



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:25 PM UTC

PDB ID : 8F4K / pdb_00008f4k
Title : RT XFEL structure of the three-flash state of Photosystem II (3F, S0-rich) at 2.16 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 : 2.16 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

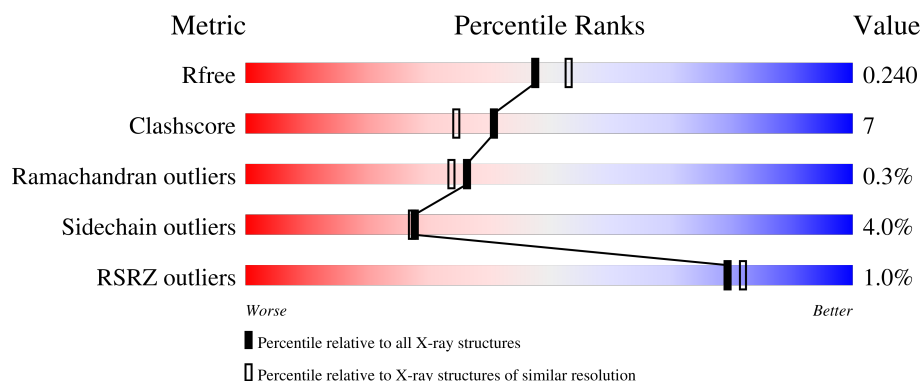
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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)

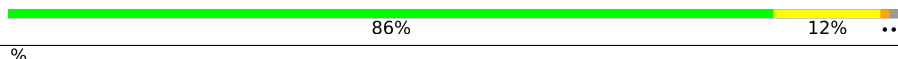
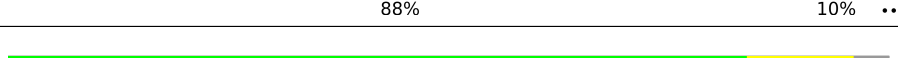
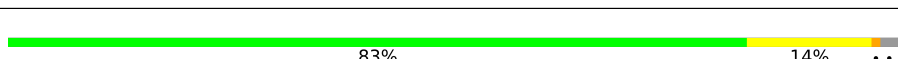
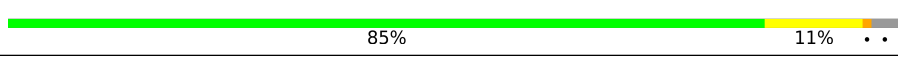
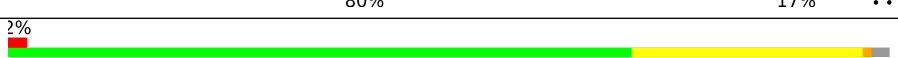
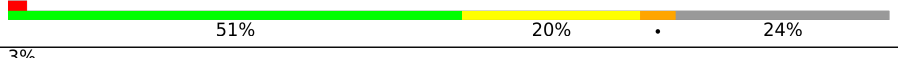
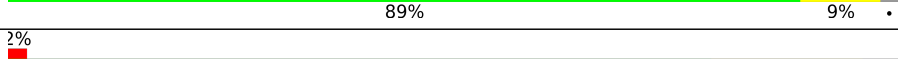
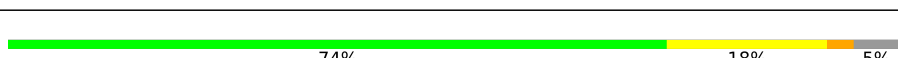
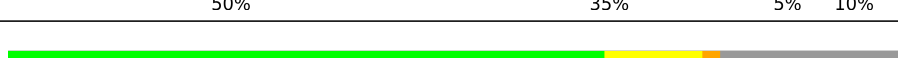
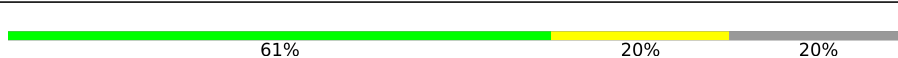
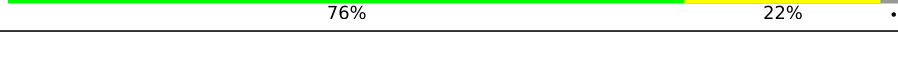
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 86% 11% ..

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	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	609	X	-	-	-
25	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	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	508	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	H	101	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	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	401	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	h	101	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 53024 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

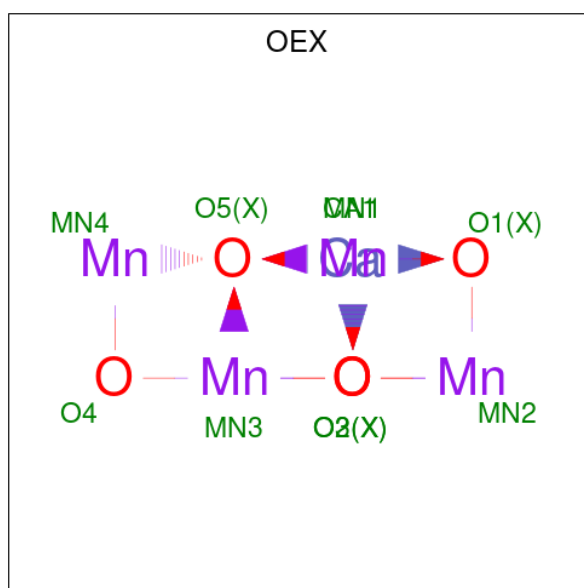
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

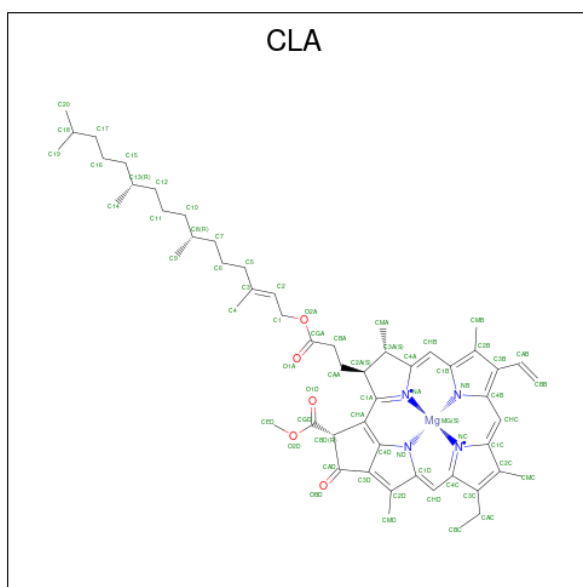
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
20	r	31	Total	C	N	O	0	0	0
			246	166	43	37			

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).

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

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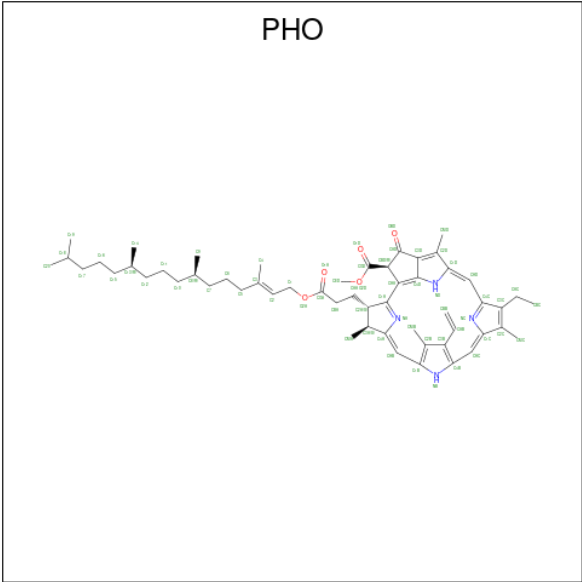
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25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 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

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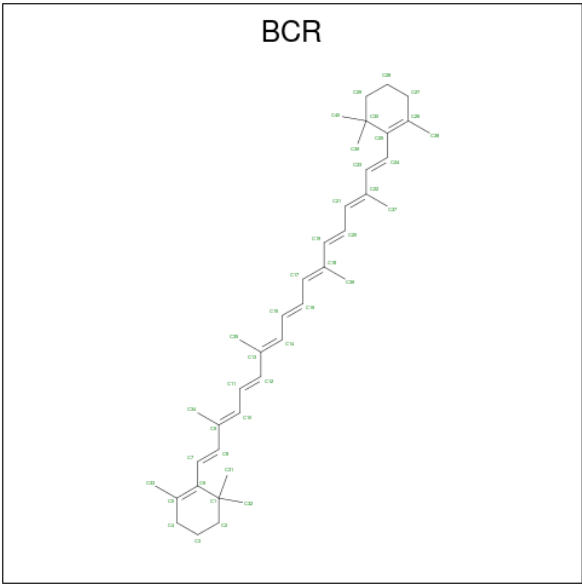
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



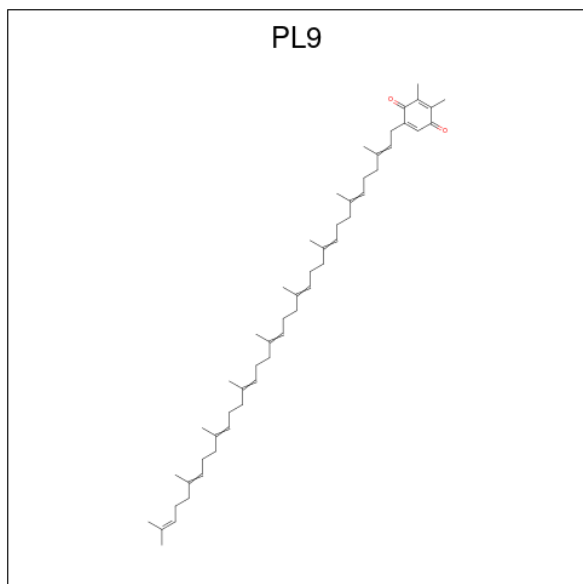
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



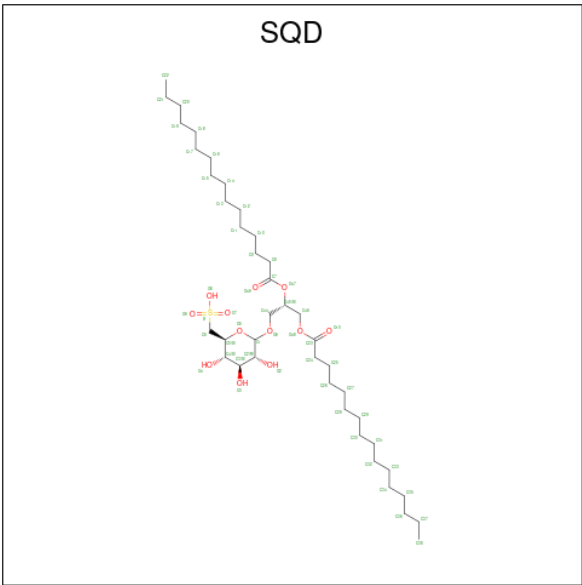
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	Z	1	Total 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
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0
27	x	1	Total C 40 40	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



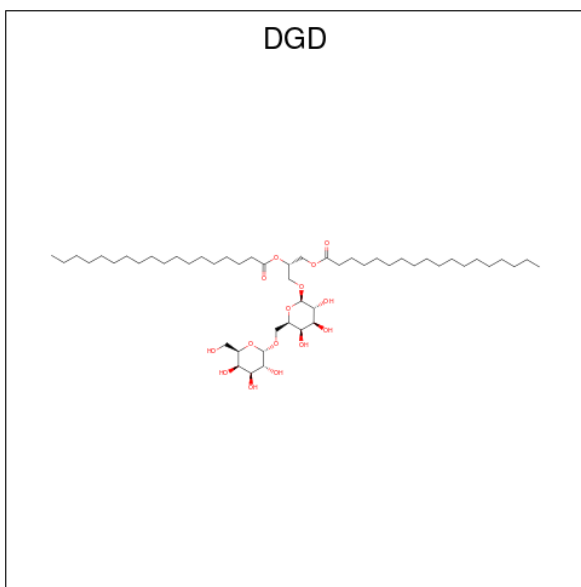
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			55	53	2		
28	D	1	Total	C	O	0	0
			55	53	2		
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

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



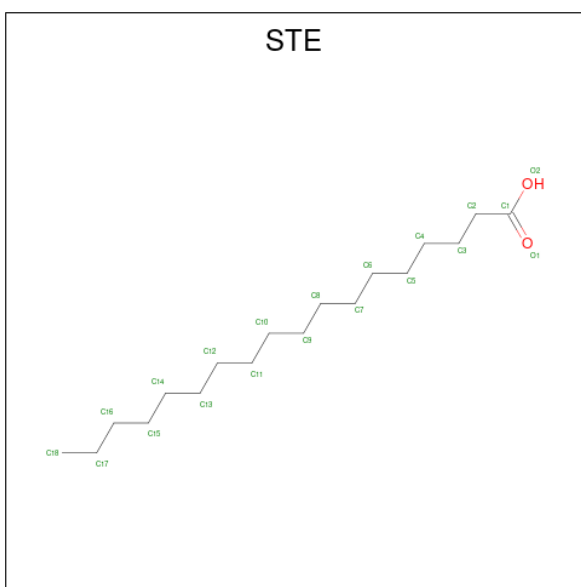
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			36	25	10	1		
29	T	1	Total	C	O		0	0
			39	35	4			
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O		0	0
			36	31	5			
29	b	1	Total	C	O	S	0	0
			49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

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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

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



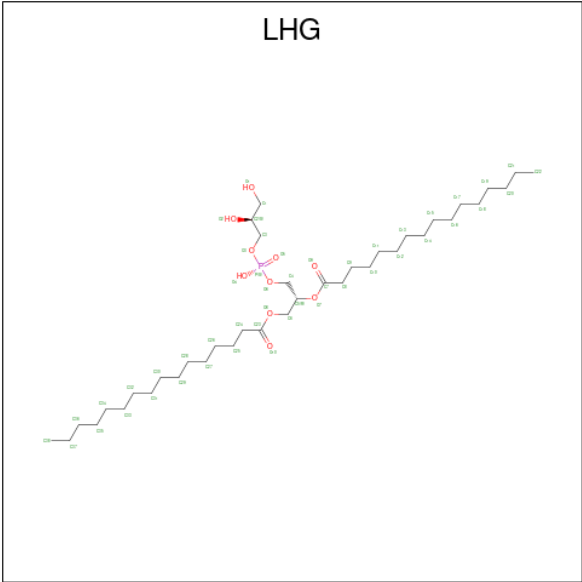
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 17	C 15	O 2	0	0
31	B	1	Total 12	C 10	O 2	0	0
31	B	1	Total 18	C 16	O 2	0	0
31	B	1	Total 12	C 10	O 2	0	0
31	B	1	Total 16	C 16		0	0
31	C	1	Total 12	C 10	O 2	0	0
31	C	1	Total 12	C 10	O 2	0	0
31	C	1	Total 16	C 16		0	0
31	D	1	Total 20	C 18	O 2	0	0
31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

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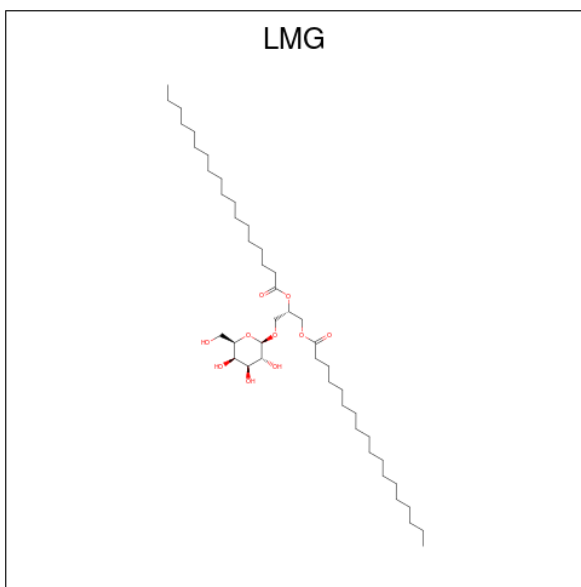
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	M	1	Total C 10 10	0	0
31	M	1	Total C 15 15	0	0
31	T	1	Total C 16 16	0	0
31	a	1	Total C O 12 10 2	0	0
31	b	1	Total C O 20 18 2	0	0
31	b	1	Total C O 16 14 2	0	0
31	b	1	Total C O 20 18 2	0	0
31	b	1	Total C 10 10	0	0
31	c	1	Total C O 20 18 2	0	0
31	c	1	Total C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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



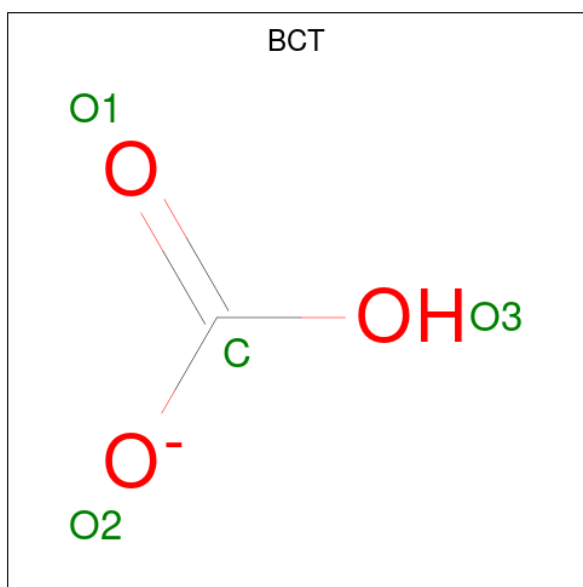
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			47	36	10	1		
32	E	1	Total	C	O	P	0	0
			49	38	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	b	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



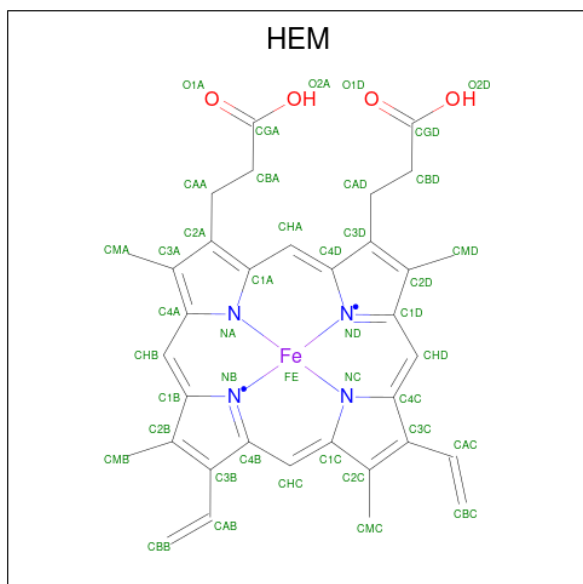
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			48	38	10		
33	C	1	Total	C	O	0	0
			48	38	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			33	27	6		
33	D	1	Total	C	O	0	0
			28	24	4		
33	M	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C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

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



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

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



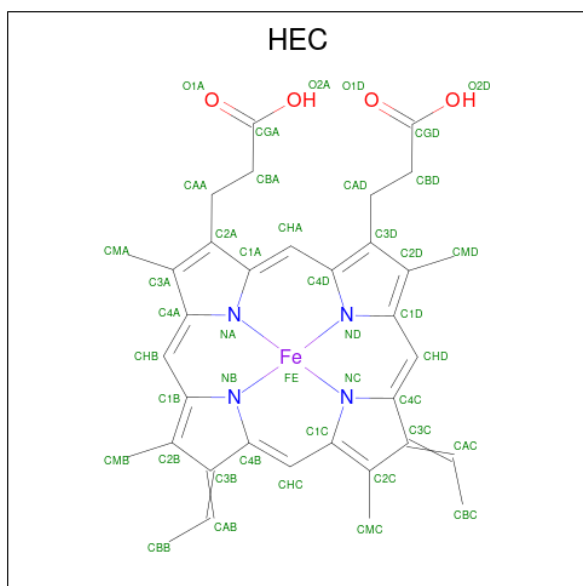
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	121	Total	O	0	4
			125	125		
37	B	161	Total	O	0	0
			161	161		
37	C	150	Total	O	0	0
			150	150		
37	D	112	Total	O	0	0
			112	112		
37	E	20	Total	O	0	0
			20	20		
37	F	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	28	Total 28	O 28	0	0
37	I	20	Total 20	O 20	0	0
37	J	17	Total 17	O 17	0	0
37	K	4	Total 4	O 4	0	0
37	L	8	Total 8	O 8	0	0
37	M	3	Total 3	O 3	0	0
37	O	76	Total 76	O 76	0	0
37	T	9	Total 9	O 9	0	0
37	U	32	Total 32	O 32	0	0
37	V	52	Total 52	O 52	0	0
37	X	7	Total 7	O 7	0	0
37	Z	2	Total 2	O 2	0	0
37	R	7	Total 7	O 7	0	0
37	a	102	Total 106	O 106	0	4
37	b	163	Total 163	O 163	0	0
37	c	145	Total 145	O 145	0	0
37	d	93	Total 93	O 93	0	0
37	e	18	Total 18	O 18	0	0
37	f	8	Total 8	O 8	0	0
37	h	18	Total 18	O 18	0	0
37	i	11	Total 11	O 11	0	0

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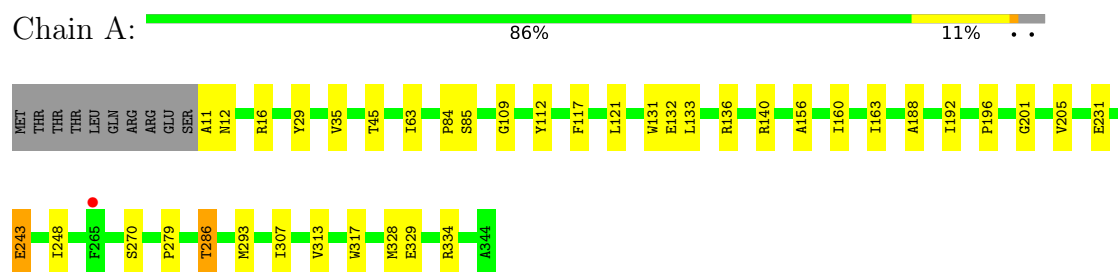
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	j	6	Total 6	O 6	0	0
37	k	4	Total 4	O 4	0	0
37	l	5	Total 5	O 5	0	0
37	m	6	Total 6	O 6	0	0
37	o	79	Total 79	O 79	0	0
37	t	9	Total 9	O 9	0	0
37	u	39	Total 39	O 39	0	0
37	v	46	Total 46	O 46	0	0
37	y	3	Total 3	O 3	0	0
37	x	2	Total 2	O 2	0	0
37	z	8	Total 8	O 8	0	0
37	r	8	Total 8	O 8	0	0

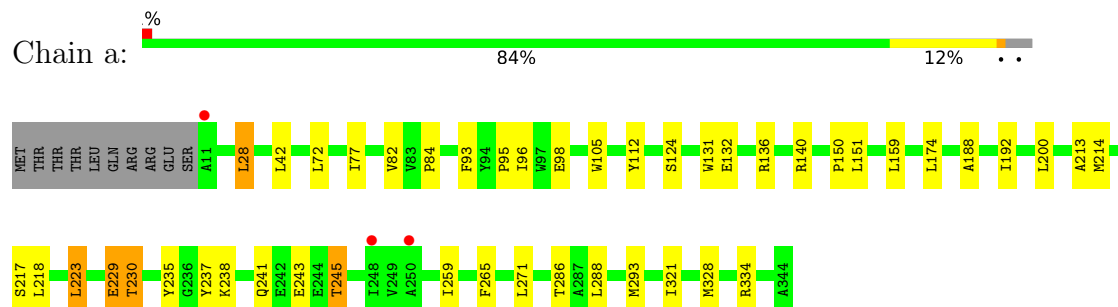
3 Residue-property plots [i](#)

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

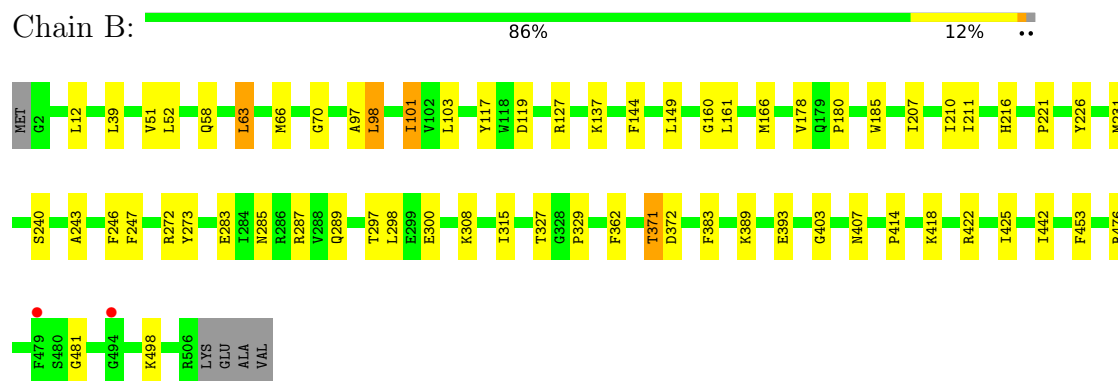
- Molecule 1: Photosystem II protein D1 1



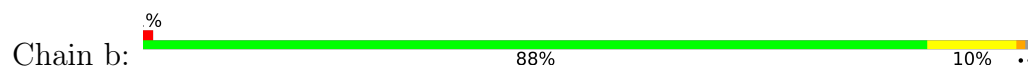
- Molecule 1: Photosystem II protein D1 1

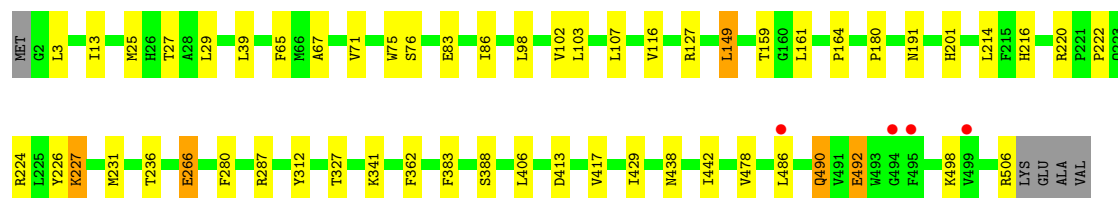


- Molecule 2: Photosystem II CP47 reaction center protein



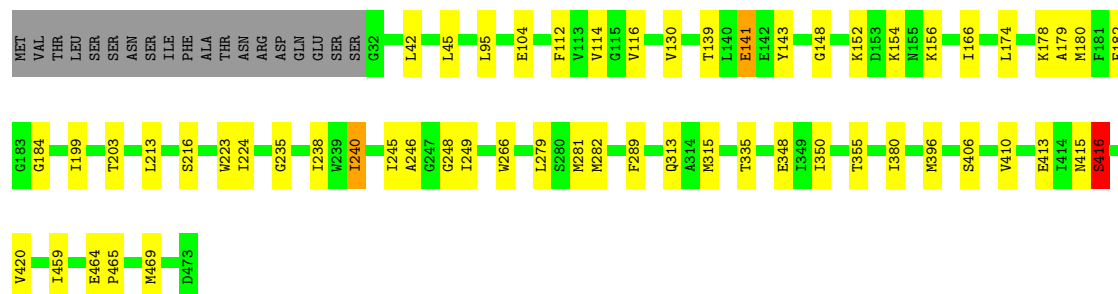
- Molecule 2: Photosystem II CP47 reaction center protein





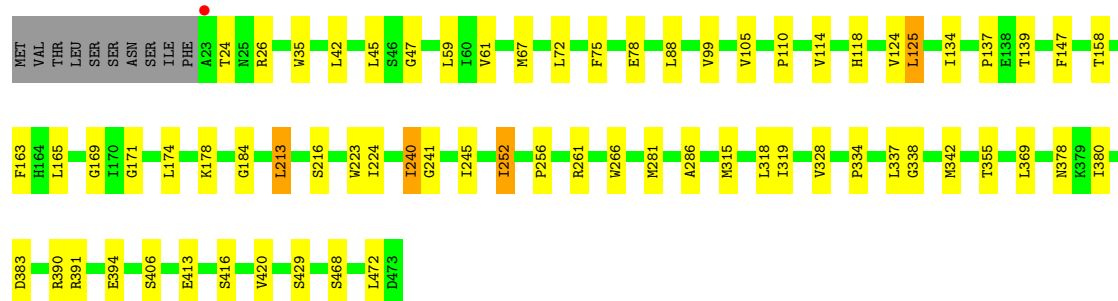
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 83% 12% .



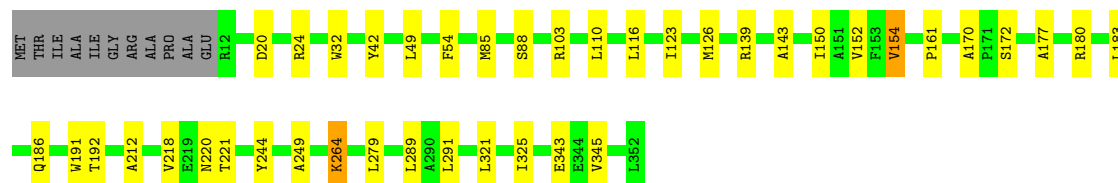
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 83% 14% ..



• Molecule 4: Photosystem II D2 protein

Chain D: 85% 11% ..



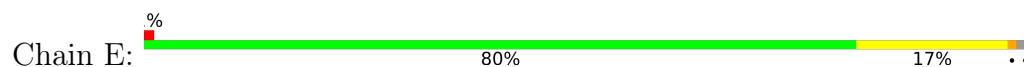
• Molecule 4: Photosystem II D2 protein

Chain d: 81% 16% .





- Molecule 5: Cytochrome b559 subunit alpha



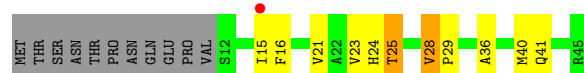
- Molecule 5: Cytochrome b559 subunit alpha



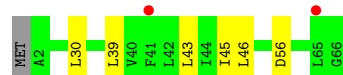
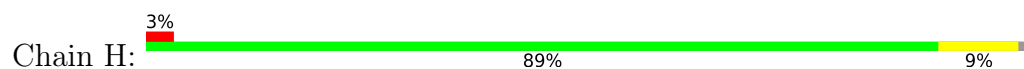
- Molecule 6: Cytochrome b559 subunit beta



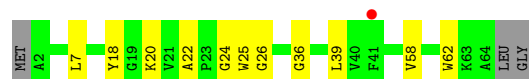
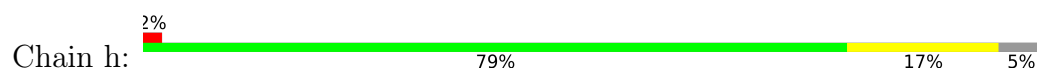
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

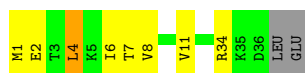


- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

Chain I:  74% 18% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  87% 8% 5%



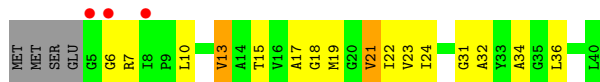
- Molecule 9: Photosystem II reaction center protein J

Chain J:  72% 18% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  8% 50% 35% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  67% 11% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  61% 20% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 



- Molecule 12: Photosystem II reaction center protein M

Chain M: 



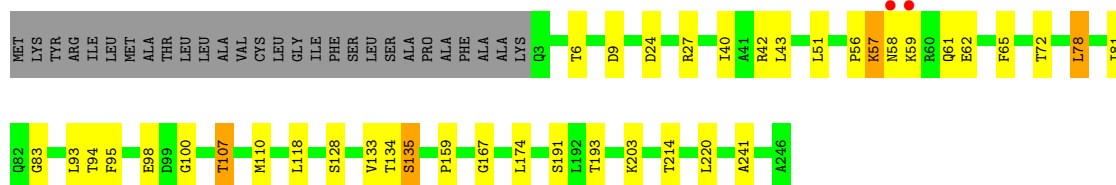
- Molecule 12: Photosystem II reaction center protein M

Chain m: 



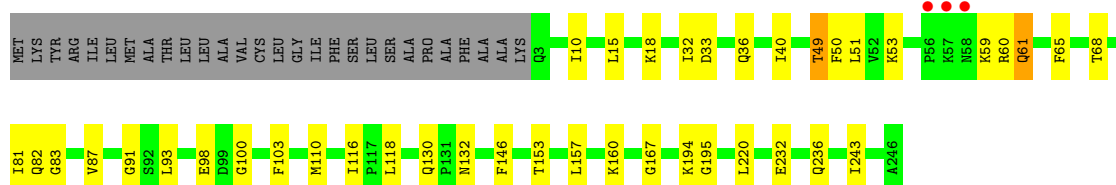
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 

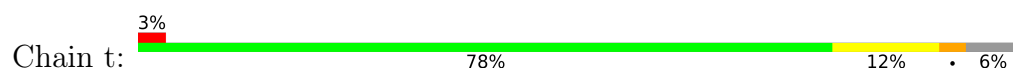


- Molecule 14: Photosystem II reaction center protein T

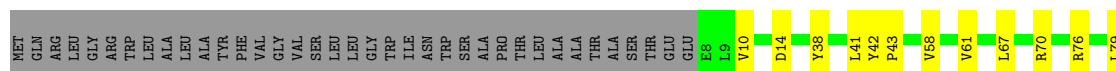
Chain T: 



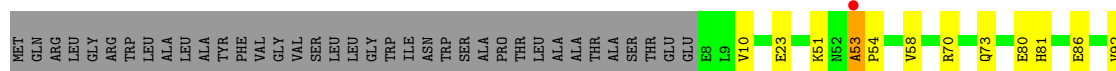
- Molecule 14: Photosystem II reaction center protein T



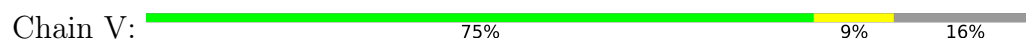
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



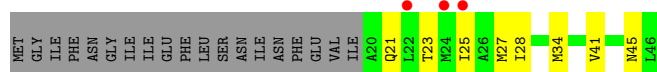
- Molecule 16: Cytochrome c-550



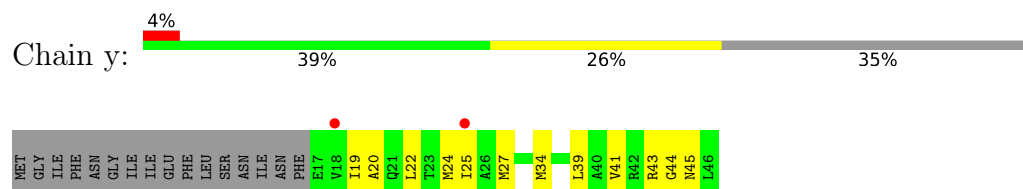
- Molecule 16: Cytochrome c-550



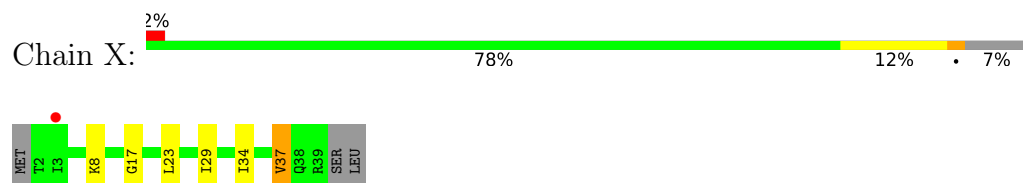
- Molecule 17: Photosystem II reaction center protein Ycf12



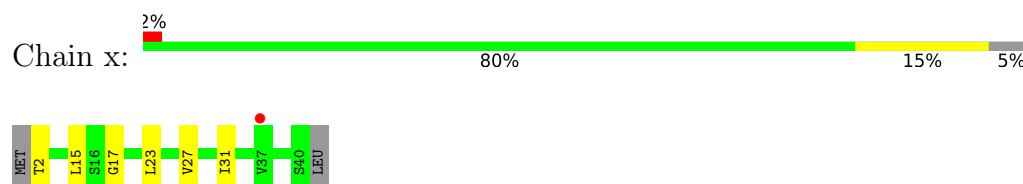
- Molecule 17: Photosystem II reaction center protein Ycf12



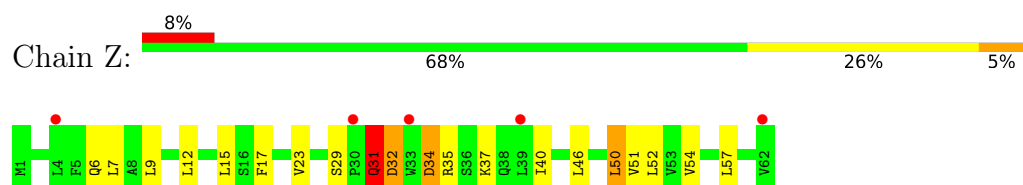
- Molecule 18: Photosystem II reaction center X protein



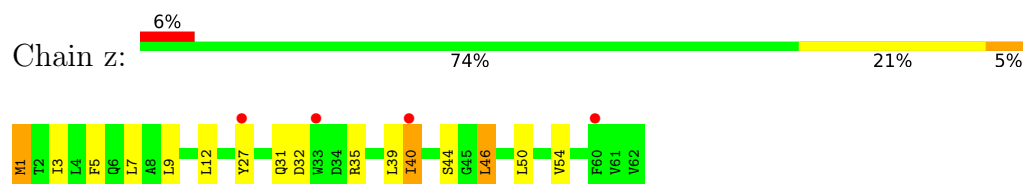
- Molecule 18: Photosystem II reaction center X protein



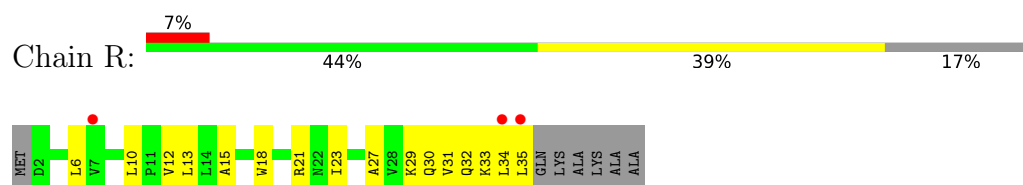
- Molecule 19: Photosystem II reaction center protein Z



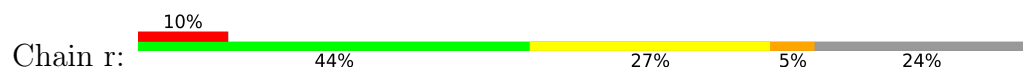
- Molecule 19: Photosystem II reaction center protein Z



- 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	116.99Å 221.75Å 307.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.52 – 2.16 33.52 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.1 (33.52-2.16) 84.7 (33.52-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.241 0.185 , 0.240	Depositor DCC
R_{free} test set	3779 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53024	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/3212	0.49	0/4376
1	a	0.29	0/3209	0.48	0/4372
2	B	0.33	0/4155	0.50	0/5661
2	b	0.31	0/4118	0.48	0/5611
3	C	0.31	0/3625	0.47	0/4935
3	c	0.29	0/3705	0.45	0/5042
4	D	0.34	0/2825	0.51	0/3847
4	d	0.33	0/2834	0.51	0/3859
5	E	0.27	0/688	0.42	0/940
5	e	0.23	0/683	0.42	0/932
6	F	0.29	0/284	0.43	0/387
6	f	0.26	0/284	0.50	0/387
7	H	0.36	0/523	0.53	0/713
7	h	0.30	0/511	0.43	0/697
8	I	0.32	0/293	0.49	0/396
8	i	0.35	0/293	0.45	0/396
9	J	0.28	0/263	0.44	0/356
9	j	0.25	0/263	0.42	0/356
10	K	0.26	0/303	0.46	0/416
10	k	0.25	0/303	0.41	0/416
11	L	0.34	0/311	0.49	0/422
11	l	0.33	0/303	0.46	0/412
12	M	0.33	0/249	0.56	0/341
12	m	0.35	0/244	0.52	0/334
13	O	0.31	0/1904	0.52	0/2585
13	o	0.33	0/1905	0.49	0/2583
14	T	0.36	0/257	0.51	0/349
14	t	0.33	0/255	0.50	0/346
15	U	0.28	0/785	0.48	0/1064
15	u	0.31	0/785	0.50	0/1064
16	V	0.31	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.28	0/1085	0.43	0/1473
17	Y	0.22	0/197	0.37	0/264
17	y	0.21	0/219	0.35	0/294
18	X	0.26	0/284	0.43	0/384
18	x	0.23	0/289	0.36	0/391
19	Z	0.21	0/490	0.38	0/669
19	z	0.18	0/488	0.32	0/666
20	R	0.28	0/277	0.55	0/380
20	r	0.24	0/252	0.37	0/347
All	All	0.30	0/44038	0.48	0/59936

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	2981	29	0
1	a	3110	0	2972	36	0
2	B	4005	0	3871	45	0
2	b	3978	0	3836	44	0
3	C	3509	0	3426	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	42	0
4	D	2731	0	2637	35	0
4	d	2737	0	2643	44	0
5	E	666	0	651	14	0
5	e	664	0	648	14	0
6	F	275	0	282	4	0
6	f	275	0	282	11	0
7	H	510	0	532	5	0
7	h	498	0	518	11	0
8	I	296	0	311	4	0
8	i	296	0	311	3	0
9	J	257	0	268	5	0
9	j	257	0	268	10	0
10	K	293	0	305	2	0
10	k	293	0	305	4	0
11	L	304	0	316	7	0
11	l	296	0	304	5	0
12	M	256	0	269	7	0
12	m	251	0	267	7	0
13	O	1870	0	1830	27	0
13	o	1874	0	1846	26	0
14	T	258	0	261	4	0
14	t	256	0	256	4	0
15	U	774	0	773	7	0
15	u	774	0	773	7	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	12	0
17	Y	196	0	217	3	0
17	y	218	0	241	5	0
18	X	281	0	312	4	0
18	x	286	0	314	3	0
19	Z	479	0	516	12	0
19	z	477	0	509	8	0
20	R	271	0	298	10	0
20	r	246	0	263	8	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	11	0	0	1	0
22	a	11	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	6	0
25	B	970	0	1067	41	0
25	C	839	0	922	24	0
25	D	130	0	144	5	0
25	H	65	0	72	3	0
25	a	195	0	216	10	0
25	b	970	0	1067	44	0
25	c	839	0	919	25	0
25	d	195	0	216	6	0
25	h	65	0	72	4	0
26	A	64	0	74	0	0
26	D	64	0	74	5	0
26	a	64	0	74	2	0
26	d	64	0	74	5	0
27	A	40	0	56	0	0
27	B	120	0	168	7	0
27	C	40	0	56	5	0
27	D	40	0	56	1	0
27	H	40	0	56	1	0
27	K	40	0	56	1	0
27	T	40	0	56	4	0
27	Y	40	0	56	1	0
27	Z	40	0	56	1	0
27	a	40	0	56	0	0
27	b	120	0	168	6	0
27	c	120	0	168	6	0
27	d	40	0	56	2	0
27	k	40	0	56	0	0
27	t	40	0	56	5	0
27	x	40	0	56	4	0
28	A	55	0	80	5	0
28	D	55	0	80	0	0
28	a	55	0	80	5	0
28	d	55	0	80	3	0
29	A	52	0	71	3	0
29	B	54	0	78	4	0
29	D	36	0	46	1	0
29	T	39	0	65	1	0
29	a	90	0	134	4	0
29	b	49	0	65	4	0
29	f	41	0	49	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	66	0	96	9	0
30	C	186	0	246	9	0
30	H	62	0	82	4	0
30	a	44	0	75	2	0
30	c	186	0	246	6	0
30	h	62	0	82	3	0
31	B	75	0	117	2	0
31	C	40	0	63	2	0
31	D	20	0	35	1	0
31	E	12	0	16	0	0
31	H	18	0	35	1	0
31	I	15	0	26	2	0
31	J	12	0	16	0	0
31	M	40	0	67	0	0
31	T	16	0	31	0	0
31	a	12	0	16	0	0
31	b	66	0	110	1	0
31	c	32	0	51	1	0
31	d	17	0	26	1	0
31	j	12	0	16	0	0
31	l	18	0	35	0	0
31	m	12	0	16	0	0
31	t	24	0	36	2	0
31	x	20	0	35	0	0
32	B	49	0	74	3	0
32	D	96	0	141	5	0
32	E	49	0	74	2	0
32	L	49	0	74	1	0
32	b	49	0	74	3	0
32	d	88	0	125	4	0
32	e	42	0	57	0	0
32	l	49	0	74	5	0
33	C	96	0	132	7	0
33	D	112	0	157	4	0
33	M	51	0	72	2	0
33	b	106	0	158	3	0
33	c	134	0	181	6	0
33	d	67	0	92	1	0
34	D	4	0	1	1	0
34	a	4	0	1	0	0
35	F	43	0	30	3	0
35	e	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	43	0	30	0	0
36	v	43	0	30	0	0
37	A	125	0	0	3	0
37	B	161	0	0	0	0
37	C	150	0	0	4	0
37	D	112	0	0	1	0
37	E	20	0	0	0	0
37	F	7	0	0	0	0
37	H	28	0	0	0	0
37	I	20	0	0	1	0
37	J	17	0	0	1	0
37	K	4	0	0	0	0
37	L	8	0	0	1	0
37	M	3	0	0	0	0
37	O	76	0	0	4	0
37	R	7	0	0	0	0
37	T	9	0	0	0	0
37	U	32	0	0	0	0
37	V	52	0	0	1	0
37	X	7	0	0	1	0
37	Z	2	0	0	0	0
37	a	106	0	0	0	0
37	b	163	0	0	2	0
37	c	145	0	0	1	0
37	d	93	0	0	0	0
37	e	18	0	0	0	0
37	f	8	0	0	0	0
37	h	18	0	0	1	0
37	i	11	0	0	0	0
37	j	6	0	0	2	0
37	k	4	0	0	0	0
37	l	5	0	0	0	0
37	m	6	0	0	0	0
37	o	79	0	0	0	0
37	r	8	0	0	1	0
37	t	9	0	0	0	0
37	u	39	0	0	1	0
37	v	46	0	0	1	0
37	x	2	0	0	0	0
37	y	3	0	0	0	0
37	z	8	0	0	0	0
All	All	53024	0	52753	681	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 (681) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:611:PL9:H361	6:F:25:THR:HG21	1.49	0.95
3:C:245:ILE:O	37:C:601:HOH:O	1.85	0.94
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.62	0.81
5:e:57:ALA:H	5:e:60:GLN:HE21	1.29	0.81
35:F:101:HEM:HBC2	35:F:101:HEM:HH2	1.64	0.79
27:T:101:BCR:H311	27:T:101:BCR:HC8	1.67	0.77
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.49	0.77
33:b:620:LMG:O10	12:m:4:ASN:ND2	2.17	0.77
25:b:614:CLA:H2	25:b:615:CLA:HBB2	1.69	0.75
22:A:602[A]:OEY:O6	22:A:602[A]:OEY:O5	2.04	0.75
3:C:148:GLY:O	3:C:156:LYS:NZ	2.20	0.74
3:C:249:ILE:N	37:C:601:HOH:O	2.04	0.74
25:C:513:CLA:H201	31:C:522:STE:H171	1.70	0.73
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.70	0.72
25:b:603:CLA:H42	25:b:604:CLA:H2	1.69	0.72
16:v:55:ARG:NH1	37:v:301:HOH:O	2.22	0.70
25:B:606:CLA:H191	32:B:620:LHG:H142	1.74	0.69
13:O:24:ASP:OD1	13:O:203:LYS:NZ	2.24	0.69
19:z:1:MET:SD	19:z:1:MET:N	2.67	0.68
9:J:15:THR:HG22	9:J:19:MET:HE2	1.74	0.68
4:D:279:LEU:HD22	26:D:402:PHO:HBC3	1.74	0.68
9:J:36:LEU:O	37:J:201:HOH:O	2.11	0.68
15:U:70:ARG:NH2	16:V:85:GLU:OE2	2.26	0.67
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.76	0.67
27:t:101:BCR:HC8	27:t:101:BCR:H311	1.76	0.67
4:d:279:LEU:HD22	26:d:402:PHO:HBC3	1.76	0.67
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.78	0.66
27:B:616:BCR:H383	29:B:621:SQD:H112	1.78	0.65
16:v:13:ASN:HD21	16:v:17:LYS:HB3	1.61	0.65
25:a:609:CLA:H52	25:a:609:CLA:H111	1.79	0.65
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.77	0.65
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.77	0.65
19:z:32:ASP:HB2	19:z:35:ARG:HB2	1.80	0.64
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.79	0.64
4:d:79:SER:HA	4:d:172:SER:HB3	1.79	0.64
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.33	0.63
35:e:101:HEM:HBC2	35:e:101:HEM:HMC2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:235:TYR:OH	11:l:11:GLU:OE2	2.15	0.63
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.79	0.63
3:C:174:LEU:HB3	25:C:502:CLA:H152	1.80	0.63
30:c:518:DGD:HA91	30:c:519:DGD:HBT2	1.79	0.63
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.81	0.63
30:A:614:DGD:HD5	2:b:75:TRP:HB3	1.81	0.62
27:T:101:BCR:H19C	27:b:617:BCR:H363	1.79	0.62
2:b:65:PHE:HE1	25:b:603:CLA:HED2	1.63	0.62
19:z:40:ILE:O	19:z:44:SER:OG	2.13	0.62
3:c:42:LEU:HD21	25:c:511:CLA:H2A	1.79	0.62
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.80	0.62
25:B:614:CLA:H2	25:B:615:CLA:HBB2	1.80	0.62
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.82	0.62
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.80	0.62
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.82	0.61
6:f:21:VAL:O	6:f:25:THR:OG1	2.17	0.61
30:A:614:DGD:HE4	2:b:76:SER:HB3	1.82	0.61
25:B:610:CLA:HBB1	25:B:610:CLA:HMB3	1.82	0.61
13:O:133:VAL:O	13:O:135:SER:N	2.33	0.60
3:c:59:LEU:HD21	27:c:516:BCR:H372	1.82	0.60
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.82	0.60
25:a:612:CLA:HED1	28:d:406:PL9:H372	1.82	0.60
2:b:39:LEU:HD22	31:b:625:STE:H62	1.83	0.60
1:A:11:ALA:O	1:A:16:ARG:NH2	2.34	0.60
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.83	0.60
4:d:36:LEU:HB2	31:d:411:STE:H111	1.83	0.60
5:e:8:ARG:NH1	5:e:12:ASP:OD1	2.34	0.60
13:o:32:ILE:HG13	13:o:93:LEU:HD11	1.82	0.60
1:A:196:PRO:HB3	30:C:518:DGD:HA92	1.84	0.60
15:U:58:VAL:O	15:U:61:VAL:HG22	2.01	0.60
25:h:101:CLA:H12	25:h:101:CLA:H72	1.84	0.60
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.82	0.59
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.65	0.59
3:c:429:SER:HB3	30:c:518:DGD:HBE1	1.85	0.59
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.84	0.59
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.38	0.58
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.30	0.58
25:b:601:CLA:H42	30:h:102:DGD:HB41	1.82	0.58
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.85	0.58
28:a:611:PL9:H503	4:d:39:PRO:HG3	1.85	0.58
25:C:504:CLA:H101	30:C:518:DGD:HBN1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:241:GLU:CD	4:d:241:GLU:H	2.10	0.58
5:e:40:THR:HB	20:r:4:ARG:HD2	1.84	0.58
6:f:16:PHE:HB2	29:f:101:SQD:H82	1.86	0.58
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.68	0.58
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.86	0.58
13:o:33:ASP:HB3	13:o:36:GLN:HB2	1.85	0.58
1:a:72:LEU:HD21	31:t:102:STE:H41	1.86	0.58
1:A:163[B]:ILE:HD11	30:C:516:DGD:HA32	1.86	0.58
30:A:614:DGD:HBE1	30:A:614:DGD:HB62	1.85	0.58
35:e:101:HEM:HBD2	6:f:23:VAL:HG21	1.85	0.58
1:a:82:VAL:HB	1:a:174[B]:LEU:HB2	1.84	0.58
25:c:510:CLA:H201	10:k:33:LEU:HD22	1.85	0.57
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.85	0.57
3:c:134:ILE:HD12	25:c:511:CLA:H43	1.86	0.57
2:B:117:TYR:HA	11:L:1:MET:HE1	1.87	0.57
32:B:620:LHG:H211	12:M:14:PHE:CE2	2.40	0.57
3:C:281:MET:HG3	33:C:515:LMG:H391	1.85	0.57
13:O:56:PRO:O	13:O:58:ASN:N	2.34	0.57
2:B:211:ILE:HG23	31:B:624:STE:H72	1.86	0.56
28:d:406:PL9:H201	32:l:101:LHG:H202	1.87	0.56
20:r:2:ASP:HB3	20:r:5:VAL:HG23	1.86	0.56
13:O:27:ARG:NH1	37:O:301:HOH:O	2.17	0.56
25:H:101:CLA:H41	31:H:104:STE:H171	1.86	0.56
25:h:101:CLA:HBB2	27:x:101:BCR:H351	1.88	0.56
32:D:410:LHG:H172	32:D:410:LHG:H341	1.86	0.56
32:B:620:LHG:H152	32:L:101:LHG:H272	1.86	0.56
6:f:16:PHE:H	20:r:30:GLN:HE22	1.53	0.56
33:C:519:LMG:H202	10:K:27:VAL:HG11	1.88	0.56
16:v:104:MET:HA	16:v:107:LEU:HD22	1.88	0.56
19:z:12:LEU:HA	19:z:50:LEU:HD13	1.87	0.56
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.87	0.56
3:C:114:VAL:HG22	31:C:522:STE:H101	1.88	0.55
13:O:133:VAL:C	13:O:135:SER:H	2.13	0.55
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.35	0.55
25:c:505:CLA:H43	27:c:515:BCR:HC7	1.88	0.55
2:b:492:GLU:OE1	5:e:3:GLY:N	2.39	0.55
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.87	0.55
2:b:116:VAL:HG21	27:b:618:BCR:H292	1.87	0.55
3:C:415:ASN:O	3:C:416:SER:HB2	2.06	0.55
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.21	0.55
25:a:607:CLA:H143	26:a:608:PHO:H61	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:614:DGD:HA22	25:b:605:CLA:H202	1.89	0.55
5:e:26:THR:HA	20:r:15:ALA:HB1	1.88	0.55
32:D:410:LHG:H322	32:D:410:LHG:H142	1.89	0.55
5:E:60:GLN:NE2	5:E:62:SER:O	2.39	0.54
19:Z:23:VAL:HG22	19:Z:40:ILE:HD12	1.89	0.54
32:D:409:LHG:H321	14:T:21:ILE:HD11	1.88	0.54
25:b:608:CLA:H203	7:h:39:LEU:HD12	1.90	0.54
33:c:522:LMG:H112	33:c:522:LMG:H292	1.90	0.54
29:D:408:SQD:H441	20:R:30:GLN:NE2	2.23	0.54
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.42	0.54
9:j:36:LEU:O	37:j:201:HOH:O	2.18	0.54
2:b:478:VAL:O	4:d:139:ARG:HG2	2.08	0.54
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.43	0.54
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.42	0.54
3:c:256:PRO:O	3:c:261:ARG:NH1	2.40	0.54
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.90	0.54
4:D:150:ILE:O	4:D:154:VAL:HG13	2.08	0.54
3:C:246:ALA:C	37:C:601:HOH:O	2.51	0.54
4:d:199:MET:HG2	28:d:406:PL9:H312	1.89	0.54
3:c:315:MET:HE3	3:c:319:ILE:HD11	1.89	0.54
25:c:506:CLA:H141	25:c:507:CLA:H141	1.90	0.54
6:f:15:ILE:H	20:r:30:GLN:NE2	2.06	0.54
4:D:152:VAL:HG21	4:D:279:LEU:HG	1.89	0.54
25:B:608:CLA:H203	7:H:39:LEU:HD12	1.88	0.53
15:u:86:GLU:H	15:u:86:GLU:CD	2.16	0.53
2:B:39:LEU:HD13	31:t:103:STE:H22	1.90	0.53
2:b:222:PRO:HB3	7:h:26:GLY:HA3	1.91	0.53
25:B:603:CLA:H42	25:B:604:CLA:H42	1.90	0.53
2:b:287:ARG:HD3	37:b:746:HOH:O	2.07	0.53
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.43	0.53
14:T:29:ILE:HG22	14:T:30:THR:HG23	1.91	0.53
1:a:28:LEU:HD23	29:a:614:SQD:H252	1.91	0.53
3:C:141:GLU:H	3:C:141:GLU:CD	2.16	0.53
4:D:49:LEU:HD21	33:D:407:LMG:H342	1.91	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
19:Z:12:LEU:HD13	19:Z:50:LEU:HB3	1.90	0.53
3:c:286:ALA:HB2	25:c:502:CLA:HMD1	1.91	0.52
11:L:14:ARG:HB3	14:T:25:GLU:HG3	1.90	0.52
5:e:68:ASP:O	5:e:72:ALA:HB2	2.09	0.52
25:C:504:CLA:H143	25:C:508:CLA:H141	1.91	0.52
2:b:341:LYS:HG3	2:b:429:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:r:20:VAL:O	20:r:24:LEU:HB2	2.10	0.52
3:c:281:MET:HG3	33:c:524:LMG:H412	1.92	0.52
1:A:329[B]:GLU:HG3	37:A:806:HOH:O	2.09	0.52
25:C:506:CLA:H8	27:C:514:BCR:H12C	1.92	0.52
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.45	0.52
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.41	0.52
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.91	0.52
1:a:245:THR:HB	4:d:265:ARG:HE	1.74	0.52
29:a:613:SQD:H291	31:c:523:STE:H82	1.92	0.52
29:f:101:SQD:H312	18:x:27:VAL:HG11	1.91	0.52
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.92	0.52
2:B:498:LYS:HD2	4:D:20:ASP:HA	1.92	0.51
2:B:371:THR:HG23	2:B:372:ASP:O	2.10	0.51
30:C:517:DGD:HB22	33:C:519:LMG:H302	1.93	0.51
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.92	0.51
25:a:607:CLA:HBB1	25:a:607:CLA:HMB3	1.92	0.51
25:c:513:CLA:HBB1	25:c:513:CLA:HMB3	1.93	0.51
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.91	0.51
16:v:13:ASN:ND2	16:v:17:LYS:HB3	2.25	0.51
2:B:283:GLU:O	2:B:287:ARG:HG3	2.10	0.51
2:B:247:PHE:HE1	25:B:601:CLA:H102	1.74	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.46	0.51
28:a:611:PL9:H452	4:d:30:VAL:HG11	1.92	0.51
32:b:623:LHG:O4	4:d:141:TYR:OH	2.17	0.51
25:b:614:CLA:H2	25:b:615:CLA:CBB	2.39	0.51
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.46	0.51
25:c:508:CLA:H192	30:c:518:DGD:HA72	1.93	0.51
4:D:103:ARG:HH21	5:E:77:GLU:CG	2.20	0.50
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.93	0.50
25:b:608:CLA:HMB1	25:b:608:CLA:HBB1	1.92	0.50
25:c:504:CLA:H91	25:c:508:CLA:H171	1.91	0.50
3:C:213:LEU:HD11	27:C:514:BCR:C20	2.41	0.50
2:b:127:ARG:NH2	7:h:18:TYR:O	2.44	0.50
5:e:14:ILE:O	5:e:20:TRP:NE1	2.43	0.50
11:l:14:ARG:HB3	14:t:25:GLU:HG2	1.93	0.50
27:d:405:BCR:H381	33:d:410:LMG:H162	1.93	0.50
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.93	0.50
13:O:27:ARG:HG3	37:O:301:HOH:O	2.12	0.50
25:b:612:CLA:H203	32:b:623:LHG:H212	1.94	0.50
3:c:171:GLY:HA2	3:c:174:LEU:HD12	1.93	0.50
18:x:27:VAL:O	18:x:31:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.93	0.50
25:a:609:CLA:H42	8:i:9:TYR:CE2	2.47	0.50
3:c:472:LEU:HD11	4:d:255:GLN:HG3	1.94	0.50
3:C:42:LEU:HD21	25:C:511:CLA:H2A	1.93	0.50
12:M:28:GLN:HB3	12:m:27:VAL:HG12	1.92	0.50
25:b:607:CLA:H203	30:h:102:DGD:HA82	1.92	0.50
6:f:36:ALA:O	6:f:40:MET:HG3	2.11	0.50
2:B:149[A]:LEU:HD21	25:B:605:CLA:HBB2	1.94	0.50
2:b:159:THR:O	2:b:180:PRO:HB3	2.11	0.50
3:c:391[B]:ARG:HH21	3:c:394:GLU:HG2	1.75	0.50
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	1.94	0.50
25:C:505:CLA:H43	27:C:514:BCR:HC7	1.94	0.50
14:t:18:PHE:HB2	27:t:101:BCR:HC8	1.94	0.50
25:B:612:CLA:HBB1	25:B:612:CLA:HMB1	1.93	0.49
25:a:612:CLA:H151	32:d:407:LHG:H222	1.93	0.49
25:d:404:CLA:H2	18:x:17:GLY:HA3	1.95	0.49
2:B:149[B]:LEU:HD11	25:B:603:CLA:H162	1.94	0.49
25:C:502:CLA:H61	25:C:512:CLA:H42	1.94	0.49
3:c:78:GLU:OE1	16:v:106:ASN:ND2	2.45	0.49
17:y:41:VAL:C	17:y:43:ARG:H	2.20	0.49
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	1.94	0.49
1:A:270:SER:HB3	29:A:613:SQD:O49	2.13	0.49
29:B:621:SQD:H161	29:B:621:SQD:H341	1.95	0.49
10:K:26:PRO:O	10:K:29:PRO:HD2	2.12	0.49
26:D:402:PHO:HBA2	25:D:403:CLA:H142	1.93	0.49
1:a:334[A]:ARG:HG3	13:o:157:LEU:HB2	1.95	0.49
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.95	0.49
31:D:413:STE:H141	18:X:17:GLY:HA2	1.94	0.49
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.47	0.49
2:B:216:HIS:HE1	25:B:608:CLA:C1A	2.26	0.49
25:B:607:CLA:H172	25:B:608:CLA:H193	1.94	0.49
1:a:229:GLU:CD	1:a:229:GLU:H	2.20	0.49
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.94	0.49
2:b:65:PHE:CE1	25:b:603:CLA:HED2	2.46	0.49
13:O:57:LYS:NZ	37:O:303:HOH:O	2.44	0.49
15:U:104:LYS:NZ	16:V:131:GLY:O	2.41	0.49
29:b:619:SQD:H242	29:b:619:SQD:H92	1.95	0.49
9:j:18:GLY:O	9:j:22:ILE:HG12	2.13	0.49
4:D:343:GLU:HG2	16:V:135:VAL:HG11	1.94	0.49
5:E:26:THR:HA	20:R:15:ALA:HB1	1.94	0.49
13:O:27:ARG:O	13:O:27:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.95	0.49
25:c:503:CLA:H203	25:c:510:CLA:HAB	1.95	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.49	0.48
3:C:406:SER:HA	3:C:420:VAL:HG23	1.94	0.48
1:a:93:PHE:HZ	25:a:609:CLA:HAA1	1.78	0.48
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.49	0.48
1:a:286:THR:HG23	25:a:607:CLA:HED3	1.95	0.48
3:C:223:TRP:CG	3:C:224:ILE:H	2.31	0.48
32:E:101:LHG:H152	32:E:101:LHG:H182	1.74	0.48
3:c:147:PHE:CE2	25:c:513:CLA:HBA1	2.48	0.48
32:b:623:LHG:H151	32:l:101:LHG:H281	1.95	0.48
3:c:35:TRP:CD1	10:k:45:PHE:HB3	2.47	0.48
3:C:465:PRO:O	3:C:469:MET:HG3	2.14	0.48
2:b:266:GLU:HB2	37:b:714:HOH:O	2.12	0.48
4:d:85:MET:HE3	4:d:107:LEU:HB3	1.95	0.48
4:d:131:GLU:O	4:d:135:LEU:HG	2.13	0.48
35:e:101:HEM:HHC	35:e:101:HEM:HBB2	1.96	0.48
10:k:24:VAL:O	10:k:27:VAL:HG22	2.13	0.48
2:B:12:LEU:HB2	25:B:611:CLA:HMC2	1.94	0.48
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.96	0.48
25:b:608:CLA:HBA1	25:b:609:CLA:CBB	2.44	0.48
4:d:246:MET:HE3	4:d:264:LYS:CG	2.43	0.48
33:D:412:LMG:O9	37:D:501:HOH:O	2.20	0.48
1:a:132:GLU:O	1:a:136:ARG:HG2	2.14	0.48
3:c:406:SER:HA	3:c:420:VAL:HG23	1.96	0.48
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.48	0.47
20:R:32:GLN:C	20:R:34:LEU:N	2.71	0.47
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.95	0.47
2:B:97:ALA:O	2:B:101:ILE:HD12	2.14	0.47
25:B:615:CLA:H61	25:B:615:CLA:H41	1.51	0.47
2:b:383:PHE:N	4:d:344:GLU:O	2.41	0.47
2:B:98:LEU:HD11	30:a:615:DGD:HBW1	1.96	0.47
16:V:87:GLU:OE1	16:V:96:ARG:NH1	2.42	0.47
18:X:34:ILE:CG2	20:R:34:LEU:HD21	2.45	0.47
25:b:609:CLA:H51	25:b:609:CLA:H8	1.75	0.47
4:d:126:MET:HE3	4:d:143:ALA:O	2.15	0.47
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.95	0.47
25:B:605:CLA:H122	25:B:605:CLA:H161	1.43	0.47
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.49	0.47
1:a:214:MET:SD	26:d:402:PHO:HED3	2.54	0.47
16:v:26:TYR:OH	16:v:122:GLU:OE1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.50	0.47
2:B:422:ARG:O	2:B:425:ILE:HG12	2.15	0.47
25:B:613:CLA:H92	25:B:613:CLA:H62	1.73	0.47
13:O:107:THR:HG22	37:O:310:HOH:O	2.14	0.47
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.97	0.47
19:Z:29:SER:HB3	19:Z:31:GLN:HE21	1.79	0.47
2:b:413:ASP:O	2:b:417:VAL:HG23	2.15	0.47
25:c:506:CLA:H62	25:c:506:CLA:H41	1.70	0.47
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.50	0.47
16:v:57:GLU:H	16:v:57:GLU:CD	2.22	0.47
2:B:52:LEU:HD12	13:o:59:LYS:HE2	1.97	0.47
29:B:621:SQD:H382	29:B:621:SQD:H352	1.67	0.47
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.96	0.47
1:a:150:PRO:HB2	25:a:607:CLA:H62	1.97	0.47
1:A:117:PHE:HD2	25:A:609:CLA:HED3	1.80	0.47
25:B:605:CLA:H72	27:B:618:BCR:H311	1.96	0.47
4:D:123:ILE:HD11	30:H:103:DGD:HAW2	1.96	0.47
2:b:149:LEU:HD12	25:b:603:CLA:H162	1.97	0.47
3:C:143:TYR:CE2	25:C:513:CLA:HED3	2.50	0.46
25:C:508:CLA:HBC3	25:C:510:CLA:H92	1.97	0.46
27:C:514:BCR:H15C	27:C:514:BCR:H351	1.73	0.46
25:b:605:CLA:H71	27:b:618:BCR:H311	1.96	0.46
27:Z:101:BCR:H371	27:Z:101:BCR:H24C	1.78	0.46
30:c:518:DGD:HD3	33:c:520:LMG:HC3	1.97	0.46
29:A:613:SQD:H272	32:D:410:LHG:H152	1.96	0.46
30:H:103:DGD:HBN1	30:H:103:DGD:HBW2	1.50	0.46
16:V:44:GLY:HA2	16:V:54:LEU:HD12	1.96	0.46
2:b:102:VAL:HG11	25:b:605:CLA:H142	1.98	0.46
4:d:85:MET:HE1	4:d:107:LEU:HD13	1.98	0.46
16:v:41:HIS:HA	16:v:45:ILE:O	2.15	0.46
2:B:119:ASP:H	11:L:1:MET:HE3	1.80	0.46
30:H:103:DGD:HB21	30:H:103:DGD:HB51	1.60	0.46
28:A:611:PL9:H33	4:D:42:TYR:HB2	1.98	0.46
4:D:192:THR:HG23	25:D:403:CLA:HBC2	1.98	0.46
2:b:164:PRO:HG3	25:b:605:CLA:O1D	2.15	0.46
2:b:201:HIS:HB2	25:b:601:CLA:CHB	2.45	0.46
25:C:504:CLA:H42	30:C:517:DGD:HB62	1.96	0.46
13:O:72:THR:HG21	13:O:107:THR:HG23	1.98	0.46
18:X:8:LYS:NZ	37:X:101:HOH:O	2.48	0.46
33:c:524:LMG:HC2	8:i:9:TYR:OH	2.15	0.46
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:607:CLA:H162	28:A:611:PL9:H221	1.98	0.46
19:Z:31:GLN:NE2	19:Z:32:ASP:HB2	2.31	0.46
1:a:82:VAL:HB	1:a:174[A]:LEU:HB2	1.97	0.46
25:b:606:CLA:H2	33:b:620:LMG:H152	1.96	0.46
2:B:221:PRO:HA	25:B:608:CLA:HED3	1.98	0.46
25:B:606:CLA:HAC2	27:t:101:BCR:H272	1.98	0.46
25:C:512:CLA:H93	25:C:512:CLA:H61	1.72	0.46
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.97	0.46
1:A:45:THR:HG21	29:T:103:SQD:H223	1.98	0.46
29:B:621:SQD:H82	29:B:621:SQD:H111	1.52	0.46
4:D:186:GLN:HB2	25:D:403:CLA:HBC1	1.98	0.46
14:T:15:ALA:HB2	27:T:101:BCR:H14C	1.97	0.46
28:a:611:PL9:H251	28:a:611:PL9:H272	1.55	0.46
2:b:224:ARG:HG2	7:h:24:GLY:O	2.16	0.46
30:A:614:DGD:HG12	31:I:101:STE:H81	1.97	0.46
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.97	0.46
13:O:83:GLY:HA2	13:O:98:GLU:HG3	1.98	0.45
25:b:602:CLA:C4D	25:b:604:CLA:H43	2.46	0.45
25:b:611:CLA:H171	25:b:611:CLA:H13	1.69	0.45
3:c:110:PRO:O	3:c:114:VAL:HG23	2.17	0.45
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.96	0.45
25:B:612:CLA:H62	25:B:612:CLA:H41	1.58	0.45
2:b:27:THR:HG22	2:b:107:LEU:HD13	1.98	0.45
13:o:160:LYS:HA	13:o:160:LYS:HD2	1.70	0.45
25:B:614:CLA:H102	25:B:614:CLA:H172	1.98	0.45
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.52	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.45
3:c:337:LEU:HD22	3:c:342:MET:HE3	1.97	0.45
3:c:391[B]:ARG:NE	3:c:391[B]:ARG:HA	2.32	0.45
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.98	0.45
15:u:80:GLU:HG3	15:u:81:HIS:CD2	2.50	0.45
20:r:2:ASP:N	37:r:101:HOH:O	2.49	0.45
28:A:611:PL9:H152	32:E:101:LHG:H372	1.98	0.45
25:C:510:CLA:HMB1	25:C:510:CLA:HBB1	1.98	0.45
20:R:34:LEU:HD23	20:R:34:LEU:O	2.15	0.45
28:a:611:PL9:H201	28:a:611:PL9:H221	1.67	0.45
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.98	0.45
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.97	0.45
2:b:327:THR:HG22	25:b:606:CLA:H12	1.98	0.45
3:c:45:LEU:HA	3:c:139:THR:HG22	1.97	0.45
25:c:509:CLA:H3A	25:c:509:CLA:HBA1	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:53:THR:O	4:d:66:SER:HB2	2.16	0.45
3:c:369:LEU:HD13	3:c:380:ILE:HG12	1.99	0.45
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.45
25:B:606:CLA:H41	25:B:606:CLA:H61	1.71	0.45
30:c:518:DGD:HAN2	30:c:519:DGD:HAT2	1.98	0.45
2:b:29:LEU:HD23	29:b:619:SQD:H222	1.98	0.45
30:c:519:DGD:HG12	9:j:32:ALA:HB1	1.99	0.45
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.72	0.45
3:C:139:THR:HB	3:C:141:GLU:OE2	2.17	0.45
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.17	0.45
25:b:613:CLA:H43	29:b:619:SQD:H102	1.99	0.45
25:b:614:CLA:H161	25:b:614:CLA:H141	1.58	0.45
25:b:614:CLA:HBA1	25:b:614:CLA:H3A	1.74	0.45
5:e:73:LYS:NZ	5:e:77:GLU:OE2	2.48	0.45
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.98	0.45
25:A:607:CLA:HED1	30:C:518:DGD:HAW1	1.99	0.45
25:b:609:CLA:H152	25:b:611:CLA:O1A	2.17	0.45
3:c:47:GLY:HA3	3:c:137:PRO:O	2.17	0.45
32:d:407:LHG:H321	14:t:21:ILE:HD11	1.99	0.45
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.53	0.44
2:b:25:MET:HG2	27:b:616:BCR:H23C	2.00	0.44
3:c:67:MET:HB3	3:c:88:LEU:HD12	1.98	0.44
13:o:59:LYS:H	13:o:59:LYS:HG3	1.50	0.44
3:C:279:LEU:HD12	25:C:509:CLA:HED2	2.00	0.44
2:B:393:GLU:OE2	15:U:14:ASP:HB3	2.18	0.44
25:B:611:CLA:H8	25:B:611:CLA:H193	1.98	0.44
25:b:604:CLA:HMA1	25:b:605:CLA:H3A	1.99	0.44
11:l:26:VAL:HG11	32:l:101:LHG:H212	1.99	0.44
30:C:518:DGD:HB62	30:C:518:DGD:HB91	1.80	0.44
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.48	0.44
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.17	0.44
13:O:93:LEU:O	13:O:128:SER:HA	2.17	0.44
4:d:35:ILE:O	25:d:404:CLA:HBB2	2.18	0.44
25:B:606:CLA:H92	25:B:606:CLA:H62	1.68	0.44
3:C:180:MET:HG2	3:C:199:ILE:O	2.18	0.44
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.99	0.44
25:b:609:CLA:H143	25:b:609:CLA:H161	1.78	0.44
25:c:508:CLA:H91	25:c:508:CLA:H112	1.84	0.44
2:B:185:TRP:HB3	25:H:101:CLA:HMA3	2.00	0.44
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.99	0.44
1:A:243:GLU:H	1:A:243:GLU:CD	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ILE:HD13	31:B:625:STE:H182	1.98	0.44
2:B:216:HIS:CE1	25:B:608:CLA:NA	2.85	0.44
30:C:518:DGD:HA31	33:D:407:LMG:H111	1.98	0.44
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.44
28:a:611:PL9:H301	28:a:611:PL9:H322	1.81	0.44
3:c:245:ILE:HG21	33:c:522:LMG:H371	2.00	0.44
4:d:191:TRP:CZ2	4:d:197:HIS:HB2	2.53	0.44
13:o:146:PHE:CZ	13:o:195:GLY:HA3	2.53	0.44
17:y:39:LEU:O	17:y:44:GLY:N	2.45	0.44
25:C:512:CLA:H93	25:C:512:CLA:H111	1.66	0.44
5:E:22[A]:ILE:HA	20:R:18:TRP:HE1	1.83	0.44
1:a:217:SER:HA	4:d:272:LEU:HD12	2.00	0.44
2:b:191:ASN:HB2	7:h:58:VAL:HG13	2.00	0.44
2:b:280:PHE:CD2	2:b:312:TYR:HB3	2.53	0.44
4:d:126:MET:HA	4:d:129:GLN:OE1	2.17	0.44
25:d:404:CLA:H122	7:h:36:GLY:HA3	2.00	0.44
35:e:101:HEM:O2A	6:f:15:ILE:HG12	2.17	0.44
27:x:101:BCR:H20C	27:x:101:BCR:H361	1.82	0.44
2:B:327:THR:HG21	33:M:101:LMG:H291	1.98	0.43
25:B:601:CLA:H43	7:H:45:ILE:HG22	1.99	0.43
13:O:94:THR:OG1	13:O:128:SER:OG	2.26	0.43
25:c:501:CLA:C2D	25:c:503:CLA:H2	2.48	0.43
8:i:18:LEU:HD23	8:i:18:LEU:HA	1.72	0.43
2:B:285:ASN:O	2:B:289:GLN:HG2	2.18	0.43
25:B:605:CLA:H91	25:B:605:CLA:H112	1.58	0.43
4:D:321:LEU:O	4:D:325:ILE:HG13	2.18	0.43
1:a:223:LEU:HD12	1:a:223:LEU:HA	1.90	0.43
30:a:615:DGD:HB51	30:a:615:DGD:HB21	1.76	0.43
13:o:153:THR:HB	37:u:230:HOH:O	2.17	0.43
16:v:26:TYR:HD2	16:v:27:LEU:HD23	1.82	0.43
19:z:3:ILE:HG22	19:z:7:LEU:HD23	2.00	0.43
25:D:404:CLA:H42	7:H:43:LEU:HD11	2.00	0.43
5:E:30:LEU:HD23	20:R:12:VAL:HG22	2.00	0.43
1:a:213:ALA:HB2	4:d:275:PRO:HG2	2.00	0.43
25:c:509:CLA:HMB1	25:c:509:CLA:HBB1	1.99	0.43
3:C:203:THR:O	3:C:235:GLY:HA3	2.19	0.43
33:C:519:LMG:H171	17:Y:25:ILE:HD13	2.00	0.43
25:b:613:CLA:H93	25:b:613:CLA:H61	1.73	0.43
27:c:515:BCR:H11C	27:c:515:BCR:H341	1.88	0.43
17:y:20:ALA:O	17:y:24:MET:HG2	2.17	0.43
2:B:119:ASP:CB	11:L:1:MET:HE3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.54	0.43
25:C:508:CLA:H203	33:C:519:LMG:H351	2.00	0.43
12:M:6:LEU:HD12	33:M:101:LMG:HC92	1.99	0.43
3:c:334:PRO:HA	13:o:153:THR:OG1	2.19	0.43
13:o:53:LYS:HD2	13:o:232:GLU:OE1	2.19	0.43
1:A:85:SER:HA	1:A:109:GLY:HA3	2.01	0.43
4:d:54:PHE:O	5:e:49:THR:OG1	2.30	0.43
26:d:402:PHO:H3A	25:d:403:CLA:H142	2.01	0.43
27:B:618:BCR:H11C	27:B:618:BCR:H341	1.85	0.43
27:B:618:BCR:H363	29:a:614:SQD:H162	2.01	0.43
3:C:179:ALA:O	3:C:184:GLY:HA2	2.19	0.43
25:b:606:CLA:H93	25:b:606:CLA:H111	1.84	0.43
13:o:32:ILE:HG21	13:o:93:LEU:HD21	2.00	0.43
27:x:101:BCR:H351	27:x:101:BCR:H15C	1.84	0.43
1:A:156:ALA:HA	1:A:160[B]:ILE:HB	2.01	0.43
2:B:119:ASP:H	11:L:1:MET:CE	2.31	0.43
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.53	0.43
3:c:163:PHE:CD1	3:c:252:ILE:HD11	2.53	0.43
3:c:338:GLY:HA2	13:o:103:PHE:HZ	1.84	0.43
4:d:49:LEU:HD13	27:d:405:BCR:C15	2.49	0.43
12:m:9:ILE:HG13	12:m:13:LEU:HD22	2.00	0.43
1:A:334[A]:ARG:NH2	13:O:159:PRO:HA	2.34	0.43
25:A:606:CLA:C19	32:D:409:LHG:H312	2.49	0.43
2:B:137:LYS:HB2	2:B:137:LYS:HE3	1.78	0.43
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.43
3:C:216:SER:HB2	33:C:515:LMG:HC8	1.99	0.43
26:D:402:PHO:H3A	25:D:403:CLA:H142	2.01	0.43
5:E:76:VAL:O	5:E:80:LEU:HG	2.18	0.43
13:O:72:THR:CG2	13:O:107:THR:HG23	2.49	0.43
25:b:606:CLA:H142	25:b:612:CLA:H171	1.99	0.43
9:j:19:MET:O	9:j:23:VAL:HG23	2.19	0.43
27:x:101:BCR:H24C	27:x:101:BCR:H371	1.89	0.43
25:B:601:CLA:H191	30:H:103:DGD:HBE1	2.00	0.43
3:C:410:VAL:HG22	3:C:413[B]:GLU:HG2	2.00	0.43
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.00	0.43
19:Z:31:GLN:NE2	19:Z:32:ASP:H	2.15	0.43
20:R:32:GLN:C	20:R:34:LEU:H	2.27	0.43
5:e:30:LEU:HD11	35:e:101:HEM:CBB	2.48	0.43
25:C:508:CLA:H142	25:C:508:CLA:H112	1.77	0.42
30:C:517:DGD:HA82	30:C:517:DGD:HAE2	1.44	0.42
33:C:519:LMG:H331	33:C:519:LMG:H361	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:178:LYS:NZ	3:c:184:GLY:O	2.49	0.42
4:d:12:ARG:HA	4:d:12:ARG:HD3	1.84	0.42
11:l:22:LEU:HD23	32:l:101:LHG:H172	2.01	0.42
1:A:328[A]:MET:HE1	4:D:183:LEU:HD13	2.00	0.42
25:B:607:CLA:H141	25:B:607:CLA:H161	1.78	0.42
27:K:101:BCR:H24C	27:K:101:BCR:H371	1.81	0.42
25:b:603:CLA:HBB1	25:b:603:CLA:HMB1	2.00	0.42
29:b:619:SQD:H142	29:b:619:SQD:H172	1.69	0.42
3:c:318:LEU:HG	3:c:328[B]:VAL:HG11	2.01	0.42
32:d:408:LHG:H242	32:d:408:LHG:H272	1.59	0.42
13:o:220:LEU:HD23	13:o:220:LEU:HA	1.81	0.42
1:A:334[A]:ARG:HD3	37:A:774:HOH:O	2.18	0.42
28:A:611:PL9:H203	26:D:402:PHO:HMA2	2.01	0.42
2:B:414:PRO:O	2:B:418:LYS:HG3	2.19	0.42
3:C:95:LEU:HD21	25:C:501:CLA:OBD	2.20	0.42
2:b:13:ILE:HG12	25:b:611:CLA:HAC2	2.00	0.42
2:b:216:HIS:HE1	25:b:608:CLA:C1A	2.32	0.42
3:c:158:THR:HG21	3:c:256:PRO:HD3	2.01	0.42
25:c:509:CLA:H142	25:c:509:CLA:H111	1.79	0.42
4:d:116:LEU:HD23	4:d:116:LEU:HA	1.80	0.42
6:f:24:HIS:O	6:f:28:VAL:HG13	2.18	0.42
27:B:617:BCR:H24C	27:B:617:BCR:H371	1.94	0.42
3:C:313:GLN:HB2	3:C:396:MET:HG3	2.02	0.42
5:E:32:ILE:HD13	5:E:32:ILE:HA	1.88	0.42
9:J:19:MET:O	9:J:23:VAL:HG23	2.19	0.42
2:b:222:PRO:HA	7:h:22:ALA:HB3	2.01	0.42
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.01	0.42
25:h:101:CLA:H141	25:h:101:CLA:H161	1.76	0.42
9:j:15:THR:HG22	9:j:19:MET:HE2	2.00	0.42
17:y:34:MET:HE3	17:y:34:MET:HB2	1.81	0.42
2:B:403:GLY:C	2:B:407:ASN:HB2	2.45	0.42
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.81	0.42
3:c:26:ARG:HA	25:c:511:CLA:OBD	2.19	0.42
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.19	0.42
13:o:53:LYS:HB2	13:o:53:LYS:HE3	1.89	0.42
25:B:609:CLA:H152	25:B:611:CLA:O1A	2.20	0.42
3:C:112:PHE:O	3:C:116:VAL:HG23	2.20	0.42
25:C:507:CLA:H142	27:C:514:BCR:H16C	2.00	0.42
12:M:12:ALA:O	12:M:16:LEU:HB2	2.20	0.42
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.01	0.42
25:b:606:CLA:H141	25:b:606:CLA:H161	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:613:CLA:H62	25:b:613:CLA:H41	1.51	0.42
3:c:213:LEU:HD21	27:c:515:BCR:C20	2.50	0.42
3:c:383:ASP:HA	37:c:659:HOH:O	2.19	0.42
27:c:515:BCR:H24C	27:c:515:BCR:H371	1.91	0.42
30:A:614:DGD:C2B	25:b:605:CLA:H201	2.50	0.42
3:C:45:LEU:HA	3:C:139:THR:HG22	2.01	0.42
4:D:116:LEU:HD23	4:D:116:LEU:HA	1.84	0.42
6:F:15:ILE:HD13	20:R:23:ILE:HD11	2.01	0.42
25:H:101:CLA:O1D	25:H:101:CLA:H2A	2.20	0.42
13:O:110:MET:HE2	13:O:110:MET:HB3	1.84	0.42
1:a:265:PHE:CD2	1:a:271:LEU:HD23	2.54	0.42
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.53	0.42
26:d:402:PHO:H152	25:d:403:CLA:H171	2.02	0.42
13:o:50:PHE:O	13:o:68:THR:OG1	2.28	0.42
13:o:110:MET:HE2	13:o:116:ILE:HD11	2.02	0.42
1:A:131:TRP:CZ3	25:C:505:CLA:HAA2	2.55	0.42
2:B:272:ARG:HG3	2:B:273:TYR:N	2.35	0.42
25:B:604:CLA:H41	25:B:604:CLA:H61	1.83	0.42
25:B:610:CLA:H72	25:B:610:CLA:H112	1.80	0.42
19:Z:35:ARG:HD3	19:Z:35:ARG:HA	1.80	0.42
15:u:51:LYS:HE2	15:u:51:LYS:HB2	1.86	0.42
30:A:614:DGD:HB61	31:I:101:STE:H51	2.02	0.42
3:C:348:GLU:O	3:C:350:ILE:HG23	2.20	0.42
16:V:69:ILE:O	16:V:73:VAL:HG23	2.20	0.42
19:Z:34:ASP:O	19:Z:37:LYS:HG2	2.19	0.42
25:b:601:CLA:CHC	25:h:101:CLA:HBB1	2.50	0.42
25:c:505:CLA:C1A	25:c:505:CLA:CGA	2.98	0.42
4:d:152:VAL:HG21	4:d:279:LEU:HG	2.02	0.42
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.55	0.42
25:A:609:CLA:H61	25:A:609:CLA:H41	1.54	0.42
25:B:602:CLA:C2D	25:B:604:CLA:H2	2.50	0.42
19:Z:29:SER:HB3	19:Z:31:GLN:NE2	2.35	0.42
2:b:486:LEU:HD11	2:b:490:GLN:NE2	2.35	0.42
25:c:507:CLA:O2A	25:c:507:CLA:HMA2	2.18	0.42
13:o:10:ILE:HG23	13:o:15:LEU:HB2	2.02	0.42
7:H:30:LEU:HD12	7:H:30:LEU:HA	1.88	0.41
27:H:102:BCR:H11C	27:H:102:BCR:H341	1.93	0.41
11:L:7:ARG:NE	37:L:202:HOH:O	2.44	0.41
15:U:76:ARG:HA	15:U:79:LEU:HG	2.01	0.41
2:b:67:ALA:HA	2:b:71:VAL:O	2.20	0.41
2:b:341:LYS:O	2:b:406:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:442:ILE:HD12	4:d:299:ILE:HG12	2.02	0.41
3:c:169:GLY:HA2	3:c:241:GLY:HA2	2.02	0.41
8:I:2:GLU:O	8:I:6:ILE:HG12	2.20	0.41
13:O:81:ILE:HA	13:O:100:GLY:HA3	2.03	0.41
29:a:613:SQD:H222	29:a:613:SQD:H192	1.81	0.41
3:c:125:LEU:HA	3:c:125:LEU:HD12	1.75	0.41
3:c:378:ASN:HD21	13:o:82:GLN:HE22	1.68	0.41
9:j:10:LEU:O	9:j:13:VAL:HG22	2.20	0.41
25:C:510:CLA:H152	25:C:510:CLA:H112	1.87	0.41
4:D:54:PHE:O	5:E:49:THR:OG1	2.31	0.41
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.08	0.41
8:I:4:LEU:O	8:I:8:VAL:HG23	2.20	0.41
16:V:55:ARG:HD2	37:V:315:HOH:O	2.20	0.41
1:a:321:ILE:HD11	4:d:179:PHE:HB2	2.02	0.41
25:b:607:CLA:HHD	25:b:607:CLA:HAC2	1.90	0.41
3:c:261:ARG:HA	3:c:266:TRP:CZ2	2.54	0.41
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.77	0.41
26:d:402:PHO:HMB1	26:d:402:PHO:HBB1	2.02	0.41
30:A:614:DGD:HB31	25:b:605:CLA:H191	2.02	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.45	0.41
25:B:611:CLA:HBB1	25:B:611:CLA:HMB1	2.02	0.41
4:D:32:TRP:CE3	33:D:411:LMG:H161	2.55	0.41
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.41
11:L:27:LEU:HD23	11:L:27:LEU:HA	1.90	0.41
9:j:34:ALA:O	37:j:201:HOH:O	2.22	0.41
32:l:101:LHG:H322	12:m:18:PRO:HB3	2.03	0.41
15:u:70:ARG:NH1	15:u:73:GLN:HB3	2.35	0.41
2:B:297:THR:HG23	2:B:300:GLU:OE1	2.20	0.41
25:B:614:CLA:H3A	25:B:614:CLA:HBA1	1.91	0.41
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.02	0.41
8:I:7:THR:O	8:I:11:VAL:HG23	2.21	0.41
1:a:124:SER:HA	1:a:151:LEU:HD21	2.02	0.41
7:h:62:TRP:HD1	30:h:102:DGD:HE62	1.84	0.41
13:o:83:GLY:HA2	13:o:98:GLU:HG3	2.01	0.41
15:u:70:ARG:NH1	15:u:73:GLN:OE1	2.53	0.41
19:z:46:LEU:HD22	19:z:46:LEU:HA	1.79	0.41
27:B:617:BCR:H15C	27:B:617:BCR:H351	1.85	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.93	0.41
3:C:249:ILE:HB	37:C:601:HOH:O	2.20	0.41
4:D:221:THR:HG21	4:D:249:ALA:HB2	2.03	0.41
4:D:264:LYS:NZ	34:D:401:BCT:O3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:27:VAL:HG12	12:m:28:GLN:HB3	2.01	0.41
1:a:218:LEU:HD23	1:a:218:LEU:HA	1.91	0.41
25:c:505:CLA:H161	25:c:505:CLA:H122	1.77	0.41
4:d:182:LEU:HD21	25:d:401:CLA:HMD2	2.02	0.41
2:B:63:LEU:HA	2:B:66:MET:HE3	2.01	0.41
25:B:601:CLA:H41	7:H:46:LEU:HA	2.03	0.41
4:D:126:MET:HE3	4:D:143:ALA:O	2.21	0.41
27:D:405:BCR:H20C	27:D:405:BCR:H361	1.87	0.41
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.38	0.41
30:A:614:DGD:HB21	25:b:605:CLA:H201	2.02	0.41
2:B:453:PHE:HB2	4:D:291:LEU:HD12	2.03	0.41
2:B:481:GLY:HA2	4:D:139:ARG:HD2	2.02	0.41
25:C:501:CLA:CBB	25:C:501:CLA:H71	2.51	0.41
25:C:505:CLA:H193	25:C:505:CLA:H162	1.83	0.41
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.01	0.41
17:Y:28:ILE:HG23	27:Y:101:BCR:H10C	2.02	0.41
2:b:71:VAL:HG23	25:b:605:CLA:HMA2	2.03	0.41
2:B:442:ILE:HD11	13:O:174:LEU:HD23	2.03	0.41
25:B:610:CLA:H41	25:B:613:CLA:HAC2	2.03	0.41
26:D:402:PHO:HBA2	26:D:402:PHO:H3A	1.89	0.41
26:a:608:PHO:H102	26:a:608:PHO:H13	1.86	0.41
2:b:103:LEU:HB2	25:b:605:CLA:H61	2.03	0.41
2:b:498:LYS:HE3	4:d:20:ASP:HA	2.03	0.41
32:d:407:LHG:HC2	11:l:15:THR:HG21	2.03	0.41
27:t:101:BCR:H15C	27:t:101:BCR:H351	1.92	0.41
20:r:9:LEU:O	20:r:13:LEU:HG	2.21	0.41
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.56	0.41
1:A:201:GLY:HA3	1:A:286:THR:HB	2.03	0.41
20:R:27:ALA:O	20:R:31:VAL:HG23	2.20	0.41
2:b:214:LEU:HD23	2:b:214:LEU:HA	1.89	0.41
27:b:617:BCR:H371	27:b:617:BCR:H24C	1.79	0.41
25:c:510:CLA:H202	25:c:510:CLA:H161	1.82	0.41
4:d:171:PRO:HG3	4:d:181:PHE:CZ	2.56	0.41
2:B:389:LYS:HD3	2:B:389:LYS:HA	1.80	0.40
25:B:602:CLA:HAB	25:B:604:CLA:H162	2.03	0.40
27:B:616:BCR:H20C	27:B:616:BCR:H361	1.87	0.40
3:C:166:ILE:HG13	3:C:248:GLY:HA3	2.03	0.40
5:E:30:LEU:HD12	35:F:101:HEM:HMC1	2.02	0.40
19:Z:12:LEU:HD21	19:Z:51:VAL:HG22	2.03	0.40
1:a:238:LYS:HB2	1:a:238:LYS:HE2	1.78	0.40
25:b:615:CLA:H142	25:b:615:CLA:H111	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:223:TRP:CG	3:c:224:ILE:H	2.38	0.40
5:e:17:VAL:HG21	9:j:7:ARG:HE	1.86	0.40
13:o:40:ILE:HD13	13:o:243:ILE:HG13	2.03	0.40
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.85	0.40
8:I:34:ARG:HB3	37:I:202:HOH:O	2.20	0.40
19:Z:50:LEU:HD12	19:Z:50:LEU:HA	1.95	0.40
25:a:609:CLA:HMA2	33:c:524:LMG:H142	2.02	0.40
7:h:58:VAL:HB	37:h:207:HOH:O	2.20	0.40
9:j:17:ALA:O	9:j:21:VAL:HG13	2.21	0.40
1:A:334[B]:ARG:NH2	37:A:717:HOH:O	2.54	0.40
25:A:612:CLA:HBA1	25:A:612:CLA:C4A	2.51	0.40
25:B:602:CLA:H142	25:B:602:CLA:H112	1.90	0.40
25:B:612:CLA:H192	25:B:612:CLA:H161	1.82	0.40
25:C:504:CLA:H62	25:C:504:CLA:H41	1.85	0.40
27:T:101:BCR:H20C	27:T:101:BCR:H361	1.93	0.40
19:Z:57:LEU:HD23	19:Z:57:LEU:HA	1.84	0.40
27:b:617:BCR:H15C	27:b:617:BCR:H351	1.83	0.40
3:c:61:VAL:HG13	3:c:118:HIS:HD2	1.85	0.40
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.52	0.40
27:t:101:BCR:H24C	27:t:101:BCR:H371	1.94	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.87	0.40
1:a:237:TYR:OH	4:d:246:MET:HG2	2.21	0.40
3:c:240:ILE:HA	3:c:240:ILE:HD13	1.86	0.40
29:A:613:SQD:H381	9:J:22:ILE:HD11	2.04	0.40
2:B:103:LEU:HD21	25:B:604:CLA:HMC3	2.04	0.40
25:B:610:CLA:HBB1	25:B:610:CLA:CMB	2.50	0.40
1:a:230:THR:O	2:b:3:LEU:HD23	2.21	0.40
33:b:620:LMG:H381	33:b:620:LMG:H412	1.77	0.40
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.84	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%)	391 (99%)	4 (1%)	0	100	100
1	a	395/344 (115%)	387 (98%)	7 (2%)	1 (0%)	36	34
2	B	507/510 (99%)	501 (99%)	6 (1%)	0	100	100
2	b	503/510 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	451/461 (98%)	441 (98%)	9 (2%)	1 (0%)	43	44
3	c	461/461 (100%)	448 (97%)	12 (3%)	1 (0%)	43	44
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
10	K	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	27 (90%)	3 (10%)	0	100	100
13	O	243/272 (89%)	231 (95%)	8 (3%)	4 (2%)	7	3
13	o	242/272 (89%)	234 (97%)	7 (3%)	1 (0%)	30	26
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	13
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	25/46 (54%)	22 (88%)	2 (8%)	1 (4%)	2	0
17	y	28/46 (61%)	25 (89%)	3 (11%)	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%)	53 (88%)	6 (10%)	1 (2%)	7	2
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
20	r	29/41 (71%)	29 (100%)	0	0	100	100
All	All	5386/5700 (94%)	5234 (97%)	138 (3%)	14 (0%)	36	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
19	Z	31	GLN
13	O	62	GLU
13	O	134	THR
17	Y	45	ASN
3	c	416	SER
15	u	53	ALA
9	j	6	GLY
13	o	61	GLN
9	J	6	GLY
13	O	57	LYS
13	O	59	LYS
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%)	314 (98%)	8 (2%)	42	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	321/280 (115%)	310 (97%)	11 (3%)	32	33
2	B	407/407 (100%)	395 (97%)	12 (3%)	37	39
2	b	402/407 (99%)	388 (96%)	14 (4%)	32	32
3	C	353/362 (98%)	341 (97%)	12 (3%)	32	33
3	c	362/362 (100%)	347 (96%)	15 (4%)	27	26
4	D	277/283 (98%)	274 (99%)	3 (1%)	65	72
4	d	278/283 (98%)	271 (98%)	7 (2%)	42	45
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	40
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	9
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	31
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	8
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	56
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	56
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	2
10	K	30/37 (81%)	26 (87%)	4 (13%)	4	1
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	39
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	5
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	3
13	O	206/228 (90%)	200 (97%)	6 (3%)	37	39
13	o	207/228 (91%)	200 (97%)	7 (3%)	32	33
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	27
15	U	84/112 (75%)	82 (98%)	2 (2%)	43	47
15	u	84/112 (75%)	81 (96%)	3 (4%)	31	31
16	V	117/138 (85%)	116 (99%)	1 (1%)	70	77
16	v	117/138 (85%)	114 (97%)	3 (3%)	40	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	19/37 (51%)	16 (84%)	3 (16%)	2	1
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	4
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	4
19	Z	52/52 (100%)	42 (81%)	10 (19%)	1	0
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
20	R	28/33 (85%)	21 (75%)	7 (25%)	0	0
20	r	25/33 (76%)	19 (76%)	6 (24%)	1	0
All	All	4450/4654 (96%)	4272 (96%)	178 (4%)	28	27

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	35	VAL
1	A	121	LEU
1	A	205	VAL
1	A	231	GLU
1	A	243	GLU
1	A	248	ILE
1	A	286	THR
2	B	63	LEU
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	161	LEU
2	B	166	MET
2	B	207	ILE
2	B	240	SER
2	B	315	ILE
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	152	LYS
3	C	238	ILE
3	C	240	ILE

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Mol	Chain	Res	Type
3	C	289	PHE
3	C	315	MET
3	C	355[A]	THR
3	C	355[B]	THR
3	C	380	ILE
3	C	416	SER
4	D	154	VAL
4	D	264	LYS
4	D	345	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	56	ASP
8	I	4	LEU
10	K	17	ILE
10	K	19	ASP
10	K	24	VAL
10	K	27	VAL
11	L	10	VAL
12	M	25	LEU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	191	SER
13	O	214	THR
15	U	10	VAL
15	U	67	LEU
16	V	3	LEU
17	Y	21	GLN
17	Y	34	MET
17	Y	41	VAL
18	X	23	LEU
18	X	29	ILE
18	X	37	VAL
19	Z	6	GLN
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	31	GLN
19	Z	32	ASP
19	Z	34	ASP

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Mol	Chain	Res	Type
19	Z	46	LEU
19	Z	50	LEU
19	Z	52	LEU
20	R	6	LEU
20	R	10	LEU
20	R	13	LEU
20	R	21	ARG
20	R	29	LYS
20	R	33	LYS
20	R	35	LEU
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	230	THR
1	a	243	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	86	ILE
2	b	98	LEU
2	b	149	LEU
2	b	161	LEU
2	b	227	LYS
2	b	236	THR
2	b	266	GLU
2	b	362	PHE
2	b	388	SER
2	b	438	ASN
2	b	490	GLN
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	213	LEU

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Mol	Chain	Res	Type
3	c	216	SER
3	c	240	ILE
3	c	252	ILE
3	c	355[A]	THR
3	c	355[B]	THR
3	c	413[A]	GLU
3	c	413[B]	GLU
3	c	468	SER
4	d	182	LEU
4	d	230	SER
4	d	233	ARG
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
5	e	4	THR
5	e	60	GLN
5	e	63	ILE
5	e	65	LEU
5	e	83	LEU
6	f	25	THR
6	f	28	VAL
7	h	7	LEU
9	j	13	VAL
9	j	21	VAL
9	j	24	ILE
10	k	10	LYS
10	k	25	LEU
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
12	m	27	VAL
13	o	18	LYS
13	o	49	THR
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN

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Mol	Chain	Res	Type
13	o	194	LYS
14	t	25	GLU
15	u	10	VAL
15	u	23	GLU
15	u	58	VAL
16	v	2	GLU
16	v	52	LEU
16	v	107	LEU
17	y	19	ILE
17	y	27	MET
17	y	45	ASN
18	x	2	THR
18	x	15	LEU
18	x	23	LEU
19	z	1	MET
19	z	27	TYR
19	z	31	GLN
19	z	39	LEU
19	z	40	ILE
19	z	46	LEU
20	r	6	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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	179	GLN
2	B	394	GLN
4	D	61	HIS
4	D	186	GLN
13	O	3	GLN
13	O	88	ASN
13	O	132	ASN
15	U	81	HIS
17	Y	21	GLN
19	Z	31	GLN
1	a	19	ASN
1	a	266	ASN

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Mol	Chain	Res	Type
1	a	296	ASN
2	b	179	GLN
2	b	338	GLN
2	b	409	GLN
2	b	490	GLN
3	c	378	ASN
3	c	382	ASN
4	d	350	ASN
5	e	60	GLN
5	e	82	GLN
7	h	59	ASN
12	m	5	GLN
13	o	155	ASN
15	u	81	HIS
16	v	118	HIS
18	x	33	GLN
19	z	31	GLN
20	r	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.99	0	8,9,11	0.82	0
12	FME	M	1	12	8,9,10	1.05	1 (12%)	8,9,11	0.99	0
8	FME	i	1	8	8,9,10	1.01	0	8,9,11	1.17	1 (12%)
8	FME	I	1	8	8,9,10	1.02	0	8,9,11	1.02	1 (12%)
12	FME	m	1	12	8,9,10	1.01	1 (12%)	8,9,11	0.63	0

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	1.13	1 (12%)	8,9,11	1.07	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	-	2/7/9/11	-
12	FME	M	1	12	-	4/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.39	1.43	1.46
12	M	1	FME	CA-N	-2.20	1.43	1.46
12	m	1	FME	CA-N	-2.16	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.69	114.70	109.50
8	I	1	FME	CB-CA-N	2.07	114.29	110.52

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
28	PL9	a	611	-	55,55,55	0.69	1 (1%)	68,69,69	1.62	12 (17%)
30	DGD	C	516	-	63,63,67	1.09	8 (12%)	77,77,81	1.33	8 (10%)
25	CLA	C	508	-	69,73,73	1.39	10 (14%)	82,113,113	1.36	8 (9%)
33	LMG	b	622	-	55,55,55	0.82	1 (1%)	63,63,63	1.39	8 (12%)
27	BCR	T	101	-	41,41,41	0.99	3 (7%)	56,56,56	1.23	4 (7%)
27	BCR	k	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.06	2 (3%)
32	LHG	D	410	-	46,46,48	0.92	2 (4%)	49,52,54	1.20	6 (12%)
25	CLA	B	615	-	64,68,73	1.33	9 (14%)	76,107,113	1.38	4 (5%)
25	CLA	C	502	-	69,73,73	1.46	9 (13%)	82,113,113	1.33	10 (12%)
35	HEM	F	101	6,5	50,50,50	1.41	7 (14%)	67,82,82	1.14	3 (4%)
31	STE	b	625	-	19,19,19	0.59	0	19,19,19	1.11	1 (5%)
25	CLA	d	401	37	69,73,73	1.19	6 (8%)	82,113,113	1.28	8 (9%)
27	BCR	B	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.35	8 (14%)
29	SQD	A	613	-	50,52,54	1.61	7 (14%)	60,63,65	1.89	11 (18%)
32	LHG	e	102	-	41,41,48	0.81	1 (2%)	44,47,54	1.33	6 (13%)
27	BCR	b	618	-	41,41,41	0.99	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	c	509	-	69,73,73	1.16	6 (8%)	82,113,113	1.35	5 (6%)
29	SQD	D	408	-	34,36,54	1.50	6 (17%)	42,45,65	2.44	12 (28%)
30	DGD	C	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.43	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	L	101	-	48,48,48	0.76	2 (4%)	51,54,54	1.19	3 (5%)
25	CLA	d	404	-	69,73,73	1.19	7 (10%)	82,113,113	1.21	9 (10%)
28	PL9	d	406	-	55,55,55	1.15	3 (5%)	68,69,69	1.55	13 (19%)
25	CLA	b	615	-	64,68,73	1.19	7 (10%)	76,107,113	1.44	7 (9%)
25	CLA	B	614	-	69,73,73	1.28	7 (10%)	82,113,113	1.28	8 (9%)
31	STE	M	104	-	14,14,19	0.35	0	13,13,19	0.82	0
25	CLA	d	403	-	69,73,73	1.22	6 (8%)	82,113,113	1.13	5 (6%)
25	CLA	B	603	-	69,73,73	1.31	7 (10%)	82,113,113	1.54	8 (9%)
25	CLA	a	612	37	69,73,73	1.32	6 (8%)	82,113,113	1.32	9 (10%)
32	LHG	d	407	-	48,48,48	0.62	0	51,54,54	1.21	3 (5%)
25	CLA	b	602	-	69,73,73	1.34	10 (14%)	82,113,113	1.46	12 (14%)
25	CLA	C	512	-	69,73,73	1.43	9 (13%)	82,113,113	1.28	7 (8%)
31	STE	x	102	-	19,19,19	0.64	0	19,19,19	1.00	1 (5%)
25	CLA	C	505	-	69,73,73	1.40	7 (10%)	82,113,113	1.26	8 (9%)
25	CLA	c	506	-	69,73,73	1.37	9 (13%)	82,113,113	1.26	5 (6%)
27	BCR	b	616	-	41,41,41	1.05	3 (7%)	56,56,56	1.27	7 (12%)
25	CLA	b	605	-	69,73,73	1.43	5 (7%)	82,113,113	1.50	8 (9%)
29	SQD	T	103	-	38,38,54	1.75	5 (13%)	40,40,65	1.23	3 (7%)
30	DGD	C	517	-	63,63,67	1.01	6 (9%)	77,77,81	1.43	13 (16%)
36	HEC	V	201	16	46,50,50	1.83	7 (15%)	58,82,82	1.97	6 (10%)
25	CLA	c	505	-	69,73,73	1.29	7 (10%)	82,113,113	1.28	7 (8%)
31	STE	B	624	-	11,11,19	0.65	0	11,11,19	1.29	1 (9%)
25	CLA	B	610	-	69,73,73	1.27	7 (10%)	82,113,113	1.42	10 (12%)
33	LMG	c	524	-	49,49,55	0.86	4 (8%)	57,57,63	1.35	7 (12%)
31	STE	m	101	-	11,11,19	0.70	0	11,11,19	1.53	2 (18%)
25	CLA	b	603	-	69,73,73	1.15	8 (11%)	82,113,113	1.65	14 (17%)
26	PHO	d	402	-	58,69,69	2.12	10 (17%)	55,99,99	1.59	9 (16%)
25	CLA	b	613	-	69,73,73	1.23	7 (10%)	82,113,113	1.29	7 (8%)
27	BCR	c	516	-	41,41,41	1.05	3 (7%)	56,56,56	1.22	6 (10%)
25	CLA	c	508	-	68,72,73	1.39	8 (11%)	80,111,113	1.35	6 (7%)
31	STE	b	624	-	15,15,19	0.74	0	15,15,19	0.97	0
31	STE	c	521	-	19,19,19	0.64	0	19,19,19	0.95	0
25	CLA	c	512	-	69,73,73	1.37	10 (14%)	82,113,113	1.31	10 (12%)
27	BCR	c	515	-	41,41,41	1.08	3 (7%)	56,56,56	1.27	5 (8%)
31	STE	B	622	-	11,11,19	0.66	0	11,11,19	1.32	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	OEY	a	602[A]	3,1,37	0,16,16	-	-	-		
27	BCR	D	405	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	4 (7%)
31	STE	t	103	-	9,9,19	0.48	0	8,8,19	0.55	0
31	STE	M	103	-	9,9,19	0.37	0	8,8,19	0.71	0
25	CLA	b	609	37	69,73,73	1.41	8 (11%)	82,113,113	1.39	12 (14%)
25	CLA	c	504	37	64,68,73	1.18	6 (9%)	76,107,113	1.31	9 (11%)
28	PL9	A	611	-	55,55,55	0.90	2 (3%)	68,69,69	1.42	12 (17%)
30	DGD	c	517	-	63,63,67	1.01	7 (11%)	77,77,81	1.36	8 (10%)
33	LMG	M	101	-	51,51,55	0.85	0	59,59,63	1.38	7 (11%)
25	CLA	C	504	37	63,67,73	1.34	7 (11%)	74,105,113	1.32	12 (16%)
25	CLA	b	608	-	69,73,73	1.26	9 (13%)	82,113,113	1.19	8 (9%)
26	PHO	A	608	-	58,69,69	1.99	8 (13%)	55,99,99	1.52	8 (14%)
31	STE	C	521	-	11,11,19	0.71	0	11,11,19	1.26	1 (9%)
25	CLA	D	403	-	69,73,73	1.29	6 (8%)	82,113,113	1.28	7 (8%)
31	STE	a	616	-	11,11,19	0.85	0	11,11,19	1.01	0
31	STE	H	104	-	17,17,19	0.43	0	16,16,19	0.66	0
27	BCR	c	514	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	6 (10%)
25	CLA	B	607	-	69,73,73	1.29	8 (11%)	82,113,113	1.34	10 (12%)
25	CLA	B	609	37	69,73,73	1.12	6 (8%)	82,113,113	1.35	9 (10%)
31	STE	t	102	-	13,13,19	0.69	0	13,13,19	1.28	2 (15%)
33	LMG	d	410	-	44,44,55	0.88	2 (4%)	52,52,63	1.34	6 (11%)
25	CLA	C	507	37	69,73,73	1.23	10 (14%)	82,113,113	1.46	8 (9%)
32	LHG	D	409	-	48,48,48	0.70	1 (2%)	51,54,54	1.24	7 (13%)
30	DGD	H	103	-	63,63,67	1.13	4 (6%)	77,77,81	1.36	9 (11%)
36	HEC	v	201	16	46,50,50	1.81	4 (8%)	58,82,82	1.85	6 (10%)
32	LHG	d	408	-	38,38,48	0.76	1 (2%)	41,44,54	1.15	3 (7%)
25	CLA	B	608	-	69,73,73	1.16	6 (8%)	82,113,113	1.27	6 (7%)
25	CLA	h	101	37	69,73,73	1.31	9 (13%)	82,113,113	1.41	7 (8%)
31	STE	b	626	-	9,9,19	0.34	0	8,8,19	0.78	0
25	CLA	b	601	-	69,73,73	1.17	7 (10%)	82,113,113	1.38	9 (10%)
27	BCR	b	617	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	6 (10%)
25	CLA	B	605	-	69,73,73	1.36	9 (13%)	82,113,113	1.48	8 (9%)
31	STE	j	101	-	11,11,19	0.73	0	11,11,19	1.28	1 (9%)
25	CLA	b	612	-	69,73,73	1.30	8 (11%)	82,113,113	1.39	12 (14%)
26	PHO	a	608	-	58,69,69	2.11	9 (15%)	55,99,99	1.38	7 (12%)
25	CLA	b	604	-	69,73,73	1.25	7 (10%)	82,113,113	1.52	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	M	102	-	14,14,19	0.64	0	14,14,19	1.13	1 (7%)
25	CLA	c	511	3	69,73,73	1.37	7 (10%)	82,113,113	1.43	5 (6%)
21	OEX	A	601[B]	3,1,37	0,15,15	-	-	-		
33	LMG	D	411	-	31,31,55	0.65	0	33,33,63	1.26	2 (6%)
31	STE	B	625	-	15,15,19	0.34	0	14,14,19	0.94	0
29	SQD	a	613	-	52,54,54	1.55	7 (13%)	62,65,65	1.86	13 (20%)
31	STE	J	101	-	11,11,19	0.71	0	11,11,19	1.19	1 (9%)
27	BCR	x	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.16	3 (5%)
33	LMG	C	519	-	48,48,55	0.85	2 (4%)	56,56,63	1.34	8 (14%)
25	CLA	H	101	37	69,73,73	1.31	9 (13%)	82,113,113	1.30	8 (9%)
25	CLA	A	606	-	69,73,73	1.08	5 (7%)	82,113,113	1.18	5 (6%)
31	STE	C	522	-	15,15,19	0.39	0	14,14,19	0.70	0
27	BCR	K	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	7 (12%)
33	LMG	c	522	-	48,48,55	0.88	2 (4%)	56,56,63	1.26	8 (14%)
25	CLA	B	612	-	69,73,73	1.44	5 (7%)	82,113,113	1.45	10 (12%)
25	CLA	C	506	-	69,73,73	1.46	10 (14%)	82,113,113	1.33	7 (8%)
25	CLA	C	510	-	69,73,73	1.23	9 (13%)	82,113,113	1.31	8 (9%)
27	BCR	d	405	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	6 (10%)
32	LHG	E	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.20	5 (9%)
31	STE	l	102	-	17,17,19	0.35	0	16,16,19	0.83	0
21	OEX	a	601[B]	3,1,37	0,15,15	-	-	-		
25	CLA	b	611	-	69,73,73	1.18	7 (10%)	82,113,113	1.37	12 (14%)
25	CLA	B	601	-	69,73,73	1.18	8 (11%)	82,113,113	1.36	10 (12%)
25	CLA	c	513	-	69,73,73	1.20	7 (10%)	82,113,113	1.27	7 (8%)
31	STE	c	523	-	11,11,19	0.75	0	11,11,19	1.21	1 (9%)
25	CLA	c	510	-	69,73,73	1.24	10 (14%)	82,113,113	1.36	9 (10%)
27	BCR	Z	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
25	CLA	c	501	-	69,73,73	1.22	8 (11%)	82,113,113	1.45	7 (8%)
29	SQD	f	101	-	39,41,54	1.69	8 (20%)	49,52,65	1.85	11 (22%)
25	CLA	b	610	-	69,73,73	1.19	8 (11%)	82,113,113	1.40	6 (7%)
25	CLA	b	607	-	69,73,73	1.40	8 (11%)	82,113,113	1.38	12 (14%)
30	DGD	A	614	-	67,67,67	1.15	8 (11%)	81,81,81	1.30	11 (13%)
33	LMG	b	620	-	51,51,55	0.94	3 (5%)	59,59,63	1.54	10 (16%)
25	CLA	C	503	-	69,73,73	1.31	8 (11%)	82,113,113	1.46	10 (12%)
27	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.25	6 (10%)
29	SQD	a	614	-	35,35,54	1.77	5 (14%)	37,37,65	1.35	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCT	a	606	23	3,3,3	1.17	0	2,3,3	2.88	1 (50%)
30	DGD	c	519	-	63,63,67	0.88	2 (3%)	77,77,81	1.45	14 (18%)
25	CLA	B	604	-	69,73,73	1.28	7 (10%)	82,113,113	1.25	9 (10%)
31	STE	B	623	-	17,17,19	0.57	0	17,17,19	1.23	1 (5%)
26	PHO	D	402	-	58,69,69	2.10	10 (17%)	55,99,99	1.61	8 (14%)
31	STE	T	102	-	15,15,19	0.35	0	14,14,19	0.95	0
30	DGD	a	615	-	43,43,67	0.84	2 (4%)	45,45,81	1.45	6 (13%)
33	LMG	c	520	-	37,37,55	0.96	1 (2%)	45,45,63	1.32	6 (13%)
22	OEY	A	602[A]	3,1,37	0,16,16	-	-	-	-	-
27	BCR	a	610	-	41,41,41	0.97	2 (4%)	56,56,56	1.12	4 (7%)
29	SQD	B	621	-	52,54,54	1.59	9 (17%)	62,65,65	1.76	12 (19%)
31	STE	D	413	-	19,19,19	0.61	0	19,19,19	1.07	0
35	HEM	e	101	6,5	50,50,50	1.44	9 (18%)	67,82,82	1.33	7 (10%)
25	CLA	c	507	37	69,73,73	1.34	9 (13%)	82,113,113	1.36	9 (10%)
25	CLA	c	502	-	69,73,73	1.23	8 (11%)	82,113,113	1.33	10 (12%)
30	DGD	h	102	-	63,63,67	0.96	4 (6%)	77,77,81	1.41	9 (11%)
25	CLA	D	404	-	69,73,73	1.30	9 (13%)	82,113,113	1.30	8 (9%)
27	BCR	B	616	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	6 (10%)
27	BCR	Y	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	5 (8%)
32	LHG	b	623	-	48,48,48	0.72	2 (4%)	51,54,54	1.31	7 (13%)
32	LHG	B	620	-	48,48,48	0.84	1 (2%)	51,54,54	1.36	7 (13%)
25	CLA	b	614	-	69,73,73	1.47	11 (15%)	82,113,113	1.29	5 (6%)
33	LMG	D	407	-	51,51,55	0.76	2 (3%)	59,59,63	1.36	7 (11%)
31	STE	b	621	-	19,19,19	0.62	0	19,19,19	1.04	1 (5%)
25	CLA	A	607	37	69,73,73	1.16	5 (7%)	82,113,113	1.28	8 (9%)
25	CLA	A	609	-	58,62,73	1.30	6 (10%)	68,99,113	1.29	9 (13%)
25	CLA	B	602	-	69,73,73	1.27	9 (13%)	82,113,113	1.29	6 (7%)
28	PL9	D	406	-	55,55,55	1.00	4 (7%)	68,69,69	1.51	14 (20%)
31	STE	B	619	-	16,16,19	0.71	0	16,16,19	1.03	0
25	CLA	a	607	-	69,73,73	1.27	9 (13%)	82,113,113	1.31	7 (8%)
25	CLA	a	609	-	69,73,73	1.24	8 (11%)	82,113,113	1.21	6 (7%)
25	CLA	c	503	-	69,73,73	1.33	9 (13%)	82,113,113	1.36	8 (9%)
25	CLA	C	509	-	69,73,73	1.31	10 (14%)	82,113,113	1.41	9 (10%)
27	BCR	H	102	-	41,41,41	0.96	1 (2%)	56,56,56	1.27	6 (10%)
31	STE	C	520	-	11,11,19	0.70	0	11,11,19	1.49	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	C	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	5 (8%)
25	CLA	b	606	37	69,73,73	1.20	9 (13%)	82,113,113	1.29	7 (8%)
32	LHG	l	101	-	48,48,48	0.65	0	51,54,54	1.23	7 (13%)
25	CLA	B	613	-	69,73,73	1.28	7 (10%)	82,113,113	1.27	7 (8%)
25	CLA	C	513	-	69,73,73	1.28	6 (8%)	82,113,113	1.32	7 (8%)
27	BCR	t	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.36	8 (14%)
33	LMG	D	412	-	26,26,55	0.55	0	26,26,63	1.36	1 (3%)
25	CLA	C	501	-	69,73,73	1.41	8 (11%)	82,113,113	1.44	10 (12%)
31	STE	d	411	-	16,16,19	0.64	0	16,16,19	1.22	1 (6%)
31	STE	E	102	-	11,11,19	0.76	0	11,11,19	1.17	0
25	CLA	C	511	3	69,73,73	1.23	8 (11%)	82,113,113	1.28	6 (7%)
25	CLA	A	612	37	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
25	CLA	B	606	37	69,73,73	1.25	7 (10%)	82,113,113	1.41	10 (12%)
25	CLA	B	611	-	69,73,73	1.16	8 (11%)	82,113,113	1.50	11 (13%)
33	LMG	C	515	-	48,48,55	0.93	2 (4%)	56,56,63	1.32	6 (10%)
33	LMG	d	409	-	21,21,55	0.50	0	20,20,63	1.23	2 (10%)
27	BCR	A	610	-	41,41,41	0.94	2 (4%)	56,56,56	1.38	6 (10%)
34	BCT	D	401	23	3,3,3	1.07	0	2,3,3	3.18	1 (50%)
30	DGD	c	518	-	63,63,67	1.03	3 (4%)	77,77,81	1.39	10 (12%)
31	STE	I	101	-	14,14,19	0.43	0	13,13,19	0.65	0
29	SQD	b	619	-	47,49,54	1.62	8 (17%)	57,60,65	1.92	14 (24%)

