CLA	CHB-C1B-NB	2.26	127.43	124.05
25	A	609	CLA	CMB-C2B-C3B	2.25	131.85	126.55
25	B	612	CLA	O1D-CGD-CBD	2.25	128.96	124.52
27	b	617	BCR	C15-C16-C17	-2.25	118.92	123.52
25	A	607	CLA	O2D-CGD-CBD	2.25	115.16	111.23
29	M	101	LMG	C40-C39-C38	-2.25	103.00	114.37
25	B	601	CLA	CHB-C4A-NA	2.25	127.64	124.40
36	v	201	HEC	CHB-C1B-NB	2.25	127.94	123.86
31	C	517	DGD	C5B-C4B-C3B	-2.25	103.01	114.37
34	D	411	LHG	C11-C10-C9	-2.25	103.02	114.37
25	C	508	CLA	CHB-C1B-NB	2.25	127.42	124.05
27	B	618	BCR	C3-C4-C5	-2.24	110.05	114.06
29	D	412	LMG	O7-C10-O9	-2.24	118.46	123.70
25	c	508	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
26	d	402	PHO	CMA-C3A-C4A	-2.24	109.78	114.61
25	C	507	CLA	O2D-CGD-CBD	2.24	115.15	111.23
25	C	504	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
25	B	608	CLA	C3B-C4B-NB	-2.24	108.53	110.53
25	a	606	CLA	O1D-CGD-CBD	2.24	128.94	124.52
25	b	603	CLA	CHB-C4A-NA	2.24	127.63	124.40
25	c	502	CLA	CHD-C1D-ND	-2.24	121.65	124.80
27	B	617	BCR	C33-C5-C6	-2.24	122.04	124.48
29	b	622	LMG	C40-C39-C38	-2.24	103.06	114.37
31	c	516	DGD	C3G-C2G-C1G	-2.24	106.57	111.78
34	l	101	LHG	O8-C23-O10	-2.24	118.04	123.63
25	b	608	CLA	CHD-C4C-C3C	-2.23	121.52	124.77
25	c	508	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	H	102	DGD	C3D-C4D-C5D	-2.23	106.18	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	609	CLA	CHB-C4A-NA	2.23	127.62	124.40
25	c	509	CLA	C1-O2A-CGA	-2.23	111.25	116.65
27	t	101	BCR	C28-C27-C26	-2.23	110.08	114.06
25	b	612	CLA	C11-C12-C13	-2.23	108.56	115.97
25	D	403	CLA	CHD-C1D-C2D	2.23	130.12	125.49
26	d	402	PHO	C16-C15-C13	-2.23	108.56	115.97
25	b	613	CLA	C2D-C1D-ND	-2.23	107.92	110.13
31	a	614	DGD	C7B-C6B-C5B	-2.23	103.12	114.37
29	D	408	LMG	C38-C37-C36	-2.22	103.12	114.37
29	c	519	LMG	O3-C3-C2	-2.22	105.13	110.38
25	B	607	CLA	CHC-C4B-NB	2.22	127.39	124.05
29	C	519	LMG	C38-C37-C36	-2.22	103.13	114.37
25	A	609	CLA	CHC-C1C-NC	2.22	127.66	124.31
25	a	609	CLA	CAA-CBA-CGA	-2.22	106.90	113.21
25	B	616	CLA	O2D-CGD-CBD	2.22	115.11	111.23
25	C	502	CLA	O1D-CGD-CBD	2.22	128.90	124.52
25	C	503	CLA	CHB-C4A-NA	2.22	127.60	124.40
25	B	614	CLA	CHA-C1A-NA	-2.22	121.37	126.39
27	K	102	BCR	C15-C14-C13	-2.22	124.17	127.28
34	l	101	LHG	C11-C10-C9	-2.22	103.16	114.37
28	d	406	PL9	O1-C4-C3	-2.22	118.39	120.73
30	L	101	SQD	O5-C1-C2	-2.22	105.82	110.37
25	C	508	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	c	503	CLA	CHD-C1D-ND	-2.21	121.69	124.80
29	c	519	LMG	C40-C39-C38	-2.21	103.19	114.37
31	C	518	DGD	O5D-C6D-C5D	-2.21	104.44	109.42
29	A	612	LMG	O6-C1-O1	-2.21	104.82	110.04
25	b	616	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
25	b	604	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
31	h	102	DGD	O6E-C5E-C4E	2.20	113.67	109.70
25	C	505	CLA	O2D-CGD-CBD	2.20	115.08	111.23
25	A	606	CLA	C7-C6-C5	-2.20	107.39	113.26
32	b	625	STE	O2-C1-C2	2.20	120.96	114.00
25	b	602	CLA	C11-C10-C8	-2.20	108.66	115.97
29	m	101	LMG	C38-C37-C36	-2.20	103.26	114.37
25	B	603	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
25	b	609	CLA	C3B-C4B-NB	-2.20	108.57	110.53
25	B	601	CLA	CHA-C4D-ND	2.20	137.08	132.55
29	c	523	LMG	O7-C10-O9	-2.19	118.58	123.70
25	d	404	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
25	C	513	CLA	CHB-C4A-NA	2.19	127.56	124.40
25	a	607	CLA	O2D-CGD-CBD	2.19	115.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	618	BCR	C30-C25-C26	-2.19	119.64	122.64
28	d	406	PL9	C12-C13-C14	-2.19	122.61	127.62
25	c	502	CLA	O2D-CGD-CBD	2.19	115.06	111.23
25	B	603	CLA	CMB-C2B-C3B	2.19	131.70	126.55
25	C	503	CLA	CHD-C1D-ND	-2.19	121.72	124.80
29	d	411	LMG	C38-C37-C36	-2.19	103.31	114.37
32	J	101	STE	O2-C1-C2	2.19	120.91	114.00
25	b	613	CLA	CMB-C2B-C3B	2.19	131.69	126.55
25	b	603	CLA	O1D-CGD-CBD	2.19	128.83	124.52
28	d	406	PL9	O2-C1-C6	2.18	123.96	120.48
30	B	622	SQD	O5-C1-C2	-2.18	105.88	110.37
25	c	505	CLA	C16-C15-C13	-2.18	108.71	115.97
27	A	610	BCR	C7-C8-C9	-2.18	123.01	126.23
29	A	612	LMG	C1-O6-C5	-2.18	109.46	113.72
29	D	408	LMG	O1-C7-C8	-2.18	105.52	110.82
25	B	605	CLA	CHD-C1D-ND	-2.18	121.74	124.80
25	B	601	CLA	CAA-CBA-CGA	-2.17	107.03	113.21
31	A	615	DGD	CAB-C9B-C8B	-2.17	103.38	114.37
25	B	609	CLA	CHD-C1D-ND	-2.17	121.75	124.80
25	B	613	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	C	502	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
31	c	518	DGD	C3D-C4D-C5D	-2.17	106.30	110.23
25	C	504	CLA	O2D-CGD-CBD	2.17	115.02	111.23
25	b	604	CLA	CBA-CAA-C2A	-2.17	107.34	113.79
25	b	615	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	c	511	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	c	510	CLA	C3B-C4B-NB	-2.17	108.60	110.53
31	C	516	DGD	C6B-C5B-C4B	-2.16	103.43	114.37
31	C	516	DGD	O2E-C2E-C1E	-2.16	104.92	110.08
26	D	402	PHO	CMD-C2D-C3D	2.16	129.00	124.68
25	c	513	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
25	C	504	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
32	c	522	STE	C3-C2-C1	-2.16	108.87	114.51
30	L	101	SQD	C9-C8-C7	-2.16	105.78	113.69
29	b	622	LMG	C3-C4-C5	-2.16	106.32	110.23
31	A	615	DGD	C8B-C7B-C6B	-2.16	103.46	114.37
25	D	404	CLA	O2D-CGD-CBD	2.16	115.00	111.23
25	B	611	CLA	CHD-C4C-NC	2.16	127.57	124.23
30	D	409	SQD	O7-S-C6	2.15	109.97	106.76
28	a	611	PL9	C27-C28-C29	-2.15	122.69	127.62
25	c	511	CLA	C1-C2-C3	-2.15	122.67	126.20
25	B	604	CLA	CAA-CBA-CGA	-2.15	107.10	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	101	LHG	C18-C17-C16	-2.15	103.50	114.37
27	T	101	BCR	C31-C1-C6	2.15	113.61	110.24
27	B	619	BCR	C34-C9-C10	-2.15	119.33	122.82
25	C	512	CLA	CHB-C1B-NB	2.15	127.27	124.05
30	A	613	SQD	O5-C1-O6	2.15	115.12	110.04
31	c	516	DGD	O5D-C6D-C5D	-2.15	104.58	109.42
25	B	601	CLA	CHA-C1A-NA	-2.15	121.53	126.39
25	C	512	CLA	CHA-C1A-NA	-2.15	121.53	126.39
34	d	408	LHG	O8-C23-O10	-2.15	118.25	123.63
27	b	618	BCR	C8-C7-C6	-2.15	121.27	127.00
28	a	611	PL9	O2-C1-C6	2.15	123.89	120.48
27	T	101	BCR	C7-C8-C9	-2.14	123.06	126.23
25	b	609	CLA	CHC-C4B-NB	2.14	127.26	124.05
25	b	609	CLA	C7-C6-C5	-2.14	107.55	113.26
29	D	408	LMG	O1-C1-C2	-2.14	105.02	108.27
32	B	624	STE	O2-C1-C2	2.14	120.76	114.00
29	D	408	LMG	O3-C3-C2	-2.14	105.33	110.38
25	b	603	CLA	CHA-C4D-ND	2.14	136.96	132.55
31	C	517	DGD	CAB-C9B-C8B	-2.14	103.57	114.37
29	c	521	LMG	O2-C2-C1	-2.13	104.99	110.08
30	a	613	SQD	O8-S-C6	2.13	110.09	105.97
25	b	614	CLA	CHC-C4B-NB	2.13	127.24	124.05
31	H	102	DGD	C5B-C4B-C3B	-2.13	103.61	114.37
25	C	512	CLA	O2D-CGD-CBD	2.13	114.95	111.23
25	a	606	CLA	C2A-C1A-CHA	2.13	127.56	123.87
25	b	613	CLA	CHA-C4D-ND	2.13	136.94	132.55
25	c	504	CLA	C3B-C4B-NB	-2.13	108.63	110.53
25	b	607	CLA	CHB-C1B-NB	2.13	127.24	124.05
30	B	622	SQD	O8-S-C6	2.13	110.08	105.97
25	C	504	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	h	102	DGD	C7B-C6B-C5B	-2.12	103.63	114.37
27	c	514	BCR	C3-C4-C5	-2.12	110.27	114.06
27	c	514	BCR	C15-C14-C13	-2.12	124.30	127.28
27	K	101	BCR	C35-C13-C14	-2.12	119.38	122.82
34	l	101	LHG	C20-C19-C18	-2.12	103.64	114.37
26	a	608	PHO	O2A-CGA-O1A	-2.12	118.32	123.63
25	b	608	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
27	c	514	BCR	C7-C8-C9	-2.12	123.10	126.23
25	B	605	CLA	CHD-C4C-NC	2.12	127.52	124.23
25	c	505	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	c	517	DGD	C6D-O5D-C1E	2.12	118.34	113.80
25	B	614	CLA	CHB-C1B-NB	2.12	127.23	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	612	CLA	CMB-C2B-C3B	2.12	131.54	126.55
25	D	405	CLA	CHD-C1D-ND	-2.12	121.82	124.80
26	A	608	PHO	CMA-C3A-C4A	-2.12	110.05	114.61
25	d	404	CLA	CHB-C1B-NB	2.12	127.22	124.05
26	D	402	PHO	C2D-C1D-ND	-2.12	107.90	109.43
25	B	608	CLA	CMB-C2B-C3B	2.12	131.53	126.55
25	C	513	CLA	O2D-CGD-CBD	2.11	114.92	111.23
25	B	610	CLA	C11-C10-C8	-2.11	108.94	115.97
27	t	101	BCR	C35-C13-C12	2.11	121.31	118.09
25	C	507	CLA	CAA-CBA-CGA	-2.11	107.22	113.21
31	h	102	DGD	CAB-C9B-C8B	-2.11	103.70	114.37
32	R	101	STE	O2-C1-C2	2.11	120.67	114.00
27	d	405	BCR	C2-C1-C6	2.11	113.50	110.44
25	B	612	CLA	CED-O2D-CGD	-2.11	111.13	115.92
25	B	609	CLA	C7-C6-C5	-2.11	107.64	113.26
25	b	603	CLA	CHB-C1B-NB	2.11	127.21	124.05
27	C	514	BCR	C3-C4-C5	-2.11	110.30	114.06
27	k	102	BCR	C11-C10-C9	-2.11	124.32	127.28
31	C	516	DGD	C3G-C2G-C1G	-2.11	106.87	111.78
25	b	609	CLA	C1-C2-C3	-2.11	122.75	126.20
25	b	608	CLA	C2A-C1A-CHA	2.10	127.52	123.87
27	h	101	BCR	C20-C21-C22	-2.10	124.33	127.28
36	v	201	HEC	CBA-CAA-C2A	-2.10	106.71	112.53
31	c	518	DGD	O5E-C6E-C5E	-2.10	104.17	111.33
25	a	612	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
25	B	613	CLA	CHA-C1A-NA	-2.10	121.63	126.39
29	M	101	LMG	O2-C2-C1	-2.10	105.07	110.08
27	B	619	BCR	C15-C16-C17	-2.10	119.22	123.52
31	c	516	DGD	CBB-CAB-C9B	-2.10	103.75	114.37
34	l	101	LHG	C27-C26-C25	-2.10	103.75	114.37
25	C	511	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
25	B	614	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
31	c	518	DGD	C8B-C7B-C6B	-2.10	103.76	114.37
31	c	517	DGD	O6E-C1E-O5D	-2.10	105.09	110.04
25	c	501	CLA	CHB-C4A-NA	2.10	127.43	124.40
27	B	618	BCR	C29-C30-C25	2.10	113.48	110.44
27	K	102	BCR	C10-C11-C12	-2.10	117.13	123.20
25	c	512	CLA	CHD-C1D-ND	-2.10	121.85	124.80
34	d	407	LHG	C18-C17-C16	-2.10	103.78	114.37
30	a	613	SQD	O5-C5-C4	2.09	113.47	109.70
25	c	511	CLA	C2A-C1A-CHA	2.09	127.50	123.87
26	a	608	PHO	CMA-C3A-C4A	-2.09	110.10	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	O2D-CGD-CBD	2.09	114.89	111.23
25	c	510	CLA	C1-C2-C3	-2.09	122.77	126.20
27	k	102	BCR	C28-C27-C26	-2.09	110.33	114.06
32	t	104	STE	C3-C2-C1	-2.09	109.05	114.51
25	c	506	CLA	CHB-C1B-NB	2.09	127.19	124.05
31	a	614	DGD	C1G-C2G-C3G	-2.09	106.98	111.80
26	D	402	PHO	OBD-CAD-C3D	2.09	131.15	127.89
31	H	102	DGD	O3E-C3E-C2E	-2.09	105.46	110.38
25	a	612	CLA	CHD-C1D-ND	-2.09	121.87	124.80
25	d	403	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
25	A	607	CLA	CHD-C1D-C2D	2.08	129.82	125.49
31	A	615	DGD	O5E-C6E-C5E	-2.08	104.24	111.33
31	C	518	DGD	C7B-C6B-C5B	-2.08	103.83	114.37
29	c	521	LMG	C42-C41-C40	-2.08	103.84	114.37
25	C	510	CLA	CMB-C2B-C3B	2.08	131.45	126.55
25	b	612	CLA	CHA-C1A-NA	-2.08	121.68	126.39
34	e	102	LHG	C5-O7-C7	-2.08	112.82	117.80
25	c	507	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
31	A	615	DGD	C5B-C4B-C3B	-2.08	103.86	114.37
25	C	502	CLA	CHD-C1D-ND	-2.08	121.88	124.80
27	h	101	BCR	C7-C8-C9	-2.08	123.16	126.23
27	h	101	BCR	C38-C26-C25	-2.07	122.22	124.48
25	C	506	CLA	C1-C2-C3	-2.07	122.80	126.20
31	A	615	DGD	O6E-C5E-C4E	2.07	113.44	109.70
25	c	505	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	c	510	CLA	C16-C15-C13	-2.07	109.09	115.97
31	c	516	DGD	C4E-C3E-C2E	-2.07	107.20	110.83
25	C	509	CLA	CHD-C1D-C2D	2.07	129.78	125.49
25	B	606	CLA	CHA-C1A-NA	-2.07	121.71	126.39
35	e	101	HEM	C1B-NB-C4B	2.07	107.65	105.21
31	c	517	DGD	C7B-C6B-C5B	-2.07	103.93	114.37
34	l	101	LHG	C29-C28-C27	-2.06	103.93	114.37
25	B	612	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
35	e	101	HEM	CHA-C4D-ND	2.06	126.92	124.37
29	A	612	LMG	O3-C3-C2	-2.06	105.52	110.38
27	B	617	BCR	C30-C25-C26	-2.06	119.82	122.64
25	C	505	CLA	C4D-CHA-C1A	-2.06	118.79	121.24
25	C	505	CLA	CHA-C1A-NA	-2.06	121.73	126.39
25	B	613	CLA	CED-O2D-CGD	2.06	120.58	115.92
32	b	621	STE	C3-C2-C1	-2.06	109.14	114.51
29	C	519	LMG	O8-C28-O10	-2.06	118.48	123.63
29	A	612	LMG	C36-C35-C34	-2.06	103.97	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	518	DGD	CBB-CAB-C9B	-2.06	103.97	114.37
25	b	607	CLA	C1D-CHD-C4C	-2.06	121.65	126.02
25	B	602	CLA	CGD-CBD-CAD	-2.06	104.19	110.85
31	C	516	DGD	O3E-C3E-C2E	-2.05	105.53	110.38
25	C	508	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
36	v	201	HEC	CMD-C2D-C1D	2.05	128.55	125.42
25	c	508	CLA	O2D-CGD-CBD	2.05	114.81	111.23
31	c	518	DGD	O6E-C5E-C4E	2.05	113.39	109.70
27	t	101	BCR	C16-C15-C14	-2.05	119.33	123.52
25	b	604	CLA	C2A-C1A-CHA	2.05	127.42	123.87
25	c	509	CLA	C11-C12-C13	-2.05	109.16	115.97
34	d	407	LHG	C27-C26-C25	-2.05	104.02	114.37
25	c	507	CLA	CHD-C1D-ND	-2.05	121.92	124.80
27	K	102	BCR	C30-C25-C26	-2.05	119.84	122.64
29	C	519	LMG	O7-C10-O9	-2.05	118.92	123.70
25	b	608	CLA	CAC-C3C-C2C	2.04	131.31	127.56
31	C	518	DGD	CAB-C9B-C8B	-2.04	104.03	114.37
25	B	608	CLA	CHB-C4A-NA	2.04	127.35	124.40
36	V	201	HEC	CAA-C2A-C3A	-2.04	124.04	127.87
27	b	618	BCR	C35-C13-C14	-2.04	119.51	122.82
27	k	102	BCR	C15-C14-C13	-2.04	124.42	127.28
25	c	508	CLA	CHD-C4C-NC	2.04	127.39	124.23
31	C	517	DGD	C7B-C6B-C5B	-2.04	104.06	114.37
28	d	406	PL9	O2-C1-C2	-2.04	117.20	121.83
29	c	519	LMG	O6-C5-C4	2.04	113.37	109.70
32	B	623	STE	O2-C1-C2	2.04	120.43	114.00
25	b	607	CLA	CHC-C4B-NB	2.04	127.10	124.05
31	A	615	DGD	CBB-CAB-C9B	-2.03	104.08	114.37
25	b	614	CLA	O2D-CGD-CBD	2.03	114.79	111.23
31	C	518	DGD	O4D-C4D-C5D	-2.03	104.31	109.32
31	c	518	DGD	C4D-C3D-C2D	-2.03	107.26	110.83
31	C	517	DGD	C4E-C3E-C2E	-2.03	107.26	110.83
25	b	602	CLA	C4-C3-C5	2.03	118.75	115.23
25	b	605	CLA	CHC-C1C-NC	2.03	127.37	124.31
25	B	606	CLA	C2A-C1A-CHA	2.03	127.39	123.87
31	C	516	DGD	C6D-O5D-C1E	2.03	118.15	113.80
25	B	613	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
31	A	615	DGD	CFB-CEB-CDB	-2.03	104.12	114.37
34	d	409	LHG	C27-C26-C25	-2.02	104.13	114.37
25	B	604	CLA	C3A-C2A-C1A	2.02	104.37	101.34
25	B	603	CLA	CHB-C4A-NA	2.02	127.32	124.40
25	B	604	CLA	O2A-CGA-O1A	-2.02	118.57	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	610	BCR	C16-C15-C14	-2.02	119.38	123.52
25	b	603	CLA	C7-C6-C5	-2.02	107.87	113.26
31	c	517	DGD	C3E-C4E-C5E	-2.02	106.57	110.23
27	K	102	BCR	C15-C16-C17	-2.02	119.39	123.52
25	a	607	CLA	CHA-C1A-NA	-2.02	121.82	126.39
25	B	613	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
27	c	514	BCR	C20-C21-C22	-2.02	124.45	127.28
34	E	101	LHG	C27-C26-C25	-2.02	104.17	114.37
31	A	615	DGD	O5D-C1E-C2E	2.02	111.34	108.27
32	B	624	STE	C3-C2-C1	-2.02	109.25	114.51
25	b	603	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
29	A	612	LMG	O1-C7-C8	-2.01	105.93	110.82
25	B	607	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
25	c	510	CLA	O1D-CGD-CBD	2.01	128.48	124.52
35	e	101	HEM	CBA-CAA-C2A	-2.01	106.98	112.53
25	C	503	CLA	CHB-C1B-NB	2.01	127.06	124.05
25	a	609	CLA	CMB-C2B-C3B	2.01	131.27	126.55
31	C	518	DGD	CBB-CAB-C9B	-2.01	104.22	114.37
25	B	606	CLA	CHD-C4C-NC	2.01	127.34	124.23
28	D	407	PL9	C42-C43-C44	-2.01	123.03	127.62
25	b	607	CLA	CHD-C1D-ND	-2.01	121.98	124.80
25	c	507	CLA	C2A-C1A-CHA	2.01	127.35	123.87
25	c	505	CLA	CHB-C4A-NA	2.01	127.30	124.40
25	b	608	CLA	CHB-C1B-NB	2.01	127.06	124.05
25	b	606	CLA	CHD-C1D-ND	-2.01	121.98	124.80
25	C	504	CLA	CHB-C4A-NA	2.01	127.29	124.40
25	C	505	CLA	CHB-C4A-NA	2.01	127.29	124.40
30	t	102	SQD	C45-O47-C7	-2.01	113.00	117.80
25	B	609	CLA	CHA-C1A-NA	-2.00	121.85	126.39
31	C	518	DGD	O5E-C6E-C5E	-2.00	104.51	111.33
34	e	102	LHG	C18-C17-C16	-2.00	104.25	114.37
34	d	408	LHG	C15-C14-C13	-2.00	104.25	114.37
29	c	519	LMG	O7-C10-O9	-2.00	119.13	122.99

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	609	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND

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Mol	Chain	Res	Type	Atom
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	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	405	CLA	ND
25	a	606	CLA	ND
25	a	607	CLA	ND
25	a	609	CLA	ND
25	a	612	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	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 (1939) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	601	CLA	C11-C12-C13-C14
25	B	605	CLA	C2B-C3B-CAB-CBB
25	B	605	CLA	C4B-C3B-CAB-CBB
25	B	613	CLA	C4-C3-C5-C6
25	C	503	CLA	C4B-C3B-CAB-CBB
25	C	512	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C4B-C3B-CAB-CBB
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	C14-C13-C15-C16
25	b	611	CLA	C14-C13-C15-C16
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	C2B-C3B-CAB-CBB
25	c	504	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	512	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
27	B	618	BCR	C7-C8-C9-C34
27	B	619	BCR	C17-C18-C19-C20
27	B	619	BCR	C20-C21-C22-C37
27	D	406	BCR	C7-C8-C9-C10
27	D	406	BCR	C16-C17-C18-C36
27	D	406	BCR	C23-C24-C25-C26
27	K	101	BCR	C11-C12-C13-C35
27	K	102	BCR	C37-C22-C23-C24
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	T	101	BCR	C7-C8-C9-C10
27	T	101	BCR	C7-C8-C9-C34
27	b	617	BCR	C21-C22-C23-C24
27	b	618	BCR	C7-C8-C9-C34
27	b	618	BCR	C20-C21-C22-C37
27	b	619	BCR	C35-C13-C14-C15
27	b	619	BCR	C37-C22-C23-C24
27	c	514	BCR	C18-C19-C20-C21
27	c	515	BCR	C20-C21-C22-C37
27	d	405	BCR	C20-C21-C22-C37
27	d	405	BCR	C22-C23-C24-C25
27	k	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C17-C18-C19-C20
27	k	102	BCR	C20-C21-C22-C37
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C5-C6-C7-C8
27	t	101	BCR	C7-C8-C9-C10
27	t	101	BCR	C7-C8-C9-C34
28	A	611	PL9	C22-C23-C24-C26
28	A	611	PL9	C37-C38-C39-C40
28	D	407	PL9	C32-C33-C34-C35
28	D	407	PL9	C33-C34-C36-C37
28	D	407	PL9	C42-C43-C44-C46
28	a	611	PL9	C12-C13-C14-C15
28	a	611	PL9	C12-C13-C14-C16
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C42-C43-C44-C46
28	d	406	PL9	C32-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
28	d	406	PL9	C42-C43-C44-C45
28	d	406	PL9	C42-C43-C44-C46
28	d	406	PL9	C47-C48-C49-C50
29	A	612	LMG	O6-C1-O1-C7
29	A	612	LMG	O9-C10-O7-C8
29	C	519	LMG	C11-C10-O7-C8
29	D	412	LMG	O1-C7-C8-C9
29	D	412	LMG	O1-C7-C8-O7
29	D	412	LMG	C11-C10-O7-C8
29	b	622	LMG	O9-C10-O7-C8
29	b	622	LMG	C11-C10-O7-C8
29	c	523	LMG	O6-C1-O1-C7
30	B	622	SQD	C2-C1-O6-C44
30	B	622	SQD	O5-C1-O6-C44
30	B	622	SQD	O6-C44-C45-O47
30	B	622	SQD	O49-C7-O47-C45
30	B	622	SQD	C8-C7-O47-C45
30	D	409	SQD	C2-C1-O6-C44
30	L	101	SQD	C8-C7-O47-C45
30	L	101	SQD	O10-C23-O48-C46
30	L	101	SQD	C24-C23-O48-C46
30	a	613	SQD	O6-C44-C45-O47
30	a	613	SQD	C5-C6-S-O7
30	a	613	SQD	C5-C6-S-O8
30	a	613	SQD	C5-C6-S-O9
30	f	101	SQD	C2-C1-O6-C44
30	f	101	SQD	O5-C1-O6-C44
30	t	102	SQD	O6-C44-C45-C46
30	t	102	SQD	O6-C44-C45-O47
30	t	102	SQD	C8-C7-O47-C45
31	A	615	DGD	O1B-C1B-O2G-C2G
31	a	614	DGD	C2B-C1B-O2G-C2G
34	D	410	LHG	O1-C1-C2-O2
34	D	410	LHG	O1-C1-C2-C3
34	D	410	LHG	C1-C2-C3-O3
34	D	410	LHG	C3-O3-P-O4
34	D	410	LHG	C3-O3-P-O6
34	D	410	LHG	C4-O6-P-O3
34	D	410	LHG	C4-O6-P-O4
34	D	411	LHG	O1-C1-C2-O2
34	D	411	LHG	O1-C1-C2-C3
34	D	411	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
34	D	411	LHG	C3-O3-P-O6
34	D	413	LHG	O1-C1-C2-C3
34	D	413	LHG	C3-O3-P-O4
34	D	413	LHG	C3-O3-P-O6
34	E	101	LHG	O1-C1-C2-O2
34	E	101	LHG	O1-C1-C2-C3
34	E	101	LHG	C4-O6-P-O3
34	E	101	LHG	C4-O6-P-O4
34	L	102	LHG	C4-O6-P-O3
34	L	102	LHG	C4-O6-P-O4
34	d	407	LHG	O1-C1-C2-C3
34	d	407	LHG	C1-C2-C3-O3
34	d	408	LHG	O1-C1-C2-C3
34	d	408	LHG	C3-O3-P-O5
34	d	408	LHG	C4-O6-P-O3
34	d	408	LHG	C4-O6-P-O4
34	e	102	LHG	C3-O3-P-O4
34	e	102	LHG	C3-O3-P-O6
34	e	102	LHG	C4-O6-P-O5
34	e	102	LHG	O10-C23-O8-C6
34	e	102	LHG	C24-C23-O8-C6
34	l	101	LHG	C4-O6-P-O5
36	V	201	HEC	C2B-C3B-CAB-CBB
36	V	201	HEC	C2C-C3C-CAC-CBC
36	V	201	HEC	C4C-C3C-CAC-CBC
36	v	201	HEC	C2B-C3B-CAB-CBB
36	v	201	HEC	C4B-C3B-CAB-CBB
36	v	201	HEC	C2C-C3C-CAC-CBC
36	v	201	HEC	C4C-C3C-CAC-CBC
25	B	601	CLA	O1D-CGD-O2D-CED
29	c	519	LMG	C11-C10-O7-C8
25	B	601	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
29	c	523	LMG	O10-C28-O8-C9
28	A	611	PL9	C47-C48-C49-C51
28	a	611	PL9	C47-C48-C49-C51
28	d	406	PL9	C47-C48-C49-C51
29	c	523	LMG	C29-C28-O8-C9
30	f	101	SQD	O10-C23-O48-C46
25	b	601	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	O1D-CGD-O2D-CED
29	D	412	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
29	c	521	LMG	O9-C10-O7-C8
30	L	101	SQD	O49-C7-O47-C45
30	f	101	SQD	O49-C7-O47-C45
30	t	102	SQD	O49-C7-O47-C45
31	a	614	DGD	O1B-C1B-O2G-C2G
25	B	604	CLA	C3-C5-C6-C7
25	B	605	CLA	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
30	f	101	SQD	C24-C23-O48-C46
26	d	402	PHO	CBD-CGD-O2D-CED
29	A	612	LMG	C11-C10-O7-C8
31	A	615	DGD	C2B-C1B-O2G-C2G
29	c	521	LMG	O10-C28-O8-C9
29	c	519	LMG	O9-C10-O7-C8
25	B	604	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	C	503	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
28	A	611	PL9	C45-C44-C46-C47
28	a	611	PL9	C20-C19-C21-C22
25	B	604	CLA	C2-C3-C5-C6
25	B	613	CLA	C2-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
28	A	611	PL9	C38-C39-C41-C42
25	b	601	CLA	C3-C5-C6-C7
28	D	407	PL9	C42-C43-C44-C45
28	a	611	PL9	C42-C43-C44-C45
28	A	611	PL9	C37-C38-C39-C41
28	D	407	PL9	C32-C33-C34-C36
29	C	519	LMG	O9-C10-O7-C8
25	b	603	CLA	C3-C5-C6-C7
25	c	503	CLA	CBD-CGD-O2D-CED
34	D	410	LHG	O2-C2-C3-O3
34	D	413	LHG	O2-C2-C3-O3
34	E	101	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
34	d	407	LHG	O2-C2-C3-O3
30	D	409	SQD	O6-C44-C45-C46
29	c	521	LMG	C29-C28-O8-C9
30	f	101	SQD	C8-C7-O47-C45
31	h	102	DGD	O6E-C5E-C6E-O5E
25	c	513	CLA	O1D-CGD-O2D-CED
25	C	512	CLA	C3-C5-C6-C7
25	B	605	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
28	A	611	PL9	C20-C19-C21-C22
28	A	611	PL9	C40-C39-C41-C42
28	a	611	PL9	C25-C24-C26-C27
28	a	611	PL9	C35-C34-C36-C37
25	B	614	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
28	a	611	PL9	C18-C19-C21-C22
28	d	406	PL9	C38-C39-C41-C42
28	A	611	PL9	C19-C21-C22-C23
28	A	611	PL9	C29-C31-C32-C33
28	A	611	PL9	C34-C36-C37-C38
28	A	611	PL9	C44-C46-C47-C48
28	D	407	PL9	C29-C31-C32-C33
28	a	611	PL9	C19-C21-C22-C23
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C39-C41-C42-C43
28	d	406	PL9	C44-C46-C47-C48
31	A	615	DGD	C4E-C5E-C6E-O5E
28	A	611	PL9	C47-C48-C49-C50
28	a	611	PL9	C47-C48-C49-C50
31	c	518	DGD	O1A-C1A-O1G-C1G
29	m	101	LMG	O6-C1-O1-C7
30	A	613	SQD	O5-C1-O6-C44
30	D	409	SQD	O5-C1-O6-C44
29	m	101	LMG	C29-C28-O8-C9
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED
30	L	101	SQD	C14-C15-C16-C17
29	D	408	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CBD-CGD-O2D-CED
25	a	607	CLA	CBD-CGD-O2D-CED
29	c	521	LMG	C11-C10-O7-C8
30	D	409	SQD	O10-C23-O48-C46
34	D	413	LHG	C1-C2-C3-O3
25	c	506	CLA	CBA-CGA-O2A-C1
30	D	409	SQD	C24-C23-O48-C46
32	B	624	STE	C4-C5-C6-C7
26	d	402	PHO	O1D-CGD-O2D-CED
34	E	101	LHG	C32-C33-C34-C35
25	A	609	CLA	C4-C3-C5-C6
28	d	406	PL9	C40-C39-C41-C42
25	A	609	CLA	C2-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	C	503	CLA	C2-C3-C5-C6
28	A	611	PL9	C18-C19-C21-C22
28	A	611	PL9	C43-C44-C46-C47
28	a	611	PL9	C23-C24-C26-C27
25	B	601	CLA	C3-C5-C6-C7
25	A	607	CLA	C14-C13-C15-C16
25	B	601	CLA	C6-C7-C8-C9
25	B	607	CLA	C11-C12-C13-C14
25	B	614	CLA	C6-C7-C8-C9
25	B	614	CLA	C14-C13-C15-C16
25	C	501	CLA	C14-C13-C15-C16
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	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	D	404	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C10-C8-C9
25	b	601	CLA	C14-C13-C15-C16
25	b	605	CLA	C11-C10-C8-C9
25	b	613	CLA	C6-C7-C8-C9
25	b	614	CLA	C6-C7-C8-C9
25	c	503	CLA	C11-C12-C13-C14
25	c	511	CLA	C14-C13-C15-C16
25	c	512	CLA	C6-C7-C8-C9
26	A	608	PHO	C14-C13-C15-C16
29	m	101	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
30	A	613	SQD	C2-C1-O6-C44
27	B	617	BCR	C7-C8-C9-C34
27	B	618	BCR	C37-C22-C23-C24
27	B	619	BCR	C11-C12-C13-C35
27	B	619	BCR	C37-C22-C23-C24
27	K	102	BCR	C7-C8-C9-C34
27	c	514	BCR	C11-C12-C13-C35
27	d	405	BCR	C37-C22-C23-C24
27	t	101	BCR	C37-C22-C23-C24
31	A	615	DGD	O6E-C5E-C6E-O5E
29	c	523	LMG	C16-C17-C18-C19
29	c	519	LMG	C28-C29-C30-C31
34	e	102	LHG	C23-C24-C25-C26
28	D	407	PL9	C47-C48-C49-C51
25	c	506	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	CBD-CGD-O2D-CED
29	B	621	LMG	C28-C29-C30-C31
31	c	516	DGD	C1B-C2B-C3B-C4B
32	C	521	STE	C1-C2-C3-C4
31	h	102	DGD	C4E-C5E-C6E-O5E
25	b	607	CLA	CBD-CGD-O2D-CED
28	d	406	PL9	C32-C33-C34-C35
25	C	513	CLA	C13-C15-C16-C17
25	c	507	CLA	C5-C6-C7-C8
29	A	612	LMG	O6-C5-C6-O5
25	c	510	CLA	C3-C5-C6-C7
30	A	614	SQD	C23-C24-C25-C26
25	B	602	CLA	C15-C16-C17-C18
25	c	510	CLA	CBD-CGD-O2D-CED
29	c	519	LMG	O6-C5-C6-O5
25	B	601	CLA	C11-C10-C8-C7
25	B	611	CLA	C12-C13-C15-C16
25	C	503	CLA	C6-C7-C8-C10
25	C	503	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	C	513	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C15
25	c	510	CLA	C6-C7-C8-C10
25	b	607	CLA	CBA-CGA-O2A-C1
31	c	517	DGD	O6E-C5E-C6E-O5E
27	k	101	BCR	C19-C20-C21-C22
28	D	407	PL9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
28	a	611	PL9	C9-C11-C12-C13
30	D	409	SQD	C45-C46-O48-C23
29	D	412	LMG	C28-C29-C30-C31
29	d	411	LMG	C28-C29-C30-C31
31	A	615	DGD	C1A-C2A-C3A-C4A
34	d	407	LHG	C23-C24-C25-C26
34	e	102	LHG	C7-C8-C9-C10
25	B	602	CLA	C13-C15-C16-C17
25	C	503	CLA	C5-C6-C7-C8
25	C	507	CLA	C10-C11-C12-C13
25	a	607	CLA	C8-C10-C11-C12
25	b	607	CLA	C5-C6-C7-C8
25	c	503	CLA	C15-C16-C17-C18
25	c	511	CLA	C15-C16-C17-C18
31	c	517	DGD	C4E-C5E-C6E-O5E
25	B	606	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	B	607	CLA	C8-C10-C11-C12
25	B	613	CLA	C5-C6-C7-C8
25	C	504	CLA	C8-C10-C11-C12
25	C	509	CLA	C10-C11-C12-C13
25	a	606	CLA	C15-C16-C17-C18
25	b	605	CLA	C5-C6-C7-C8
25	b	611	CLA	C8-C10-C11-C12
25	c	511	CLA	C13-C15-C16-C17
25	c	512	CLA	C13-C15-C16-C17
29	C	519	LMG	C28-C29-C30-C31
31	a	614	DGD	C1A-C2A-C3A-C4A
25	A	606	CLA	C2C-C3C-CAC-CBC
27	B	619	BCR	C22-C23-C24-C25
30	L	101	SQD	C11-C10-C9-C8
25	B	613	CLA	C8-C10-C11-C12
25	B	616	CLA	C5-C6-C7-C8
25	C	506	CLA	C8-C10-C11-C12
25	D	403	CLA	C15-C16-C17-C18
25	a	609	CLA	C5-C6-C7-C8
25	b	603	CLA	C10-C11-C12-C13
25	b	608	CLA	C8-C10-C11-C12
25	b	614	CLA	C5-C6-C7-C8
25	c	504	CLA	C10-C11-C12-C13
34	e	102	LHG	O2-C2-C3-O3
25	B	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	C13-C15-C16-C17
25	B	603	CLA	C5-C6-C7-C8
25	B	606	CLA	C8-C10-C11-C12
25	b	613	CLA	CBD-CGD-O2D-CED
29	c	521	LMG	C10-C11-C12-C13
32	X	101	STE	C3-C4-C5-C6
25	c	503	CLA	O1D-CGD-O2D-CED
25	b	608	CLA	C2C-C3C-CAC-CBC
25	B	603	CLA	C15-C16-C17-C18
25	B	614	CLA	C8-C10-C11-C12
25	b	615	CLA	C15-C16-C17-C18
25	c	512	CLA	CBA-CGA-O2A-C1
31	c	518	DGD	C2A-C1A-O1G-C1G
34	E	101	LHG	C24-C23-O8-C6
25	b	607	CLA	O1A-CGA-O2A-C1
25	B	601	CLA	C15-C16-C17-C18
25	B	615	CLA	C15-C16-C17-C18
25	a	609	CLA	C10-C11-C12-C13
30	A	614	SQD	C7-C8-C9-C10
30	a	613	SQD	C7-C8-C9-C10
34	E	101	LHG	C1-C2-C3-O3
34	e	102	LHG	C1-C2-C3-O3
25	B	604	CLA	CBA-CGA-O2A-C1
25	C	502	CLA	C15-C16-C17-C18
25	C	505	CLA	C10-C11-C12-C13
25	C	507	CLA	C13-C15-C16-C17
25	a	607	CLA	C13-C15-C16-C17
25	b	606	CLA	C15-C16-C17-C18
25	B	611	CLA	C13-C15-C16-C17
25	C	506	CLA	C15-C16-C17-C18
25	C	508	CLA	C10-C11-C12-C13
25	C	513	CLA	C8-C10-C11-C12
25	C	513	CLA	C15-C16-C17-C18
25	D	403	CLA	C13-C15-C16-C17
25	D	404	CLA	C15-C16-C17-C18
25	b	607	CLA	C8-C10-C11-C12
25	b	613	CLA	C10-C11-C12-C13
29	c	523	LMG	C4-C5-C6-O5
25	A	607	CLA	C8-C10-C11-C12
25	B	607	CLA	C5-C6-C7-C8
25	B	611	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	b	622	LMG	C28-C29-C30-C31
31	c	517	DGD	C2E-C1E-O5D-C6D
25	b	611	CLA	C13-C15-C16-C17
25	B	603	CLA	C16-C17-C18-C20
25	C	502	CLA	C16-C17-C18-C19
27	B	618	BCR	C16-C17-C18-C36
27	C	515	BCR	C11-C10-C9-C34
27	C	515	BCR	C16-C17-C18-C36
27	C	515	BCR	C20-C21-C22-C37
27	D	406	BCR	C11-C10-C9-C34
27	D	406	BCR	C20-C21-C22-C37
27	K	102	BCR	C20-C21-C22-C37
27	T	101	BCR	C20-C21-C22-C37
27	b	617	BCR	C35-C13-C14-C15
27	b	617	BCR	C20-C21-C22-C37
27	b	619	BCR	C20-C21-C22-C37
27	t	101	BCR	C35-C13-C14-C15
29	C	519	LMG	C10-C11-C12-C13
27	C	514	BCR	C7-C8-C9-C34
27	d	405	BCR	C7-C8-C9-C34
27	h	101	BCR	C7-C8-C9-C34
27	k	101	BCR	C7-C8-C9-C34
25	b	606	CLA	C2A-CAA-CBA-CGA
25	c	503	CLA	C5-C6-C7-C8
34	d	409	LHG	O1-C1-C2-C3
34	e	102	LHG	O1-C1-C2-C3
25	b	616	CLA	O1D-CGD-O2D-CED
29	D	412	LMG	C9-C8-O7-C10
30	L	101	SQD	C46-C45-O47-C7
31	C	518	DGD	C8A-C9A-CAA-CBA
25	A	607	CLA	C16-C17-C18-C20
25	B	614	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C20
25	c	512	CLA	O1A-CGA-O2A-C1
27	B	618	BCR	C11-C10-C9-C8
27	H	101	BCR	C11-C10-C9-C8
27	b	618	BCR	C11-C10-C9-C8
27	b	618	BCR	C20-C21-C22-C23
27	b	619	BCR	C12-C13-C14-C15
27	c	514	BCR	C20-C21-C22-C23
27	c	515	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	c	515	BCR	C20-C21-C22-C23
27	h	101	BCR	C11-C10-C9-C8
27	k	102	BCR	C20-C21-C22-C23
29	b	622	LMG	O6-C1-O1-C7
31	c	517	DGD	O6E-C1E-O5D-C6D
31	C	516	DGD	C1B-C2B-C3B-C4B
25	b	615	CLA	C5-C6-C7-C8
25	C	511	CLA	CBA-CGA-O2A-C1
25	B	603	CLA	C13-C15-C16-C17
29	b	622	LMG	C15-C16-C17-C18
25	B	605	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C20
25	B	604	CLA	O1A-CGA-O2A-C1
29	D	408	LMG	C13-C14-C15-C16
30	B	622	SQD	C16-C17-C18-C19
30	f	101	SQD	C25-C26-C27-C28
31	c	517	DGD	CCA-CDA-CEA-CFA
34	E	101	LHG	C17-C18-C19-C20
34	l	101	LHG	C34-C35-C36-C37
27	b	619	BCR	C14-C15-C16-C17
29	C	519	LMG	C32-C33-C34-C35
30	A	614	SQD	C15-C16-C17-C18
30	f	101	SQD	C28-C29-C30-C31
31	A	615	DGD	CBA-CCA-CDA-CEA
31	C	517	DGD	C2B-C3B-C4B-C5B
31	c	516	DGD	C5B-C6B-C7B-C8B
31	h	102	DGD	C7A-C8A-C9A-CAA
32	d	413	STE	C2-C3-C4-C5
32	l	102	STE	C5-C6-C7-C8
32	l	102	STE	C7-C8-C9-C10
25	b	615	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	C13-C15-C16-C17
29	b	622	LMG	C16-C17-C18-C19
29	c	521	LMG	C33-C34-C35-C36
31	a	614	DGD	C9B-CAB-CBB-CCB
32	B	620	STE	C7-C8-C9-C10
32	R	101	STE	C6-C7-C8-C9
34	D	411	LHG	C29-C30-C31-C32
29	M	101	LMG	C19-C20-C21-C22
30	L	101	SQD	C29-C30-C31-C32
31	A	615	DGD	CCB-CDB-CEB-CFB
31	H	102	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
31	h	102	DGD	C6B-C7B-C8B-C9B
32	H	103	STE	C6-C7-C8-C9
32	J	101	STE	C5-C6-C7-C8
32	b	625	STE	C12-C13-C14-C15
34	D	411	LHG	C9-C10-C11-C12
34	D	413	LHG	O1-C1-C2-O2
34	d	407	LHG	O1-C1-C2-O2
34	d	408	LHG	O1-C1-C2-O2
29	c	519	LMG	C39-C40-C41-C42
30	B	622	SQD	C34-C35-C36-C37
31	a	614	DGD	CBA-CCA-CDA-CEA
31	c	516	DGD	C4B-C5B-C6B-C7B
32	c	520	STE	C9-C10-C11-C12
34	L	102	LHG	C12-C13-C14-C15
34	d	407	LHG	C25-C26-C27-C28
25	C	506	CLA	O1D-CGD-O2D-CED
25	C	507	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
32	B	623	STE	C1-C2-C3-C4
32	d	413	STE	C1-C2-C3-C4
29	c	523	LMG	C14-C15-C16-C17
29	m	101	LMG	C16-C17-C18-C19
31	h	102	DGD	C5B-C6B-C7B-C8B
31	c	516	DGD	O6E-C5E-C6E-O5E
25	B	603	CLA	C16-C17-C18-C19
25	b	601	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C19
28	A	611	PL9	C12-C13-C14-C16
31	c	516	DGD	CBB-CCB-CDB-CEB
34	E	101	LHG	C25-C26-C27-C28
25	c	503	CLA	C8-C10-C11-C12
34	e	102	LHG	C8-C7-O7-C5
29	D	408	LMG	C15-C16-C17-C18
25	B	615	CLA	C11-C10-C8-C7
29	c	523	LMG	C15-C16-C17-C18
30	A	613	SQD	C16-C17-C18-C19
31	a	614	DGD	C4B-C5B-C6B-C7B
30	L	101	SQD	C7-C8-C9-C10
25	b	612	CLA	C15-C16-C17-C18
31	A	615	DGD	C2B-C3B-C4B-C5B
31	c	516	DGD	CCB-CDB-CEB-CFB
31	c	518	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
34	l	101	LHG	C15-C16-C17-C18
25	D	405	CLA	C4-C3-C5-C6
25	b	601	CLA	C3A-C2A-CAA-CBA
25	c	512	CLA	C3A-C2A-CAA-CBA
29	c	523	LMG	C30-C31-C32-C33
30	A	614	SQD	C11-C12-C13-C14
30	a	613	SQD	C25-C26-C27-C28
32	d	412	STE	C3-C4-C5-C6
34	d	407	LHG	C28-C29-C30-C31
34	l	101	LHG	C25-C26-C27-C28
29	D	408	LMG	C38-C39-C40-C41
29	c	521	LMG	C31-C32-C33-C34
25	C	502	CLA	O1D-CGD-O2D-CED
29	C	519	LMG	C11-C12-C13-C14
30	f	101	SQD	C30-C31-C32-C33
31	a	614	DGD	C2A-C3A-C4A-C5A
32	l	102	STE	C4-C5-C6-C7
25	B	614	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C20
25	c	509	CLA	C16-C17-C18-C19
29	c	521	LMG	C36-C37-C38-C39
31	A	615	DGD	C7A-C8A-C9A-CAA
31	C	517	DGD	C5A-C6A-C7A-C8A
31	H	102	DGD	CCA-CDA-CEA-CFA
31	a	614	DGD	C4A-C5A-C6A-C7A
32	H	103	STE	C14-C15-C16-C17
29	d	411	LMG	C12-C13-C14-C15
32	d	412	STE	C5-C6-C7-C8
31	a	614	DGD	C2A-C1A-O1G-C1G
31	C	518	DGD	C5A-C6A-C7A-C8A
32	R	101	STE	C4-C5-C6-C7
32	b	625	STE	C14-C15-C16-C17
32	t	103	STE	C5-C6-C7-C8
34	D	413	LHG	C28-C29-C30-C31
34	L	102	LHG	C34-C35-C36-C37
29	d	410	LMG	C30-C31-C32-C33
29	d	410	LMG	C35-C36-C37-C38
31	C	517	DGD	C5B-C6B-C7B-C8B
31	c	516	DGD	C3B-C4B-C5B-C6B
31	h	102	DGD	C2B-C3B-C4B-C5B
32	B	620	STE	C6-C7-C8-C9
32	H	103	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
32	d	413	STE	C4-C5-C6-C7
34	D	411	LHG	C24-C25-C26-C27
34	d	409	LHG	C27-C28-C29-C30
25	C	511	CLA	O1A-CGA-O2A-C1
29	m	101	LMG	O10-C28-O8-C9
29	D	408	LMG	C18-C19-C20-C21
31	h	102	DGD	C3B-C4B-C5B-C6B
32	B	623	STE	C4-C5-C6-C7
32	H	103	STE	C7-C8-C9-C10
32	a	615	STE	C5-C6-C7-C8
34	L	102	LHG	C27-C28-C29-C30
34	d	407	LHG	C15-C16-C17-C18
29	D	412	LMG	C33-C34-C35-C36
30	a	613	SQD	C28-C29-C30-C31
32	b	621	STE	C13-C14-C15-C16
25	B	616	CLA	O1D-CGD-O2D-CED
25	C	510	CLA	O1D-CGD-O2D-CED
31	H	102	DGD	C3B-C4B-C5B-C6B
31	a	614	DGD	C5A-C6A-C7A-C8A
31	c	516	DGD	C9B-CAB-CBB-CCB
32	a	616	STE	C5-C6-C7-C8
25	B	605	CLA	C16-C17-C18-C20
28	D	407	PL9	C47-C48-C49-C50
25	C	503	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C2B-C3B-CAB-CBB
27	D	406	BCR	C23-C24-C25-C30
27	K	102	BCR	C1-C6-C7-C8
27	K	102	BCR	C5-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
29	c	519	LMG	C31-C32-C33-C34
30	B	622	SQD	C11-C12-C13-C14
34	d	408	LHG	C29-C30-C31-C32
25	D	404	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	C	501	CLA	CBA-CGA-O2A-C1
29	C	519	LMG	C17-C18-C19-C20
29	M	101	LMG	C31-C32-C33-C34
29	c	521	LMG	C11-C12-C13-C14
29	c	523	LMG	C13-C14-C15-C16
29	c	523	LMG	C18-C19-C20-C21
30	a	613	SQD	C17-C18-C19-C20
31	c	518	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
32	a	616	STE	C4-C5-C6-C7
34	d	408	LHG	C11-C12-C13-C14
34	d	408	LHG	C28-C29-C30-C31
30	L	101	SQD	C16-C17-C18-C19
31	A	615	DGD	C4B-C5B-C6B-C7B
32	b	623	STE	C11-C10-C9-C8
32	b	624	STE	C10-C11-C12-C13
34	L	102	LHG	C32-C33-C34-C35
34	d	408	LHG	C12-C13-C14-C15
29	D	408	LMG	C20-C21-C22-C23
29	D	408	LMG	C21-C22-C23-C24
31	C	517	DGD	C6A-C7A-C8A-C9A
32	L	103	STE	C5-C6-C7-C8
32	d	413	STE	C3-C4-C5-C6
34	D	413	LHG	C11-C12-C13-C14
29	M	101	LMG	C34-C35-C36-C37
31	C	518	DGD	CCA-CDA-CEA-CFA
34	d	408	LHG	C15-C16-C17-C18
28	d	406	PL9	C20-C19-C21-C22
30	L	101	SQD	C25-C26-C27-C28
31	c	517	DGD	CBA-CCA-CDA-CEA
31	c	518	DGD	CBA-CCA-CDA-CEA
32	b	623	STE	C9-C10-C11-C12
32	b	623	STE	C10-C11-C12-C13
27	d	405	BCR	C18-C19-C20-C21
27	t	101	BCR	C18-C19-C20-C21
25	c	505	CLA	C10-C11-C12-C13
29	D	408	LMG	C39-C40-C41-C42
30	A	614	SQD	C18-C19-C20-C21
30	A	614	SQD	C31-C32-C33-C34
31	c	516	DGD	CAB-CBB-CCB-CDB
34	D	411	LHG	C25-C26-C27-C28
34	L	102	LHG	C31-C32-C33-C34
34	d	408	LHG	C32-C33-C34-C35
31	a	614	DGD	C1B-C2B-C3B-C4B
30	B	622	SQD	C24-C23-O48-C46
25	B	614	CLA	C11-C12-C13-C14
34	d	409	LHG	C24-C25-C26-C27
34	e	102	LHG	C11-C10-C9-C8
34	e	102	LHG	C11-C12-C13-C14
25	B	615	CLA	C13-C15-C16-C17
25	D	404	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	B	621	LMG	C29-C30-C31-C32
29	c	519	LMG	C37-C38-C39-C40
29	c	521	LMG	C16-C17-C18-C19
29	c	521	LMG	C30-C31-C32-C33
29	d	410	LMG	C38-C39-C40-C41
31	A	615	DGD	C2A-C3A-C4A-C5A
31	H	102	DGD	C7B-C8B-C9B-CAB
31	c	516	DGD	C8A-C9A-CAA-CBA
29	C	519	LMG	C31-C32-C33-C34
29	c	521	LMG	C29-C30-C31-C32
29	c	523	LMG	C31-C32-C33-C34
29	m	101	LMG	C18-C19-C20-C21
30	B	622	SQD	C13-C14-C15-C16
32	c	522	STE	C3-C4-C5-C6
34	d	408	LHG	C10-C11-C12-C13
29	b	622	LMG	C2-C1-O1-C7
29	c	523	LMG	C2-C1-O1-C7
25	B	607	CLA	C10-C11-C12-C13
25	B	612	CLA	C10-C11-C12-C13
29	D	408	LMG	C36-C37-C38-C39
30	B	622	SQD	C17-C18-C19-C20
32	b	625	STE	C10-C11-C12-C13
29	A	612	LMG	C36-C37-C38-C39
30	A	613	SQD	C27-C28-C29-C30
30	D	409	SQD	C31-C32-C33-C34
29	D	412	LMG	C11-C12-C13-C14
29	c	521	LMG	C32-C33-C34-C35
31	C	518	DGD	C2B-C3B-C4B-C5B
34	d	409	LHG	C32-C33-C34-C35
25	C	503	CLA	C15-C16-C17-C18
34	D	411	LHG	C11-C12-C13-C14
29	c	523	LMG	C11-C10-O7-C8
30	A	613	SQD	C8-C7-O47-C45
29	D	408	LMG	C28-C29-C30-C31
32	B	620	STE	C1-C2-C3-C4
25	a	607	CLA	C15-C16-C17-C18
25	c	505	CLA	C5-C6-C7-C8
30	A	613	SQD	O49-C7-O47-C45
29	C	519	LMG	C30-C31-C32-C33
29	M	101	LMG	C13-C14-C15-C16
29	b	622	LMG	C23-C24-C25-C26
32	c	520	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	b	622	LMG	C31-C32-C33-C34
32	H	103	STE	C11-C12-C13-C14
30	D	409	SQD	C32-C33-C34-C35
25	A	607	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
30	B	622	SQD	C9-C10-C11-C12
31	c	518	DGD	C5B-C6B-C7B-C8B
32	X	101	STE	C9-C10-C11-C12
34	D	410	LHG	C12-C13-C14-C15
34	d	409	LHG	C26-C27-C28-C29
30	A	613	SQD	C7-C8-C9-C10
29	B	621	LMG	C16-C17-C18-C19
30	B	622	SQD	C28-C29-C30-C31
32	C	520	STE	C4-C5-C6-C7
30	a	613	SQD	C34-C35-C36-C37
25	a	607	CLA	O1D-CGD-O2D-CED
30	D	409	SQD	C25-C26-C27-C28
30	a	613	SQD	C24-C25-C26-C27
25	b	602	CLA	C3-C5-C6-C7
29	d	411	LMG	O6-C5-C6-O5
25	C	509	CLA	C13-C15-C16-C17
25	c	511	CLA	C10-C11-C12-C13
32	I	101	STE	C11-C10-C9-C8
32	c	520	STE	C11-C12-C13-C14
30	A	613	SQD	C23-C24-C25-C26
31	c	517	DGD	C1B-C2B-C3B-C4B
31	A	615	DGD	CCA-CDA-CEA-CFA
34	e	102	LHG	O6-C4-C5-O7
30	a	613	SQD	C11-C10-C9-C8
34	l	101	LHG	C17-C18-C19-C20
25	b	614	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C19
30	t	102	SQD	C11-C12-C13-C14
32	M	102	STE	C2-C3-C4-C5
32	b	624	STE	C11-C12-C13-C14
32	d	413	STE	C11-C12-C13-C14
34	D	413	LHG	C27-C28-C29-C30
34	e	102	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	C	501	CLA	O1A-CGA-O2A-C1
31	c	516	DGD	C8B-C9B-CAB-CBB
32	b	621	STE	C3-C4-C5-C6
32	b	623	STE	C1-C2-C3-C4
25	b	611	CLA	C15-C16-C17-C18
30	B	622	SQD	C33-C34-C35-C36
32	C	521	STE	C5-C6-C7-C8
29	c	523	LMG	O6-C5-C6-O5
31	A	615	DGD	O2G-C2G-C3G-O3G
29	A	612	LMG	C16-C17-C18-C19
32	X	101	STE	C4-C5-C6-C7
30	A	613	SQD	C34-C35-C36-C37
34	L	102	LHG	C15-C16-C17-C18
34	l	101	LHG	C9-C10-C11-C12
31	C	516	DGD	O6E-C5E-C6E-O5E
29	b	622	LMG	C11-C12-C13-C14
30	a	613	SQD	C15-C16-C17-C18
32	J	101	STE	C6-C7-C8-C9
32	b	621	STE	C6-C7-C8-C9
34	l	101	LHG	C27-C28-C29-C30
29	M	101	LMG	C35-C36-C37-C38
30	a	613	SQD	C29-C30-C31-C32
31	C	516	DGD	C5B-C6B-C7B-C8B
31	a	614	DGD	CCB-CDB-CEB-CFB
32	C	520	STE	C5-C6-C7-C8
32	X	101	STE	C5-C6-C7-C8
30	t	102	SQD	C11-C10-C9-C8
32	b	621	STE	C14-C15-C16-C17
25	b	609	CLA	C3-C5-C6-C7
34	l	101	LHG	C7-C8-C9-C10
25	C	505	CLA	C2-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
28	d	406	PL9	C13-C14-C16-C17
28	d	406	PL9	C43-C44-C46-C47
29	M	101	LMG	C33-C34-C35-C36
31	c	518	DGD	C2A-C3A-C4A-C5A
32	b	624	STE	C14-C15-C16-C17
34	D	413	LHG	C14-C15-C16-C17
25	C	501	CLA	C2A-CAA-CBA-CGA
25	b	609	CLA	CBD-CGD-O2D-CED
29	A	612	LMG	C17-C18-C19-C20
29	b	622	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	c	516	DGD	C7A-C8A-C9A-CAA
32	b	625	STE	C4-C5-C6-C7
34	d	407	LHG	C30-C31-C32-C33
25	A	606	CLA	C4C-C3C-CAC-CBC
32	L	103	STE	C6-C7-C8-C9
30	A	613	SQD	C10-C11-C12-C13
29	d	411	LMG	C14-C15-C16-C17
29	m	101	LMG	C12-C13-C14-C15
31	c	517	DGD	C6A-C7A-C8A-C9A
32	X	101	STE	C11-C12-C13-C14
25	B	604	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C13-C15-C16-C17
25	b	610	CLA	C5-C6-C7-C8
30	f	101	SQD	C31-C32-C33-C34
30	t	102	SQD	C17-C18-C19-C20
32	b	624	STE	C11-C10-C9-C8
34	d	407	LHG	C11-C10-C9-C8
34	e	102	LHG	O9-C7-O7-C5
29	D	408	LMG	C31-C32-C33-C34
29	M	101	LMG	C12-C13-C14-C15
29	d	410	LMG	C11-C12-C13-C14
32	t	104	STE	C7-C8-C9-C10
34	L	102	LHG	C13-C14-C15-C16
25	B	601	CLA	C11-C12-C13-C15
25	B	604	CLA	C11-C10-C8-C7
25	B	604	CLA	C11-C12-C13-C15
25	B	604	CLA	C12-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C10
25	C	501	CLA	C12-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C7
25	C	505	CLA	C12-C13-C15-C16
25	C	506	CLA	C12-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C12-C13-C15
25	b	604	CLA	C12-C13-C15-C16
25	b	605	CLA	C11-C12-C13-C15
25	b	605	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C12-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C10
25	b	614	CLA	C11-C12-C13-C15
25	c	506	CLA	C11-C12-C13-C15
25	c	510	CLA	C12-C13-C15-C16
25	c	512	CLA	C12-C13-C15-C16
31	A	615	DGD	C5B-C6B-C7B-C8B
31	H	102	DGD	C5A-C6A-C7A-C8A
32	c	520	STE	C12-C13-C14-C15
25	b	613	CLA	C5-C6-C7-C8
25	b	610	CLA	C13-C15-C16-C17
25	b	612	CLA	C10-C11-C12-C13
32	t	104	STE	C1-C2-C3-C4
32	R	101	STE	C2-C3-C4-C5
25	B	601	CLA	C2-C3-C5-C6
25	D	405	CLA	C2-C3-C5-C6
31	a	614	DGD	CEA-CFA-CGA-CHA
34	D	411	LHG	C16-C17-C18-C19
34	L	102	LHG	C11-C12-C13-C14
25	c	501	CLA	C2A-CAA-CBA-CGA
25	B	604	CLA	C11-C12-C13-C14
25	B	606	CLA	C11-C10-C8-C9
25	B	616	CLA	C6-C7-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	a	607	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	604	CLA	C14-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C14
25	b	616	CLA	C11-C10-C8-C9
25	B	610	CLA	C16-C17-C18-C20
32	a	616	STE	C3-C4-C5-C6
25	C	505	CLA	O1D-CGD-O2D-CED
34	d	407	LHG	C16-C17-C18-C19
29	c	521	LMG	C7-C8-C9-O8
30	B	622	SQD	O6-C44-C45-C46
31	C	518	DGD	C3A-C4A-C5A-C6A
32	j	101	STE	C6-C7-C8-C9
25	c	510	CLA	O1D-CGD-O2D-CED
25	B	612	CLA	CBD-CGD-O2D-CED
29	M	101	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
32	d	412	STE	C11-C12-C13-C14
31	a	614	DGD	C6B-C7B-C8B-C9B
34	l	101	LHG	C24-C23-O8-C6
29	D	412	LMG	C10-C11-C12-C13
25	c	506	CLA	C16-C17-C18-C20
29	A	612	LMG	C11-C12-C13-C14
31	H	102	DGD	CCB-CDB-CEB-CFB
31	c	518	DGD	C9A-CAA-CBA-CCA
34	d	409	LHG	C30-C31-C32-C33
31	h	102	DGD	CCA-CDA-CEA-CFA
34	l	101	LHG	C32-C33-C34-C35
29	D	408	LMG	O6-C5-C6-O5
31	a	614	DGD	O1A-C1A-O1G-C1G
31	C	518	DGD	C9A-CAA-CBA-CCA
25	B	601	CLA	C4-C3-C5-C6
25	C	505	CLA	C4-C3-C5-C6
25	C	506	CLA	C4-C3-C5-C6
29	c	519	LMG	C30-C31-C32-C33
25	C	505	CLA	C15-C16-C17-C18
25	b	608	CLA	C13-C15-C16-C17
31	c	517	DGD	CAA-CBA-CCA-CDA
30	B	622	SQD	O10-C23-O48-C46
25	A	606	CLA	C15-C16-C17-C18
25	b	601	CLA	C2A-CAA-CBA-CGA
29	b	622	LMG	O6-C5-C6-O5
29	D	412	LMG	C34-C35-C36-C37
31	A	615	DGD	C7B-C8B-C9B-CAB
30	B	622	SQD	C23-C24-C25-C26
31	H	102	DGD	C9A-CAA-CBA-CCA
31	c	518	DGD	CCB-CDB-CEB-CFB
32	a	615	STE	C3-C4-C5-C6
30	A	614	SQD	C27-C28-C29-C30
30	B	622	SQD	C25-C26-C27-C28
32	B	620	STE	C2-C3-C4-C5
25	b	601	CLA	C10-C11-C12-C13
31	c	517	DGD	C8B-C9B-CAB-CBB
32	C	522	STE	C5-C6-C7-C8
34	D	413	LHG	C29-C30-C31-C32
25	c	511	CLA	C16-C17-C18-C20
25	C	512	CLA	C8-C10-C11-C12
30	f	101	SQD	C27-C28-C29-C30
31	a	614	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C24-C25-C26-C27
27	d	405	BCR	C20-C21-C22-C23
31	C	516	DGD	C6A-C7A-C8A-C9A
27	T	101	BCR	C6-C7-C8-C9
25	D	405	CLA	C10-C11-C12-C13
29	c	523	LMG	C37-C38-C39-C40
30	A	614	SQD	C14-C15-C16-C17
30	D	409	SQD	C30-C31-C32-C33
31	a	614	DGD	CFB-CGB-CHB-CIB
34	D	411	LHG	C34-C35-C36-C37
25	B	614	CLA	O1D-CGD-O2D-CED
31	c	518	DGD	C3A-C4A-C5A-C6A
34	D	410	LHG	C13-C14-C15-C16
34	d	407	LHG	C18-C19-C20-C21
25	C	510	CLA	C2-C3-C5-C6
29	b	622	LMG	C18-C19-C20-C21
29	c	519	LMG	C34-C35-C36-C37
30	A	613	SQD	C9-C10-C11-C12
30	t	102	SQD	C16-C17-C18-C19
32	B	620	STE	C11-C12-C13-C14
29	D	412	LMG	C16-C17-C18-C19
29	b	622	LMG	C22-C23-C24-C25
31	c	516	DGD	C6B-C7B-C8B-C9B
32	a	615	STE	C2-C3-C4-C5
34	l	101	LHG	C13-C14-C15-C16
31	C	517	DGD	C8B-C9B-CAB-CBB
32	b	626	STE	C4-C5-C6-C7
32	c	522	STE	C5-C6-C7-C8
29	A	612	LMG	O1-C7-C8-O7
32	M	102	STE	C11-C10-C9-C8
34	D	411	LHG	C11-C10-C9-C8
34	l	101	LHG	C33-C34-C35-C36
29	M	101	LMG	C40-C41-C42-C43
29	d	410	LMG	C32-C33-C34-C35
31	C	516	DGD	CCB-CDB-CEB-CFB
25	B	601	CLA	C2A-CAA-CBA-CGA
34	d	409	LHG	C35-C36-C37-C38
25	C	505	CLA	C5-C6-C7-C8
29	D	408	LMG	C11-C12-C13-C14
29	M	101	LMG	C39-C40-C41-C42
29	c	523	LMG	C19-C20-C21-C22
31	c	517	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
32	L	103	STE	C7-C8-C9-C10
29	B	621	LMG	C31-C32-C33-C34
30	L	101	SQD	C27-C28-C29-C30
34	D	411	LHG	C30-C31-C32-C33
25	A	609	CLA	CBA-CGA-O2A-C1
30	a	613	SQD	C19-C20-C21-C22
30	f	101	SQD	C35-C36-C37-C38
31	c	518	DGD	CDA-CEA-CFA-CGA
32	t	104	STE	C13-C14-C15-C16
32	d	413	STE	C15-C16-C17-C18
29	c	523	LMG	C11-C12-C13-C14
25	a	607	CLA	C3-C5-C6-C7
29	M	101	LMG	C38-C39-C40-C41
31	C	516	DGD	C4B-C5B-C6B-C7B
32	b	624	STE	C15-C16-C17-C18
34	D	411	LHG	C17-C18-C19-C20
25	c	510	CLA	C2-C3-C5-C6
29	d	411	LMG	C38-C39-C40-C41
34	E	101	LHG	C14-C15-C16-C17
25	B	606	CLA	C15-C16-C17-C18
25	C	506	CLA	C13-C15-C16-C17
34	d	408	LHG	C16-C17-C18-C19
29	A	612	LMG	C14-C15-C16-C17
30	t	102	SQD	C10-C11-C12-C13
31	C	518	DGD	C4B-C5B-C6B-C7B
31	c	517	DGD	C8A-C9A-CAA-CBA
32	a	615	STE	C4-C5-C6-C7
34	e	102	LHG	O1-C1-C2-O2
25	B	602	CLA	C6-C7-C8-C9
25	B	602	CLA	C11-C12-C13-C14
25	B	604	CLA	C14-C13-C15-C16
25	B	607	CLA	C14-C13-C15-C16
25	B	611	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	C	508	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C14
25	D	405	CLA	C11-C12-C13-C14
25	b	605	CLA	C14-C13-C15-C16
25	b	607	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C10-C8-C9
25	b	615	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	c	505	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	512	CLA	C14-C13-C15-C16
29	c	523	LMG	C33-C34-C35-C36
31	A	615	DGD	CEB-CFB-CGB-CHB
25	C	501	CLA	O1D-CGD-O2D-CED
25	b	607	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	C13-C15-C16-C17
25	B	614	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
25	C	502	CLA	C4B-C3B-CAB-CBB
25	D	404	CLA	C4B-C3B-CAB-CBB
25	b	610	CLA	C4B-C3B-CAB-CBB
25	b	615	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
29	b	622	LMG	C34-C35-C36-C37
32	C	521	STE	C6-C7-C8-C9
32	t	104	STE	C9-C10-C11-C12
25	b	608	CLA	C4C-C3C-CAC-CBC
34	e	102	LHG	C14-C15-C16-C17
25	b	614	CLA	C8-C10-C11-C12
29	d	410	LMG	C34-C35-C36-C37
31	a	614	DGD	CBB-CCB-CDB-CEB
31	c	516	DGD	CBA-CCA-CDA-CEA
34	D	410	LHG	C10-C11-C12-C13
34	d	409	LHG	C25-C26-C27-C28
29	d	410	LMG	C40-C41-C42-C43
30	B	622	SQD	C19-C20-C21-C22
34	D	413	LHG	C19-C20-C21-C22
34	e	102	LHG	O6-C4-C5-C6
34	l	101	LHG	O6-C4-C5-C6
30	a	613	SQD	C33-C34-C35-C36
34	d	408	LHG	C33-C34-C35-C36
25	B	606	CLA	O1D-CGD-O2D-CED
31	c	516	DGD	CDB-CEB-CFB-CGB
34	D	410	LHG	C35-C36-C37-C38
29	c	523	LMG	C34-C35-C36-C37
25	B	602	CLA	C11-C12-C13-C15
25	B	607	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C6-C7-C8-C10
25	C	510	CLA	C11-C10-C8-C7
25	a	607	CLA	C6-C7-C8-C10
25	b	601	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C12-C13-C15
25	b	604	CLA	C11-C12-C13-C15
25	b	605	CLA	C11-C10-C8-C7
25	b	607	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	c	505	CLA	C6-C7-C8-C10
25	c	506	CLA	C6-C7-C8-C10
32	c	520	STE	C1-C2-C3-C4
34	d	407	LHG	C14-C15-C16-C17
25	c	511	CLA	C16-C17-C18-C19
29	c	521	LMG	C15-C16-C17-C18
29	c	521	LMG	C37-C38-C39-C40
30	a	613	SQD	C18-C19-C20-C21
29	B	621	LMG	C17-C18-C19-C20
25	a	607	CLA	C3A-C2A-CAA-CBA
25	b	609	CLA	C3A-C2A-CAA-CBA
31	a	614	DGD	C3A-C4A-C5A-C6A
25	B	601	CLA	CAA-CBA-CGA-O2A
29	A	612	LMG	C13-C14-C15-C16
31	a	614	DGD	CAB-CBB-CCB-CDB
31	C	517	DGD	CDA-CEA-CFA-CGA
32	c	520	STE	C4-C5-C6-C7
34	E	101	LHG	O10-C23-O8-C6
25	B	612	CLA	C8-C10-C11-C12
29	C	519	LMG	C37-C38-C39-C40
25	C	513	CLA	CBA-CGA-O2A-C1
25	d	404	CLA	CBA-CGA-O2A-C1
32	H	103	STE	C1-C2-C3-C4
25	b	616	CLA	C5-C6-C7-C8
34	e	102	LHG	C16-C17-C18-C19
25	c	512	CLA	O1D-CGD-O2D-CED
31	C	516	DGD	C9B-CAB-CBB-CCB
32	b	621	STE	C5-C6-C7-C8
26	A	608	PHO	CBD-CGD-O2D-CED
29	D	408	LMG	C14-C15-C16-C17
32	C	522	STE	C6-C7-C8-C9
29	M	101	LMG	C29-C28-O8-C9
29	C	519	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	c	523	LMG	O1-C7-C8-C9
30	a	613	SQD	O6-C44-C45-C46
31	A	615	DGD	O1G-C1G-C2G-C3G
31	A	615	DGD	C1G-C2G-C3G-O3G
30	t	102	SQD	C12-C13-C14-C15
25	b	601	CLA	C16-C17-C18-C19
25	C	512	CLA	C10-C11-C12-C13
25	b	607	CLA	C10-C11-C12-C13
25	D	404	CLA	C2C-C3C-CAC-CBC
30	A	614	SQD	C19-C20-C21-C22
29	c	523	LMG	C39-C40-C41-C42
29	m	101	LMG	C13-C14-C15-C16
32	C	522	STE	C7-C8-C9-C10
32	c	520	STE	C3-C4-C5-C6
29	d	411	LMG	C32-C33-C34-C35
25	C	510	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
28	D	407	PL9	C40-C39-C41-C42
28	a	611	PL9	C30-C29-C31-C32
28	d	406	PL9	C15-C14-C16-C17
28	d	406	PL9	C45-C44-C46-C47
31	c	517	DGD	C5B-C6B-C7B-C8B
32	d	413	STE	C14-C15-C16-C17
26	A	608	PHO	C15-C16-C17-C18
25	b	603	CLA	CBD-CGD-O2D-CED
30	L	101	SQD	C19-C20-C21-C22
29	D	412	LMG	C30-C31-C32-C33
25	B	610	CLA	C16-C17-C18-C19
32	B	624	STE	C3-C4-C5-C6
34	D	413	LHG	C25-C26-C27-C28
34	d	408	LHG	C34-C35-C36-C37
25	B	601	CLA	C2B-C3B-CAB-CBB
27	B	617	BCR	C1-C6-C7-C8
27	H	101	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C30
27	k	102	BCR	C23-C24-C25-C30
29	m	101	LMG	C14-C15-C16-C17
32	I	101	STE	C10-C11-C12-C13
25	c	511	CLA	CBD-CGD-O2D-CED
30	t	102	SQD	C28-C29-C30-C31
32	b	621	STE	C11-C10-C9-C8
32	B	620	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
34	D	410	LHG	C25-C26-C27-C28
29	c	521	LMG	O7-C8-C9-O8
29	m	101	LMG	O1-C7-C8-O7
28	A	611	PL9	C4-C3-C7-C8
28	a	611	PL9	C4-C3-C7-C8
28	d	406	PL9	C4-C3-C7-C8
32	M	103	STE	C4-C5-C6-C7
26	A	608	PHO	O1D-CGD-O2D-CED
31	c	516	DGD	O6D-C5D-C6D-O5D
31	c	517	DGD	C1A-C2A-C3A-C4A
32	d	412	STE	C2-C3-C4-C5
34	l	101	LHG	C26-C27-C28-C29
27	B	618	BCR	C10-C11-C12-C13
32	B	623	STE	C3-C4-C5-C6
25	B	602	CLA	C16-C17-C18-C20
29	A	612	LMG	C37-C38-C39-C40
29	B	621	LMG	C34-C35-C36-C37
32	b	625	STE	C6-C7-C8-C9
30	f	101	SQD	C23-C24-C25-C26
32	L	103	STE	C1-C2-C3-C4
31	A	615	DGD	C2A-C1A-O1G-C1G
34	e	102	LHG	C27-C28-C29-C30
25	b	601	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C10-C8-C9
32	t	104	STE	C4-C5-C6-C7
29	b	622	LMG	C24-C25-C26-C27
29	m	101	LMG	C30-C31-C32-C33
29	C	519	LMG	O6-C1-O1-C7
30	L	101	SQD	O5-C1-O6-C44
34	L	102	LHG	C18-C19-C20-C21
32	c	520	STE	C10-C11-C12-C13
29	b	622	LMG	C38-C39-C40-C41
30	D	409	SQD	C27-C28-C29-C30
30	t	102	SQD	C14-C15-C16-C17
32	X	101	STE	C13-C14-C15-C16
34	D	410	LHG	C33-C34-C35-C36
32	B	624	STE	C7-C8-C9-C10
32	B	620	STE	C12-C13-C14-C15
32	d	412	STE	C12-C13-C14-C15
25	D	404	CLA	O1D-CGD-O2D-CED
25	B	609	CLA	C15-C16-C17-C18
29	c	523	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
34	L	102	LHG	C33-C34-C35-C36
34	d	409	LHG	C34-C35-C36-C37
34	d	409	LHG	O1-C1-C2-O2
25	c	505	CLA	C4-C3-C5-C6
25	c	506	CLA	C16-C17-C18-C19
31	c	518	DGD	C6B-C7B-C8B-C9B
34	d	408	LHG	C18-C19-C20-C21
25	b	615	CLA	C13-C15-C16-C17
30	A	613	SQD	C29-C30-C31-C32
32	B	620	STE	C9-C10-C11-C12
32	d	413	STE	C12-C13-C14-C15
27	A	610	BCR	C35-C13-C14-C15
27	A	610	BCR	C20-C21-C22-C37
27	a	610	BCR	C20-C21-C22-C37
27	k	101	BCR	C20-C21-C22-C37
30	B	622	SQD	C35-C36-C37-C38
31	C	516	DGD	O1G-C1A-C2A-C3A
25	c	503	CLA	CBA-CGA-O2A-C1
29	M	101	LMG	C37-C38-C39-C40
25	B	611	CLA	C15-C16-C17-C18
25	C	508	CLA	C16-C17-C18-C19
32	b	620	STE	C11-C12-C13-C14
25	C	509	CLA	C8-C10-C11-C12
27	b	619	BCR	C7-C8-C9-C34
30	f	101	SQD	C34-C35-C36-C37
25	B	601	CLA	C6-C7-C8-C10
25	B	604	CLA	C6-C7-C8-C10
25	B	608	CLA	C6-C7-C8-C10
25	B	613	CLA	C12-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C10
25	B	614	CLA	C12-C13-C15-C16
25	a	607	CLA	C12-C13-C15-C16
25	b	601	CLA	C12-C13-C15-C16
25	b	612	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C7
25	c	510	CLA	C11-C10-C8-C7
25	c	511	CLA	C6-C7-C8-C10
25	c	511	CLA	C11-C10-C8-C7
25	c	511	CLA	C12-C13-C15-C16
31	H	102	DGD	O2G-C1B-C2B-C3B
31	c	517	DGD	C3A-C4A-C5A-C6A
34	L	102	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
34	d	407	LHG	C9-C10-C11-C12
31	C	516	DGD	CDB-CEB-CFB-CGB
27	T	101	BCR	C21-C22-C23-C24
32	b	620	STE	C5-C6-C7-C8
25	C	513	CLA	O1A-CGA-O2A-C1
31	C	517	DGD	C2G-C3G-O3G-C1D
31	C	517	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C5D-C6D-O5D-C1E
25	c	509	CLA	C13-C15-C16-C17
29	D	412	LMG	C37-C38-C39-C40
29	M	101	LMG	C11-C12-C13-C14
32	c	520	STE	C2-C3-C4-C5
25	B	613	CLA	CBD-CGD-O2D-CED
30	a	613	SQD	C14-C15-C16-C17
32	b	620	STE	C7-C8-C9-C10
25	d	404	CLA	O1A-CGA-O2A-C1
29	B	621	LMG	C35-C36-C37-C38
29	c	521	LMG	C17-C18-C19-C20
25	b	601	CLA	C8-C10-C11-C12
25	A	609	CLA	O1A-CGA-O2A-C1
25	c	507	CLA	C8-C10-C11-C12
27	K	101	BCR	C14-C15-C16-C17
29	b	622	LMG	C32-C33-C34-C35
34	D	413	LHG	C24-C25-C26-C27
25	B	602	CLA	C16-C17-C18-C19
25	B	607	CLA	C16-C17-C18-C20
32	I	101	STE	C1-C2-C3-C4
25	c	502	CLA	C3-C5-C6-C7
29	b	622	LMG	C12-C13-C14-C15
34	E	101	LHG	C30-C31-C32-C33
27	b	617	BCR	C12-C13-C14-C15
29	m	101	LMG	C36-C37-C38-C39
34	E	101	LHG	O6-C4-C5-O7
34	l	101	LHG	O6-C4-C5-O7
30	a	613	SQD	C27-C28-C29-C30
32	B	620	STE	C5-C6-C7-C8
31	C	517	DGD	O6E-C1E-O5D-C6D
28	A	611	PL9	C9-C11-C12-C13
29	m	101	LMG	O1-C7-C8-C9
31	c	516	DGD	O1G-C1G-C2G-C3G
32	c	522	STE	C1-C2-C3-C4
25	B	606	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	L	101	SQD	C11-C12-C13-C14
31	H	102	DGD	C6B-C7B-C8B-C9B
32	B	620	STE	C3-C4-C5-C6
32	X	101	STE	C10-C11-C12-C13
28	D	407	PL9	C15-C14-C16-C17
32	a	616	STE	C2-C3-C4-C5
29	c	521	LMG	C38-C39-C40-C41
30	L	101	SQD	C28-C29-C30-C31
29	C	519	LMG	O1-C7-C8-O7
29	c	523	LMG	O1-C7-C8-O7
30	L	101	SQD	O6-C44-C45-O47
31	A	615	DGD	O1G-C1G-C2G-O2G
31	C	516	DGD	O1G-C1G-C2G-O2G
31	c	516	DGD	O1G-C1G-C2G-O2G
25	c	507	CLA	C15-C16-C17-C18
25	B	604	CLA	C11-C10-C8-C9
25	B	608	CLA	C6-C7-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	b	605	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C9
25	c	507	CLA	C6-C7-C8-C9
25	c	510	CLA	C11-C12-C13-C14
25	c	511	CLA	C6-C7-C8-C9
29	c	523	LMG	O9-C10-O7-C8
29	B	621	LMG	C37-C38-C39-C40
29	D	412	LMG	C36-C37-C38-C39
29	b	622	LMG	C35-C36-C37-C38
30	A	614	SQD	C28-C29-C30-C31
31	A	615	DGD	C5A-C6A-C7A-C8A
34	d	407	LHG	C10-C11-C12-C13
31	C	517	DGD	CBA-CCA-CDA-CEA
29	A	612	LMG	C35-C36-C37-C38
29	d	411	LMG	C34-C35-C36-C37
31	H	102	DGD	C1A-C2A-C3A-C4A
34	D	413	LHG	C32-C33-C34-C35
34	l	101	LHG	C31-C32-C33-C34
32	H	103	STE	C5-C6-C7-C8
31	C	517	DGD	C2E-C1E-O5D-C6D
25	C	513	CLA	C16-C17-C18-C19
25	b	607	CLA	C16-C17-C18-C20
25	b	602	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C11-C10-C9-C8
25	B	612	CLA	CBA-CGA-O2A-C1
25	B	606	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C19
31	A	615	DGD	CEA-CFA-CGA-CHA
32	b	621	STE	C11-C12-C13-C14
25	c	503	CLA	O1A-CGA-O2A-C1
30	t	102	SQD	C30-C31-C32-C33
31	c	516	DGD	C6A-C7A-C8A-C9A
29	A	612	LMG	C32-C33-C34-C35
31	c	516	DGD	C5A-C6A-C7A-C8A
32	B	625	STE	C11-C10-C9-C8
25	B	612	CLA	C16-C17-C18-C19
25	D	404	CLA	C16-C17-C18-C19
31	C	516	DGD	CBA-CCA-CDA-CEA
27	C	515	BCR	C7-C8-C9-C34
25	B	601	CLA	C4B-C3B-CAB-CBB
25	B	609	CLA	C4B-C3B-CAB-CBB
25	B	610	CLA	C4B-C3B-CAB-CBB
25	B	615	CLA	C4B-C3B-CAB-CBB
25	C	503	CLA	C1A-C2A-CAA-CBA
25	a	607	CLA	C4B-C3B-CAB-CBB
25	a	609	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	C4B-C3B-CAB-CBB
25	B	612	CLA	O1D-CGD-O2D-CED
25	B	607	CLA	CBA-CGA-O2A-C1
29	c	521	LMG	C39-C40-C41-C42
31	C	517	DGD	CBB-CCB-CDB-CEB
30	a	613	SQD	C23-C24-C25-C26
27	a	610	BCR	C22-C23-C24-C25
28	a	611	PL9	C28-C29-C31-C32
27	K	101	BCR	C11-C12-C13-C14
31	C	516	DGD	CAB-CBB-CCB-CDB
31	c	516	DGD	C4D-C5D-C6D-O5D
30	B	622	SQD	C29-C30-C31-C32
31	c	516	DGD	C4A-C5A-C6A-C7A
25	b	604	CLA	C13-C15-C16-C17
34	E	101	LHG	O6-C4-C5-C6
29	m	101	LMG	C34-C35-C36-C37
31	C	516	DGD	C4A-C5A-C6A-C7A
34	E	101	LHG	O9-C7-O7-C5
29	A	612	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C12-C13-C15-C16
25	B	607	CLA	C6-C7-C8-C10
25	B	607	CLA	C11-C12-C13-C15
25	D	404	CLA	C6-C7-C8-C10
25	b	602	CLA	C6-C7-C8-C10
25	b	608	CLA	C11-C10-C8-C7
25	b	615	CLA	C12-C13-C15-C16
25	c	507	CLA	C11-C12-C13-C15
25	c	513	CLA	C11-C12-C13-C15
25	B	613	CLA	C16-C17-C18-C19
25	C	509	CLA	C16-C17-C18-C19
25	a	606	CLA	C16-C17-C18-C19
25	b	608	CLA	C16-C17-C18-C19
25	b	604	CLA	C15-C16-C17-C18
25	a	609	CLA	CBA-CGA-O2A-C1
34	E	101	LHG	C18-C19-C20-C21
25	C	507	CLA	C15-C16-C17-C18
30	A	614	SQD	C10-C11-C12-C13
30	L	101	SQD	C23-C24-C25-C26
29	D	408	LMG	C30-C31-C32-C33
31	C	518	DGD	CBB-CCB-CDB-CEB
34	D	411	LHG	C27-C28-C29-C30
34	L	102	LHG	C30-C31-C32-C33
26	A	608	PHO	C4-C3-C5-C6
36	V	201	HEC	C4B-C3B-CAB-CBB
29	D	408	LMG	C37-C38-C39-C40
29	m	101	LMG	C32-C33-C34-C35
32	X	101	STE	C7-C8-C9-C10
28	d	406	PL9	C18-C19-C21-C22
32	I	101	STE	C3-C4-C5-C6
25	B	603	CLA	C2A-CAA-CBA-CGA
25	B	604	CLA	C6-C7-C8-C9
25	B	613	CLA	C14-C13-C15-C16
25	b	612	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C10-C8-C9
30	A	613	SQD	C14-C15-C16-C17
30	A	613	SQD	C24-C25-C26-C27
32	b	624	STE	C12-C13-C14-C15
31	C	518	DGD	CDA-CEA-CFA-CGA
32	b	625	STE	C2-C3-C4-C5
30	B	622	SQD	O5-C5-C6-S
31	C	518	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
32	l	102	STE	C3-C4-C5-C6
31	c	518	DGD	C4A-C5A-C6A-C7A
32	b	620	STE	C15-C16-C17-C18
29	C	519	LMG	O10-C28-O8-C9
25	C	509	CLA	C5-C6-C7-C8
25	c	511	CLA	C8-C10-C11-C12
29	c	521	LMG	O1-C7-C8-C9
31	C	516	DGD	O1G-C1G-C2G-C3G
32	J	101	STE	C3-C4-C5-C6
34	E	101	LHG	C27-C28-C29-C30
29	c	523	LMG	C10-C11-C12-C13
25	B	612	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
32	X	101	STE	C6-C7-C8-C9
32	H	103	STE	C4-C5-C6-C7
29	M	101	LMG	C28-C29-C30-C31
34	E	101	LHG	C13-C14-C15-C16
31	C	517	DGD	C9A-CAA-CBA-CCA
25	c	506	CLA	C8-C10-C11-C12
25	B	607	CLA	O1A-CGA-O2A-C1
25	B	612	CLA	O1A-CGA-O2A-C1
34	d	408	LHG	O9-C7-O7-C5
31	c	517	DGD	C5A-C6A-C7A-C8A
32	C	522	STE	C9-C10-C11-C12
25	c	511	CLA	O1D-CGD-O2D-CED
29	c	521	LMG	C14-C15-C16-C17
32	a	615	STE	C1-C2-C3-C4
30	B	622	SQD	C26-C27-C28-C29
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	CAD-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O2D
27	K	101	BCR	C13-C14-C15-C16
27	d	405	BCR	C16-C17-C18-C36
30	A	614	SQD	C46-C45-O47-C7
34	D	410	LHG	C4-O6-P-O5
34	D	413	LHG	C3-O3-P-O5
34	E	101	LHG	C4-O6-P-O5
34	L	102	LHG	C4-O6-P-O5
34	e	102	LHG	C4-O6-P-O3
25	b	616	CLA	C10-C11-C12-C13
25	c	505	CLA	C15-C16-C17-C18
34	d	407	LHG	C32-C33-C34-C35
29	b	622	LMG	C40-C41-C42-C43
30	A	613	SQD	C17-C18-C19-C20
25	B	615	CLA	C2B-C3B-CAB-CBB
25	a	607	CLA	C2B-C3B-CAB-CBB
31	C	518	DGD	C6A-C7A-C8A-C9A
31	a	614	DGD	CEB-CFB-CGB-CHB
34	D	411	LHG	C32-C33-C34-C35
27	H	101	BCR	C7-C8-C9-C34
29	D	412	LMG	C29-C30-C31-C32
29	D	412	LMG	C17-C18-C19-C20
31	c	518	DGD	C8A-C9A-CAA-CBA
25	a	606	CLA	C16-C17-C18-C20
32	b	624	STE	C4-C5-C6-C7
31	a	614	DGD	CDA-CEA-CFA-CGA
34	D	410	LHG	C15-C16-C17-C18
34	L	102	LHG	C35-C36-C37-C38
25	c	511	CLA	C5-C6-C7-C8
25	c	505	CLA	C2-C3-C5-C6
26	A	608	PHO	C2-C3-C5-C6
32	c	520	STE	C5-C6-C7-C8
32	j	101	STE	C4-C5-C6-C7
25	B	612	CLA	C16-C17-C18-C20
25	c	506	CLA	C15-C16-C17-C18
30	a	613	SQD	C12-C13-C14-C15
29	D	412	LMG	C31-C32-C33-C34
25	B	607	CLA	C6-C7-C8-C9
25	D	404	CLA	C14-C13-C15-C16
25	a	607	CLA	C11-C10-C8-C9
25	a	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	C11-C10-C8-C9
25	c	506	CLA	C6-C7-C8-C9
25	c	513	CLA	C6-C7-C8-C9
25	B	609	CLA	C11-C12-C13-C15
25	B	613	CLA	C6-C7-C8-C10
25	C	503	CLA	C11-C10-C8-C7
25	D	404	CLA	C11-C12-C13-C15
25	a	607	CLA	C11-C10-C8-C7
25	b	607	CLA	C6-C7-C8-C10
25	c	502	CLA	C11-C12-C13-C15
25	c	504	CLA	C11-C10-C8-C7
27	C	514	BCR	C12-C13-C14-C15
27	D	406	BCR	C16-C17-C18-C19
27	k	101	BCR	C20-C21-C22-C23
30	L	101	SQD	C24-C25-C26-C27
34	D	410	LHG	C11-C12-C13-C14
31	H	102	DGD	C9B-CAB-CBB-CCB
29	B	621	LMG	C10-C11-C12-C13
25	d	404	CLA	C5-C6-C7-C8
30	B	622	SQD	C24-C25-C26-C27
25	B	613	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C20
25	B	601	CLA	C13-C15-C16-C17
30	A	613	SQD	O47-C45-C46-O48
31	h	102	DGD	O2G-C1B-C2B-C3B
30	t	102	SQD	C31-C32-C33-C34
34	E	101	LHG	C10-C11-C12-C13
30	t	102	SQD	C24-C23-O48-C46
34	l	101	LHG	C23-C24-C25-C26
27	c	514	BCR	C13-C14-C15-C16
29	c	523	LMG	C12-C13-C14-C15
25	b	607	CLA	C16-C17-C18-C19
32	b	625	STE	C5-C6-C7-C8
34	l	101	LHG	C24-C25-C26-C27
25	a	609	CLA	O1A-CGA-O2A-C1
29	A	612	LMG	C4-C5-C6-O5
34	D	413	LHG	C18-C19-C20-C21
25	b	616	CLA	C2-C1-O2A-CGA
28	A	611	PL9	C25-C24-C26-C27
30	A	613	SQD	C26-C27-C28-C29
25	C	508	CLA	C16-C17-C18-C20
29	A	612	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	L	101	SQD	O6-C44-C45-C46
25	c	509	CLA	CAA-CBA-CGA-O2A
25	B	614	CLA	C15-C16-C17-C18
29	M	101	LMG	C32-C33-C34-C35
32	b	625	STE	C3-C4-C5-C6
25	b	604	CLA	C16-C17-C18-C19
31	C	517	DGD	CAA-CBA-CCA-CDA
31	C	516	DGD	C5D-C6D-O5D-C1E
32	b	623	STE	C5-C6-C7-C8
32	c	520	STE	C7-C8-C9-C10
25	B	610	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C16-C17-C18-C20
32	b	625	STE	C11-C12-C13-C14
25	c	513	CLA	C4-C3-C5-C6
31	h	102	DGD	C9A-CAA-CBA-CCA
32	I	101	STE	C5-C6-C7-C8
25	B	613	CLA	O1D-CGD-O2D-CED
30	D	409	SQD	C45-C44-O6-C1
25	B	609	CLA	C11-C12-C13-C14
25	C	505	CLA	C6-C7-C8-C9
25	b	602	CLA	C6-C7-C8-C9
25	b	608	CLA	C11-C10-C8-C9
25	c	502	CLA	C11-C12-C13-C14
31	h	102	DGD	C7B-C8B-C9B-CAB
32	b	626	STE	C3-C4-C5-C6
26	A	608	PHO	CBA-CGA-O2A-C1
31	C	516	DGD	CDA-CEA-CFA-CGA
29	m	101	LMG	C17-C18-C19-C20
25	B	606	CLA	C4B-C3B-CAB-CBB
25	b	614	CLA	C4B-C3B-CAB-CBB
25	b	616	CLA	C4B-C3B-CAB-CBB
30	t	102	SQD	C15-C16-C17-C18
35	e	101	HEM	C2A-CAA-CBA-CGA
34	D	410	LHG	C23-C24-C25-C26
29	c	519	LMG	C4-C5-C6-O5
34	D	413	LHG	C16-C17-C18-C19
29	d	410	LMG	C31-C32-C33-C34
29	d	410	LMG	C29-C30-C31-C32
34	E	101	LHG	C11-C12-C13-C14
31	c	518	DGD	O6E-C5E-C6E-O5E
30	a	613	SQD	C10-C11-C12-C13
25	B	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	B	611	CLA	C11-C10-C8-C7
25	b	611	CLA	C12-C13-C15-C16
25	c	511	CLA	C11-C12-C13-C15
30	a	613	SQD	C16-C17-C18-C19
27	C	514	BCR	C14-C15-C16-C17
29	d	410	LMG	C33-C34-C35-C36
32	B	625	STE	C5-C6-C7-C8
34	L	102	LHG	C11-C10-C9-C8
29	c	521	LMG	O1-C7-C8-O7
28	D	407	PL9	C12-C13-C14-C15
25	B	602	CLA	C3A-C2A-CAA-CBA
25	c	512	CLA	C4-C3-C5-C6
32	M	102	STE	C5-C6-C7-C8
32	c	520	STE	C11-C10-C9-C8
25	B	615	CLA	C16-C17-C18-C19
27	C	514	BCR	C20-C21-C22-C37
31	c	517	DGD	O6D-C1D-O3G-C3G
25	b	602	CLA	C8-C10-C11-C12
25	b	610	CLA	C4C-C3C-CAC-CBC
25	B	613	CLA	C2-C1-O2A-CGA
27	B	619	BCR	C15-C16-C17-C18
29	m	101	LMG	C33-C34-C35-C36
25	b	603	CLA	C13-C15-C16-C17
31	C	517	DGD	C4A-C5A-C6A-C7A
29	B	621	LMG	O7-C10-C11-C12
30	D	409	SQD	O48-C23-C24-C25
25	B	611	CLA	C10-C11-C12-C13
32	b	625	STE	O1-C1-C2-C3
28	D	407	PL9	C39-C41-C42-C43
25	C	509	CLA	C3-C5-C6-C7
25	b	616	CLA	C8-C10-C11-C12
25	b	610	CLA	C2C-C3C-CAC-CBC
25	B	603	CLA	C6-C7-C8-C9
25	B	615	CLA	C11-C12-C13-C14
25	C	506	CLA	C11-C12-C13-C14
25	C	511	CLA	C6-C7-C8-C9
25	C	511	CLA	C14-C13-C15-C16
25	D	404	CLA	C6-C7-C8-C9
25	b	603	CLA	C14-C13-C15-C16
25	b	615	CLA	C14-C13-C15-C16
25	c	512	CLA	C11-C12-C13-C14
25	d	403	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
32	t	104	STE	C12-C13-C14-C15
29	C	519	LMG	C12-C13-C14-C15
32	B	623	STE	O1-C1-C2-C3
32	d	412	STE	O2-C1-C2-C3
29	A	612	LMG	C7-C8-O7-C10
31	H	102	DGD	CAA-CBA-CCA-CDA
32	B	623	STE	O2-C1-C2-C3
32	b	621	STE	O2-C1-C2-C3
29	D	408	LMG	C19-C20-C21-C22
32	H	103	STE	C9-C10-C11-C12
32	t	104	STE	C10-C11-C12-C13
29	m	101	LMG	C20-C21-C22-C23
32	C	521	STE	O1-C1-C2-C3
31	H	102	DGD	CBB-CCB-CDB-CEB
25	b	610	CLA	C2A-CAA-CBA-CGA
32	d	413	STE	C10-C11-C12-C13
25	B	602	CLA	C1A-C2A-CAA-CBA
25	a	607	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C1A-C2A-CAA-CBA
32	b	624	STE	C5-C6-C7-C8
25	B	607	CLA	C16-C17-C18-C19
34	D	413	LHG	C23-C24-C25-C26
25	C	507	CLA	C8-C10-C11-C12
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	609	CLA	C2B-C3B-CAB-CBB
25	D	404	CLA	C2B-C3B-CAB-CBB
25	b	601	CLA	C2B-C3B-CAB-CBB
25	b	615	CLA	C2B-C3B-CAB-CBB
25	c	503	CLA	C2B-C3B-CAB-CBB
25	d	404	CLA	C2B-C3B-CAB-CBB
27	B	617	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C1-C6-C7-C8
27	H	101	BCR	C23-C24-C25-C26
27	K	101	BCR	C1-C6-C7-C8
27	K	101	BCR	C5-C6-C7-C8
27	b	617	BCR	C1-C6-C7-C8
27	c	514	BCR	C1-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C26
27	h	101	BCR	C23-C24-C25-C30
27	k	102	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
32	b	621	STE	C12-C13-C14-C15
32	b	625	STE	O2-C1-C2-C3
25	B	604	CLA	C15-C16-C17-C18
25	c	513	CLA	C8-C10-C11-C12
31	C	517	DGD	C8A-C9A-CAA-CBA
25	b	606	CLA	C4-C3-C5-C6
29	d	410	LMG	C36-C37-C38-C39
32	B	624	STE	C6-C7-C8-C9
34	d	408	LHG	C11-C10-C9-C8
29	D	408	LMG	C35-C36-C37-C38
29	B	621	LMG	O8-C28-C29-C30
25	B	606	CLA	C6-C7-C8-C10
25	B	615	CLA	C11-C12-C13-C15
25	C	507	CLA	C6-C7-C8-C10
25	C	511	CLA	C6-C7-C8-C10
25	b	610	CLA	C11-C12-C13-C15
25	b	614	CLA	C6-C7-C8-C10
25	c	508	CLA	C11-C10-C8-C7
26	A	608	PHO	C12-C13-C15-C16
25	b	616	CLA	C11-C12-C13-C15
31	C	516	DGD	O6D-C5D-C6D-O5D
30	t	102	SQD	O10-C23-O48-C46
32	c	522	STE	C2-C3-C4-C5
32	j	101	STE	C5-C6-C7-C8
34	l	101	LHG	C29-C30-C31-C32
28	D	407	PL9	C4-C3-C7-C8
29	B	621	LMG	C12-C13-C14-C15
30	A	614	SQD	C33-C34-C35-C36
30	t	102	SQD	C25-C26-C27-C28
31	H	102	DGD	C6A-C7A-C8A-C9A
29	B	621	LMG	O9-C10-C11-C12
29	d	411	LMG	C33-C34-C35-C36
29	c	521	LMG	C12-C13-C14-C15
25	d	403	CLA	C4-C3-C5-C6
34	E	101	LHG	C31-C32-C33-C34
25	a	609	CLA	C15-C16-C17-C18
25	c	512	CLA	C2-C3-C5-C6
28	A	611	PL9	C33-C34-C36-C37
29	B	621	LMG	O10-C28-C29-C30
36	v	201	HEC	CAD-CBD-CGD-O2D
25	c	505	CLA	C11-C10-C8-C9
25	c	508	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
34	d	409	LHG	C33-C34-C35-C36
32	M	102	STE	O1-C1-C2-C3
32	b	621	STE	O1-C1-C2-C3
25	c	510	CLA	C10-C11-C12-C13
31	C	516	DGD	C4D-C5D-C6D-O5D
25	B	607	CLA	C4-C3-C5-C6
36	v	201	HEC	CAD-CBD-CGD-O1D
34	D	411	LHG	C2-C3-O3-P
34	d	409	LHG	C2-C3-O3-P
26	A	608	PHO	O1A-CGA-O2A-C1
25	b	613	CLA	C8-C10-C11-C12
25	c	503	CLA	C10-C11-C12-C13
32	l	102	STE	C9-C10-C11-C12
34	D	411	LHG	C26-C27-C28-C29
29	C	519	LMG	C2-C1-O1-C7
34	d	407	LHG	C34-C35-C36-C37
29	D	412	LMG	C7-C8-C9-O8
31	c	518	DGD	O1G-C1G-C2G-C3G
25	B	601	CLA	CAA-CBA-CGA-O1A
31	C	516	DGD	CCA-CDA-CEA-CFA
32	C	521	STE	O2-C1-C2-C3
25	B	604	CLA	C10-C11-C12-C13
32	d	412	STE	O1-C1-C2-C3
31	h	102	DGD	CDA-CEA-CFA-CGA
31	C	517	DGD	C2A-C3A-C4A-C5A
25	B	606	CLA	C16-C17-C18-C20
31	C	516	DGD	C2B-C3B-C4B-C5B
25	C	513	CLA	C4B-C3B-CAB-CBB
29	d	410	LMG	C39-C40-C41-C42
30	L	101	SQD	C9-C10-C11-C12
26	D	402	PHO	CHA-CBD-CGD-O2D
26	d	402	PHO	CHA-CBD-CGD-O1D
27	K	101	BCR	C20-C21-C22-C37
27	k	101	BCR	C16-C17-C18-C36
31	H	102	DGD	CDB-CEB-CFB-CGB
32	b	623	STE	C7-C8-C9-C10
32	X	101	STE	O1-C1-C2-C3
31	a	614	DGD	O2G-C1B-C2B-C3B
34	E	101	LHG	C2-C3-O3-P
29	c	521	LMG	C41-C42-C43-C44
25	c	503	CLA	C11-C10-C8-C7
25	c	512	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
34	L	102	LHG	C7-C8-C9-C10
32	M	102	STE	C9-C10-C11-C12
31	C	518	DGD	C3B-C4B-C5B-C6B
31	c	517	DGD	CBB-CCB-CDB-CEB
31	C	517	DGD	C1A-C2A-C3A-C4A
25	B	603	CLA	C14-C13-C15-C16
25	B	613	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C12-C13-C14
25	c	513	CLA	C11-C12-C13-C14
30	L	101	SQD	C45-C44-O6-C1
30	L	101	SQD	C5-C6-S-O8
30	L	101	SQD	C26-C27-C28-C29
25	d	403	CLA	C2-C1-O2A-CGA
25	b	609	CLA	C16-C17-C18-C20
29	M	101	LMG	O9-C10-O7-C8
34	L	102	LHG	C23-C24-C25-C26
25	A	609	CLA	C3A-C2A-CAA-CBA
30	f	101	SQD	C32-C33-C34-C35
25	B	607	CLA	C2-C3-C5-C6
28	a	611	PL9	C38-C39-C41-C42
25	b	610	CLA	C3-C5-C6-C7
32	b	620	STE	C10-C11-C12-C13
30	t	102	SQD	C29-C30-C31-C32
25	B	605	CLA	CBA-CGA-O2A-C1
31	C	518	DGD	CBA-CCA-CDA-CEA
31	h	102	DGD	C1A-C2A-C3A-C4A
25	C	513	CLA	O2A-C1-C2-C3
29	A	612	LMG	C9-C8-O7-C10
32	b	623	STE	O2-C1-C2-C3
29	b	622	LMG	C19-C20-C21-C22
32	C	520	STE	C3-C4-C5-C6
32	c	522	STE	C6-C7-C8-C9
34	l	101	LHG	C16-C17-C18-C19
25	B	615	CLA	C16-C17-C18-C20
32	c	520	STE	O2-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O2D
25	D	404	CLA	C16-C17-C18-C20
32	M	103	STE	C3-C4-C5-C6
27	B	617	BCR	C6-C7-C8-C9
32	M	102	STE	O2-C1-C2-C3
31	C	516	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
25	B	610	CLA	C15-C16-C17-C18
25	b	615	CLA	C8-C10-C11-C12
32	b	624	STE	C7-C8-C9-C10
25	B	605	CLA	O1A-CGA-O2A-C1
32	M	102	STE	C1-C2-C3-C4
32	l	102	STE	C14-C15-C16-C17
25	c	508	CLA	C4-C3-C5-C6
35	e	101	HEM	CAD-CBD-CGD-O1D
32	j	101	STE	O1-C1-C2-C3
32	j	101	STE	O2-C1-C2-C3
32	t	104	STE	O1-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O1D
30	D	409	SQD	C23-C24-C25-C26
25	b	603	CLA	C8-C10-C11-C12
25	B	611	CLA	C11-C12-C13-C14
25	C	510	CLA	C6-C7-C8-C9
25	C	511	CLA	C11-C10-C8-C9
25	c	507	CLA	C11-C12-C13-C14
31	a	614	DGD	C8A-C9A-CAA-CBA
32	c	520	STE	O1-C1-C2-C3
27	B	619	BCR	C21-C22-C23-C24
31	a	614	DGD	C5B-C6B-C7B-C8B
25	B	616	CLA	O1A-CGA-O2A-C1
32	t	104	STE	O2-C1-C2-C3
25	A	607	CLA	C12-C13-C15-C16
25	B	614	CLA	C11-C12-C13-C15
25	C	502	CLA	C12-C13-C15-C16
25	C	506	CLA	C11-C12-C13-C15
25	C	510	CLA	C6-C7-C8-C10
25	C	513	CLA	C11-C10-C8-C7
25	D	405	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C12-C13-C15
25	b	606	CLA	C6-C7-C8-C10
25	b	612	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C10-C8-C7
25	c	507	CLA	C11-C10-C8-C7
25	c	508	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C7
26	a	608	PHO	C6-C7-C8-C10
32	M	102	STE	C10-C11-C12-C13
25	b	612	CLA	O1A-CGA-O2A-C1
32	L	103	STE	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	b	623	STE	O1-C1-C2-C3
25	C	502	CLA	C2B-C3B-CAB-CBB
25	C	507	CLA	C2B-C3B-CAB-CBB
25	b	610	CLA	C2B-C3B-CAB-CBB
25	b	611	CLA	C2B-C3B-CAB-CBB
25	b	614	CLA	C2B-C3B-CAB-CBB
25	b	616	CLA	C2B-C3B-CAB-CBB
25	c	501	CLA	C2B-C3B-CAB-CBB
25	c	502	CLA	C2B-C3B-CAB-CBB
25	c	510	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
27	B	618	BCR	C23-C24-C25-C26
27	B	619	BCR	C23-C24-C25-C30
27	C	514	BCR	C5-C6-C7-C8
27	C	514	BCR	C23-C24-C25-C30
27	C	515	BCR	C1-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C30
27	b	617	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C26
27	h	101	BCR	C23-C24-C25-C26
34	D	413	LHG	O9-C7-O7-C5
29	c	523	LMG	C38-C39-C40-C41
34	D	413	LHG	C34-C35-C36-C37
32	H	103	STE	C10-C11-C12-C13
34	E	101	LHG	C26-C27-C28-C29
34	d	408	LHG	C30-C31-C32-C33
25	b	616	CLA	C11-C12-C13-C14
25	B	609	CLA	C2-C3-C5-C6
25	D	405	CLA	C13-C15-C16-C17
31	a	614	DGD	CCA-CDA-CEA-CFA
29	d	411	LMG	C37-C38-C39-C40
32	d	413	STE	C13-C14-C15-C16
25	B	613	CLA	CAA-CBA-CGA-O2A
25	B	609	CLA	C4-C3-C5-C6
25	c	509	CLA	C4-C3-C5-C6
28	a	611	PL9	C45-C44-C46-C47
29	M	101	LMG	C10-C11-C12-C13
29	m	101	LMG	O6-C5-C6-O5
25	c	513	CLA	C2-C3-C5-C6
28	D	407	PL9	C43-C44-C46-C47
25	C	506	CLA	C2C-C3C-CAC-CBC
31	c	516	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C14-C13-C15-C16
25	B	605	CLA	C6-C7-C8-C9
25	c	507	CLA	C11-C10-C8-C9
29	D	408	LMG	C12-C13-C14-C15
30	A	613	SQD	C44-C45-C46-O48
31	c	516	DGD	C1G-C2G-C3G-O3G
25	b	611	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
25	d	404	CLA	C4B-C3B-CAB-CBB
32	X	101	STE	O2-C1-C2-C3
25	c	504	CLA	C4-C3-C5-C6
31	C	517	DGD	O6D-C1D-O3G-C3G
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	612	CLA	CAA-CBA-CGA-O2A
25	c	513	CLA	CAA-CBA-CGA-O2A
34	E	101	LHG	O8-C23-C24-C25
29	b	622	LMG	O7-C8-C9-O8
27	B	618	BCR	C17-C18-C19-C20
27	k	102	BCR	C21-C22-C23-C24
25	d	404	CLA	C16-C17-C18-C19
25	b	603	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	CAA-CBA-CGA-O2A
32	l	102	STE	C2-C3-C4-C5
29	d	410	LMG	C37-C38-C39-C40
29	D	408	LMG	C16-C17-C18-C19
28	A	611	PL9	C27-C28-C29-C30
29	m	101	LMG	O8-C28-C29-C30
34	d	408	LHG	C19-C20-C21-C22
30	L	101	SQD	C5-C6-S-O7
25	c	513	CLA	C2-C1-O2A-CGA
25	C	509	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C10-C8-C7
25	B	608	CLA	CBA-CGA-O2A-C1
34	L	102	LHG	C29-C30-C31-C32
32	L	103	STE	O1-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O1D
28	a	611	PL9	C7-C8-C9-C10
26	a	608	PHO	C3A-C2A-CAA-CBA
25	c	513	CLA	CAA-CBA-CGA-O1A
25	d	404	CLA	C8-C10-C11-C12
25	B	608	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C16-C17-C18-C19
32	t	103	STE	O2-C1-C2-C3
35	e	101	HEM	CAD-CBD-CGD-O2D
32	M	103	STE	C6-C7-C8-C9
32	d	413	STE	C7-C8-C9-C10
34	d	407	LHG	C24-C23-O8-C6
29	D	412	LMG	C12-C13-C14-C15
25	b	614	CLA	C2A-CAA-CBA-CGA
25	a	612	CLA	C4C-C3C-CAC-CBC
25	B	615	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C12-C13-C14
25	C	510	CLA	C14-C13-C15-C16
25	D	404	CLA	C11-C12-C13-C14
25	b	612	CLA	C11-C10-C8-C9
25	c	503	CLA	C11-C10-C8-C9
25	c	508	CLA	C11-C10-C8-C9
26	D	402	PHO	C14-C13-C15-C16
31	C	518	DGD	C4E-C5E-C6E-O5E
34	D	411	LHG	O10-C23-C24-C25
25	b	613	CLA	CAA-CBA-CGA-O2A
26	a	608	PHO	C8-C10-C11-C12
29	M	101	LMG	C30-C31-C32-C33
25	B	613	CLA	CAA-CBA-CGA-O1A
31	C	517	DGD	O1B-C1B-C2B-C3B
32	R	101	STE	C5-C6-C7-C8
25	d	403	CLA	C2C-C3C-CAC-CBC
25	B	608	CLA	O1A-CGA-O2A-C1
29	M	101	LMG	O8-C28-C29-C30
25	B	601	CLA	C8-C10-C11-C12
27	C	515	BCR	C17-C18-C19-C20
31	C	516	DGD	O1B-C1B-C2B-C3B
25	B	601	CLA	C5-C6-C7-C8
29	c	523	LMG	C8-C7-O1-C1
29	C	519	LMG	C19-C20-C21-C22
34	D	413	LHG	C31-C32-C33-C34
34	E	101	LHG	O10-C23-C24-C25
25	b	615	CLA	C10-C11-C12-C13
25	c	510	CLA	C5-C6-C7-C8
25	a	612	CLA	C2C-C3C-CAC-CBC
29	b	622	LMG	O8-C28-C29-C30
31	c	516	DGD	O1G-C1A-C2A-C3A
25	b	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	601	CLA	CAA-CBA-CGA-O1A
29	C	519	LMG	O9-C10-C11-C12
29	d	411	LMG	O9-C10-C11-C12
25	B	607	CLA	CAD-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O2D
26	a	608	PHO	CAD-CBD-CGD-O2D
32	C	522	STE	C4-C5-C6-C7
31	h	102	DGD	O1B-C1B-C2B-C3B
26	d	402	PHO	C8-C10-C11-C12
25	B	616	CLA	CBA-CGA-O2A-C1
25	C	506	CLA	C2-C1-O2A-CGA
25	D	404	CLA	C2-C1-O2A-CGA
31	C	517	DGD	C6B-C7B-C8B-C9B
34	D	413	LHG	C33-C34-C35-C36
30	A	614	SQD	C29-C30-C31-C32
25	b	613	CLA	CAA-CBA-CGA-O1A
29	D	408	LMG	O7-C10-C11-C12
30	A	613	SQD	O47-C7-C8-C9
34	D	410	LHG	C32-C33-C34-C35
32	t	103	STE	O1-C1-C2-C3
31	C	516	DGD	C9A-CAA-CBA-CCA
31	c	518	DGD	C7A-C8A-C9A-CAA
25	c	501	CLA	CAA-CBA-CGA-O2A
31	c	516	DGD	O1A-C1A-O1G-C1G
35	F	101	HEM	CAD-CBD-CGD-O2D
25	b	612	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