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
28	PL9	a	611	-	-	28/53/73/73	0/1/1/1
30	DGD	C	516	-	-	24/51/91/95	0/2/2/2
25	CLA	C	508	-	1/1/15/20	6/39/115/115	-
33	LMG	b	622	-	-	18/50/70/70	0/1/1/1
27	BCR	T	101	-	-	11/29/63/63	0/2/2/2
27	BCR	k	101	-	-	7/29/63/63	0/2/2/2
32	LHG	D	410	-	-	17/51/51/53	-
25	CLA	B	615	-	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	502	-	1/1/15/20	8/39/115/115	-
35	HEM	F	101	6,5	-	3/14/54/54	-
31	STE	b	625	-	-	11/17/17/17	-
25	CLA	d	401	37	1/1/15/20	12/39/115/115	-
27	BCR	B	618	-	-	7/29/63/63	0/2/2/2
29	SQD	A	613	-	-	18/47/67/69	0/1/1/1
32	LHG	e	102	-	-	22/46/46/53	-
27	BCR	b	618	-	-	5/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	9/39/115/115	-
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
30	DGD	C	518	-	-	20/51/91/95	0/2/2/2
32	LHG	L	101	-	-	22/53/53/53	-
25	CLA	d	404	-	1/1/15/20	8/39/115/115	-
28	PL9	d	406	-	-	8/53/73/73	0/1/1/1
25	CLA	b	615	-	1/1/14/20	10/33/109/115	-
25	CLA	B	614	-	1/1/15/20	11/39/115/115	-
31	STE	M	104	-	-	8/12/12/17	-
25	CLA	d	403	-	1/1/15/20	12/39/115/115	-
25	CLA	B	603	-	1/1/15/20	11/39/115/115	-
25	CLA	a	612	37	1/1/15/20	14/39/115/115	-
32	LHG	d	407	-	-	19/53/53/53	-
25	CLA	b	602	-	1/1/15/20	6/39/115/115	-
25	CLA	C	512	-	1/1/15/20	12/39/115/115	-
31	STE	x	102	-	-	10/17/17/17	-
25	CLA	C	505	-	1/1/15/20	11/39/115/115	-
25	CLA	c	506	-	1/1/15/20	15/39/115/115	-
27	BCR	b	616	-	-	4/29/63/63	0/2/2/2
25	CLA	b	605	-	1/1/15/20	7/39/115/115	-
29	SQD	T	103	-	-	13/39/39/69	-
30	DGD	C	517	-	-	23/51/91/95	0/2/2/2
36	HEC	V	201	16	-	6/14/54/54	-
25	CLA	c	505	-	1/1/15/20	10/39/115/115	-
31	STE	B	624	-	-	4/9/9/17	-
25	CLA	B	610	-	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	c	524	-	-	26/44/64/70	0/1/1/1
31	STE	m	101	-	-	3/9/9/17	-
25	CLA	b	603	-	1/1/15/20	9/39/115/115	-
26	PHO	d	402	-	-	7/37/103/103	0/5/6/6
25	CLA	b	613	-	1/1/15/20	14/39/115/115	-
27	BCR	c	516	-	-	5/29/63/63	0/2/2/2
25	CLA	c	508	-	-	6/38/114/115	-
31	STE	b	624	-	-	11/13/13/17	-
31	STE	c	521	-	-	12/17/17/17	-
25	CLA	c	512	-	1/1/15/20	25/39/115/115	-
27	BCR	c	515	-	-	5/29/63/63	0/2/2/2
31	STE	B	622	-	-	6/9/9/17	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
31	STE	t	103	-	-	3/7/7/17	-
31	STE	M	103	-	-	3/7/7/17	-
25	CLA	b	609	37	1/1/15/20	7/39/115/115	-
25	CLA	c	504	37	1/1/14/20	10/33/109/115	-
28	PL9	A	611	-	-	29/53/73/73	0/1/1/1
30	DGD	c	517	-	-	28/51/91/95	0/2/2/2
33	LMG	M	101	-	-	28/46/66/70	0/1/1/1
25	CLA	C	504	37	1/1/13/20	8/32/108/115	-
25	CLA	b	608	-	1/1/15/20	3/39/115/115	-
26	PHO	A	608	-	-	4/37/103/103	0/5/6/6
31	STE	C	521	-	-	2/9/9/17	-
25	CLA	D	403	-	1/1/15/20	10/39/115/115	-
31	STE	a	616	-	-	2/9/9/17	-
31	STE	H	104	-	-	7/15/15/17	-
27	BCR	c	514	-	-	9/29/63/63	0/2/2/2
25	CLA	B	607	-	1/1/15/20	4/39/115/115	-
25	CLA	B	609	37	1/1/15/20	5/39/115/115	-
31	STE	t	102	-	-	6/11/11/17	-
33	LMG	d	410	-	-	11/39/59/70	0/1/1/1
25	CLA	C	507	37	1/1/15/20	10/39/115/115	-
32	LHG	D	409	-	-	26/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	H	103	-	-	17/51/91/95	0/2/2/2
36	HEC	v	201	16	-	6/14/54/54	-
32	LHG	d	408	-	-	15/43/43/53	-
25	CLA	B	608	-	-	5/39/115/115	-
25	CLA	h	101	37	1/1/15/20	19/39/115/115	-
31	STE	b	626	-	-	5/7/7/17	-
25	CLA	b	601	-	1/1/15/20	11/39/115/115	-
27	BCR	b	617	-	-	4/29/63/63	0/2/2/2
25	CLA	B	605	-	1/1/15/20	16/39/115/115	-
31	STE	j	101	-	-	3/9/9/17	-
25	CLA	b	612	-	1/1/15/20	11/39/115/115	-
26	PHO	a	608	-	-	5/37/103/103	0/5/6/6
25	CLA	b	604	-	1/1/15/20	9/39/115/115	-
31	STE	M	102	-	-	7/12/12/17	-
25	CLA	c	511	3	1/1/15/20	9/39/115/115	-
33	LMG	D	411	-	-	15/33/33/70	-
31	STE	B	625	-	-	8/13/13/17	-
29	SQD	a	613	-	-	25/49/69/69	0/1/1/1
31	STE	J	101	-	-	6/9/9/17	-
27	BCR	x	101	-	-	8/29/63/63	0/2/2/2
33	LMG	C	519	-	-	23/43/63/70	0/1/1/1
25	CLA	H	101	37	1/1/15/20	20/39/115/115	-
25	CLA	A	606	-	1/1/15/20	9/39/115/115	-
31	STE	C	522	-	-	3/13/13/17	-
27	BCR	K	101	-	-	9/29/63/63	0/2/2/2
33	LMG	c	522	-	-	23/43/63/70	0/1/1/1
25	CLA	B	612	-	1/1/15/20	19/39/115/115	-
25	CLA	C	506	-	1/1/15/20	13/39/115/115	-
25	CLA	C	510	-	1/1/15/20	12/39/115/115	-
27	BCR	d	405	-	-	10/29/63/63	0/2/2/2
32	LHG	E	101	-	-	24/53/53/53	-
31	STE	l	102	-	-	10/15/15/17	-
25	CLA	b	611	-	1/1/15/20	8/39/115/115	-
25	CLA	B	601	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	513	-	1/1/15/20	7/39/115/115	-
31	STE	c	523	-	-	3/9/9/17	-
25	CLA	c	510	-	1/1/15/20	9/39/115/115	-
27	BCR	Z	101	-	-	11/29/63/63	0/2/2/2
25	CLA	c	501	-	1/1/15/20	3/39/115/115	-
29	SQD	f	101	-	-	16/36/56/69	0/1/1/1
25	CLA	b	610	-	1/1/15/20	5/39/115/115	-
25	CLA	b	607	-	1/1/15/20	7/39/115/115	-
30	DGD	A	614	-	-	26/55/95/95	0/2/2/2
33	LMG	b	620	-	-	16/46/66/70	0/1/1/1
25	CLA	C	503	-	1/1/15/20	6/39/115/115	-
27	BCR	B	617	-	-	5/29/63/63	0/2/2/2
29	SQD	a	614	-	-	14/37/37/69	-
30	DGD	c	519	-	-	17/51/91/95	0/2/2/2
25	CLA	B	604	-	1/1/15/20	12/39/115/115	-
31	STE	B	623	-	-	10/15/15/17	-
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
31	STE	T	102	-	-	8/13/13/17	-
30	DGD	a	615	-	-	24/45/45/95	-
33	LMG	c	520	-	-	22/31/51/70	0/1/1/1
27	BCR	a	610	-	-	3/29/63/63	0/2/2/2
29	SQD	B	621	-	-	30/49/69/69	0/1/1/1
31	STE	D	413	-	-	9/17/17/17	-
35	HEM	e	101	6,5	-	2/14/54/54	-
25	CLA	c	507	37	1/1/15/20	9/39/115/115	-
25	CLA	c	502	-	1/1/15/20	5/39/115/115	-
30	DGD	h	102	-	-	17/51/91/95	0/2/2/2
25	CLA	D	404	-	-	6/39/115/115	-
27	BCR	B	616	-	-	4/29/63/63	0/2/2/2
27	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
32	LHG	b	623	-	-	22/53/53/53	-
32	LHG	B	620	-	-	14/53/53/53	-
25	CLA	b	614	-	1/1/15/20	9/39/115/115	-
33	LMG	D	407	-	-	16/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	b	621	-	-	10/17/17/17	-
25	CLA	A	607	37	1/1/15/20	9/39/115/115	-
25	CLA	A	609	-	1/1/12/20	3/26/102/115	-
25	CLA	B	602	-	1/1/15/20	12/39/115/115	-
28	PL9	D	406	-	-	8/53/73/73	0/1/1/1
31	STE	B	619	-	-	6/14/14/17	-
25	CLA	a	607	-	1/1/15/20	6/39/115/115	-
25	CLA	a	609	-	1/1/15/20	9/39/115/115	-
25	CLA	c	503	-	-	14/39/115/115	-
25	CLA	C	509	-	1/1/15/20	14/39/115/115	-
27	BCR	H	102	-	-	3/29/63/63	0/2/2/2
31	STE	C	520	-	-	5/9/9/17	-
27	BCR	C	514	-	-	7/29/63/63	0/2/2/2
25	CLA	b	606	37	1/1/15/20	18/39/115/115	-
32	LHG	l	101	-	-	19/53/53/53	-
25	CLA	B	613	-	1/1/15/20	10/39/115/115	-
25	CLA	C	513	-	1/1/15/20	14/39/115/115	-
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
33	LMG	D	412	-	-	15/22/22/70	-
25	CLA	C	501	-	1/1/15/20	6/39/115/115	-
31	STE	d	411	-	-	11/14/14/17	-
31	STE	E	102	-	-	5/9/9/17	-
25	CLA	C	511	3	1/1/15/20	3/39/115/115	-
25	CLA	A	612	37	1/1/15/20	9/39/115/115	-
25	CLA	B	606	37	1/1/15/20	11/39/115/115	-
25	CLA	B	611	-	1/1/15/20	9/39/115/115	-
33	LMG	C	515	-	-	26/43/63/70	0/1/1/1
33	LMG	d	409	-	-	10/17/17/70	-
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
30	DGD	c	518	-	-	15/51/91/95	0/2/2/2
31	STE	I	101	-	-	6/12/12/17	-
29	SQD	b	619	-	-	21/44/64/69	0/1/1/1

All (795) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	608	PHO	C1B-C2B	10.33	1.50	1.39
26	D	402	PHO	C1B-C2B	9.19	1.49	1.39
26	d	402	PHO	C1B-C2B	9.02	1.49	1.39
26	d	402	PHO	C3B-C4B	8.75	1.50	1.41
26	D	402	PHO	C3B-C4B	8.58	1.50	1.41
26	A	608	PHO	C1B-C2B	8.44	1.48	1.39
25	b	605	CLA	MG-NA	8.32	2.26	2.06
26	A	608	PHO	C3B-C4B	7.80	1.49	1.41
26	a	608	PHO	C3B-C4B	7.08	1.48	1.41
25	C	502	CLA	MG-NA	6.75	2.22	2.06
36	V	201	HEC	CAC-C3C	6.47	1.56	1.35
25	B	605	CLA	MG-NA	6.35	2.21	2.06
36	v	201	HEC	CAC-C3C	6.20	1.55	1.35
25	b	614	CLA	MG-NA	6.16	2.20	2.06
25	c	511	CLA	MG-NA	6.16	2.20	2.06
36	v	201	HEC	CAB-C3B	6.14	1.55	1.35
25	B	612	CLA	MG-ND	-6.05	1.93	2.05
25	C	501	CLA	MG-NA	6.05	2.20	2.06
25	C	506	CLA	MG-ND	-6.02	1.93	2.05
25	C	508	CLA	MG-NA	6.02	2.20	2.06
36	V	201	HEC	CAB-C3B	5.82	1.53	1.35
25	B	603	CLA	MG-NC	5.68	2.19	2.06
25	C	505	CLA	MG-NA	5.51	2.19	2.06
29	T	103	SQD	O47-C45	-5.48	1.37	1.47
25	D	403	CLA	MG-NA	5.45	2.19	2.06
25	b	609	CLA	MG-NB	-5.43	1.95	2.05
25	c	508	CLA	MG-NC	5.41	2.19	2.06
36	v	201	HEC	C3D-C2D	5.34	1.52	1.38
36	V	201	HEC	C3D-C2D	5.34	1.52	1.38
25	C	512	CLA	MG-NA	5.23	2.18	2.06
25	b	602	CLA	MG-NA	5.12	2.18	2.06
25	b	612	CLA	MG-NA	5.07	2.18	2.06
25	h	101	CLA	MG-NA	5.02	2.18	2.06
29	b	619	SQD	O48-C23	5.00	1.47	1.33
25	B	604	CLA	MG-NA	4.93	2.18	2.06
29	B	621	SQD	O48-C23	4.92	1.47	1.33
25	C	509	CLA	MG-NA	4.87	2.17	2.06
29	a	613	SQD	O48-C23	4.87	1.47	1.33
25	B	613	CLA	MG-ND	-4.80	1.96	2.05
29	T	103	SQD	O48-C23	4.76	1.47	1.33
29	D	408	SQD	O48-C23	4.73	1.47	1.33
25	c	506	CLA	MG-ND	-4.72	1.96	2.05
29	A	613	SQD	O48-C23	4.71	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	MG-NA	4.71	2.17	2.06
29	a	614	SQD	O48-C23	4.65	1.46	1.33
25	b	614	CLA	MG-NB	4.64	2.15	2.05
26	a	608	PHO	C1D-C2D	4.62	1.44	1.39
26	d	402	PHO	C1D-C2D	4.61	1.44	1.39
25	c	503	CLA	MG-NB	4.60	2.14	2.05
25	b	607	CLA	MG-NA	4.60	2.17	2.06
29	f	101	SQD	O48-C23	4.59	1.46	1.33
25	B	612	CLA	C1D-ND	4.50	1.43	1.37
25	c	507	CLA	MG-NA	4.42	2.16	2.06
25	a	612	CLA	MG-NA	4.40	2.16	2.06
25	c	512	CLA	MG-NB	4.35	2.14	2.05
28	d	406	PL9	C3-C4	-4.32	1.42	1.49
25	B	612	CLA	MG-NA	4.29	2.16	2.06
25	d	403	CLA	C1D-ND	4.23	1.43	1.37
25	H	101	CLA	MG-NA	4.22	2.16	2.06
27	b	617	BCR	C30-C25	-4.22	1.48	1.53
25	C	512	CLA	MG-NB	4.21	2.14	2.05
25	B	610	CLA	MG-ND	4.18	2.14	2.05
29	a	614	SQD	O47-C7	4.13	1.45	1.34
25	b	609	CLA	MG-NA	4.12	2.16	2.06
25	c	505	CLA	MG-NA	4.11	2.16	2.06
25	C	501	CLA	C1D-ND	4.09	1.43	1.37
25	B	606	CLA	MG-ND	-4.02	1.97	2.05
25	b	609	CLA	C1D-ND	4.02	1.43	1.37
25	C	510	CLA	MG-NA	3.99	2.15	2.06
25	c	510	CLA	MG-NA	3.98	2.15	2.06
25	c	505	CLA	MG-NB	-3.97	1.97	2.05
25	b	607	CLA	MG-ND	-3.93	1.98	2.05
25	C	504	CLA	MG-NA	3.92	2.15	2.06
25	a	612	CLA	C1D-ND	3.90	1.43	1.37
25	c	507	CLA	C1D-ND	3.89	1.43	1.37
35	e	101	HEM	FE-NB	3.86	2.06	1.94
25	D	404	CLA	C1D-ND	3.85	1.42	1.37
25	B	606	CLA	C1D-ND	3.84	1.42	1.37
25	B	602	CLA	MG-NA	3.83	2.15	2.06
25	B	607	CLA	C4B-NB	3.83	1.42	1.37
25	a	607	CLA	MG-NC	3.83	2.15	2.06
25	c	508	CLA	C1D-ND	3.82	1.42	1.37
27	C	514	BCR	C1-C6	-3.82	1.48	1.53
25	b	604	CLA	C1D-ND	3.79	1.42	1.37
25	b	601	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	C1D-ND	3.78	1.42	1.37
25	b	615	CLA	C1D-ND	3.76	1.42	1.37
25	b	610	CLA	MG-NA	3.74	2.15	2.06
27	B	616	BCR	C1-C6	-3.73	1.49	1.53
25	C	512	CLA	MG-ND	-3.73	1.98	2.05
25	b	612	CLA	C1D-ND	3.71	1.42	1.37
26	A	608	PHO	C1D-C2D	3.71	1.43	1.39
25	C	502	CLA	MG-NB	-3.69	1.98	2.05
25	b	607	CLA	C1D-ND	3.68	1.42	1.37
25	a	607	CLA	C1D-ND	3.67	1.42	1.37
25	C	505	CLA	MG-ND	-3.67	1.98	2.05
25	B	614	CLA	MG-NA	3.65	2.14	2.06
25	c	512	CLA	C1D-ND	3.64	1.42	1.37
25	c	502	CLA	MG-NB	-3.64	1.98	2.05
25	b	613	CLA	C4B-NB	3.63	1.42	1.37
29	A	613	SQD	O47-C7	3.62	1.44	1.34
25	C	502	CLA	C1D-ND	3.62	1.42	1.37
29	B	621	SQD	O47-C7	3.62	1.44	1.34
27	c	515	BCR	C1-C6	-3.61	1.49	1.53
25	C	506	CLA	C1D-ND	3.61	1.42	1.37
25	B	614	CLA	C4B-NB	3.60	1.42	1.37
25	B	604	CLA	C1D-ND	3.60	1.42	1.37
25	B	608	CLA	C1D-ND	3.59	1.42	1.37
25	C	504	CLA	C4B-NB	3.59	1.42	1.37
25	B	615	CLA	C1D-ND	3.57	1.42	1.37
25	c	511	CLA	C1D-ND	3.56	1.42	1.37
25	b	604	CLA	C4B-NB	3.56	1.42	1.37
25	B	611	CLA	MG-NA	3.56	2.14	2.06
25	a	609	CLA	C1D-ND	3.55	1.42	1.37
25	C	505	CLA	C4B-NB	3.55	1.42	1.37
25	b	608	CLA	MG-NC	3.54	2.14	2.06
25	a	609	CLA	MG-ND	-3.54	1.98	2.05
25	C	506	CLA	MG-NA	3.54	2.14	2.06
35	F	101	HEM	FE-NA	3.52	2.06	1.95
25	c	506	CLA	C1D-ND	3.52	1.42	1.37
30	a	615	DGD	O1G-C1A	3.52	1.43	1.33
25	c	503	CLA	MG-NC	3.51	2.14	2.06
25	d	401	CLA	C4B-NB	3.50	1.42	1.37
29	a	613	SQD	O47-C45	-3.50	1.38	1.46
25	b	611	CLA	C1D-ND	3.49	1.42	1.37
25	d	404	CLA	C4B-NB	3.49	1.42	1.37
25	c	506	CLA	MG-NA	3.49	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	MG-NB	-3.49	1.98	2.05
25	A	607	CLA	C4B-NB	3.48	1.42	1.37
27	k	101	BCR	C1-C6	-3.47	1.49	1.53
29	f	101	SQD	O47-C7	3.47	1.44	1.34
25	c	510	CLA	C1D-ND	3.47	1.42	1.37
25	c	512	CLA	MG-ND	-3.47	1.98	2.05
25	b	608	CLA	C1D-ND	3.46	1.42	1.37
25	C	505	CLA	C1D-ND	3.46	1.42	1.37
25	c	501	CLA	C1D-ND	3.45	1.42	1.37
29	f	101	SQD	O47-C45	-3.45	1.38	1.46
26	D	402	PHO	C1D-C2D	3.45	1.43	1.39
25	b	606	CLA	C4B-NB	3.44	1.42	1.37
25	H	101	CLA	C1D-ND	3.44	1.42	1.37
25	C	508	CLA	C1D-ND	3.44	1.42	1.37
29	B	621	SQD	O47-C45	-3.43	1.38	1.46
28	d	406	PL9	C6-C1	-3.43	1.42	1.48
25	B	615	CLA	MG-NA	3.43	2.14	2.06
25	D	404	CLA	MG-NA	3.42	2.14	2.06
25	B	613	CLA	C4B-NB	3.42	1.42	1.37
25	c	513	CLA	C1D-ND	3.42	1.42	1.37
27	K	101	BCR	C30-C25	-3.42	1.49	1.53
26	A	608	PHO	C4D-CHA	3.42	1.44	1.39
25	C	503	CLA	C4B-NB	3.41	1.42	1.37
25	c	509	CLA	C1D-ND	3.41	1.42	1.37
25	c	503	CLA	C1D-ND	3.41	1.42	1.37
25	A	609	CLA	C1D-ND	3.40	1.42	1.37
32	B	620	LHG	O7-C5	-3.40	1.38	1.46
29	T	103	SQD	O47-C7	3.40	1.43	1.34
29	a	614	SQD	C24-C23	3.39	1.60	1.50
32	D	410	LHG	P-O6	3.39	1.72	1.59
26	a	608	PHO	C4D-CHA	3.39	1.44	1.39
25	H	101	CLA	C4B-NB	3.39	1.42	1.37
29	f	101	SQD	C24-C23	3.38	1.60	1.50
29	b	619	SQD	O47-C7	3.38	1.43	1.34
29	a	613	SQD	O47-C7	3.36	1.43	1.34
25	b	602	CLA	C1D-ND	3.35	1.42	1.37
25	a	609	CLA	C4B-NB	3.35	1.42	1.37
27	c	514	BCR	C1-C6	-3.35	1.49	1.53
25	C	512	CLA	C1D-ND	3.33	1.42	1.37
25	c	508	CLA	C4B-NB	3.33	1.42	1.37
27	Z	101	BCR	C30-C25	-3.33	1.49	1.53
30	H	103	DGD	C4D-C5D	3.32	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	C4B-NB	3.32	1.42	1.37
25	b	603	CLA	MG-NA	3.31	2.14	2.06
25	d	401	CLA	C1D-ND	3.31	1.42	1.37
27	Y	101	BCR	C30-C25	-3.31	1.49	1.53
27	Y	101	BCR	C1-C6	-3.31	1.49	1.53
27	d	405	BCR	C1-C6	-3.30	1.49	1.53
25	h	101	CLA	C1D-ND	3.29	1.42	1.37
25	C	504	CLA	C1D-ND	3.29	1.42	1.37
25	B	610	CLA	MG-NA	3.28	2.14	2.06
25	B	603	CLA	C1D-ND	3.28	1.42	1.37
29	D	408	SQD	C24-C23	3.28	1.60	1.50
25	b	610	CLA	C1B-C2B	3.28	1.50	1.43
25	C	507	CLA	MG-NB	-3.27	1.99	2.05
25	a	612	CLA	C1B-C2B	3.27	1.50	1.43
25	C	509	CLA	C1D-ND	3.27	1.42	1.37
27	Z	101	BCR	C1-C6	-3.27	1.49	1.53
25	b	611	CLA	MG-ND	-3.27	1.99	2.05
25	C	503	CLA	C1D-ND	3.27	1.42	1.37
25	C	503	CLA	MG-ND	3.26	2.12	2.05
25	B	601	CLA	C1D-ND	3.25	1.42	1.37
25	b	606	CLA	C1D-ND	3.25	1.42	1.37
25	B	614	CLA	C1B-C2B	3.24	1.50	1.43
29	A	613	SQD	O47-C45	-3.22	1.39	1.46
26	D	402	PHO	C4D-CHA	3.22	1.44	1.39
25	D	403	CLA	C1D-ND	3.22	1.42	1.37
33	b	620	LMG	O1-C7	-3.22	1.38	1.43
25	b	605	CLA	C1D-ND	3.22	1.42	1.37
25	c	512	CLA	C1B-C2B	3.22	1.50	1.43
25	a	607	CLA	C1B-C2B	3.21	1.50	1.43
25	B	607	CLA	MG-ND	-3.21	1.99	2.05
29	b	619	SQD	O47-C45	-3.21	1.39	1.46
29	A	613	SQD	C24-C23	3.21	1.60	1.50
25	B	615	CLA	C1B-C2B	3.20	1.50	1.43
27	D	405	BCR	C30-C25	-3.20	1.49	1.53
25	B	604	CLA	C1B-C2B	3.19	1.50	1.43
25	C	511	CLA	C1D-ND	3.19	1.42	1.37
25	C	511	CLA	MG-NA	3.18	2.13	2.06
25	b	613	CLA	C1D-ND	3.18	1.42	1.37
27	B	616	BCR	C30-C25	-3.18	1.49	1.53
27	d	405	BCR	C30-C25	-3.18	1.49	1.53
25	b	610	CLA	C1D-ND	3.17	1.42	1.37
30	C	516	DGD	O2G-C2G	-3.17	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	C4B-NB	3.16	1.42	1.37
25	B	615	CLA	MG-NB	-3.16	1.99	2.05
25	a	609	CLA	C1B-C2B	3.15	1.50	1.43
25	B	607	CLA	C1D-ND	3.14	1.42	1.37
25	A	607	CLA	C1D-ND	3.14	1.42	1.37
29	a	614	SQD	O47-C45	-3.14	1.39	1.46
25	C	511	CLA	C1B-C2B	3.14	1.50	1.43
25	b	604	CLA	C1B-C2B	3.13	1.50	1.43
35	e	101	HEM	CAC-C3C	3.13	1.55	1.47
35	F	101	HEM	FE-NC	3.13	2.05	1.95
26	D	402	PHO	CMC-C2C	-3.12	1.45	1.50
25	C	507	CLA	MG-NC	3.12	2.13	2.06
25	C	501	CLA	C4B-NB	3.12	1.42	1.37
25	A	607	CLA	CHC-C1C	3.12	1.44	1.38
29	T	103	SQD	C24-C23	3.12	1.59	1.50
25	d	401	CLA	CHC-C1C	3.11	1.44	1.38
25	c	504	CLA	C4B-NB	3.11	1.41	1.37
27	D	405	BCR	C1-C6	-3.10	1.49	1.53
25	d	404	CLA	C1D-ND	3.10	1.41	1.37
26	A	608	PHO	CMC-C2C	-3.10	1.45	1.50
29	a	613	SQD	C24-C23	3.09	1.59	1.50
25	B	601	CLA	C1B-C2B	3.08	1.50	1.43
25	A	612	CLA	C1D-ND	3.08	1.41	1.37
25	B	614	CLA	C1D-ND	3.08	1.41	1.37
25	c	509	CLA	C1B-C2B	3.08	1.50	1.43
25	b	608	CLA	C4B-NB	3.08	1.41	1.37
25	C	503	CLA	MG-NA	3.07	2.13	2.06
25	B	602	CLA	MG-ND	3.07	2.11	2.05
25	C	511	CLA	C4B-NB	3.07	1.41	1.37
25	c	512	CLA	C4B-NB	3.07	1.41	1.37
25	b	614	CLA	C1D-ND	3.06	1.41	1.37
27	c	516	BCR	C30-C25	-3.06	1.49	1.53
25	c	513	CLA	C4B-NB	3.06	1.41	1.37
25	b	607	CLA	C4B-NB	3.06	1.41	1.37
25	b	612	CLA	C4B-NB	3.06	1.41	1.37
35	e	101	HEM	FE-NA	3.06	2.05	1.95
25	C	503	CLA	C1B-C2B	3.06	1.50	1.43
25	b	606	CLA	MG-NA	3.05	2.13	2.06
27	H	102	BCR	C30-C25	-3.04	1.49	1.53
25	B	602	CLA	C1D-ND	3.04	1.41	1.37
25	b	607	CLA	CHC-C1C	3.03	1.44	1.38
29	b	619	SQD	O5-C1	3.03	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	C4B-NB	3.03	1.41	1.37
27	K	101	BCR	C1-C6	-3.03	1.49	1.53
26	d	402	PHO	CMC-C2C	-3.03	1.45	1.50
25	B	610	CLA	C1D-ND	3.02	1.41	1.37
25	c	504	CLA	C1D-ND	3.02	1.41	1.37
25	b	615	CLA	C4B-NB	3.01	1.41	1.37
25	C	513	CLA	C1B-C2B	3.01	1.50	1.43
25	H	101	CLA	C1B-C2B	3.01	1.50	1.43
25	c	513	CLA	MG-NA	3.01	2.13	2.06
30	A	614	DGD	C4D-C5D	3.00	1.59	1.53
35	F	101	HEM	CAB-C3B	3.00	1.55	1.47
25	C	507	CLA	C1B-C2B	2.99	1.50	1.43
26	d	402	PHO	C4D-CHA	2.99	1.44	1.39
25	A	609	CLA	C4B-NB	2.98	1.41	1.37
25	C	505	CLA	C1B-C2B	2.98	1.50	1.43
25	C	510	CLA	CHC-C1C	2.98	1.44	1.38
29	B	621	SQD	C24-C23	2.97	1.59	1.50
25	b	601	CLA	C1B-C2B	2.97	1.50	1.43
25	b	604	CLA	C3B-C4B	2.97	1.51	1.42
25	h	101	CLA	C4B-NB	2.97	1.41	1.37
25	B	608	CLA	C1B-C2B	2.97	1.50	1.43
25	A	606	CLA	C1B-C2B	2.97	1.50	1.43
25	B	607	CLA	MG-NB	-2.96	1.99	2.05
27	c	516	BCR	C1-C6	-2.96	1.50	1.53
25	c	507	CLA	C1B-C2B	2.96	1.50	1.43
25	c	507	CLA	C4B-NB	2.96	1.41	1.37
25	c	513	CLA	CHC-C1C	2.96	1.44	1.38
27	b	618	BCR	C1-C6	-2.96	1.50	1.53
25	B	607	CLA	MG-NA	2.95	2.13	2.06
25	d	403	CLA	MG-NB	-2.95	1.99	2.05
25	b	604	CLA	MG-NB	2.95	2.11	2.05
25	c	506	CLA	C4B-NB	2.94	1.41	1.37
25	B	612	CLA	C1B-C2B	2.94	1.50	1.43
27	T	101	BCR	C1-C6	-2.94	1.50	1.53
27	b	617	BCR	C1-C6	-2.94	1.50	1.53
27	k	101	BCR	C30-C25	-2.94	1.50	1.53
25	B	605	CLA	C1D-ND	2.94	1.41	1.37
25	B	611	CLA	C4B-NB	2.93	1.41	1.37
25	c	508	CLA	MG-ND	2.92	2.11	2.05
29	f	101	SQD	O5-C1	2.92	1.49	1.41
25	D	404	CLA	MG-NB	-2.91	2.00	2.05
25	C	507	CLA	C1D-ND	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	C4B-NB	2.91	1.41	1.37
25	B	609	CLA	C4B-NB	2.90	1.41	1.37
25	C	506	CLA	C1B-C2B	2.90	1.49	1.43
25	C	505	CLA	CHC-C1C	2.90	1.44	1.38
25	B	611	CLA	C1D-ND	2.90	1.41	1.37
25	B	609	CLA	C3B-C4B	2.90	1.51	1.42
27	b	616	BCR	C30-C25	-2.89	1.50	1.53
25	c	511	CLA	C1B-C2B	2.89	1.49	1.43
25	B	613	CLA	MG-NB	2.89	2.11	2.05
27	A	610	BCR	C1-C6	-2.88	1.50	1.53
25	C	504	CLA	C3B-C4B	2.88	1.51	1.42
25	C	504	CLA	CHC-C1C	2.87	1.44	1.38
25	c	502	CLA	C1D-ND	2.87	1.41	1.37
29	A	613	SQD	O5-C1	2.86	1.49	1.41
30	A	614	DGD	O5D-C1E	2.86	1.45	1.40
25	b	613	CLA	C1B-C2B	2.86	1.49	1.43
25	b	602	CLA	C4B-NB	2.86	1.41	1.37
25	c	513	CLA	C3B-C4B	2.86	1.51	1.42
25	c	501	CLA	C1B-C2B	2.86	1.49	1.43
25	C	502	CLA	C4B-NB	2.85	1.41	1.37
35	e	101	HEM	FE-NC	2.85	2.04	1.95
27	b	616	BCR	C1-C6	-2.84	1.50	1.53
25	b	615	CLA	C1B-C2B	2.84	1.49	1.43
25	c	505	CLA	C4B-NB	2.84	1.41	1.37
25	C	509	CLA	C4B-NB	2.84	1.41	1.37
25	C	508	CLA	C4B-NB	2.84	1.41	1.37
35	F	101	HEM	CAC-C3C	2.83	1.54	1.47
25	A	606	CLA	C1D-ND	2.83	1.41	1.37
25	b	603	CLA	C1B-C2B	2.83	1.49	1.43
33	b	620	LMG	O7-C8	-2.83	1.39	1.46
25	d	401	CLA	C1B-C2B	2.82	1.49	1.43
25	C	501	CLA	CHC-C1C	2.82	1.44	1.38
29	D	408	SQD	O5-C1	2.82	1.49	1.41
28	D	406	PL9	C6-C1	-2.82	1.43	1.48
25	C	507	CLA	MG-NA	2.81	2.12	2.06
25	A	609	CLA	C1B-C2B	2.80	1.49	1.43
25	D	403	CLA	C1B-C2B	2.80	1.49	1.43
29	b	619	SQD	C24-C23	2.80	1.58	1.50
25	c	505	CLA	C1B-C2B	2.79	1.49	1.43
27	B	617	BCR	C30-C25	-2.79	1.50	1.53
25	B	611	CLA	CHC-C1C	2.78	1.44	1.38
25	c	501	CLA	C4B-NB	2.78	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	502	CLA	C4B-NB	2.78	1.41	1.37
25	b	609	CLA	C1B-C2B	2.78	1.49	1.43
25	C	508	CLA	C1B-C2B	2.77	1.49	1.43
29	B	621	SQD	O5-C1	2.77	1.49	1.41
25	h	101	CLA	C1B-C2B	2.77	1.49	1.43
25	b	607	CLA	C3B-C4B	2.77	1.50	1.42
27	x	101	BCR	C30-C25	-2.76	1.50	1.53
25	c	510	CLA	C1B-C2B	2.76	1.49	1.43
25	c	501	CLA	CHC-C1C	2.76	1.44	1.38
25	b	602	CLA	CMD-C2D	-2.75	1.45	1.50
25	c	501	CLA	MG-NC	2.75	2.12	2.06
25	C	503	CLA	MG-NC	2.75	2.12	2.06
25	B	610	CLA	CHC-C1C	2.75	1.44	1.38
26	A	608	PHO	C3D-C4D	2.74	1.45	1.41
25	a	607	CLA	C4B-NB	2.74	1.41	1.37
27	c	514	BCR	C30-C25	-2.74	1.50	1.53
30	C	516	DGD	C3D-C2D	2.73	1.59	1.52
25	B	605	CLA	C4B-NB	2.73	1.41	1.37
27	t	101	BCR	C30-C25	-2.73	1.50	1.53
30	A	614	DGD	C4E-C5E	2.72	1.58	1.53
25	C	511	CLA	C3B-C4B	2.72	1.50	1.42
28	D	406	PL9	C52-C5	-2.71	1.45	1.50
25	B	605	CLA	CHC-C1C	2.71	1.43	1.38
30	c	518	DGD	C4D-C3D	2.71	1.59	1.52
28	A	611	PL9	C7-C3	-2.71	1.47	1.51
25	b	613	CLA	C3B-C4B	2.71	1.50	1.42
28	D	406	PL9	C3-C4	-2.71	1.45	1.49
25	B	609	CLA	C1D-ND	2.71	1.41	1.37
25	c	505	CLA	C3B-C4B	2.70	1.50	1.42
25	c	506	CLA	CHC-C1C	2.70	1.43	1.38
25	B	609	CLA	CHC-C1C	2.70	1.43	1.38
25	C	503	CLA	CHC-C1C	2.70	1.43	1.38
25	d	403	CLA	C1B-C2B	2.69	1.49	1.43
30	C	517	DGD	O2G-C2G	-2.69	1.40	1.46
25	B	613	CLA	C1B-C2B	2.69	1.49	1.43
25	b	601	CLA	MG-ND	-2.69	2.00	2.05
25	B	605	CLA	MG-NB	2.69	2.11	2.05
30	A	614	DGD	C6E-C5E	2.68	1.60	1.51
27	B	618	BCR	C1-C6	-2.68	1.50	1.53
25	A	607	CLA	C3B-C4B	2.67	1.50	1.42
25	c	505	CLA	C1D-ND	2.67	1.41	1.37
25	b	614	CLA	C3B-C4B	2.67	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	601	CLA	C4B-NB	2.67	1.41	1.37
32	e	102	LHG	P-O6	2.67	1.69	1.59
25	b	607	CLA	MG-NB	2.67	2.11	2.05
25	B	608	CLA	C4B-NB	2.66	1.41	1.37
26	D	402	PHO	CMD-C2D	-2.66	1.46	1.51
25	D	404	CLA	C1B-C2B	2.66	1.49	1.43
25	C	508	CLA	C3B-C4B	2.66	1.50	1.42
25	A	612	CLA	C4B-NB	2.65	1.41	1.37
25	B	602	CLA	C4B-NB	2.65	1.41	1.37
25	C	510	CLA	C1D-ND	2.65	1.41	1.37
25	b	602	CLA	C1B-C2B	2.65	1.49	1.43
25	C	501	CLA	C3B-C4B	2.64	1.50	1.42
25	B	613	CLA	MG-NC	2.64	2.12	2.06
29	a	613	SQD	O5-C1	2.64	1.48	1.41
35	F	101	HEM	FE-ND	2.64	2.03	1.94
25	c	508	CLA	CHC-C1C	2.64	1.43	1.38
25	D	403	CLA	C4B-NB	2.64	1.41	1.37
32	E	101	LHG	P-O6	2.63	1.69	1.59
30	h	102	DGD	O1G-C1G	-2.63	1.39	1.45
25	c	503	CLA	CHC-C1C	2.63	1.43	1.38
30	C	516	DGD	C4E-C3E	2.62	1.59	1.52
25	c	511	CLA	CHC-C1C	2.62	1.43	1.38
25	A	607	CLA	C1B-C2B	2.62	1.49	1.43
27	a	610	BCR	C1-C6	-2.62	1.50	1.53
30	C	517	DGD	O1G-C1G	-2.62	1.39	1.45
25	b	603	CLA	C1D-ND	2.62	1.41	1.37
25	A	612	CLA	MG-NA	2.62	2.12	2.06
25	C	502	CLA	C1B-C2B	2.61	1.49	1.43
25	C	509	CLA	C1B-C2B	2.61	1.49	1.43
25	B	610	CLA	C3B-C4B	2.61	1.50	1.42
25	c	509	CLA	C4B-NB	2.61	1.41	1.37
27	a	610	BCR	C30-C25	-2.61	1.50	1.53
33	C	515	LMG	C4-C3	2.61	1.59	1.52
25	d	404	CLA	C1B-C2B	2.61	1.49	1.43
25	c	511	CLA	C4B-NB	2.61	1.41	1.37
25	b	604	CLA	MG-NA	2.60	2.12	2.06
26	D	402	PHO	C4D-ND	-2.59	1.34	1.38
28	d	406	PL9	C31-C29	-2.59	1.45	1.51
25	b	606	CLA	CHC-C1C	2.59	1.43	1.38
25	C	512	CLA	C4B-NB	2.59	1.41	1.37
26	D	402	PHO	CMB-C2B	-2.59	1.46	1.51
25	c	503	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	C4B-NB	2.59	1.41	1.37
25	B	607	CLA	C1B-C2B	2.59	1.49	1.43
25	C	513	CLA	C4B-NB	2.59	1.41	1.37
25	c	510	CLA	C4B-NB	2.59	1.41	1.37
25	B	605	CLA	C1B-C2B	2.59	1.49	1.43
25	C	512	CLA	CHC-C1C	2.58	1.43	1.38
26	a	608	PHO	C3D-C4D	2.58	1.44	1.41
25	c	508	CLA	C3B-C4B	2.58	1.50	1.42
27	b	618	BCR	C30-C25	-2.58	1.50	1.53
25	D	404	CLA	MG-ND	-2.57	2.00	2.05
30	c	517	DGD	O2G-C2G	-2.57	1.40	1.46
25	b	604	CLA	CHC-C1C	2.57	1.43	1.38
25	B	609	CLA	CMB-C2B	-2.57	1.45	1.50
25	c	512	CLA	C3B-C4B	2.57	1.50	1.42
25	c	506	CLA	C1B-C2B	2.56	1.49	1.43
25	B	602	CLA	CMD-C2D	-2.56	1.45	1.50
25	b	607	CLA	C1B-C2B	2.55	1.49	1.43
25	b	614	CLA	CMD-C2D	-2.55	1.45	1.50
25	c	513	CLA	C1B-C2B	2.55	1.49	1.43
25	B	604	CLA	C4B-NB	2.55	1.41	1.37
25	b	609	CLA	C4B-NB	2.55	1.41	1.37
25	c	504	CLA	C1B-C2B	2.55	1.49	1.43
25	c	508	CLA	C1B-C2B	2.55	1.49	1.43
30	C	518	DGD	O3G-C3G	-2.55	1.39	1.43
27	B	617	BCR	C1-C6	-2.55	1.50	1.53
25	A	612	CLA	C1B-C2B	2.55	1.49	1.43
25	A	606	CLA	C3B-C4B	2.55	1.50	1.42
25	C	501	CLA	C1B-C2B	2.54	1.49	1.43
33	b	620	LMG	C4-C3	2.54	1.58	1.52
25	c	512	CLA	CHC-C1C	2.54	1.43	1.38
25	h	101	CLA	CHC-C1C	2.54	1.43	1.38
25	d	403	CLA	MG-NA	2.54	2.12	2.06
25	b	606	CLA	C1B-C2B	2.53	1.49	1.43
25	H	101	CLA	MG-NB	-2.53	2.00	2.05
27	C	514	BCR	C30-C25	-2.53	1.50	1.53
25	d	401	CLA	C3B-C4B	2.53	1.50	1.42
25	c	502	CLA	C1B-C2B	2.52	1.49	1.43
25	B	601	CLA	MG-NC	2.52	2.12	2.06
33	C	515	LMG	C4-C5	2.52	1.58	1.53
27	c	515	BCR	C30-C25	-2.52	1.50	1.53
25	b	612	CLA	CMD-C2D	-2.51	1.45	1.50
25	b	608	CLA	CMB-C2B	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	520	LMG	C4-C5	2.51	1.58	1.53
26	d	402	PHO	CMD-C2D	-2.51	1.46	1.51
30	C	517	DGD	C4D-C3D	2.50	1.58	1.52
25	b	612	CLA	C1B-C2B	2.50	1.49	1.43
25	C	507	CLA	C4B-NB	2.50	1.41	1.37
30	A	614	DGD	C1E-C2E	2.50	1.59	1.52
29	a	614	SQD	C44-C45	2.50	1.57	1.51
25	C	512	CLA	C1B-C2B	2.50	1.49	1.43
25	C	509	CLA	C3B-C4B	2.50	1.50	1.42
35	e	101	HEM	CAB-C3B	2.50	1.54	1.47
26	d	402	PHO	C3D-C4D	2.50	1.44	1.41
25	B	614	CLA	CHC-C1C	2.50	1.43	1.38
25	b	614	CLA	C1B-C2B	2.49	1.49	1.43
25	C	503	CLA	C3B-C4B	2.49	1.50	1.42
25	b	613	CLA	CMC-C2C	-2.49	1.45	1.50
25	A	606	CLA	MG-NA	2.49	2.12	2.06
30	H	103	DGD	C1E-C2E	2.48	1.59	1.52
25	B	609	CLA	C1B-C2B	2.48	1.49	1.43
29	b	619	SQD	O9-S	2.48	1.52	1.45
33	c	524	LMG	O7-C8	-2.48	1.40	1.46
25	B	612	CLA	C4B-NB	2.47	1.41	1.37
29	A	613	SQD	O9-S	2.47	1.52	1.45
25	C	501	CLA	CMD-C2D	-2.47	1.45	1.50
32	L	101	LHG	O7-C5	-2.47	1.40	1.46
33	d	410	LMG	O1-C7	-2.47	1.39	1.43
25	b	608	CLA	C1B-C2B	2.46	1.48	1.43
25	c	509	CLA	CHC-C1C	2.46	1.43	1.38
25	c	505	CLA	CHC-C1C	2.46	1.43	1.38
25	a	607	CLA	C3B-C4B	2.46	1.49	1.42
25	c	510	CLA	C3B-C4B	2.46	1.49	1.42
25	C	502	CLA	C3B-C4B	2.45	1.49	1.42
32	b	623	LHG	O7-C5	-2.45	1.40	1.46
25	B	606	CLA	C1B-C2B	2.45	1.48	1.43
25	B	613	CLA	C1D-ND	2.45	1.41	1.37
33	d	410	LMG	C4-C5	2.44	1.58	1.53
25	D	403	CLA	CHC-C1C	2.44	1.43	1.38
25	B	603	CLA	C1B-C2B	2.44	1.48	1.43
25	c	509	CLA	MG-NC	2.43	2.12	2.06
25	H	101	CLA	CHC-C1C	2.43	1.43	1.38
35	F	101	HEM	FE-NB	2.43	2.02	1.94
25	b	602	CLA	MG-NB	-2.43	2.01	2.05
25	b	611	CLA	CMC-C2C	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	MG-NA	2.42	2.12	2.06
25	B	602	CLA	C3B-C4B	2.42	1.49	1.42
25	a	609	CLA	CMC-C2C	-2.42	1.45	1.50
25	H	101	CLA	C3B-C4B	2.42	1.49	1.42
25	b	608	CLA	C3B-C4B	2.42	1.49	1.42
29	T	103	SQD	C46-C45	2.42	1.56	1.50
25	B	603	CLA	C4B-NB	2.41	1.41	1.37
29	B	621	SQD	O9-S	2.41	1.51	1.45
25	C	513	CLA	C3B-C4B	2.41	1.49	1.42
25	a	607	CLA	CHC-C1C	2.41	1.43	1.38
30	C	517	DGD	C1E-C2E	2.40	1.59	1.52
25	B	602	CLA	C1B-C2B	2.40	1.48	1.43
30	C	516	DGD	O5D-C1E	2.40	1.44	1.40
33	c	524	LMG	O8-C9	-2.39	1.39	1.45
25	d	404	CLA	CHC-C1C	2.39	1.43	1.38
25	D	404	CLA	CMD-C2D	-2.39	1.45	1.50
25	b	611	CLA	C1B-C2B	2.39	1.48	1.43
25	B	605	CLA	C3B-C4B	2.39	1.49	1.42
25	c	503	CLA	C3B-C4B	2.39	1.49	1.42
25	b	605	CLA	C1B-C2B	2.39	1.48	1.43
25	b	601	CLA	C3B-C4B	2.39	1.49	1.42
25	b	603	CLA	C3B-C4B	2.38	1.49	1.42
30	c	517	DGD	O4D-C4D	-2.38	1.37	1.43
26	a	608	PHO	C4D-ND	-2.38	1.35	1.38
25	B	607	CLA	CMD-C2D	-2.38	1.45	1.50
25	b	606	CLA	C3B-C4B	2.38	1.49	1.42
25	b	606	CLA	CMB-C2B	-2.38	1.45	1.50
25	C	509	CLA	CHC-C1C	2.38	1.43	1.38
25	C	502	CLA	CMC-C2C	-2.38	1.45	1.50
25	B	603	CLA	C3B-C4B	2.37	1.49	1.42
36	v	201	HEC	C3B-C2B	-2.37	1.33	1.41
25	C	507	CLA	C3B-C4B	2.37	1.49	1.42
25	C	510	CLA	C3B-C4B	2.37	1.49	1.42
26	d	402	PHO	C4D-ND	-2.37	1.35	1.38
25	B	603	CLA	CHC-C1C	2.37	1.43	1.38
25	b	614	CLA	CHC-C1C	2.37	1.43	1.38
26	d	402	PHO	CAC-C3C	-2.37	1.47	1.51
29	f	101	SQD	O7-S	2.37	1.51	1.45
30	C	518	DGD	O2G-C2G	-2.36	1.41	1.46
25	B	610	CLA	C1B-C2B	2.36	1.48	1.43
26	a	608	PHO	O2D-CGD	2.36	1.39	1.33
25	D	403	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	C4B-NB	2.35	1.41	1.37
25	c	502	CLA	C3B-C4B	2.35	1.49	1.42
25	B	615	CLA	C4B-NB	2.34	1.40	1.37
30	a	615	DGD	C1G-C2G	2.34	1.58	1.50
25	A	609	CLA	MG-NB	-2.34	2.01	2.05
25	d	404	CLA	MG-ND	-2.34	2.01	2.05
25	B	607	CLA	MG-NC	2.34	2.11	2.06
33	c	524	LMG	C1-C2	2.34	1.59	1.52
25	C	504	CLA	C1B-C2B	2.34	1.48	1.43
25	a	609	CLA	C1B-NB	-2.34	1.34	1.37
25	b	608	CLA	MG-ND	-2.34	2.01	2.05
25	b	611	CLA	C3B-C4B	2.33	1.49	1.42
33	c	522	LMG	C4-C5	2.33	1.58	1.53
30	h	102	DGD	C4E-C3E	2.33	1.58	1.52
30	c	517	DGD	C6D-C5D	2.33	1.58	1.51
25	C	512	CLA	C3B-C4B	2.33	1.49	1.42
25	A	612	CLA	CHC-C1C	2.32	1.43	1.38
25	c	509	CLA	C3B-C4B	2.32	1.49	1.42
25	b	615	CLA	CMC-C2C	-2.32	1.46	1.50
25	B	608	CLA	CMD-C2D	-2.32	1.46	1.50
25	h	101	CLA	C3B-C4B	2.32	1.49	1.42
30	c	517	DGD	O1G-C1G	-2.32	1.40	1.45
25	C	512	CLA	CMD-C2D	-2.32	1.46	1.50
25	b	606	CLA	CMD-C2D	-2.31	1.46	1.50
25	C	511	CLA	CMB-C2B	-2.31	1.46	1.50
25	B	601	CLA	C3B-C4B	2.31	1.49	1.42
25	B	604	CLA	C3B-C4B	2.30	1.49	1.42
30	C	516	DGD	C4D-C3D	2.30	1.58	1.52
25	b	615	CLA	CHC-C1C	2.30	1.43	1.38
25	c	510	CLA	CHC-C1C	2.30	1.43	1.38
25	B	606	CLA	MG-NA	2.30	2.11	2.06
25	B	602	CLA	CHC-C1C	2.30	1.43	1.38
27	b	616	BCR	C33-C5	-2.30	1.47	1.50
25	B	611	CLA	C1B-C2B	2.30	1.48	1.43
25	C	508	CLA	MG-ND	-2.30	2.01	2.05
29	A	613	SQD	C8-C7	2.30	1.57	1.50
25	C	505	CLA	C3B-C4B	2.30	1.49	1.42
30	A	614	DGD	C4D-C3D	2.30	1.58	1.52
25	C	511	CLA	MG-ND	-2.29	2.01	2.05
25	B	606	CLA	C4B-NB	2.29	1.40	1.37
25	a	607	CLA	MG-NA	2.29	2.11	2.06
25	b	606	CLA	CMC-C2C	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	C1B-C2B	2.28	1.48	1.43
25	b	609	CLA	C3B-C4B	2.28	1.49	1.42
25	B	606	CLA	CMC-C2C	-2.28	1.46	1.50
30	C	516	DGD	C3G-C2G	2.28	1.57	1.50
25	b	613	CLA	CMB-C2B	-2.27	1.46	1.50
25	B	602	CLA	CMC-C2C	-2.27	1.46	1.50
25	h	101	CLA	CMC-C2C	-2.27	1.46	1.50
25	b	613	CLA	CHC-C1C	2.27	1.43	1.38
26	a	608	PHO	CAC-C3C	-2.27	1.47	1.51
25	D	404	CLA	CMB-C2B	-2.26	1.46	1.50
29	f	101	SQD	O9-S	2.25	1.51	1.45
25	B	603	CLA	MG-NA	2.25	2.11	2.06
25	C	506	CLA	CMC-C2C	-2.25	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.25	1.46	1.50
25	b	602	CLA	C3B-C4B	2.25	1.49	1.42
25	b	610	CLA	CMC-C2C	-2.25	1.46	1.50
25	a	609	CLA	C3B-C4B	2.24	1.49	1.42
25	a	612	CLA	C4B-NB	2.24	1.40	1.37
25	C	506	CLA	C3B-C4B	2.24	1.49	1.42
25	B	601	CLA	CHC-C1C	2.24	1.43	1.38
25	B	611	CLA	CMC-C2C	-2.24	1.46	1.50
25	D	404	CLA	CMC-C2C	-2.24	1.46	1.50
32	D	410	LHG	O7-C7	2.24	1.40	1.34
25	B	611	CLA	C3B-C4B	2.24	1.49	1.42
25	b	608	CLA	CHC-C1C	2.24	1.43	1.38
25	a	607	CLA	CMC-C2C	-2.24	1.46	1.50
35	e	101	HEM	C3B-C2B	-2.24	1.32	1.37
26	A	608	PHO	CMD-C2D	-2.24	1.47	1.51
25	C	509	CLA	CMD-C2D	-2.23	1.46	1.50
29	D	408	SQD	O7-S	2.23	1.51	1.45
25	b	605	CLA	C3B-C4B	2.23	1.49	1.42
35	e	101	HEM	C2A-C3A	-2.23	1.33	1.38
25	b	610	CLA	C4B-NB	2.23	1.40	1.37
30	C	517	DGD	O6D-C5D	-2.22	1.38	1.44
25	b	612	CLA	CMB-C2B	-2.22	1.46	1.50
29	a	613	SQD	O7-S	2.22	1.51	1.45
25	b	614	CLA	CMC-C2C	-2.22	1.46	1.50
35	e	101	HEM	CMA-C3A	2.22	1.55	1.50
25	A	609	CLA	CMC-C2C	-2.22	1.46	1.50
25	b	614	CLA	MG-ND	-2.22	2.01	2.05
25	b	612	CLA	C3B-C4B	2.22	1.49	1.42
26	D	402	PHO	CAC-C3C	-2.22	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	408	SQD	O9-S	2.21	1.51	1.45
30	H	103	DGD	C4E-C5E	2.21	1.57	1.53
25	b	615	CLA	C3B-C4B	2.21	1.49	1.42
25	c	511	CLA	C3B-C4B	2.21	1.49	1.42
25	B	614	CLA	CMB-C2B	-2.21	1.46	1.50
32	d	408	LHG	O8-C23	2.21	1.39	1.33
33	D	407	LMG	C4-C5	2.21	1.57	1.53
25	c	504	CLA	MG-ND	-2.21	2.01	2.05
29	B	621	SQD	O7-S	2.21	1.51	1.45
25	C	506	CLA	CHC-C1C	2.21	1.42	1.38
25	d	403	CLA	CMD-C2D	-2.20	1.46	1.50
25	H	101	CLA	CMB-C2B	-2.20	1.46	1.50
25	a	607	CLA	CMB-C2B	-2.20	1.46	1.50
25	c	502	CLA	CMD-C2D	-2.20	1.46	1.50
30	h	102	DGD	C1E-C2E	2.20	1.59	1.52
25	C	502	CLA	CHC-C1C	2.20	1.42	1.38
26	d	402	PHO	CMB-C2B	-2.20	1.47	1.51
25	B	613	CLA	CHC-C1C	2.20	1.42	1.38
25	b	605	CLA	C4B-NB	2.20	1.40	1.37
32	b	623	LHG	P-O6	2.20	1.68	1.59
25	d	403	CLA	C4B-NB	2.20	1.40	1.37
25	c	502	CLA	MG-ND	2.20	2.10	2.05
25	c	506	CLA	C3B-C4B	2.20	1.49	1.42
25	C	509	CLA	MG-ND	2.19	2.10	2.05
25	b	603	CLA	CHC-C1C	2.19	1.42	1.38
25	C	506	CLA	CMD-C2D	-2.19	1.46	1.50
25	b	610	CLA	C3B-C4B	2.19	1.49	1.42
26	a	608	PHO	CMD-C2D	-2.18	1.47	1.51
36	V	201	HEC	CMB-C2B	2.18	1.55	1.50
25	c	512	CLA	CMD-C2D	-2.18	1.46	1.50
25	c	502	CLA	CHC-C1C	2.18	1.42	1.38
25	c	504	CLA	C3B-C4B	2.18	1.49	1.42
33	c	522	LMG	C3-C2	2.17	1.58	1.52
25	B	610	CLA	CMD-C2D	-2.17	1.46	1.50
25	c	512	CLA	C1D-C2D	2.17	1.49	1.45
25	c	503	CLA	CMC-C2C	-2.17	1.46	1.50
29	B	621	SQD	C8-C7	2.17	1.57	1.50
25	D	404	CLA	C4B-NB	2.17	1.40	1.37
30	c	517	DGD	C4D-C5D	2.17	1.57	1.53
25	A	612	CLA	CMD-C2D	-2.17	1.46	1.50
25	b	610	CLA	CMD-C2D	-2.16	1.46	1.50
25	c	510	CLA	CMC-C2C	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	CMB-C2B	-2.16	1.46	1.50
25	c	501	CLA	MG-NB	-2.16	2.01	2.05
25	B	615	CLA	C3B-C4B	2.16	1.49	1.42
25	c	510	CLA	CMB-C2B	-2.16	1.46	1.50
27	A	610	BCR	C33-C5	-2.16	1.47	1.50
25	B	615	CLA	CMD-C2D	-2.16	1.46	1.50
29	b	619	SQD	C46-C45	2.16	1.57	1.50
25	c	501	CLA	C3B-C4B	2.16	1.49	1.42
30	A	614	DGD	C3E-C2E	2.16	1.57	1.52
25	h	101	CLA	C3D-C4D	2.16	1.49	1.44
27	B	616	BCR	C33-C5	-2.16	1.47	1.50
30	c	517	DGD	C4E-C3E	2.15	1.57	1.52
25	C	508	CLA	CMD-C2D	-2.15	1.46	1.50
35	e	101	HEM	CMC-C2C	2.15	1.55	1.50
25	b	609	CLA	CMD-C2D	-2.15	1.46	1.50
33	b	622	LMG	C3-C2	2.15	1.57	1.52
25	b	611	CLA	CHC-C1C	2.14	1.42	1.38
25	c	510	CLA	CMD-C2D	-2.14	1.46	1.50
27	T	101	BCR	C30-C25	-2.14	1.51	1.53
25	C	510	CLA	CMC-C2C	-2.14	1.46	1.50
26	A	608	PHO	CMB-C2B	-2.14	1.47	1.51
25	d	404	CLA	CMB-C2B	-2.14	1.46	1.50
30	c	517	DGD	C3G-C2G	2.14	1.57	1.50
29	f	101	SQD	O5-C5	2.13	1.49	1.44
25	C	509	CLA	O2D-CGD	2.13	1.38	1.33
25	B	611	CLA	C1B-NB	-2.13	1.35	1.37
25	B	608	CLA	CMC-C2C	-2.13	1.46	1.50
36	V	201	HEC	C3B-C2B	-2.13	1.34	1.41
25	b	612	CLA	C3C-C2C	2.13	1.41	1.36
25	C	511	CLA	CHC-C1C	2.12	1.42	1.38
25	c	507	CLA	C3D-C4D	2.12	1.49	1.44
27	k	101	BCR	C33-C5	-2.12	1.47	1.50
25	c	507	CLA	CMC-C2C	-2.12	1.46	1.50
25	C	506	CLA	C1B-NB	-2.12	1.35	1.37
25	a	612	CLA	MG-NC	-2.12	2.01	2.06
27	c	515	BCR	C38-C26	-2.12	1.47	1.50
28	D	406	PL9	C31-C29	-2.12	1.46	1.51
30	C	516	DGD	C3E-C2E	2.12	1.57	1.52
25	b	603	CLA	CMC-C2C	-2.11	1.46	1.50
25	B	605	CLA	CMD-C2D	-2.11	1.46	1.50
25	c	507	CLA	CHC-C1C	2.11	1.42	1.38
25	b	608	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	x	101	BCR	C1-C6	-2.11	1.51	1.53
30	c	519	DGD	C6D-C5D	2.11	1.57	1.51
33	C	519	LMG	O7-C8	-2.11	1.41	1.46
25	C	510	CLA	CMD-C2D	-2.11	1.46	1.50
32	D	409	LHG	P-O6	2.11	1.67	1.59
30	C	516	DGD	O2E-C2E	-2.10	1.37	1.43
27	T	101	BCR	C38-C26	-2.10	1.47	1.50
30	C	518	DGD	O1G-C1G	-2.10	1.40	1.45
30	c	518	DGD	O2G-C2G	-2.10	1.41	1.46
25	b	602	CLA	CMB-C2B	-2.09	1.46	1.50
25	B	604	CLA	CMC-C2C	-2.09	1.46	1.50
25	C	504	CLA	CMC-C2C	-2.09	1.46	1.50
25	b	609	CLA	CMB-C2B	-2.09	1.46	1.50
29	D	408	SQD	O5-C5	2.09	1.49	1.44
25	c	504	CLA	CHC-C1C	2.09	1.42	1.38
25	B	604	CLA	CHC-C1C	2.09	1.42	1.38
36	V	201	HEC	CMD-C2D	2.09	1.55	1.50
25	C	508	CLA	C1D-C2D	2.08	1.49	1.45
30	A	614	DGD	C3G-C2G	2.08	1.57	1.50
25	c	503	CLA	CMD-C2D	-2.08	1.46	1.50
25	a	609	CLA	CMD-C2D	-2.08	1.46	1.50
27	c	516	BCR	C38-C26	-2.08	1.47	1.50
30	c	519	DGD	O2G-C2G	-2.08	1.41	1.46
29	b	619	SQD	O7-S	2.08	1.51	1.45
25	C	507	CLA	CHC-C1C	2.07	1.42	1.38
25	c	510	CLA	MG-NB	-2.07	2.01	2.05
25	c	501	CLA	MG-NA	2.07	2.11	2.06
25	C	508	CLA	MG-NB	2.07	2.09	2.05
25	B	614	CLA	MG-NC	2.07	2.11	2.06
33	c	524	LMG	C4-C3	2.07	1.57	1.52
25	C	513	CLA	CHC-C1C	2.07	1.42	1.38
25	b	611	CLA	CMB-C2B	-2.07	1.46	1.50
25	B	615	CLA	CMC-C2C	-2.06	1.46	1.50
25	c	508	CLA	CMD-C2D	-2.06	1.46	1.50
29	a	613	SQD	O9-S	2.06	1.50	1.45
25	B	605	CLA	CMB-C2B	-2.06	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.05	1.46	1.50
25	C	507	CLA	CMB-C2B	-2.05	1.46	1.50
25	C	501	CLA	C1D-C2D	2.05	1.49	1.45
25	C	510	CLA	CMB-C2B	-2.05	1.46	1.50
25	c	507	CLA	CMB-C2B	-2.05	1.46	1.50
25	b	601	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	V	201	HEC	CMC-C2C	2.05	1.55	1.50
33	C	519	LMG	O8-C9	-2.05	1.40	1.45
28	a	611	PL9	C53-C6	-2.04	1.46	1.50
30	c	518	DGD	O5D-C6D	-2.04	1.40	1.43
25	B	606	CLA	C3D-C4D	2.04	1.48	1.44
25	A	609	CLA	CMD-C2D	-2.04	1.46	1.50
25	c	512	CLA	CMB-C2B	-2.04	1.46	1.50
29	B	621	SQD	C46-C45	2.04	1.57	1.50
25	d	404	CLA	C3B-C4B	2.04	1.48	1.42
25	b	602	CLA	C3D-C4D	2.03	1.48	1.44
30	H	103	DGD	O2D-C2D	-2.03	1.37	1.43
25	b	614	CLA	CMB-C2B	-2.03	1.46	1.50
25	C	509	CLA	CMB-C2B	-2.03	1.46	1.50
25	c	513	CLA	CMC-C2C	-2.03	1.46	1.50
25	c	506	CLA	CMB-C2B	-2.03	1.46	1.50
25	b	601	CLA	CHC-C1C	2.03	1.42	1.38
25	b	615	CLA	CMB-C2B	-2.03	1.46	1.50
25	a	612	CLA	CHC-C1C	2.03	1.42	1.38
25	B	615	CLA	CHC-C4B	-2.03	1.34	1.39
25	b	602	CLA	CMC-C2C	-2.03	1.46	1.50
32	L	101	LHG	P-O6	2.03	1.67	1.59
25	b	610	CLA	CHC-C1C	2.02	1.42	1.38
25	d	401	CLA	CMB-C2B	-2.02	1.46	1.50
25	h	101	CLA	CMD-C2D	-2.02	1.46	1.50
25	B	601	CLA	CMB-C2B	-2.02	1.46	1.50
30	h	102	DGD	C4E-C5E	2.02	1.57	1.53
25	C	502	CLA	CMB-C2B	-2.01	1.46	1.50
30	C	517	DGD	O3E-C3E	-2.01	1.38	1.43
35	F	101	HEM	CMA-C3A	2.01	1.54	1.50
25	C	507	CLA	CMC-C2C	-2.01	1.46	1.50
27	t	101	BCR	C1-C6	-2.01	1.51	1.53
25	H	101	CLA	CMC-C2C	-2.01	1.46	1.50
26	D	402	PHO	C3D-C4D	2.01	1.44	1.41
33	D	407	LMG	O3-C3	-2.01	1.38	1.43
25	A	606	CLA	CHC-C1C	2.01	1.42	1.38
25	C	508	CLA	CHC-C1C	2.01	1.42	1.38
28	A	611	PL9	C53-C6	-2.00	1.46	1.50
25	B	601	CLA	C1D-C2D	2.00	1.49	1.45

All (1129) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	201	HEC	CBB-CAB-C3B	-10.01	107.42	127.43
25	c	511	CLA	C4A-NA-C1A	8.71	110.66	106.68
25	C	507	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	B	603	CLA	C4A-NA-C1A	8.04	110.35	106.68
25	b	603	CLA	C4A-NA-C1A	7.96	110.31	106.68
25	h	101	CLA	C4A-NA-C1A	7.96	110.31	106.68
25	B	606	CLA	C4A-NA-C1A	7.67	110.18	106.68
36	v	201	HEC	CBB-CAB-C3B	-7.65	112.14	127.43
25	C	506	CLA	C4A-NA-C1A	7.61	110.15	106.68
29	D	408	SQD	C1-O5-C5	-7.50	99.07	113.72
36	v	201	HEC	CBC-CAC-C3C	-7.41	112.61	127.43
25	c	509	CLA	C4A-NA-C1A	7.33	110.02	106.68
25	b	604	CLA	C4A-NA-C1A	7.33	110.02	106.68
25	c	501	CLA	C4A-NA-C1A	7.29	110.00	106.68
25	B	605	CLA	C4A-NA-C1A	7.25	109.98	106.68
25	c	507	CLA	C4A-NA-C1A	7.18	109.96	106.68
25	b	605	CLA	C4A-NA-C1A	7.17	109.95	106.68
25	b	610	CLA	C4A-NA-C1A	7.12	109.93	106.68
25	C	509	CLA	C4A-NA-C1A	7.06	109.90	106.68
25	C	513	CLA	C4A-NA-C1A	6.95	109.85	106.68
29	a	613	SQD	O6-C1-C2	6.91	118.77	108.27
25	C	501	CLA	C4A-NA-C1A	6.87	109.81	106.68
25	b	615	CLA	C4A-NA-C1A	6.81	109.79	106.68
25	c	510	CLA	C4A-NA-C1A	6.75	109.76	106.68
29	D	408	SQD	O6-C1-C2	6.69	118.43	108.27
25	B	614	CLA	C4A-NA-C1A	6.67	109.72	106.68
25	C	503	CLA	C4A-NA-C1A	6.65	109.72	106.68
25	B	615	CLA	C4A-NA-C1A	6.56	109.67	106.68
25	C	511	CLA	C4A-NA-C1A	6.47	109.63	106.68
25	b	606	CLA	C4A-NA-C1A	6.42	109.61	106.68
25	c	503	CLA	C4A-NA-C1A	6.42	109.61	106.68
25	b	602	CLA	C4A-NA-C1A	6.40	109.60	106.68
25	C	502	CLA	C4A-NA-C1A	6.34	109.57	106.68
28	a	611	PL9	C7-C3-C4	6.26	122.07	116.91
36	V	201	HEC	CBC-CAC-C3C	-6.23	114.99	127.43
29	b	619	SQD	O6-C1-C2	6.20	117.68	108.27
25	B	612	CLA	C4A-NA-C1A	6.19	109.50	106.68
25	C	508	CLA	C4A-NA-C1A	6.12	109.47	106.68
25	b	613	CLA	C4A-NA-C1A	6.07	109.45	106.68
25	c	513	CLA	C4A-NA-C1A	6.05	109.44	106.68
25	b	609	CLA	C4A-NA-C1A	5.94	109.39	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	608	CLA	C4A-NA-C1A	5.86	109.35	106.68
25	b	614	CLA	C4A-NA-C1A	5.85	109.35	106.68
29	A	613	SQD	O6-C1-C2	5.83	117.12	108.27
29	A	613	SQD	C1-O5-C5	-5.81	102.38	113.72
25	c	506	CLA	C4A-NA-C1A	5.81	109.33	106.68
26	d	402	PHO	C4D-CHA-CBD	-5.73	105.71	108.45
25	c	502	CLA	C4A-NA-C1A	5.62	109.24	106.68
25	B	610	CLA	C4A-NA-C1A	5.59	109.23	106.68
25	d	401	CLA	C4A-NA-C1A	5.58	109.23	106.68
25	B	611	CLA	C4A-NA-C1A	5.57	109.22	106.68
25	b	612	CLA	C4A-NA-C1A	5.57	109.22	106.68
25	c	508	CLA	C4A-NA-C1A	5.49	109.18	106.68
25	c	504	CLA	C4A-NA-C1A	5.46	109.17	106.68
29	a	613	SQD	C1-O5-C5	-5.43	103.12	113.72
25	a	607	CLA	C4A-NA-C1A	5.37	109.13	106.68
29	a	614	SQD	O47-C7-C8	5.37	123.09	111.48
25	c	505	CLA	C4A-NA-C1A	5.36	109.13	106.68
25	C	510	CLA	C4A-NA-C1A	5.16	109.03	106.68
25	C	505	CLA	C4A-NA-C1A	5.14	109.03	106.68
25	B	604	CLA	C4A-NA-C1A	5.12	109.02	106.68
25	A	606	CLA	C4A-NA-C1A	5.09	109.00	106.68
26	D	402	PHO	C1-C2-C3	-5.05	117.92	126.20
26	A	608	PHO	C4D-CHA-CBD	-4.96	106.07	108.45
25	c	512	CLA	C4A-NA-C1A	4.95	108.94	106.68
29	D	408	SQD	C1-C2-C3	-4.94	99.61	110.01
25	C	512	CLA	C4A-NA-C1A	4.92	108.92	106.68
25	D	404	CLA	C4A-NA-C1A	4.86	108.89	106.68
29	B	621	SQD	O47-C7-C8	4.86	121.98	111.48
25	a	612	CLA	C4A-NA-C1A	4.85	108.89	106.68
25	B	613	CLA	C4A-NA-C1A	4.80	108.87	106.68
30	C	518	DGD	O3G-C3G-C2G	-4.78	99.20	110.82
29	A	613	SQD	O47-C7-C8	4.77	121.81	111.48
25	B	607	CLA	C4A-NA-C1A	4.77	108.85	106.68
30	a	615	DGD	O3G-C3G-C2G	-4.76	99.54	111.77
25	B	601	CLA	C4A-NA-C1A	4.76	108.85	106.68
28	a	611	PL9	C7-C3-C2	-4.76	117.78	123.39
25	D	403	CLA	C4A-NA-C1A	4.73	108.84	106.68
25	b	605	CLA	O2D-CGD-O1D	-4.72	114.65	123.85
25	H	101	CLA	C4A-NA-C1A	4.63	108.79	106.68
25	b	603	CLA	C1-C2-C3	-4.59	118.67	126.20
28	D	406	PL9	C7-C3-C4	4.57	120.68	116.91
25	b	608	CLA	C4A-NA-C1A	4.53	108.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	602	CLA	C4A-NA-C1A	4.50	108.73	106.68
29	f	101	SQD	O6-C1-C2	4.48	115.07	108.27
32	B	620	LHG	O4-P-O5	4.47	133.24	112.44
26	D	402	PHO	C2B-C1B-NB	-4.46	106.21	109.43
29	f	101	SQD	O9-S-O7	-4.45	99.36	113.82
32	d	407	LHG	O4-P-O5	4.39	132.88	112.44
25	b	607	CLA	C3B-C4B-NB	-4.38	106.62	110.53
32	e	102	LHG	O4-P-O5	4.36	132.75	112.44
25	B	602	CLA	C3B-C4B-NB	-4.36	106.64	110.53
25	b	601	CLA	C4A-NA-C1A	4.35	108.66	106.68
25	b	615	CLA	O2D-CGD-O1D	-4.34	115.39	123.85
28	d	406	PL9	C7-C3-C4	4.34	120.48	116.91
32	E	101	LHG	O4-P-O5	4.32	132.52	112.44
29	B	621	SQD	O7-S-C6	4.31	113.19	106.76
25	B	611	CLA	C1-C2-C3	-4.30	119.16	126.20
25	b	607	CLA	C4A-NA-C1A	4.30	108.64	106.68
25	b	611	CLA	C1-C2-C3	-4.29	119.17	126.20
26	d	402	PHO	C1-C2-C3	-4.28	119.18	126.20
25	b	602	CLA	O2D-CGD-O1D	-4.27	115.54	123.85
25	B	601	CLA	O2D-CGD-CBD	4.26	118.67	111.23
33	b	620	LMG	O1-C1-C2	-4.25	101.82	108.27
32	L	101	LHG	O4-P-O5	4.20	131.99	112.44
28	d	406	PL9	C22-C23-C24	-4.19	118.03	127.62
26	A	608	PHO	C2B-C1B-NB	-4.19	106.40	109.43
25	A	607	CLA	C4A-NA-C1A	4.19	108.59	106.68
32	b	623	LHG	O4-P-O5	4.19	131.92	112.44
25	b	604	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
25	A	609	CLA	C4A-NA-C1A	4.17	108.58	106.68
30	C	517	DGD	O3G-C3G-C2G	-4.15	100.71	110.82
32	D	410	LHG	O4-P-O5	4.15	131.73	112.44
25	c	501	CLA	O2D-CGD-O1D	-4.14	115.80	123.85
26	a	608	PHO	C4D-CHA-CBD	-4.13	106.47	108.45
29	A	613	SQD	O9-S-O7	-4.11	100.44	113.82
34	D	401	BCT	O2-C-O1	4.11	130.20	119.68
32	l	101	LHG	O4-P-O5	4.09	131.49	112.44
30	h	102	DGD	O3G-C3G-C2G	-4.09	100.87	110.82
32	d	408	LHG	O4-P-O5	4.08	131.45	112.44
30	c	519	DGD	O3G-C3G-C2G	-4.08	100.90	110.82
25	d	403	CLA	C4A-NA-C1A	4.07	108.54	106.68
29	B	621	SQD	C3-C4-C5	4.07	117.61	110.23
25	B	613	CLA	O2D-CGD-O1D	-4.06	115.94	123.85
25	b	609	CLA	CAC-C3C-C4C	4.06	130.07	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	101	SQD	O7-S-C6	4.06	112.81	106.76
25	B	605	CLA	C3B-C4B-NB	-4.05	106.91	110.53
27	B	616	BCR	C2-C1-C6	4.05	116.33	110.44
30	H	103	DGD	O3G-C3G-C2G	-4.05	100.96	110.82
29	B	621	SQD	O6-C1-C2	4.05	114.42	108.27
32	D	409	LHG	O4-P-O5	4.04	131.25	112.44
25	B	611	CLA	O2D-CGD-O1D	-4.04	115.99	123.85
25	C	504	CLA	C4A-NA-C1A	4.03	108.52	106.68
29	D	408	SQD	O9-S-C6	4.00	112.73	106.76
25	c	512	CLA	C1-C2-C3	-3.99	119.65	126.20
29	f	101	SQD	C1-O5-C5	-3.99	105.92	113.72
25	b	610	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
34	a	606	BCT	O2-C-O1	3.96	129.82	119.68
29	a	613	SQD	O47-C7-C8	3.96	120.05	111.48
30	c	518	DGD	O3G-C3G-C2G	-3.95	101.22	110.82
25	b	601	CLA	O2D-CGD-O1D	-3.94	116.18	123.85
25	B	607	CLA	CMB-C2B-C1B	-3.93	119.43	125.42
28	A	611	PL9	C7-C3-C4	3.92	120.14	116.91
29	a	613	SQD	O9-S-O7	-3.89	101.17	113.82
25	B	609	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
35	e	101	HEM	CBD-CAD-C3D	-3.84	101.90	112.53
25	B	603	CLA	C3B-C4B-NB	-3.84	107.11	110.53
25	D	403	CLA	C3B-C4B-NB	-3.83	107.11	110.53
25	B	612	CLA	C1-C2-C3	-3.82	119.94	126.20
25	a	609	CLA	C4A-NA-C1A	3.82	108.42	106.68
30	c	517	DGD	O3G-C3G-C2G	-3.81	101.56	110.82
29	D	408	SQD	C44-O6-C1	3.80	120.16	113.68
25	B	610	CLA	C3B-C4B-NB	-3.77	107.17	110.53
29	D	408	SQD	O9-S-O7	-3.76	101.60	113.82
25	b	604	CLA	O1D-CGD-CBD	3.74	131.90	124.52
25	B	604	CLA	O2D-CGD-O1D	-3.74	116.58	123.85
25	H	101	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
25	C	510	CLA	C3B-C4B-NB	-3.73	107.20	110.53
25	b	614	CLA	C3B-C4B-NB	-3.72	107.21	110.53
25	c	505	CLA	C3B-C4B-NB	-3.71	107.22	110.53
25	c	513	CLA	C3B-C4B-NB	-3.71	107.22	110.53
29	b	619	SQD	C3-C4-C5	3.70	116.95	110.23
36	v	201	HEC	CBD-CAD-C3D	-3.70	102.30	112.53
25	d	401	CLA	C3B-C4B-NB	-3.70	107.23	110.53
29	B	621	SQD	O48-C23-C24	3.70	123.10	111.83
26	D	402	PHO	O1D-CGD-CBD	3.69	130.32	124.72
29	b	619	SQD	O7-S-C6	3.69	112.26	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	613	SQD	O5-C1-C2	-3.68	102.81	110.37
25	b	611	CLA	C4A-NA-C1A	3.68	108.36	106.68
29	D	408	SQD	O5-C1-O6	3.67	118.72	110.04
25	b	606	CLA	C3B-C4B-NB	-3.66	107.27	110.53
25	B	609	CLA	CHB-C4A-NA	3.66	129.68	124.40
25	c	509	CLA	O2A-CGA-O1A	-3.66	114.48	123.63
25	d	404	CLA	C4A-NA-C1A	3.64	108.34	106.68
25	C	501	CLA	C3B-C4B-NB	-3.63	107.29	110.53
27	T	101	BCR	C2-C1-C6	3.62	115.70	110.44
25	A	607	CLA	C3B-C4B-NB	-3.61	107.30	110.53
26	A	608	PHO	CMB-C2B-C3B	3.61	131.90	124.68
29	B	621	SQD	O9-S-O7	-3.61	102.09	113.82
25	B	603	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
25	b	611	CLA	O2D-CGD-O1D	-3.57	116.91	123.85
25	c	503	CLA	C3B-C4B-NB	-3.57	107.35	110.53
33	b	620	LMG	O1-C7-C8	-3.57	102.14	110.82
25	b	612	CLA	C1-C2-C3	-3.57	120.36	126.20
29	b	619	SQD	C1-O5-C5	-3.56	106.77	113.72
27	b	616	BCR	C2-C1-C6	3.56	115.60	110.44
25	B	601	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
29	b	619	SQD	O48-C23-C24	3.55	122.65	111.83
26	D	402	PHO	C4D-CHA-CBD	-3.52	106.77	108.45
25	d	401	CLA	CHB-C4A-NA	3.52	129.48	124.40
25	c	508	CLA	C1-C2-C3	-3.51	120.44	126.20
29	b	619	SQD	O47-C7-C8	3.51	119.07	111.48
25	B	602	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
25	c	508	CLA	C3B-C4B-NB	-3.49	107.41	110.53
25	b	601	CLA	C1-C2-C3	-3.48	120.49	126.20
29	f	101	SQD	O9-S-C6	3.48	111.95	106.76
25	B	613	CLA	C3B-C4B-NB	-3.47	107.43	110.53
26	a	608	PHO	C1-C2-C3	-3.47	120.52	126.20
25	C	503	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
25	C	503	CLA	C3B-C4B-NB	-3.46	107.44	110.53
26	a	608	PHO	C2B-C1B-NB	-3.46	106.93	109.43
29	A	613	SQD	C1-C2-C3	-3.46	102.73	110.01
36	v	201	HEC	C4D-ND-C1D	3.45	111.45	105.82
25	b	604	CLA	C1-C2-C3	-3.45	120.55	126.20
25	b	601	CLA	CHB-C4A-NA	3.44	129.37	124.40
25	C	505	CLA	C3B-C4B-NB	-3.44	107.46	110.53
25	h	101	CLA	C3B-C4B-NB	-3.44	107.46	110.53
25	b	603	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
28	A	611	PL9	C7-C8-C9	-3.44	120.91	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	610	BCR	C11-C10-C9	-3.43	122.46	127.28
28	d	406	PL9	C37-C38-C39	-3.43	119.78	127.62
25	A	607	CLA	C1-C2-C3	-3.42	120.59	126.20
27	C	514	BCR	C15-C14-C13	-3.41	122.49	127.28
25	C	510	CLA	CMB-C2B-C1B	-3.40	120.25	125.42
26	d	402	PHO	CMB-C2B-C3B	3.40	131.47	124.68
33	b	622	LMG	C1-O6-C5	-3.39	107.09	113.72
25	c	513	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
25	C	509	CLA	C3B-C4B-NB	-3.39	107.50	110.53
27	t	101	BCR	C3-C4-C5	-3.39	108.02	114.06
25	A	612	CLA	C3B-C4B-NB	-3.38	107.51	110.53
25	c	508	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
27	A	610	BCR	C27-C26-C25	3.36	127.24	122.70
25	b	605	CLA	O2D-CGD-CBD	3.35	117.09	111.23
29	T	103	SQD	O47-C7-C8	3.35	118.73	111.48
25	C	504	CLA	C3B-C4B-NB	-3.35	107.54	110.53
30	c	518	DGD	O6D-C1D-O3G	-3.35	102.13	110.04
25	C	501	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
25	B	611	CLA	C3B-C4B-NB	-3.34	107.54	110.53
25	C	507	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
27	B	618	BCR	C2-C1-C6	3.32	115.27	110.44
25	c	504	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
25	B	609	CLA	C3B-C4B-NB	-3.31	107.57	110.53
32	B	620	LHG	O8-C23-C24	3.31	121.91	111.83
32	b	623	LHG	O8-C23-C24	3.29	121.87	111.83
36	V	201	HEC	C4D-ND-C1D	3.29	111.18	105.82
27	b	617	BCR	C15-C14-C13	-3.29	122.67	127.28
25	B	601	CLA	CHB-C4A-NA	3.29	129.14	124.40
25	A	612	CLA	C4A-NA-C1A	3.28	108.17	106.68
25	A	606	CLA	CHB-C4A-NA	3.26	129.11	124.40
25	B	607	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
25	b	613	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	C	512	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	C	502	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
25	a	612	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
29	b	619	SQD	O9-S-O7	-3.23	103.31	113.82
35	e	101	HEM	C3B-C4B-NB	-3.23	107.15	109.47
25	c	510	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
25	B	601	CLA	O2A-CGA-O1A	-3.21	115.59	123.63
25	B	607	CLA	O2D-CGD-CBD	3.21	116.85	111.23
29	a	613	SQD	C1-C2-C3	-3.21	103.26	110.01
29	a	613	SQD	O48-C23-C24	3.21	121.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	408	SQD	O7-S-C6	3.21	111.55	106.76
25	B	605	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
25	A	609	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
29	f	101	SQD	O5-C5-C4	3.20	115.47	109.70
25	A	607	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
25	A	606	CLA	C3B-C4B-NB	-3.20	107.67	110.53
30	H	103	DGD	C3E-C4E-C5E	-3.20	104.43	110.23
29	A	613	SQD	O7-S-C6	3.19	111.52	106.76
25	C	512	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
30	A	614	DGD	O6D-C1D-O3G	-3.19	102.51	110.04
25	b	613	CLA	O2A-CGA-O1A	-3.19	115.65	123.63
33	b	620	LMG	O6-C1-O1	-3.19	102.51	110.04
33	d	410	LMG	O6-C1-O1	-3.18	102.52	110.04
25	b	601	CLA	O2D-CGD-CBD	3.18	116.79	111.23
25	b	603	CLA	CHB-C4A-NA	3.18	128.99	124.40
25	b	612	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
25	b	608	CLA	C3B-C4B-NB	-3.16	107.71	110.53
33	D	407	LMG	O6-C1-O1	-3.15	102.59	110.04
25	a	609	CLA	O2D-CGD-CBD	3.15	116.74	111.23
28	d	406	PL9	C40-C39-C41	3.14	120.68	115.23
25	c	502	CLA	C3B-C4B-NB	-3.14	107.73	110.53
27	H	102	BCR	C27-C26-C25	3.14	126.95	122.70
25	B	606	CLA	CHB-C4A-NA	3.14	128.93	124.40
28	A	611	PL9	C7-C3-C2	-3.14	119.69	123.39
35	e	101	HEM	CBA-CAA-C2A	-3.14	103.86	112.53
25	B	608	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
25	C	504	CLA	CMB-C2B-C1B	-3.13	120.65	125.42
27	D	405	BCR	C2-C1-C6	3.13	114.98	110.44
25	D	404	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
27	D	405	BCR	C7-C8-C9	-3.12	121.61	126.23
27	B	617	BCR	C35-C13-C14	-3.12	117.76	122.82
25	B	611	CLA	O2A-CGA-O1A	-3.12	115.83	123.63
25	c	501	CLA	O2D-CGD-CBD	3.10	116.66	111.23
25	c	511	CLA	C3B-C4B-NB	-3.10	107.76	110.53
25	B	615	CLA	C1-O2A-CGA	3.10	124.16	116.65
26	d	402	PHO	C2B-C1B-NB	-3.10	107.19	109.43
25	b	604	CLA	C3B-C4B-NB	-3.09	107.77	110.53
35	F	101	HEM	CBD-CAD-C3D	-3.09	104.00	112.53
29	a	613	SQD	O7-S-C6	3.08	111.36	106.76
32	D	409	LHG	O8-C23-C24	3.08	121.24	111.83
27	b	617	BCR	C11-C10-C9	-3.08	122.95	127.28
25	h	101	CLA	O2D-CGD-O1D	-3.08	117.85	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	m	101	STE	O2-C1-C2	3.08	123.73	114.00
30	C	518	DGD	O6D-C1D-O3G	-3.08	102.78	110.04
33	D	411	LMG	O1-C7-C8	-3.07	103.87	111.77
27	t	101	BCR	C2-C1-C6	3.07	114.90	110.44
25	b	606	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
25	B	609	CLA	C4A-NA-C1A	3.07	108.08	106.68
25	H	101	CLA	C3B-C4B-NB	-3.07	107.79	110.53
25	b	612	CLA	O2D-CGD-CBD	3.06	116.58	111.23
25	b	610	CLA	O2D-CGD-CBD	3.06	116.57	111.23
25	C	502	CLA	C3B-C4B-NB	-3.05	107.80	110.53
30	C	516	DGD	O3G-C3G-C2G	-3.05	103.39	110.82
27	Z	101	BCR	C15-C16-C17	-3.05	117.27	123.52
25	b	609	CLA	C1-C2-C3	-3.05	121.20	126.20
25	c	501	CLA	C3B-C4B-NB	-3.03	107.82	110.53
25	b	611	CLA	C11-C10-C8	-3.03	105.90	115.97
25	B	601	CLA	C3B-C4B-NB	-3.03	107.83	110.53
27	T	101	BCR	C3-C4-C5	-3.02	108.66	114.06
25	c	505	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
29	A	613	SQD	O48-C23-C24	3.02	121.03	111.83
25	b	615	CLA	CHB-C4A-NA	3.01	128.75	124.40
30	h	102	DGD	O6D-C1D-O3G	-3.01	102.92	110.04
25	c	503	CLA	CHB-C4A-NA	3.01	128.74	124.40
25	b	612	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
25	B	611	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
25	c	509	CLA	CHB-C4A-NA	2.99	128.72	124.40
31	b	625	STE	C3-C2-C1	-2.99	106.70	114.51
30	c	518	DGD	CDB-CCB-CBB	-2.99	99.26	114.37
25	b	602	CLA	C3B-C4B-NB	-2.98	107.87	110.53
25	b	610	CLA	C1-C2-C3	-2.98	121.32	126.20
25	c	512	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
25	C	506	CLA	C1-C2-C3	-2.97	121.33	126.20
25	b	613	CLA	CHB-C4A-NA	2.96	128.68	124.40
25	b	607	CLA	O2D-CGD-CBD	2.96	116.41	111.23
26	D	402	PHO	CMB-C2B-C3B	2.96	130.60	124.68
29	a	614	SQD	O48-C23-C24	2.96	120.86	111.83
25	c	507	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
25	D	403	CLA	C4-C3-C5	2.96	120.36	115.23
30	C	517	DGD	O6D-C1D-O3G	-2.95	103.07	110.04
27	B	616	BCR	C3-C4-C5	-2.95	108.79	114.06
25	d	404	CLA	C3B-C4B-NB	-2.95	107.90	110.53
25	a	609	CLA	CHB-C4A-NA	2.94	128.65	124.40
32	l	101	LHG	O8-C23-C24	2.94	120.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	614	CLA	CHB-C4A-NA	2.94	128.64	124.40
25	a	607	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
32	d	407	LHG	O8-C23-C24	2.93	120.77	111.83
30	c	519	DGD	O6D-C1D-O3G	-2.93	103.12	110.04
28	d	406	PL9	C36-C34-C33	-2.93	114.60	121.17
26	D	402	PHO	O2D-CGD-O1D	-2.92	118.16	123.85
29	B	621	SQD	O5-C5-C4	2.92	114.97	109.70
25	B	607	CLA	CMB-C2B-C3B	2.92	133.42	126.55
28	a	611	PL9	C22-C23-C24	-2.92	120.94	127.62
25	B	609	CLA	O2A-CGA-O1A	-2.92	116.33	123.63
27	c	514	BCR	C33-C5-C6	-2.92	121.30	124.48
25	c	502	CLA	CHD-C1D-ND	-2.92	120.70	124.80
27	B	617	BCR	C15-C14-C13	-2.91	123.19	127.28
25	B	612	CLA	CAC-C3C-C4C	2.91	128.58	124.79
25	b	615	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	b	613	CLA	C1-C2-C3	-2.90	121.44	126.20
31	x	102	STE	C3-C2-C1	-2.90	106.93	114.51
25	C	507	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	a	612	CLA	CHB-C4A-NA	2.90	128.58	124.40
25	A	609	CLA	O2D-CGD-CBD	2.89	116.29	111.23
30	h	102	DGD	C1D-C2D-C3D	-2.89	103.92	110.01
32	b	623	LHG	O8-C23-O10	-2.89	116.40	123.63
25	C	508	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
27	C	514	BCR	C35-C13-C14	-2.89	118.14	122.82
25	b	607	CLA	CHB-C4A-NA	2.89	128.57	124.40
32	e	102	LHG	O8-C23-C24	2.89	120.63	111.83
27	c	515	BCR	C27-C26-C25	2.89	126.60	122.70
25	C	508	CLA	C3B-C4B-NB	-2.88	107.95	110.53
33	b	622	LMG	O7-C10-O9	-2.88	116.97	123.70
27	Y	101	BCR	C27-C26-C25	2.88	126.59	122.70
27	T	101	BCR	C27-C26-C25	2.88	126.59	122.70
25	c	512	CLA	CHB-C4A-NA	2.88	128.55	124.40
33	b	622	LMG	C3-C4-C5	-2.87	105.02	110.23
27	Z	101	BCR	C24-C23-C22	-2.87	121.99	126.23
25	d	401	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
27	B	617	BCR	C27-C26-C25	2.86	126.57	122.70
28	d	406	PL9	C7-C3-C2	-2.86	120.02	123.39
25	C	505	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
30	C	516	DGD	O6D-C1D-O3G	-2.85	103.30	110.04
25	A	607	CLA	CHB-C4A-NA	2.85	128.52	124.40
25	b	605	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
25	c	502	CLA	O2A-CGA-O1A	-2.85	116.51	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	408	SQD	O48-C23-C24	2.84	120.49	111.83
30	A	614	DGD	C3G-C2G-C1G	-2.84	105.17	111.78
25	B	611	CLA	C11-C12-C13	-2.83	106.54	115.97
25	a	612	CLA	C1-C2-C3	-2.83	121.55	126.20
25	C	509	CLA	CHD-C1D-ND	-2.83	120.82	124.80
27	B	617	BCR	C2-C1-C6	2.83	114.55	110.44
25	c	504	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
25	c	513	CLA	CHB-C4A-NA	2.83	128.48	124.40
25	c	504	CLA	CMB-C2B-C1B	-2.83	121.12	125.42
25	b	605	CLA	C3B-C4B-NB	-2.83	108.01	110.53
25	c	509	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
25	C	501	CLA	O2D-CGD-CBD	2.82	116.17	111.23
32	E	101	LHG	O8-C23-C24	2.82	120.45	111.83
25	B	610	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
27	c	514	BCR	C11-C10-C9	-2.82	123.32	127.28
29	f	101	SQD	O5-C1-C2	-2.82	104.57	110.37
25	a	607	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
25	H	101	CLA	CAA-CBA-CGA	-2.82	105.21	113.21
30	c	517	DGD	C3G-C2G-C1G	-2.81	105.22	111.78
25	c	505	CLA	O2D-CGD-CBD	2.81	116.15	111.23
25	c	510	CLA	C1-C2-C3	-2.81	121.60	126.20
25	C	511	CLA	CHB-C4A-NA	2.81	128.45	124.40
28	A	611	PL9	O1-C4-C3	-2.80	117.77	120.73
27	c	515	BCR	C15-C16-C17	-2.80	117.78	123.52
25	b	615	CLA	O1D-CGD-CBD	2.80	130.04	124.52
28	D	406	PL9	C27-C28-C29	-2.80	121.22	127.62
25	B	610	CLA	CHD-C1D-ND	-2.80	120.87	124.80
25	a	609	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
30	c	519	DGD	C3G-C2G-C1G	-2.79	105.28	111.78
33	C	515	LMG	C1-O6-C5	-2.79	108.28	113.72
30	A	614	DGD	CDB-CCB-CBB	-2.79	100.28	114.37
25	C	510	CLA	CMB-C2B-C3B	2.78	133.10	126.55
25	B	609	CLA	O2D-CGD-CBD	2.78	116.09	111.23
27	c	516	BCR	C24-C23-C22	-2.78	122.12	126.23
25	d	403	CLA	C1-C2-C3	-2.78	121.64	126.20
29	a	613	SQD	C44-O6-C1	-2.78	107.83	113.80
25	C	513	CLA	O2A-CGA-O1A	-2.78	116.68	123.63
30	C	517	DGD	O5D-C6D-C5D	-2.78	103.16	109.42
31	j	101	STE	O2-C1-C2	2.77	122.77	114.00
27	c	515	BCR	C11-C10-C9	-2.77	123.39	127.28
25	B	614	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
29	B	621	SQD	C1-O5-C5	-2.77	108.31	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	520	STE	C3-C2-C1	-2.76	107.30	114.51
30	C	517	DGD	O3G-C1D-C2D	-2.76	104.08	108.27
25	C	508	CLA	O2D-CGD-CBD	2.76	116.06	111.23
25	b	602	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
25	C	512	CLA	CHB-C4A-NA	2.76	128.38	124.40
30	C	518	DGD	C3G-C2G-C1G	-2.76	105.35	111.78
25	B	608	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
27	c	515	BCR	C2-C1-C6	2.76	114.44	110.44
25	d	404	CLA	CMB-C2B-C1B	-2.75	121.22	125.42
25	C	513	CLA	CHB-C4A-NA	2.75	128.38	124.40
29	A	613	SQD	O8-S-C6	2.75	111.29	105.97
25	D	403	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
25	c	509	CLA	C3B-C4B-NB	-2.75	108.08	110.53
25	A	612	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	d	401	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
25	c	508	CLA	O2A-CGA-O1A	-2.75	116.76	123.63
25	B	610	CLA	CHB-C4A-NA	2.75	128.36	124.40
25	d	403	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
25	c	508	CLA	O2D-CGD-CBD	2.74	116.03	111.23
29	b	619	SQD	O5-C5-C4	2.74	114.64	109.70
27	K	101	BCR	C15-C14-C13	-2.74	123.44	127.28
25	B	606	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
25	D	404	CLA	CHB-C4A-NA	2.74	128.35	124.40
25	c	503	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
28	a	611	PL9	C37-C38-C39	-2.73	121.36	127.62
25	c	512	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
33	d	410	LMG	O1-C1-C2	-2.73	104.12	108.27
28	D	406	PL9	C7-C3-C2	-2.73	120.17	123.39
33	c	520	LMG	O8-C28-O10	-2.73	116.80	123.63
28	d	406	PL9	O1-C4-C3	-2.73	117.86	120.73
33	C	519	LMG	O6-C1-O1	-2.72	103.61	110.04
25	b	604	CLA	CHB-C4A-NA	2.72	128.33	124.40
25	C	508	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
27	B	618	BCR	C15-C16-C17	-2.72	117.95	123.52
36	v	201	HEC	CHA-C4D-ND	2.72	128.79	123.86
27	b	617	BCR	C24-C23-C22	-2.72	122.21	126.23
27	x	101	BCR	C2-C1-C6	2.72	114.39	110.44
25	B	605	CLA	CHB-C4A-NA	2.71	128.31	124.40
25	c	512	CLA	C3B-C4B-NB	-2.71	108.11	110.53
30	c	518	DGD	O2D-C2D-C1D	-2.71	103.62	110.08
32	d	408	LHG	O8-C23-C24	2.71	120.09	111.83
27	A	610	BCR	C15-C16-C17	-2.71	117.98	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	410	LMG	O2-C2-C1	-2.70	103.63	110.08
31	C	521	STE	C3-C2-C1	-2.70	107.45	114.51
30	h	102	DGD	C7B-C6B-C5B	-2.70	100.71	114.37
25	c	506	CLA	C3B-C4B-NB	-2.70	108.12	110.53
27	C	514	BCR	C27-C26-C25	2.70	126.35	122.70
28	d	406	PL9	C42-C43-C44	-2.70	121.45	127.62
28	a	611	PL9	O2-C1-C6	2.70	124.77	120.48
25	c	507	CLA	CHC-C4B-NB	2.70	128.09	124.05
27	C	514	BCR	C2-C1-C6	2.69	114.35	110.44
27	Z	101	BCR	C27-C26-C25	2.69	126.34	122.70
25	B	611	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	C	513	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
25	B	611	CLA	O1D-CGD-CBD	2.69	129.82	124.52
27	d	405	BCR	C27-C26-C25	2.69	126.34	122.70
25	b	602	CLA	CHC-C4B-NB	2.69	128.08	124.05
33	c	524	LMG	C1-O6-C5	-2.69	108.47	113.72
28	D	406	PL9	C20-C19-C21	2.69	119.89	115.23
25	d	404	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
29	f	101	SQD	C1-C2-C3	-2.68	104.37	110.01
28	A	611	PL9	C22-C23-C24	-2.68	121.49	127.62
26	d	402	PHO	O1D-CGD-CBD	2.68	128.79	124.72
27	x	101	BCR	C27-C26-C25	2.68	126.32	122.70
25	b	611	CLA	CAC-C3C-C4C	2.68	128.27	124.79
28	D	406	PL9	O1-C4-C3	-2.67	117.92	120.73
25	C	509	CLA	CED-O2D-CGD	2.67	121.97	115.92
25	B	611	CLA	CMB-C2B-C3B	2.67	132.82	126.55
25	b	614	CLA	CHB-C4A-NA	2.67	128.25	124.40
25	B	603	CLA	CHB-C4A-NA	2.66	128.24	124.40
27	b	618	BCR	C11-C10-C9	-2.66	123.55	127.28
25	c	505	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
27	k	101	BCR	C27-C26-C25	2.66	126.30	122.70
25	b	604	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
29	f	101	SQD	O47-C7-C8	2.65	120.68	110.93
27	b	616	BCR	C27-C26-C25	2.65	126.29	122.70
27	t	101	BCR	C29-C30-C25	2.65	114.29	110.44
27	K	101	BCR	C27-C26-C25	2.65	126.29	122.70
27	d	405	BCR	C38-C26-C25	-2.65	121.59	124.48
25	c	502	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
30	C	517	DGD	O2D-C2D-C1D	-2.65	103.77	110.08
27	K	101	BCR	C24-C23-C22	-2.64	122.32	126.23
25	C	504	CLA	CHB-C1B-NB	2.64	128.01	124.05
27	Z	101	BCR	C2-C1-C6	2.64	114.28	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	614	DGD	O3G-C3G-C2G	-2.64	104.40	110.82
27	Z	101	BCR	C15-C14-C13	-2.64	123.58	127.28
30	H	103	DGD	O2D-C2D-C1D	-2.64	103.79	110.08
25	B	605	CLA	C4-C3-C5	2.64	119.81	115.23
27	A	610	BCR	C2-C1-C6	2.63	114.27	110.44
30	C	516	DGD	CDB-CCB-CBB	-2.63	101.05	114.37
25	h	101	CLA	CHB-C4A-NA	2.63	128.20	124.40
28	D	406	PL9	C37-C38-C39	-2.63	121.60	127.62
25	d	404	CLA	CHB-C4A-NA	2.63	128.20	124.40
25	c	510	CLA	C3B-C4B-NB	-2.63	108.18	110.53
26	d	402	PHO	CMA-C3A-C4A	-2.63	108.95	114.61
29	D	408	SQD	C46-C45-C44	-2.63	105.17	113.67
27	c	516	BCR	C27-C26-C25	2.63	126.25	122.70
25	C	512	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
27	H	102	BCR	C16-C15-C14	-2.63	118.15	123.52
28	D	406	PL9	C40-C39-C41	2.62	119.78	115.23
27	a	610	BCR	C27-C26-C25	2.62	126.25	122.70
27	H	102	BCR	C24-C23-C22	-2.62	122.36	126.23
30	C	518	DGD	CDB-CCB-CBB	-2.62	101.13	114.37
29	b	619	SQD	C4-C3-C2	2.62	115.42	110.83
25	A	609	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
25	B	614	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	D	405	BCR	C27-C26-C25	2.61	126.23	122.70
27	c	514	BCR	C27-C26-C25	2.61	126.23	122.70
25	B	613	CLA	CHB-C4A-NA	2.61	128.17	124.40
33	d	410	LMG	C40-C39-C38	-2.61	101.18	114.37
25	B	612	CLA	C6-C5-C3	-2.61	107.11	113.47
25	C	503	CLA	C4-C3-C5	2.61	119.76	115.23
29	B	621	SQD	C4-C3-C2	2.61	115.41	110.83
25	B	612	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
25	C	510	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
29	f	101	SQD	O48-C23-C24	2.61	119.78	111.83
29	B	621	SQD	C25-C24-C23	-2.60	104.16	113.69
25	A	606	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
30	C	516	DGD	O2D-C2D-C1D	-2.59	103.90	110.08
25	C	503	CLA	CHD-C1D-ND	-2.59	121.16	124.80
29	b	619	SQD	O8-S-C6	2.59	110.97	105.97
25	c	507	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	C	506	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
30	H	103	DGD	C4E-C3E-C2E	-2.58	106.30	110.83
25	c	511	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
25	b	611	CLA	CHB-C4A-NA	2.58	128.13	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	CHD-C1D-ND	-2.58	121.18	124.80
32	B	620	LHG	C11-C10-C9	-2.57	101.36	114.37
35	e	101	HEM	CHB-C1B-NB	2.57	127.55	124.37
25	b	606	CLA	CHB-C4A-NA	2.57	128.11	124.40
27	H	102	BCR	C2-C1-C6	2.57	114.17	110.44
33	b	622	LMG	O1-C1-C2	-2.57	104.37	108.27
25	C	509	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	a	608	PHO	CMB-C2B-C3B	2.57	129.82	124.68
25	c	504	CLA	O2D-CGD-CBD	2.57	115.72	111.23
33	b	620	LMG	O3-C3-C2	-2.57	104.32	110.38
27	Y	101	BCR	C33-C5-C6	-2.57	121.68	124.48
30	H	103	DGD	CDB-CCB-CBB	-2.57	101.39	114.37
32	L	101	LHG	C20-C19-C18	-2.57	101.40	114.37
30	c	519	DGD	CDB-CCB-CBB	-2.56	101.41	114.37
27	Y	101	BCR	C16-C15-C14	-2.56	118.28	123.52
25	d	404	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
30	A	614	DGD	O6D-C5D-C6D	-2.56	101.62	106.69
31	B	624	STE	O2-C1-C2	2.56	122.08	114.00
33	C	519	LMG	O2-C2-C1	-2.56	103.98	110.08
27	B	616	BCR	C29-C30-C25	2.56	114.15	110.44
25	b	602	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
25	b	605	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
25	B	604	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
28	D	406	PL9	C42-C43-C44	-2.55	121.79	127.62
25	B	602	CLA	CHD-C4C-NC	2.55	128.18	124.23
25	c	501	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
27	b	618	BCR	C29-C30-C25	2.54	114.13	110.44
29	a	613	SQD	O8-S-C6	2.54	110.88	105.97
25	b	609	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
25	b	602	CLA	O2D-CGD-CBD	2.54	115.67	111.23
25	c	510	CLA	C16-C15-C13	-2.54	107.53	115.97
25	a	612	CLA	O2D-CGD-CBD	2.53	115.66	111.23
25	C	502	CLA	CHB-C1B-NB	2.53	127.85	124.05
25	b	610	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	c	504	CLA	C1-C2-C3	-2.53	122.05	126.20
33	M	101	LMG	C38-C37-C36	-2.53	101.58	114.37
25	C	512	CLA	C1-C2-C3	-2.53	122.05	126.20
25	c	503	CLA	C4-C3-C5	2.53	119.61	115.23
25	B	615	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
25	D	404	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
25	C	508	CLA	CHB-C1B-NB	2.52	127.84	124.05
25	A	612	CLA	O2D-CGD-O1D	-2.52	118.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	511	CLA	C1-C2-C3	-2.52	122.07	126.20
25	D	403	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
25	b	605	CLA	CHB-C1B-NB	2.52	127.82	124.05
25	b	611	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	B	613	CLA	CHC-C4B-NB	2.51	127.82	124.05
25	c	513	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
25	B	604	CLA	CHD-C1D-ND	-2.51	121.27	124.80
25	b	607	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
27	b	617	BCR	C27-C26-C25	2.51	126.09	122.70
25	B	603	CLA	C1-C2-C3	-2.51	122.09	126.20
30	c	517	DGD	O6D-C1D-O3G	-2.51	104.12	110.04
27	A	610	BCR	C33-C5-C6	-2.51	121.75	124.48
25	C	512	CLA	O2D-CGD-CBD	2.50	115.61	111.23
26	d	402	PHO	O2D-CGD-O1D	-2.50	118.98	123.85
25	b	604	CLA	C4-C3-C5	2.50	119.56	115.23
25	B	603	CLA	C6-C5-C3	-2.50	107.39	113.47
27	b	617	BCR	C8-C7-C6	-2.50	120.33	127.00
30	A	614	DGD	O5D-C1E-C2E	2.49	112.06	108.27
31	t	102	STE	C3-C2-C1	-2.49	108.00	114.51
25	B	606	CLA	C2A-C1A-CHA	2.49	128.19	123.87
25	b	603	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
28	a	611	PL9	C20-C19-C21	2.49	119.55	115.23
32	e	102	LHG	C11-C10-C9	-2.49	101.79	114.37
25	b	605	CLA	CMB-C2B-C3B	2.49	132.40	126.55
25	C	507	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
30	C	517	DGD	C4E-C3E-C2E	-2.49	106.47	110.83
30	c	517	DGD	CDB-CCB-CBB	-2.48	101.82	114.37
25	b	607	CLA	CHB-C1B-NB	2.48	127.77	124.05
28	A	611	PL9	C36-C34-C33	-2.48	115.60	121.17
25	B	610	CLA	CHD-C4C-NC	2.48	128.07	124.23
25	b	601	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
28	A	611	PL9	C40-C39-C41	2.47	119.52	115.23
25	C	511	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
25	B	606	CLA	C3B-C4B-NB	-2.47	108.32	110.53
36	v	201	HEC	CMD-C2D-C1D	2.47	129.18	125.42
25	b	608	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
25	B	606	CLA	CMB-C2B-C3B	2.47	132.36	126.55
32	B	620	LHG	C18-C17-C16	-2.47	101.89	114.37
25	H	101	CLA	O2D-CGD-CBD	2.47	115.54	111.23
33	C	519	LMG	C40-C39-C38	-2.47	101.90	114.37
27	Z	101	BCR	C33-C5-C6	-2.47	121.79	124.48
25	B	609	CLA	CAC-C3C-C4C	2.46	127.99	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
25	B	602	CLA	O2D-CGD-CBD	2.46	115.53	111.23
30	C	517	DGD	C1D-C2D-C3D	-2.46	104.84	110.01
29	T	103	SQD	O48-C23-C24	2.46	119.33	111.83
25	C	504	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
32	b	623	LHG	C11-C10-C9	-2.45	101.97	114.37
25	C	507	CLA	C1-C2-C3	-2.45	122.18	126.20
27	k	101	BCR	C33-C5-C6	-2.45	121.81	124.48
25	b	606	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
25	a	607	CLA	C11-C12-C13	-2.45	107.83	115.97
28	D	406	PL9	C22-C23-C24	-2.45	122.03	127.62
28	a	611	PL9	C40-C39-C41	2.44	119.47	115.23
27	b	616	BCR	C33-C5-C6	-2.44	121.82	124.48
26	a	608	PHO	O2A-CGA-O1A	-2.44	117.53	123.63
30	C	516	DGD	C5B-C4B-C3B	-2.44	102.04	114.37
27	d	405	BCR	C11-C10-C9	-2.44	123.86	127.28
25	C	504	CLA	CHD-C4C-NC	2.44	128.01	124.23
27	c	514	BCR	C24-C23-C22	-2.44	122.63	126.23
27	B	618	BCR	C34-C9-C10	-2.43	118.87	122.82
30	h	102	DGD	O3E-C3E-C2E	-2.43	104.64	110.38
30	c	518	DGD	CBB-CAB-C9B	-2.43	102.07	114.37
25	b	602	CLA	CHB-C1B-NB	2.43	127.70	124.05
30	c	517	DGD	C4D-C3D-C2D	-2.43	106.56	110.83
32	B	620	LHG	O8-C23-O10	-2.43	117.55	123.63
25	b	609	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
25	b	609	CLA	CAA-CBA-CGA	-2.43	106.31	113.21
28	a	611	PL9	C27-C28-C29	-2.43	122.06	127.62
25	c	510	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
28	a	611	PL9	O2-C1-C2	-2.43	116.31	121.83
30	a	615	DGD	CDB-CCB-CBB	-2.43	102.11	114.37
33	b	622	LMG	O2-C2-C1	-2.42	104.30	110.08
28	A	611	PL9	O2-C1-C2	-2.42	116.32	121.83
33	M	101	LMG	C40-C39-C38	-2.42	102.14	114.37
27	c	514	BCR	C2-C1-C6	2.42	113.95	110.44
25	b	607	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
32	l	101	LHG	C5-O7-C7	-2.42	112.01	117.80
27	b	618	BCR	C27-C26-C25	2.42	125.97	122.70
33	b	620	LMG	C40-C39-C38	-2.42	102.16	114.37
25	A	606	CLA	O2A-CGA-O1A	-2.42	117.59	123.63
33	c	522	LMG	C40-C39-C38	-2.41	102.17	114.37
25	B	610	CLA	CHD-C1D-C2D	2.41	130.50	125.49
25	C	509	CLA	CMB-C2B-C1B	-2.41	121.75	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
25	a	607	CLA	CHB-C4A-NA	2.41	127.87	124.40
27	B	618	BCR	C11-C10-C9	-2.41	123.90	127.28
33	c	524	LMG	O6-C1-O1	-2.40	104.36	110.04
28	D	406	PL9	C12-C13-C14	-2.40	122.13	127.62
35	e	101	HEM	CAB-C3B-C2B	-2.40	120.64	128.43
25	c	507	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
33	c	522	LMG	O2-C2-C1	-2.39	104.37	110.08
30	C	517	DGD	CDB-CCB-CBB	-2.39	102.28	114.37
25	C	510	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
25	B	612	CLA	C2A-C1A-CHA	2.39	128.01	123.87
25	A	612	CLA	CMB-C2B-C3B	2.39	132.17	126.55
25	C	508	CLA	CMB-C2B-C3B	2.39	132.16	126.55
25	b	603	CLA	O2D-CGD-CBD	2.39	115.40	111.23
25	b	612	CLA	CHB-C4A-NA	2.38	127.84	124.40
29	f	101	SQD	C3-C4-C5	2.38	114.56	110.23
33	C	515	LMG	C40-C39-C38	-2.38	102.32	114.37
25	C	506	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
28	a	611	PL9	C45-C44-C46	-2.38	111.09	115.23
25	B	613	CLA	O2D-CGD-CBD	2.38	115.39	111.23
25	A	609	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	b	609	CLA	C3B-C4B-NB	-2.38	108.41	110.53
25	C	506	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	C	505	CLA	CHB-C1B-NB	2.37	127.61	124.05
25	b	612	CLA	CMB-C2B-C3B	2.37	132.13	126.55
33	c	520	LMG	C38-C37-C36	-2.37	102.39	114.37
32	D	409	LHG	C11-C10-C9	-2.37	102.39	114.37
33	C	519	LMG	O1-C7-C8	-2.37	105.06	110.82
33	D	412	LMG	C38-C37-C36	-2.37	102.39	114.37
26	A	608	PHO	C1-C2-C3	-2.37	122.32	126.20
25	C	511	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
33	D	407	LMG	C38-C37-C36	-2.37	102.41	114.37
32	b	623	LHG	C27-C26-C25	-2.36	102.42	114.37
30	c	519	DGD	O5D-C6D-C5D	-2.36	104.09	109.42
25	C	508	CLA	CHD-C1D-ND	-2.36	121.48	124.80
33	c	520	LMG	C40-C39-C38	-2.36	102.42	114.37
25	B	604	CLA	O1D-CGD-CBD	2.36	129.17	124.52
25	d	401	CLA	O2D-CGD-CBD	2.36	115.36	111.23
26	D	402	PHO	C3B-C4B-NB	-2.36	105.93	107.46
33	C	515	LMG	C38-C37-C36	-2.36	102.46	114.37
25	B	609	CLA	C1-C2-C3	-2.36	122.34	126.20
27	b	616	BCR	C11-C10-C9	-2.36	123.97	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	l	101	LHG	C18-C17-C16	-2.35	102.47	114.37
25	A	612	CLA	CHD-C1D-ND	-2.35	121.49	124.80
27	B	618	BCR	C1-C6-C5	-2.35	119.42	122.64
25	C	504	CLA	CHD-C1D-ND	-2.35	121.49	124.80
25	b	612	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
27	K	101	BCR	C15-C16-C17	-2.35	118.71	123.52
25	B	610	CLA	C1-C2-C3	-2.35	122.35	126.20
26	d	402	PHO	C3B-C4B-NB	-2.35	105.93	107.46
25	c	504	CLA	CMB-C2B-C3B	2.35	132.07	126.55
28	D	406	PL9	C35-C34-C36	2.35	119.30	115.23
33	c	524	LMG	O1-C7-C8	-2.35	105.11	110.82
33	c	522	LMG	C3-C4-C5	-2.34	105.98	110.23
31	b	621	STE	C3-C2-C1	-2.34	108.39	114.51
25	C	503	CLA	O1D-CGD-CBD	2.34	129.14	124.52
30	h	102	DGD	CDB-CCB-CBB	-2.34	102.55	114.37
32	E	101	LHG	C11-C10-C9	-2.34	102.55	114.37
25	d	404	CLA	CMB-C2B-C3B	2.34	132.05	126.55
25	C	506	CLA	C3B-C4B-NB	-2.34	108.44	110.53
25	B	607	CLA	CHB-C1B-NB	2.34	127.56	124.05
29	b	619	SQD	O5-C1-C2	-2.34	105.57	110.37
30	a	615	DGD	C5B-C4B-C3B	-2.34	102.56	114.37
25	A	607	CLA	O2D-CGD-CBD	2.33	115.31	111.23
25	C	502	CLA	C4D-CHA-C1A	2.33	124.02	121.24
25	c	501	CLA	C1-C2-C3	-2.33	122.38	126.20
31	d	411	STE	O2-C1-C2	2.33	121.35	114.00
33	d	410	LMG	O1-C7-C8	-2.33	105.16	110.82
32	e	102	LHG	C20-C19-C18	-2.33	102.61	114.37
25	B	612	CLA	CHA-C1A-NA	-2.33	121.12	126.39
25	B	608	CLA	CHB-C4A-NA	2.33	127.76	124.40
33	b	620	LMG	O7-C10-O9	-2.33	118.27	123.70
32	D	409	LHG	C20-C19-C18	-2.33	102.61	114.37
35	e	101	HEM	C3B-C2B-C1B	2.33	108.16	106.41
25	A	607	CLA	CHD-C1D-ND	-2.32	121.53	124.80
25	C	513	CLA	C3B-C4B-NB	-2.32	108.45	110.53
29	b	619	SQD	C9-C8-C7	-2.32	105.18	113.69
25	b	603	CLA	CHD-C1D-ND	-2.32	121.53	124.80
33	M	101	LMG	C1-O6-C5	-2.32	109.18	113.72
25	B	607	CLA	CHC-C4B-NB	2.32	127.53	124.05
25	A	609	CLA	CMB-C2B-C3B	2.32	132.00	126.55
27	Y	101	BCR	C8-C7-C6	-2.32	120.81	127.00
25	B	612	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	b	603	CLA	C3B-C4B-NB	-2.32	108.46	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	516	BCR	C33-C5-C6	-2.32	121.96	124.48
26	A	608	PHO	C3B-C4B-NB	-2.32	105.95	107.46
25	B	609	CLA	CHC-C1C-NC	2.31	127.80	124.31
25	B	606	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
27	B	616	BCR	C27-C26-C25	2.31	125.82	122.70
28	d	406	PL9	C27-C28-C29	-2.31	122.34	127.62
29	a	613	SQD	C3-C4-C5	2.31	114.42	110.23
25	H	101	CLA	C1-C2-C3	-2.31	122.42	126.20
30	C	516	DGD	CAB-C9B-C8B	-2.31	102.71	114.37
25	D	403	CLA	C1-C2-C3	-2.31	122.42	126.20
25	A	612	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
30	A	614	DGD	C8B-C7B-C6B	-2.30	102.72	114.37
27	C	514	BCR	C15-C16-C17	-2.30	118.81	123.52
33	b	622	LMG	C40-C39-C38	-2.30	102.73	114.37
25	b	601	CLA	C3B-C4B-NB	-2.30	108.48	110.53
25	B	614	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
33	C	519	LMG	C6-C5-C4	-2.30	107.38	113.02
25	b	601	CLA	C4-C3-C5	2.30	119.21	115.23
33	d	410	LMG	C38-C37-C36	-2.29	102.77	114.37
25	a	609	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
35	F	101	HEM	CHC-C4B-NB	2.29	126.89	124.42
25	C	507	CLA	CHB-C4A-NA	2.29	127.70	124.40
28	A	611	PL9	C20-C19-C21	2.29	119.20	115.23
25	c	504	CLA	C3B-C4B-NB	-2.29	108.49	110.53
25	b	612	CLA	C7-C6-C5	-2.29	107.17	113.26
25	B	605	CLA	O2D-CGD-CBD	2.28	115.22	111.23
29	D	408	SQD	C3-C4-C5	2.28	114.37	110.23
33	b	622	LMG	O6-C5-C6	2.28	112.09	106.44
27	d	405	BCR	C2-C1-C6	2.28	113.75	110.44
25	H	101	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
25	c	503	CLA	C1-C2-C3	-2.28	122.46	126.20
25	c	503	CLA	CHD-C1D-ND	-2.28	121.60	124.80
25	B	612	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
29	B	621	SQD	O8-S-C6	2.28	110.36	105.97
36	V	201	HEC	CBD-CAD-C3D	-2.27	106.24	112.53
25	B	608	CLA	CHC-C4B-NB	2.27	127.46	124.05
31	t	102	STE	O2-C1-C2	2.27	121.18	114.00
25	C	503	CLA	C7-C6-C5	-2.27	107.20	113.26
30	c	517	DGD	C4E-C3E-C2E	-2.27	106.84	110.83
25	c	510	CLA	CHB-C4A-NA	2.27	127.68	124.40
27	b	616	BCR	C15-C14-C13	-2.27	124.09	127.28
25	b	611	CLA	O2A-CGA-O1A	-2.27	117.95	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	510	CLA	O2D-CGD-CBD	2.27	115.20	111.23
25	C	504	CLA	CED-O2D-CGD	2.27	121.06	115.92
33	C	519	LMG	C38-C37-C36	-2.27	102.91	114.37
31	B	623	STE	C3-C2-C1	-2.27	108.59	114.51
30	A	614	DGD	CBB-CAB-C9B	-2.27	102.91	114.37
33	C	515	LMG	O1-C7-C8	-2.27	105.31	110.82
31	m	101	STE	C3-C2-C1	-2.26	108.60	114.51
27	t	101	BCR	C30-C25-C26	-2.26	119.54	122.64
30	C	517	DGD	C3E-C4E-C5E	-2.26	106.13	110.23
25	h	101	CLA	CHD-C1D-ND	-2.26	121.62	124.80
25	B	610	CLA	CMB-C2B-C3B	2.26	131.87	126.55
27	t	101	BCR	C27-C26-C25	2.26	125.76	122.70
25	c	512	CLA	CHC-C1C-NC	2.26	127.71	124.31
26	A	608	PHO	O2D-CGD-CBD	2.26	113.43	110.95
25	B	602	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
25	d	401	CLA	CHD-C1D-ND	-2.25	121.63	124.80
31	M	102	STE	C3-C2-C1	-2.25	108.63	114.51
25	b	607	CLA	CMB-C2B-C3B	2.25	131.85	126.55
27	c	516	BCR	C11-C10-C9	-2.25	124.12	127.28
25	b	615	CLA	CMB-C2B-C3B	2.25	131.85	126.55
29	D	408	SQD	O8-S-C6	2.25	110.32	105.97
26	D	402	PHO	CMA-C3A-C4A	-2.25	109.77	114.61
26	a	608	PHO	C1A-C2A-C3A	-2.25	100.70	102.84
27	B	618	BCR	C29-C30-C25	2.24	113.69	110.44
27	x	101	BCR	C15-C14-C13	-2.24	124.14	127.28
25	B	604	CLA	C3B-C4B-NB	-2.24	108.53	110.53
28	A	611	PL9	O2-C1-C6	2.24	124.04	120.48
25	B	605	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
25	C	502	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
30	a	615	DGD	CFB-CEB-CDB	-2.24	103.06	114.37
27	t	101	BCR	C31-C1-C6	2.24	113.75	110.24
33	c	522	LMG	O7-C10-O9	-2.23	118.49	123.70
32	B	620	LHG	C20-C19-C18	-2.23	103.11	114.37
32	D	410	LHG	C27-C26-C25	-2.23	103.11	114.37
25	C	509	CLA	CMB-C2B-C3B	2.23	131.79	126.55
25	D	403	CLA	C6-C5-C3	2.23	118.89	113.47
29	a	613	SQD	O5-C1-C2	-2.23	105.80	110.37
32	D	409	LHG	C27-C26-C25	-2.22	103.12	114.37
25	b	607	CLA	C2A-C1A-CHA	2.22	127.72	123.87
25	a	612	CLA	CHD-C1D-ND	-2.22	121.68	124.80
27	D	405	BCR	C3-C4-C5	-2.22	110.10	114.06
25	A	609	CLA	CHD-C1D-ND	-2.22	121.68	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	518	DGD	O5D-C6D-C5D	-2.22	104.42	109.42
33	b	620	LMG	C38-C37-C36	-2.22	103.16	114.37
25	b	601	CLA	CAC-C3C-C4C	2.22	127.67	124.79
25	c	502	CLA	O2D-CGD-CBD	2.21	115.10	111.23
27	b	616	BCR	C24-C23-C22	-2.21	122.96	126.23
29	B	621	SQD	O5-C1-C2	-2.21	105.83	110.37
30	c	518	DGD	C8B-C7B-C6B	-2.21	103.19	114.37
25	b	612	CLA	CHC-C4B-NB	2.21	127.36	124.05
27	K	101	BCR	C2-C1-C6	2.21	113.65	110.44
25	b	614	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
25	A	609	CLA	C3B-C4B-NB	-2.20	108.56	110.53
33	C	519	LMG	O7-C10-O9	-2.20	118.55	123.70
25	B	607	CLA	CHA-C1A-NA	-2.20	121.40	126.39
25	D	404	CLA	C1-C2-C3	-2.20	122.59	126.20
25	b	609	CLA	CHB-C4A-NA	2.20	127.58	124.40
33	D	407	LMG	O3-C3-C2	-2.20	105.19	110.38
25	c	513	CLA	O2D-CGD-CBD	2.20	115.08	111.23
25	B	615	CLA	CHB-C4A-NA	2.20	127.58	124.40
33	D	411	LMG	C38-C37-C36	-2.20	103.25	114.37
25	B	604	CLA	CHD-C4C-NC	2.20	127.64	124.23
25	c	504	CLA	CHB-C4A-NA	2.20	127.57	124.40
25	H	101	CLA	C4-C3-C5	2.20	119.04	115.23
25	C	504	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
25	C	503	CLA	CHB-C4A-NA	2.20	127.57	124.40
25	b	611	CLA	C16-C15-C13	-2.20	108.67	115.97
27	B	617	BCR	C30-C25-C26	-2.19	119.64	122.64
25	b	611	CLA	O1D-CGD-CBD	2.19	128.84	124.52
30	H	103	DGD	O6D-C1D-O3G	-2.19	104.87	110.04
25	B	606	CLA	CED-O2D-CGD	2.19	120.88	115.92
27	c	514	BCR	C7-C8-C9	-2.19	123.00	126.23
27	c	516	BCR	C2-C1-C6	2.19	113.62	110.44
27	d	405	BCR	C24-C23-C22	-2.19	123.00	126.23
30	c	518	DGD	O2E-C2E-C1E	-2.19	104.86	110.08
33	d	409	LMG	C38-C37-C36	-2.19	103.31	114.37
25	b	610	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
25	b	611	CLA	CMB-C2B-C3B	2.19	131.69	126.55
30	c	518	DGD	O2G-C1B-O1B	-2.18	118.60	123.70
32	D	410	LHG	O8-C23-C24	2.18	118.49	111.83
30	c	519	DGD	O3G-C1D-C2D	-2.18	104.96	108.27
25	C	507	CLA	C2A-C1A-CHA	2.18	127.65	123.87
25	h	101	CLA	O2D-CGD-CBD	2.18	115.04	111.23
25	b	613	CLA	O2D-CGD-O1D	-2.18	119.61	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	522	LMG	O8-C28-O10	-2.18	118.18	123.63
25	A	609	CLA	CHD-C4C-NC	2.18	127.61	124.23
26	A	608	PHO	OBD-CAD-C3D	2.18	131.29	127.89
33	c	522	LMG	O6-C1-O1	-2.18	104.90	110.04
25	a	612	CLA	C3B-C4B-NB	-2.18	108.59	110.53
27	d	405	BCR	C3-C4-C5	-2.18	110.17	114.06
27	A	610	BCR	C38-C26-C25	-2.18	122.11	124.48
30	A	614	DGD	O2D-C2D-C1D	-2.18	104.89	110.08
25	a	607	CLA	C3B-C4B-NB	-2.17	108.59	110.53
25	c	513	CLA	CMB-C2B-C3B	2.17	131.66	126.55
25	B	612	CLA	CHC-C4B-NB	2.17	127.31	124.05
31	c	523	STE	O2-C1-C2	2.17	120.86	114.00
25	d	401	CLA	CHC-C1C-NC	2.17	127.58	124.31
25	C	502	CLA	CHA-C1A-NA	-2.17	121.48	126.39
29	b	619	SQD	C1-C2-C3	-2.17	105.45	110.01
29	b	619	SQD	O9-S-C6	2.17	109.99	106.76
32	E	101	LHG	C20-C19-C18	-2.17	103.41	114.37
25	b	606	CLA	O1D-CGD-CBD	2.17	128.79	124.52
28	a	611	PL9	C35-C34-C36	2.17	118.99	115.23
25	B	605	CLA	CHD-C4C-NC	2.17	127.59	124.23
30	H	103	DGD	CAB-C9B-C8B	-2.17	103.42	114.37
25	d	403	CLA	O2D-CGD-CBD	2.16	115.01	111.23
25	C	501	CLA	C1-C2-C3	-2.16	122.65	126.20
30	h	102	DGD	O6E-C5E-C4E	2.16	113.59	109.70
30	c	517	DGD	C6D-O5D-C1E	2.16	118.43	113.80
25	C	504	CLA	CHB-C4A-NA	2.16	127.52	124.40
33	M	101	LMG	C8-O7-C10	2.16	122.96	117.80
25	b	609	CLA	C11-C10-C8	-2.16	108.80	115.97
25	b	602	CLA	O1D-CGD-CBD	2.16	128.77	124.52
33	c	524	LMG	C40-C39-C38	-2.16	103.47	114.37
28	a	611	PL9	C32-C33-C34	-2.16	122.69	127.62
25	b	607	CLA	CHA-C1A-NA	-2.16	121.51	126.39
25	b	603	CLA	C1D-ND-C4D	2.15	107.82	106.31
25	d	404	CLA	CHA-C1A-NA	-2.15	121.51	126.39
25	B	611	CLA	C16-C15-C13	-2.15	108.81	115.97
25	b	608	CLA	CHB-C4A-NA	2.15	127.51	124.40
30	C	517	DGD	C5B-C4B-C3B	-2.15	103.50	114.37
25	B	604	CLA	CHD-C1D-C2D	2.15	129.96	125.49
25	b	608	CLA	CHA-C1A-NA	-2.15	121.52	126.39
33	c	520	LMG	O6-C1-O1	-2.15	104.97	110.04
25	C	513	CLA	C2A-C1A-CHA	2.15	127.59	123.87
28	D	406	PL9	C32-C33-C34	-2.15	122.71	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	608	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
25	c	511	CLA	CHB-C4A-NA	2.15	127.50	124.40
25	b	607	CLA	CAC-C3C-C2C	2.15	131.50	127.56
30	H	103	DGD	C3G-C2G-C1G	-2.15	106.78	111.78
30	A	614	DGD	CAB-C9B-C8B	-2.14	103.53	114.37
25	B	608	CLA	CHA-C1A-NA	-2.14	121.53	126.39
28	d	406	PL9	C32-C33-C34	-2.14	122.72	127.62
26	d	402	PHO	O2A-CGA-O1A	-2.14	118.27	123.63
25	C	504	CLA	CHA-C1A-NA	-2.14	121.54	126.39
30	h	102	DGD	C3G-C2G-C1G	-2.14	106.79	111.78
25	c	507	CLA	CHB-C4A-NA	2.14	127.49	124.40
30	C	518	DGD	C6D-C5D-C4D	2.14	116.56	112.07
25	c	510	CLA	C4-C3-C5	2.14	118.94	115.23
33	b	620	LMG	O2-C2-C1	-2.14	104.98	110.08
25	C	501	CLA	C11-C12-C13	-2.14	108.86	115.97
25	B	601	CLA	CMB-C2B-C3B	2.14	131.57	126.55
33	D	407	LMG	O1-C1-C2	-2.13	105.03	108.27
25	C	502	CLA	O1D-CGD-CBD	2.13	128.72	124.52
25	B	614	CLA	C6-C7-C8	-2.13	108.88	115.97
25	C	511	CLA	C3B-C4B-NB	-2.13	108.63	110.53
25	B	603	CLA	C2D-C1D-ND	-2.13	108.02	110.13
25	C	513	CLA	O1D-CGD-CBD	2.13	128.71	124.52
25	C	504	CLA	CMB-C2B-C3B	2.13	131.55	126.55
25	B	610	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
25	c	502	CLA	CHB-C1B-NB	2.13	127.24	124.05
27	B	617	BCR	C3-C4-C5	-2.13	110.27	114.06
25	C	509	CLA	CHD-C4C-NC	2.12	127.53	124.23
27	c	516	BCR	C38-C26-C25	-2.12	122.17	124.48
32	b	623	LHG	C20-C19-C18	-2.12	103.63	114.37
25	c	502	CLA	CHD-C1D-C2D	2.12	129.91	125.49
25	b	603	CLA	CBA-CAA-C2A	-2.12	107.48	113.79
27	t	101	BCR	C11-C10-C9	-2.12	124.30	127.28
29	a	614	SQD	O48-C23-O10	-2.12	118.32	123.63
25	C	505	CLA	CHB-C4A-NA	2.12	127.46	124.40
30	C	517	DGD	O2G-C1B-O1B	-2.12	118.75	123.70
25	b	611	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
32	E	101	LHG	C27-C26-C25	-2.12	103.67	114.37
25	b	604	CLA	CHD-C4C-NC	2.12	127.51	124.23
30	C	516	DGD	O2E-C2E-C1E	-2.12	105.03	110.08
30	c	519	DGD	O2D-C2D-C1D	-2.12	105.03	110.08
25	b	603	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
27	K	101	BCR	C21-C20-C19	-2.11	117.08	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	101	HEM	O2D-CGD-CBD	2.11	120.67	114.00
27	H	102	BCR	C30-C25-C26	-2.11	119.75	122.64
33	c	522	LMG	C42-C41-C40	-2.11	103.70	114.37
32	d	407	LHG	O8-C23-O10	-2.11	118.36	123.63
25	C	501	CLA	CAA-CBA-CGA	-2.11	107.22	113.21
32	l	101	LHG	C27-C26-C25	-2.11	103.72	114.37
25	b	614	CLA	CHB-C1B-NB	2.11	127.21	124.05
25	B	613	CLA	O1D-CGD-CBD	2.10	128.67	124.52
30	C	516	DGD	C7B-C6B-C5B	-2.10	103.74	114.37
36	V	201	HEC	C2A-C1A-NA	-2.10	108.29	110.32
25	b	609	CLA	CAC-C3C-C2C	-2.10	123.69	127.56
33	M	101	LMG	O6-C1-O1	-2.10	105.08	110.04
33	c	520	LMG	O3-C3-C2	-2.10	105.42	110.38
25	b	602	CLA	CMB-C2B-C3B	2.10	131.49	126.55
33	d	409	LMG	O7-C10-O9	-2.10	117.94	123.33
25	B	606	CLA	C4-C3-C5	2.10	118.87	115.23
36	V	201	HEC	CAA-C2A-C3A	-2.10	123.94	127.87
33	C	515	LMG	O3-C3-C2	-2.10	105.43	110.38
25	b	609	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	B	601	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
25	b	612	CLA	C16-C15-C13	-2.09	109.00	115.97
31	B	622	STE	O2-C1-C2	2.09	120.62	114.00
27	B	618	BCR	C33-C5-C6	-2.09	122.20	124.48
30	c	518	DGD	C1D-O6D-C5D	-2.09	109.64	113.72
30	h	102	DGD	CBB-CAB-C9B	-2.09	103.81	114.37
25	c	506	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
27	Z	101	BCR	C11-C10-C9	-2.09	124.35	127.28
32	l	101	LHG	C20-C19-C18	-2.09	103.82	114.37
25	C	505	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
30	c	519	DGD	CBB-CAB-C9B	-2.09	103.83	114.37
25	c	512	CLA	O1D-CGD-CBD	2.08	128.63	124.52
25	B	603	CLA	O2D-CGD-CBD	2.08	114.87	111.23
25	b	609	CLA	CHA-C4D-ND	2.08	136.85	132.55
25	c	501	CLA	CHB-C4A-NA	2.08	127.41	124.40
32	L	101	LHG	O8-C23-C24	2.08	118.18	111.83
25	B	601	CLA	C1-C2-C3	-2.08	122.79	126.20
28	D	406	PL9	C41-C39-C38	-2.08	116.50	121.17
27	B	616	BCR	C24-C23-C22	-2.08	123.16	126.23
26	a	608	PHO	C3D-C4D-ND	2.08	110.37	107.71
27	Y	101	BCR	C10-C11-C12	-2.08	117.17	123.20
25	b	608	CLA	O1D-CGD-CBD	2.08	128.62	124.52
25	d	403	CLA	O2A-CGA-O1A	-2.08	118.43	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	613	SQD	O47-C7-O49	-2.08	118.85	123.70
25	A	607	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
26	A	608	PHO	O2D-CGD-O1D	-2.08	119.81	123.85
25	c	507	CLA	O2D-CGD-CBD	2.08	114.86	111.23
25	a	609	CLA	CHA-C1A-NA	-2.07	121.69	126.39
25	b	612	CLA	C3B-C4B-NB	-2.07	108.68	110.53
32	D	410	LHG	C11-C10-C9	-2.07	103.89	114.37
27	a	610	BCR	C11-C10-C9	-2.07	124.37	127.28
27	a	610	BCR	C8-C7-C6	-2.07	121.46	127.00
25	C	509	CLA	CHD-C1D-C2D	2.07	129.80	125.49
29	a	613	SQD	O9-S-C6	2.07	109.85	106.76
25	c	511	CLA	C2A-C1A-CHA	2.07	127.46	123.87
32	D	409	LHG	C18-C17-C16	-2.07	103.90	114.37
33	b	620	LMG	C22-C21-C20	-2.07	103.91	114.37
33	c	522	LMG	C38-C37-C36	-2.07	103.91	114.37
28	d	406	PL9	C8-C7-C3	2.07	117.38	112.03
25	c	510	CLA	CMB-C2B-C3B	2.07	131.42	126.55
30	C	517	DGD	CAB-C9B-C8B	-2.07	103.92	114.37
25	b	602	CLA	C1-C2-C3	-2.07	122.81	126.20
30	H	103	DGD	C1D-O6D-C5D	-2.07	109.68	113.72
27	c	515	BCR	C33-C5-C6	-2.06	122.23	124.48
29	a	613	SQD	O5-C5-C4	2.06	113.42	109.70
25	c	502	CLA	CHD-C4C-NC	2.06	127.43	124.23
30	c	519	DGD	O6E-C1E-O5D	-2.06	105.17	110.04
33	D	407	LMG	O7-C10-O9	-2.06	118.88	123.70
30	A	614	DGD	C5B-C4B-C3B	-2.06	103.94	114.37
30	c	519	DGD	CAB-C9B-C8B	-2.06	103.94	114.37
30	a	615	DGD	C1G-C2G-C3G	-2.06	107.04	111.80
27	b	616	BCR	C29-C30-C25	2.06	113.43	110.44
25	c	503	CLA	C7-C6-C5	-2.06	107.78	113.26
25	C	510	CLA	CHB-C1B-NB	2.06	127.14	124.05
27	K	101	BCR	C11-C10-C9	-2.06	124.39	127.28
32	e	102	LHG	C18-C17-C16	-2.06	103.97	114.37
27	H	102	BCR	C1-C6-C5	-2.06	119.83	122.64
30	c	519	DGD	O3E-C3E-C2E	-2.06	105.53	110.38
25	C	506	CLA	CHA-C1A-NA	-2.05	121.74	126.39
25	C	503	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
30	a	615	DGD	CBB-CAB-C9B	-2.05	103.99	114.37
25	B	606	CLA	CHA-C1A-NA	-2.05	121.74	126.39
25	c	507	CLA	CHB-C1B-NB	2.05	127.13	124.05
27	b	618	BCR	C16-C17-C18	-2.05	124.40	127.28
32	D	410	LHG	O10-C23-C24	-2.05	115.76	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	614	CLA	C4-C3-C5	2.05	118.79	115.23
33	c	524	LMG	C9-C8-C7	-2.05	107.00	111.78
31	J	101	STE	O2-C1-C2	2.05	120.48	114.00
25	B	614	CLA	O2D-CGD-CBD	2.05	114.81	111.23
32	l	101	LHG	C11-C10-C9	-2.05	104.01	114.37
32	D	410	LHG	C18-C17-C16	-2.05	104.01	114.37
25	b	606	CLA	C6-C7-C8	-2.05	109.16	115.97
28	d	406	PL9	C7-C8-C9	-2.05	123.30	126.83
27	b	618	BCR	C2-C1-C6	2.05	113.41	110.44
25	D	404	CLA	CHA-C4D-ND	2.05	136.77	132.55
30	C	517	DGD	CBB-CAB-C9B	-2.05	104.02	114.37
25	b	604	CLA	O1A-CGA-CBA	2.05	131.79	123.78
32	B	620	LHG	C27-C26-C25	-2.05	104.03	114.37
25	c	505	CLA	CHA-C1A-NA	-2.04	121.76	126.39
27	B	618	BCR	C27-C26-C25	2.04	125.47	122.70
25	C	501	CLA	CHA-C4D-ND	2.04	136.76	132.55
30	c	519	DGD	C1D-C2D-C3D	-2.04	105.71	110.01
25	C	507	CLA	CHC-C4B-NB	2.04	127.11	124.05
33	c	520	LMG	O2-C2-C1	-2.04	105.21	110.08
28	A	611	PL9	C12-C13-C14	-2.04	122.95	127.62
25	a	607	CLA	C11-C10-C8	-2.04	109.18	115.97
25	B	601	CLA	CHC-C4B-NB	2.04	127.11	124.05
28	d	406	PL9	C12-C13-C14	-2.04	122.95	127.62
25	c	507	CLA	C2A-C1A-CHA	2.04	127.41	123.87
25	h	101	CLA	CHB-C1B-NB	2.04	127.11	124.05
25	a	612	CLA	CHD-C1D-C2D	2.04	129.73	125.49
25	c	502	CLA	C1-C2-C3	-2.04	122.86	126.20
25	B	607	CLA	C3B-C4B-NB	-2.04	108.71	110.53
25	b	603	CLA	C11-C10-C8	-2.04	109.19	115.97
27	T	101	BCR	C7-C8-C9	-2.04	123.22	126.23
25	B	607	CLA	C11-C12-C13	-2.04	109.19	115.97
30	C	518	DGD	CBB-CAB-C9B	-2.04	104.08	114.37
33	c	524	LMG	O8-C28-O10	-2.04	118.54	123.63
28	A	611	PL9	C27-C28-C29	-2.04	122.97	127.62
33	C	519	LMG	O3-C3-C2	-2.03	105.58	110.38
25	c	506	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
27	b	617	BCR	C38-C26-C25	-2.03	122.27	124.48
29	A	613	SQD	O9-S-C6	2.03	109.79	106.76
32	d	408	LHG	C27-C26-C25	-2.03	104.10	114.37
33	D	407	LMG	O1-C7-C8	-2.03	105.88	110.82
25	c	505	CLA	CHB-C1B-NB	2.03	127.09	124.05
27	B	616	BCR	C33-C5-C6	-2.03	122.27	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	503	CLA	CHD-C1D-C2D	2.03	129.71	125.49
28	D	406	PL9	C7-C8-C9	-2.03	123.34	126.83
25	b	613	CLA	CHD-C1D-ND	-2.03	121.95	124.80
30	c	519	DGD	C5B-C4B-C3B	-2.03	104.12	114.37
33	b	620	LMG	O8-C28-O10	-2.03	118.56	123.63
25	D	404	CLA	CHA-C1A-NA	-2.02	121.81	126.39
29	T	103	SQD	C9-C8-C7	-2.02	106.30	113.69
25	C	505	CLA	CHA-C1A-NA	-2.02	121.82	126.39
25	C	501	CLA	CHD-C1D-C2D	2.02	129.69	125.49
33	D	407	LMG	O2-C2-C1	-2.02	105.27	110.08
25	c	506	CLA	CHA-C1A-NA	-2.02	121.82	126.39
33	M	101	LMG	C31-C30-C29	-2.02	105.72	113.13
30	c	517	DGD	CBB-CAB-C9B	-2.02	104.18	114.37
32	b	623	LHG	C18-C17-C16	-2.02	104.18	114.37
25	C	502	CLA	CHA-C4D-ND	2.02	136.71	132.55
25	D	404	CLA	C2D-C1D-ND	-2.01	108.13	110.13
25	b	602	CLA	CHD-C1D-ND	-2.01	121.97	124.80
25	b	608	CLA	C1-C2-C3	-2.01	122.90	126.20
35	e	101	HEM	C1B-NB-C4B	2.01	107.59	105.21
25	c	512	CLA	CHD-C1D-C2D	2.01	129.66	125.49
33	M	101	LMG	C22-C21-C20	-2.01	104.22	114.37
25	d	404	CLA	C1-C2-C3	-2.01	122.91	126.20
33	C	515	LMG	C1-C2-C3	-2.01	105.79	110.01
33	c	524	LMG	O5-C6-C5	-2.01	104.50	111.33
30	c	519	DGD	C7A-C6A-C5A	-2.00	104.23	114.37
25	C	502	CLA	C1-C2-C3	-2.00	122.91	126.20
29	a	614	SQD	O49-C7-C8	-2.00	115.94	123.78
25	b	603	CLA	CHD-C1D-C2D	2.00	129.66	125.49
27	t	101	BCR	C15-C16-C17	-2.00	119.42	123.52
32	e	102	LHG	O8-C23-O10	-2.00	118.62	123.63
33	b	622	LMG	C24-C23-C22	-2.00	104.25	114.37
25	a	612	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
25	b	607	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
32	D	409	LHG	O8-C23-O10	-2.00	118.62	123.63
25	b	603	CLA	C2A-C1A-CHA	2.00	127.34	123.87
25	B	604	CLA	C7-C6-C5	-2.00	107.93	113.26
27	a	610	BCR	C2-C1-C6	2.00	113.35	110.44
25	C	505	CLA	C11-C12-C13	-2.00	109.31	115.97

All (66) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
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	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	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	H	101	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

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Mol	Chain	Res	Type	Atom
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	c	501	CLA	ND
25	c	502	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	401	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND
25	h	101	CLA	ND

All (1946) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C12-C13-C15-C16
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C2B-C3B-CAB-CBB
25	B	614	CLA	C4B-C3B-CAB-CBB
25	B	615	CLA	C2-C3-C5-C6
25	B	615	CLA	C4-C3-C5-C6
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	C2-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C4B-C3B-CAB-CBB
25	H	101	CLA	C1A-C2A-CAA-CBA
25	H	101	CLA	CAD-CBD-CGD-O1D
25	H	101	CLA	CAD-CBD-CGD-O2D
25	b	609	CLA	C2B-C3B-CAB-CBB
25	b	609	CLA	C4B-C3B-CAB-CBB
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	b	615	CLA	CHA-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O2D
25	c	506	CLA	C2-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C6-C7-C8-C9
25	c	512	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
25	c	512	CLA	C6-C7-C8-C9
25	d	404	CLA	C6-C7-C8-C9
25	h	101	CLA	C2B-C3B-CAB-CBB
25	h	101	CLA	C4B-C3B-CAB-CBB
27	A	610	BCR	C20-C21-C22-C37
27	B	618	BCR	C11-C12-C13-C35
27	B	618	BCR	C37-C22-C23-C24
27	C	514	BCR	C7-C8-C9-C34
27	C	514	BCR	C11-C12-C13-C14
27	C	514	BCR	C11-C12-C13-C35
27	D	405	BCR	C23-C24-C25-C26
27	K	101	BCR	C18-C19-C20-C21
27	K	101	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
27	T	101	BCR	C11-C12-C13-C14
27	Y	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C37-C22-C23-C24
27	Z	101	BCR	C7-C8-C9-C34
27	Z	101	BCR	C11-C12-C13-C14
27	b	616	BCR	C21-C22-C23-C24
27	c	515	BCR	C7-C8-C9-C10
27	d	405	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	d	405	BCR	C21-C22-C23-C24
27	d	405	BCR	C37-C22-C23-C24
27	k	101	BCR	C7-C8-C9-C10
27	k	101	BCR	C7-C8-C9-C34
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	C27-C28-C29-C30
28	A	611	PL9	C32-C33-C34-C36
28	A	611	PL9	C37-C38-C39-C41
28	D	406	PL9	C32-C33-C34-C35
28	D	406	PL9	C32-C33-C34-C36
28	a	611	PL9	C12-C13-C14-C15
28	a	611	PL9	C12-C13-C14-C16
28	a	611	PL9	C17-C18-C19-C20
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C37-C38-C39-C40
28	a	611	PL9	C37-C38-C39-C41
28	a	611	PL9	C41-C42-C43-C44
28	a	611	PL9	C42-C43-C44-C45
28	a	611	PL9	C42-C43-C44-C46
28	a	611	PL9	C47-C48-C49-C50
28	a	611	PL9	C47-C48-C49-C51
28	d	406	PL9	C32-C33-C34-C36
28	d	406	PL9	C42-C43-C44-C46
29	B	621	SQD	C2-C1-O6-C44
29	B	621	SQD	O5-C1-O6-C44
29	B	621	SQD	O6-C44-C45-O47
29	B	621	SQD	O49-C7-O47-C45
29	B	621	SQD	C8-C7-O47-C45
29	D	408	SQD	C2-C1-O6-C44
29	a	613	SQD	O6-C44-C45-O47
29	a	614	SQD	O6-C44-C45-C46
29	a	614	SQD	O6-C44-C45-O47
29	a	614	SQD	O49-C7-O47-C45
29	b	619	SQD	C8-C7-O47-C45
30	A	614	DGD	O1B-C1B-O2G-C2G
30	A	614	DGD	O2G-C2G-C3G-O3G
32	B	620	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
32	B	620	LHG	C3-O3-P-O5
32	B	620	LHG	C3-O3-P-O6
32	D	409	LHG	O1-C1-C2-C3
32	D	409	LHG	C3-O3-P-O4
32	D	409	LHG	C3-O3-P-O5
32	D	409	LHG	C3-O3-P-O6
32	D	409	LHG	C4-O6-P-O3
32	D	409	LHG	C4-O6-P-O4
32	D	409	LHG	C4-O6-P-O5
32	D	410	LHG	C3-O3-P-O6
32	L	101	LHG	C3-O3-P-O4
32	L	101	LHG	C4-O6-P-O4
32	b	623	LHG	O1-C1-C2-C3
32	b	623	LHG	C1-C2-C3-O3
32	b	623	LHG	C3-O3-P-O5
32	b	623	LHG	C3-O3-P-O6
32	d	407	LHG	O1-C1-C2-C3
32	d	407	LHG	C1-C2-C3-O3
32	d	408	LHG	C4-O6-P-O4
32	e	102	LHG	C1-C2-C3-O3
32	e	102	LHG	C3-O3-P-O5
32	e	102	LHG	C3-O3-P-O6
32	e	102	LHG	O6-C4-C5-O7
32	e	102	LHG	O10-C23-O8-C6
32	l	101	LHG	C3-O3-P-O4
32	l	101	LHG	C4-O6-P-O3
32	l	101	LHG	C4-O6-P-O4
32	l	101	LHG	C4-O6-P-O5
33	C	515	LMG	O6-C1-O1-C7
33	C	515	LMG	O1-C7-C8-O7
33	C	515	LMG	O9-C10-O7-C8
33	b	622	LMG	C11-C10-O7-C8
33	c	524	LMG	O6-C1-O1-C7
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
33	c	520	LMG	C11-C10-O7-C8
25	b	615	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	c	502	CLA	CBD-CGD-O2D-CED
26	d	402	PHO	CBD-CGD-O2D-CED
29	D	408	SQD	O10-C23-O48-C46
29	b	619	SQD	O10-C23-O48-C46
33	M	101	LMG	O10-C28-O8-C9
29	b	619	SQD	C24-C23-O48-C46
32	e	102	LHG	C24-C23-O8-C6
25	C	509	CLA	CBD-CGD-O2D-CED
29	f	101	SQD	O10-C23-O48-C46
32	E	101	LHG	O10-C23-O8-C6
33	c	522	LMG	O10-C28-O8-C9
33	c	524	LMG	O10-C28-O8-C9
33	c	520	LMG	O9-C10-O7-C8
29	b	619	SQD	O49-C7-O47-C45
33	D	411	LMG	O9-C10-O7-C8
33	b	622	LMG	O9-C10-O7-C8
33	c	522	LMG	O9-C10-O7-C8
25	B	607	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	d	404	CLA	C3-C5-C6-C7
25	h	101	CLA	C3-C5-C6-C7
26	d	402	PHO	O1D-CGD-O2D-CED
29	D	408	SQD	C24-C23-O48-C46
25	C	513	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	h	101	CLA	CBD-CGD-O2D-CED
29	a	614	SQD	C8-C7-O47-C45
30	A	614	DGD	C2B-C1B-O2G-C2G
33	C	515	LMG	C11-C10-O7-C8
33	D	411	LMG	C11-C10-O7-C8
33	c	522	LMG	C11-C10-O7-C8
25	B	606	CLA	C4-C3-C5-C6
25	b	613	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
28	A	611	PL9	C45-C44-C46-C47
28	a	611	PL9	C20-C19-C21-C22
28	a	611	PL9	C35-C34-C36-C37
25	b	613	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
28	A	611	PL9	C12-C11-C9-C8
28	D	406	PL9	C38-C39-C41-C42
28	a	611	PL9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	C3-C5-C6-C7
29	f	101	SQD	C24-C23-O48-C46
32	E	101	LHG	C24-C23-O8-C6
33	c	524	LMG	C29-C28-O8-C9
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C7-C8-C9-C11
28	A	611	PL9	C27-C28-C29-C31
25	B	604	CLA	C3-C5-C6-C7
25	B	606	CLA	C3-C5-C6-C7
25	B	615	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	b	612	CLA	CBD-CGD-O2D-CED
25	c	510	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	b	607	CLA	C2C-C3C-CAC-CBC
32	b	623	LHG	O2-C2-C3-O3
32	e	102	LHG	O2-C2-C3-O3
25	c	502	CLA	O1D-CGD-O2D-CED
25	C	513	CLA	CBA-CGA-O2A-C1
33	M	101	LMG	C29-C28-O8-C9
33	c	522	LMG	C29-C28-O8-C9
25	c	510	CLA	C3-C5-C6-C7
25	b	615	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	CBA-CGA-O2A-C1
28	A	611	PL9	C20-C19-C21-C22
28	A	611	PL9	C18-C19-C21-C22
28	A	611	PL9	C38-C39-C41-C42
28	a	611	PL9	C18-C19-C21-C22
28	a	611	PL9	C33-C34-C36-C37
30	c	519	DGD	O1A-C1A-O1G-C1G
28	A	611	PL9	C19-C21-C22-C23
28	A	611	PL9	C24-C26-C27-C28
28	A	611	PL9	C34-C36-C37-C38
28	A	611	PL9	C44-C46-C47-C48
28	a	611	PL9	C9-C11-C12-C13
28	a	611	PL9	C14-C16-C17-C18
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C34-C36-C37-C38
29	B	621	SQD	C11-C10-C9-C8
33	C	515	LMG	O6-C5-C6-O5
25	C	513	CLA	O1A-CGA-O2A-C1
25	c	506	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	f	101	SQD	O5-C1-O6-C44
29	B	621	SQD	C24-C23-O48-C46
25	B	612	CLA	CBD-CGD-O2D-CED
25	C	501	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
33	M	101	LMG	O6-C5-C6-O5
25	C	509	CLA	O1D-CGD-O2D-CED
25	h	101	CLA	O1D-CGD-O2D-CED
28	D	406	PL9	C47-C48-C49-C50
28	d	406	PL9	C47-C48-C49-C51
29	B	621	SQD	O10-C23-O48-C46
25	H	101	CLA	CBA-CGA-O2A-C1
25	b	606	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
33	c	520	LMG	O6-C5-C6-O5
32	d	408	LHG	C24-C25-C26-C27
33	c	524	LMG	C4-C5-C6-O5
25	A	609	CLA	C4-C3-C5-C6
28	A	611	PL9	C40-C39-C41-C42
25	A	609	CLA	C2-C3-C5-C6
25	B	606	CLA	C2-C3-C5-C6
25	c	501	CLA	CBD-CGD-O2D-CED
25	A	607	CLA	C14-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C14
25	B	606	CLA	C11-C12-C13-C14
25	B	613	CLA	C14-C13-C15-C16
25	C	502	CLA	C14-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	H	101	CLA	C11-C12-C13-C14
25	b	601	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C9
25	b	614	CLA	C6-C7-C8-C9
25	b	615	CLA	C6-C7-C8-C9
25	c	504	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	511	CLA	C14-C13-C15-C16
25	h	101	CLA	C14-C13-C15-C16
29	f	101	SQD	C2-C1-O6-C44
31	x	102	STE	C1-C2-C3-C4
32	B	620	LHG	O2-C2-C3-O3
32	D	409	LHG	O2-C2-C3-O3
32	d	407	LHG	O2-C2-C3-O3
27	D	405	BCR	C37-C22-C23-C24
27	Y	101	BCR	C7-C8-C9-C34
27	b	617	BCR	C7-C8-C9-C34
27	b	618	BCR	C11-C12-C13-C35
27	b	618	BCR	C37-C22-C23-C24
27	c	515	BCR	C7-C8-C9-C34
27	t	101	BCR	C36-C18-C19-C20
27	x	101	BCR	C7-C8-C9-C34
25	c	512	CLA	C2A-CAA-CBA-CGA
31	d	411	STE	C1-C2-C3-C4
25	c	511	CLA	C15-C16-C17-C18
33	C	519	LMG	C11-C10-O7-C8
33	d	410	LMG	C10-C11-C12-C13
25	B	615	CLA	C2-C1-O2A-CGA
25	c	512	CLA	O1D-CGD-O2D-CED
28	A	611	PL9	C7-C8-C9-C10
31	b	621	STE	C11-C12-C13-C14
25	B	604	CLA	C13-C15-C16-C17
25	b	610	CLA	C8-C10-C11-C12
25	c	511	CLA	C13-C15-C16-C17
25	C	513	CLA	O1D-CGD-O2D-CED
32	d	408	LHG	C23-C24-C25-C26
33	D	411	LMG	C28-C29-C30-C31
33	c	520	LMG	C28-C29-C30-C31
25	C	506	CLA	C13-C15-C16-C17
33	c	524	LMG	O6-C5-C6-O5
25	C	506	CLA	C11-C12-C13-C15
25	C	508	CLA	C12-C13-C15-C16
25	a	612	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C15
25	a	607	CLA	C15-C16-C17-C18
32	E	101	LHG	C7-C8-C9-C10
33	d	410	LMG	C28-C29-C30-C31
28	A	611	PL9	C9-C11-C12-C13
28	A	611	PL9	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	a	611	PL9	C39-C41-C42-C43
25	b	606	CLA	C8-C10-C11-C12
25	A	606	CLA	C2C-C3C-CAC-CBC
29	b	619	SQD	C7-C8-C9-C10
32	b	623	LHG	C23-C24-C25-C26
33	C	519	LMG	C28-C29-C30-C31
33	D	407	LMG	C10-C11-C12-C13
33	b	622	LMG	C28-C29-C30-C31
25	C	509	CLA	C10-C11-C12-C13
25	b	613	CLA	C13-C15-C16-C17
30	c	517	DGD	O6E-C5E-C6E-O5E
25	b	607	CLA	C4C-C3C-CAC-CBC
25	B	612	CLA	C5-C6-C7-C8
25	C	512	CLA	C8-C10-C11-C12
25	c	512	CLA	C15-C16-C17-C18
29	B	621	SQD	C23-C24-C25-C26
30	a	615	DGD	C1A-C2A-C3A-C4A
30	c	517	DGD	C1A-C2A-C3A-C4A
31	B	619	STE	C1-C2-C3-C4
32	d	408	LHG	C7-C8-C9-C10
32	l	101	LHG	C23-C24-C25-C26
33	D	412	LMG	C28-C29-C30-C31
33	b	620	LMG	C10-C11-C12-C13
25	H	101	CLA	O1A-CGA-O2A-C1
25	b	606	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
25	a	612	CLA	CBD-CGD-O2D-CED
30	H	103	DGD	C2B-C3B-C4B-C5B
25	A	612	CLA	C13-C15-C16-C17
25	B	612	CLA	C8-C10-C11-C12
25	C	503	CLA	C5-C6-C7-C8
25	C	509	CLA	C5-C6-C7-C8
25	C	509	CLA	C8-C10-C11-C12
25	b	610	CLA	C13-C15-C16-C17
25	b	612	CLA	C10-C11-C12-C13
33	M	101	LMG	C4-C5-C6-O5
30	c	518	DGD	C1B-C2B-C3B-C4B
31	b	624	STE	C1-C2-C3-C4
25	B	605	CLA	C13-C15-C16-C17
25	B	613	CLA	C5-C6-C7-C8
25	C	505	CLA	C5-C6-C7-C8
25	C	510	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C10-C11-C12-C13
25	b	603	CLA	C15-C16-C17-C18
25	c	508	CLA	C13-C15-C16-C17
25	h	101	CLA	C8-C10-C11-C12
25	C	504	CLA	C8-C10-C11-C12
25	C	512	CLA	C13-C15-C16-C17
29	f	101	SQD	C23-C24-C25-C26
32	B	620	LHG	C7-C8-C9-C10
25	b	612	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	O1D-CGD-O2D-CED
25	B	615	CLA	C5-C6-C7-C8
25	c	503	CLA	C5-C6-C7-C8
25	c	506	CLA	C13-C15-C16-C17
25	c	510	CLA	C10-C11-C12-C13
30	c	519	DGD	C2A-C1A-O1G-C1G
25	b	603	CLA	C3-C5-C6-C7
25	d	404	CLA	C10-C11-C12-C13
29	a	613	SQD	C11-C12-C13-C14
33	M	101	LMG	C10-C11-C12-C13
25	B	605	CLA	C2A-CAA-CBA-CGA
25	b	605	CLA	C2A-CAA-CBA-CGA
27	d	405	BCR	C14-C15-C16-C17
30	C	517	DGD	C8A-C9A-CAA-CBA
25	B	602	CLA	C8-C10-C11-C12
25	B	603	CLA	C15-C16-C17-C18
25	B	608	CLA	C15-C16-C17-C18
25	C	509	CLA	C13-C15-C16-C17
25	b	604	CLA	C5-C6-C7-C8
25	b	606	CLA	C5-C6-C7-C8
25	b	614	CLA	C10-C11-C12-C13
25	c	506	CLA	C8-C10-C11-C12
25	c	509	CLA	C10-C11-C12-C13
26	a	608	PHO	CBD-CGD-O2D-CED
25	B	611	CLA	C13-C15-C16-C17
25	b	601	CLA	C10-C11-C12-C13
25	b	614	CLA	C15-C16-C17-C18
25	c	512	CLA	C13-C15-C16-C17
25	B	606	CLA	C8-C10-C11-C12
25	C	505	CLA	C10-C11-C12-C13
25	C	513	CLA	C13-C15-C16-C17
25	H	101	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	b	613	CLA	C5-C6-C7-C8
25	b	613	CLA	C8-C10-C11-C12
30	a	615	DGD	C2B-C3B-C4B-C5B
28	A	611	PL9	C22-C23-C24-C25
30	a	615	DGD	O1B-C1B-O2G-C2G
32	e	102	LHG	O9-C7-O7-C5
30	C	517	DGD	C2E-C1E-O5D-C6D
30	c	518	DGD	C2E-C1E-O5D-C6D
33	C	515	LMG	C2-C1-O1-C7
25	A	607	CLA	C15-C16-C17-C18
33	c	522	LMG	C10-C11-C12-C13
32	D	410	LHG	O2-C2-C3-O3
25	c	511	CLA	C16-C17-C18-C20
27	B	618	BCR	C16-C17-C18-C36
27	D	405	BCR	C20-C21-C22-C37
27	H	102	BCR	C20-C21-C22-C37
27	T	101	BCR	C35-C13-C14-C15
27	Y	101	BCR	C16-C17-C18-C36
27	b	616	BCR	C20-C21-C22-C37
27	b	618	BCR	C16-C17-C18-C36
27	b	618	BCR	C20-C21-C22-C37
27	c	514	BCR	C16-C17-C18-C36
27	c	515	BCR	C16-C17-C18-C36
27	c	516	BCR	C20-C21-C22-C37
27	d	405	BCR	C16-C17-C18-C36
27	k	101	BCR	C20-C21-C22-C37
25	b	614	CLA	C13-C15-C16-C17
27	T	101	BCR	C37-C22-C23-C24
25	a	609	CLA	C5-C6-C7-C8
25	b	615	CLA	C10-C11-C12-C13
32	d	408	LHG	O1-C1-C2-C3
29	b	619	SQD	C46-C45-O47-C7
25	B	603	CLA	C16-C17-C18-C19
25	B	605	CLA	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C20
25	C	512	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
25	c	507	CLA	C3-C5-C6-C7
25	b	612	CLA	C8-C10-C11-C12
25	d	401	CLA	C8-C10-C11-C12
27	A	610	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
27	B	617	BCR	C12-C13-C14-C15
27	B	618	BCR	C12-C13-C14-C15
27	B	618	BCR	C16-C17-C18-C19
27	Z	101	BCR	C11-C10-C9-C8
27	b	618	BCR	C16-C17-C18-C19
27	k	101	BCR	C20-C21-C22-C23
27	x	101	BCR	C11-C10-C9-C8
30	C	517	DGD	O6E-C1E-O5D-C6D
30	c	518	DGD	O6E-C1E-O5D-C6D
25	b	606	CLA	C10-C11-C12-C13
28	a	611	PL9	C38-C39-C41-C42
25	C	510	CLA	O1D-CGD-O2D-CED
33	C	519	LMG	C29-C28-O8-C9
25	c	504	CLA	O1D-CGD-O2D-CED
25	b	615	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
25	A	612	CLA	C16-C17-C18-C20
25	B	604	CLA	C16-C17-C18-C20
25	b	601	CLA	C16-C17-C18-C19
25	b	601	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C20
25	h	101	CLA	C13-C15-C16-C17
30	H	103	DGD	C9B-CAB-CBB-CCB
30	c	517	DGD	C8B-C9B-CAB-CBB
33	c	524	LMG	C18-C19-C20-C21
30	C	518	DGD	C9A-CAA-CBA-CCA
30	a	615	DGD	C4A-C5A-C6A-C7A
30	a	615	DGD	C8A-C9A-CAA-CBA
30	c	517	DGD	CAA-CBA-CCA-CDA
31	D	413	STE	C5-C6-C7-C8
31	I	101	STE	C10-C11-C12-C13
31	M	102	STE	C3-C4-C5-C6
31	T	102	STE	C7-C8-C9-C10
31	b	621	STE	C14-C15-C16-C17
31	c	521	STE	C9-C10-C11-C12
31	l	102	STE	C3-C4-C5-C6
31	l	102	STE	C14-C15-C16-C17
31	t	102	STE	C11-C10-C9-C8
31	x	102	STE	C5-C6-C7-C8
32	L	101	LHG	C27-C28-C29-C30
32	b	623	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
33	D	412	LMG	C30-C31-C32-C33
33	M	101	LMG	C18-C19-C20-C21
33	c	522	LMG	C36-C37-C38-C39
25	D	404	CLA	C10-C11-C12-C13
29	f	101	SQD	C30-C31-C32-C33
31	b	625	STE	C12-C13-C14-C15
33	c	522	LMG	C30-C31-C32-C33
30	a	615	DGD	C2A-C1A-O1G-C1G
29	A	613	SQD	C11-C10-C9-C8
29	A	613	SQD	C12-C13-C14-C15
30	C	518	DGD	C6A-C7A-C8A-C9A
30	a	615	DGD	CBB-CCB-CDB-CEB
30	c	517	DGD	C7A-C8A-C9A-CAA
31	B	622	STE	C2-C3-C4-C5
32	D	410	LHG	C30-C31-C32-C33
32	l	101	LHG	C15-C16-C17-C18
33	C	519	LMG	C18-C19-C20-C21
33	c	522	LMG	C16-C17-C18-C19
33	d	409	LMG	C33-C34-C35-C36
33	d	410	LMG	C33-C34-C35-C36
32	D	409	LHG	O1-C1-C2-O2
32	b	623	LHG	O1-C1-C2-O2
32	d	407	LHG	O1-C1-C2-O2
29	B	621	SQD	C13-C14-C15-C16
29	D	408	SQD	C30-C31-C32-C33
29	b	619	SQD	C29-C30-C31-C32
30	A	614	DGD	C8B-C9B-CAB-CBB
30	A	614	DGD	CCB-CDB-CEB-CFB
30	h	102	DGD	C9A-CAA-CBA-CCA
31	M	102	STE	C6-C7-C8-C9
31	M	102	STE	C7-C8-C9-C10
25	B	605	CLA	C4B-C3B-CAB-CBB
25	C	503	CLA	C4B-C3B-CAB-CBB
30	A	614	DGD	C2A-C3A-C4A-C5A
31	b	625	STE	C10-C11-C12-C13
33	b	620	LMG	C30-C31-C32-C33
33	c	524	LMG	C32-C33-C34-C35
25	B	603	CLA	C16-C17-C18-C20
25	B	605	CLA	C16-C17-C18-C20
25	B	608	CLA	C16-C17-C18-C19
25	B	608	CLA	C16-C17-C18-C20
25	B	611	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C16-C17-C18-C19
25	b	606	CLA	C16-C17-C18-C20
32	D	410	LHG	C34-C35-C36-C37
33	c	524	LMG	C15-C16-C17-C18
29	T	103	SQD	C8-C7-O47-C45
29	f	101	SQD	C32-C33-C34-C35
30	c	519	DGD	C3A-C4A-C5A-C6A
30	c	519	DGD	CCA-CDA-CEA-CFA
30	h	102	DGD	CAB-CBB-CCB-CDB
31	I	101	STE	C2-C3-C4-C5
31	b	621	STE	C10-C11-C12-C13
33	c	524	LMG	C31-C32-C33-C34
25	d	404	CLA	C11-C12-C13-C15
29	f	101	SQD	C28-C29-C30-C31
30	c	519	DGD	C4B-C5B-C6B-C7B
29	A	613	SQD	C7-C8-C9-C10
30	A	614	DGD	C1A-C2A-C3A-C4A
30	c	517	DGD	C3A-C4A-C5A-C6A
31	B	622	STE	C3-C4-C5-C6
31	I	101	STE	C9-C10-C11-C12
32	d	408	LHG	C32-C33-C34-C35
33	C	515	LMG	C29-C30-C31-C32
33	M	101	LMG	C33-C34-C35-C36
33	b	620	LMG	C17-C18-C19-C20
33	d	410	LMG	C32-C33-C34-C35
32	D	410	LHG	O10-C23-O8-C6
25	c	512	CLA	C3A-C2A-CAA-CBA
26	d	402	PHO	C3A-C2A-CAA-CBA
29	a	613	SQD	C30-C31-C32-C33
33	C	519	LMG	C32-C33-C34-C35
33	M	101	LMG	C32-C33-C34-C35
33	c	522	LMG	C33-C34-C35-C36
29	a	613	SQD	C29-C30-C31-C32
30	C	518	DGD	CAA-CBA-CCA-CDA
30	c	519	DGD	C8B-C9B-CAB-CBB
31	x	102	STE	C3-C4-C5-C6
32	l	101	LHG	C17-C18-C19-C20
25	B	609	CLA	C13-C15-C16-C17
32	b	623	LHG	C16-C17-C18-C19
33	D	407	LMG	C15-C16-C17-C18
30	C	518	DGD	C4A-C5A-C6A-C7A
30	c	518	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
30	c	519	DGD	CBA-CCA-CDA-CEA
32	e	102	LHG	C24-C25-C26-C27
25	B	612	CLA	O1D-CGD-O2D-CED
33	D	411	LMG	C7-C8-C9-O8
31	H	104	STE	C10-C11-C12-C13
33	b	620	LMG	C18-C19-C20-C21
33	b	620	LMG	C34-C35-C36-C37
33	d	409	LMG	C32-C33-C34-C35
30	H	103	DGD	C3B-C4B-C5B-C6B
30	c	517	DGD	CBB-CCB-CDB-CEB
31	D	413	STE	C11-C12-C13-C14
32	D	409	LHG	C10-C11-C12-C13
32	D	409	LHG	C11-C12-C13-C14
32	D	409	LHG	C30-C31-C32-C33
32	L	101	LHG	C17-C18-C19-C20
33	D	407	LMG	C12-C13-C14-C15
33	M	101	LMG	C36-C37-C38-C39
33	c	522	LMG	C39-C40-C41-C42
33	c	524	LMG	C38-C39-C40-C41
30	C	518	DGD	CBA-CCA-CDA-CEA
30	a	615	DGD	CBA-CCA-CDA-CEA
31	b	624	STE	C3-C4-C5-C6
32	D	410	LHG	C24-C25-C26-C27
32	L	101	LHG	C12-C13-C14-C15
32	b	623	LHG	C32-C33-C34-C35
32	d	407	LHG	C29-C30-C31-C32
25	C	511	CLA	O1D-CGD-O2D-CED
29	a	613	SQD	C24-C25-C26-C27
30	h	102	DGD	CCA-CDA-CEA-CFA
31	E	102	STE	C5-C6-C7-C8
31	I	101	STE	C7-C8-C9-C10
31	d	411	STE	C5-C6-C7-C8
33	C	519	LMG	C31-C32-C33-C34
33	D	412	LMG	C36-C37-C38-C39
25	C	513	CLA	C10-C11-C12-C13
29	A	613	SQD	C16-C17-C18-C19
30	h	102	DGD	C2B-C3B-C4B-C5B
31	b	624	STE	C5-C6-C7-C8
25	H	101	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C19
30	C	518	DGD	C1A-C2A-C3A-C4A
27	D	405	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
27	Y	101	BCR	C1-C6-C7-C8
27	Y	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
31	x	102	STE	C7-C8-C9-C10
32	L	101	LHG	C32-C33-C34-C35
33	D	412	LMG	C29-C30-C31-C32
33	c	522	LMG	C15-C16-C17-C18
32	e	102	LHG	C8-C7-O7-C5
25	b	605	CLA	C10-C11-C12-C13
29	a	613	SQD	C34-C35-C36-C37
33	c	522	LMG	C31-C32-C33-C34
33	c	524	LMG	C36-C37-C38-C39
32	L	101	LHG	C11-C12-C13-C14
32	L	101	LHG	C33-C34-C35-C36
29	a	614	SQD	C10-C11-C12-C13
33	c	520	LMG	C36-C37-C38-C39
29	T	103	SQD	C13-C14-C15-C16
30	C	517	DGD	C6B-C7B-C8B-C9B
30	H	103	DGD	C5B-C6B-C7B-C8B
30	c	517	DGD	C6B-C7B-C8B-C9B
31	H	104	STE	C14-C15-C16-C17
31	M	104	STE	C7-C8-C9-C10
31	b	626	STE	C5-C6-C7-C8
32	d	407	LHG	C10-C11-C12-C13
33	d	409	LMG	C31-C32-C33-C34
29	T	103	SQD	O49-C7-O47-C45
25	B	602	CLA	C4-C3-C5-C6
28	a	611	PL9	C25-C24-C26-C27
31	B	619	STE	C7-C8-C9-C10
33	D	412	LMG	C31-C32-C33-C34
28	A	611	PL9	C42-C43-C44-C46
27	A	610	BCR	C18-C19-C20-C21
27	B	618	BCR	C10-C11-C12-C13
27	t	101	BCR	C18-C19-C20-C21
25	B	602	CLA	C2-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	c	506	CLA	C16-C17-C18-C20
30	c	517	DGD	C4B-C5B-C6B-C7B
31	D	413	STE	C4-C5-C6-C7
32	E	101	LHG	C24-C25-C26-C27
33	b	622	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	b	622	LMG	C16-C17-C18-C19
33	d	409	LMG	C38-C39-C40-C41
25	c	503	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
29	b	619	SQD	C16-C17-C18-C19
31	c	521	STE	C6-C7-C8-C9
31	x	102	STE	C4-C5-C6-C7
33	d	409	LMG	C35-C36-C37-C38
31	d	411	STE	C9-C10-C11-C12
32	l	101	LHG	C11-C12-C13-C14
30	c	518	DGD	O6D-C1D-O3G-C3G
33	C	519	LMG	O6-C1-O1-C7
33	M	101	LMG	O6-C1-O1-C7
33	c	520	LMG	O6-C1-O1-C7
31	M	103	STE	C4-C5-C6-C7
33	M	101	LMG	C21-C22-C23-C24
33	c	524	LMG	C39-C40-C41-C42
33	c	524	LMG	C2-C1-O1-C7
29	b	619	SQD	C13-C14-C15-C16
30	c	517	DGD	C8A-C9A-CAA-CBA
30	c	519	DGD	C9A-CAA-CBA-CCA
32	d	408	LHG	C27-C28-C29-C30
31	C	522	STE	C4-C5-C6-C7
31	H	104	STE	C4-C5-C6-C7
31	c	521	STE	C11-C12-C13-C14
31	d	411	STE	C10-C11-C12-C13
32	D	410	LHG	C11-C12-C13-C14
32	l	101	LHG	C28-C29-C30-C31
29	D	408	SQD	C25-C26-C27-C28
29	a	613	SQD	C13-C14-C15-C16
30	C	517	DGD	C7B-C8B-C9B-CAB
30	c	517	DGD	C2A-C3A-C4A-C5A
33	M	101	LMG	C20-C21-C22-C23
33	b	622	LMG	C40-C41-C42-C43
33	d	409	LMG	C36-C37-C38-C39
25	c	511	CLA	C16-C17-C18-C19
31	d	411	STE	C11-C12-C13-C14
32	E	101	LHG	C8-C7-O7-C5
32	l	101	LHG	C24-C25-C26-C27
33	c	524	LMG	C12-C13-C14-C15
25	b	610	CLA	C15-C16-C17-C18
25	c	510	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	A	613	SQD	C34-C35-C36-C37
30	A	614	DGD	CCA-CDA-CEA-CFA
31	b	621	STE	C3-C4-C5-C6
30	c	517	DGD	CAB-CBB-CCB-CDB
25	b	606	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	C15-C16-C17-C18
25	c	506	CLA	C5-C6-C7-C8
31	t	103	STE	C2-C3-C4-C5
32	B	620	LHG	C23-C24-C25-C26
32	E	101	LHG	C23-C24-C25-C26
32	l	101	LHG	C7-C8-C9-C10
32	B	620	LHG	C27-C28-C29-C30
32	D	410	LHG	C9-C10-C11-C12
32	e	102	LHG	C11-C10-C9-C8
30	C	518	DGD	C5A-C6A-C7A-C8A
25	h	101	CLA	C2A-CAA-CBA-CGA
25	C	513	CLA	C16-C17-C18-C19
25	C	513	CLA	C16-C17-C18-C20
25	h	101	CLA	C16-C17-C18-C20
29	D	408	SQD	C33-C34-C35-C36
31	T	102	STE	C6-C7-C8-C9
33	D	407	LMG	C17-C18-C19-C20
33	b	622	LMG	C17-C18-C19-C20
30	A	614	DGD	CEA-CFA-CGA-CHA
33	c	524	LMG	C11-C12-C13-C14
29	B	621	SQD	C19-C20-C21-C22
25	A	612	CLA	C15-C16-C17-C18
25	a	609	CLA	C10-C11-C12-C13
25	c	503	CLA	C15-C16-C17-C18
29	b	619	SQD	C10-C11-C12-C13
30	H	103	DGD	C4B-C5B-C6B-C7B
32	E	101	LHG	C16-C17-C18-C19
33	D	407	LMG	C39-C40-C41-C42
25	A	607	CLA	C8-C10-C11-C12
30	A	614	DGD	C2B-C3B-C4B-C5B
32	D	409	LHG	C33-C34-C35-C36
33	C	515	LMG	C35-C36-C37-C38
25	c	513	CLA	O1D-CGD-O2D-CED
32	E	101	LHG	C32-C33-C34-C35
32	d	408	LHG	C26-C27-C28-C29
30	c	517	DGD	CCB-CDB-CEB-CFB
32	l	101	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C15-C16-C17-C18
25	b	603	CLA	C10-C11-C12-C13
25	c	503	CLA	C13-C15-C16-C17
25	B	604	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C20
30	C	517	DGD	C9A-CAA-CBA-CCA
32	b	623	LHG	C7-C8-C9-C10
25	B	606	CLA	C10-C11-C12-C13
25	C	505	CLA	C15-C16-C17-C18
25	c	512	CLA	C8-C10-C11-C12
29	A	613	SQD	C14-C15-C16-C17
30	A	614	DGD	CBA-CCA-CDA-CEA
30	C	516	DGD	C2A-C3A-C4A-C5A
31	B	625	STE	C5-C6-C7-C8
32	D	409	LHG	C14-C15-C16-C17
32	d	407	LHG	C33-C34-C35-C36
29	A	613	SQD	O6-C44-C45-O47
29	B	621	SQD	C9-C10-C11-C12
29	D	408	SQD	C34-C35-C36-C37
30	C	518	DGD	C3A-C4A-C5A-C6A
31	j	101	STE	C2-C3-C4-C5
29	a	614	SQD	C14-C15-C16-C17
25	b	601	CLA	C5-C6-C7-C8
31	C	520	STE	C6-C7-C8-C9
31	T	102	STE	C4-C5-C6-C7
32	L	101	LHG	C16-C17-C18-C19
32	d	407	LHG	C11-C12-C13-C14
33	b	622	LMG	C31-C32-C33-C34
33	c	524	LMG	C30-C31-C32-C33
30	H	103	DGD	C6A-C7A-C8A-C9A
30	H	103	DGD	CBA-CCA-CDA-CEA
30	c	519	DGD	CCB-CDB-CEB-CFB
30	h	102	DGD	C3A-C4A-C5A-C6A
31	M	104	STE	C14-C15-C16-C17
32	L	101	LHG	C9-C10-C11-C12
33	b	622	LMG	O6-C5-C6-O5
25	D	404	CLA	C16-C17-C18-C19
29	a	613	SQD	C28-C29-C30-C31
29	a	614	SQD	C24-C25-C26-C27
29	b	619	SQD	C18-C19-C20-C21
30	C	517	DGD	C6A-C7A-C8A-C9A
31	B	623	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	D	413	STE	C6-C7-C8-C9
31	D	413	STE	C9-C10-C11-C12
33	c	520	LMG	C35-C36-C37-C38
31	x	102	STE	C11-C10-C9-C8
25	D	403	CLA	C3-C5-C6-C7
29	D	408	SQD	C28-C29-C30-C31
32	E	101	LHG	C27-C28-C29-C30
32	b	623	LHG	C15-C16-C17-C18
33	d	409	LMG	C39-C40-C41-C42
25	B	605	CLA	CBD-CGD-O2D-CED
29	B	621	SQD	C17-C18-C19-C20
30	C	517	DGD	C4B-C5B-C6B-C7B
32	l	101	LHG	C9-C10-C11-C12
32	l	101	LHG	C34-C35-C36-C37
30	C	516	DGD	C2B-C3B-C4B-C5B
33	C	519	LMG	C16-C17-C18-C19
29	B	621	SQD	C11-C12-C13-C14
31	b	626	STE	C6-C7-C8-C9
33	c	522	LMG	C34-C35-C36-C37
28	A	611	PL9	C47-C48-C49-C51
29	A	613	SQD	C8-C7-O47-C45
31	B	623	STE	C6-C7-C8-C9
31	T	102	STE	C9-C10-C11-C12
33	M	101	LMG	C31-C32-C33-C34
33	d	409	LMG	C34-C35-C36-C37
25	C	510	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
30	a	615	DGD	O1A-C1A-O1G-C1G
32	b	623	LHG	C10-C11-C12-C13
33	C	515	LMG	C33-C34-C35-C36
29	a	613	SQD	C26-C27-C28-C29
31	B	622	STE	C4-C5-C6-C7
32	B	620	LHG	C29-C30-C31-C32
33	D	411	LMG	C34-C35-C36-C37
25	C	503	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	CBA-CGA-O2A-C1
29	f	101	SQD	C25-C26-C27-C28
31	C	521	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	C	519	LMG	C15-C16-C17-C18
31	b	624	STE	C6-C7-C8-C9
32	D	410	LHG	C32-C33-C34-C35
32	b	623	LHG	C14-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
31	B	624	STE	C2-C3-C4-C5
32	d	407	LHG	C32-C33-C34-C35
33	c	520	LMG	C37-C38-C39-C40
25	A	612	CLA	C11-C12-C13-C15
25	B	609	CLA	C11-C10-C8-C7
25	B	614	CLA	C11-C12-C13-C15
25	C	502	CLA	C12-C13-C15-C16
25	C	508	CLA	C11-C10-C8-C7
25	a	607	CLA	C12-C13-C15-C16
25	b	603	CLA	C11-C12-C13-C15
25	b	603	CLA	C12-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C10
25	b	608	CLA	C12-C13-C15-C16
25	b	612	CLA	C6-C7-C8-C10
25	b	615	CLA	C6-C7-C8-C10
25	c	504	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	509	CLA	C6-C7-C8-C10
25	d	401	CLA	C6-C7-C8-C10
25	h	101	CLA	C11-C12-C13-C15
31	H	104	STE	C12-C13-C14-C15
31	t	102	STE	C4-C5-C6-C7
32	b	623	LHG	C27-C28-C29-C30
25	H	101	CLA	C16-C17-C18-C19
25	a	612	CLA	C16-C17-C18-C19
30	H	103	DGD	C5A-C6A-C7A-C8A
25	b	605	CLA	O1D-CGD-O2D-CED
25	b	602	CLA	C10-C11-C12-C13
30	H	103	DGD	C1A-C2A-C3A-C4A
31	B	619	STE	C6-C7-C8-C9
31	b	624	STE	C11-C10-C9-C8
25	C	505	CLA	C4-C3-C5-C6
31	T	102	STE	C12-C13-C14-C15
31	b	626	STE	C7-C8-C9-C10
30	c	519	DGD	C5B-C6B-C7B-C8B
25	A	612	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C11-C12-C13-C14
25	C	506	CLA	C14-C13-C15-C16
25	D	404	CLA	C6-C7-C8-C9
25	b	603	CLA	C14-C13-C15-C16
25	b	608	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	508	CLA	C14-C13-C15-C16
25	c	512	CLA	C14-C13-C15-C16
25	h	101	CLA	C11-C12-C13-C14
30	C	516	DGD	C5A-C6A-C7A-C8A
30	c	518	DGD	CCB-CDB-CEB-CFB
31	H	104	STE	C5-C6-C7-C8
30	C	516	DGD	O6E-C5E-C6E-O5E
33	d	410	LMG	O6-C5-C6-O5
30	A	614	DGD	C1B-C2B-C3B-C4B
29	a	613	SQD	C17-C18-C19-C20
25	C	505	CLA	CBA-CGA-O2A-C1
31	m	101	STE	C5-C6-C7-C8
33	C	519	LMG	O9-C10-O7-C8
33	C	519	LMG	C2-C1-O1-C7
25	B	601	CLA	C15-C16-C17-C18
31	l	102	STE	C12-C13-C14-C15
32	E	101	LHG	C11-C10-C9-C8
30	h	102	DGD	O6E-C5E-C6E-O5E
29	B	621	SQD	O6-C44-C45-C46
30	A	614	DGD	O1G-C1G-C2G-C3G
32	E	101	LHG	C4-C5-C6-O8
33	C	515	LMG	O1-C7-C8-C9
33	C	519	LMG	O1-C7-C8-C9
33	c	522	LMG	C7-C8-C9-O8
33	c	524	LMG	C7-C8-C9-O8
30	C	518	DGD	CCB-CDB-CEB-CFB
33	C	519	LMG	C30-C31-C32-C33
25	C	505	CLA	O1A-CGA-O2A-C1
32	D	409	LHG	C25-C26-C27-C28
32	L	101	LHG	C30-C31-C32-C33
33	c	522	LMG	C13-C14-C15-C16
31	d	411	STE	C12-C13-C14-C15
25	c	513	CLA	C10-C11-C12-C13
33	C	515	LMG	C38-C39-C40-C41
33	b	620	LMG	C29-C28-O8-C9
25	D	404	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	a	612	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C19
29	b	619	SQD	C12-C13-C14-C15
32	E	101	LHG	C25-C26-C27-C28
33	D	407	LMG	O6-C5-C6-O5
31	x	102	STE	C2-C3-C4-C5
33	c	520	LMG	C38-C39-C40-C41
27	Z	101	BCR	C16-C17-C18-C36
25	b	614	CLA	C8-C10-C11-C12
30	C	516	DGD	C6B-C7B-C8B-C9B
30	c	517	DGD	C9B-CAB-CBB-CCB
33	c	524	LMG	C37-C38-C39-C40
25	C	505	CLA	C2-C3-C5-C6
30	A	614	DGD	C2A-C1A-O1G-C1G
25	c	510	CLA	C8-C10-C11-C12
29	B	621	SQD	C15-C16-C17-C18
31	b	621	STE	C5-C6-C7-C8
31	b	621	STE	C6-C7-C8-C9
31	b	624	STE	C9-C10-C11-C12
29	a	613	SQD	C27-C28-C29-C30
30	C	516	DGD	C3B-C4B-C5B-C6B
31	B	623	STE	C4-C5-C6-C7
33	b	622	LMG	C13-C14-C15-C16
27	x	101	BCR	C11-C12-C13-C14
30	C	518	DGD	O6D-C5D-C6D-O5D
25	c	503	CLA	O1A-CGA-O2A-C1
30	C	517	DGD	C5A-C6A-C7A-C8A
25	c	501	CLA	C2A-CAA-CBA-CGA
31	C	522	STE	C11-C10-C9-C8
29	A	613	SQD	C11-C12-C13-C14
30	c	518	DGD	C7A-C8A-C9A-CAA
32	B	620	LHG	C11-C12-C13-C14
33	C	519	LMG	C38-C39-C40-C41
29	B	621	SQD	C7-C8-C9-C10
31	J	101	STE	C1-C2-C3-C4
29	b	619	SQD	C25-C26-C27-C28
31	C	521	STE	C4-C5-C6-C7
31	b	625	STE	C5-C6-C7-C8
32	E	101	LHG	C30-C31-C32-C33
33	D	407	LMG	C31-C32-C33-C34
29	a	613	SQD	C24-C23-O48-C46
33	c	520	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
25	A	606	CLA	C4C-C3C-CAC-CBC
33	D	411	LMG	C9-C8-O7-C10
33	C	515	LMG	C16-C17-C18-C19
27	K	101	BCR	C10-C11-C12-C13
27	c	515	BCR	C18-C19-C20-C21
28	A	611	PL9	C47-C48-C49-C50
28	d	406	PL9	C47-C48-C49-C50
29	B	621	SQD	C32-C33-C34-C35
29	T	103	SQD	C18-C19-C20-C21
31	J	101	STE	C6-C7-C8-C9
29	B	621	SQD	C35-C36-C37-C38
30	a	615	DGD	CCB-CDB-CEB-CFB
25	C	501	CLA	O1D-CGD-O2D-CED
27	B	616	BCR	C12-C13-C14-C15
27	T	101	BCR	C12-C13-C14-C15
27	Z	101	BCR	C20-C21-C22-C23
27	c	516	BCR	C11-C10-C9-C8
31	d	411	STE	C4-C5-C6-C7
30	c	517	DGD	C2B-C3B-C4B-C5B
31	C	520	STE	C3-C4-C5-C6
33	b	622	LMG	C38-C39-C40-C41
32	l	101	LHG	C14-C15-C16-C17
29	A	613	SQD	C17-C18-C19-C20
29	a	614	SQD	C17-C18-C19-C20
29	b	619	SQD	C9-C10-C11-C12
31	b	621	STE	C11-C10-C9-C8
25	B	604	CLA	C4-C3-C5-C6
25	B	612	CLA	C4-C3-C5-C6
28	d	406	PL9	C15-C14-C16-C17
28	d	406	PL9	C28-C29-C31-C32
31	T	102	STE	C3-C4-C5-C6
31	l	102	STE	C15-C16-C17-C18
32	E	101	LHG	C17-C18-C19-C20
33	D	407	LMG	C30-C31-C32-C33
29	T	103	SQD	C9-C10-C11-C12
31	B	623	STE	C12-C13-C14-C15
31	x	102	STE	C9-C10-C11-C12
33	D	411	LMG	C31-C32-C33-C34
33	b	620	LMG	C12-C13-C14-C15
28	a	611	PL9	C17-C18-C19-C21
30	h	102	DGD	C6B-C7B-C8B-C9B
31	B	625	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	M	101	LMG	O1-C7-C8-O7
30	A	614	DGD	C5B-C6B-C7B-C8B
31	B	624	STE	C7-C8-C9-C10
29	f	101	SQD	C33-C34-C35-C36
33	b	622	LMG	C11-C12-C13-C14
33	c	520	LMG	C30-C31-C32-C33
32	B	620	LHG	C28-C29-C30-C31
25	C	509	CLA	C3-C5-C6-C7
29	B	621	SQD	C10-C11-C12-C13
32	D	409	LHG	C35-C36-C37-C38
33	D	412	LMG	C37-C38-C39-C40
30	H	103	DGD	C7A-C8A-C9A-CAA
33	D	411	LMG	C36-C37-C38-C39
30	a	615	DGD	CFB-CGB-CHB-CIB
31	H	104	STE	C11-C12-C13-C14
33	D	407	LMG	C37-C38-C39-C40
25	a	609	CLA	CBA-CGA-O2A-C1
33	c	520	LMG	C4-C5-C6-O5
30	a	615	DGD	C2A-C3A-C4A-C5A
31	b	624	STE	C7-C8-C9-C10
33	D	407	LMG	C35-C36-C37-C38
32	d	407	LHG	C12-C13-C14-C15
29	a	614	SQD	C31-C32-C33-C34
25	B	612	CLA	C15-C16-C17-C18
26	a	608	PHO	O1D-CGD-O2D-CED
30	C	516	DGD	C4B-C5B-C6B-C7B
25	B	614	CLA	C13-C15-C16-C17
30	A	614	DGD	CFA-CGA-CHA-CIA
31	b	624	STE	C4-C5-C6-C7
32	b	623	LHG	C31-C32-C33-C34
31	b	625	STE	C11-C10-C9-C8
32	e	102	LHG	C12-C13-C14-C15
33	C	515	LMG	C36-C37-C38-C39
33	c	524	LMG	C14-C15-C16-C17
25	B	605	CLA	C11-C12-C13-C14
25	B	612	CLA	C11-C12-C13-C14
25	B	614	CLA	C11-C12-C13-C14
25	C	508	CLA	C11-C10-C8-C9
25	C	510	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C12-C13-C14
25	C	513	CLA	C11-C10-C8-C9
25	a	612	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	603	CLA	C11-C12-C13-C14
25	b	606	CLA	C6-C7-C8-C9
25	b	606	CLA	C11-C12-C13-C14
25	b	608	CLA	C14-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C9
25	d	401	CLA	C6-C7-C8-C9
25	d	401	CLA	C11-C10-C8-C9
25	d	401	CLA	C11-C12-C13-C14
25	d	404	CLA	C11-C12-C13-C14
33	M	101	LMG	C38-C39-C40-C41
25	B	605	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	C8-C10-C11-C12
25	c	506	CLA	C15-C16-C17-C18
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	604	CLA	C4B-C3B-CAB-CBB
25	C	502	CLA	C4B-C3B-CAB-CBB
25	D	403	CLA	C4B-C3B-CAB-CBB
25	H	101	CLA	C4B-C3B-CAB-CBB
25	a	612	CLA	C4B-C3B-CAB-CBB
25	c	502	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
32	L	101	LHG	C10-C11-C12-C13
31	J	101	STE	C7-C8-C9-C10
33	C	519	LMG	C19-C20-C21-C22
33	C	515	LMG	C12-C13-C14-C15
25	B	602	CLA	C10-C11-C12-C13
25	B	613	CLA	C13-C15-C16-C17
25	c	506	CLA	C16-C17-C18-C19
30	c	518	DGD	C2D-C1D-O3G-C3G
30	h	102	DGD	C9B-CAB-CBB-CCB
31	b	625	STE	C4-C5-C6-C7
32	D	410	LHG	C28-C29-C30-C31
33	c	522	LMG	C11-C12-C13-C14
25	d	401	CLA	C3-C5-C6-C7
31	B	625	STE	C3-C4-C5-C6
31	t	103	STE	C6-C7-C8-C9
32	D	409	LHG	C29-C30-C31-C32
32	D	409	LHG	C34-C35-C36-C37
25	c	501	CLA	O1D-CGD-O2D-CED
31	B	622	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	d	408	LHG	C35-C36-C37-C38
25	B	603	CLA	C11-C12-C13-C15
25	B	605	CLA	C11-C12-C13-C15
25	C	503	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C10-C8-C7
25	C	506	CLA	C12-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C10-C8-C7
25	D	403	CLA	C6-C7-C8-C10
25	D	404	CLA	C6-C7-C8-C10
25	H	101	CLA	C12-C13-C15-C16
25	a	609	CLA	C12-C13-C15-C16
25	b	603	CLA	C11-C10-C8-C7
25	b	604	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C12-C13-C15
25	c	505	CLA	C6-C7-C8-C10
25	c	508	CLA	C12-C13-C15-C16
25	c	512	CLA	C6-C7-C8-C10
25	c	512	CLA	C11-C10-C8-C7
25	c	512	CLA	C12-C13-C15-C16
25	d	401	CLA	C11-C10-C8-C7
25	d	401	CLA	C11-C12-C13-C15
30	C	518	DGD	C2A-C3A-C4A-C5A
30	C	516	DGD	CDA-CEA-CFA-CGA
33	b	620	LMG	C32-C33-C34-C35
33	c	522	LMG	C38-C39-C40-C41
25	C	506	CLA	C16-C17-C18-C20
33	c	522	LMG	C42-C43-C44-C45
31	M	104	STE	C12-C13-C14-C15
31	c	521	STE	C4-C5-C6-C7
31	B	625	STE	C6-C7-C8-C9
25	C	510	CLA	C4-C3-C5-C6
25	c	513	CLA	C3A-C2A-CAA-CBA
25	a	612	CLA	C10-C11-C12-C13
25	c	503	CLA	C8-C10-C11-C12
30	C	516	DGD	O6D-C5D-C6D-O5D
25	C	510	CLA	C2-C3-C5-C6
30	C	517	DGD	C9B-CAB-CBB-CCB
25	B	611	CLA	C10-C11-C12-C13
25	b	611	CLA	C15-C16-C17-C18
25	c	513	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	C	515	LMG	C4-C5-C6-O5
30	C	516	DGD	C4D-C5D-C6D-O5D
33	C	515	LMG	C29-C28-O8-C9
29	D	408	SQD	C27-C28-C29-C30
27	Z	101	BCR	C13-C14-C15-C16
27	Z	101	BCR	C11-C12-C13-C35
29	B	621	SQD	C16-C17-C18-C19
30	C	517	DGD	C8B-C9B-CAB-CBB
32	B	620	LHG	C32-C33-C34-C35
33	b	620	LMG	O6-C5-C6-O5
25	D	404	CLA	C5-C6-C7-C8
31	c	521	STE	C2-C3-C4-C5
25	B	608	CLA	C13-C15-C16-C17
29	A	613	SQD	O6-C44-C45-C46
33	M	101	LMG	O1-C7-C8-C9
33	M	101	LMG	C7-C8-C9-O8
33	c	520	LMG	O1-C7-C8-C9
33	c	520	LMG	C7-C8-C9-O8
25	C	507	CLA	C10-C11-C12-C13
30	H	103	DGD	C4A-C5A-C6A-C7A
31	m	101	STE	C4-C5-C6-C7
25	b	606	CLA	C13-C15-C16-C17
31	D	413	STE	C14-C15-C16-C17
33	D	411	LMG	C14-C15-C16-C17
30	c	517	DGD	O6D-C5D-C6D-O5D
25	B	613	CLA	C4-C3-C5-C6
28	d	406	PL9	C30-C29-C31-C32
31	a	616	STE	C4-C5-C6-C7
29	b	619	SQD	C14-C15-C16-C17
30	a	615	DGD	C3A-C4A-C5A-C6A
32	e	102	LHG	C23-C24-C25-C26
31	t	102	STE	C3-C4-C5-C6
29	a	613	SQD	O10-C23-O48-C46
25	a	612	CLA	O1D-CGD-O2D-CED
25	c	505	CLA	C2B-C3B-CAB-CBB
27	B	616	BCR	C1-C6-C7-C8
27	C	514	BCR	C23-C24-C25-C30
27	H	102	BCR	C23-C24-C25-C30
27	K	101	BCR	C1-C6-C7-C8
25	C	504	CLA	C11-C12-C13-C14
31	M	102	STE	C4-C5-C6-C7
31	C	520	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	e	102	LHG	C18-C19-C20-C21
25	b	604	CLA	C15-C16-C17-C18
25	c	507	CLA	C15-C16-C17-C18
30	A	614	DGD	C7B-C8B-C9B-CAB
30	C	518	DGD	C2B-C3B-C4B-C5B
30	a	615	DGD	C6B-C7B-C8B-C9B
33	b	622	LMG	C18-C19-C20-C21
33	c	520	LMG	C40-C41-C42-C43
29	f	101	SQD	C31-C32-C33-C34
31	B	623	STE	C9-C10-C11-C12
32	L	101	LHG	C13-C14-C15-C16
25	B	614	CLA	C10-C11-C12-C13
29	f	101	SQD	O6-C44-C45-O47
33	M	101	LMG	O7-C8-C9-O8
33	c	520	LMG	O1-C7-C8-O7
33	c	522	LMG	O7-C8-C9-O8
28	A	611	PL9	C4-C3-C7-C8
28	d	406	PL9	C4-C3-C7-C8
32	B	620	LHG	C25-C26-C27-C28
33	C	515	LMG	C14-C15-C16-C17
31	M	102	STE	C9-C10-C11-C12
31	B	623	STE	C13-C14-C15-C16
29	a	613	SQD	C7-C8-C9-C10
31	D	413	STE	C12-C13-C14-C15
32	d	407	LHG	C13-C14-C15-C16
33	D	411	LMG	C13-C14-C15-C16
27	A	610	BCR	C10-C11-C12-C13
27	c	514	BCR	C18-C19-C20-C21
25	h	101	CLA	C10-C11-C12-C13
30	A	614	DGD	C4B-C5B-C6B-C7B
30	C	518	DGD	C4B-C5B-C6B-C7B
25	c	503	CLA	C16-C17-C18-C19
32	E	101	LHG	C31-C32-C33-C34
31	M	102	STE	C1-C2-C3-C4
33	M	101	LMG	C28-C29-C30-C31
25	C	506	CLA	C6-C7-C8-C9
25	H	101	CLA	C14-C13-C15-C16
25	b	612	CLA	C6-C7-C8-C9
25	c	505	CLA	C6-C7-C8-C9
30	C	518	DGD	CCA-CDA-CEA-CFA
33	C	519	LMG	C40-C41-C42-C43
29	a	613	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	c	519	DGD	CDA-CEA-CFA-CGA
32	L	101	LHG	C34-C35-C36-C37
30	C	516	DGD	O6E-C1E-O5D-C6D
25	b	602	CLA	CBD-CGD-O2D-CED
30	A	614	DGD	CAB-CBB-CCB-CDB
31	B	619	STE	C2-C3-C4-C5
32	L	101	LHG	C31-C32-C33-C34
25	A	612	CLA	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C19
25	h	101	CLA	C16-C17-C18-C19
33	M	101	LMG	C11-C12-C13-C14
31	B	625	STE	C4-C5-C6-C7
32	B	620	LHG	C19-C20-C21-C22
25	b	611	CLA	C10-C11-C12-C13
32	E	101	LHG	C33-C34-C35-C36
27	T	101	BCR	C9-C10-C11-C12
25	C	506	CLA	C16-C17-C18-C19
31	M	104	STE	C11-C12-C13-C14
32	e	102	LHG	C28-C29-C30-C31
29	T	103	SQD	C15-C16-C17-C18
31	j	101	STE	C4-C5-C6-C7
32	b	623	LHG	C17-C18-C19-C20
32	L	101	LHG	C18-C19-C20-C21
25	B	607	CLA	C15-C16-C17-C18
29	a	613	SQD	C9-C10-C11-C12
30	A	614	DGD	C5A-C6A-C7A-C8A
30	C	518	DGD	C3B-C4B-C5B-C6B
30	a	615	DGD	CAB-CBB-CCB-CDB
30	c	518	DGD	C9A-CAA-CBA-CCA
31	M	104	STE	C11-C10-C9-C8
31	c	521	STE	C7-C8-C9-C10
33	D	412	LMG	C32-C33-C34-C35
27	B	617	BCR	C20-C21-C22-C37
27	B	618	BCR	C20-C21-C22-C37
27	C	514	BCR	C20-C21-C22-C37
27	K	101	BCR	C11-C10-C9-C34
27	K	101	BCR	C16-C17-C18-C36
27	Y	101	BCR	C35-C13-C14-C15
27	b	617	BCR	C20-C21-C22-C37
27	c	515	BCR	C35-C13-C14-C15
27	d	405	BCR	C20-C21-C22-C37
27	x	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
33	D	411	LMG	C37-C38-C39-C40
31	c	521	STE	C10-C11-C12-C13
32	d	407	LHG	C25-C26-C27-C28
32	e	102	LHG	C27-C28-C29-C30
33	M	101	LMG	C14-C15-C16-C17
32	D	409	LHG	O6-C4-C5-C6
32	e	102	LHG	O6-C4-C5-C6
25	C	508	CLA	C16-C17-C18-C19
25	A	606	CLA	C13-C15-C16-C17
25	B	606	CLA	C12-C13-C15-C16
25	B	609	CLA	C11-C12-C13-C15
25	B	612	CLA	C12-C13-C15-C16
25	B	614	CLA	C12-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C10
25	c	503	CLA	C11-C10-C8-C7
25	c	510	CLA	C12-C13-C15-C16
25	c	511	CLA	C12-C13-C15-C16
25	d	404	CLA	C6-C7-C8-C10
25	h	101	CLA	C12-C13-C15-C16
33	C	515	LMG	C30-C31-C32-C33
33	C	519	LMG	C37-C38-C39-C40
29	f	101	SQD	C24-C25-C26-C27
32	B	620	LHG	C18-C19-C20-C21
33	b	622	LMG	C39-C40-C41-C42
27	B	617	BCR	C17-C18-C19-C20
27	Z	101	BCR	C17-C18-C19-C20
31	c	523	STE	C5-C6-C7-C8
32	l	101	LHG	C32-C33-C34-C35
30	C	517	DGD	C2G-C3G-O3G-C1D
30	C	517	DGD	C5D-C6D-O5D-C1E
30	c	518	DGD	C5D-C6D-O5D-C1E
25	c	513	CLA	C2A-CAA-CBA-CGA
29	A	613	SQD	O49-C7-O47-C45
32	d	407	LHG	C9-C10-C11-C12
33	D	407	LMG	C19-C20-C21-C22
25	a	609	CLA	O1A-CGA-O2A-C1
25	b	610	CLA	C2-C3-C5-C6
32	d	407	LHG	C14-C15-C16-C17
30	C	516	DGD	C6A-C7A-C8A-C9A
33	M	101	LMG	C7-C8-O7-C10
32	d	408	LHG	C29-C30-C31-C32
32	e	102	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C8-C10-C11-C12
29	B	621	SQD	C33-C34-C35-C36
32	b	623	LHG	C25-C26-C27-C28
27	D	405	BCR	C16-C17-C18-C19
32	D	409	LHG	O6-C4-C5-O7
30	C	517	DGD	C3A-C4A-C5A-C6A
31	a	616	STE	C6-C7-C8-C9
33	M	101	LMG	C40-C41-C42-C43
29	D	408	SQD	O5-C1-O6-C44
28	A	611	PL9	C39-C41-C42-C43
29	a	613	SQD	O6-C44-C45-C46
30	A	614	DGD	C1G-C2G-C3G-O3G
32	L	101	LHG	C5-C6-O8-C23
30	a	615	DGD	C2B-C1B-O2G-C2G
33	C	515	LMG	C28-C29-C30-C31
25	H	101	CLA	C15-C16-C17-C18
35	F	101	HEM	C4C-C3C-CAC-CBC
25	B	614	CLA	C16-C17-C18-C19
29	b	619	SQD	C26-C27-C28-C29
25	C	506	CLA	C4-C3-C5-C6
25	b	610	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
28	D	406	PL9	C47-C48-C49-C51
32	E	101	LHG	O7-C5-C6-O8
33	C	519	LMG	O1-C7-C8-O7
33	c	520	LMG	O7-C8-C9-O8
33	c	524	LMG	O7-C8-C9-O8
25	B	601	CLA	C13-C15-C16-C17
25	b	607	CLA	C5-C6-C7-C8
25	B	601	CLA	C6-C7-C8-C9
25	B	606	CLA	C6-C7-C8-C9
25	B	609	CLA	C11-C12-C13-C14
25	B	614	CLA	C14-C13-C15-C16
25	C	512	CLA	C6-C7-C8-C9
25	C	507	CLA	C16-C17-C18-C19
31	T	102	STE	C10-C11-C12-C13
33	D	411	LMG	C30-C31-C32-C33
33	d	410	LMG	C14-C15-C16-C17
31	M	103	STE	C5-C6-C7-C8
31	l	102	STE	C7-C8-C9-C10
32	L	101	LHG	C28-C29-C30-C31
33	c	522	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
30	a	615	DGD	C6A-C7A-C8A-C9A
32	b	623	LHG	C33-C34-C35-C36
31	E	102	STE	C7-C8-C9-C10
31	H	104	STE	C7-C8-C9-C10
30	C	517	DGD	C4A-C5A-C6A-C7A
32	D	409	LHG	C11-C10-C9-C8
33	D	407	LMG	C38-C39-C40-C41
25	b	605	CLA	C3-C5-C6-C7
30	h	102	DGD	O2G-C1B-C2B-C3B
25	c	512	CLA	C2-C3-C5-C6
25	C	510	CLA	C13-C15-C16-C17
25	b	609	CLA	C2A-CAA-CBA-CGA
25	b	613	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C20
30	C	517	DGD	CBA-CCA-CDA-CEA
25	b	605	CLA	C15-C16-C17-C18
30	C	516	DGD	O1B-C1B-O2G-C2G
30	c	518	DGD	C4E-C5E-C6E-O5E
27	K	101	BCR	C37-C22-C23-C24
27	T	101	BCR	C11-C12-C13-C35
30	c	517	DGD	C4D-C5D-C6D-O5D
25	B	603	CLA	C1A-C2A-CAA-CBA
25	C	501	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA
32	d	408	LHG	C24-C23-O8-C6
33	M	101	LMG	C37-C38-C39-C40
33	b	620	LMG	C38-C39-C40-C41
33	d	410	LMG	C30-C31-C32-C33
30	h	102	DGD	C6A-C7A-C8A-C9A
27	Z	101	BCR	C7-C8-C9-C10
33	d	410	LMG	C37-C38-C39-C40
29	a	614	SQD	C9-C10-C11-C12
30	C	517	DGD	CDA-CEA-CFA-CGA
25	a	609	CLA	C15-C16-C17-C18
33	c	520	LMG	C39-C40-C41-C42
25	A	607	CLA	C12-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C11-C10-C8-C7
25	B	606	CLA	C11-C12-C13-C15
25	B	612	CLA	C6-C7-C8-C10
25	B	615	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C6-C7-C8-C10
25	C	507	CLA	C11-C12-C13-C15
25	H	101	CLA	C11-C10-C8-C7
25	H	101	CLA	C11-C12-C13-C15
25	a	607	CLA	C11-C12-C13-C15
25	b	613	CLA	C6-C7-C8-C10
25	d	401	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
26	a	608	PHO	C6-C7-C8-C10
30	a	615	DGD	CEB-CFB-CGB-CHB
31	b	621	STE	C9-C10-C11-C12
31	b	625	STE	C7-C8-C9-C10
29	T	103	SQD	C10-C11-C12-C13
30	c	517	DGD	C6A-C7A-C8A-C9A
31	j	101	STE	C5-C6-C7-C8
36	V	201	HEC	C4B-C3B-CAB-CBB
33	D	411	LMG	C15-C16-C17-C18
33	D	412	LMG	C13-C14-C15-C16
33	C	519	LMG	C11-C12-C13-C14
25	B	606	CLA	C14-C13-C15-C16
25	B	612	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	c	510	CLA	C14-C13-C15-C16
25	B	605	CLA	C15-C16-C17-C18
27	Z	101	BCR	C15-C16-C17-C18
27	c	516	BCR	C13-C14-C15-C16
25	b	606	CLA	O1D-CGD-O2D-CED
29	a	614	SQD	C29-C30-C31-C32
31	C	520	STE	C2-C3-C4-C5
31	E	102	STE	C6-C7-C8-C9
33	D	412	LMG	C34-C35-C36-C37
30	C	516	DGD	O1G-C1G-C2G-O2G
33	D	411	LMG	O7-C8-C9-O8
30	C	517	DGD	C7A-C8A-C9A-CAA
30	c	517	DGD	C3B-C4B-C5B-C6B
25	B	610	CLA	C15-C16-C17-C18
25	b	613	CLA	C16-C17-C18-C20
30	C	516	DGD	O1G-C1G-C2G-C3G
28	a	611	PL9	C30-C29-C31-C32
30	c	519	DGD	C3B-C4B-C5B-C6B
25	C	506	CLA	C2-C3-C5-C6
32	l	101	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
25	B	611	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	h	101	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	C15-C16-C17-C18
25	B	603	CLA	O1A-CGA-O2A-C1
33	c	524	LMG	C19-C20-C21-C22
32	E	101	LHG	C35-C36-C37-C38
30	C	517	DGD	C2A-C3A-C4A-C5A
31	m	101	STE	C3-C4-C5-C6
33	b	622	LMG	C15-C16-C17-C18
31	b	624	STE	C10-C11-C12-C13
25	B	611	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	513	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O2D
25	h	101	CLA	CAD-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O2D
27	b	617	BCR	C35-C13-C14-C15
27	c	514	BCR	C19-C20-C21-C22
27	k	101	BCR	C19-C20-C21-C22
32	D	410	LHG	C3-O3-P-O5
32	L	101	LHG	C3-O3-P-O6
32	d	407	LHG	C3-O3-P-O5
25	B	601	CLA	C16-C17-C18-C20
25	C	507	CLA	C16-C17-C18-C20
30	A	614	DGD	C8A-C9A-CAA-CBA
25	c	509	CLA	C8-C10-C11-C12
26	D	402	PHO	C2C-C3C-CAC-CBC
25	C	502	CLA	C2B-C3B-CAB-CBB
25	H	101	CLA	C2B-C3B-CAB-CBB
25	a	612	CLA	C2B-C3B-CAB-CBB
27	B	616	BCR	C7-C8-C9-C34
30	C	517	DGD	CDB-CEB-CFB-CGB
25	B	602	CLA	C5-C6-C7-C8
25	c	504	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	b	609	CLA	C2C-C3C-CAC-CBC
26	D	402	PHO	O1D-CGD-O2D-CED
29	T	103	SQD	C32-C33-C34-C35
33	C	515	LMG	C37-C38-C39-C40
29	A	613	SQD	C25-C26-C27-C28
28	a	611	PL9	C4-C3-C7-C8
33	M	101	LMG	C13-C14-C15-C16
33	C	515	LMG	C9-C8-O7-C10
31	B	624	STE	C1-C2-C3-C4
31	D	413	STE	C10-C11-C12-C13
25	B	610	CLA	C16-C17-C18-C19
25	B	610	CLA	C16-C17-C18-C20
25	B	614	CLA	C16-C17-C18-C20
26	A	608	PHO	C16-C17-C18-C20
25	b	609	CLA	C13-C15-C16-C17
32	d	407	LHG	C26-C27-C28-C29
30	C	518	DGD	CAB-CBB-CCB-CDB
25	c	505	CLA	C15-C16-C17-C18
25	B	604	CLA	C6-C7-C8-C9
25	B	612	CLA	C6-C7-C8-C9
25	B	615	CLA	C6-C7-C8-C9
25	D	403	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C10-C8-C9
25	b	604	CLA	C14-C13-C15-C16
25	c	507	CLA	C6-C7-C8-C9
25	c	512	CLA	C11-C10-C8-C9
25	h	101	CLA	C11-C10-C8-C9
26	a	608	PHO	C11-C10-C8-C9
27	A	610	BCR	C11-C10-C9-C8
27	x	101	BCR	C16-C17-C18-C19
32	D	410	LHG	C29-C30-C31-C32
25	B	601	CLA	C16-C17-C18-C19
25	c	505	CLA	C10-C11-C12-C13
30	a	615	DGD	C8B-C9B-CAB-CBB
29	T	103	SQD	C24-C23-O48-C46
30	C	516	DGD	C2E-C1E-O5D-C6D
33	M	101	LMG	C2-C1-O1-C7
33	c	520	LMG	C2-C1-O1-C7
25	B	612	CLA	C2-C3-C5-C6
31	l	102	STE	C10-C11-C12-C13
30	c	518	DGD	O1B-C1B-O2G-C2G
32	d	408	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
33	c	522	LMG	O6-C5-C6-O5
30	A	614	DGD	O1G-C1G-C2G-O2G
32	d	407	LHG	C31-C32-C33-C34
25	B	603	CLA	CBA-CGA-O2A-C1
30	c	517	DGD	C1B-C2B-C3B-C4B
27	a	610	BCR	C19-C20-C21-C22
27	c	516	BCR	C15-C16-C17-C18
33	M	101	LMG	C17-C18-C19-C20
25	c	504	CLA	C11-C12-C13-C14
25	B	613	CLA	C8-C10-C11-C12
29	T	103	SQD	O10-C23-O48-C46
30	H	103	DGD	O2G-C1B-C2B-C3B
28	a	611	PL9	C19-C21-C22-C23
29	D	408	SQD	C44-C45-C46-O48
33	C	515	LMG	C34-C35-C36-C37
33	c	520	LMG	C31-C32-C33-C34
29	a	613	SQD	C16-C17-C18-C19
25	B	612	CLA	C16-C17-C18-C19
32	E	101	LHG	C29-C30-C31-C32
31	M	102	STE	C11-C10-C9-C8
30	c	517	DGD	C5D-C6D-O5D-C1E
33	c	524	LMG	C8-C7-O1-C1
25	B	601	CLA	C2A-CAA-CBA-CGA
25	c	509	CLA	O1D-CGD-O2D-CED
27	c	514	BCR	C15-C16-C17-C18
33	b	620	LMG	C16-C17-C18-C19
25	b	604	CLA	C4-C3-C5-C6
31	b	625	STE	C1-C2-C3-C4
32	l	101	LHG	C29-C30-C31-C32
33	D	407	LMG	C33-C34-C35-C36
25	B	601	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C10-C8-C9
25	a	609	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
31	b	626	STE	C3-C4-C5-C6
31	l	102	STE	C13-C14-C15-C16
25	b	613	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
25	d	401	CLA	C4B-C3B-CAB-CBB
32	L	101	LHG	C7-C8-C9-C10
25	C	508	CLA	C16-C17-C18-C20
33	C	519	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
30	C	516	DGD	CCB-CDB-CEB-CFB
31	l	102	STE	C11-C12-C13-C14
31	B	624	STE	C4-C5-C6-C7
30	H	103	DGD	C4D-C5D-C6D-O5D
25	B	603	CLA	C10-C11-C12-C13
32	b	623	LHG	C11-C10-C9-C8
25	c	509	CLA	CAA-CBA-CGA-O2A
33	c	520	LMG	C32-C33-C34-C35
25	A	607	CLA	C6-C7-C8-C10
25	B	607	CLA	C6-C7-C8-C10
25	C	512	CLA	C11-C10-C8-C7
25	D	403	CLA	C12-C13-C15-C16
25	a	612	CLA	C11-C12-C13-C15
25	b	602	CLA	C11-C12-C13-C15
25	b	605	CLA	C11-C10-C8-C7
25	c	512	CLA	C5-C6-C7-C8
31	b	624	STE	C11-C12-C13-C14
25	c	511	CLA	C8-C10-C11-C12
30	c	519	DGD	CBB-CCB-CDB-CEB
32	d	408	LHG	C28-C29-C30-C31
26	D	402	PHO	CBD-CGD-O2D-CED
25	A	612	CLA	C4C-C3C-CAC-CBC
31	l	102	STE	C5-C6-C7-C8
25	H	101	CLA	C3A-C2A-CAA-CBA
33	b	620	LMG	C15-C16-C17-C18
32	E	101	LHG	C18-C19-C20-C21
27	T	101	BCR	C16-C17-C18-C36
27	a	610	BCR	C35-C13-C14-C15
27	a	610	BCR	C20-C21-C22-C37
29	b	619	SQD	O5-C1-O6-C44
33	b	622	LMG	C24-C25-C26-C27
30	C	517	DGD	CCA-CDA-CEA-CFA
25	C	506	CLA	C15-C16-C17-C18
29	f	101	SQD	C27-C28-C29-C30
25	d	403	CLA	C2-C1-O2A-CGA
31	t	103	STE	C4-C5-C6-C7
25	B	610	CLA	C8-C10-C11-C12
25	C	509	CLA	C15-C16-C17-C18
31	d	411	STE	C6-C7-C8-C9
29	A	613	SQD	C29-C30-C31-C32
29	f	101	SQD	C34-C35-C36-C37
31	I	101	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	b	625	STE	O1-C1-C2-C3
35	e	101	HEM	C2A-CAA-CBA-CGA
25	A	612	CLA	C2C-C3C-CAC-CBC
30	a	615	DGD	CAA-CBA-CCA-CDA
30	c	519	DGD	C6B-C7B-C8B-C9B
30	H	103	DGD	CDA-CEA-CFA-CGA
30	C	516	DGD	O1A-C1A-C2A-C3A
31	B	622	STE	O1-C1-C2-C3
25	A	607	CLA	C6-C7-C8-C9
25	B	602	CLA	C11-C10-C8-C9
25	B	605	CLA	C11-C10-C8-C9
25	B	607	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	a	612	CLA	C11-C12-C13-C14
25	b	601	CLA	C6-C7-C8-C9
25	b	612	CLA	C14-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C14
25	c	503	CLA	C11-C10-C8-C9
25	c	512	CLA	C11-C12-C13-C14
25	d	401	CLA	C14-C13-C15-C16
26	D	402	PHO	C6-C7-C8-C9
29	a	613	SQD	C10-C11-C12-C13
31	b	626	STE	C1-C2-C3-C4
31	c	523	STE	C7-C8-C9-C10
31	B	623	STE	O2-C1-C2-C3
25	A	607	CLA	C3-C5-C6-C7
26	d	402	PHO	C1A-C2A-CAA-CBA
30	C	518	DGD	O6E-C5E-C6E-O5E
32	D	410	LHG	C11-C10-C9-C8
25	d	401	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	C1A-C2A-CAA-CBA
27	b	616	BCR	C12-C13-C14-C15
27	d	405	BCR	C16-C17-C18-C19
36	V	201	HEC	CAD-CBD-CGD-O1D
30	C	516	DGD	C8A-C9A-CAA-CBA
32	D	409	LHG	C13-C14-C15-C16
25	A	607	CLA	C2B-C3B-CAB-CBB
25	B	604	CLA	C2B-C3B-CAB-CBB
25	B	605	CLA	C2B-C3B-CAB-CBB
25	C	501	CLA	C2B-C3B-CAB-CBB
25	C	503	CLA	C2B-C3B-CAB-CBB
25	b	613	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	c	502	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
27	B	616	BCR	C5-C6-C7-C8
27	B	617	BCR	C23-C24-C25-C30
27	H	102	BCR	C23-C24-C25-C26
27	K	101	BCR	C5-C6-C7-C8
27	b	616	BCR	C1-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C30
27	x	101	BCR	C23-C24-C25-C30
31	b	621	STE	O1-C1-C2-C3
31	t	102	STE	O2-C1-C2-C3
30	h	102	DGD	C7B-C8B-C9B-CAB
29	B	621	SQD	C28-C29-C30-C31
29	T	103	SQD	C16-C17-C18-C19
31	c	521	STE	C3-C4-C5-C6
25	B	612	CLA	C13-C15-C16-C17
31	b	625	STE	O2-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O1D
36	v	201	HEC	CAD-CBD-CGD-O2D
25	c	508	CLA	C4-C3-C5-C6
25	d	403	CLA	C4-C3-C5-C6
29	A	613	SQD	C9-C10-C11-C12
31	x	102	STE	C12-C13-C14-C15
33	c	520	LMG	C34-C35-C36-C37
31	B	622	STE	O2-C1-C2-C3
25	B	601	CLA	C11-C12-C13-C15
25	B	605	CLA	C6-C7-C8-C10
25	C	505	CLA	C6-C7-C8-C10
25	C	509	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C12-C13-C15
25	D	403	CLA	C11-C12-C13-C15
29	B	621	SQD	C14-C15-C16-C17
25	d	404	CLA	C16-C17-C18-C19
25	B	613	CLA	C2A-CAA-CBA-CGA
25	C	501	CLA	C2A-CAA-CBA-CGA
25	C	502	CLA	C13-C15-C16-C17
29	a	613	SQD	O47-C45-C46-O48
30	a	615	DGD	C5B-C6B-C7B-C8B
33	M	101	LMG	C34-C35-C36-C37
31	C	520	STE	C7-C8-C9-C10
27	x	101	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
31	B	625	STE	C11-C12-C13-C14
30	c	517	DGD	O1G-C1A-C2A-C3A
28	D	406	PL9	C33-C34-C36-C37
33	c	524	LMG	C33-C34-C35-C36
25	c	509	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	C10-C11-C12-C13
25	b	611	CLA	C8-C10-C11-C12
31	B	623	STE	O1-C1-C2-C3
31	t	102	STE	O1-C1-C2-C3
31	b	625	STE	C11-C12-C13-C14
33	C	515	LMG	C17-C18-C19-C20
25	c	505	CLA	C11-C10-C8-C9
33	b	622	LMG	C32-C33-C34-C35
30	h	102	DGD	C4B-C5B-C6B-C7B
31	c	521	STE	C5-C6-C7-C8
32	D	410	LHG	C15-C16-C17-C18
33	C	515	LMG	C18-C19-C20-C21
25	B	612	CLA	C16-C17-C18-C20
25	a	609	CLA	C16-C17-C18-C20
30	A	614	DGD	CEB-CFB-CGB-CHB
33	D	412	LMG	O9-C10-C11-C12
35	F	101	HEM	CAD-CBD-CGD-O2D
30	c	517	DGD	CDB-CEB-CFB-CGB
27	Z	101	BCR	C6-C7-C8-C9
31	E	102	STE	C3-C4-C5-C6
25	b	612	CLA	C4-C3-C5-C6
28	A	611	PL9	C15-C14-C16-C17
25	B	613	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
36	v	201	HEC	CAD-CBD-CGD-O1D
32	d	407	LHG	C28-C29-C30-C31
33	D	407	LMG	C11-C12-C13-C14
30	C	518	DGD	O1G-C1G-C2G-C3G
30	c	517	DGD	O1G-C1G-C2G-C3G
33	c	522	LMG	C29-C30-C31-C32
30	h	102	DGD	CBA-CCA-CDA-CEA
31	c	523	STE	C2-C3-C4-C5
33	D	412	LMG	O7-C10-C11-C12
30	C	518	DGD	C7A-C8A-C9A-CAA
31	M	104	STE	C13-C14-C15-C16
30	C	516	DGD	O1G-C1A-C2A-C3A
32	b	623	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
32	d	408	LHG	C9-C10-C11-C12
25	A	606	CLA	C15-C16-C17-C18
25	C	507	CLA	C5-C6-C7-C8
33	C	519	LMG	C36-C37-C38-C39
25	C	507	CLA	C4B-C3B-CAB-CBB
30	H	103	DGD	O1B-C1B-C2B-C3B
32	D	409	LHG	C1-C2-C3-O3
30	h	102	DGD	C7A-C8A-C9A-CAA
26	d	402	PHO	CHA-CBD-CGD-O1D
25	c	504	CLA	C8-C10-C11-C12
36	V	201	HEC	CAD-CBD-CGD-O2D
33	D	412	LMG	C17-C18-C19-C20
29	B	621	SQD	C25-C26-C27-C28
29	T	103	SQD	C25-C26-C27-C28
32	D	409	LHG	C15-C16-C17-C18
32	l	101	LHG	O6-C4-C5-C6
25	b	607	CLA	C16-C17-C18-C19
30	c	517	DGD	O1G-C1G-C2G-O2G
33	D	411	LMG	C10-C11-C12-C13
33	C	515	LMG	C39-C40-C41-C42
25	c	508	CLA	C2-C3-C5-C6
25	b	602	CLA	O1D-CGD-O2D-CED
32	D	410	LHG	C2-C3-O3-P
33	C	519	LMG	C33-C34-C35-C36
25	b	602	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C10-C8-C7
32	E	101	LHG	C15-C16-C17-C18
31	M	103	STE	C1-C2-C3-C4
30	A	614	DGD	C6A-C7A-C8A-C9A
32	L	101	LHG	C25-C26-C27-C28
33	d	410	LMG	C34-C35-C36-C37
31	c	521	STE	O1-C1-C2-C3
25	A	606	CLA	C11-C10-C8-C9
25	A	606	CLA	C14-C13-C15-C16
25	B	603	CLA	C11-C10-C8-C9
25	B	605	CLA	C14-C13-C15-C16
25	C	505	CLA	C14-C13-C15-C16
25	H	101	CLA	C11-C10-C8-C9
25	b	602	CLA	C11-C10-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	d	403	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	c	518	DGD	C7B-C8B-C9B-CAB
33	D	412	LMG	C12-C13-C14-C15
29	b	619	SQD	C45-C44-O6-C1
33	C	515	LMG	C8-C7-O1-C1
25	H	101	CLA	C2-C1-O2A-CGA
25	A	609	CLA	C3A-C2A-CAA-CBA
31	c	521	STE	O2-C1-C2-C3
25	c	506	CLA	C10-C11-C12-C13
25	C	510	CLA	C8-C10-C11-C12
31	b	621	STE	O2-C1-C2-C3
31	T	102	STE	C15-C16-C17-C18
31	B	623	STE	C11-C12-C13-C14
33	b	622	LMG	C19-C20-C21-C22
31	J	101	STE	C3-C4-C5-C6
30	a	615	DGD	C1G-C2G-O2G-C1B
26	d	402	PHO	C8-C10-C11-C12
32	e	102	LHG	C14-C15-C16-C17
31	d	411	STE	C7-C8-C9-C10
31	E	102	STE	C4-C5-C6-C7
31	M	104	STE	C15-C16-C17-C18
32	D	410	LHG	C1-C2-C3-O3
32	b	623	LHG	C9-C10-C11-C12
30	C	517	DGD	O6D-C1D-O3G-C3G
30	c	518	DGD	O6E-C5E-C6E-O5E
28	D	406	PL9	C24-C26-C27-C28
29	f	101	SQD	O6-C44-C45-C46
30	C	516	DGD	C1G-C2G-C3G-O3G
33	D	412	LMG	O10-C28-C29-C30
31	M	104	STE	C10-C11-C12-C13
25	a	612	CLA	C2C-C3C-CAC-CBC
28	A	611	PL9	C43-C44-C46-C47
30	c	517	DGD	C5B-C6B-C7B-C8B
31	I	101	STE	C1-C2-C3-C4
25	b	615	CLA	O1A-CGA-O2A-C1
30	a	615	DGD	O1G-C1G-C2G-O2G
25	c	510	CLA	C15-C16-C17-C18
25	C	505	CLA	C11-C10-C8-C9
25	C	507	CLA	C6-C7-C8-C9
25	C	509	CLA	C11-C12-C13-C14
25	a	607	CLA	C14-C13-C15-C16
29	a	614	SQD	C18-C19-C20-C21
32	e	102	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	d	403	CLA	C2-C3-C5-C6
25	A	606	CLA	C12-C13-C15-C16
25	B	603	CLA	C11-C10-C8-C7
25	B	614	CLA	C6-C7-C8-C10
25	b	601	CLA	C6-C7-C8-C10
25	b	601	CLA	C11-C10-C8-C7
25	b	606	CLA	C11-C10-C8-C7
25	b	607	CLA	C11-C10-C8-C7
25	b	611	CLA	C12-C13-C15-C16
25	b	612	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C12-C13-C15
25	d	403	CLA	C6-C7-C8-C10
25	C	502	CLA	C10-C11-C12-C13
25	B	610	CLA	C2B-C3B-CAB-CBB
25	D	403	CLA	C2B-C3B-CAB-CBB
25	c	503	CLA	C2B-C3B-CAB-CBB
27	B	617	BCR	C23-C24-C25-C26
27	C	514	BCR	C23-C24-C25-C26
27	Y	101	BCR	C23-C24-C25-C30
27	b	617	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
27	c	514	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C26
27	d	405	BCR	C23-C24-C25-C26
27	x	101	BCR	C23-C24-C25-C26
31	b	625	STE	C2-C3-C4-C5
31	x	102	STE	C14-C15-C16-C17
29	a	613	SQD	O47-C7-C8-C9
31	B	619	STE	C4-C5-C6-C7
25	b	607	CLA	C2-C1-O2A-CGA
29	a	614	SQD	C25-C26-C27-C28
29	B	621	SQD	C45-C46-O48-C23
30	A	614	DGD	CBB-CCB-CDB-CEB
25	a	607	CLA	C13-C15-C16-C17
26	A	608	PHO	C2-C3-C5-C6
25	D	403	CLA	C13-C15-C16-C17
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	601	CLA	C2A-CAA-CBA-CGA
33	b	620	LMG	C11-C10-O7-C8
33	d	409	LMG	C40-C41-C42-C43
31	t	102	STE	C7-C8-C9-C10
25	d	404	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	D	407	LMG	C22-C23-C24-C25
28	A	611	PL9	C25-C24-C26-C27
32	D	409	LHG	C12-C13-C14-C15
30	H	103	DGD	C3A-C4A-C5A-C6A
33	c	524	LMG	O9-C10-O7-C8
25	b	615	CLA	CBA-CGA-O2A-C1
31	J	101	STE	O2-C1-C2-C3
25	C	505	CLA	C6-C7-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	a	607	CLA	C11-C12-C13-C14
25	b	612	CLA	CAA-CBA-CGA-O2A
29	A	613	SQD	O47-C7-C8-C9
33	c	524	LMG	O1-C7-C8-C9
25	C	511	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	d	403	CLA	C1A-C2A-CAA-CBA
30	c	517	DGD	O6E-C1E-O5D-C6D
25	B	611	CLA	CAA-CBA-CGA-O2A
27	K	101	BCR	C11-C12-C13-C14
27	D	405	BCR	C19-C20-C21-C22
25	b	607	CLA	C13-C15-C16-C17
31	B	625	STE	C13-C14-C15-C16
32	L	101	LHG	C24-C25-C26-C27
32	D	410	LHG	O8-C23-C24-C25
33	b	620	LMG	O8-C28-C29-C30
29	a	613	SQD	C12-C13-C14-C15
31	B	625	STE	C12-C13-C14-C15
25	c	502	CLA	O1A-CGA-O2A-C1
30	C	518	DGD	C1B-C2B-C3B-C4B
25	A	606	CLA	C16-C17-C18-C20
28	D	406	PL9	C42-C43-C44-C45
29	B	621	SQD	O47-C7-C8-C9
31	l	102	STE	C9-C10-C11-C12
32	d	407	LHG	C24-C25-C26-C27
26	A	608	PHO	C4-C3-C5-C6
29	D	408	SQD	C31-C32-C33-C34
30	h	102	DGD	CCB-CDB-CEB-CFB
25	A	606	CLA	C11-C10-C8-C7
25	A	612	CLA	C12-C13-C15-C16
25	B	602	CLA	C12-C13-C15-C16
25	a	612	CLA	C6-C7-C8-C10
25	b	604	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	C12-C13-C15-C16
29	B	621	SQD	C31-C32-C33-C34
25	B	612	CLA	CAA-CBA-CGA-O2A
29	T	103	SQD	C28-C29-C30-C31
25	B	612	CLA	C10-C11-C12-C13
32	E	101	LHG	C12-C13-C14-C15
25	B	602	CLA	C13-C15-C16-C17
30	a	615	DGD	C4B-C5B-C6B-C7B
32	E	101	LHG	O7-C7-C8-C9
29	a	613	SQD	C25-C26-C27-C28
25	B	611	CLA	C8-C10-C11-C12
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	613	CLA	C16-C17-C18-C20
25	c	505	CLA	C16-C17-C18-C19
27	C	514	BCR	C11-C10-C9-C8
25	b	609	CLA	C5-C6-C7-C8
25	B	609	CLA	C8-C10-C11-C12
32	D	409	LHG	C17-C18-C19-C20
33	d	410	LMG	O7-C10-C11-C12
32	e	102	LHG	C7-C8-C9-C10
25	a	612	CLA	C4C-C3C-CAC-CBC
25	a	609	CLA	C6-C7-C8-C9
26	a	608	PHO	C6-C7-C8-C9
30	C	516	DGD	CAB-CBB-CCB-CDB
29	a	613	SQD	O49-C7-C8-C9
32	e	102	LHG	C9-C10-C11-C12
25	b	601	CLA	C15-C16-C17-C18
25	b	611	CLA	CAA-CBA-CGA-O2A
29	B	621	SQD	O5-C5-C6-S
33	d	409	LMG	O7-C10-C11-C12
30	h	102	DGD	C2A-C3A-C4A-C5A
31	D	413	STE	C11-C10-C9-C8
30	C	516	DGD	CDB-CEB-CFB-CGB
33	C	519	LMG	C39-C40-C41-C42
30	c	519	DGD	C7B-C8B-C9B-CAB
26	A	608	PHO	C16-C17-C18-C19
31	J	101	STE	O1-C1-C2-C3
27	c	514	BCR	C17-C18-C19-C20
27	c	516	BCR	C17-C18-C19-C20
27	d	405	BCR	C7-C8-C9-C10
25	B	611	CLA	CAA-CBA-CGA-O1A
29	B	621	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	c	517	DGD	O1B-C1B-C2B-C3B
33	c	524	LMG	O10-C28-C29-C30
25	b	604	CLA	C10-C11-C12-C13
30	H	103	DGD	C2G-C3G-O3G-C1D
30	h	102	DGD	C2G-C3G-O3G-C1D
33	b	620	LMG	C8-C7-O1-C1
29	b	619	SQD	O6-C44-C45-O47
29	b	619	SQD	O47-C45-C46-O48
31	B	623	STE	C7-C8-C9-C10
32	E	101	LHG	O9-C7-C8-C9
30	C	517	DGD	C2B-C3B-C4B-C5B
31	b	624	STE	C2-C3-C4-C5
29	b	619	SQD	C44-C45-C46-O48
30	C	516	DGD	O1B-C1B-C2B-C3B
33	b	620	LMG	O10-C28-C29-C30
29	a	614	SQD	C11-C12-C13-C14
31	B	619	STE	C11-C10-C9-C8
25	h	101	CLA	CAA-CBA-CGA-O2A
31	d	411	STE	O2-C1-C2-C3
25	B	608	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
29	A	613	SQD	O49-C7-C8-C9
25	D	403	CLA	C15-C16-C17-C18
33	c	522	LMG	O6-C1-O1-C7
25	B	612	CLA	C2-C1-O2A-CGA
25	C	501	CLA	C16-C17-C18-C20
31	C	522	STE	C12-C13-C14-C15
33	D	407	LMG	C18-C19-C20-C21
33	d	410	LMG	C38-C39-C40-C41
35	e	101	HEM	CAA-CBA-CGA-O2A
30	c	518	DGD	C1A-C2A-C3A-C4A
25	B	601	CLA	CAA-CBA-CGA-O2A
30	c	519	DGD	O1G-C1A-C2A-C3A
29	a	613	SQD	C19-C20-C21-C22
33	D	412	LMG	O8-C28-C29-C30
30	c	519	DGD	O6D-C5D-C6D-O5D
25	H	101	CLA	CAA-CBA-CGA-O2A
32	d	408	LHG	O10-C23-O8-C6
31	d	411	STE	O1-C1-C2-C3
31	c	521	STE	C1-C2-C3-C4
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	611	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	A	613	SQD	C30-C31-C32-C33

There are no ring outliers.