148 monomers are involved in 314 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	514	BCR	5	0
34	D	413	LHG	2	0
32	C	520	STE	1	0
27	C	515	BCR	1	0
25	B	607	CLA	1	0
27	d	405	BCR	2	0
25	C	513	CLA	3	0
25	b	606	CLA	3	0
32	C	522	STE	2	0
25	a	612	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	606	CLA	4	0
25	B	615	CLA	5	0
25	c	501	CLA	4	0
27	a	610	BCR	2	0
28	d	406	PL9	2	0
25	c	507	CLA	3	0
25	B	601	CLA	5	0
26	A	608	PHO	1	0
29	c	521	LMG	4	0
32	B	625	STE	1	0
27	c	514	BCR	1	0
30	t	102	SQD	3	0
32	X	101	STE	4	0
32	b	621	STE	1	0
34	E	101	LHG	4	0
25	A	609	CLA	1	0
25	a	606	CLA	2	0
27	b	618	BCR	2	0
25	B	611	CLA	3	0
25	c	510	CLA	3	0
25	D	405	CLA	1	0
25	d	403	CLA	2	0
26	d	402	PHO	4	0
29	B	621	LMG	1	0
32	d	413	STE	2	0
21	a	601[B]	OEY	1	0
29	c	519	LMG	2	0
32	B	624	STE	2	0
34	D	411	LHG	2	0
34	d	407	LHG	5	0
25	c	513	CLA	2	0
25	B	604	CLA	6	0
25	C	507	CLA	1	0
32	d	412	STE	1	0
30	B	622	SQD	2	0
25	b	605	CLA	4	0
31	C	516	DGD	1	0
25	B	602	CLA	3	0
29	b	622	LMG	3	0
25	B	610	CLA	1	0
25	c	512	CLA	3	0
27	B	617	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	518	DGD	5	0
25	b	613	CLA	3	0
26	D	402	PHO	1	0
25	B	605	CLA	7	0
25	B	609	CLA	2	0
25	b	608	CLA	4	0
25	C	502	CLA	3	0
25	b	611	CLA	1	0
31	h	102	DGD	1	0
32	t	104	STE	1	0
25	B	613	CLA	3	0
26	a	608	PHO	1	0
27	K	101	BCR	1	0
30	A	613	SQD	2	0
27	B	619	BCR	2	0
34	D	410	LHG	6	0
27	T	101	BCR	5	0
25	C	506	CLA	3	0
29	D	412	LMG	1	0
25	C	501	CLA	3	0
34	d	409	LHG	2	0
25	C	512	CLA	3	0
28	a	611	PL9	7	0
25	b	609	CLA	3	0
25	b	604	CLA	5	0
29	c	523	LMG	5	0
31	C	517	DGD	5	0
25	B	614	CLA	4	0
27	c	515	BCR	4	0
25	b	603	CLA	1	0
35	F	101	HEM	4	0
25	C	509	CLA	3	0
27	k	101	BCR	2	0
29	m	101	LMG	3	0
31	c	517	DGD	3	0
27	t	101	BCR	3	0
25	c	508	CLA	1	0
25	C	508	CLA	4	0
25	A	606	CLA	2	0
31	a	614	DGD	1	0
25	a	609	CLA	2	0
25	B	612	CLA	3	0

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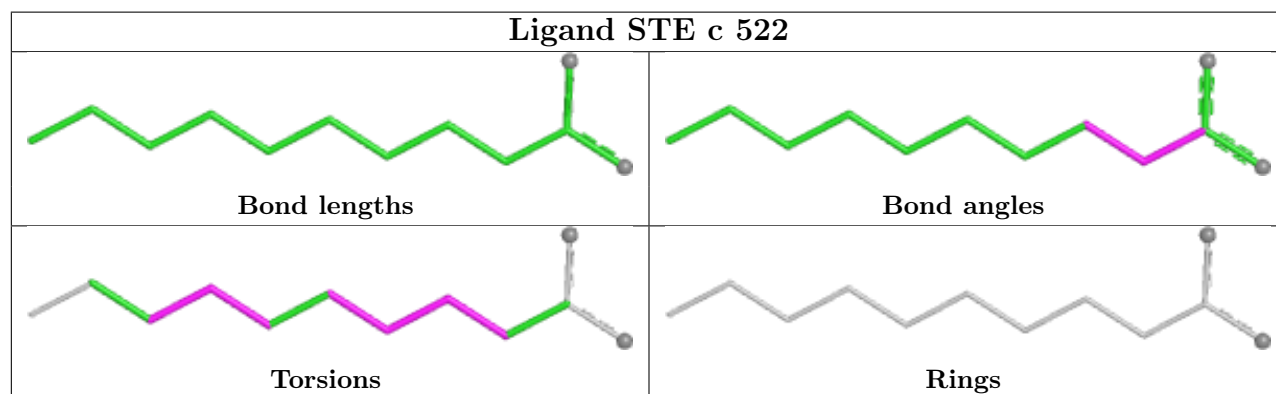
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	602	CLA	4	0
32	l	102	STE	2	0
29	C	519	LMG	2	0
25	b	615	CLA	3	0
31	c	516	DGD	2	0
25	c	511	CLA	4	0
29	d	411	LMG	1	0
27	b	617	BCR	2	0
25	B	608	CLA	1	0
25	c	503	CLA	3	0
27	B	618	BCR	2	0
29	D	408	LMG	3	0
25	C	511	CLA	2	0
25	c	505	CLA	4	0
31	C	518	DGD	2	0
32	J	101	STE	1	0
25	C	505	CLA	3	0
29	M	101	LMG	1	0
25	b	616	CLA	2	0
32	H	103	STE	3	0
27	b	619	BCR	3	0
32	L	103	STE	1	0
34	L	102	LHG	3	0
25	d	404	CLA	3	0
25	c	509	CLA	2	0
25	b	601	CLA	3	0
35	e	101	HEM	2	0
34	e	102	LHG	4	0
30	A	614	SQD	5	0
25	C	504	CLA	2	0
25	B	603	CLA	3	0
25	A	607	CLA	2	0
32	I	101	STE	3	0
32	b	620	STE	2	0
30	L	101	SQD	4	0
25	D	404	CLA	3	0
28	A	611	PL9	8	0
25	C	503	CLA	5	0
28	D	407	PL9	1	0
21	A	601[B]	OEY	1	0
25	b	614	CLA	5	0
32	b	623	STE	1	0

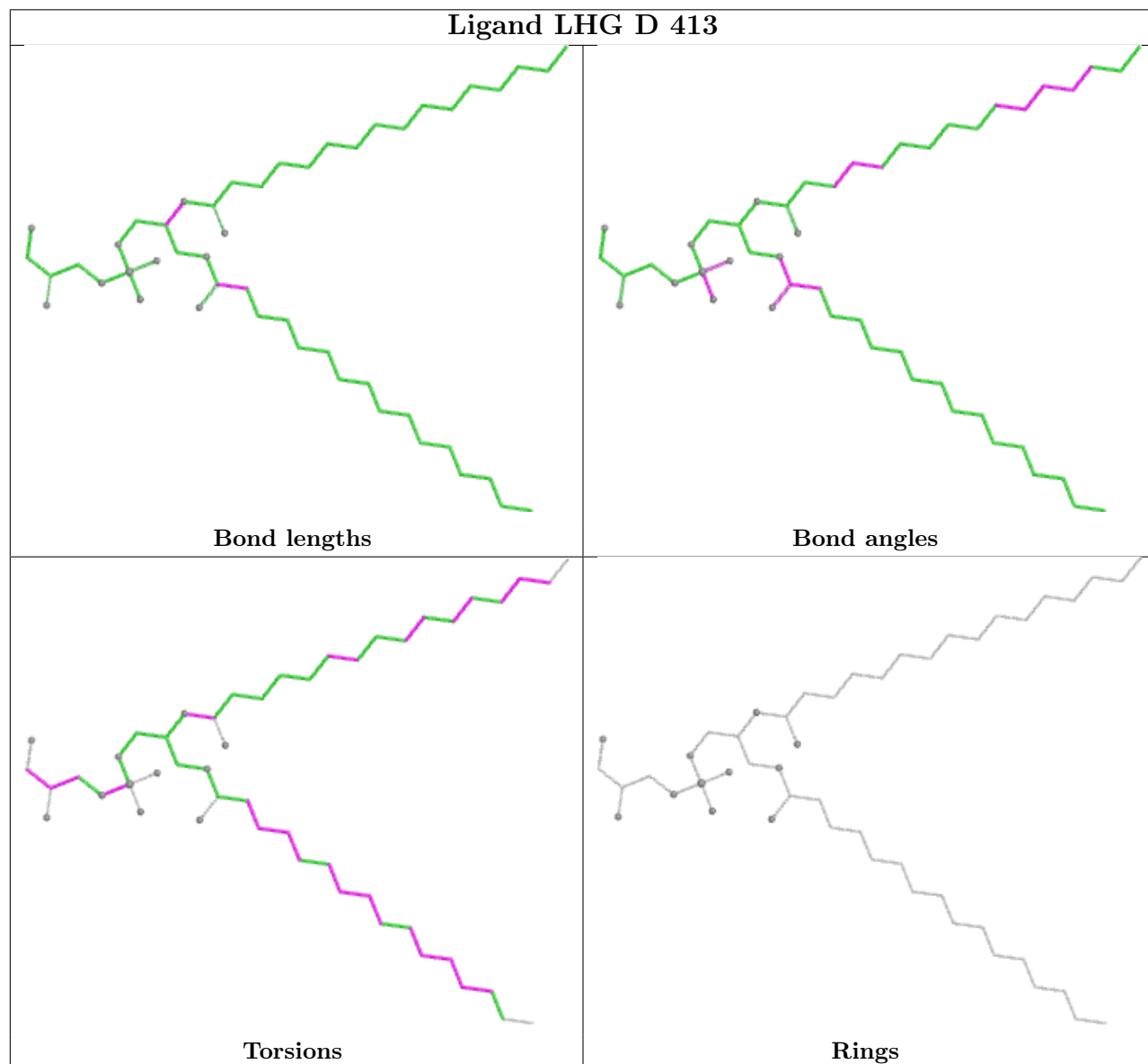
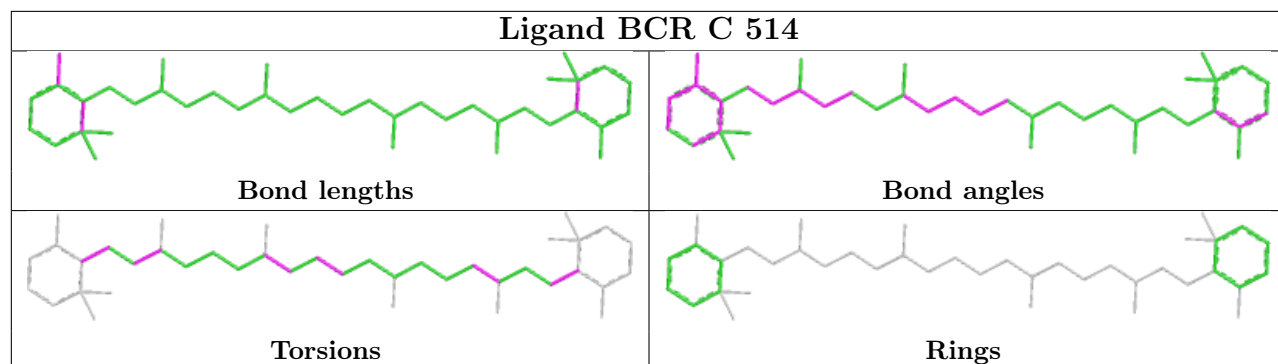
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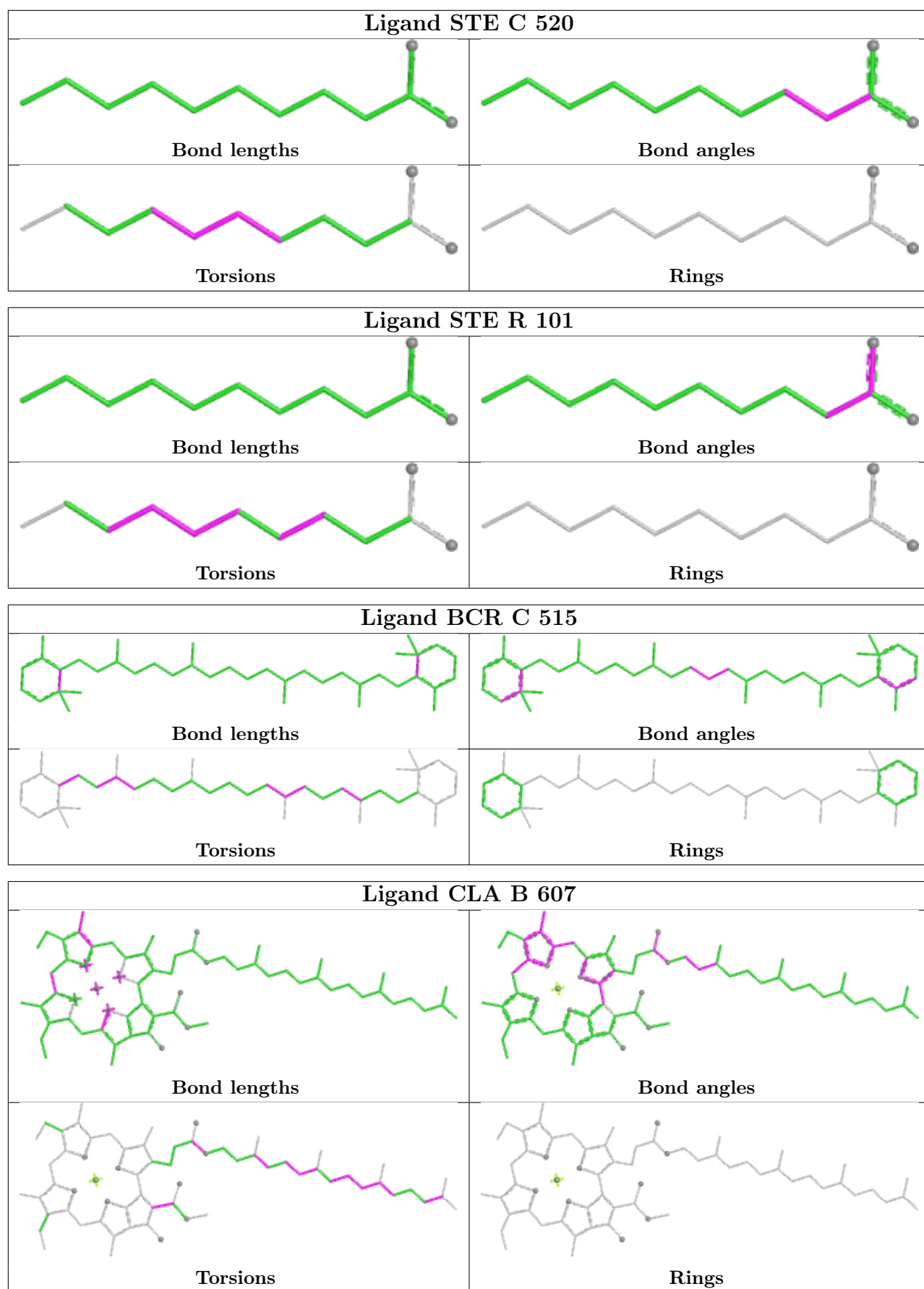
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	l	101	LHG	2	0
27	h	101	BCR	2	0
27	k	102	BCR	4	0
31	H	102	DGD	3	0
31	A	615	DGD	6	0
25	b	612	CLA	3	0
25	b	610	CLA	2	0
32	b	624	STE	2	0
32	c	520	STE	2	0
30	a	613	SQD	3	0
25	D	403	CLA	2	0
25	b	607	CLA	1	0

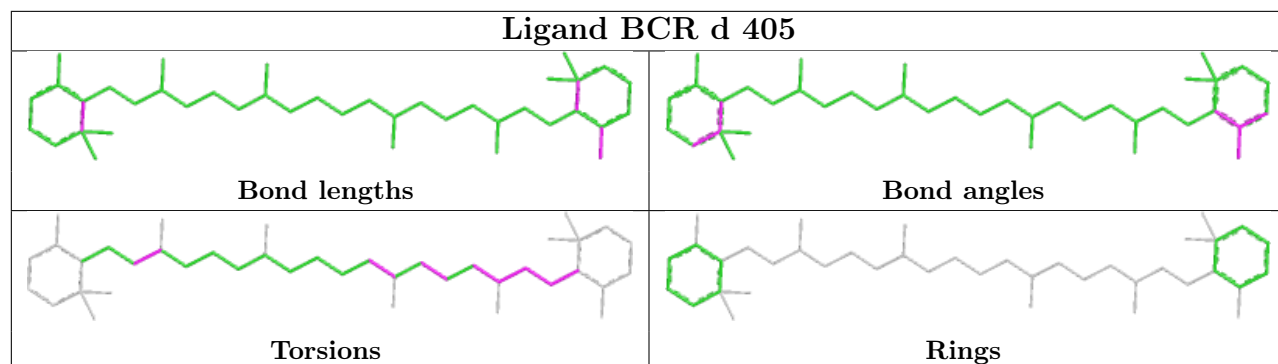
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



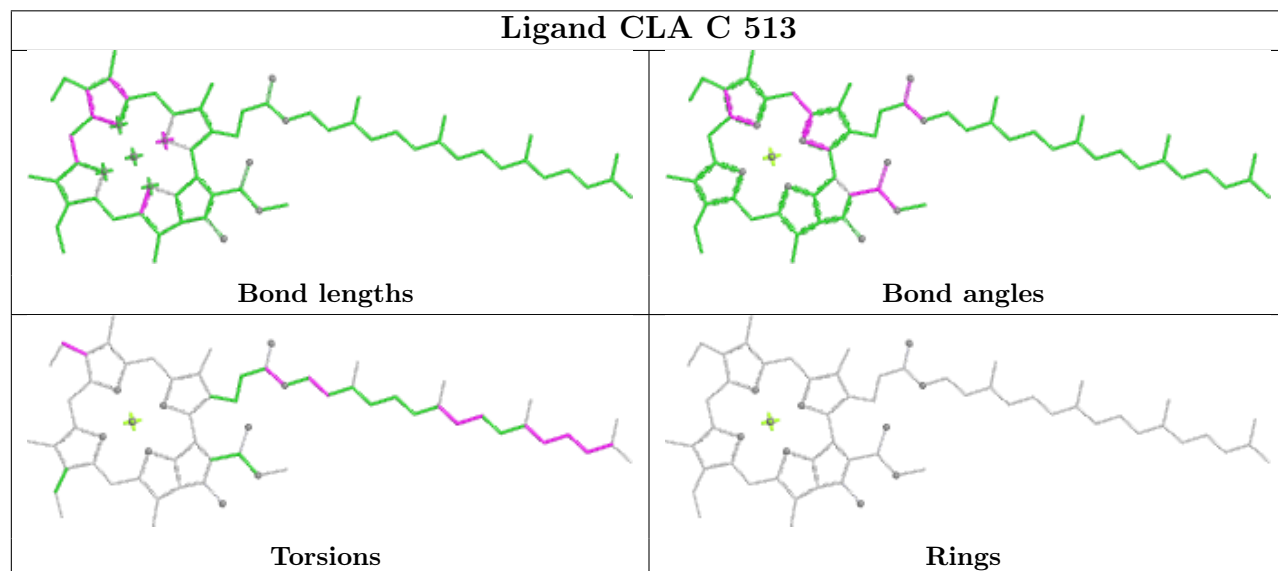




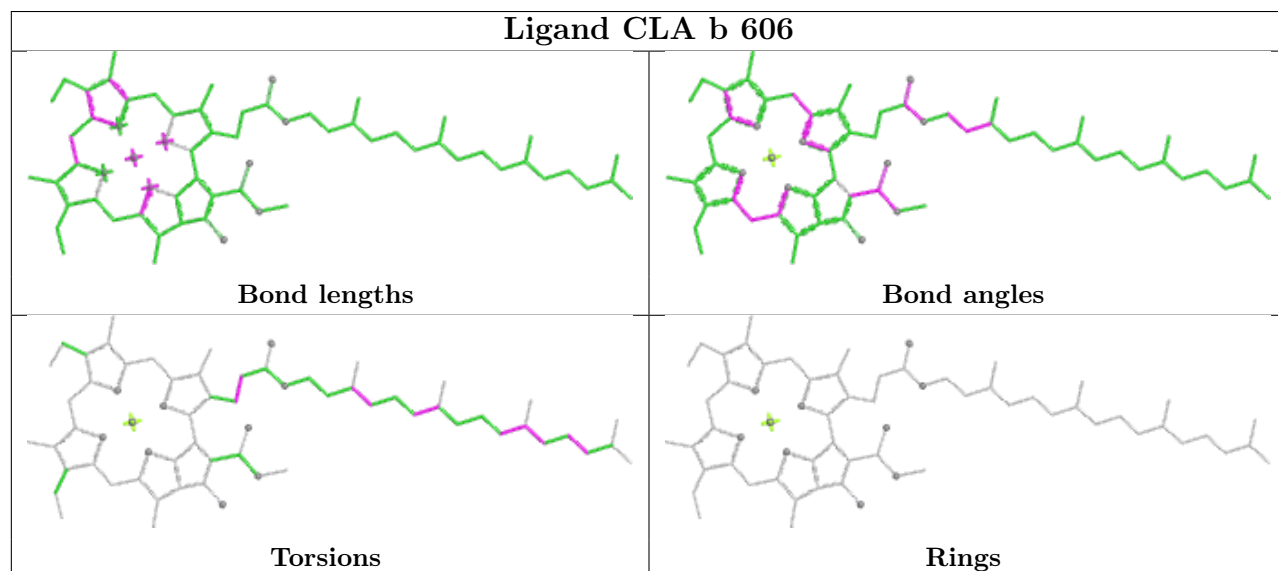
Ligand BCR d 405



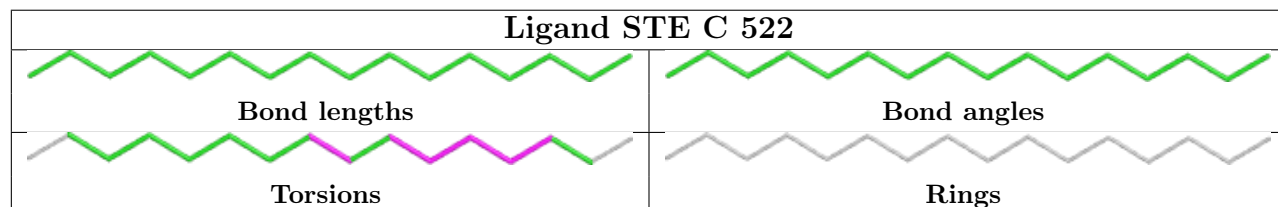
Ligand CLA C 513

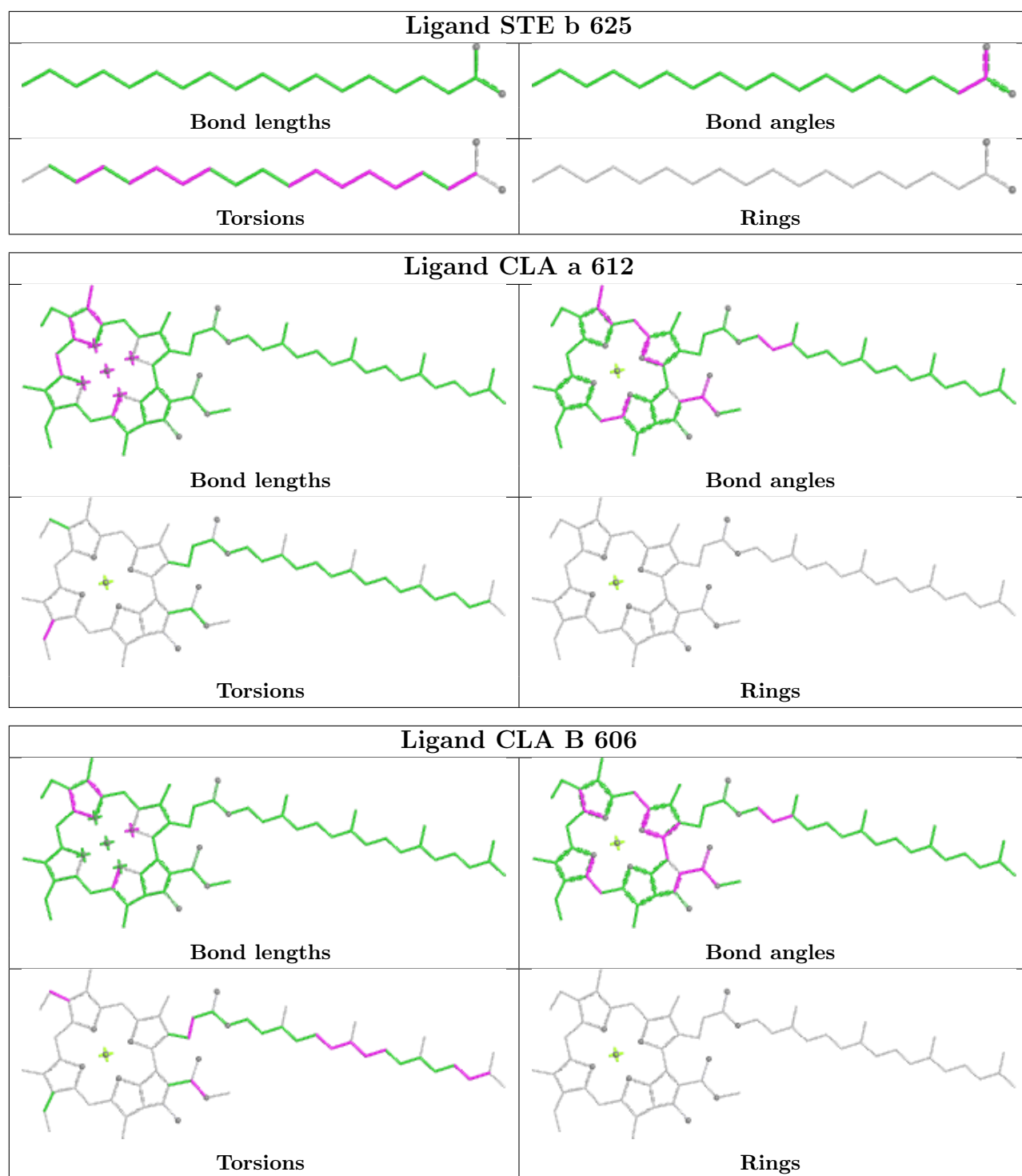


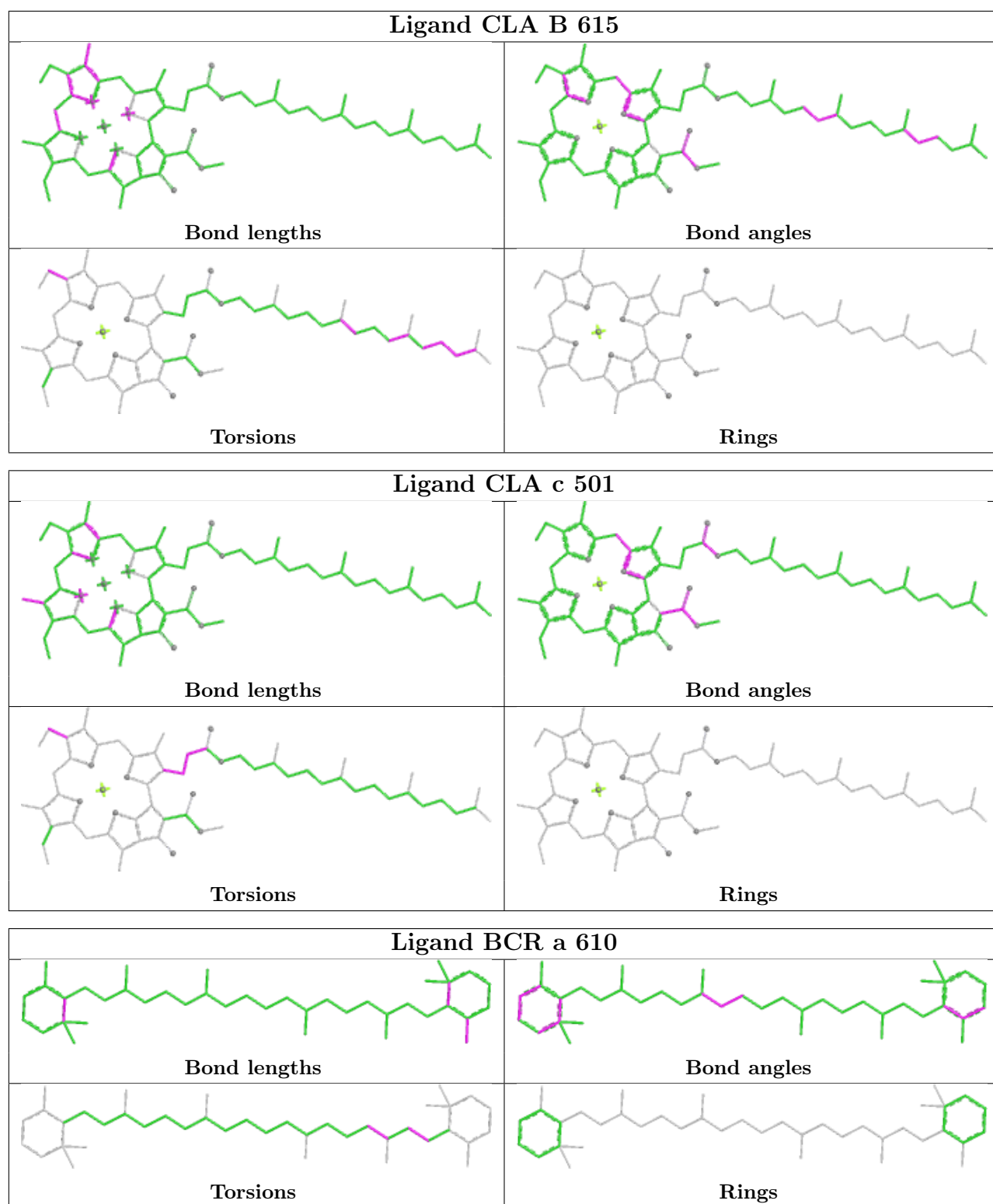
Ligand CLA b 606

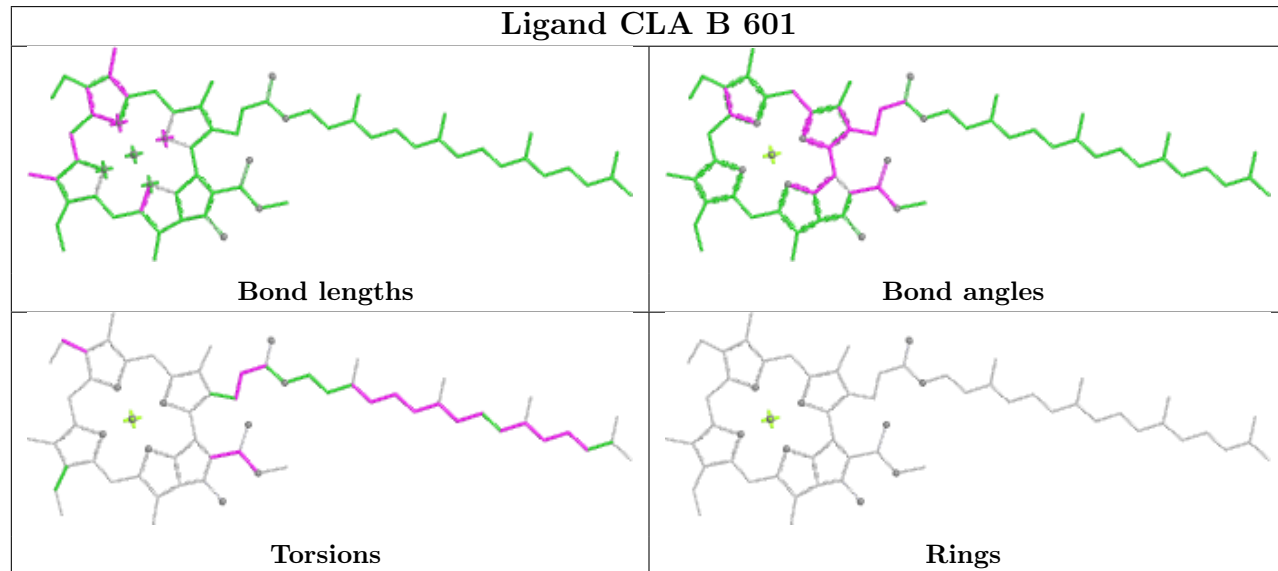
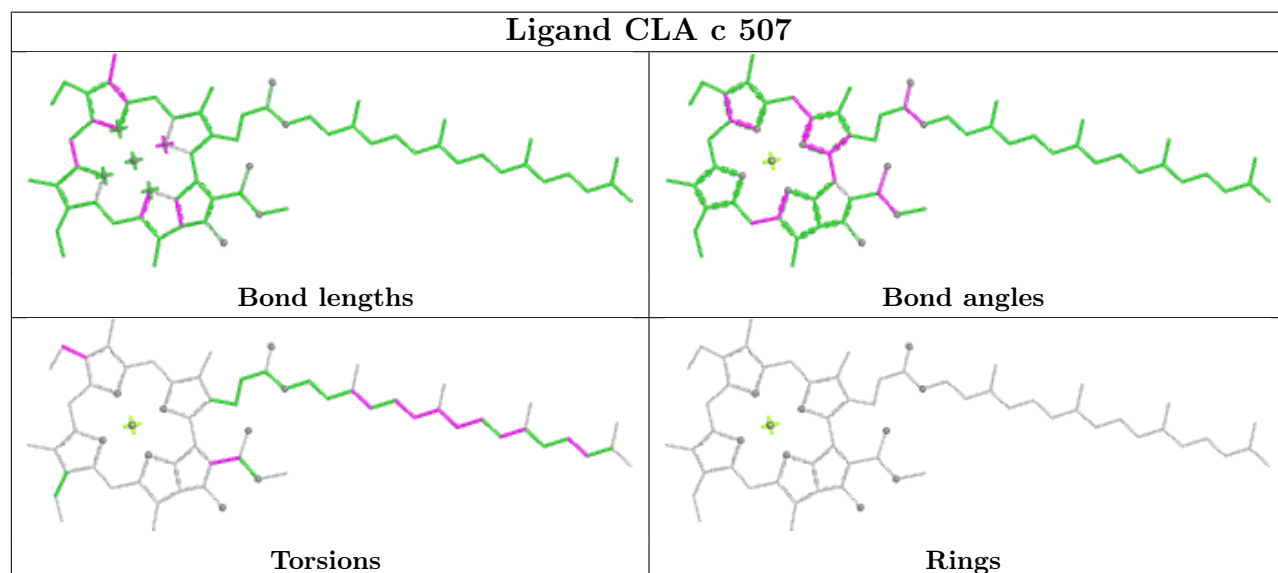
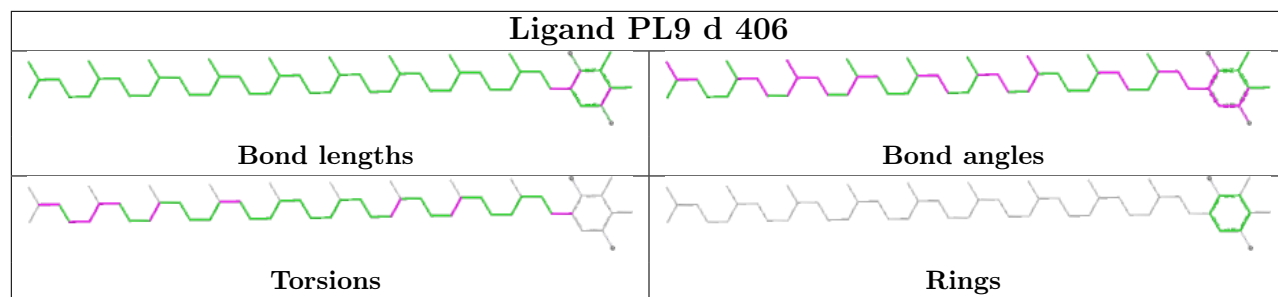


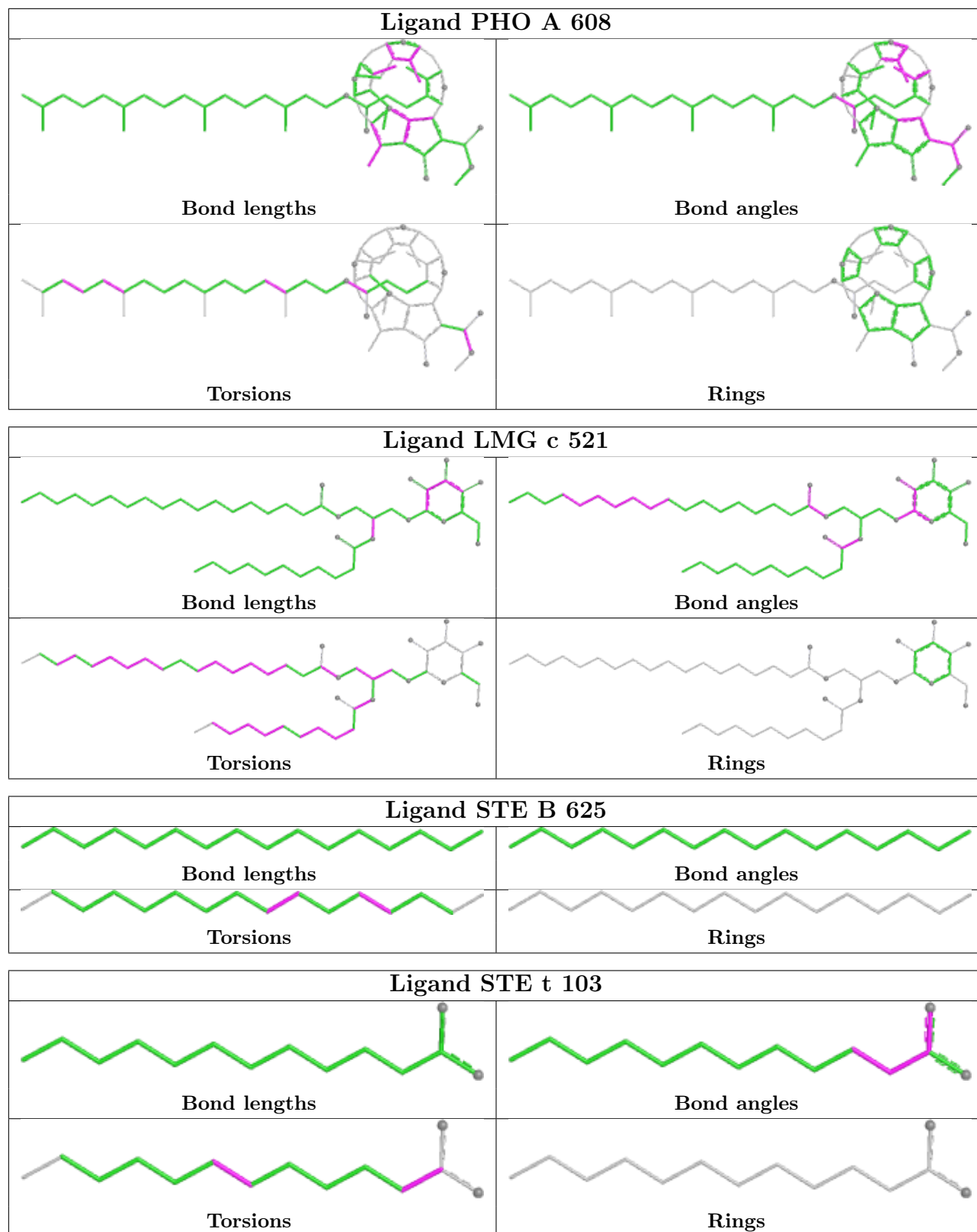
Ligand STE C 522

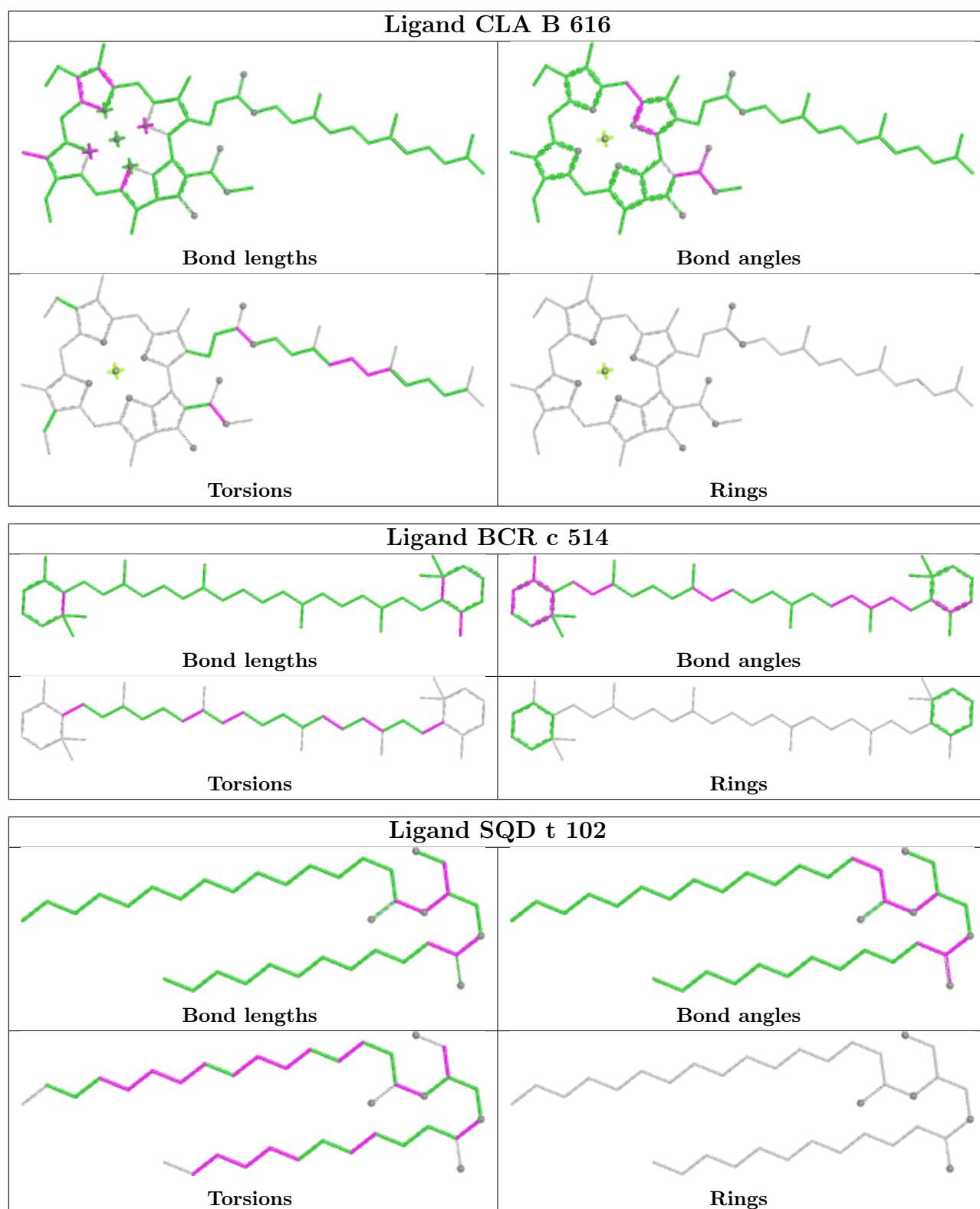


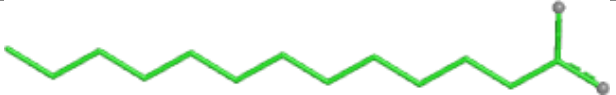
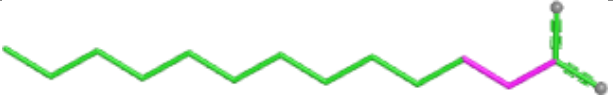
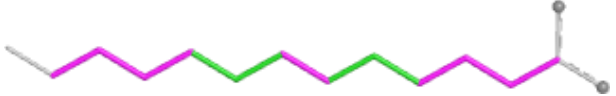
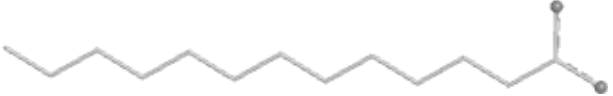


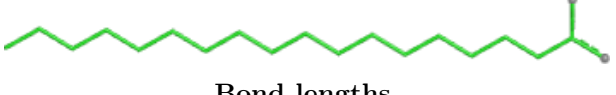
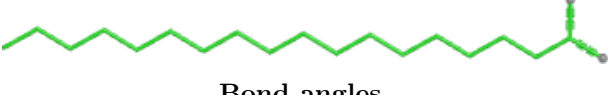
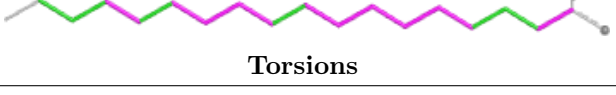


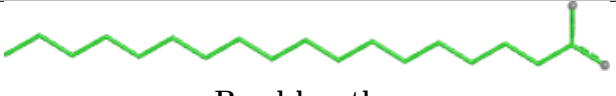
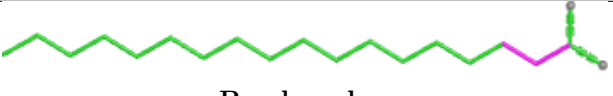


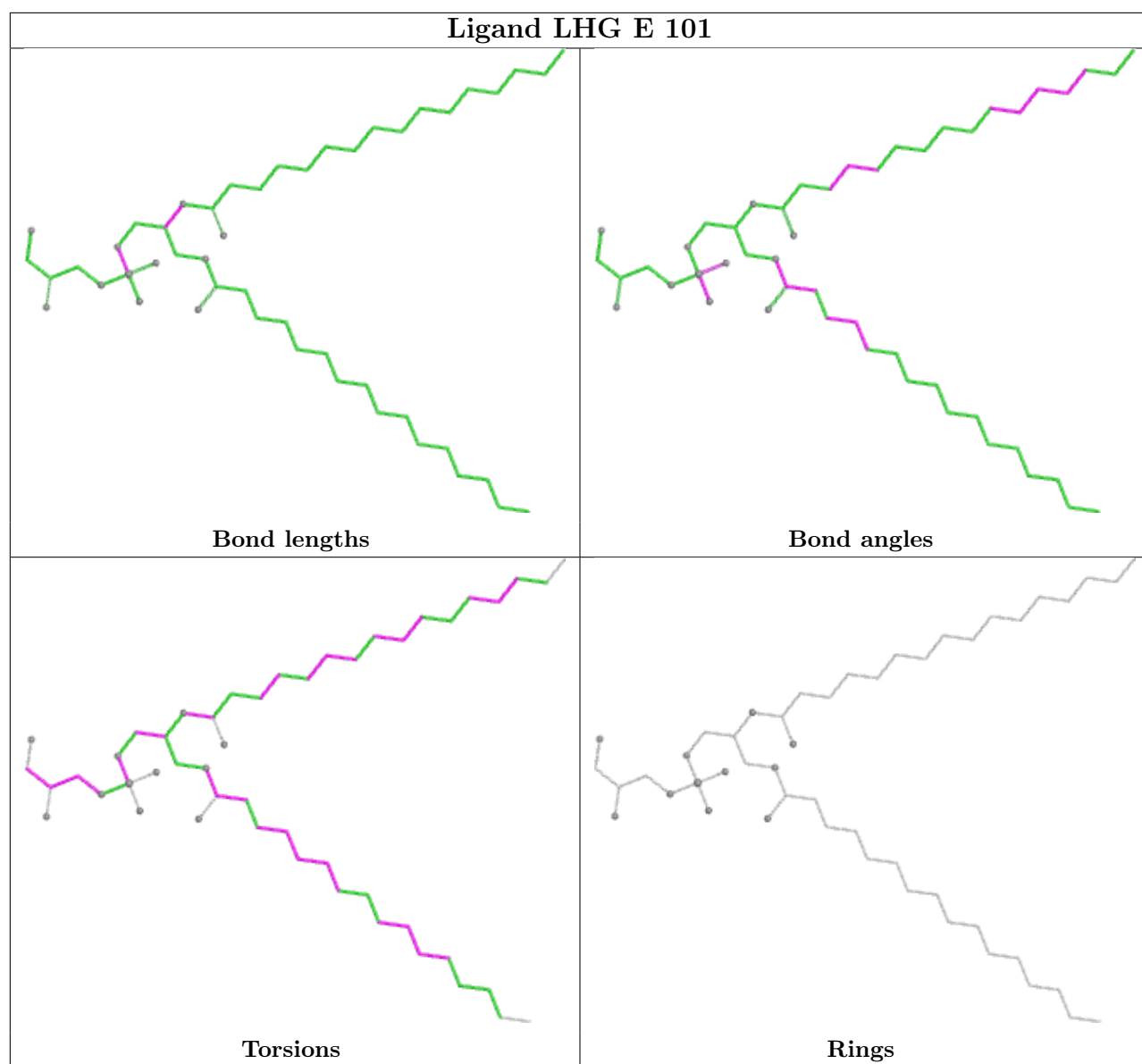


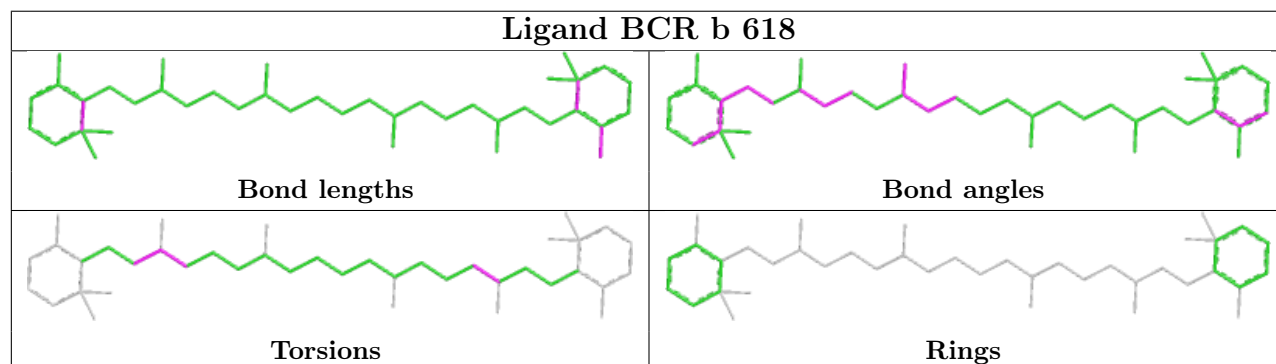
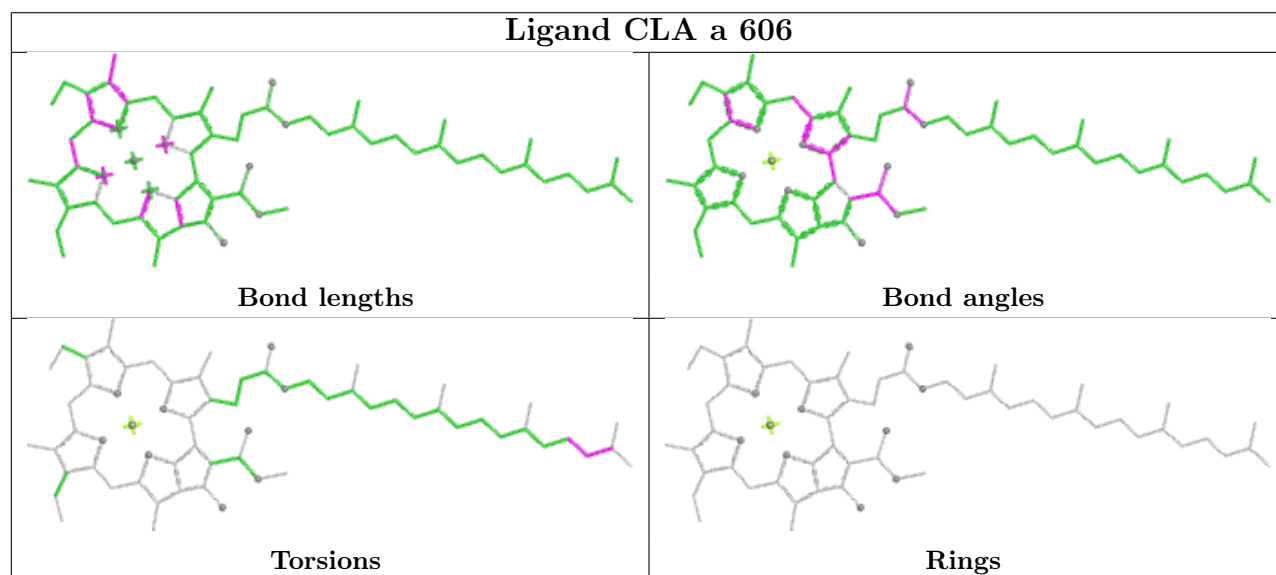
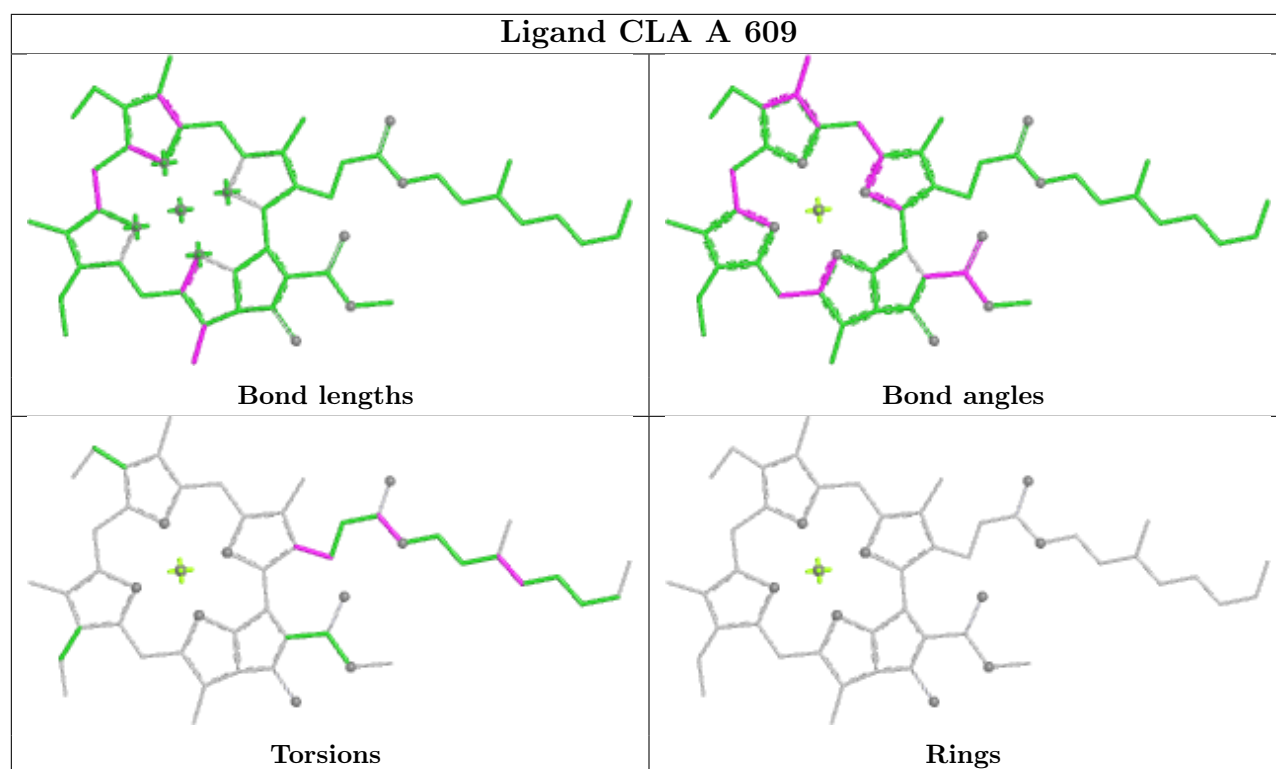


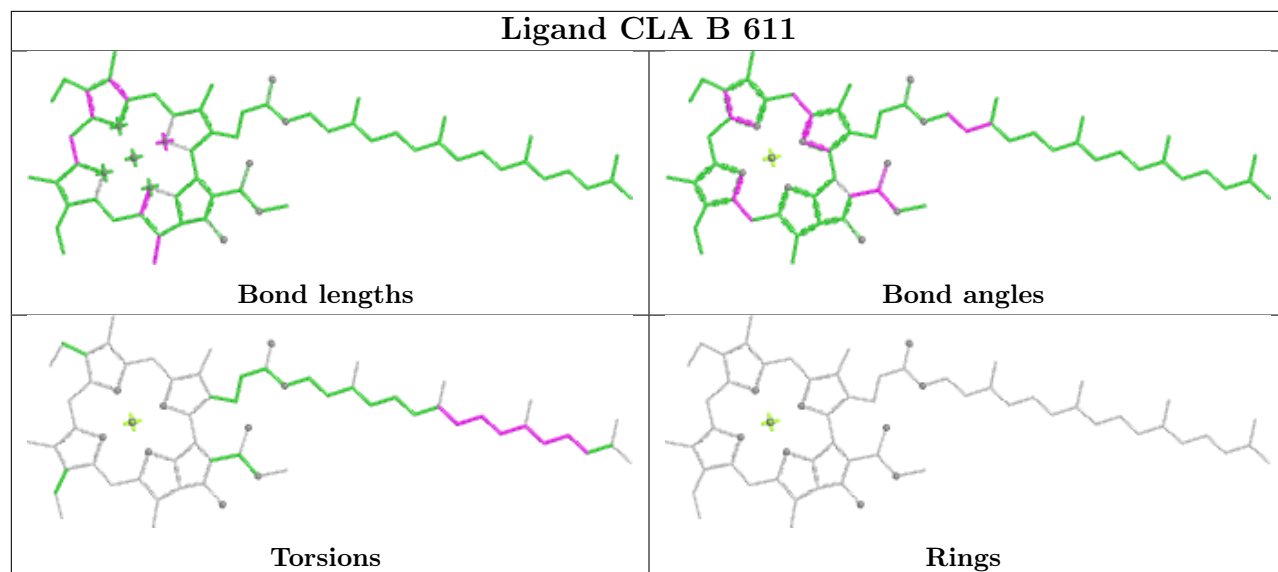
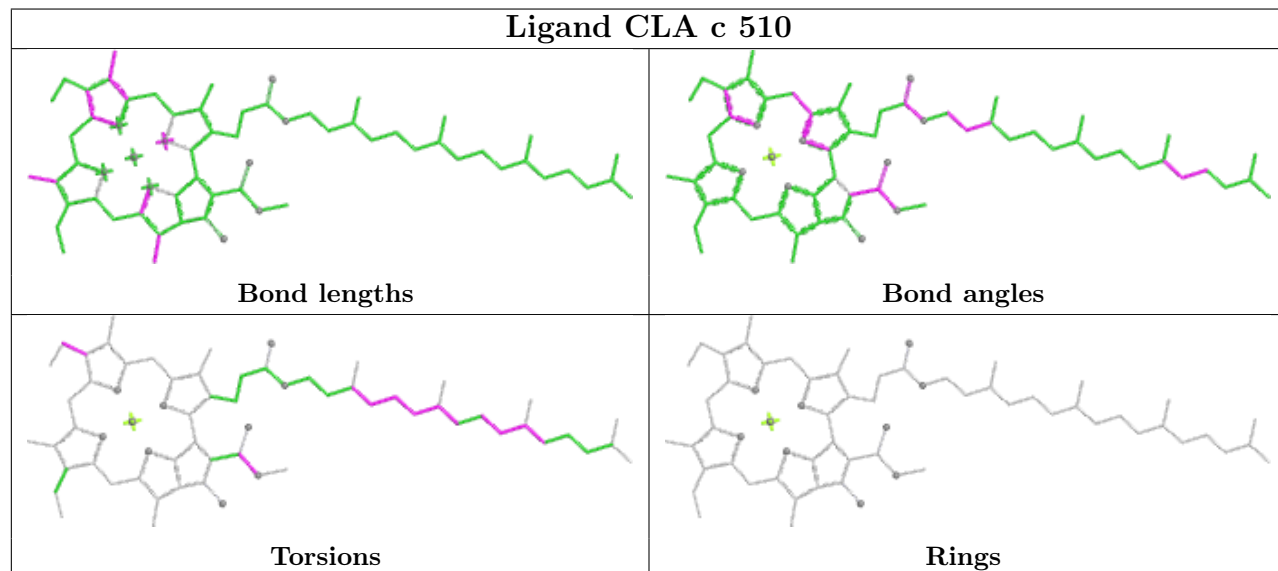
Ligand STE M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

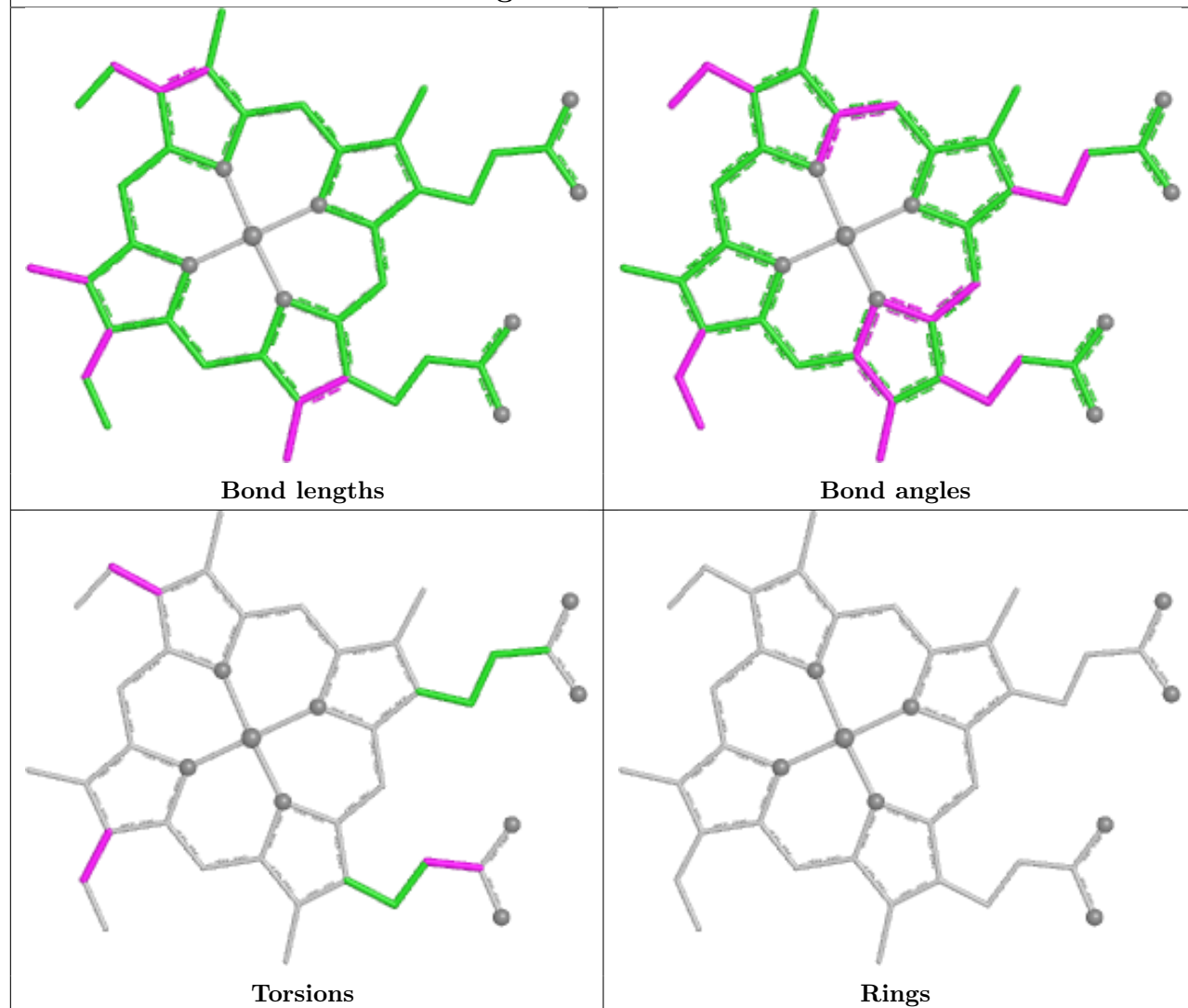
Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings



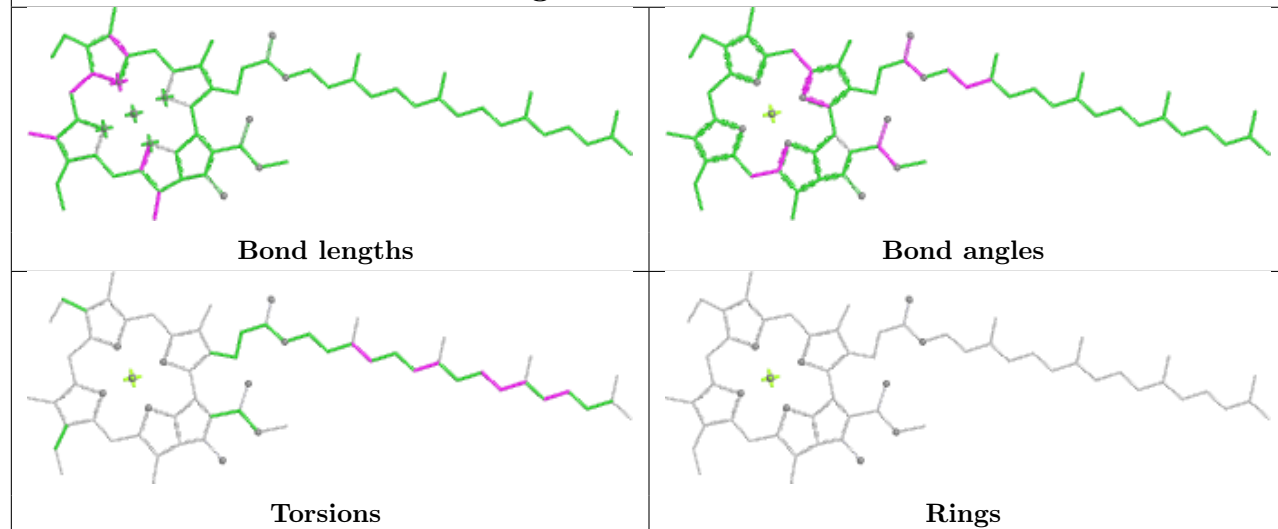


Ligand CLA B 611**Ligand CLA c 510**

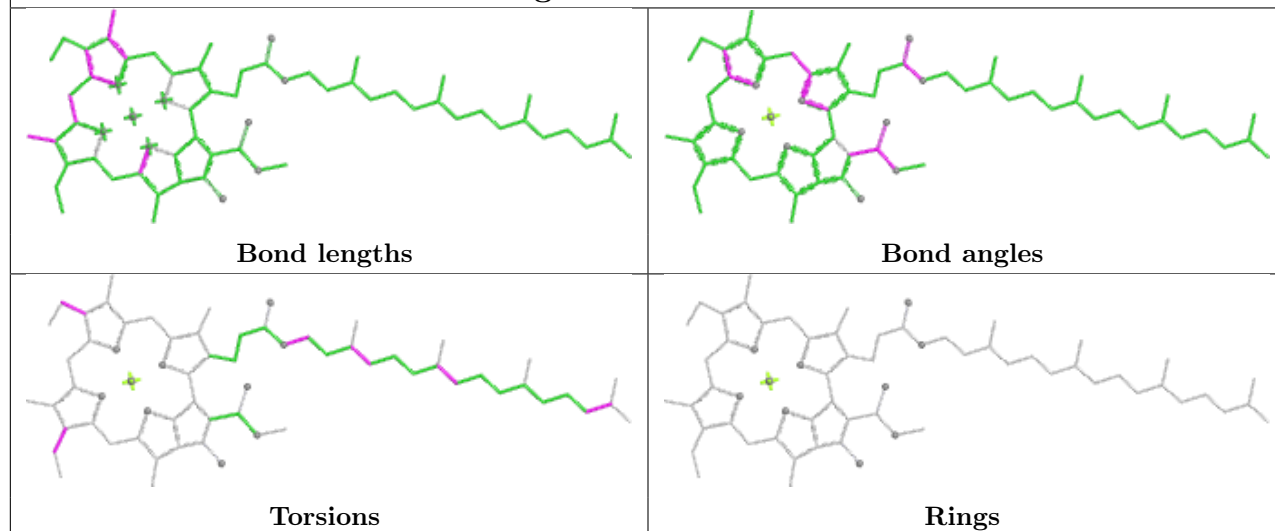
Ligand HEC v 201



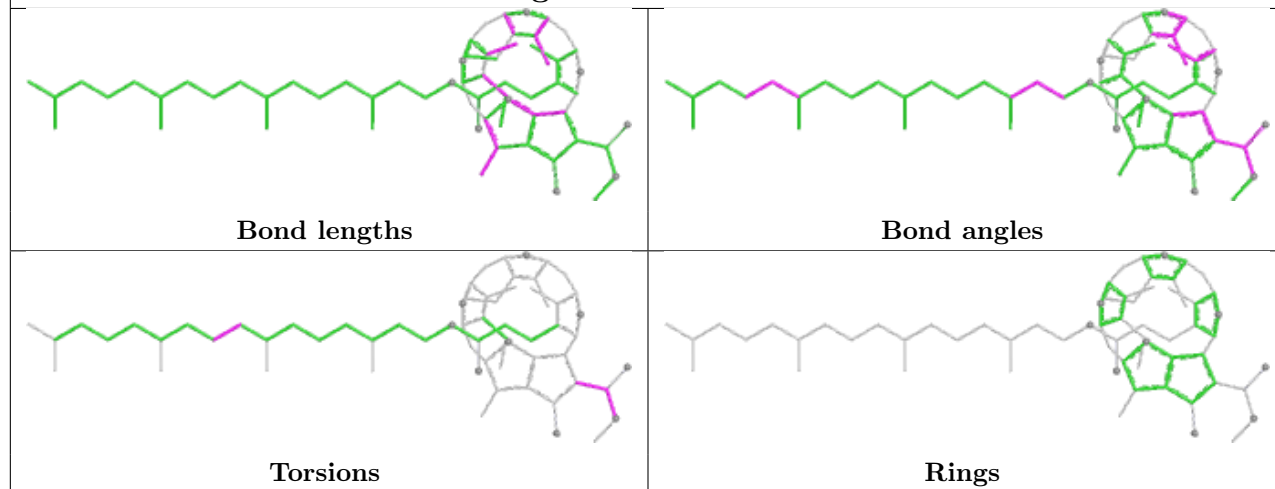
Ligand CLA D 405



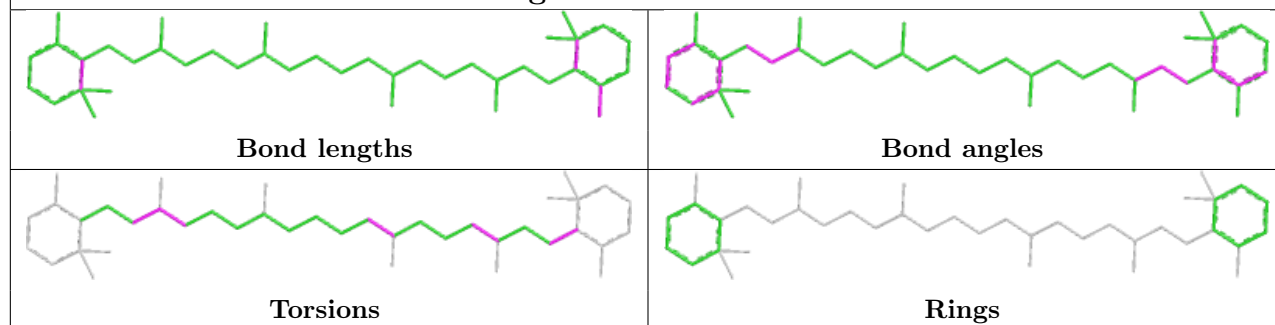
Ligand CLA d 403

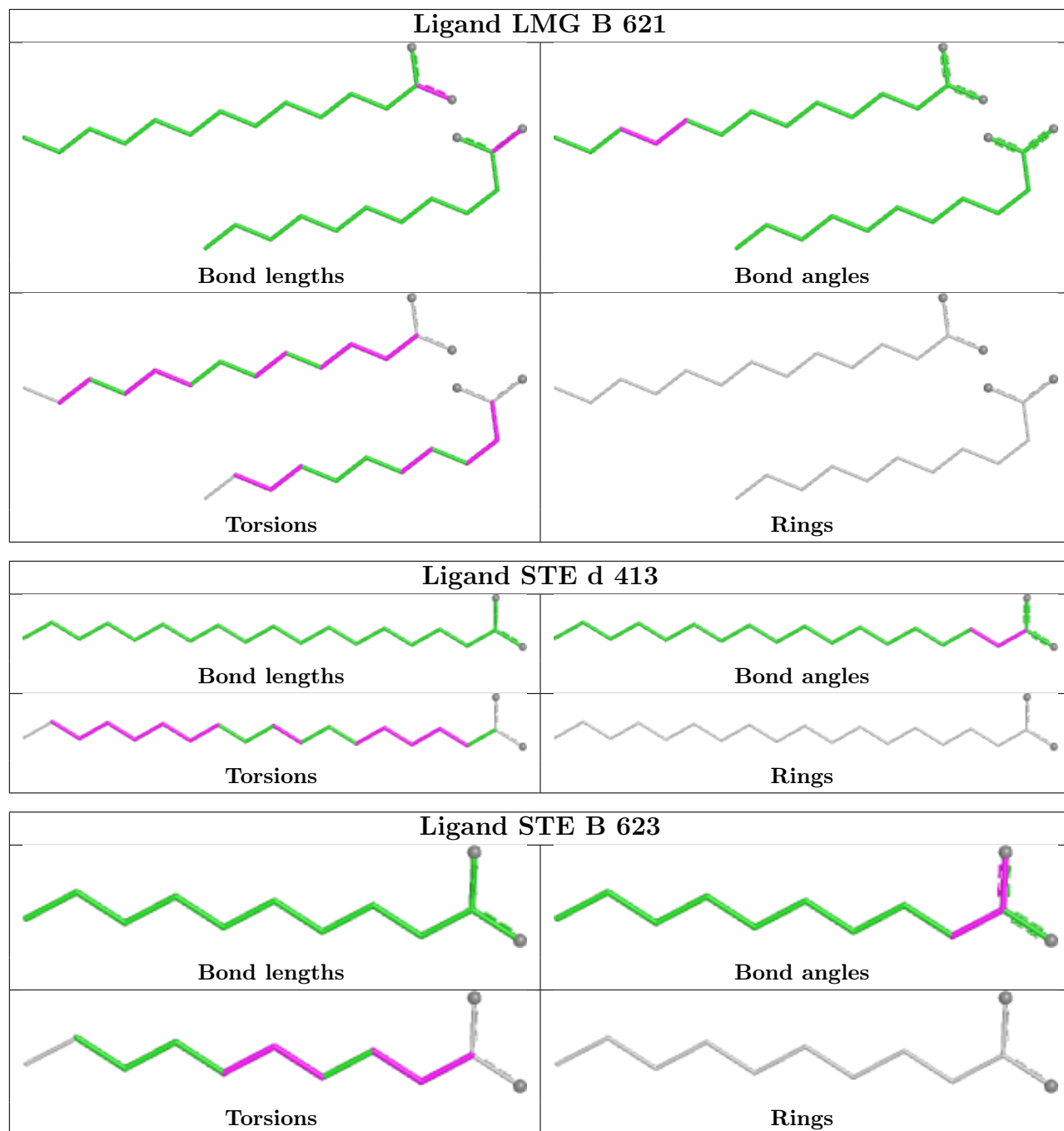


Ligand PHO d 402

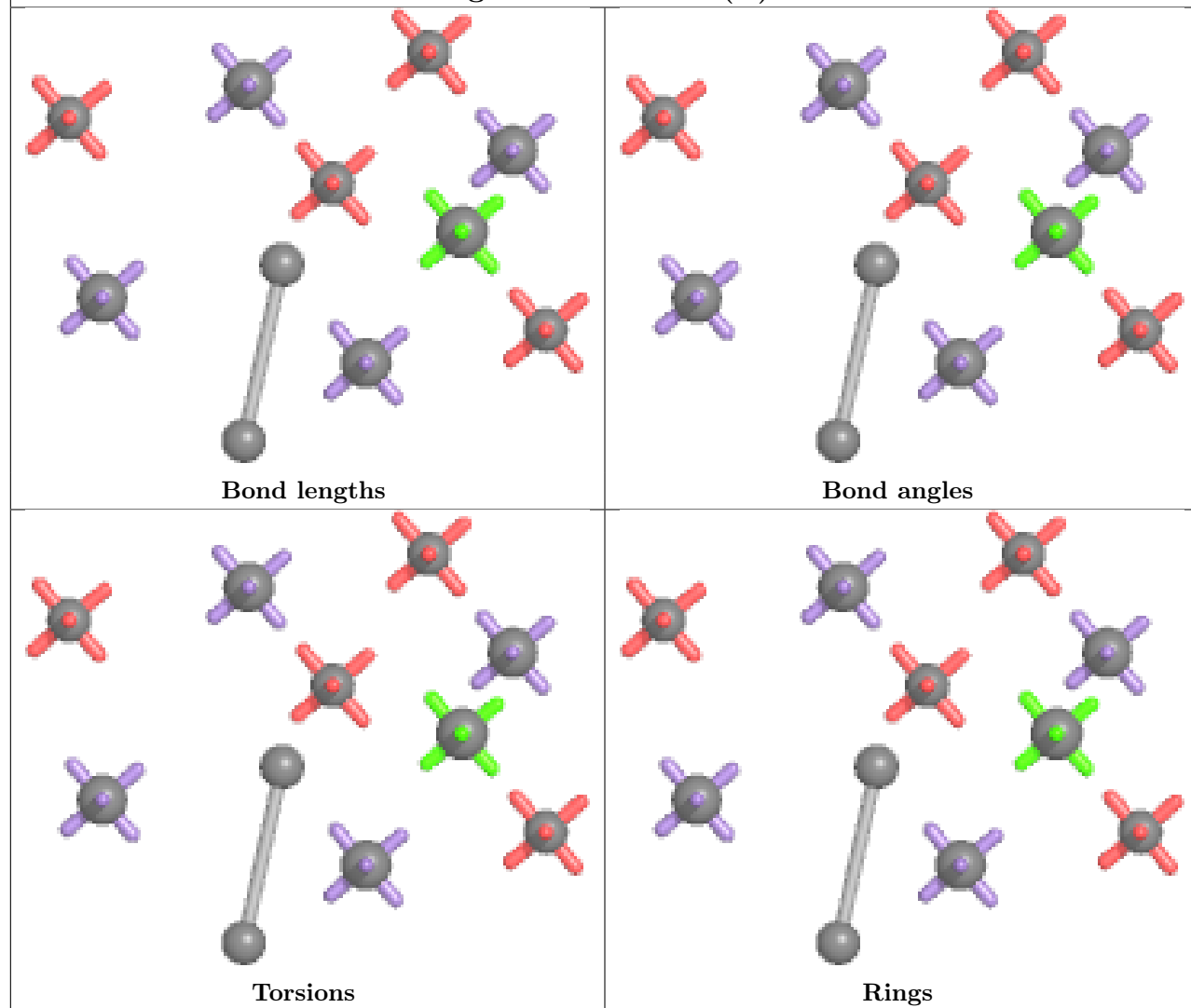


Ligand BCR D 406

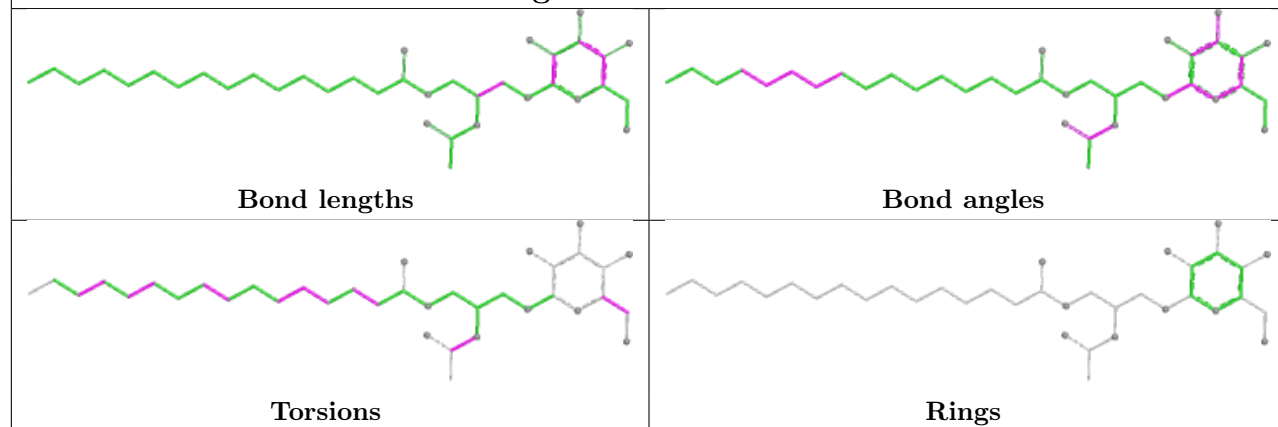


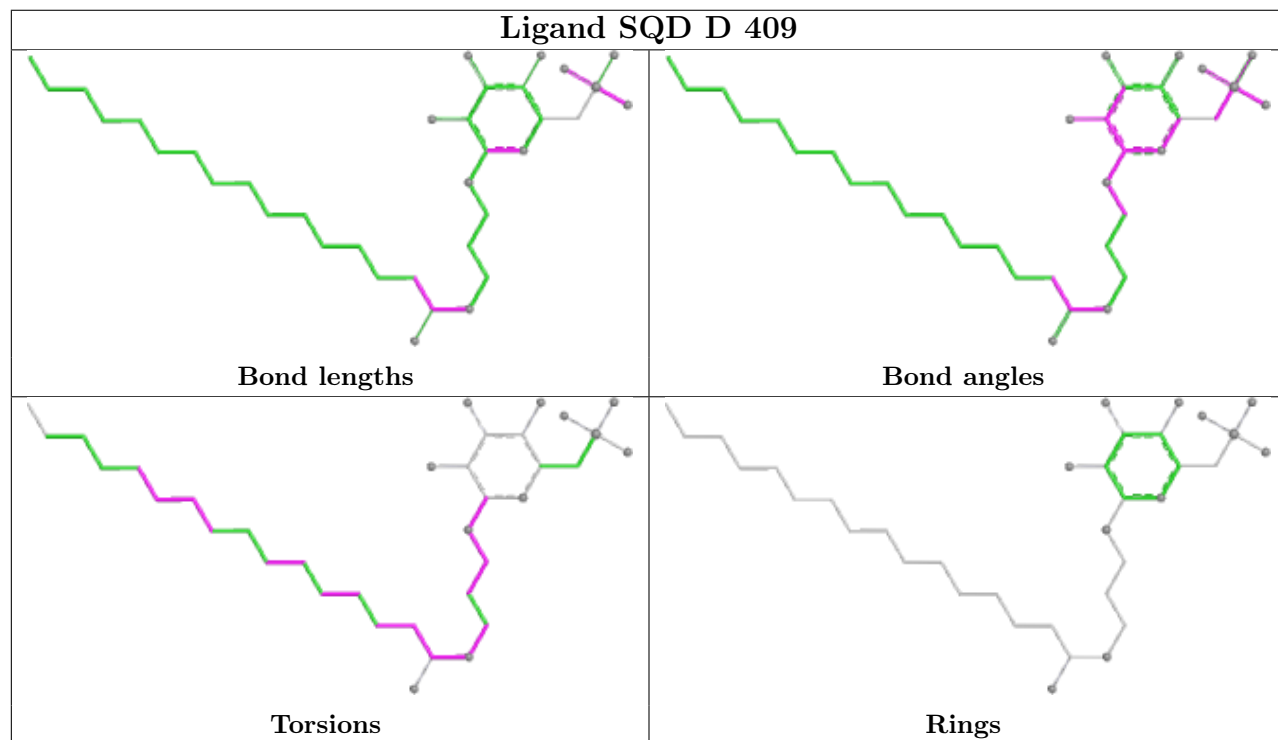
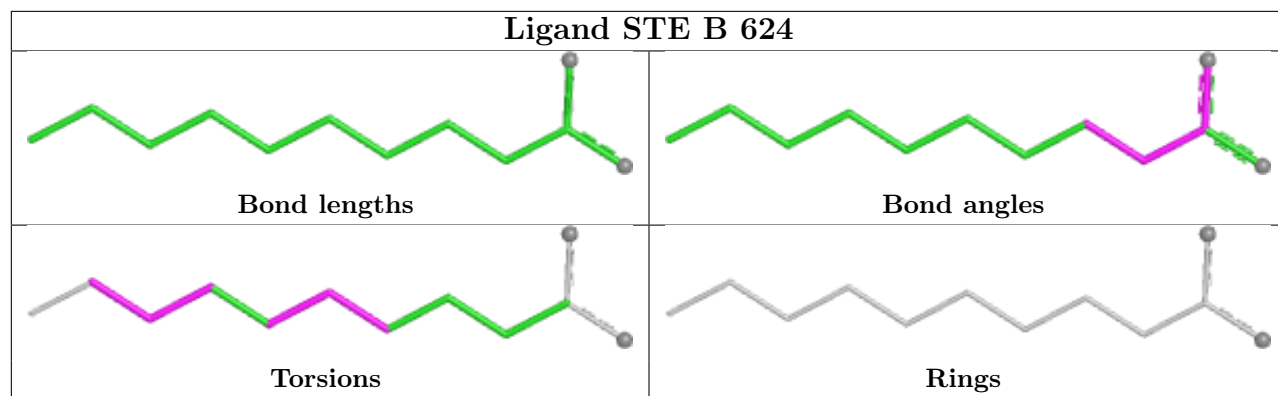


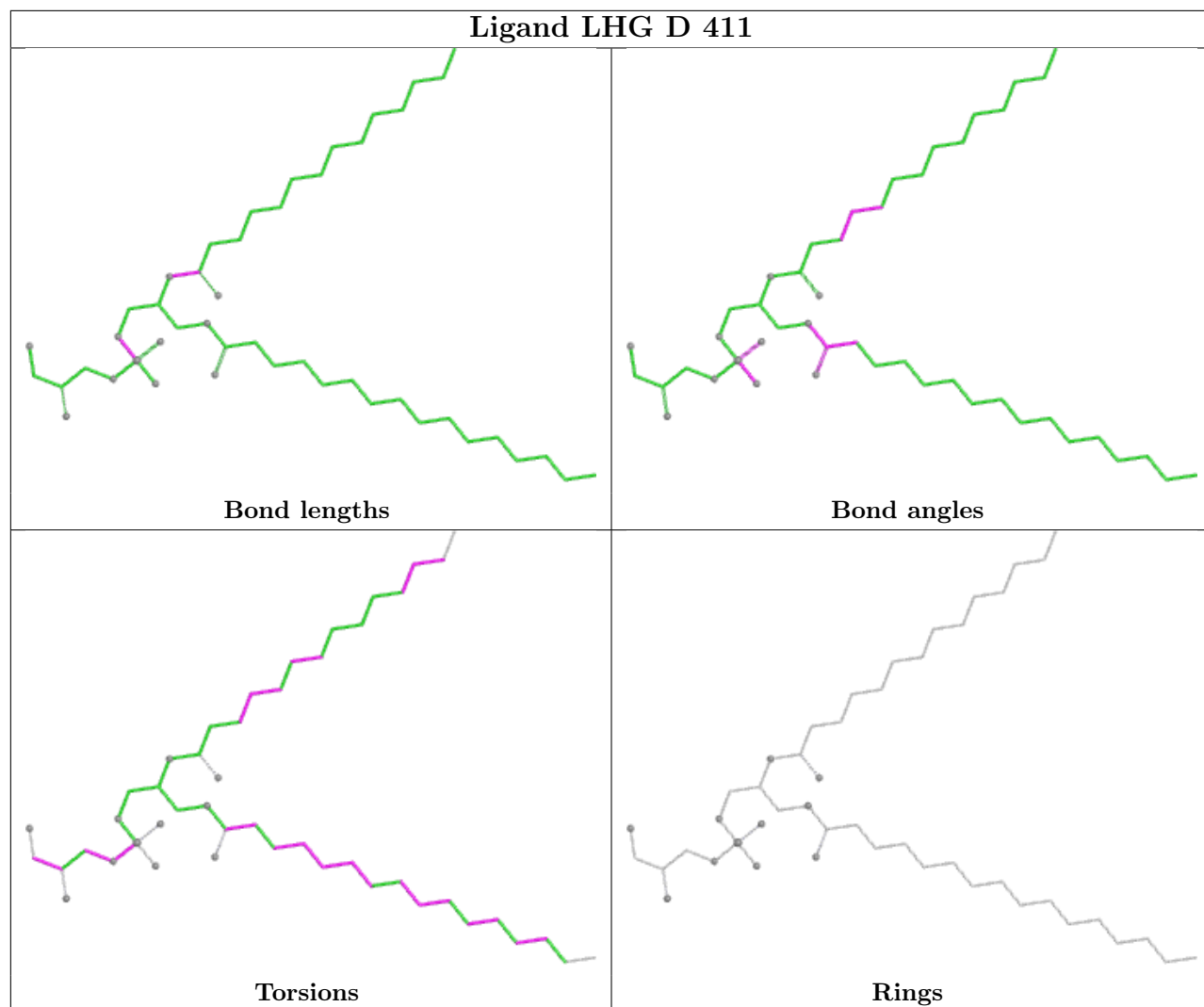
Ligand OEY a 601 (B)

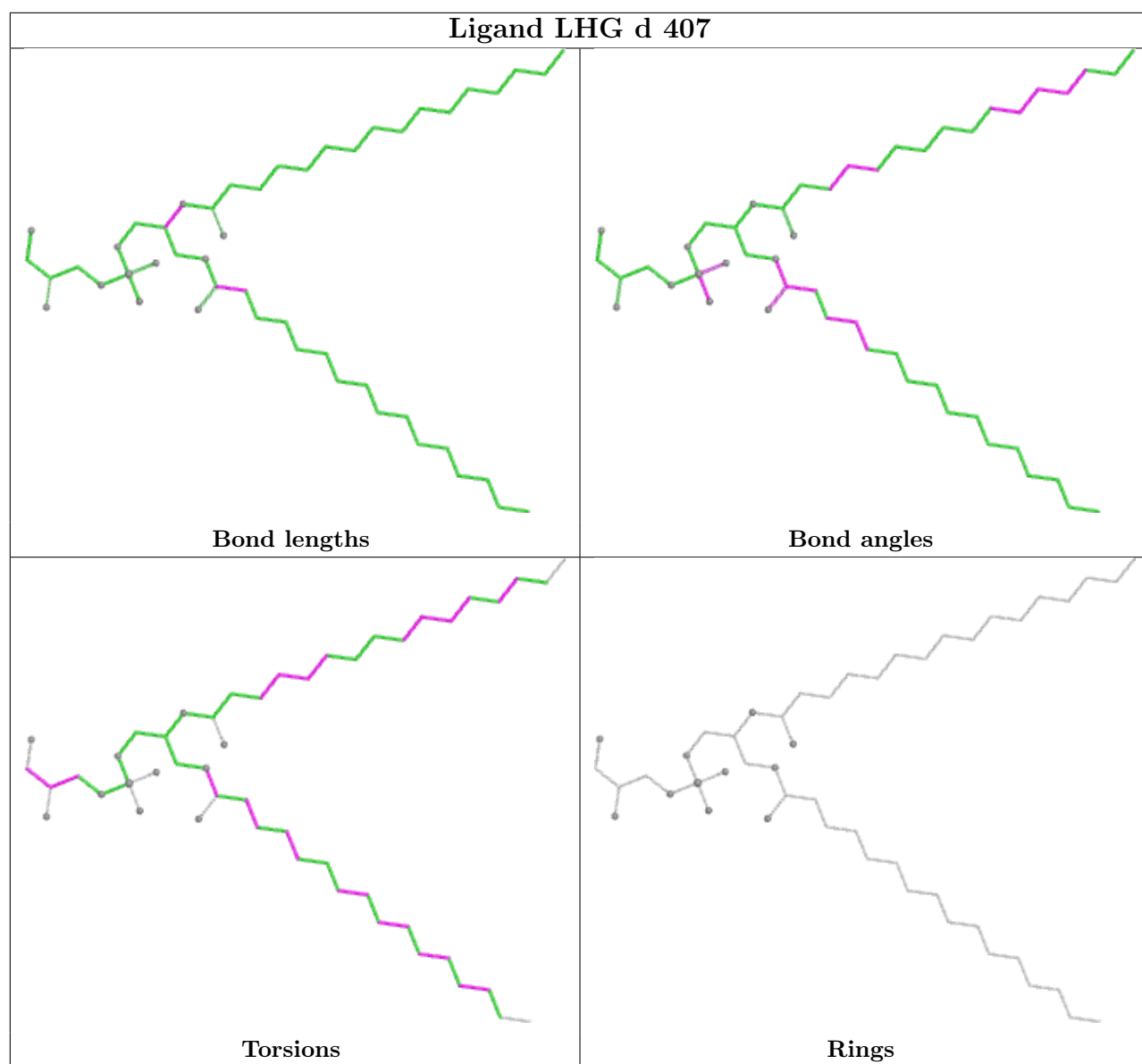


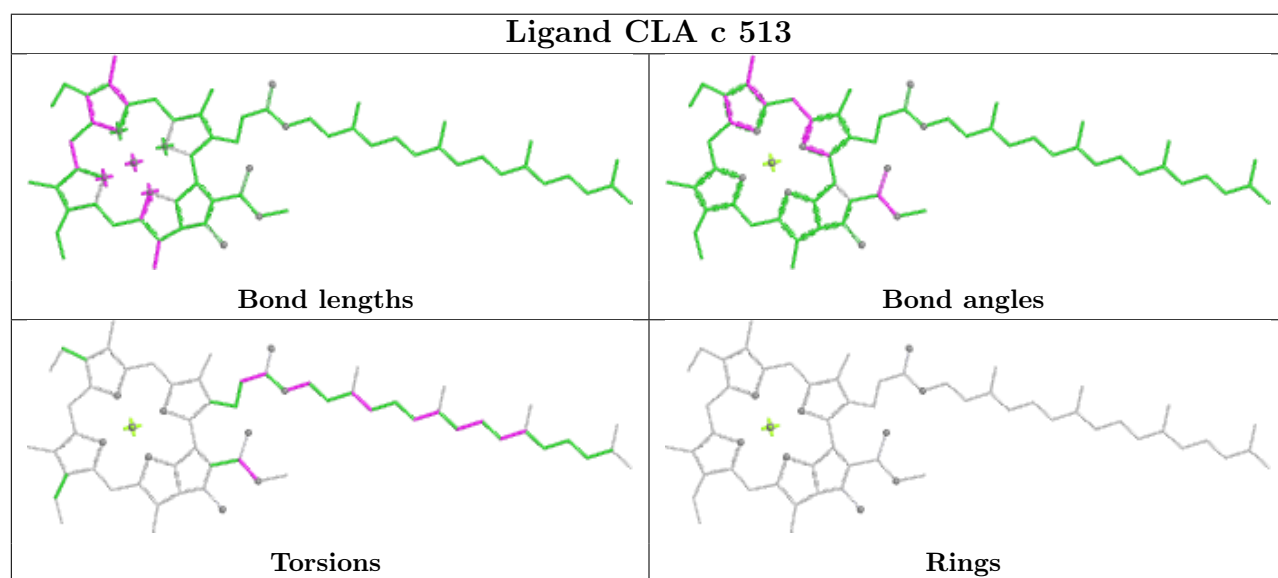
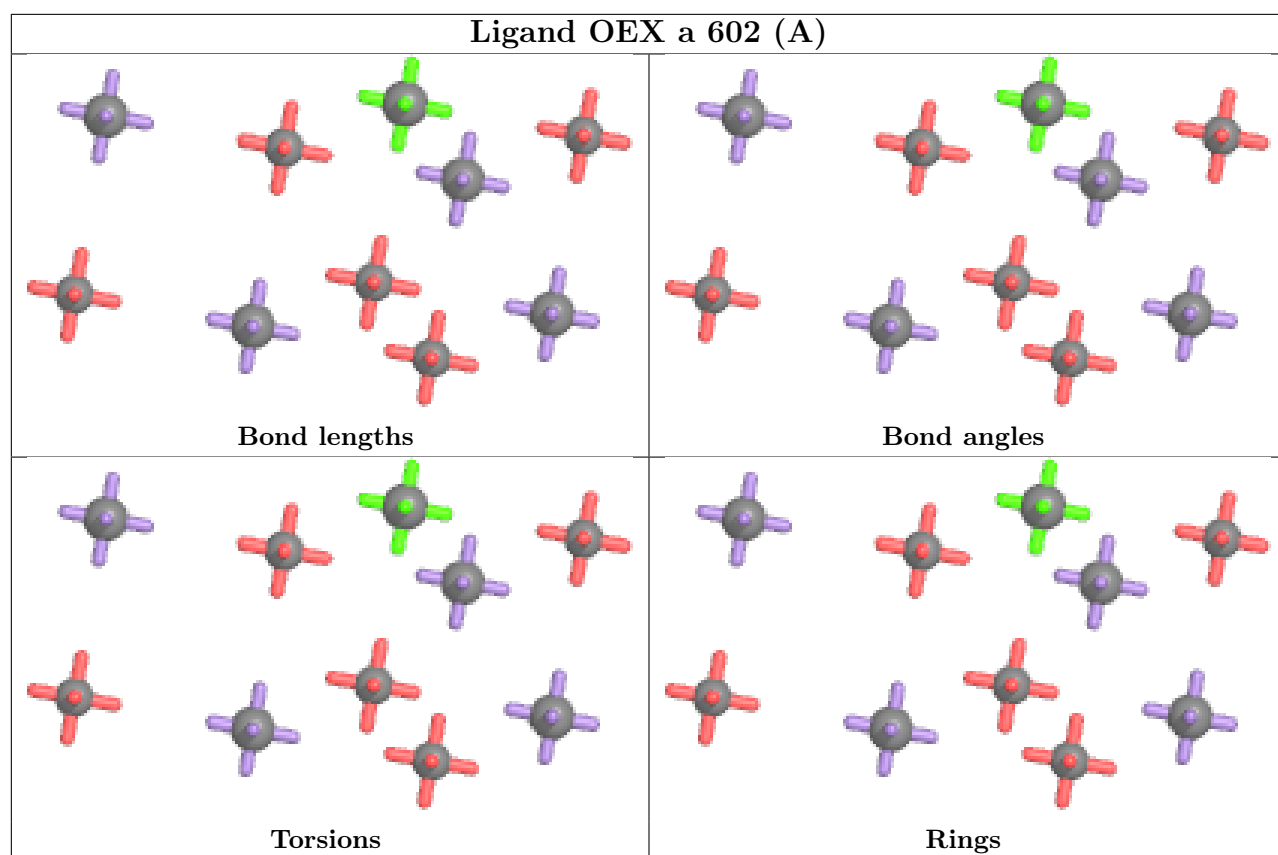
Ligand LMG c 519

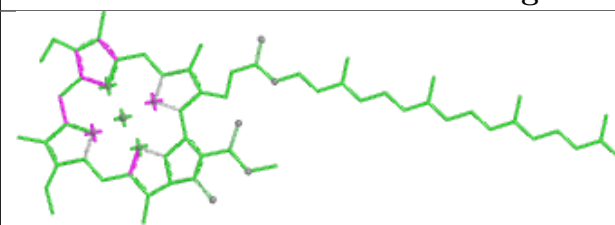
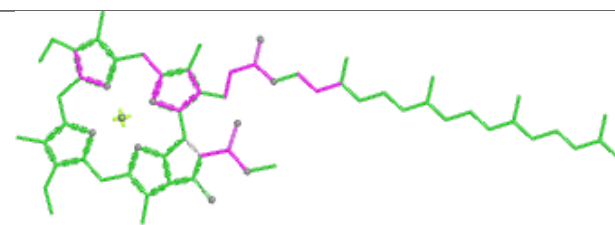
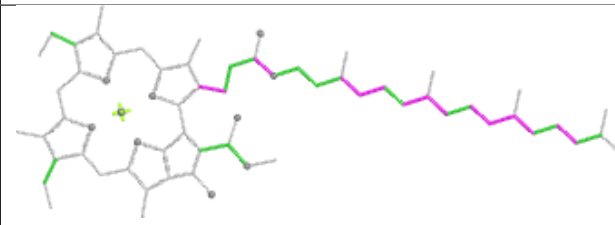
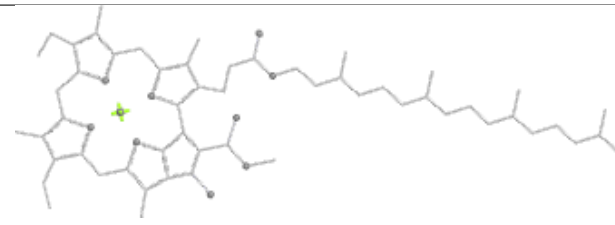


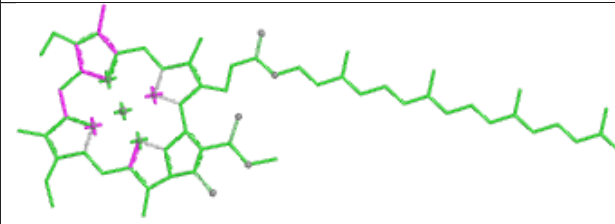
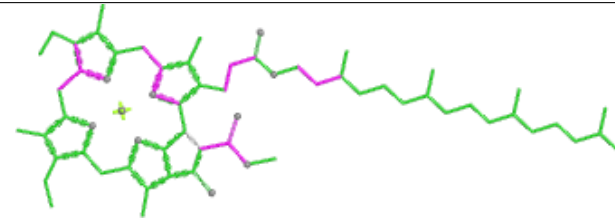
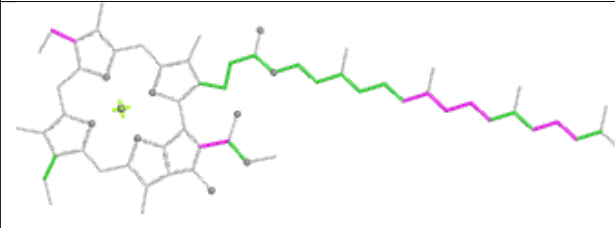
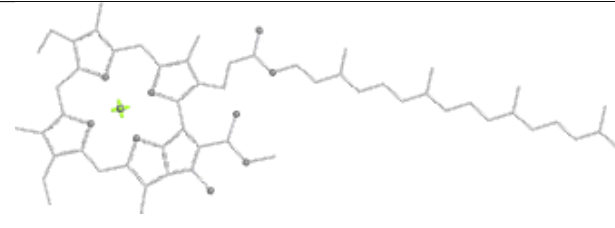


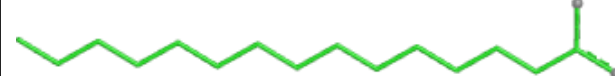
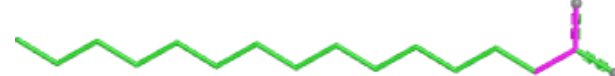
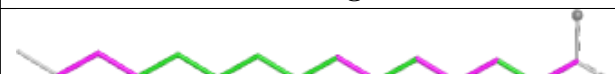




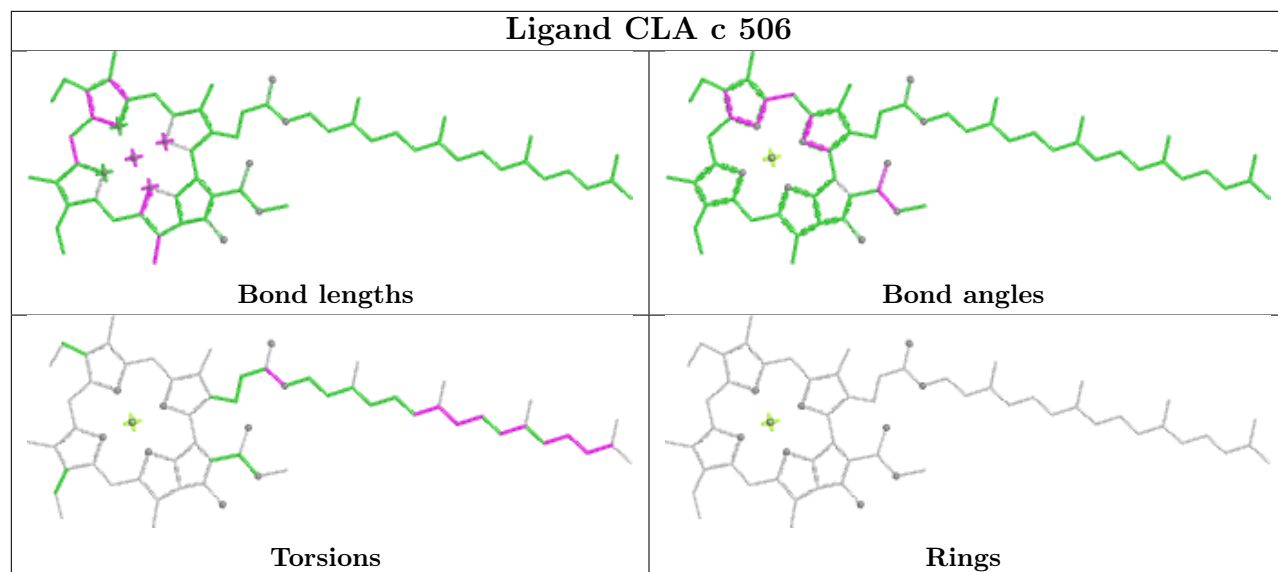


Ligand CLA B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

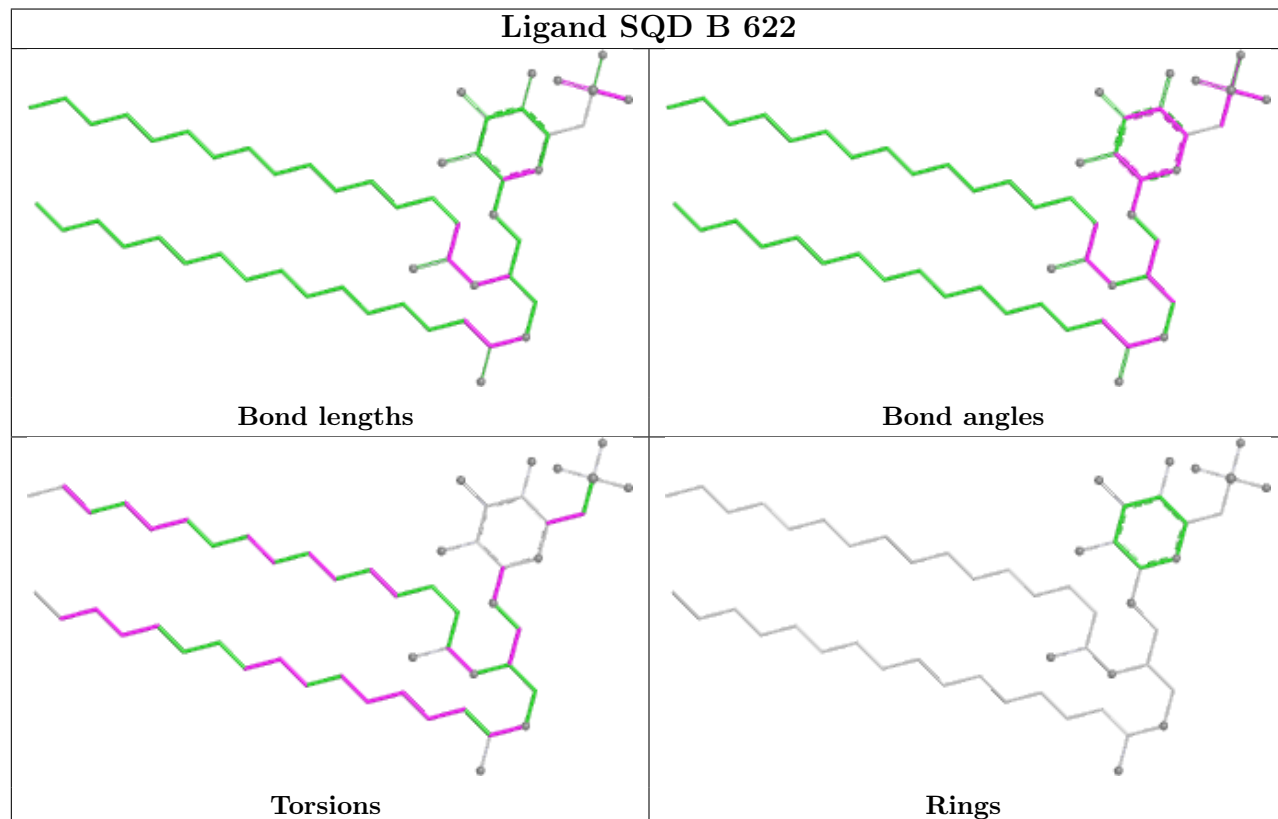
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

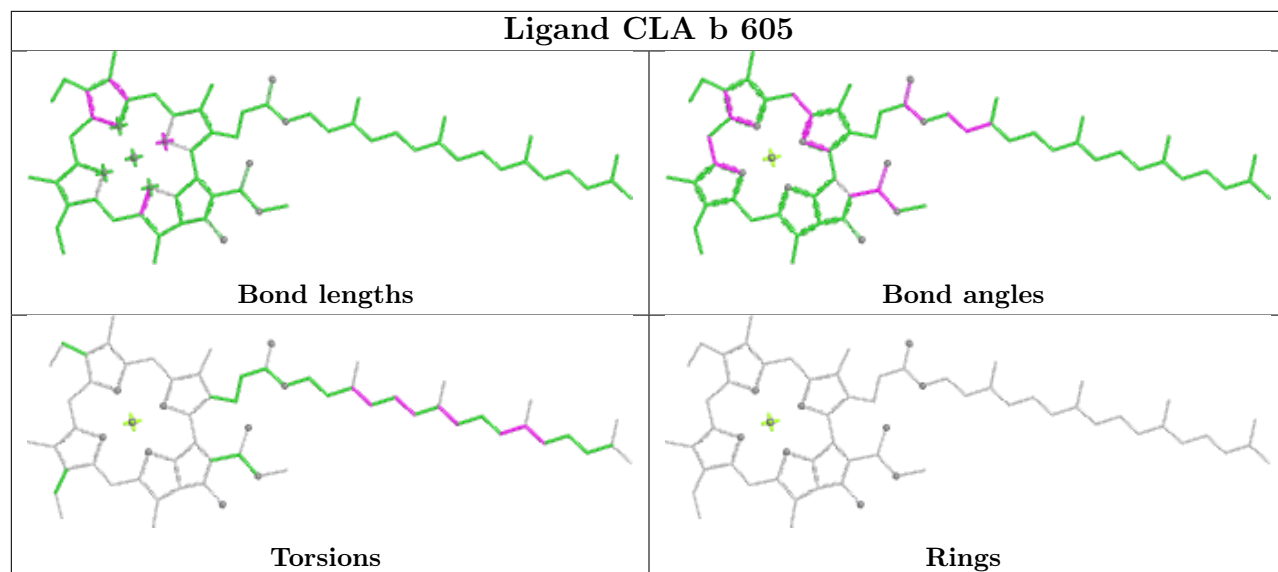
Ligand CLA c 506



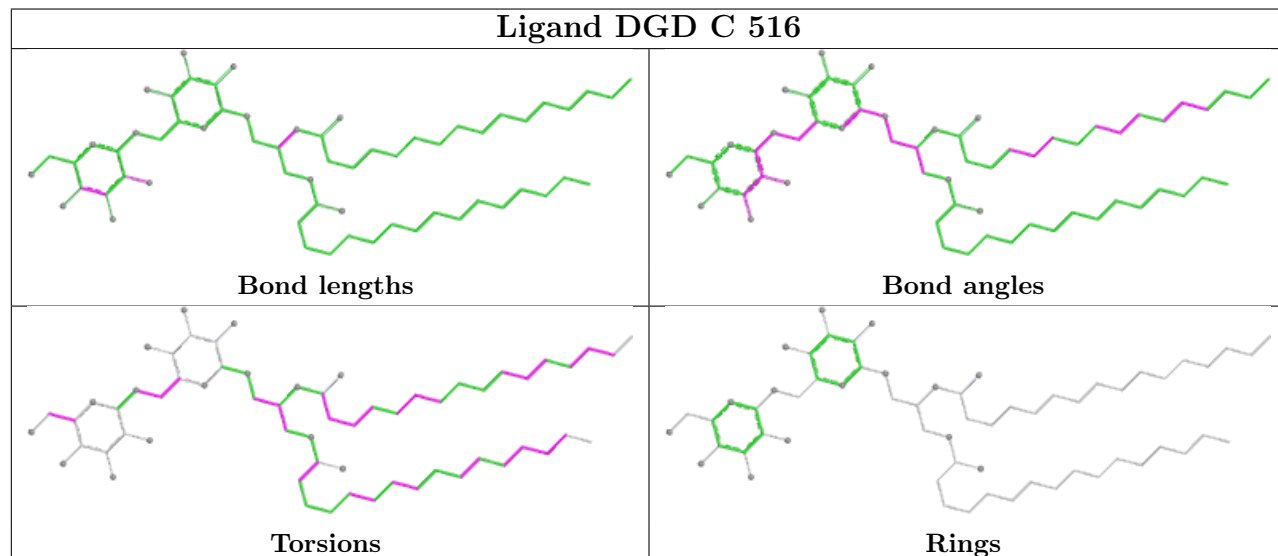
Ligand SQD B 622



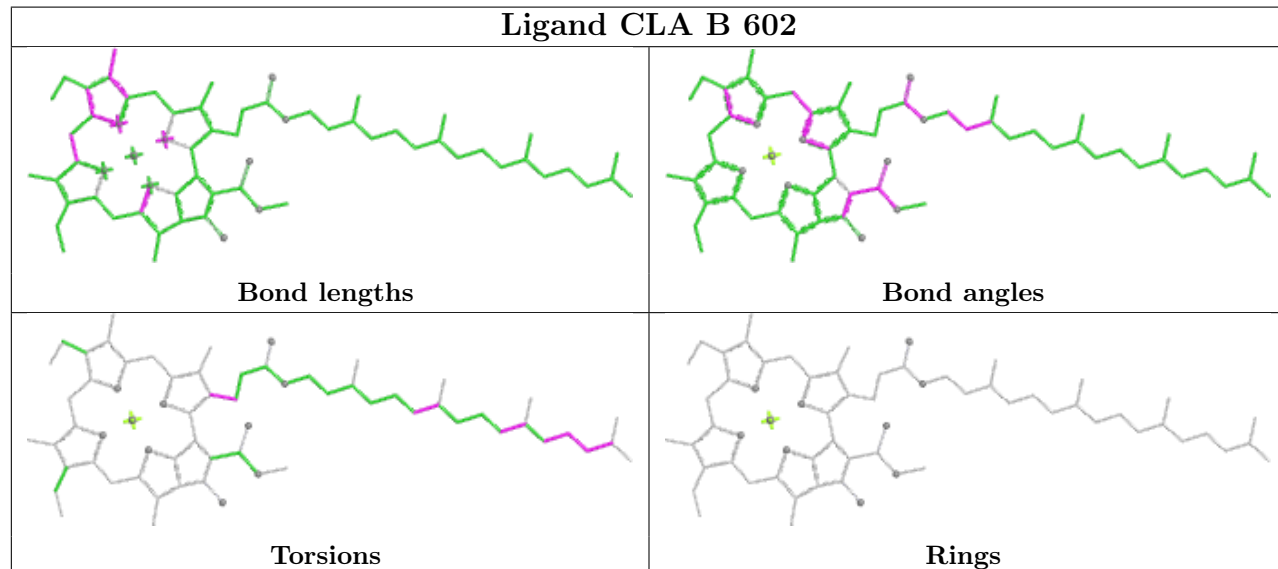
Ligand CLA b 605

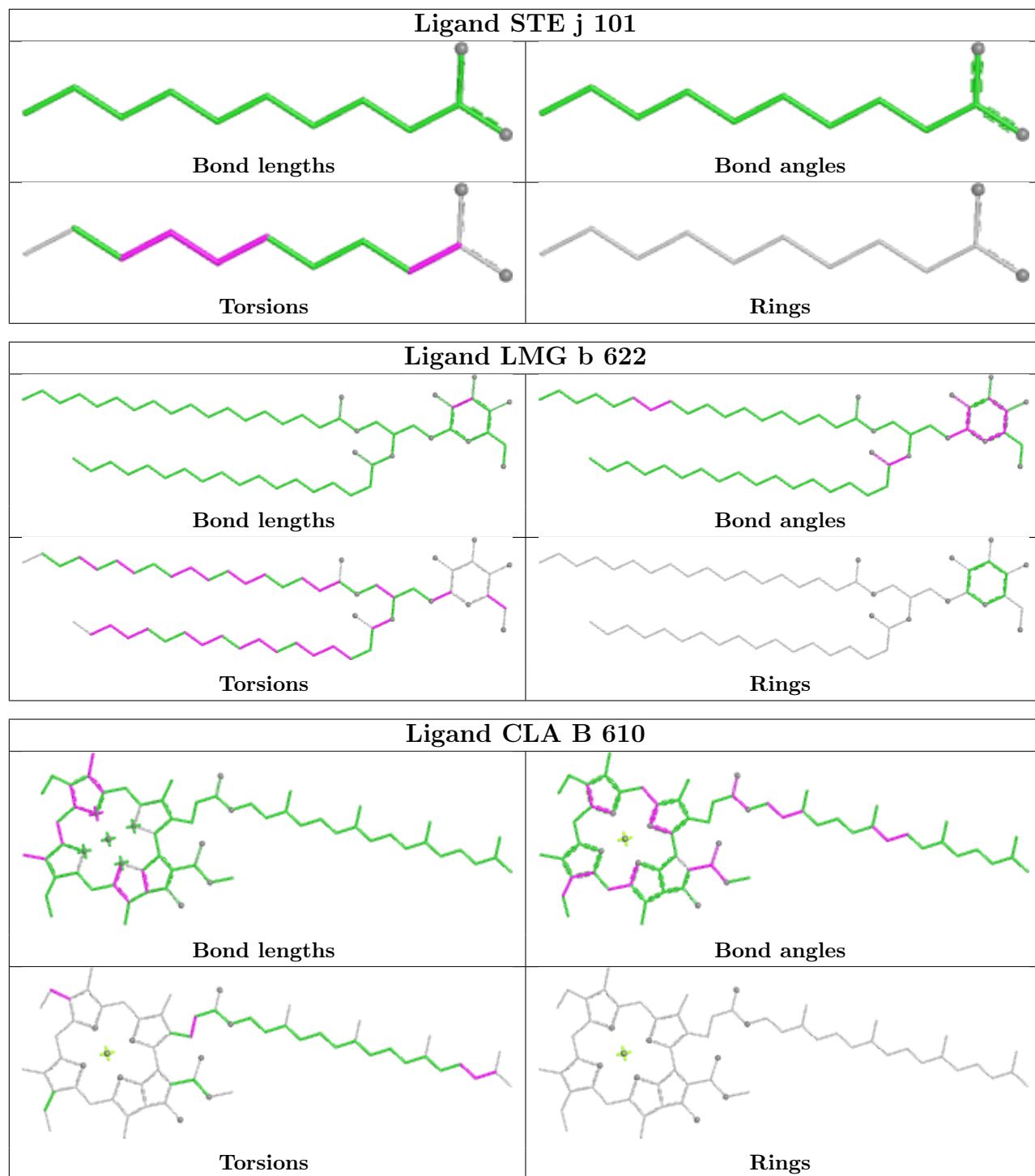


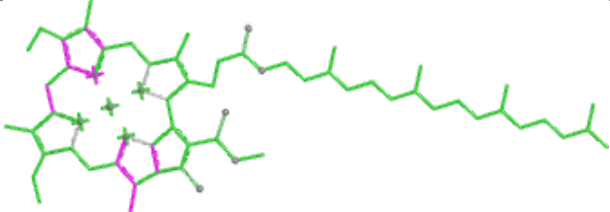
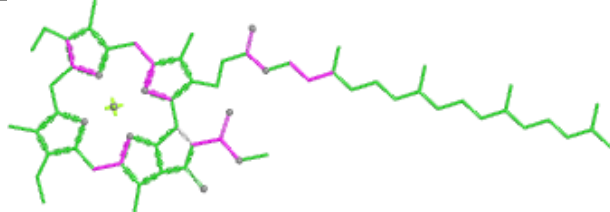
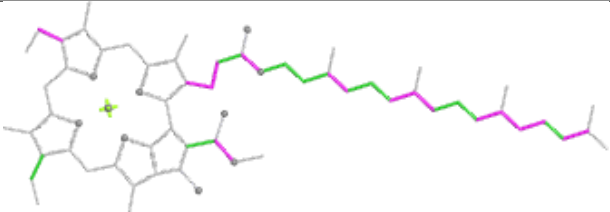
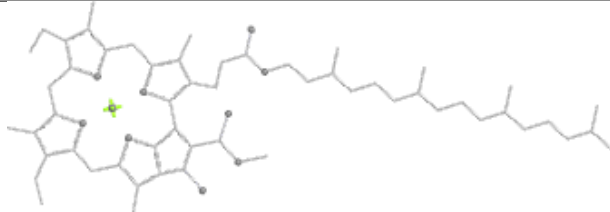
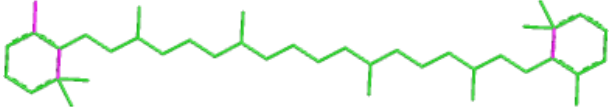
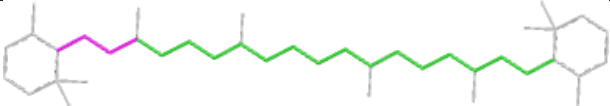
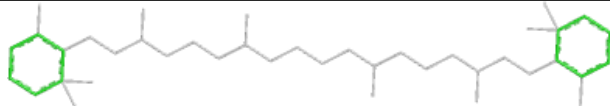
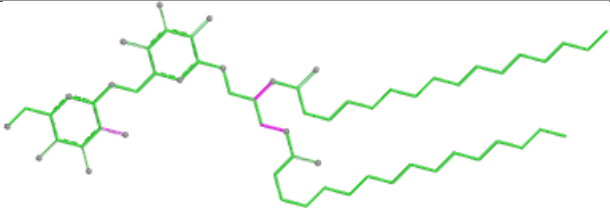
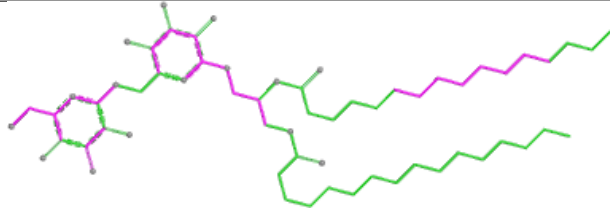
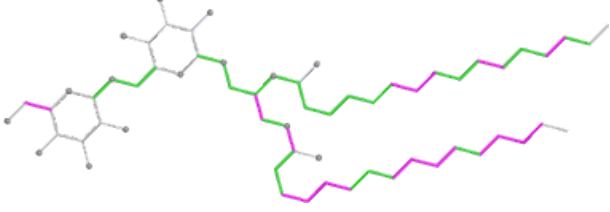
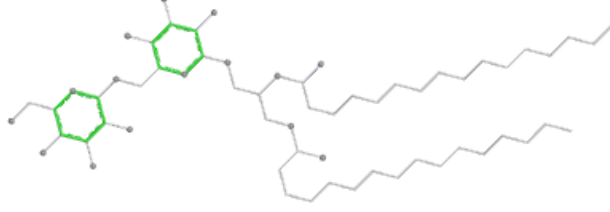
Ligand DGD C 516



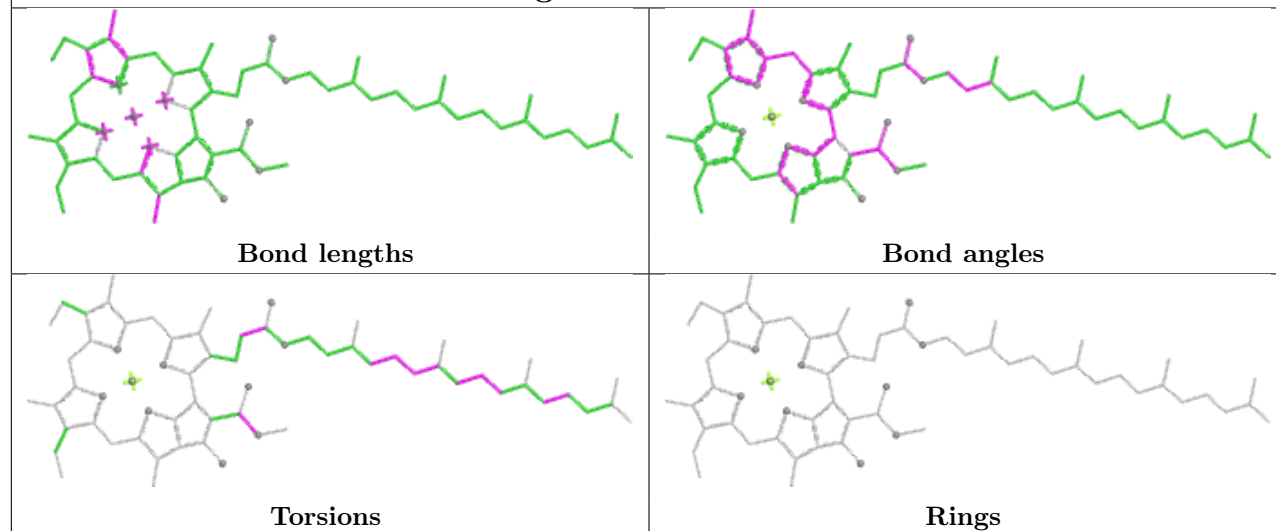
Ligand CLA B 602



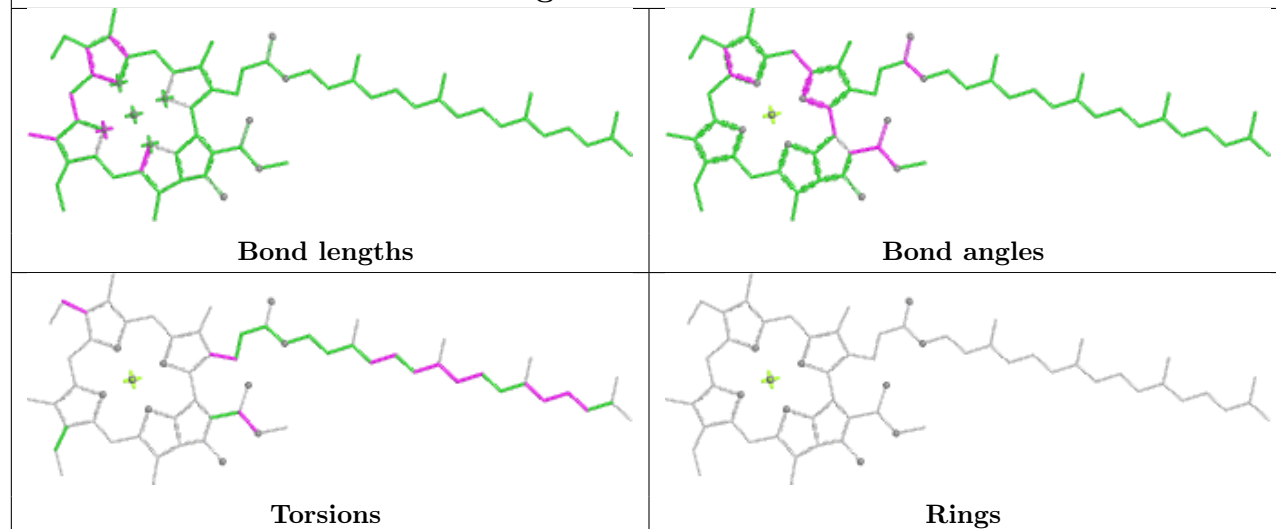


Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

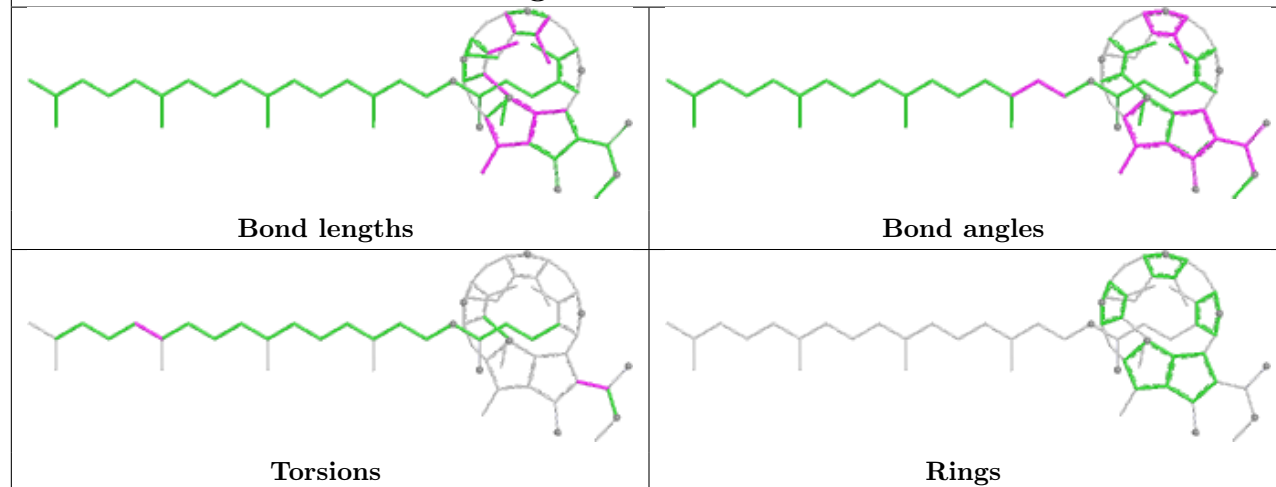
Ligand CLA b 613



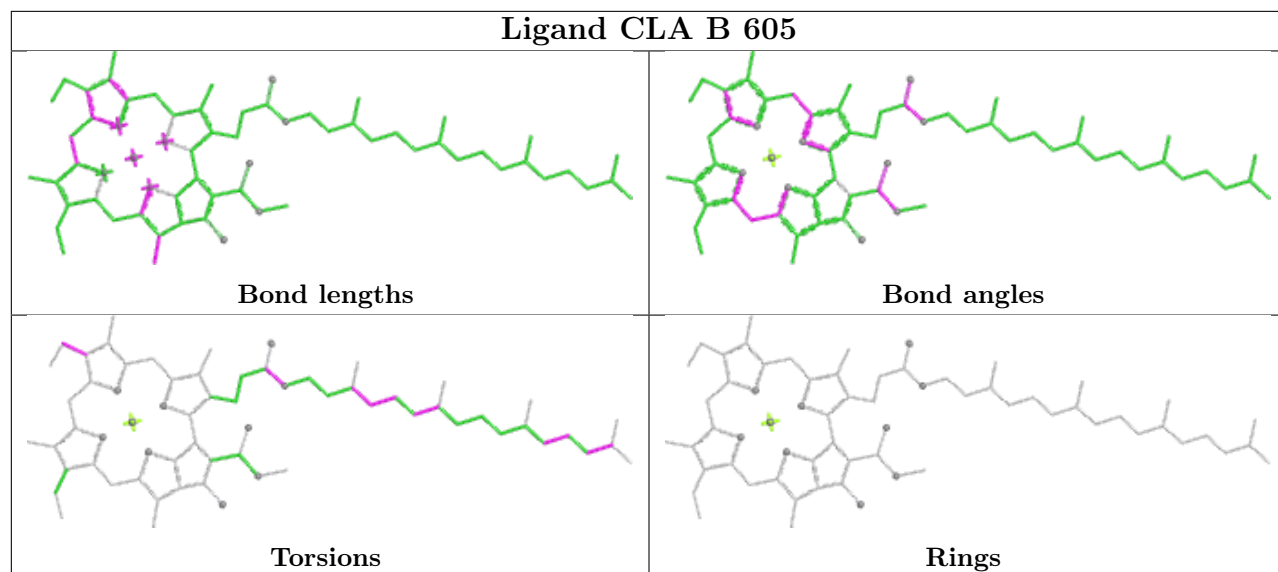
Ligand CLA a 607



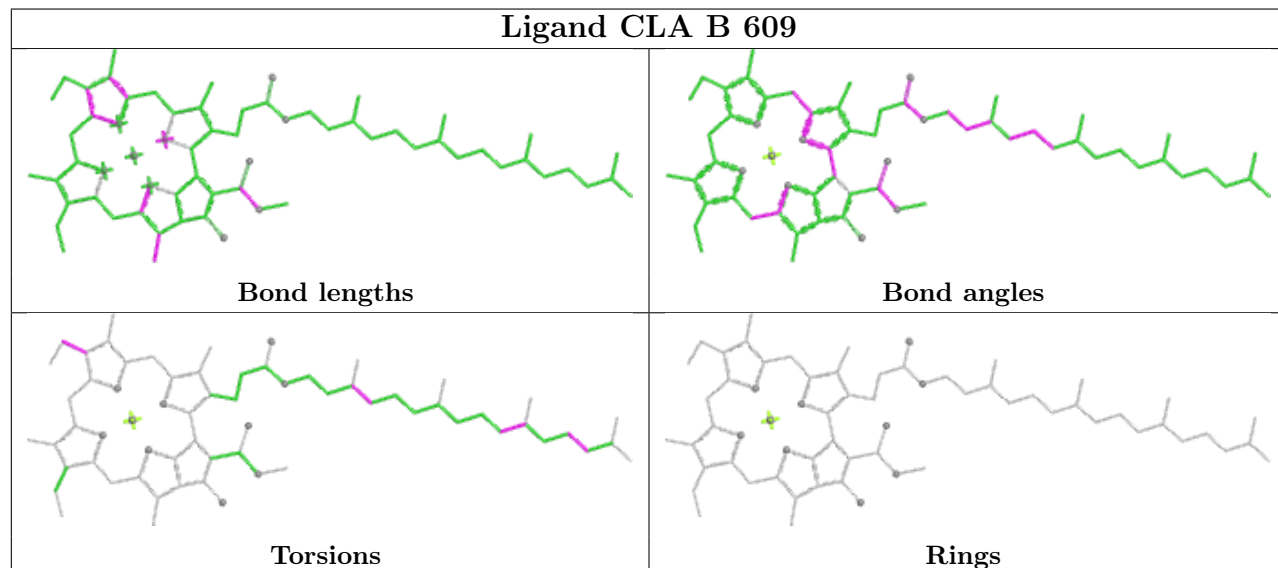
Ligand PHO D 402



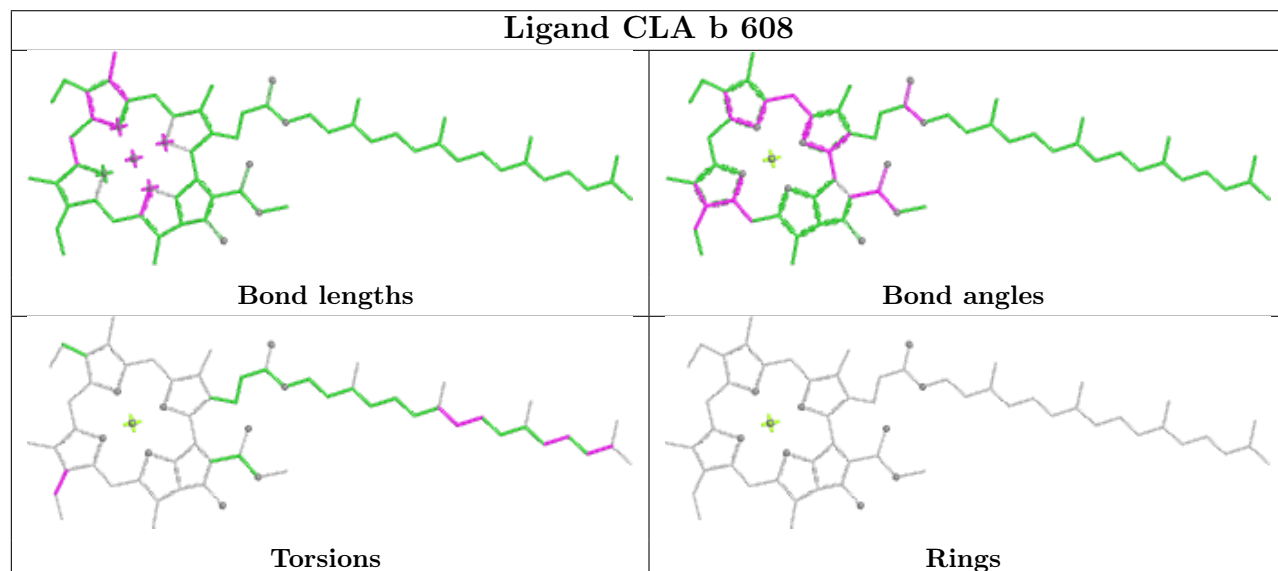
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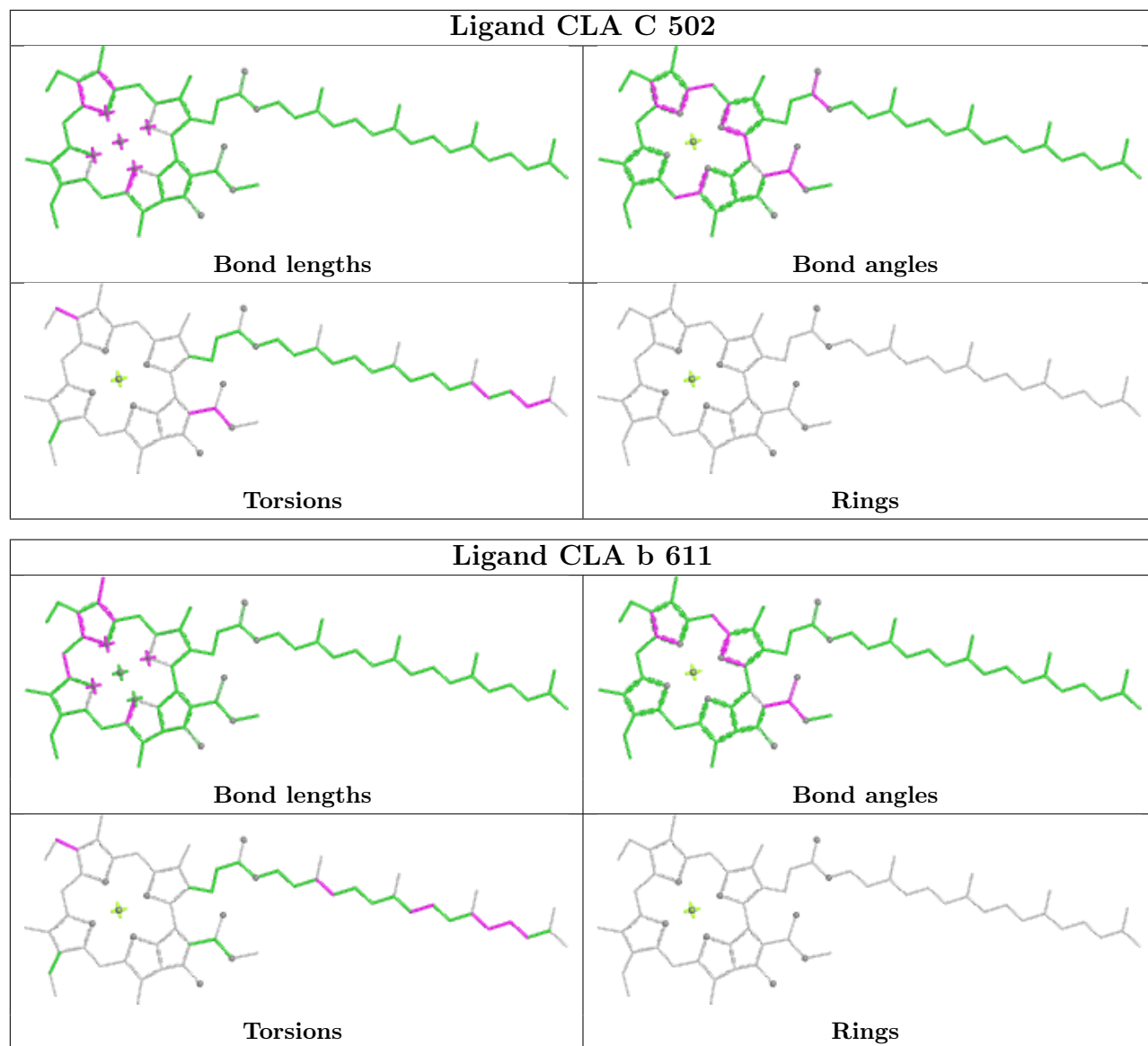


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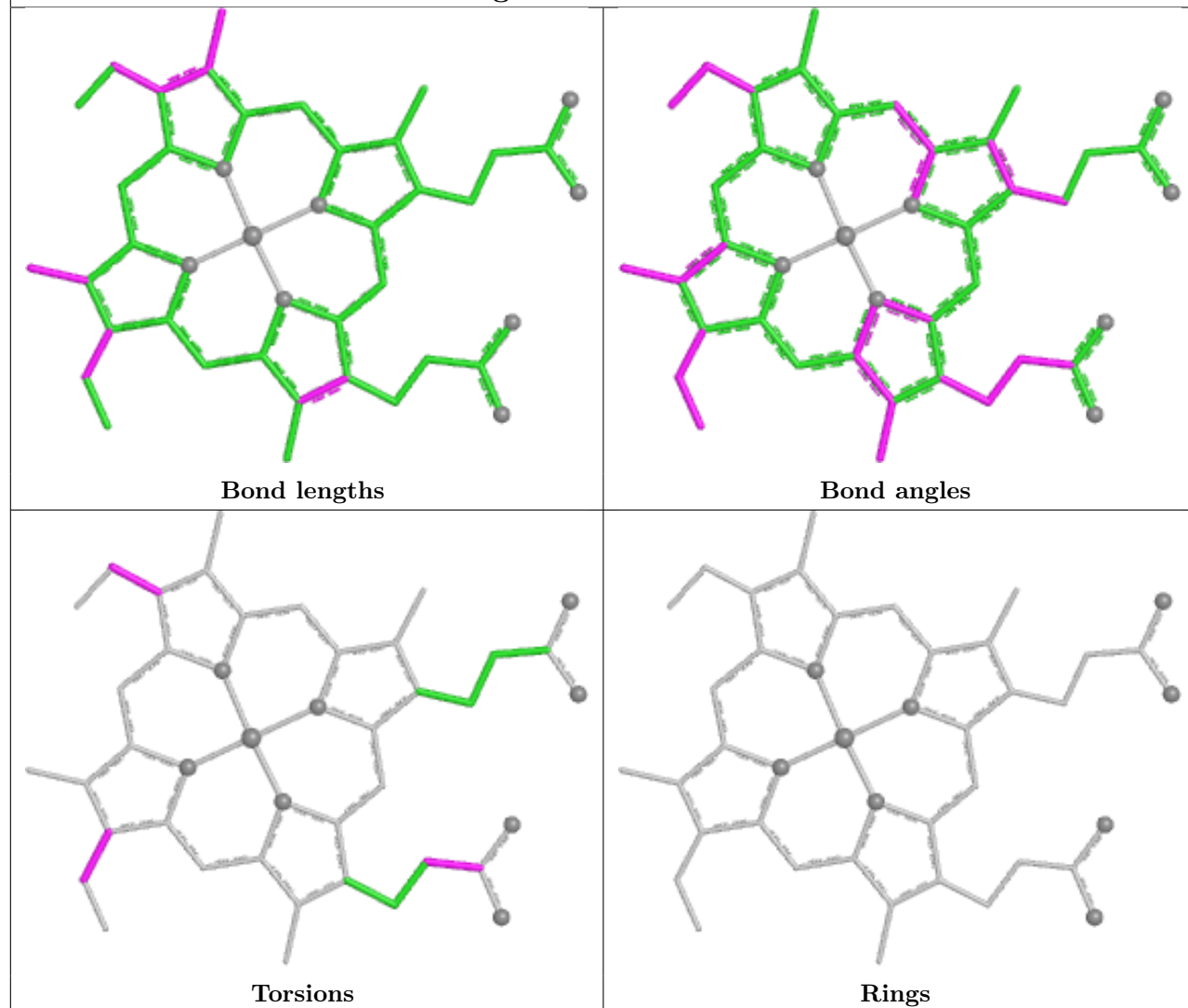


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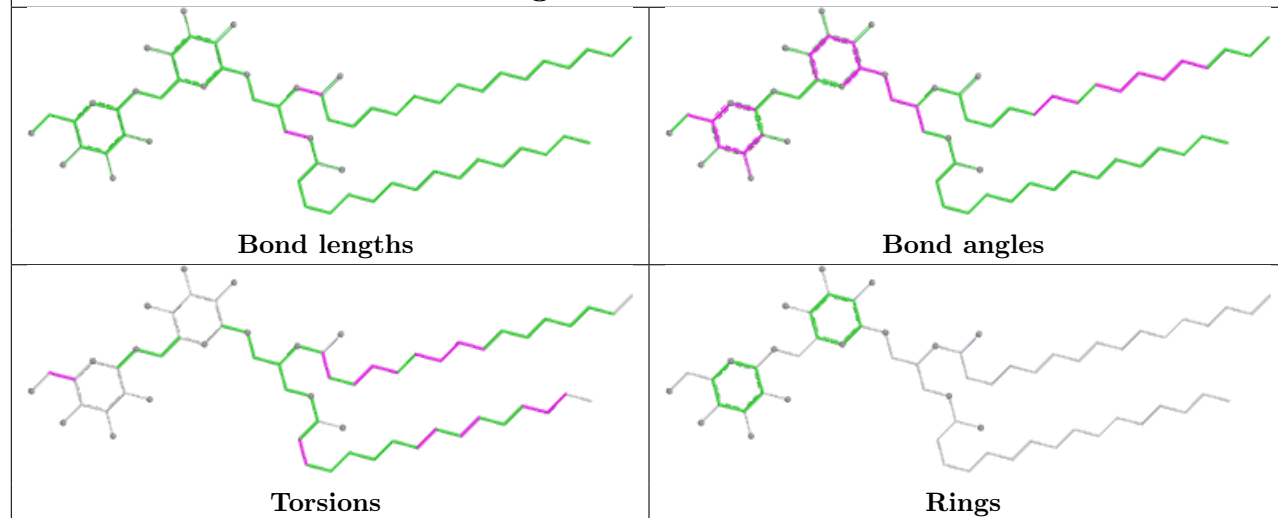


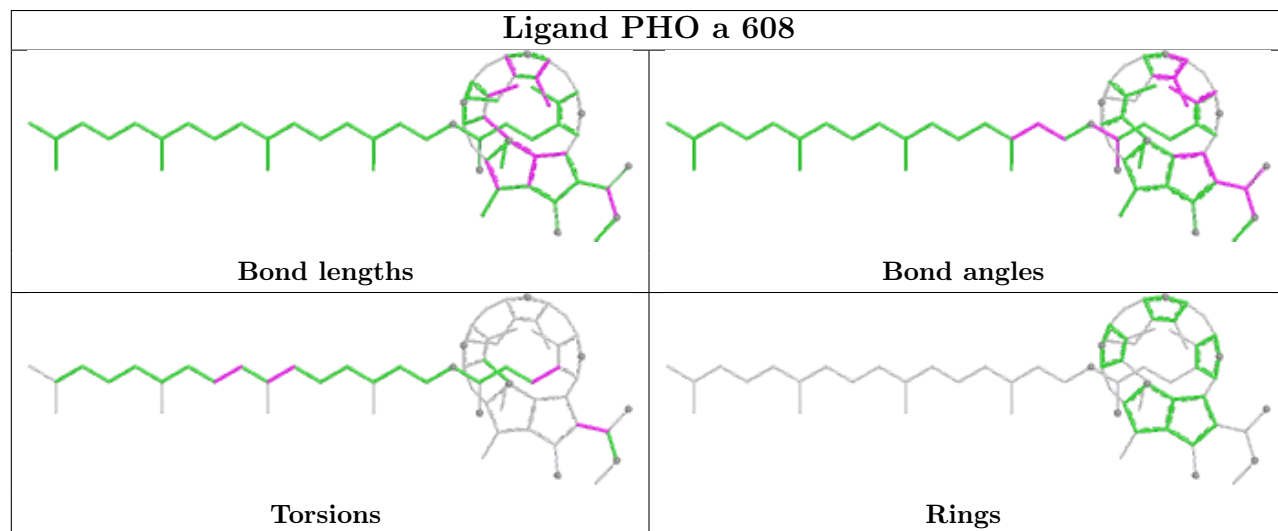
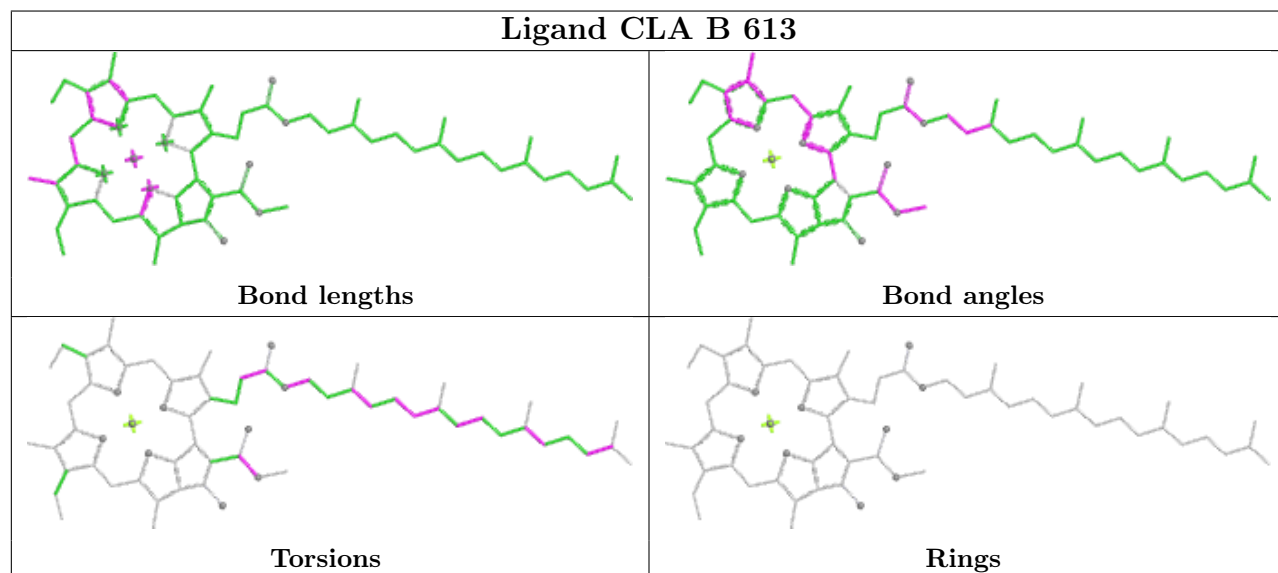
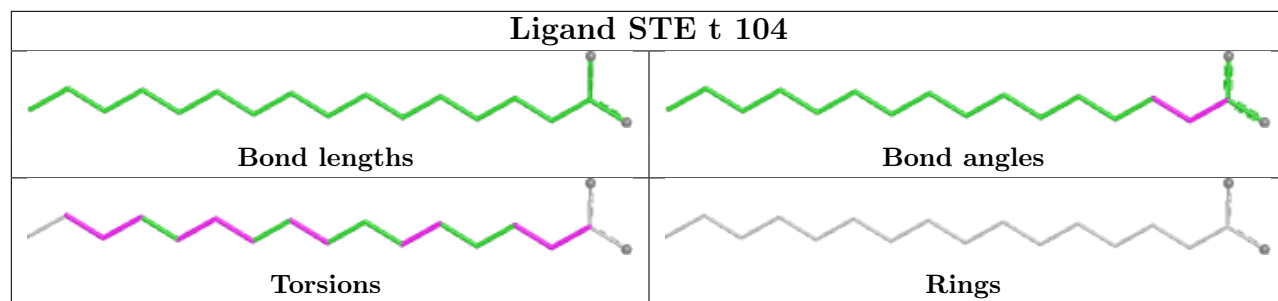


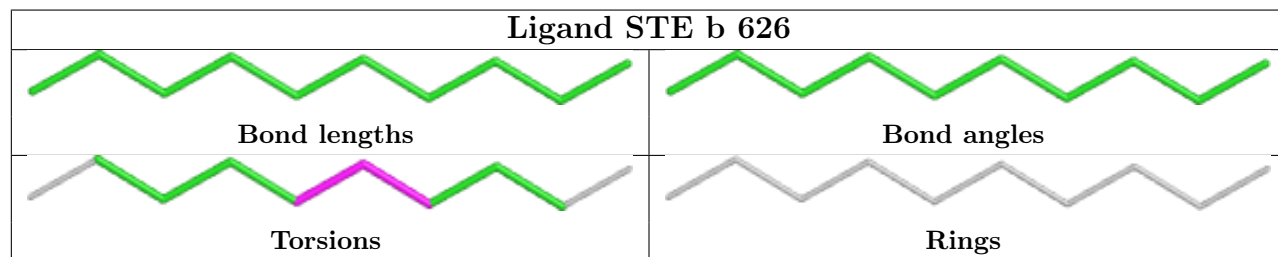
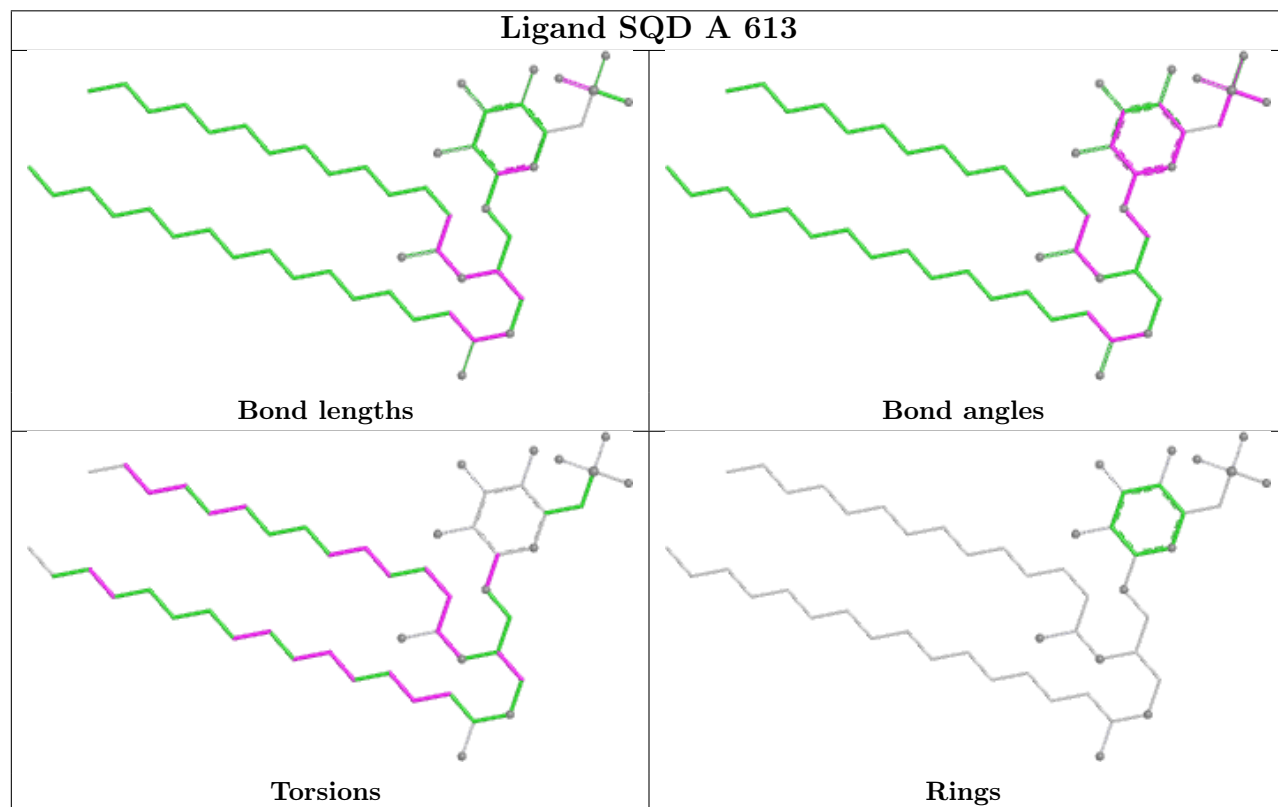
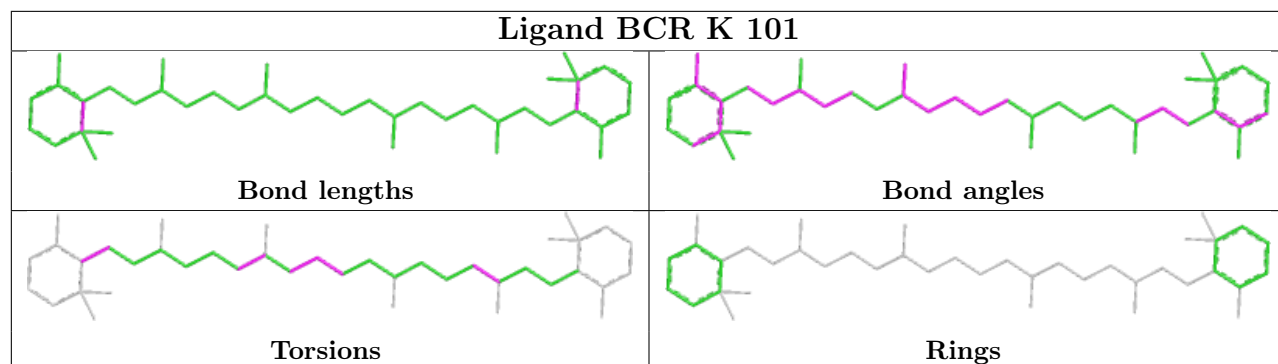
Ligand HEC V 201