144 monomers are involved in 305 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	611	PL9	5	0
30	C	516	DGD	1	0
25	C	508	CLA	4	0
27	T	101	BCR	4	0
32	D	410	LHG	3	0
25	B	615	CLA	2	0
25	C	502	CLA	2	0
35	F	101	HEM	3	0
31	b	625	STE	1	0
25	d	401	CLA	1	0
27	B	618	BCR	3	0
29	A	613	SQD	3	0
27	b	618	BCR	2	0
25	c	509	CLA	3	0
29	D	408	SQD	1	0
30	C	518	DGD	5	0
32	L	101	LHG	1	0
25	d	404	CLA	3	0
28	d	406	PL9	3	0
25	b	615	CLA	3	0
25	B	614	CLA	3	0
25	d	403	CLA	2	0
25	B	603	CLA	2	0
25	a	612	CLA	2	0
32	d	407	LHG	3	0
25	b	602	CLA	1	0
25	C	512	CLA	3	0
25	C	505	CLA	3	0
25	c	506	CLA	2	0
27	b	616	BCR	1	0
25	b	605	CLA	10	0
29	T	103	SQD	1	0
30	C	517	DGD	3	0
25	c	505	CLA	4	0
31	B	624	STE	1	0
25	B	610	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	c	524	LMG	3	0
25	b	603	CLA	5	0
26	d	402	PHO	5	0
25	b	613	CLA	3	0
27	c	516	BCR	1	0
25	c	508	CLA	3	0
27	c	515	BCR	4	0
27	D	405	BCR	1	0
31	t	103	STE	1	0
25	b	609	CLA	4	0
25	c	504	CLA	1	0
28	A	611	PL9	5	0
33	M	101	LMG	2	0
25	C	504	CLA	4	0
25	b	608	CLA	4	0
25	D	403	CLA	4	0
31	H	104	STE	1	0
27	c	514	BCR	1	0
25	B	607	CLA	2	0
25	B	609	CLA	1	0
31	t	102	STE	1	0
33	d	410	LMG	1	0
25	C	507	CLA	1	0
32	D	409	LHG	2	0
30	H	103	DGD	4	0
32	d	408	LHG	1	0
25	B	608	CLA	5	0
25	h	101	CLA	4	0
25	b	601	CLA	3	0
27	b	617	BCR	3	0
25	B	605	CLA	4	0
25	b	612	CLA	2	0
26	a	608	PHO	2	0
25	b	604	CLA	3	0
25	c	511	CLA	3	0
33	D	411	LMG	1	0
31	B	625	STE	1	0
29	a	613	SQD	2	0
27	x	101	BCR	4	0
33	C	519	LMG	5	0
25	H	101	CLA	3	0
25	A	606	CLA	1	0

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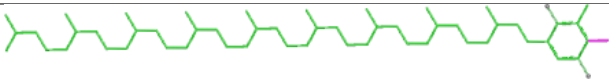
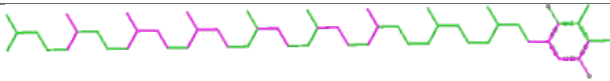
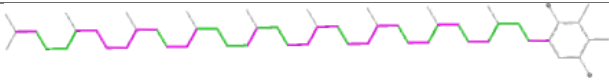
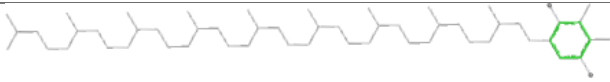
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	C	522	STE	2	0
27	K	101	BCR	1	0
33	c	522	LMG	2	0
25	B	612	CLA	3	0
25	C	506	CLA	1	0
25	C	510	CLA	3	0
27	d	405	BCR	2	0
32	E	101	LHG	2	0
25	b	611	CLA	3	0
25	B	601	CLA	4	0
25	c	513	CLA	2	0
31	c	523	STE	1	0
25	c	510	CLA	3	0
27	Z	101	BCR	1	0
25	c	501	CLA	3	0
29	f	101	SQD	2	0
25	b	607	CLA	2	0
30	A	614	DGD	9	0
33	b	620	LMG	3	0
27	B	617	BCR	2	0
29	a	614	SQD	2	0
30	c	519	DGD	3	0
25	B	604	CLA	5	0
26	D	402	PHO	5	0
30	a	615	DGD	2	0
33	c	520	LMG	1	0
22	A	602[A]	OEY	1	0
29	B	621	SQD	4	0
31	D	413	STE	1	0
35	e	101	HEM	5	0
25	c	507	CLA	3	0
25	c	502	CLA	1	0
30	h	102	DGD	3	0
25	D	404	CLA	1	0
27	B	616	BCR	2	0
27	Y	101	BCR	1	0
32	b	623	LHG	3	0
32	B	620	LHG	3	0
25	b	614	CLA	4	0
33	D	407	LMG	2	0
25	A	607	CLA	2	0
25	A	609	CLA	2	0

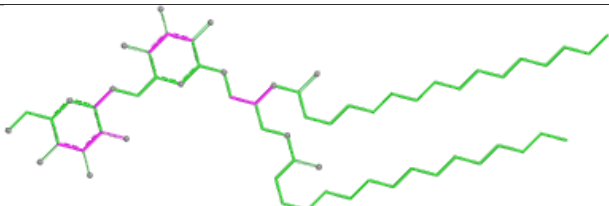
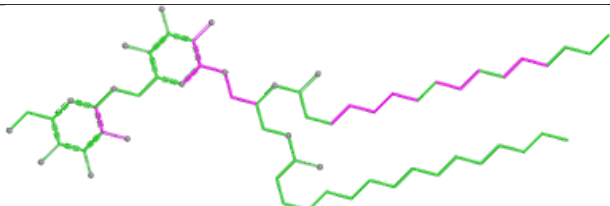
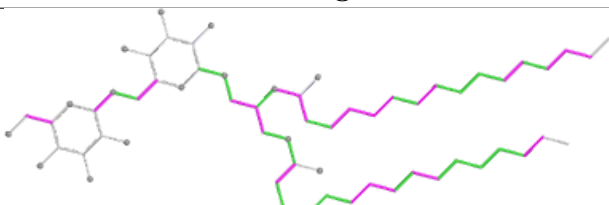
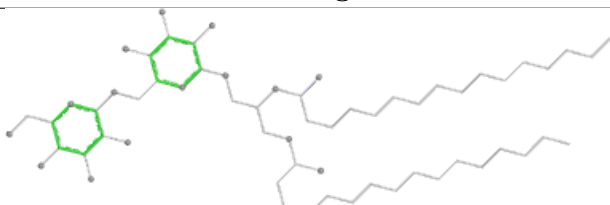
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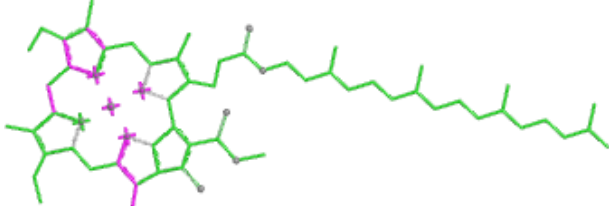
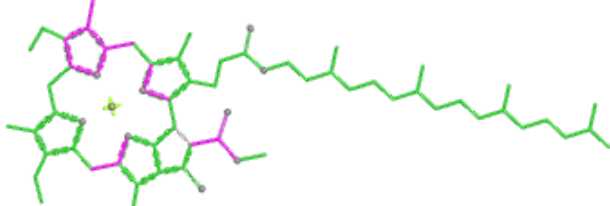
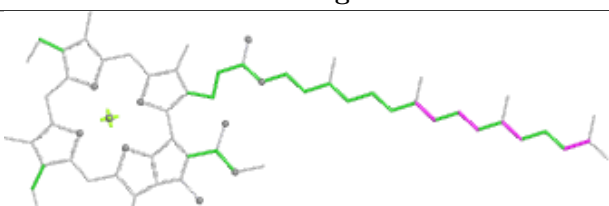
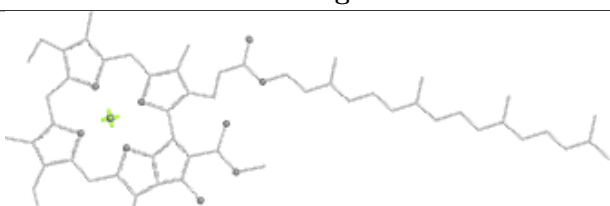
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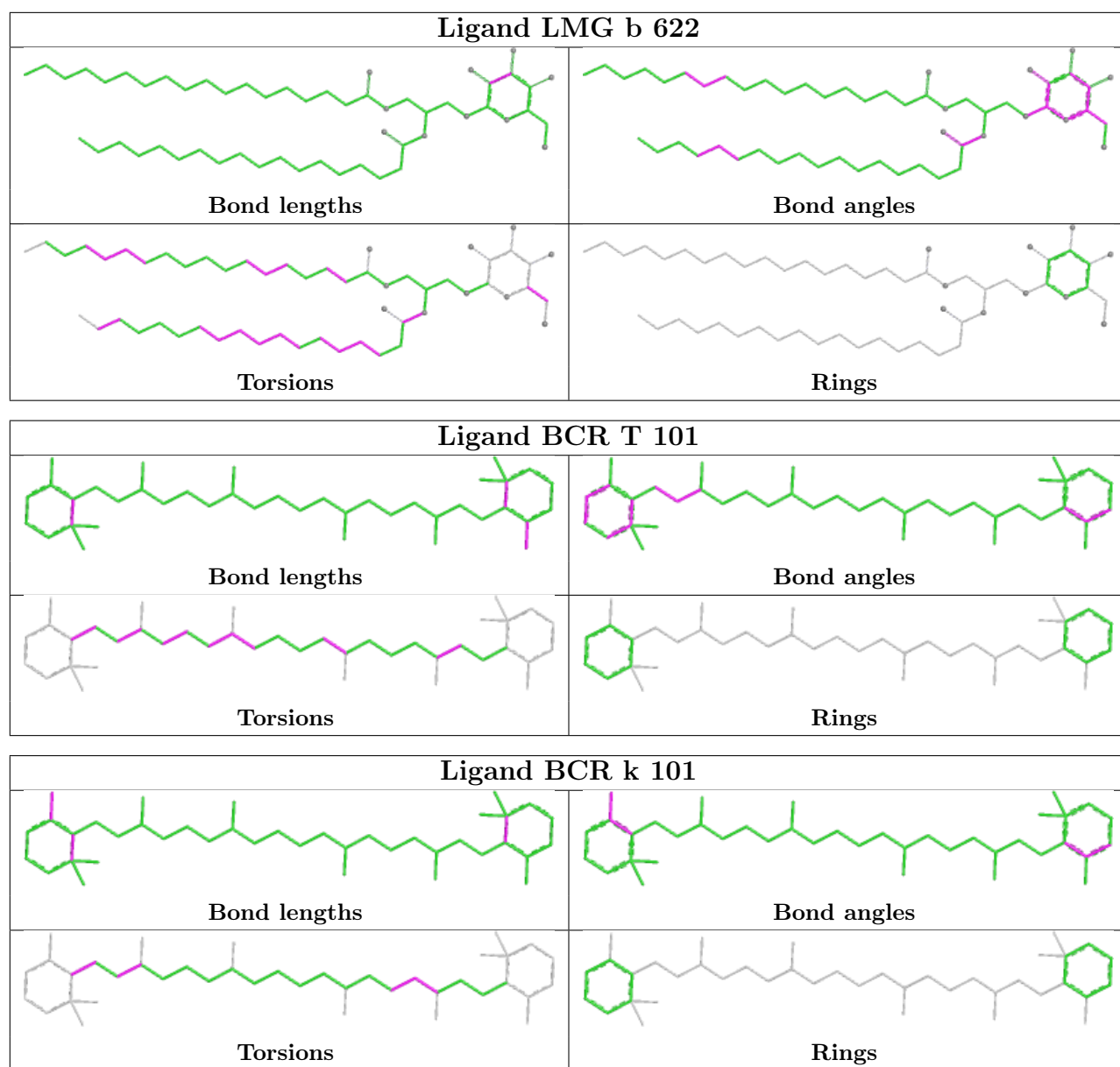
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	602	CLA	3	0
25	a	607	CLA	4	0
25	a	609	CLA	4	0
25	c	503	CLA	3	0
25	C	509	CLA	1	0
27	H	102	BCR	1	0
27	C	514	BCR	5	0
25	b	606	CLA	5	0
32	l	101	LHG	5	0
25	B	613	CLA	2	0
25	C	513	CLA	2	0
27	t	101	BCR	5	0
33	D	412	LMG	1	0
25	C	501	CLA	2	0
31	d	411	STE	1	0
25	C	511	CLA	1	0
25	A	612	CLA	1	0
25	B	606	CLA	4	0
25	B	611	CLA	4	0
33	C	515	LMG	2	0
34	D	401	BCT	1	0
30	c	518	DGD	5	0
31	I	101	STE	2	0
29	b	619	SQD	4	0

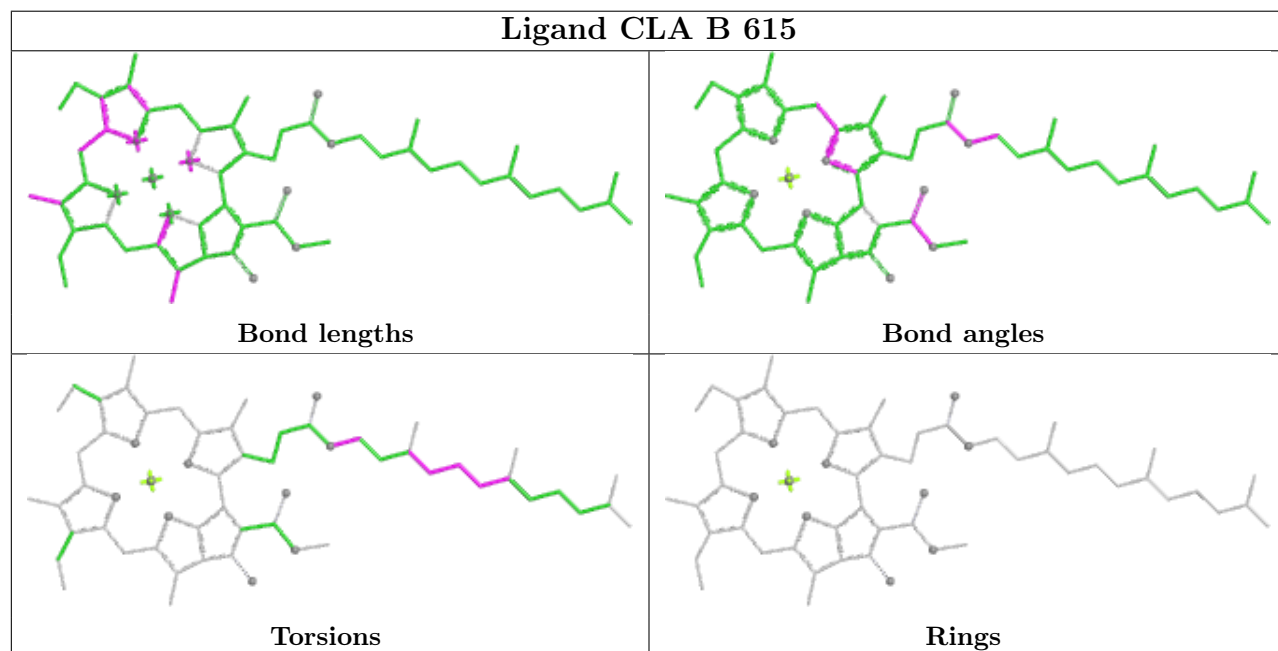
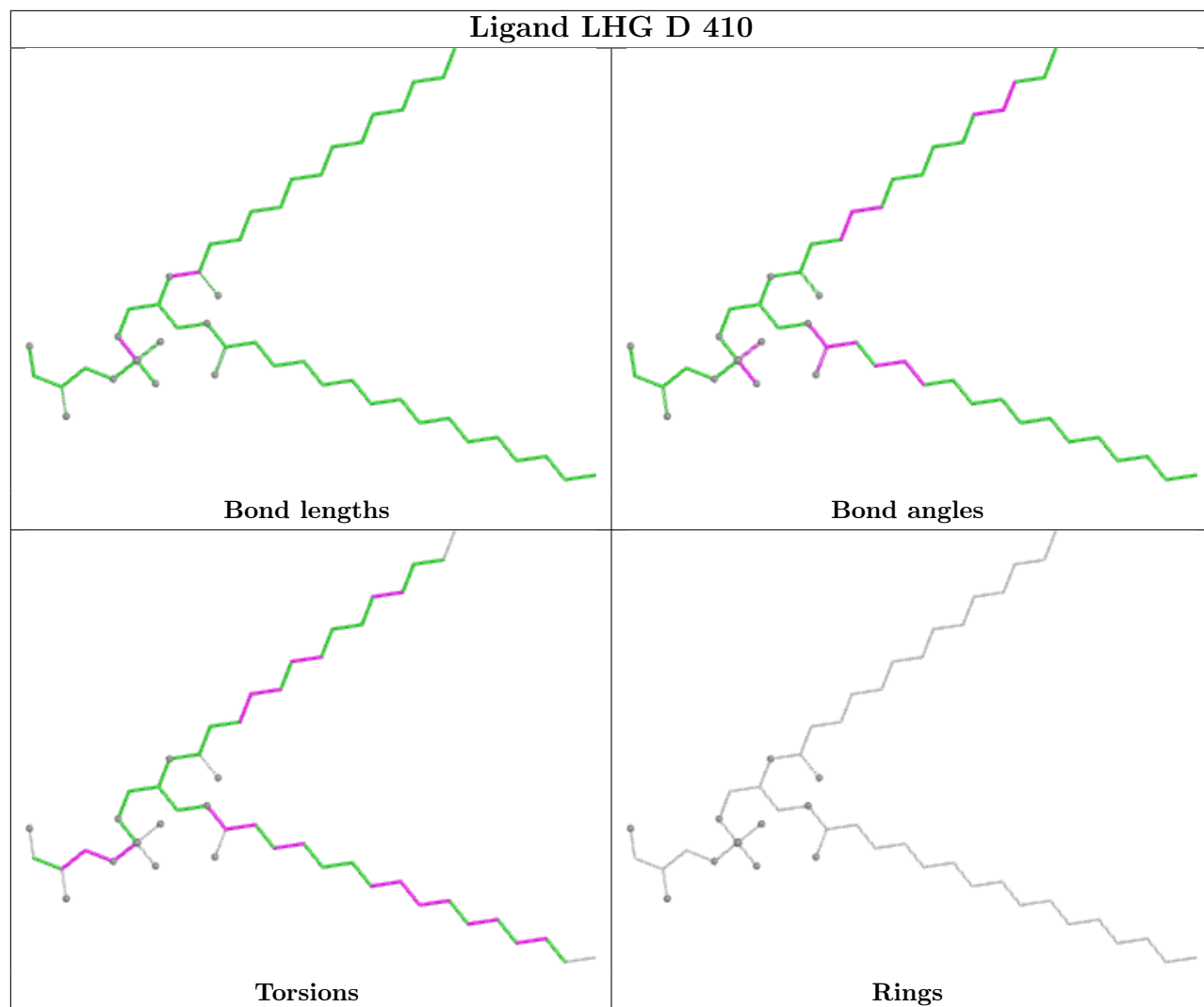
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand PL9 a 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

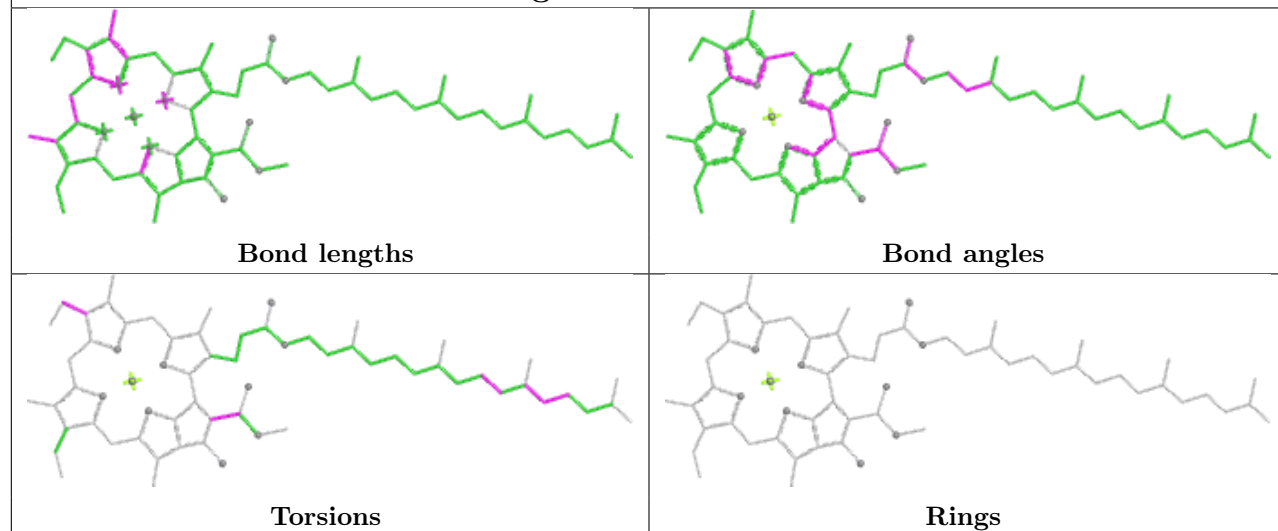
Ligand DGD C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

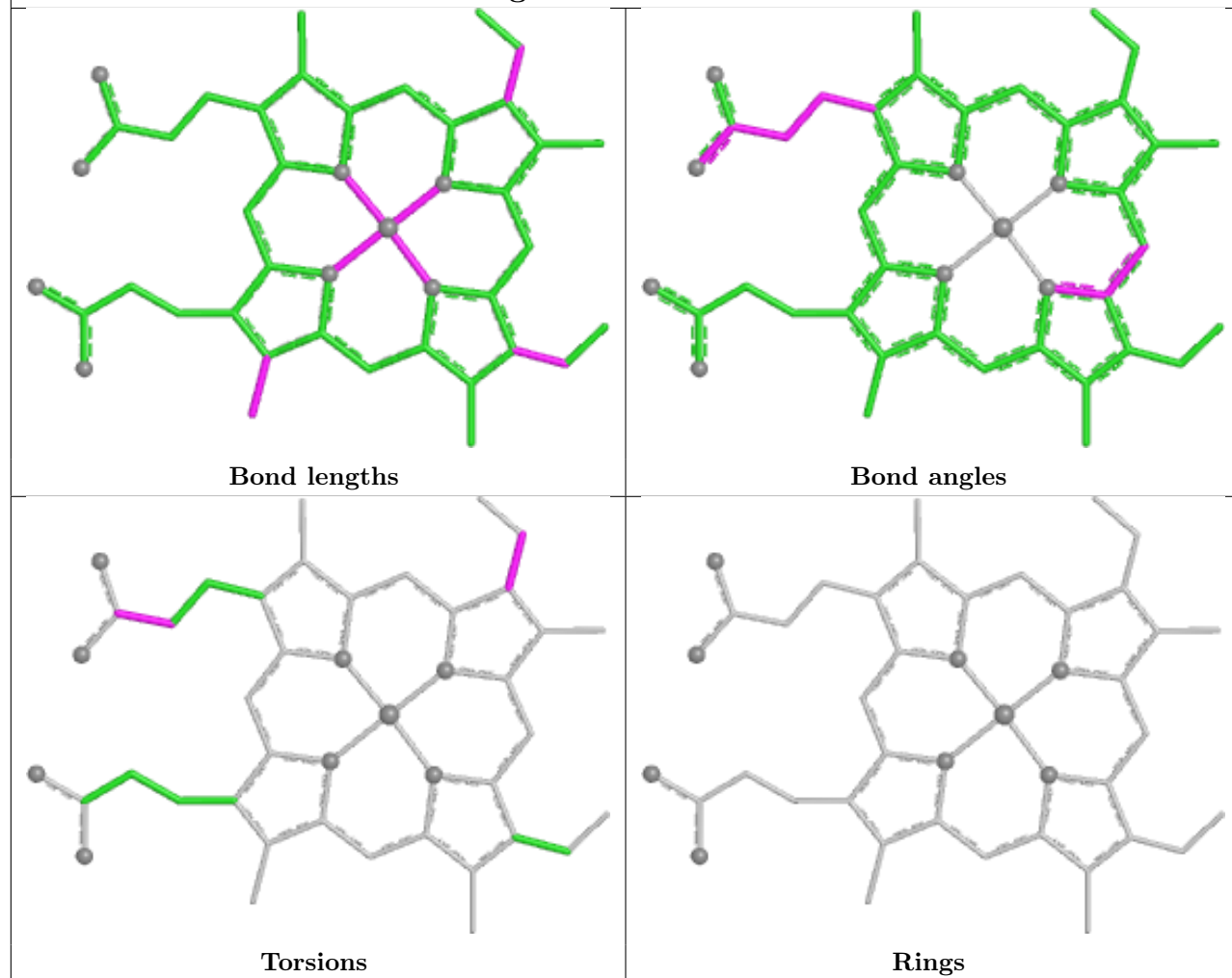


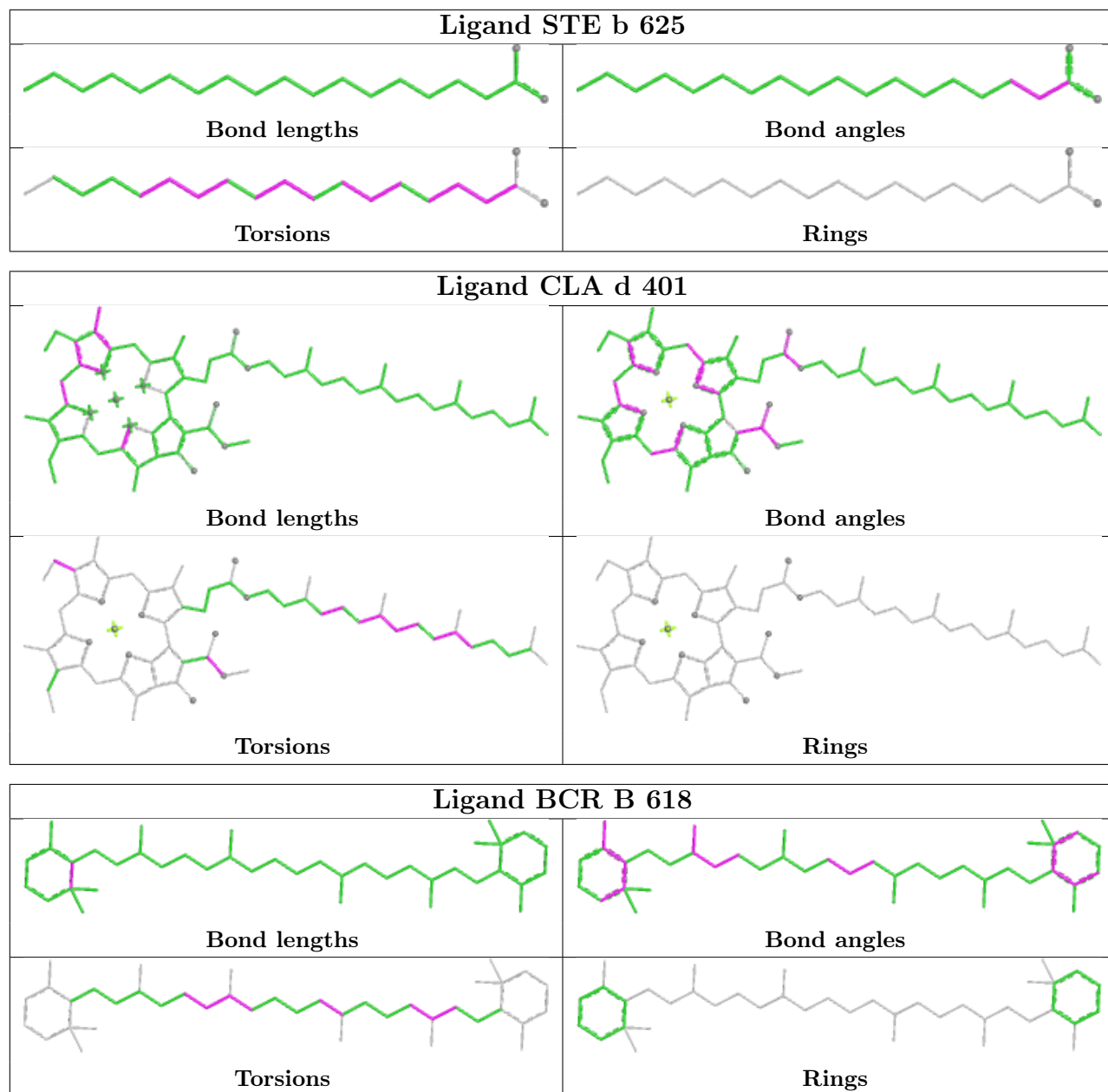


Ligand CLA C 502

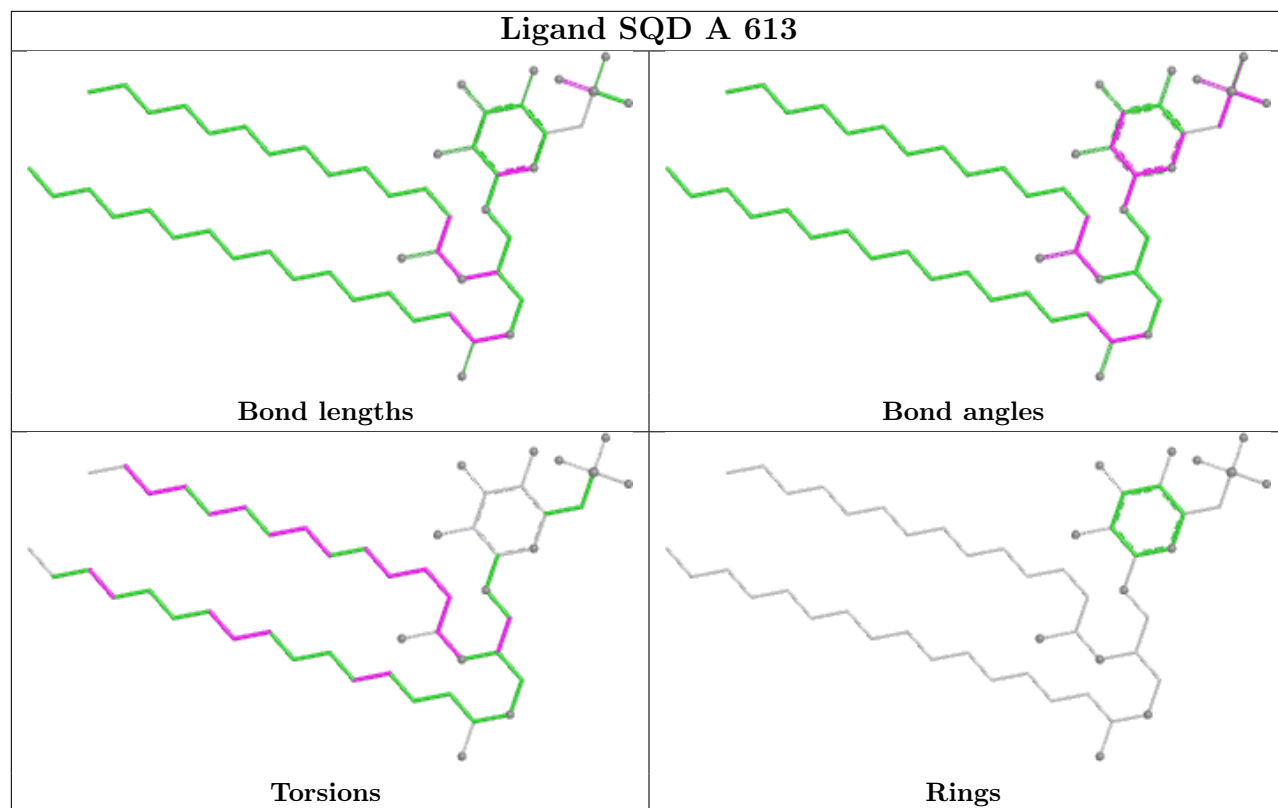


Ligand HEM F 101

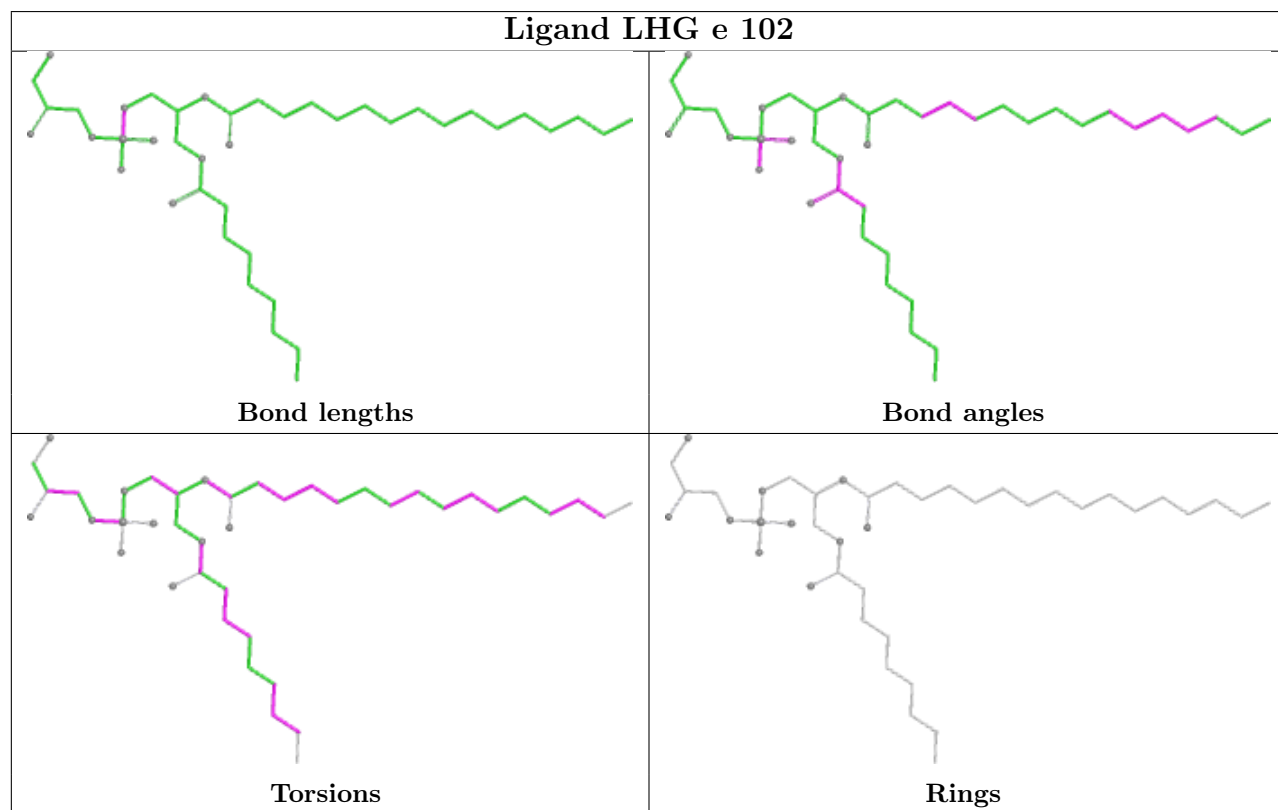




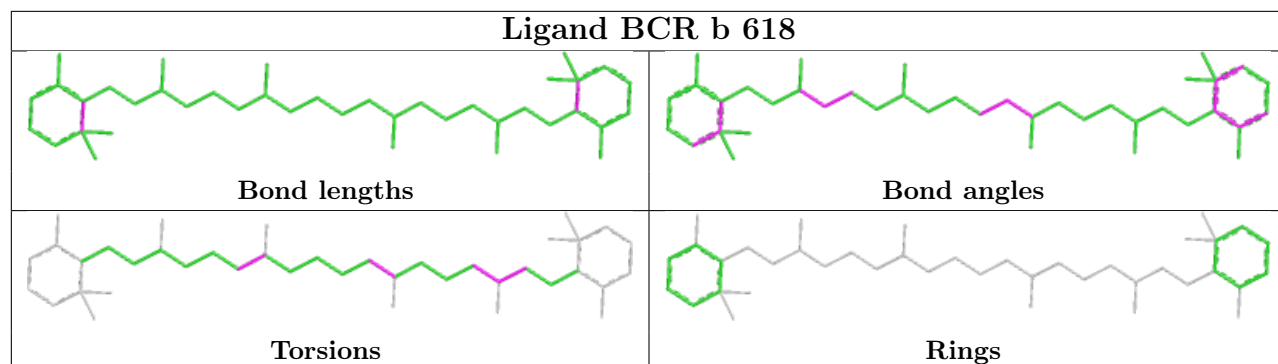
Ligand SQD A 613



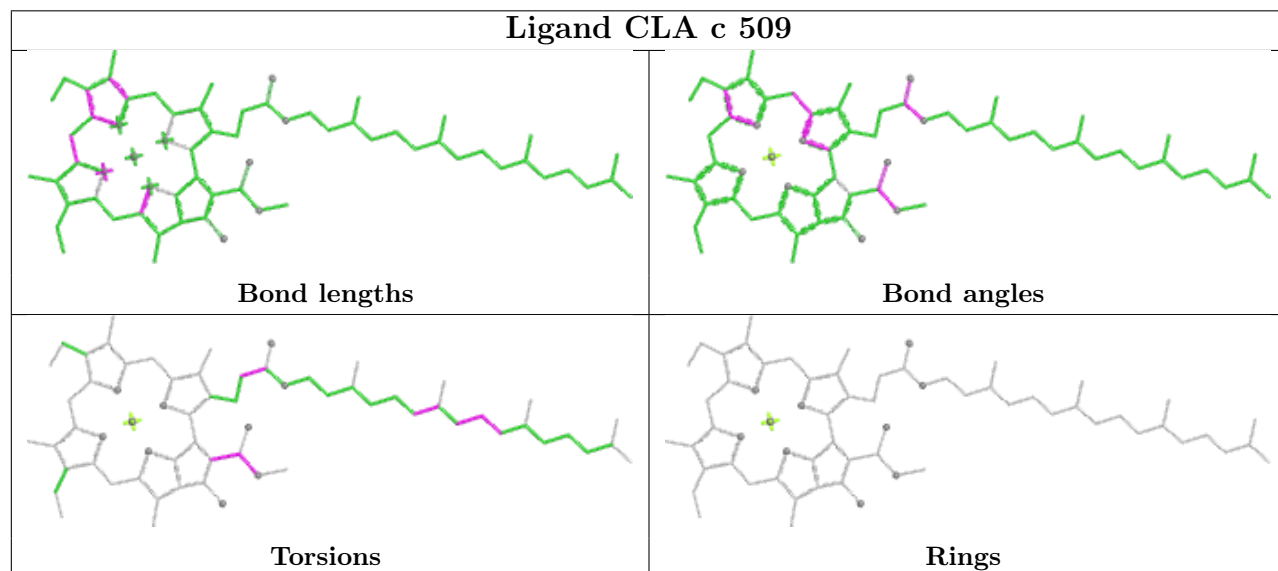
Ligand LHG e 102



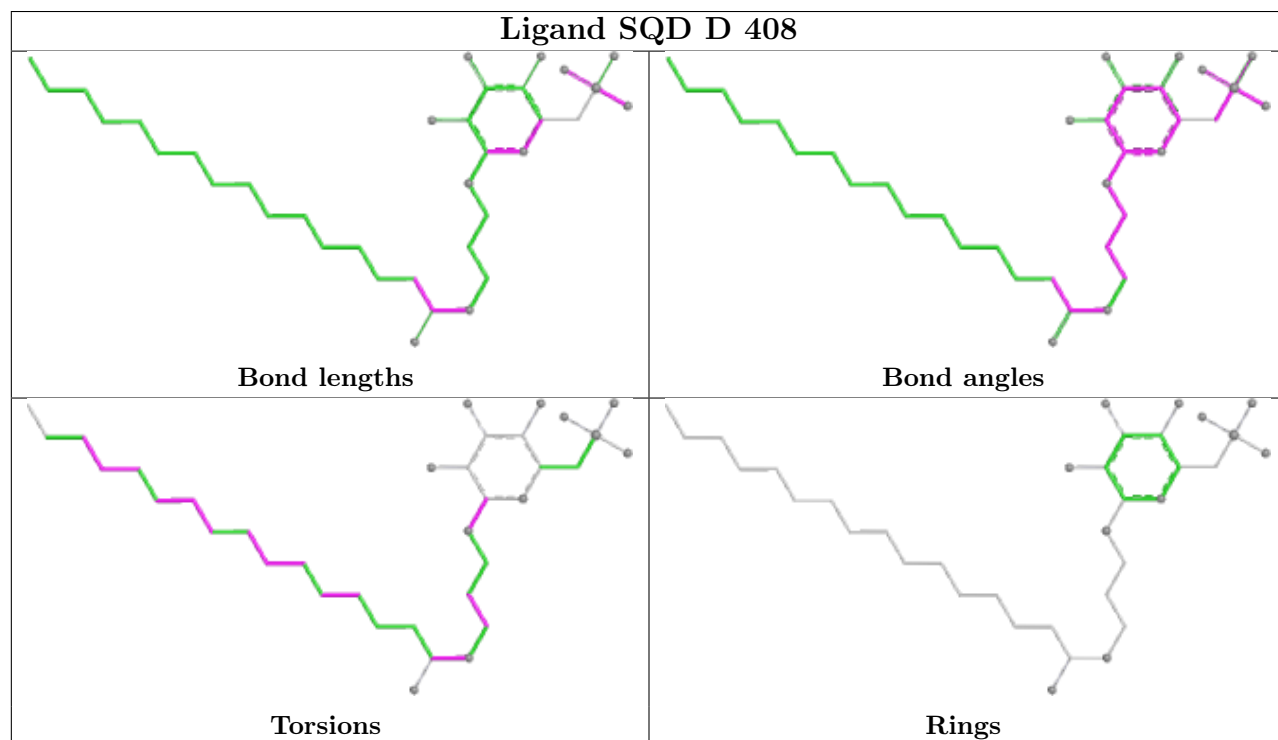
Ligand BCR b 618

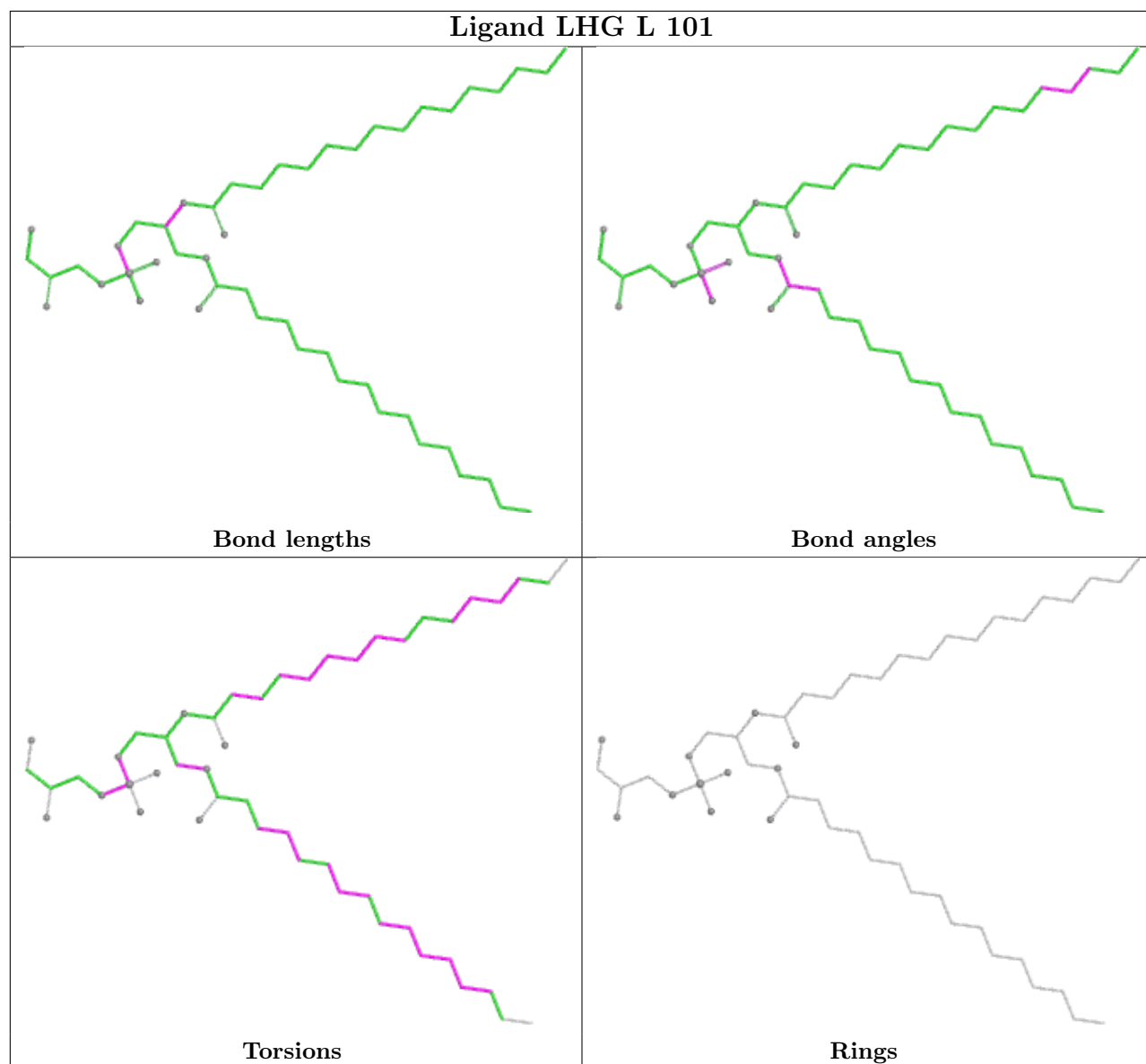
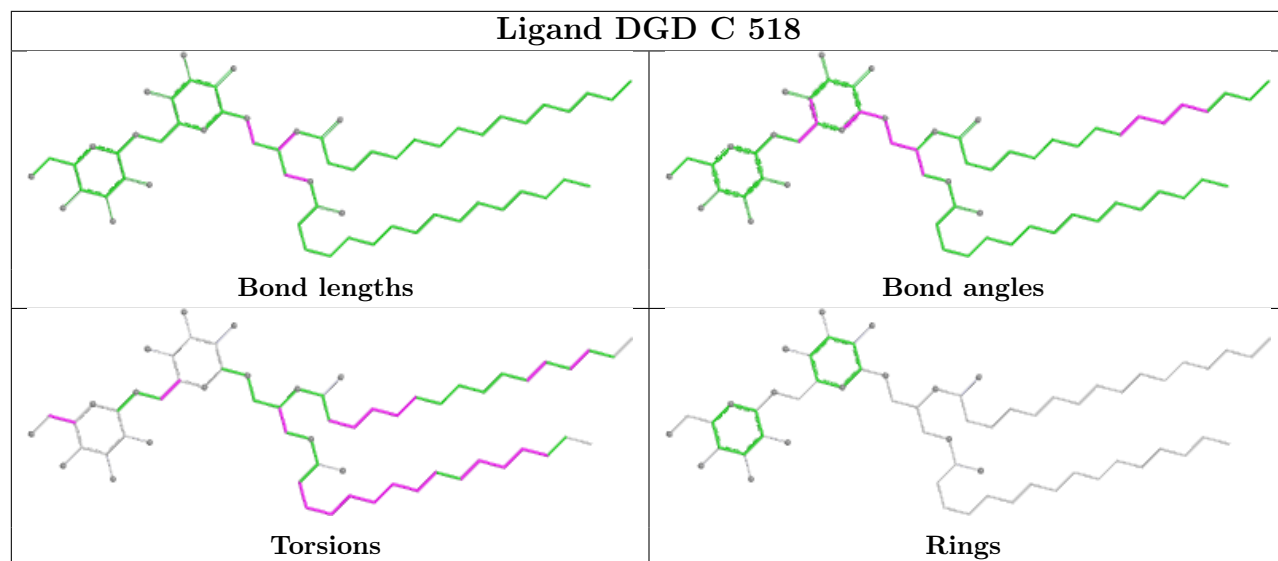


Ligand CLA c 509

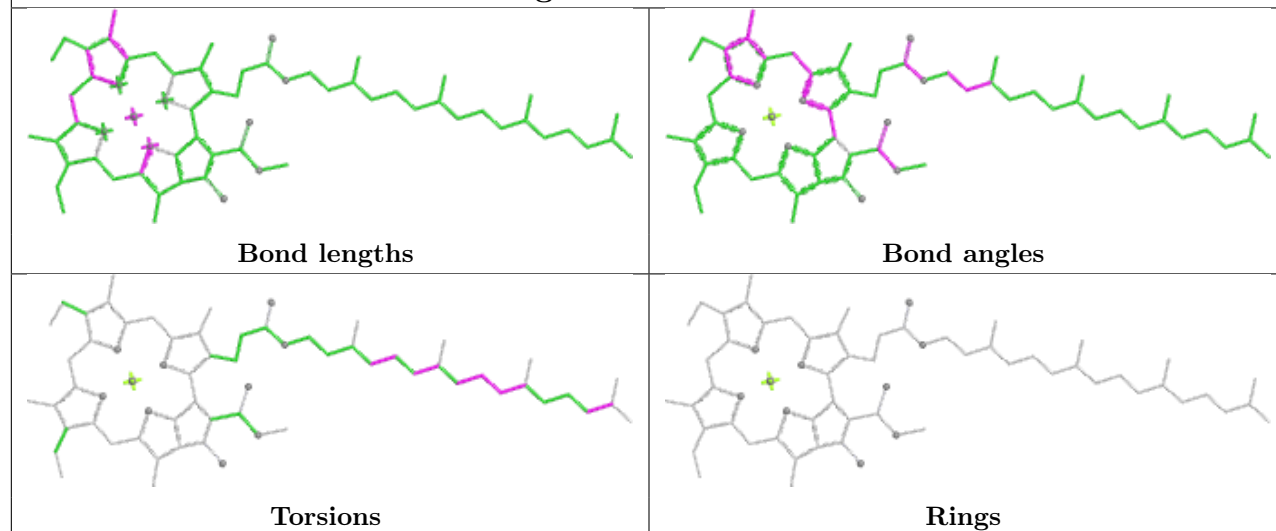


Ligand SQD D 408

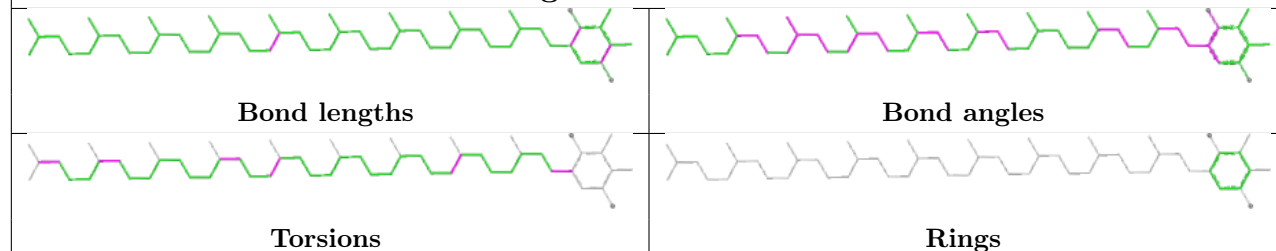




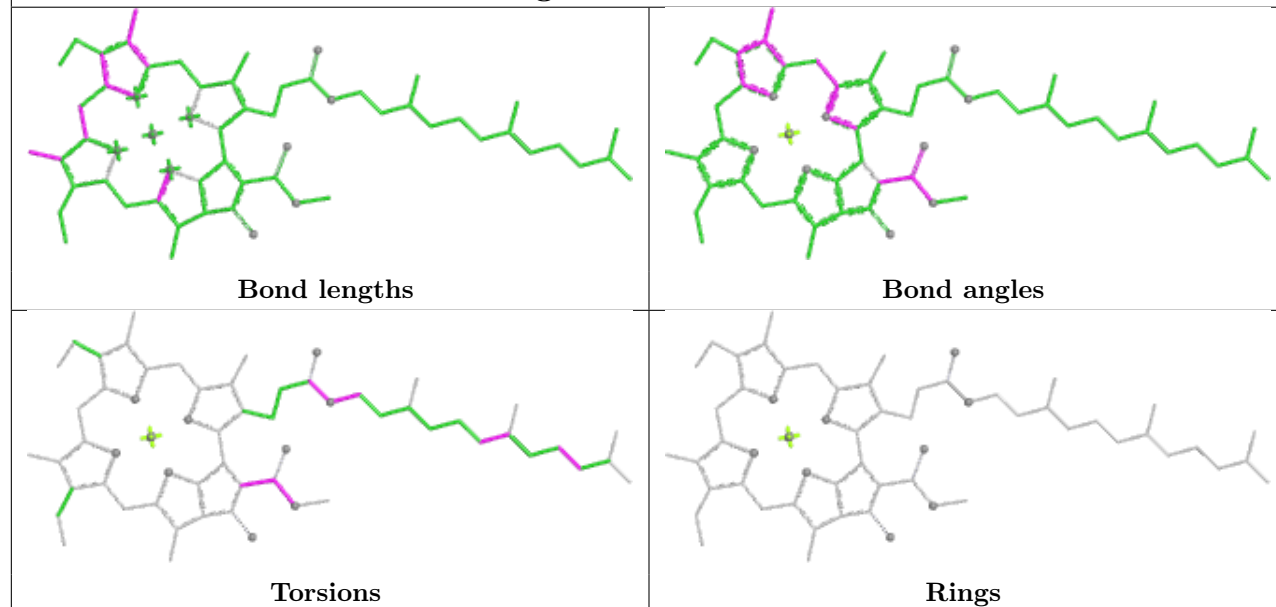
Ligand CLA d 404

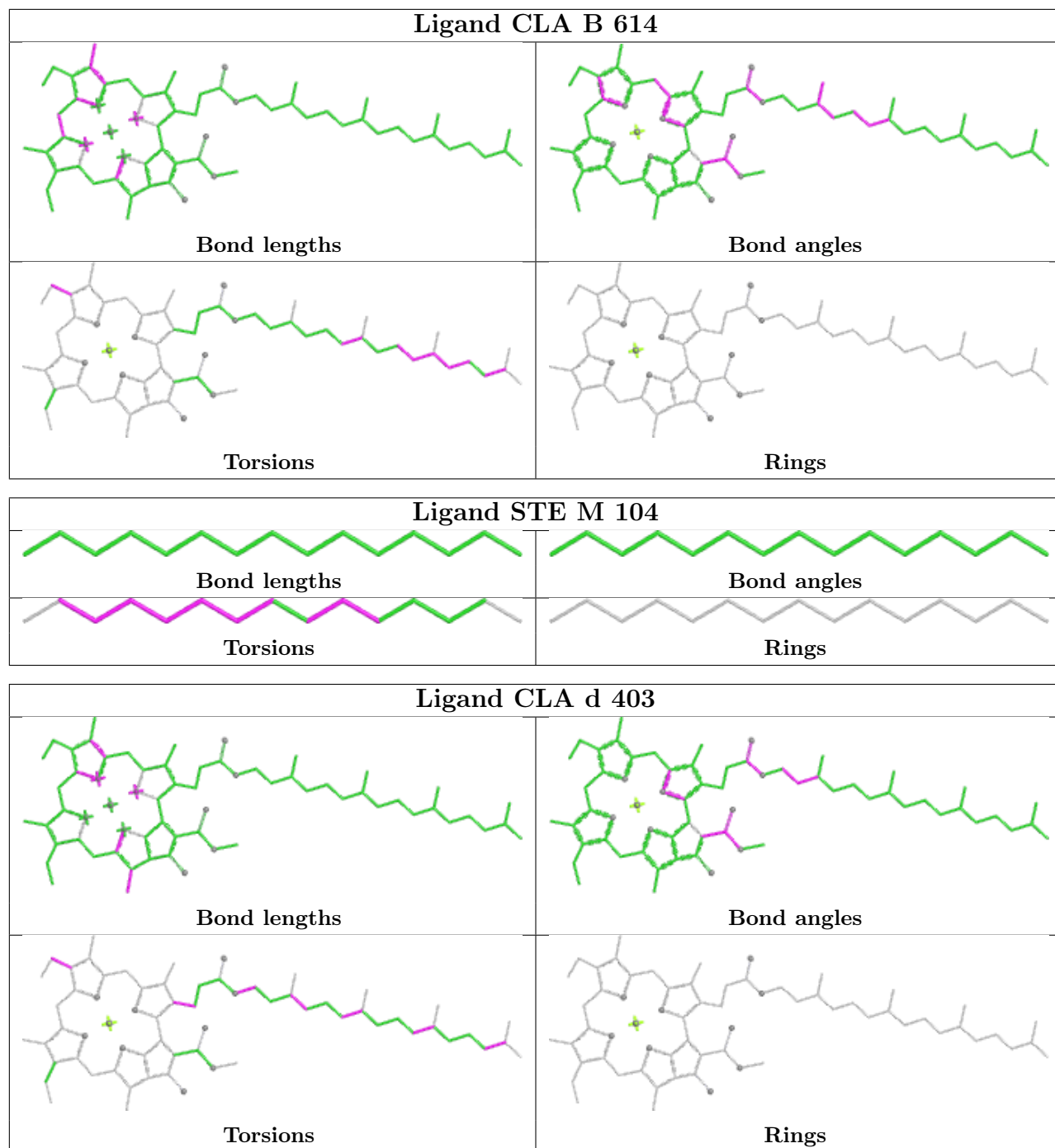


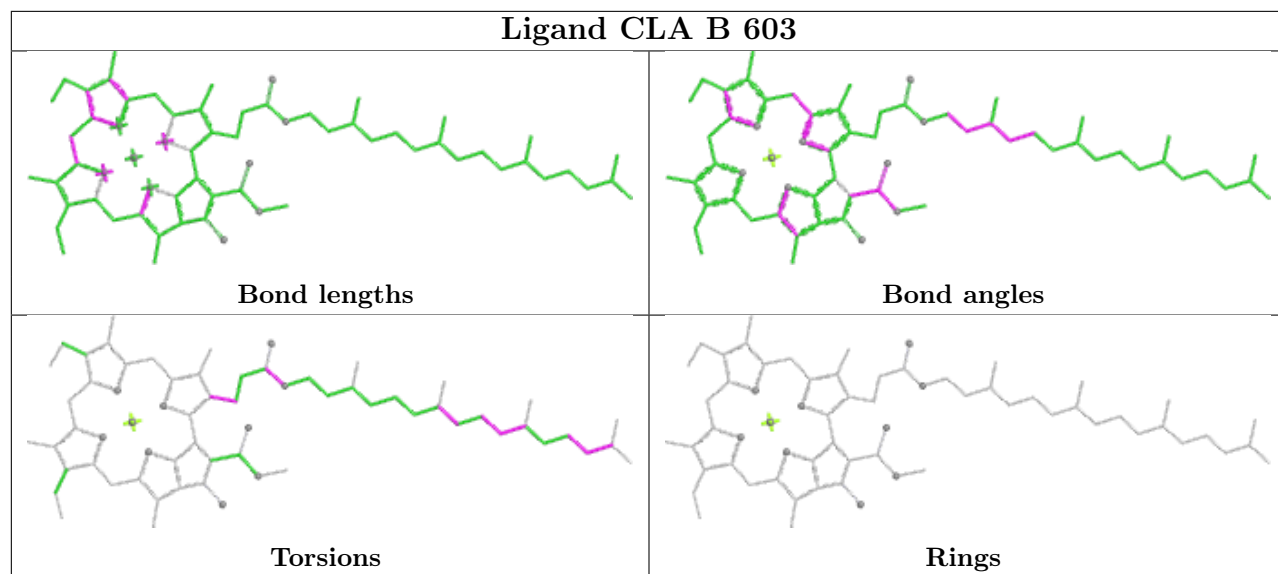
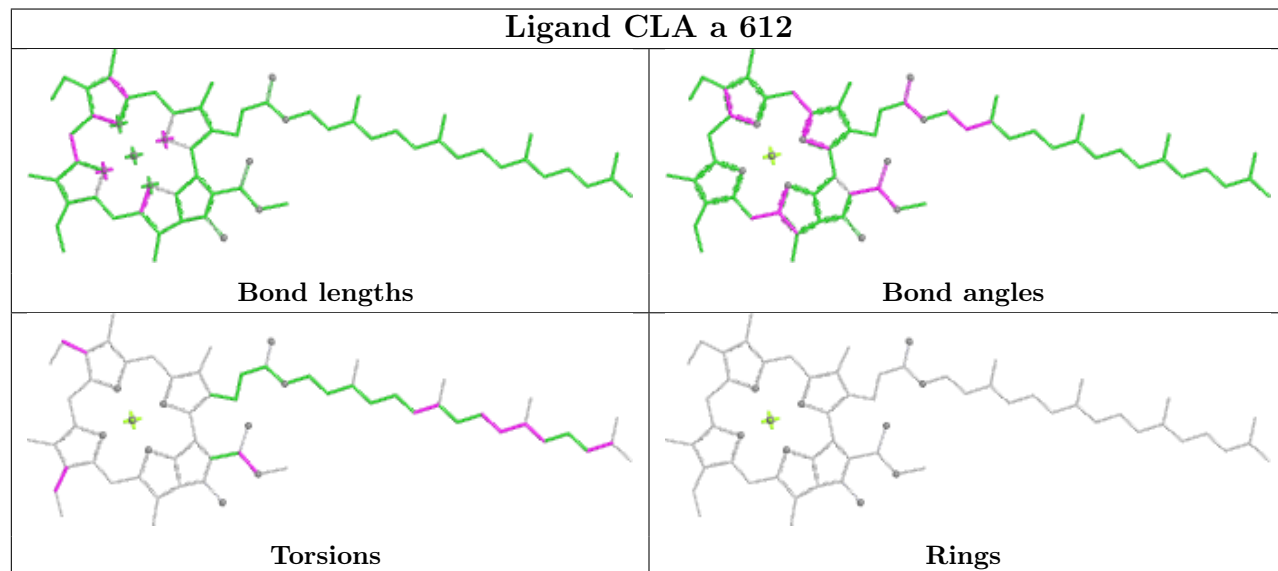
Ligand PL9 d 406

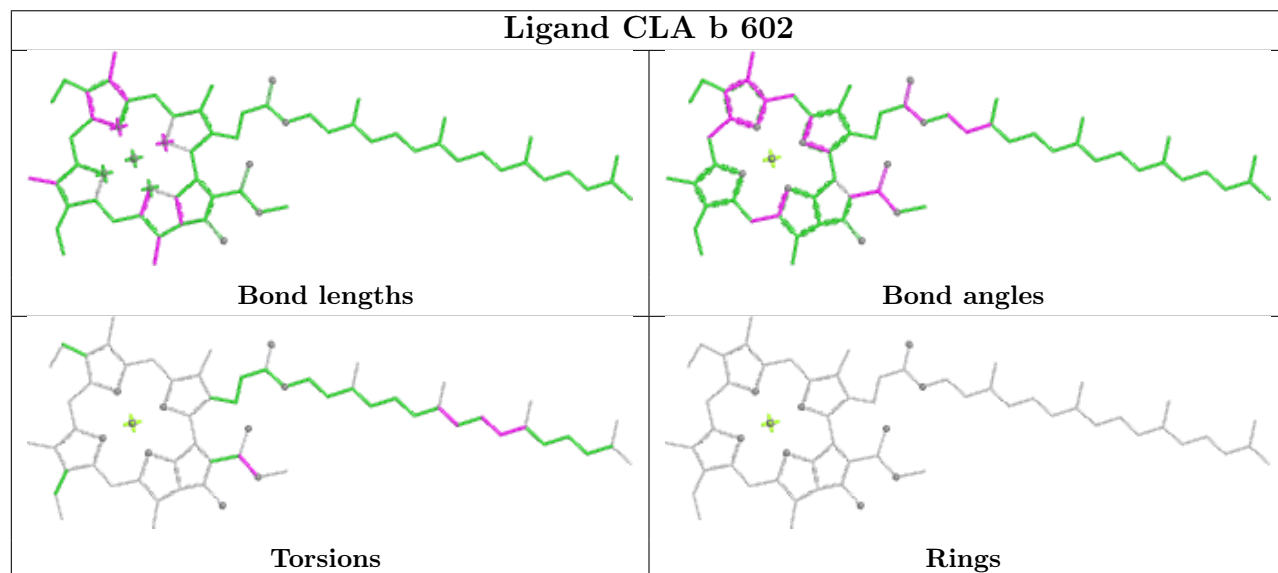
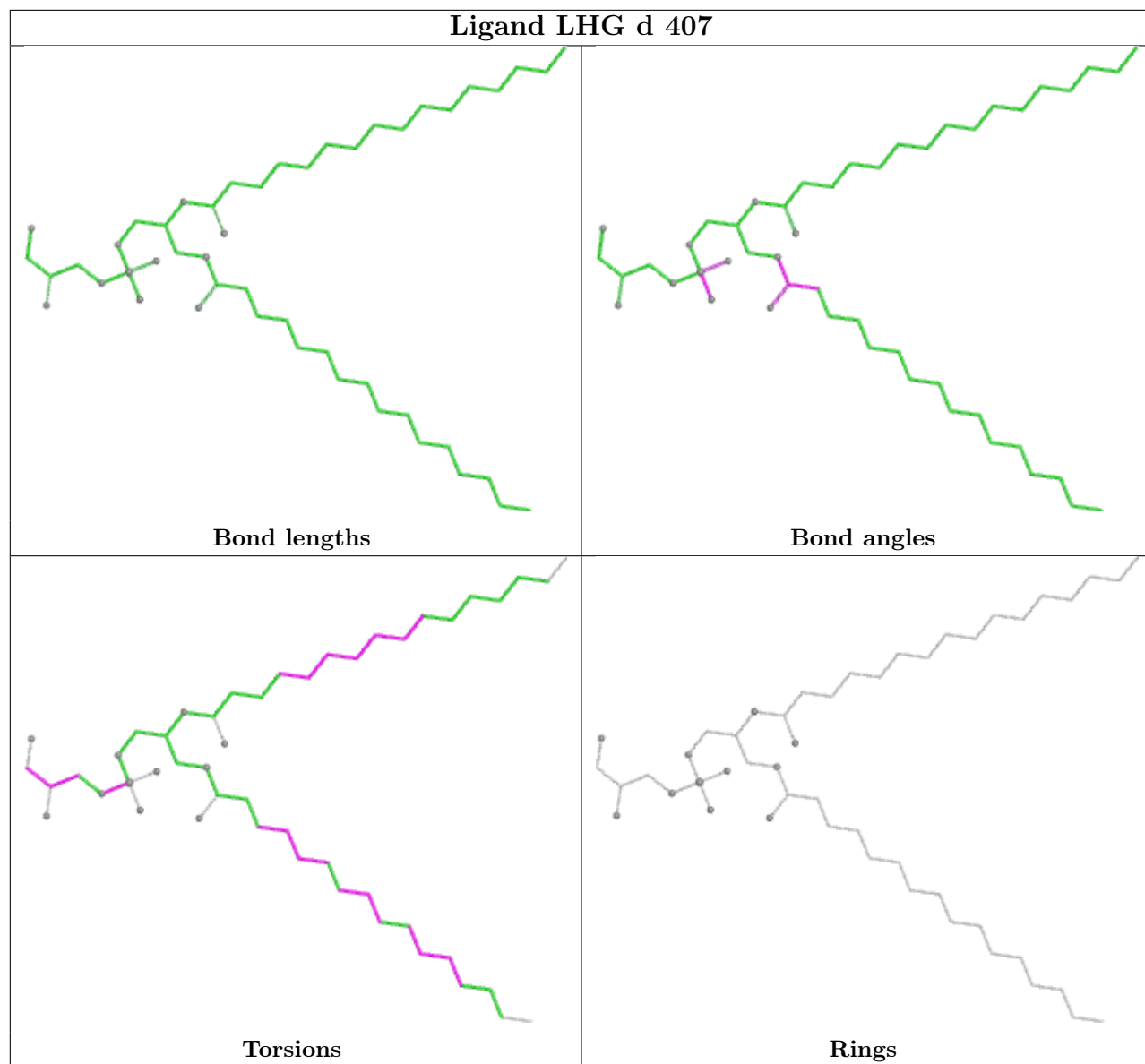


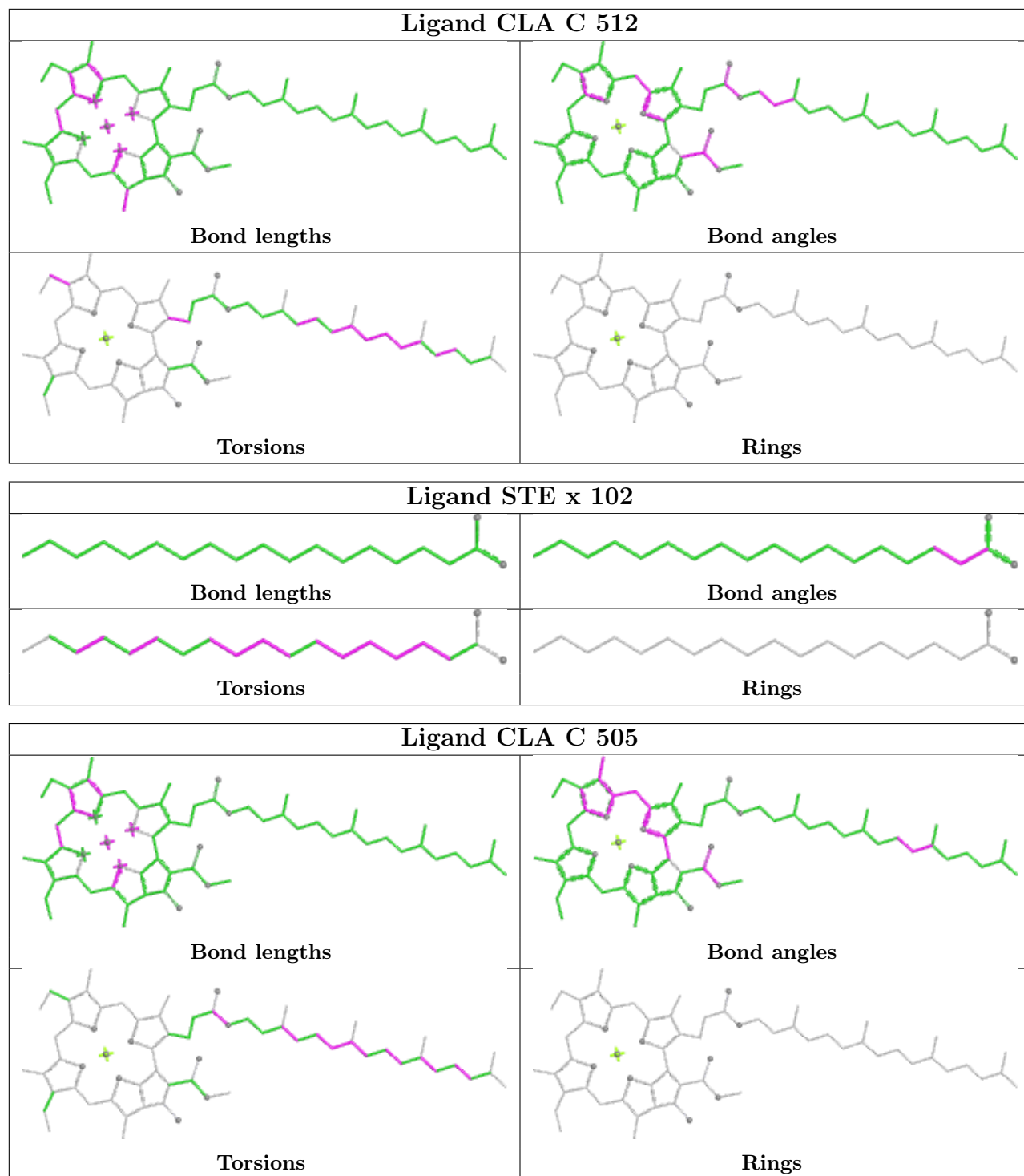
Ligand CLA b 615



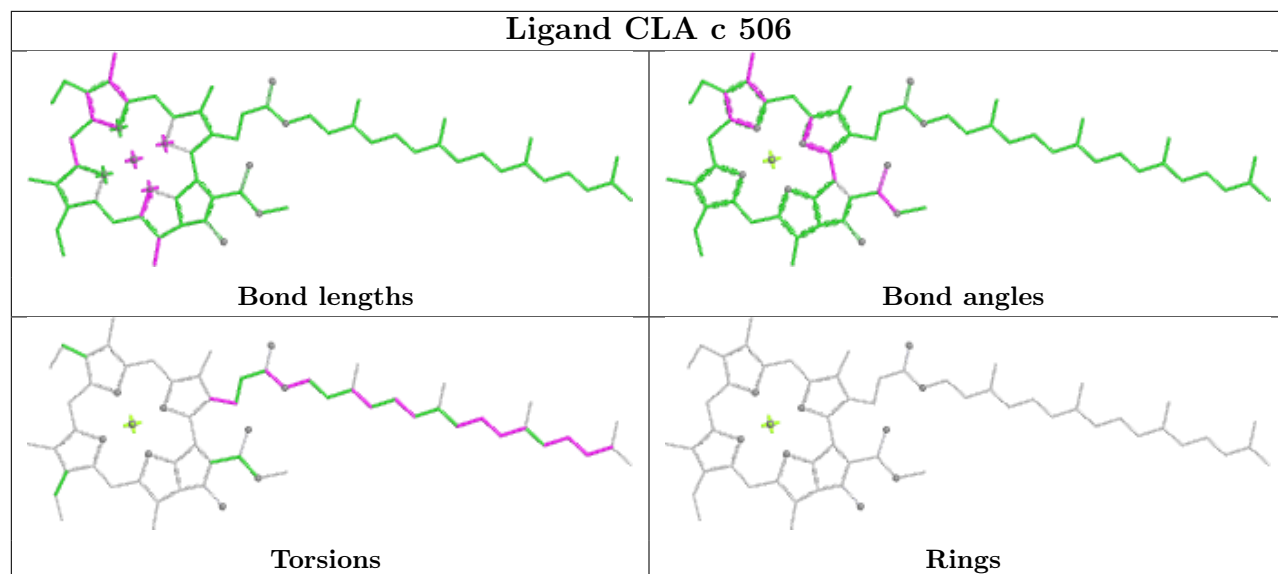


Ligand CLA B 603**Ligand CLA a 612**

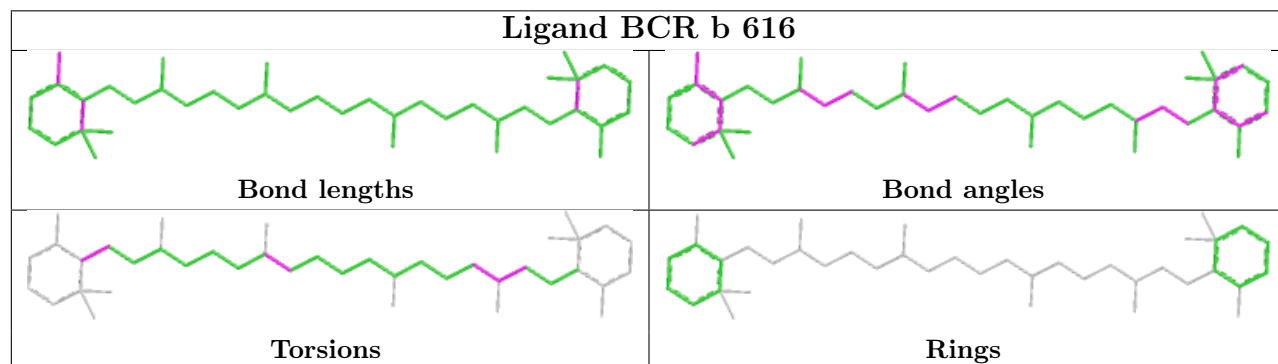




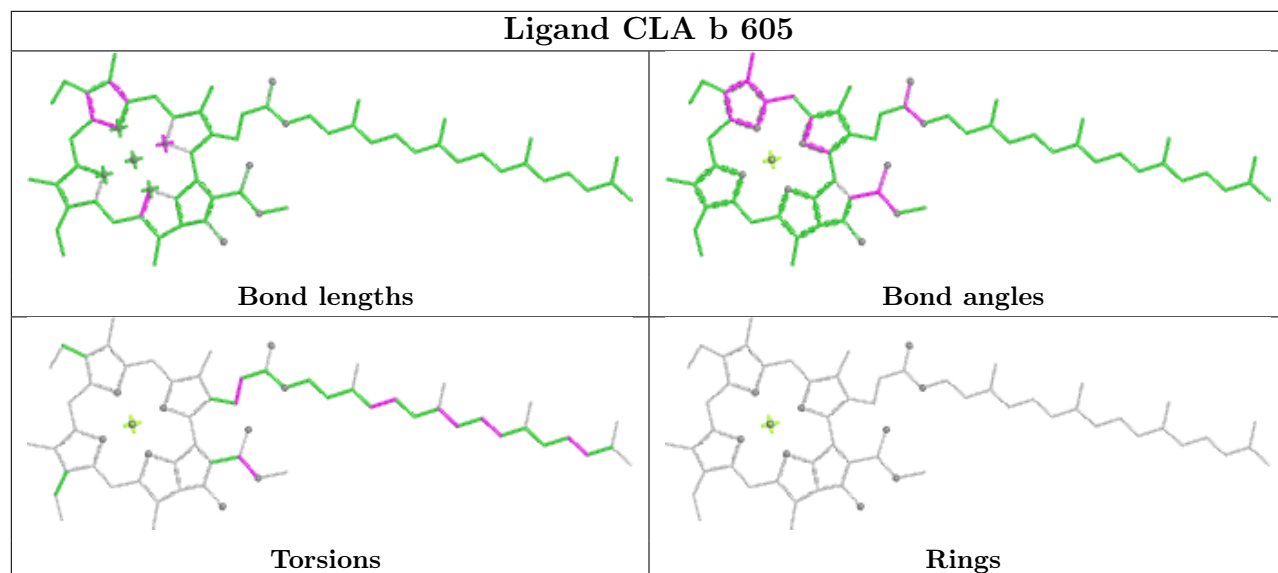
Ligand CLA c 506

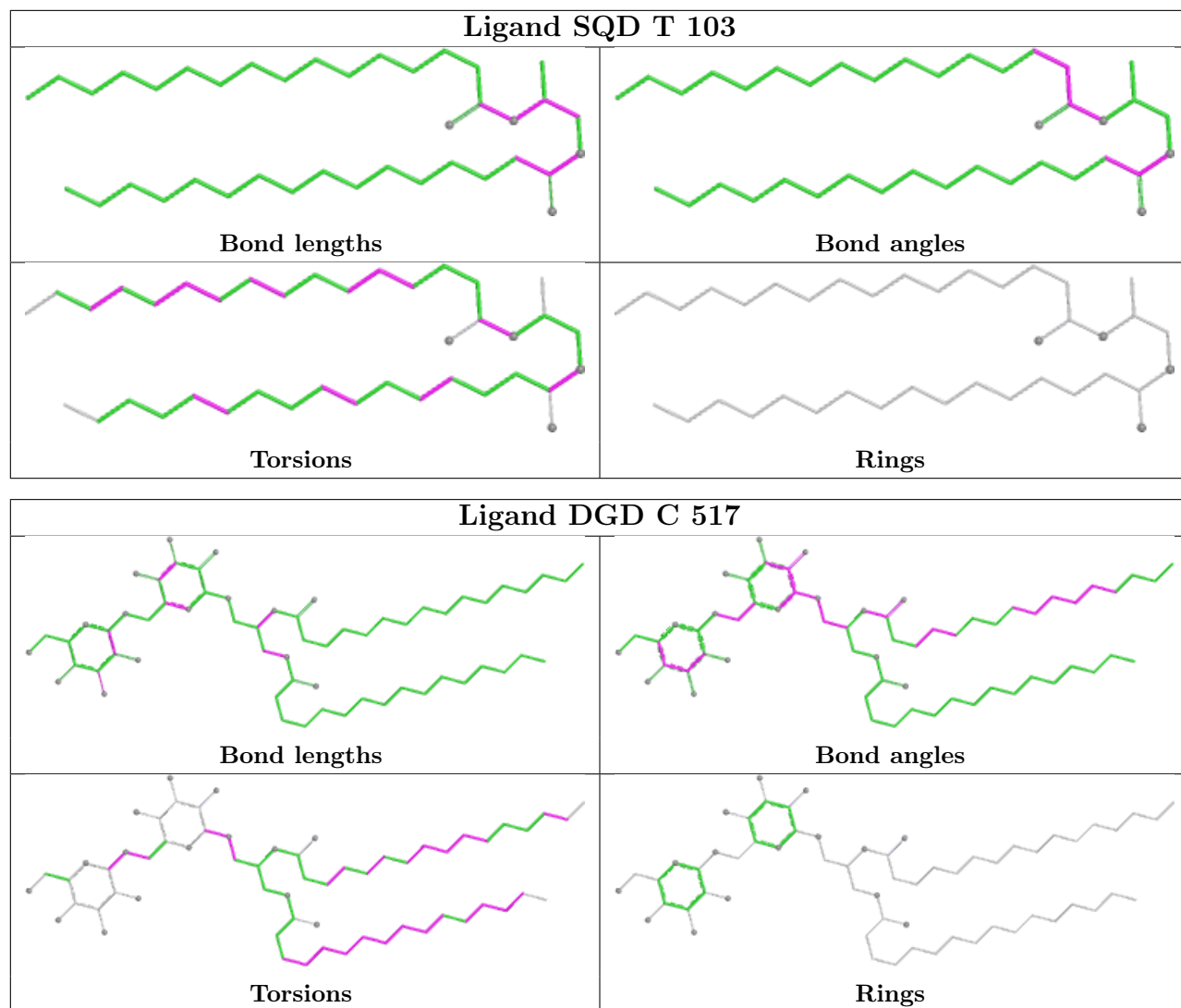


Ligand BCR b 616

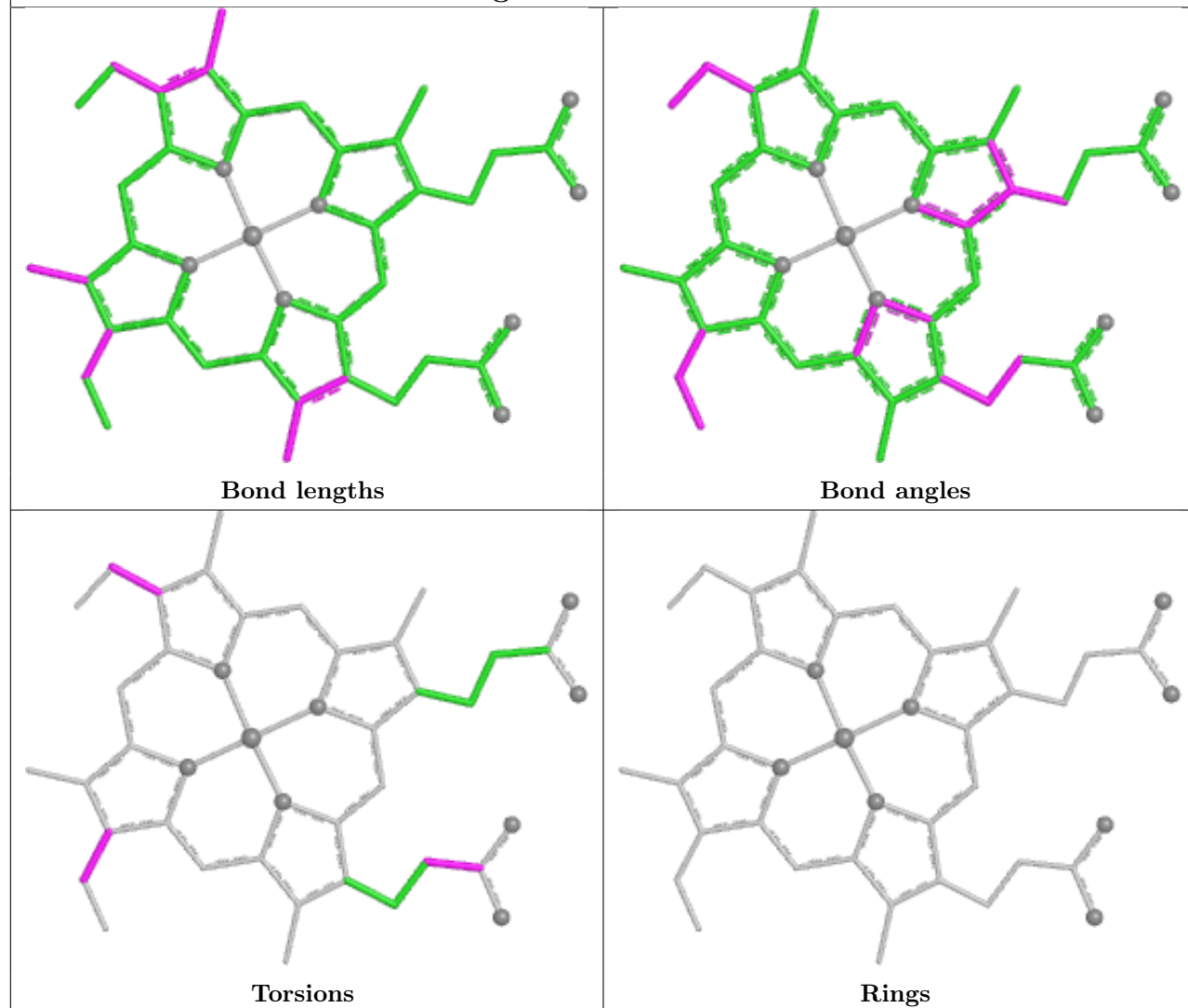


Ligand CLA b 605

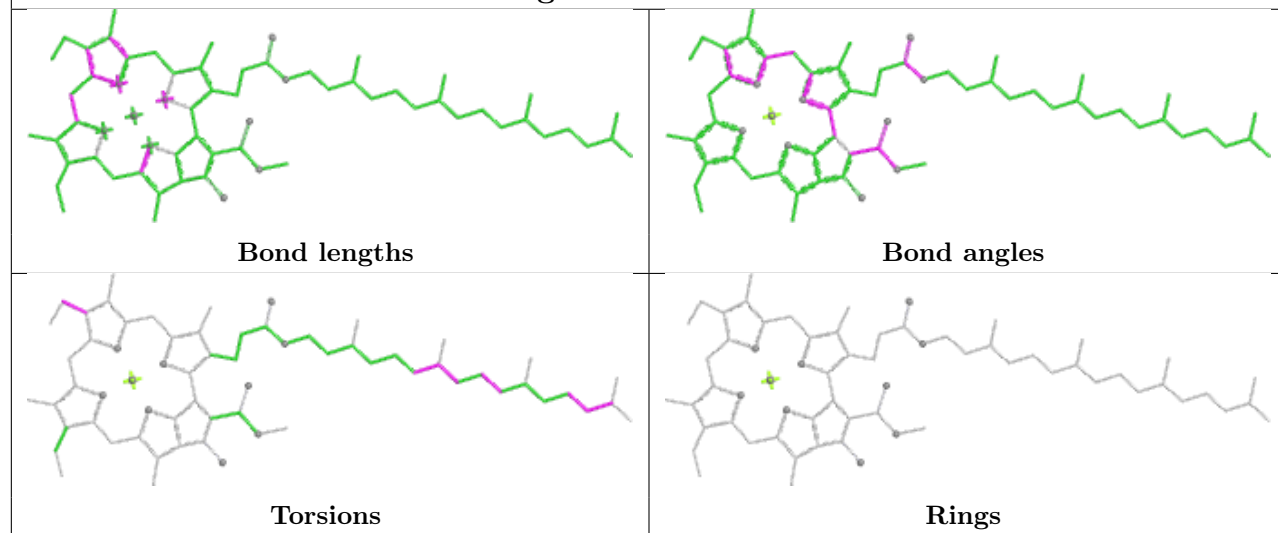


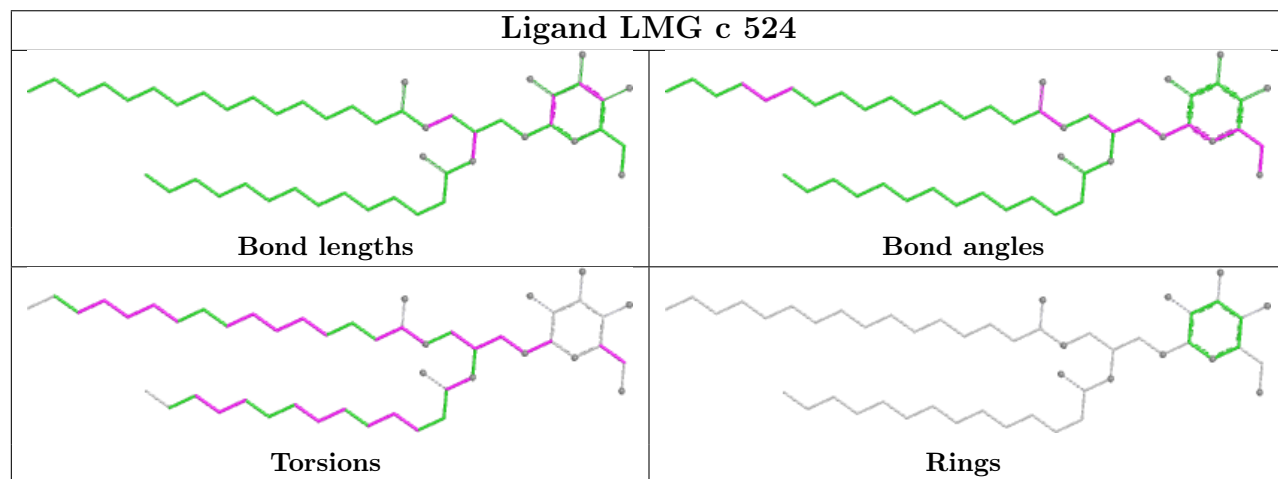
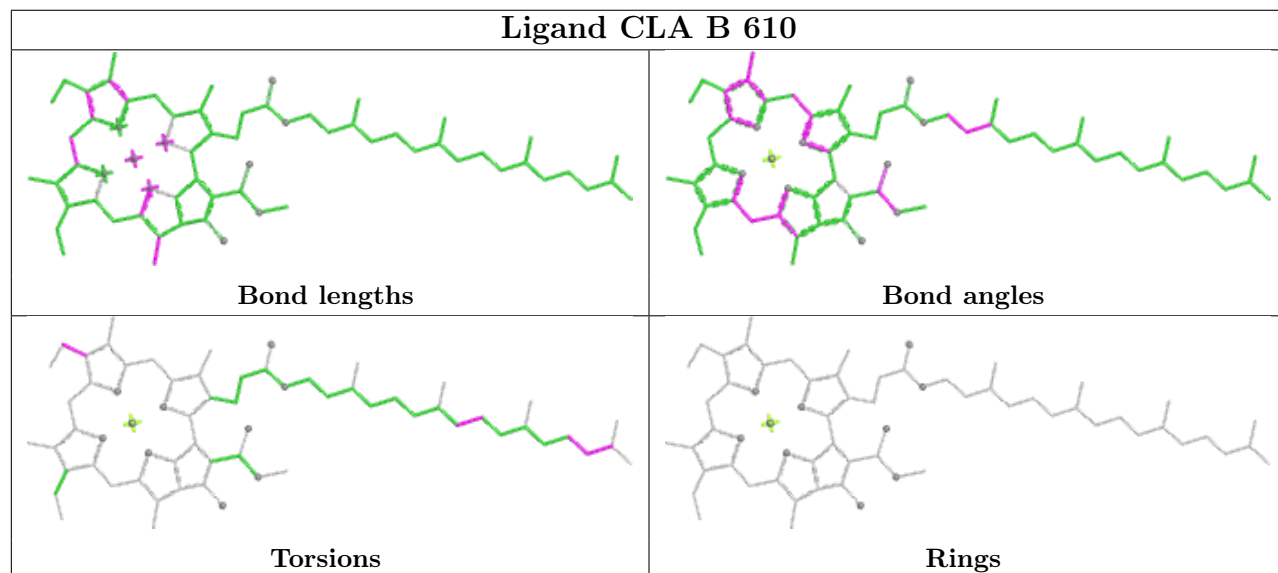
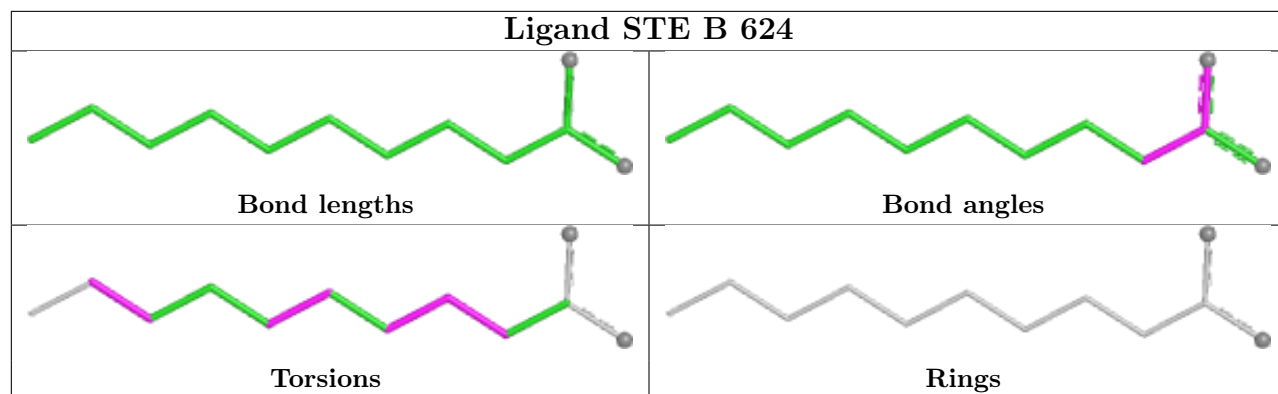


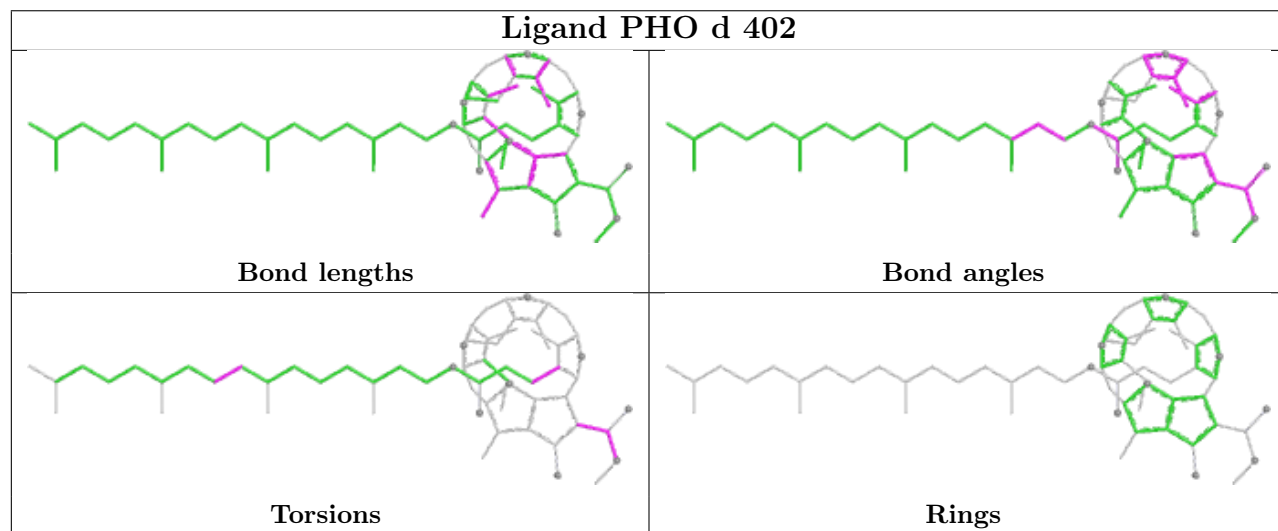
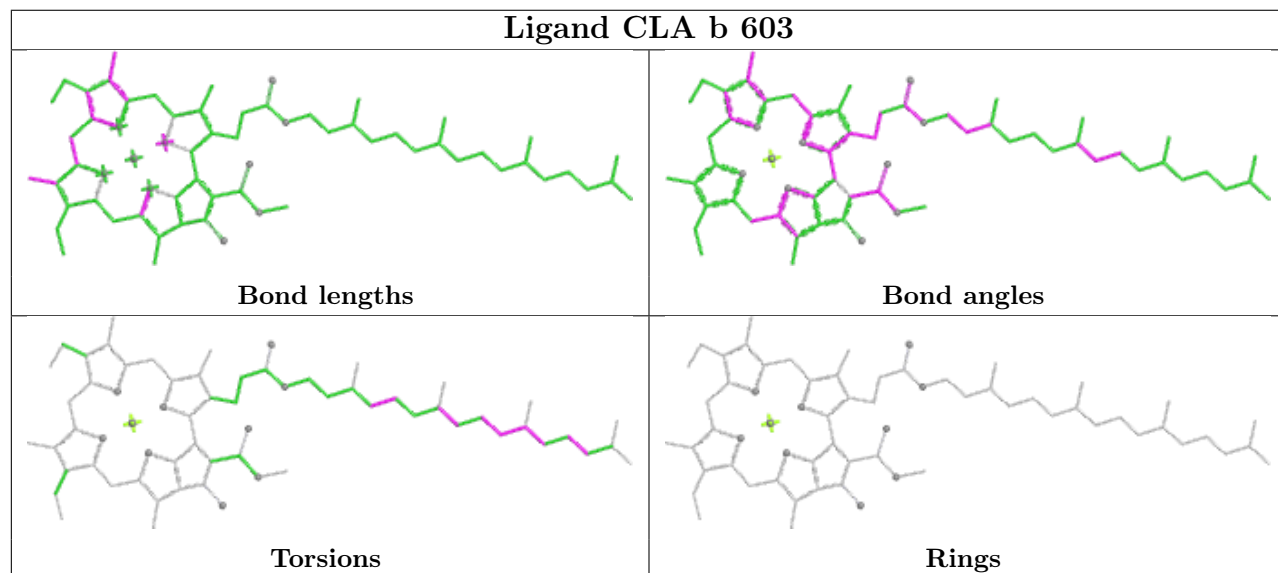
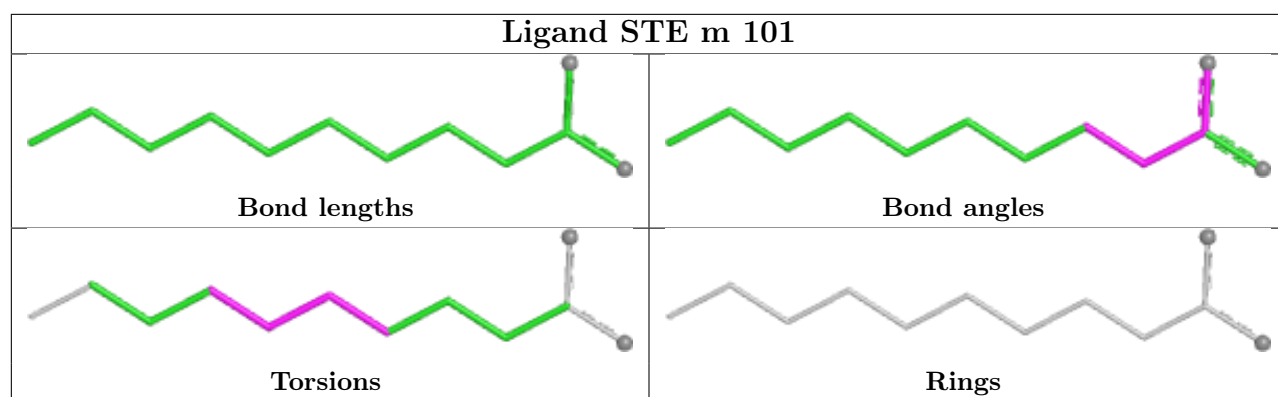
Ligand HEC V 201

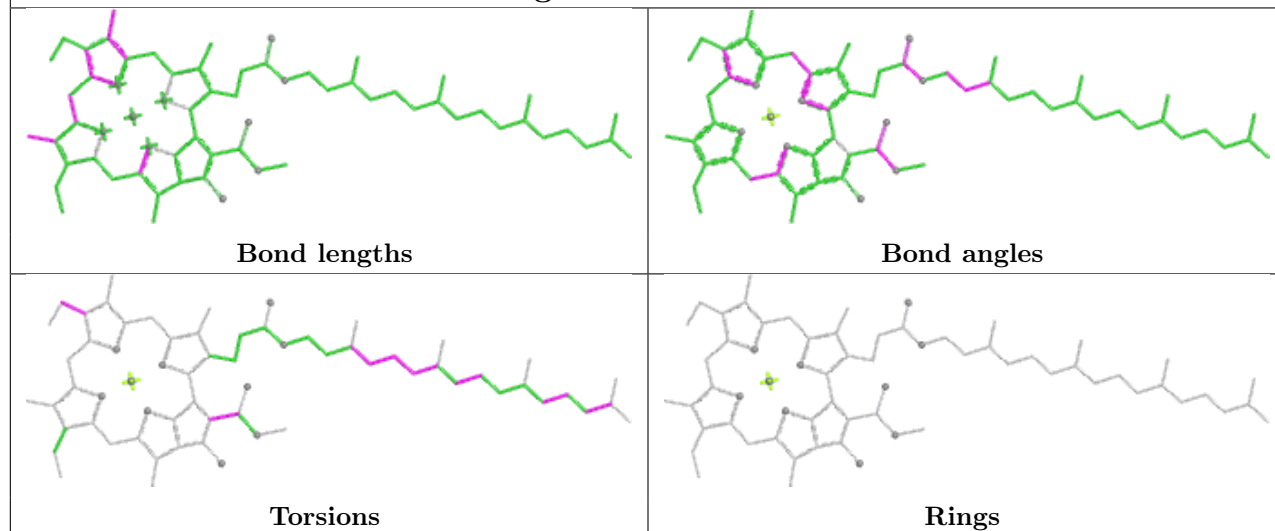
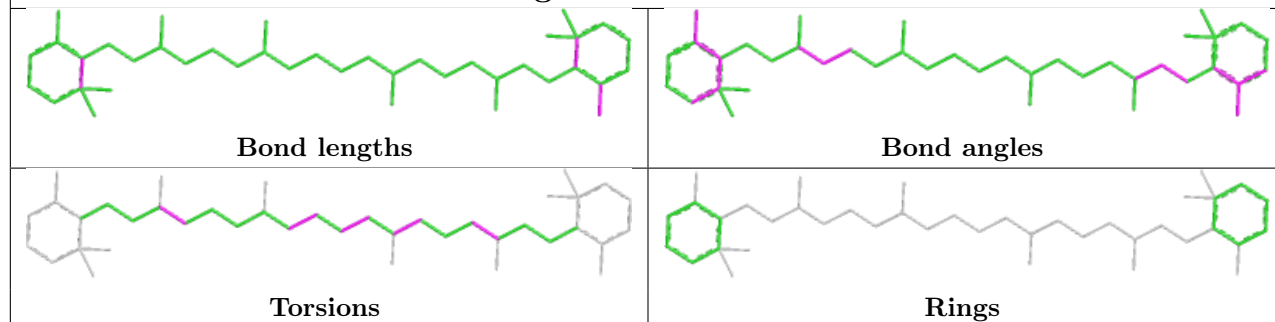
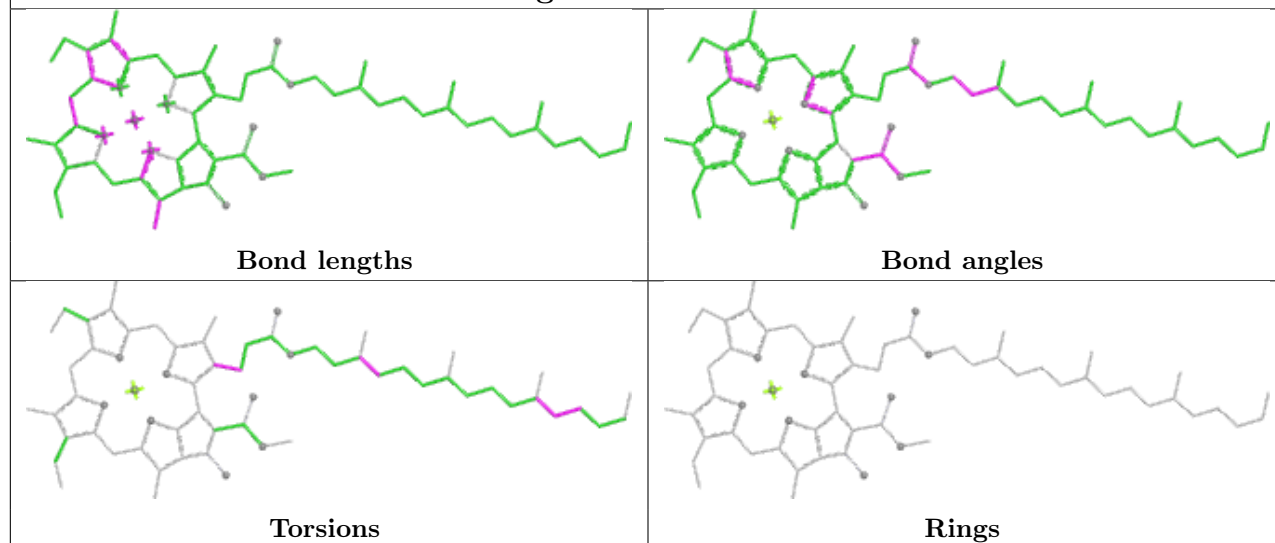


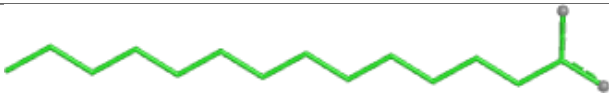
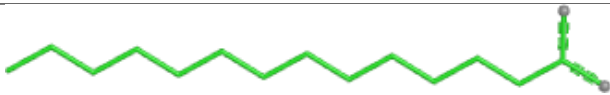
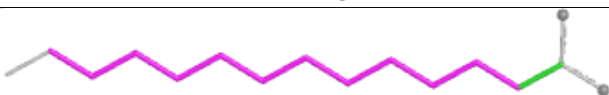
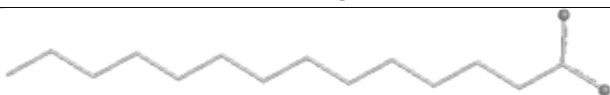
Ligand CLA c 505

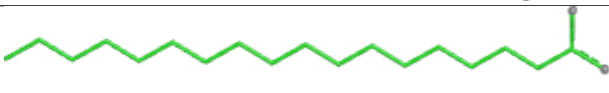
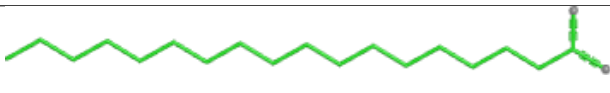
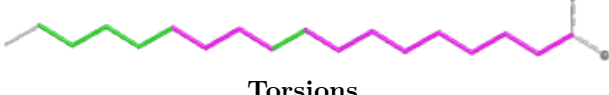


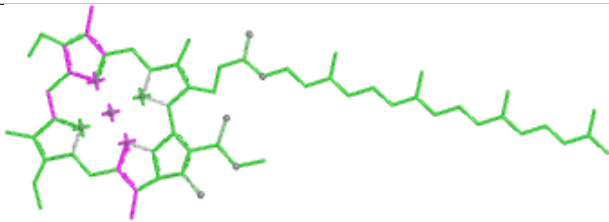
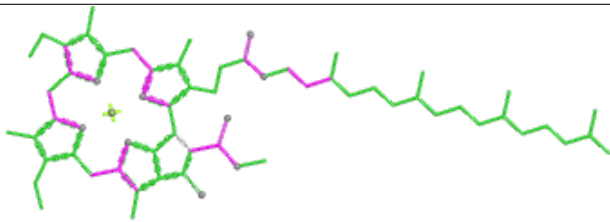
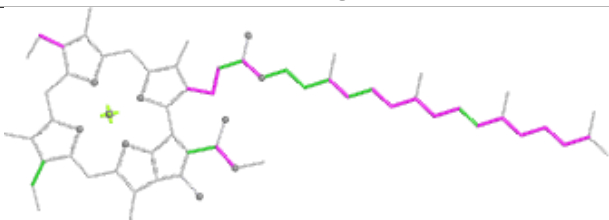
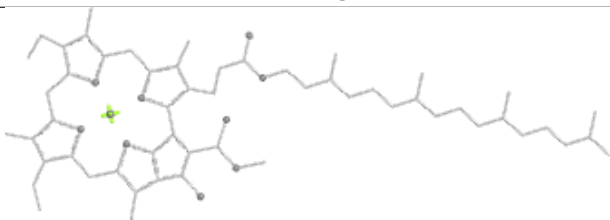


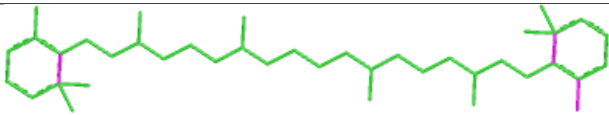
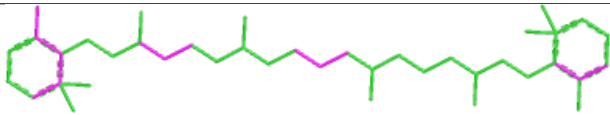
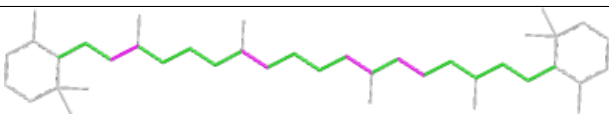
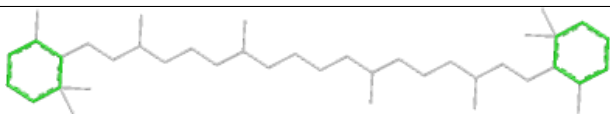


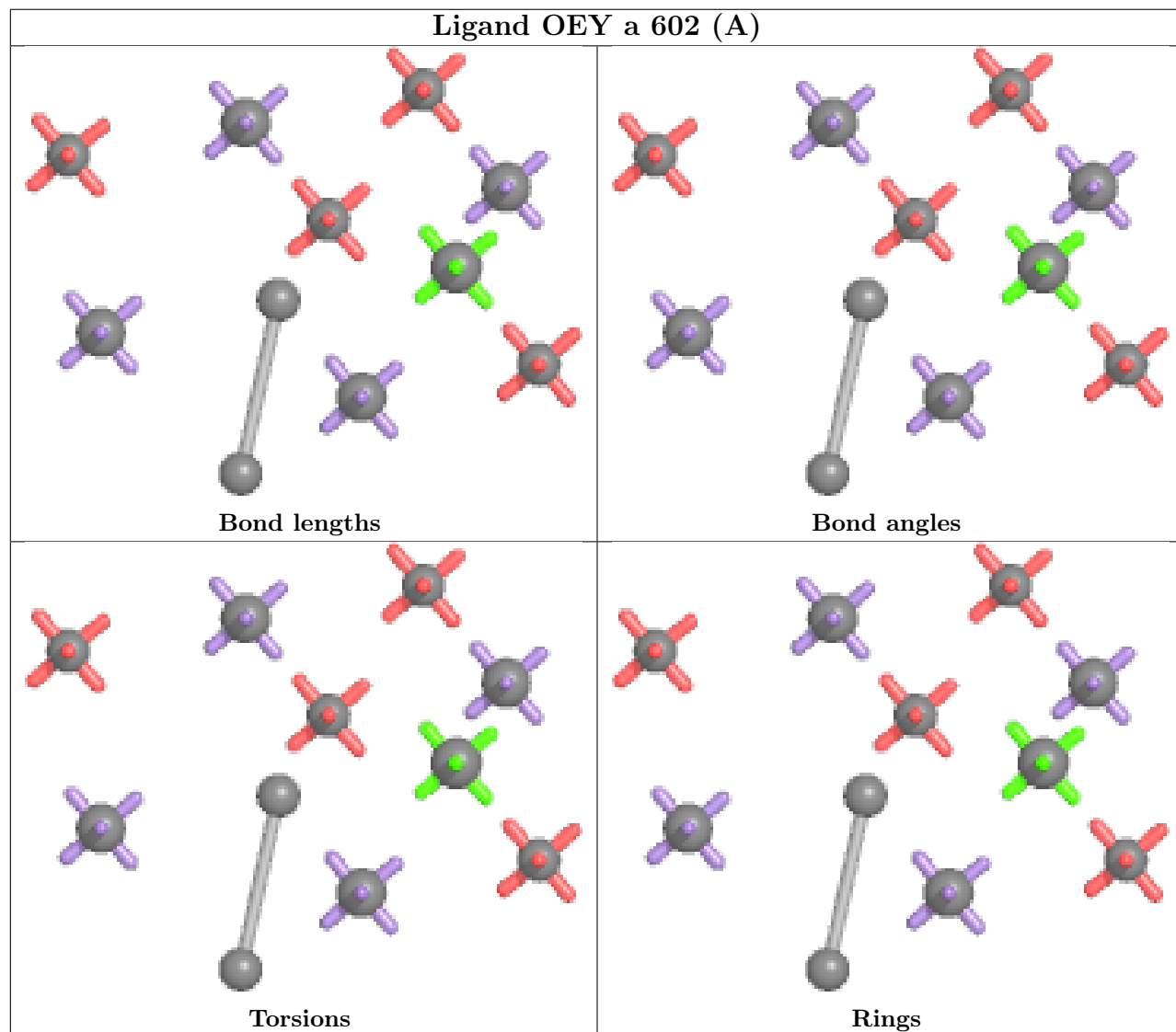
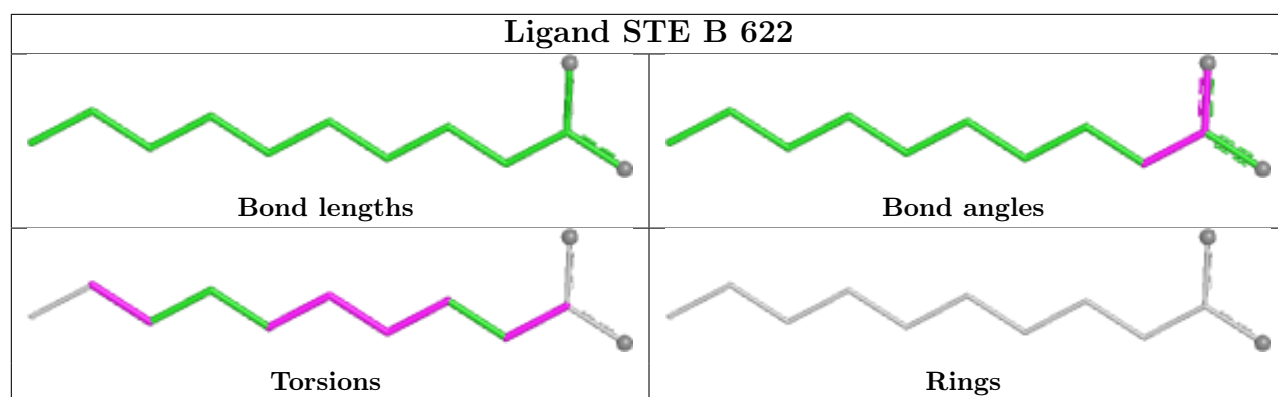
Ligand CLA b 613**Ligand BCR c 516****Ligand CLA c 508**

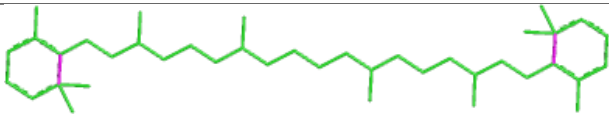
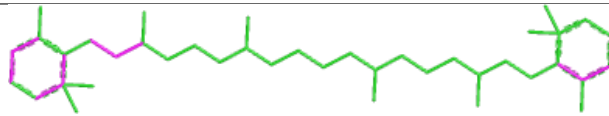
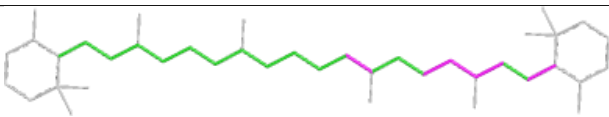
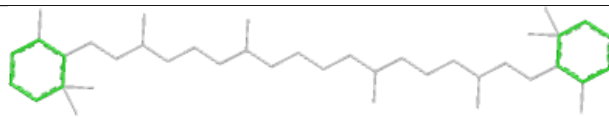
Ligand STE b 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

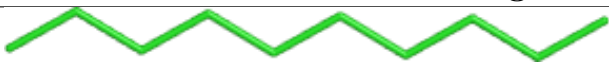
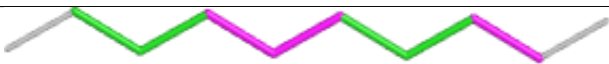
Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

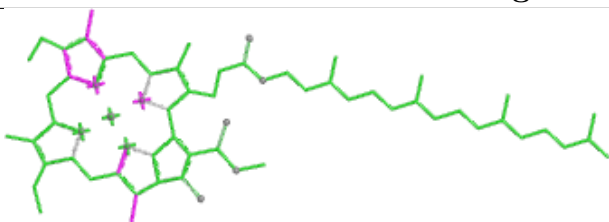
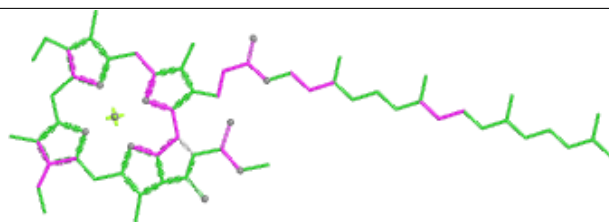
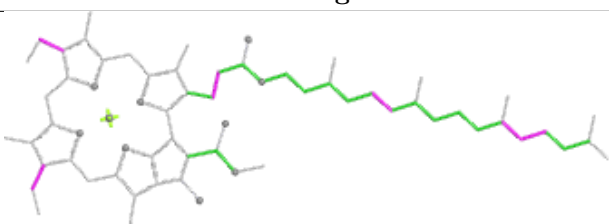
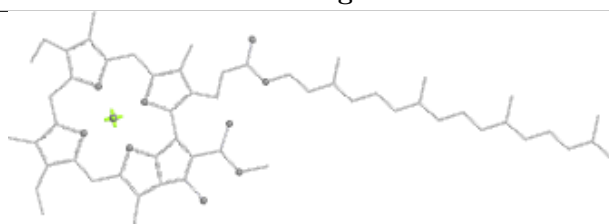
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings



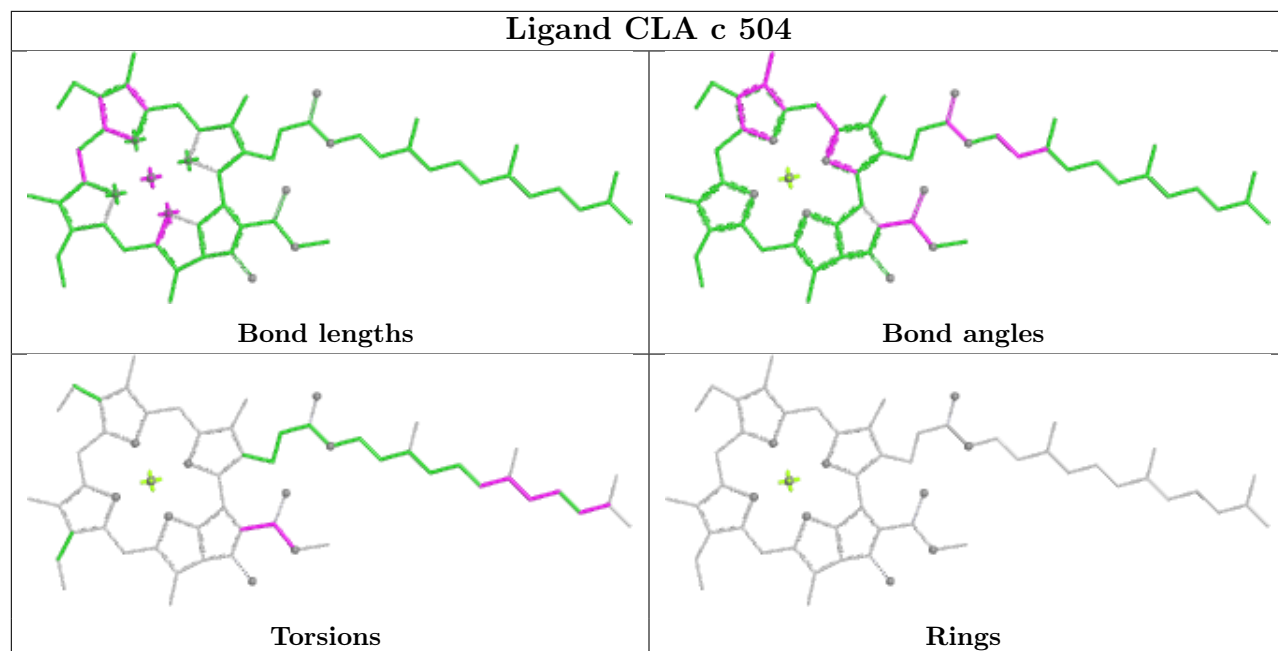
Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE t 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

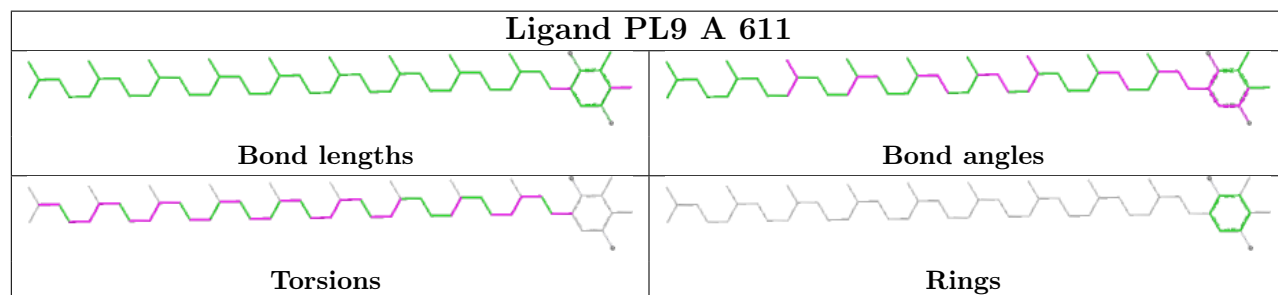
Ligand STE M 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

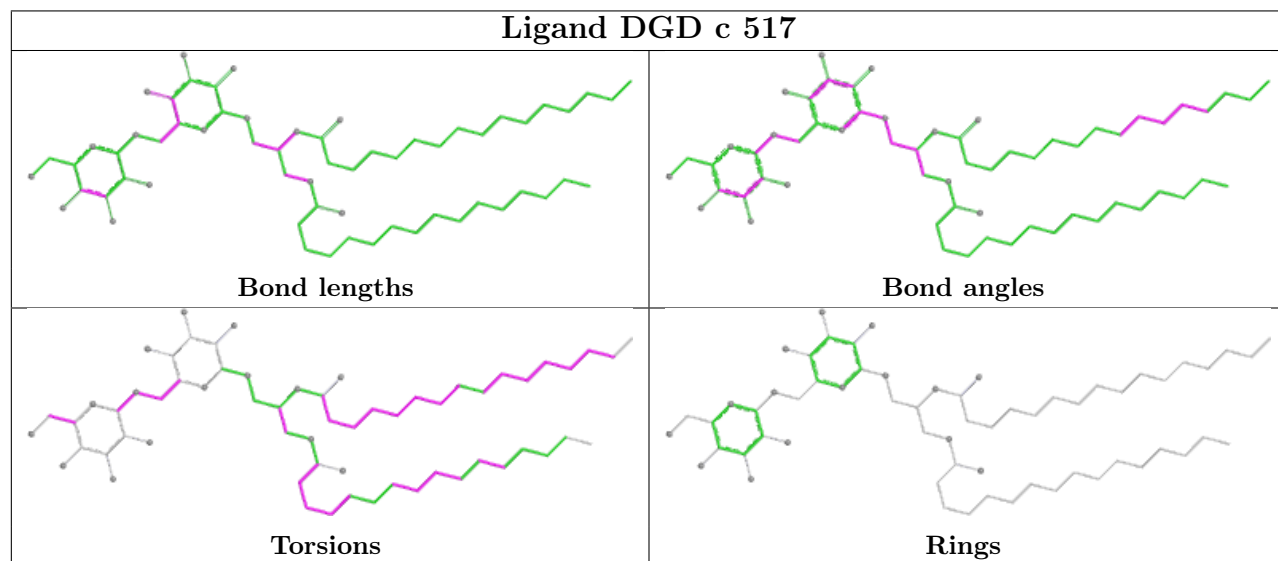
Ligand CLA c 504

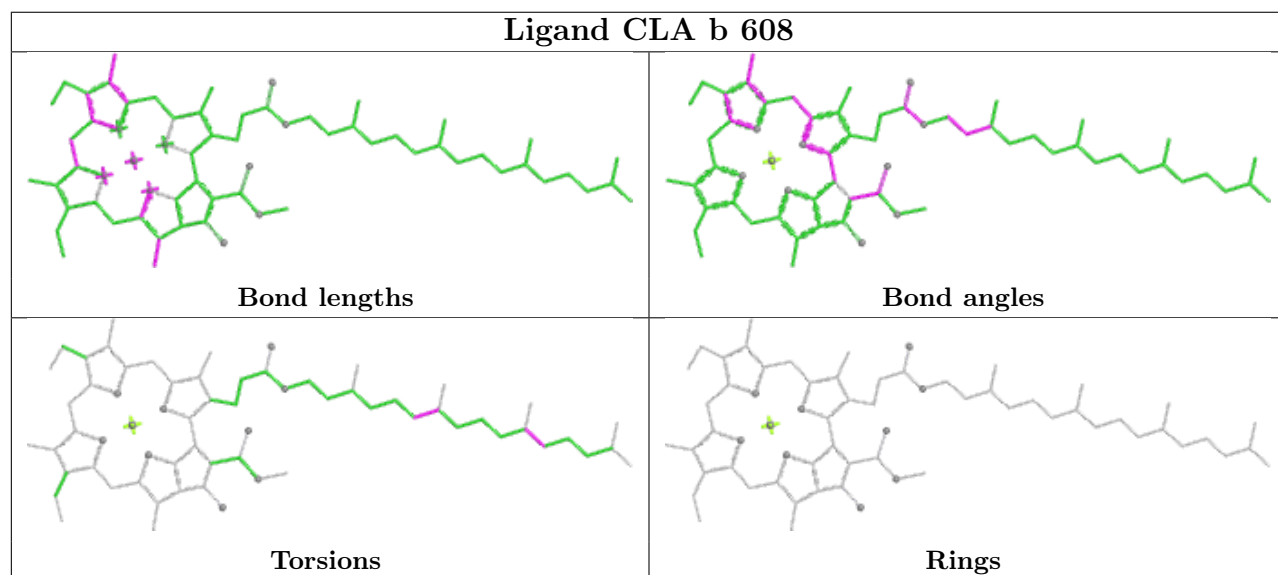
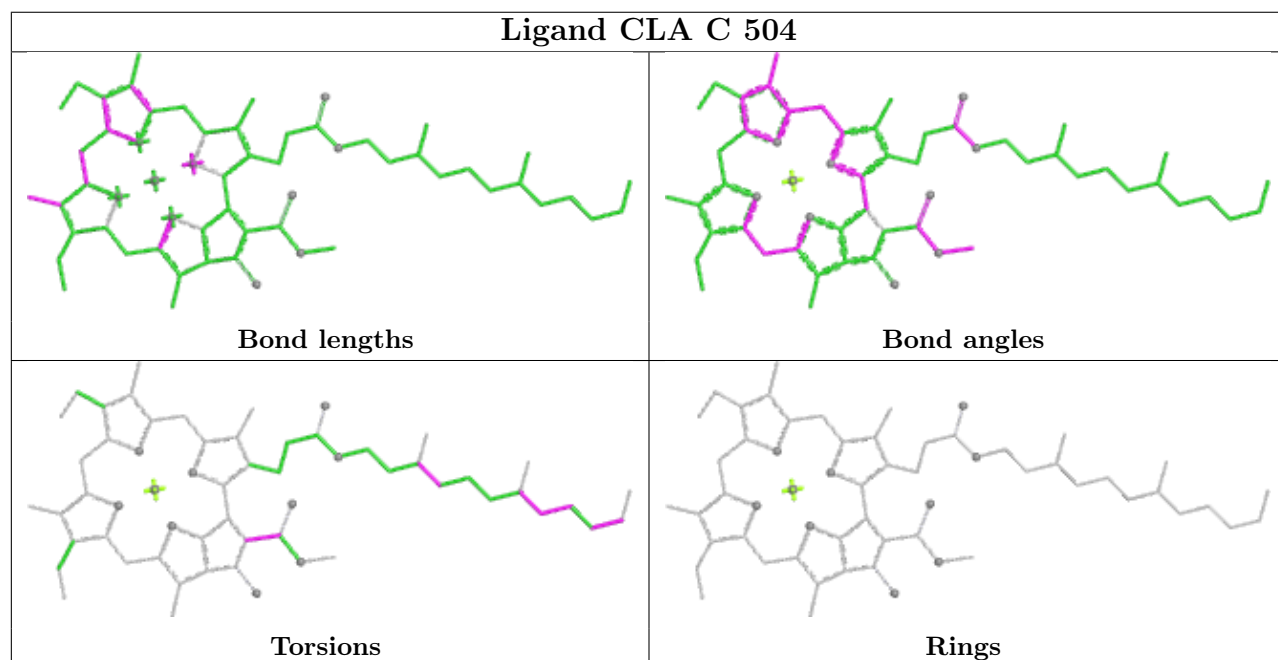
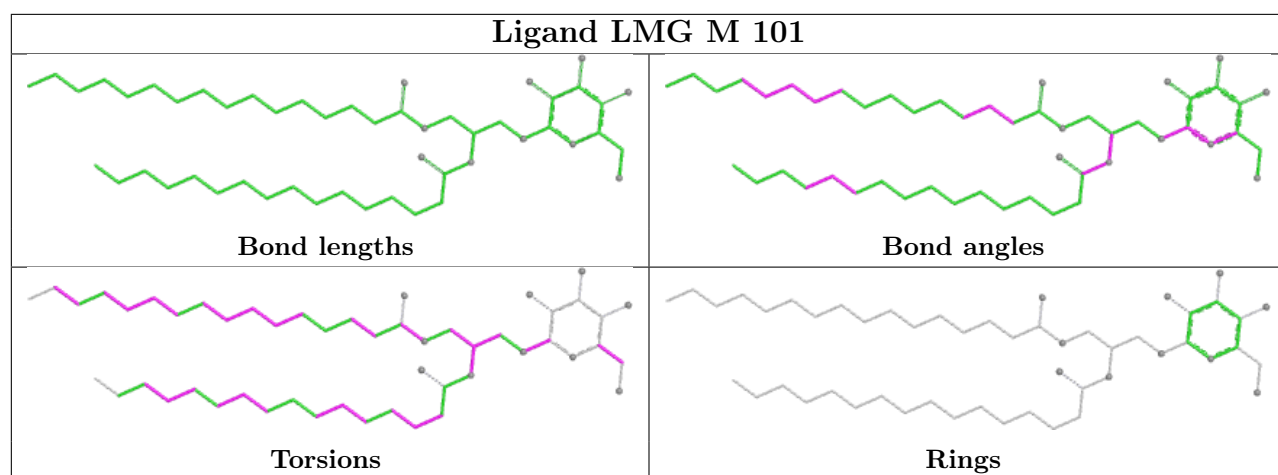