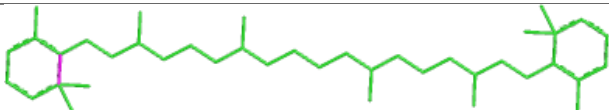
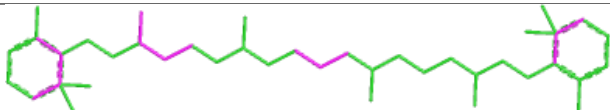
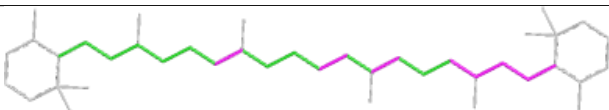
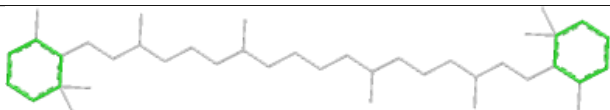


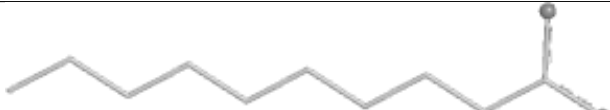
Ligand DGD h 102

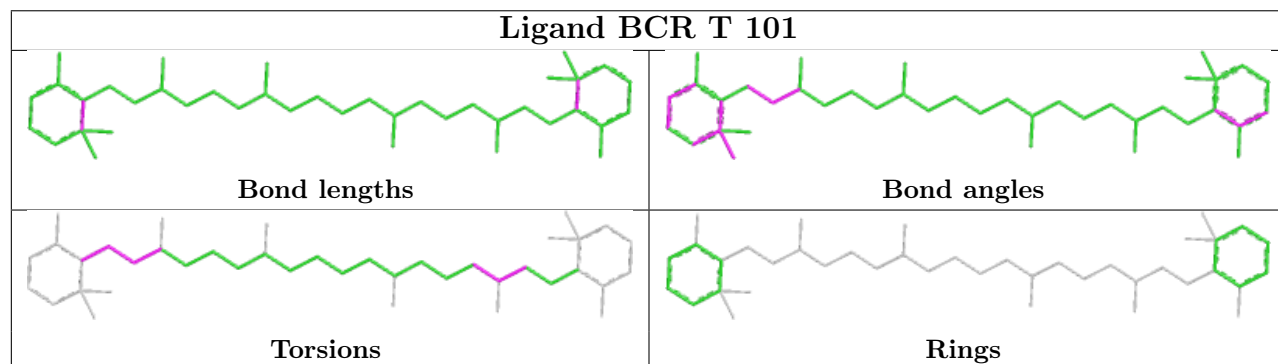
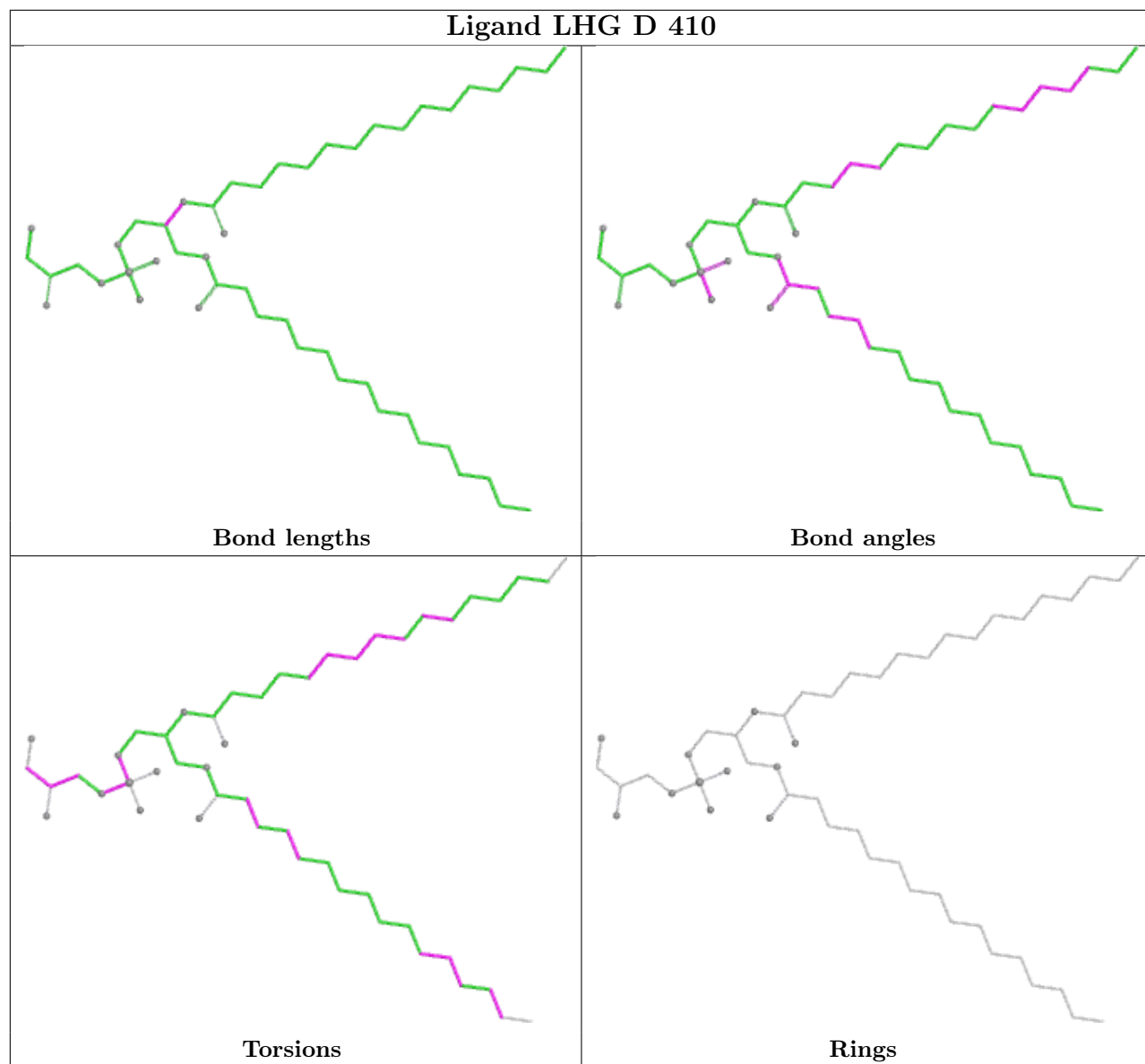




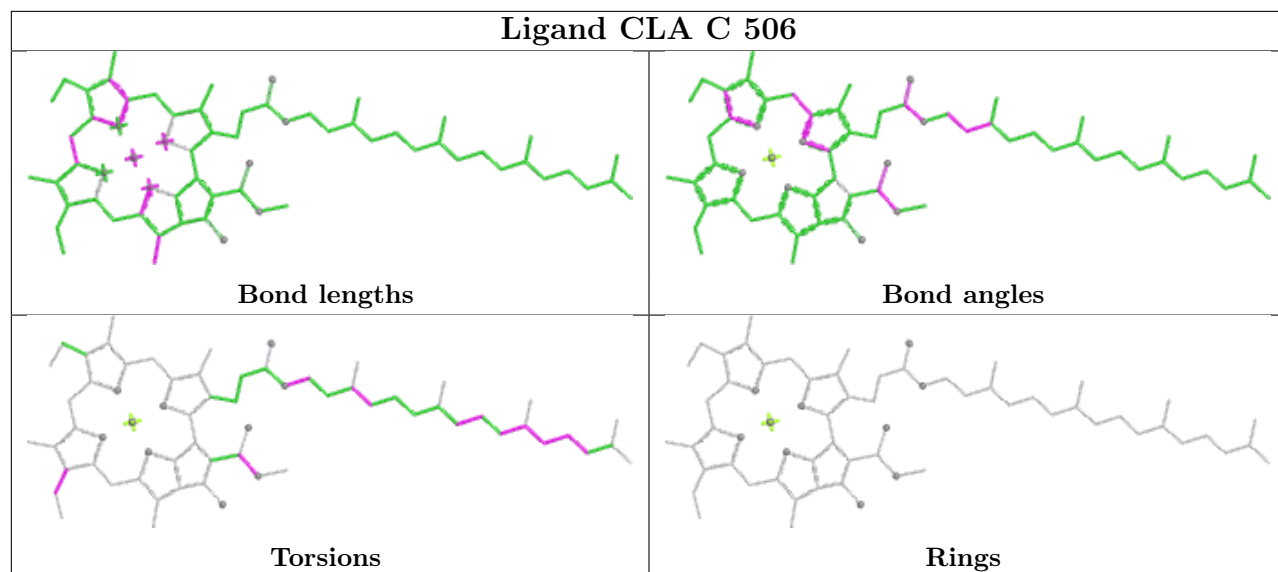


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

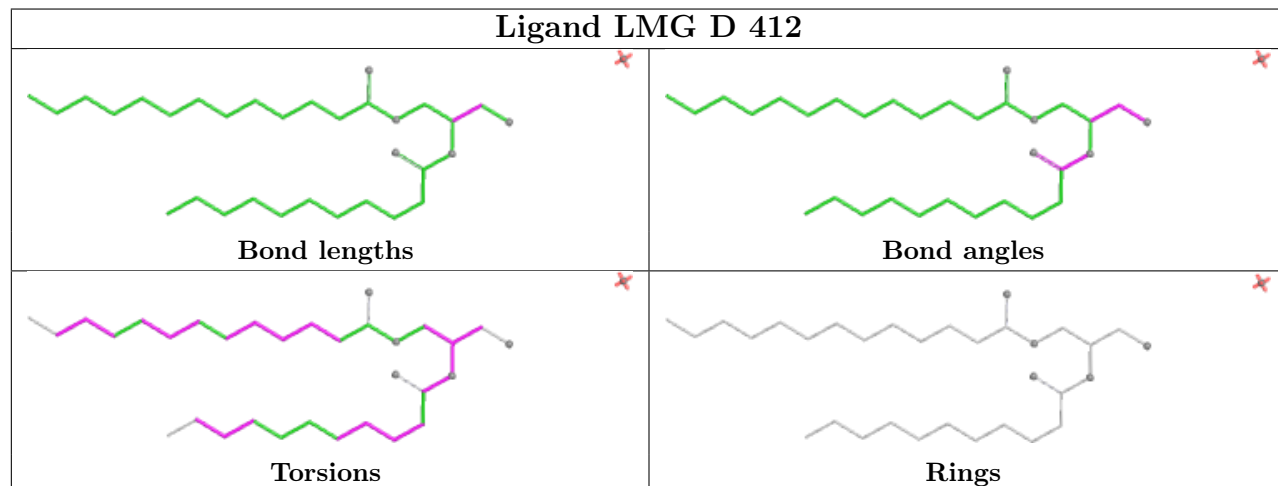
Ligand STE a 616	
	
Bond lengths	Bond angles
	
Torsions	Rings



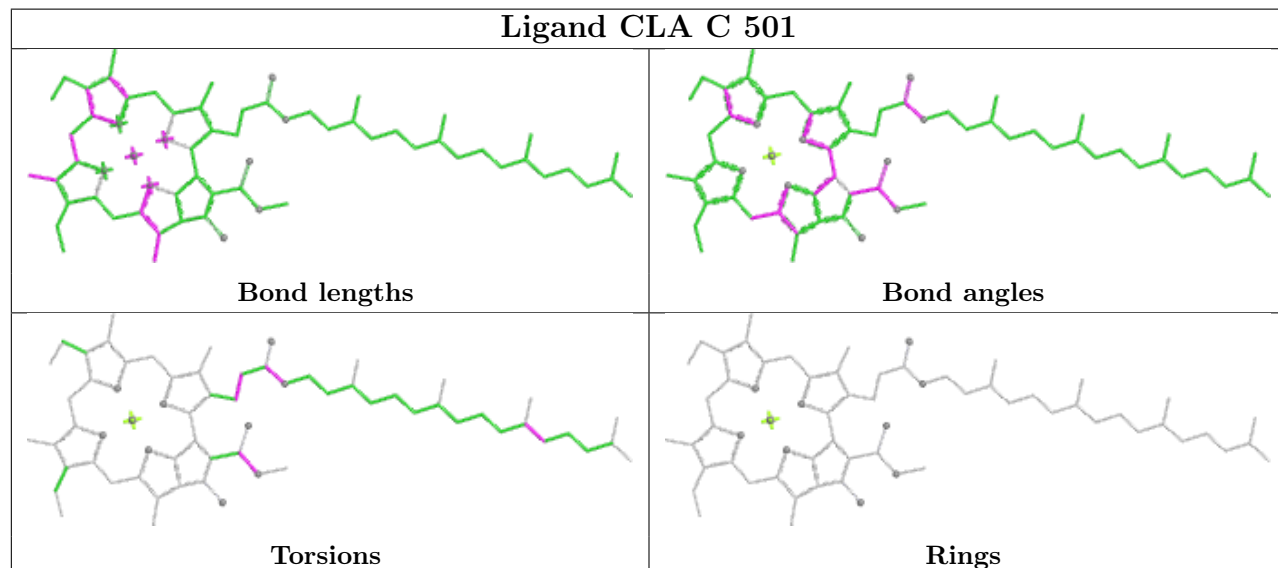
Ligand CLA C 506

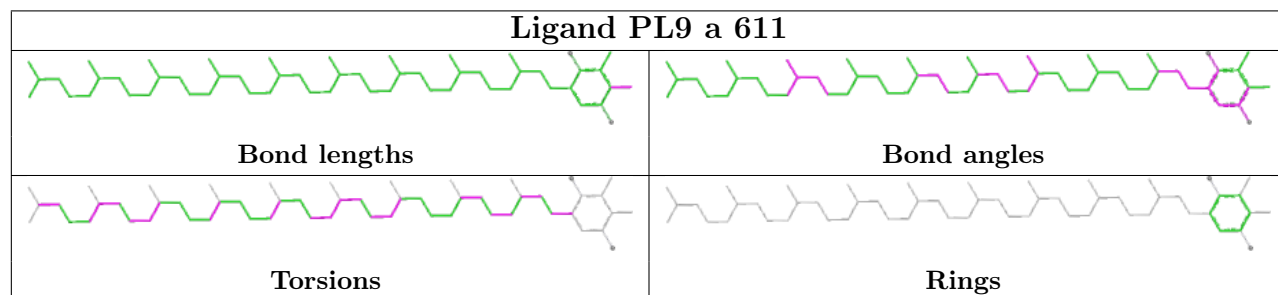
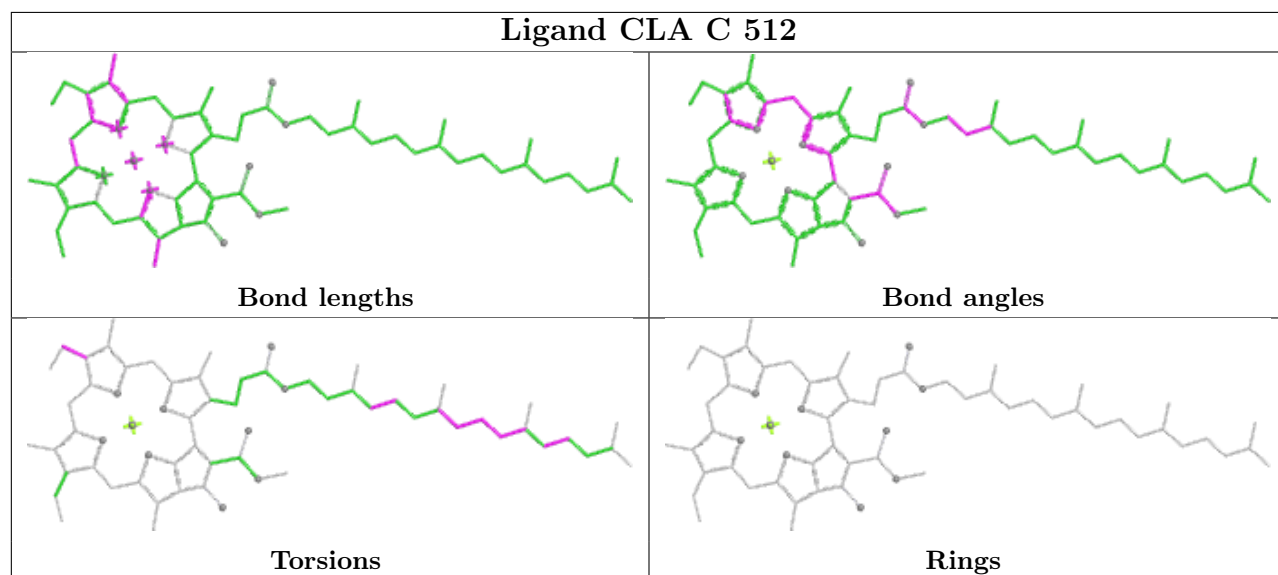
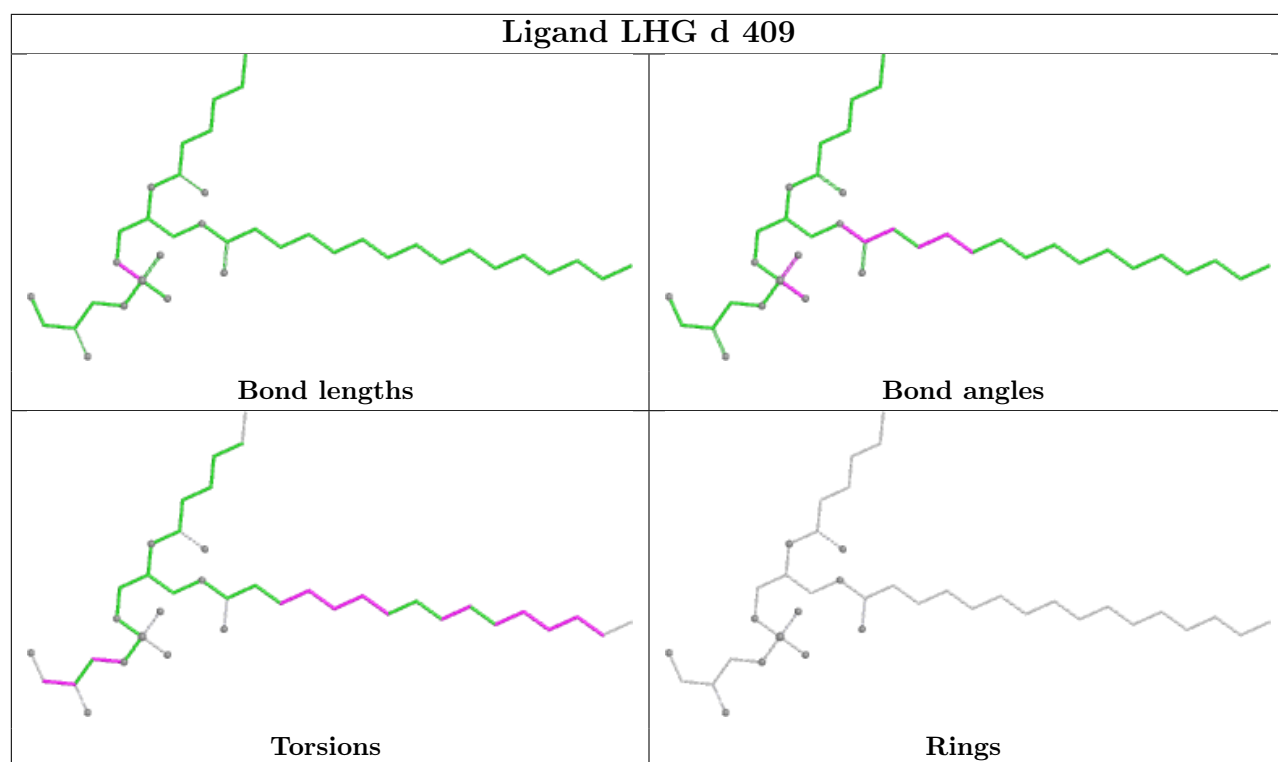


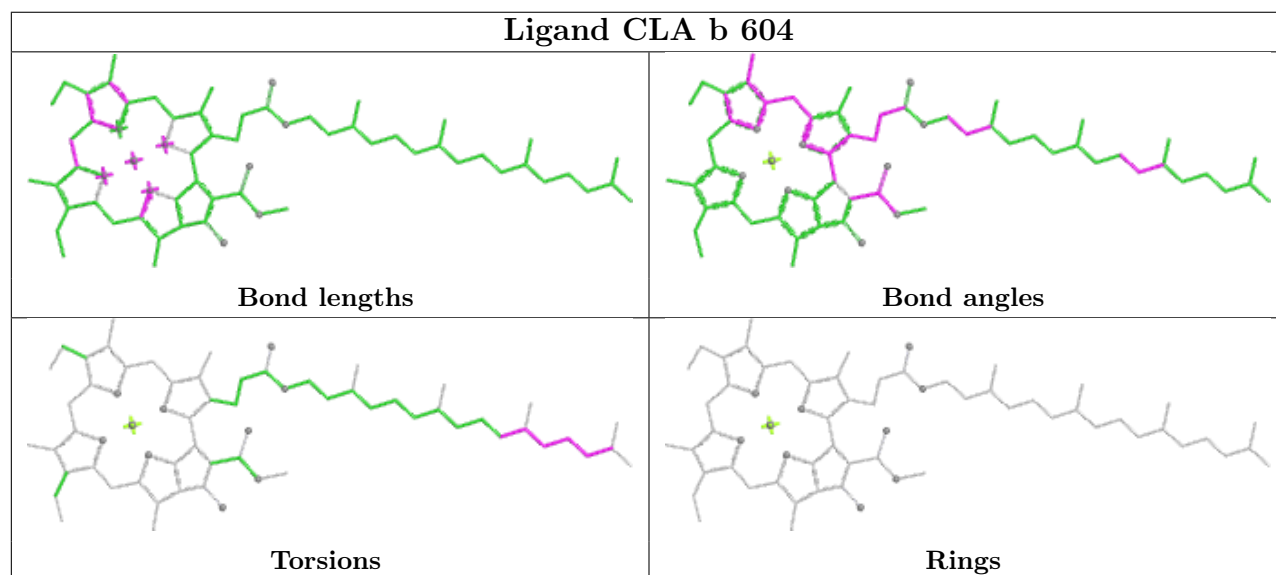
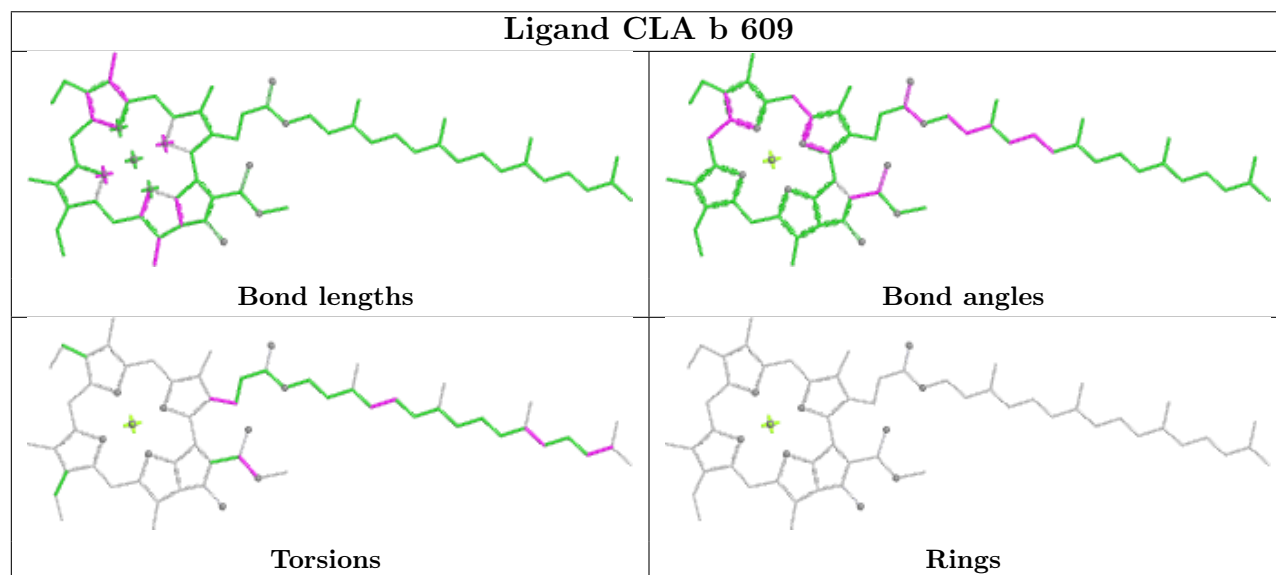
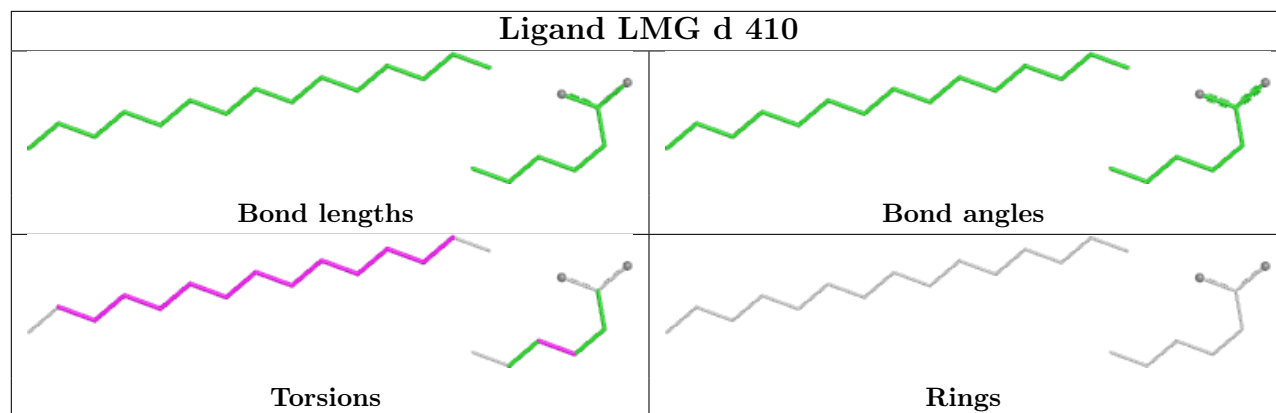
Ligand LMG D 412



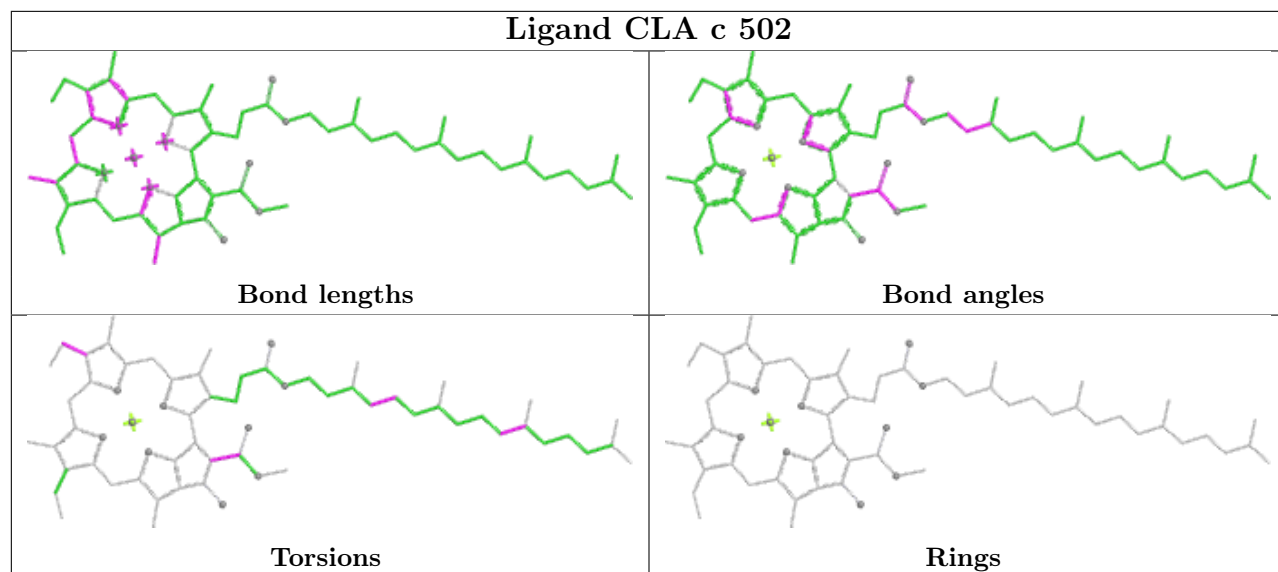
Ligand CLA C 501



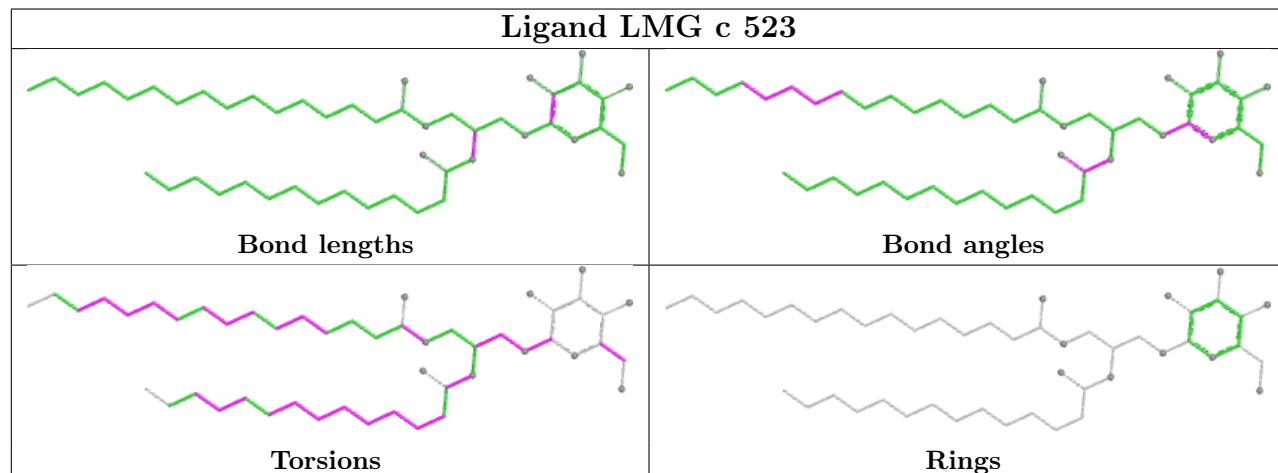




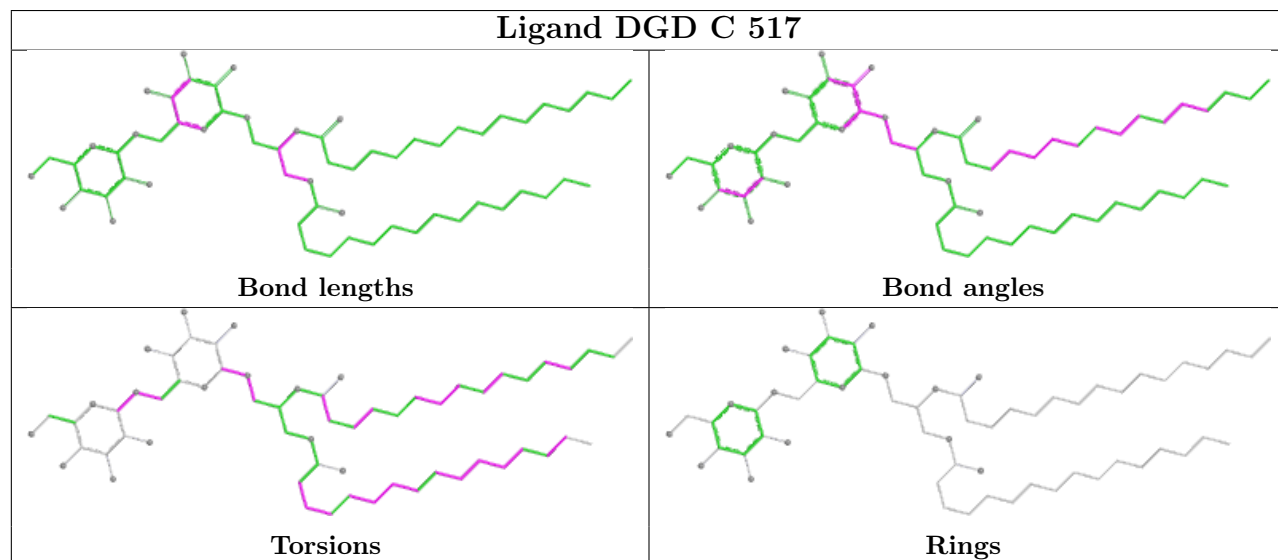
Ligand CLA c 502

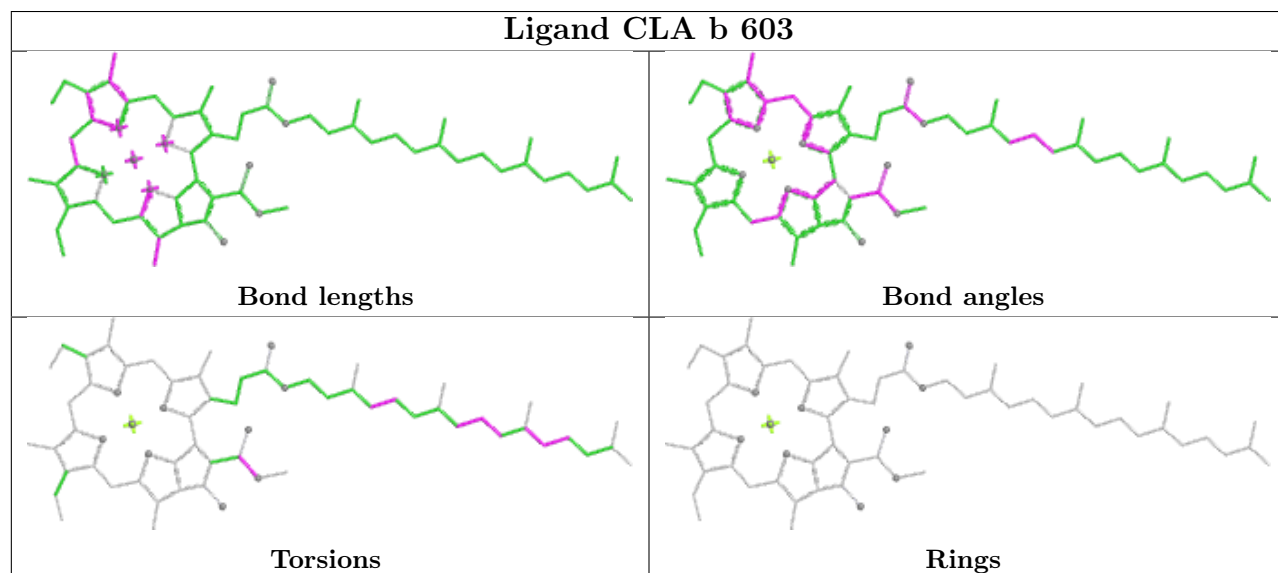
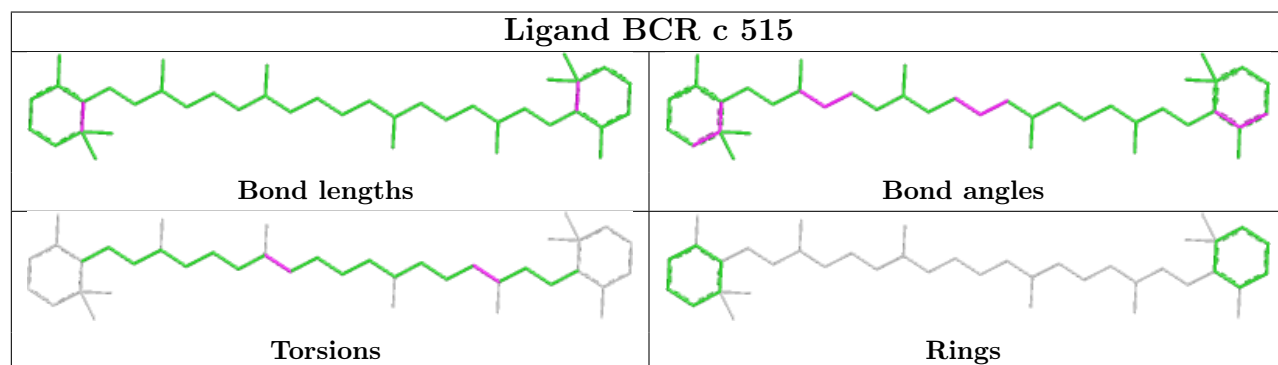
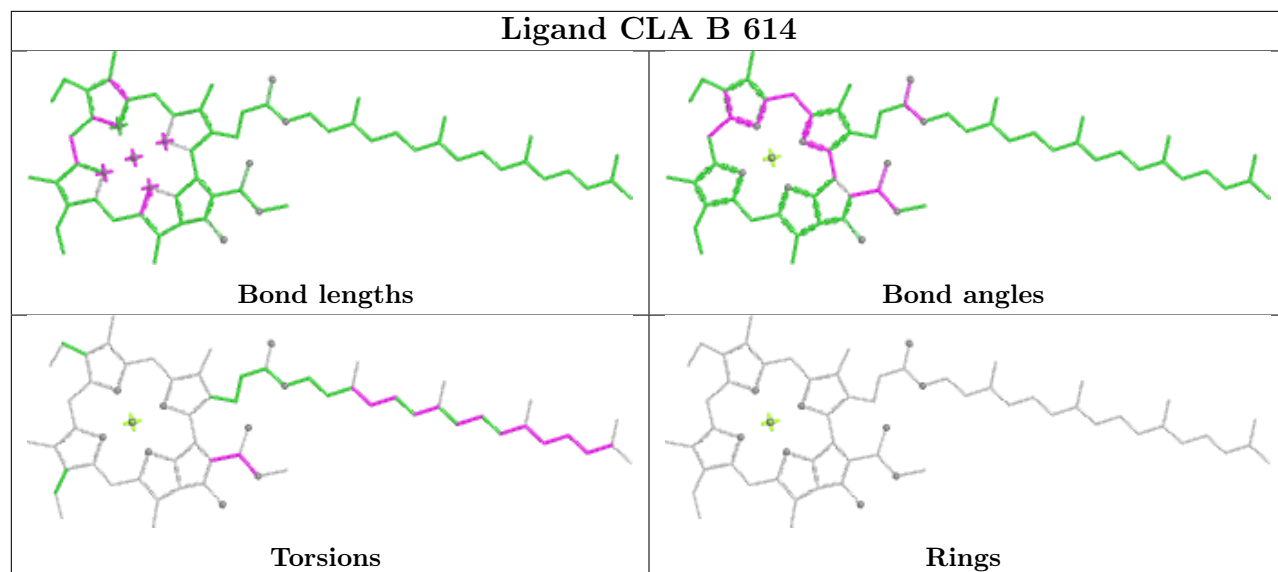


Ligand LMG c 523

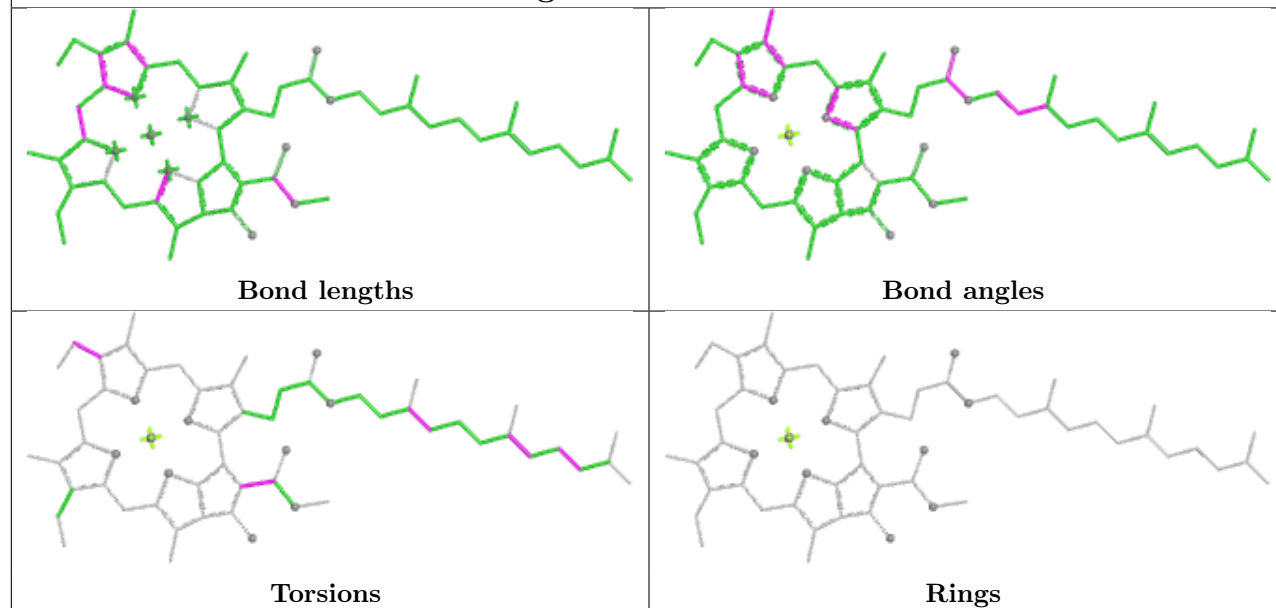


Ligand DGD C 517

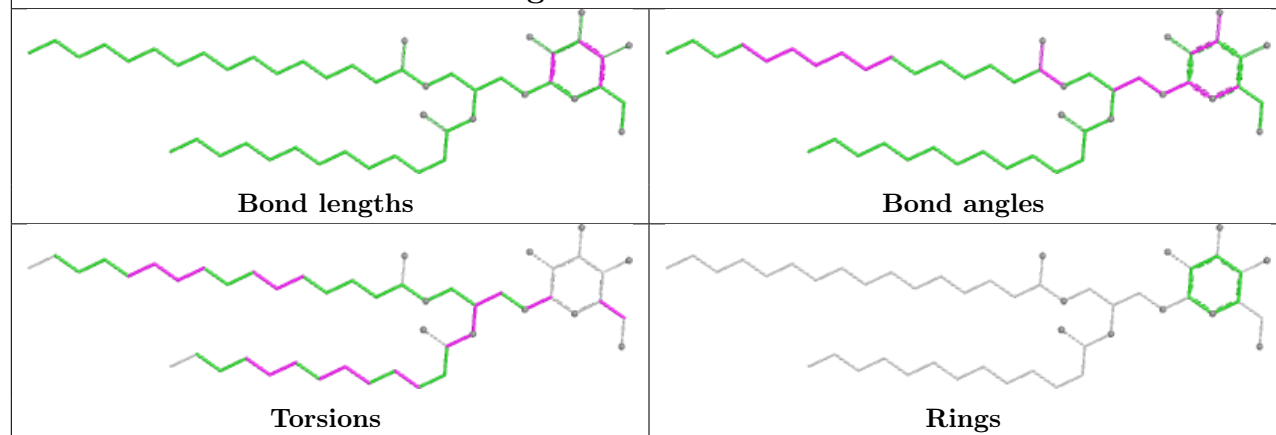


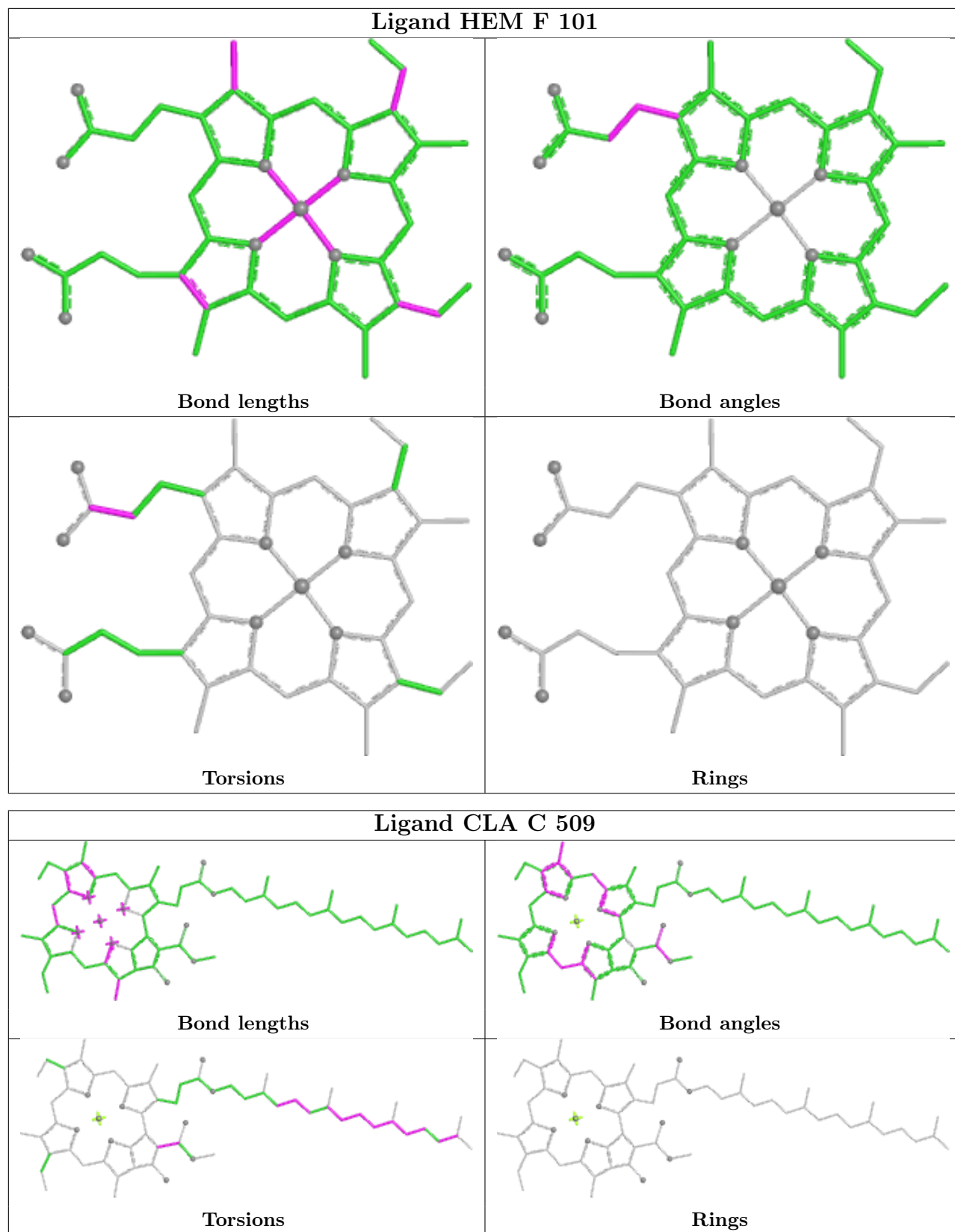


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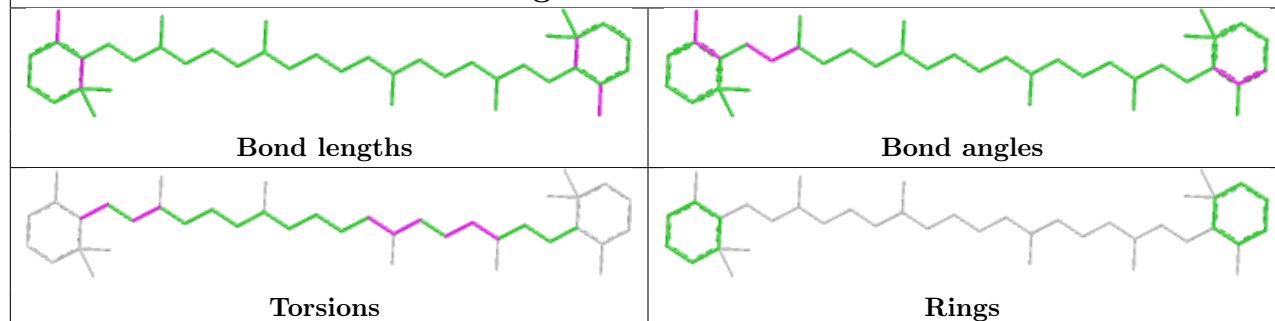


Ligand LMG A 612

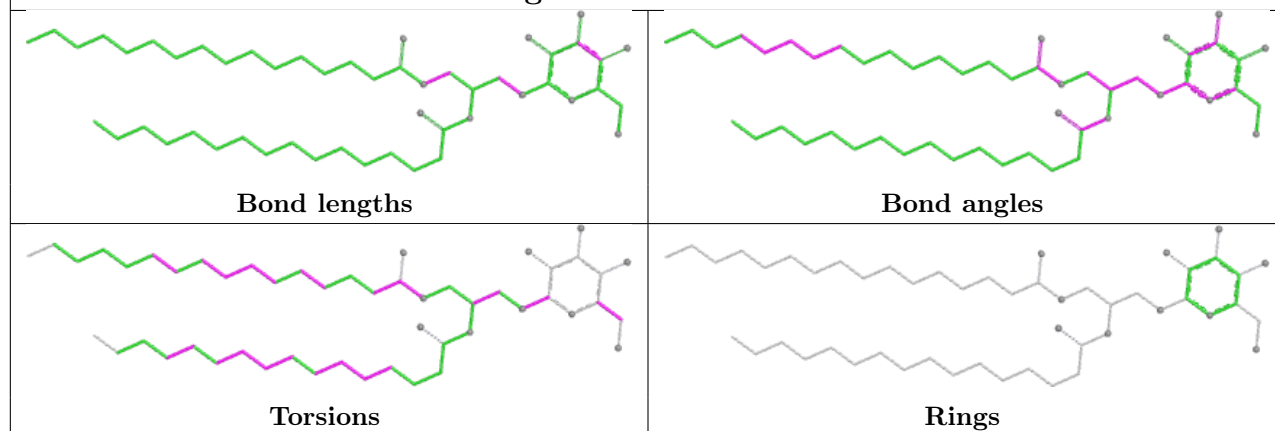




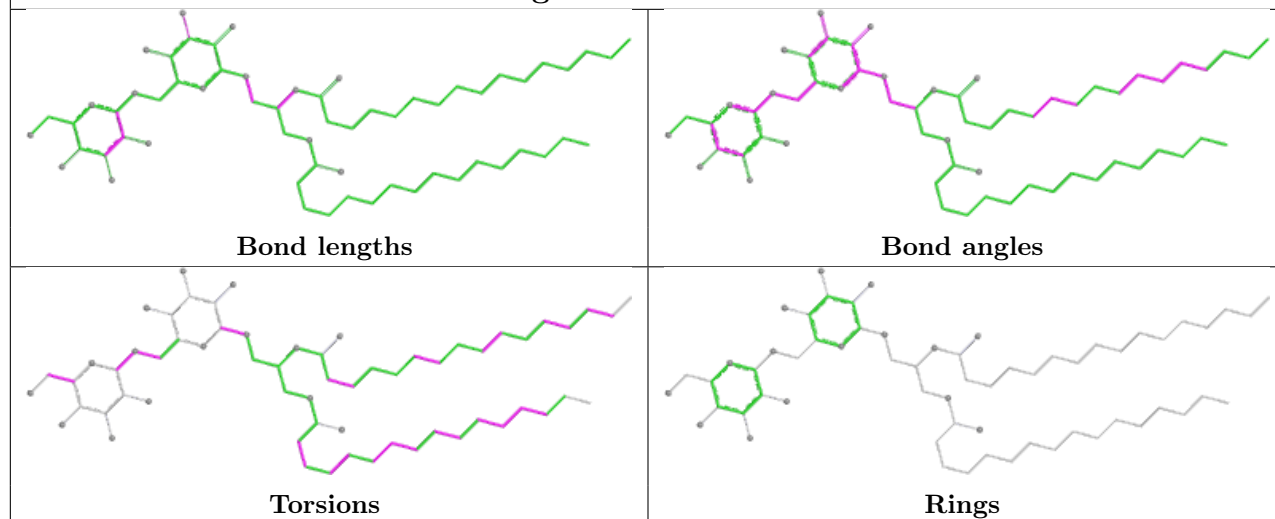
Ligand BCR k 101



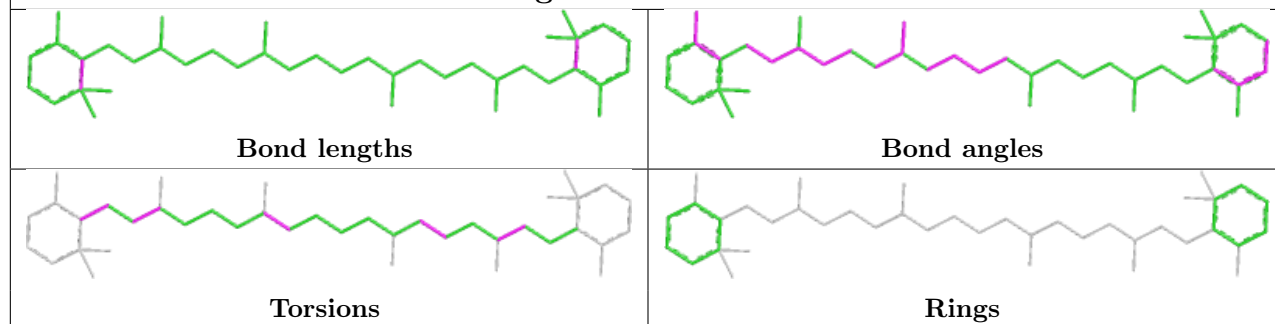
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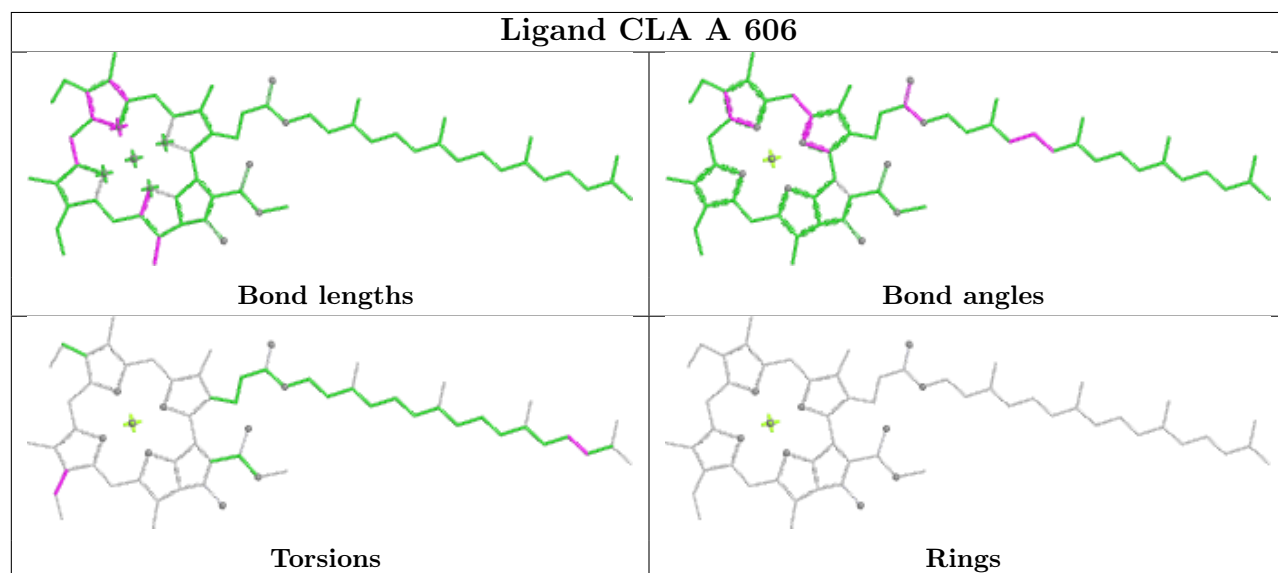
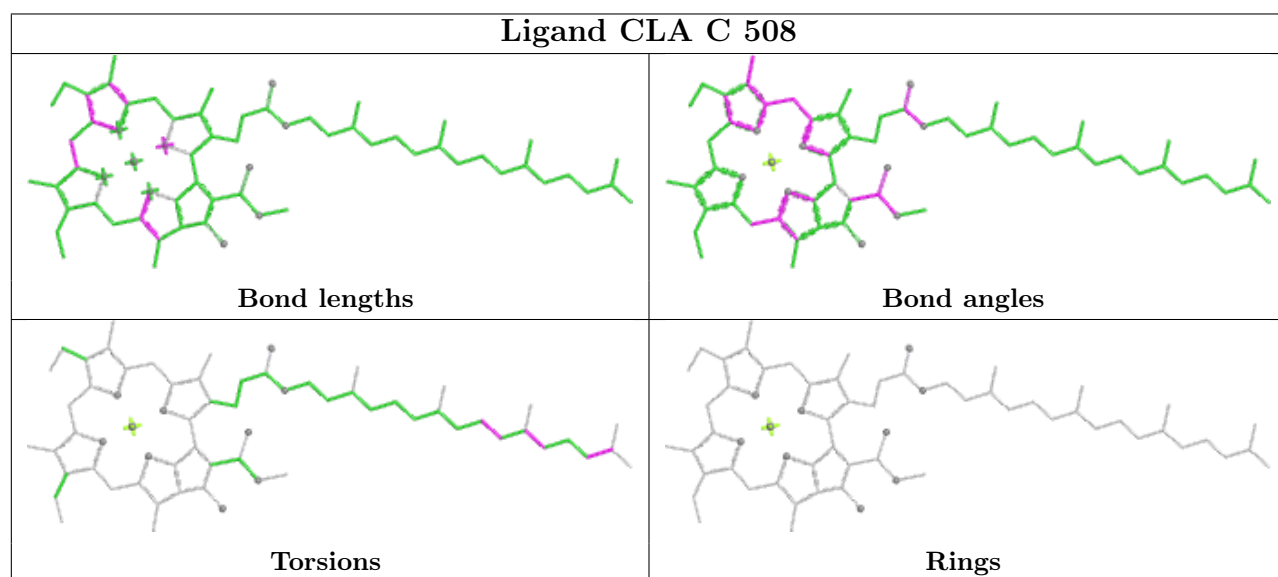
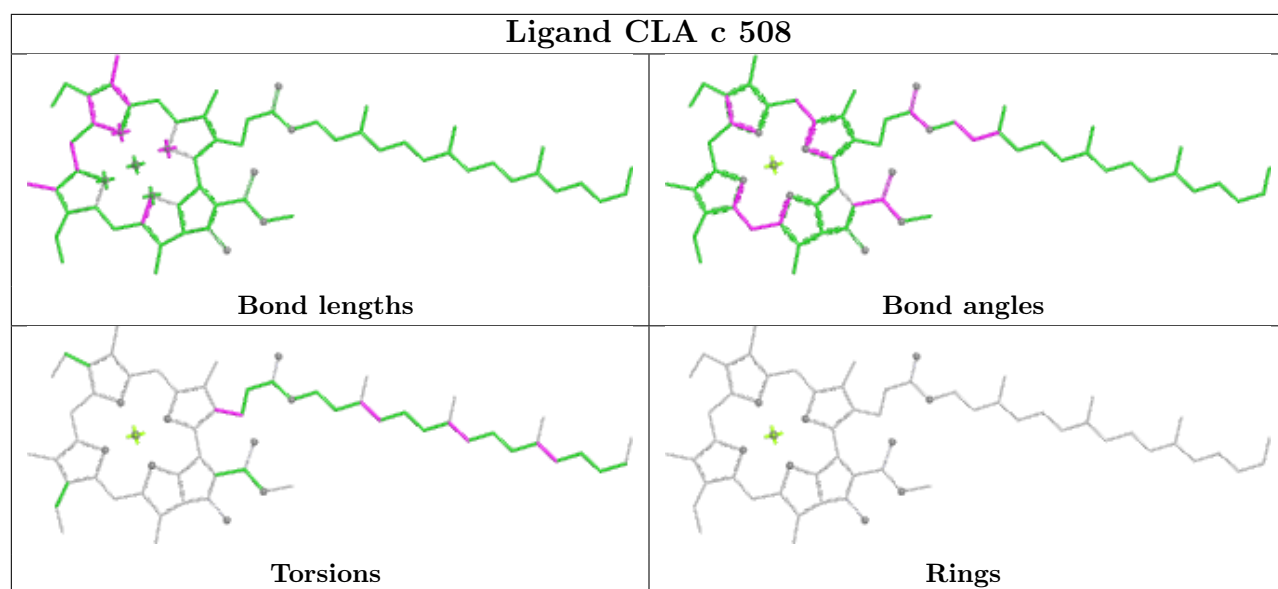


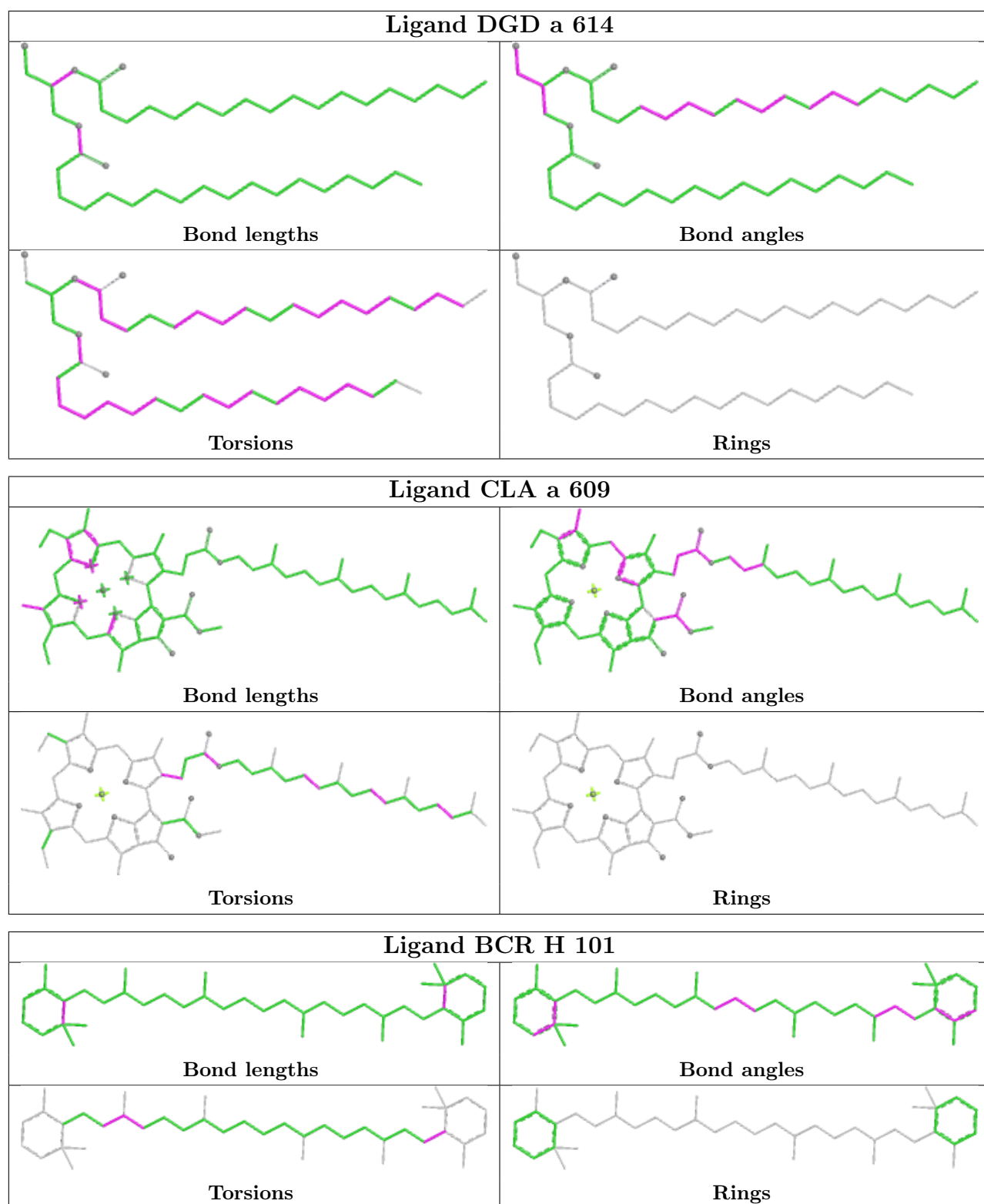
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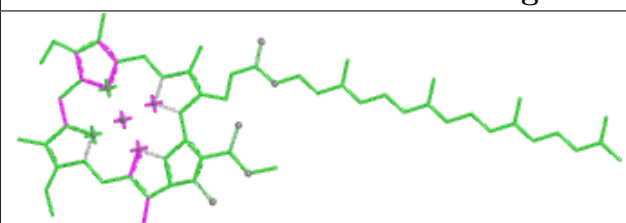
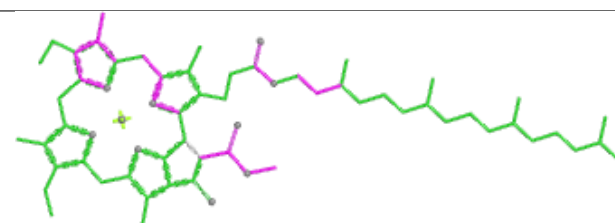
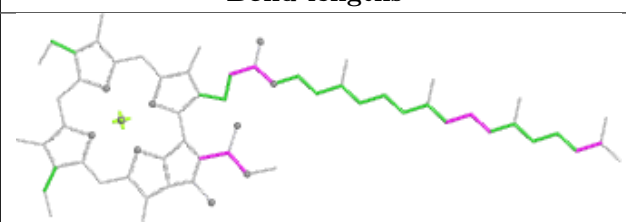
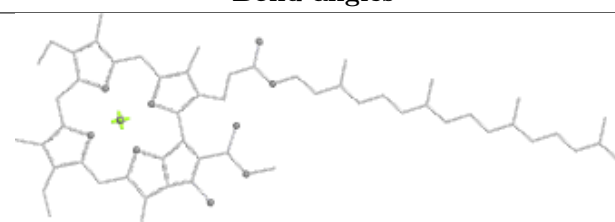


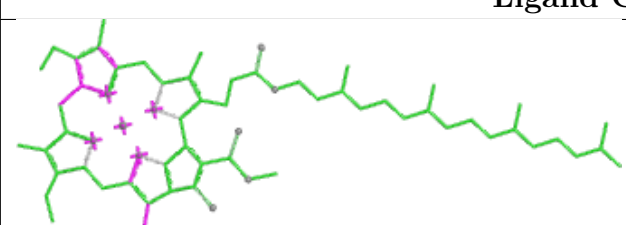
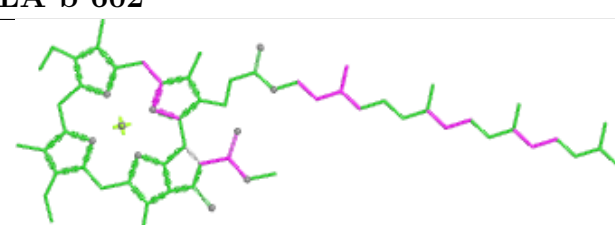
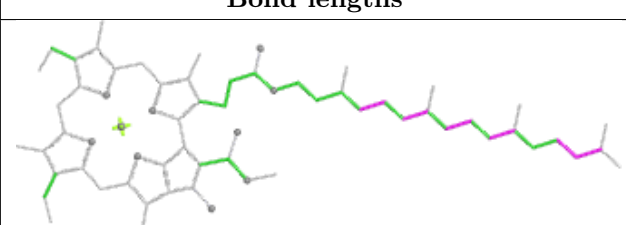
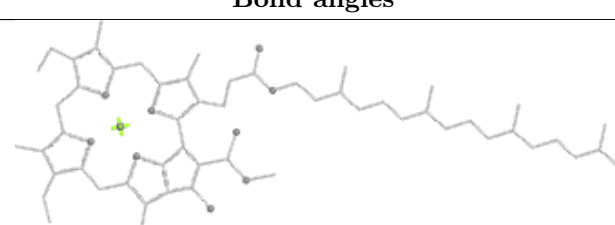
Ligand BCR t 101



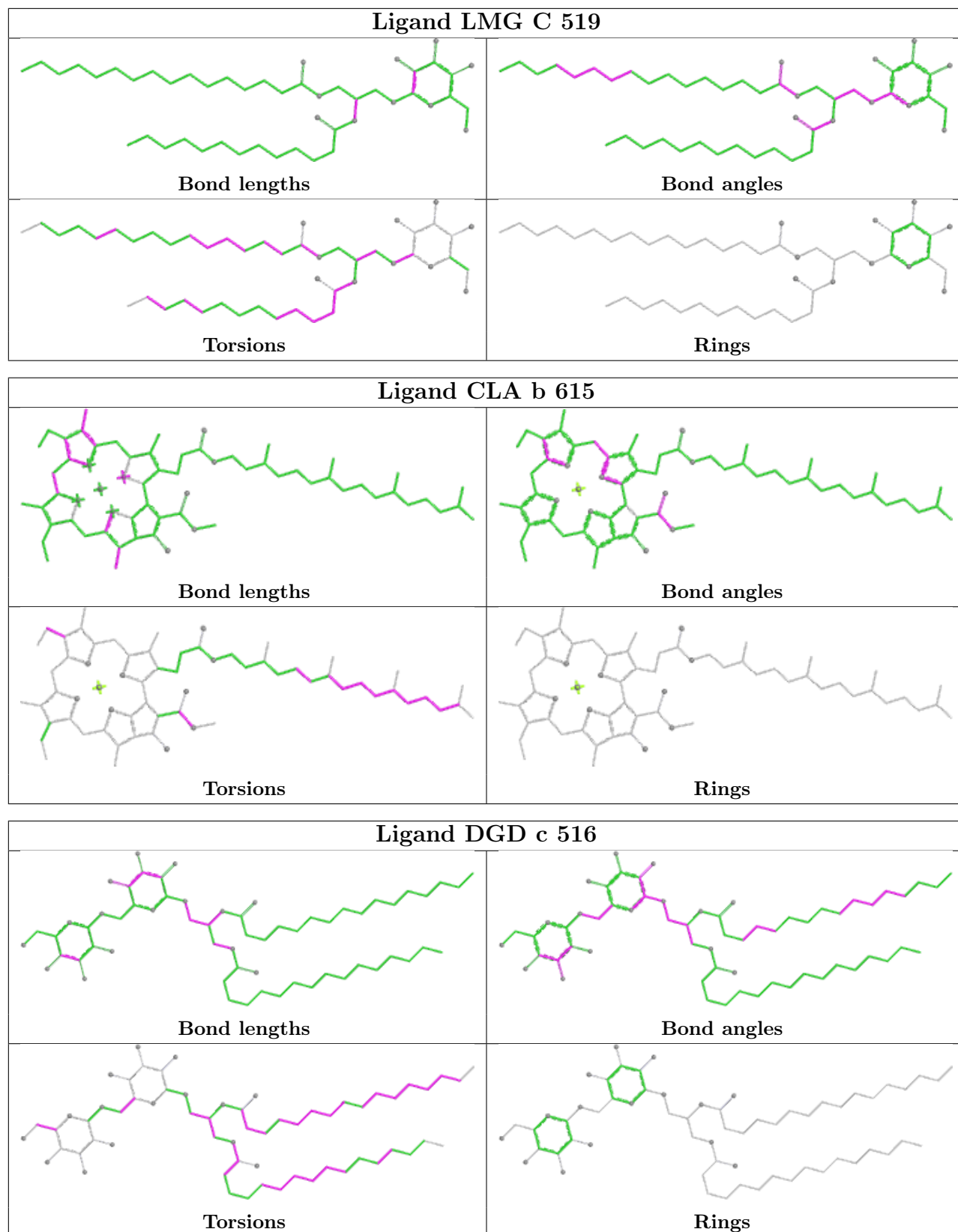


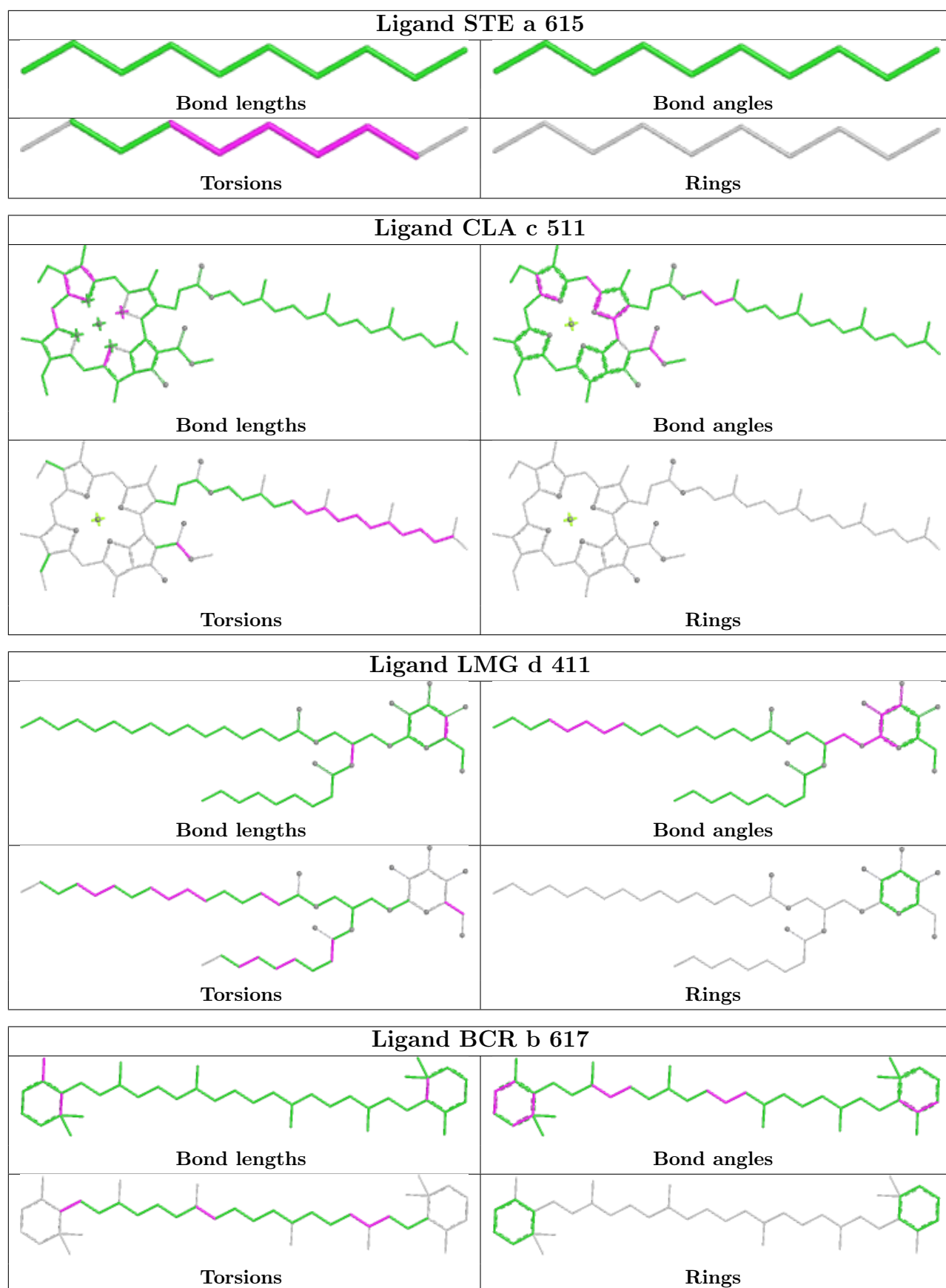


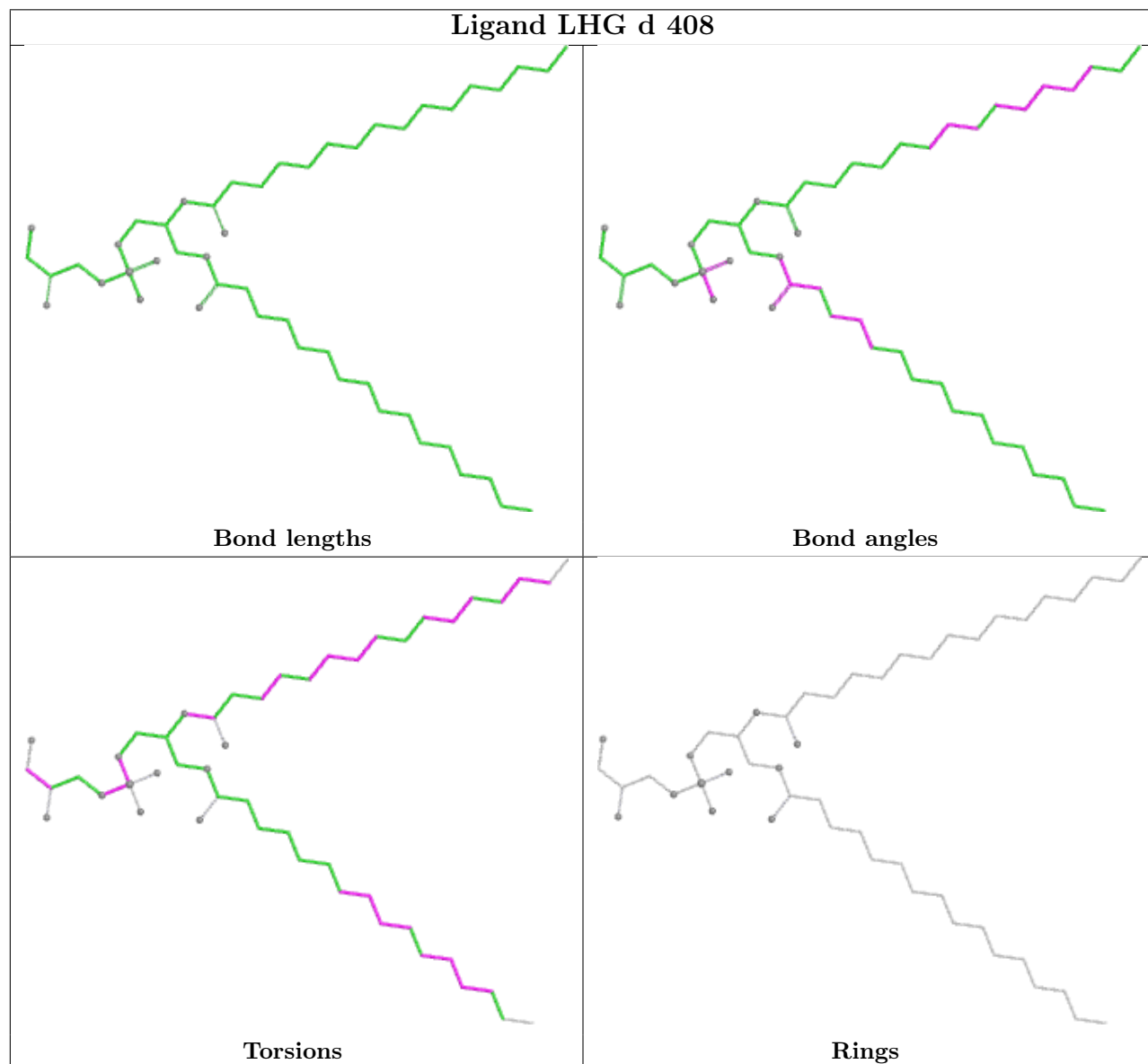
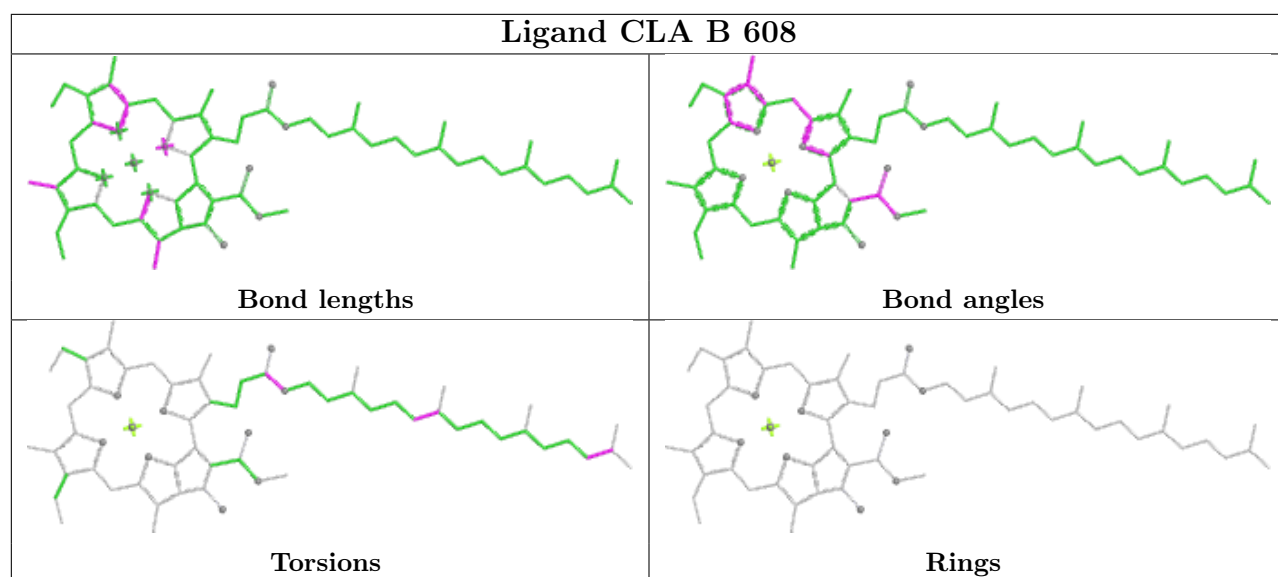
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

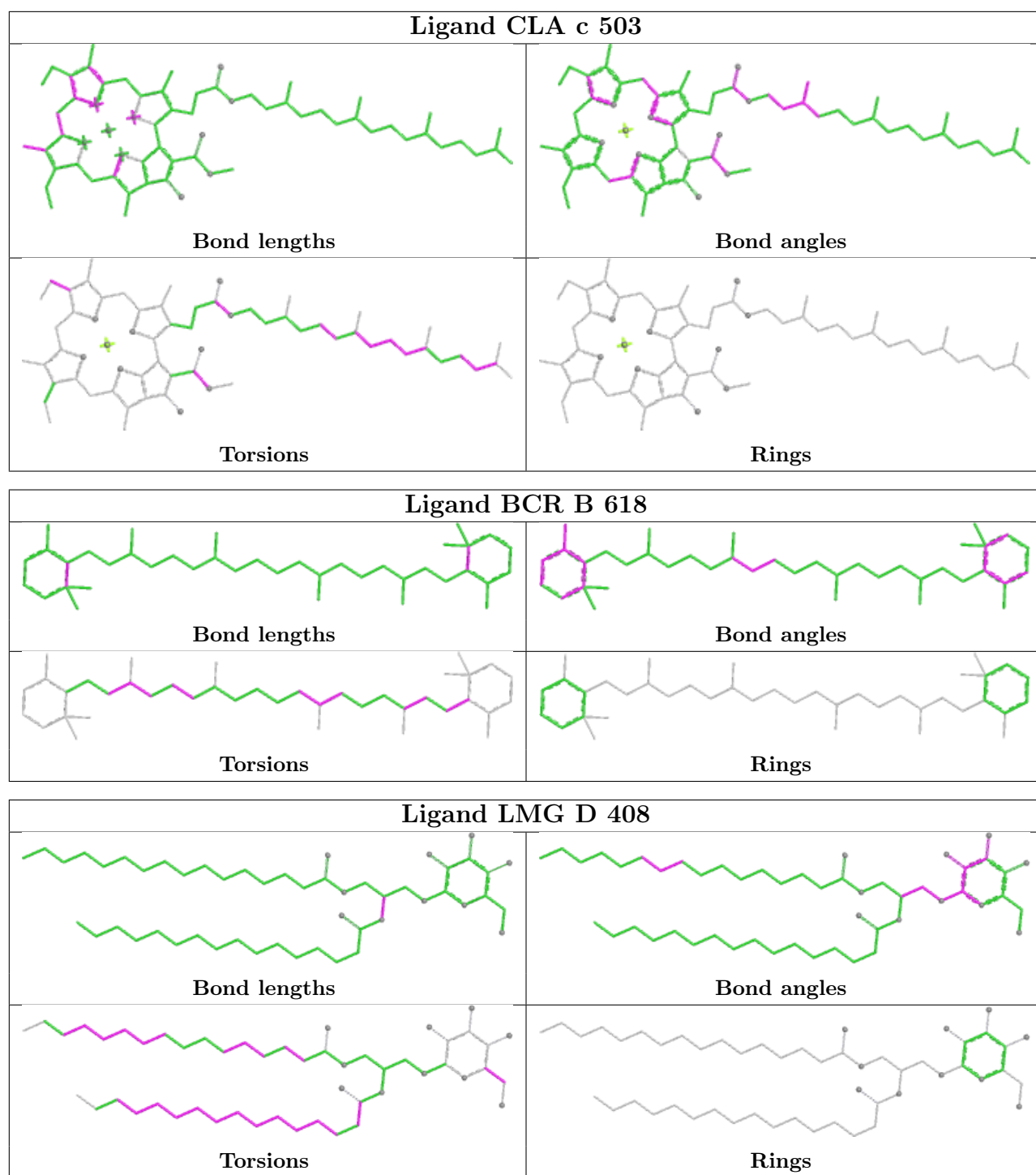
Ligand CLA b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE 1 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

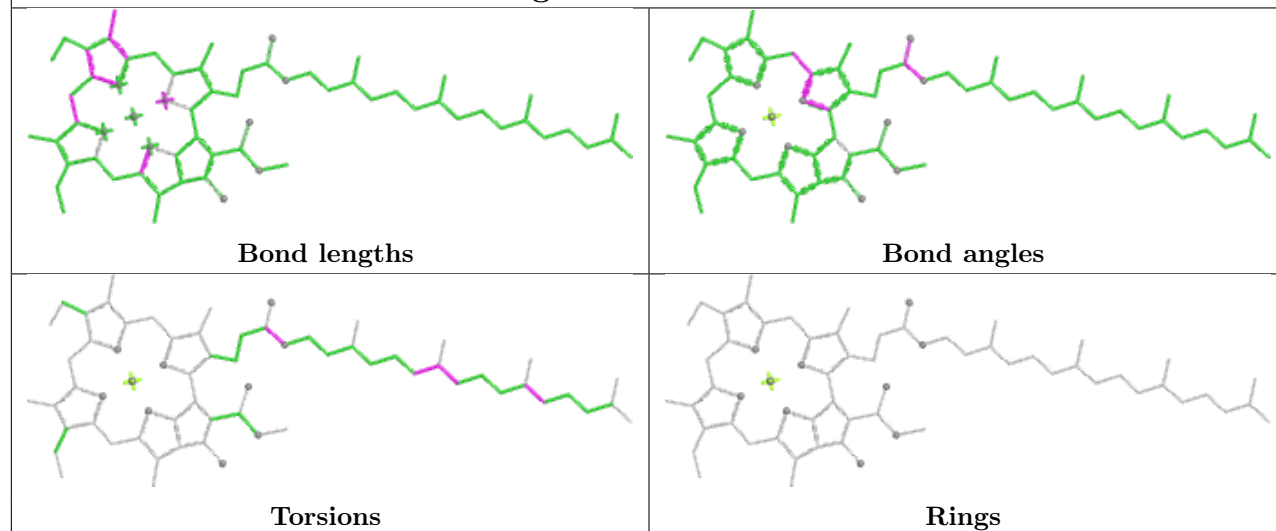




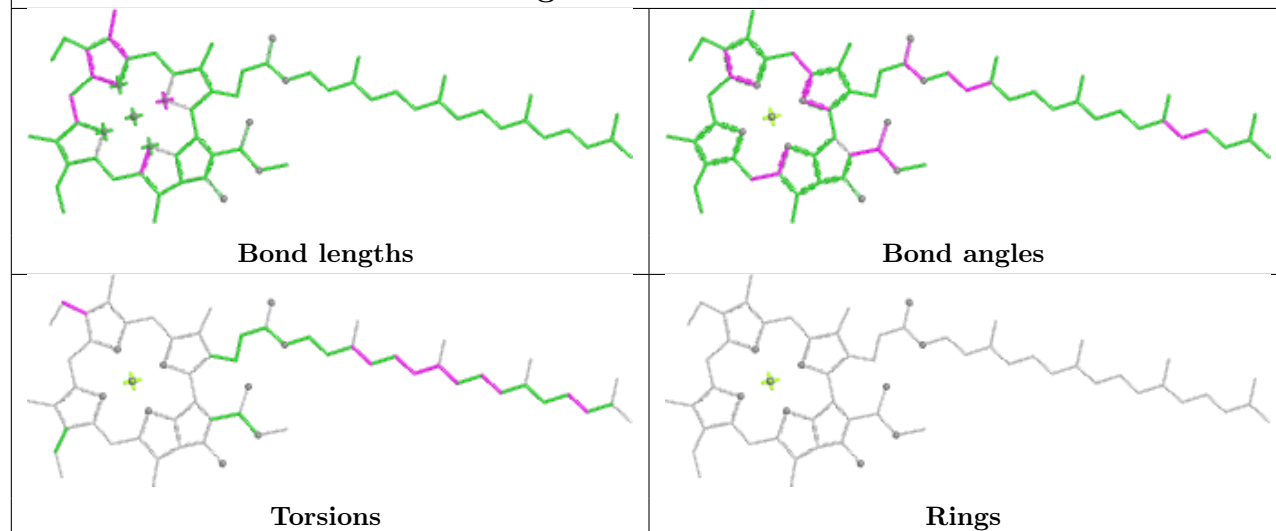


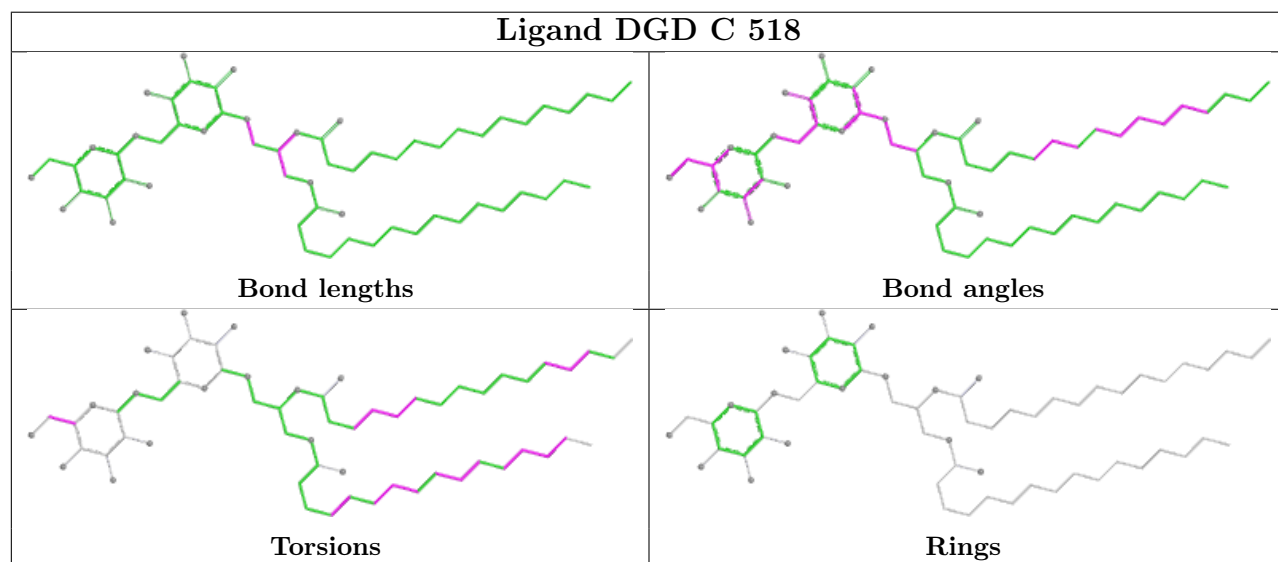
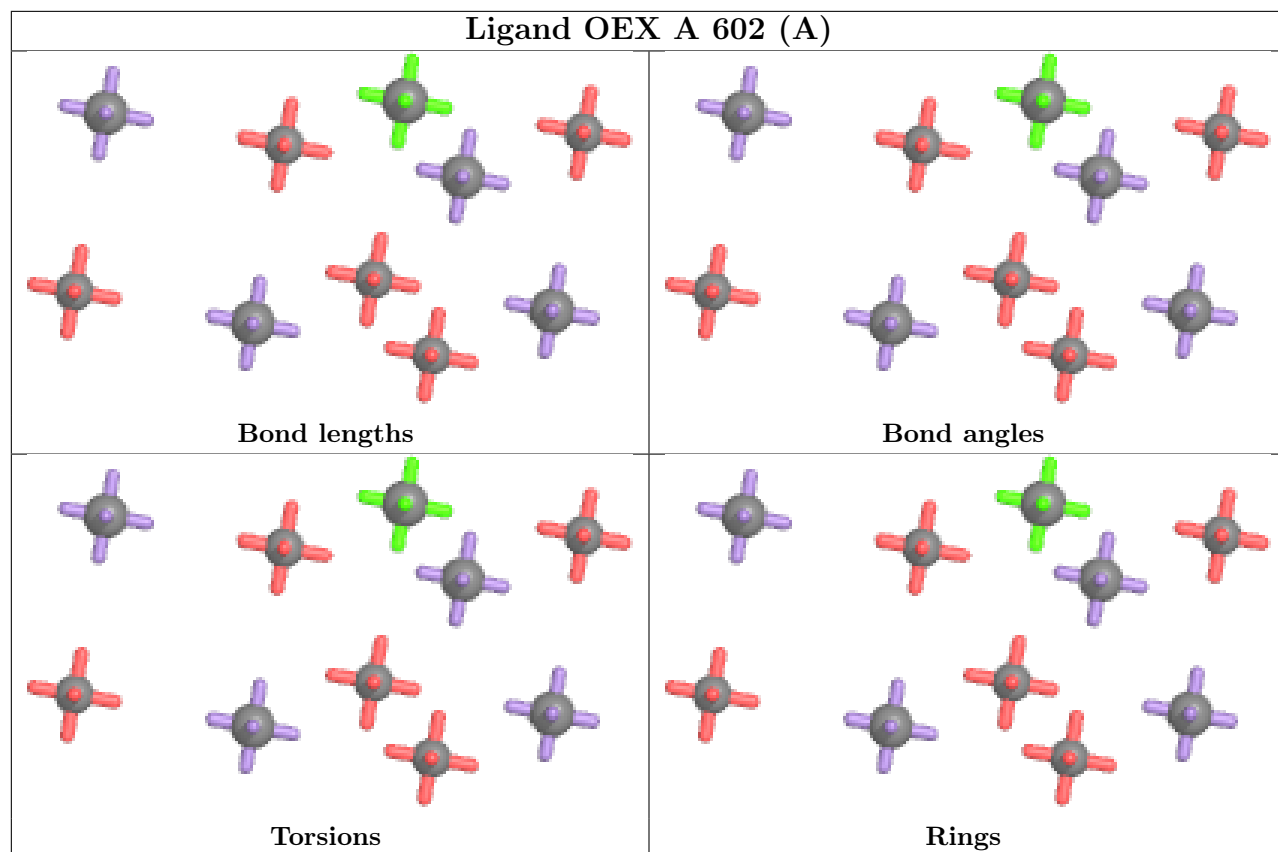


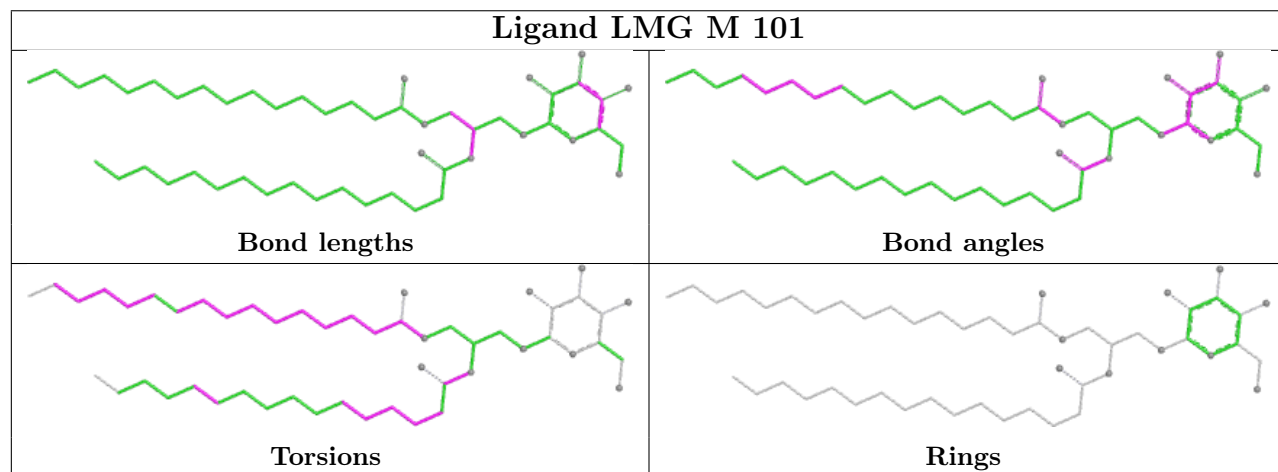
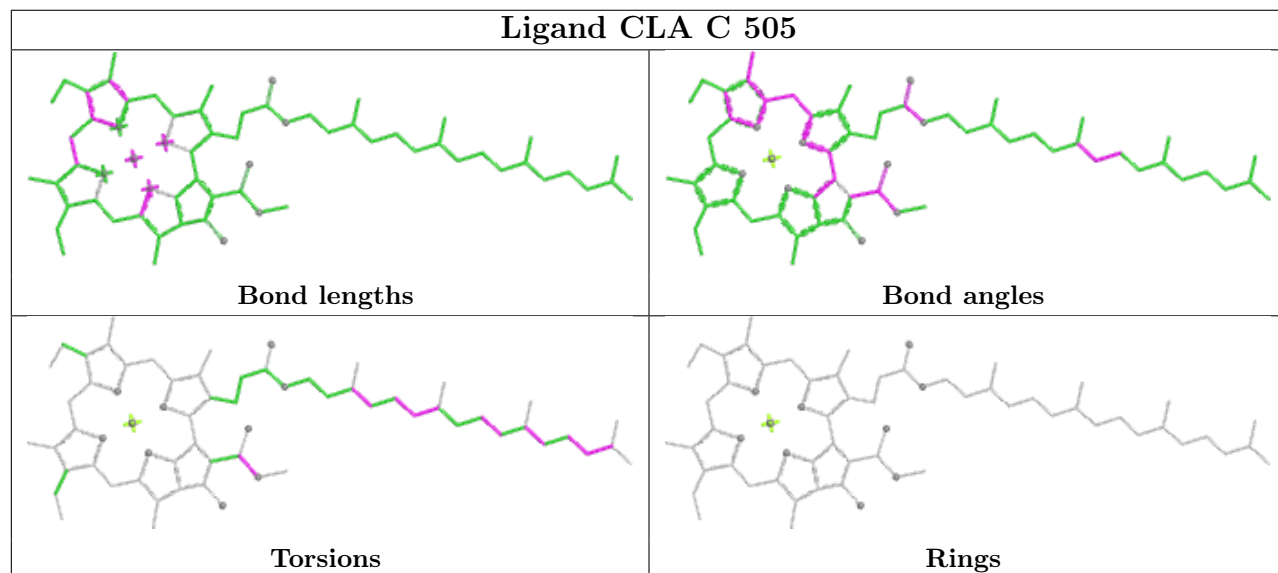
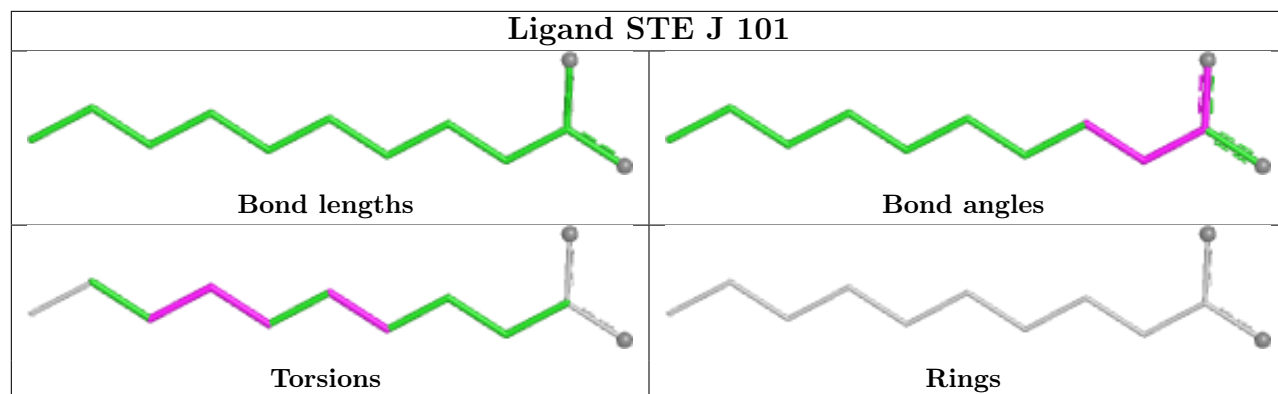
Ligand CLA C 511

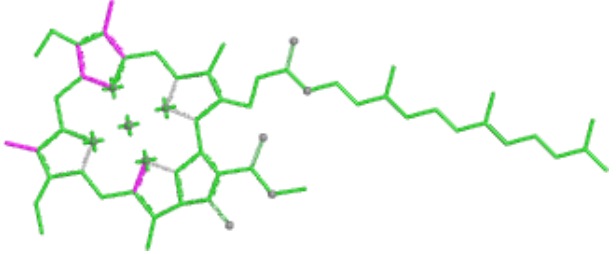
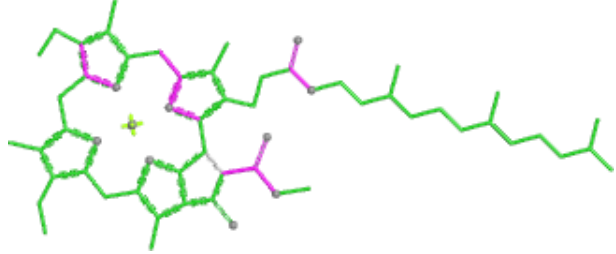
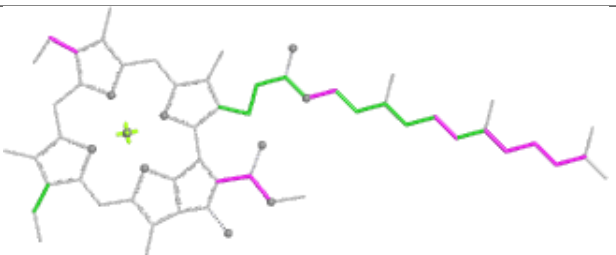
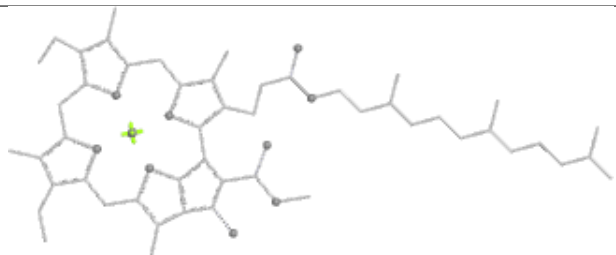
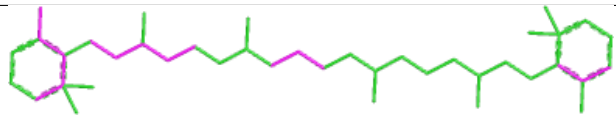
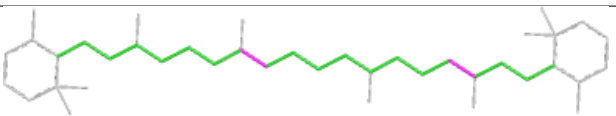
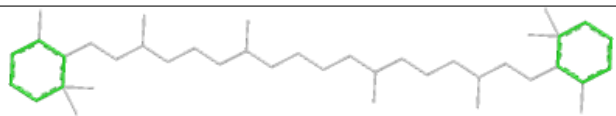
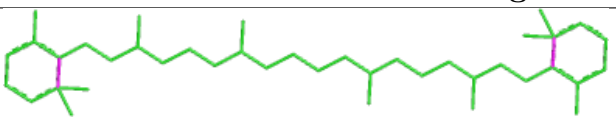
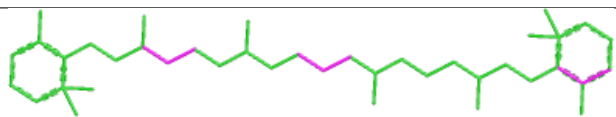
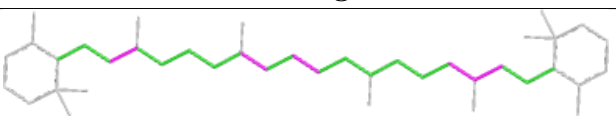
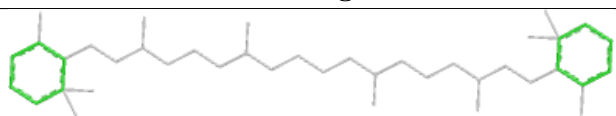


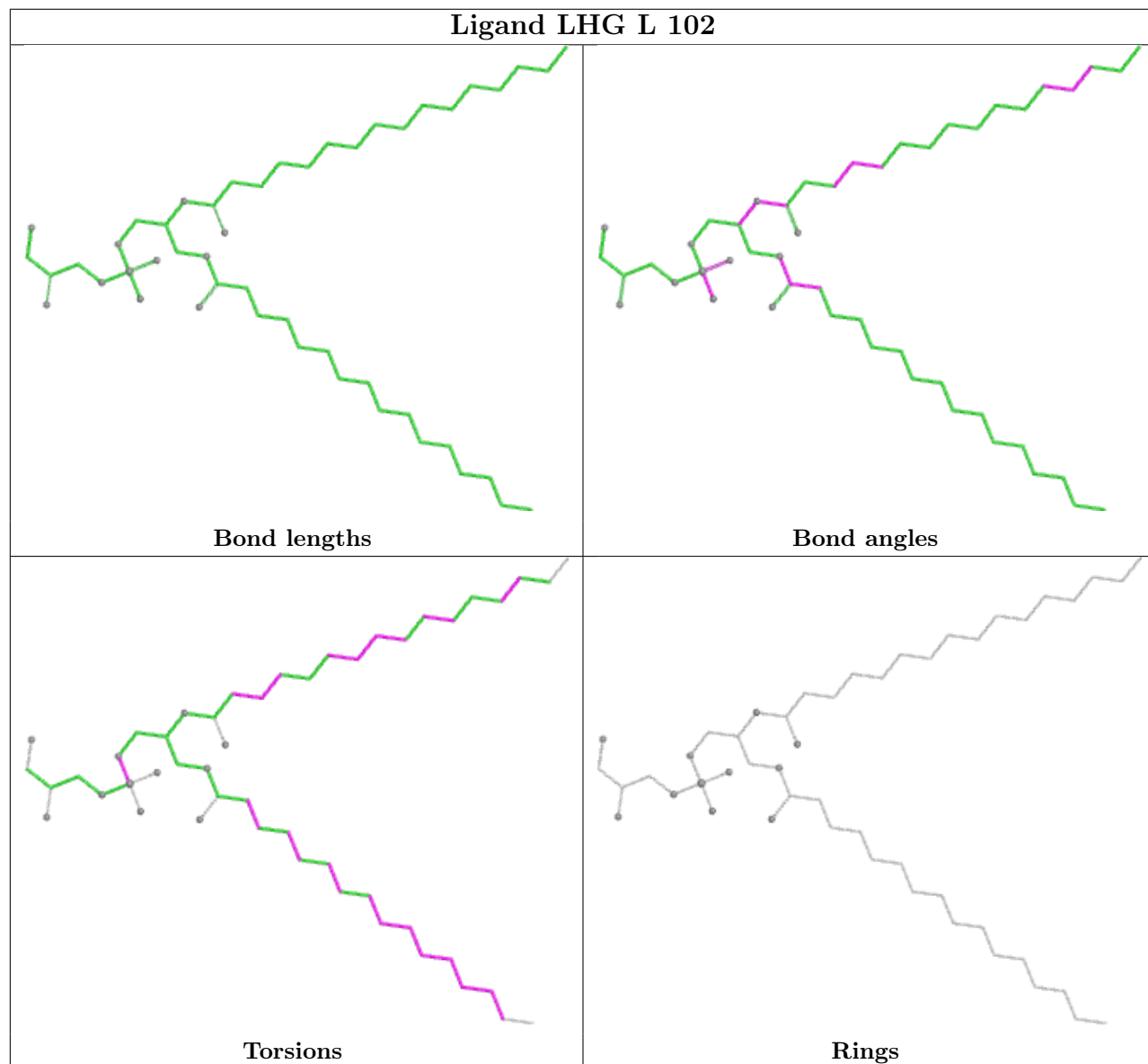
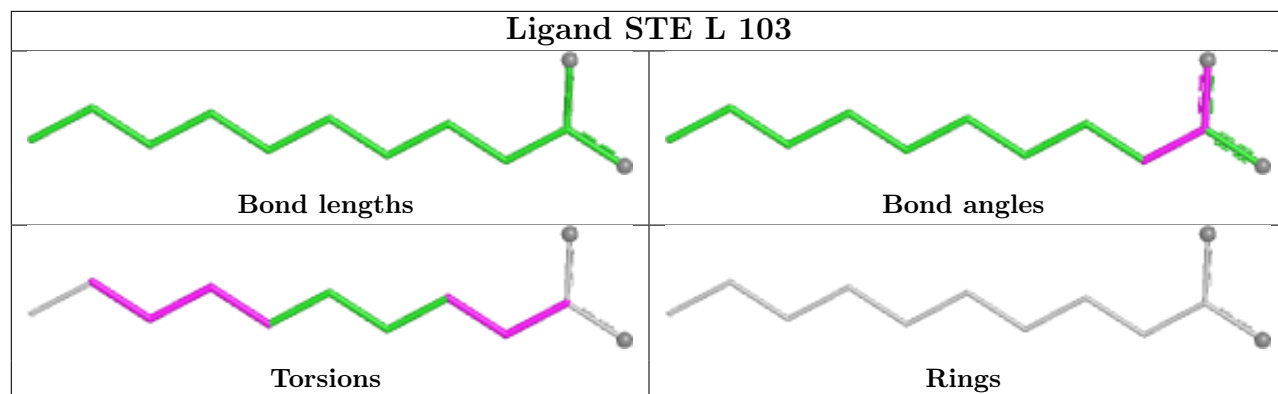
Ligand CLA c 505



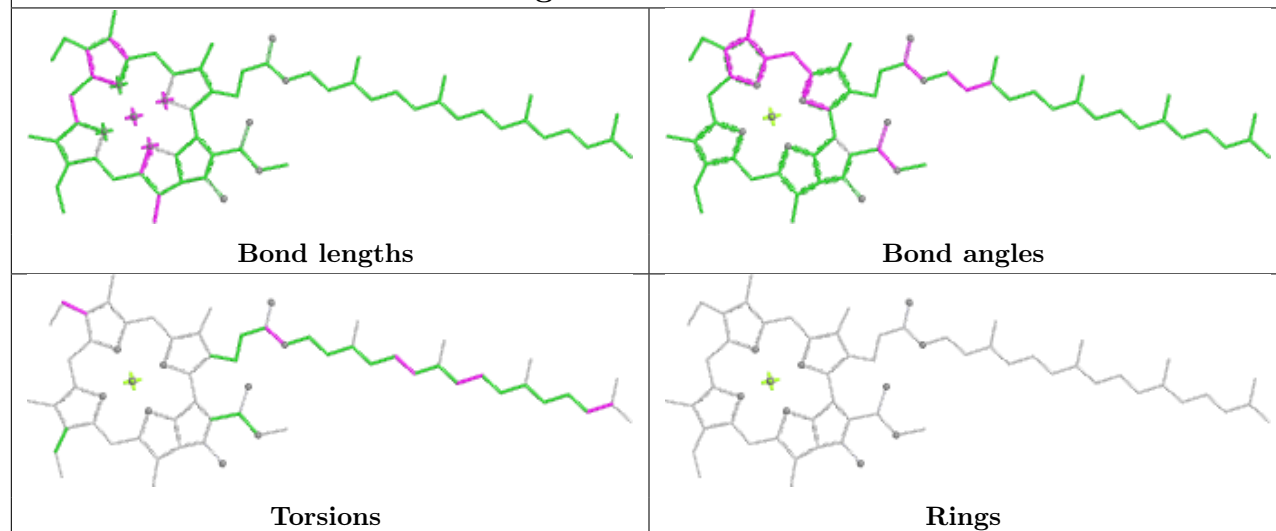




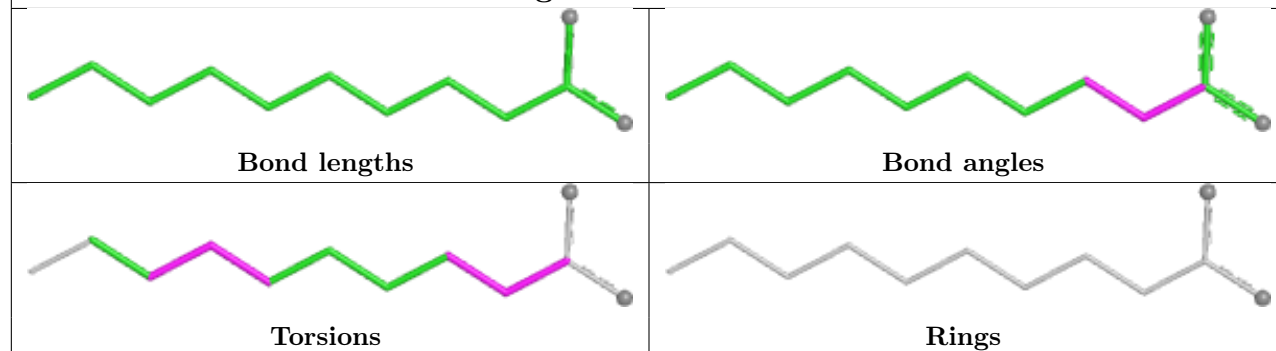
Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings



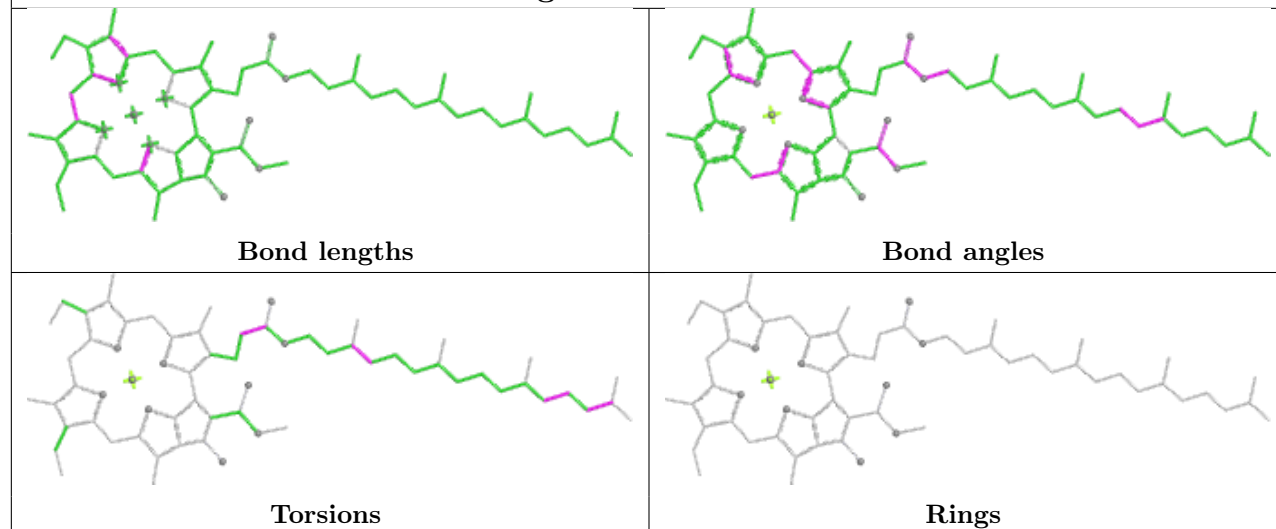
Ligand CLA d 404



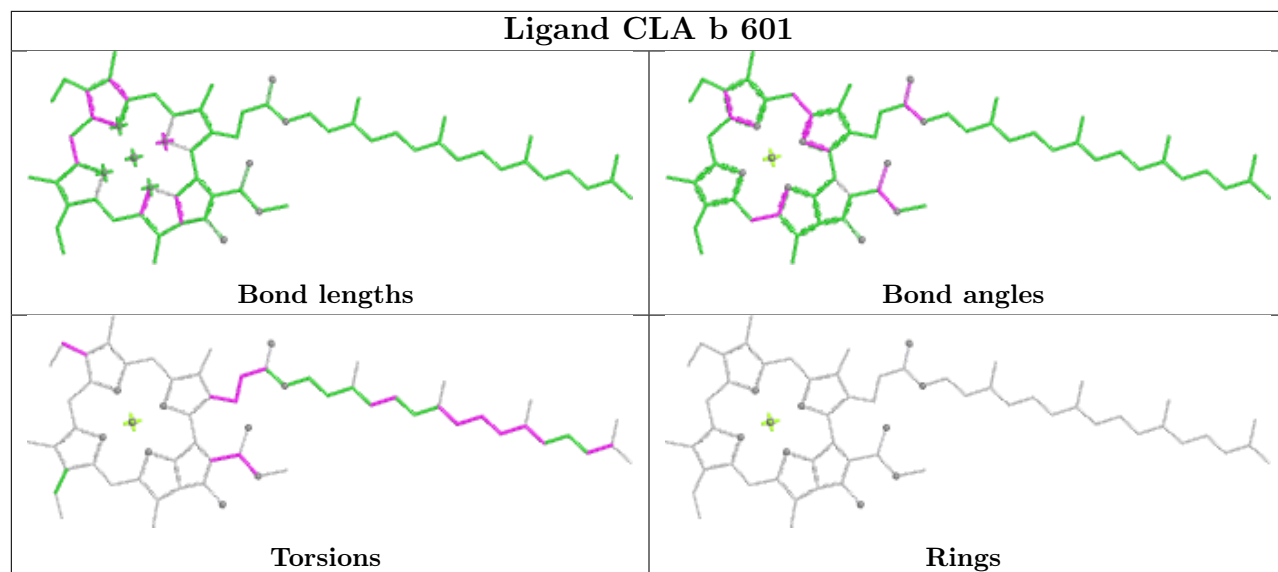
Ligand STE C 521



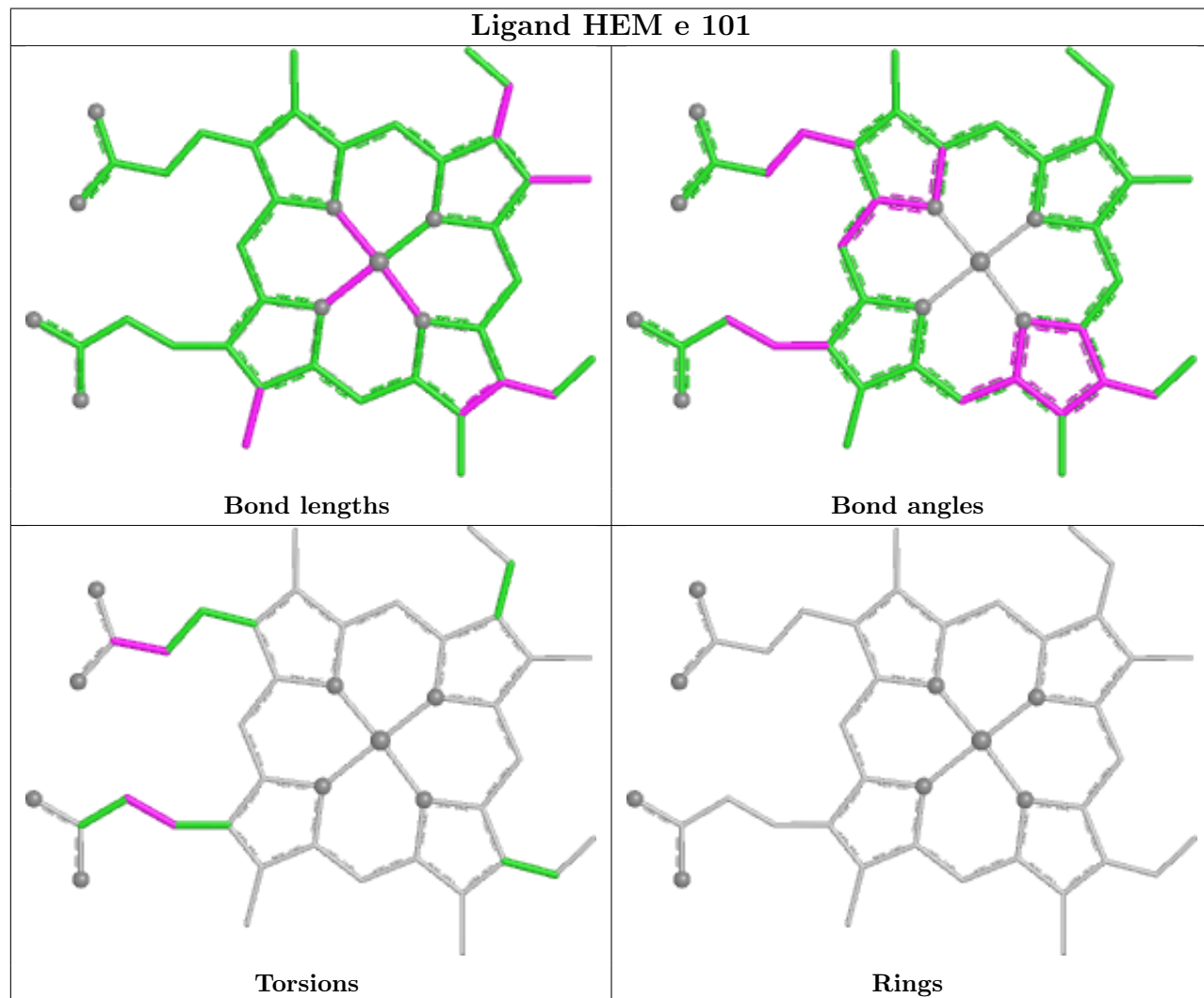
Ligand CLA c 509

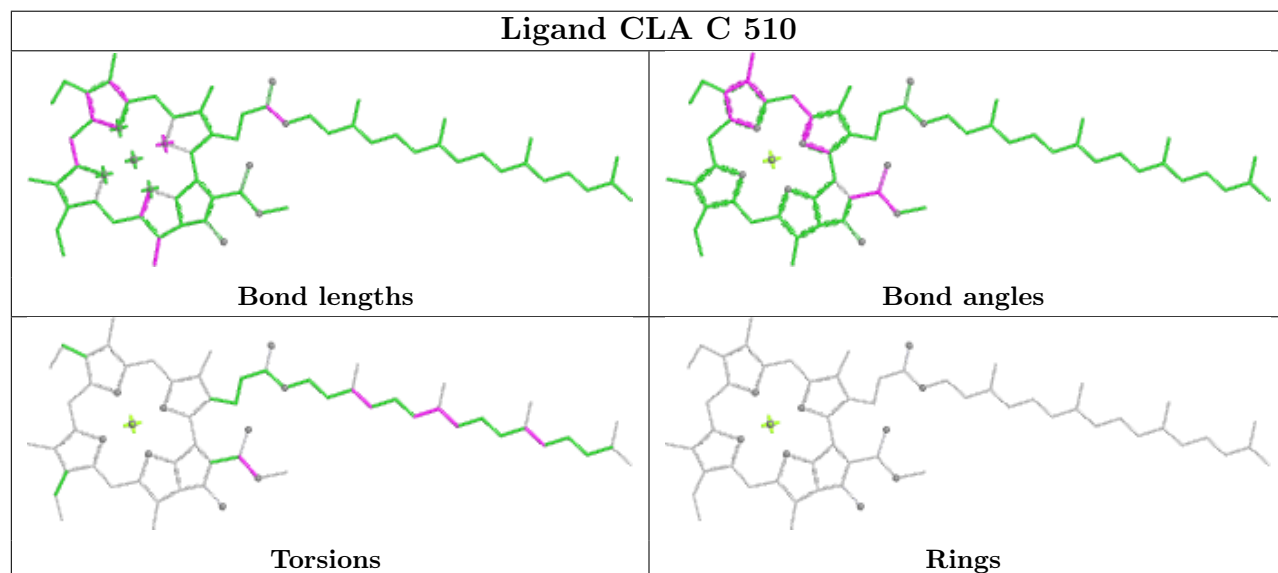
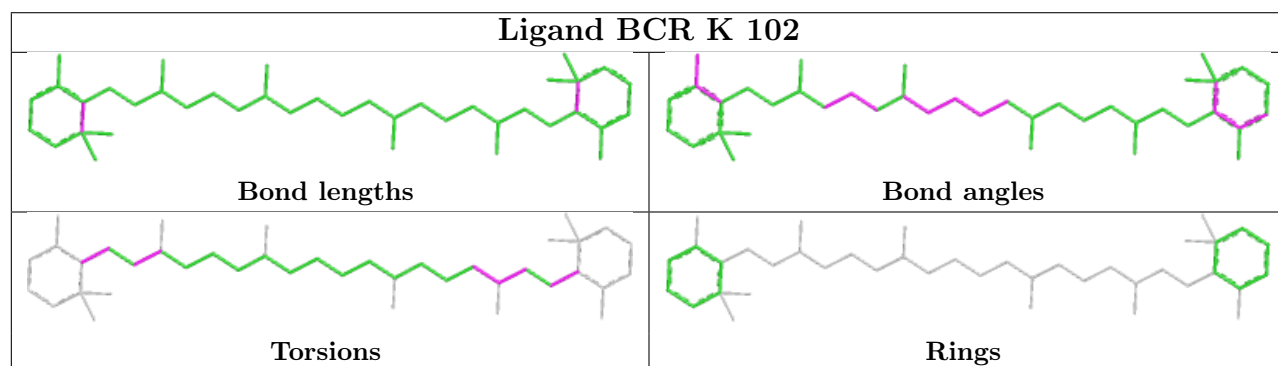
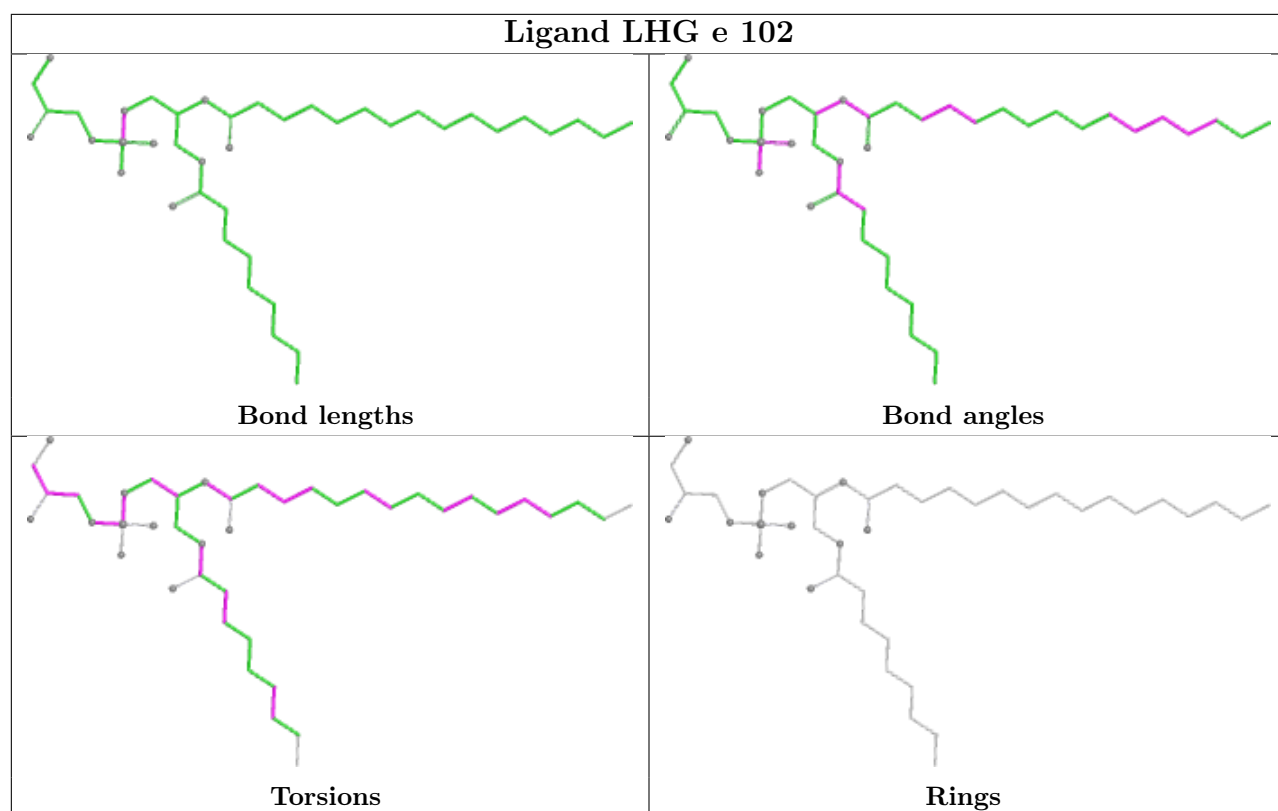


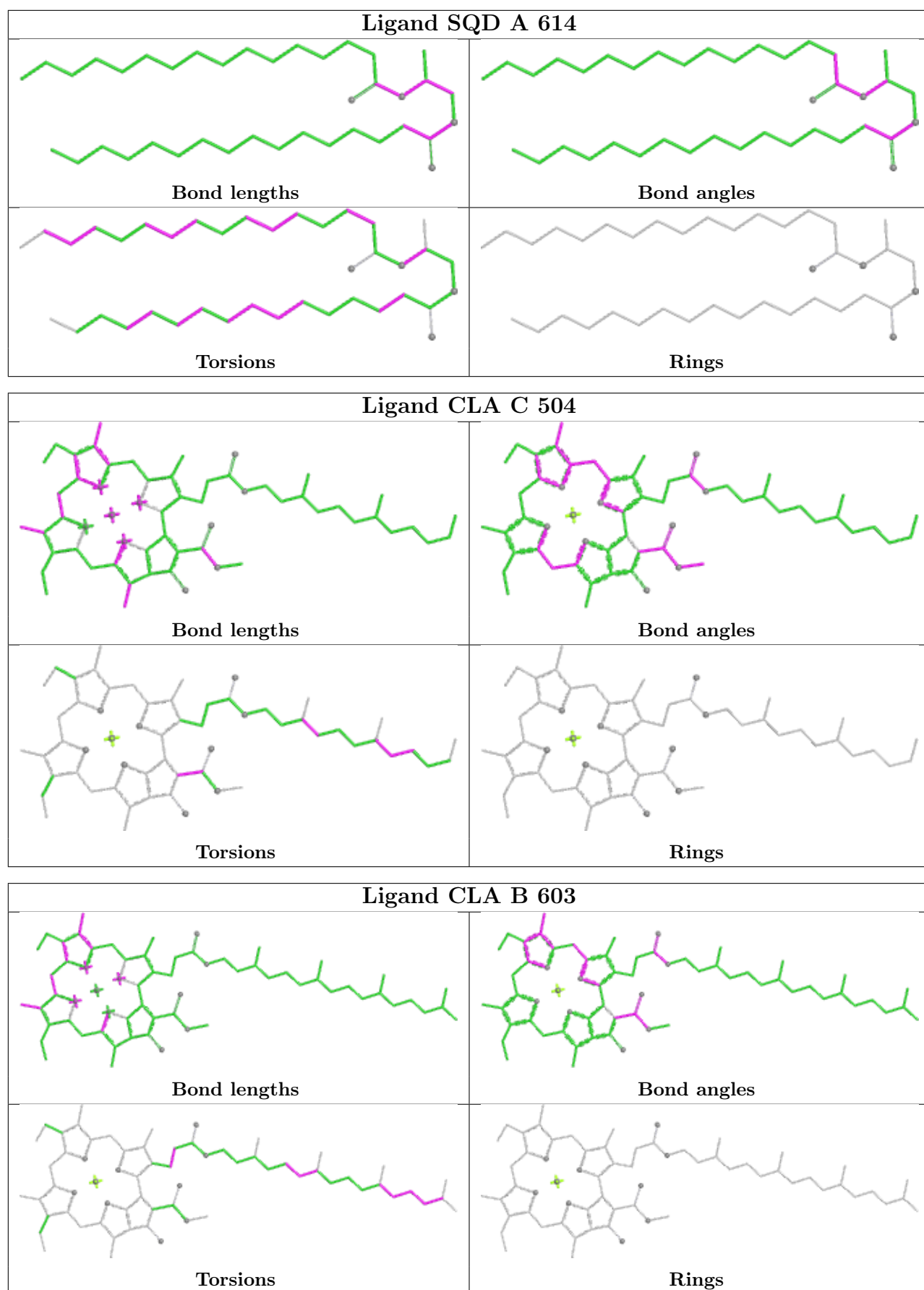
Ligand CLA b 601

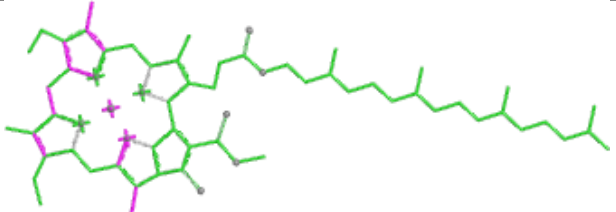
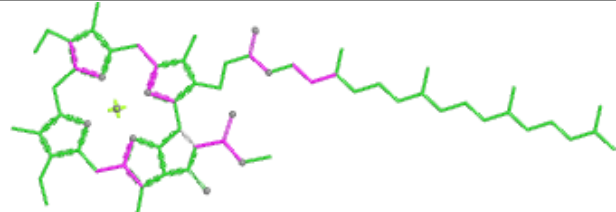
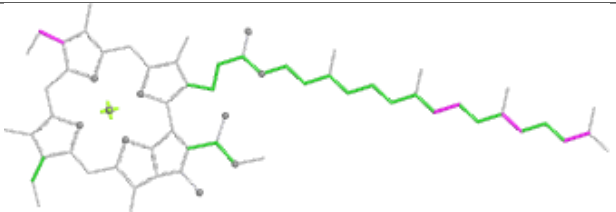
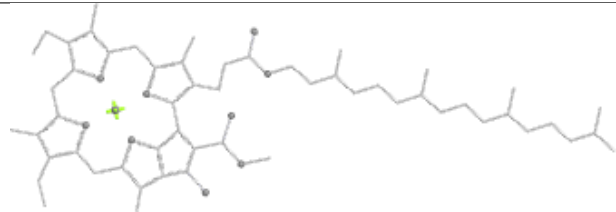


Ligand HEM e 101

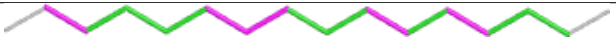
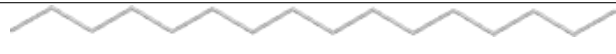


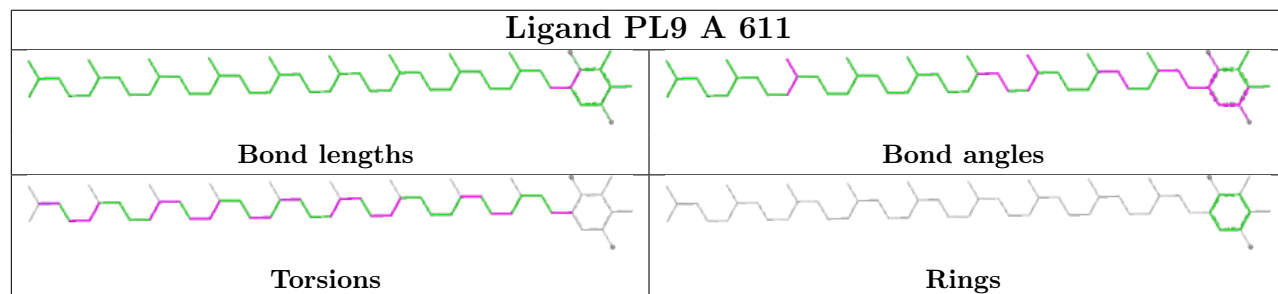
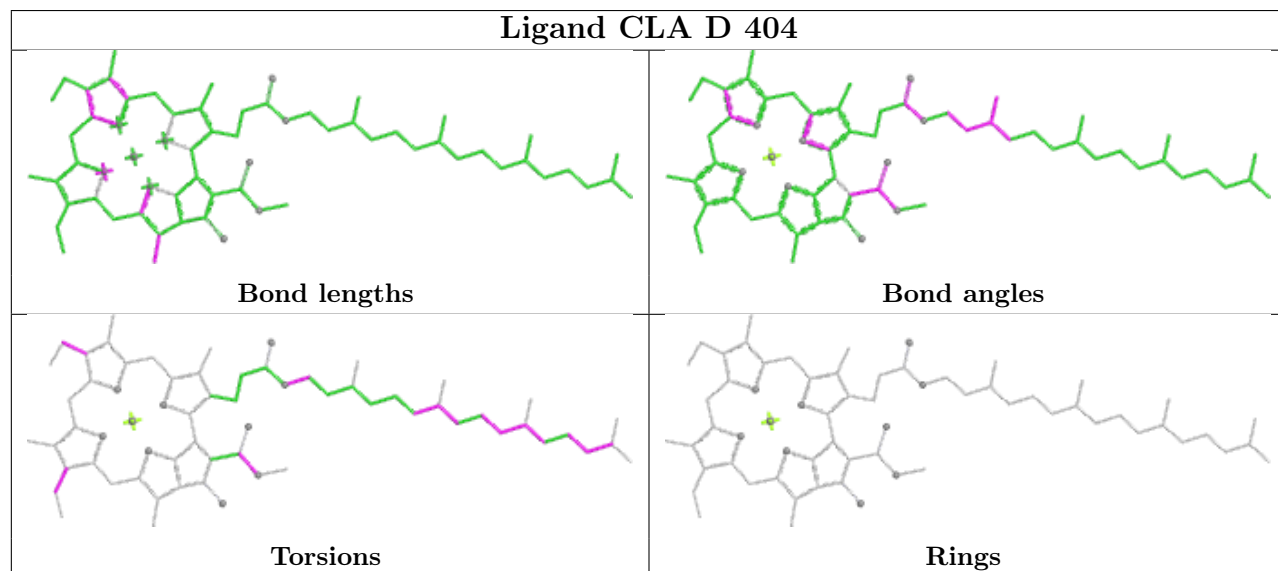
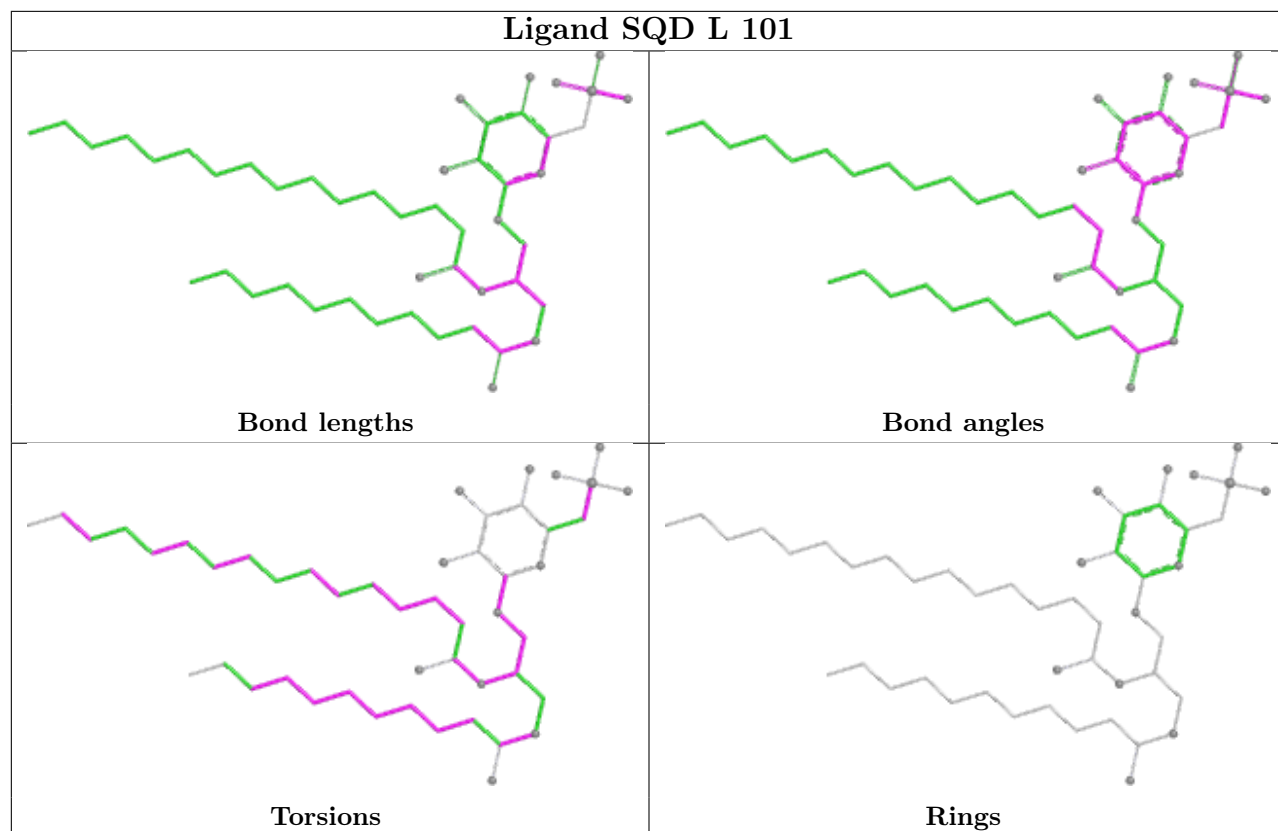


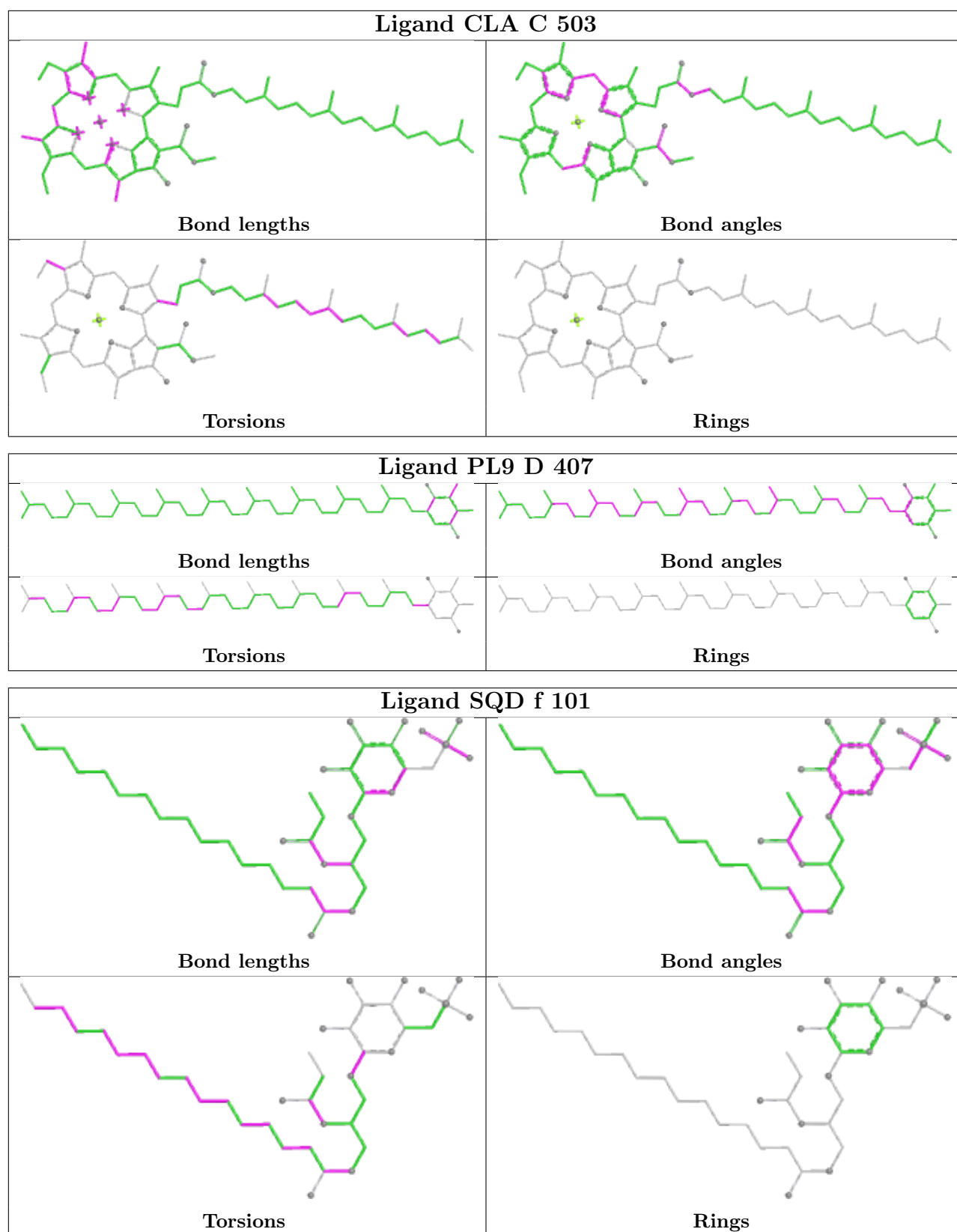


Ligand CLA A 607			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

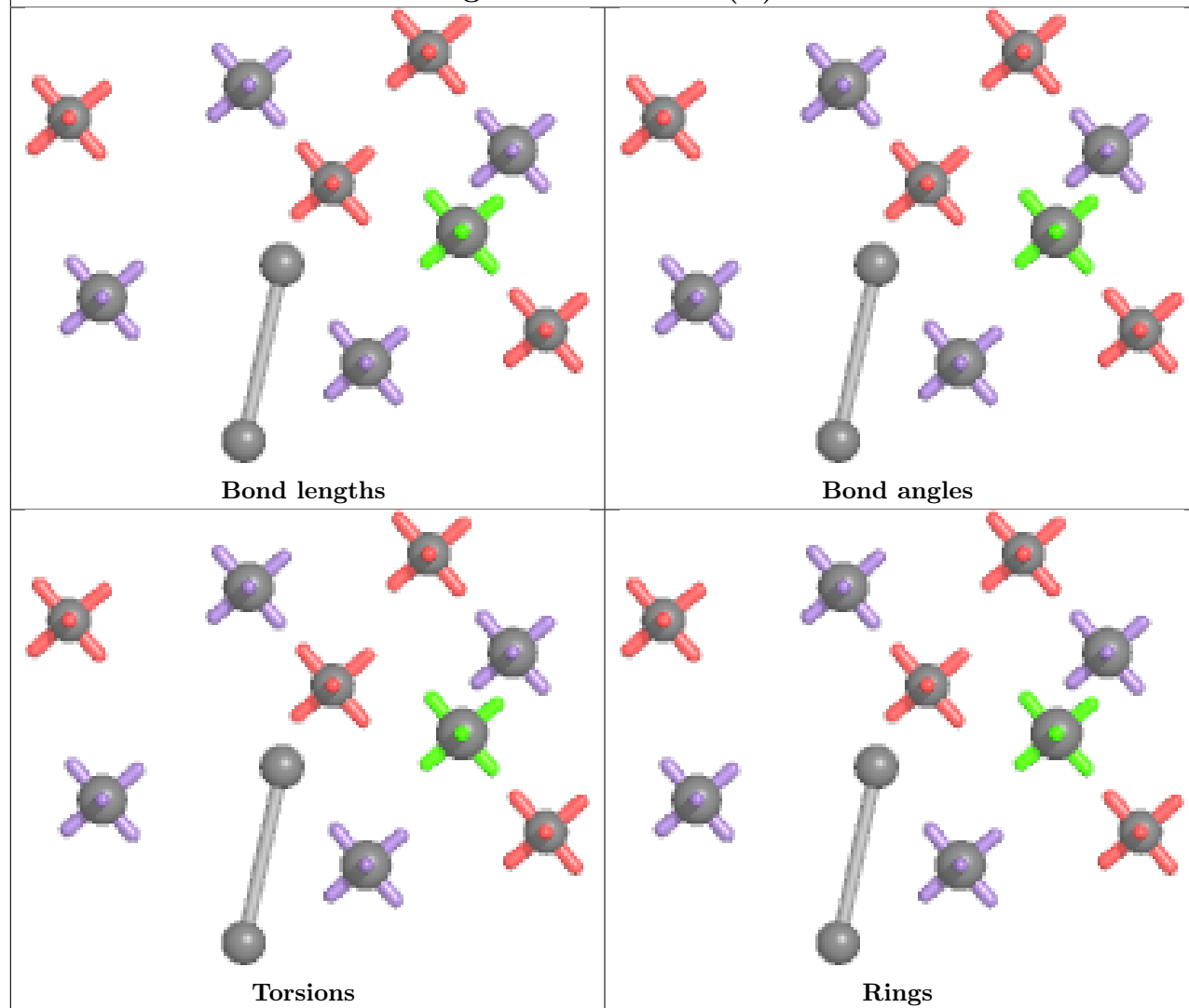
Ligand STE I 101			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand STE b 620			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

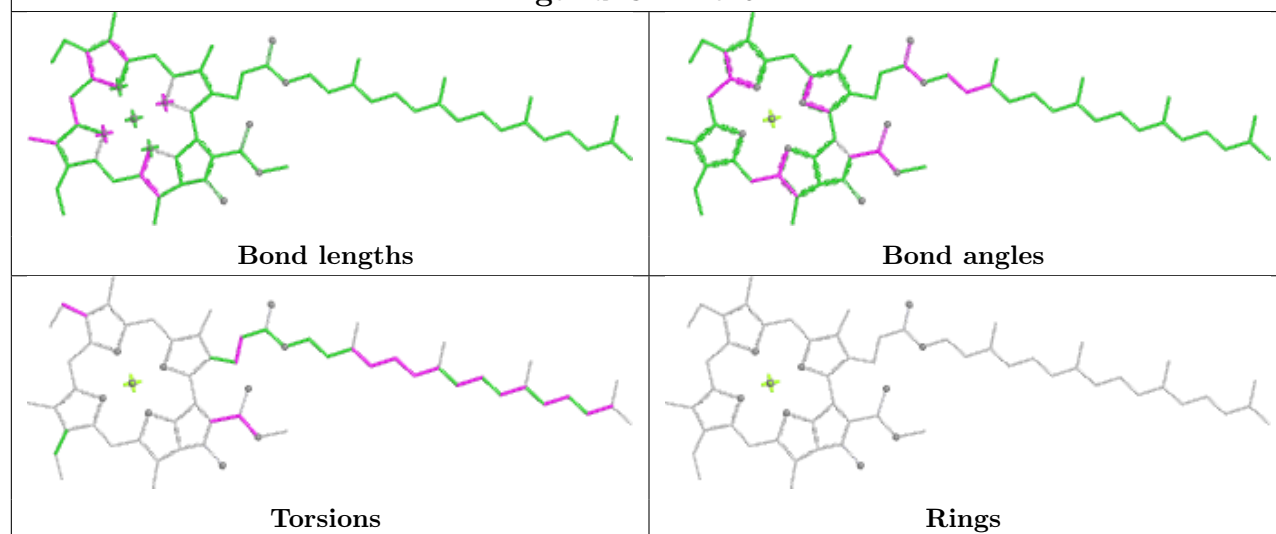


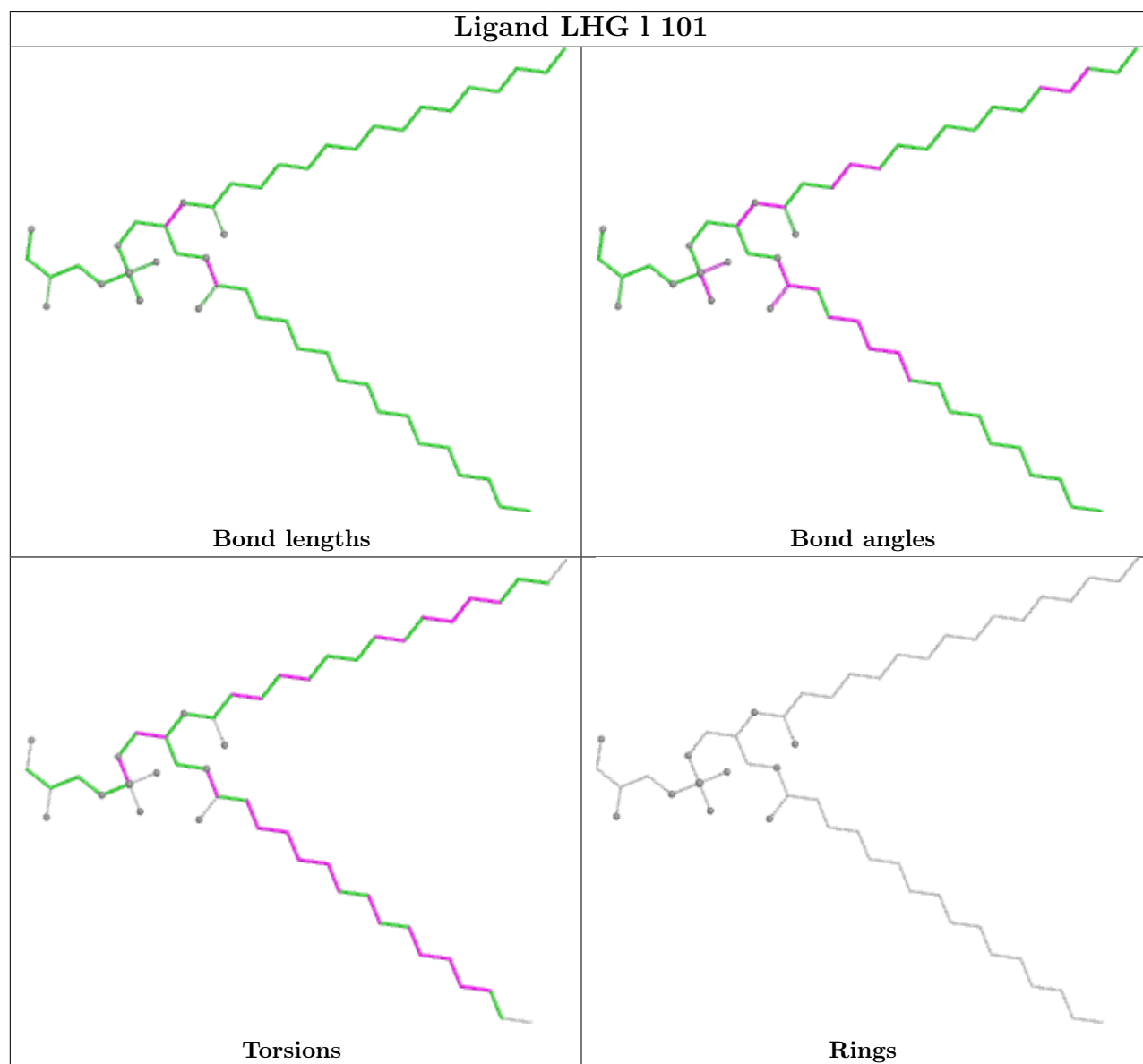
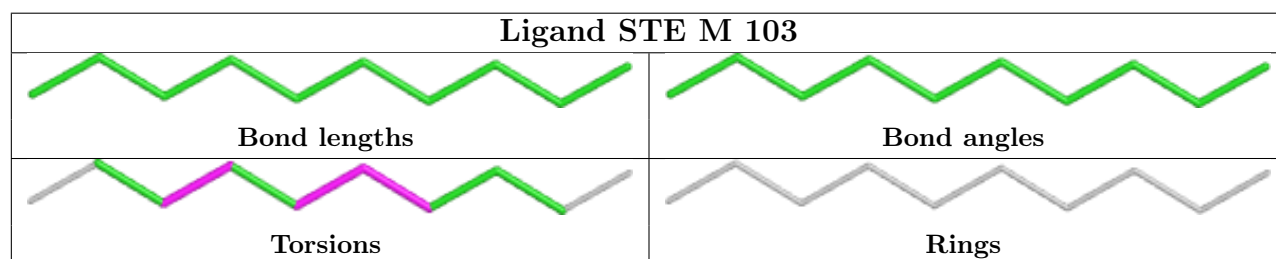
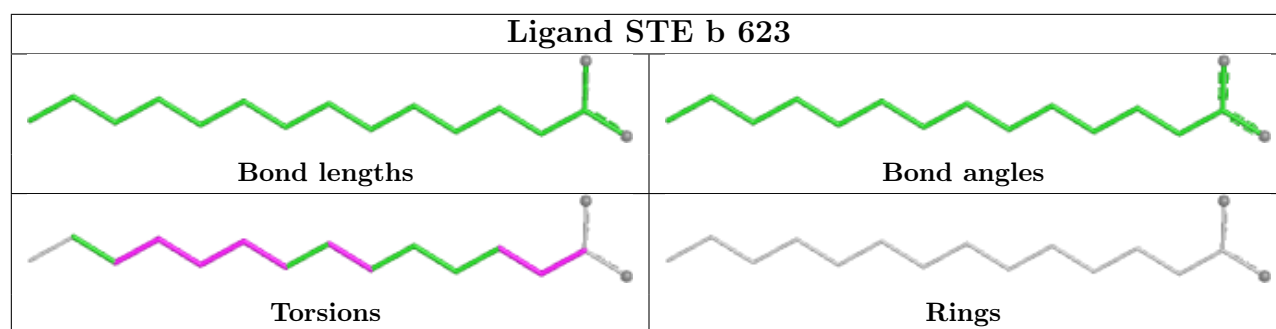


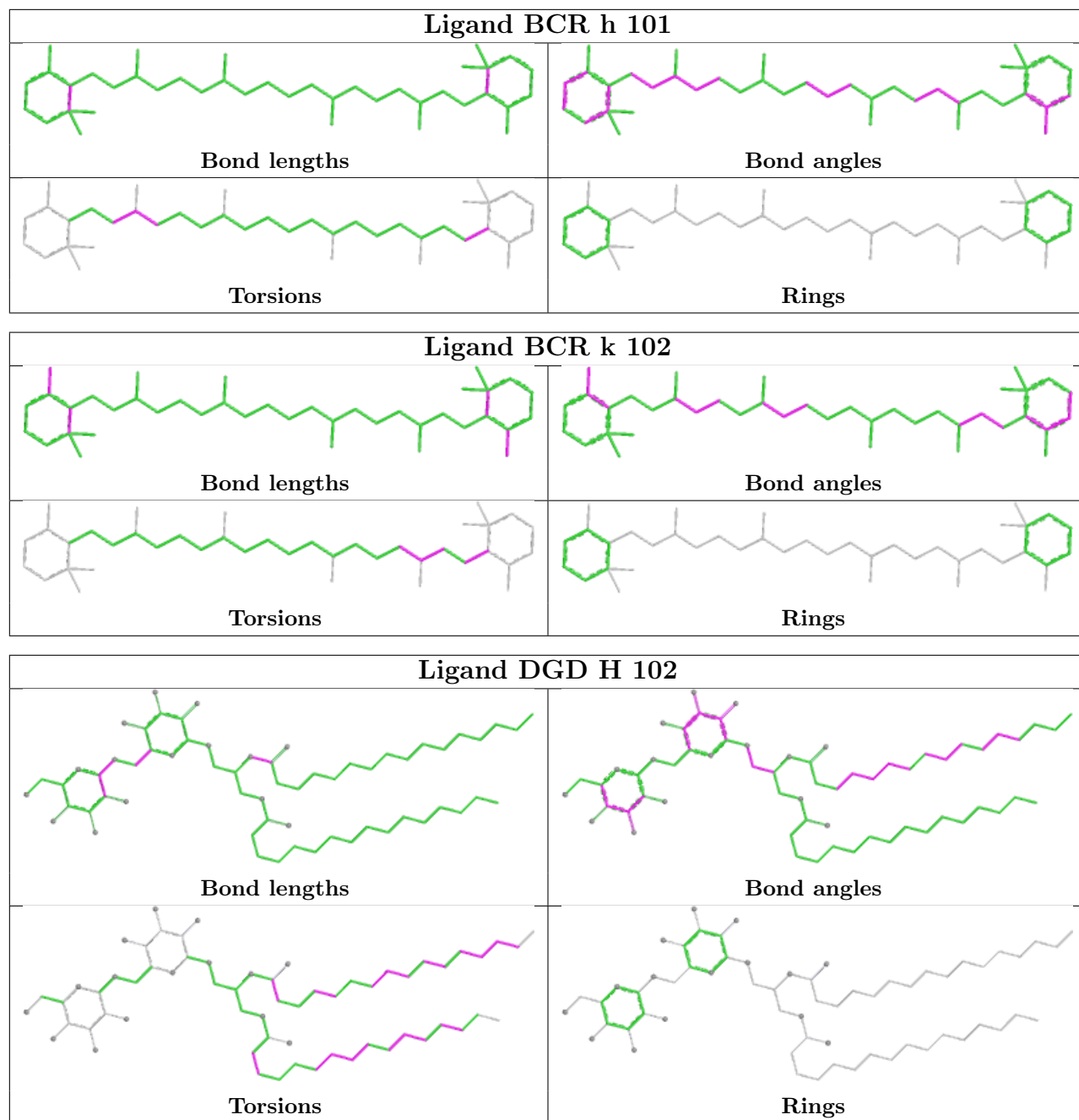
Ligand OEY A 601 (B)

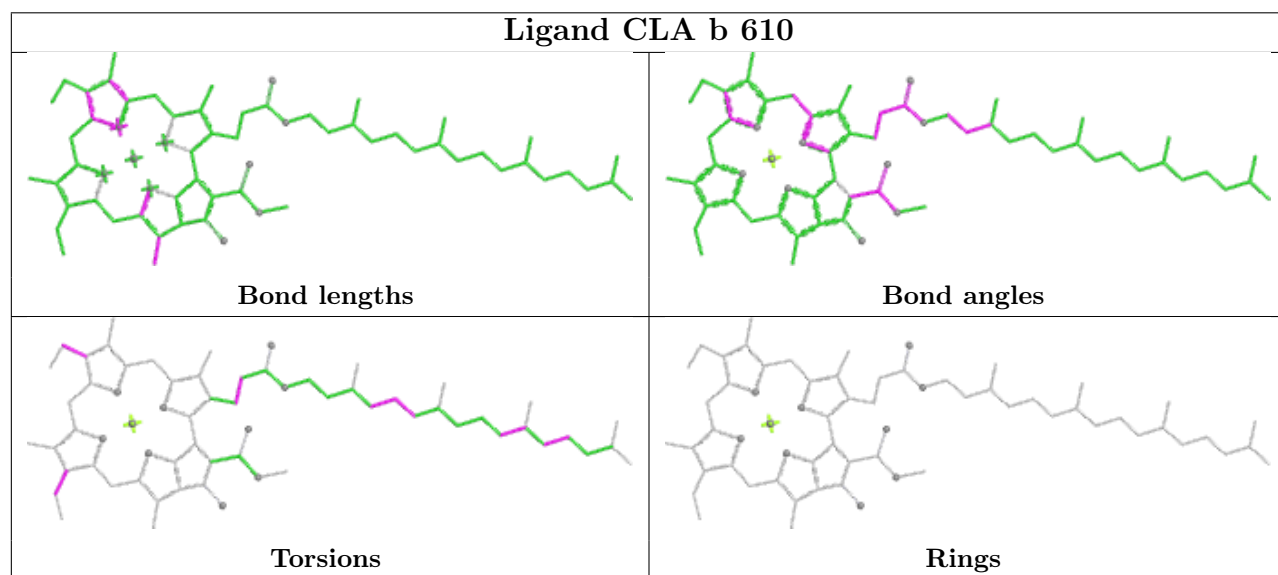
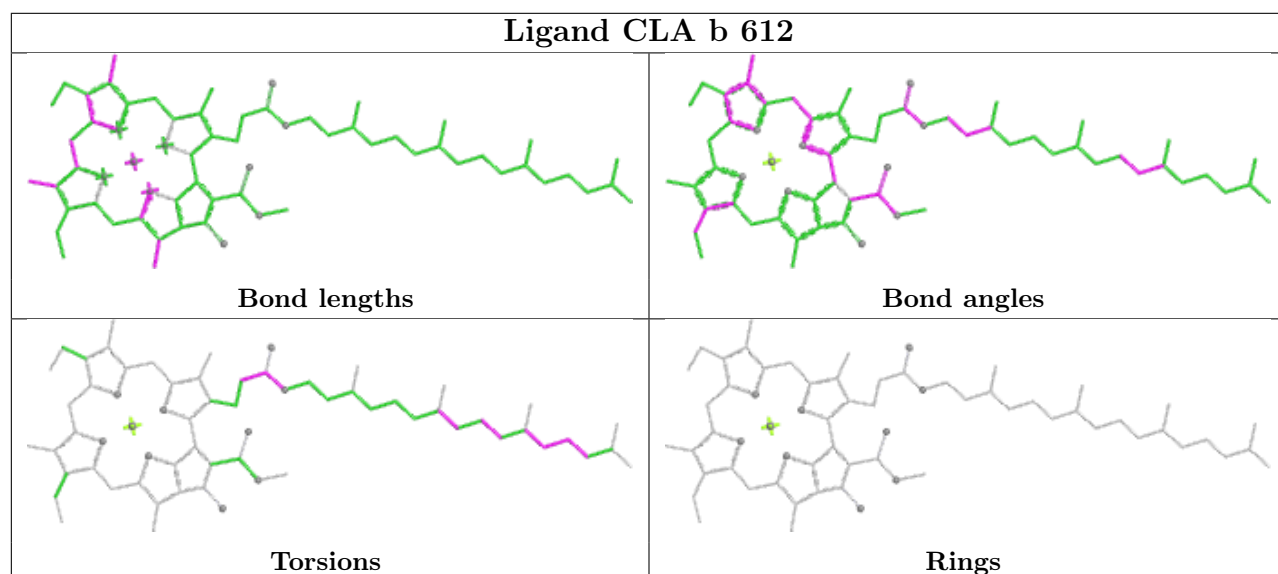
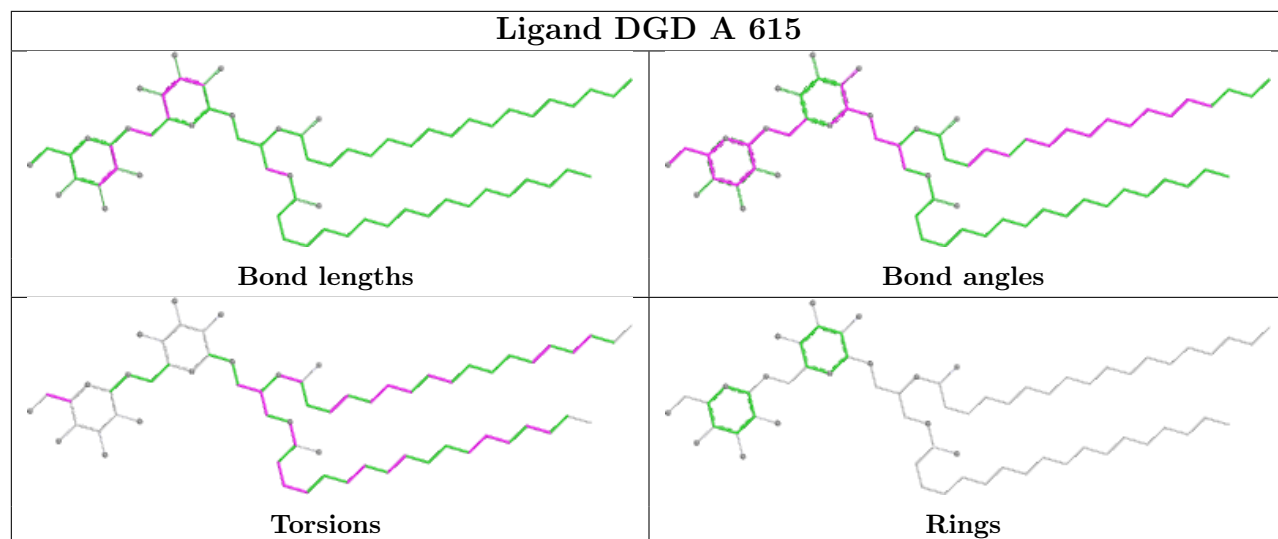


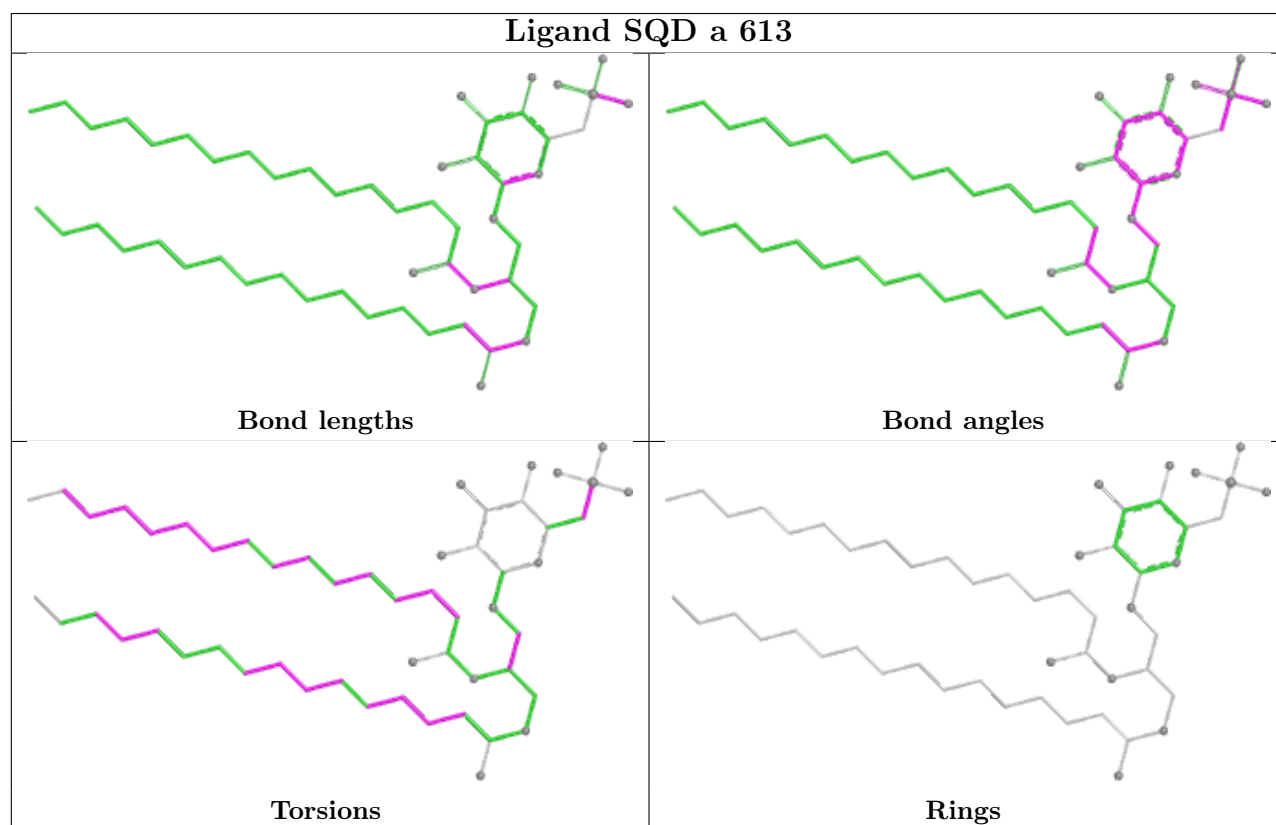
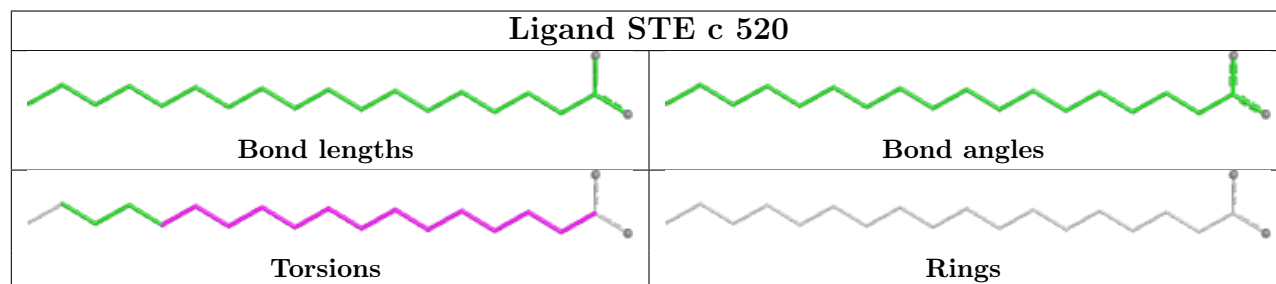
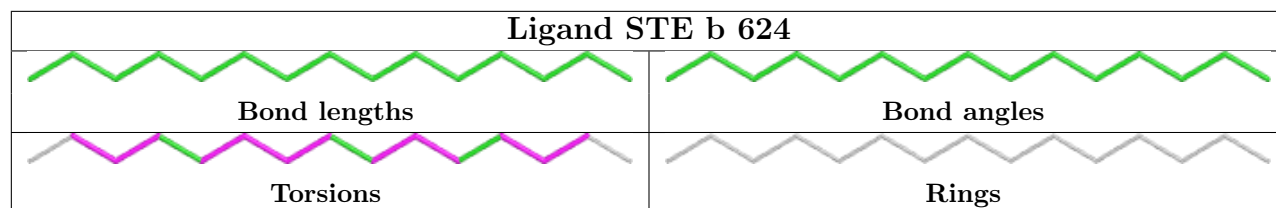
Ligand CLA b 614