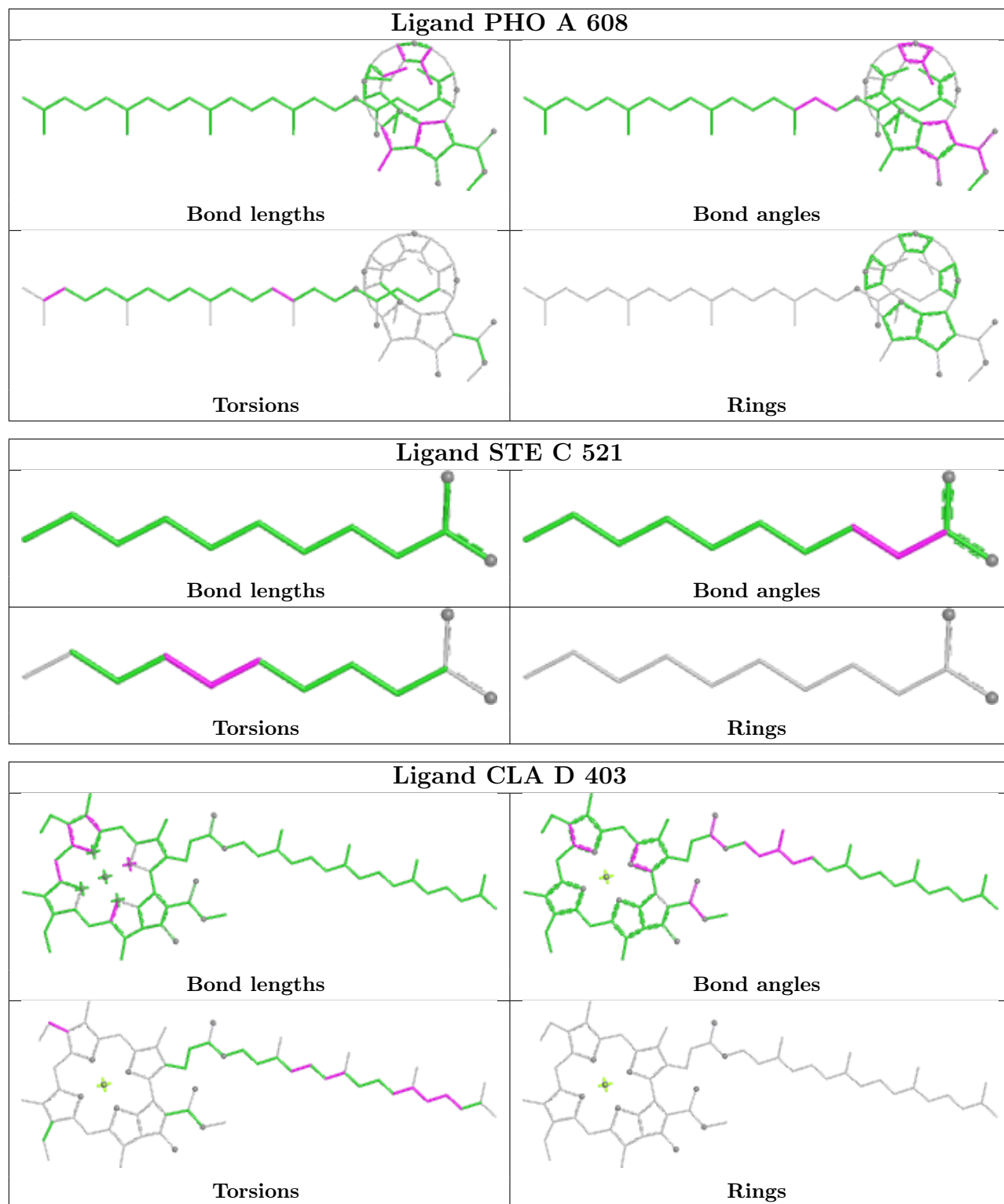
Ligand PL9 A 611

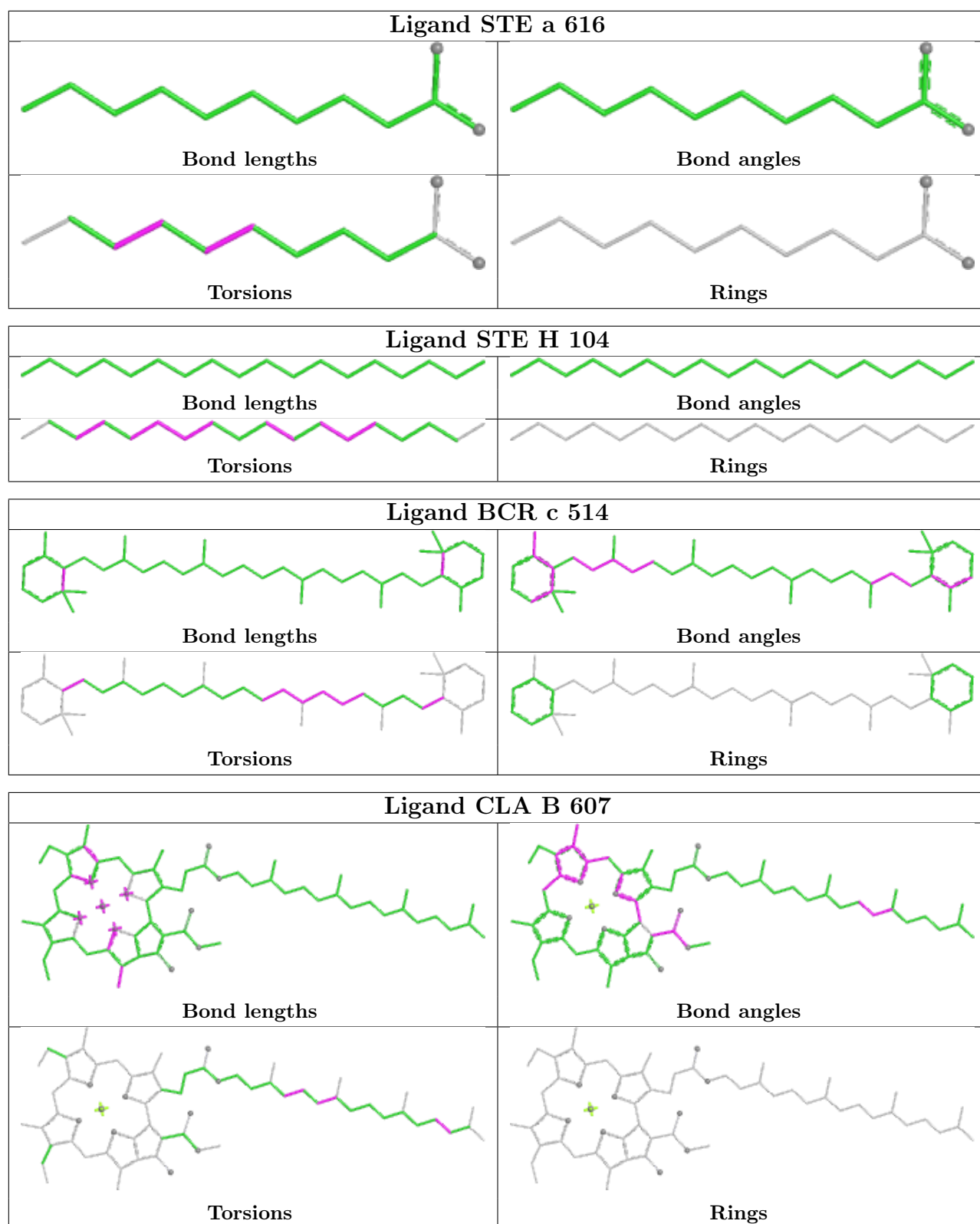


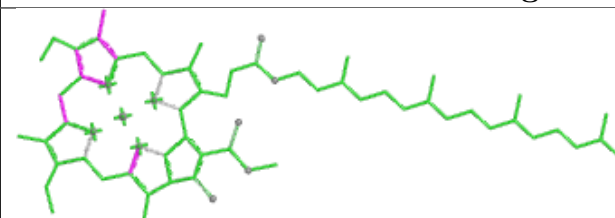
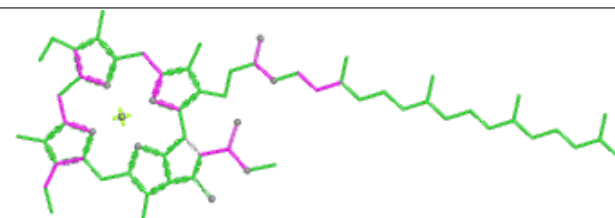
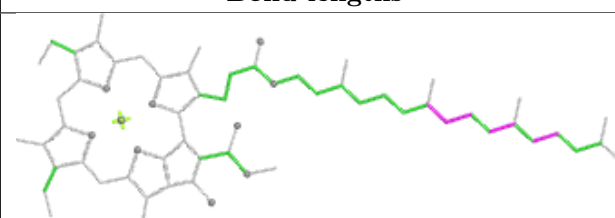
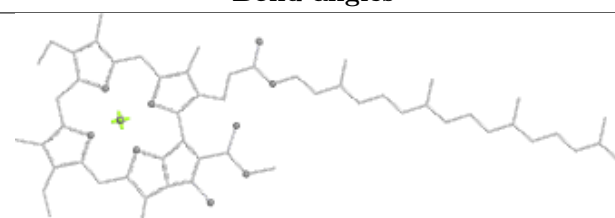
Ligand DGD c 517

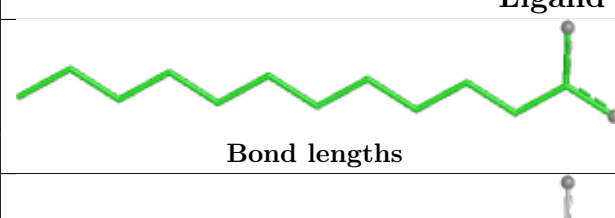
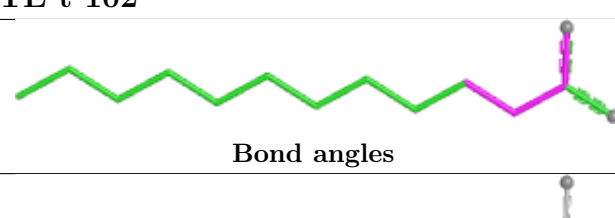
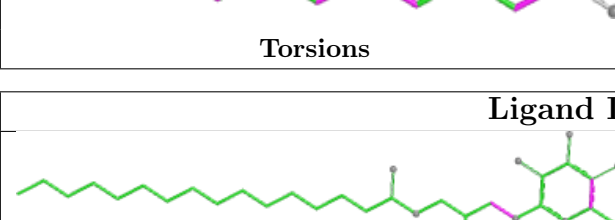
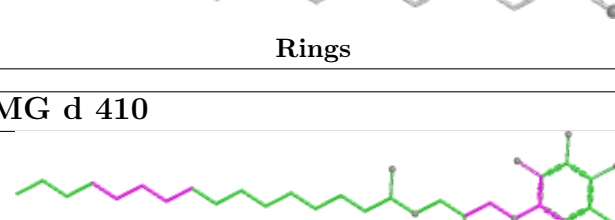


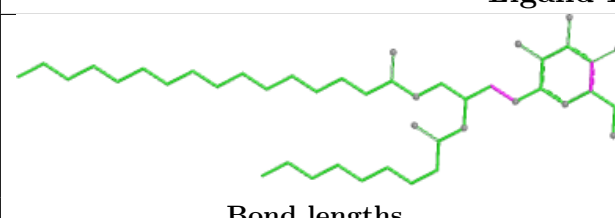
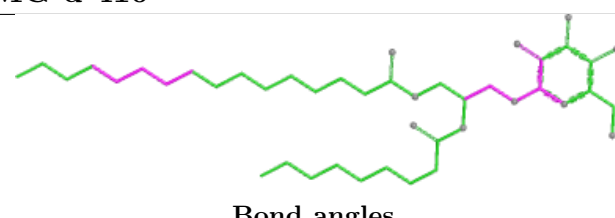
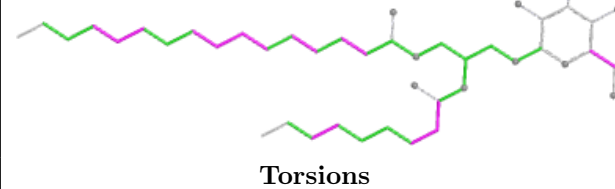
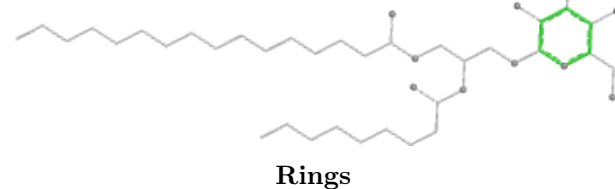




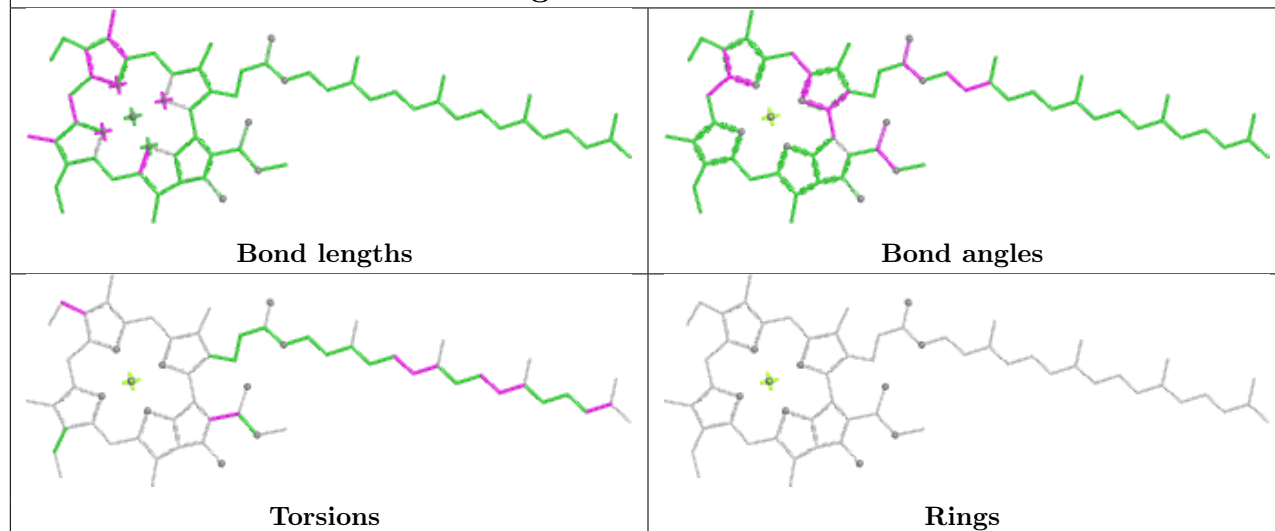


Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

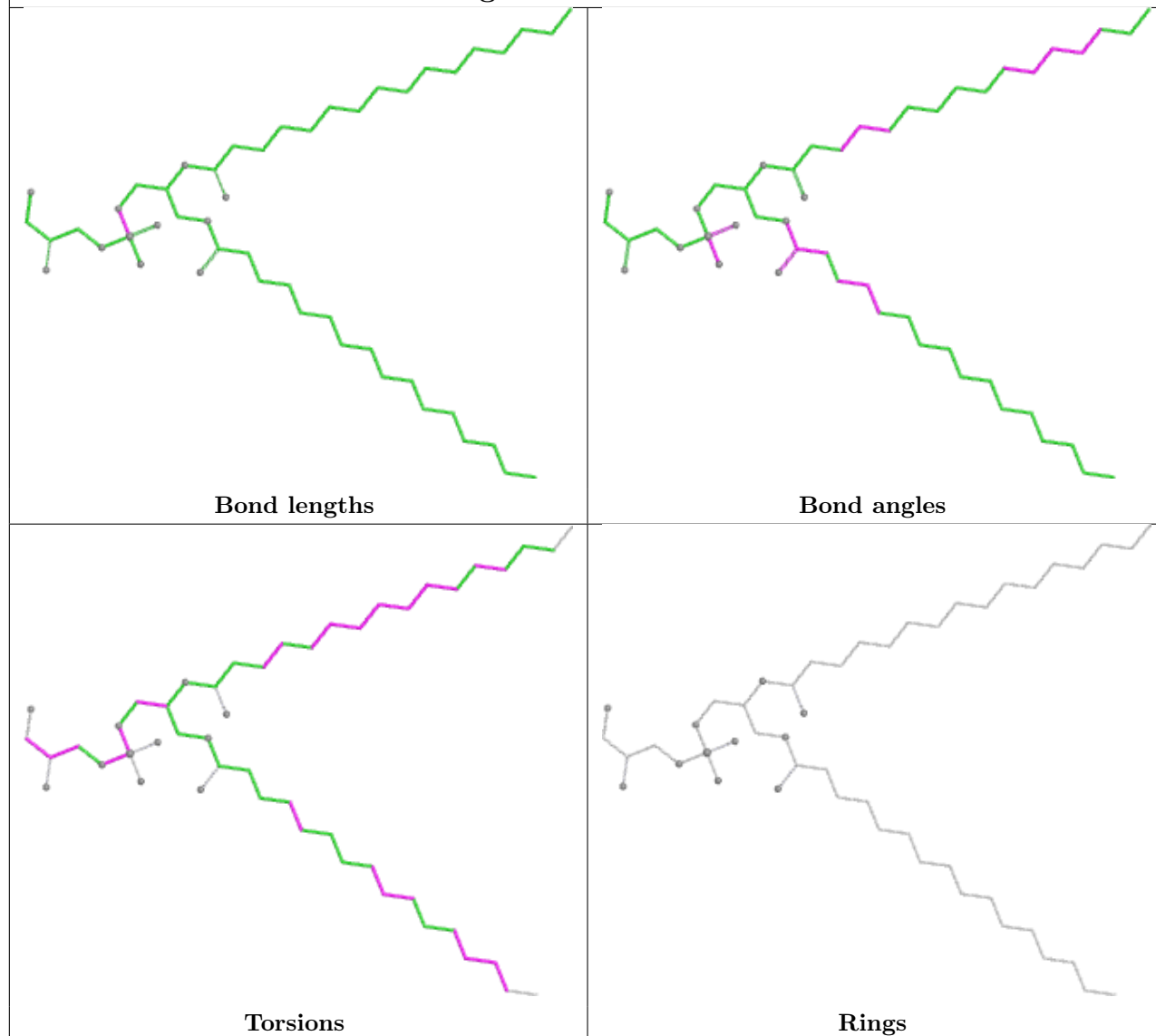
Ligand STE t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

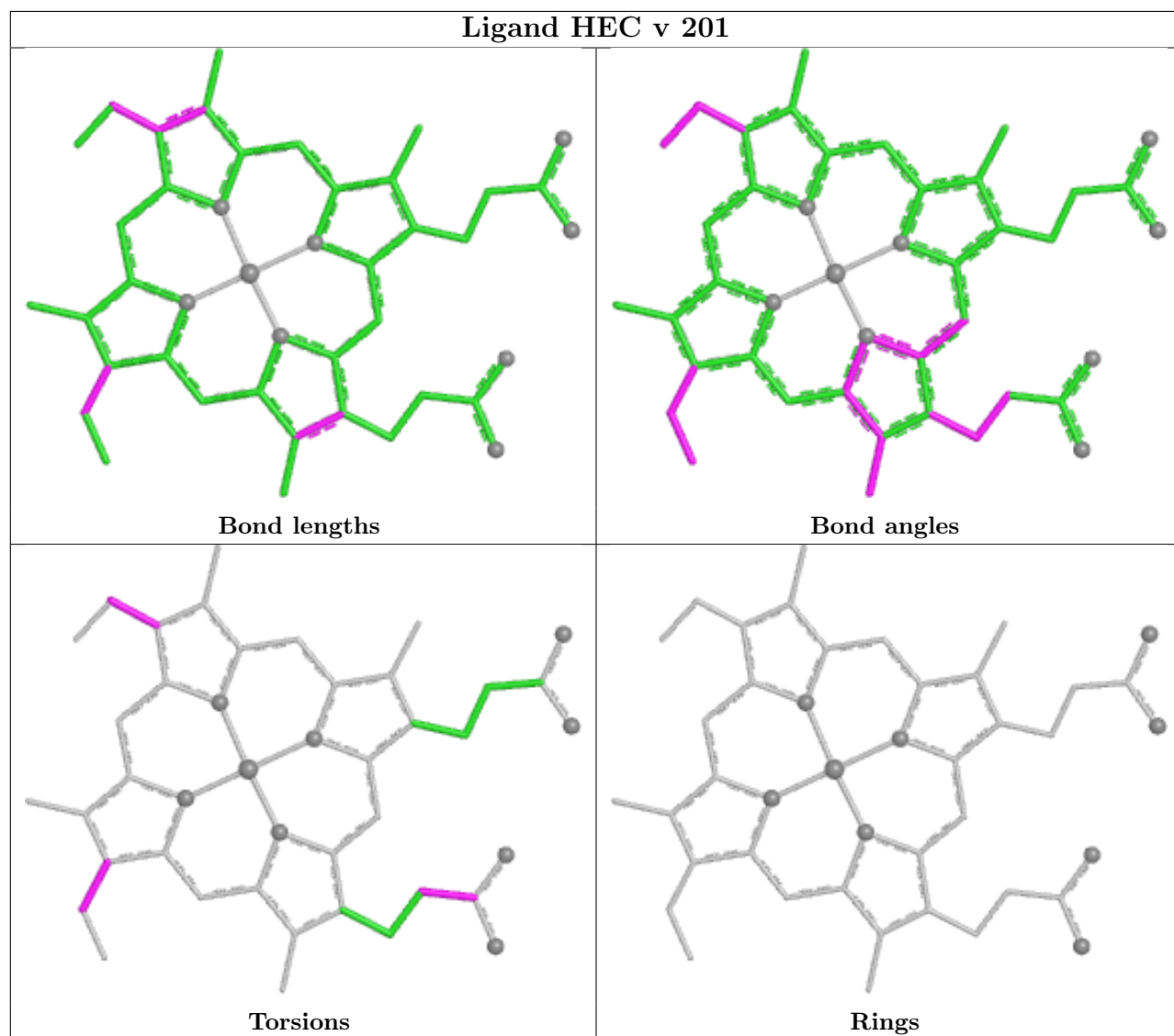
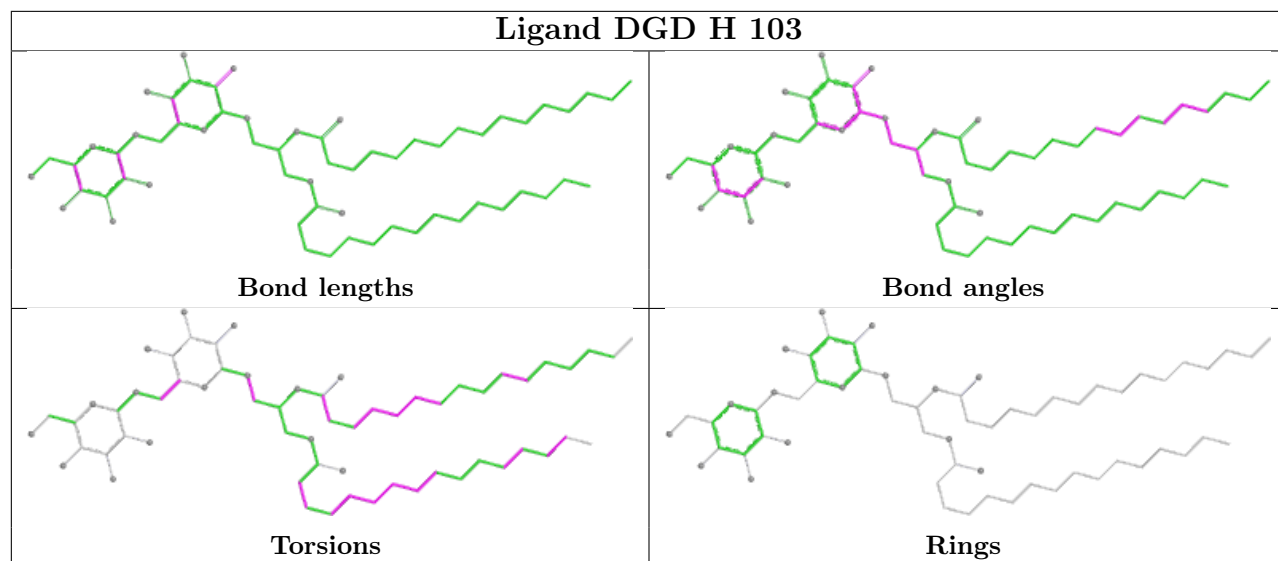
Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

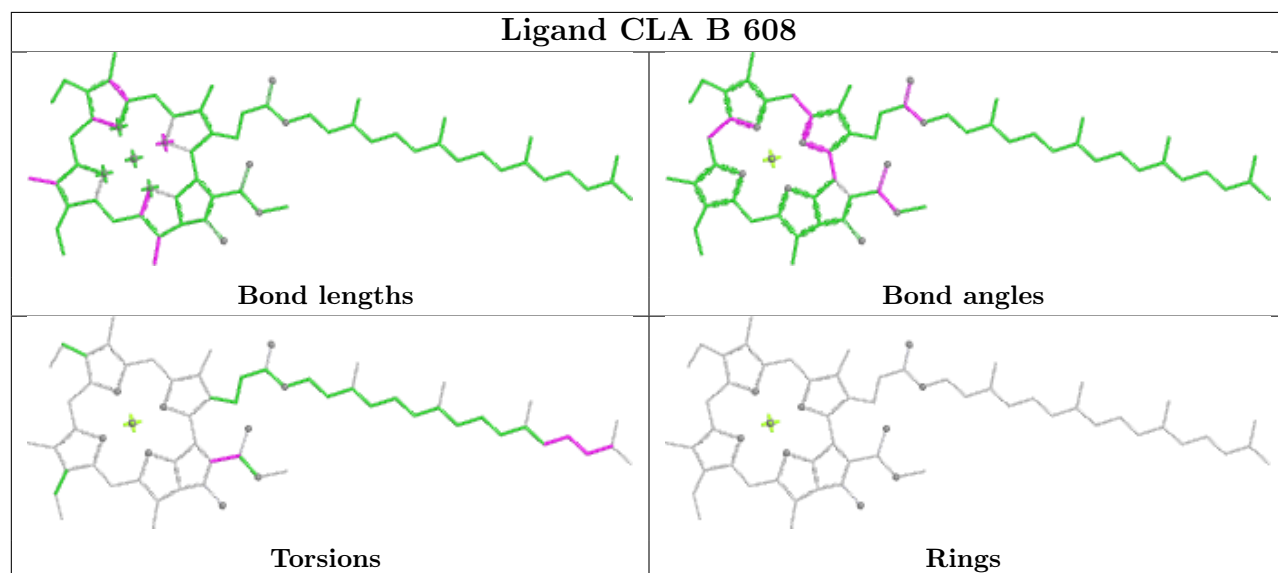
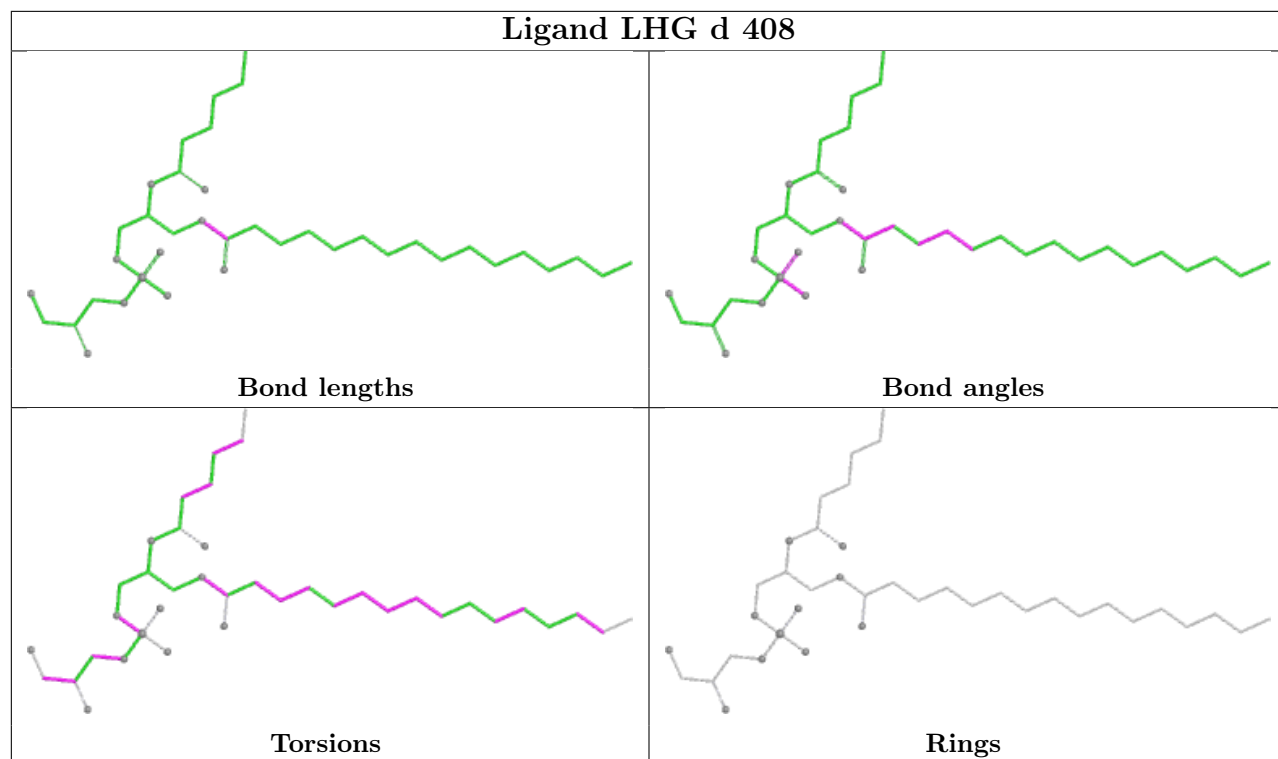
Ligand CLA C 507



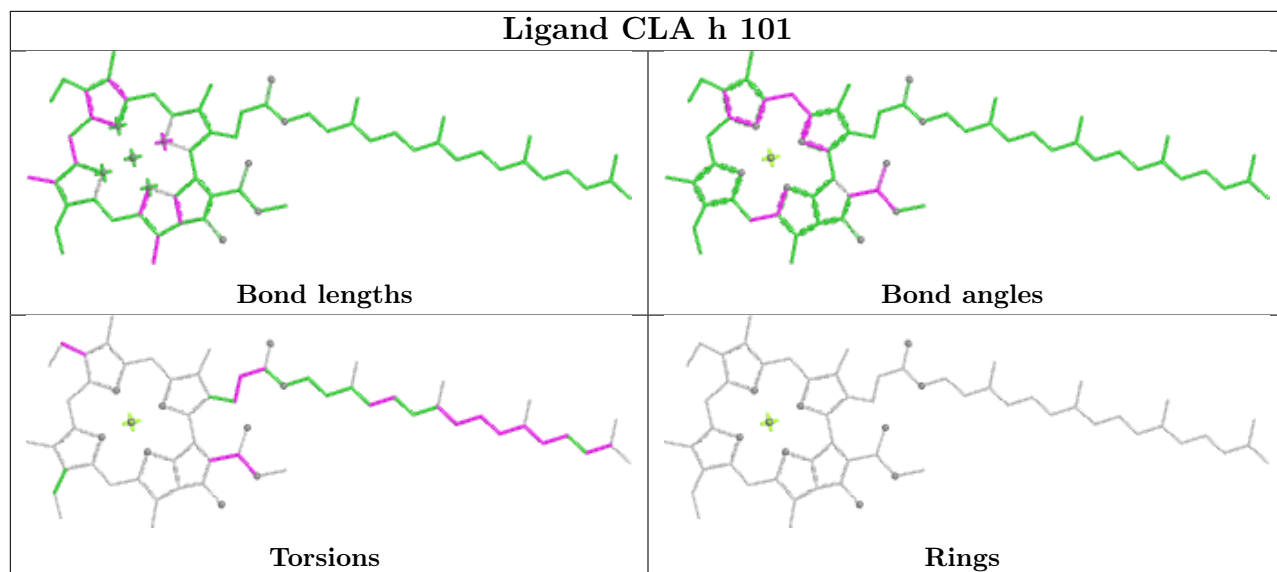
Ligand LHG D 409



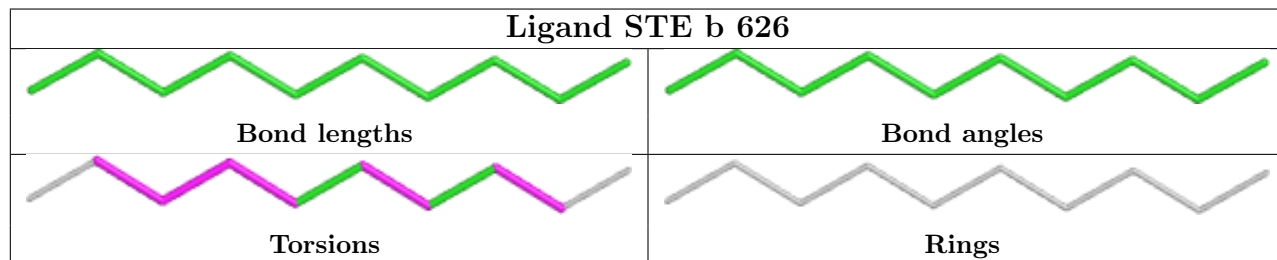




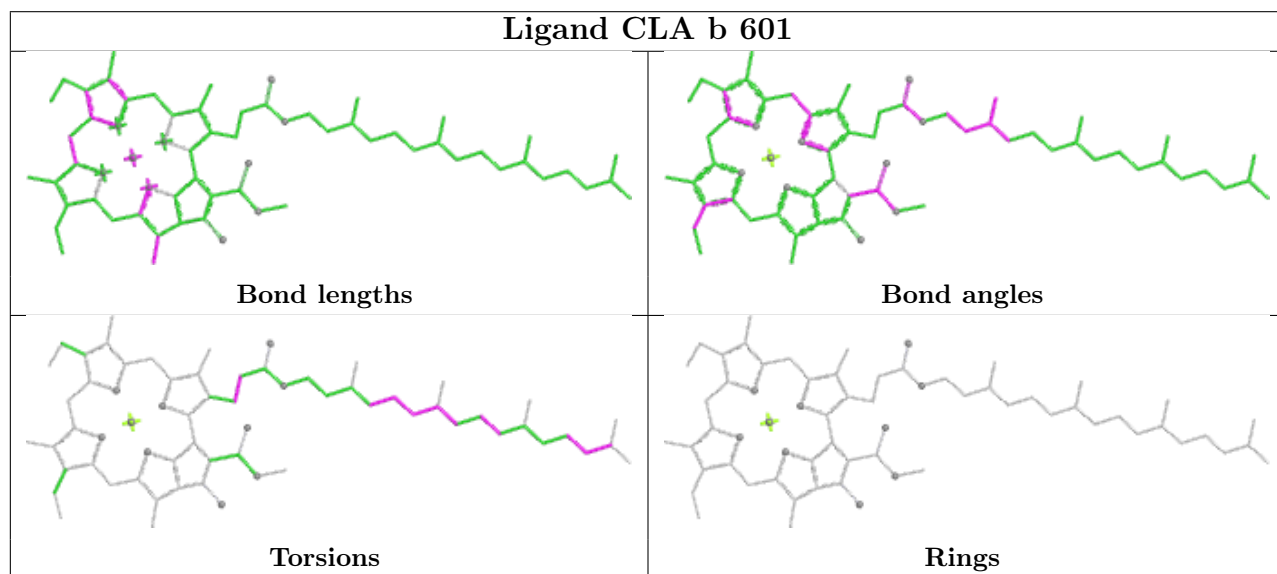
Ligand CLA h 101



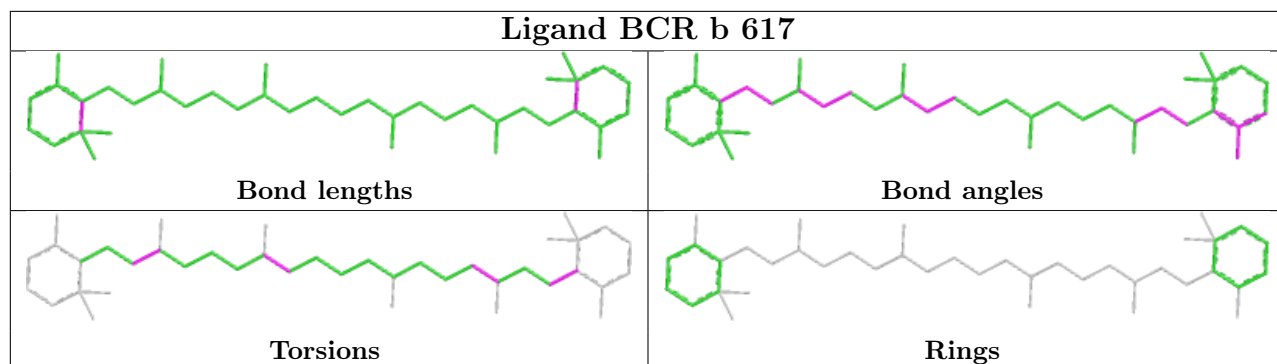
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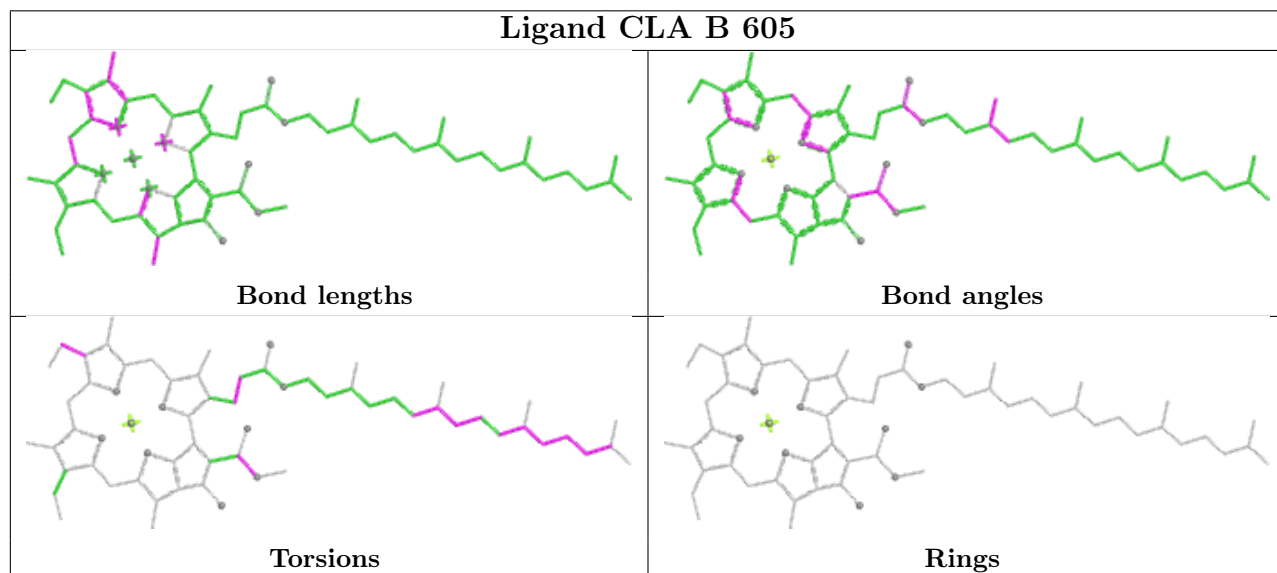
Ligand CLA b 601



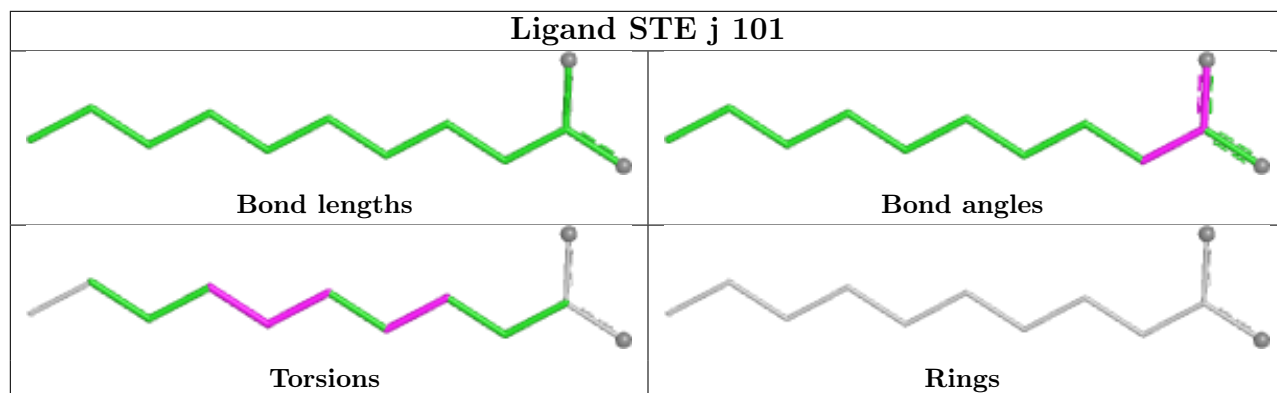
Ligand BCR b 617



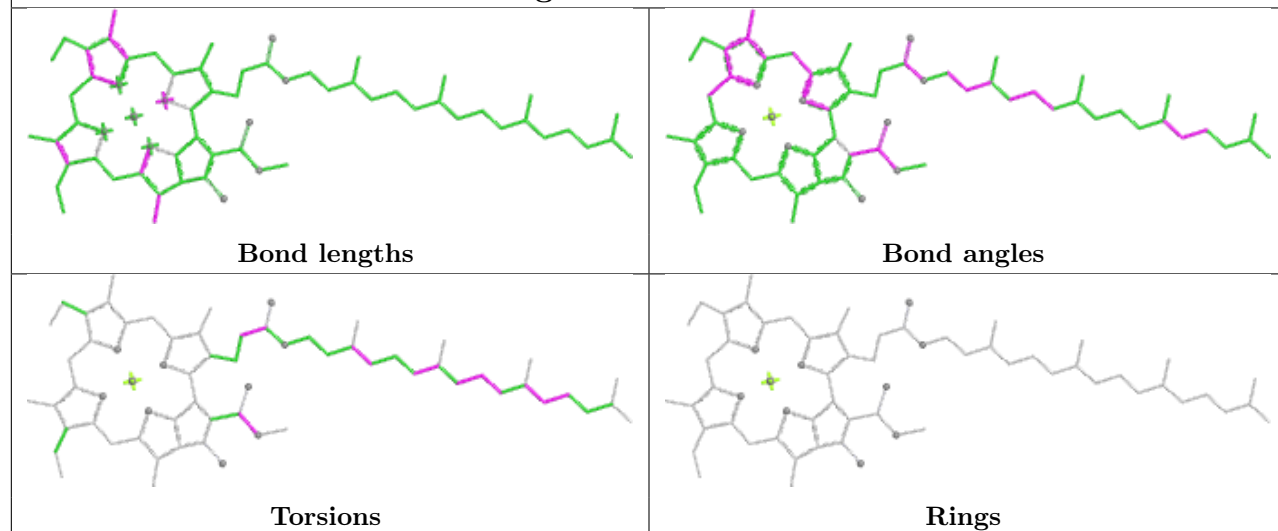
Ligand CLA B 605



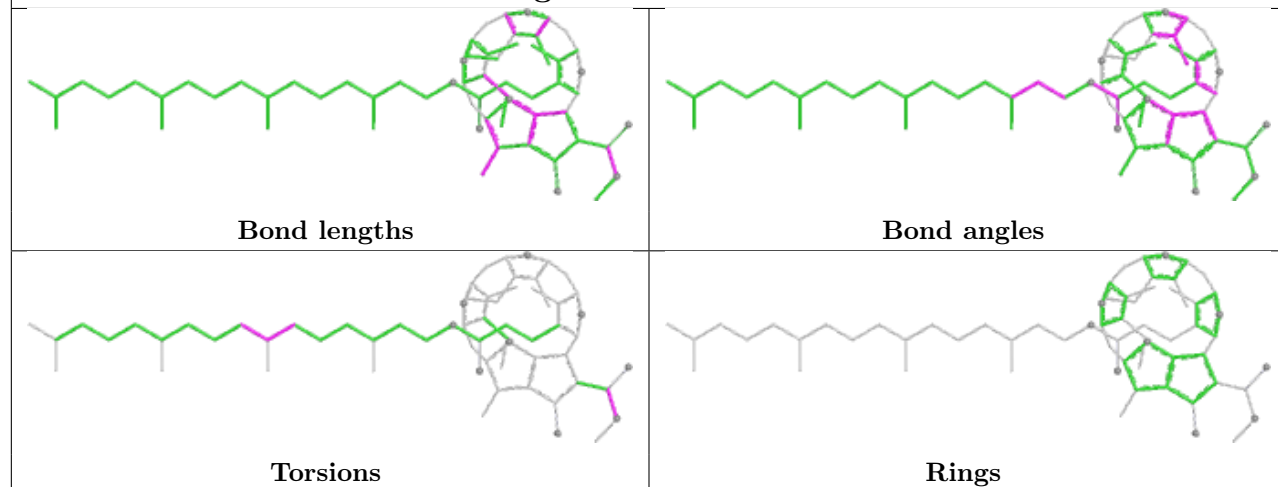
Ligand STE j 101



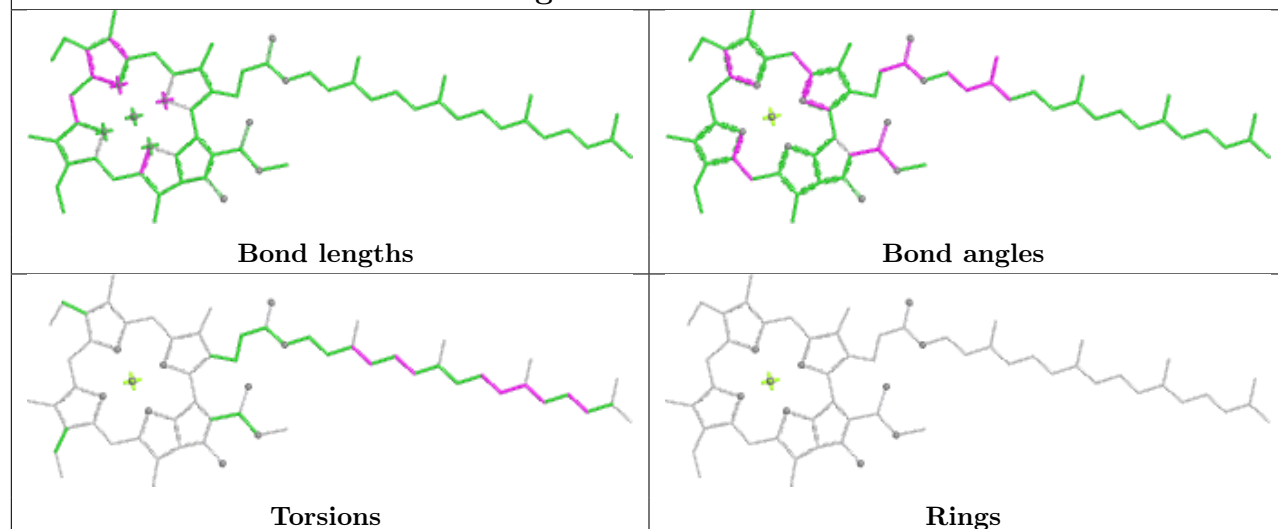
Ligand CLA b 612

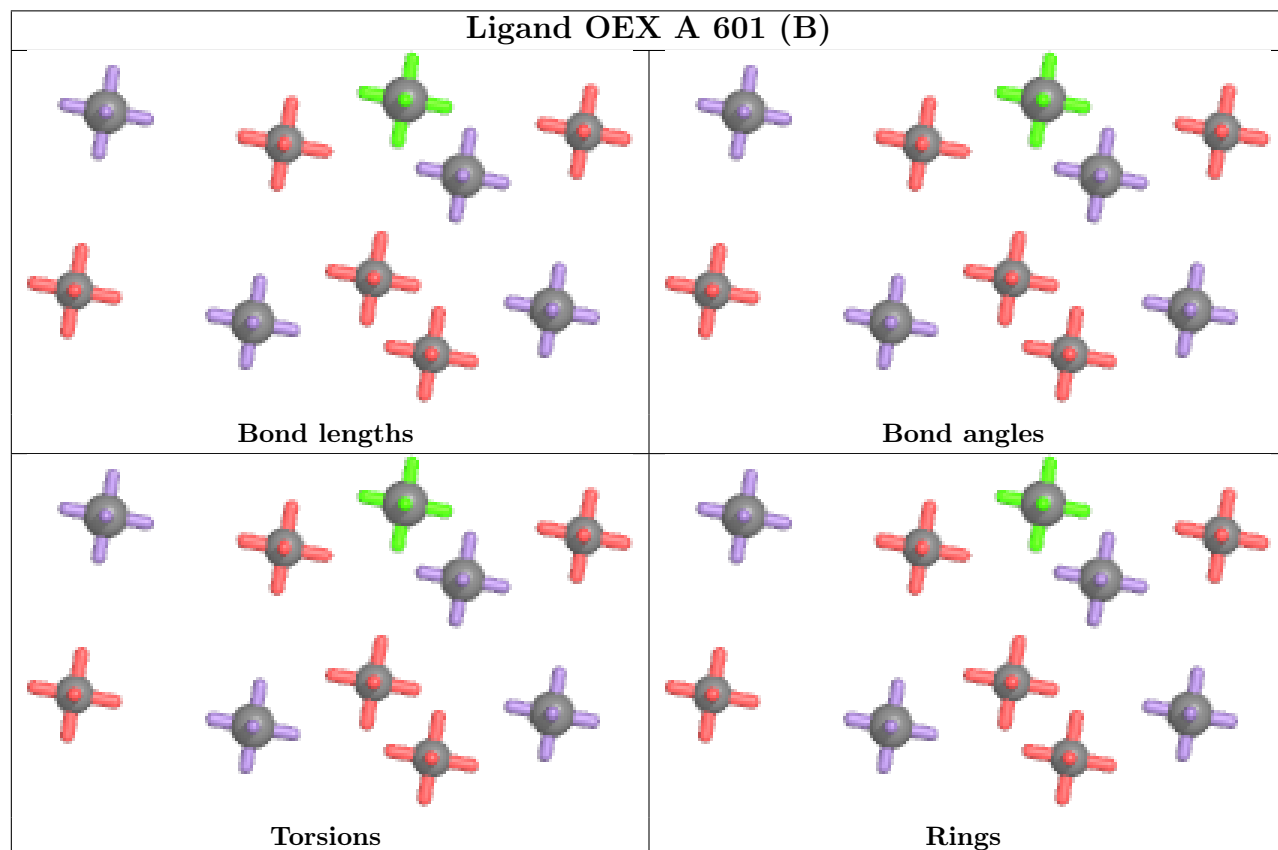
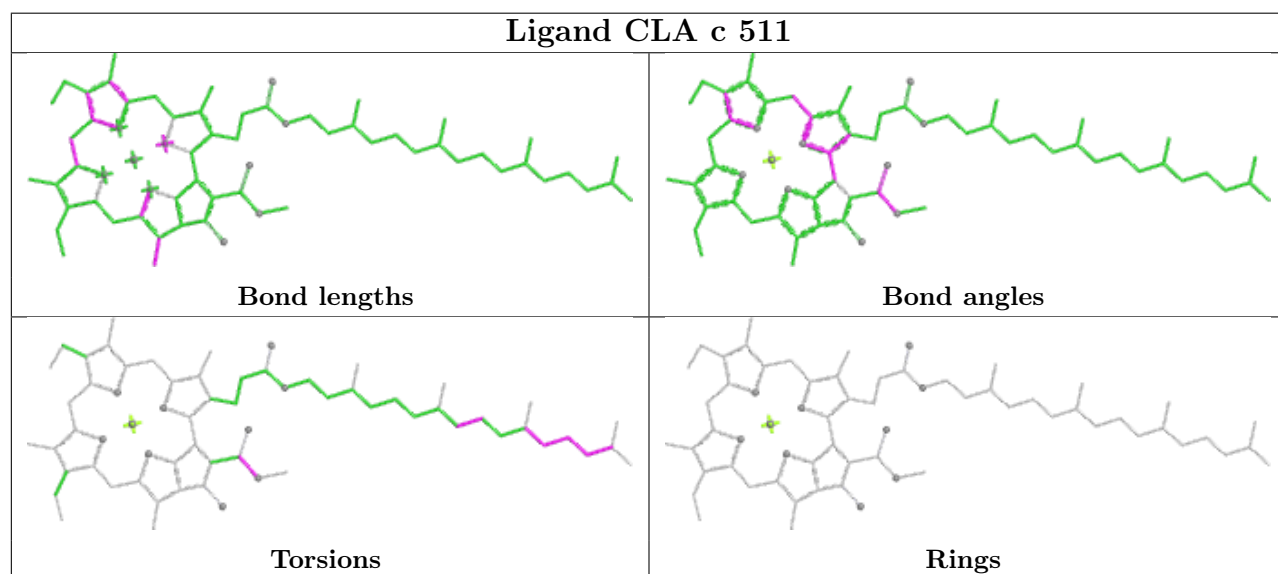
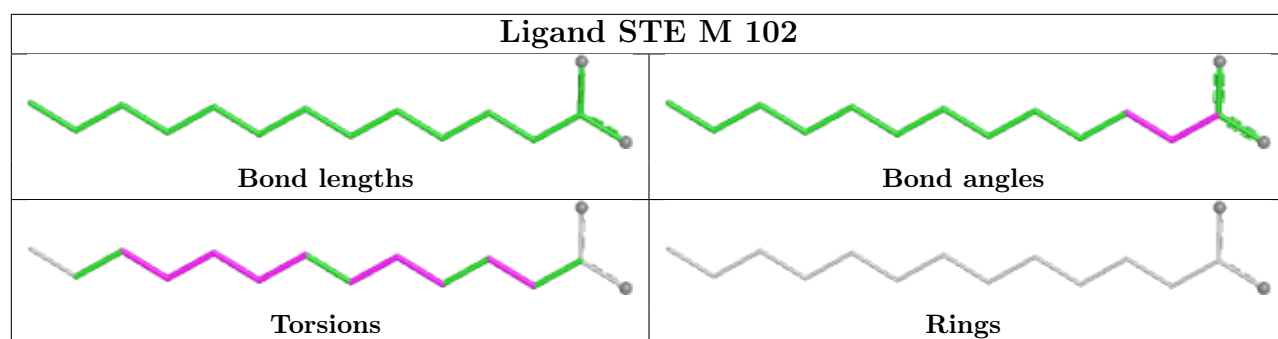


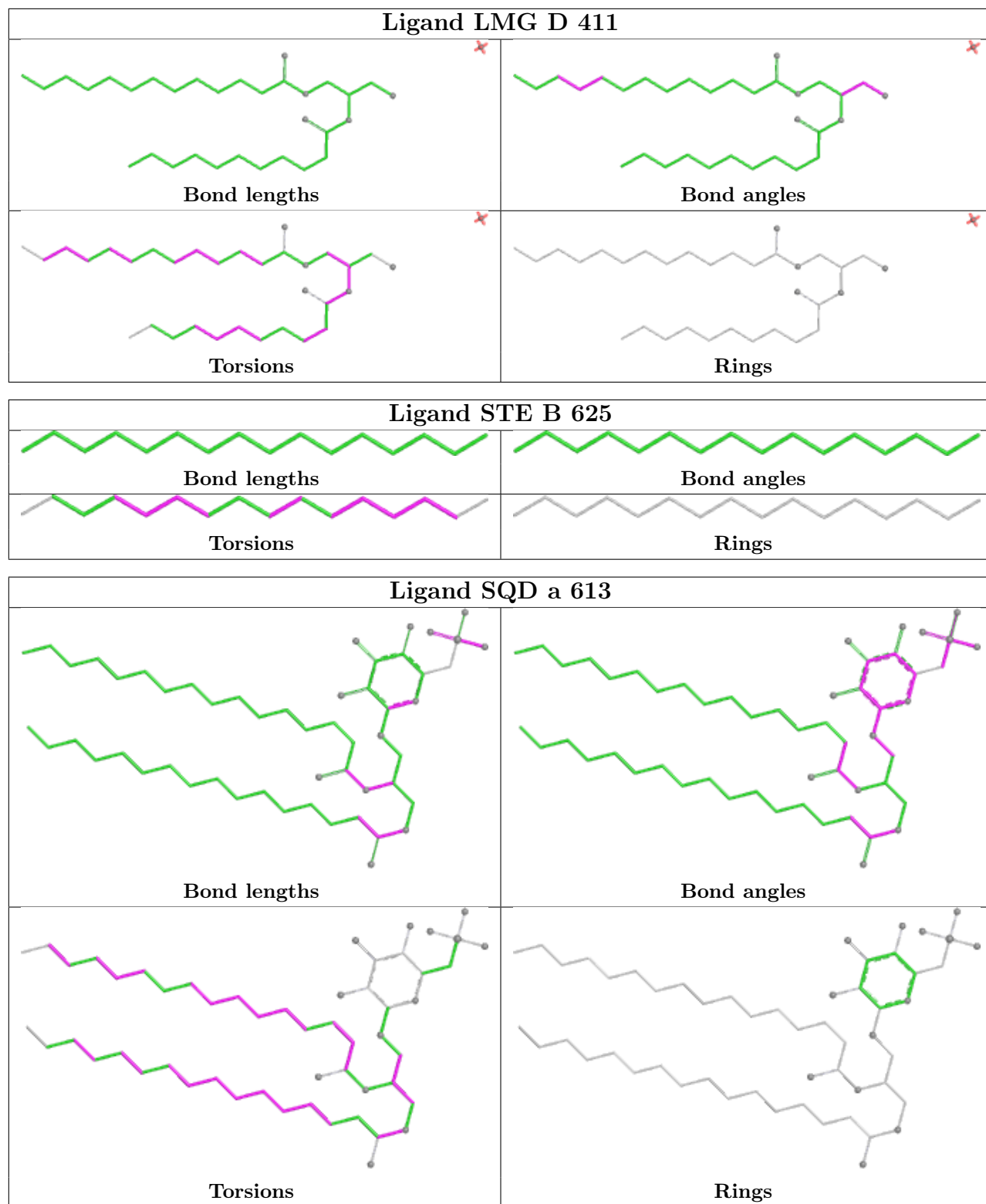
Ligand PHO a 608

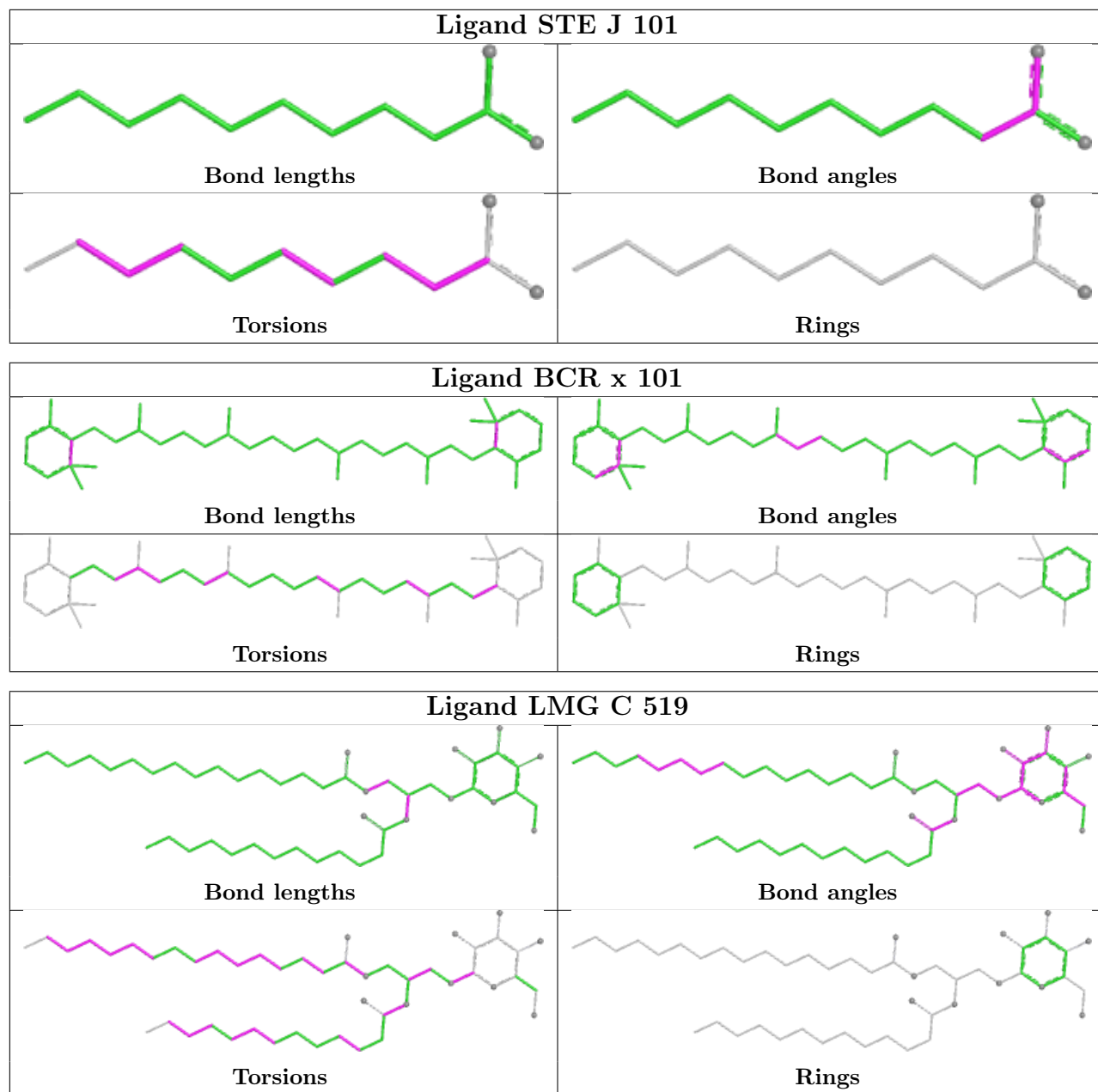


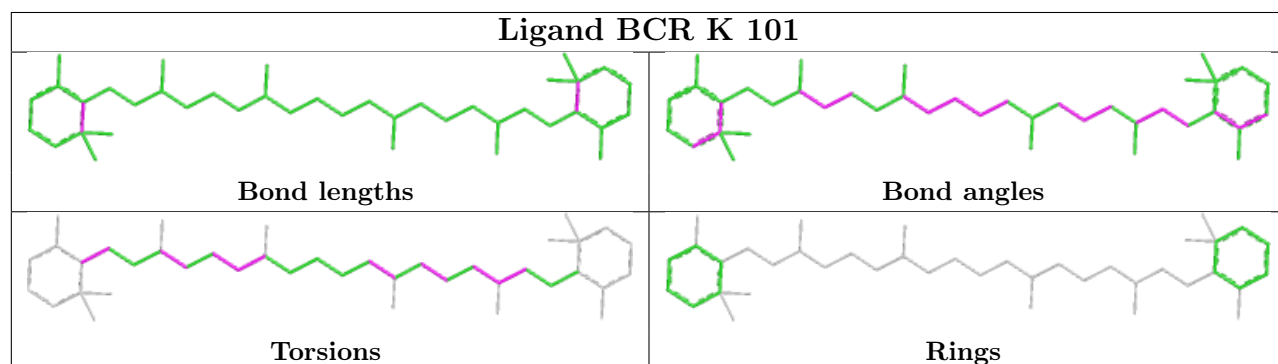
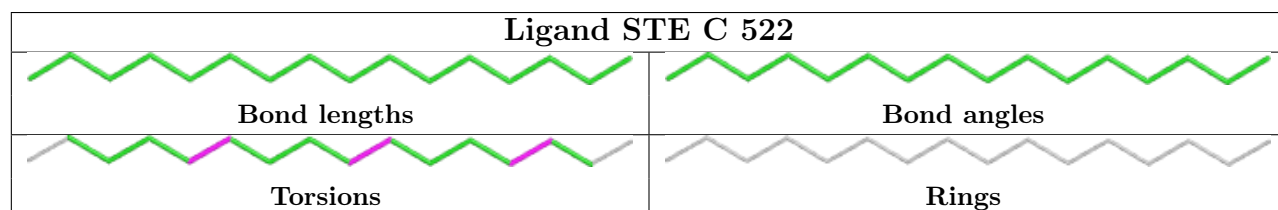
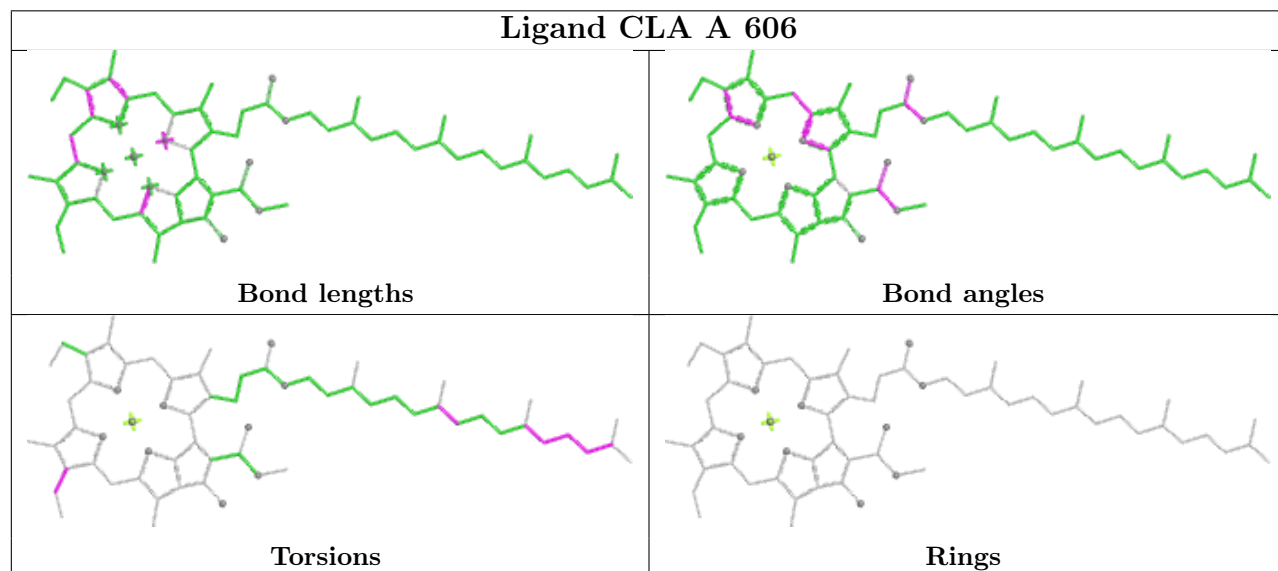
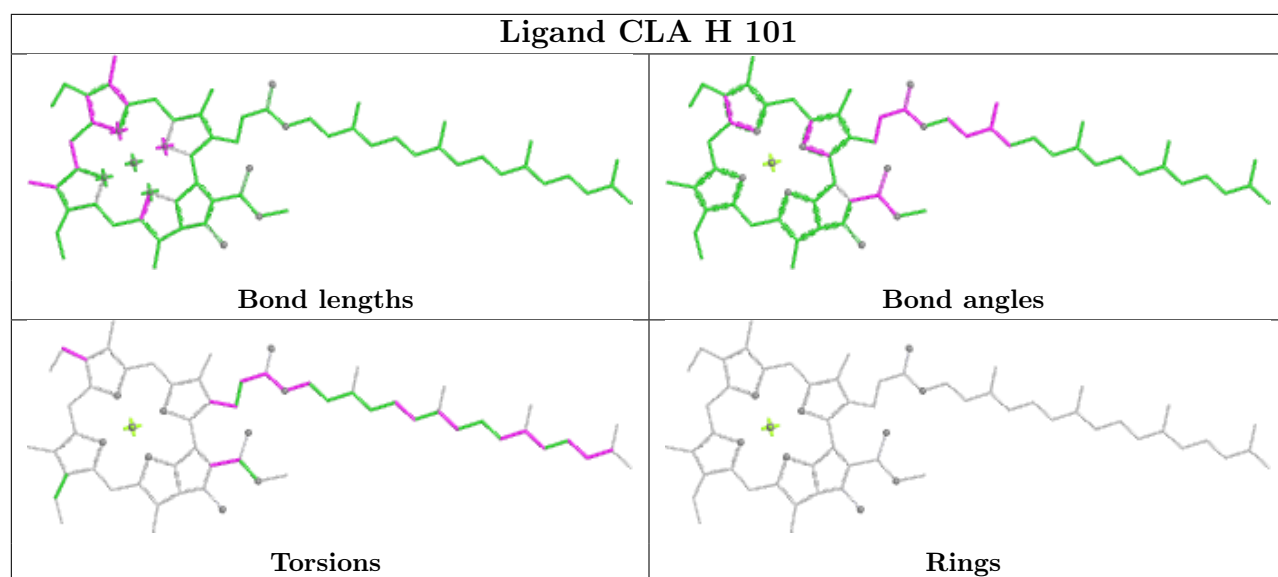
Ligand CLA b 604

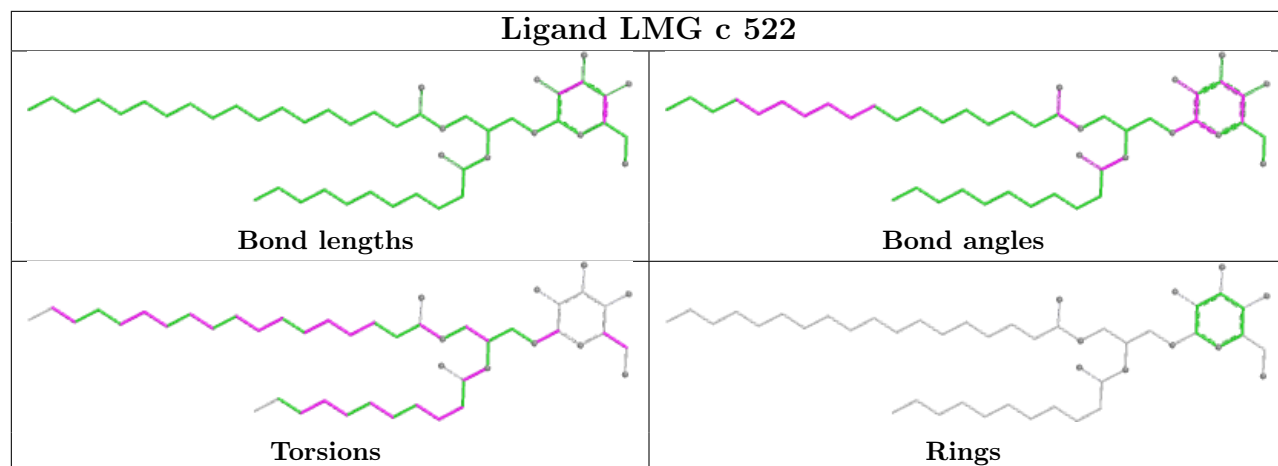
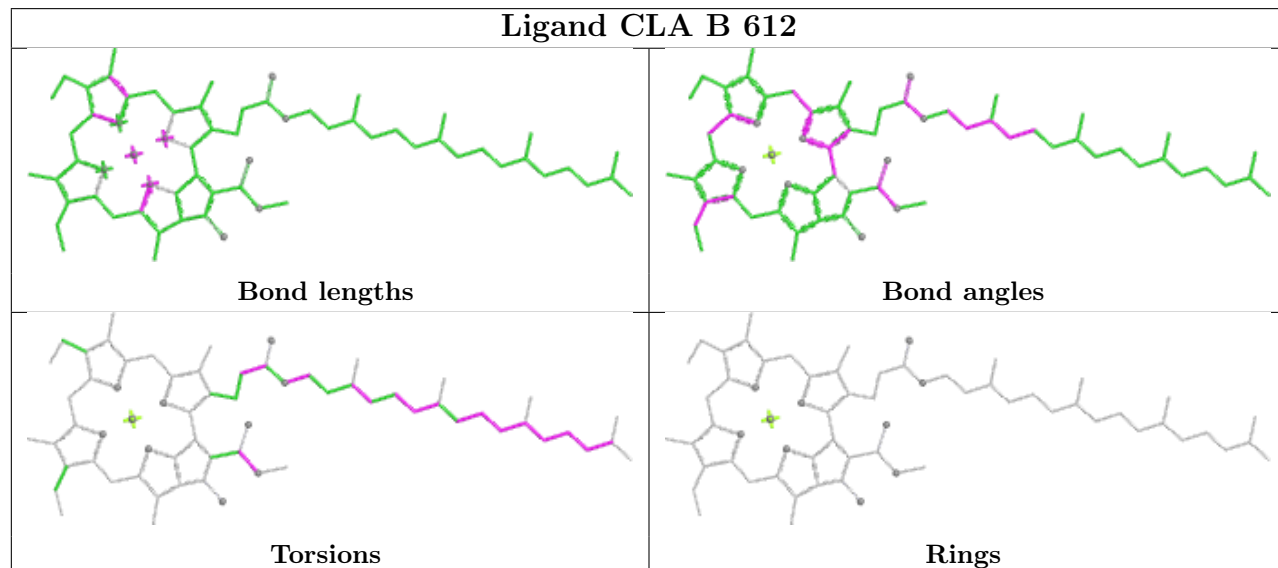
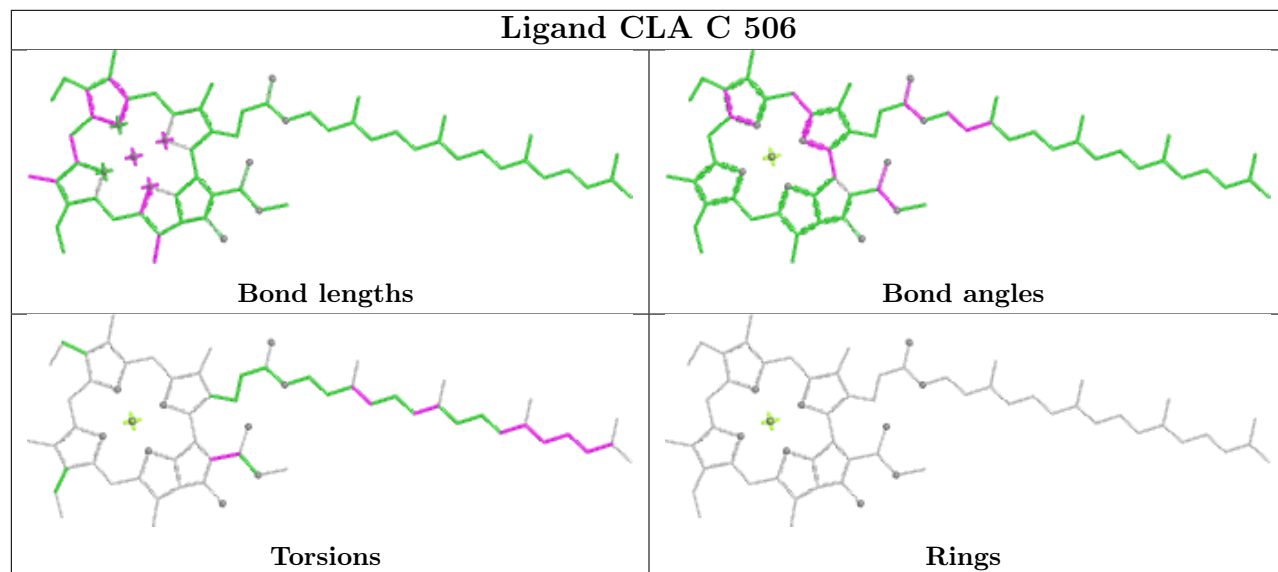


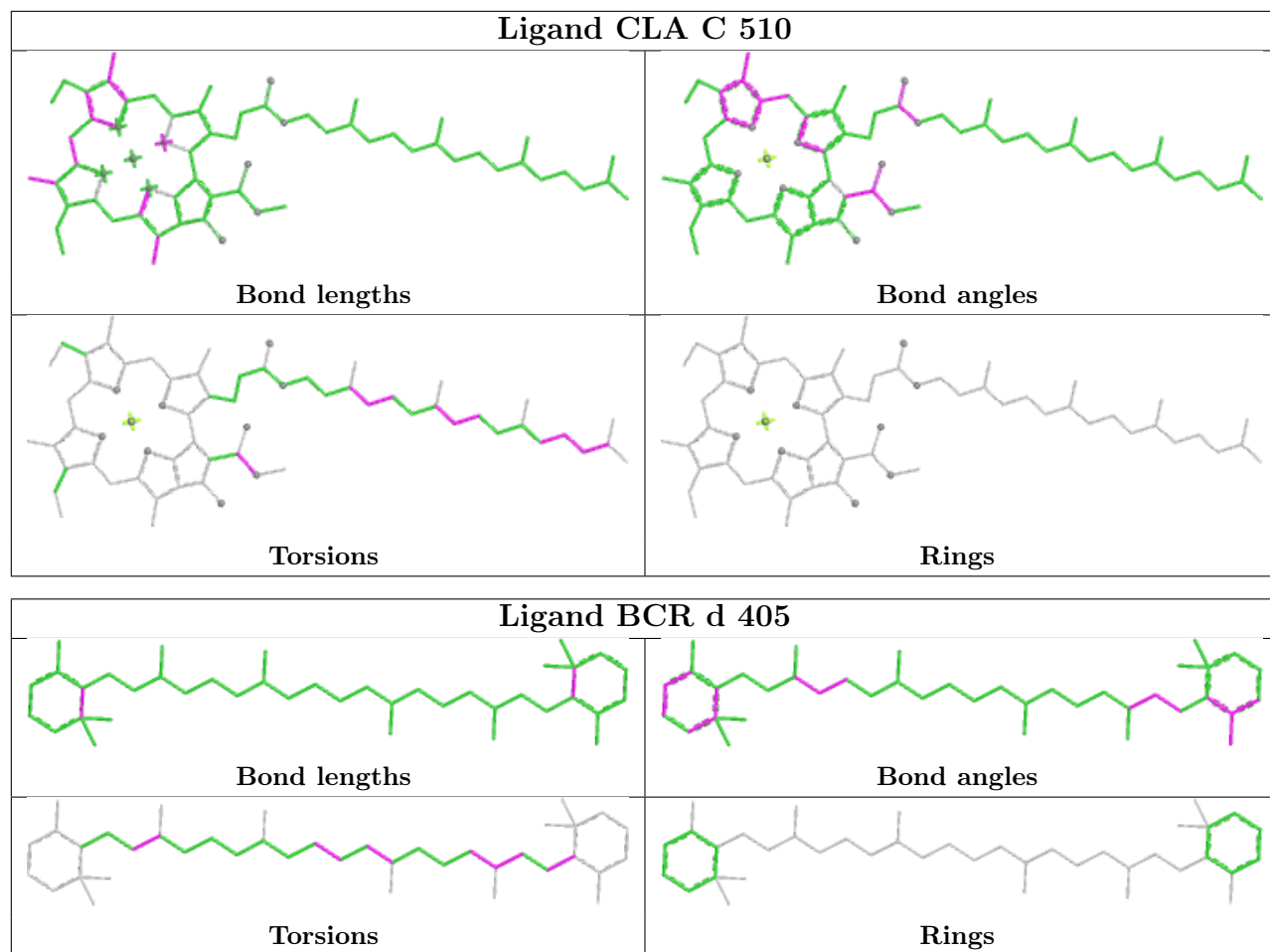


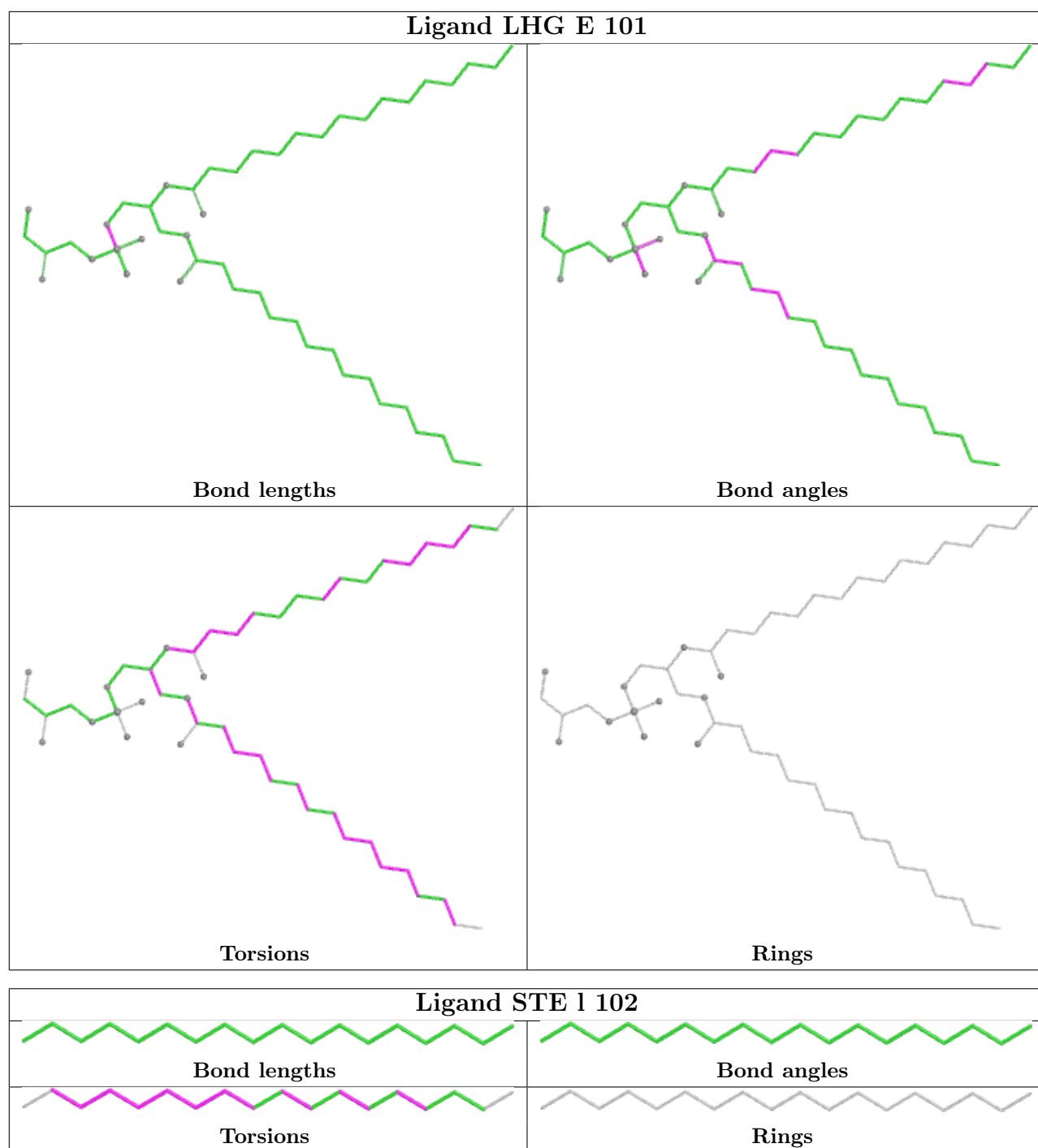


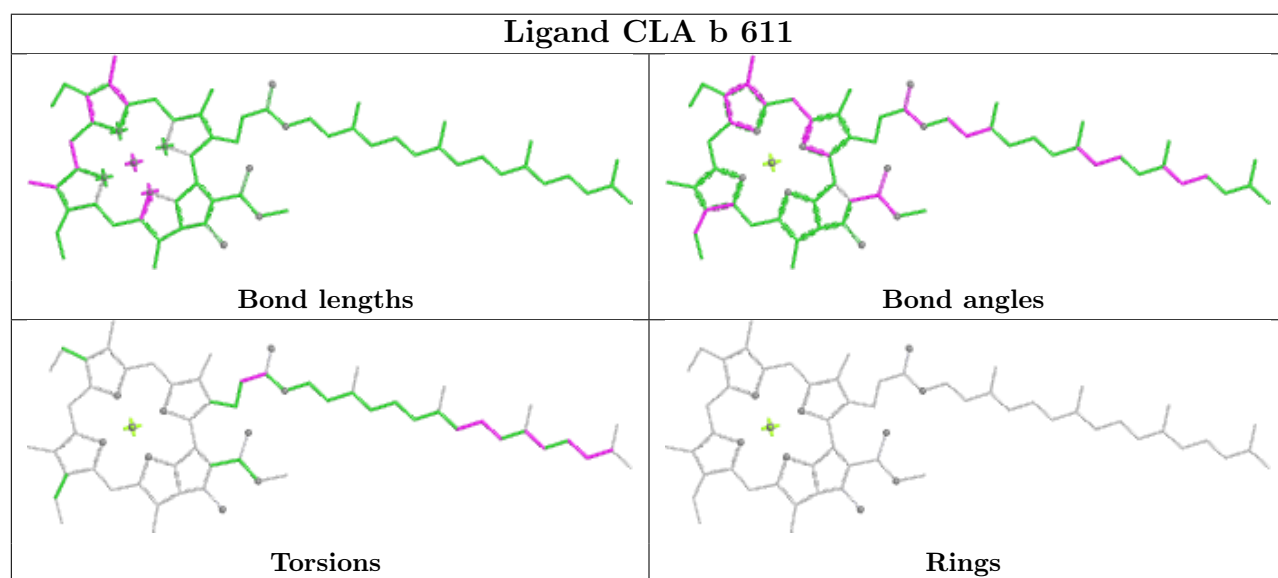
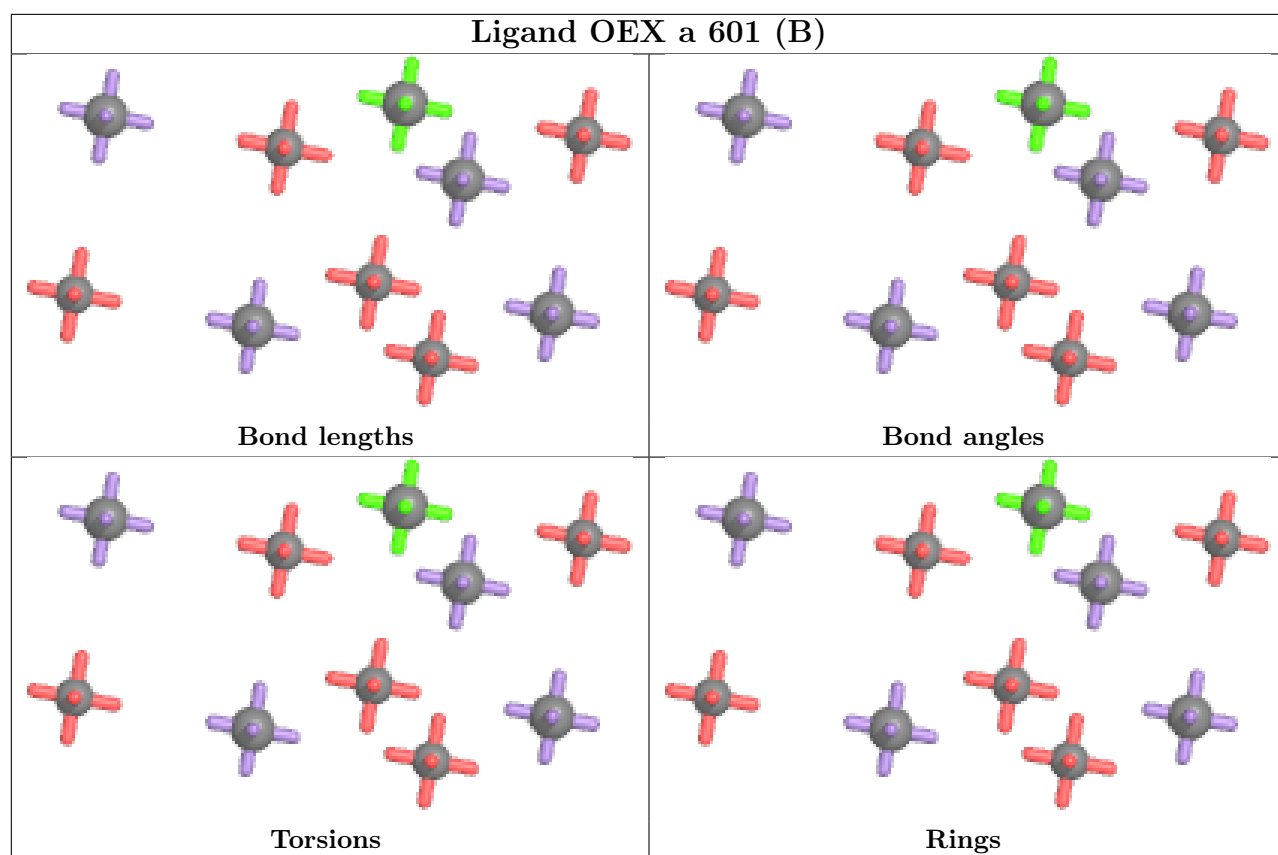




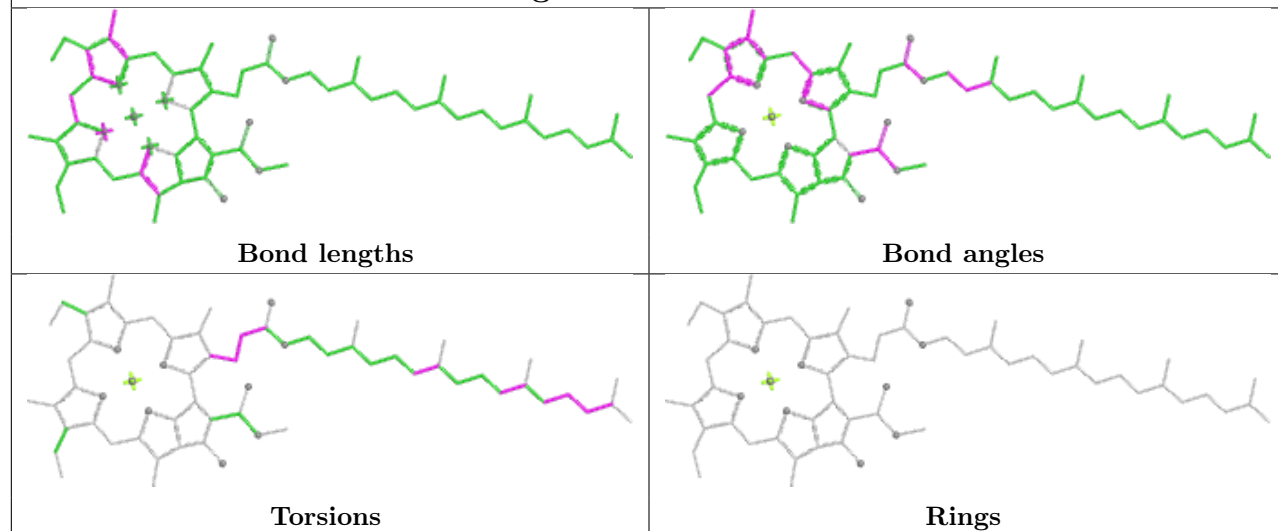
Ligand LMG c 522**Ligand CLA B 612****Ligand CLA C 506**



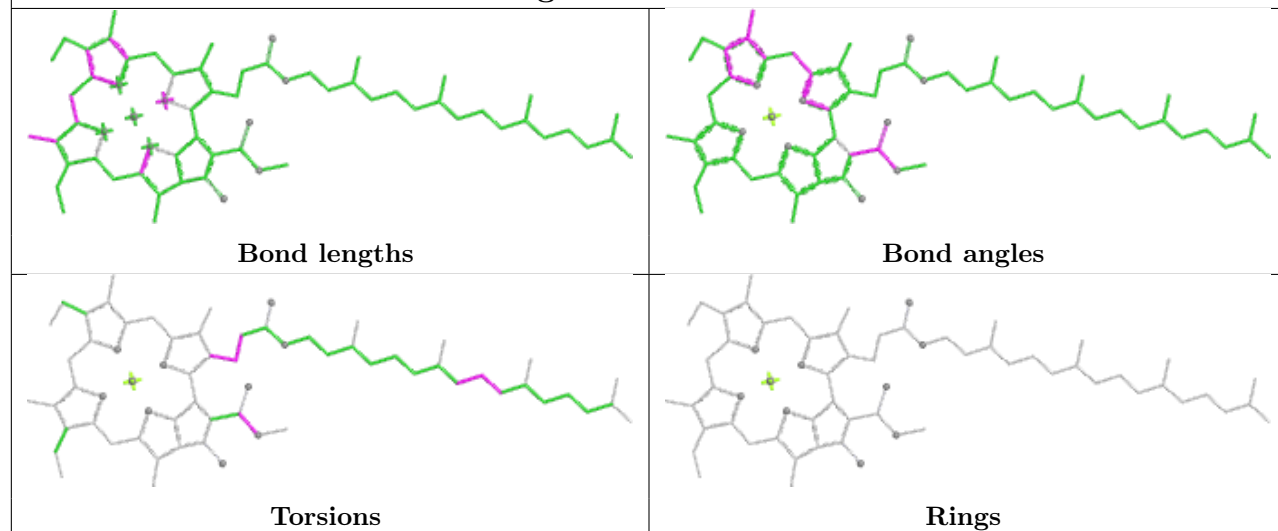




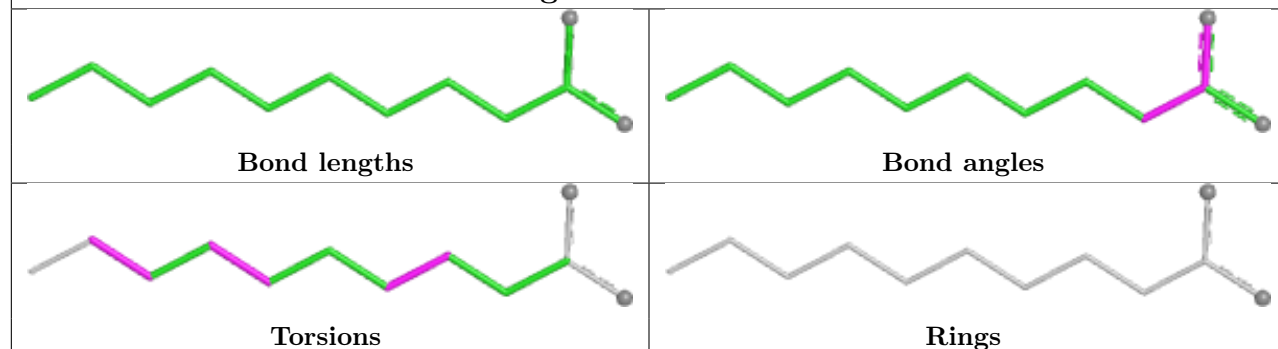
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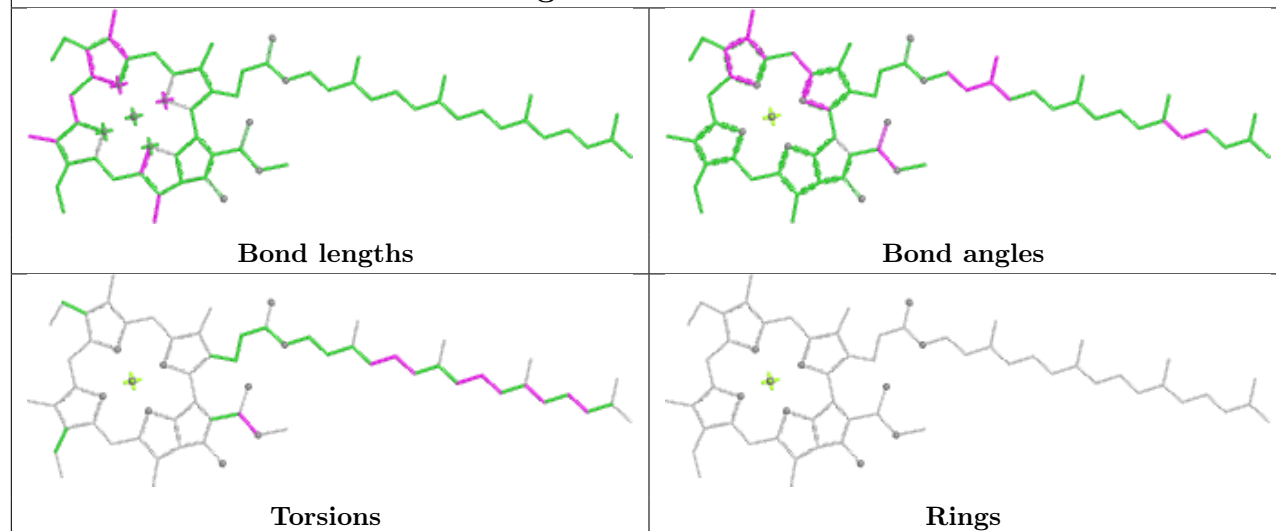
Ligand CLA c 513



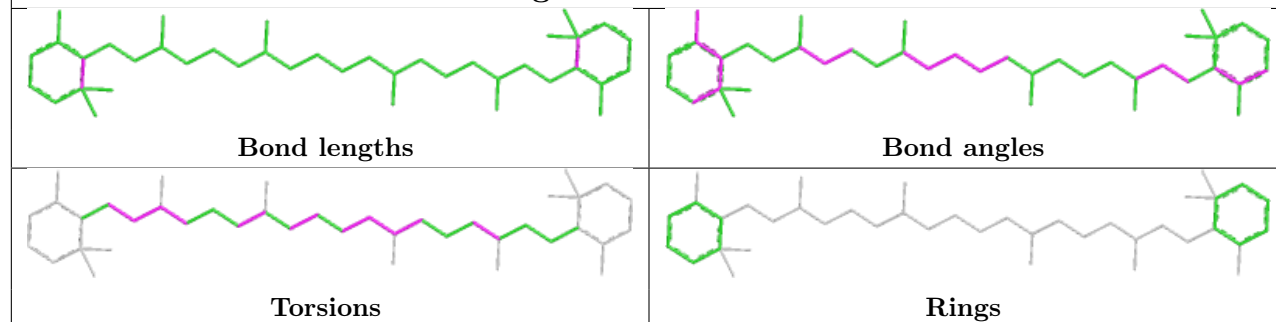
Ligand STE c 523



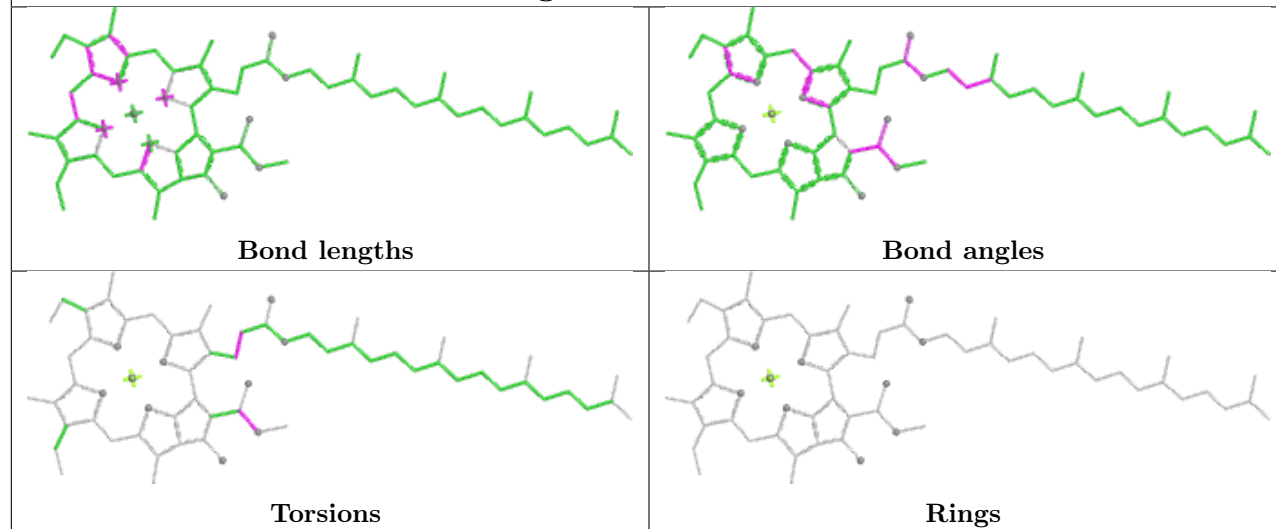
Ligand CLA c 510

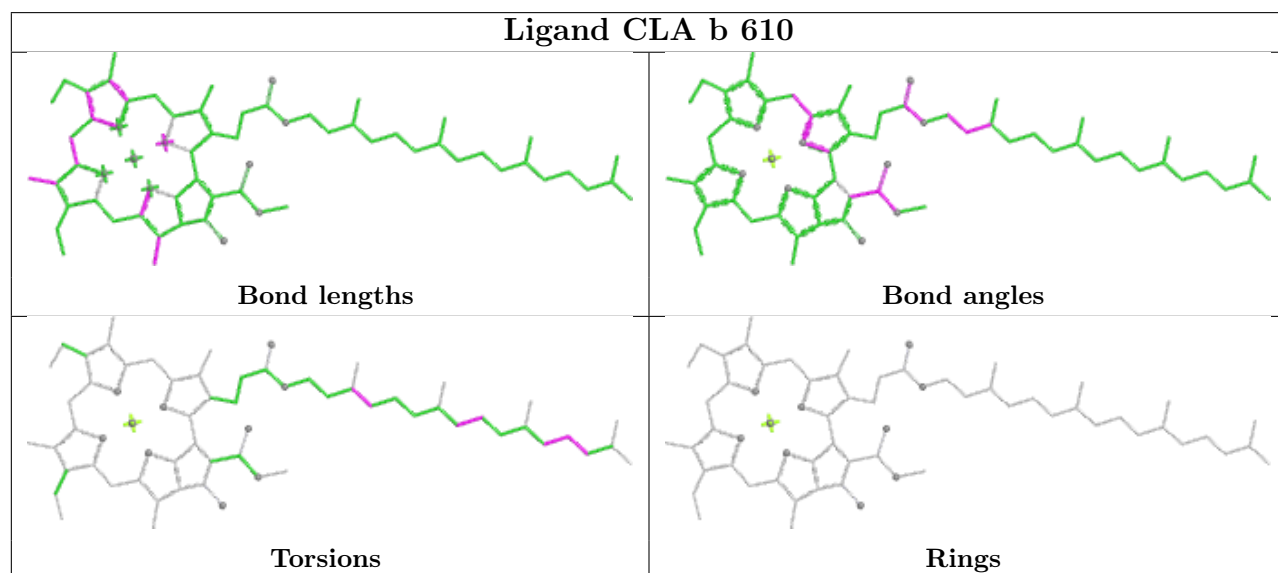
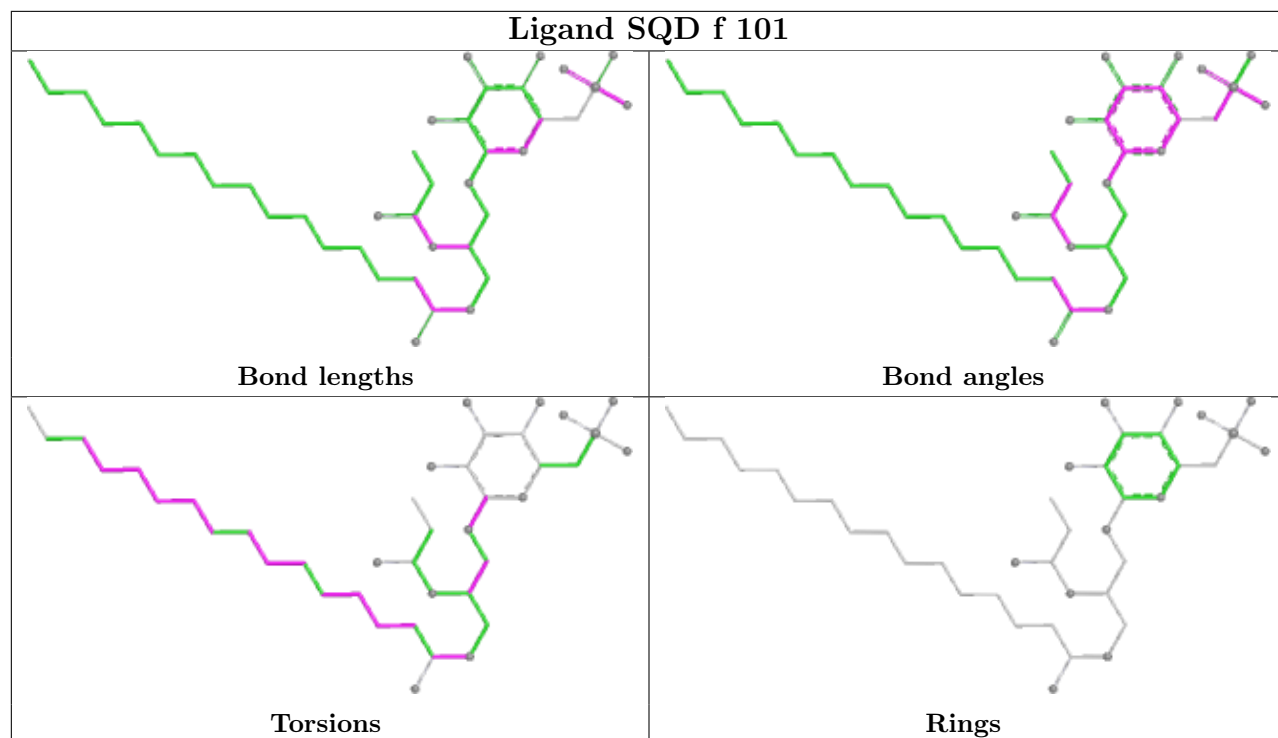


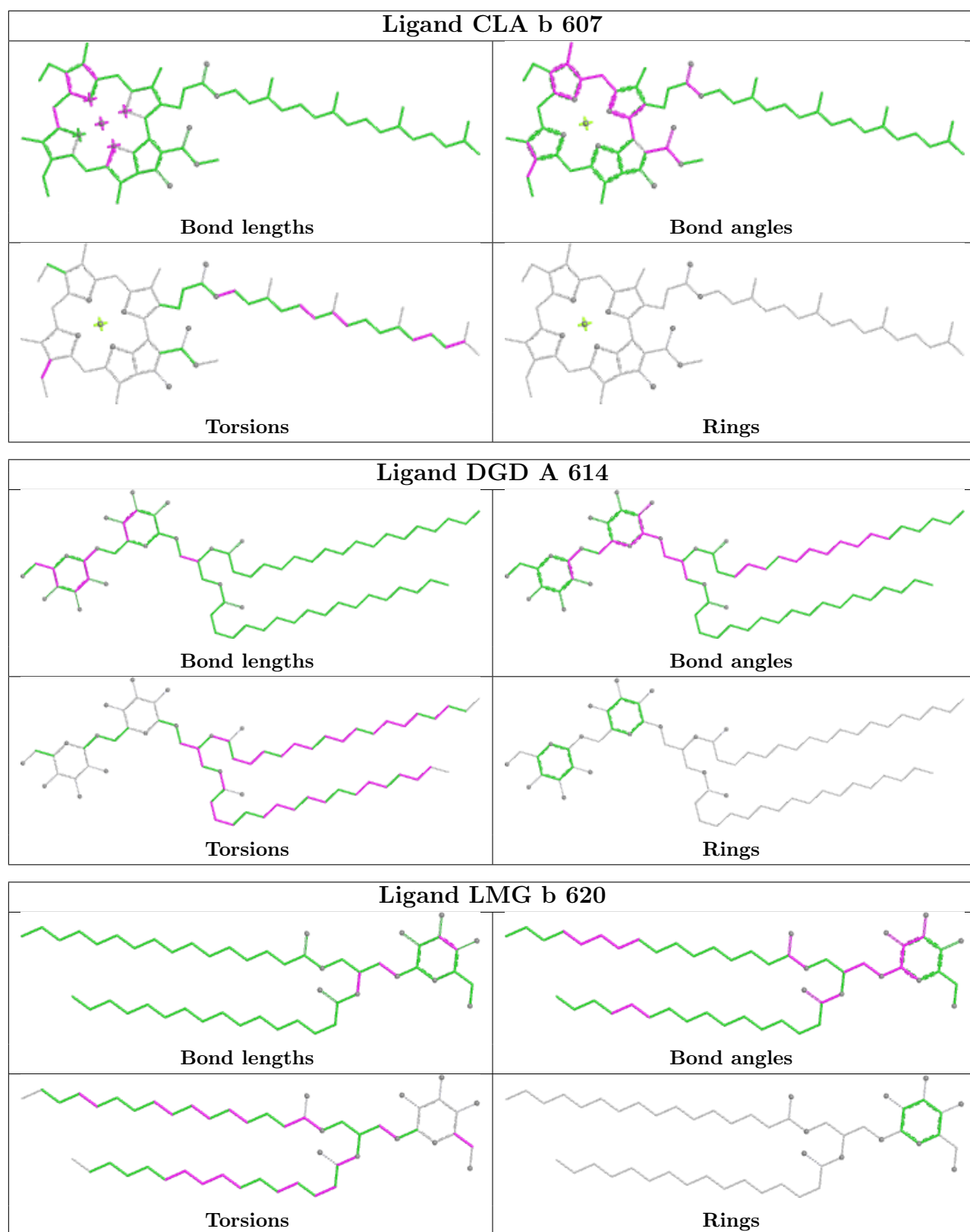
Ligand BCR Z 101

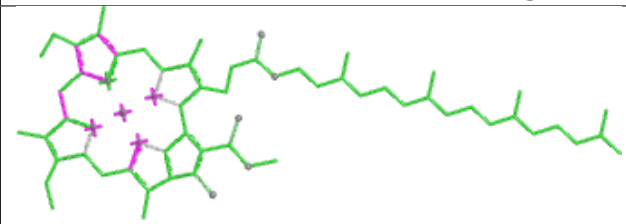
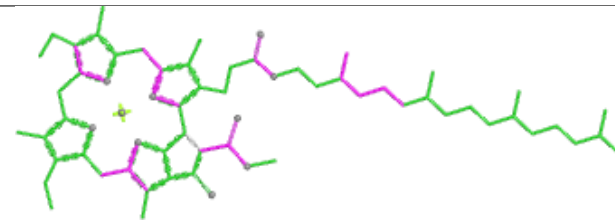
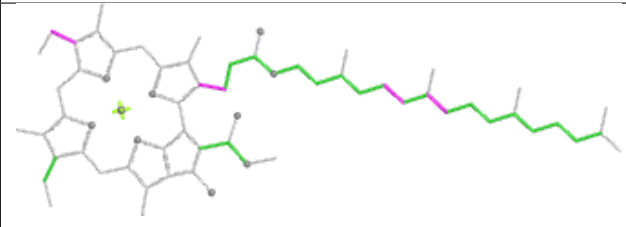
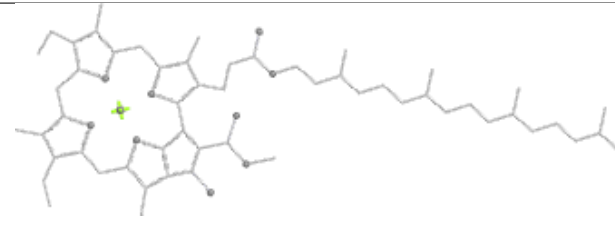


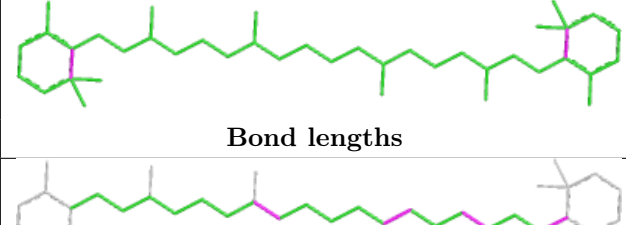
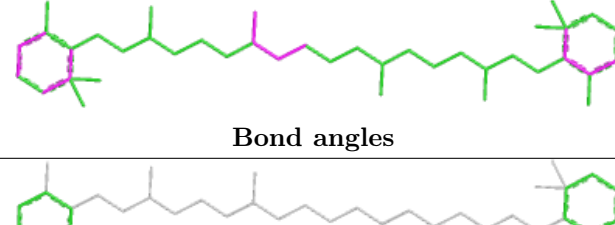
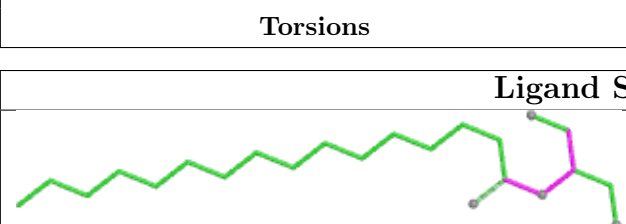
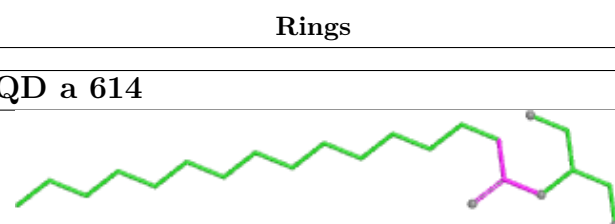
Ligand CLA c 501

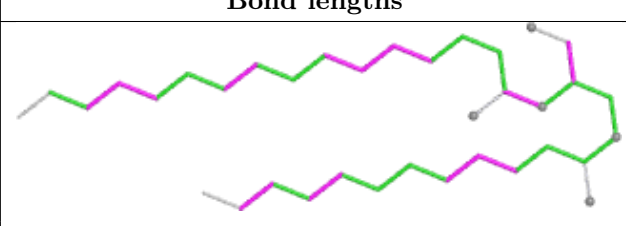
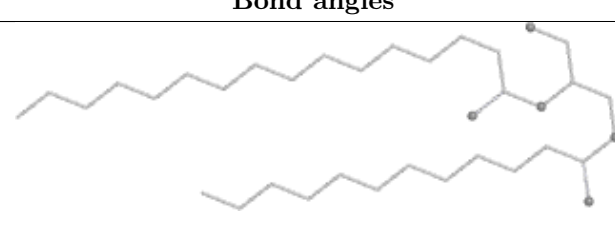