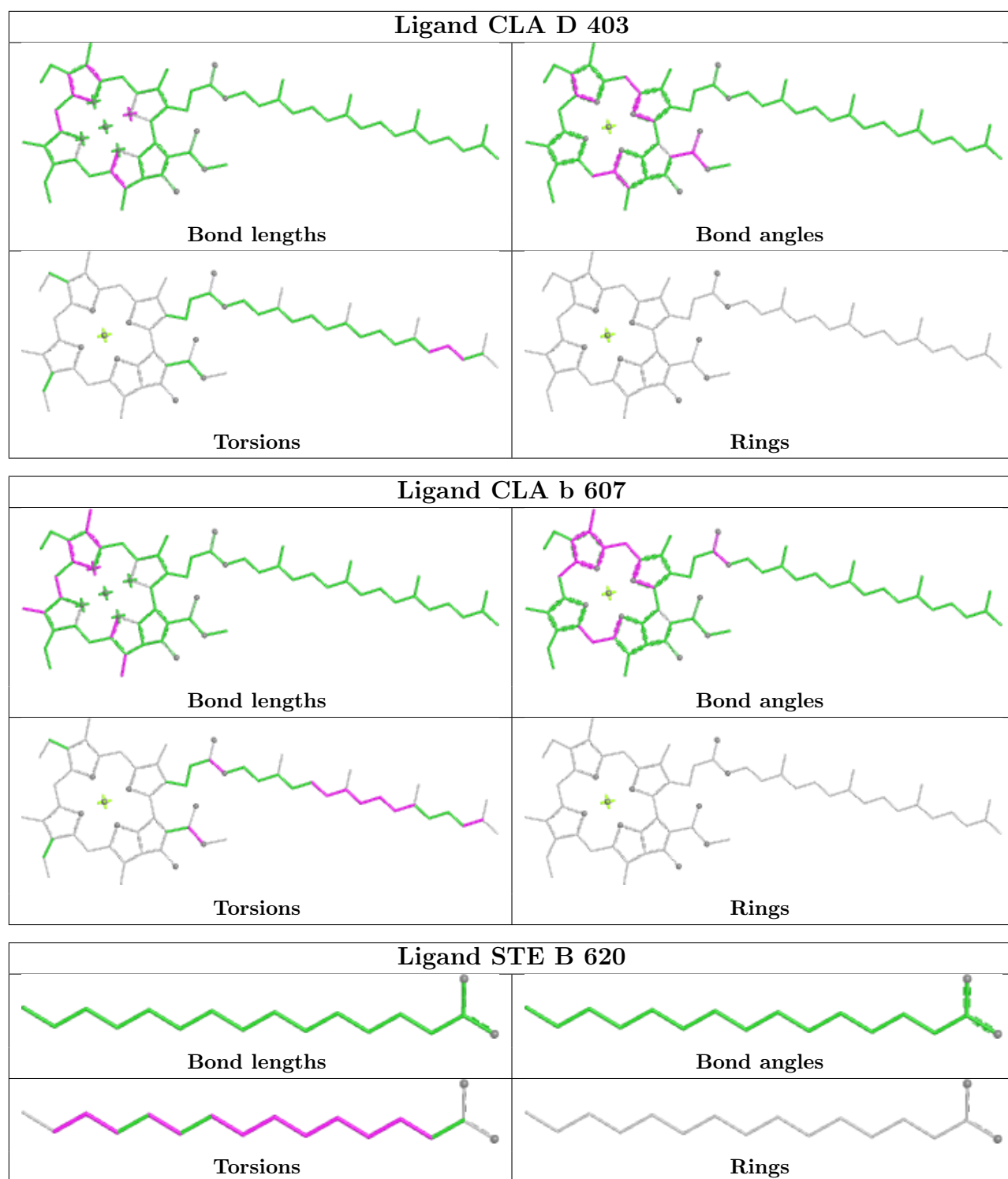












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.37	0 100 100	12, 31, 50, 83	64 (19%)
1	a	334/344 (97%)	-0.26	1 (0%) 90 91	14, 33, 59, 81	64 (19%)
2	B	505/510 (99%)	-0.25	3 (0%) 85 87	21, 35, 63, 86	4 (0%)
2	b	505/510 (99%)	-0.14	4 (0%) 82 84	28, 39, 70, 108	0
3	C	442/461 (95%)	-0.22	0 100 100	15, 38, 54, 78	11 (2%)
3	c	451/461 (97%)	-0.08	3 (0%) 84 85	15, 42, 63, 101	12 (2%)
4	D	341/352 (96%)	-0.39	0 100 100	16, 33, 49, 81	2 (0%)
4	d	341/352 (96%)	-0.25	0 100 100	17, 37, 60, 83	3 (0%)
5	E	82/84 (97%)	0.35	3 (3%) 45 49	35, 53, 70, 84	1 (1%)
5	e	82/84 (97%)	0.48	1 (1%) 76 79	41, 60, 81, 90	0
6	F	34/45 (75%)	-0.04	0 100 100	38, 46, 62, 86	0
6	f	34/45 (75%)	0.25	0 100 100	45, 53, 79, 90	0
7	H	65/66 (98%)	-0.03	2 (3%) 51 55	34, 42, 57, 74	0
7	h	63/66 (95%)	0.28	1 (1%) 70 74	43, 53, 64, 67	0
8	I	35/38 (92%)	-0.14	0 100 100	34, 41, 66, 78	0
8	i	35/38 (92%)	-0.03	0 100 100	35, 42, 70, 89	0
9	J	36/40 (90%)	0.22	1 (2%) 55 59	36, 50, 82, 91	0
9	j	36/40 (90%)	0.35	2 (5%) 30 34	40, 57, 91, 102	0
10	K	37/46 (80%)	0.16	0 100 100	44, 52, 66, 72	0
10	k	37/46 (80%)	0.28	0 100 100	53, 57, 76, 83	0
11	L	37/37 (100%)	-0.35	0 100 100	27, 32, 61, 64	0
11	l	36/37 (97%)	-0.43	0 100 100	28, 33, 72, 92	0
12	M	32/36 (88%)	-0.33	0 100 100	30, 35, 62, 72	0
12	m	31/36 (86%)	-0.36	0 100 100	30, 36, 57, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.01	4 (1%) 70 74	29, 45, 82, 141	1 (0%)
13	o	244/272 (89%)	-0.01	3 (1%) 76 79	30, 44, 79, 131	0
14	T	29/32 (90%)	-0.38	1 (3%) 48 52	29, 34, 60, 78	0
14	t	29/32 (90%)	-0.32	1 (3%) 48 52	31, 35, 70, 88	0
15	U	97/134 (72%)	-0.03	0 100 100	34, 46, 71, 98	0
15	u	97/134 (72%)	-0.12	0 100 100	34, 43, 58, 83	0
16	V	137/163 (84%)	-0.16	0 100 100	32, 43, 56, 76	0
16	v	137/163 (84%)	0.12	0 100 100	37, 49, 71, 88	0
17	Y	27/46 (58%)	0.98	0 100 100	52, 71, 95, 98	0
17	y	30/46 (65%)	0.85	0 100 100	64, 77, 85, 100	0
18	X	38/41 (92%)	0.13	1 (2%) 57 61	44, 52, 68, 71	0
18	x	39/41 (95%)	0.32	0 100 100	50, 61, 85, 100	0
19	Z	62/62 (100%)	0.90	4 (6%) 25 28	55, 69, 112, 127	0
19	z	62/62 (100%)	0.92	4 (6%) 25 28	63, 77, 115, 117	0
20	R	34/41 (82%)	0.94	1 (2%) 53 57	61, 70, 81, 89	0
20	r	31/41 (75%)	1.30	5 (16%) 4 5	72, 88, 113, 121	0
All	All	5302/5700 (93%)	-0.09	45 (0%) 82 84	12, 40, 75, 141	162 (3%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.8
20	R	35	LEU	4.0
5	e	79	PHE	3.7
14	T	30	THR	3.4
19	Z	33	TRP	3.3
19	Z	41	PHE	3.2
7	h	64	ALA	3.1
13	O	60	ARG	3.0
3	c	23	ALA	3.0
18	X	2	THR	2.9
13	O	59	LYS	2.9
19	Z	62	VAL	2.8
5	E	3	GLY	2.8
3	c	24	THR	2.8
2	b	491	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
14	t	30	THR	2.6
5	E	79	PHE	2.5
7	H	41	PHE	2.5
19	z	33	TRP	2.5
3	c	143	TYR	2.5
13	O	58	ASN	2.5
9	j	6	GLY	2.5
2	B	479[A]	PHE	2.5
7	H	65	LEU	2.4
1	a	248	ILE	2.4
20	r	28	VAL	2.3
19	z	27	TYR	2.3
20	r	14	LEU	2.3
2	b	495	PHE	2.2
2	b	486	LEU	2.2
19	z	30	PRO	2.1
2	B	495	PHE	2.1
13	o	57	LYS	2.1
20	r	3	TRP	2.1
13	o	56	PRO	2.1
5	E	22[A]	ILE	2.1
9	J	5	GLY	2.1
2	B	293	ALA	2.1
20	r	26	TYR	2.1
9	j	8	ILE	2.1
19	z	40	ILE	2.1
19	Z	40	ILE	2.0
2	b	499	VAL	2.0
13	O	133	VAL	2.0
20	r	12	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.93	0.12	41,53,66,68	0
12	FME	m	1	10/11	0.93	0.10	32,53,69,70	0
14	FME	t	1	10/11	0.93	0.09	35,42,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.95	0.08	38,52,60,65	0
8	FME	I	1	10/11	0.95	0.07	39,52,59,61	0
14	FME	T	1	10/11	0.95	0.08	36,44,53,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	H	103	18/20	0.75	0.18	56,63,72,72	0
29	LMG	b	622	55/55	0.78	0.17	53,66,81,85	0
32	STE	L	103	12/20	0.79	0.18	48,53,65,67	0
32	STE	a	616	12/20	0.79	0.13	41,57,67,73	0
32	STE	b	621	20/20	0.79	0.15	42,56,70,72	0
29	LMG	d	410	23/55	0.80	0.18	51,61,75,75	0
32	STE	b	625	20/20	0.80	0.14	49,58,70,73	0
25	CLA	b	601	65/65	0.81	0.13	46,66,83,93	0
28	PL9	A	611	55/55	0.81	0.17	43,59,72,76	0
31	DGD	a	614	44/66	0.81	0.15	40,54,74,82	0
32	STE	b	623	16/20	0.81	0.16	50,60,78,82	0
28	PL9	a	611	55/55	0.81	0.17	45,63,78,82	0
32	STE	c	522	12/20	0.81	0.12	58,68,79,85	0
34	LHG	E	101	49/49	0.81	0.15	46,74,91,94	0
29	LMG	c	521	48/55	0.82	0.15	41,68,89,92	0
32	STE	d	413	20/20	0.82	0.14	45,55,66,67	0
32	STE	t	104	18/20	0.82	0.14	43,52,77,83	0
32	STE	b	626	10/20	0.82	0.14	47,49,57,58	0
32	STE	I	101	15/20	0.83	0.14	43,53,69,73	0
32	STE	B	625	16/20	0.83	0.16	46,60,71,71	0
32	STE	a	615	10/20	0.83	0.14	43,51,57,58	0
29	LMG	D	412	33/55	0.83	0.14	36,52,75,79	0
32	STE	J	101	12/20	0.84	0.13	50,59,67,68	0
34	LHG	e	102	42/49	0.84	0.13	62,79,89,95	0
32	STE	B	620	17/20	0.85	0.11	39,49,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	DGD	A	615	66/66	0.85	0.12	47,59,68,71	0
32	STE	b	620	16/20	0.85	0.17	38,49,62,63	0
29	LMG	c	519	37/55	0.85	0.12	47,62,72,74	0
32	STE	C	520	12/20	0.86	0.13	38,44,61,64	0
32	STE	C	521	12/20	0.86	0.12	44,51,56,56	0
32	STE	X	101	20/20	0.86	0.12	38,48,68,69	0
32	STE	R	101	12/20	0.86	0.13	61,68,87,87	0
30	SQD	f	101	41/54	0.87	0.13	63,74,84,88	0
32	STE	c	520	20/20	0.87	0.11	50,54,77,81	0
32	STE	B	624	12/20	0.87	0.12	51,55,65,71	0
32	STE	d	412	17/20	0.87	0.13	44,54,69,70	0
30	SQD	t	102	36/54	0.87	0.12	34,53,67,70	0
32	STE	t	103	14/20	0.87	0.11	39,46,53,62	0
29	LMG	C	519	48/55	0.87	0.12	44,62,77,82	0
30	SQD	A	614	39/54	0.87	0.12	39,53,69,74	0
32	STE	C	522	16/20	0.87	0.13	44,49,57,59	0
25	CLA	B	601	65/65	0.88	0.11	38,54,75,79	0
30	SQD	B	622	54/54	0.88	0.11	38,58,78,81	0
32	STE	B	623	12/20	0.88	0.12	37,49,57,59	0
30	SQD	L	101	49/54	0.88	0.10	37,53,76,83	0
32	STE	j	101	12/20	0.88	0.12	51,59,64,67	0
32	STE	l	102	18/20	0.88	0.14	32,44,65,68	0
29	LMG	c	523	49/55	0.88	0.10	36,50,78,82	0
32	STE	b	624	15/20	0.88	0.13	45,52,70,74	0
29	LMG	A	612	48/55	0.88	0.11	43,54,65,71	0
29	LMG	m	101	51/55	0.88	0.11	33,47,64,67	0
29	LMG	B	621	28/55	0.89	0.12	37,49,60,61	0
27	BCR	k	101	40/40	0.89	0.13	52,61,69,72	0
27	BCR	K	102	40/40	0.89	0.11	40,50,58,62	0
29	LMG	M	101	51/55	0.89	0.10	30,49,64,69	0
27	BCR	d	405	40/40	0.90	0.11	43,49,83,87	0
27	BCR	h	101	40/40	0.90	0.11	40,52,63,66	0
30	SQD	D	409	36/54	0.90	0.12	45,62,74,79	0
32	STE	M	103	10/20	0.91	0.12	30,45,53,58	0
25	CLA	c	512	65/65	0.91	0.11	41,55,79,83	0
27	BCR	c	514	40/40	0.91	0.10	48,57,63,67	0
30	SQD	a	613	54/54	0.91	0.11	38,55,77,82	0
27	BCR	B	618	40/40	0.91	0.09	28,38,49,52	0
27	BCR	D	406	40/40	0.91	0.11	32,43,69,72	0
27	BCR	H	101	40/40	0.91	0.10	33,44,52,55	0
27	BCR	b	619	40/40	0.92	0.10	33,47,61,63	0
29	LMG	d	411	44/55	0.92	0.10	43,52,72,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	c	513	65/65	0.92	0.10	48,62,83,88	0
25	CLA	C	513	65/65	0.92	0.10	48,56,82,87	0
31	DGD	C	517	62/66	0.92	0.10	35,46,84,99	0
31	DGD	H	102	62/66	0.92	0.09	31,41,52,54	0
27	BCR	K	101	40/40	0.92	0.11	37,54,60,63	0
31	DGD	c	517	62/66	0.92	0.09	42,48,78,81	0
27	BCR	B	619	40/40	0.92	0.08	31,40,53,54	0
29	LMG	D	408	51/55	0.92	0.11	34,46,66,70	0
27	BCR	T	101	40/40	0.93	0.07	31,40,46,50	0
27	BCR	b	617	40/40	0.93	0.08	35,43,49,51	0
27	BCR	b	618	40/40	0.93	0.08	25,36,47,48	0
31	DGD	h	102	62/66	0.93	0.08	32,44,53,56	0
27	BCR	k	102	40/40	0.93	0.12	49,53,60,67	0
27	BCR	t	101	40/40	0.93	0.08	27,38,45,48	0
25	CLA	C	512	65/65	0.93	0.10	35,46,77,84	0
30	SQD	A	613	52/54	0.93	0.10	36,52,71,78	0
34	LHG	d	407	49/49	0.93	0.10	33,46,62,63	0
34	LHG	d	409	39/49	0.93	0.10	36,43,58,59	0
27	BCR	C	514	40/40	0.93	0.09	31,39,45,54	0
25	CLA	B	606	65/65	0.94	0.08	27,37,57,68	0
31	DGD	c	518	62/66	0.94	0.09	34,46,69,77	0
25	CLA	C	501	65/65	0.94	0.07	27,35,44,46	0
27	BCR	C	515	40/40	0.94	0.10	35,47,57,62	0
25	CLA	C	502	65/65	0.94	0.08	31,38,46,54	0
25	CLA	b	616	60/65	0.94	0.09	31,42,75,83	0
25	CLA	c	503	65/65	0.94	0.08	36,44,48,54	0
25	CLA	c	504	60/65	0.94	0.08	29,43,64,72	0
25	CLA	c	505	65/65	0.94	0.08	32,38,54,55	0
25	CLA	c	506	65/65	0.94	0.09	40,46,72,75	0
25	CLA	c	511	65/65	0.94	0.10	41,55,63,66	0
25	CLA	C	503	65/65	0.94	0.07	34,42,46,51	0
25	CLA	C	510	65/65	0.94	0.07	31,42,51,67	0
31	DGD	C	516	62/66	0.94	0.09	26,34,66,70	0
32	STE	M	102	15/20	0.94	0.09	40,46,55,60	0
33	BCT	d	401	4/4	0.94	0.08	36,36,40,46	0
34	LHG	D	411	47/49	0.94	0.10	30,42,63,74	0
27	BCR	c	515	40/40	0.94	0.09	33,45,54,56	0
31	DGD	C	518	62/66	0.94	0.08	33,43,68,70	0
27	BCR	B	617	40/40	0.94	0.07	26,39,45,49	0
25	CLA	C	511	65/65	0.94	0.09	31,46,58,60	0
25	CLA	b	614	65/65	0.95	0.08	30,38,66,71	0
25	CLA	b	615	65/65	0.95	0.07	28,38,50,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	506	65/65	0.95	0.09	32,43,72,77	0
25	CLA	c	502	65/65	0.95	0.07	33,40,48,57	0
25	CLA	C	508	65/65	0.95	0.08	32,38,86,92	0
25	CLA	C	509	65/65	0.95	0.08	32,39,52,56	0
25	CLA	B	610	65/65	0.95	0.07	23,31,38,41	0
25	CLA	B	612	65/65	0.95	0.07	24,31,37,46	0
25	CLA	c	507	65/65	0.95	0.08	34,41,51,56	0
25	CLA	c	508	64/65	0.95	0.08	35,43,81,94	0
25	CLA	c	509	65/65	0.95	0.09	37,45,57,59	0
25	CLA	c	510	65/65	0.95	0.07	36,45,51,58	0
25	CLA	B	616	60/65	0.95	0.09	28,36,71,73	0
25	CLA	C	504	59/65	0.95	0.07	31,38,68,74	0
25	CLA	a	606	65/65	0.95	0.07	23,30,37,48	0
28	PL9	D	407	55/55	0.95	0.07	23,31,40,43	0
25	CLA	d	404	65/65	0.95	0.08	33,41,71,83	0
31	DGD	c	516	62/66	0.95	0.09	30,41,60,64	0
28	PL9	d	406	55/55	0.95	0.07	23,34,38,42	0
26	PHO	D	402	64/64	0.95	0.07	27,34,39,41	0
26	PHO	a	608	64/64	0.95	0.07	24,30,36,41	0
26	PHO	d	402	64/64	0.95	0.07	32,38,44,46	0
27	BCR	A	610	40/40	0.95	0.07	24,33,38,41	0
33	BCT	D	401	4/4	0.95	0.07	35,35,38,38	0
25	CLA	a	607	65/65	0.95	0.09	28,38,82,87	0
25	CLA	a	609	65/65	0.95	0.08	23,30,69,73	0
34	LHG	D	413	49/49	0.95	0.09	30,39,58,61	0
25	CLA	C	505	65/65	0.95	0.08	23,36,60,62	0
25	CLA	b	602	65/65	0.95	0.08	30,40,52,56	0
25	CLA	b	606	65/65	0.95	0.08	30,38,62,71	0
25	CLA	b	609	65/65	0.95	0.08	30,42,55,66	0
34	LHG	l	101	49/49	0.95	0.08	28,41,49,52	0
35	HEM	e	101	43/43	0.95	0.10	53,59,76,87	0
27	BCR	a	610	40/40	0.96	0.06	23,33,43,49	0
25	CLA	B	615	65/65	0.96	0.07	28,36,53,59	0
25	CLA	B	603	65/65	0.96	0.07	23,31,46,51	0
25	CLA	D	403	65/65	0.96	0.06	21,29,38,41	0
25	CLA	D	404	65/65	0.96	0.07	22,28,48,52	0
25	CLA	B	604	65/65	0.96	0.07	24,31,59,63	0
25	CLA	B	605	65/65	0.96	0.07	25,31,42,46	0
25	CLA	A	607	65/65	0.96	0.08	23,33,70,78	0
25	CLA	a	612	65/65	0.96	0.06	24,31,38,46	0
25	CLA	B	607	65/65	0.96	0.07	21,30,55,65	0
25	CLA	B	608	65/65	0.96	0.06	26,32,48,53	0

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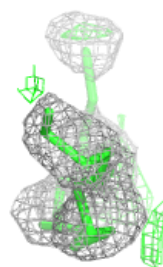
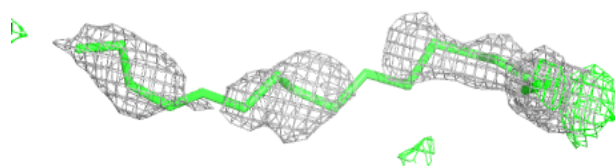
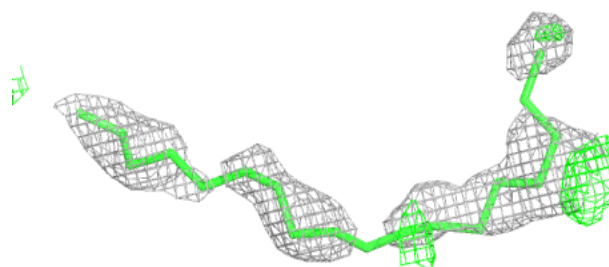
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	CLA	b	603	65/65	0.96	0.07	26,32,58,66	0
25	CLA	d	403	65/65	0.96	0.07	25,33,49,61	0
25	CLA	b	604	65/65	0.96	0.07	26,33,58,73	0
26	PHO	A	608	64/64	0.96	0.06	23,29,35,38	0
25	CLA	b	605	65/65	0.96	0.07	24,34,43,50	0
25	CLA	B	609	65/65	0.96	0.07	27,38,47,55	0
25	CLA	b	607	65/65	0.96	0.07	23,31,58,62	0
25	CLA	b	608	65/65	0.96	0.07	33,39,54,58	0
25	CLA	C	507	65/65	0.96	0.07	29,37,49,56	0
25	CLA	b	610	65/65	0.96	0.08	29,36,44,53	0
34	LHG	D	410	49/49	0.96	0.07	30,36,46,55	0
25	CLA	b	611	65/65	0.96	0.06	25,33,48,51	0
25	CLA	b	612	65/65	0.96	0.07	21,34,39,47	0
25	CLA	b	613	65/65	0.96	0.08	25,31,66,71	0
34	LHG	L	102	49/49	0.96	0.08	30,38,48,57	0
25	CLA	A	606	65/65	0.96	0.06	20,28,39,42	0
34	LHG	d	408	49/49	0.96	0.08	30,39,46,48	0
25	CLA	B	611	65/65	0.96	0.06	23,30,43,47	0
25	CLA	B	602	65/65	0.96	0.07	30,37,48,56	0
25	CLA	c	501	65/65	0.96	0.07	32,37,48,50	0
25	CLA	B	614	65/65	0.96	0.08	25,33,63,67	0
25	CLA	D	405	65/65	0.97	0.07	27,33,90,96	0
25	CLA	A	609	54/65	0.97	0.06	25,30,57,59	0
35	HEM	F	101	43/43	0.97	0.08	37,49,58,66	0
25	CLA	B	613	65/65	0.97	0.06	22,29,60,64	0
24	CL	a	605	1/1	0.98	0.07	38,38,38,38	0
24	CL	A	604	1/1	0.98	0.04	36,36,36,36	0
24	CL	a	604	1/1	0.98	0.05	38,38,38,38	0
36	HEC	V	201	43/43	0.98	0.06	28,34,39,49	0
36	HEC	v	201	43/43	0.98	0.06	32,38,45,48	0
21	OEY	a	601[B]	11/11	0.99	0.02	28,32,34,35	11
22	OEX	A	602[A]	10/10	0.99	0.03	26,36,38,39	10
22	OEX	a	602[A]	10/10	0.99	0.03	29,35,38,43	10
21	OEY	A	601[B]	11/11	0.99	0.03	29,32,34,34	11
24	CL	A	605	1/1	0.99	0.06	36,36,36,36	0
23	FE2	A	603	1/1	1.00	0.01	34,34,34,34	0
23	FE2	a	603	1/1	1.00	0.02	36,36,36,36	0

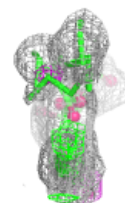
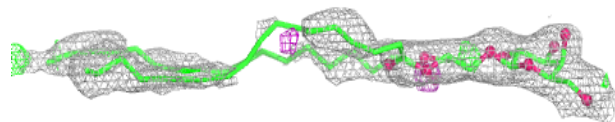
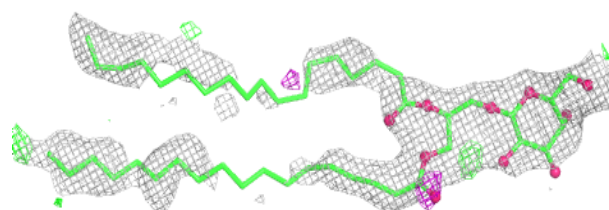
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

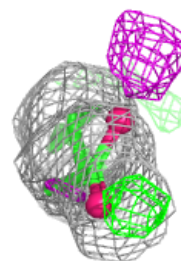
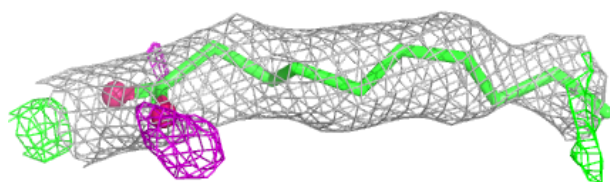
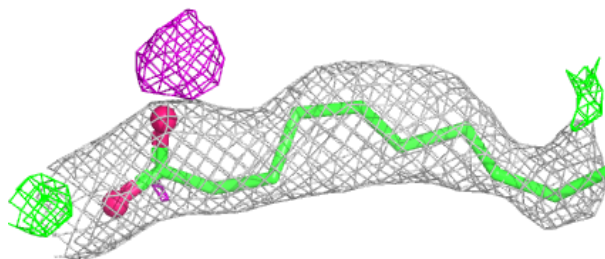
**Electron density around LMG b 622:**

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

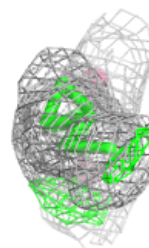
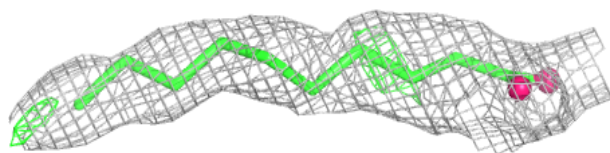
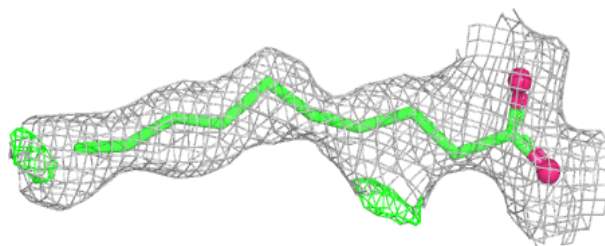


Electron density around STE L 103:

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

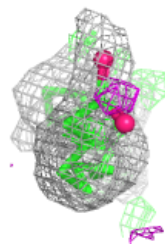
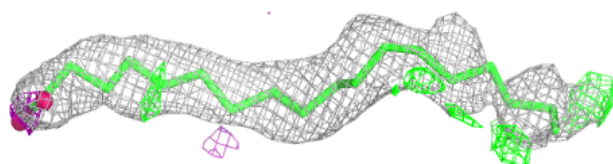
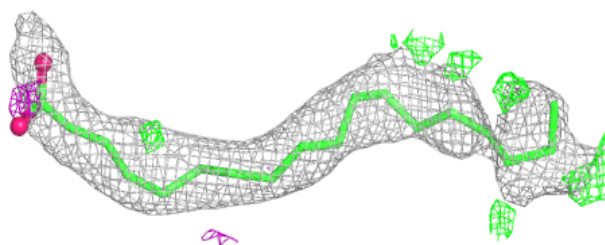
**Electron density around STE a 616:**

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

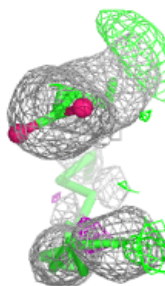
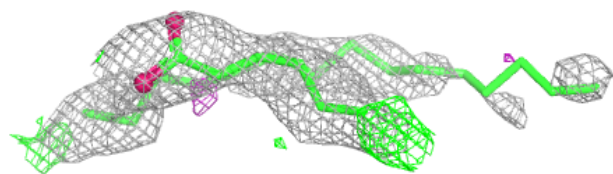
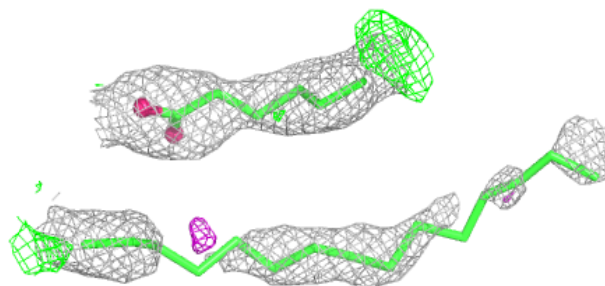


Electron density around STE b 621:

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

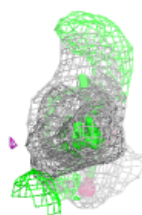
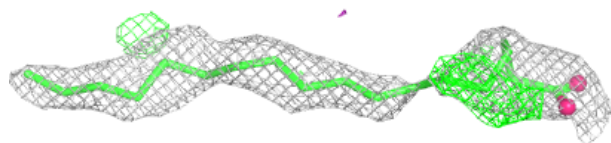
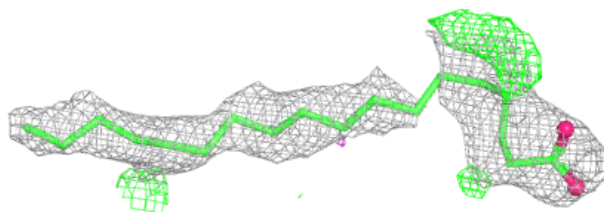
**Electron density around LMG d 410:**

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

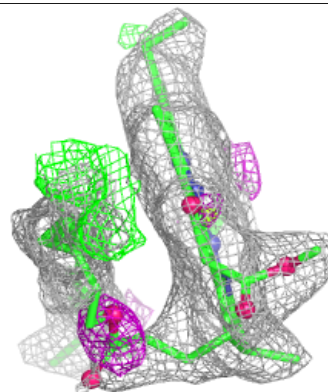
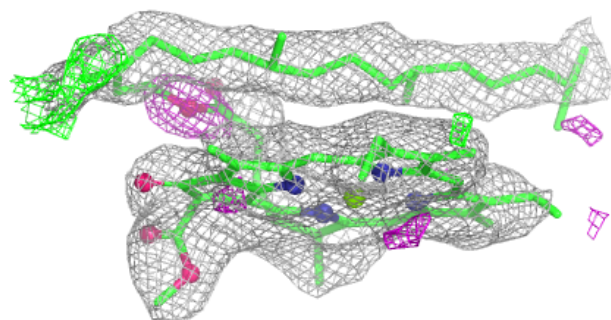
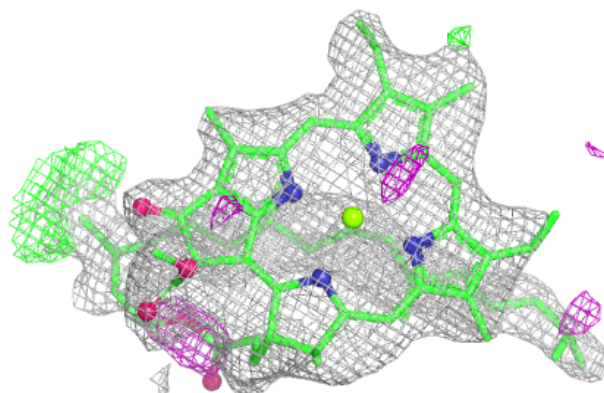


Electron density around STE b 625:

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

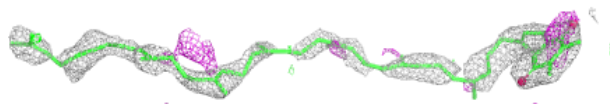
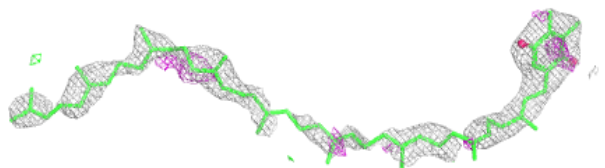
**Electron density around CLA b 601:**

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

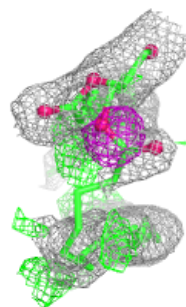
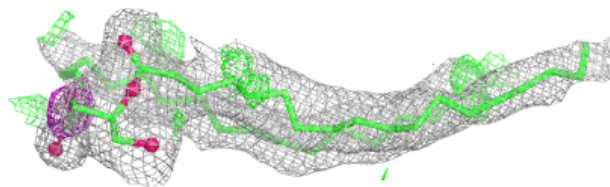
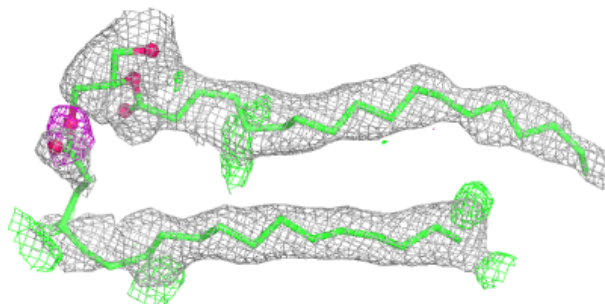


Electron density around PL9 A 611:

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

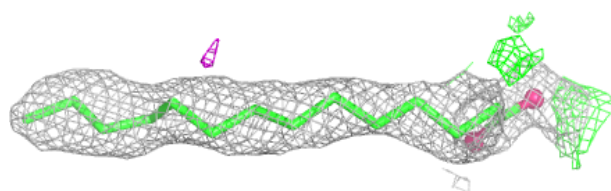
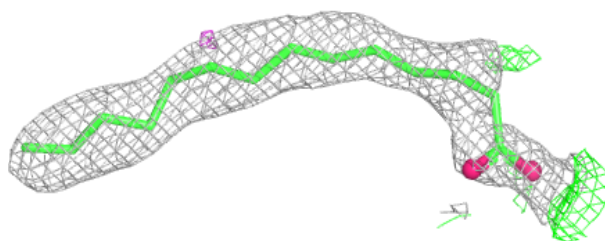
**Electron density around DGD a 614:**

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

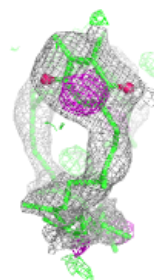
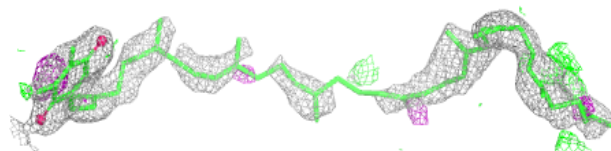
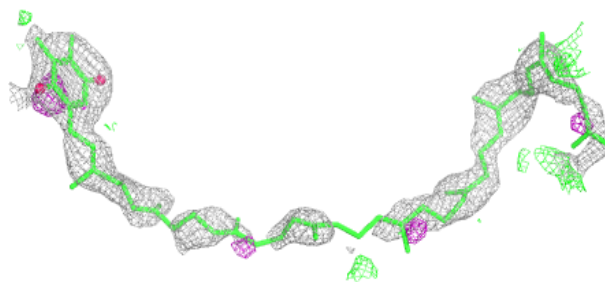


Electron density around STE b 623:

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

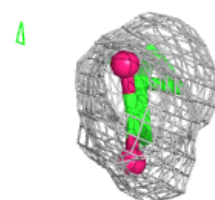
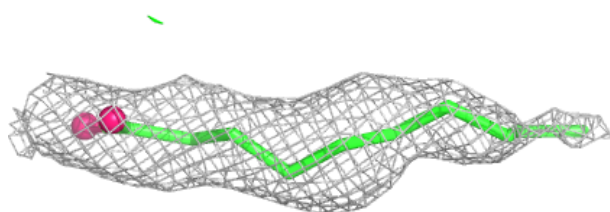
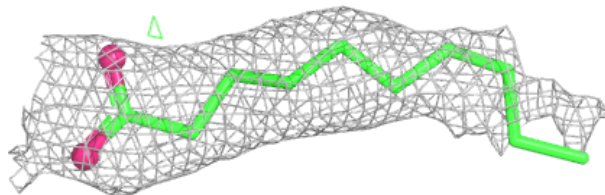
**Electron density around PL9 a 611:**

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

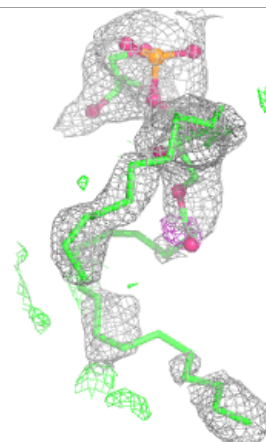
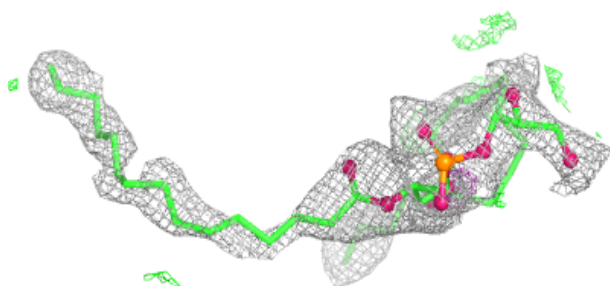
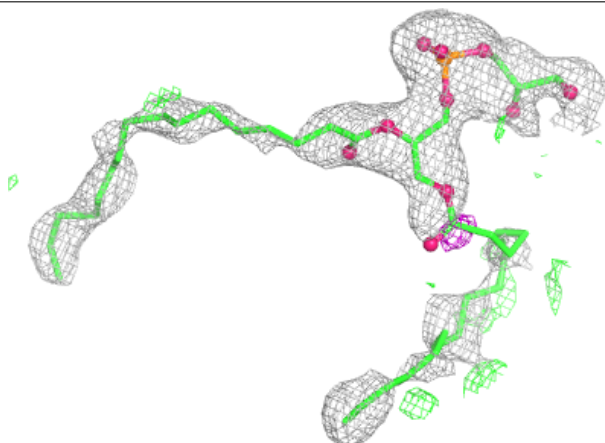


Electron density around STE c 522:

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

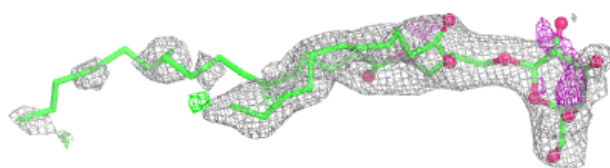
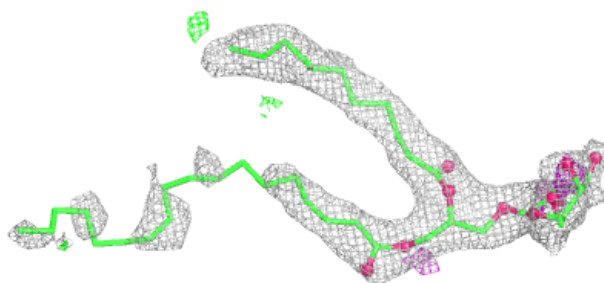
**Electron density around LHG E 101:**

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

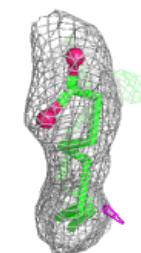
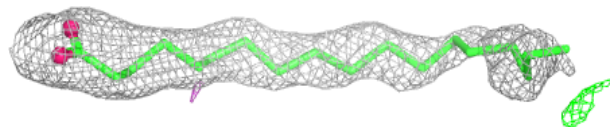
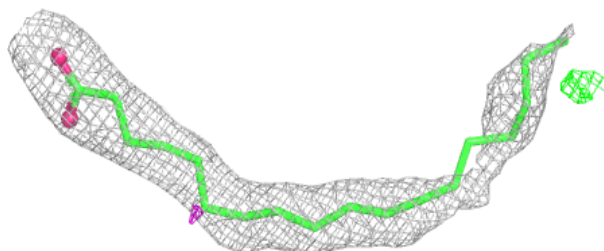


Electron density around LMG c 521:

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

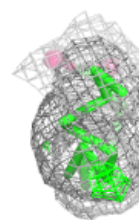
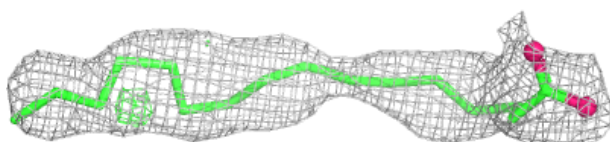
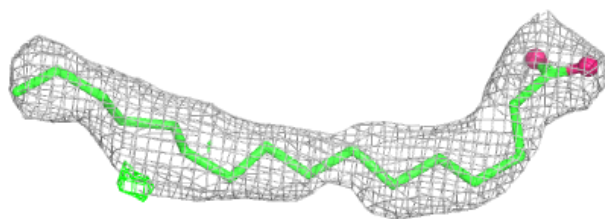
**Electron density around STE d 413:**

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

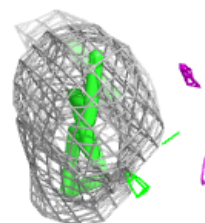
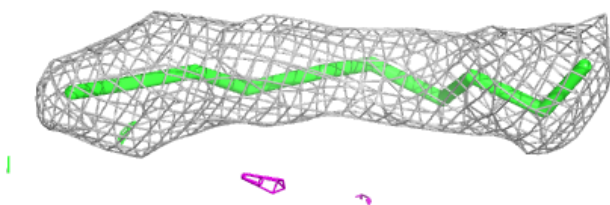
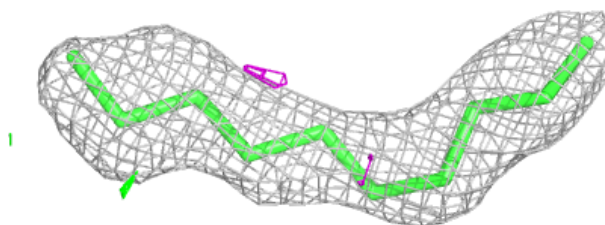


Electron density around STE t 104:

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

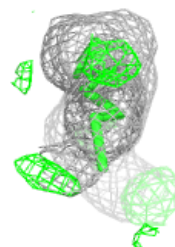
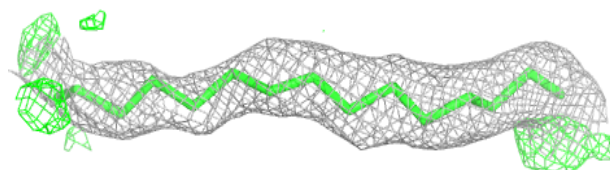
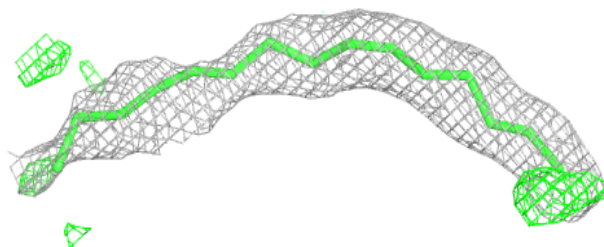
**Electron density around STE b 626:**

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

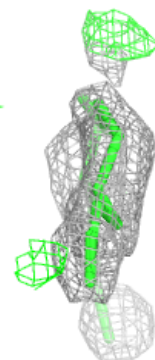
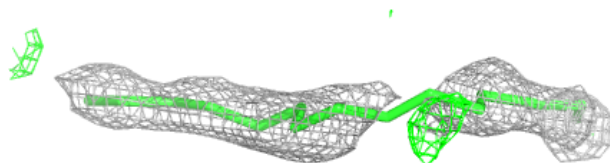
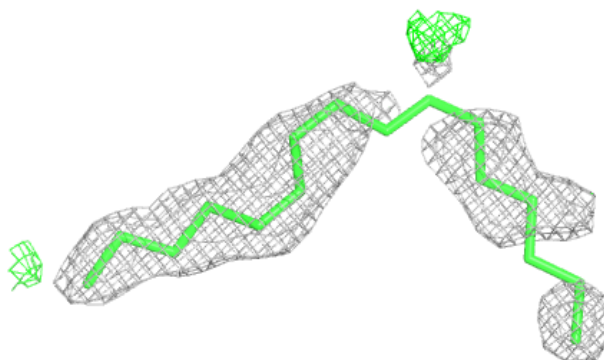


Electron density around STE I 101:

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

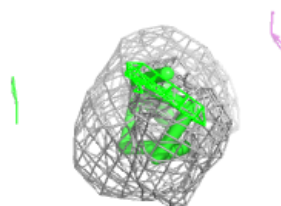
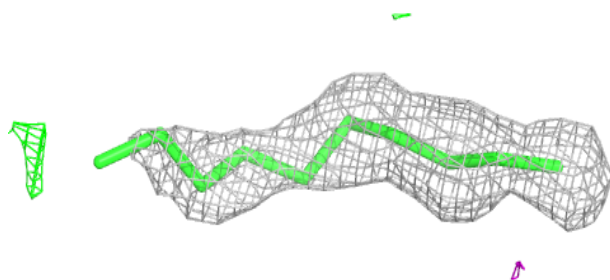
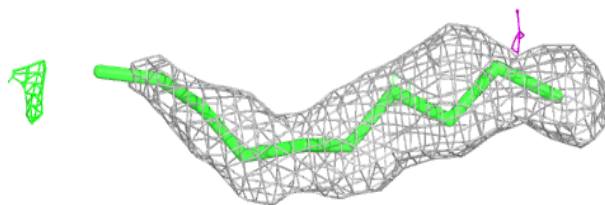
**Electron density around STE B 625:**

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

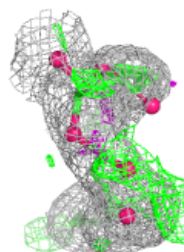
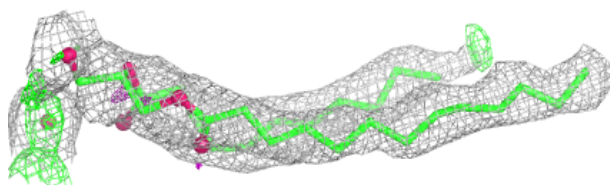
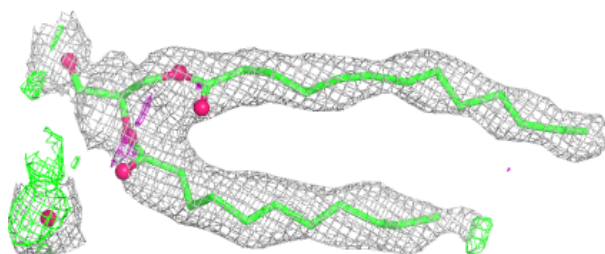


Electron density around STE a 615:

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

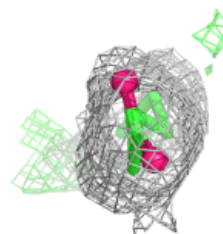
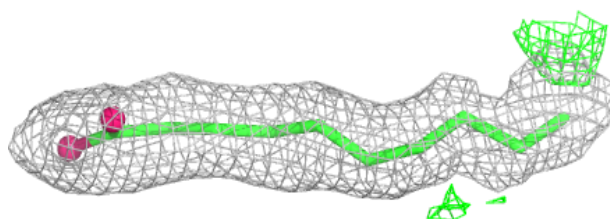
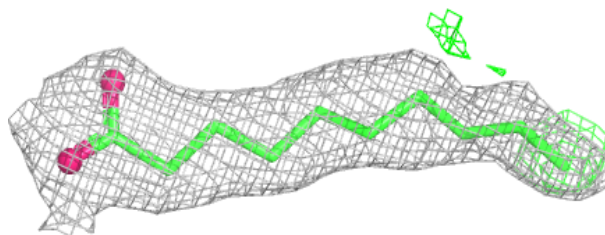
**Electron density around LMG D 412:**

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

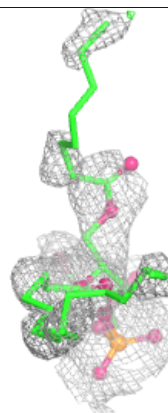
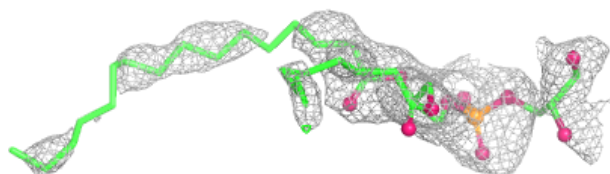
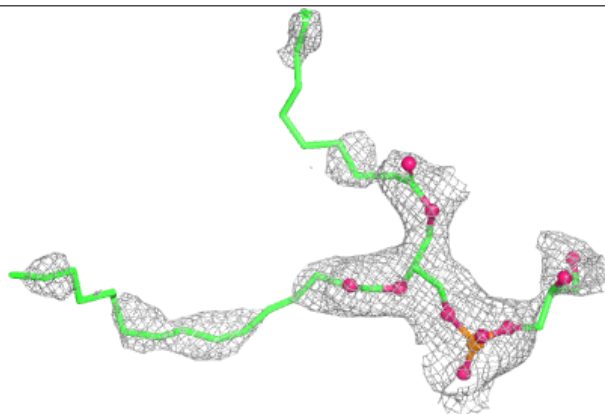


Electron density around STE J 101:

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

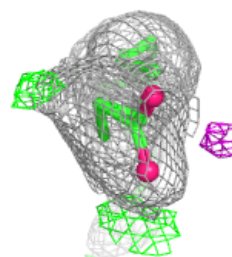
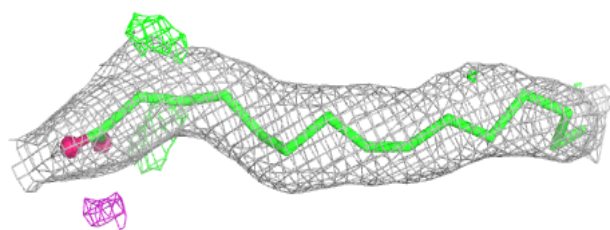
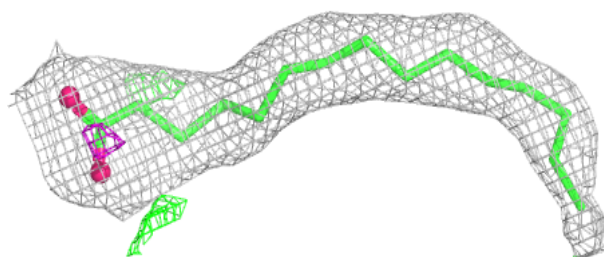
**Electron density around LHG e 102:**

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

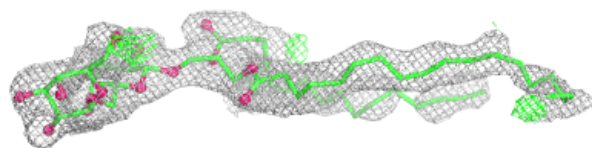
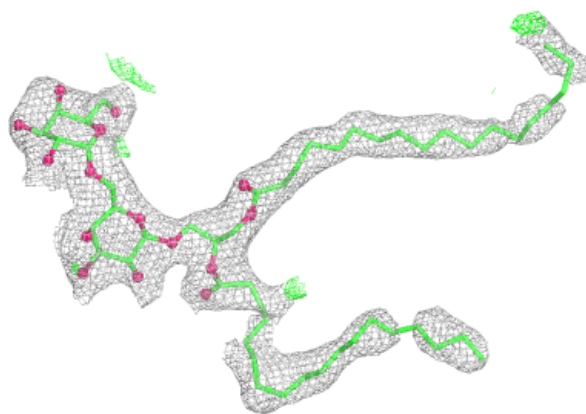


Electron density around STE B 620:

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

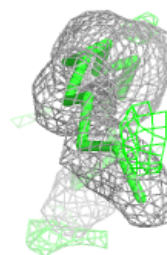
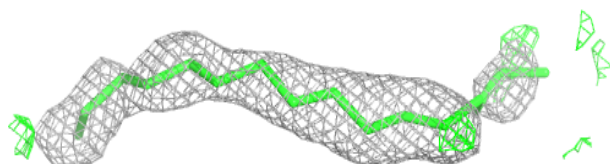
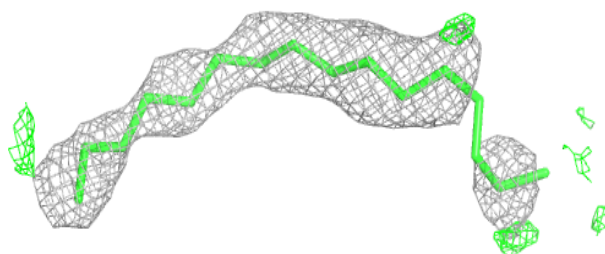
**Electron density around DGD A 615:**

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

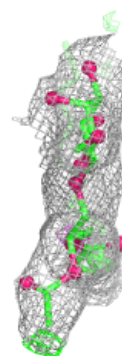
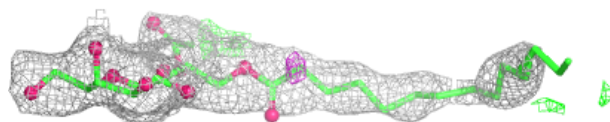
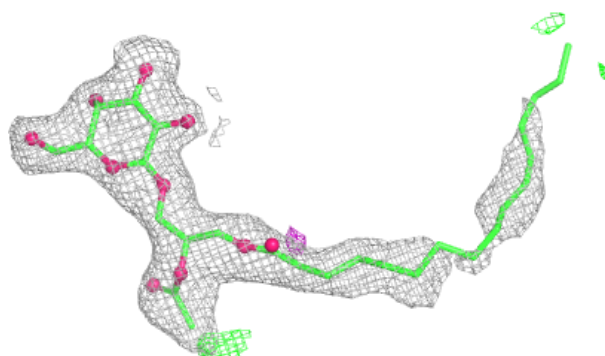


Electron density around STE b 620:

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

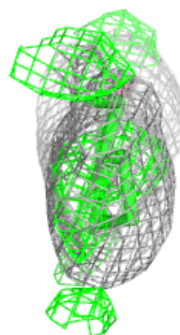
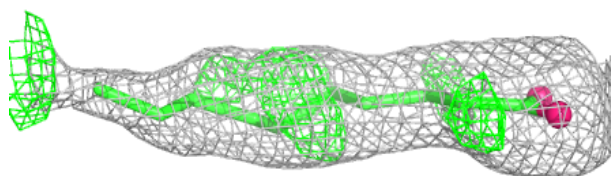
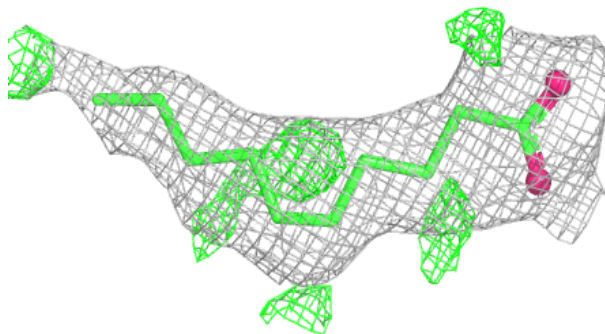
**Electron density around LMG c 519:**

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

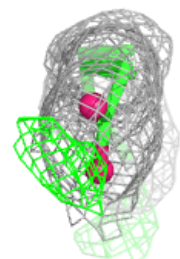
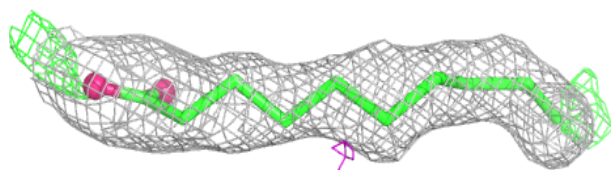
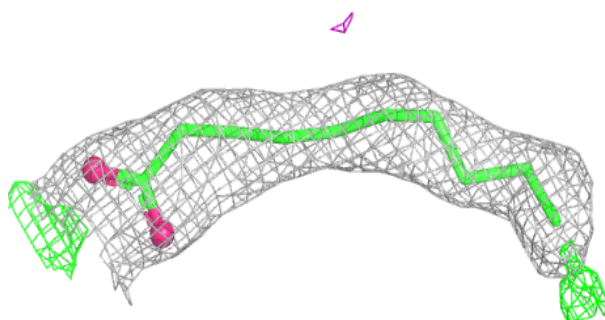


Electron density around STE C 520:

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

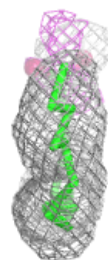
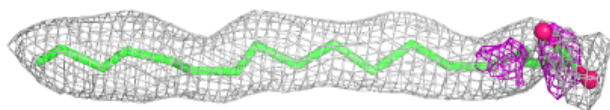
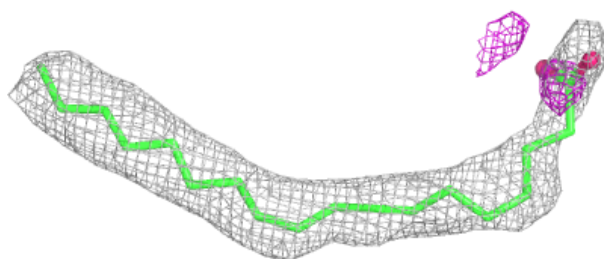
**Electron density around STE C 521:**

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

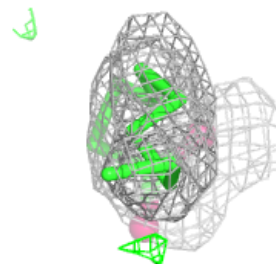
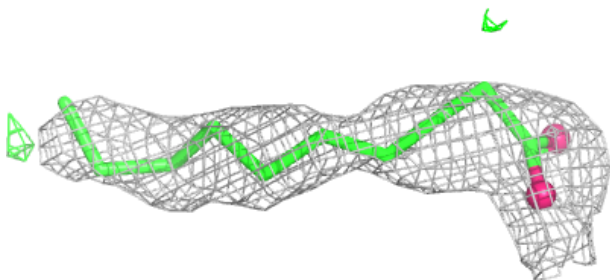
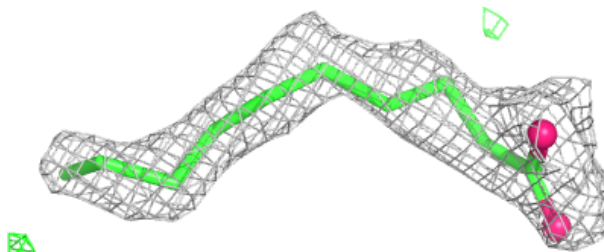


Electron density around STE X 101:

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

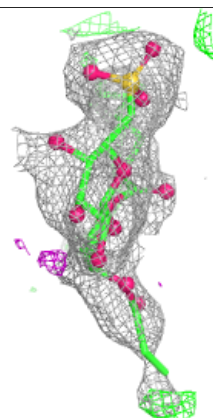
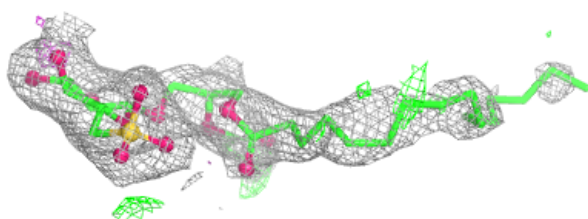
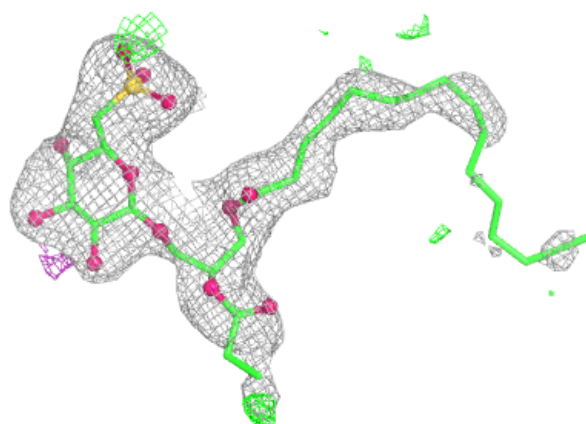
**Electron density around STE R 101:**

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

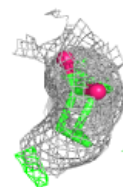
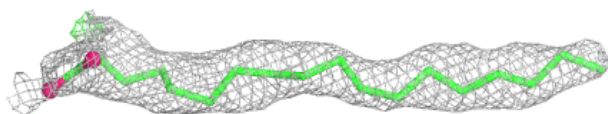
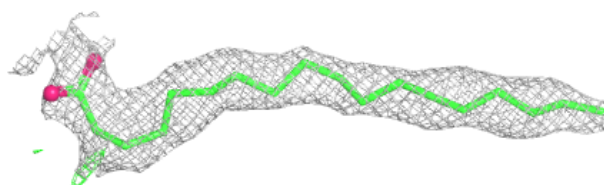


Electron density around SQD f 101:

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

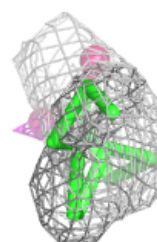
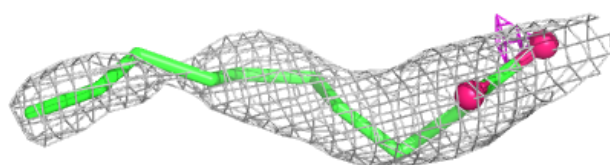
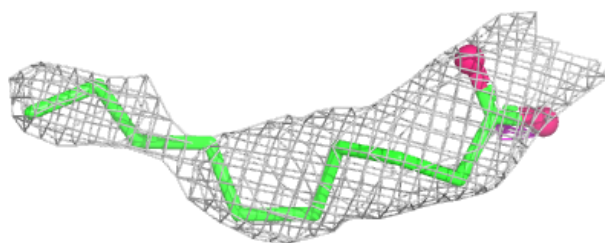
**Electron density around STE c 520:**

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

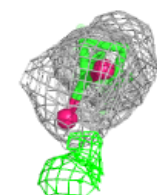
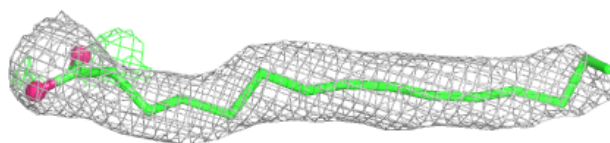
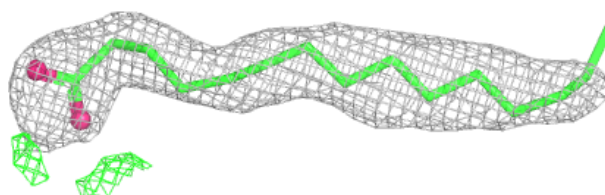


Electron density around STE B 624:

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

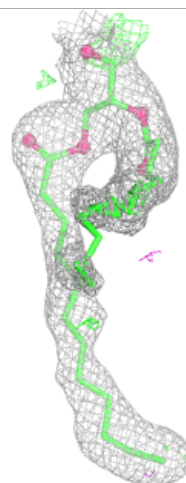
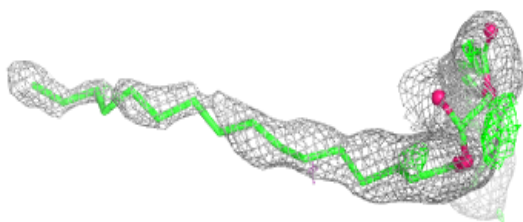
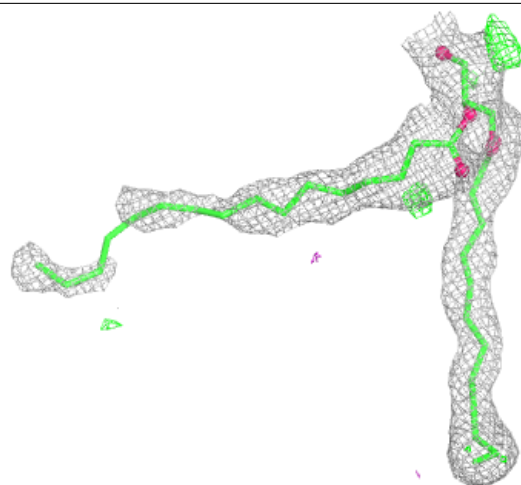
**Electron density around STE d 412:**

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



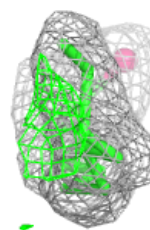
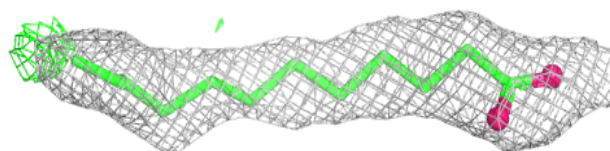
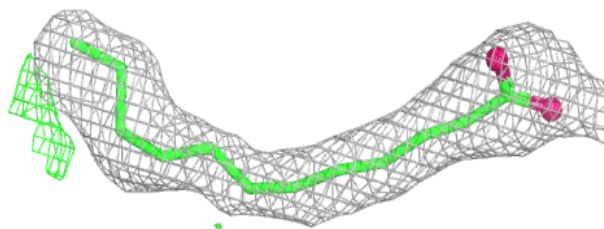
Electron density around SQD t 102:

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

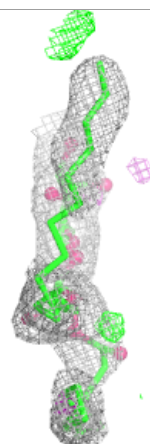
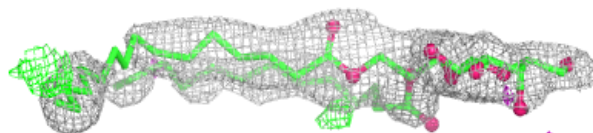
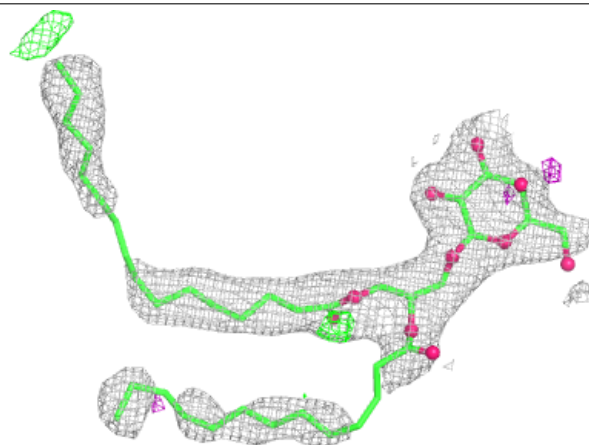


Electron density around STE t 103:

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

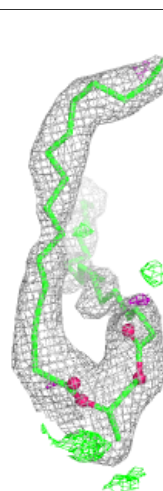
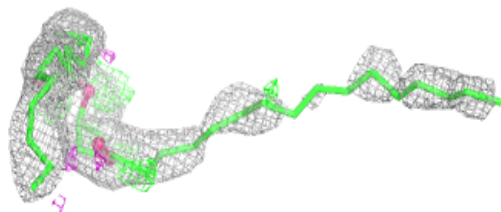
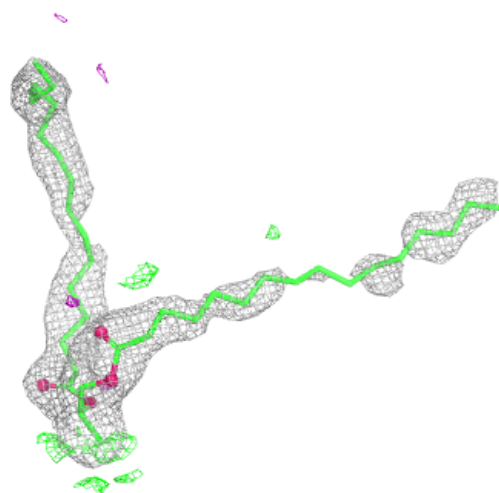
**Electron density around LMG C 519:**

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



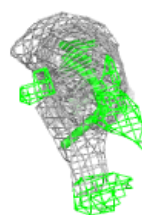
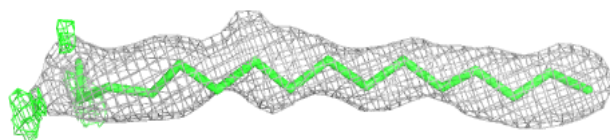
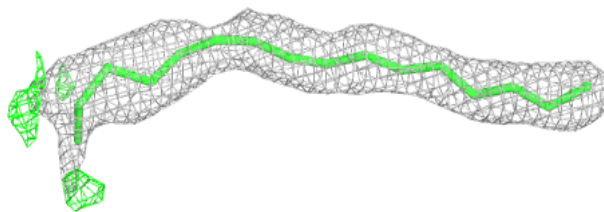
Electron density around SQD A 614:

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



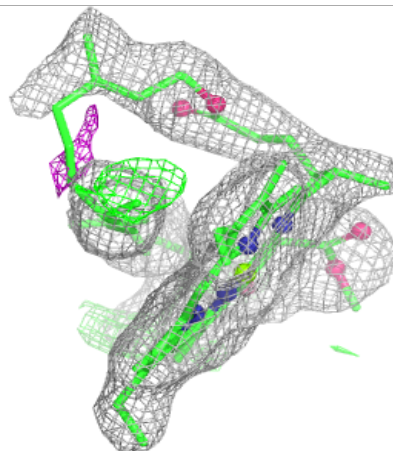
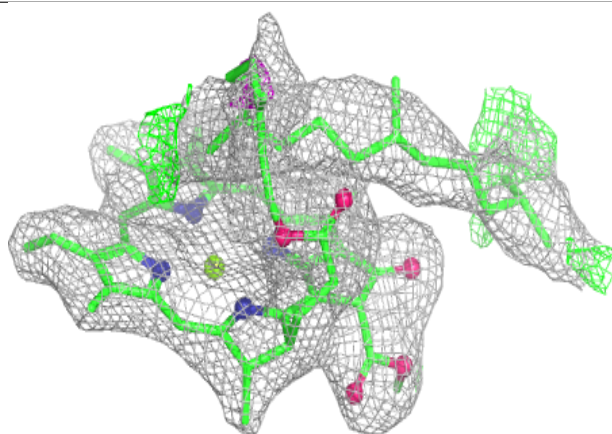
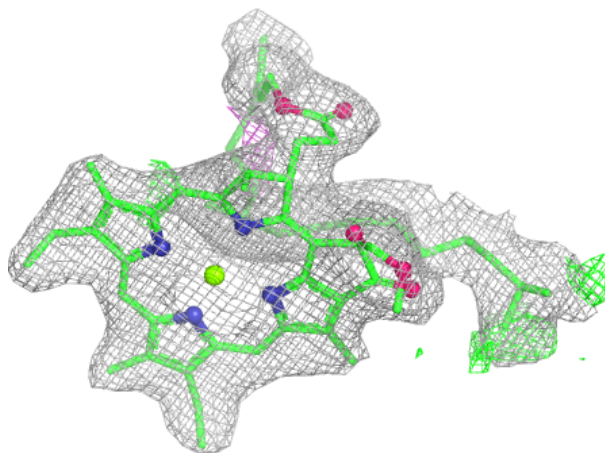
Electron density around STE C 522:

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



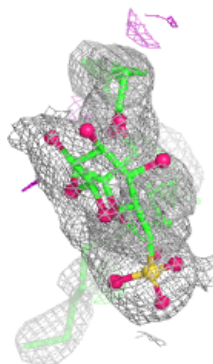
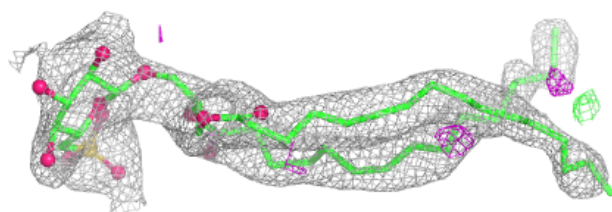
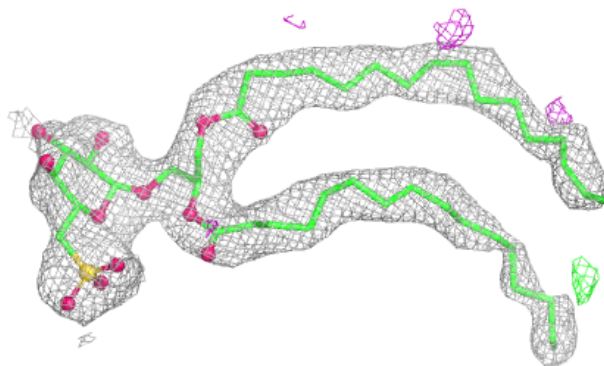
Electron density around CLA B 601:

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

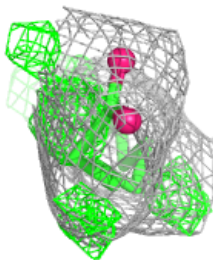
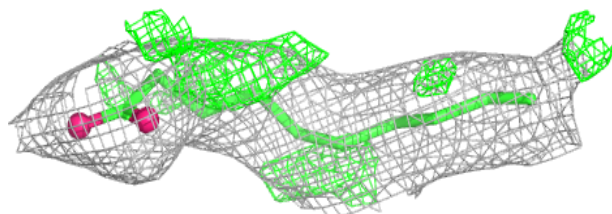
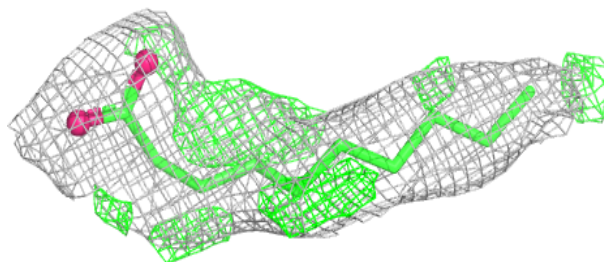


Electron density around SQD B 622:

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

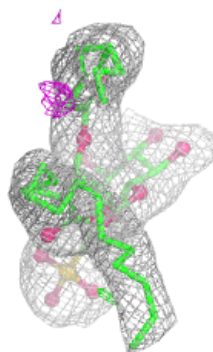
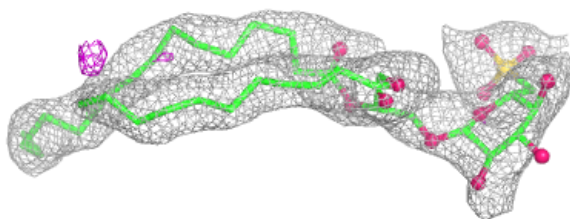
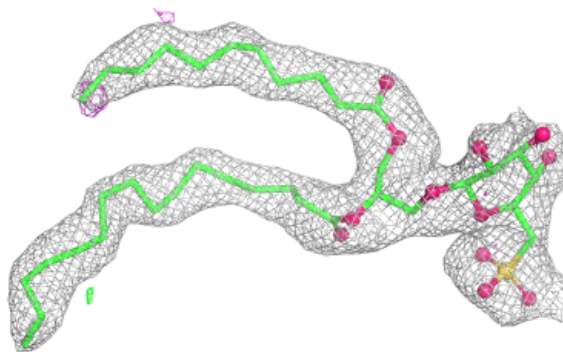
**Electron density around STE B 623:**

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

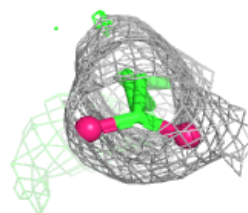
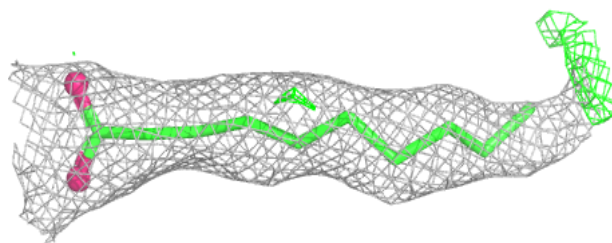
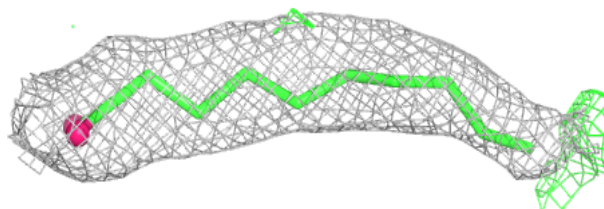


Electron density around SQD L 101:

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

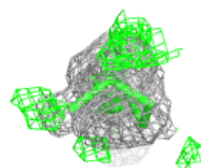
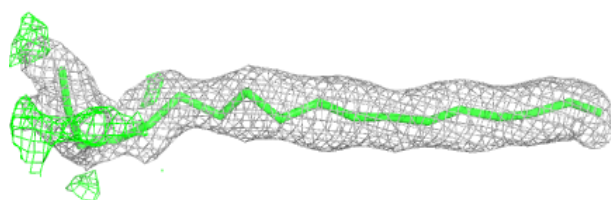
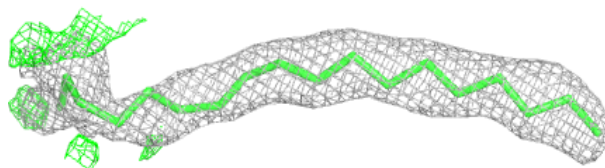
**Electron density around STE j 101:**

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

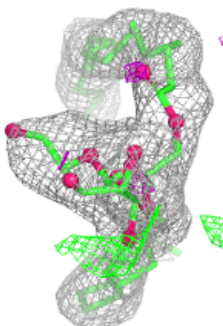
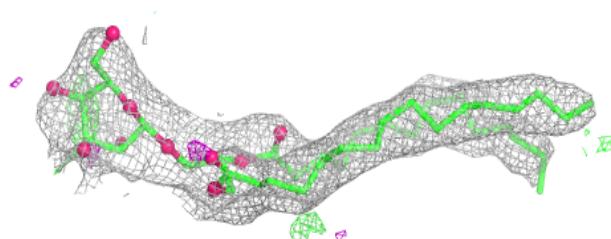
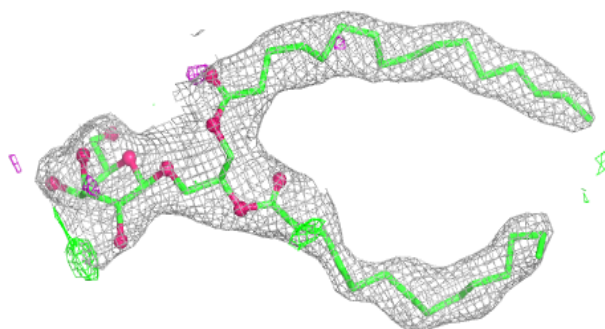


Electron density around STE 1 102:

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

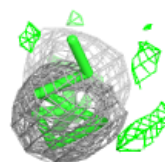
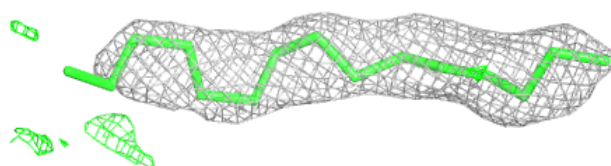
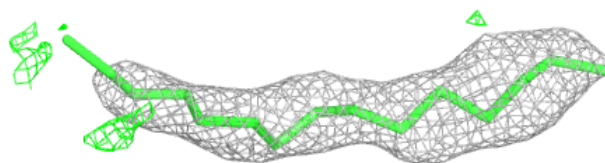
**Electron density around LMG c 523:**

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

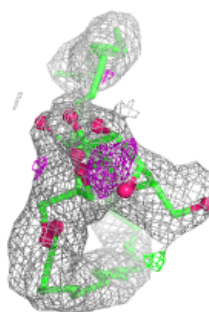
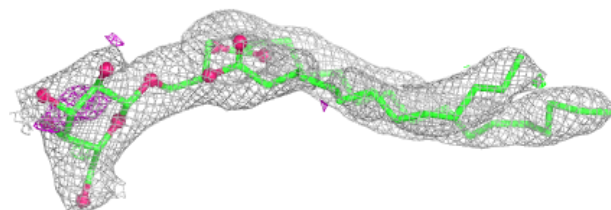
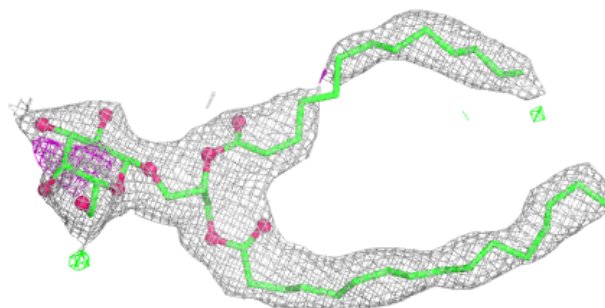


Electron density around STE b 624:

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

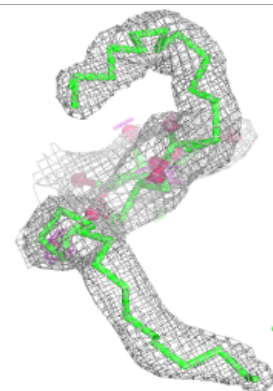
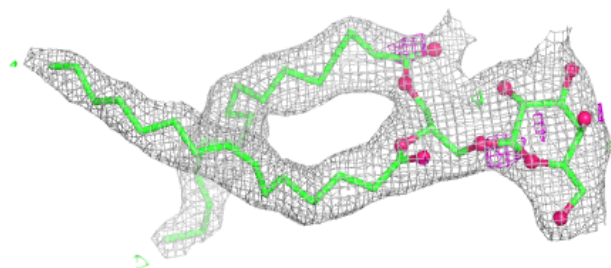
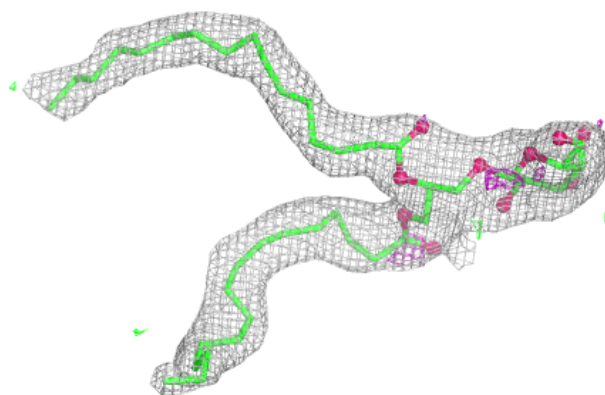
**Electron density around LMG A 612:**

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

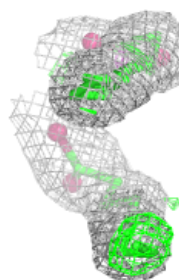
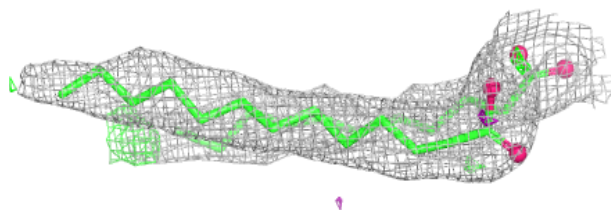
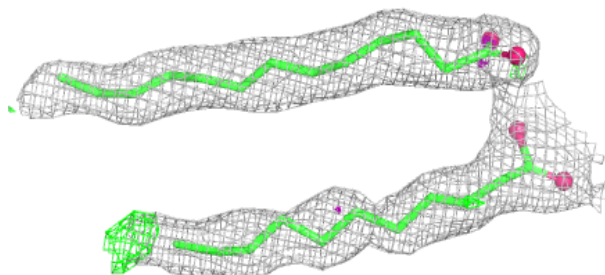


Electron density around LMG m 101:

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

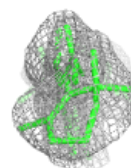
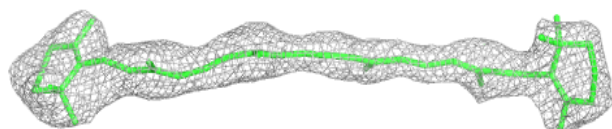
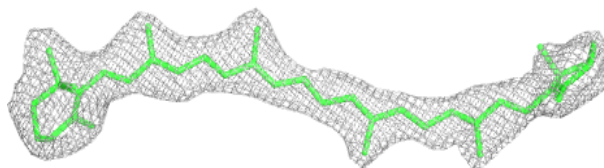
**Electron density around LMG B 621:**

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

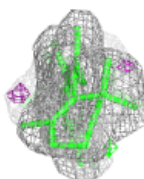
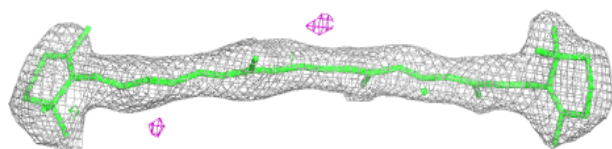


Electron density around BCR k 101:

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

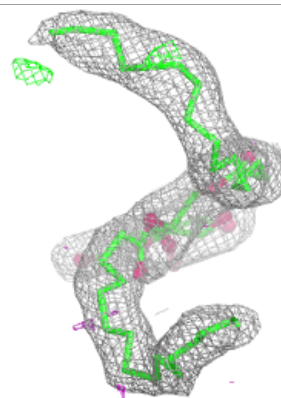
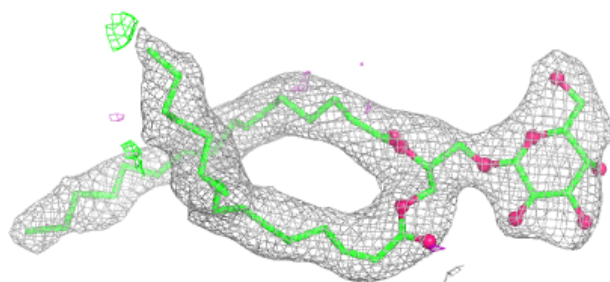
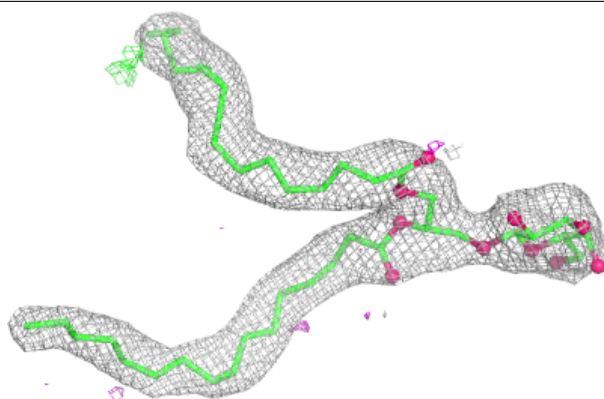
**Electron density around BCR K 102:**

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

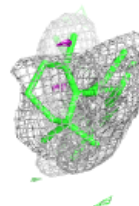
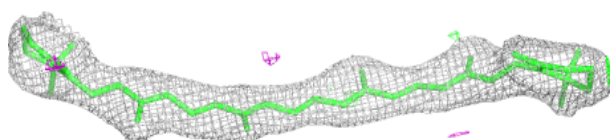
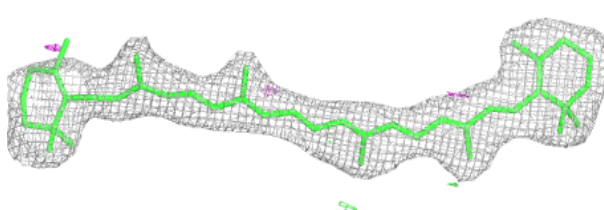


Electron density around LMG M 101:

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

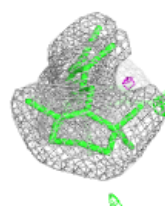
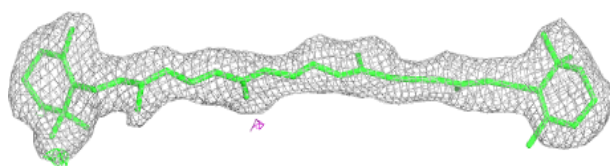
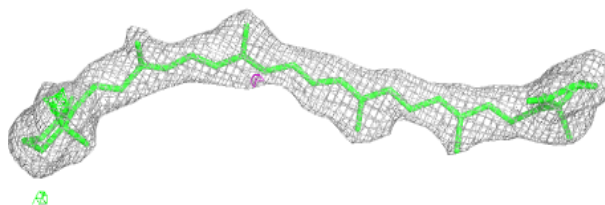
**Electron density around BCR d 405:**

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

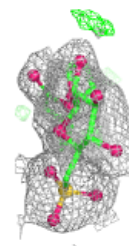
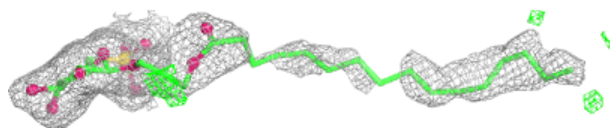
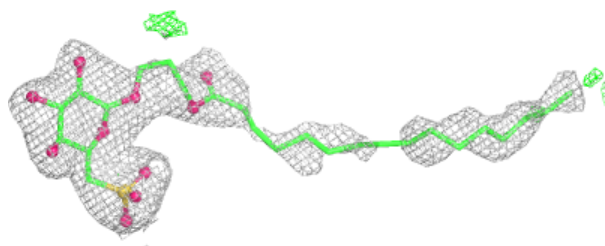


Electron density around BCR h 101:

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

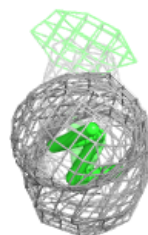
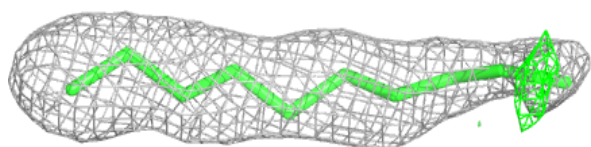
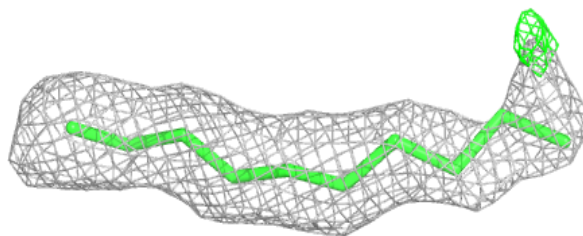
**Electron density around SQD D 409:**

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



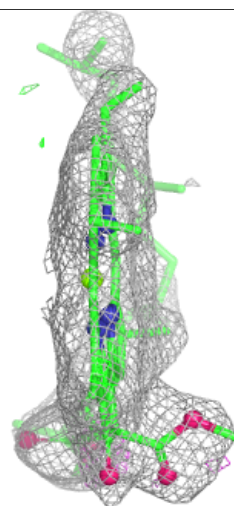
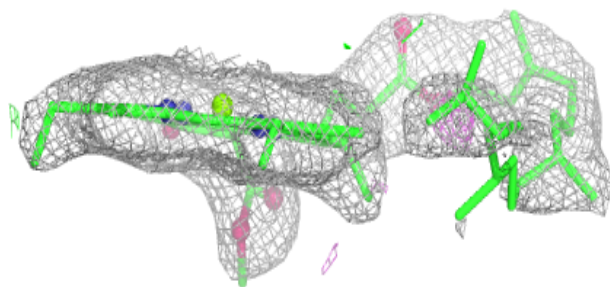
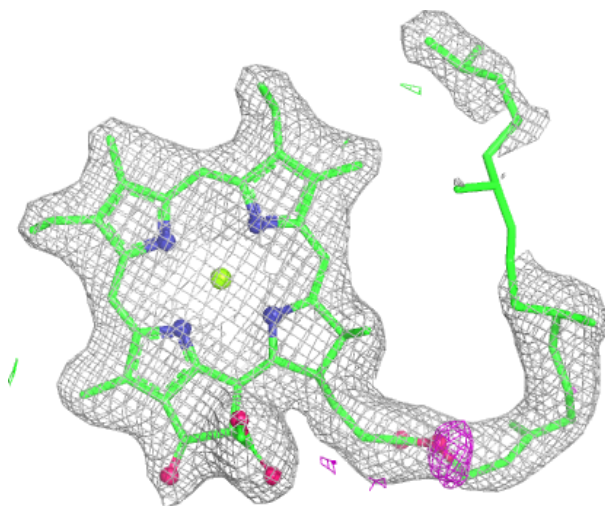
Electron density around STE M 103:

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



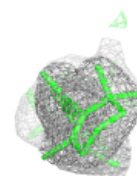
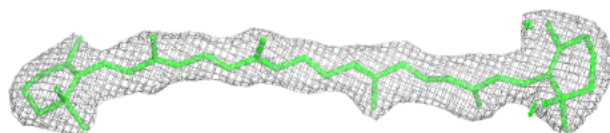
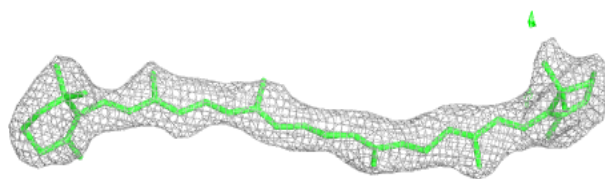
Electron density around CLA c 512:

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

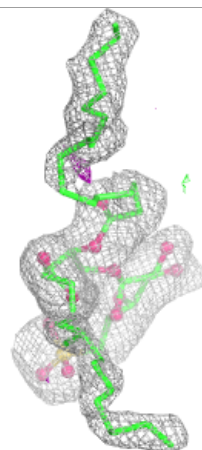
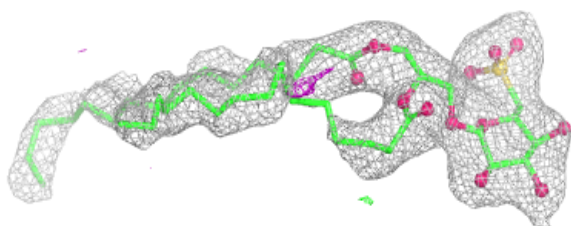
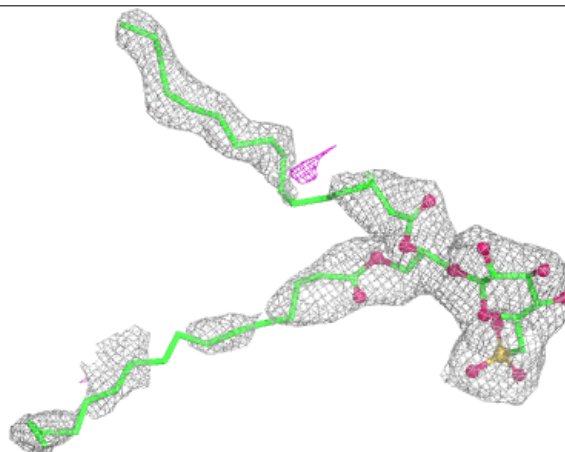


Electron density around BCR c 514:

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

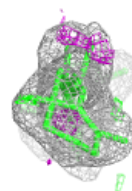
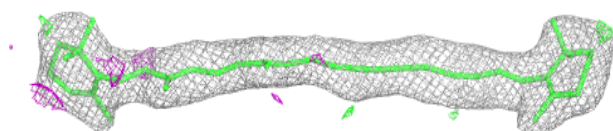
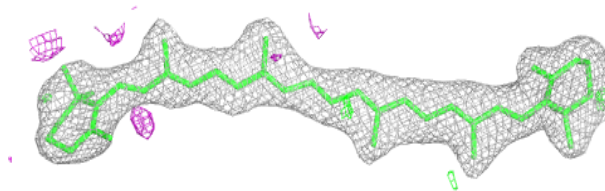
**Electron density around SQD a 613:**

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

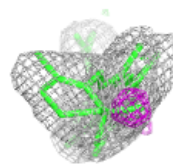
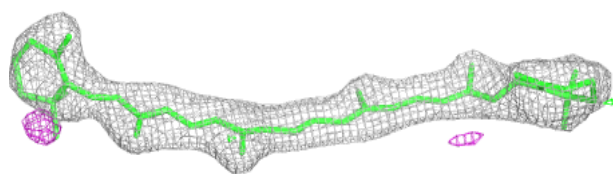
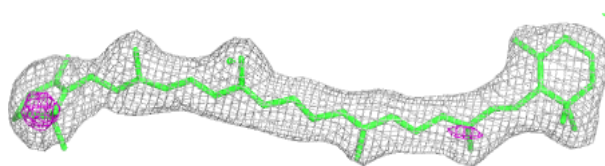


Electron density around BCR B 618:

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

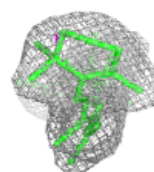
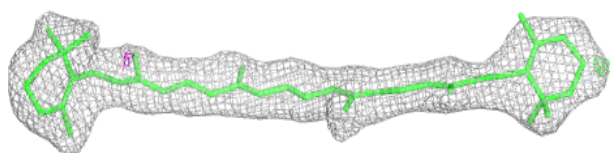
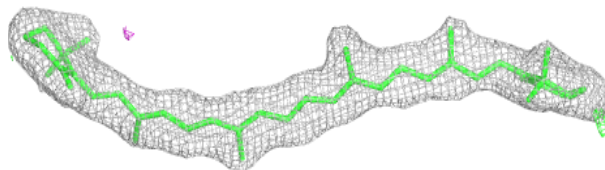
**Electron density around BCR D 406:**

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

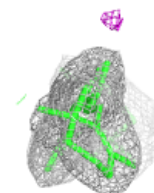
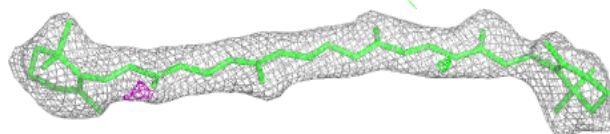
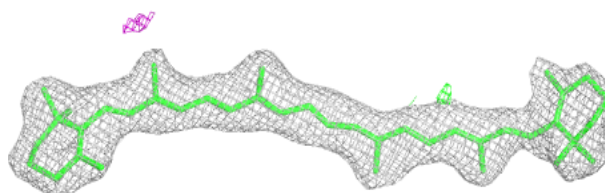


Electron density around BCR H 101:

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

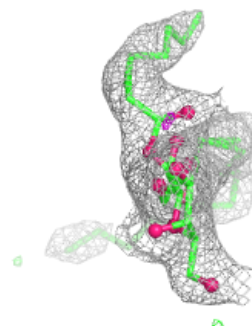
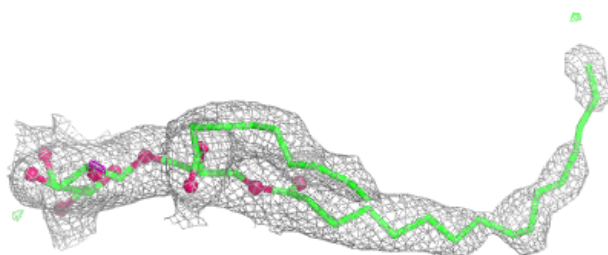
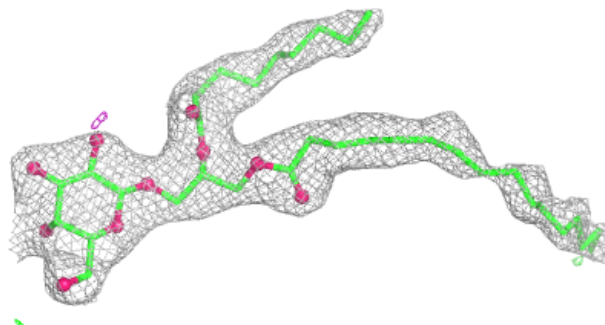
**Electron density around BCR b 619:**

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

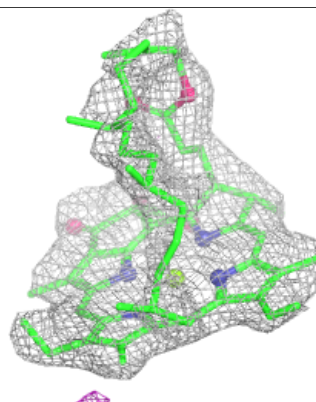
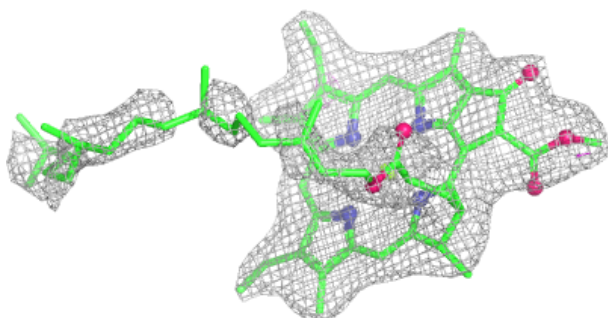
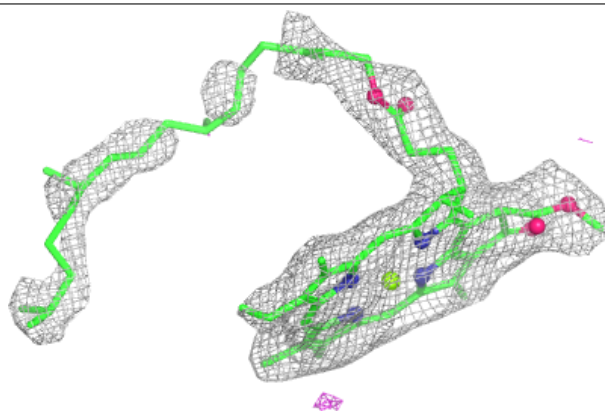


Electron density around LMG d 411:

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

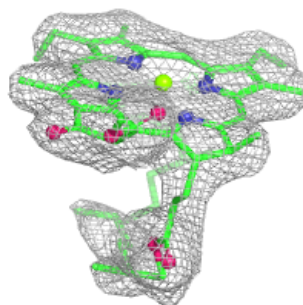
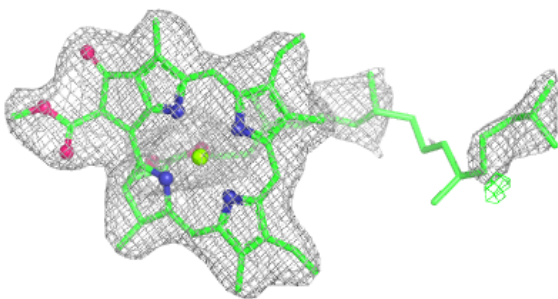
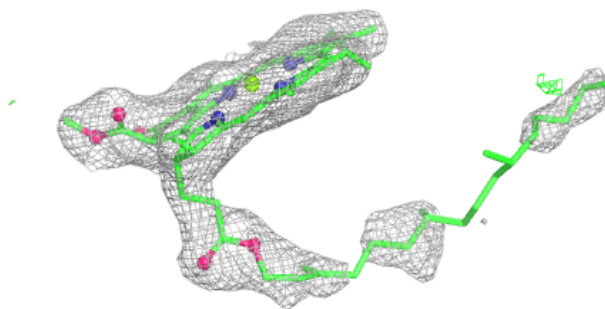
**Electron density around CLA c 513:**

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

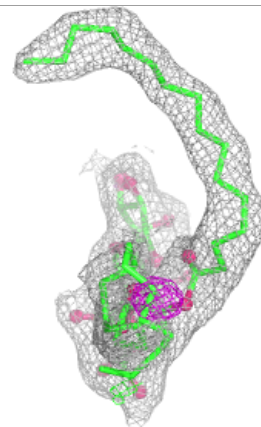
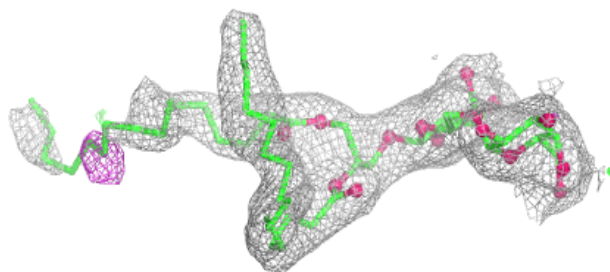
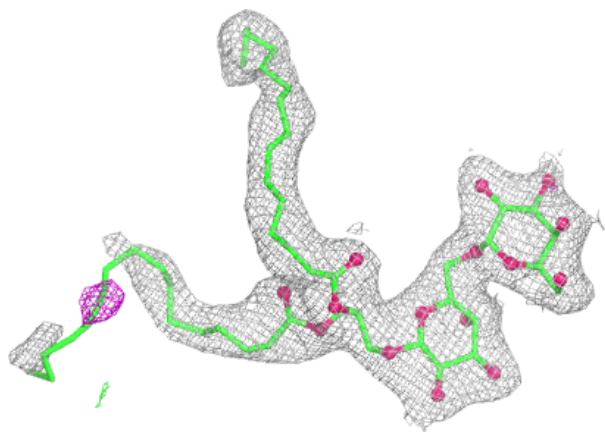


Electron density around CLA C 513:

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

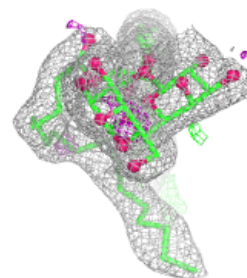
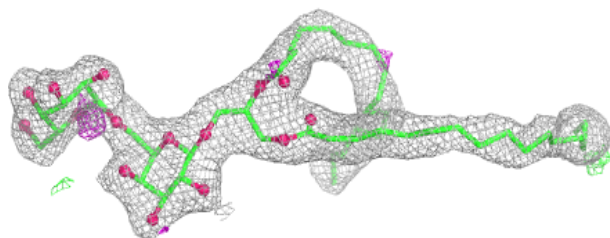
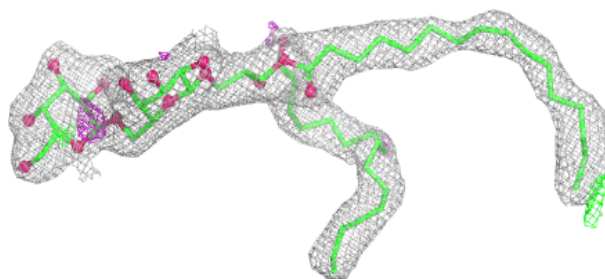
**Electron density around DGD C 517:**

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

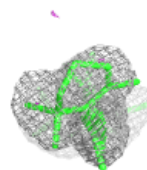
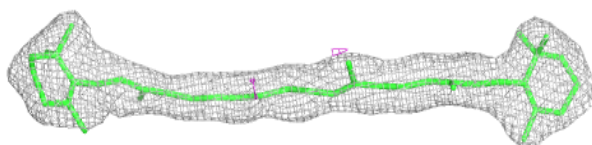
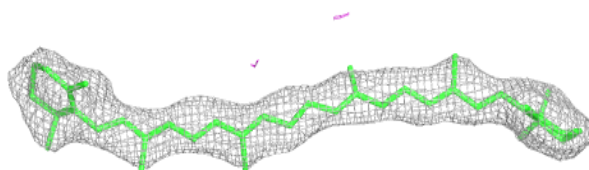


Electron density around DGD H 102:

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

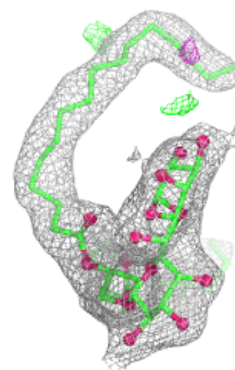
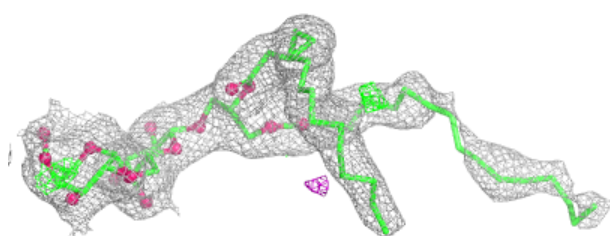
**Electron density around BCR K 101:**

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

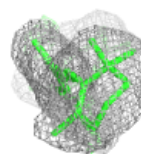
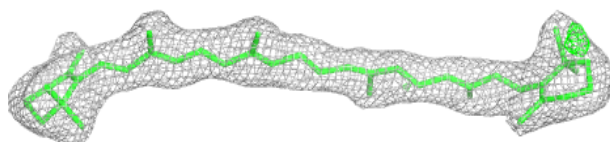
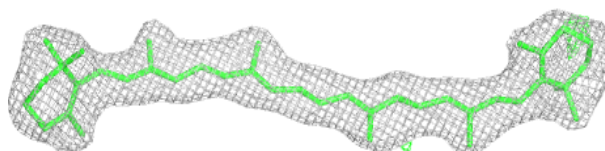


Electron density around DGD c 517:

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

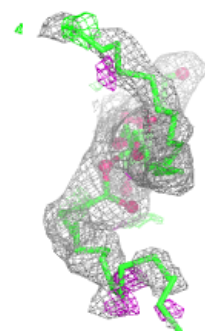
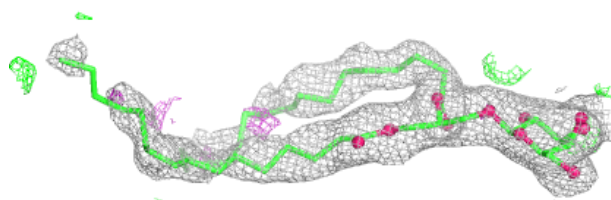
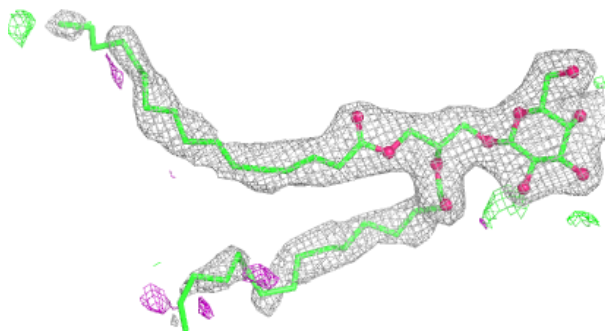
**Electron density around BCR B 619:**

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

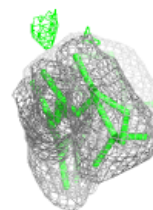
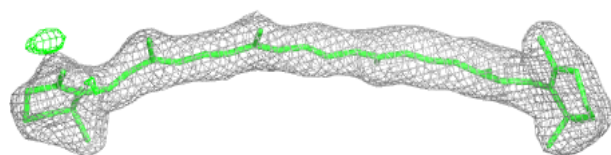
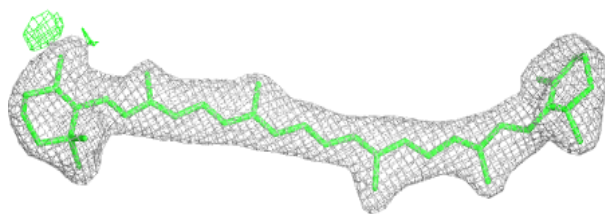


Electron density around LMG D 408:

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

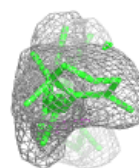
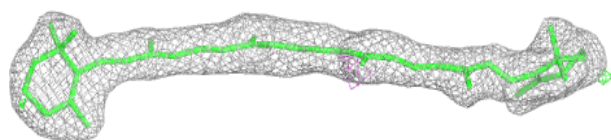
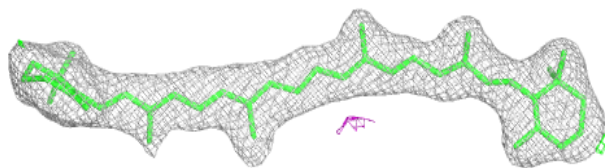
**Electron density around BCR T 101:**

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

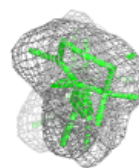
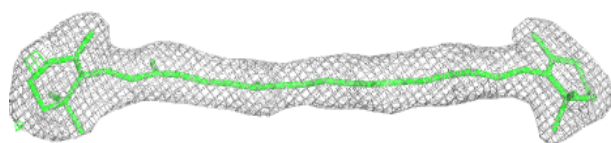
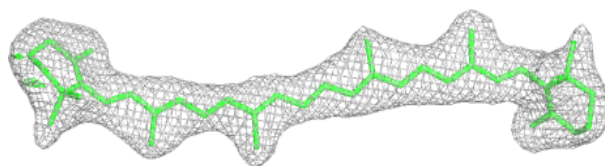


Electron density around BCR b 617:

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

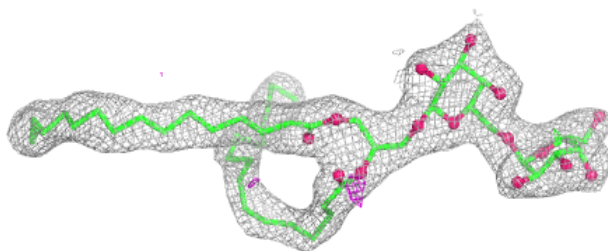
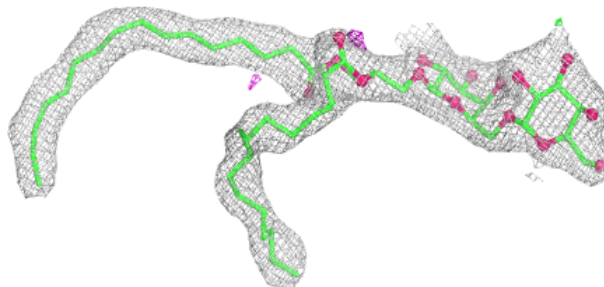
**Electron density around BCR b 618:**

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

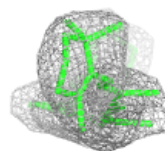
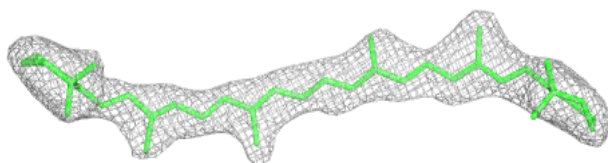
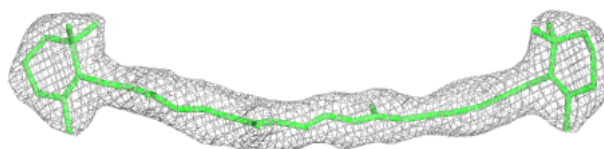


Electron density around DGD h 102:

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

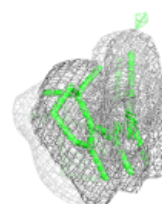
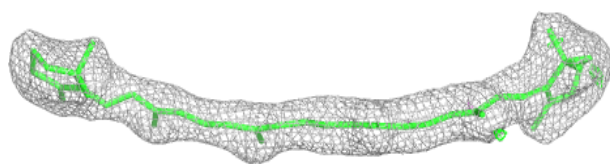
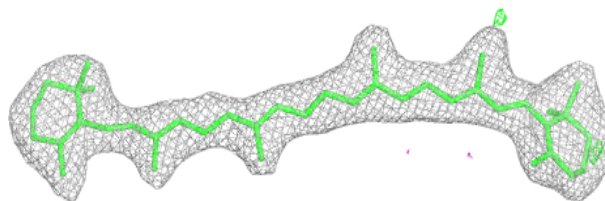
**Electron density around BCR k 102:**

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



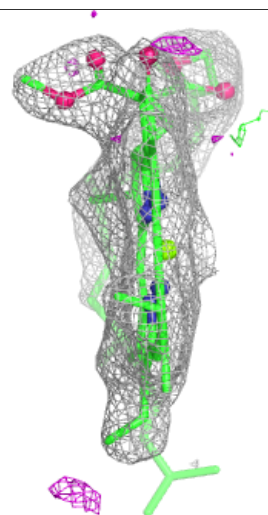
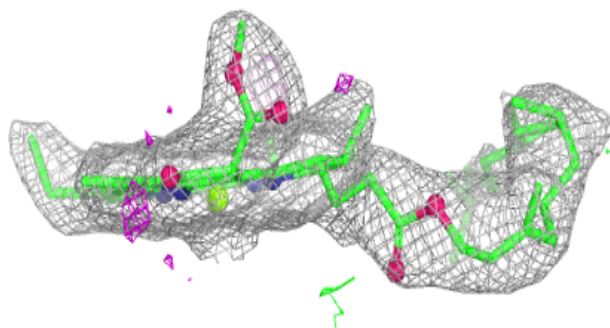
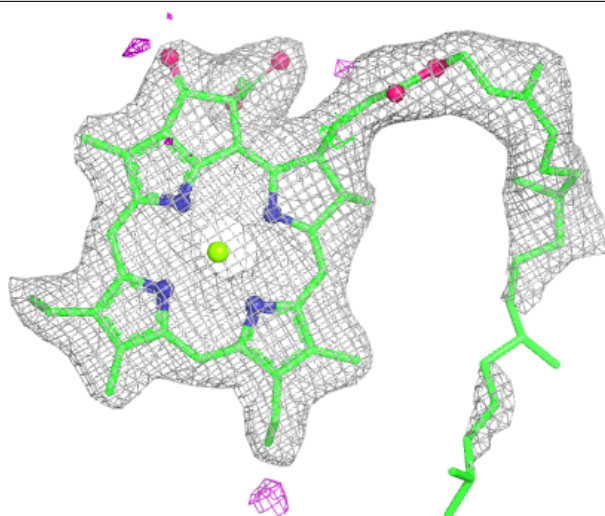
Electron density around BCR t 101:

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



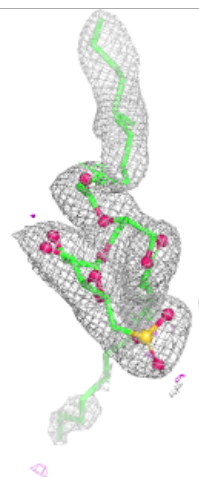
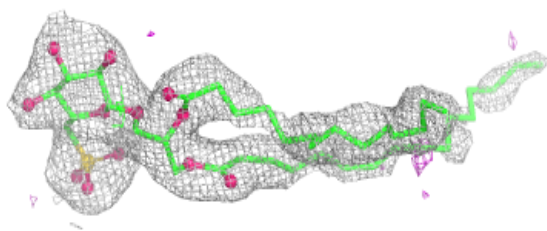
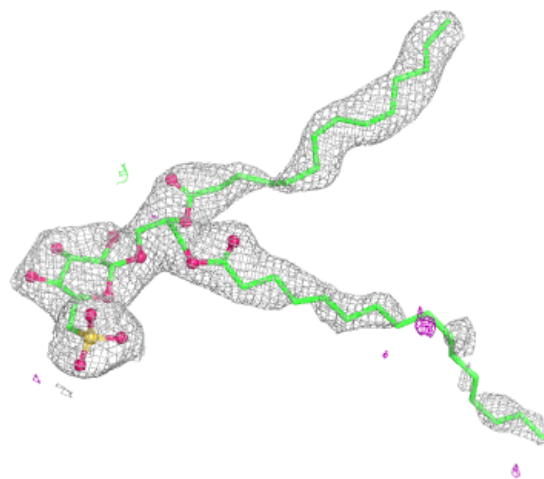
Electron density around CLA C 512:

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



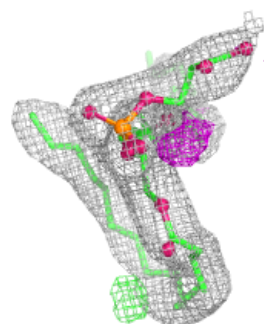
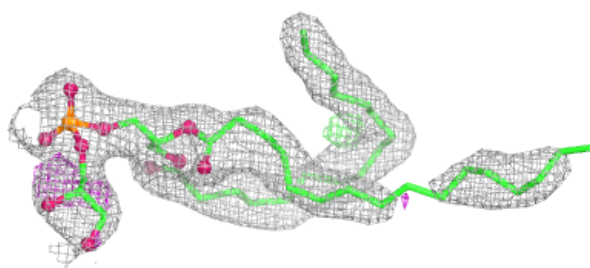
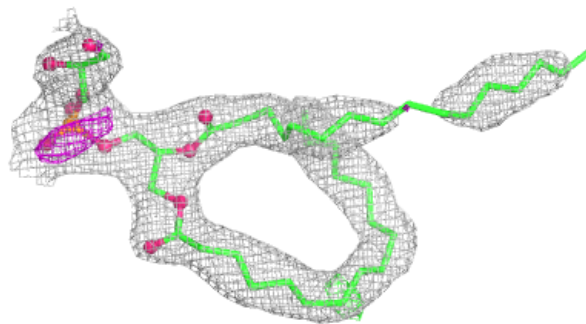
Electron density around SQD A 613:

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

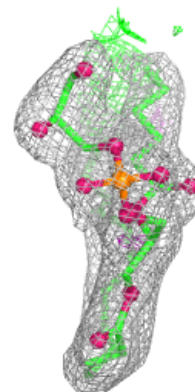
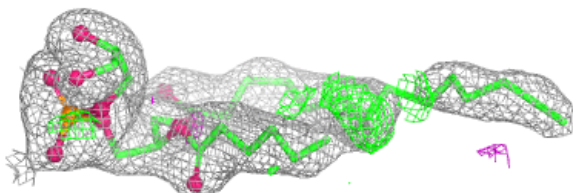
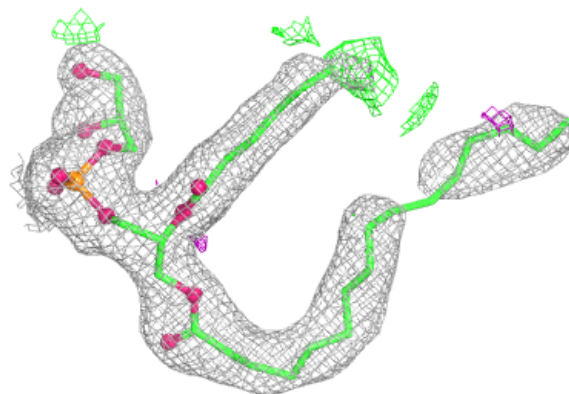


Electron density around LHG d 407:

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

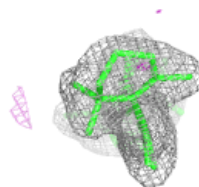
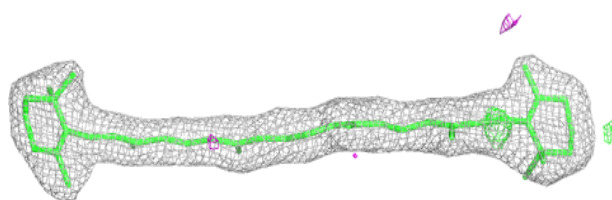
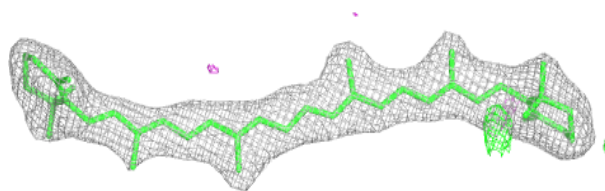
**Electron density around LHG d 409:**

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



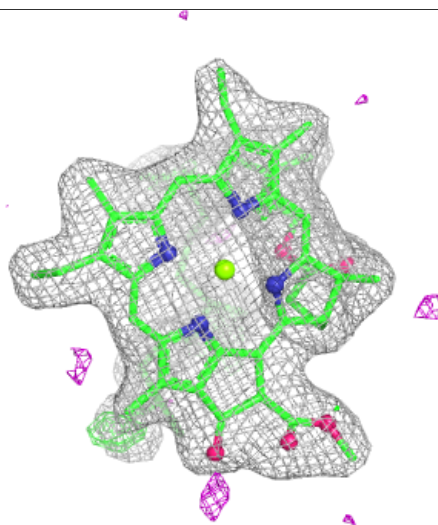
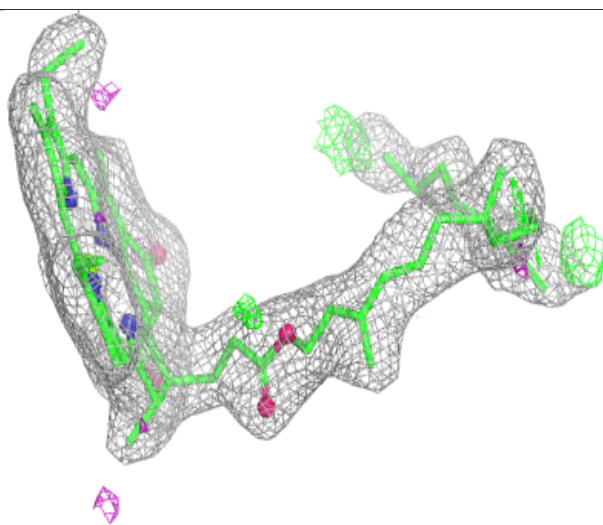
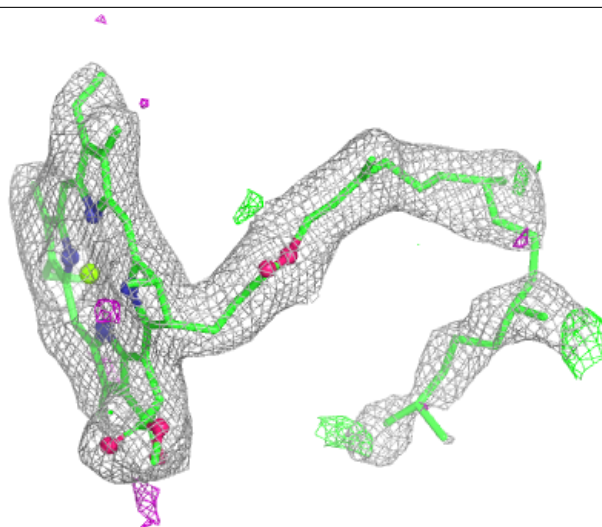
Electron density around BCR C 514:

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



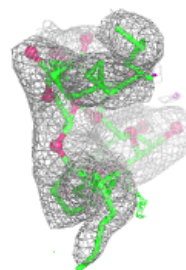
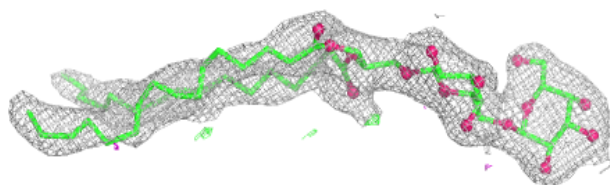
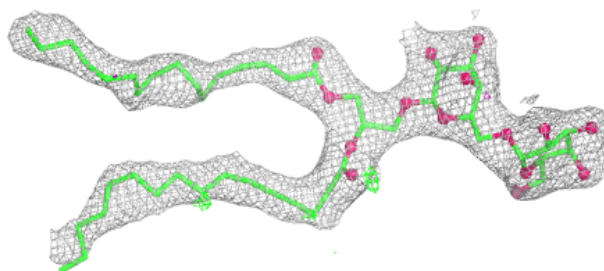
Electron density around CLA B 606:

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

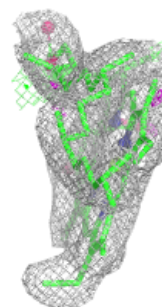
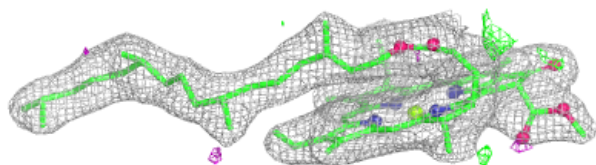
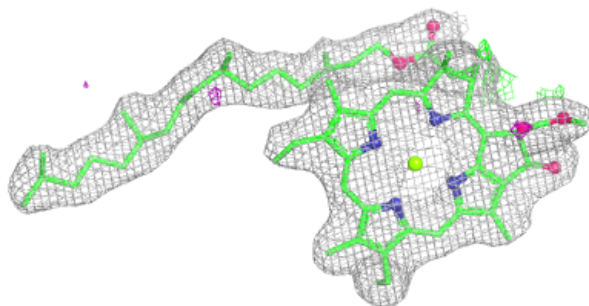


Electron density around DGD c 518:

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

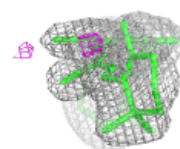
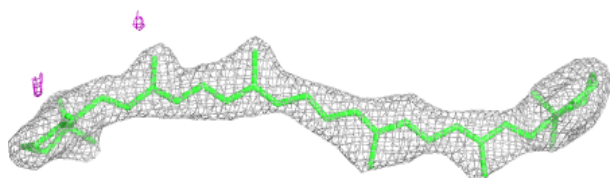
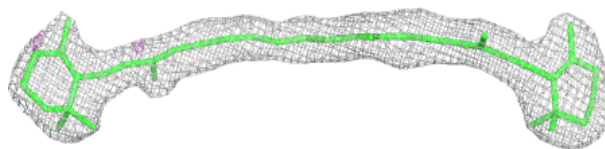
**Electron density around CLA C 501:**

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

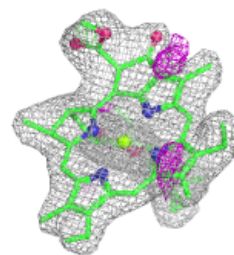
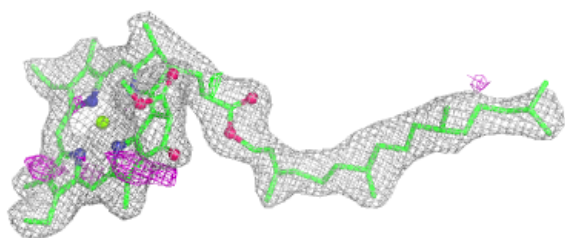
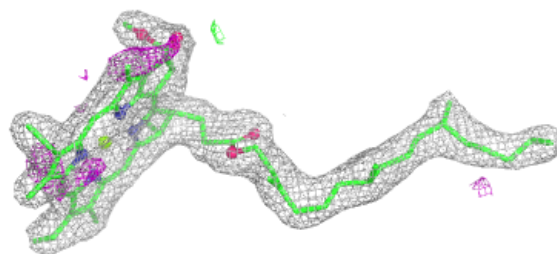


Electron density around BCR C 515:

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

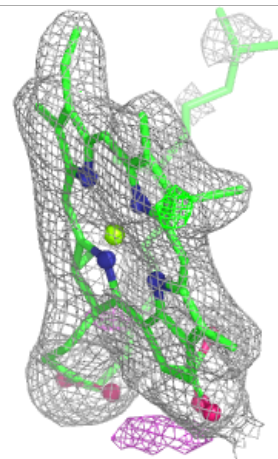
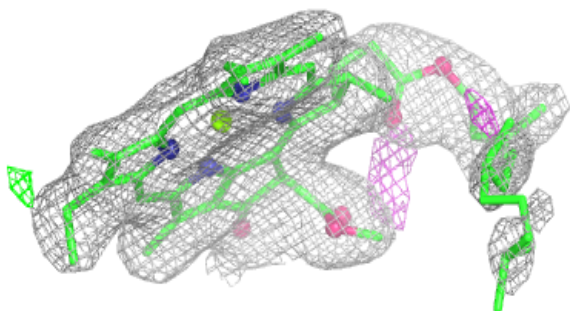
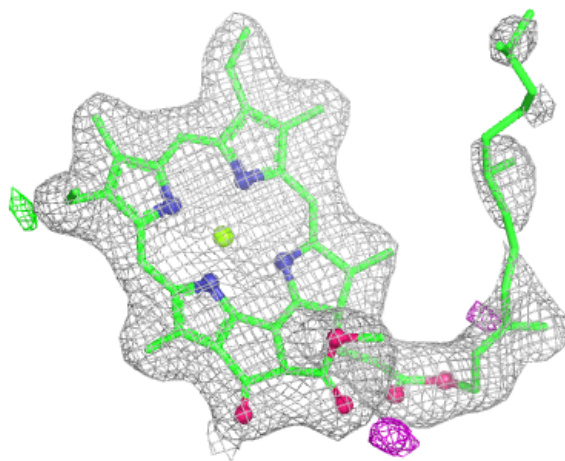
**Electron density around CLA C 502:**

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



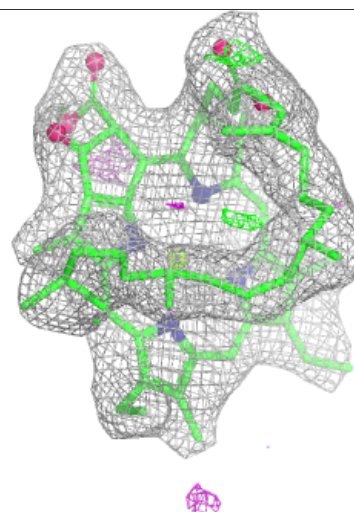
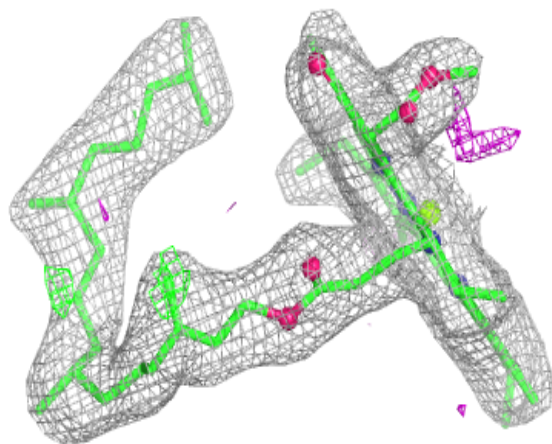
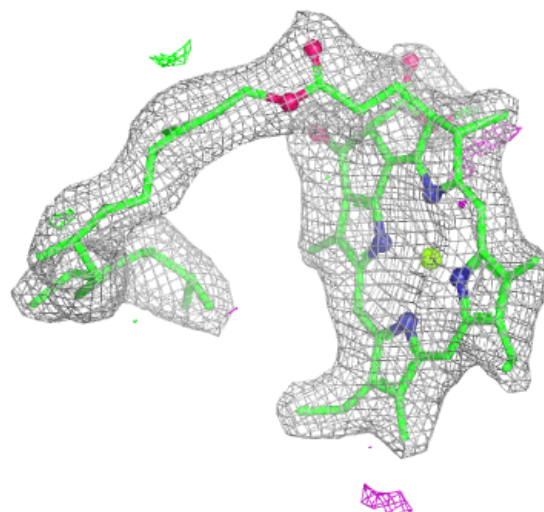
Electron density around CLA b 616:

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



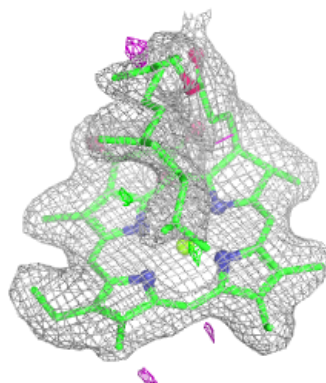
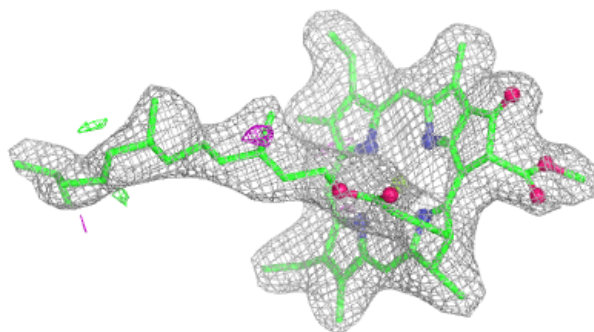
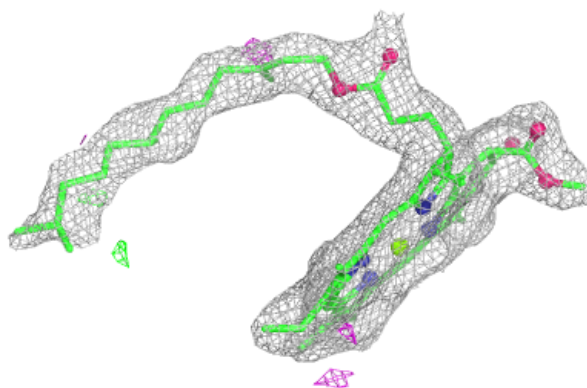
Electron density around CLA c 503:

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

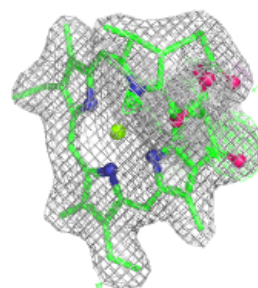
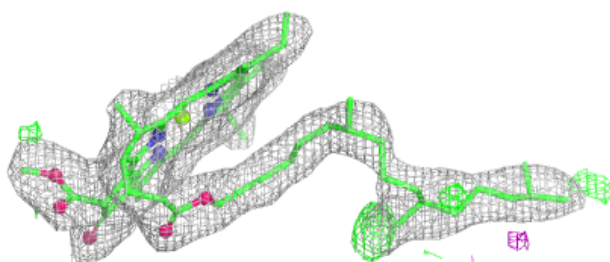
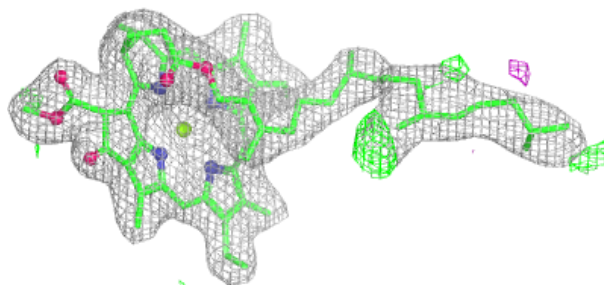


Electron density around CLA c 504:

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

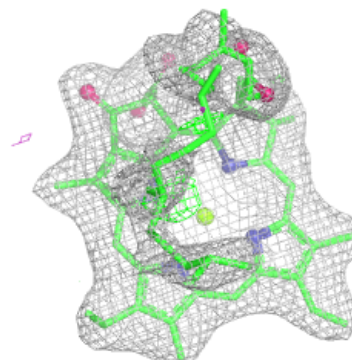
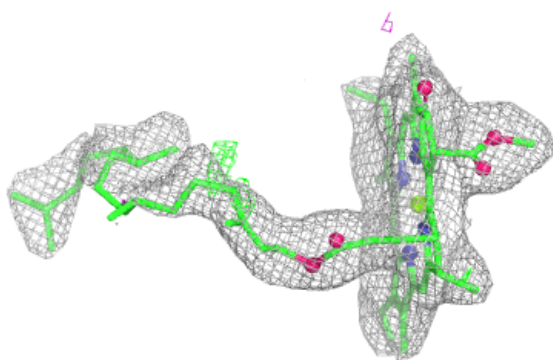
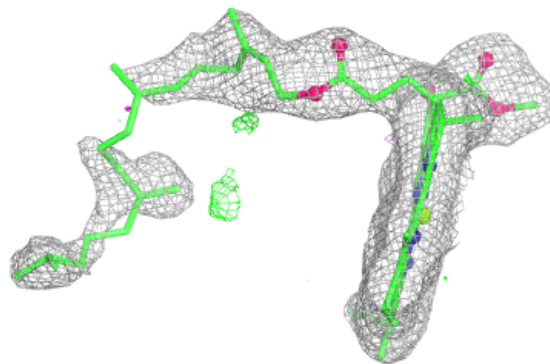
**Electron density around CLA c 505:**

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

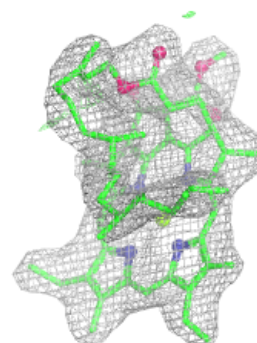
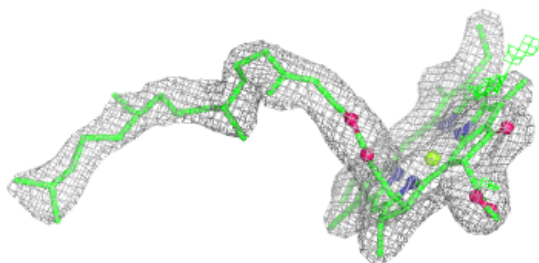
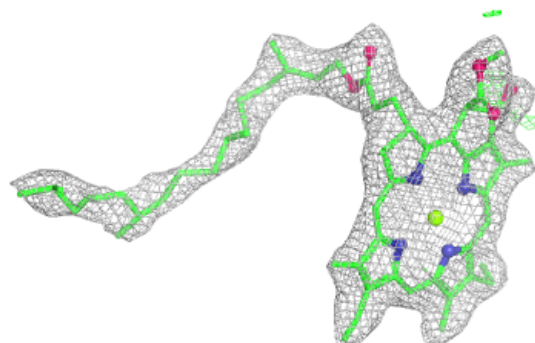


Electron density around CLA c 506:

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

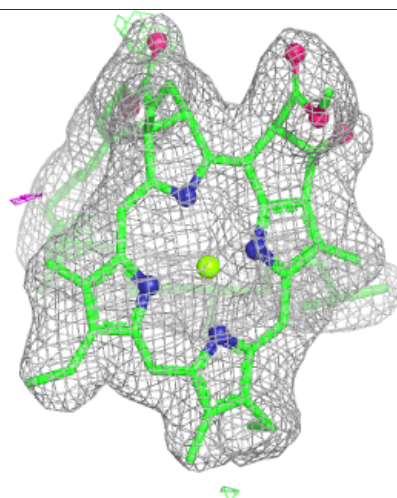
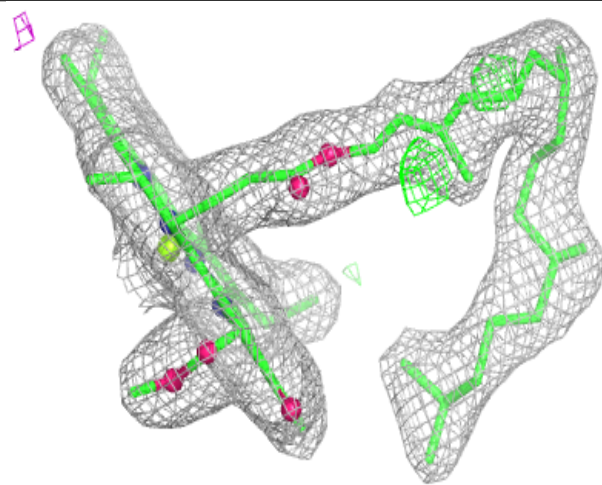
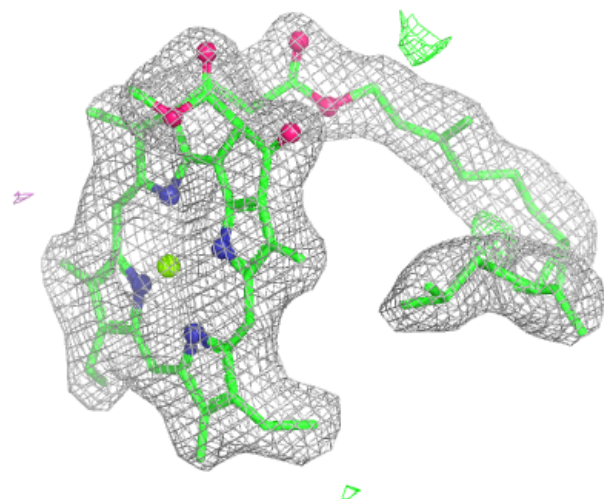
**Electron density around CLA c 511:**

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



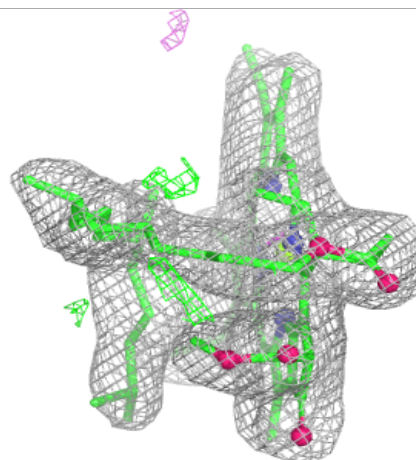
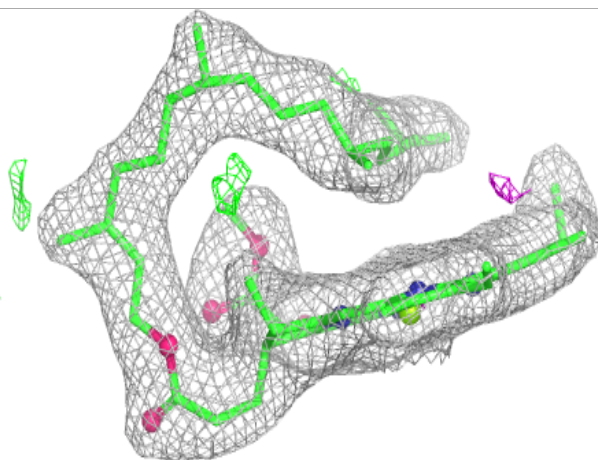
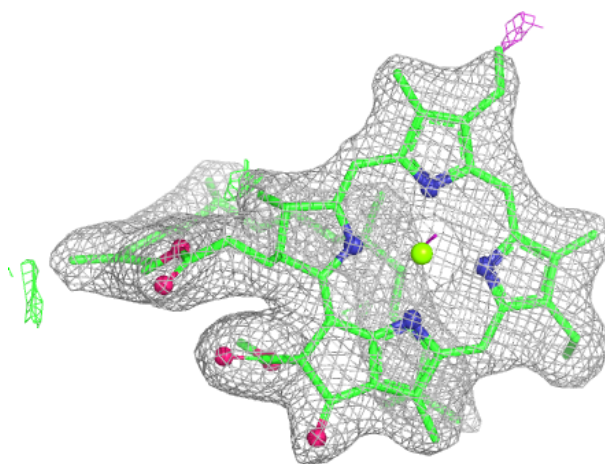
Electron density around CLA C 503:

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



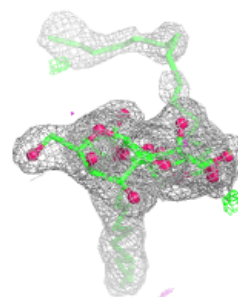
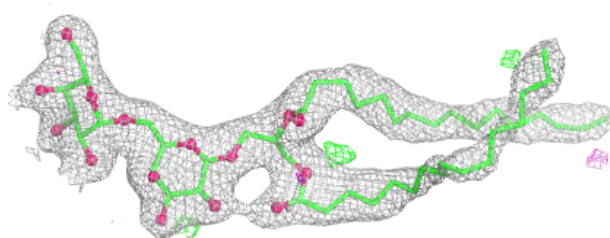
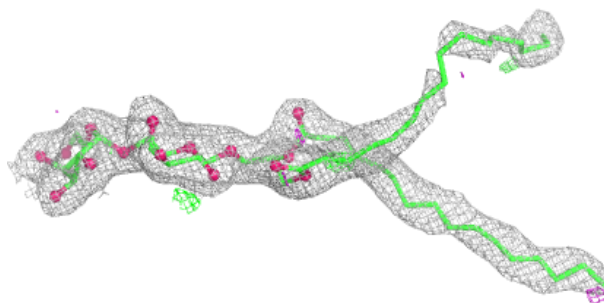
Electron density around CLA C 510:

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

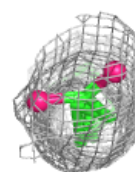
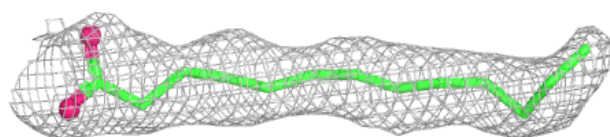
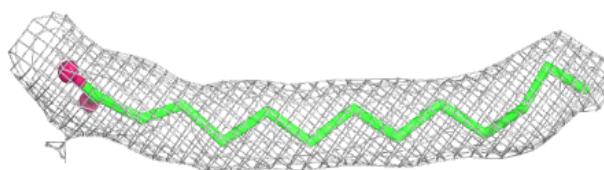


Electron density around DGD C 516:

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

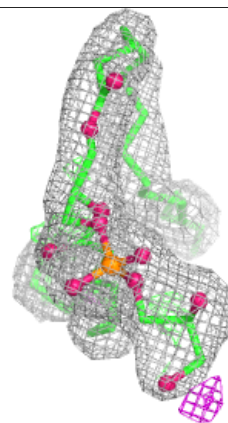
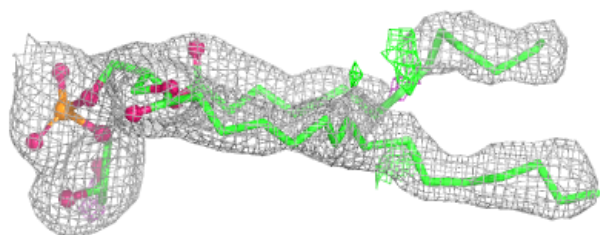
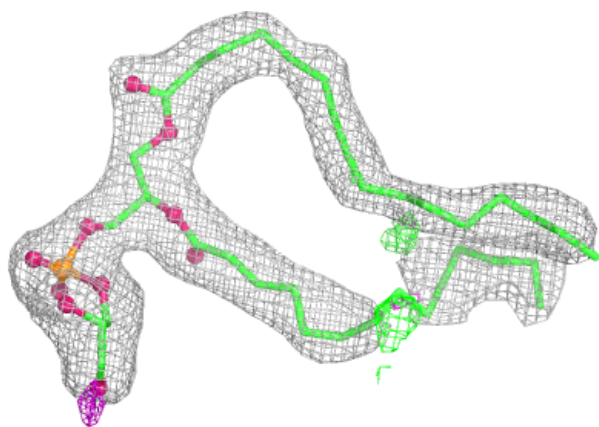
**Electron density around STE M 102:**

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

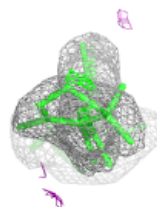
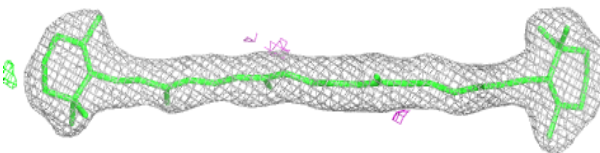
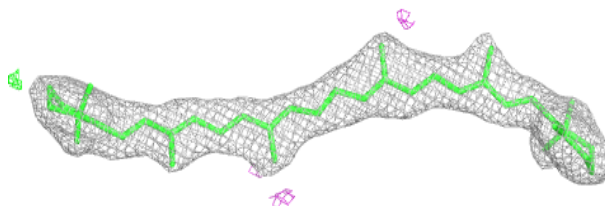


Electron density around LHG D 411:

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

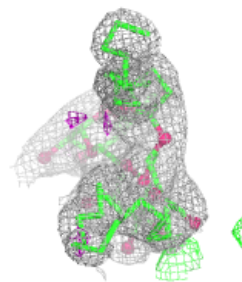
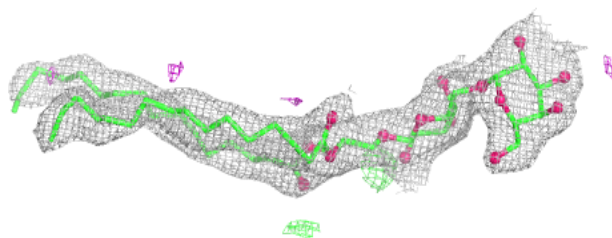
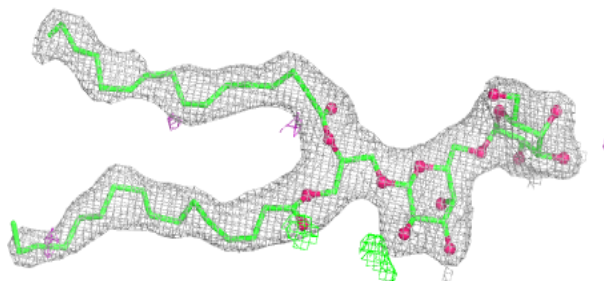
**Electron density around BCR c 515:**

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

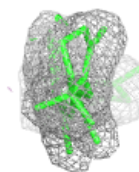
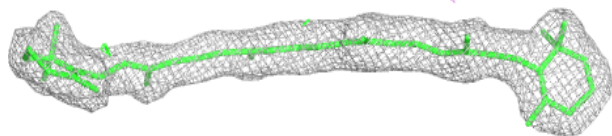
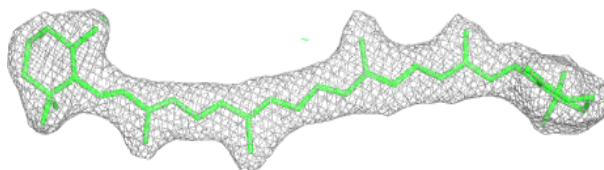


Electron density around DGD C 518:

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

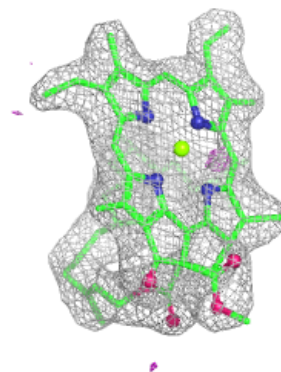
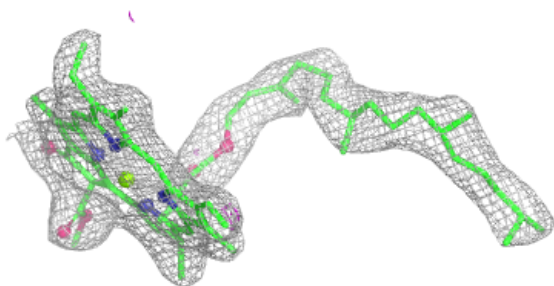
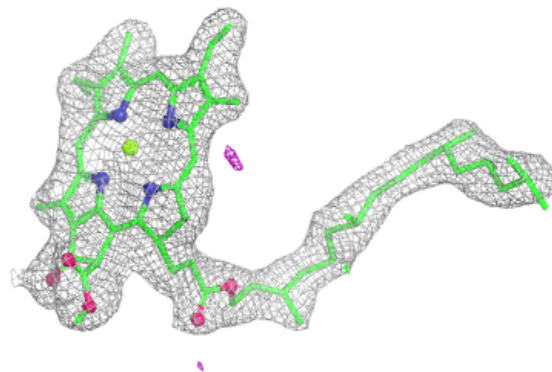
**Electron density around BCR B 617:**

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

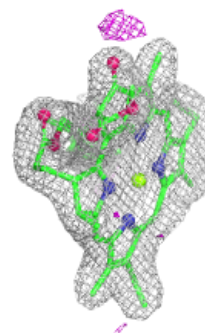
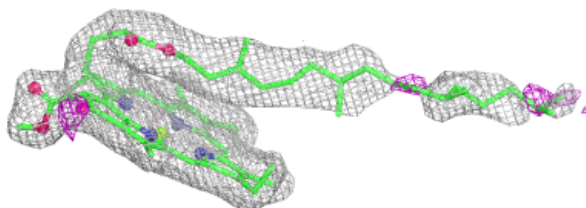
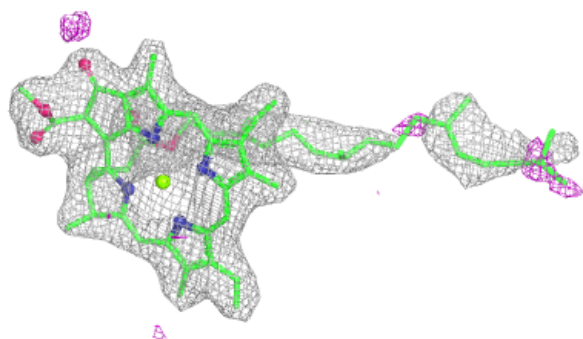


Electron density around CLA C 511:

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

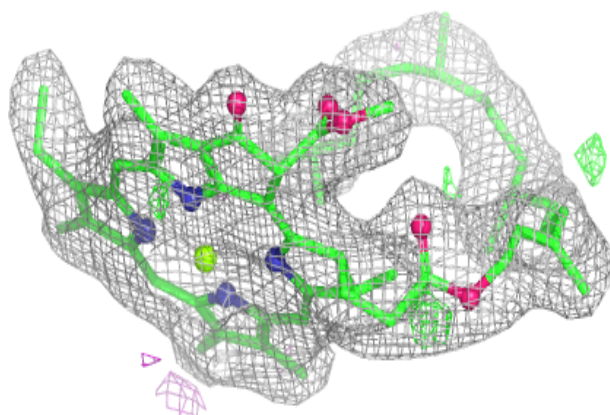
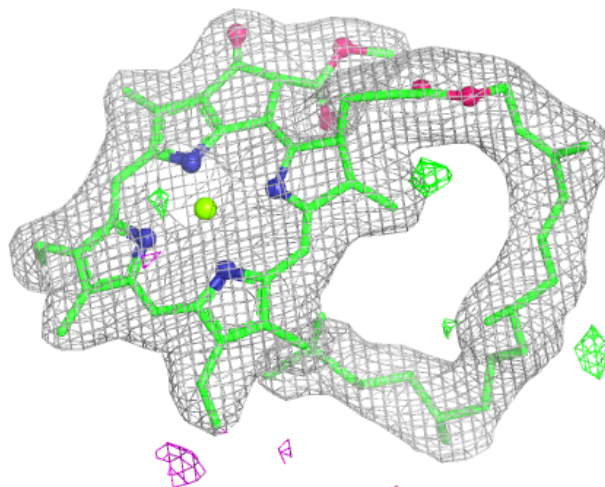
**Electron density around CLA b 614:**

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



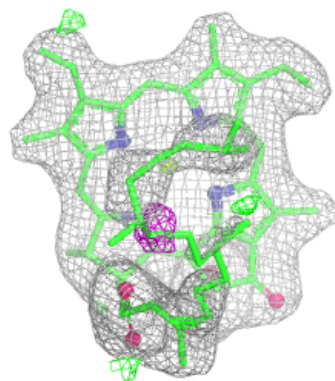
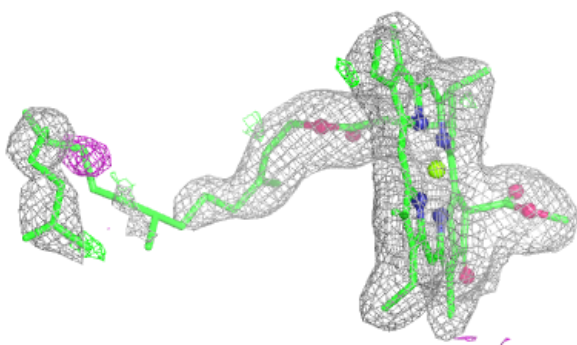
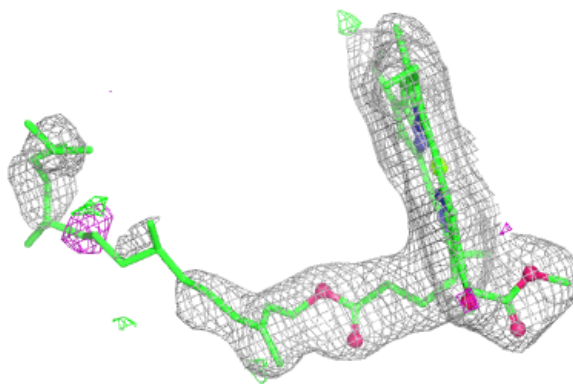
Electron density around CLA b 615:

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

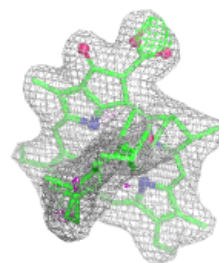
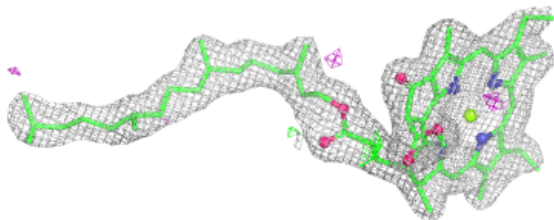
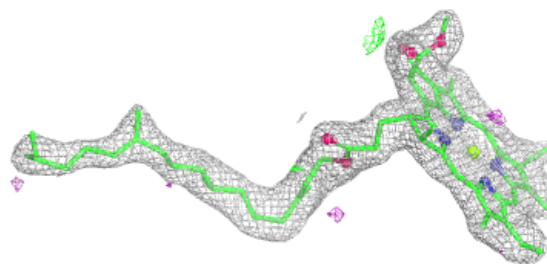


Electron density around CLA C 506:

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

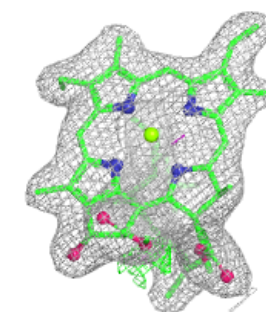
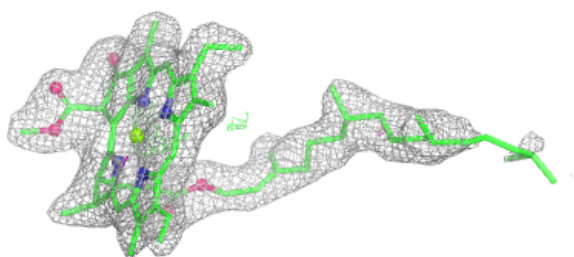
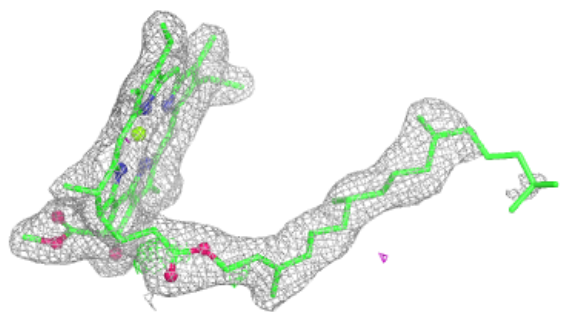
**Electron density around CLA c 502:**

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



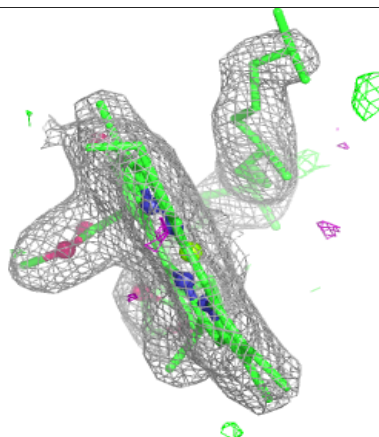
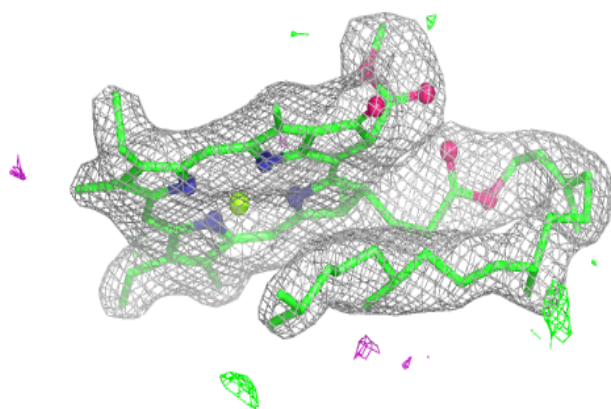
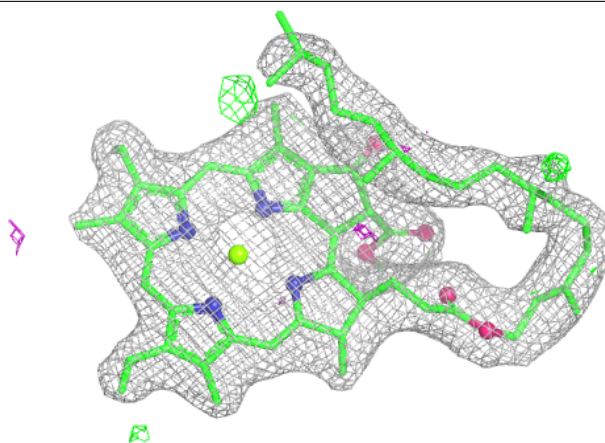
Electron density around CLA C 508:

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



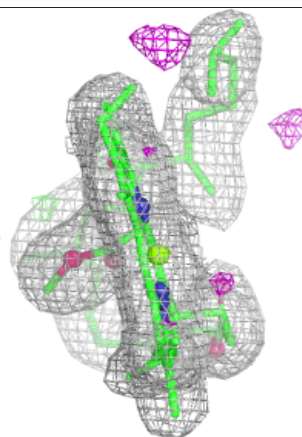
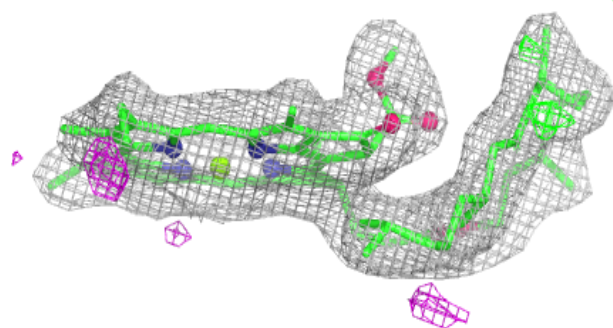
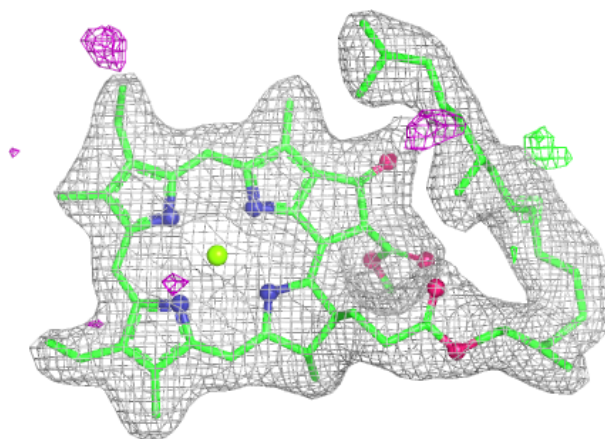
Electron density around CLA C 509:

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

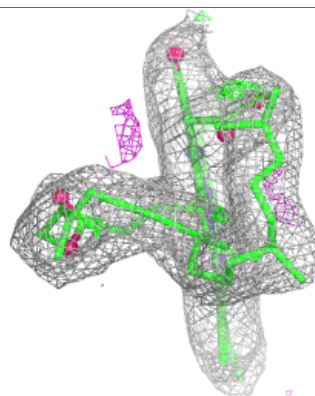
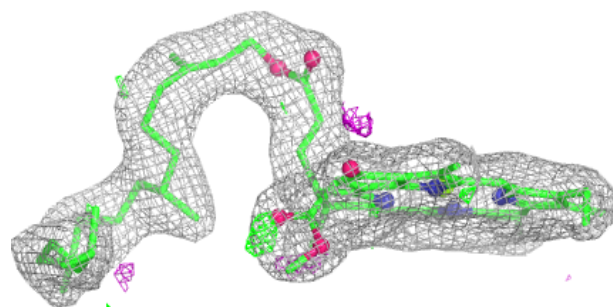
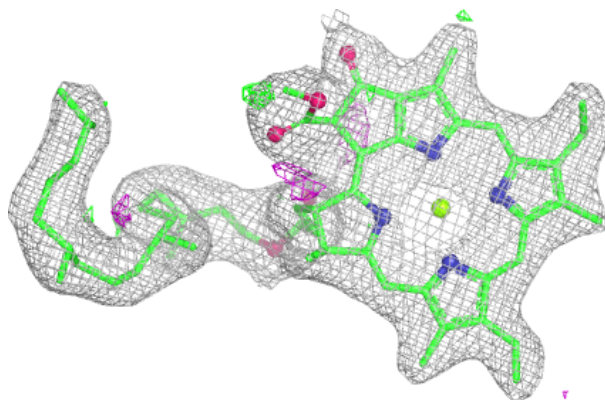


Electron density around CLA B 610:

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

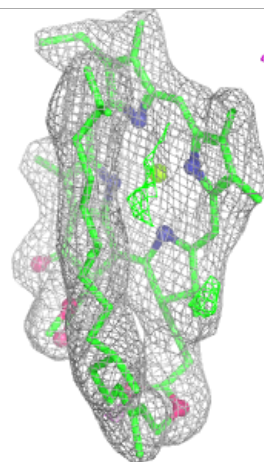
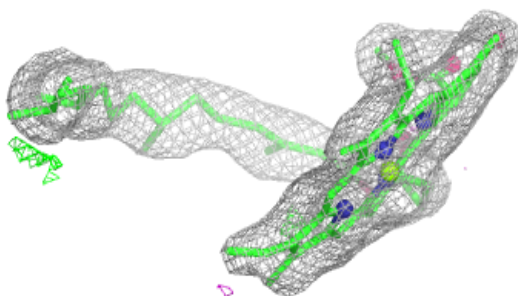
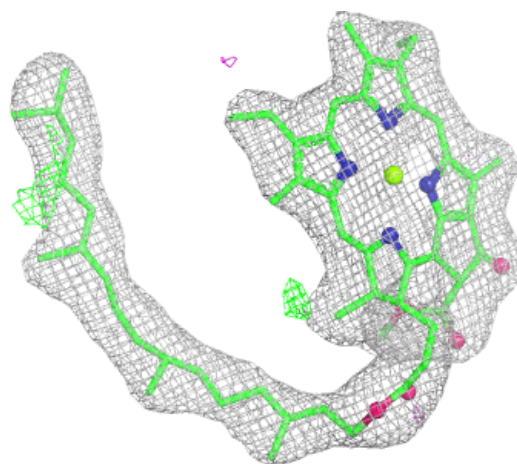
**Electron density around CLA B 612:**

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



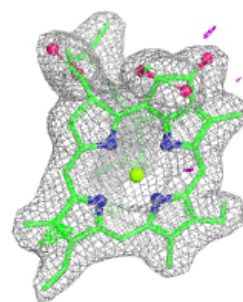
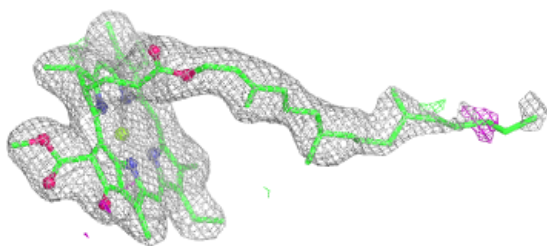
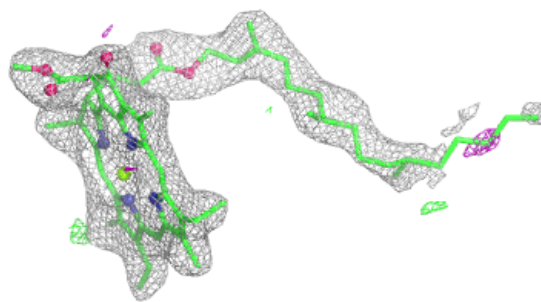
Electron density around CLA c 507:

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



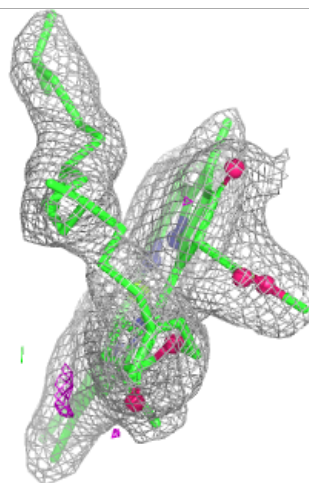
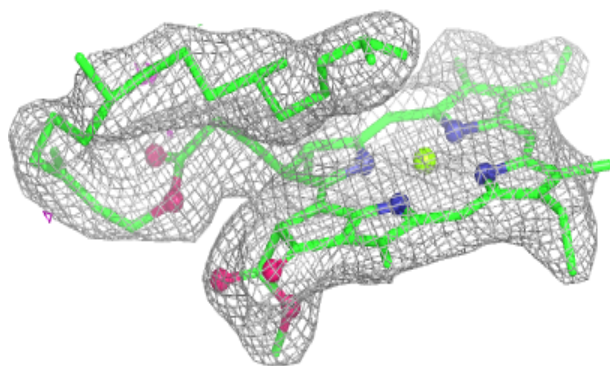
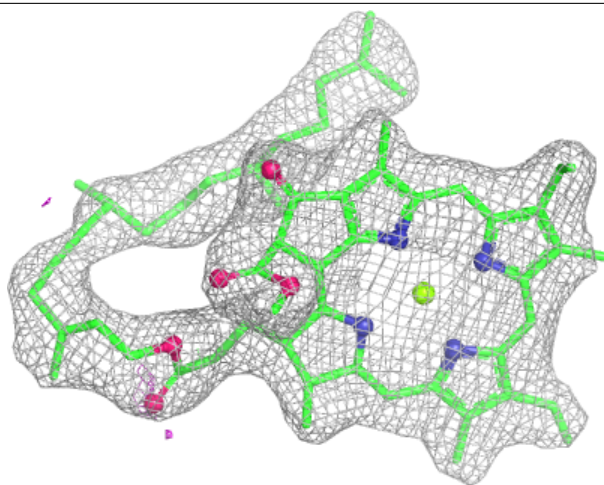
Electron density around CLA c 508:

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



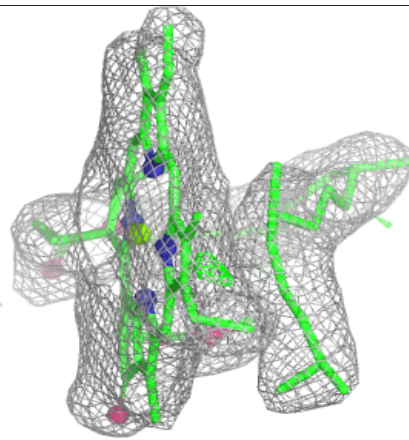
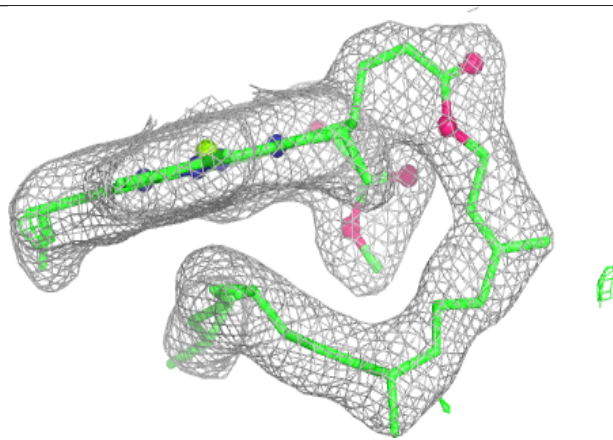
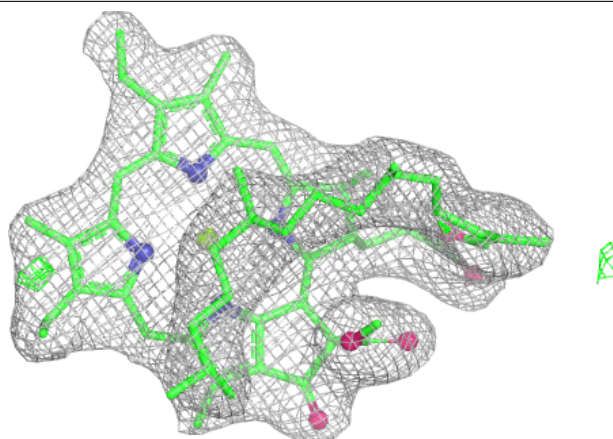
Electron density around CLA c 509:

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



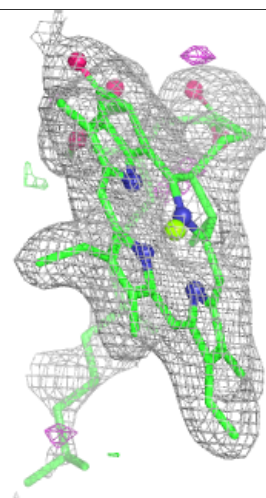
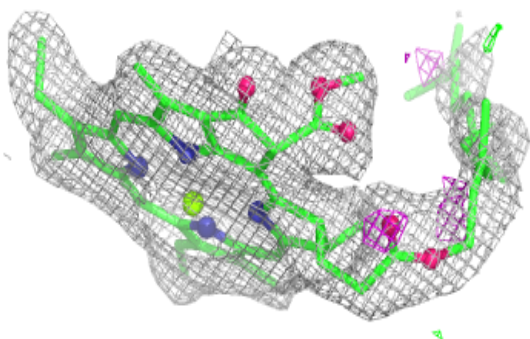
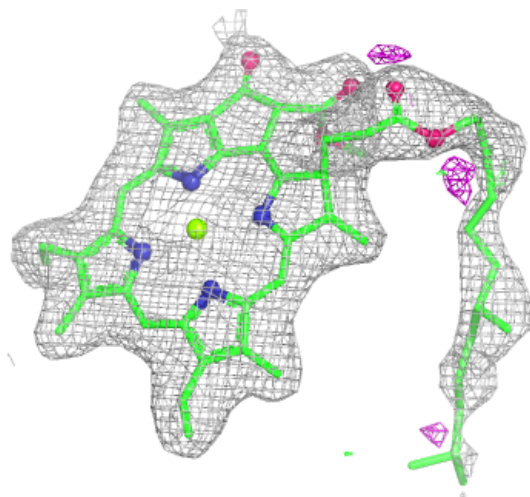
Electron density around CLA c 510:

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



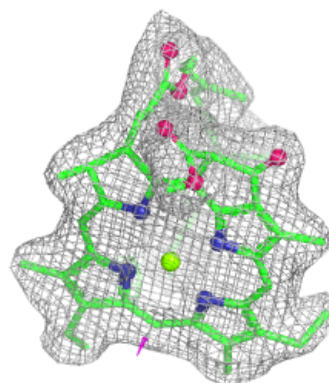
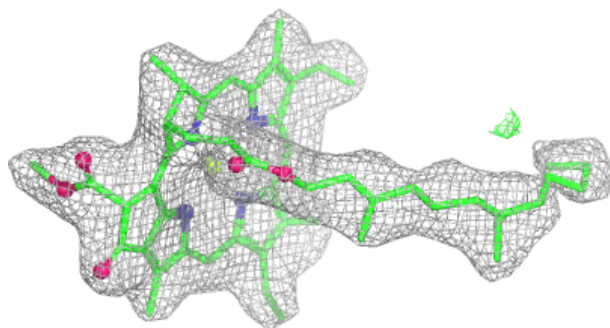
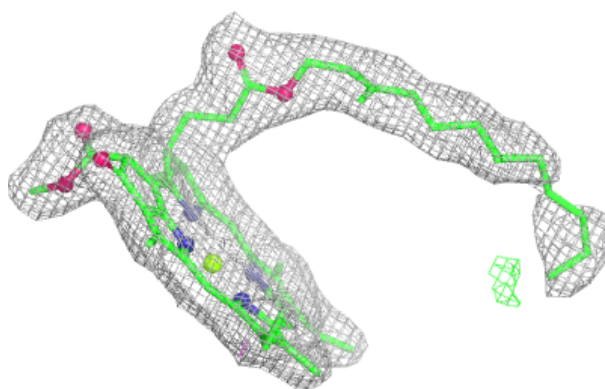
Electron density around CLA B 616:

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

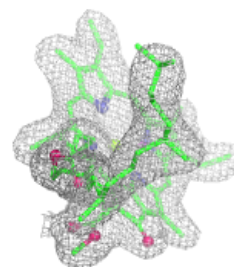
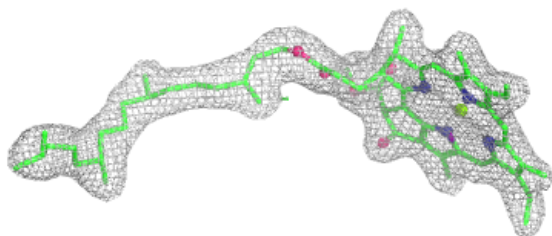
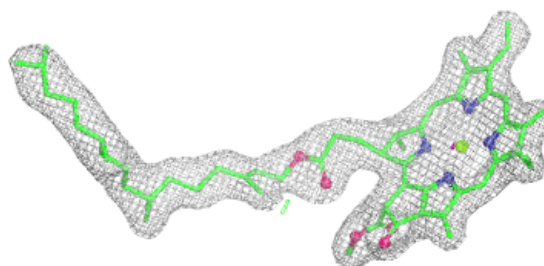


Electron density around CLA C 504:

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

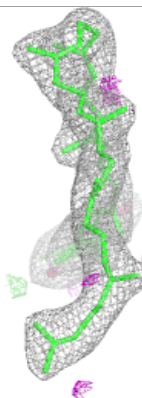
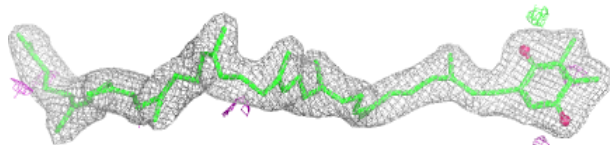
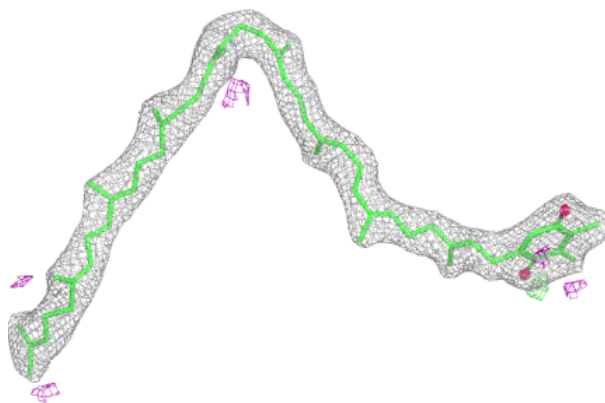
**Electron density around CLA a 606:**

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

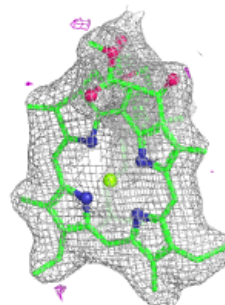
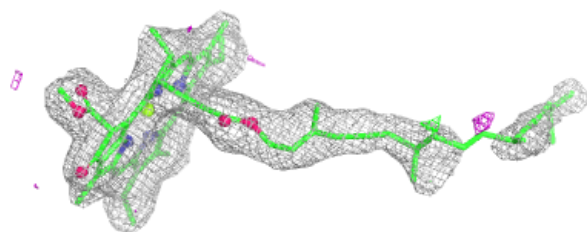
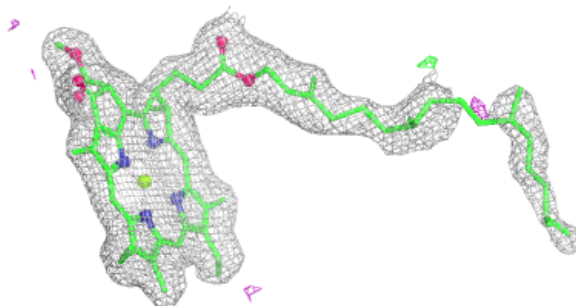


Electron density around PL9 D 407:

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

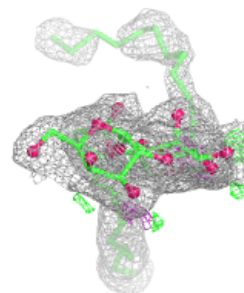
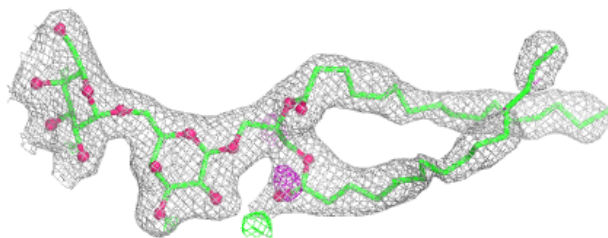
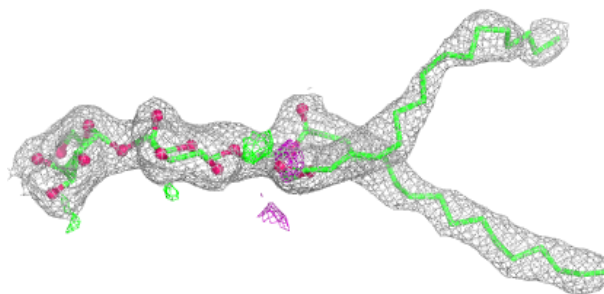
**Electron density around CLA d 404:**

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

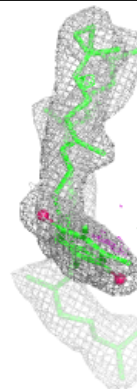
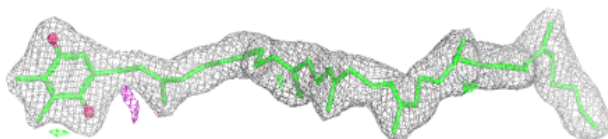
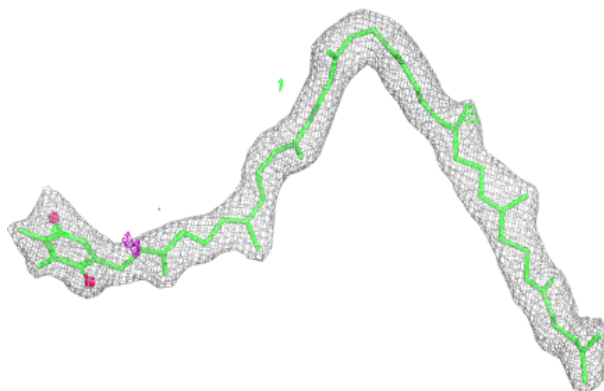


Electron density around DGD c 516:

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

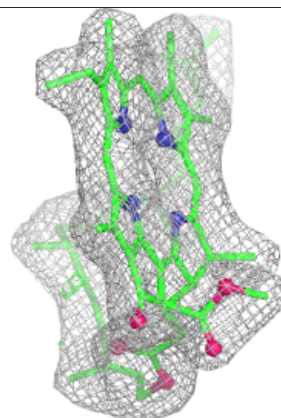
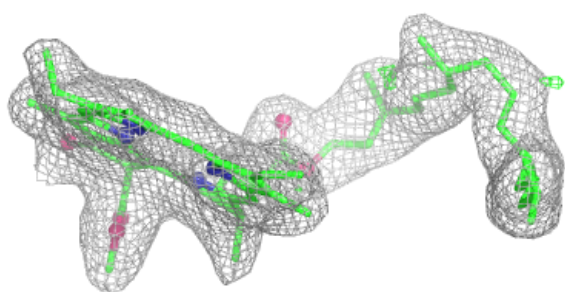
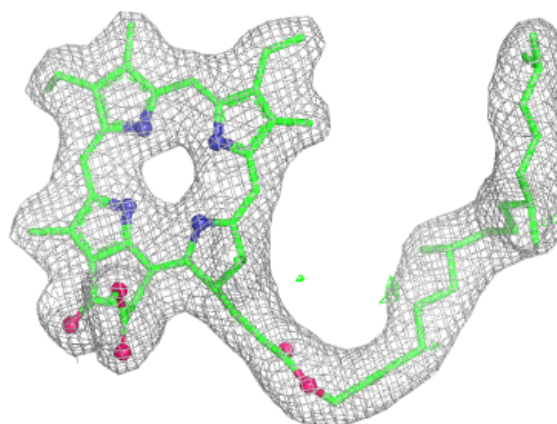
**Electron density around PL9 d 406:**

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



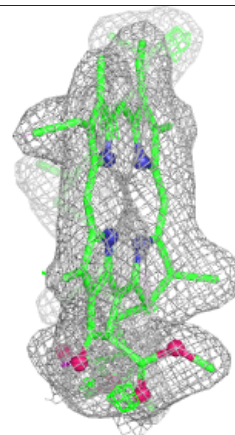
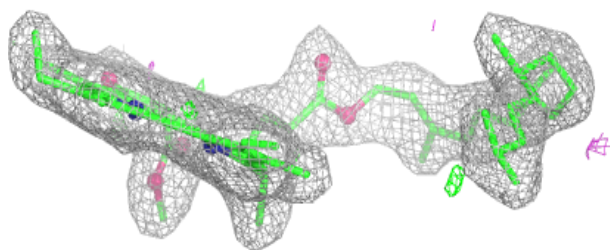
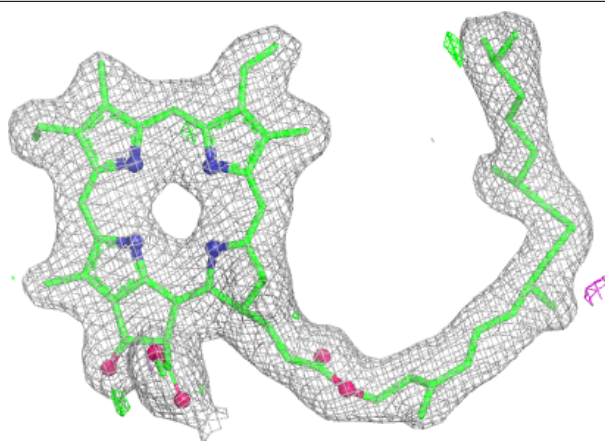
Electron density around PHO D 402:

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



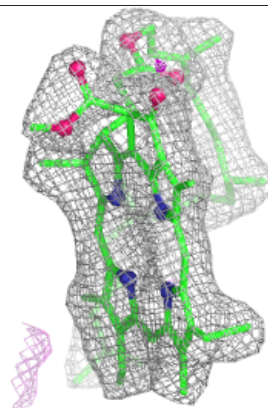
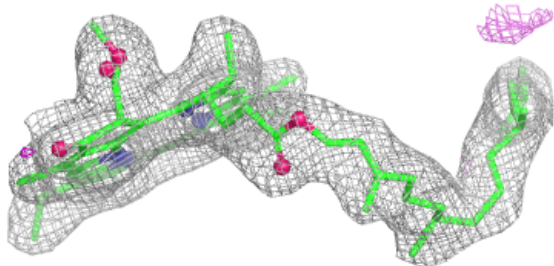
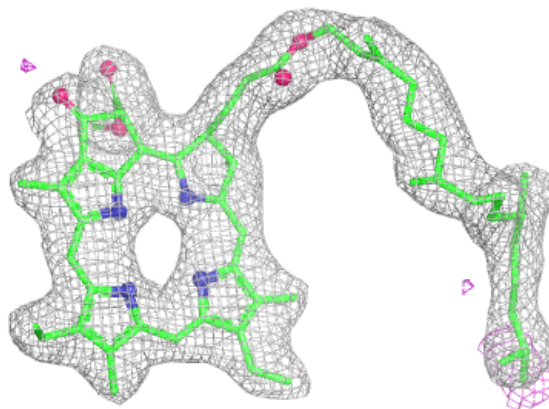
Electron density around PHO a 608:

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

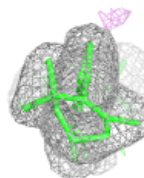
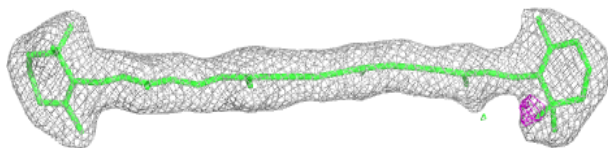
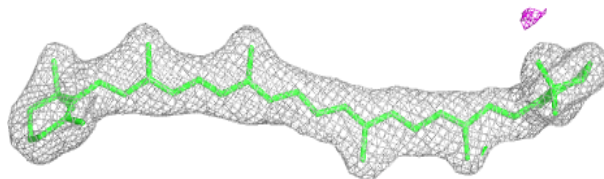


Electron density around PHO d 402:

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

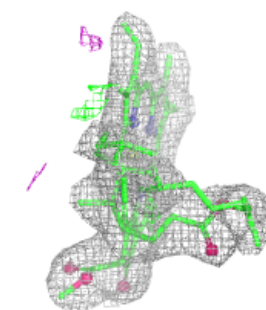
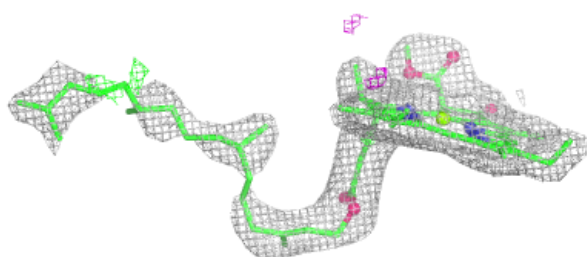
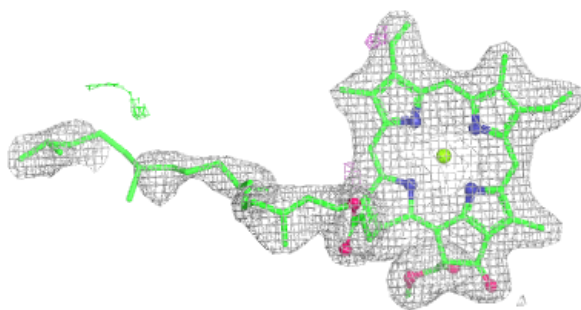
**Electron density around BCR A 610:**

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

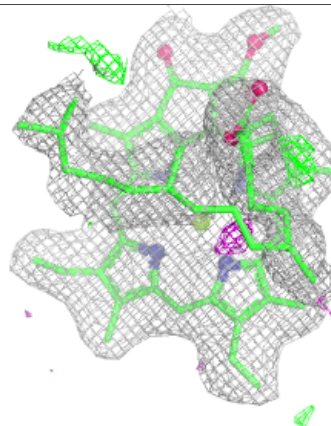
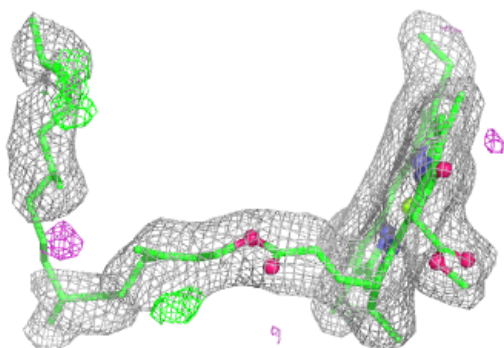
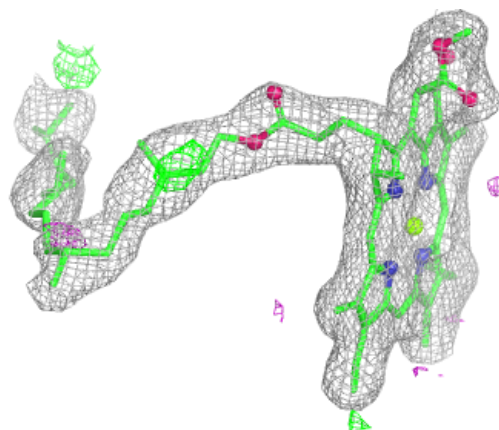


Electron density around CLA a 607:

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

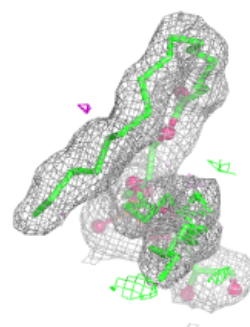
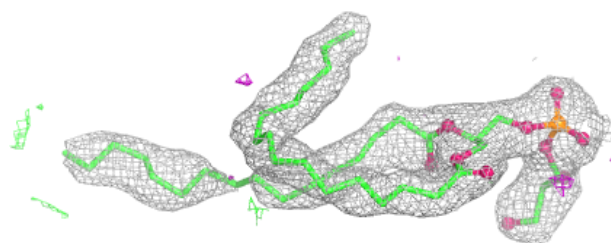
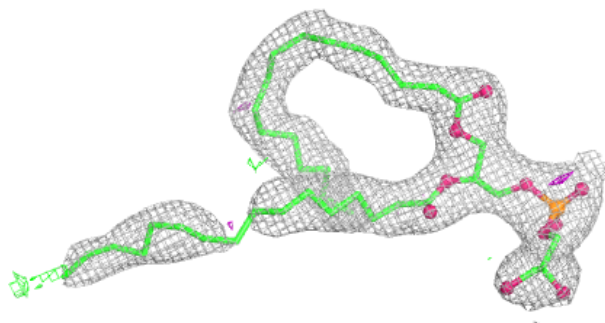
**Electron density around CLA a 609:**

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

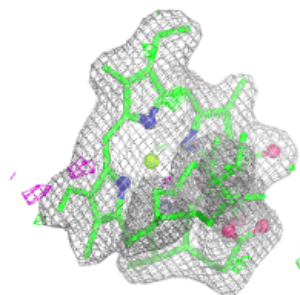
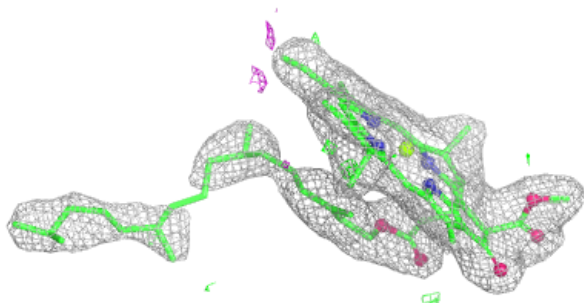
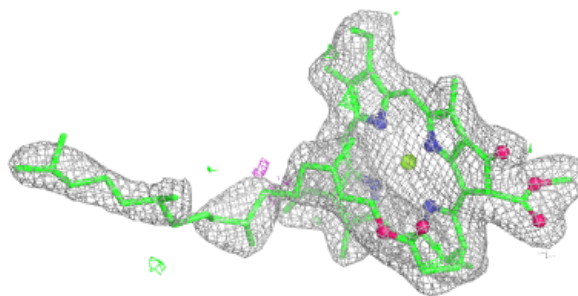


Electron density around LHG D 413:

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

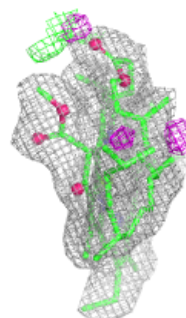
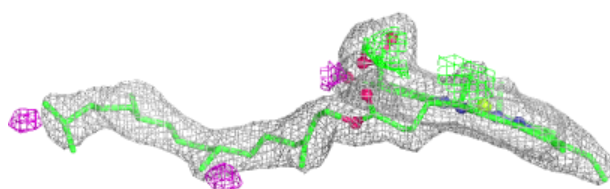
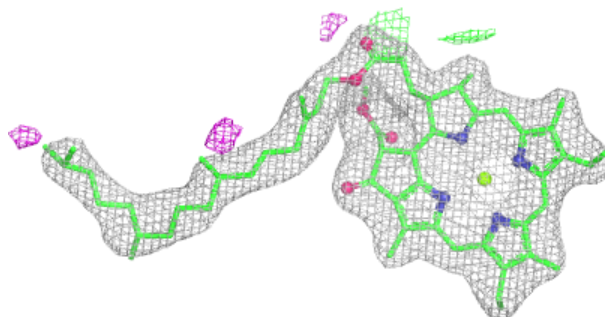
**Electron density around CLA C 505:**

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

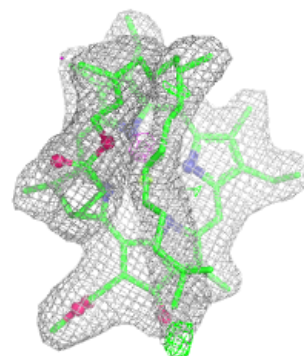
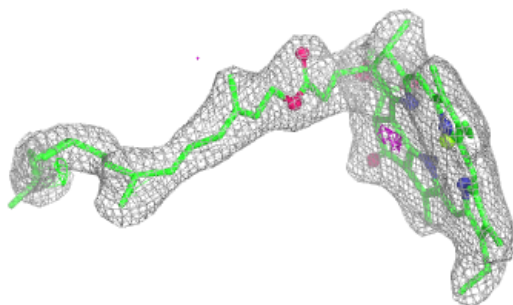
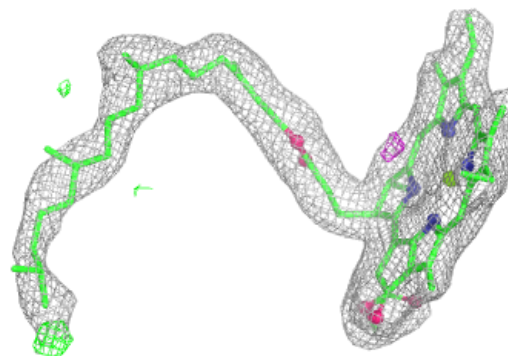


Electron density around CLA b 602:

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

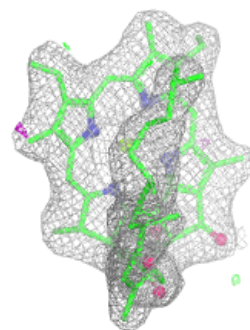
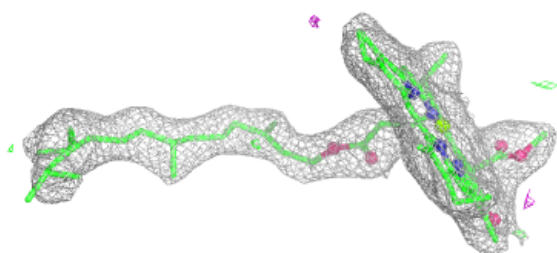
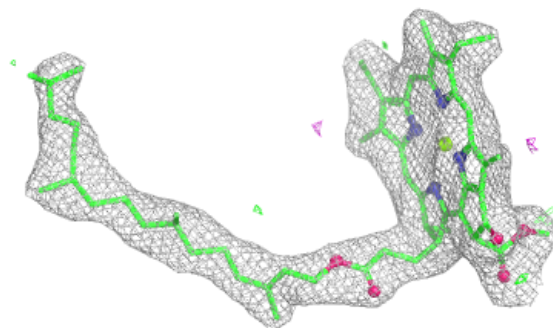
**Electron density around CLA b 606:**

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



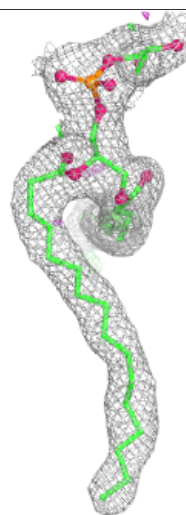
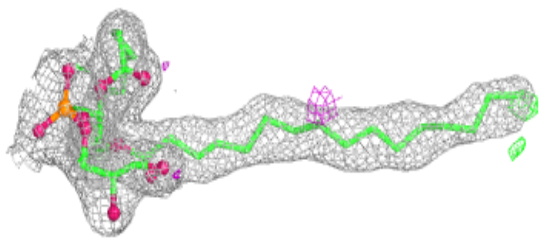
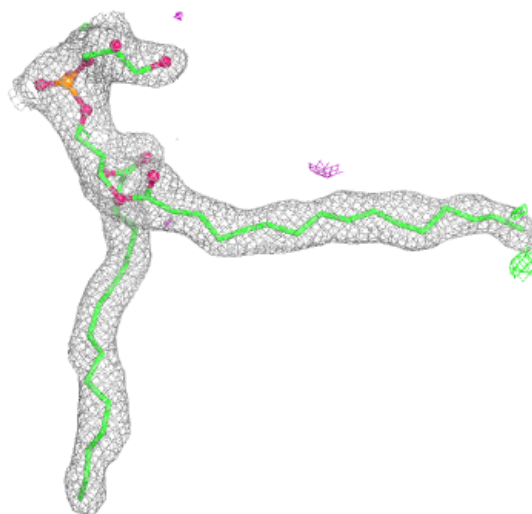
Electron density around CLA b 609:

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



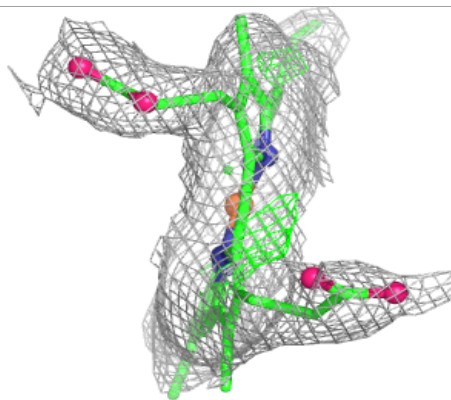
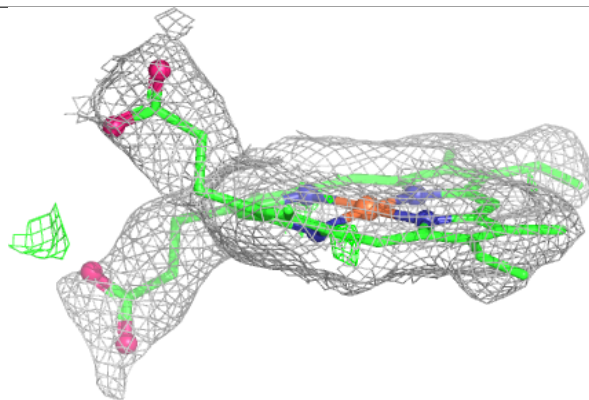
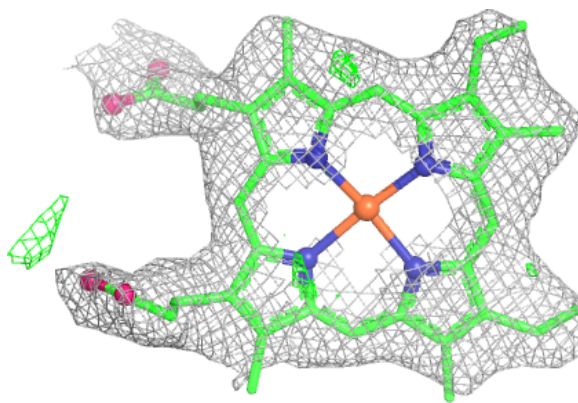
Electron density around LHG 1 101:

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

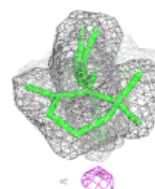
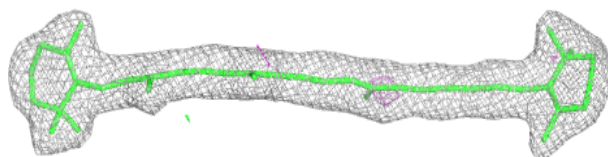
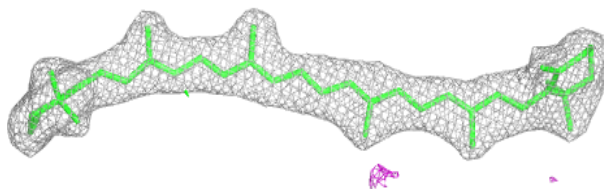


Electron density around HEM e 101:

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

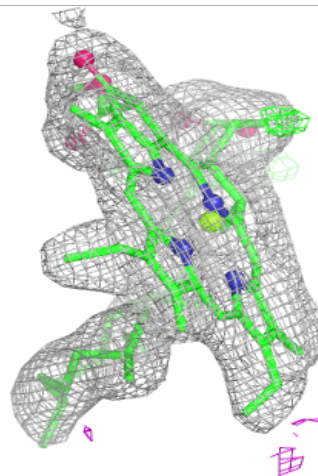
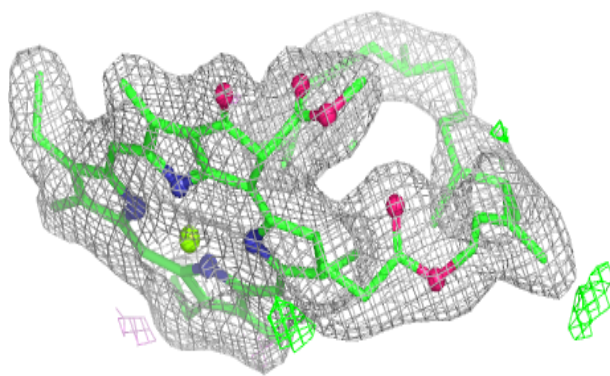
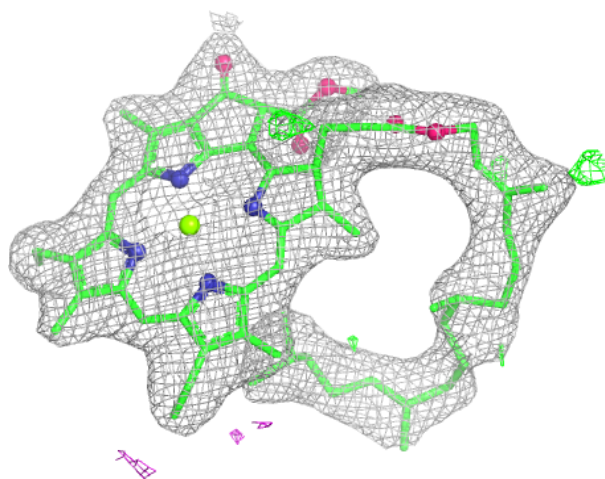
**Electron density around BCR a 610:**

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



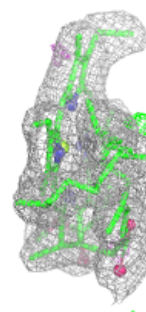
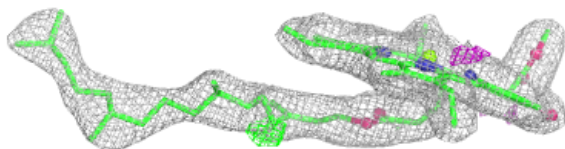
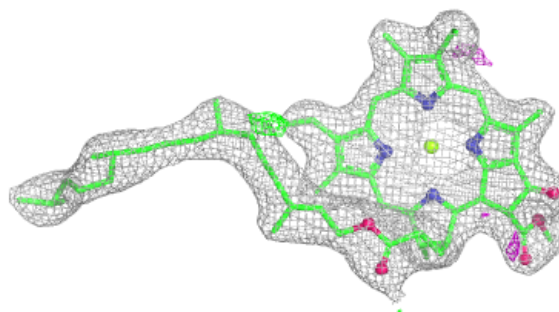
Electron density around CLA B 615:

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

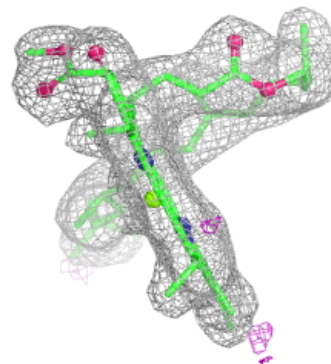
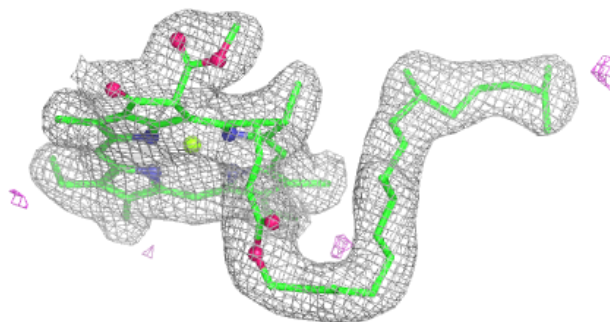
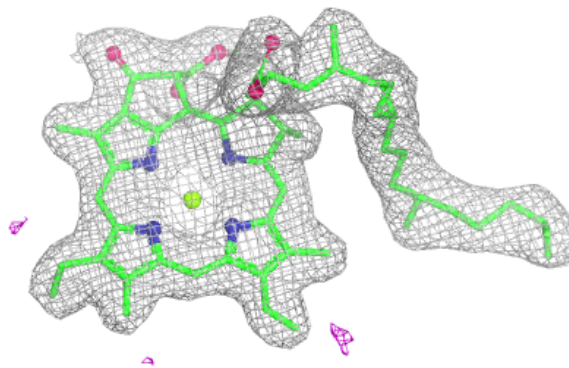


Electron density around CLA B 603:

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

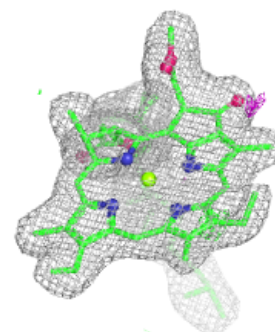
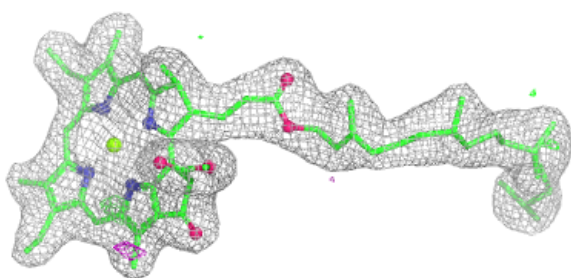
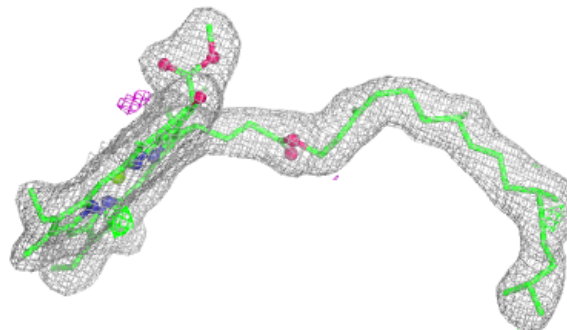
**Electron density around CLA D 403:**

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

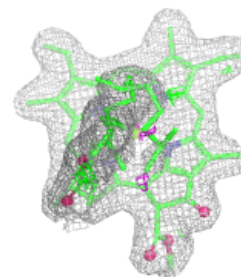
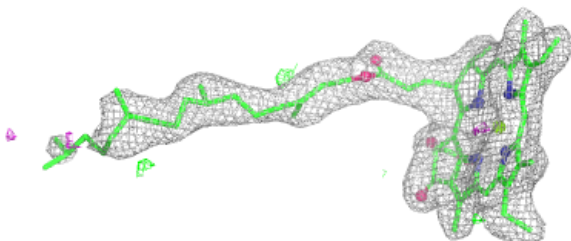
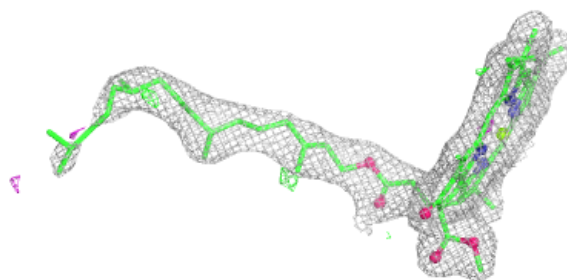


Electron density around CLA D 404:

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

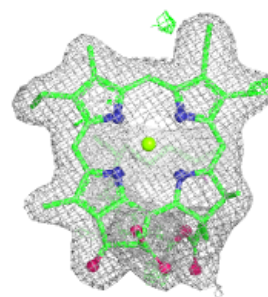
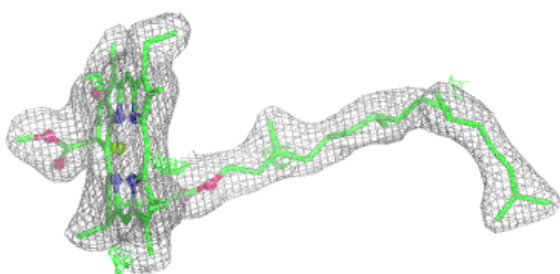
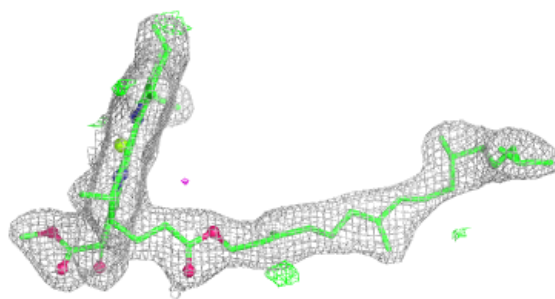
**Electron density around CLA B 604:**

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

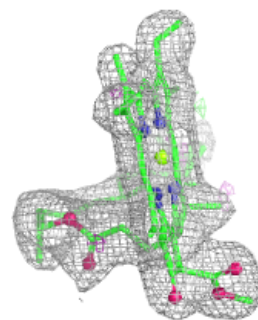
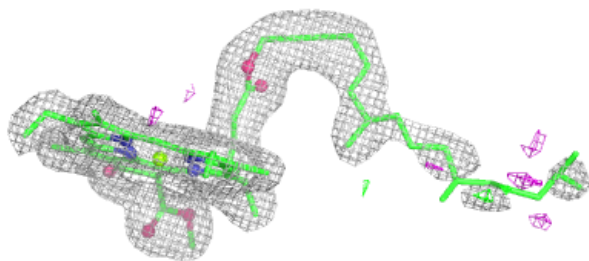
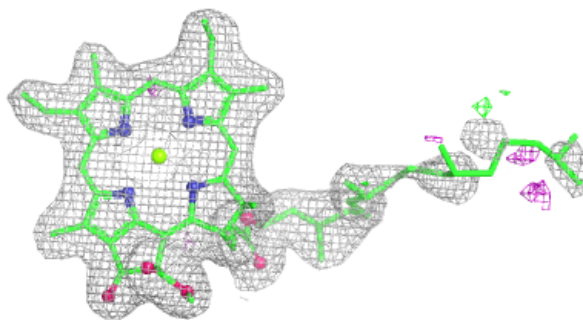


Electron density around CLA B 605:

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

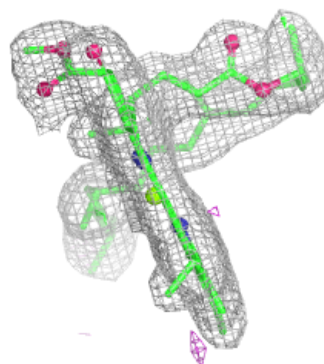
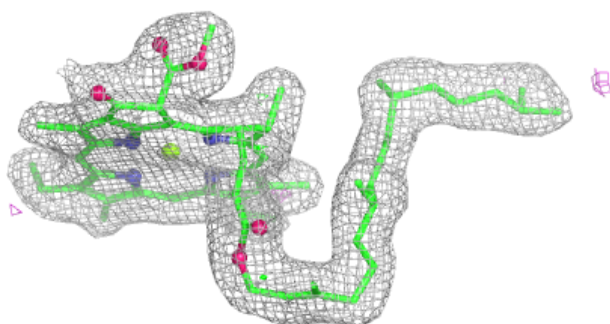
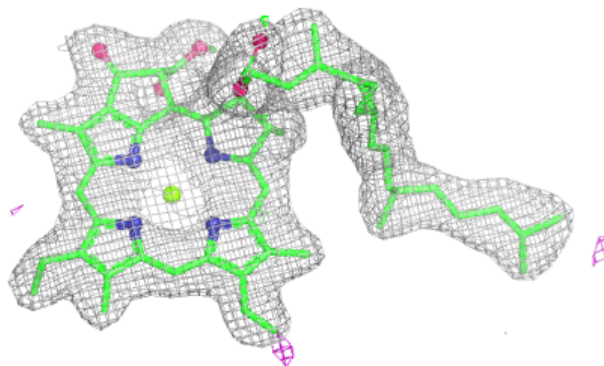
**Electron density around CLA A 607:**

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

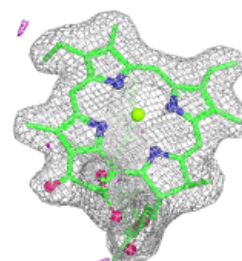
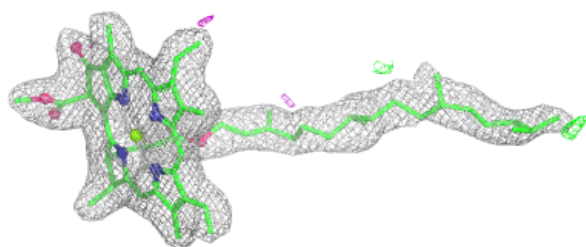
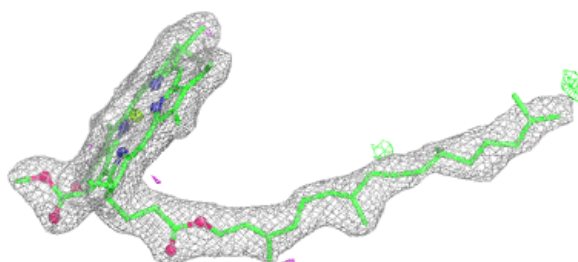


Electron density around CLA a 612:

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

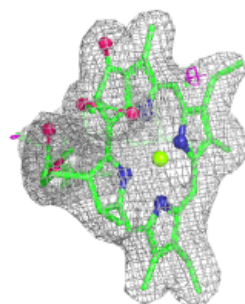
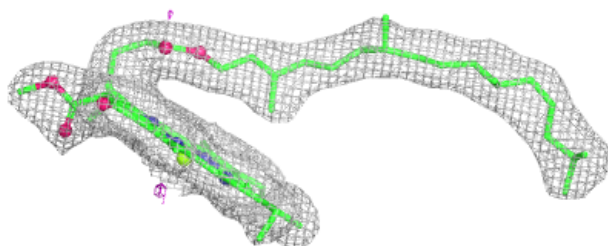
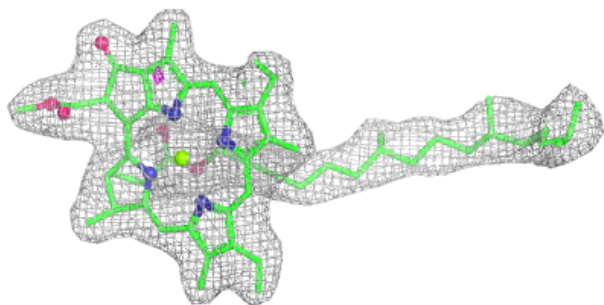
**Electron density around CLA B 607:**

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

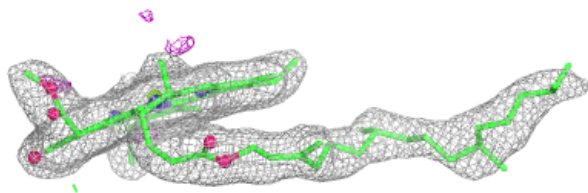
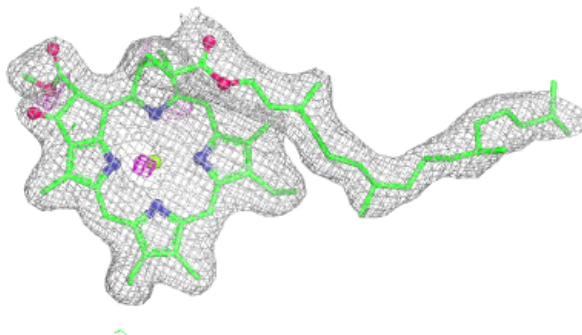


Electron density around CLA B 608:

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

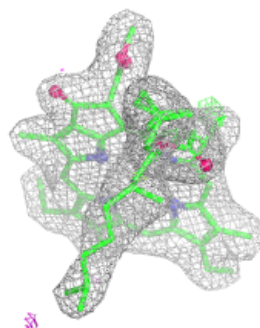
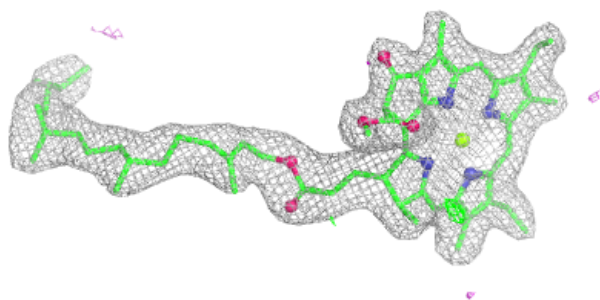
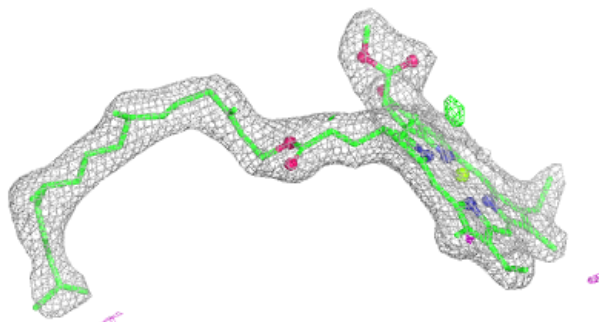
**Electron density around CLA b 603:**

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

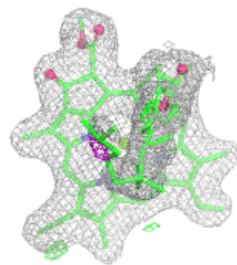
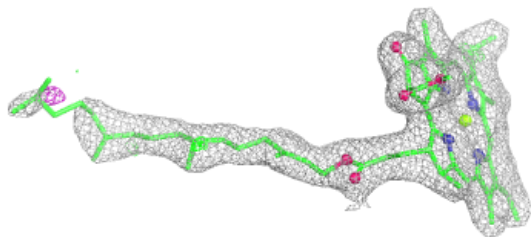
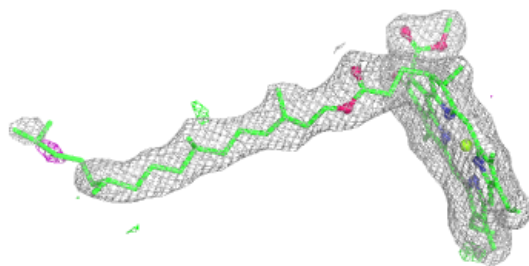


Electron density around CLA d 403:

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

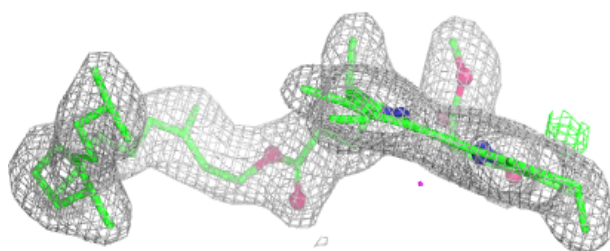
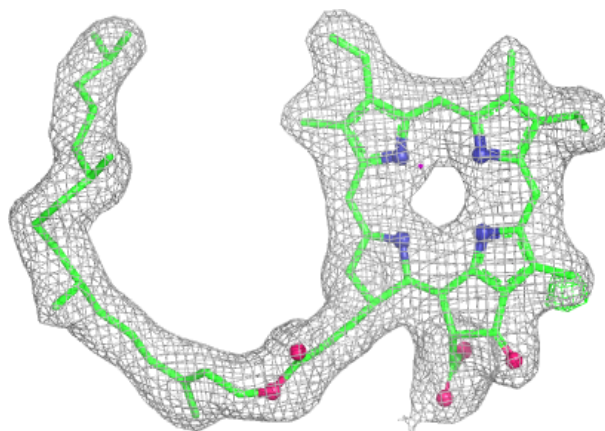
**Electron density around CLA b 604:**

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

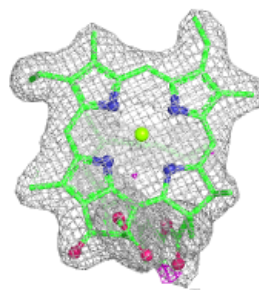
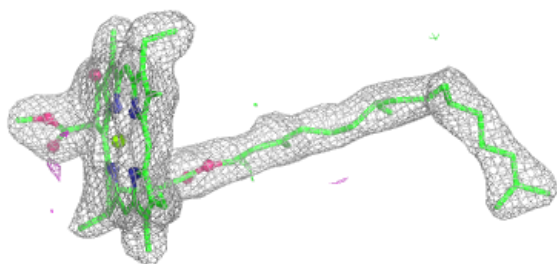
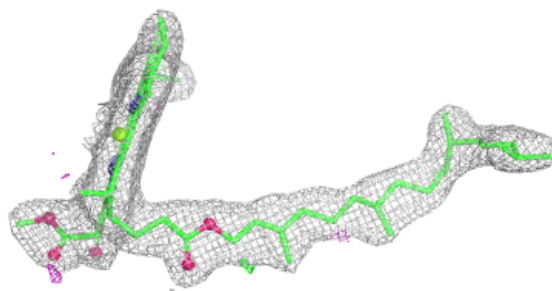


Electron density around PHO A 608:

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

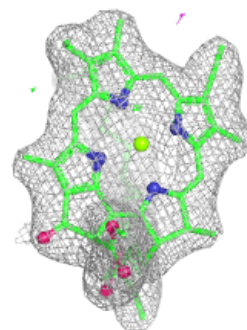
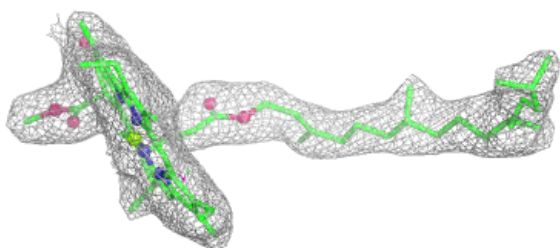
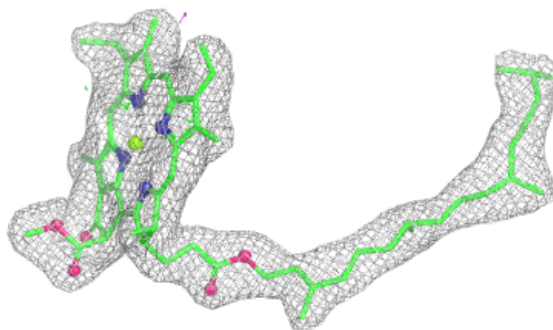
**Electron density around CLA b 605:**

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

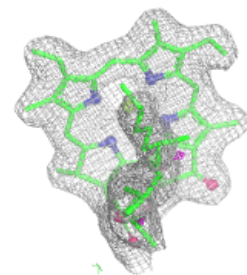
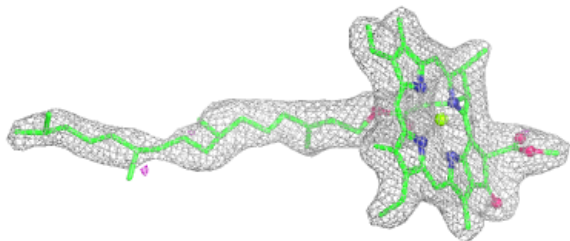
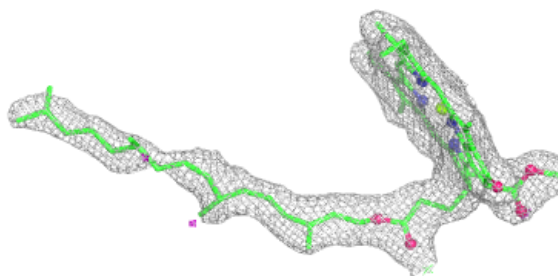


Electron density around CLA B 609:

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

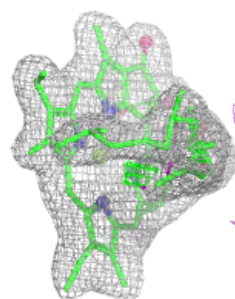
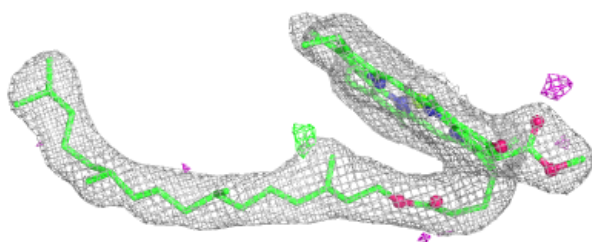
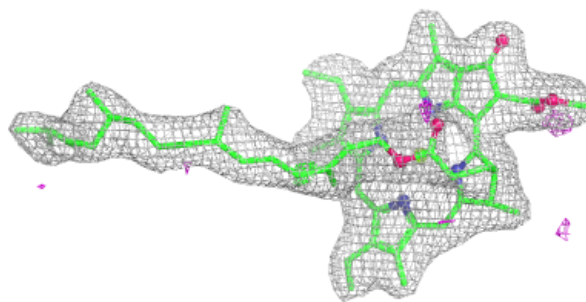
**Electron density around CLA b 607:**

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



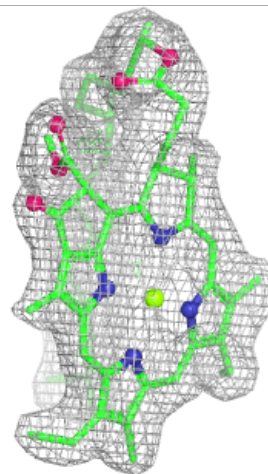
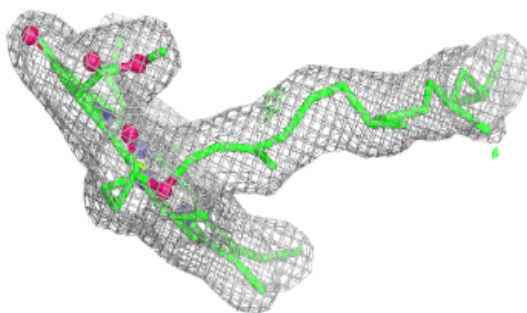
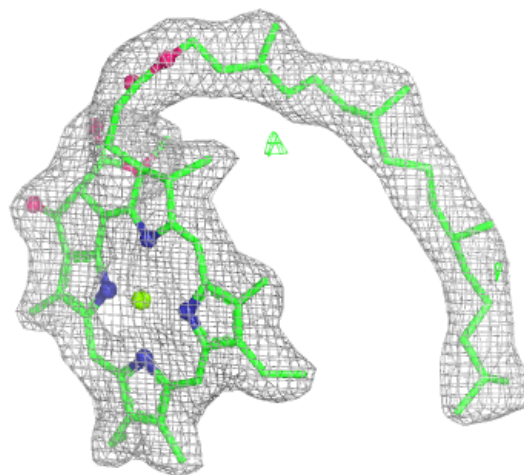
Electron density around CLA b 608:

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



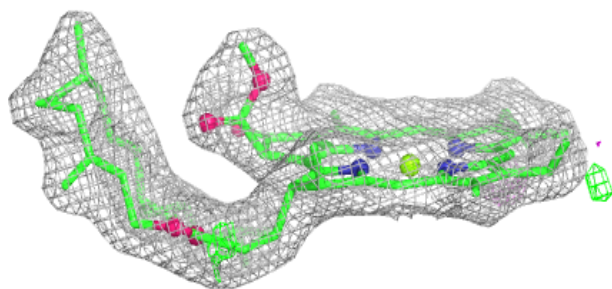
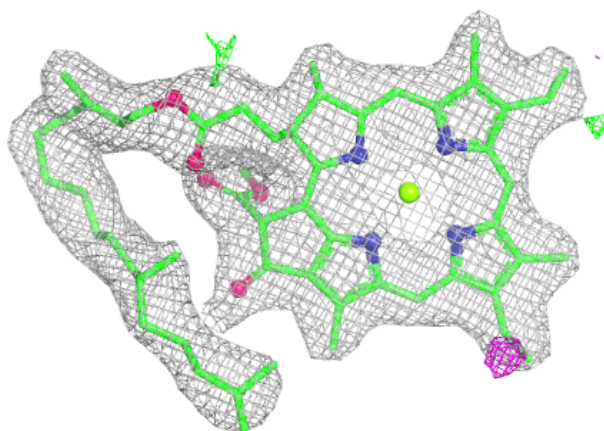
Electron density around CLA C 507:

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



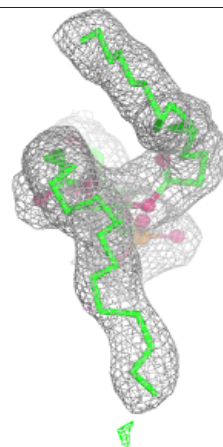
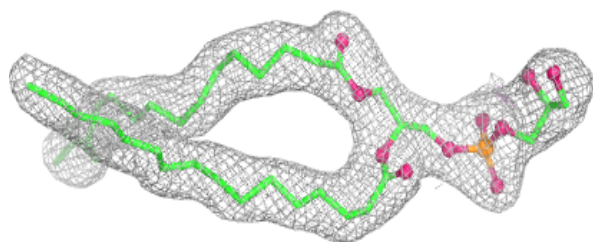
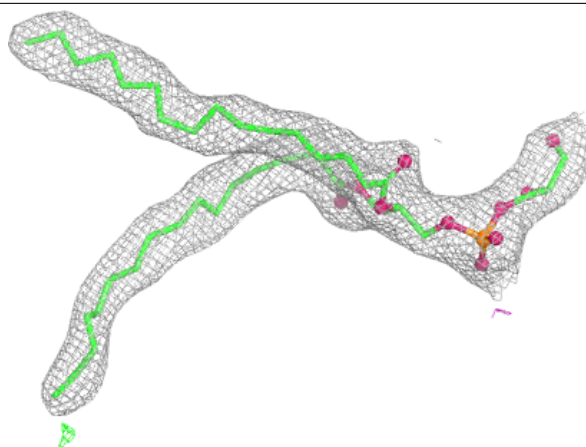
Electron density around CLA b 610:

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



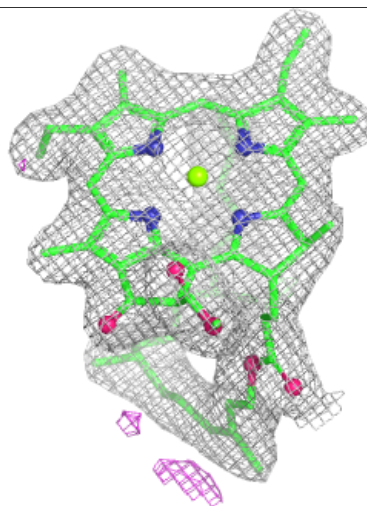
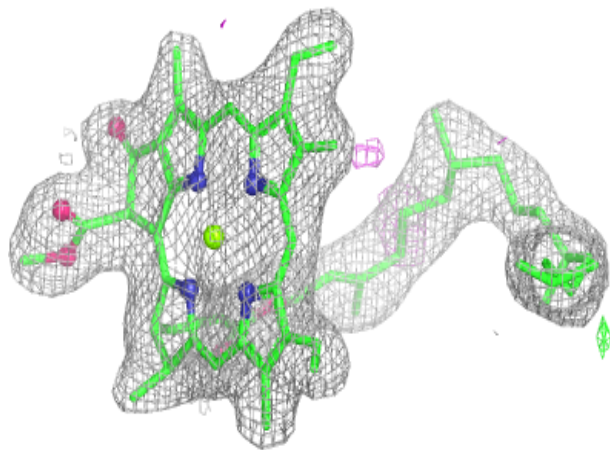
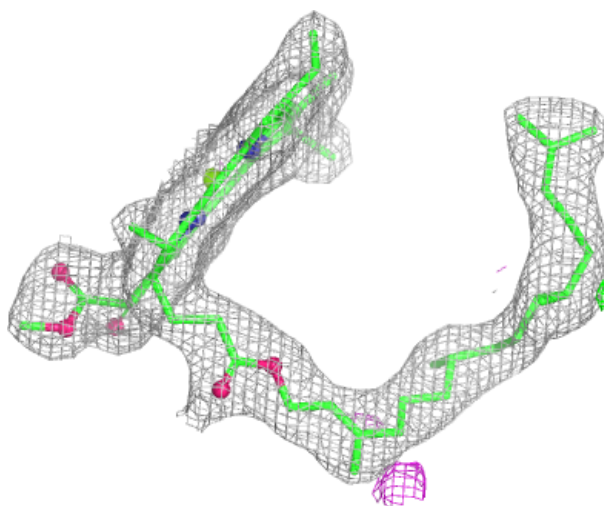
Electron density around LHG D 410:

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



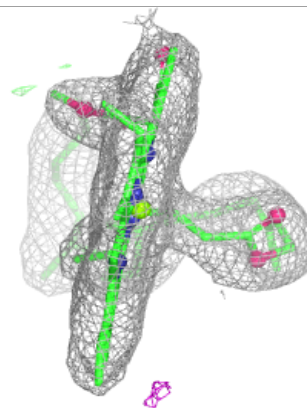
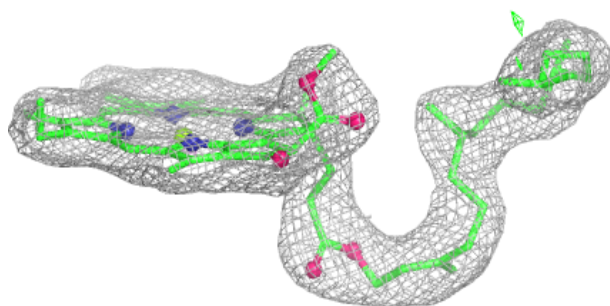
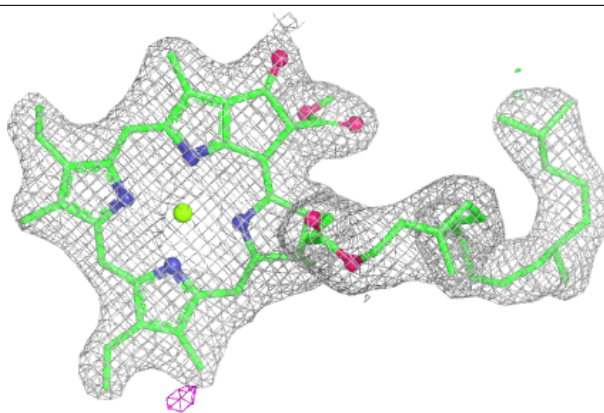
Electron density around CLA b 611:

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



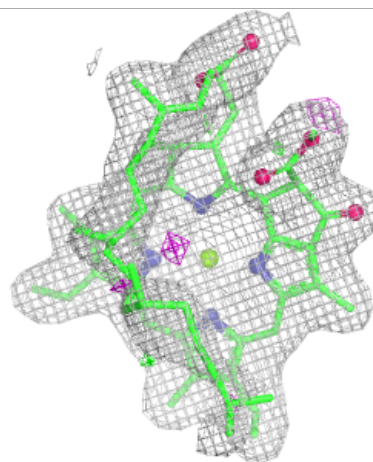
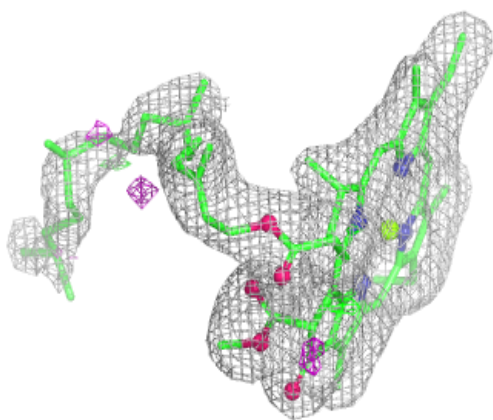
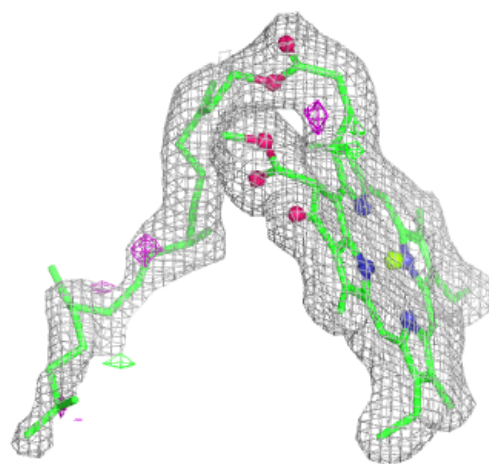
Electron density around CLA b 612:

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



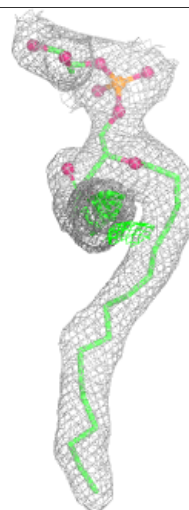
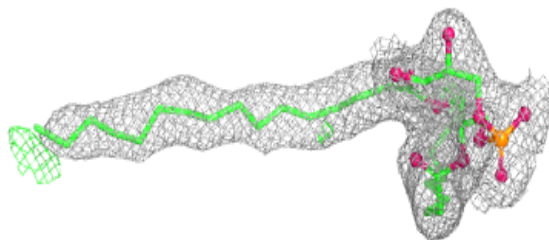
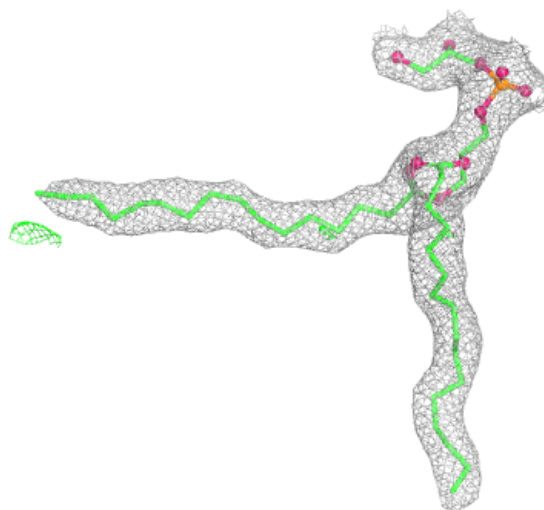
Electron density around CLA b 613:

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



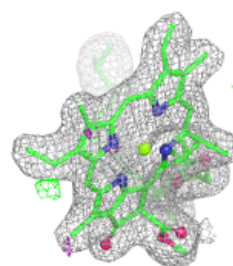
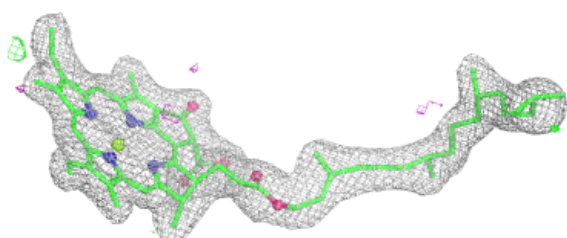
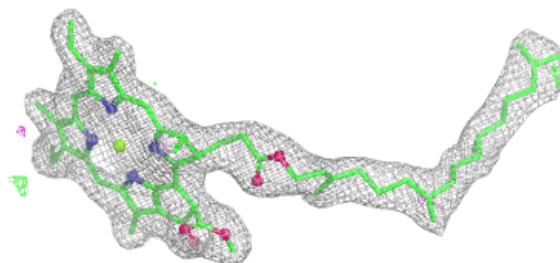
Electron density around LHG L 102:

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

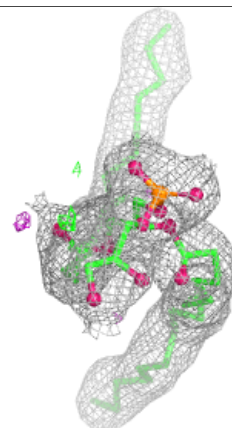
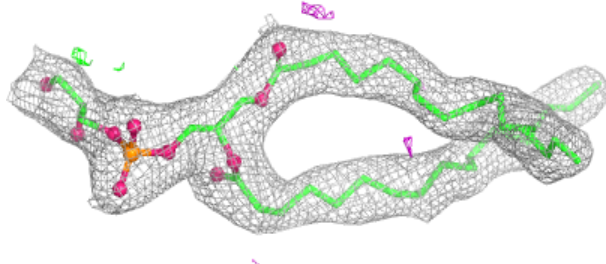
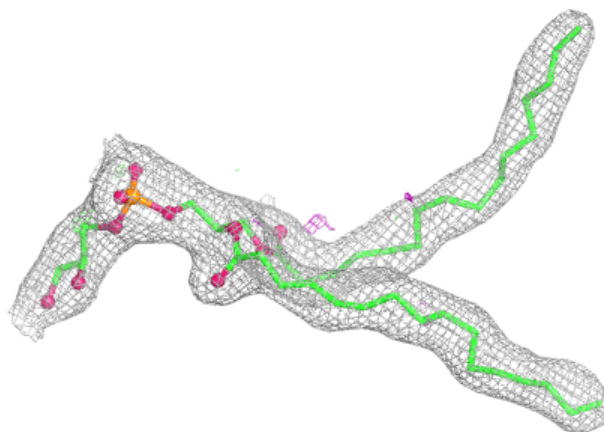


Electron density around CLA A 606:

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

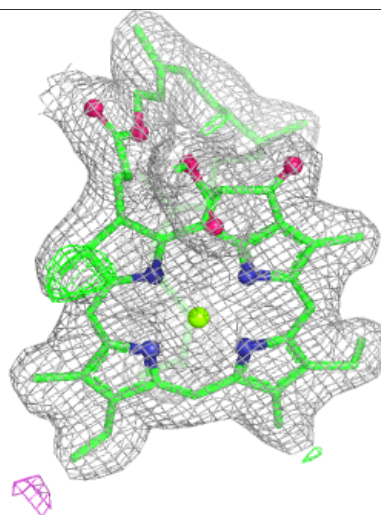
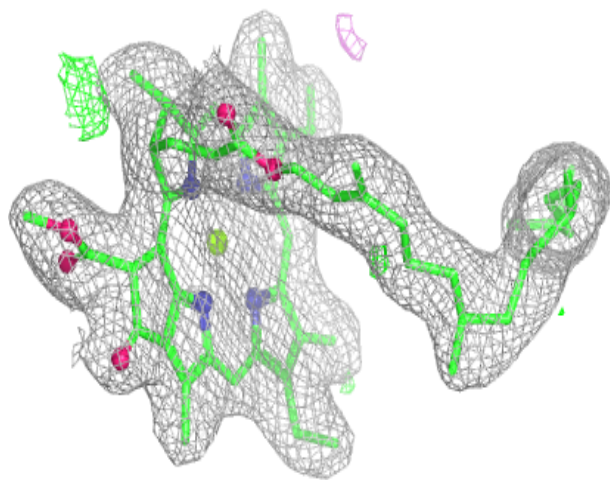
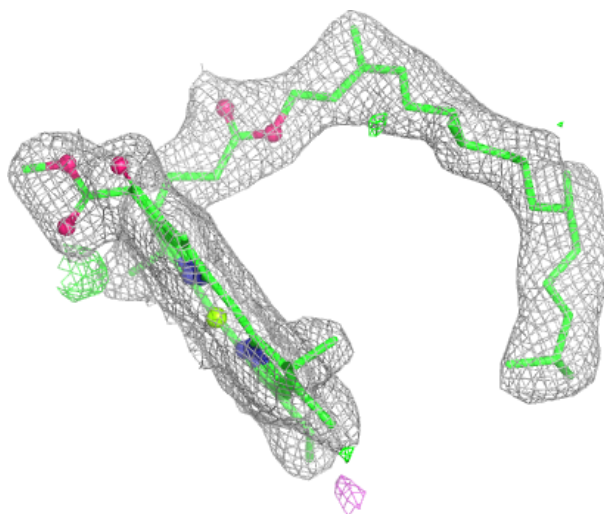
**Electron density around LHG d 408:**

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



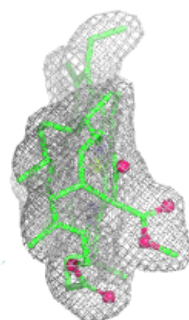
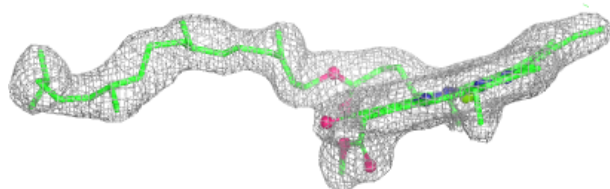
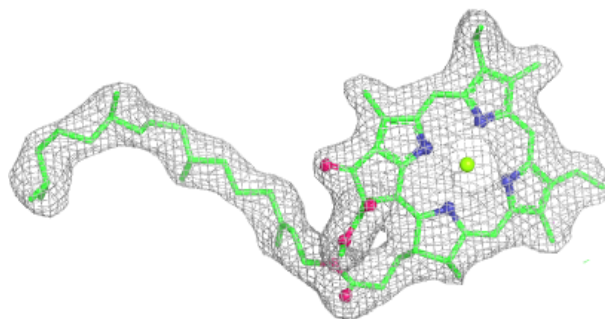
Electron density around CLA B 611:

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

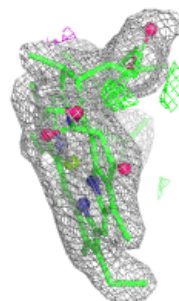
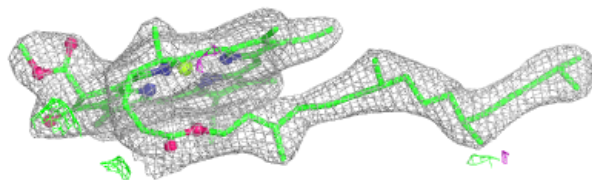
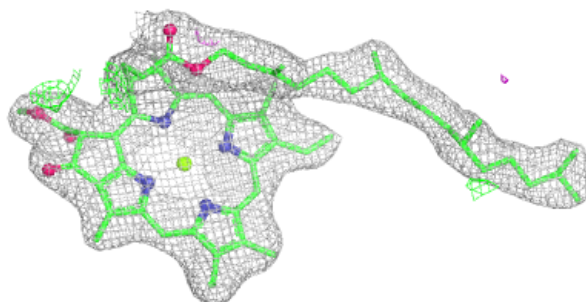


Electron density around CLA B 602:

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

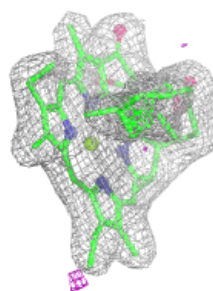
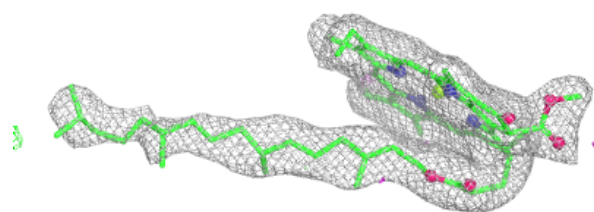
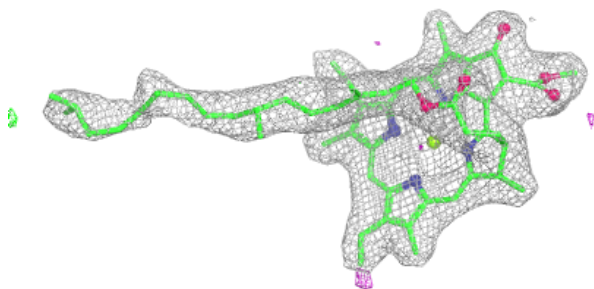
**Electron density around CLA c 501:**

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

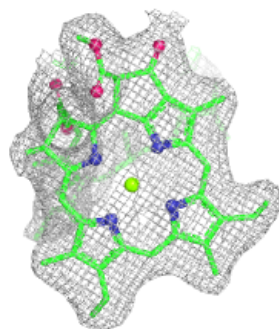
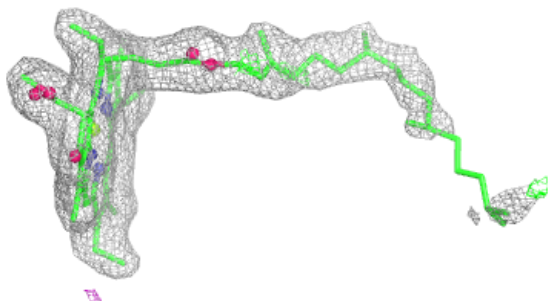
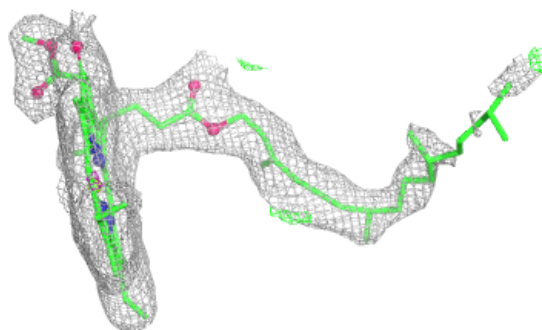


Electron density around CLA B 614:

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

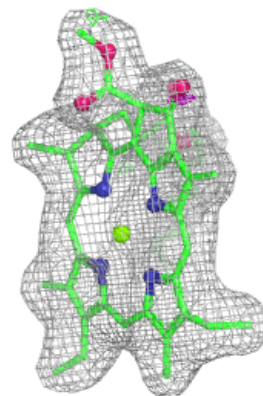
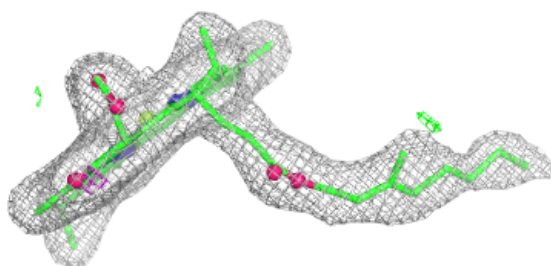
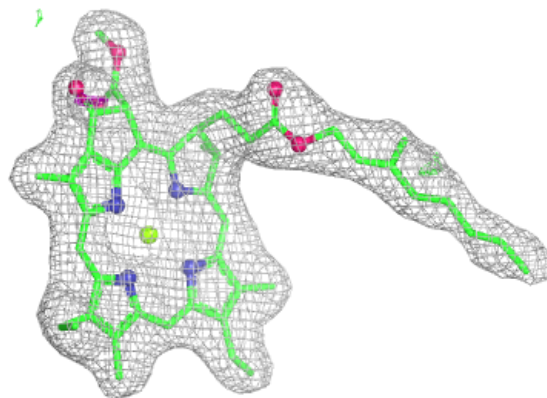
**Electron density around CLA D 405:**

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



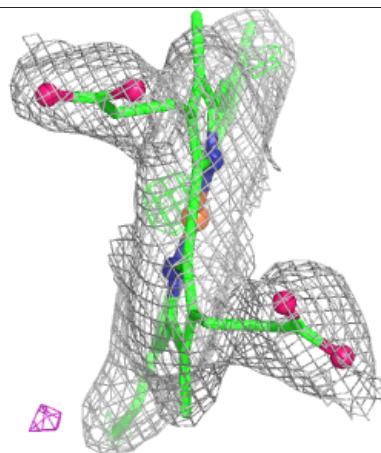
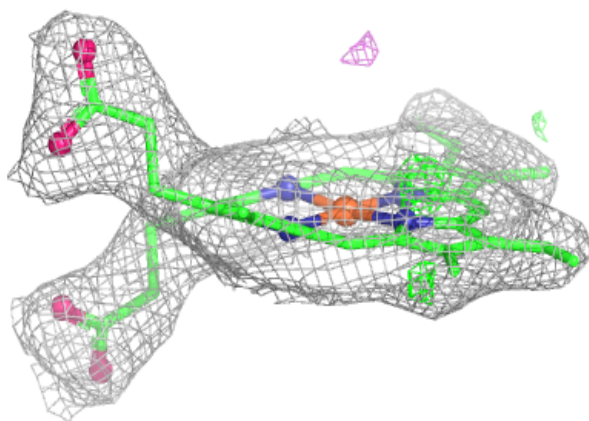
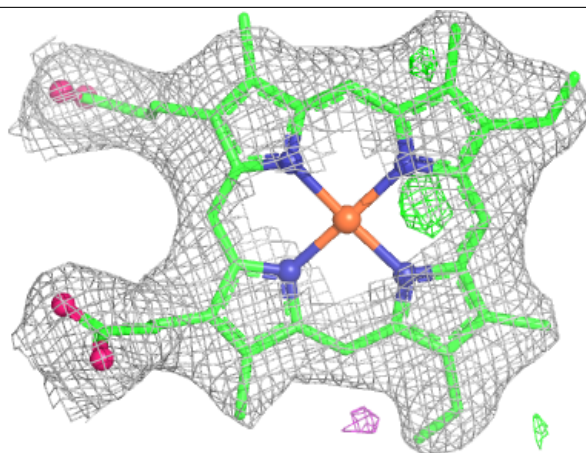
Electron density around CLA A 609:

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



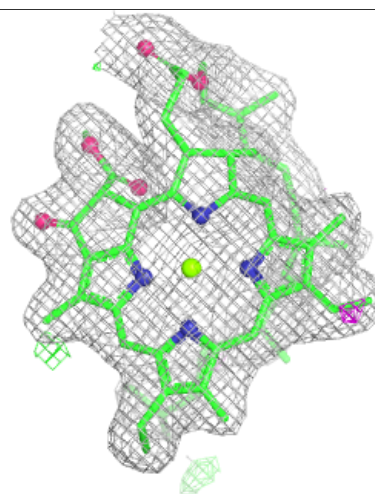
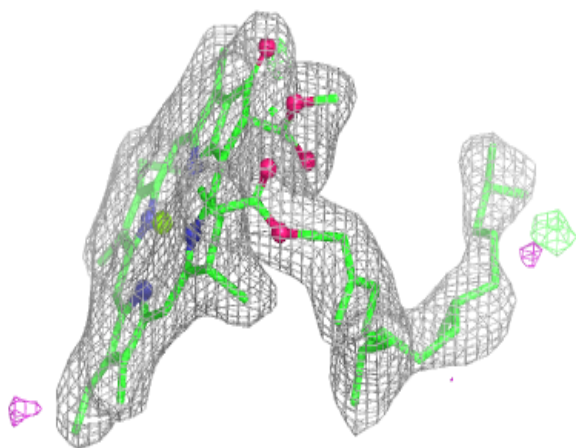
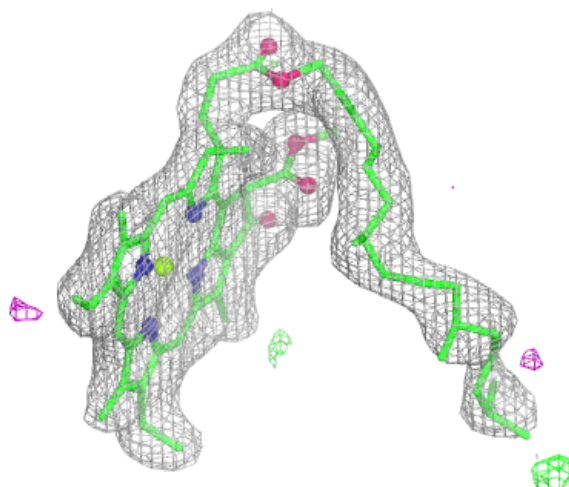
Electron density around HEM F 101:

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



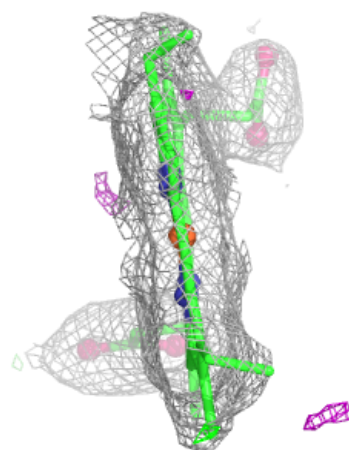
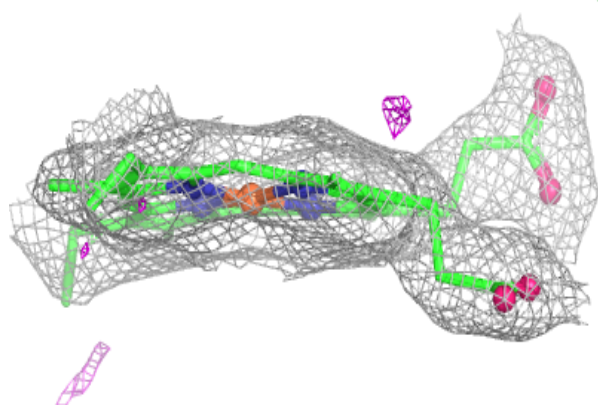
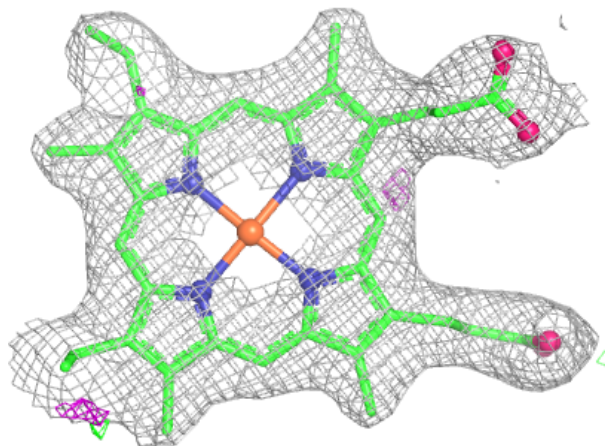
Electron density around CLA B 613:

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



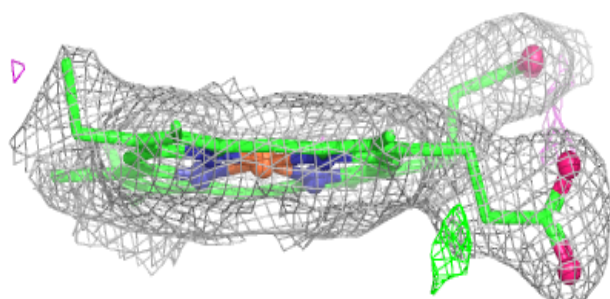
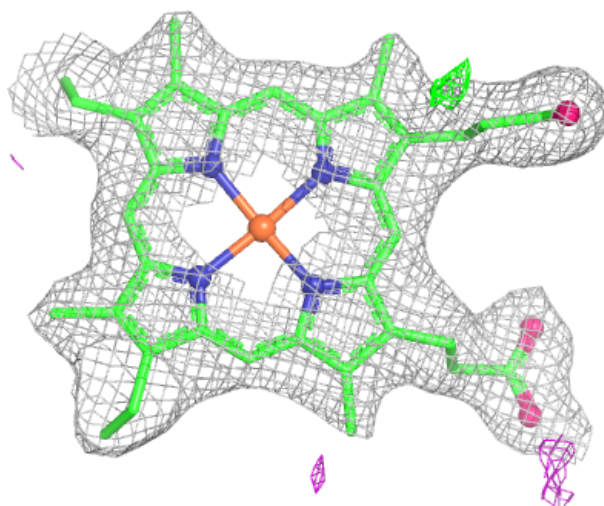
Electron density around HEC V 201:

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



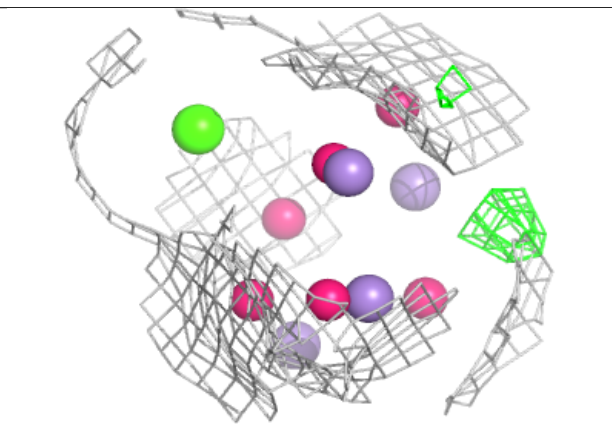
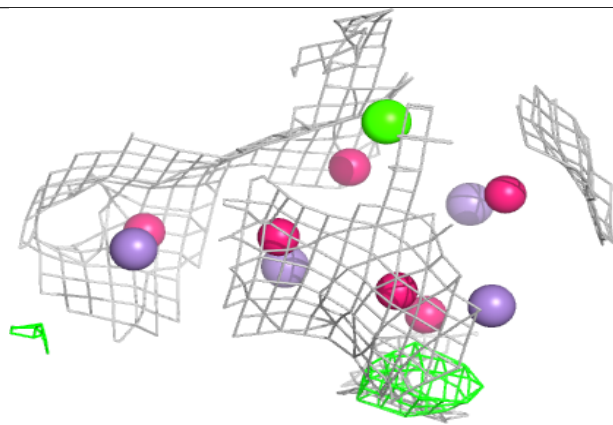
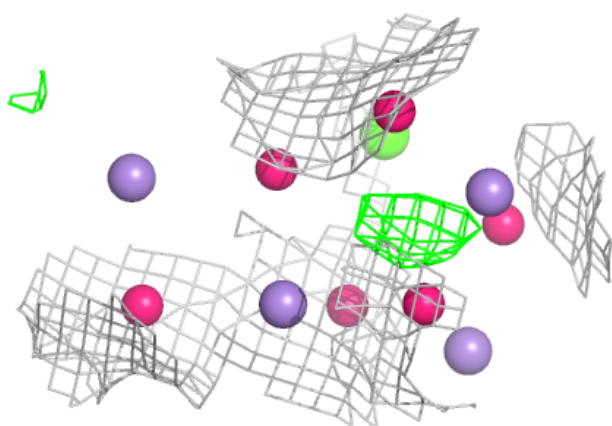
Electron density around HEC v 201:

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



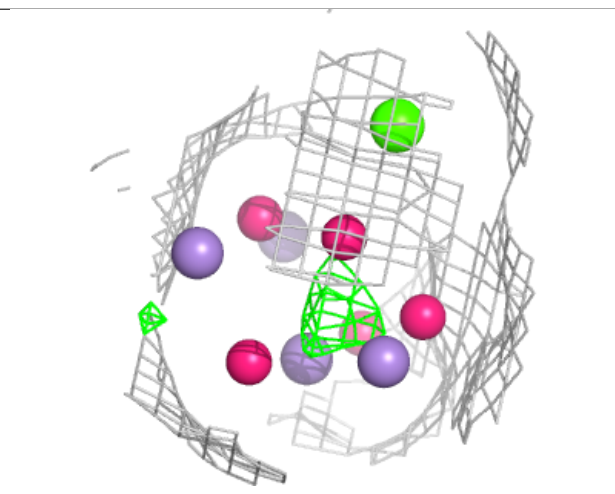
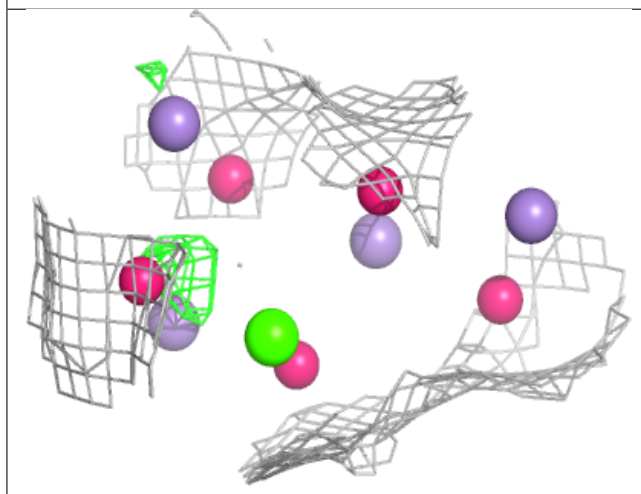
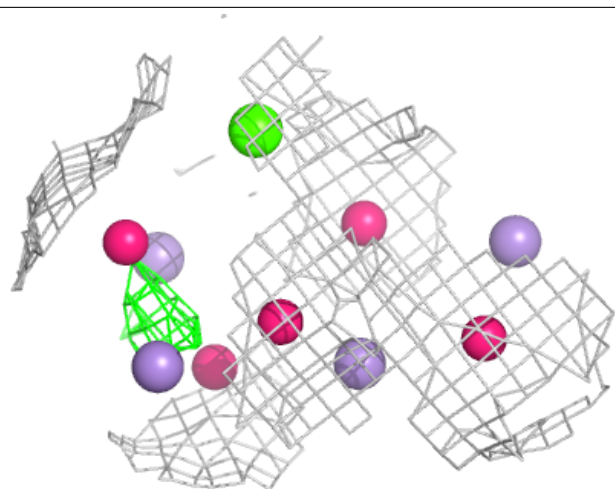
Electron density around OEY a 601 (B):

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



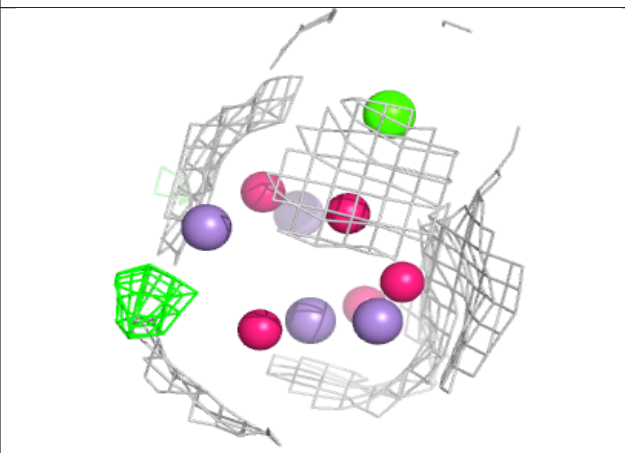
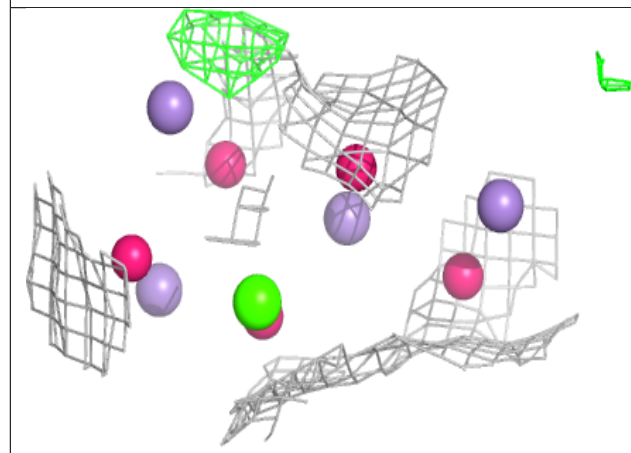
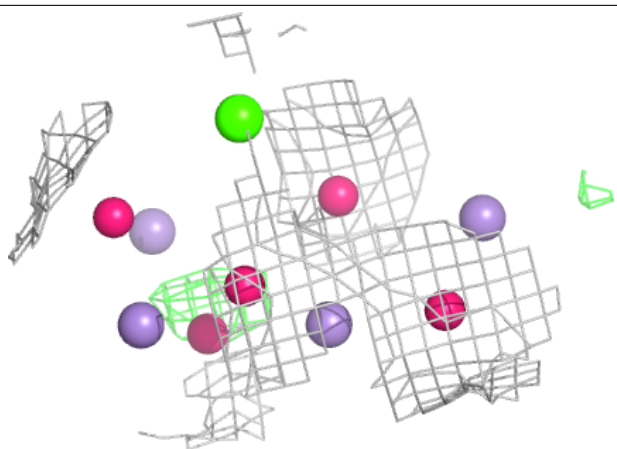
Electron density around OEX A 602 (A):

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



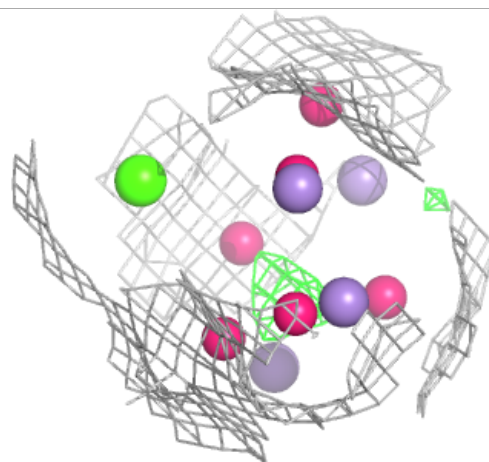
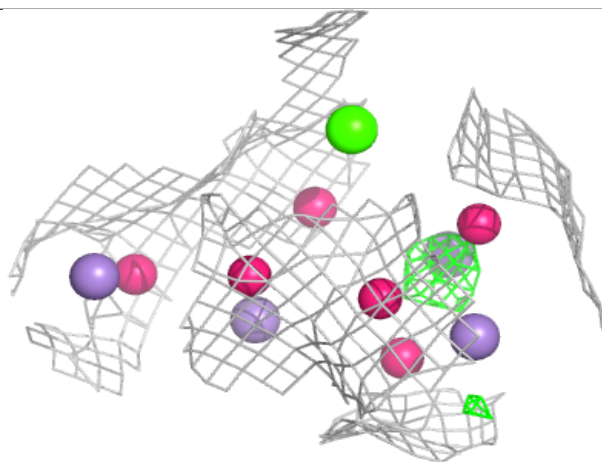
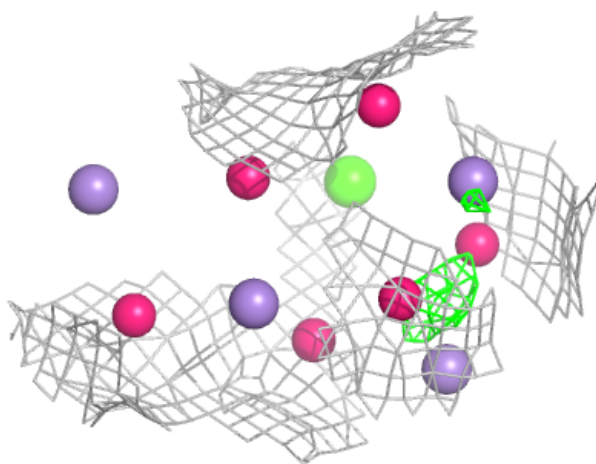
Electron density around OEX a 602 (Å):

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



Electron density around OEY A 601 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.