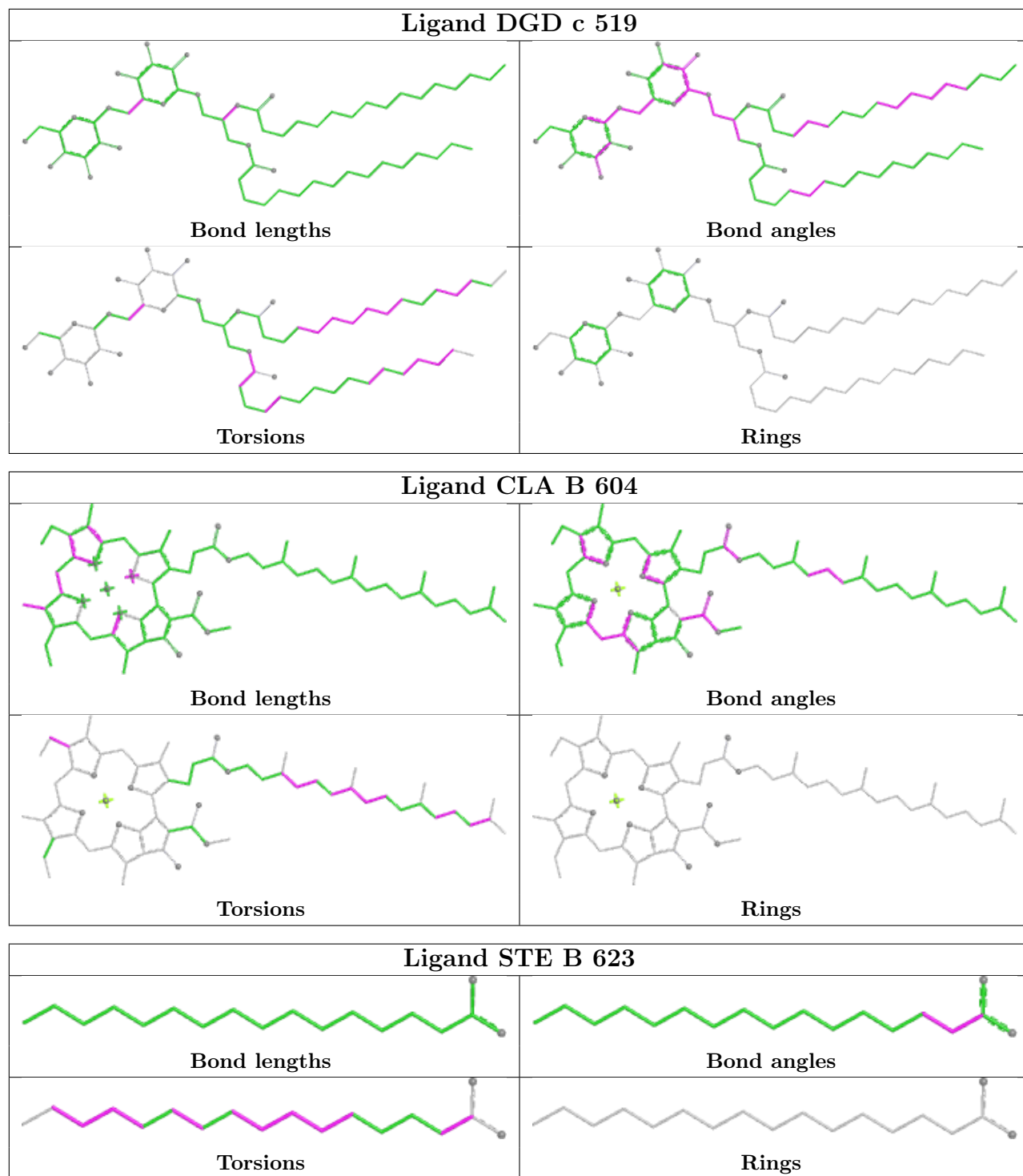


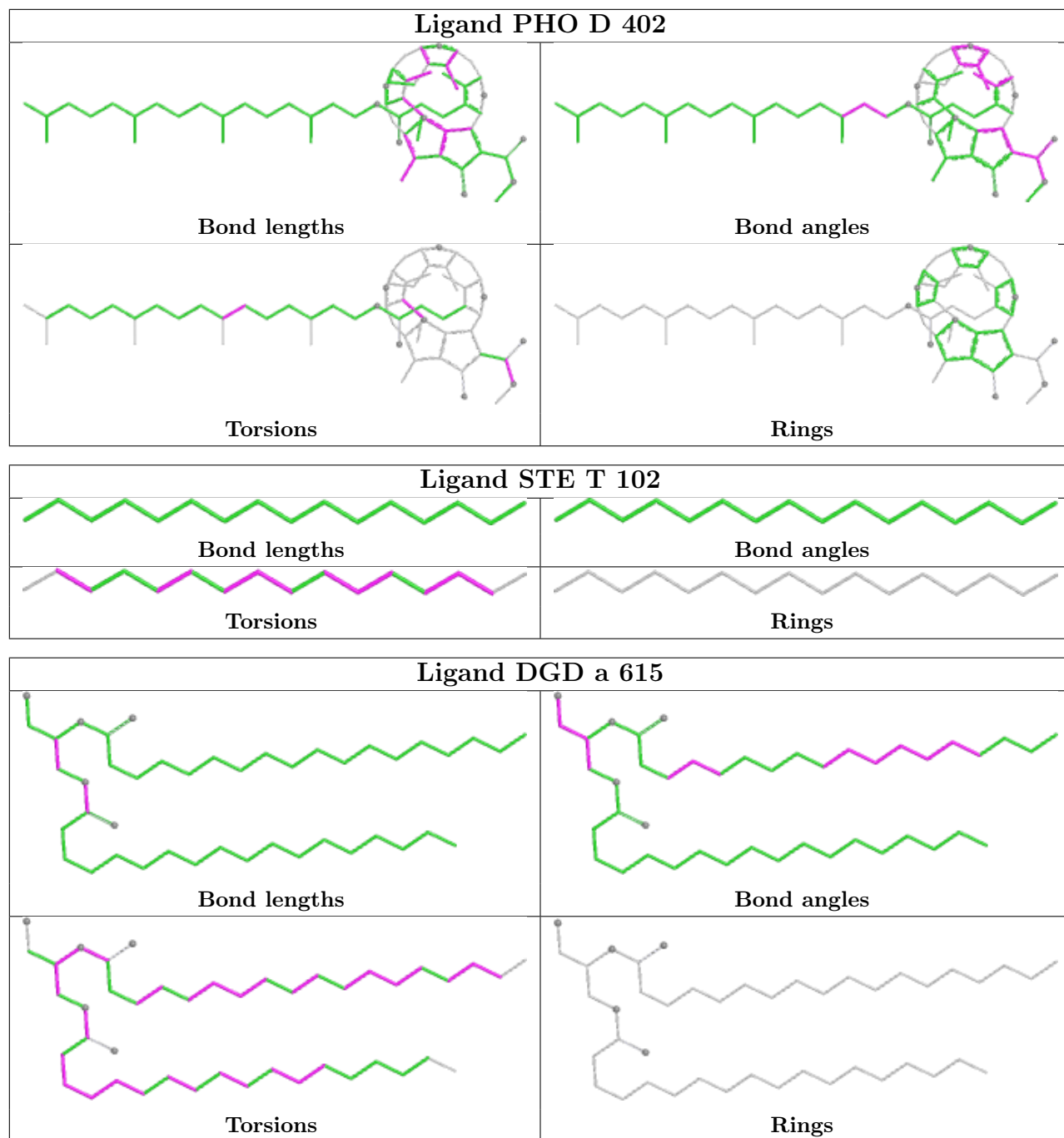


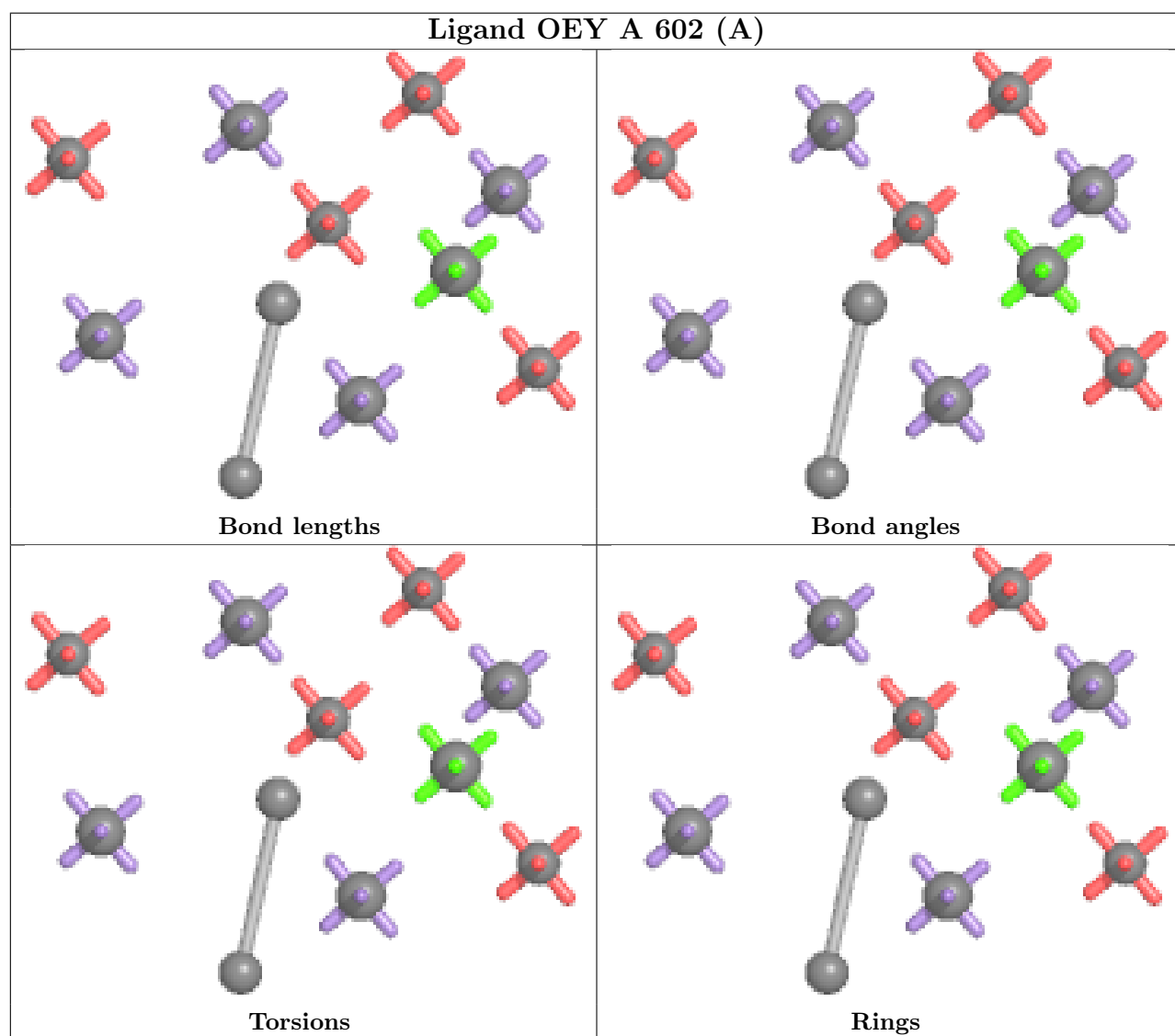
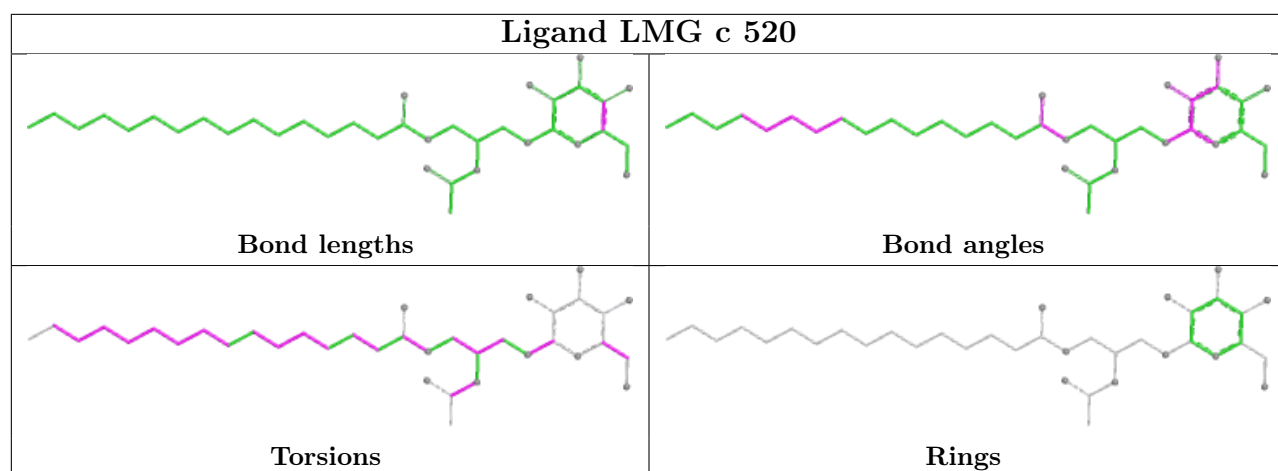
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

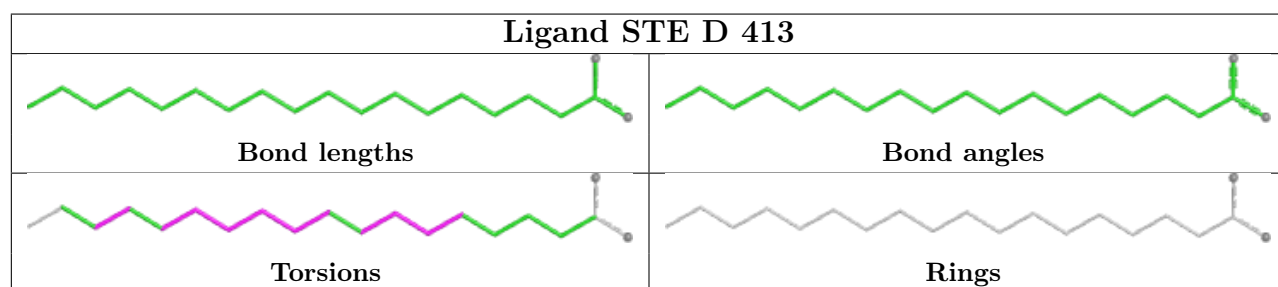
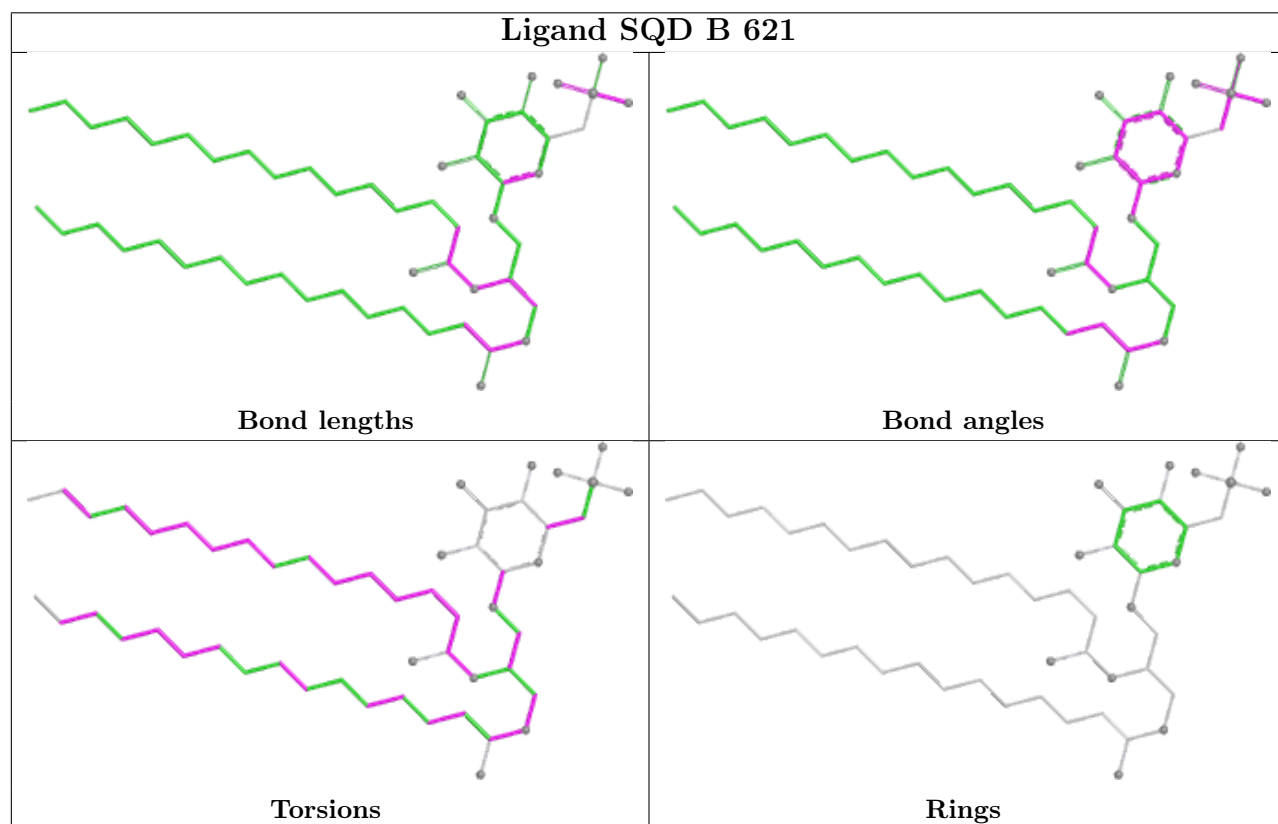
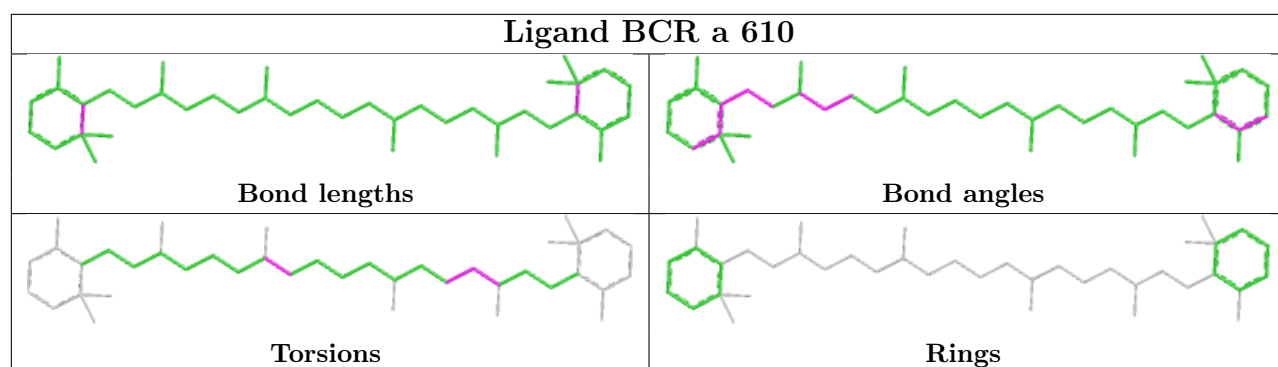
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SQD a 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

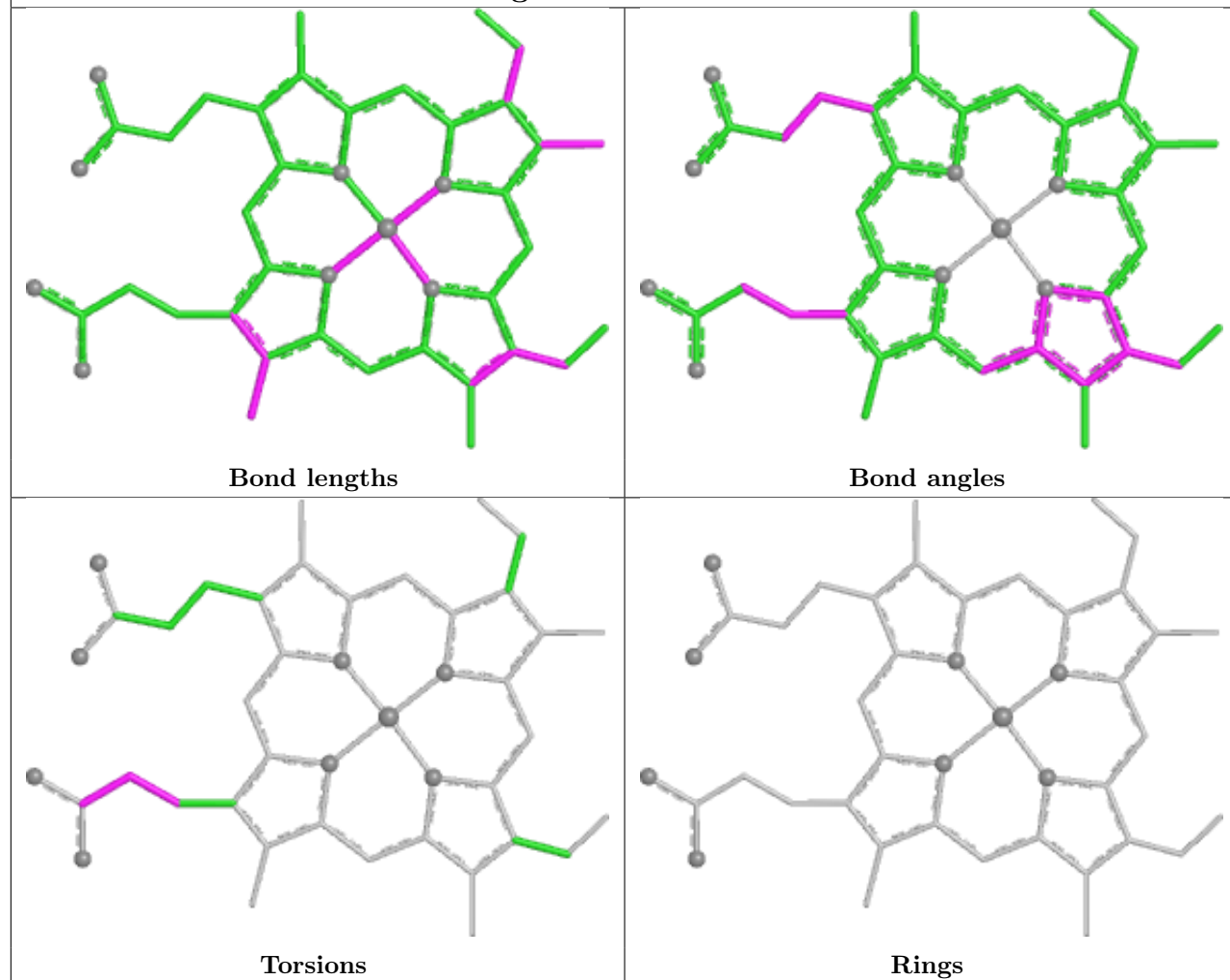




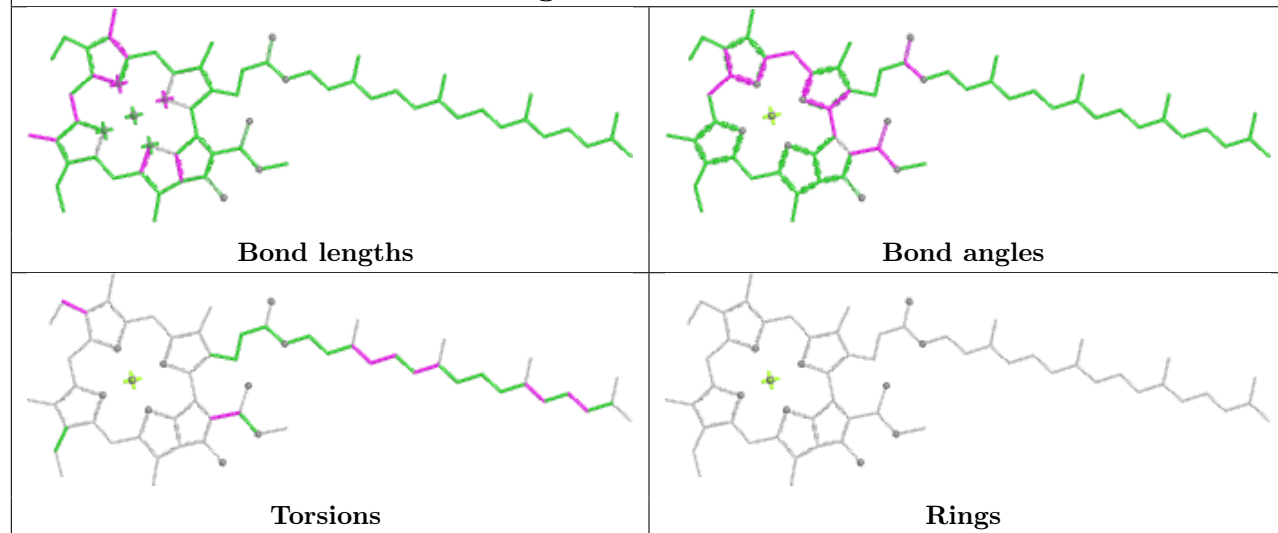




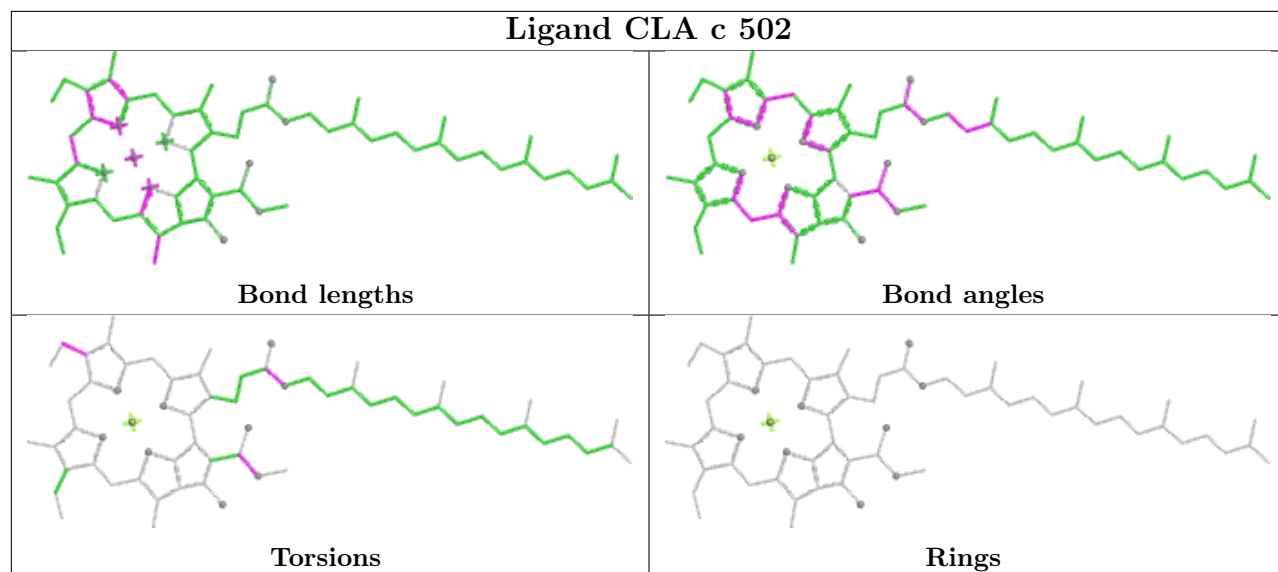
Ligand HEM e 101



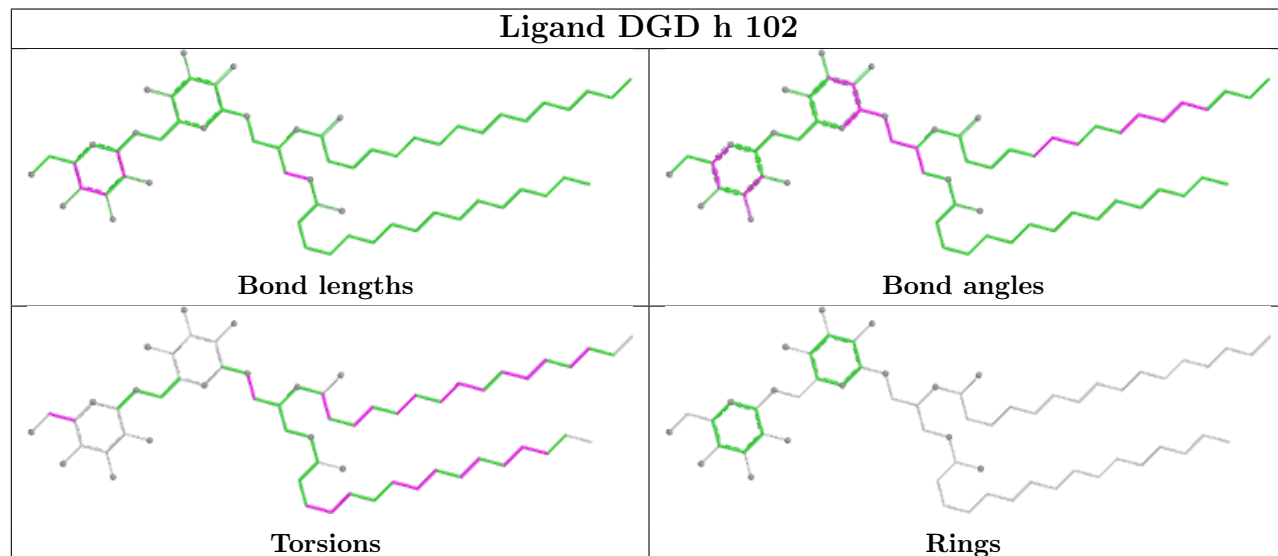
Ligand CLA c 507



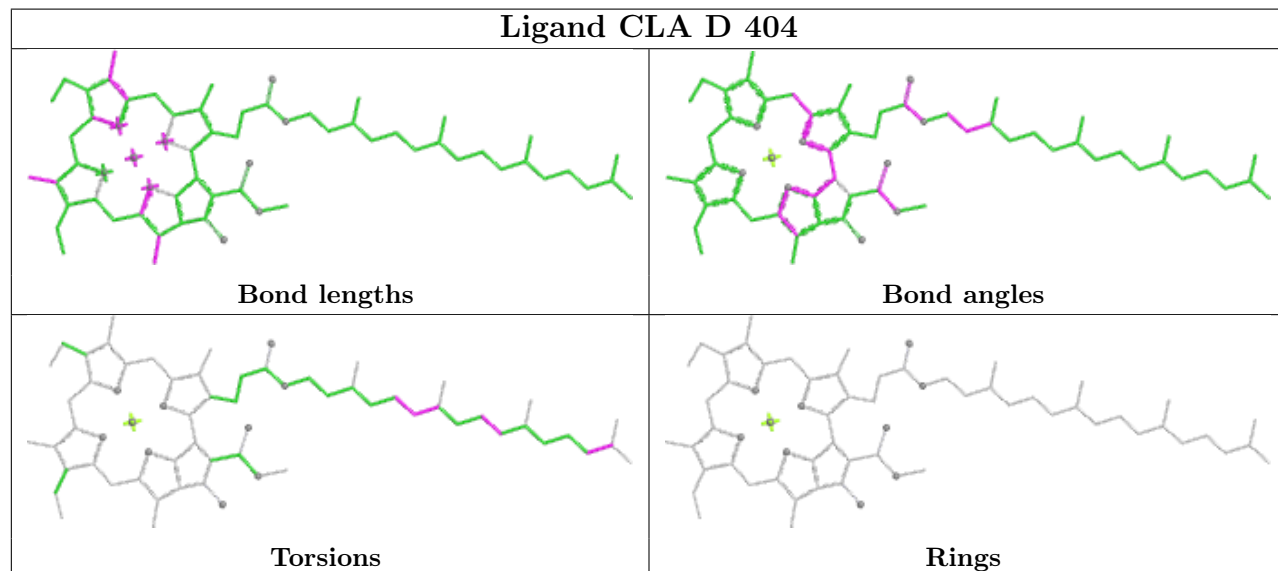
Ligand CLA c 502

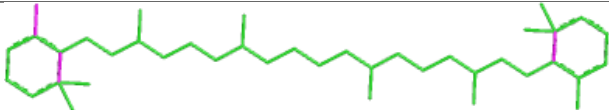
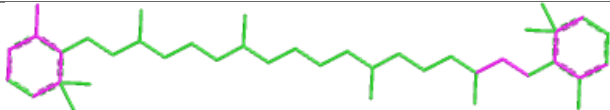
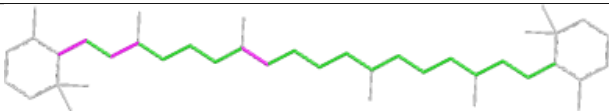
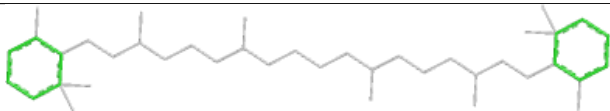


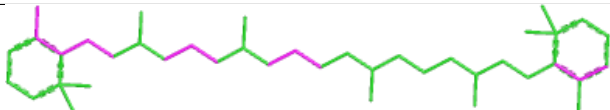
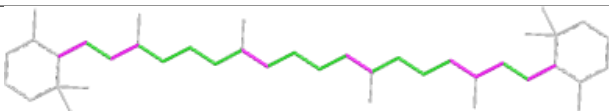
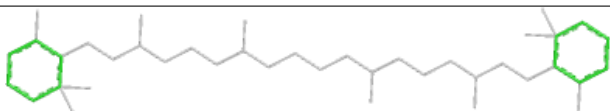
Ligand DGD h 102

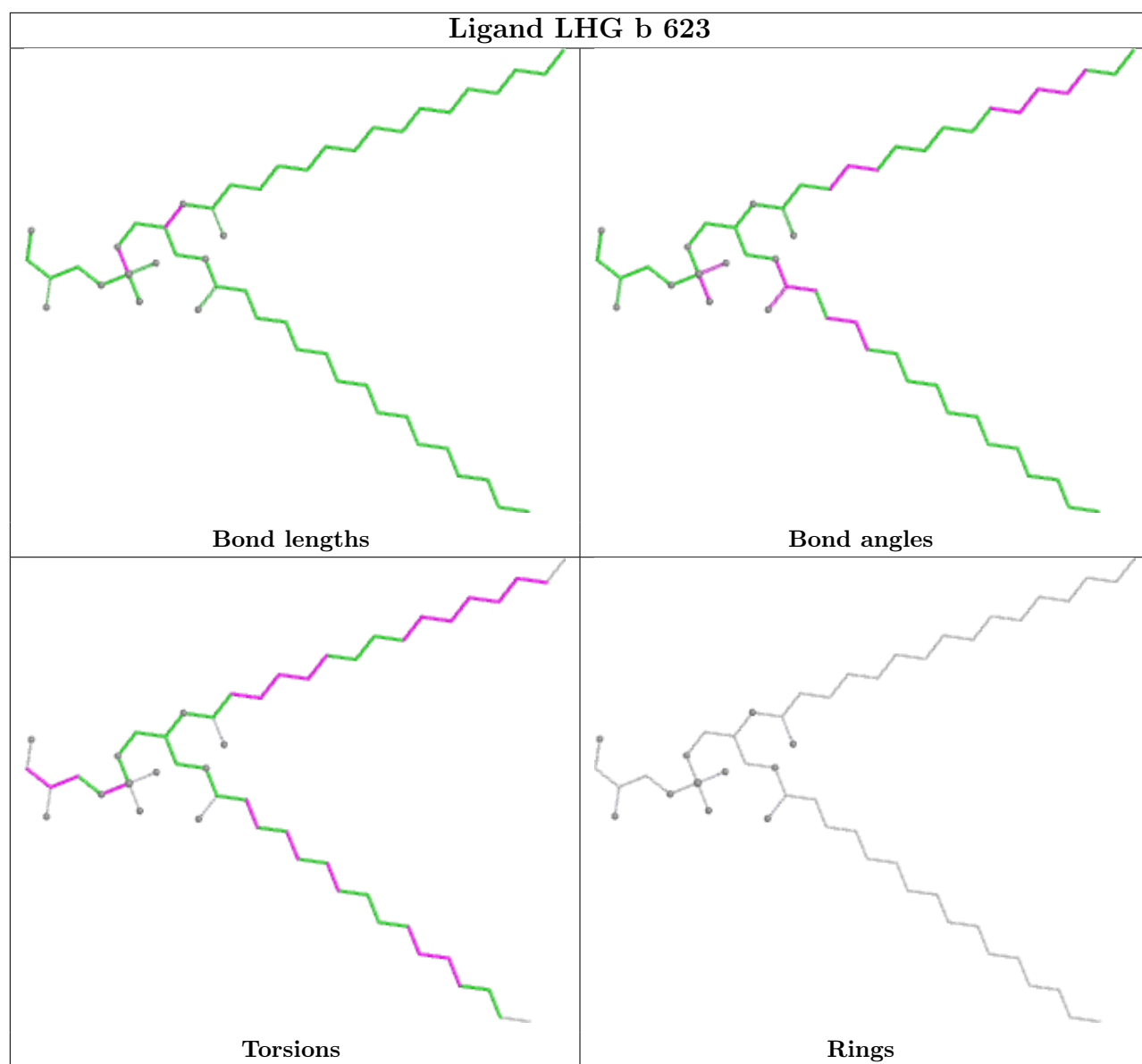


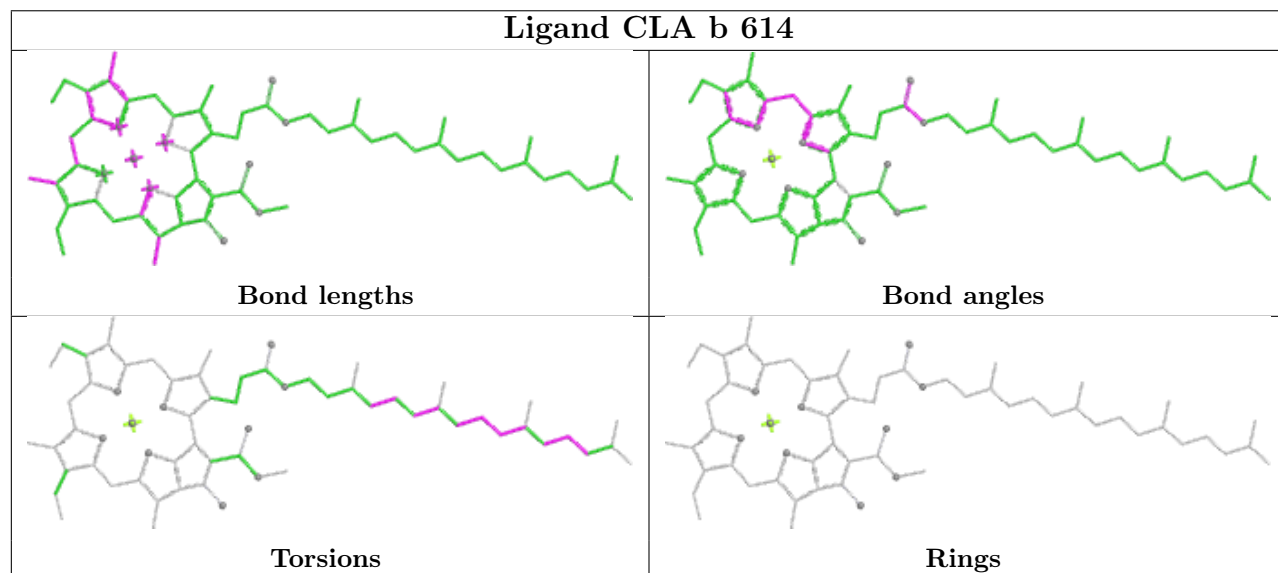
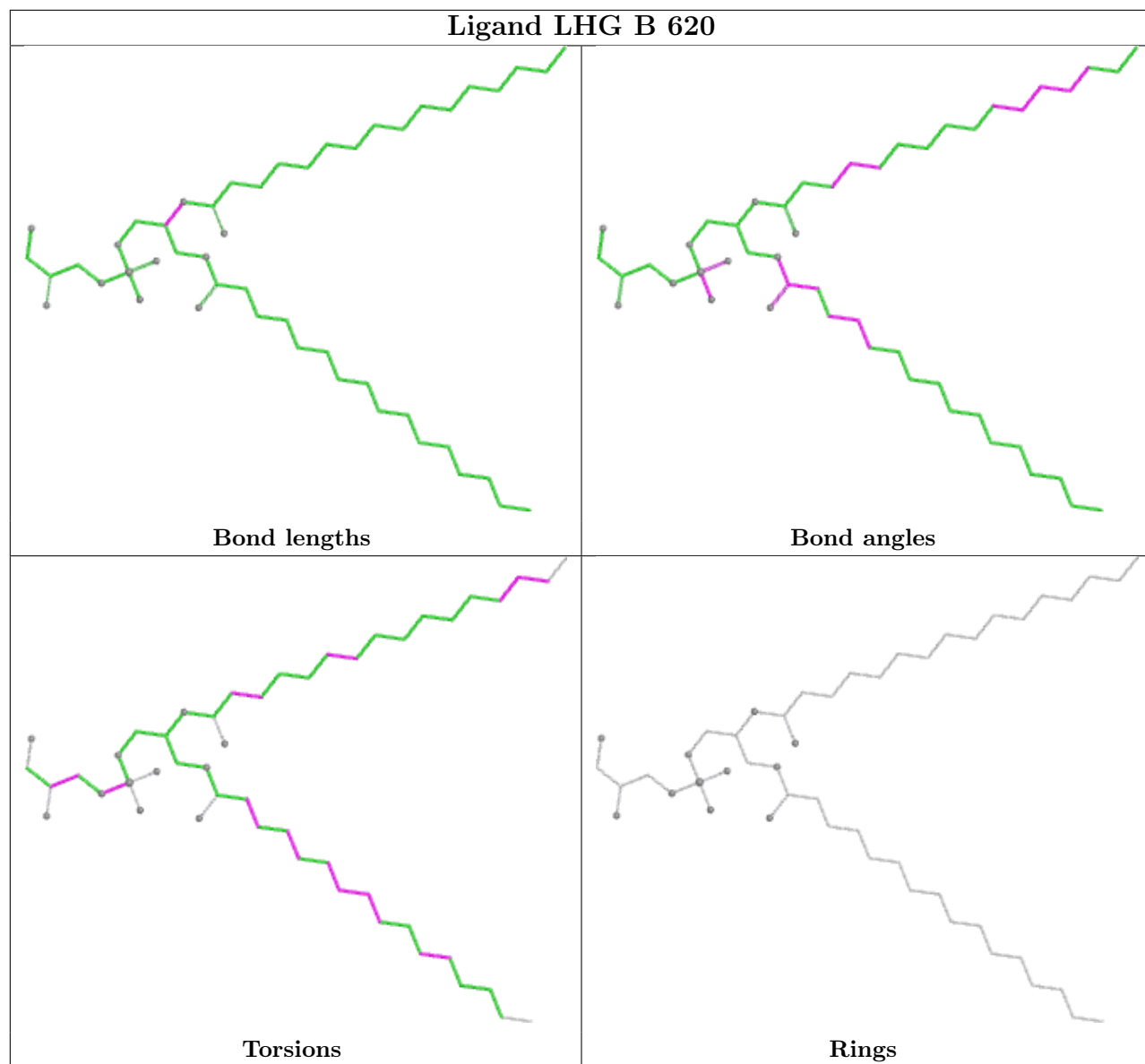
Ligand CLA D 404

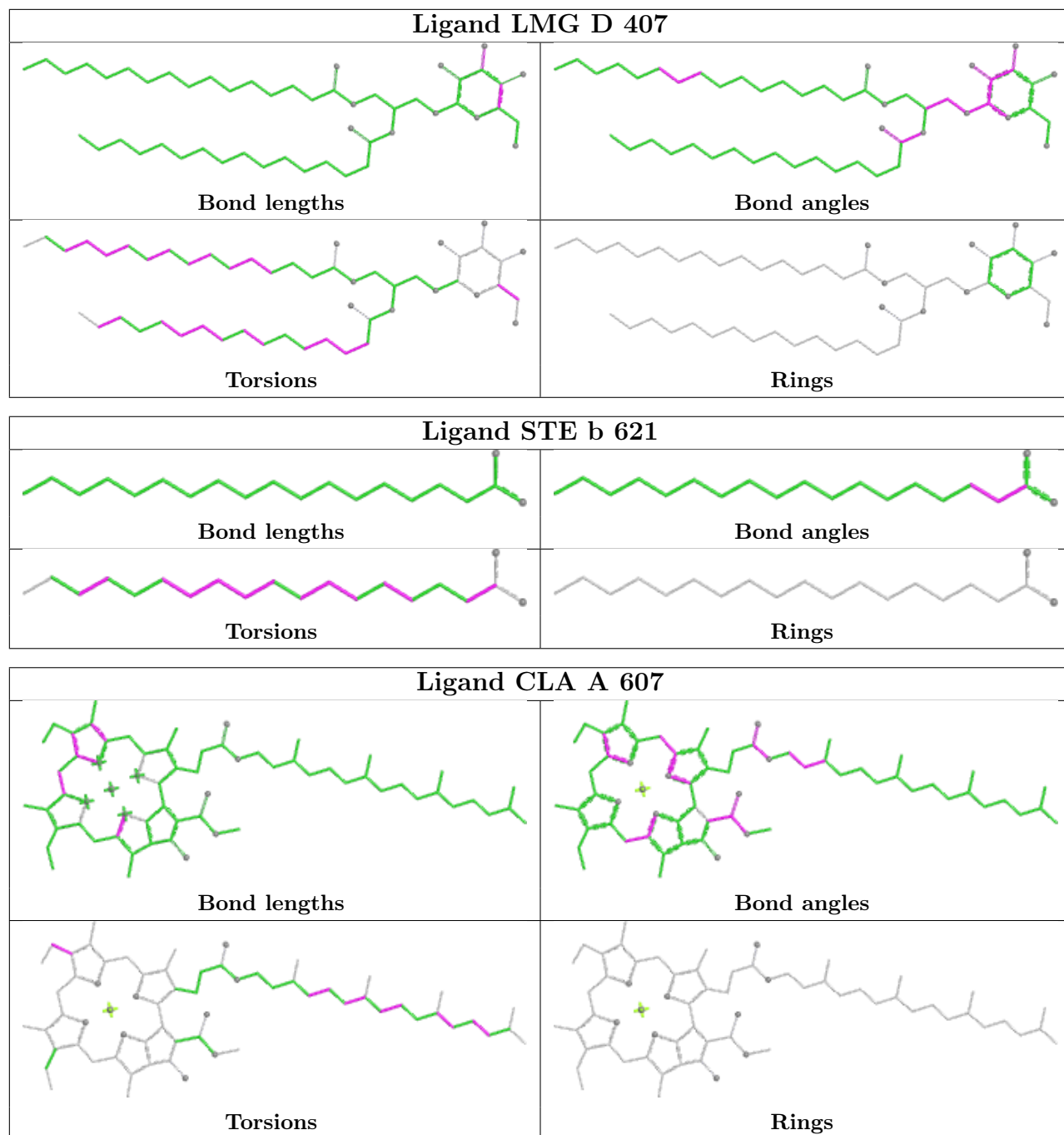


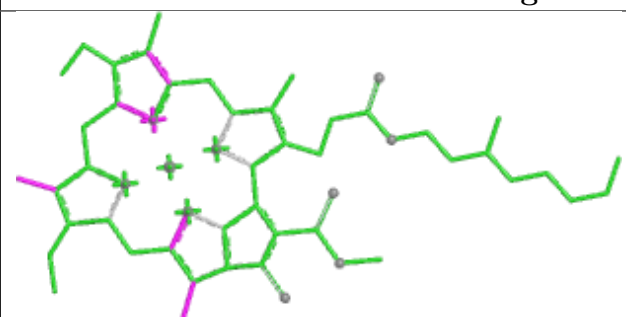
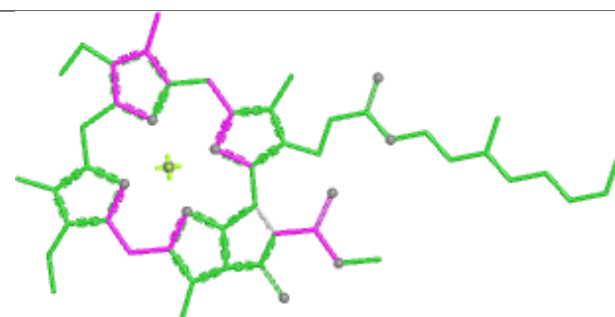
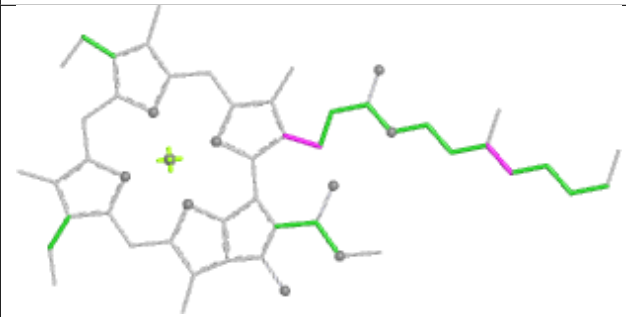
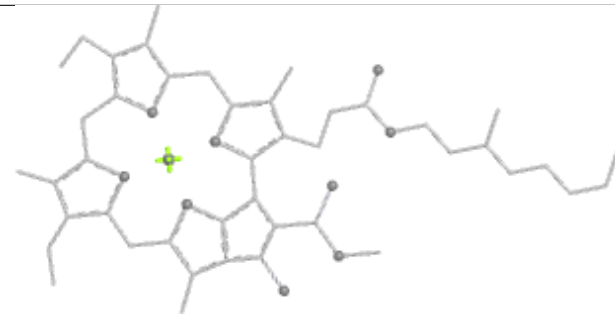
Ligand BCR B 616	
	Bond lengths
	Bond angles
	Torsions
	Rings

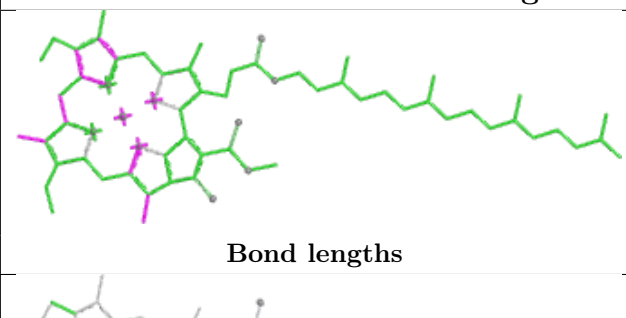
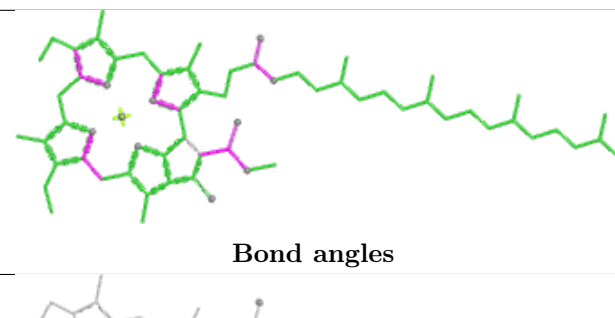
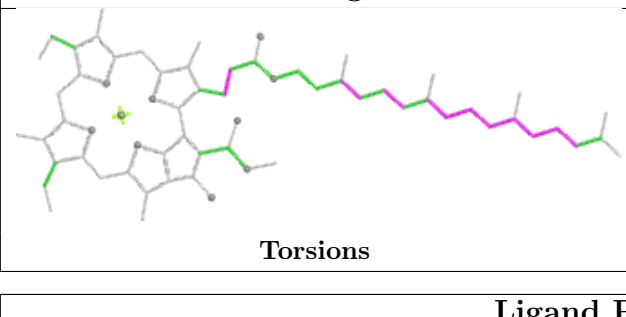
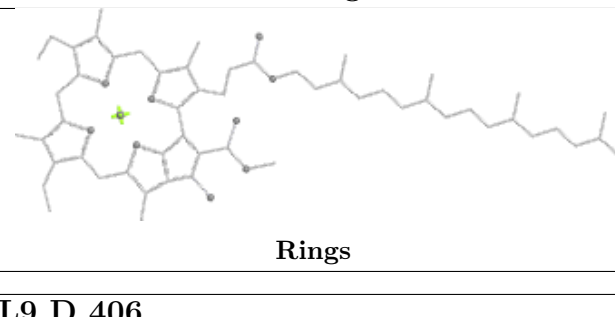
Ligand BCR Y 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

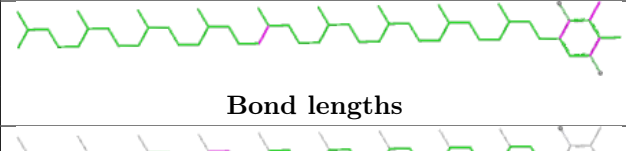
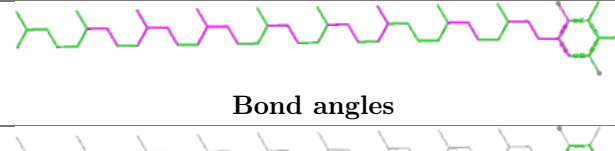
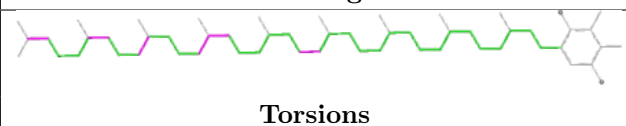
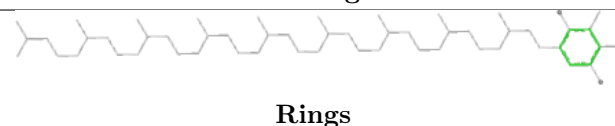


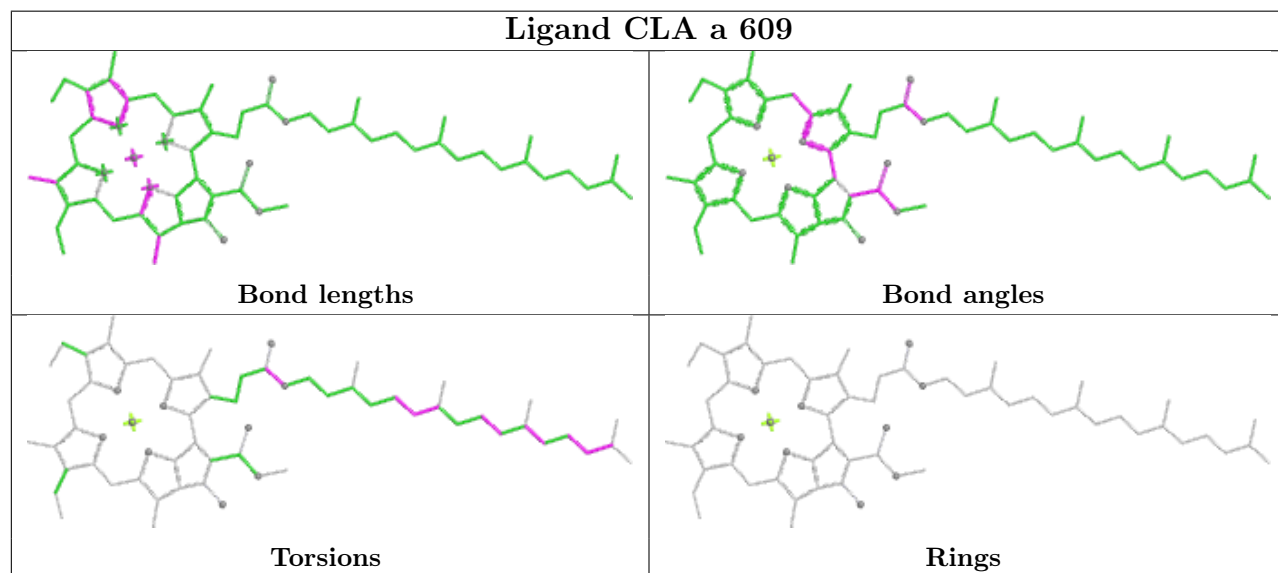
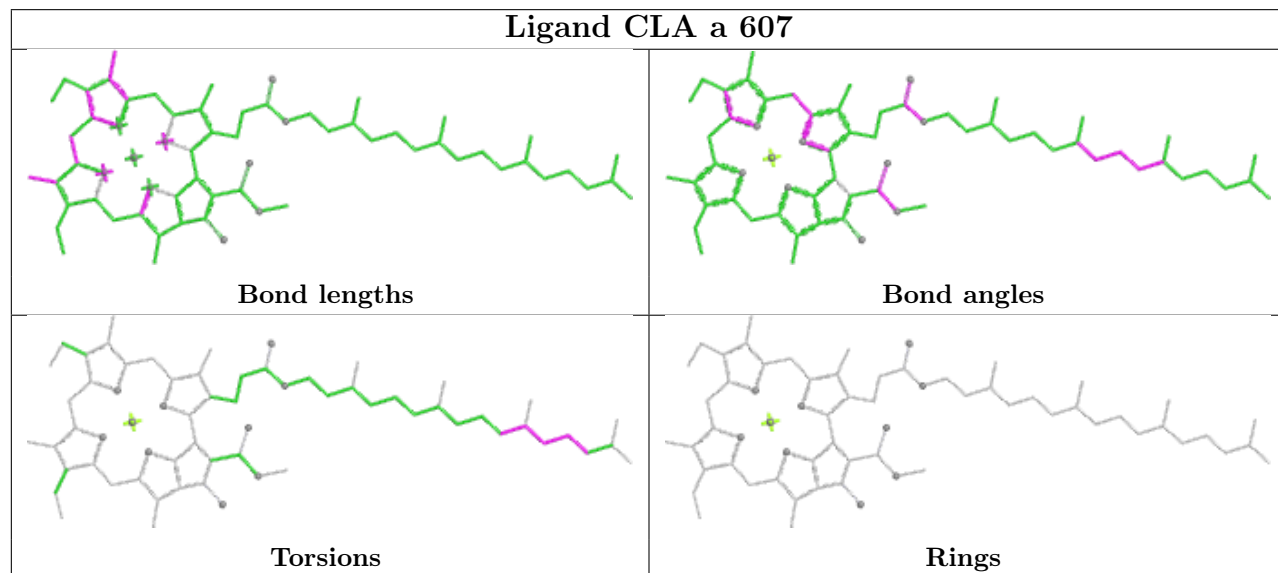
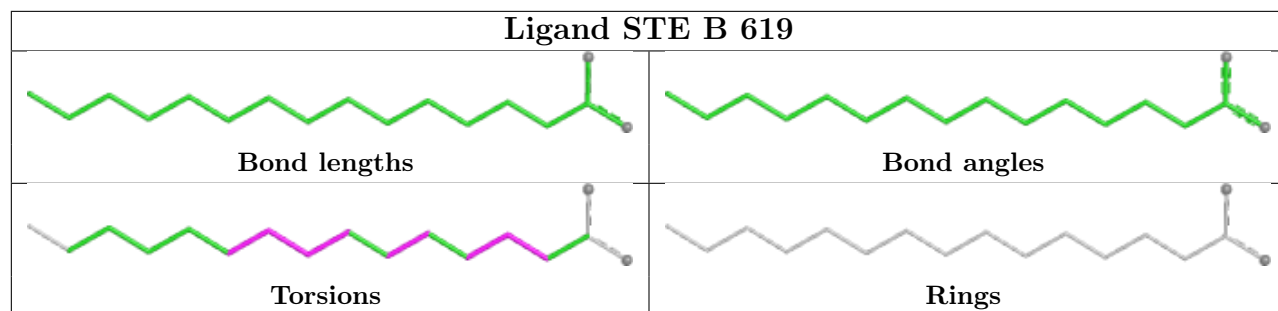




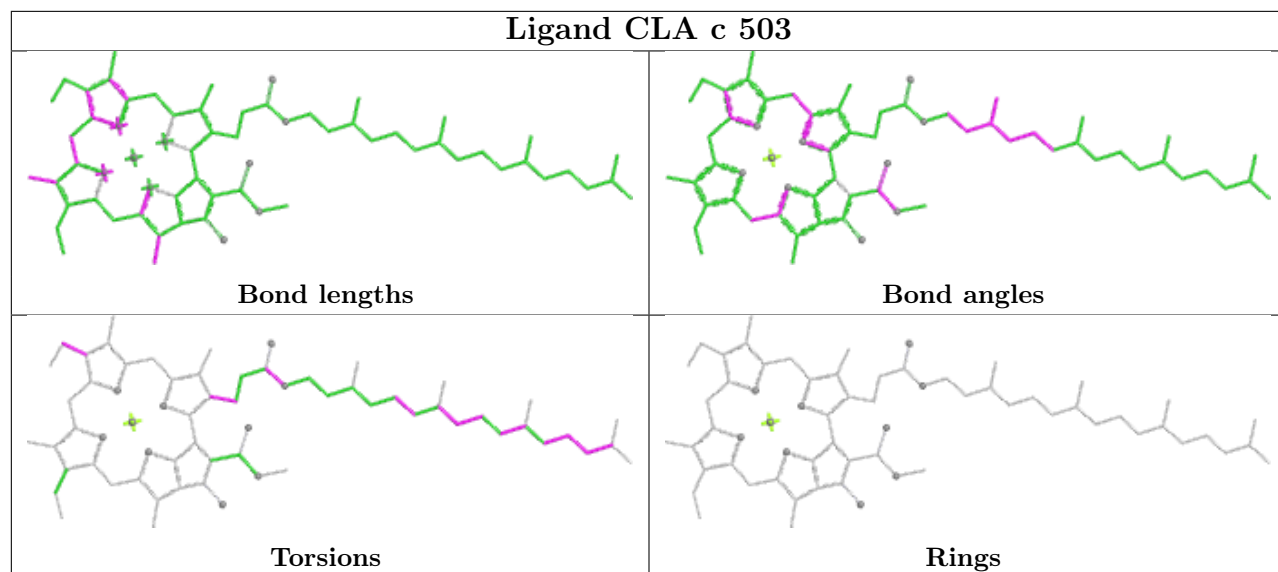
Ligand CLA A 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

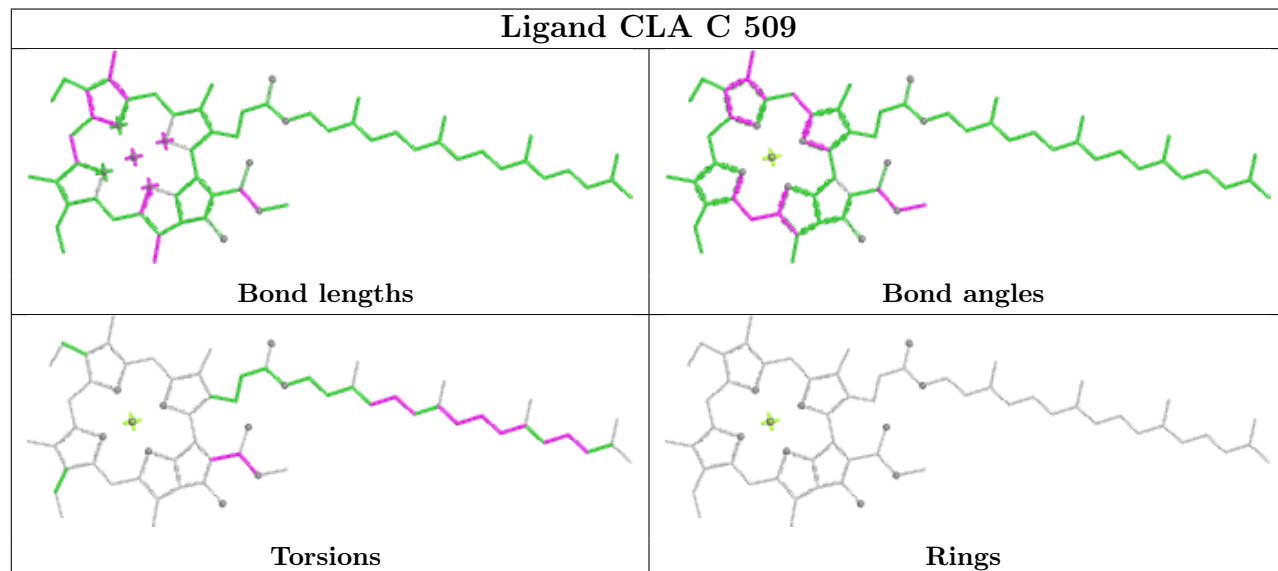
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings



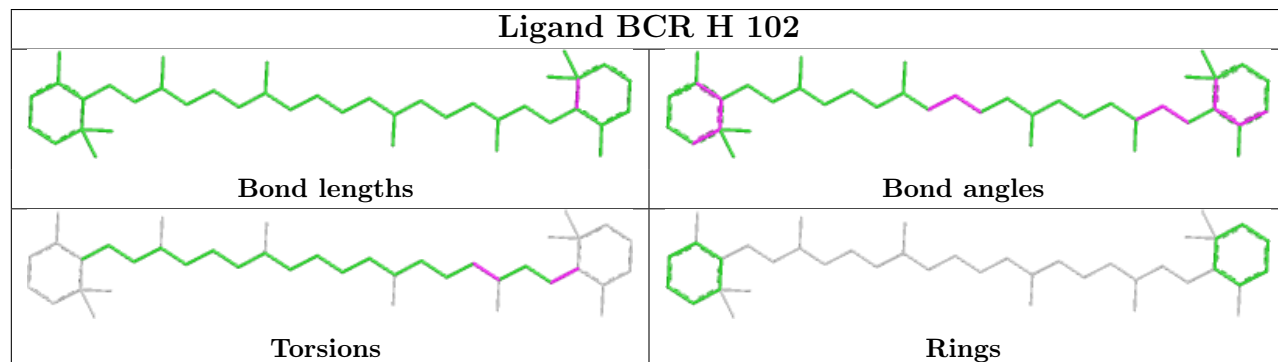
Ligand CLA c 503

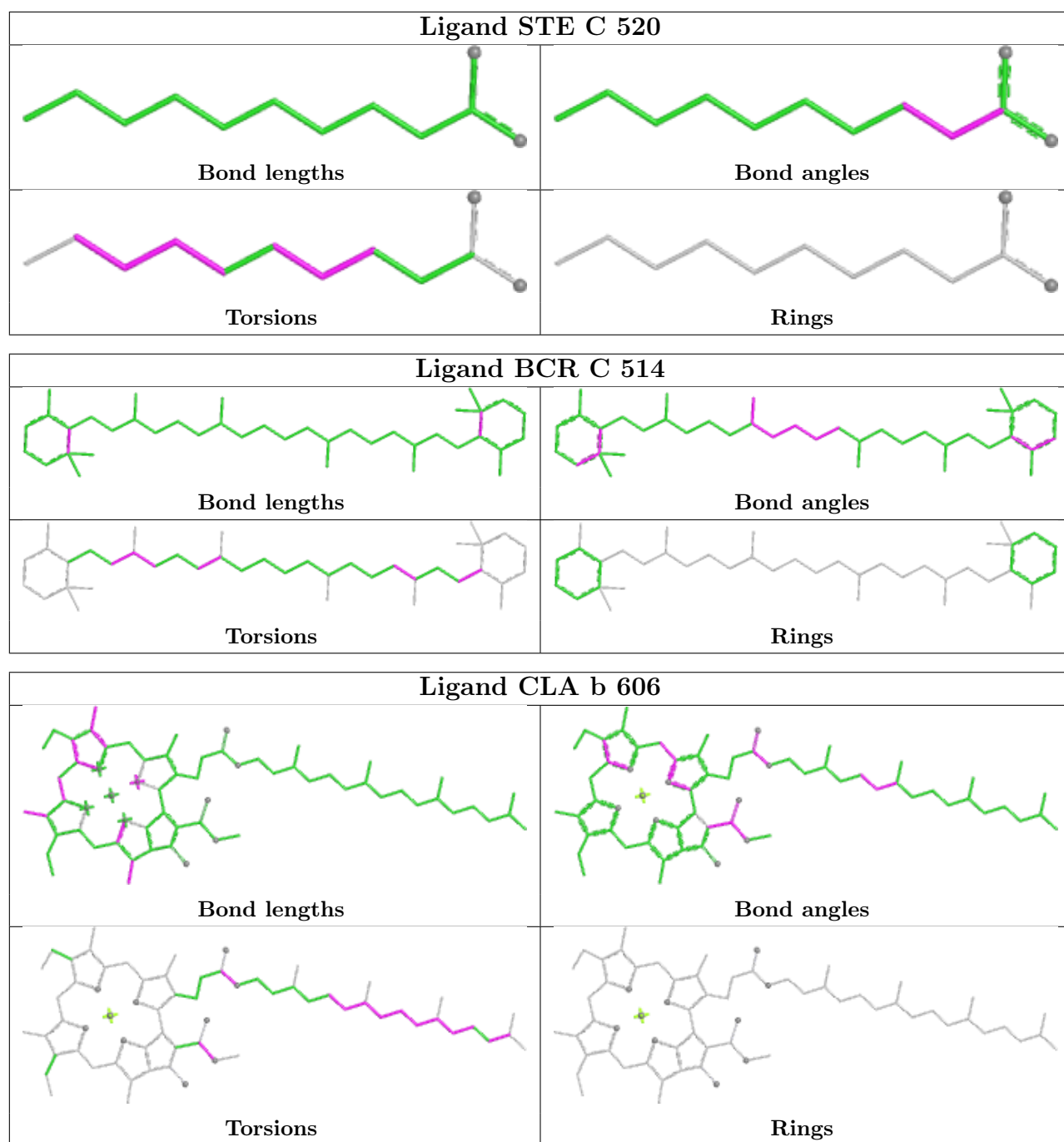


Ligand CLA C 509

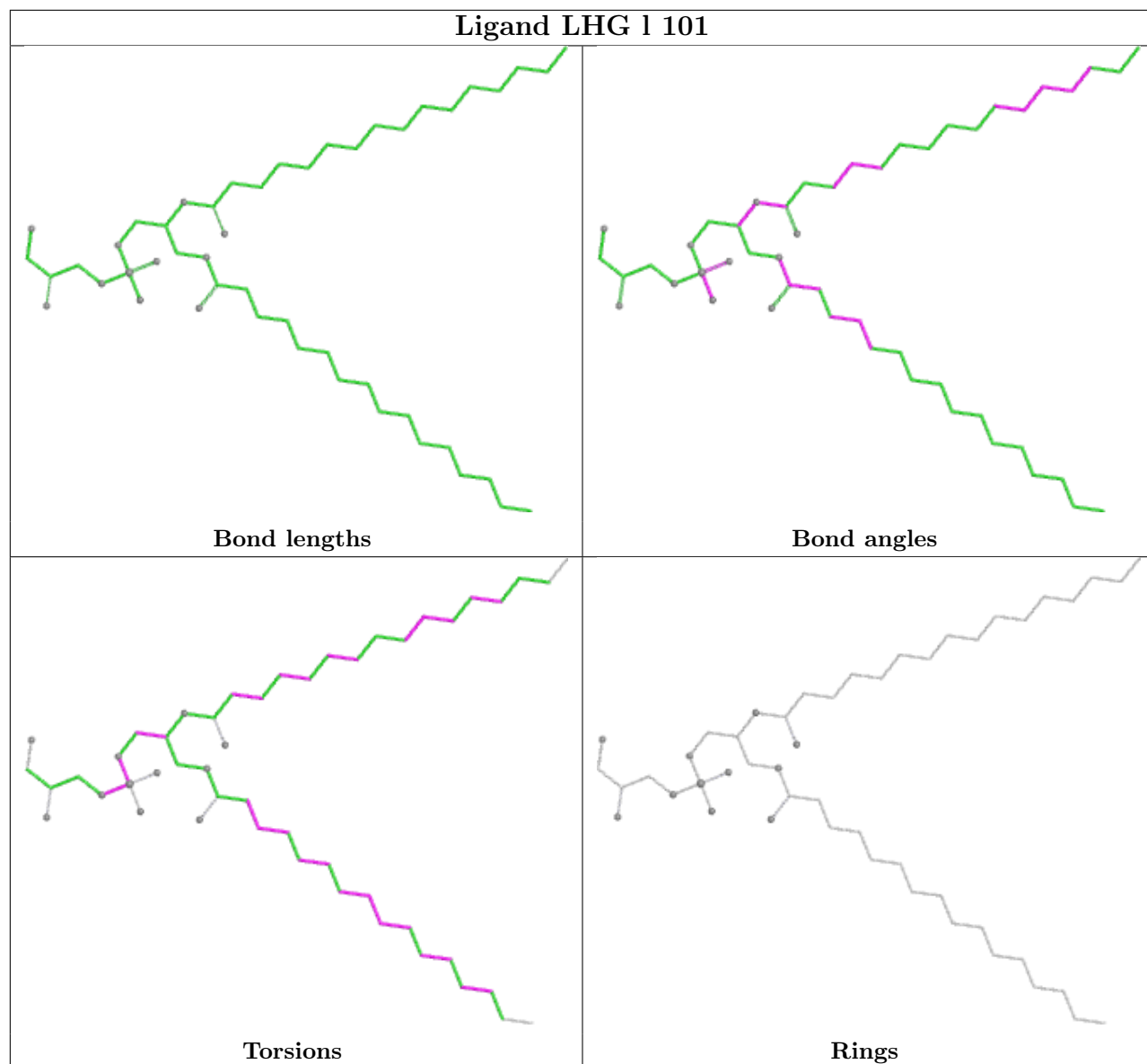


Ligand BCR H 102

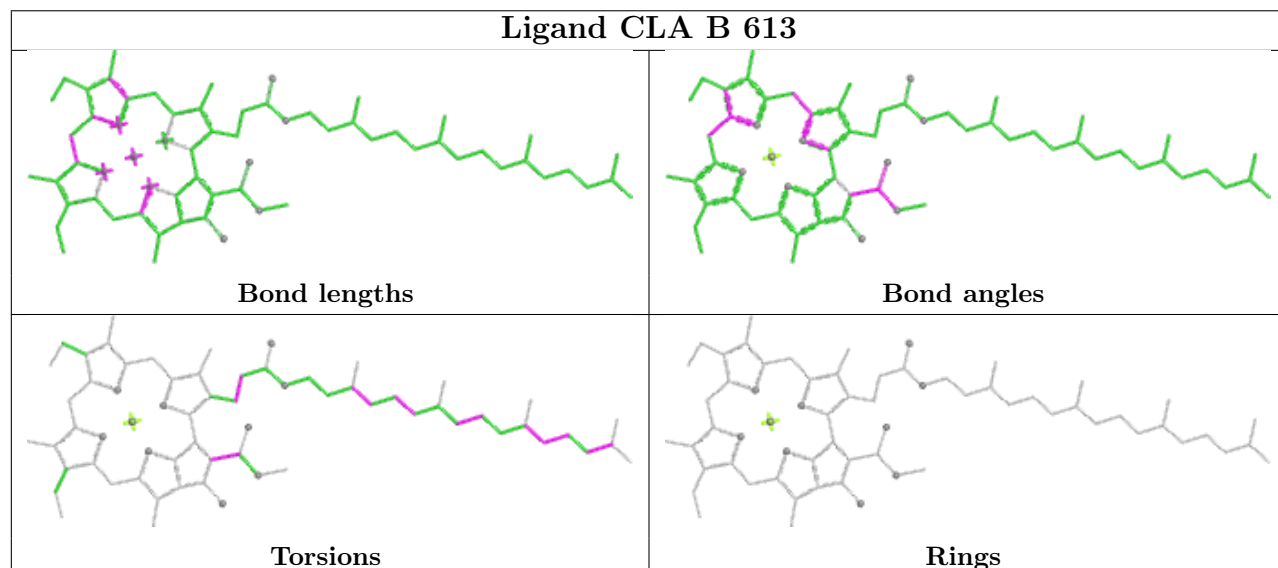


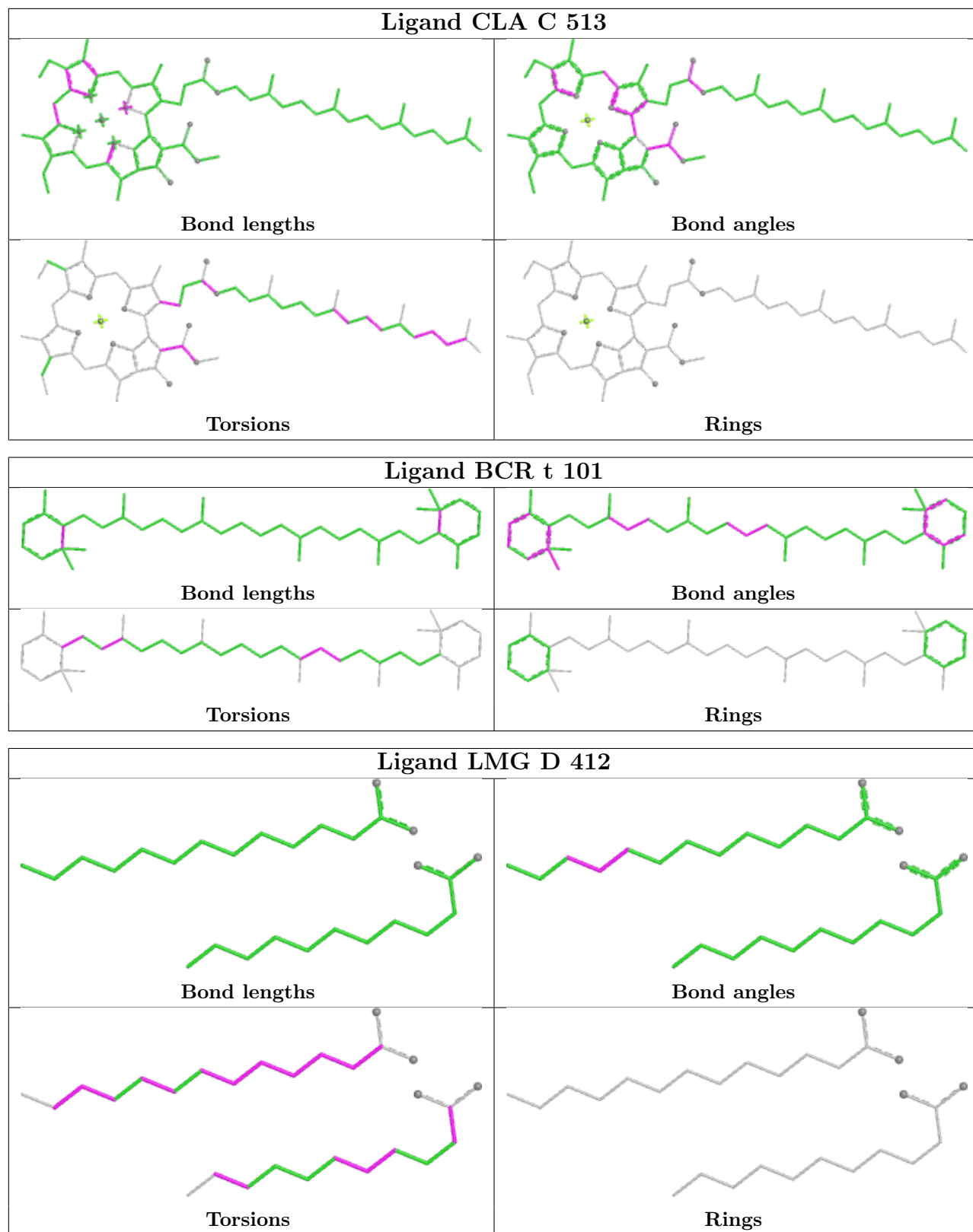


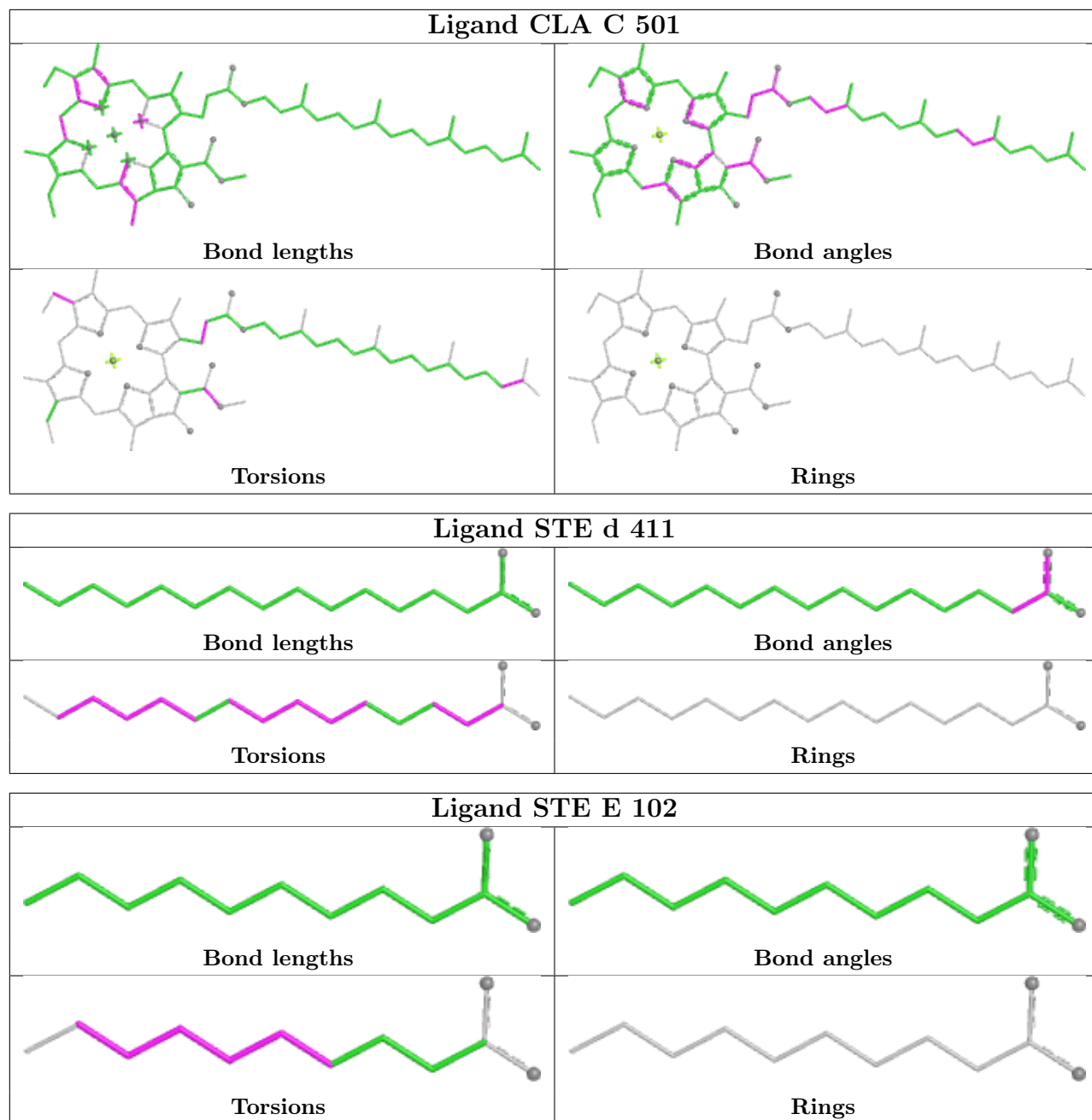
Ligand LHG 1 101



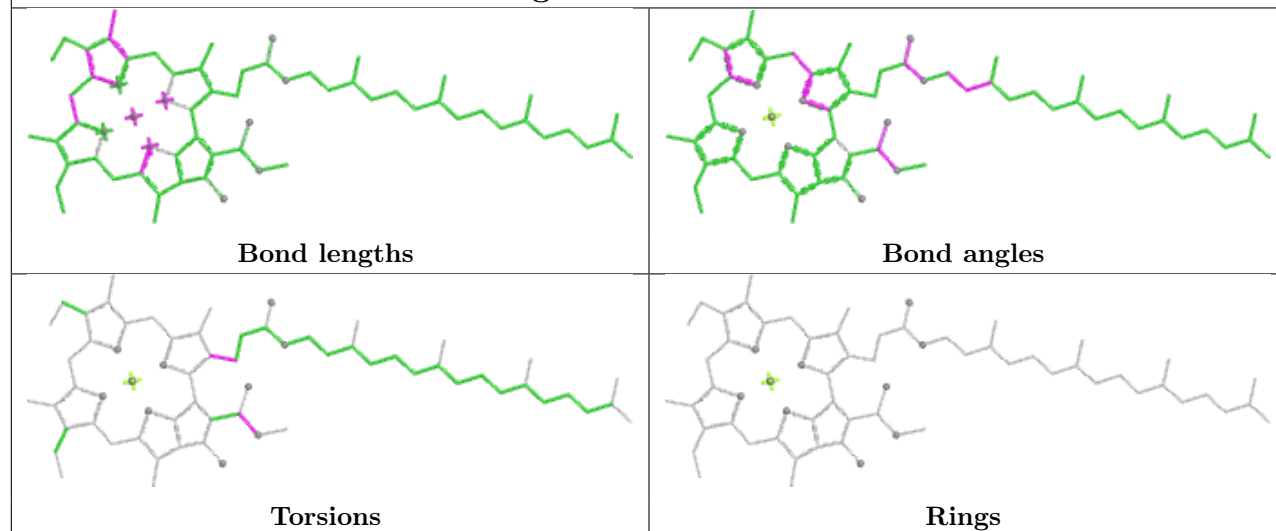
Ligand CLA B 613



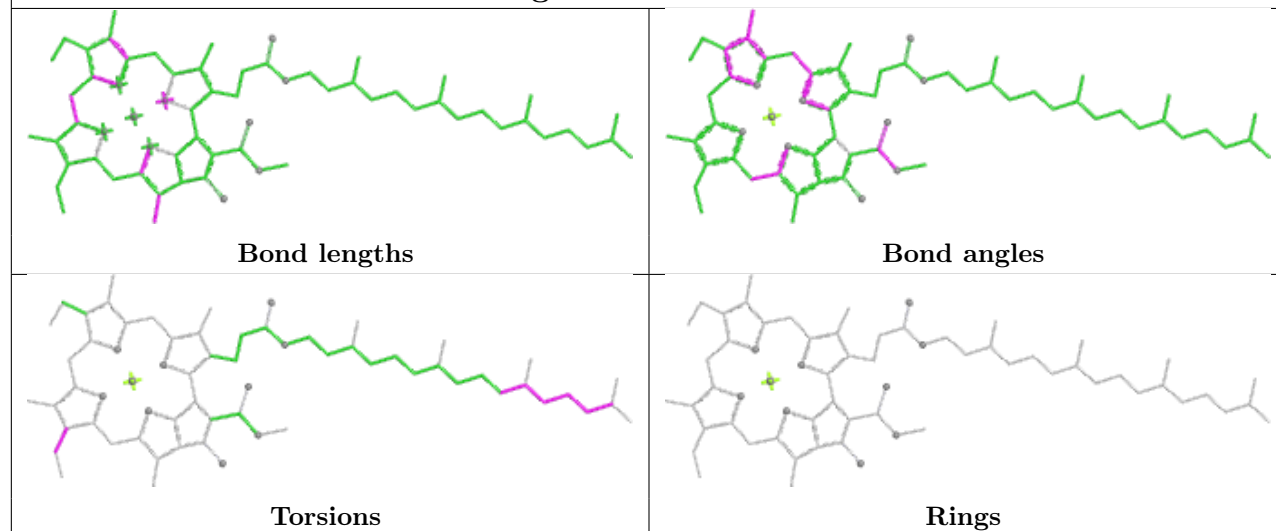




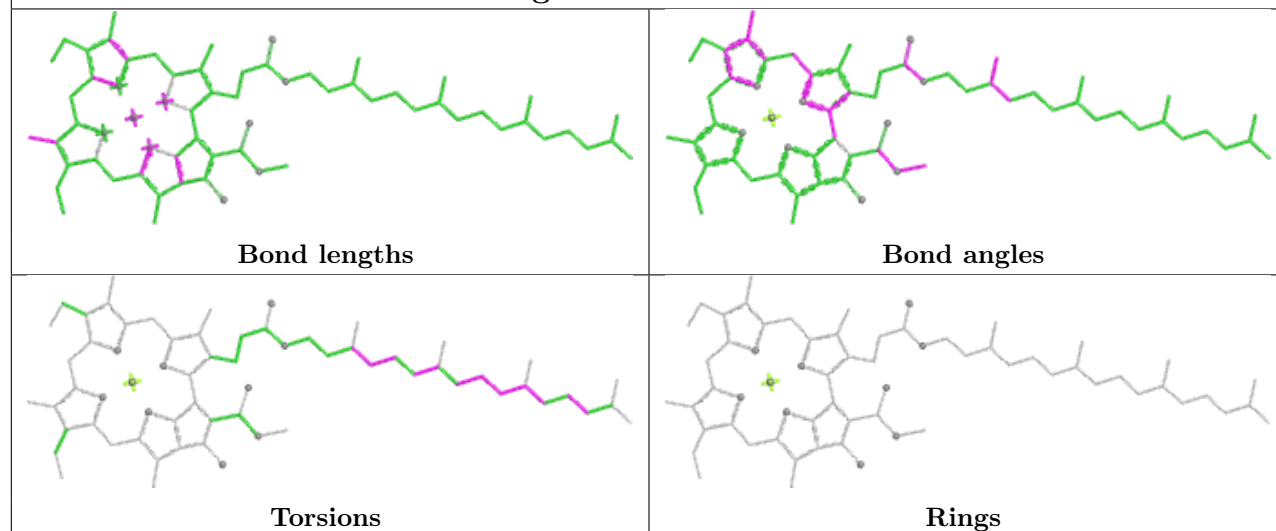
Ligand CLA C 511

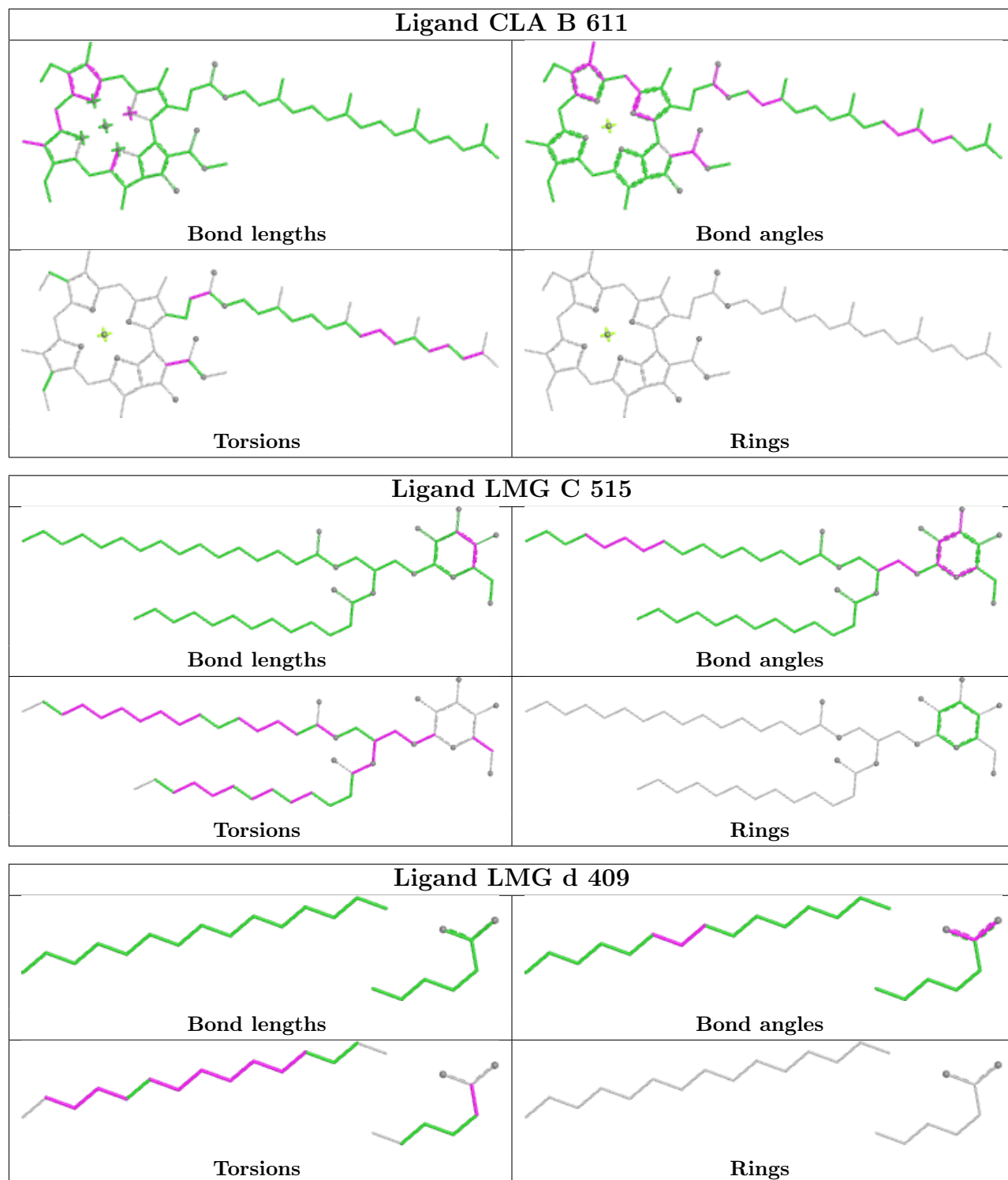


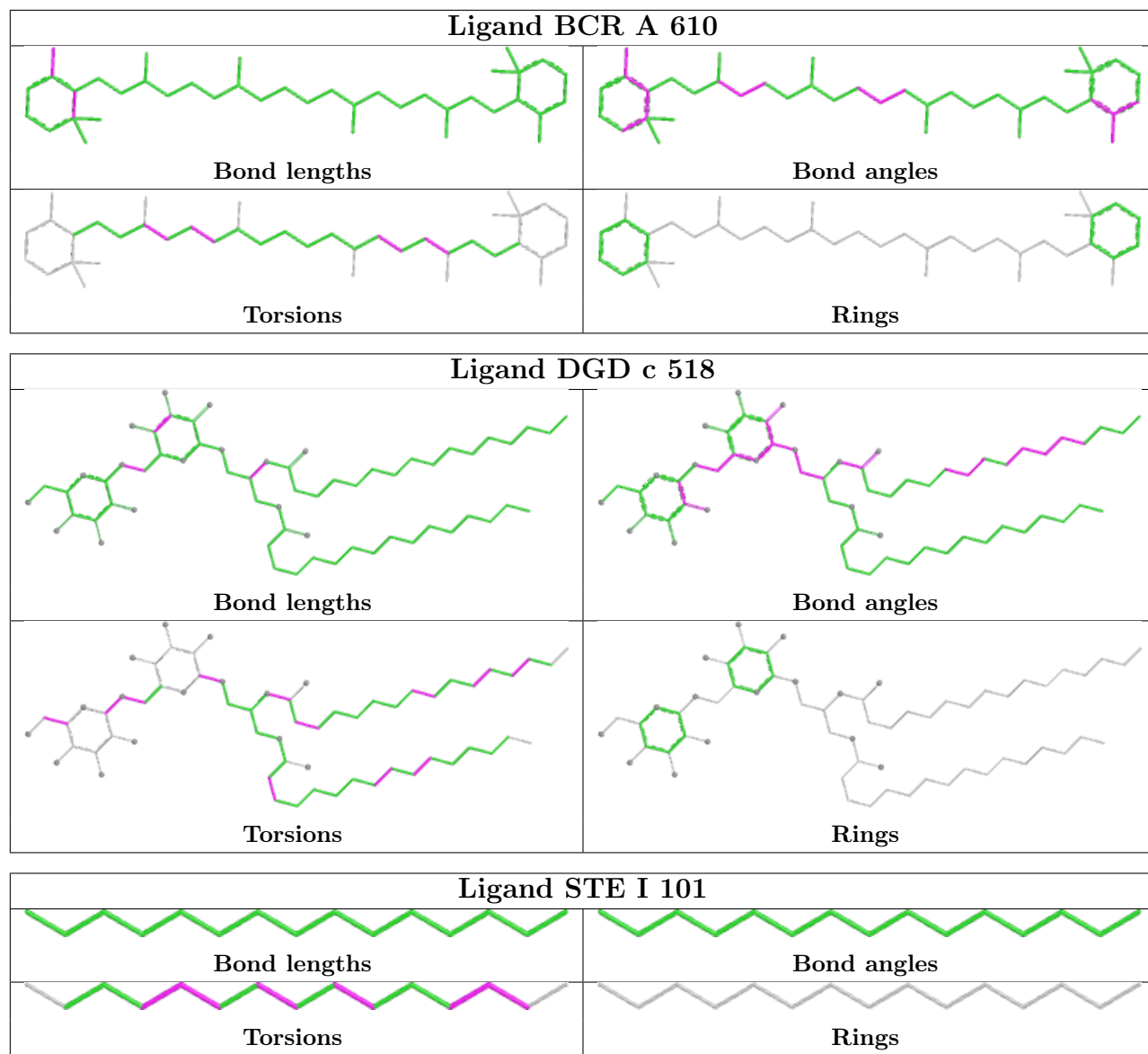
Ligand CLA A 612

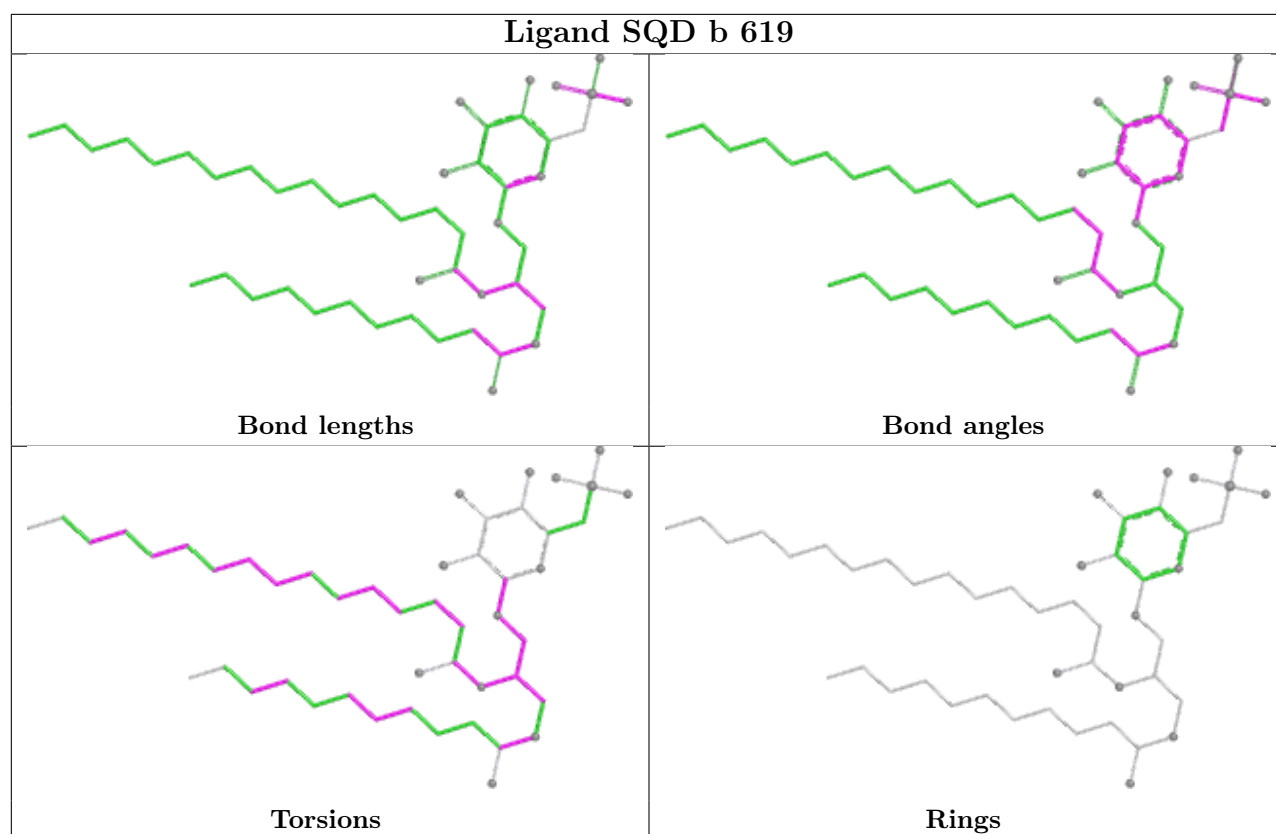


Ligand CLA B 606









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.25	1 (0%) 90 91	14, 33, 54, 92	64 (19%)
1	a	334/344 (97%)	-0.17	3 (0%) 81 83	15, 35, 60, 81	64 (19%)
2	B	505/510 (99%)	-0.22	2 (0%) 88 90	21, 38, 66, 91	4 (0%)
2	b	505/510 (99%)	-0.08	4 (0%) 82 84	30, 41, 73, 115	0
3	C	442/461 (95%)	-0.14	0 100 100	16, 41, 55, 78	11 (2%)
3	c	451/461 (97%)	-0.06	1 (0%) 91 92	16, 44, 63, 104	12 (2%)
4	D	341/352 (96%)	-0.32	0 100 100	16, 35, 52, 77	2 (0%)
4	d	341/352 (96%)	-0.17	0 100 100	18, 39, 62, 82	3 (0%)
5	E	82/84 (97%)	0.32	1 (1%) 76 79	35, 55, 72, 86	1 (1%)
5	e	82/84 (97%)	0.42	2 (2%) 59 63	44, 62, 81, 90	0
6	F	34/45 (75%)	0.07	0 100 100	40, 50, 63, 89	0
6	f	34/45 (75%)	0.36	1 (2%) 53 57	47, 54, 79, 88	0
7	H	65/66 (98%)	0.02	2 (3%) 51 55	39, 44, 60, 74	0
7	h	63/66 (95%)	0.30	1 (1%) 70 74	45, 54, 64, 70	0
8	I	35/38 (92%)	-0.09	0 100 100	37, 44, 70, 89	0
8	i	35/38 (92%)	-0.06	0 100 100	34, 44, 74, 88	0
9	J	36/40 (90%)	0.31	0 100 100	42, 55, 78, 87	0
9	j	36/40 (90%)	0.35	3 (8%) 17 19	44, 57, 90, 100	0
10	K	37/46 (80%)	0.17	0 100 100	47, 56, 74, 85	0
10	k	37/46 (80%)	0.33	0 100 100	52, 59, 73, 83	0
11	L	37/37 (100%)	-0.33	0 100 100	30, 34, 65, 75	0
11	l	36/37 (97%)	-0.36	0 100 100	30, 35, 69, 92	0
12	M	32/36 (88%)	-0.37	0 100 100	32, 37, 58, 75	0
12	m	31/36 (86%)	-0.29	0 100 100	32, 38, 56, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.01	2 (0%) 82 84	31, 46, 83, 138	1 (0%)
13	o	244/272 (89%)	0.02	3 (1%) 76 79	31, 45, 85, 119	0
14	T	29/32 (90%)	-0.38	0 100 100	31, 36, 62, 74	0
14	t	29/32 (90%)	-0.20	1 (3%) 48 52	32, 36, 75, 92	0
15	U	97/134 (72%)	0.01	0 100 100	36, 48, 71, 92	0
15	u	97/134 (72%)	-0.08	1 (1%) 79 82	35, 44, 60, 89	0
16	V	137/163 (84%)	-0.14	0 100 100	35, 44, 58, 80	0
16	v	137/163 (84%)	0.09	0 100 100	37, 51, 69, 84	0
17	Y	27/46 (58%)	0.99	3 (11%) 10 11	58, 73, 96, 106	0
17	y	30/46 (65%)	0.98	2 (6%) 24 27	66, 78, 96, 104	0
18	X	38/41 (92%)	0.17	1 (2%) 57 61	43, 55, 72, 81	0
18	x	39/41 (95%)	0.38	1 (2%) 57 61	53, 63, 87, 101	0
19	Z	62/62 (100%)	0.90	5 (8%) 18 19	57, 71, 119, 132	0
19	z	62/62 (100%)	0.81	4 (6%) 25 28	64, 74, 112, 125	0
20	R	34/41 (82%)	0.99	3 (8%) 15 17	65, 72, 85, 92	0
20	r	31/41 (75%)	1.31	4 (12%) 7 8	76, 92, 110, 126	0
All	All	5302/5700 (93%)	-0.04	51 (0%) 79 82	14, 42, 76, 138	162 (3%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	4.1
13	o	58	ASN	3.8
20	R	35	LEU	3.7
19	Z	33	TRP	3.1
14	t	30	THR	3.0
17	Y	25	ILE	3.0
6	f	15	ILE	2.9
3	c	23	ALA	2.9
13	O	59	LYS	2.8
5	E	79	PHE	2.8
7	H	41	PHE	2.8
2	B	479[A]	PHE	2.7
19	z	33	TRP	2.7
20	r	14	LEU	2.6
20	r	31	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
9	j	5	GLY	2.6
9	j	6	GLY	2.6
2	b	499	VAL	2.5
5	e	79	PHE	2.5
20	r	28	VAL	2.4
13	o	56	PRO	2.4
2	b	494	GLY	2.4
15	u	53	ALA	2.4
18	x	37	VAL	2.4
1	a	250	ALA	2.3
17	Y	22	LEU	2.3
2	b	495	PHE	2.3
20	R	7	VAL	2.3
19	Z	30	PRO	2.3
18	X	3	ILE	2.3
13	o	57	LYS	2.2
7	h	41	PHE	2.2
17	y	18	VAL	2.2
7	H	65	LEU	2.2
13	O	58	ASN	2.2
9	j	8	ILE	2.1
19	z	40	ILE	2.1
20	R	34	LEU	2.1
20	r	23	ILE	2.1
2	B	494	GLY	2.1
17	Y	24	MET	2.1
1	a	248	ILE	2.1
19	z	60	PHE	2.1
2	b	486	LEU	2.0
19	Z	4	LEU	2.0
19	Z	39	LEU	2.0
19	z	27	TYR	2.0
5	e	14	ILE	2.0
17	y	25	ILE	2.0
1	A	265	PHE	2.0
1	a	11	ALA	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($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.90	0.09	37,41,52,69	0
12	FME	M	1	10/11	0.91	0.10	40,54,65,70	0
14	FME	T	1	10/11	0.94	0.09	39,43,55,62	0
12	FME	m	1	10/11	0.94	0.10	31,45,64,68	0
8	FME	i	1	10/11	0.95	0.10	44,51,53,54	0
8	FME	I	1	10/11	0.97	0.06	42,46,52,55	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	LHG	e	102	42/49	0.75	0.16	61,81,102,104	0
31	STE	H	104	18/20	0.77	0.17	53,65,74,79	0
31	STE	m	101	12/20	0.78	0.19	54,58,69,70	0
31	STE	c	523	12/20	0.78	0.14	60,71,84,87	0
31	STE	I	101	15/20	0.79	0.18	45,50,65,70	0
31	STE	E	102	12/20	0.79	0.17	62,72,82,85	0
33	LMG	b	622	55/55	0.79	0.17	50,67,82,84	0
31	STE	b	625	20/20	0.80	0.14	45,51,64,70	0
31	STE	x	102	20/20	0.80	0.15	48,56,62,63	0
31	STE	t	103	10/20	0.81	0.14	42,55,59,59	0
33	LMG	D	411	33/55	0.81	0.15	40,56,72,74	0
32	LHG	E	101	49/49	0.81	0.14	51,76,99,106	0
33	LMG	d	409	23/55	0.81	0.17	51,63,69,70	0
33	LMG	c	522	48/55	0.83	0.14	43,71,91,96	0
30	DGD	a	615	44/66	0.83	0.14	37,52,71,73	0
31	STE	j	101	12/20	0.84	0.14	51,59,67,68	0
31	STE	B	623	18/20	0.84	0.13	42,48,81,84	0
31	STE	a	616	12/20	0.84	0.12	53,62,68,70	0
29	SQD	a	614	36/54	0.84	0.14	33,56,70,76	0
29	SQD	T	103	39/54	0.84	0.14	39,56,79,80	0
31	STE	b	626	10/20	0.85	0.14	46,50,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	h	101	65/65	0.85	0.12	55,68,83,89	0
28	PL9	A	611	55/55	0.85	0.15	40,60,74,83	0
31	STE	T	102	16/20	0.85	0.15	41,47,60,63	0
31	STE	B	624	12/20	0.85	0.12	46,54,64,67	0
30	DGD	A	614	66/66	0.85	0.12	51,58,67,73	0
31	STE	d	411	17/20	0.86	0.15	45,55,69,71	0
33	LMG	C	515	48/55	0.86	0.12	42,55,67,75	0
31	STE	C	520	12/20	0.86	0.12	38,42,57,61	0
31	STE	M	104	15/20	0.87	0.14	43,54,69,75	0
29	SQD	f	101	41/54	0.87	0.14	63,77,86,93	0
31	STE	B	625	16/20	0.87	0.14	43,57,63,66	0
31	STE	b	621	20/20	0.87	0.11	42,51,67,68	0
25	CLA	H	101	65/65	0.87	0.11	42,55,81,96	0
31	STE	D	413	20/20	0.87	0.13	38,51,73,83	0
33	LMG	C	519	48/55	0.87	0.13	48,67,78,86	0
31	STE	c	521	20/20	0.87	0.12	44,57,80,82	0
28	PL9	a	611	55/55	0.87	0.14	49,64,73,77	0
33	LMG	c	520	37/55	0.87	0.11	48,61,74,78	0
31	STE	B	619	17/20	0.87	0.12	42,50,66,69	0
29	SQD	b	619	49/54	0.87	0.11	42,57,78,80	0
33	LMG	b	620	51/55	0.88	0.10	36,49,65,66	0
31	STE	B	622	12/20	0.88	0.12	42,52,59,66	0
31	STE	b	624	16/20	0.88	0.13	54,59,76,79	0
31	STE	C	522	16/20	0.88	0.14	43,52,58,66	0
31	STE	J	101	12/20	0.88	0.13	54,60,72,72	0
29	SQD	D	408	36/54	0.89	0.13	53,65,78,82	0
27	BCR	c	514	40/40	0.89	0.12	49,60,68,71	0
33	LMG	D	412	28/55	0.89	0.11	36,47,59,65	0
33	LMG	c	524	49/55	0.89	0.10	40,55,72,79	0
29	SQD	B	621	54/54	0.89	0.11	39,61,82,91	0
27	BCR	Y	101	40/40	0.90	0.10	46,56,63,65	0
31	STE	M	102	15/20	0.90	0.10	46,48,61,65	0
33	LMG	M	101	51/55	0.90	0.10	32,47,63,65	0
25	CLA	c	512	65/65	0.91	0.11	44,59,83,89	0
27	BCR	H	102	40/40	0.91	0.09	36,47,56,62	0
27	BCR	d	405	40/40	0.91	0.11	39,49,81,89	0
27	BCR	k	101	40/40	0.91	0.11	51,61,71,73	0
31	STE	M	103	10/20	0.91	0.13	30,45,57,63	0
30	DGD	H	103	62/66	0.91	0.10	35,43,52,58	0
31	STE	l	102	18/20	0.91	0.12	34,45,68,72	0
31	STE	C	521	12/20	0.91	0.11	46,53,59,63	0
31	STE	t	102	14/20	0.91	0.09	38,48,52,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	BCR	x	101	40/40	0.91	0.10	43,55,66,69	0
30	DGD	h	102	62/66	0.91	0.10	37,47,54,59	0
29	SQD	a	613	54/54	0.91	0.11	46,61,75,81	0
30	DGD	C	517	62/66	0.92	0.09	37,49,86,99	0
27	BCR	B	618	40/40	0.92	0.09	35,44,52,54	0
27	BCR	C	514	40/40	0.92	0.10	35,42,52,53	0
27	BCR	D	405	40/40	0.92	0.10	33,46,70,78	0
25	CLA	c	513	65/65	0.92	0.10	41,61,87,92	0
25	CLA	C	513	65/65	0.92	0.10	47,55,82,86	0
27	BCR	Z	101	40/40	0.92	0.11	49,56,63,65	0
27	BCR	b	617	40/40	0.92	0.08	32,40,49,53	0
25	CLA	b	615	60/65	0.93	0.09	34,44,71,75	0
27	BCR	b	618	40/40	0.93	0.09	34,47,58,62	0
33	LMG	D	407	51/55	0.93	0.10	35,49,69,72	0
29	SQD	A	613	52/54	0.93	0.10	34,53,74,76	0
27	BCR	A	610	40/40	0.93	0.07	28,34,40,42	0
27	BCR	c	516	40/40	0.93	0.12	47,53,61,69	0
30	DGD	c	518	62/66	0.93	0.09	41,49,78,82	0
27	BCR	T	101	40/40	0.93	0.07	32,40,54,59	0
25	CLA	C	503	65/65	0.93	0.09	37,44,50,59	0
32	LHG	D	410	47/49	0.93	0.10	33,43,68,78	0
27	BCR	t	101	40/40	0.93	0.07	30,39,48,51	0
25	CLA	C	512	65/65	0.93	0.10	43,53,74,86	0
33	LMG	d	410	44/55	0.93	0.10	41,49,68,79	0
34	BCT	a	606	4/4	0.93	0.08	38,40,49,51	0
25	CLA	c	511	65/65	0.94	0.10	47,55,63,66	0
27	BCR	b	616	40/40	0.94	0.08	31,42,49,51	0
25	CLA	C	511	65/65	0.94	0.10	38,51,61,67	0
32	LHG	B	620	49/49	0.94	0.09	36,43,55,59	0
25	CLA	B	605	65/65	0.94	0.08	26,39,59,63	0
25	CLA	C	506	65/65	0.94	0.09	30,43,74,79	0
32	LHG	b	623	49/49	0.94	0.10	37,47,58,62	0
30	DGD	C	516	62/66	0.94	0.10	29,38,67,72	0
27	BCR	c	515	40/40	0.94	0.09	33,46,52,58	0
26	PHO	d	402	64/64	0.94	0.07	32,40,45,49	0
25	CLA	C	508	65/65	0.94	0.09	35,44,87,96	0
27	BCR	B	616	40/40	0.94	0.07	32,40,47,50	0
30	DGD	c	519	62/66	0.94	0.09	34,49,71,78	0
27	BCR	B	617	40/40	0.94	0.07	27,36,47,49	0
25	CLA	b	607	65/65	0.94	0.08	32,42,54,57	0
25	CLA	C	510	65/65	0.94	0.08	33,44,53,57	0
28	PL9	D	406	55/55	0.94	0.08	24,34,42,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	c	502	65/65	0.94	0.08	37,44,54,62	0
25	CLA	c	503	65/65	0.94	0.08	39,47,52,53	0
27	BCR	K	101	40/40	0.94	0.10	43,52,57,59	0
25	CLA	c	508	64/65	0.94	0.09	36,46,77,98	0
25	CLA	c	509	65/65	0.94	0.10	41,48,59,62	0
25	CLA	A	607	65/65	0.95	0.09	28,37,84,87	0
25	CLA	c	510	65/65	0.95	0.08	40,48,55,63	0
25	CLA	C	509	65/65	0.95	0.09	33,43,54,62	0
28	PL9	d	406	55/55	0.95	0.07	29,35,40,42	0
25	CLA	B	608	65/65	0.95	0.07	28,39,48,52	0
25	CLA	B	609	65/65	0.95	0.07	25,33,41,43	0
25	CLA	d	401	65/65	0.95	0.09	33,40,73,82	0
25	CLA	d	404	65/65	0.95	0.08	34,43,76,78	0
25	CLA	B	614	65/65	0.95	0.07	29,38,57,65	0
26	PHO	D	402	64/64	0.95	0.06	26,35,40,43	0
26	PHO	a	608	64/64	0.95	0.07	29,34,38,43	0
25	CLA	B	615	60/65	0.95	0.09	31,39,74,77	0
25	CLA	C	501	65/65	0.95	0.07	29,36,45,53	0
25	CLA	a	607	65/65	0.95	0.07	26,33,39,42	0
25	CLA	a	609	65/65	0.95	0.09	23,35,70,74	0
30	DGD	C	518	62/66	0.95	0.08	33,46,68,75	0
25	CLA	b	601	65/65	0.95	0.08	32,43,50,53	0
25	CLA	b	602	65/65	0.95	0.08	29,37,58,66	0
30	DGD	c	517	62/66	0.95	0.08	31,39,61,70	0
25	CLA	b	604	65/65	0.95	0.07	26,36,44,49	0
25	CLA	b	605	65/65	0.95	0.08	31,39,60,63	0
32	LHG	d	408	39/49	0.95	0.08	34,46,57,58	0
25	CLA	C	502	65/65	0.95	0.07	36,42,52,59	0
32	LHG	l	101	49/49	0.95	0.08	33,43,50,53	0
25	CLA	b	608	65/65	0.95	0.08	34,45,56,67	0
25	CLA	b	609	65/65	0.95	0.08	30,38,48,57	0
25	CLA	b	613	65/65	0.95	0.08	31,41,61,73	0
27	BCR	a	610	40/40	0.95	0.07	24,32,42,46	0
25	CLA	b	614	65/65	0.95	0.08	31,41,52,54	0
25	CLA	B	601	65/65	0.95	0.07	30,39,51,53	0
25	CLA	c	501	65/65	0.95	0.08	28,41,48,52	0
25	CLA	C	504	59/65	0.95	0.07	35,41,63,67	0
25	CLA	C	505	65/65	0.95	0.08	30,39,54,60	0
25	CLA	c	504	60/65	0.95	0.08	37,47,76,79	0
25	CLA	c	505	65/65	0.95	0.08	33,41,54,59	0
25	CLA	c	506	65/65	0.95	0.08	38,45,71,75	0
25	CLA	c	507	65/65	0.95	0.08	35,44,54,62	0

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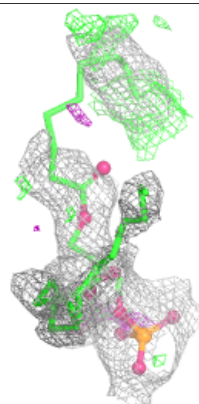
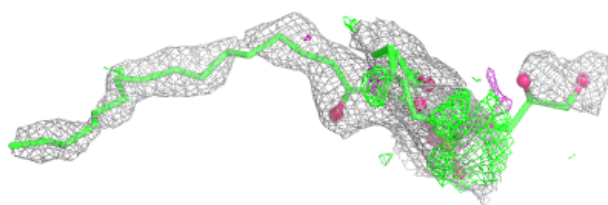
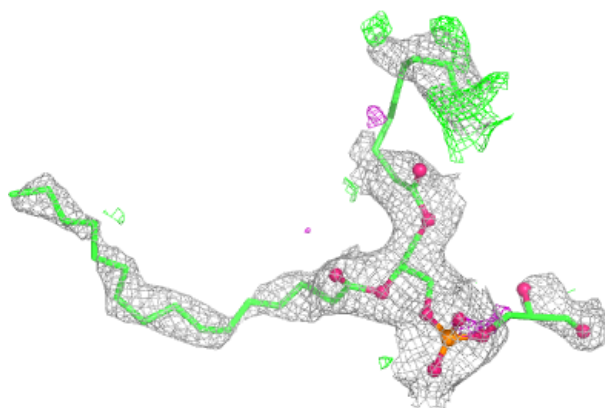
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	603	65/65	0.95	0.08	25,34,58,62	0
25	CLA	B	606	65/65	0.96	0.07	20,33,52,59	0
32	LHG	D	409	49/49	0.96	0.07	30,38,46,48	0
25	CLA	b	610	65/65	0.96	0.07	28,37,44,50	0
25	CLA	d	403	65/65	0.96	0.07	27,35,50,61	0
32	LHG	L	101	49/49	0.96	0.07	30,39,47,58	0
25	CLA	b	611	65/65	0.96	0.07	27,36,43,49	0
32	LHG	d	407	49/49	0.96	0.08	30,41,48,53	0
25	CLA	b	612	65/65	0.96	0.07	24,34,57,65	0
26	PHO	A	608	64/64	0.96	0.06	24,30,36,40	0
25	CLA	B	607	65/65	0.96	0.06	25,35,48,52	0
25	CLA	D	403	65/65	0.96	0.06	25,31,46,50	0
25	CLA	D	404	65/65	0.96	0.07	29,39,86,94	0
25	CLA	B	602	65/65	0.96	0.07	24,34,49,56	0
25	CLA	A	612	65/65	0.96	0.06	23,30,42,47	0
25	CLA	B	610	65/65	0.96	0.06	25,33,44,48	0
25	CLA	a	612	65/65	0.96	0.06	28,33,39,43	0
25	CLA	B	611	65/65	0.96	0.07	25,33,41,44	0
25	CLA	C	507	65/65	0.96	0.07	31,40,50,55	0
25	CLA	b	603	65/65	0.96	0.08	28,34,59,72	0
25	CLA	B	612	65/65	0.96	0.07	24,33,58,64	0
25	CLA	B	613	65/65	0.96	0.08	28,36,64,70	0
25	CLA	b	606	65/65	0.96	0.07	27,35,50,60	0
25	CLA	B	604	65/65	0.96	0.07	25,32,42,46	0
34	BCT	D	401	4/4	0.96	0.06	33,38,41,42	0
25	CLA	A	606	65/65	0.96	0.06	22,29,39,46	0
35	HEM	e	101	43/43	0.96	0.09	52,59,73,80	0
35	HEM	F	101	43/43	0.97	0.09	46,52,61,71	0
25	CLA	A	609	54/65	0.97	0.06	26,32,59,61	0
24	CL	A	604	1/1	0.98	0.04	33,33,33,33	0
24	CL	a	604	1/1	0.98	0.04	34,34,34,34	0
36	HEC	V	201	43/43	0.98	0.07	32,38,45,51	0
36	HEC	v	201	43/43	0.98	0.07	36,41,47,50	0
21	OEX	a	601[B]	10/10	0.99	0.03	29,32,36,36	10
24	CL	a	605	1/1	0.99	0.10	35,35,35,35	0
22	OEY	A	602[A]	11/11	0.99	0.03	32,36,39,40	11
22	OEY	a	602[A]	11/11	0.99	0.03	35,37,40,43	11
21	OEX	A	601[B]	10/10	0.99	0.03	29,32,32,36	10
24	CL	A	605	1/1	0.99	0.04	33,33,33,33	0
23	FE2	A	603	1/1	1.00	0.01	35,35,35,35	0
23	FE2	a	603	1/1	1.00	0.02	39,39,39,39	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.

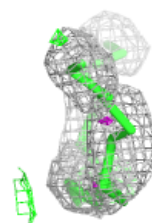
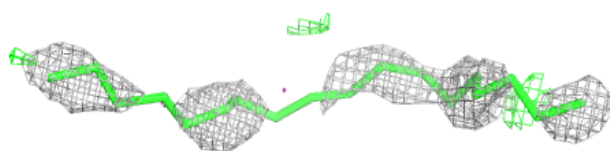
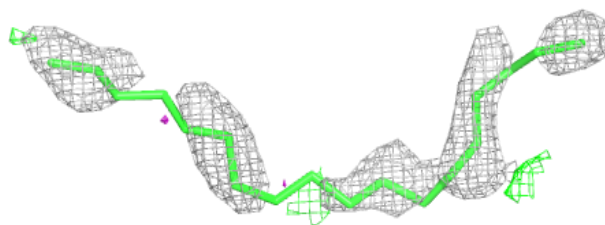
Electron density around LHG e 102:

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

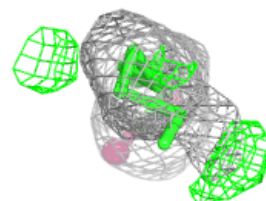
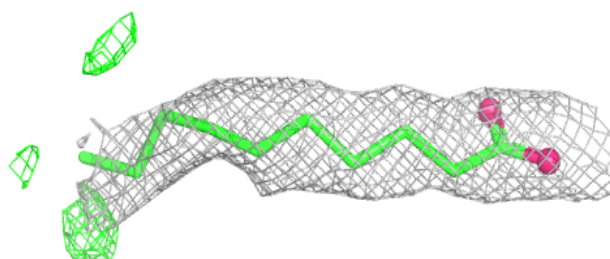
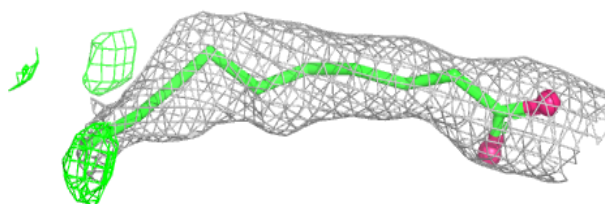


Electron density around STE H 104:

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

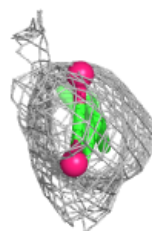
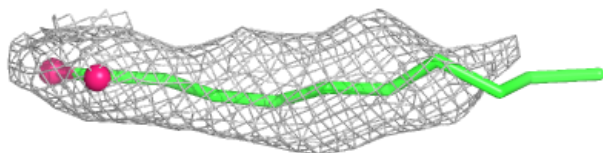
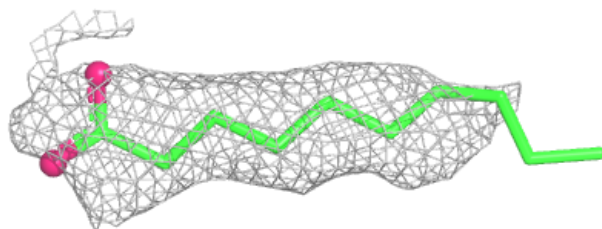
**Electron density around STE m 101:**

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

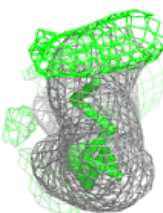
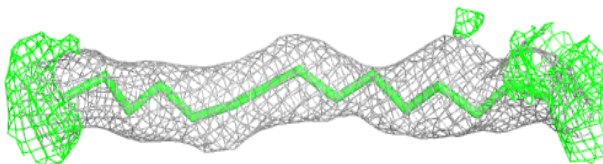
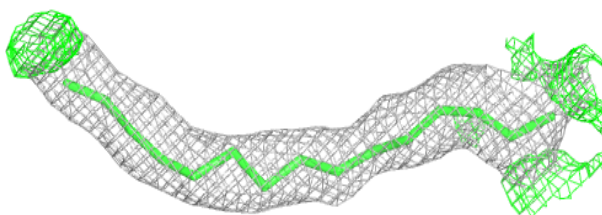


Electron density around STE c 523:

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

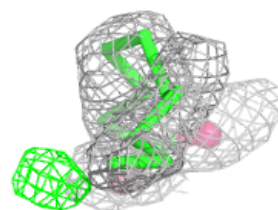
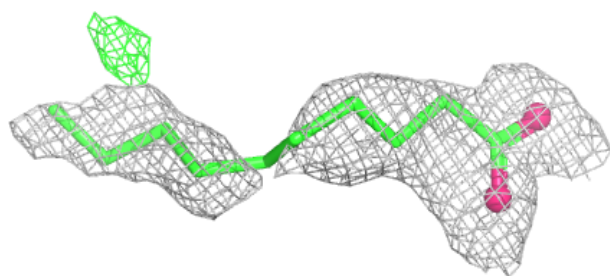
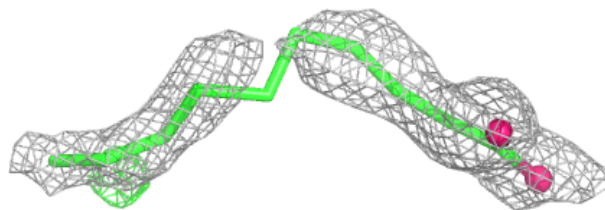
**Electron density around STE I 101:**

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

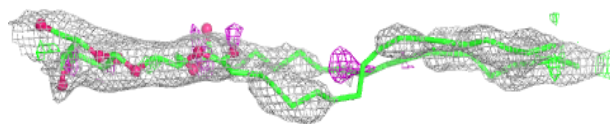
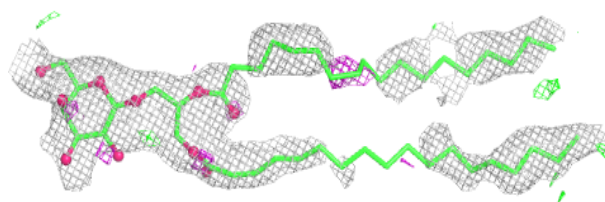


Electron density around STE E 102:

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

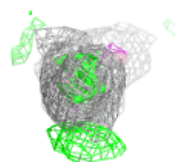
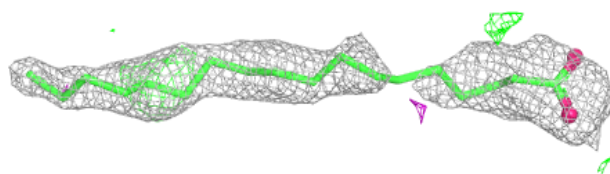
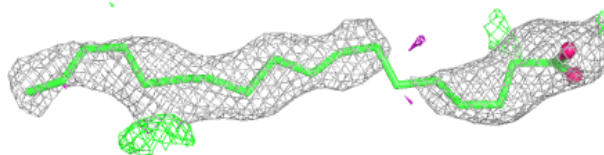
**Electron density around LMG b 622:**

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

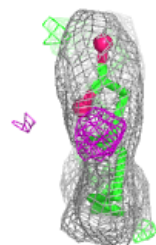
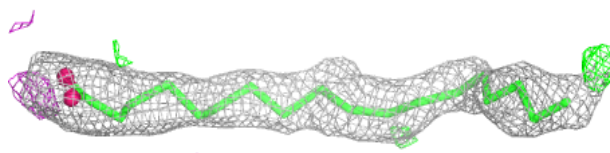
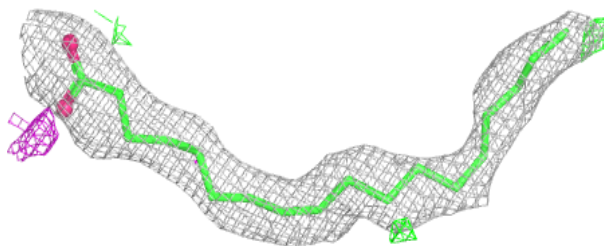


Electron density around STE b 625:

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

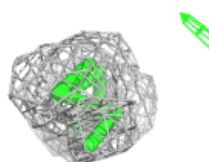
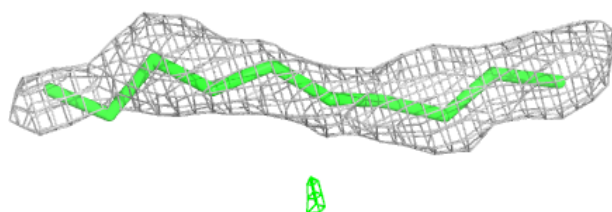
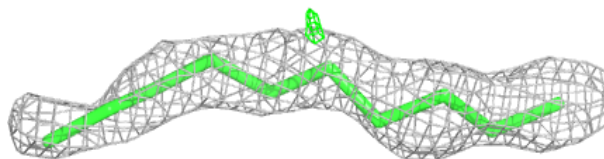
**Electron density around STE x 102:**

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

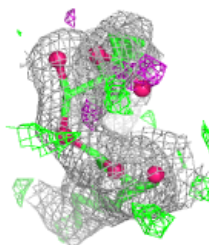
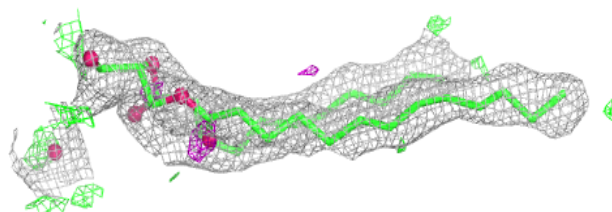
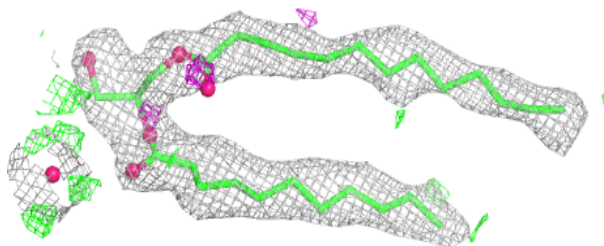


Electron density around STE t 103:

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and green (positive)

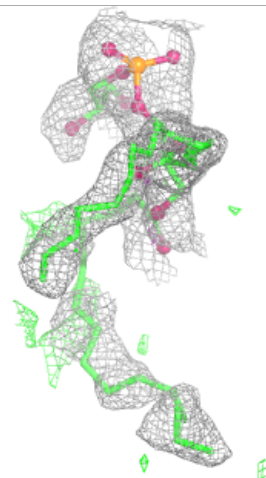
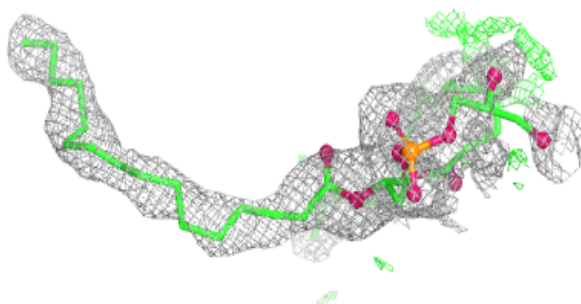
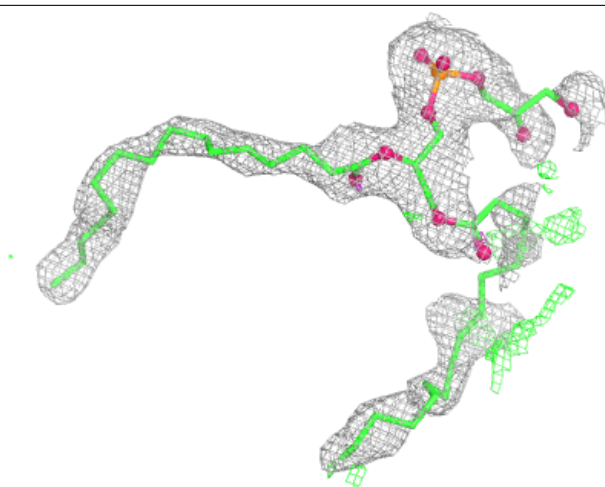
**Electron density around LMG D 411:**

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



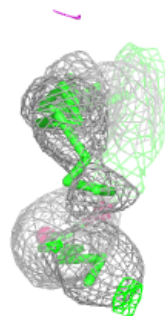
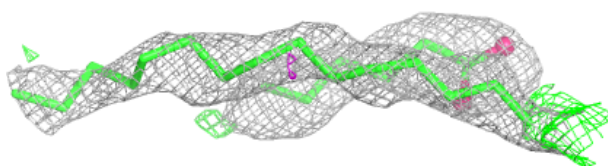
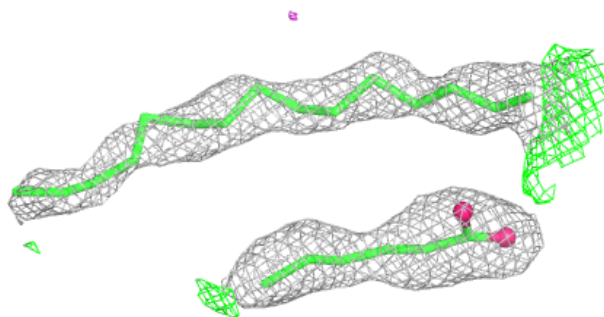
Electron density around LHG E 101:

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and green (positive)

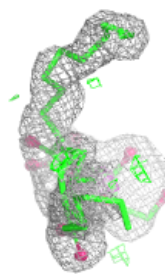
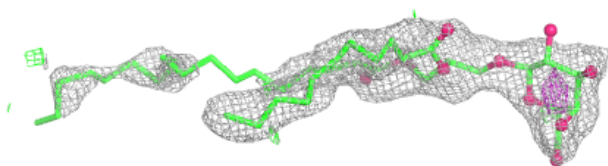
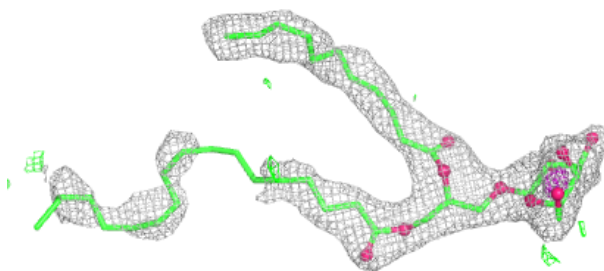


Electron density around LMG d 409:

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

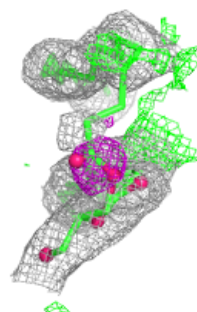
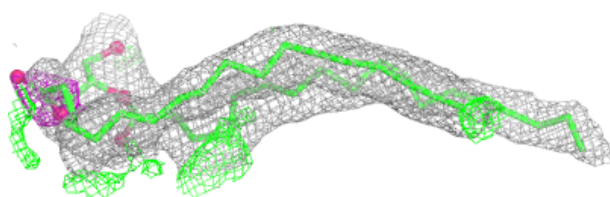
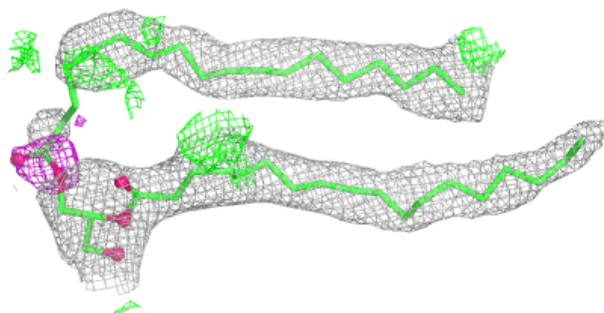
**Electron density around LMG c 522:**

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

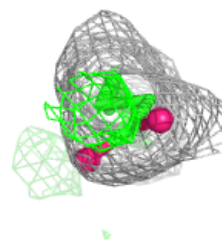
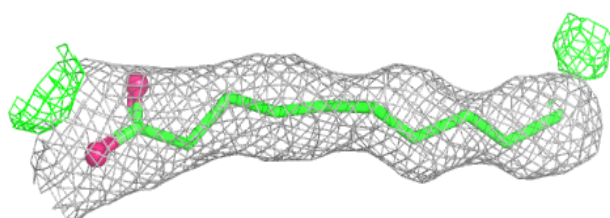
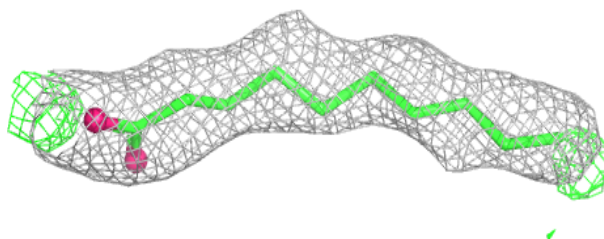


Electron density around DGD a 615:

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

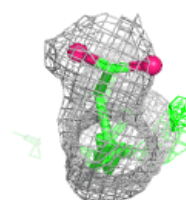
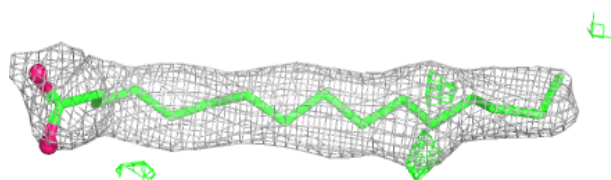
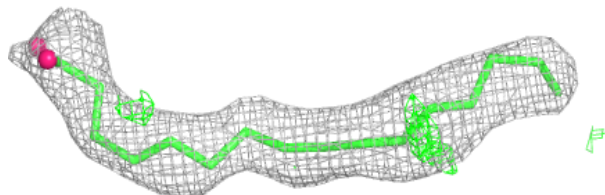
**Electron density around STE j 101:**

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

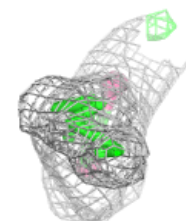
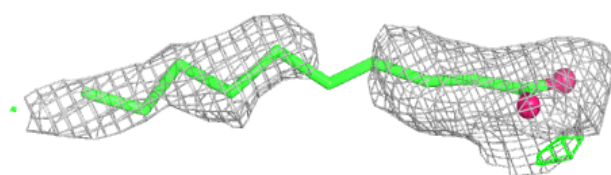
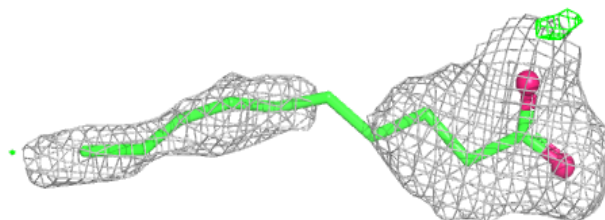


Electron density around STE B 623:

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

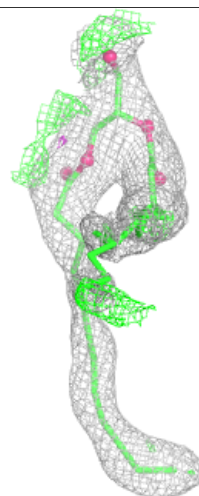
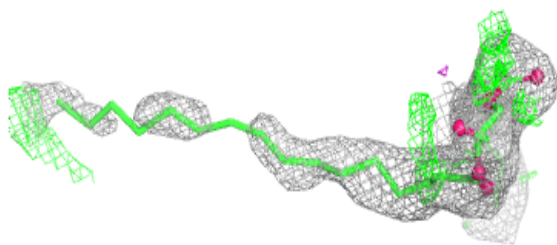
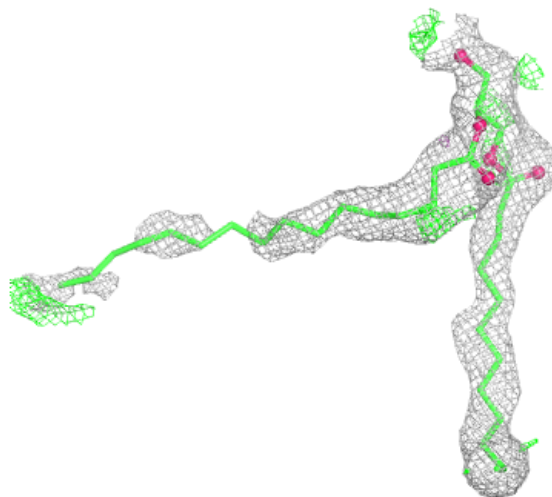
**Electron density around STE a 616:**

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



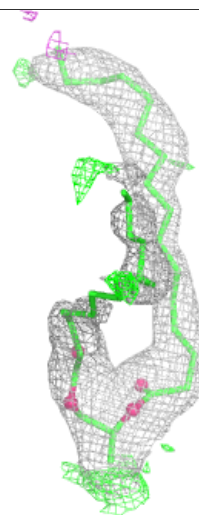
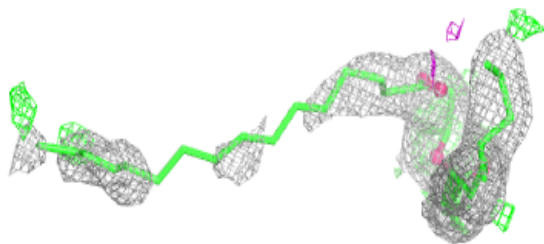
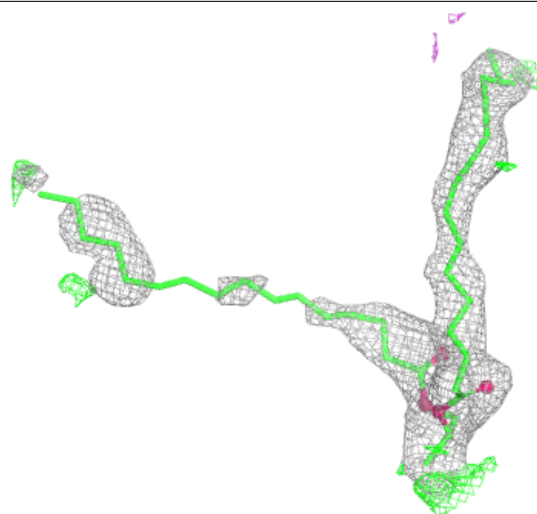
Electron density around SQD a 614:

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



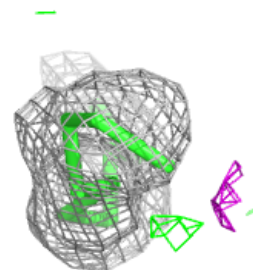
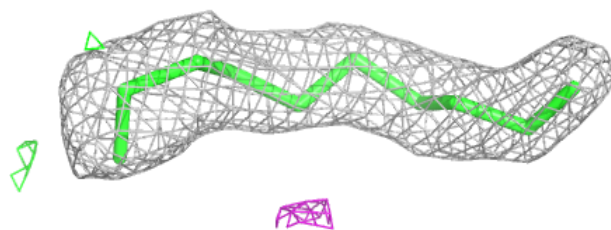
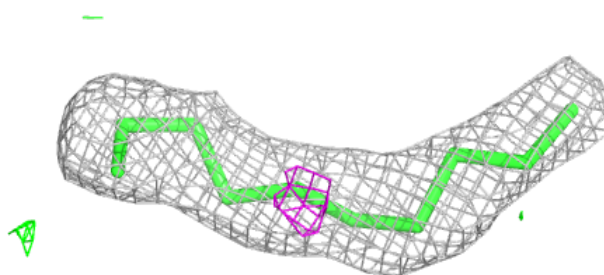
Electron density around SQD T 103:

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

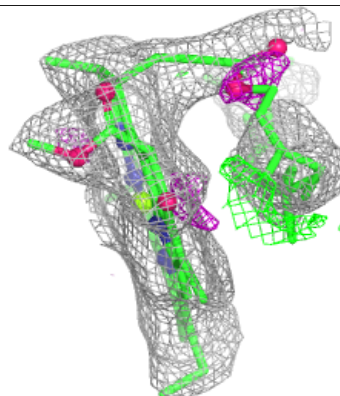
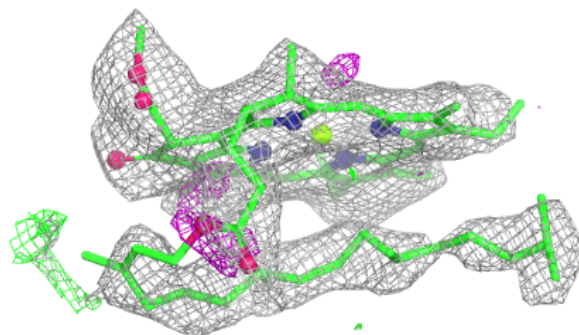
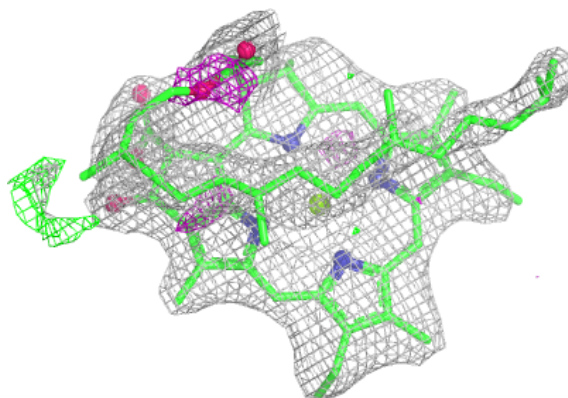


Electron density around STE b 626:

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

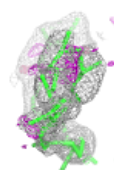
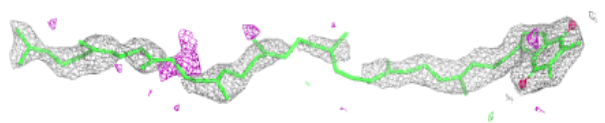
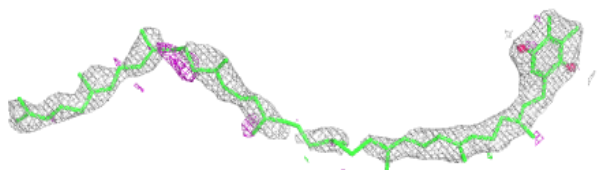
**Electron density around CLA h 101:**

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

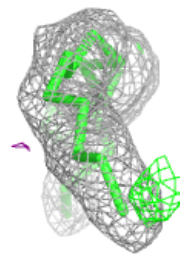
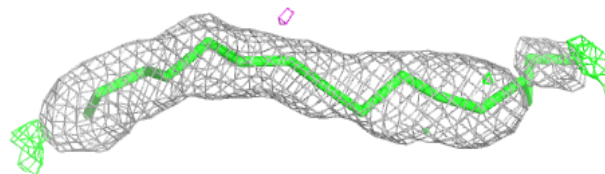
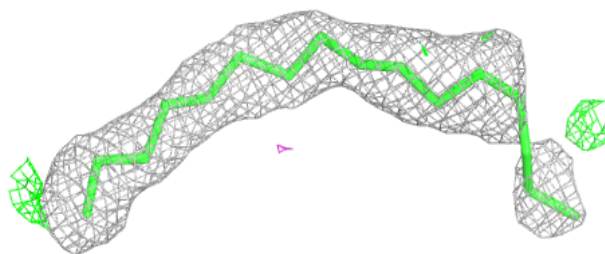


Electron density around PL9 A 611:

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

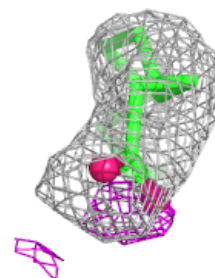
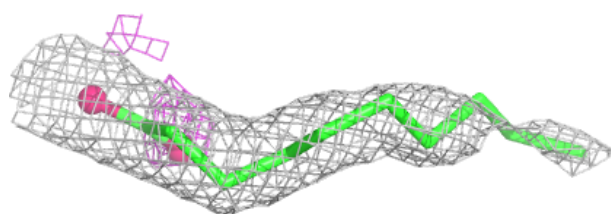
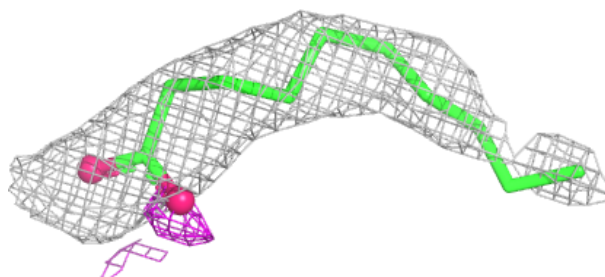
**Electron density around STE T 102:**

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

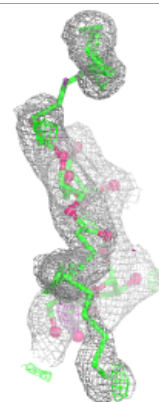
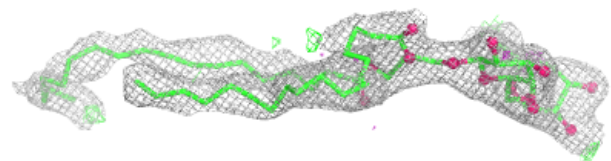
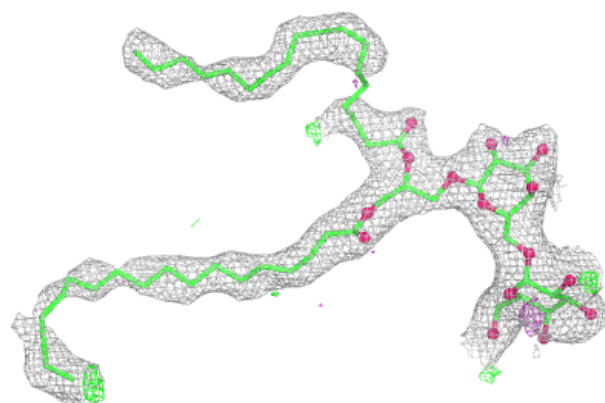


Electron density around STE B 624:

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

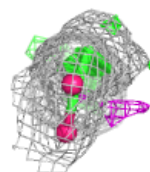
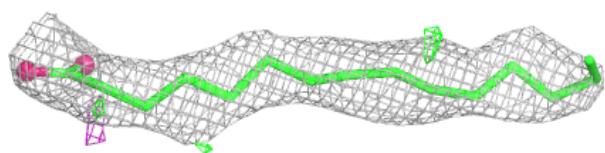
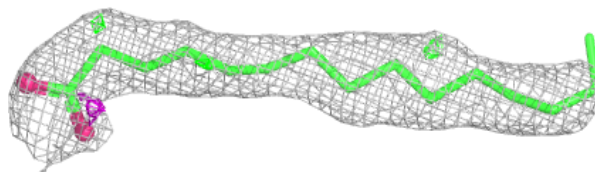
**Electron density around DGD A 614:**

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

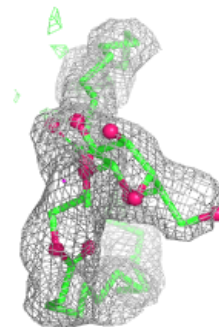
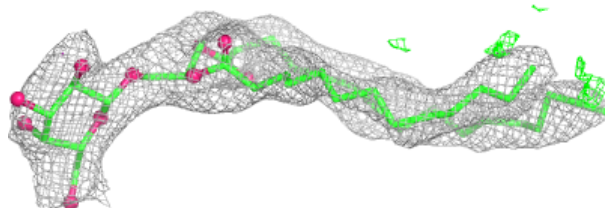
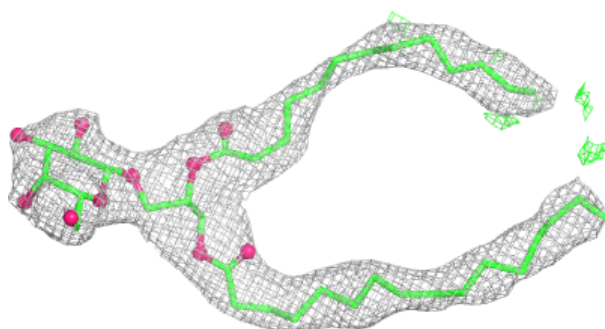


Electron density around STE d 411:

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

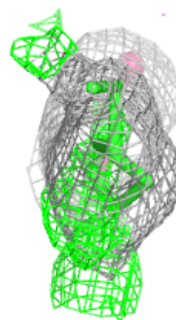
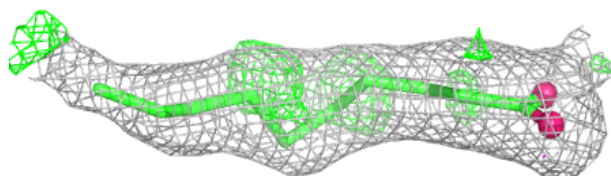
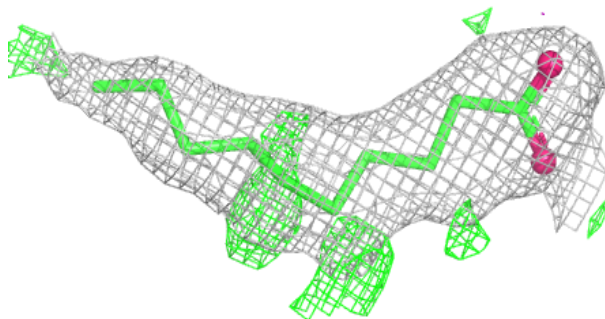
**Electron density around LMG C 515:**

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

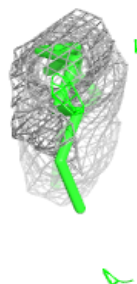
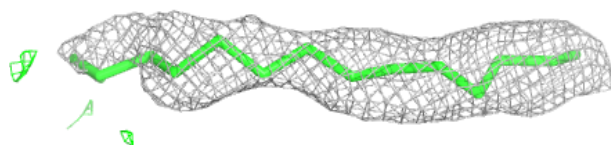
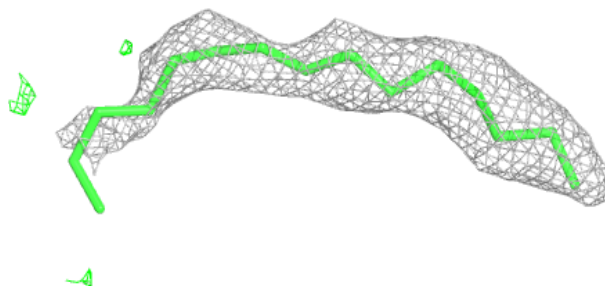


Electron density around STE C 520:

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

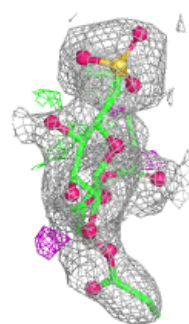
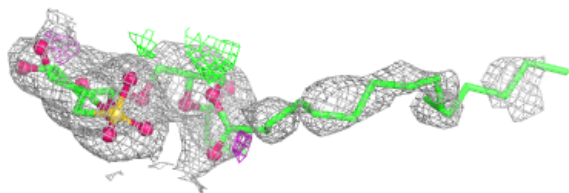
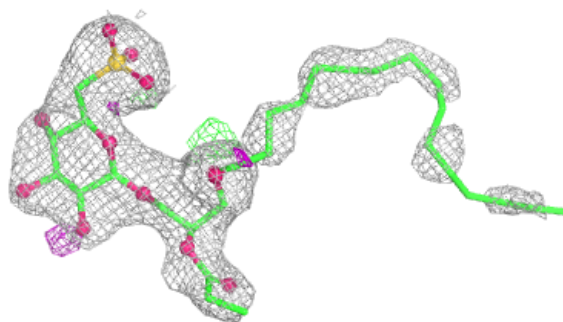
**Electron density around STE M 104:**

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

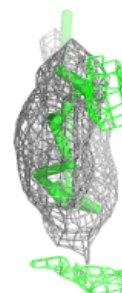
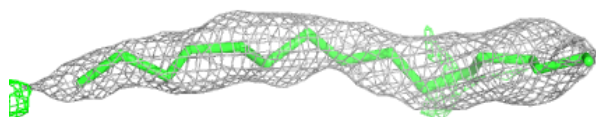
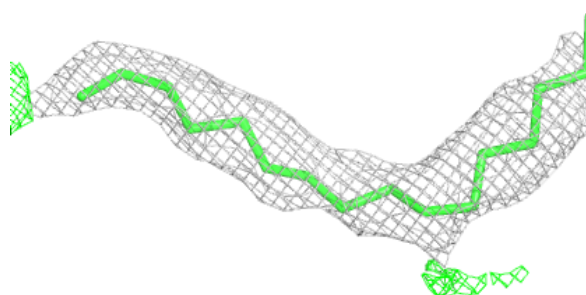


Electron density around SQD f 101:

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

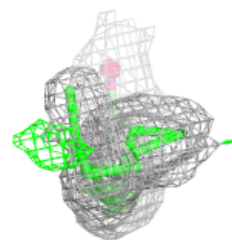
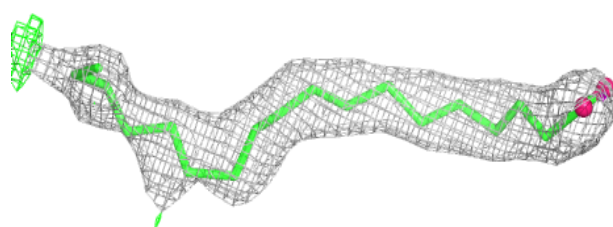
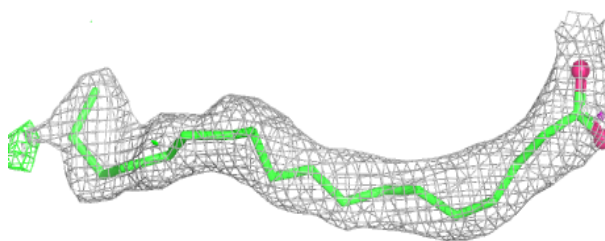
**Electron density around STE B 625:**

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

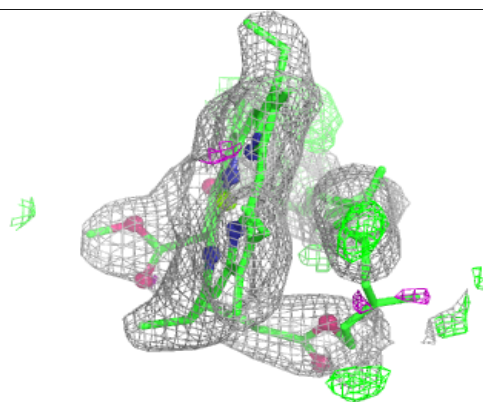
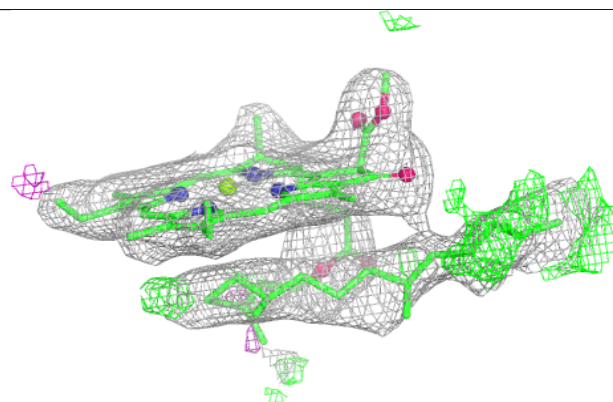
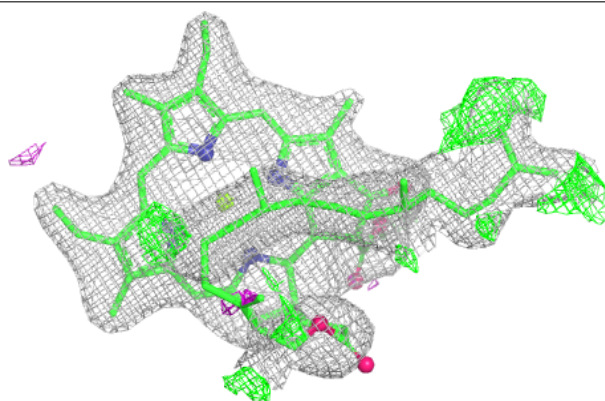


Electron density around STE b 621:

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

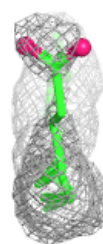
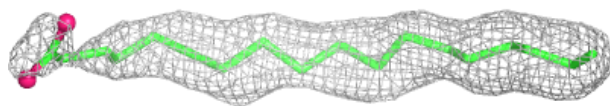
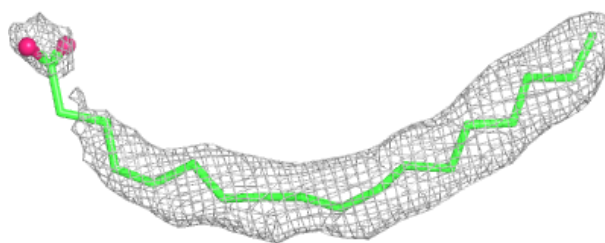
**Electron density around CLA H 101:**

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

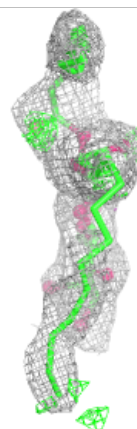
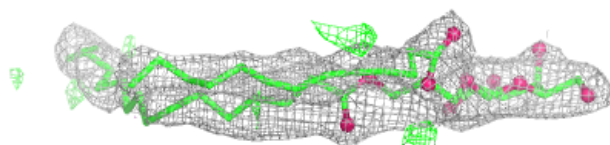
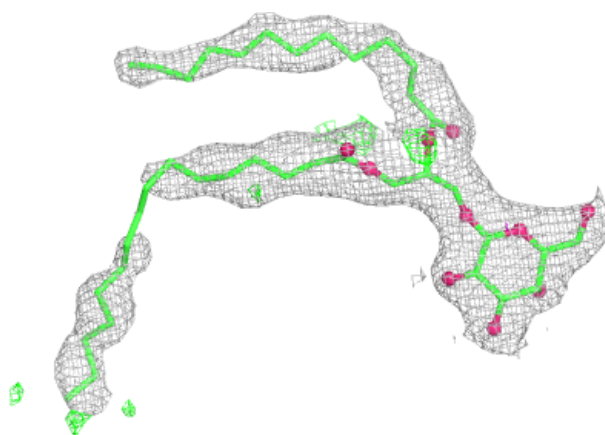


Electron density around STE D 413:

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

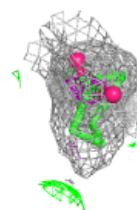
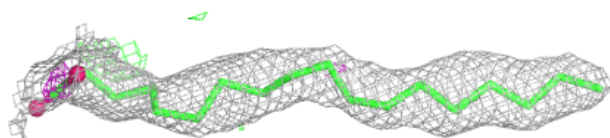
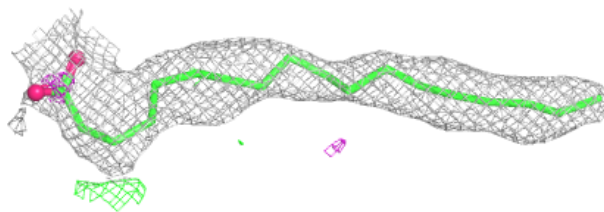
**Electron density around LMG C 519:**

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

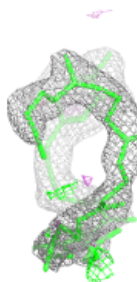
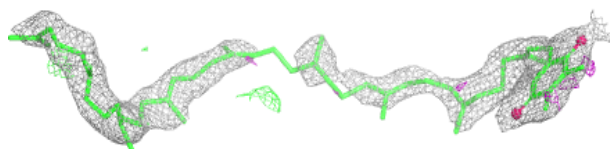
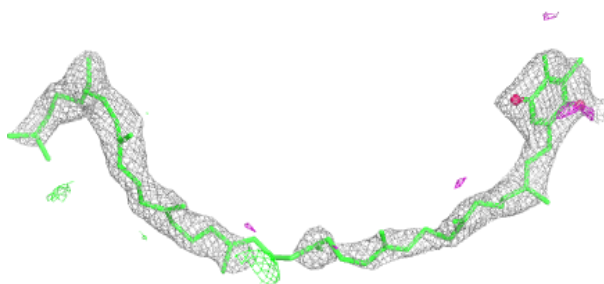


Electron density around STE c 521:

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

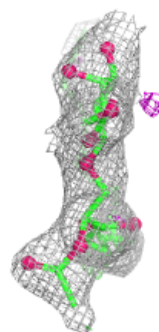
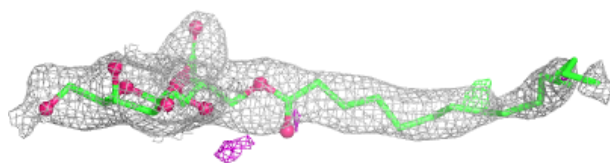
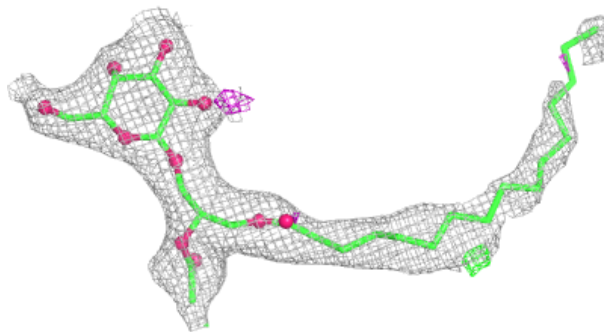
**Electron density around PL9 a 611:**

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

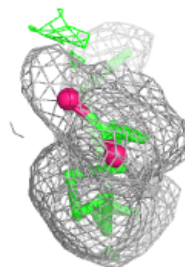
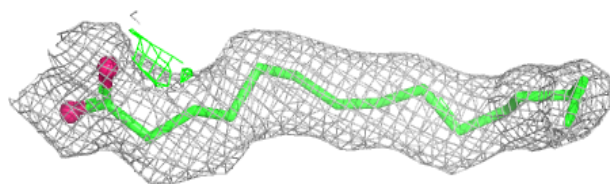
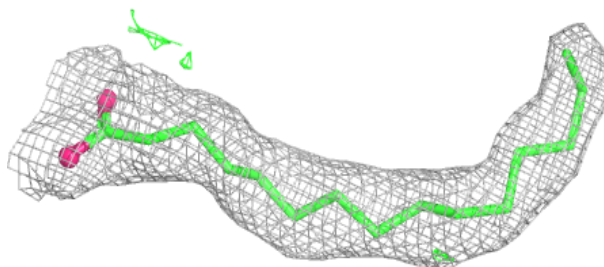


Electron density around LMG c 520:

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

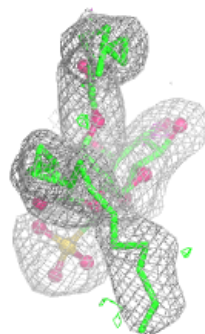
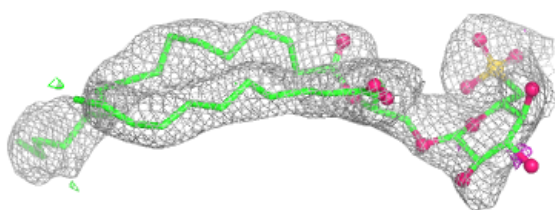
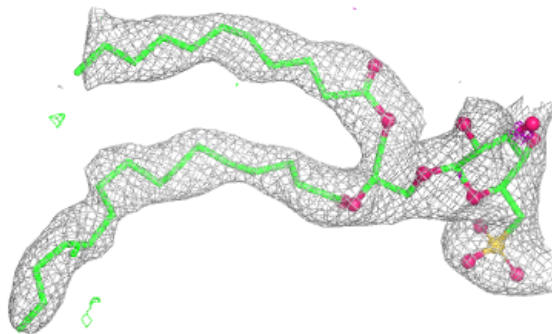
**Electron density around STE B 619:**

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

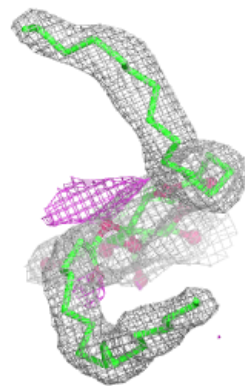
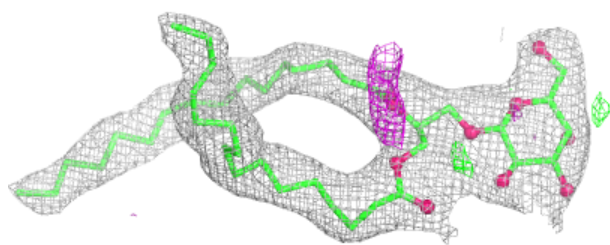
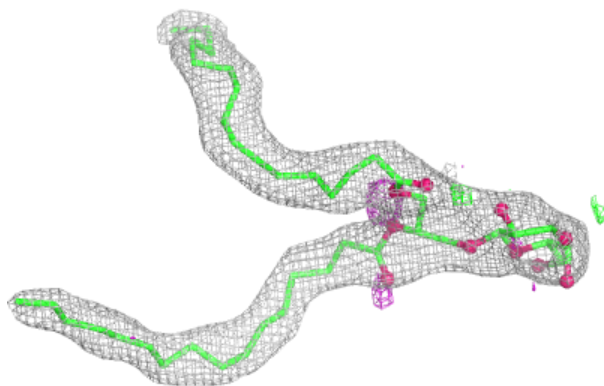


Electron density around SQD b 619:

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

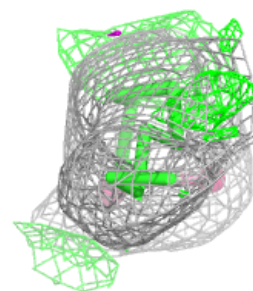
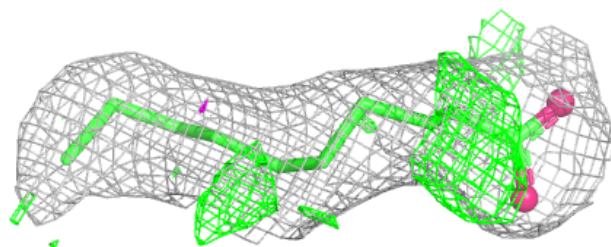
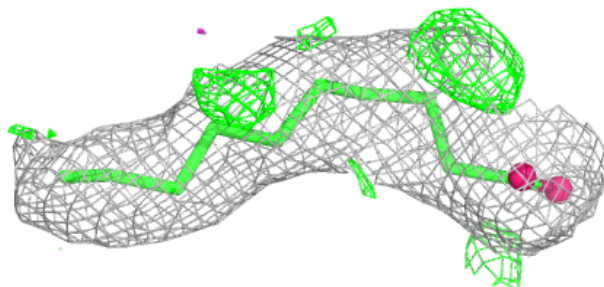
**Electron density around LMG b 620:**

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

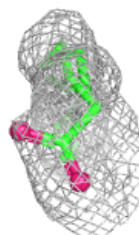
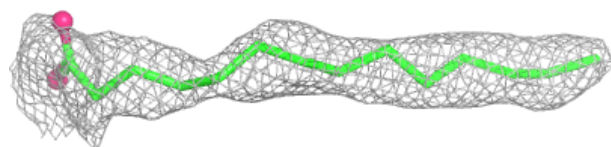
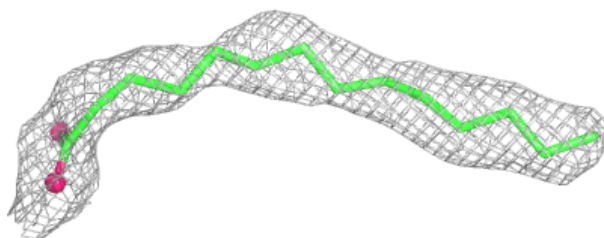


Electron density around STE B 622:

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

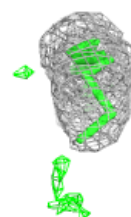
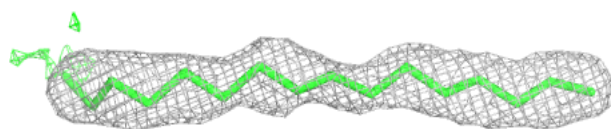
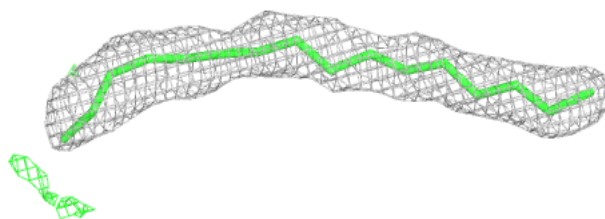
**Electron density around STE b 624:**

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

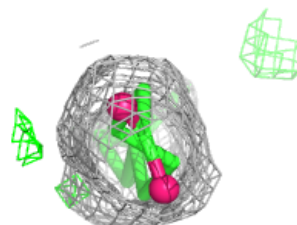
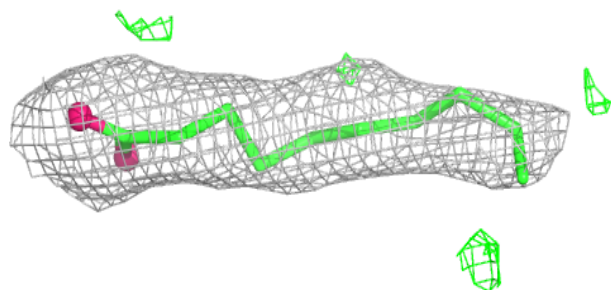
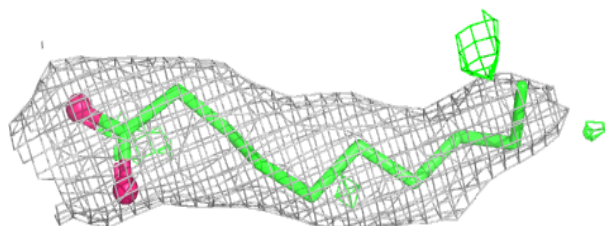


Electron density around STE C 522:

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

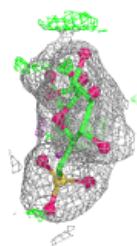
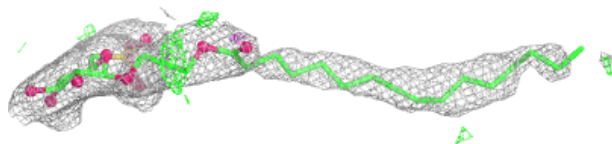
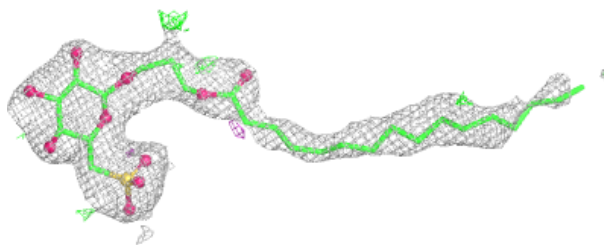
**Electron density around STE J 101:**

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

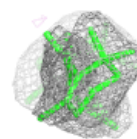
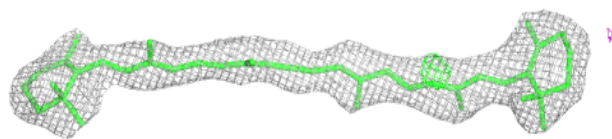
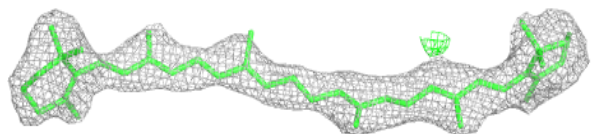


Electron density around SQD D 408:

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

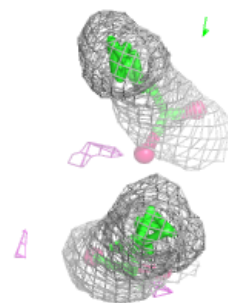
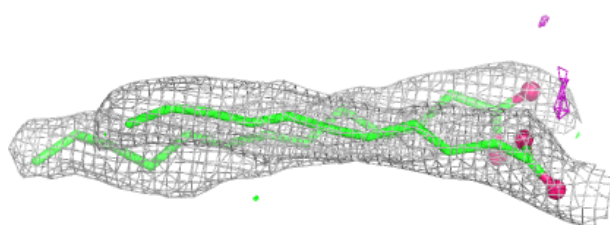
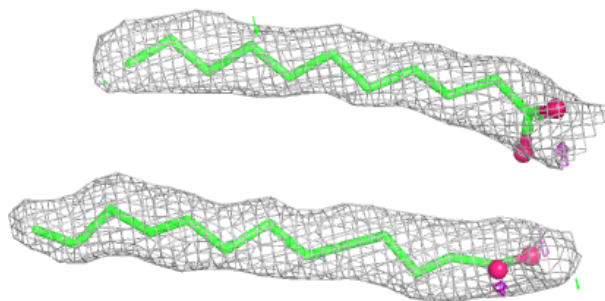
**Electron density around BCR c 514:**

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

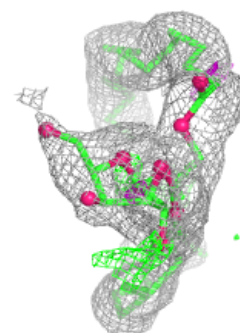
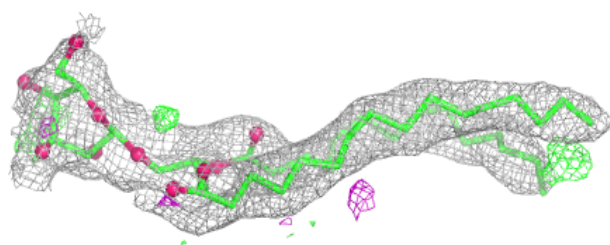
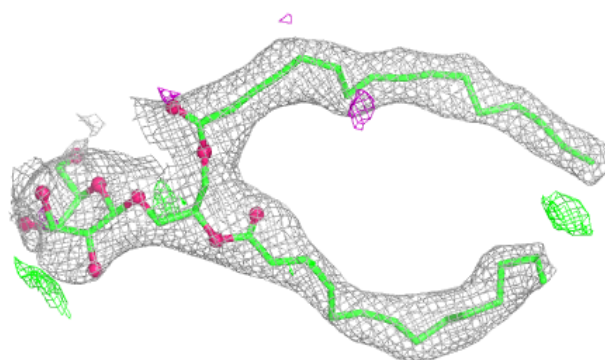


Electron density around LMG D 412:

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

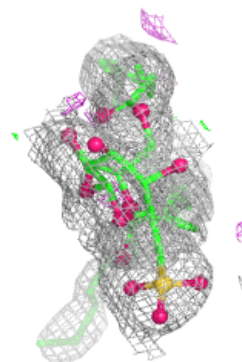
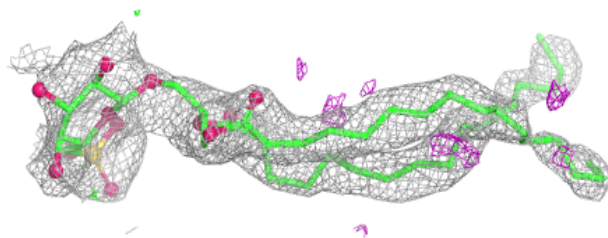
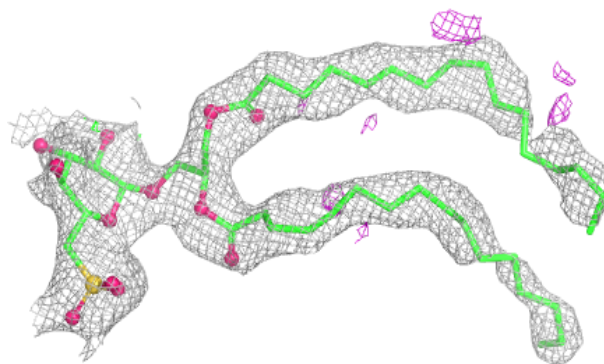
**Electron density around LMG c 524:**

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

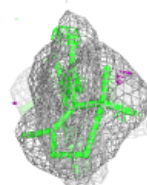
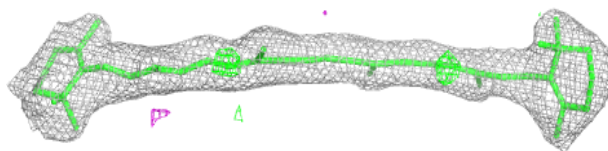
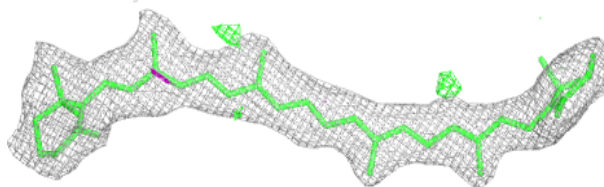


Electron density around SQD B 621:

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

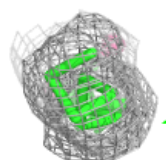
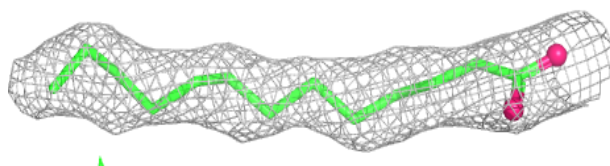
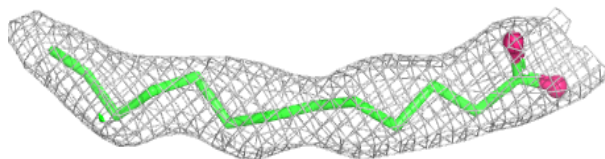
**Electron density around BCR Y 101:**

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

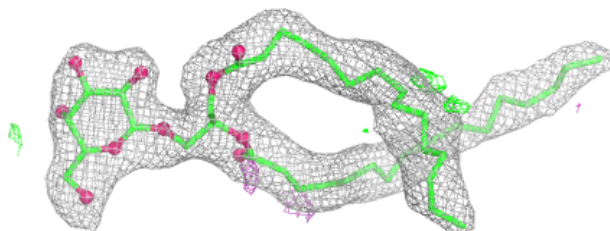
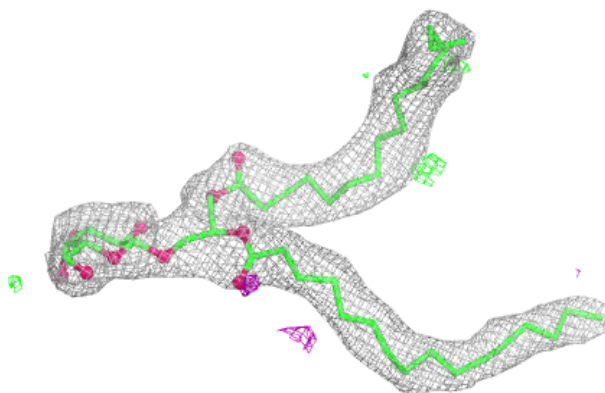


Electron density around STE M 102:

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

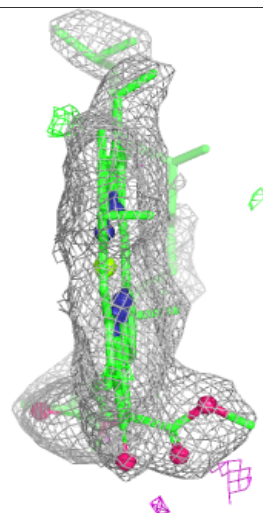
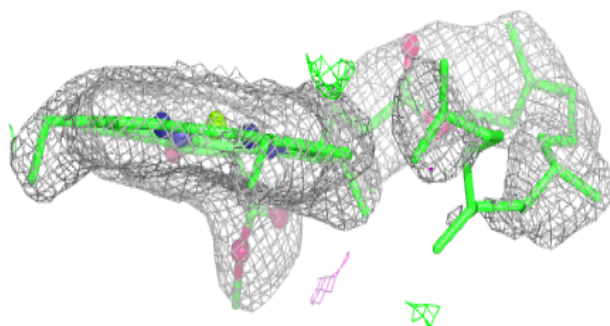
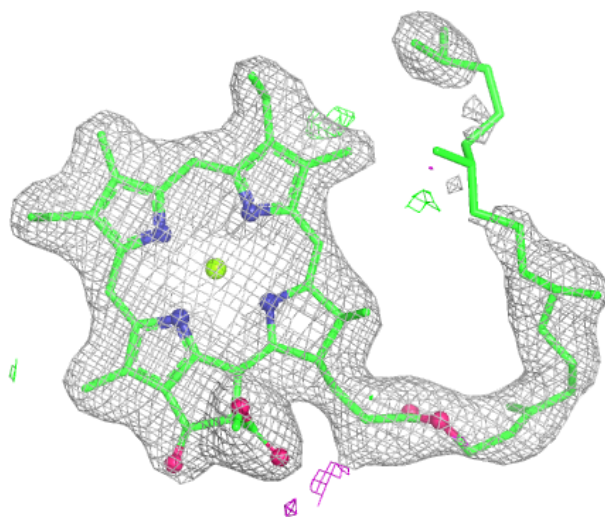
**Electron density around LMG M 101:**

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



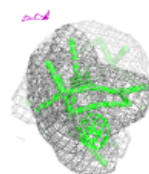
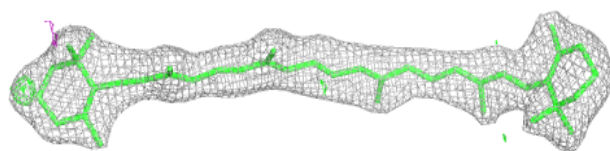
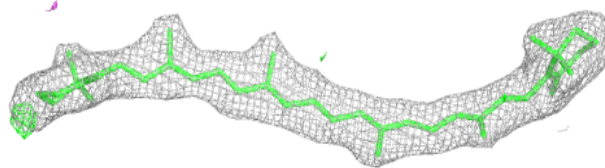
Electron density around CLA c 512:

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

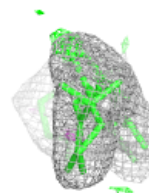
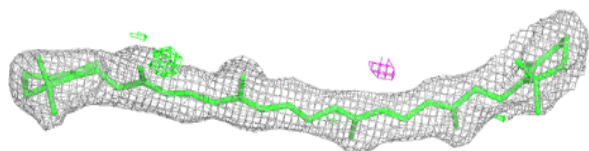
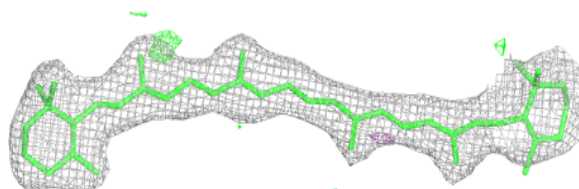


Electron density around BCR H 102:

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

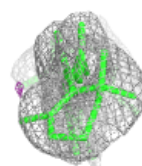
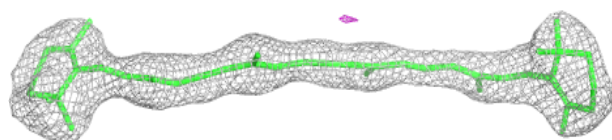
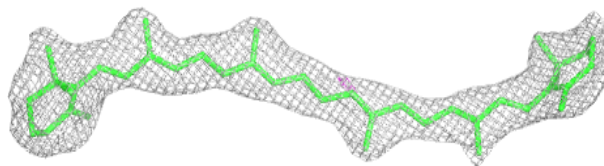
**Electron density around BCR d 405:**

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

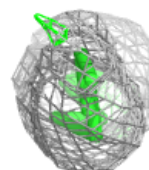
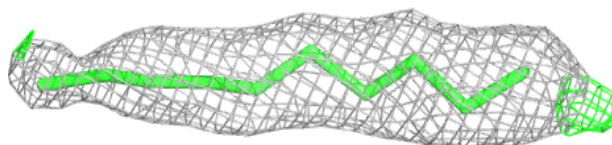
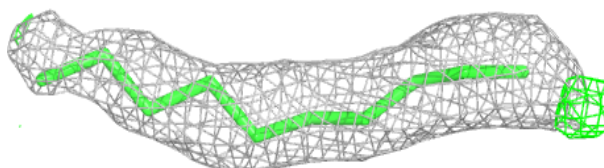


Electron density around BCR k 101:

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

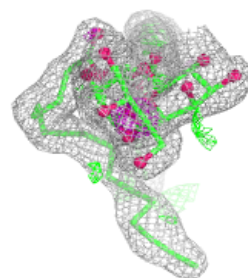
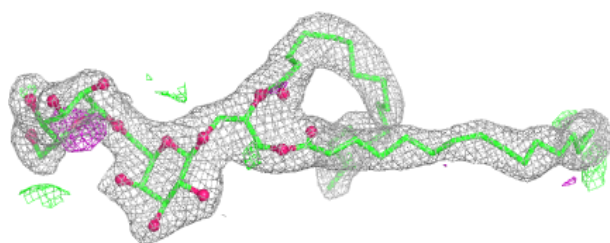
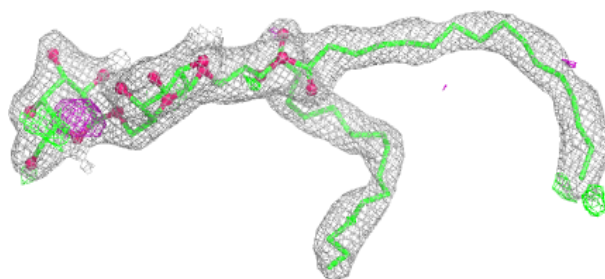
**Electron density around STE M 103:**

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

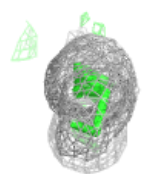
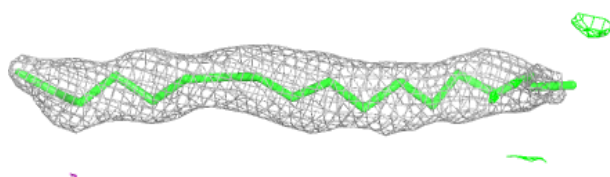
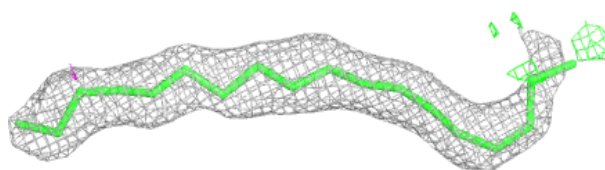


Electron density around DGD H 103:

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

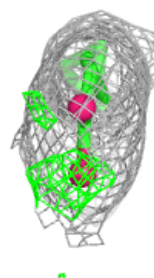
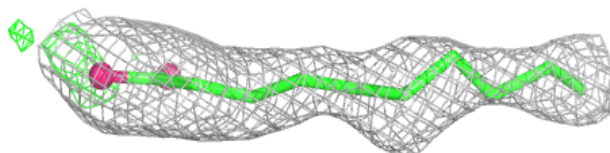
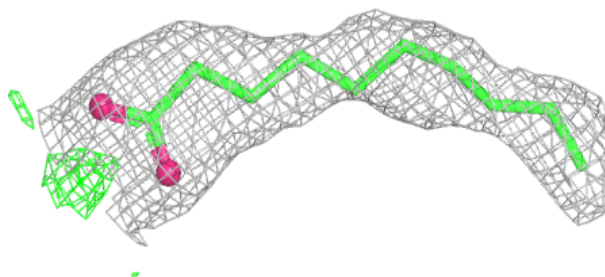
**Electron density around STE I 102:**

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

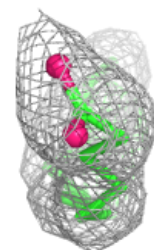
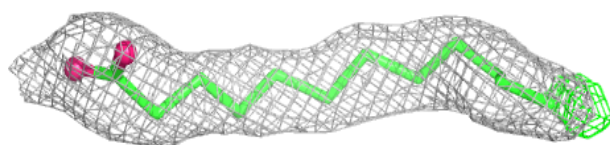
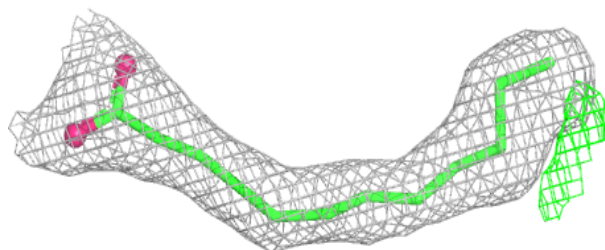


Electron density around STE C 521:

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

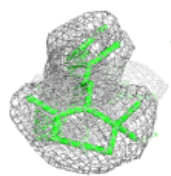
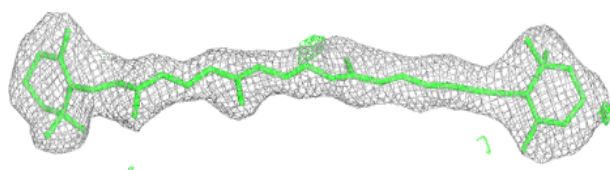
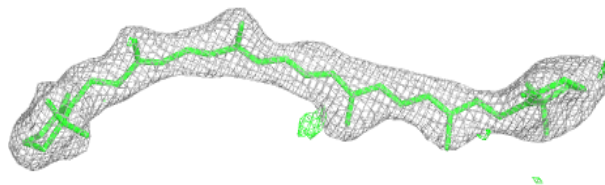
**Electron density around STE t 102:**

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

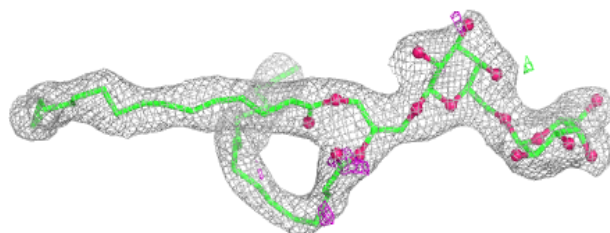
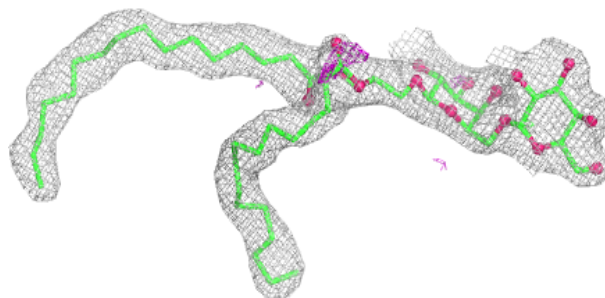


Electron density around BCR x 101:

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

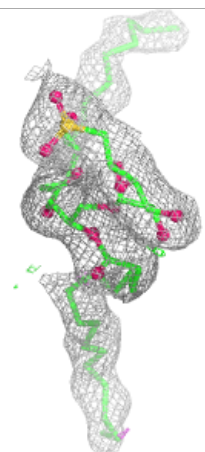
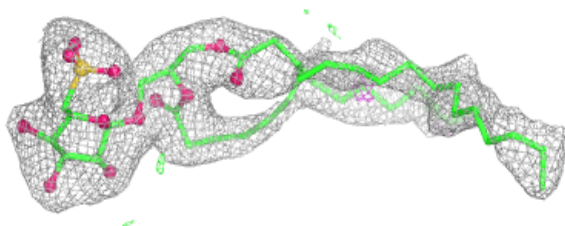
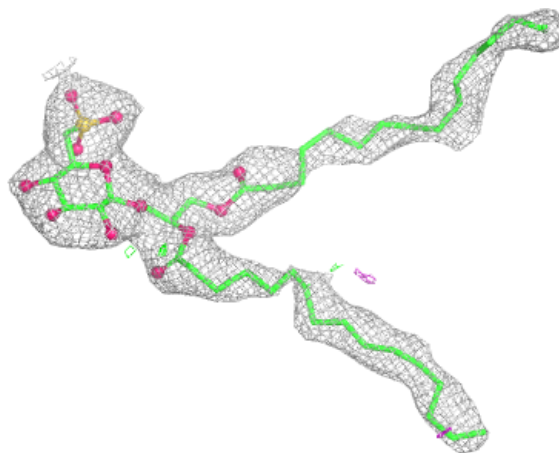
**Electron density around DGD h 102:**

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



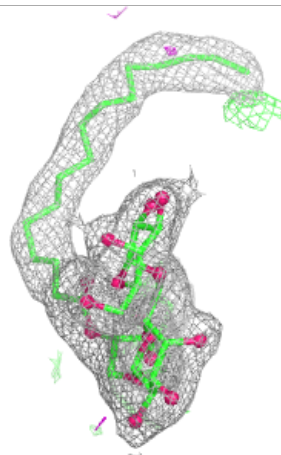
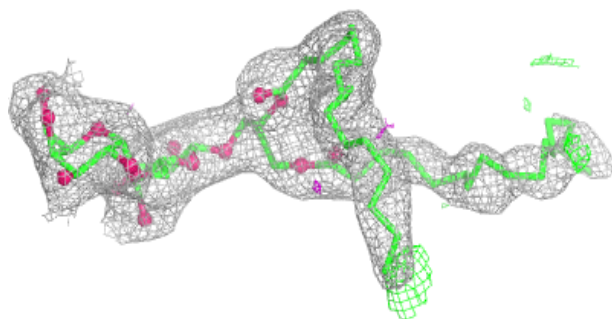
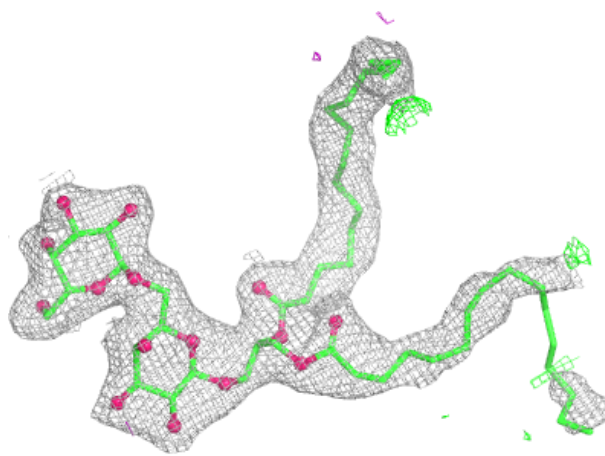
Electron density around SQD a 613:

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



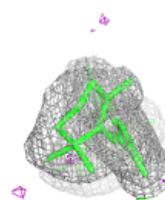
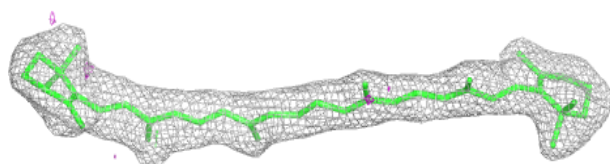
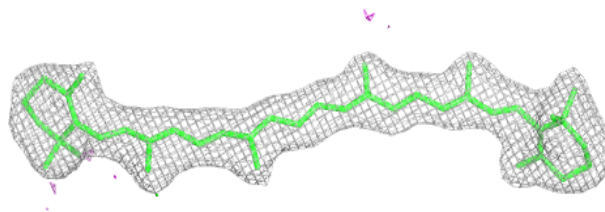
Electron density around DGD C 517:

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

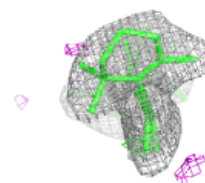
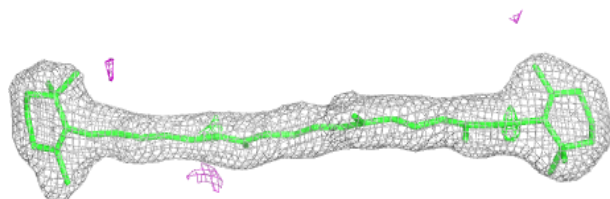
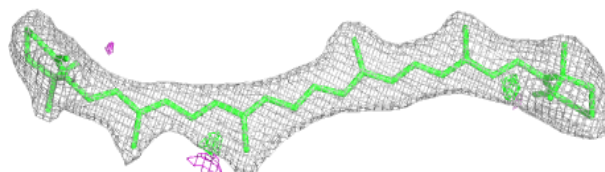


Electron density around BCR B 618:

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

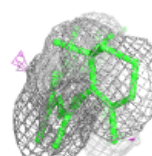
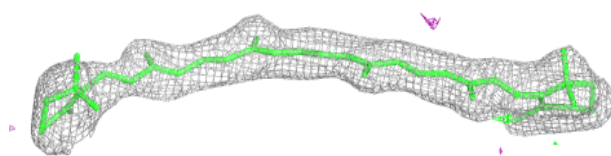
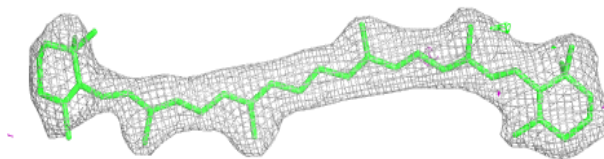
**Electron density around BCR C 514:**

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

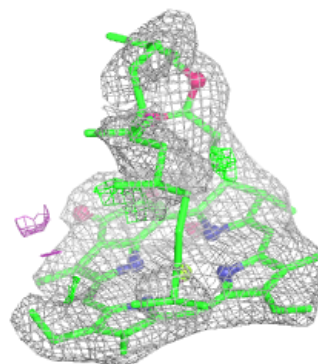
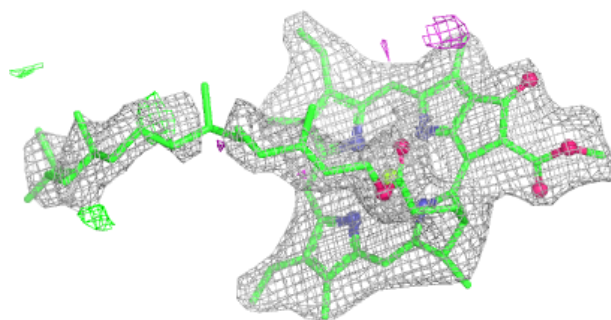
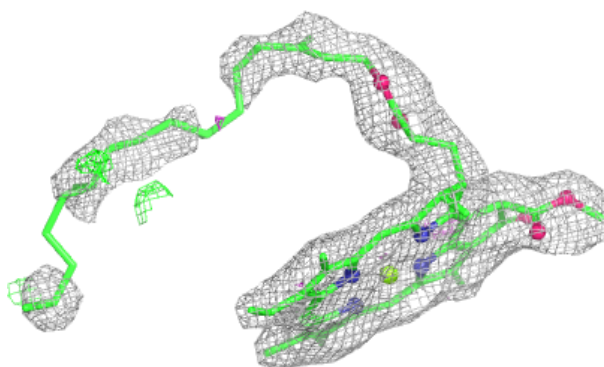


Electron density around BCR D 405:

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

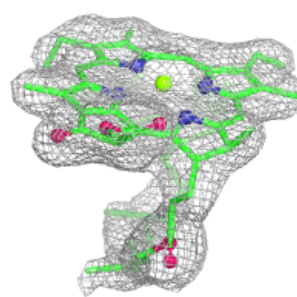
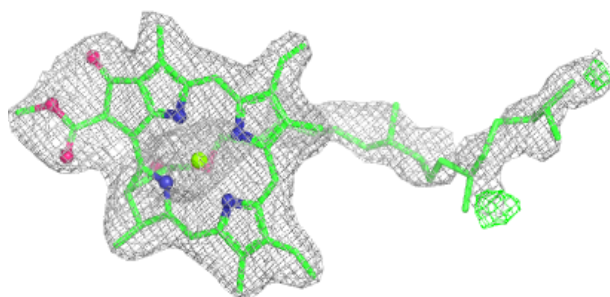
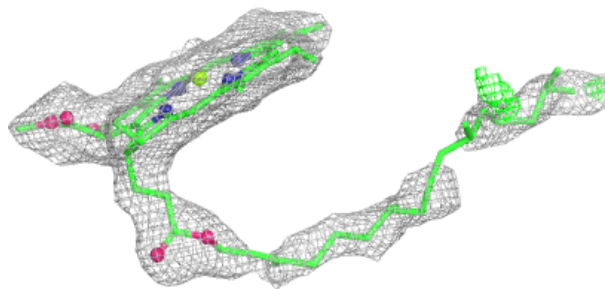
**Electron density around CLA c 513:**

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

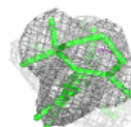
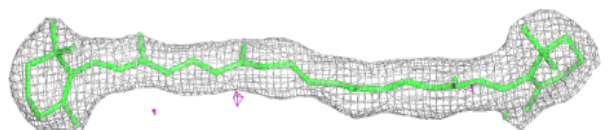


Electron density around CLA C 513:

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

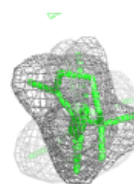
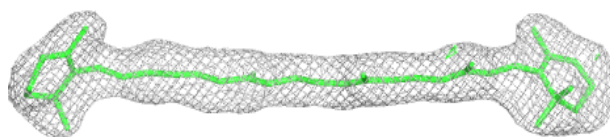
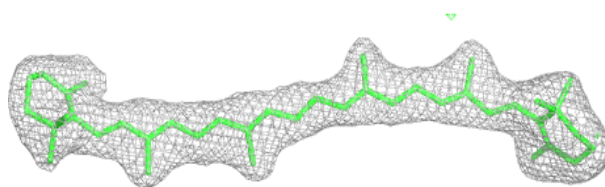
**Electron density around BCR Z 101:**

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

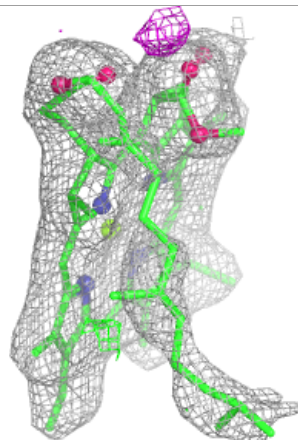
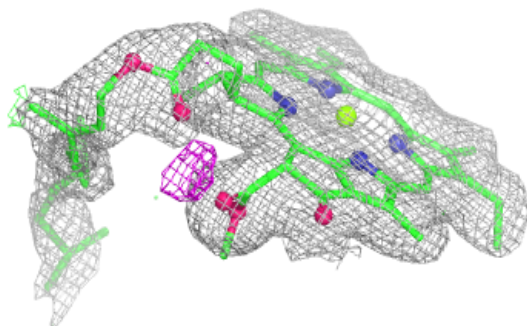
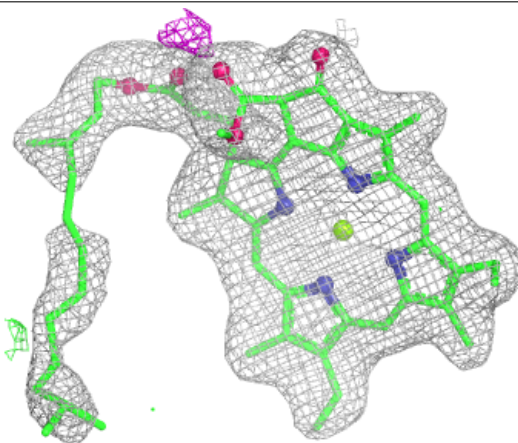


Electron density around BCR b 617:

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

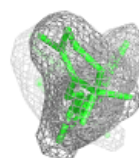
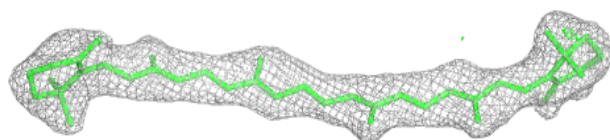
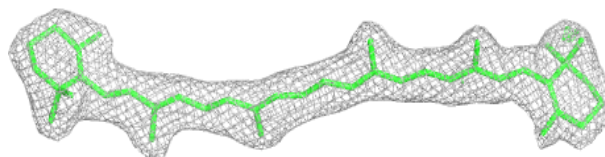
**Electron density around CLA b 615:**

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

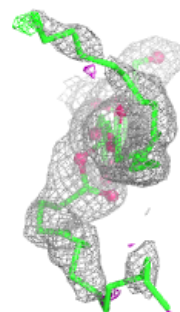
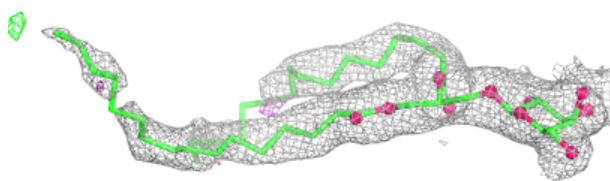
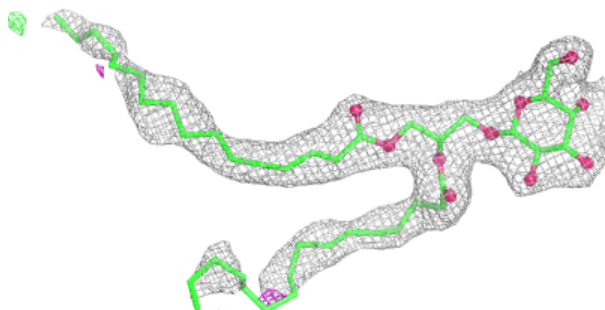


Electron density around BCR b 618:

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

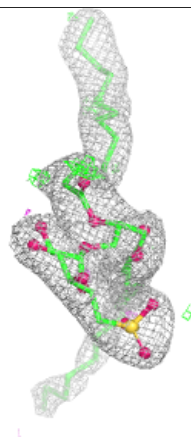
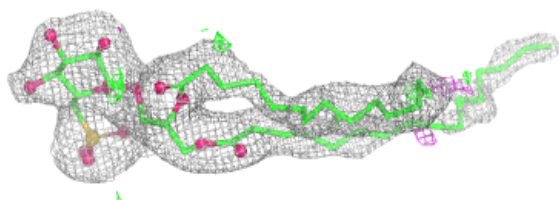
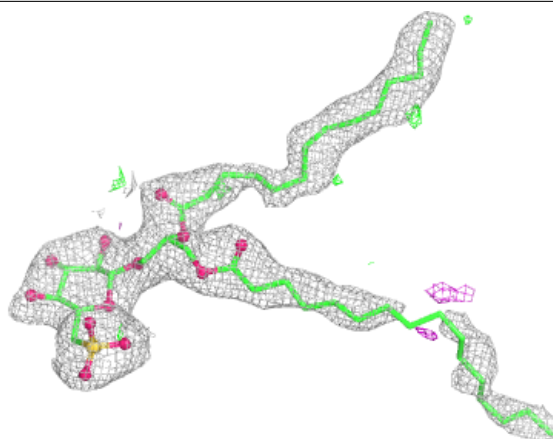
**Electron density around LMG D 407:**

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

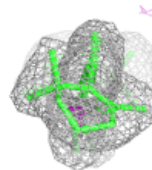
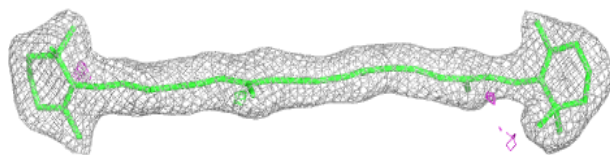
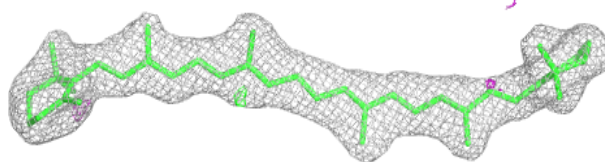


Electron density around SQD A 613:

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

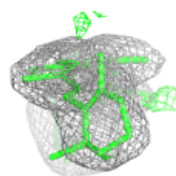
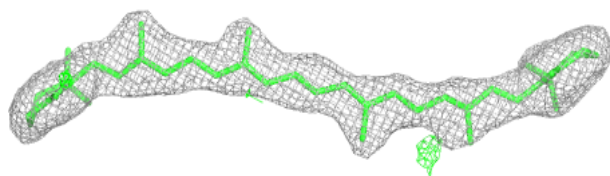
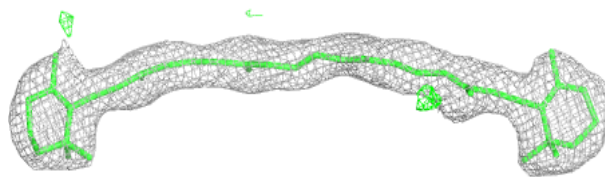
**Electron density around BCR A 610:**

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

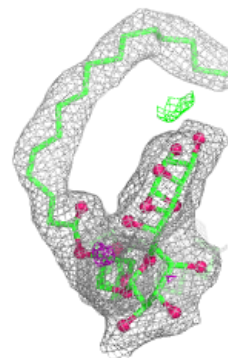
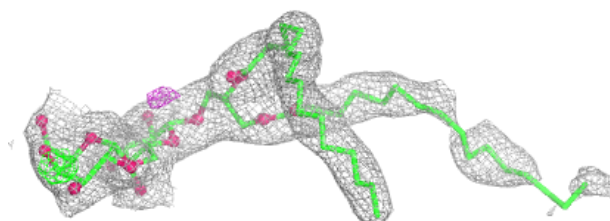


Electron density around BCR c 516:

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

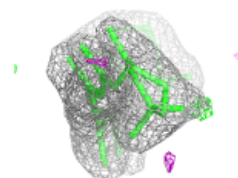
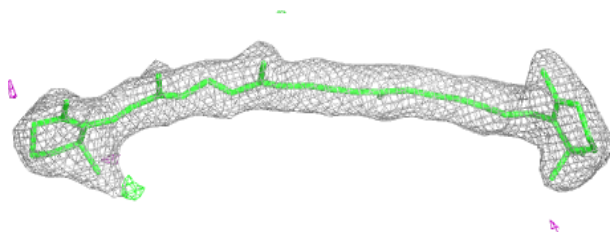
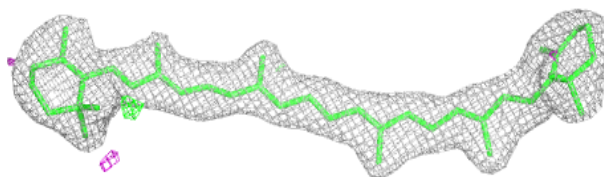
**Electron density around DGD c 518:**

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



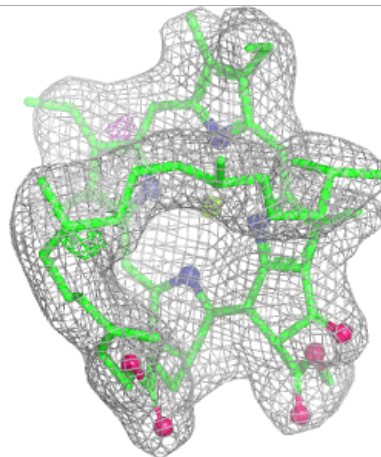
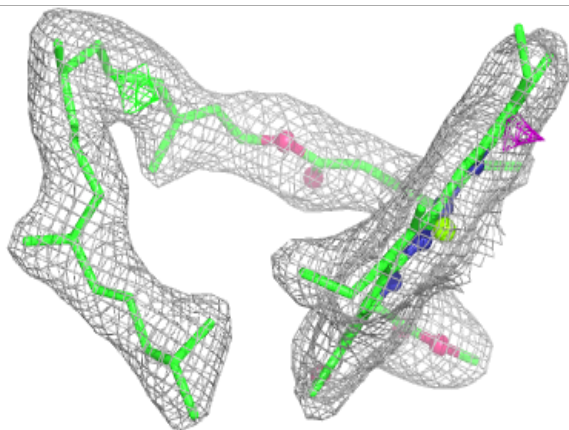
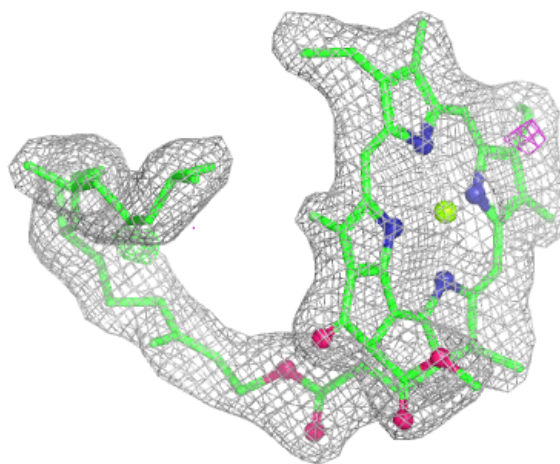
Electron density around BCR T 101:

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



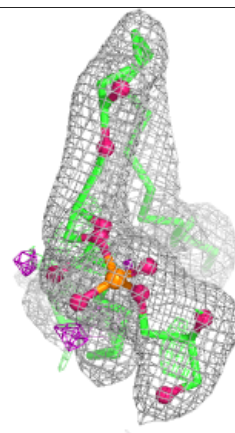
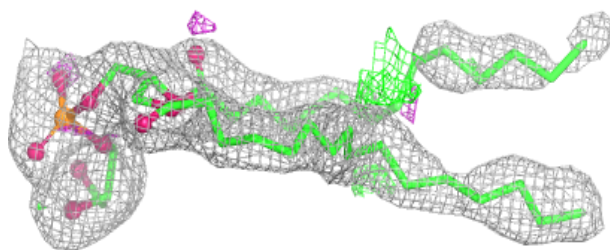
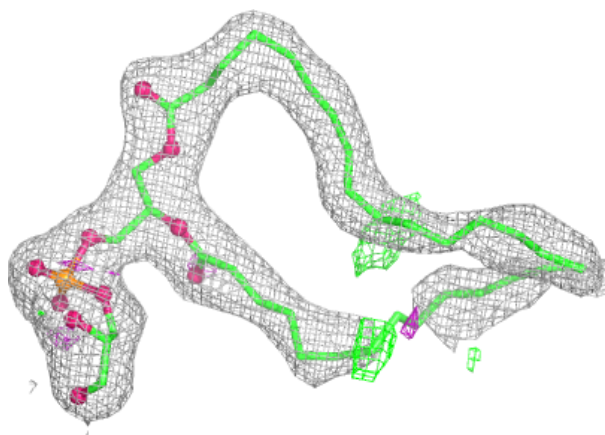
Electron density around CLA C 503:

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

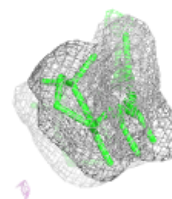
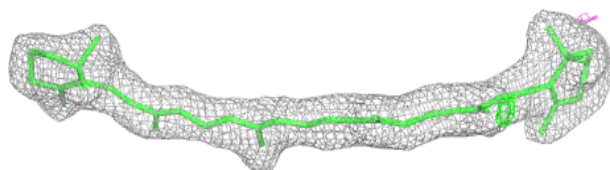
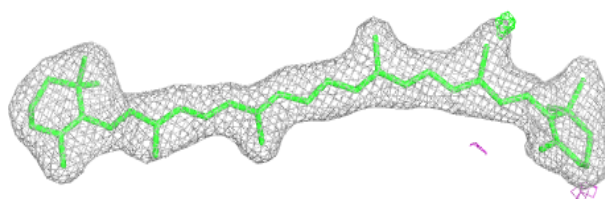


Electron density around LHG D 410:

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

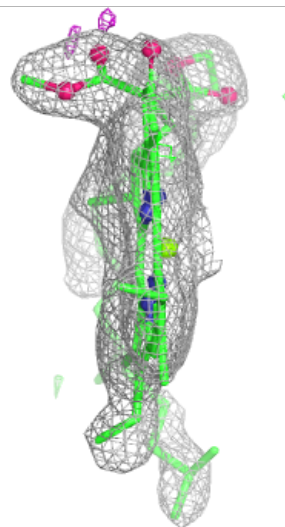
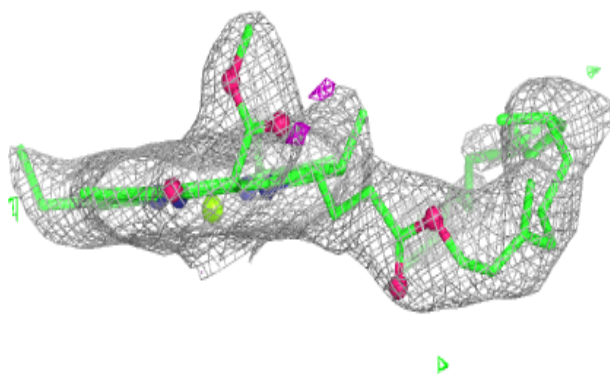
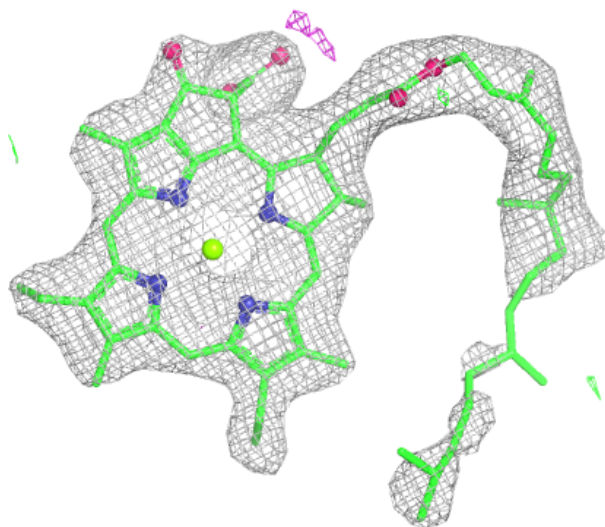
**Electron density around BCR t 101:**

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



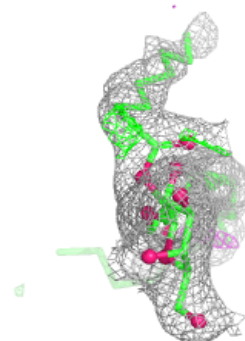
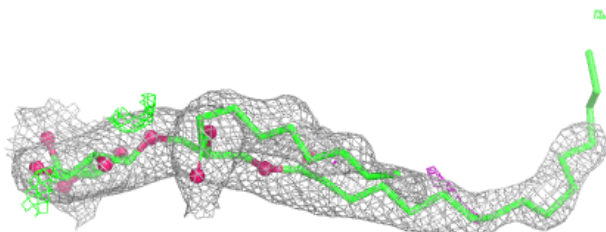
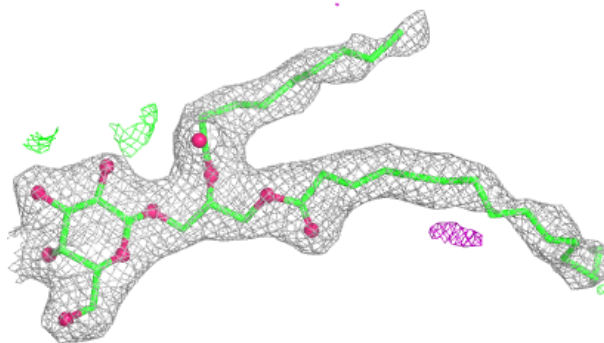
Electron density around CLA C 512:

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

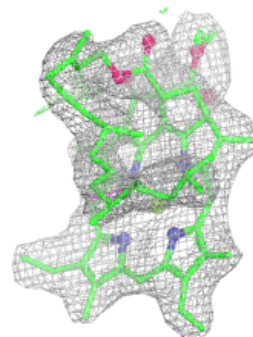
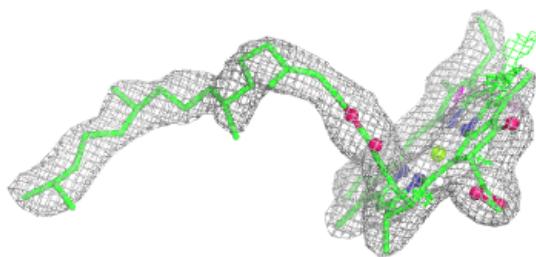
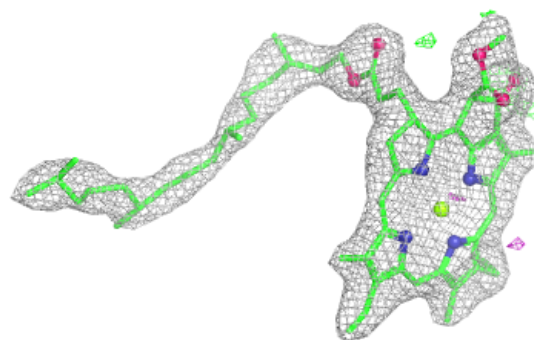


Electron density around LMG d 410:

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

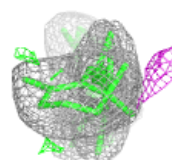
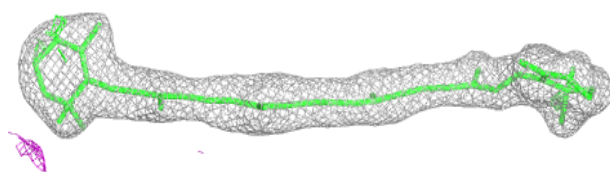
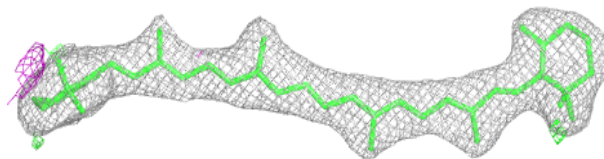
**Electron density around CLA c 511:**

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

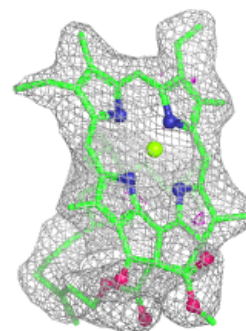
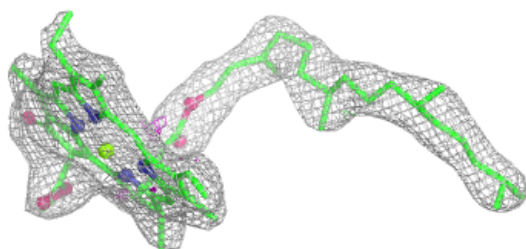
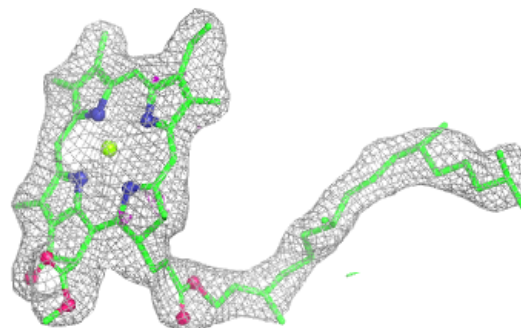


Electron density around BCR b 616:

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

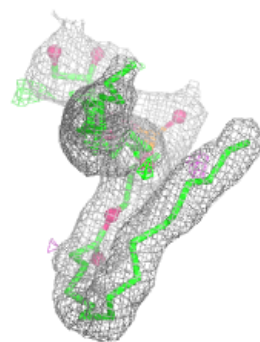
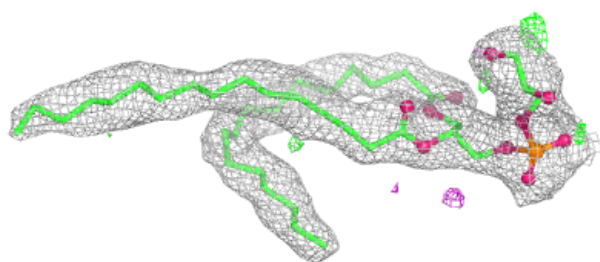
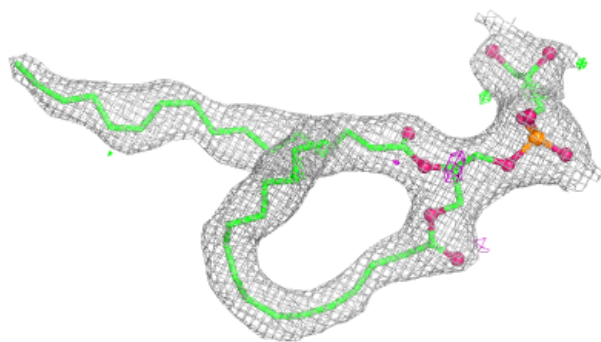
**Electron density around CLA C 511:**

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



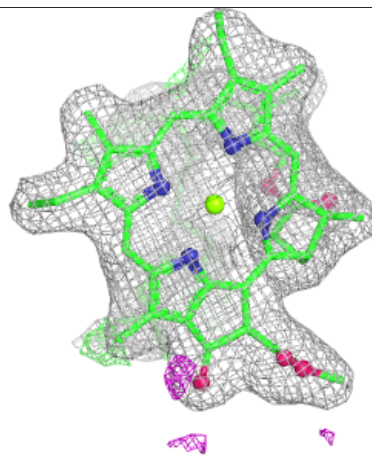
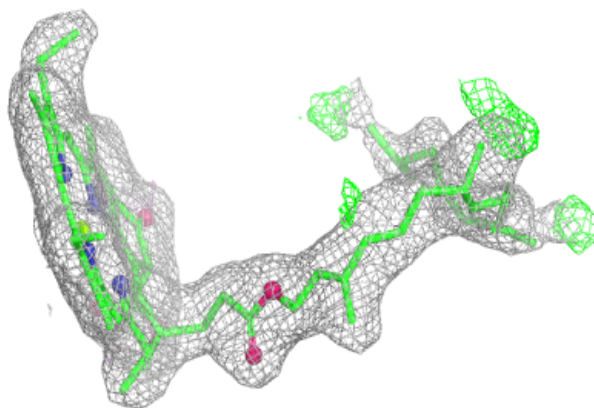
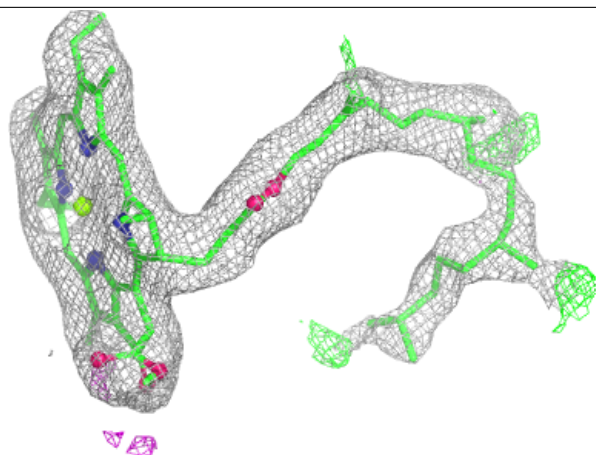
Electron density around LHG B 620:

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



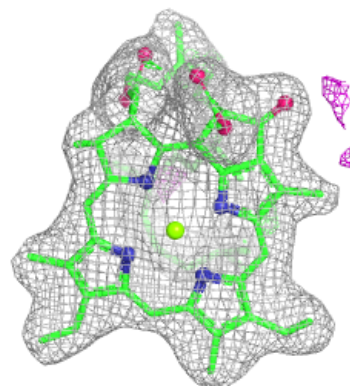
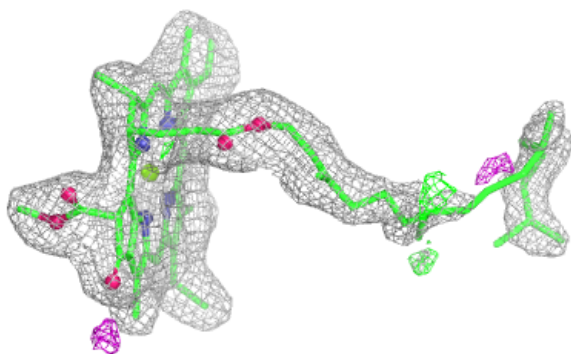
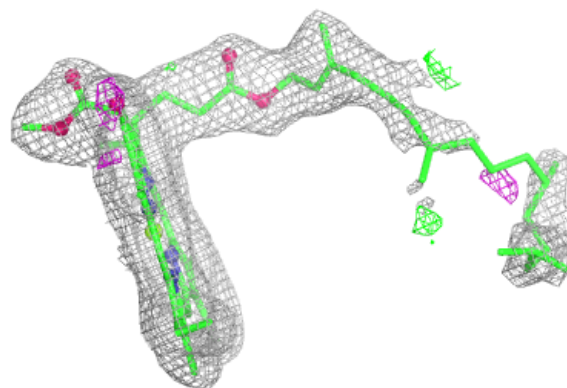
Electron density around CLA B 605:

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

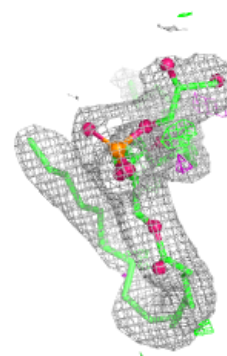
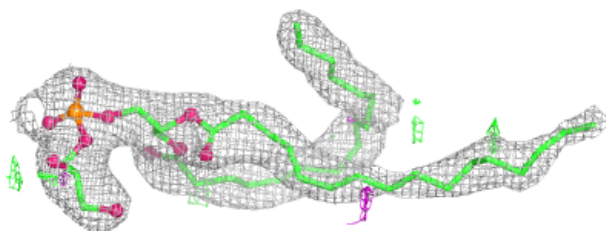
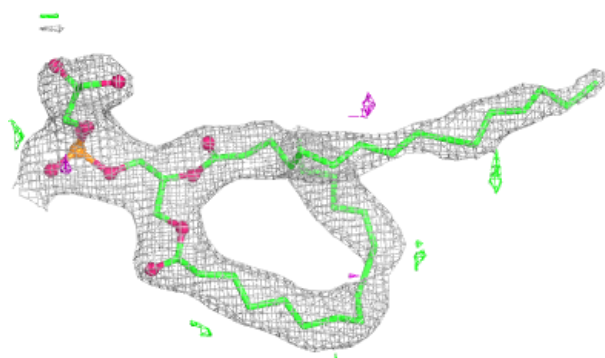


Electron density around CLA C 506:

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

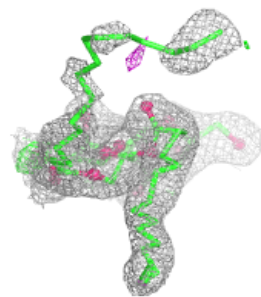
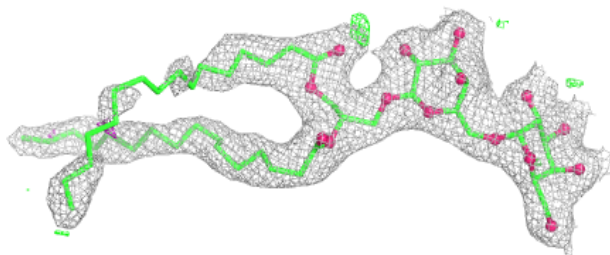
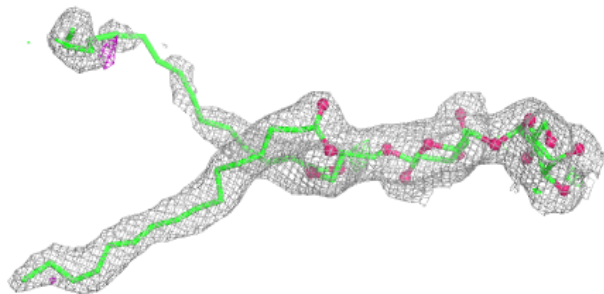
**Electron density around LHG b 623:**

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

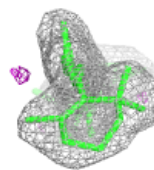
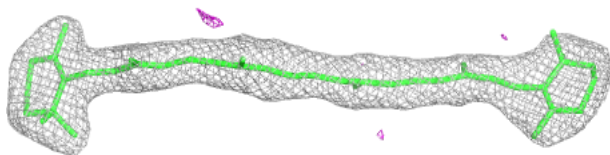
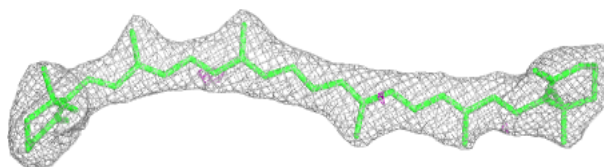


Electron density around DGD C 516:

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

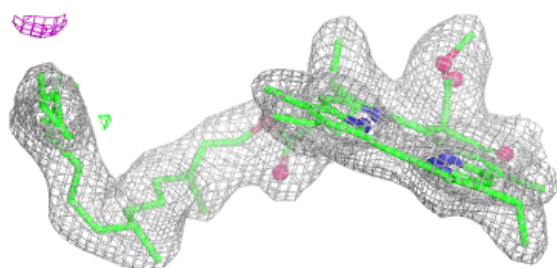
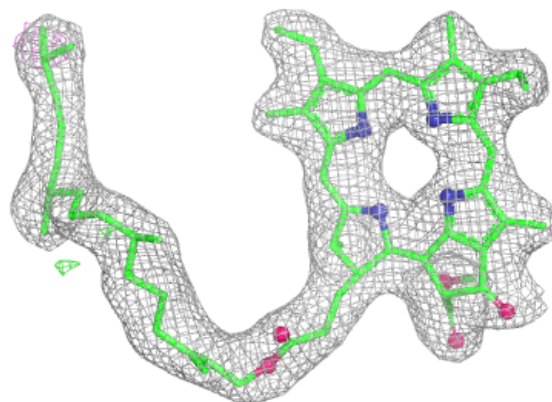
**Electron density around BCR c 515:**

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

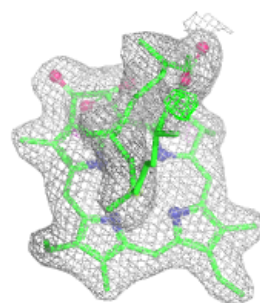
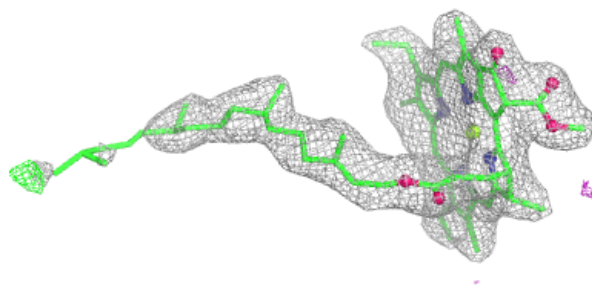
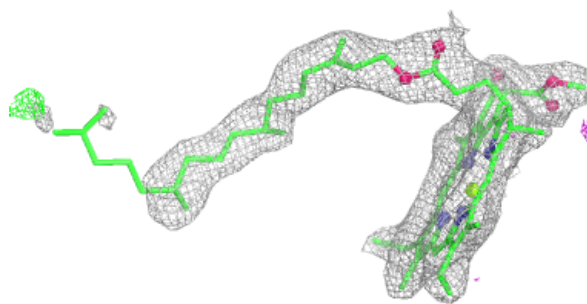


Electron density around PHO d 402:

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

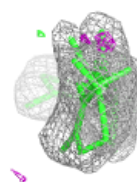
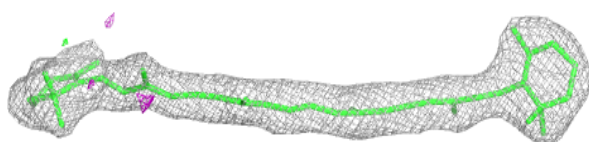
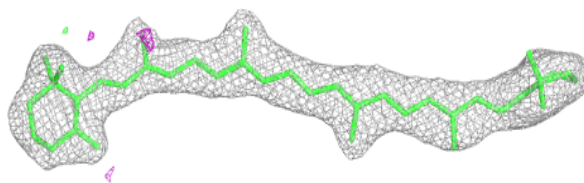
**Electron density around CLA C 508:**

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

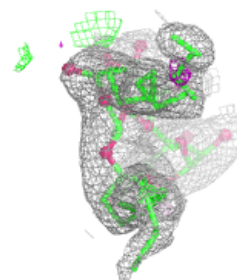
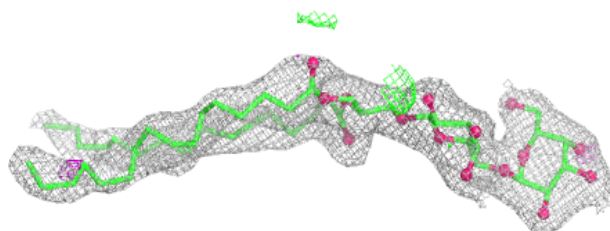
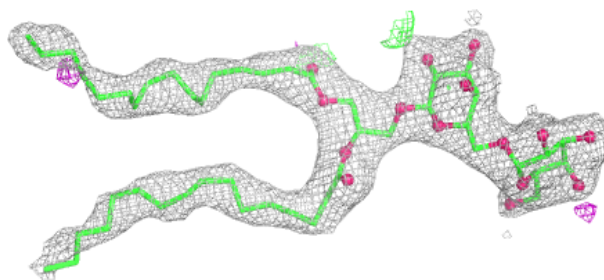


Electron density around BCR B 616:

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

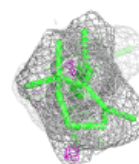
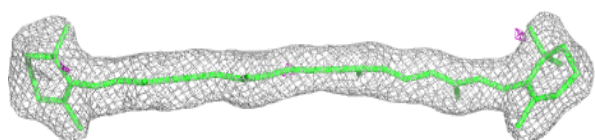
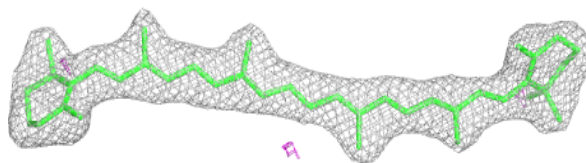
**Electron density around DGD c 519:**

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

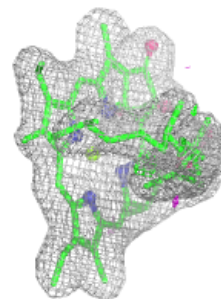
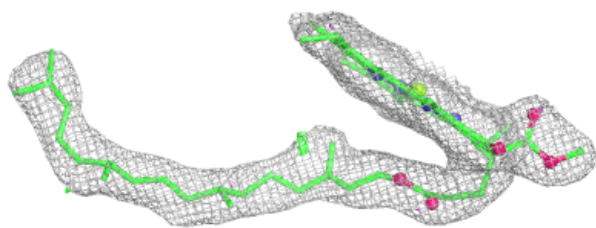
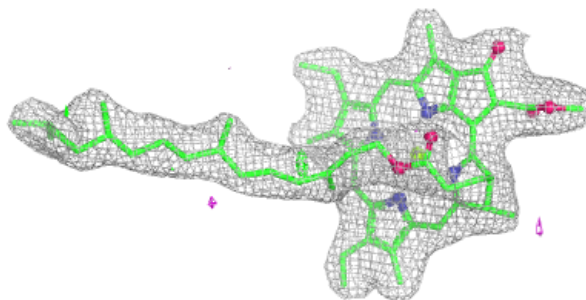


Electron density around BCR B 617:

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

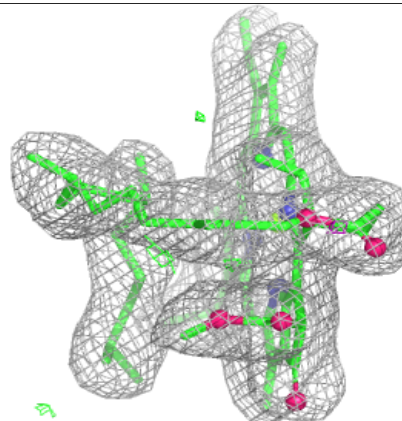
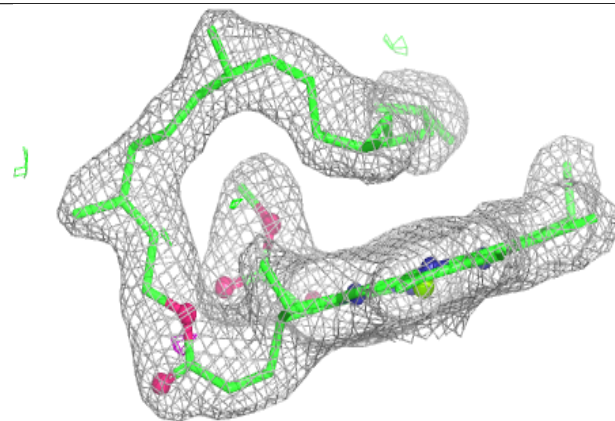
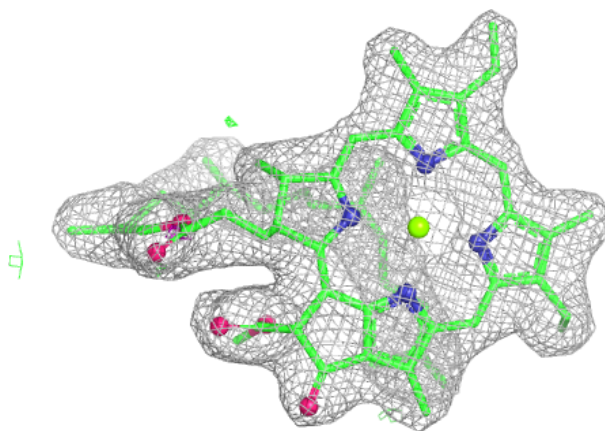
**Electron density around CLA b 607:**

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

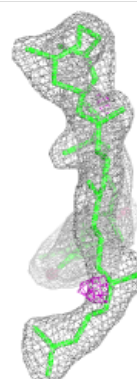
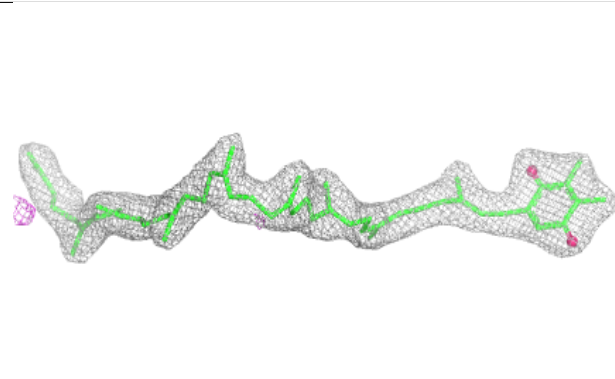
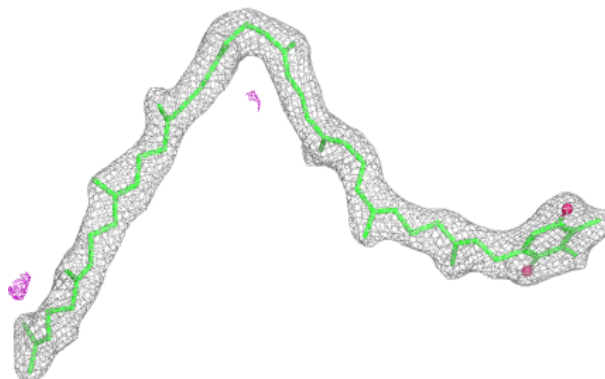


Electron density around CLA C 510:

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

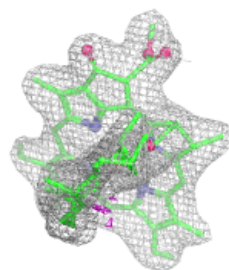
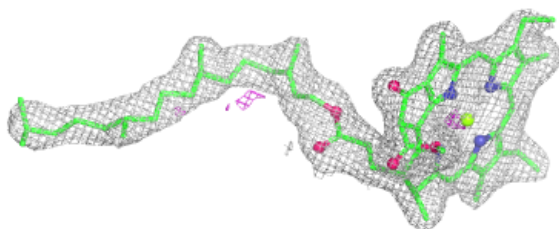
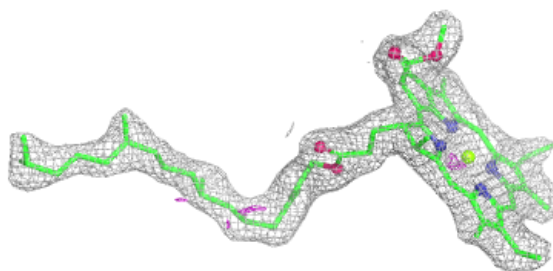
**Electron density around PL9 D 406:**

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



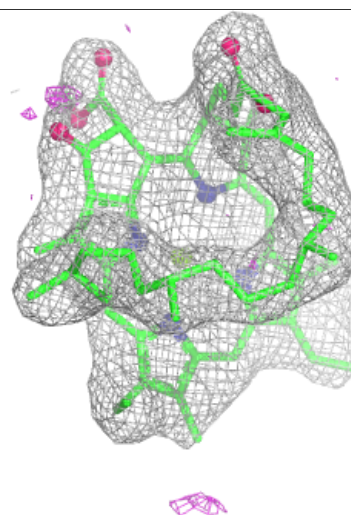
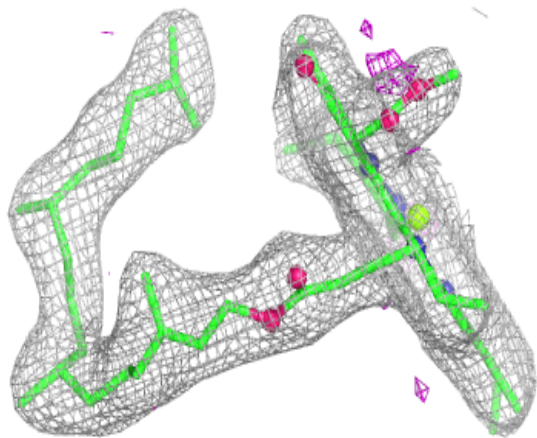
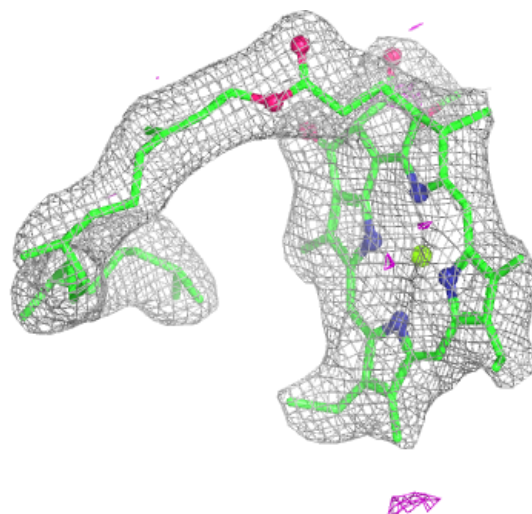
Electron density around CLA c 502:

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



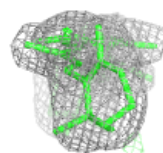
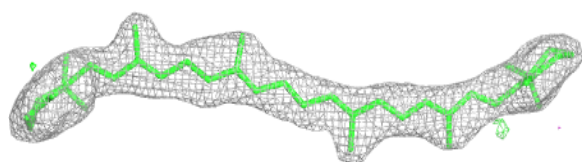
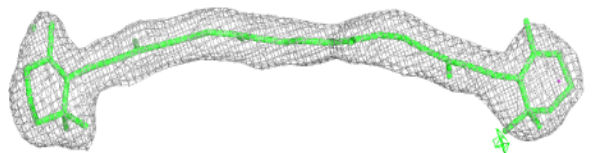
Electron density around CLA c 503:

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

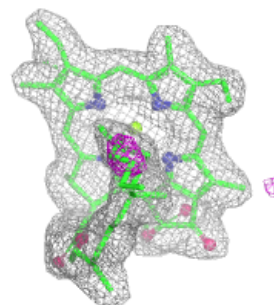
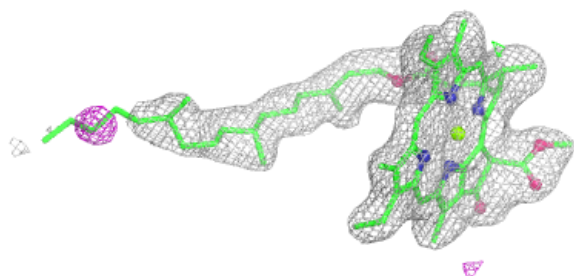
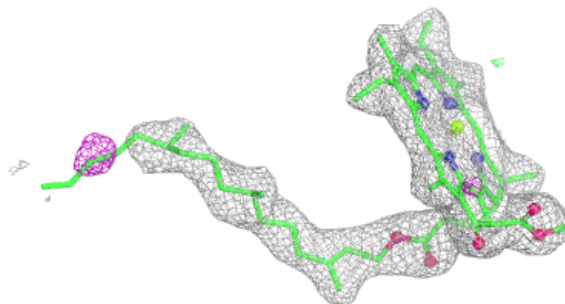


Electron density around BCR K 101:

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

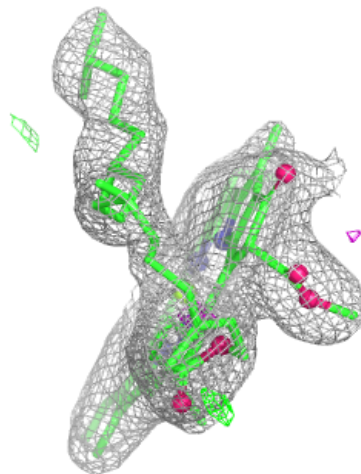
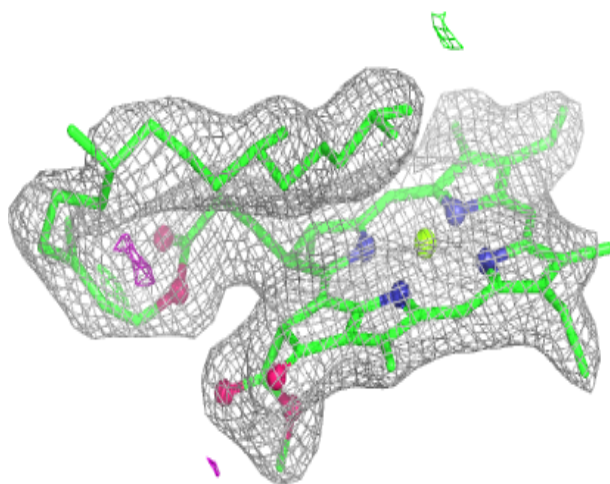
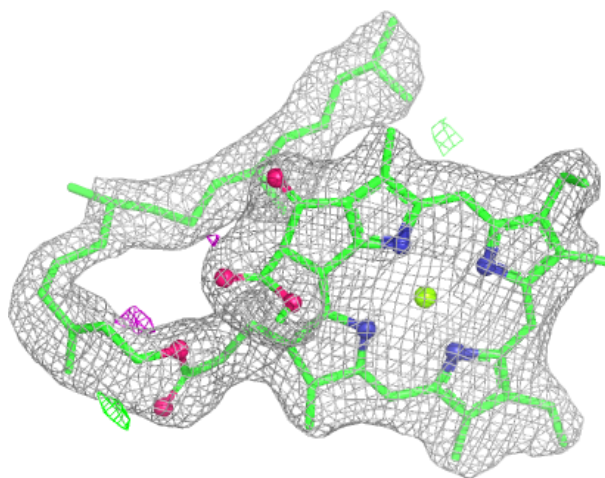
**Electron density around CLA c 508:**

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



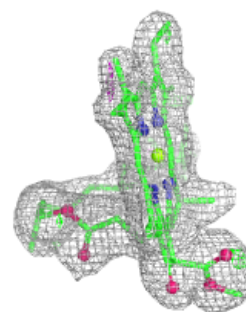
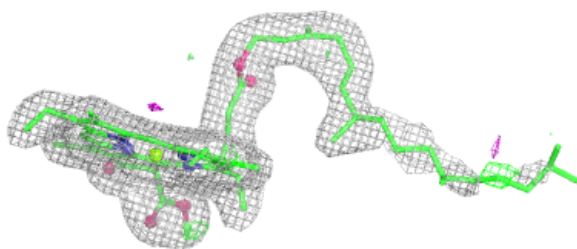
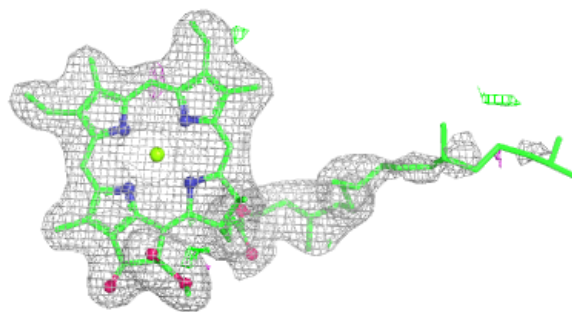
Electron density around CLA c 509:

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



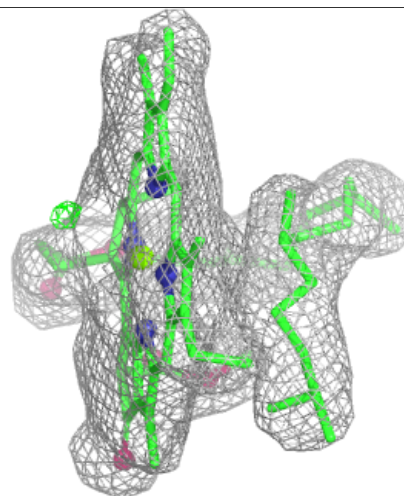
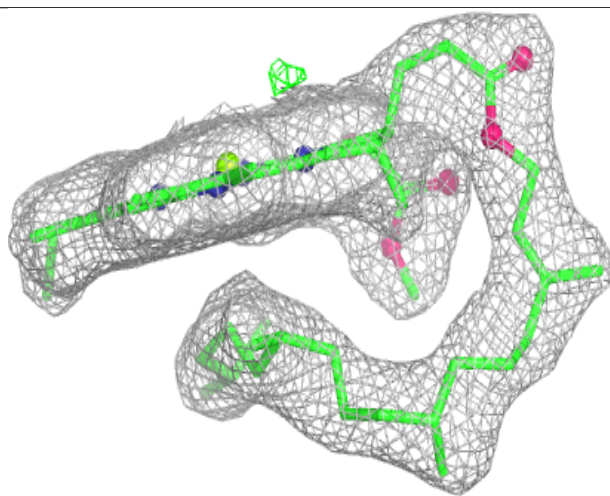
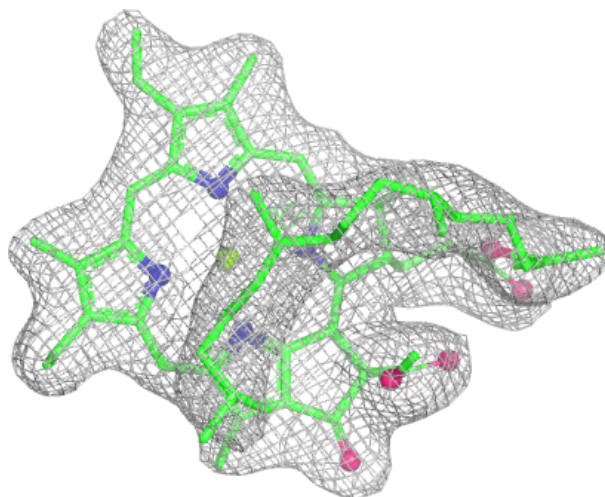
Electron density around CLA A 607:

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



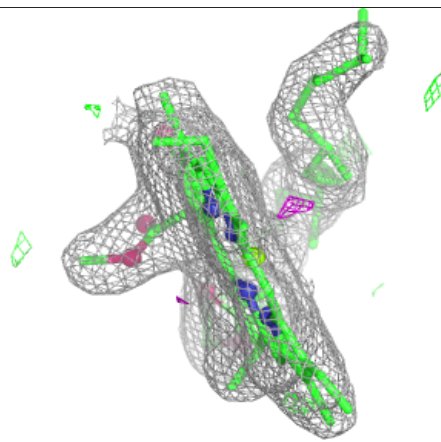
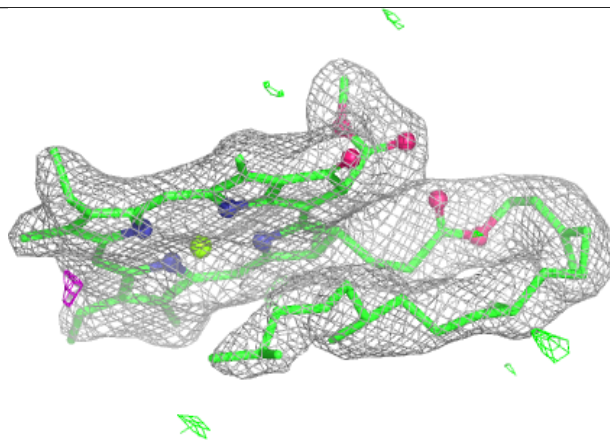
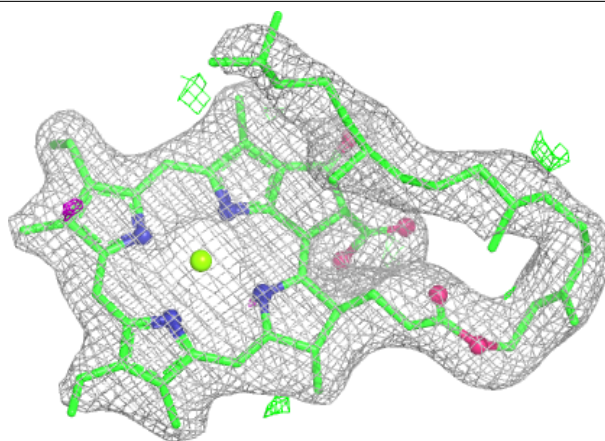
Electron density around CLA c 510:

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

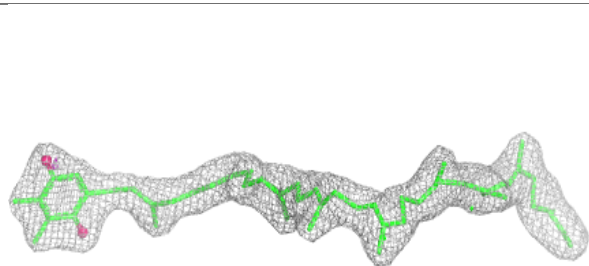
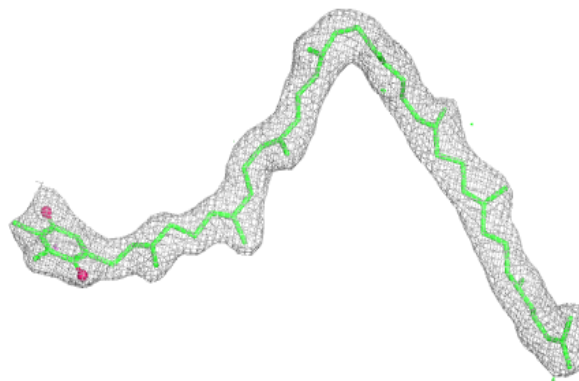


Electron density around CLA C 509:

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

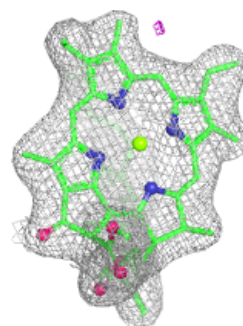
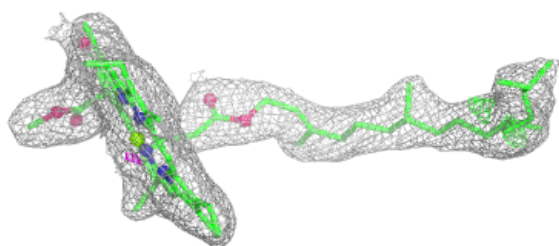
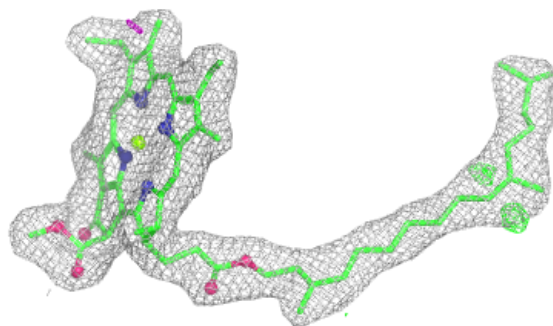
**Electron density around PL9 d 406:**

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



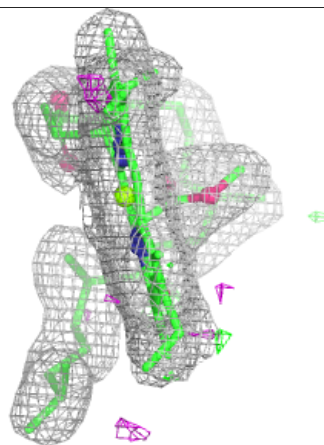
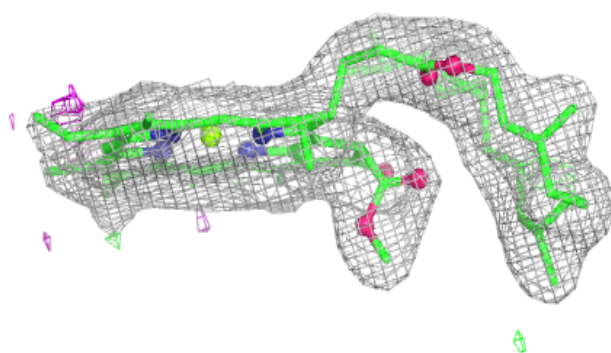
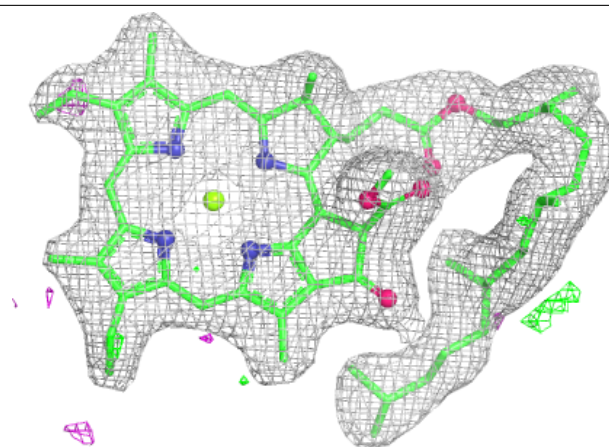
Electron density around CLA B 608:

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



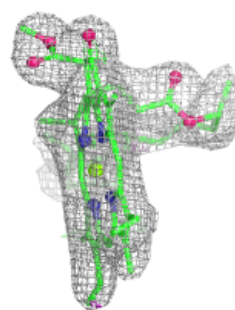
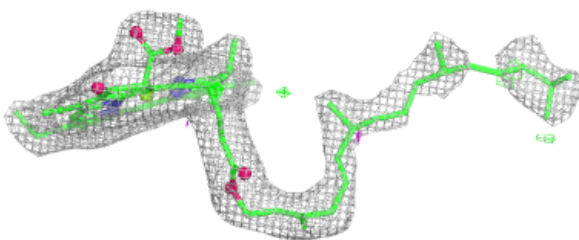
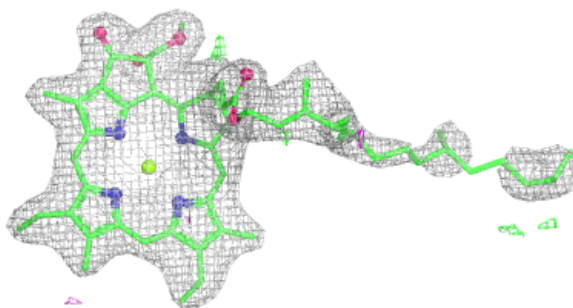
Electron density around CLA B 609:

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

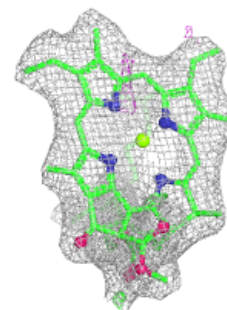
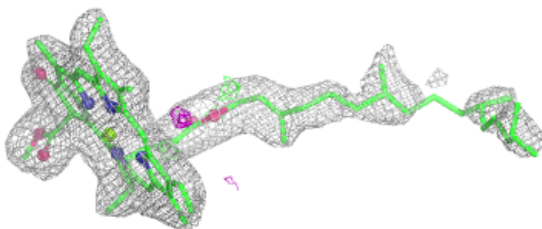
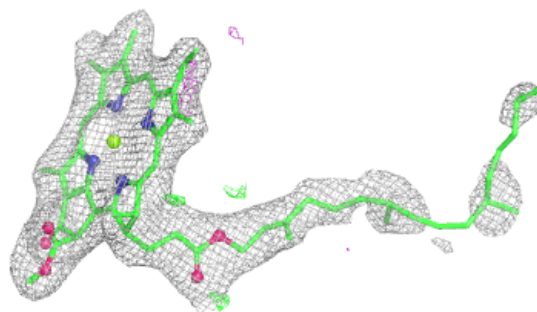


Electron density around CLA d 401:

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

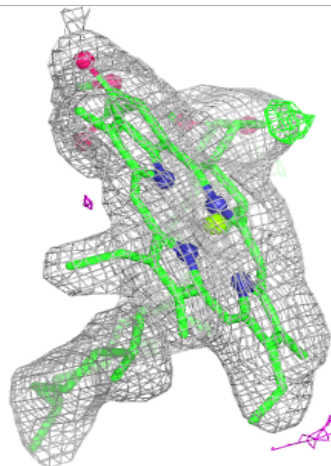
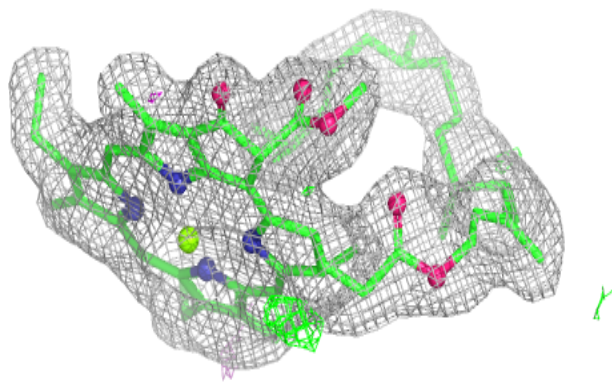
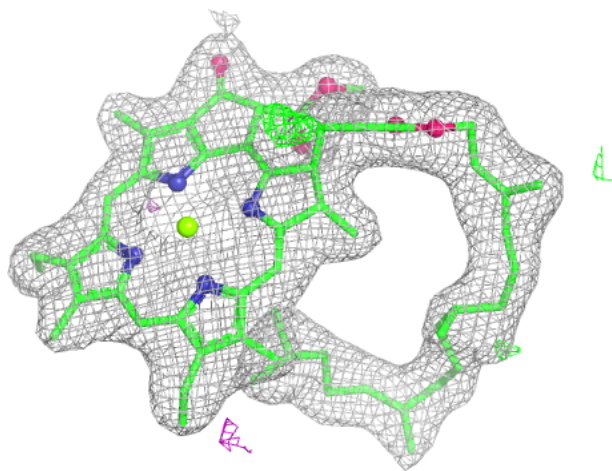
**Electron density around CLA d 404:**

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



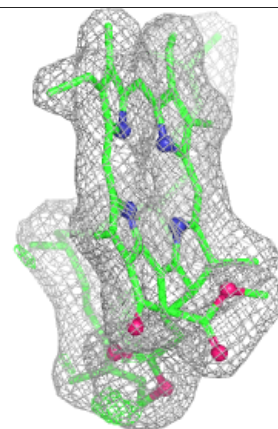
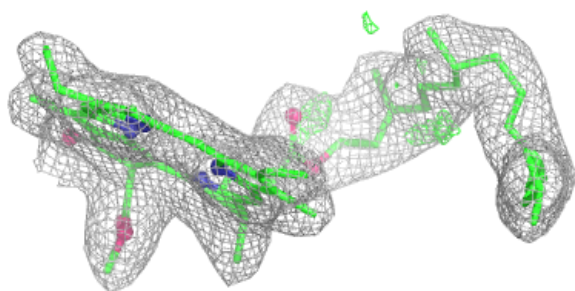
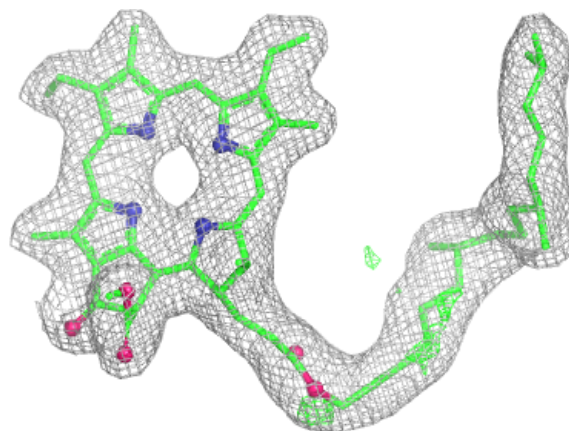
Electron density around CLA B 614:

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



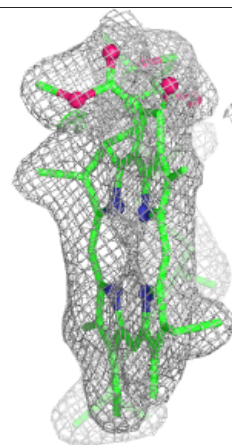
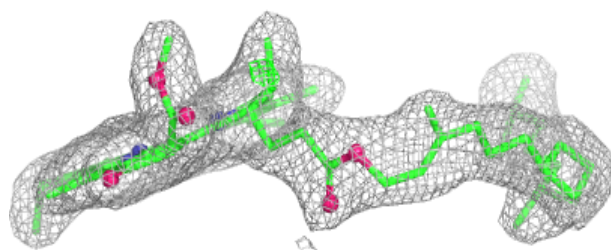
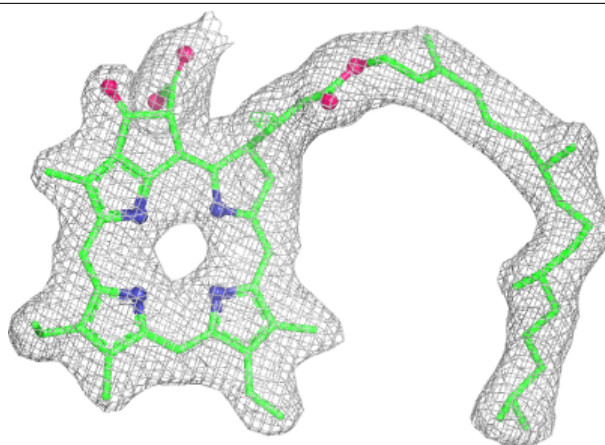
Electron density around PHO D 402:

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



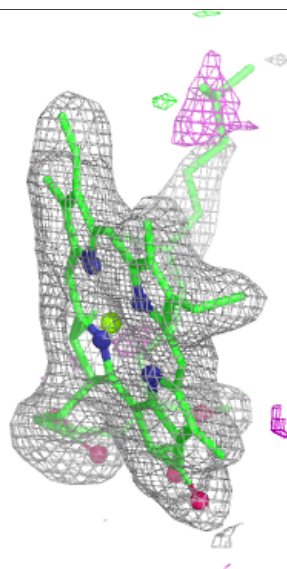
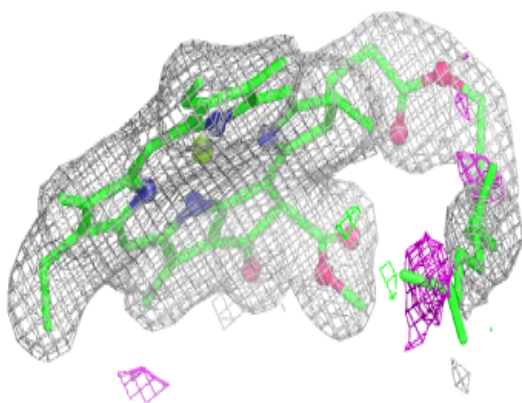
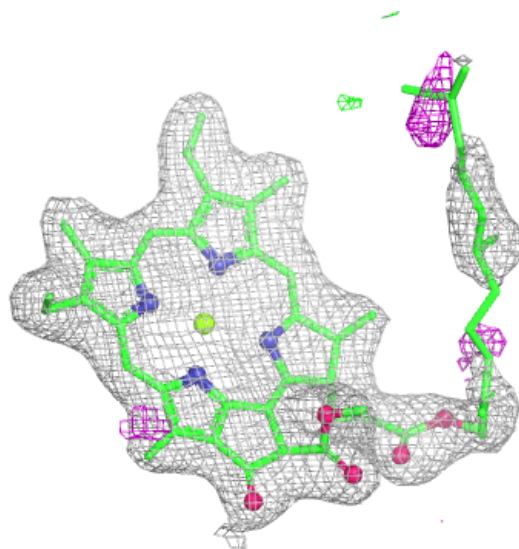
Electron density around PHO a 608:

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



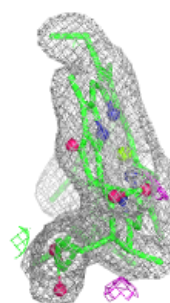
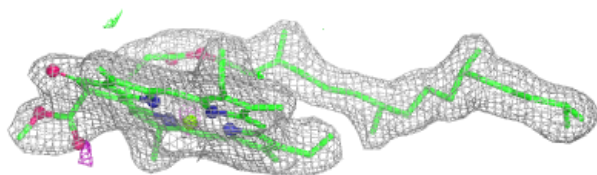
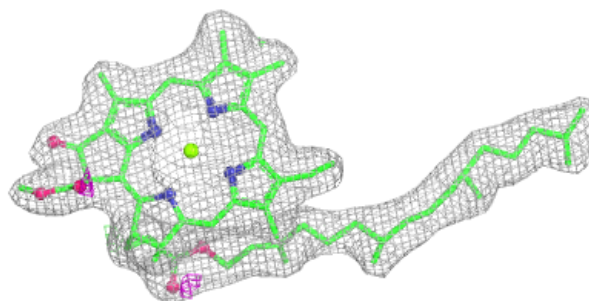
Electron density around CLA B 615:

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

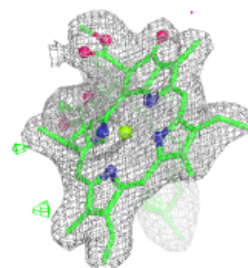
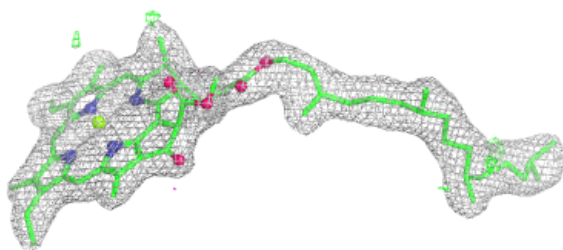
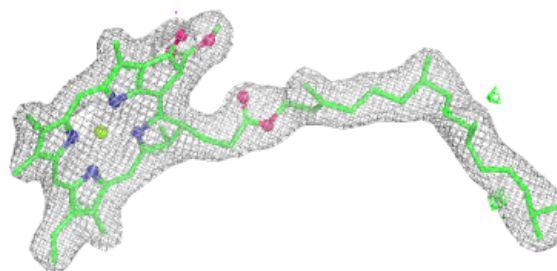


Electron density around CLA C 501:

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

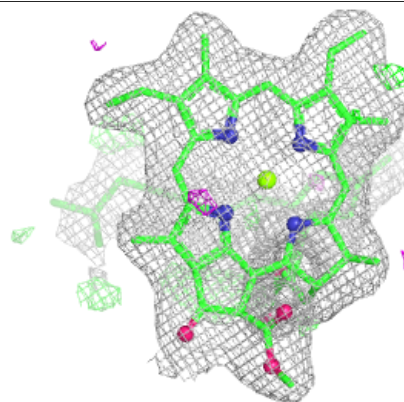
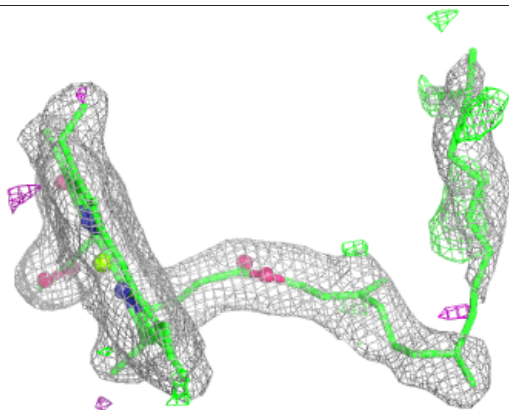
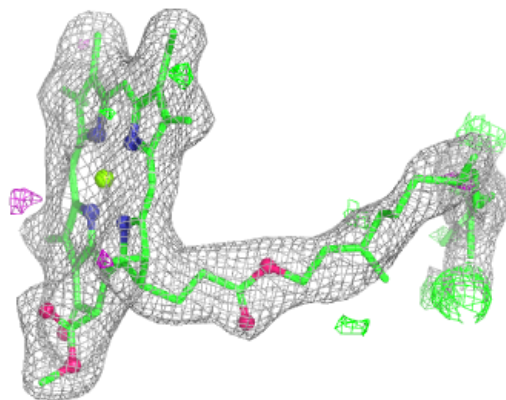
**Electron density around CLA a 607:**

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

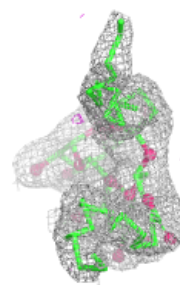
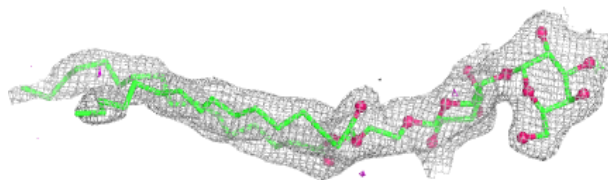
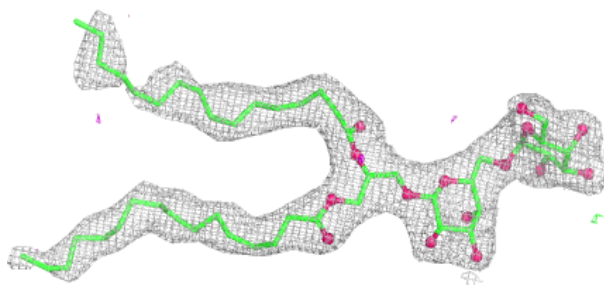


Electron density around CLA a 609:

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

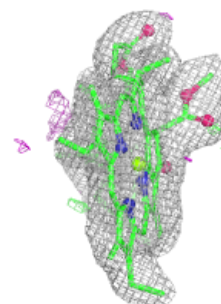
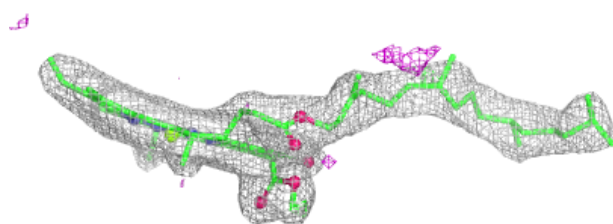
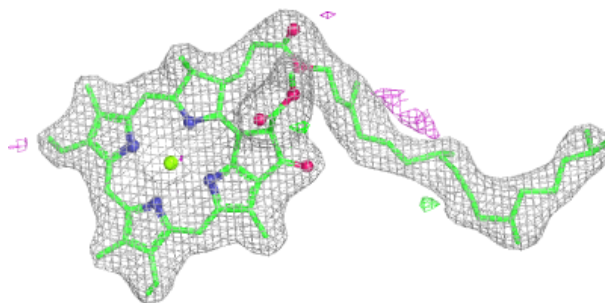
**Electron density around DGD C 518:**

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

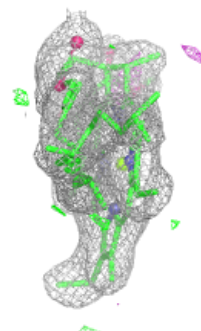
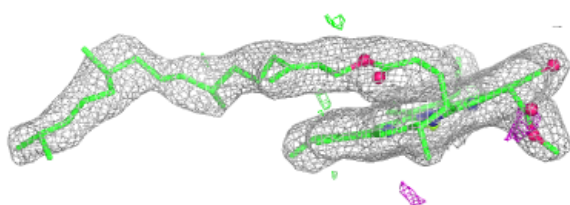
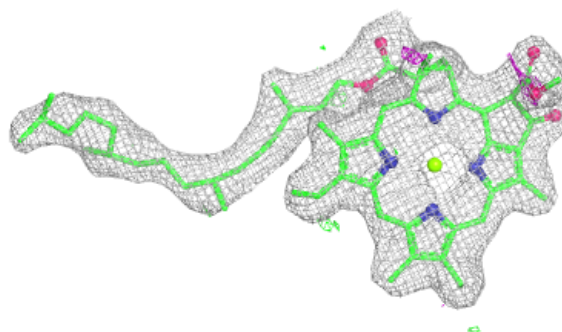


Electron density around CLA b 601:

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

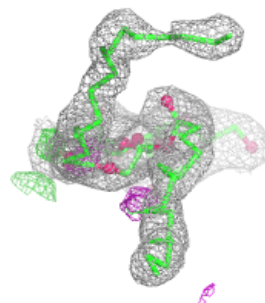
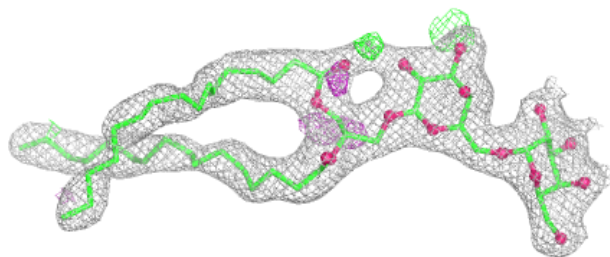
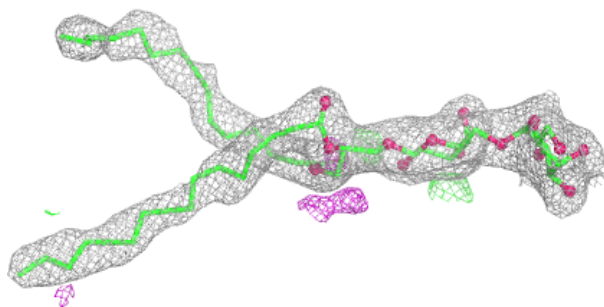
**Electron density around CLA b 602:**

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

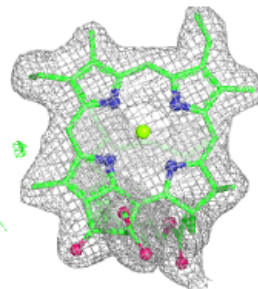
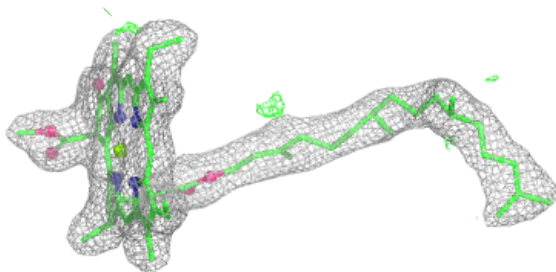
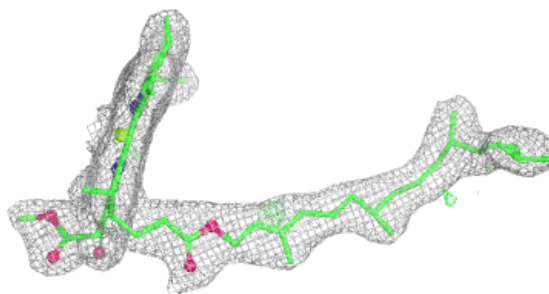


Electron density around DGD c 517:

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

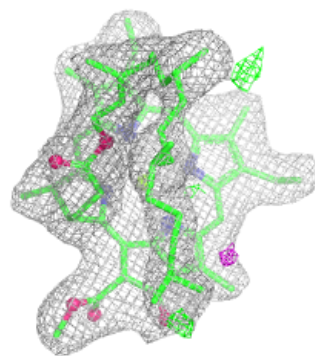
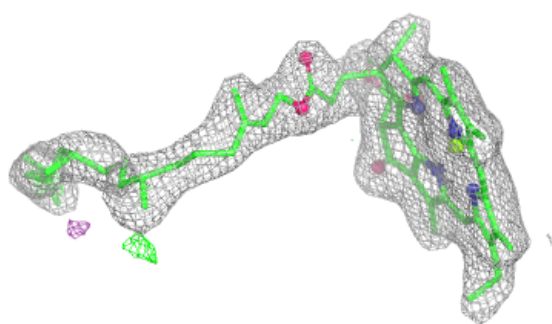
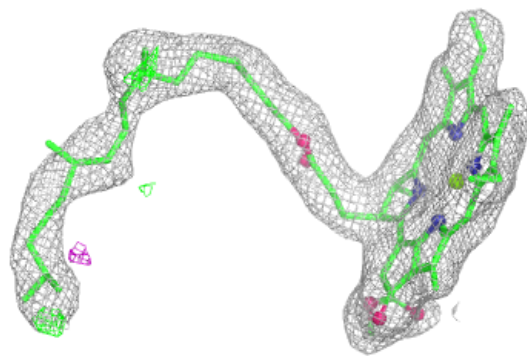
**Electron density around CLA b 604:**

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

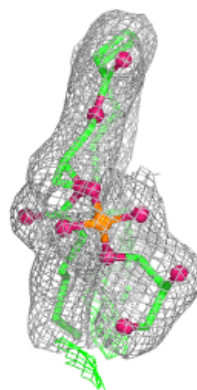
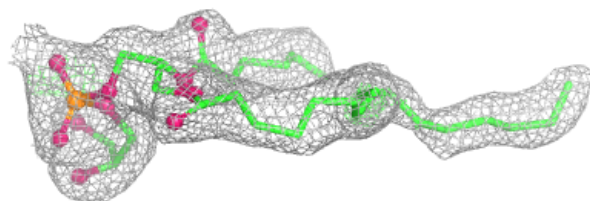
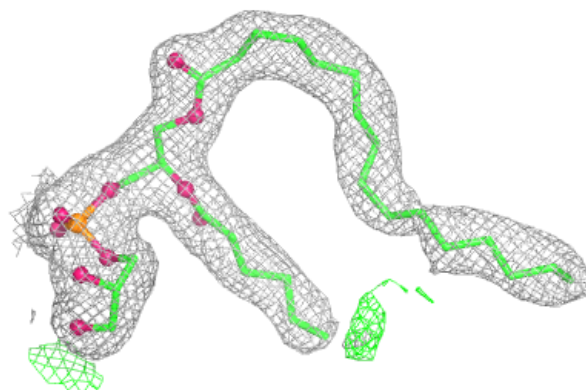


Electron density around CLA b 605:

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

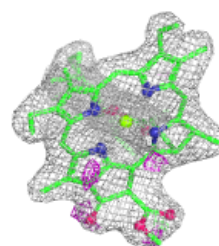
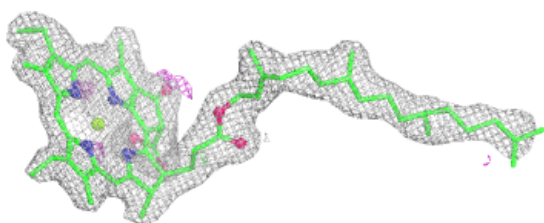
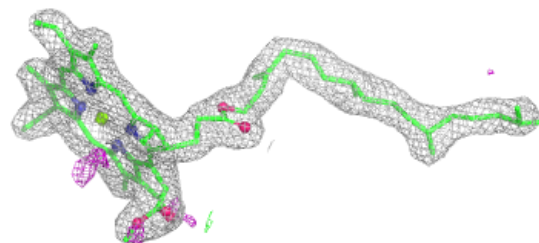
**Electron density around LHG d 408:**

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



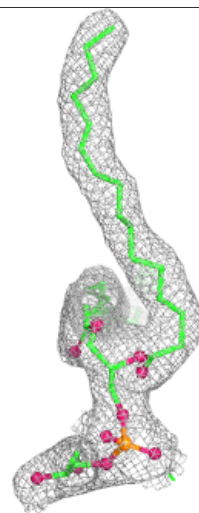
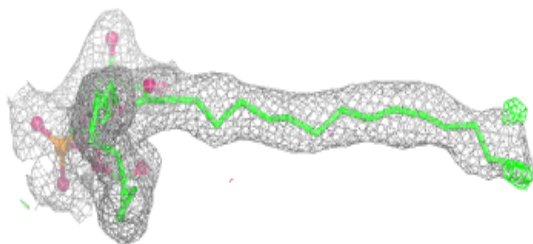
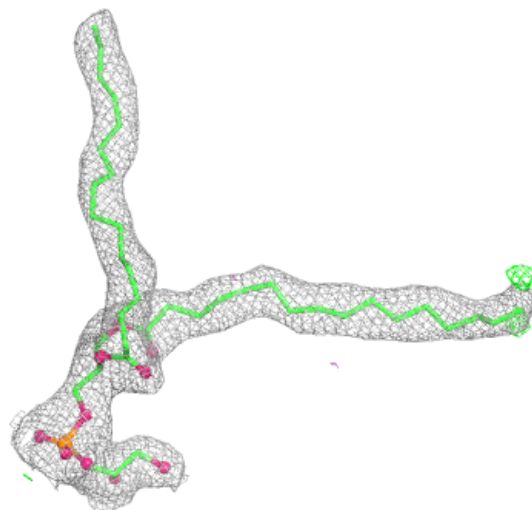
Electron density around CLA C 502:

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



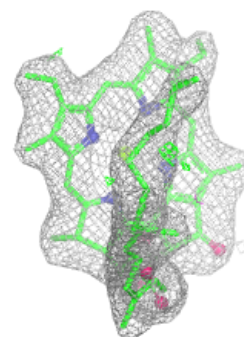
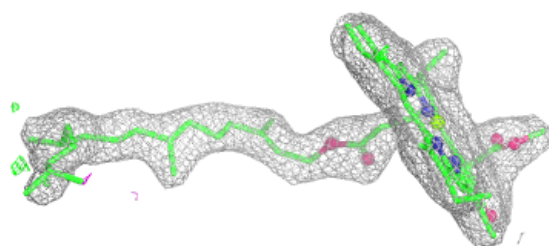
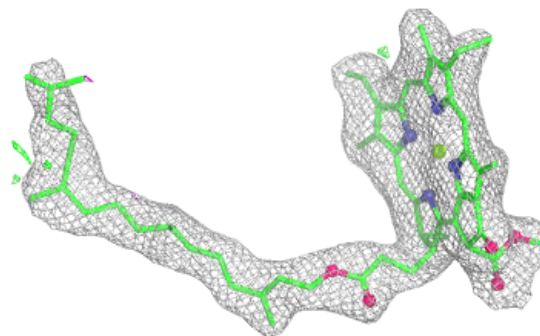
Electron density around LHG 1 101:

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

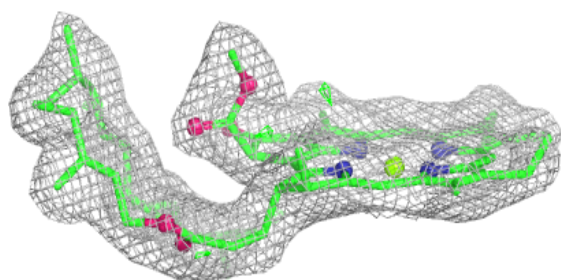
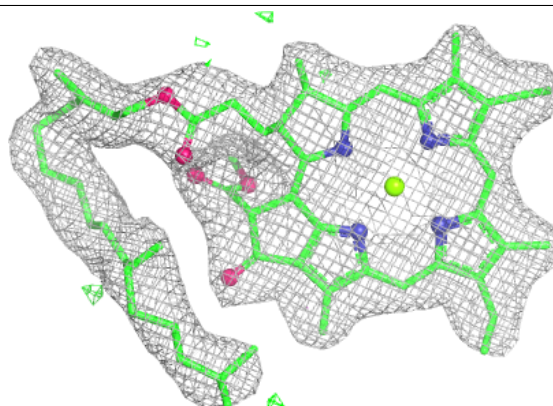


Electron density around CLA b 608:

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

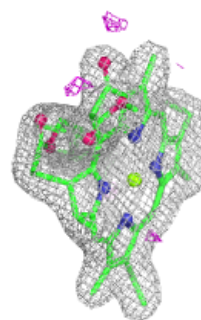
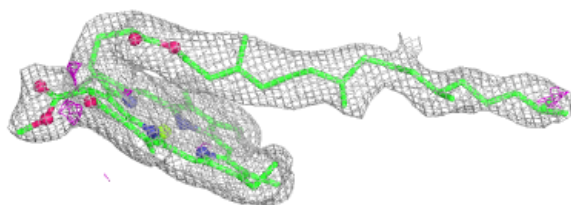
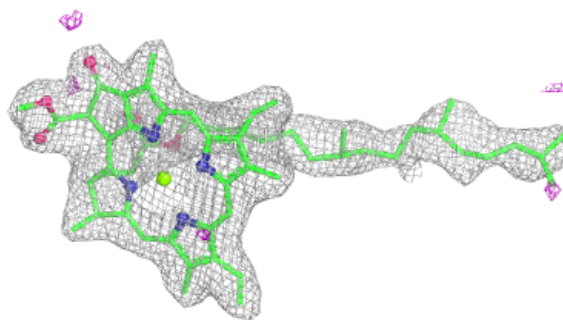
**Electron density around CLA b 609:**

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

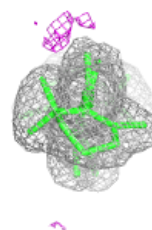
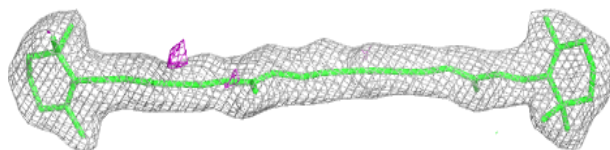
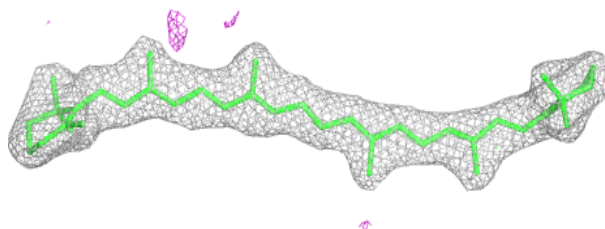


Electron density around CLA b 613:

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

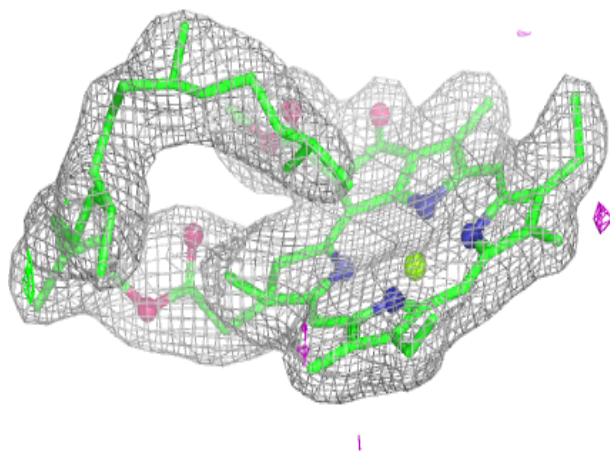
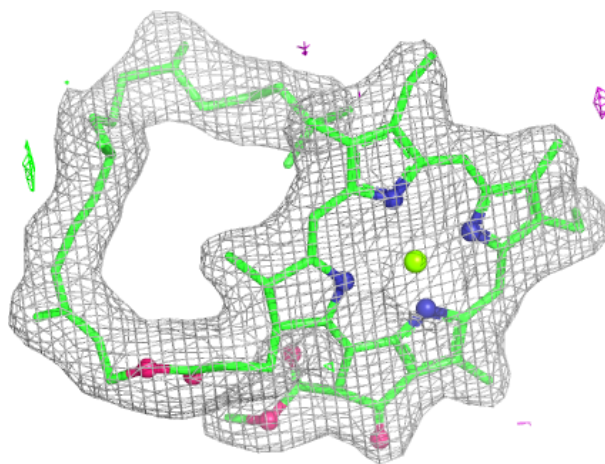
**Electron density around BCR a 610:**

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



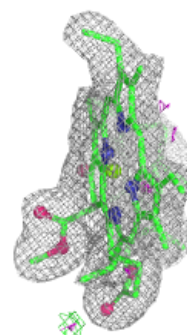
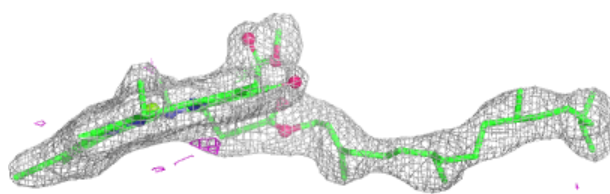
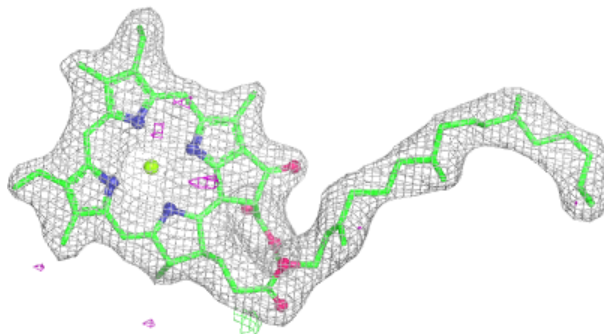
Electron density around CLA b 614:

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

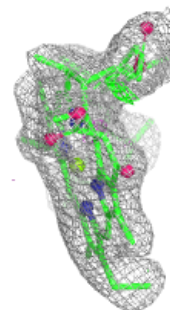
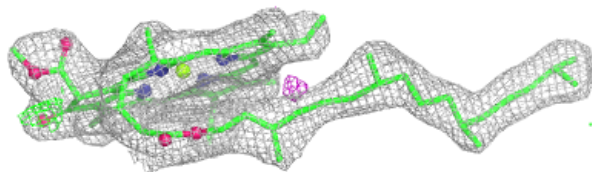
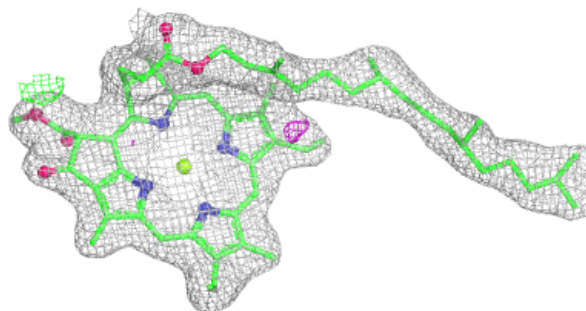


Electron density around CLA B 601:

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

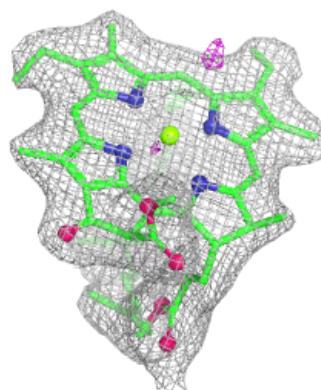
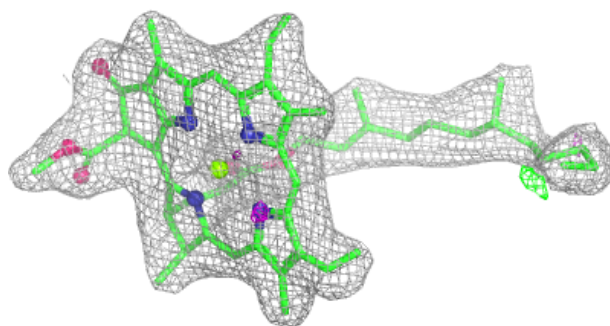
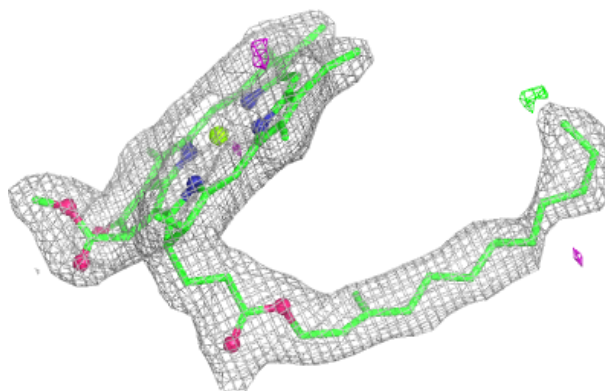
**Electron density around CLA c 501:**

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

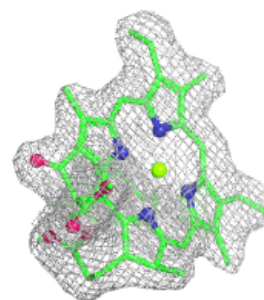
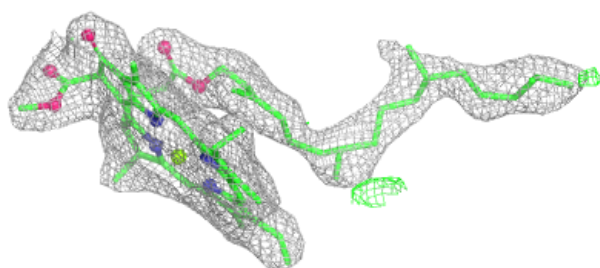
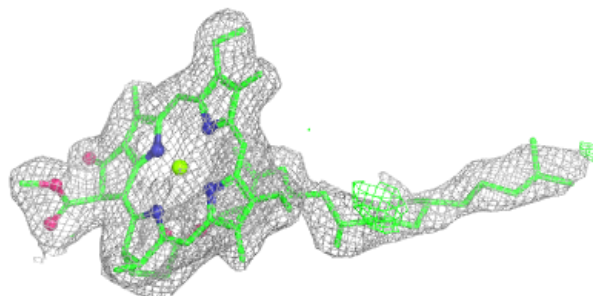


Electron density around CLA C 504:

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

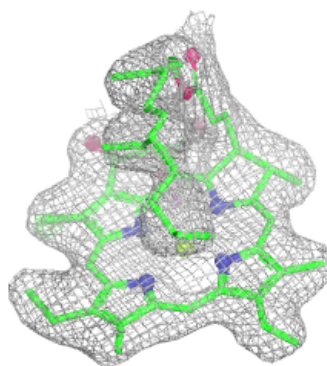
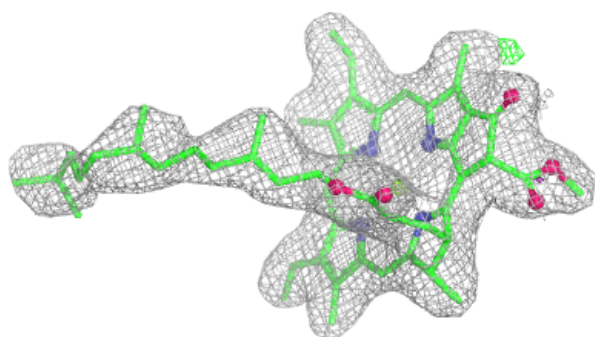
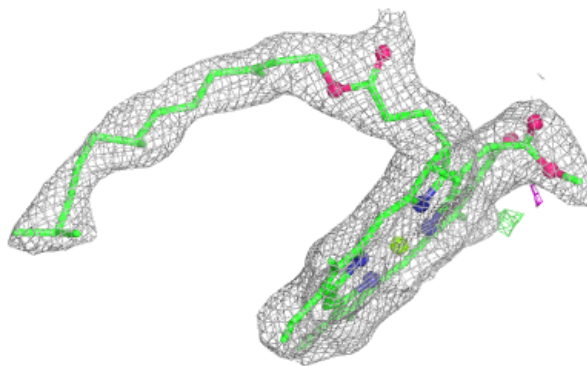
**Electron density around CLA C 505:**

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

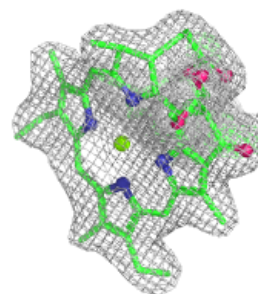
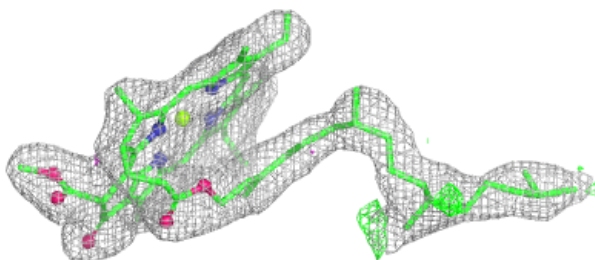
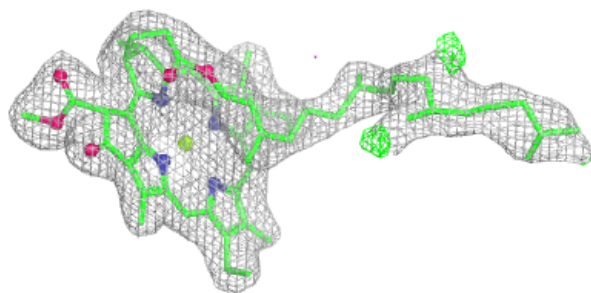


Electron density around CLA c 504:

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

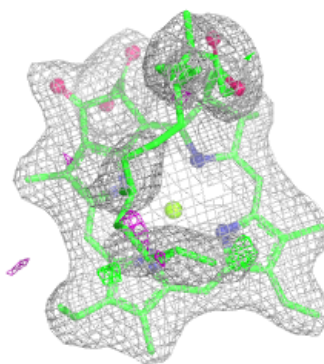
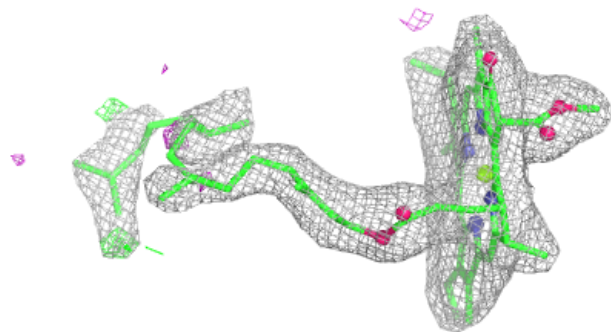
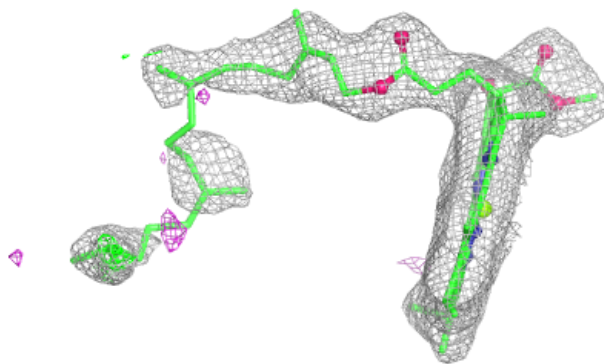
**Electron density around CLA c 505:**

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



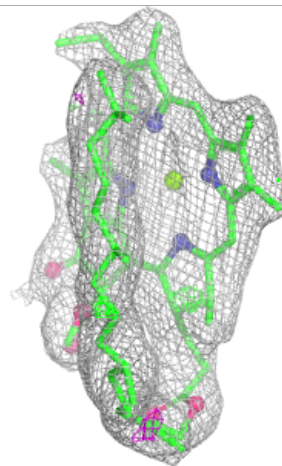
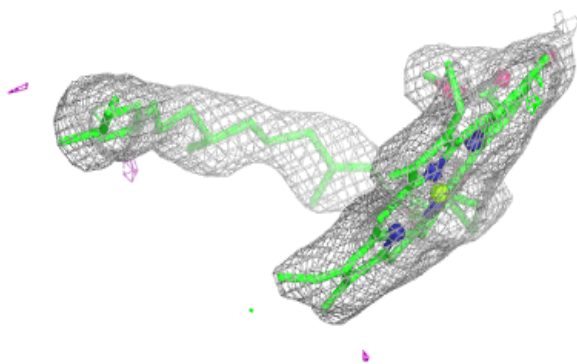
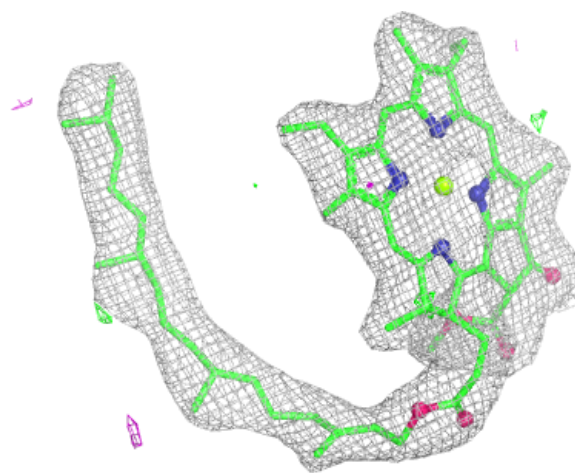
Electron density around CLA c 506:

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



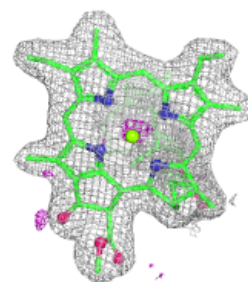
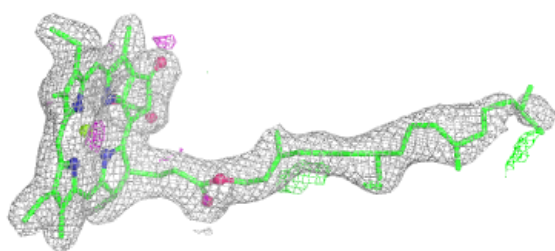
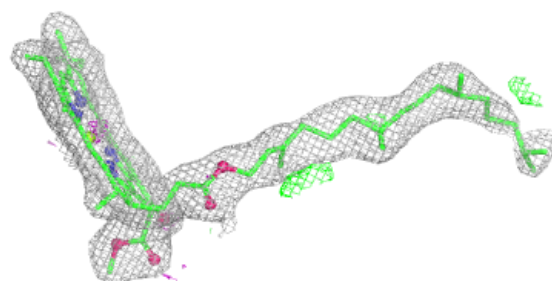
Electron density around CLA c 507:

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

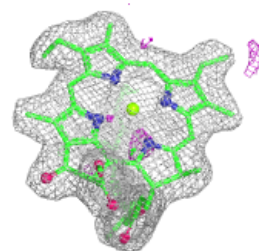
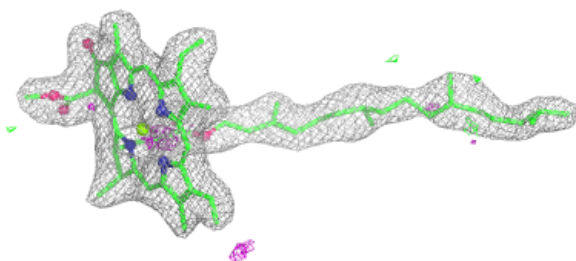
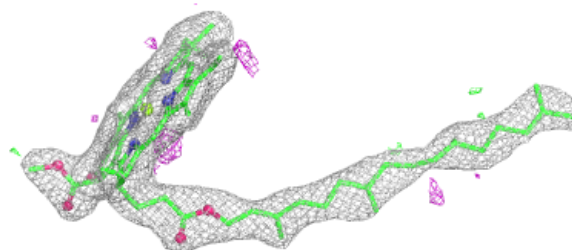


Electron density around CLA B 603:

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

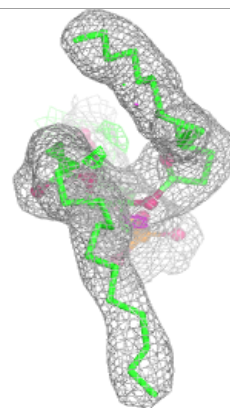
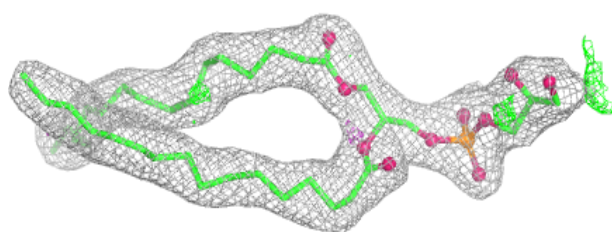
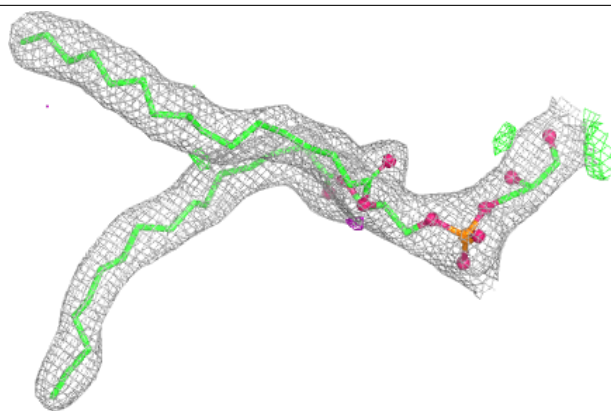
**Electron density around CLA B 606:**

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



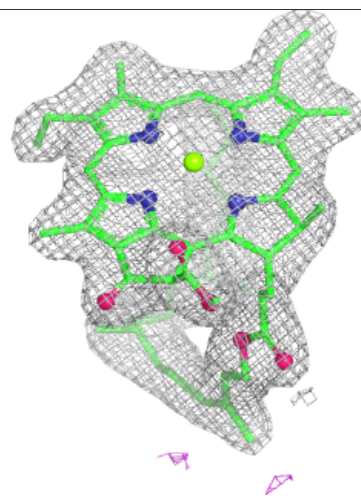
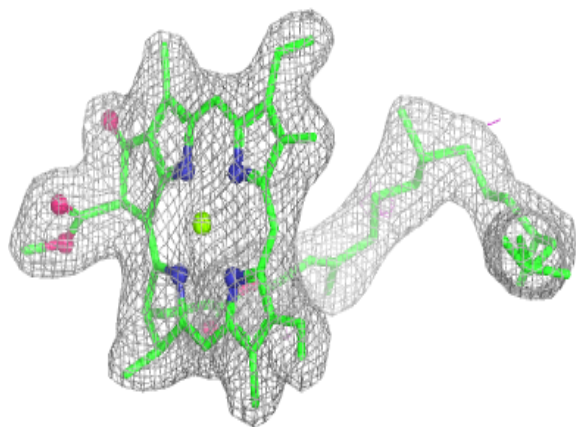
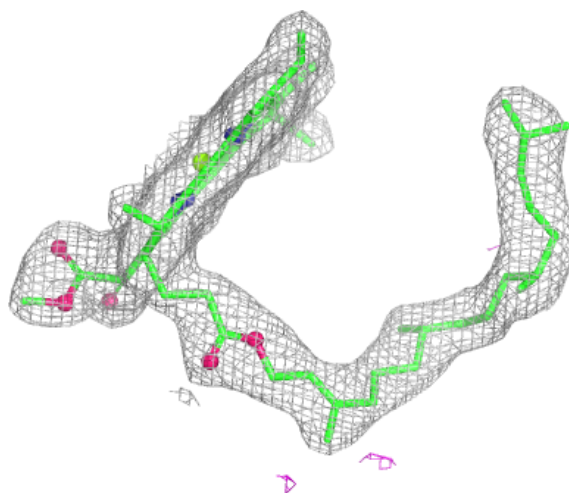
Electron density around LHG D 409:

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



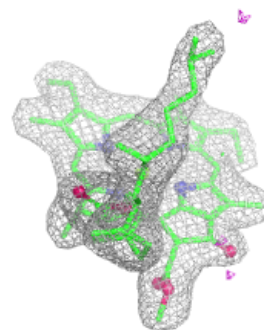
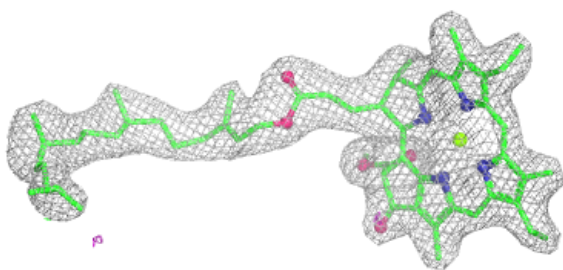
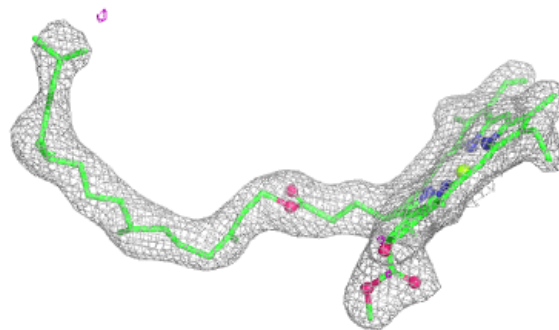
Electron density around CLA b 610:

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



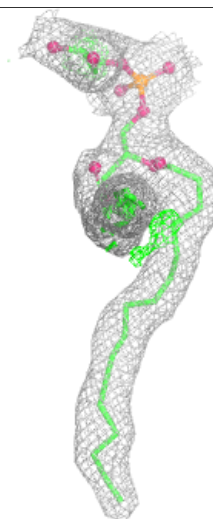
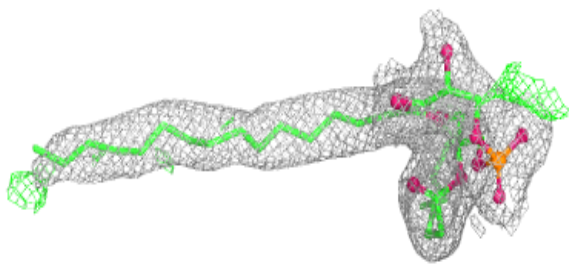
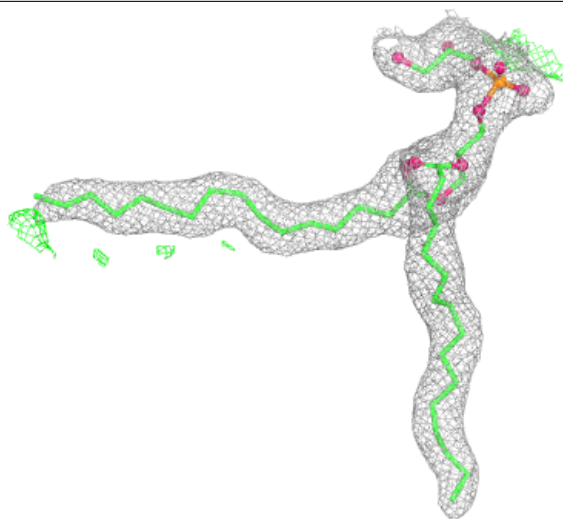
Electron density around CLA d 403:

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



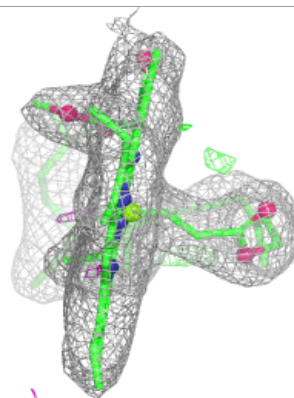
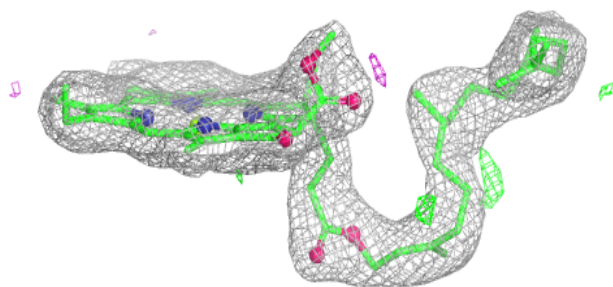
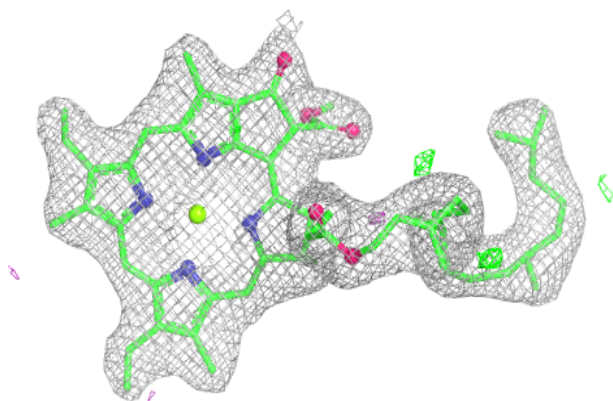
Electron density around LHG L 101:

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

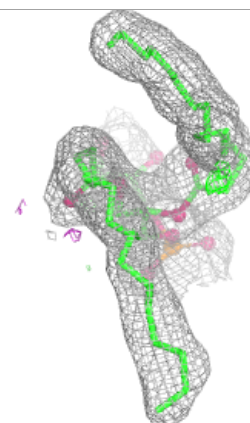
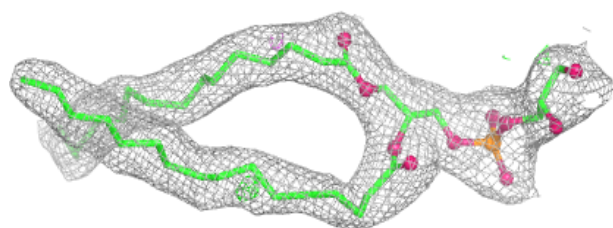
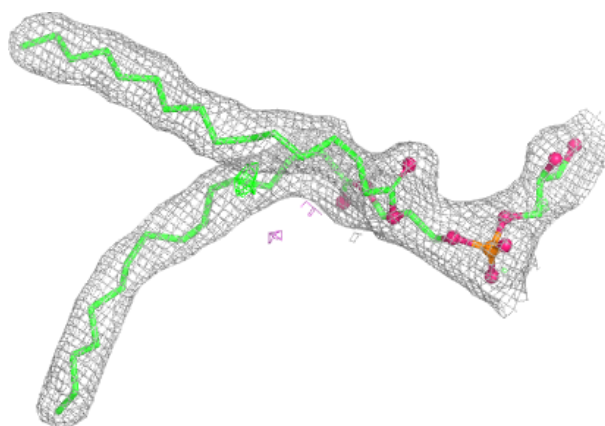


Electron density around CLA b 611:

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

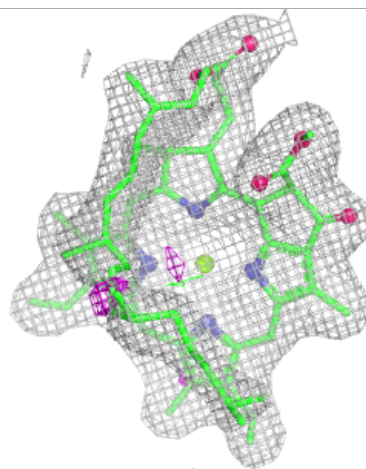
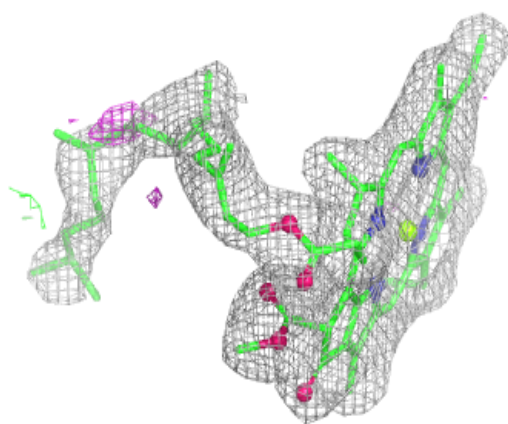
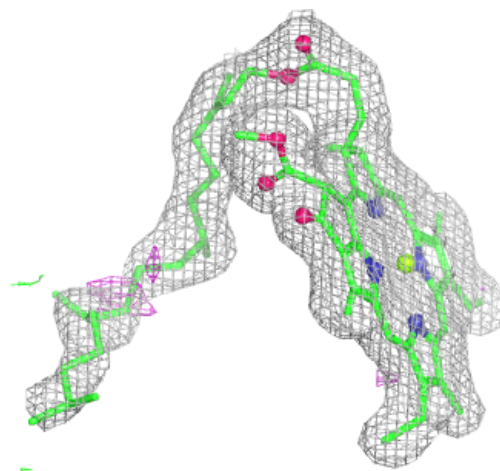
**Electron density around LHG d 407:**

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



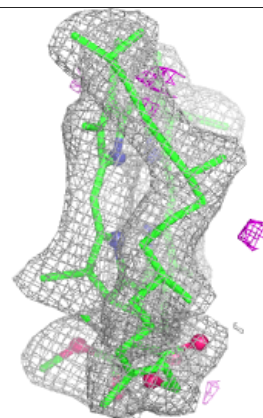
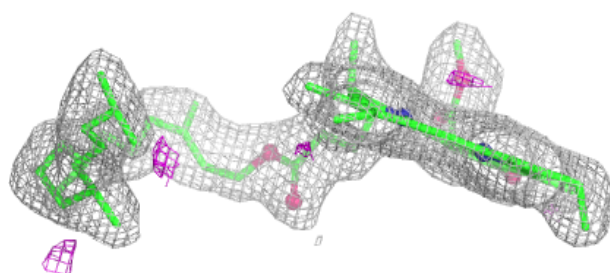
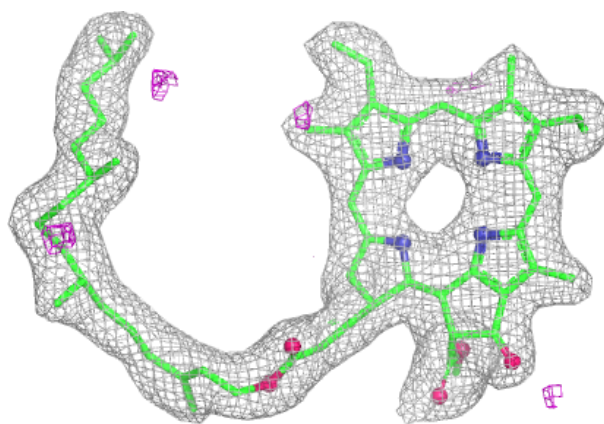
Electron density around CLA b 612:

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

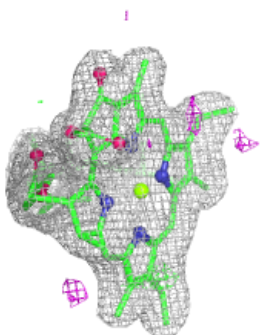
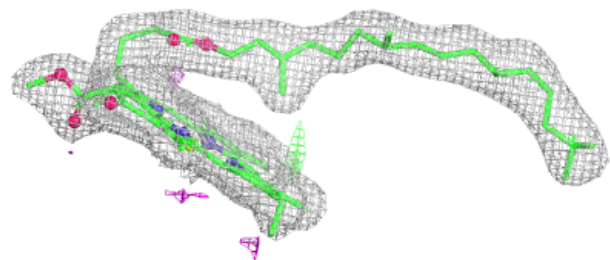
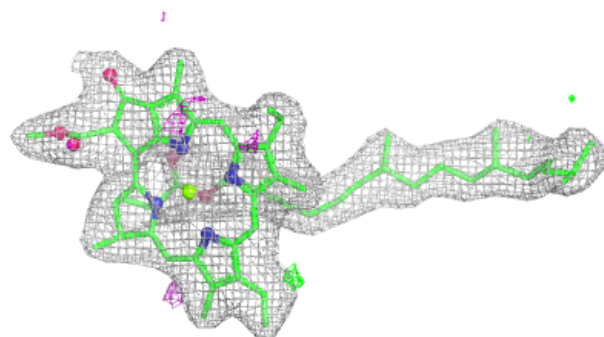


Electron density around PHO A 608:

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

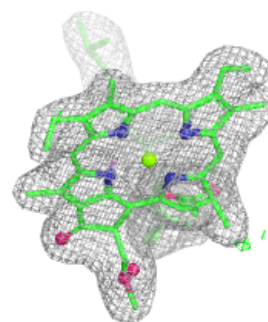
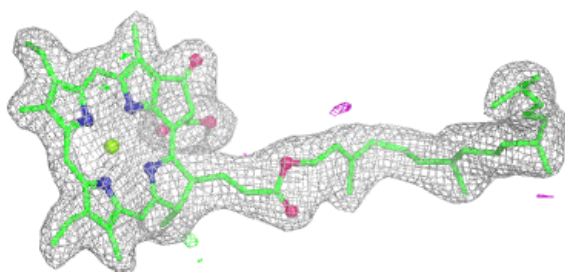
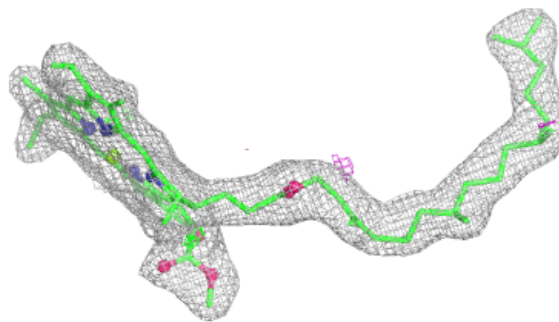
**Electron density around CLA B 607:**

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

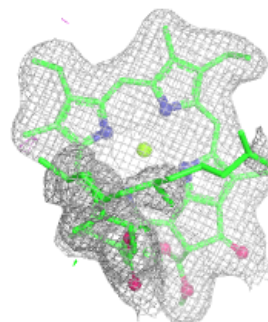
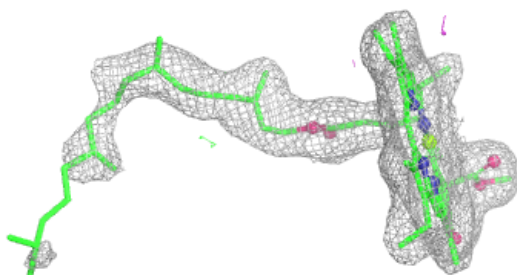
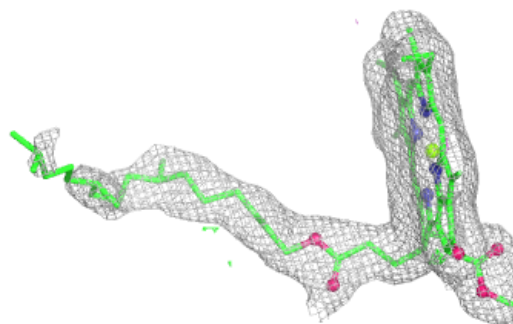


Electron density around CLA D 403:

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

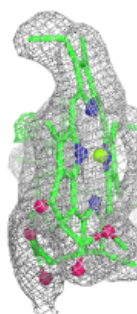
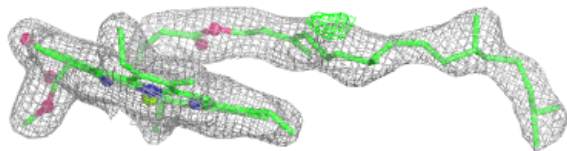
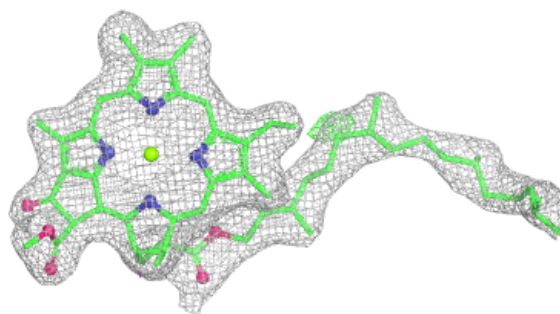
**Electron density around CLA D 404:**

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

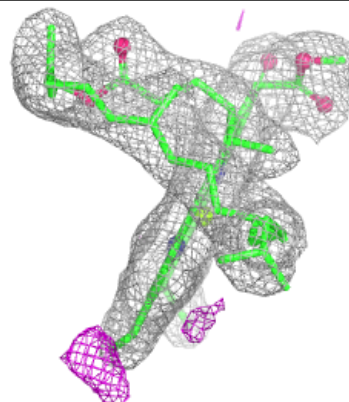
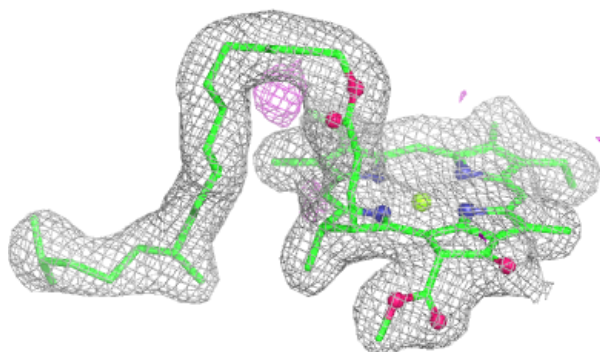
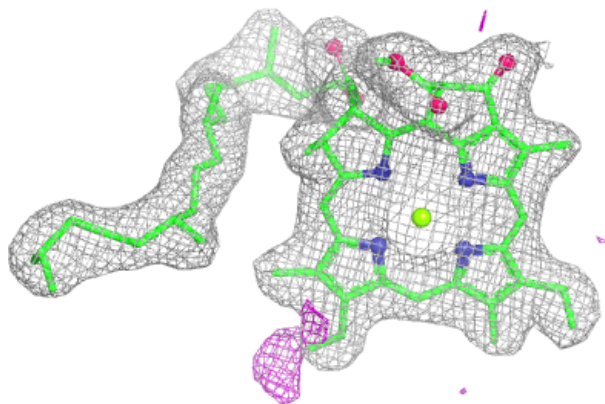


Electron density around CLA B 602:

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

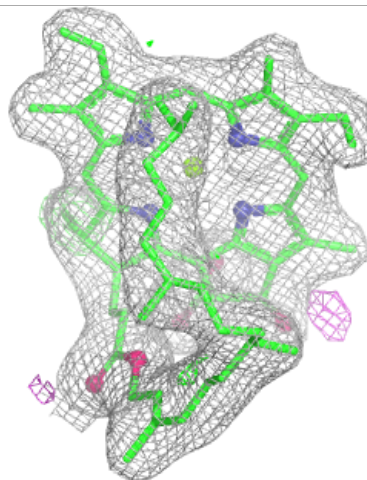
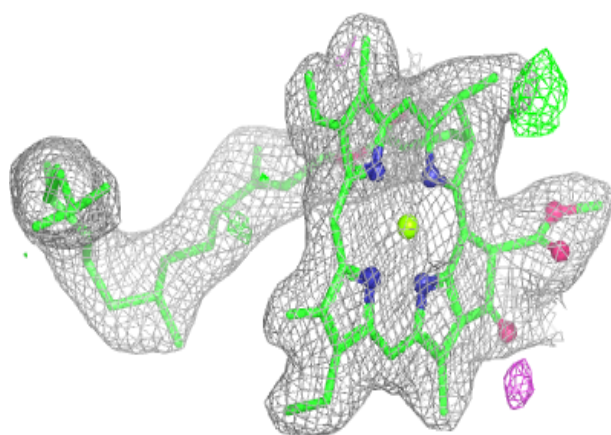
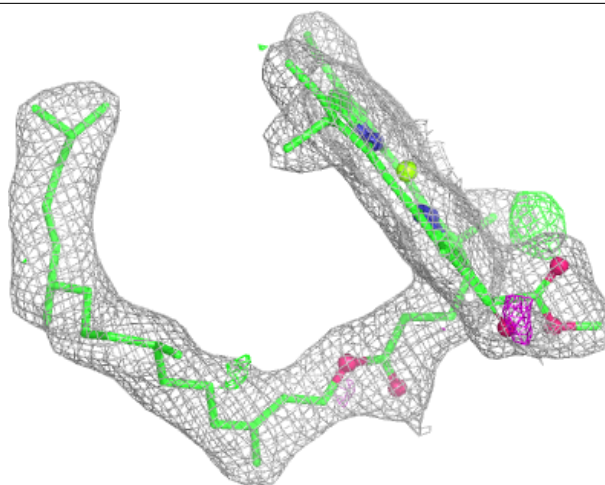
**Electron density around CLA A 612:**

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



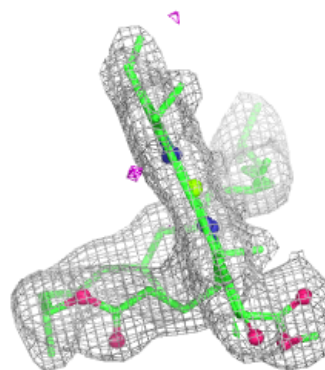
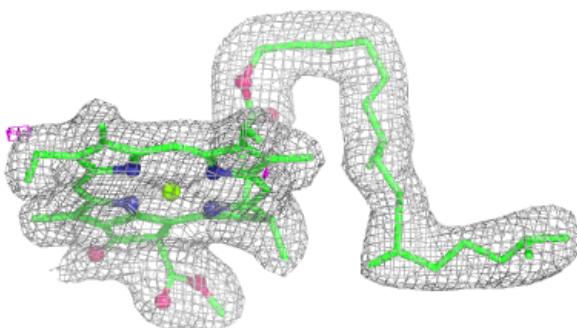
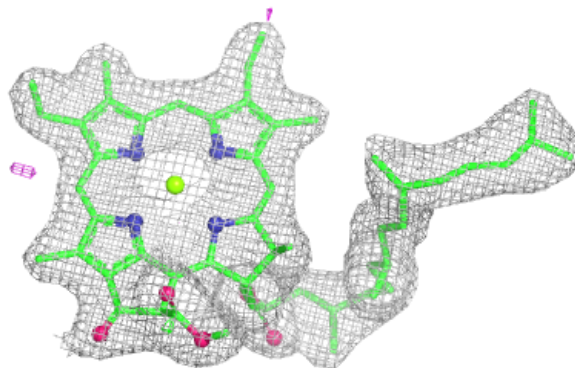
Electron density around CLA B 610:

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

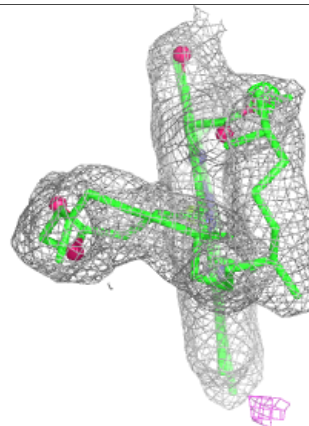
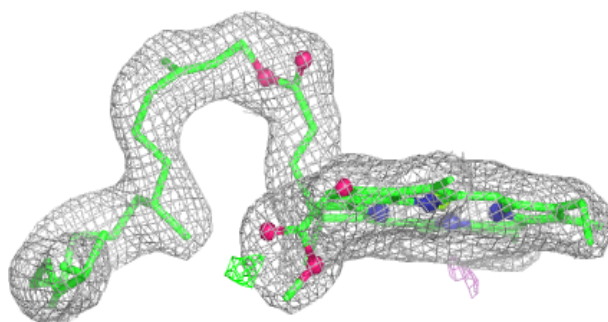
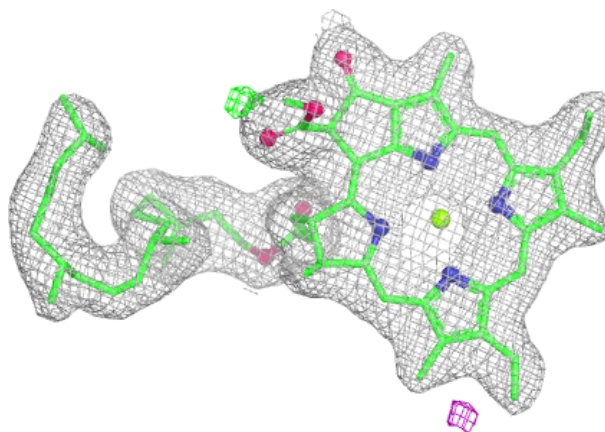


Electron density around CLA a 612:

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

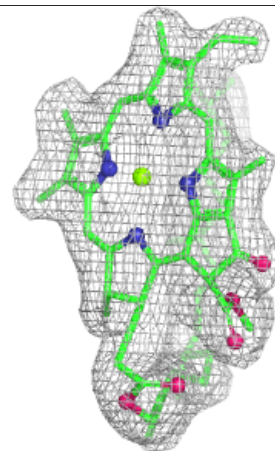
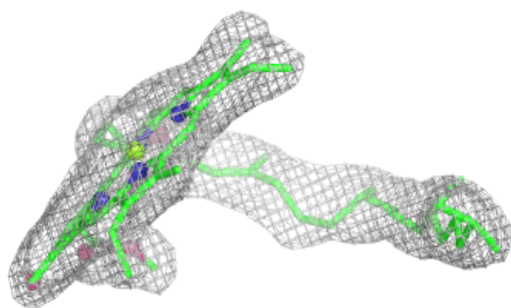
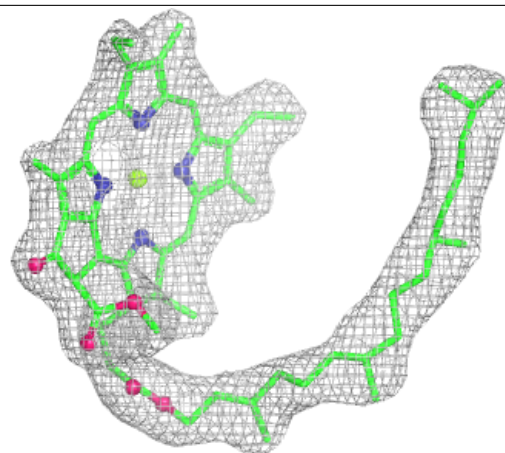
**Electron density around CLA B 611:**

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



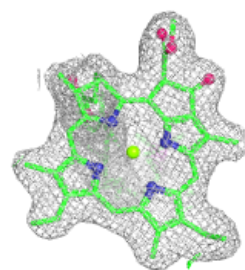
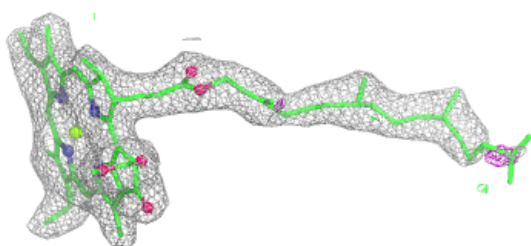
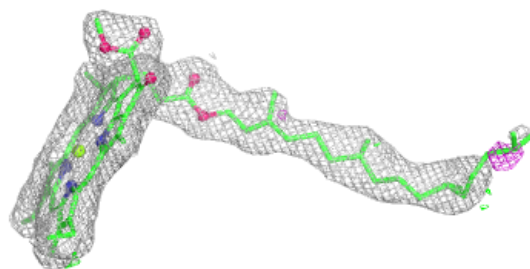
Electron density around CLA C 507:

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



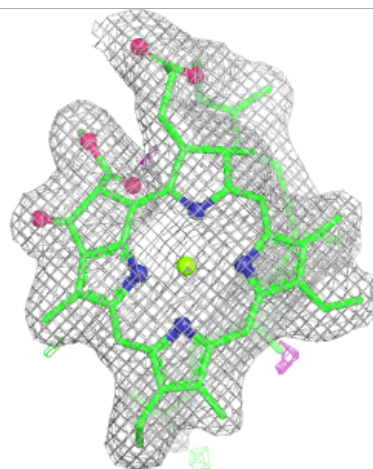
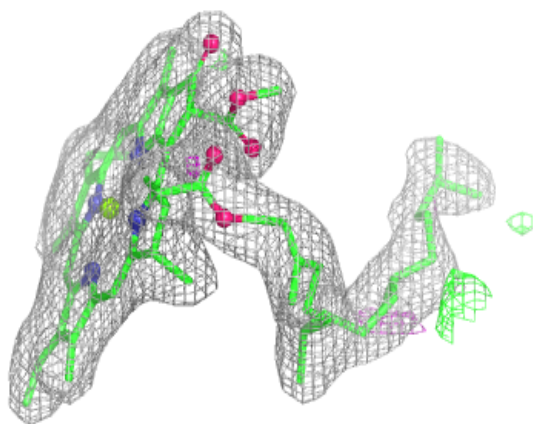
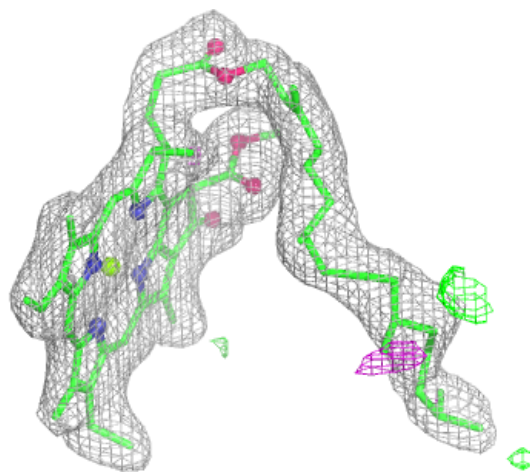
Electron density around CLA b 603:

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



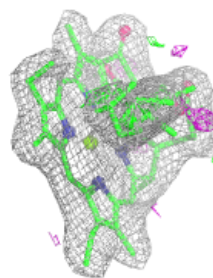
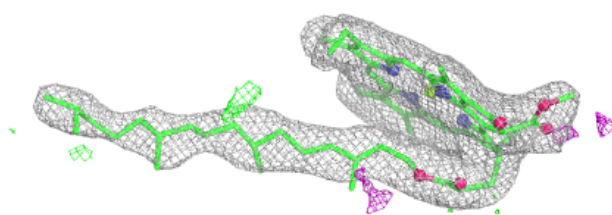
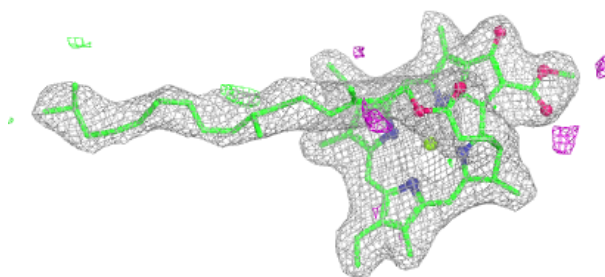
Electron density around CLA B 612:

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

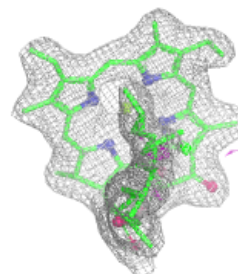
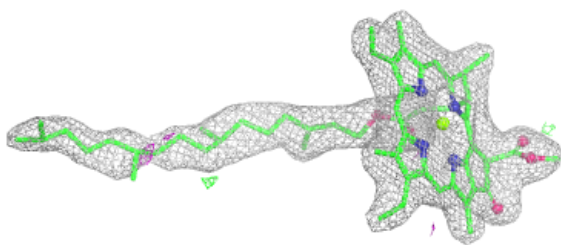
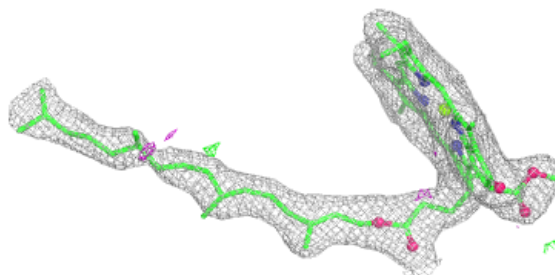


Electron density around CLA B 613:

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

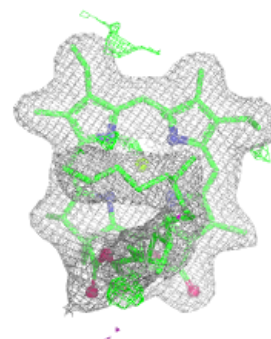
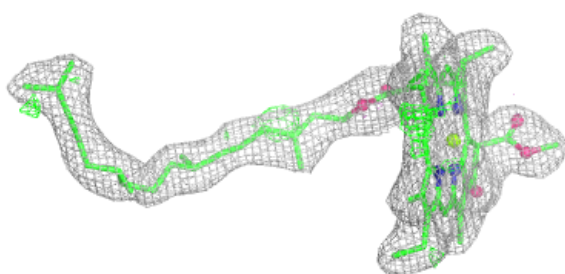
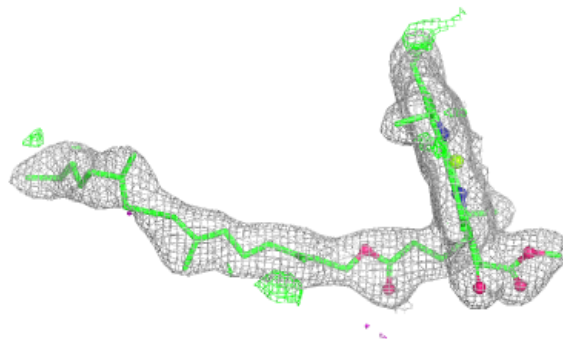
**Electron density around CLA b 606:**

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

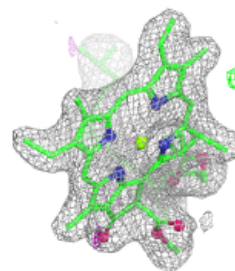
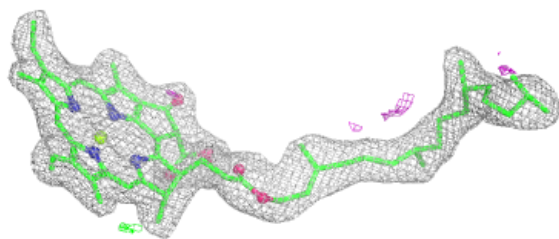
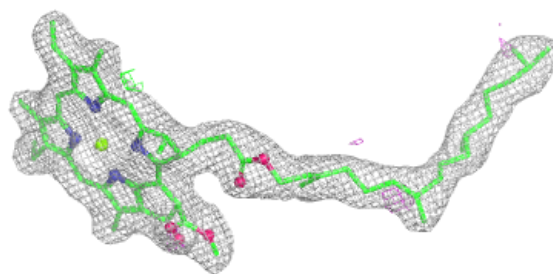


Electron density around CLA B 604:

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

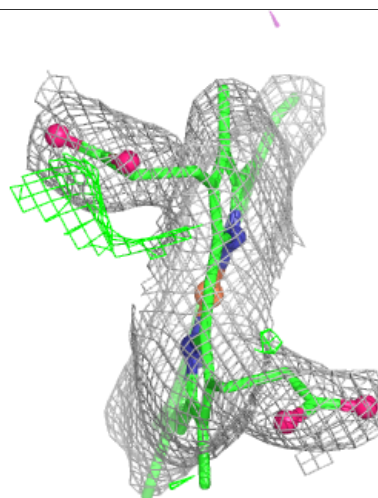
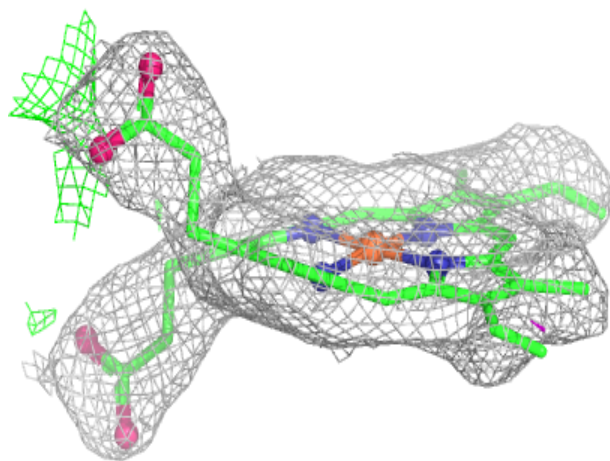
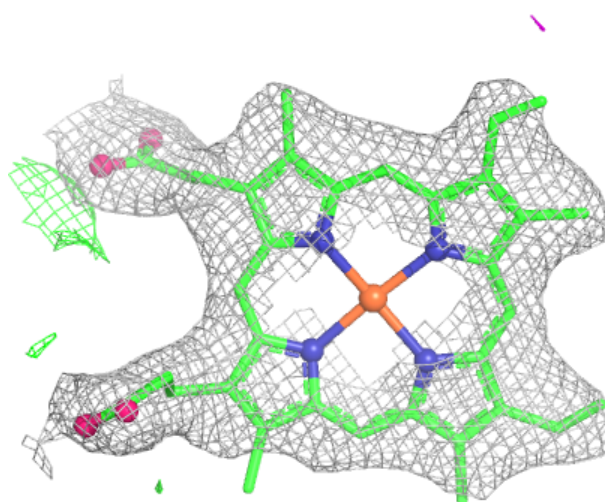
**Electron density around CLA A 606:**

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



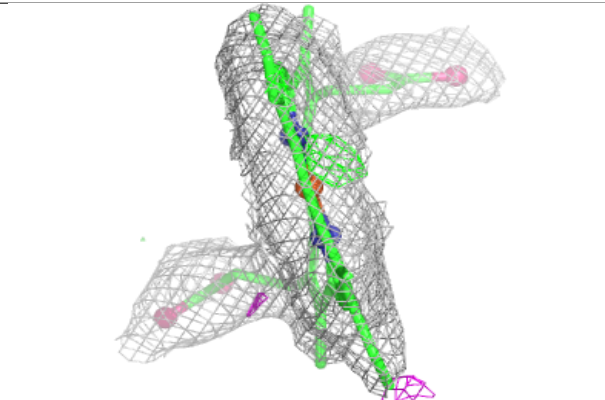
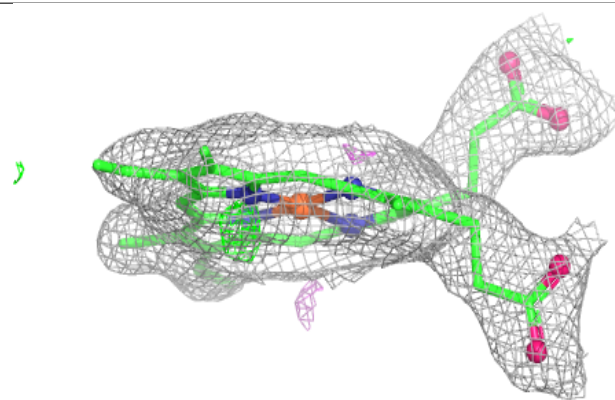
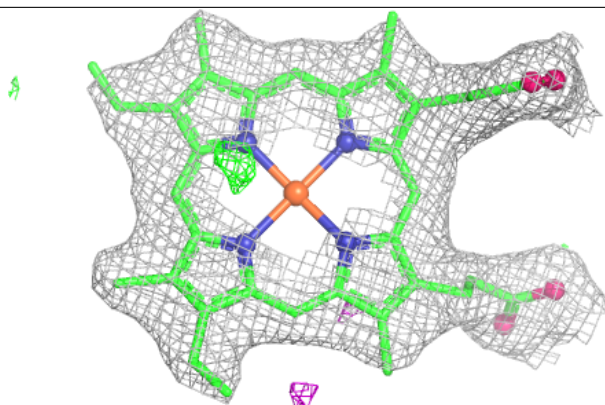
Electron density around HEM e 101:

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

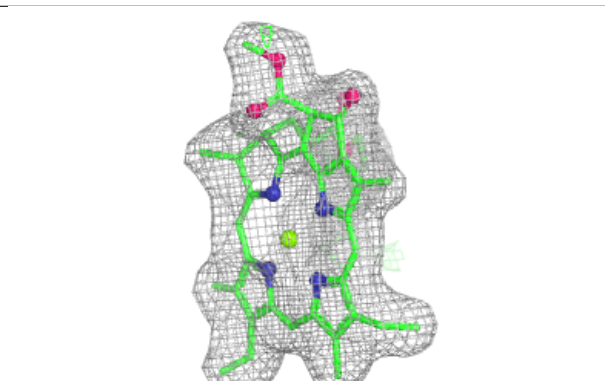
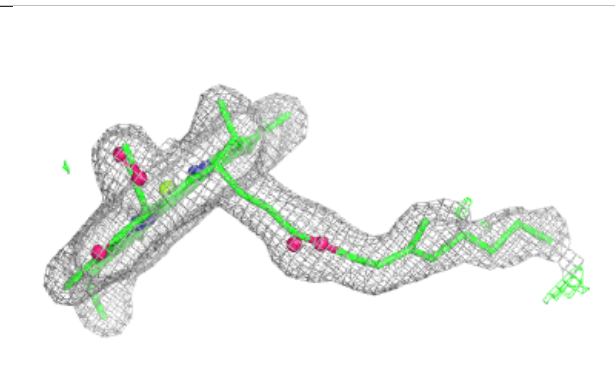
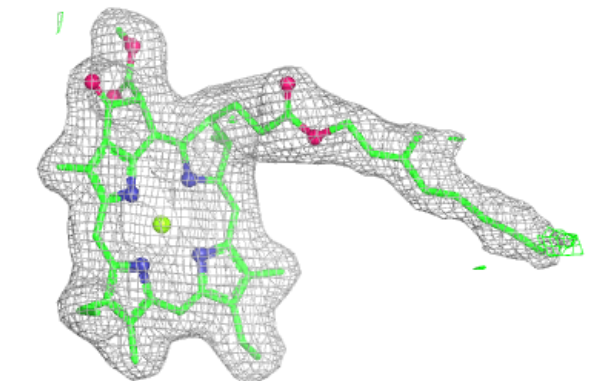


Electron density around HEM F 101:

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

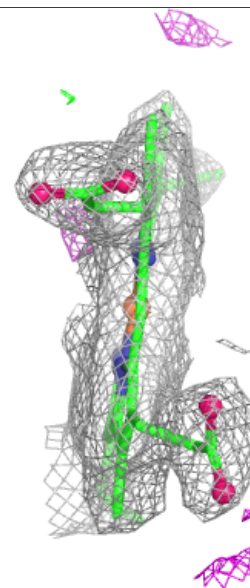
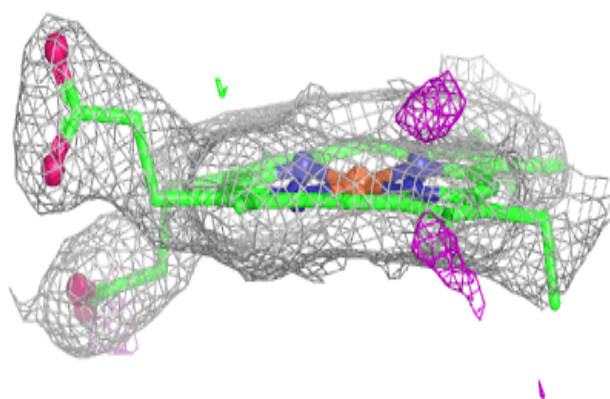
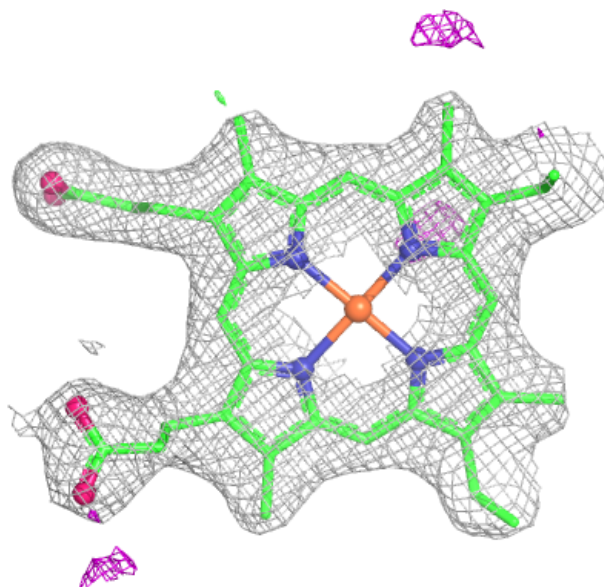
**Electron density around CLA A 609:**

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



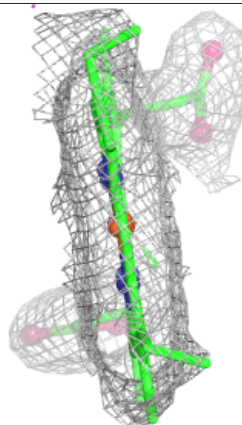
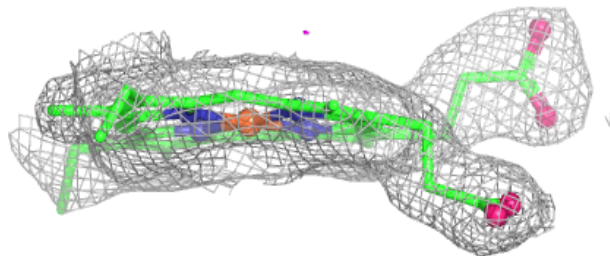
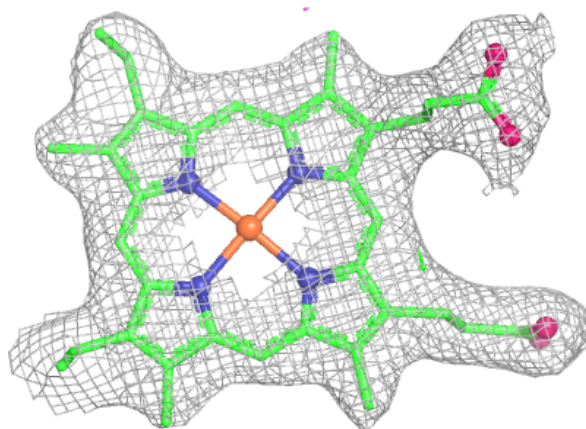
Electron density around HEC V 201:

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



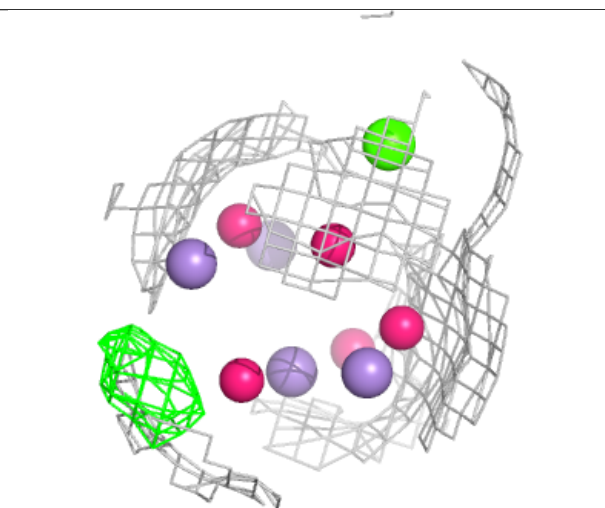
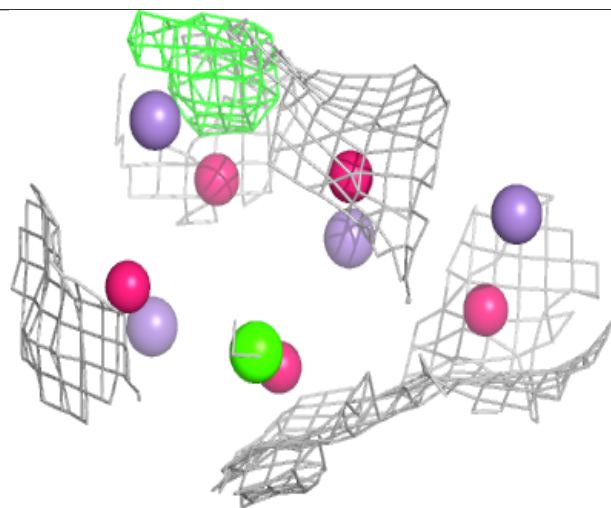
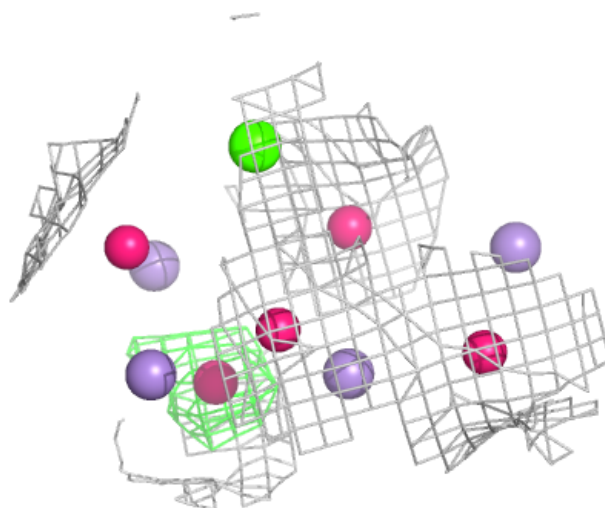
Electron density around HEC v 201:

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



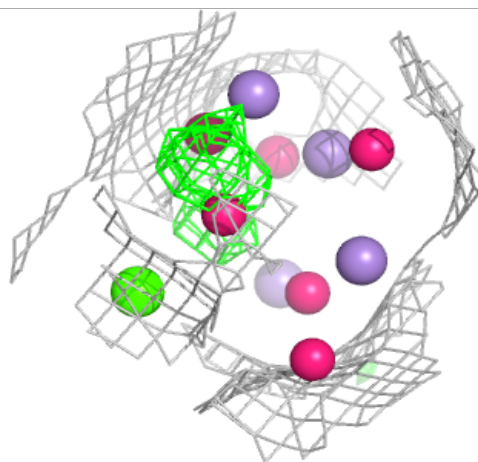
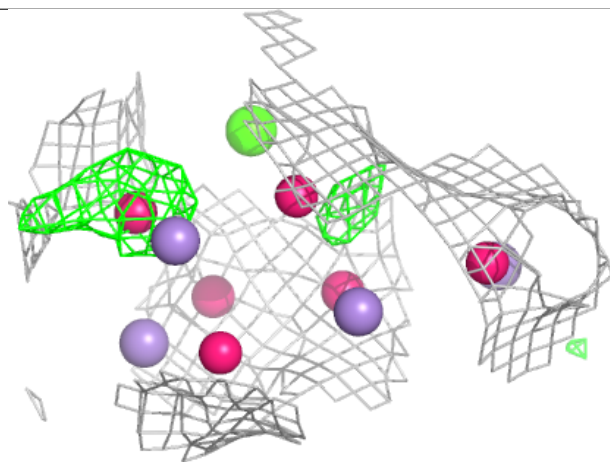
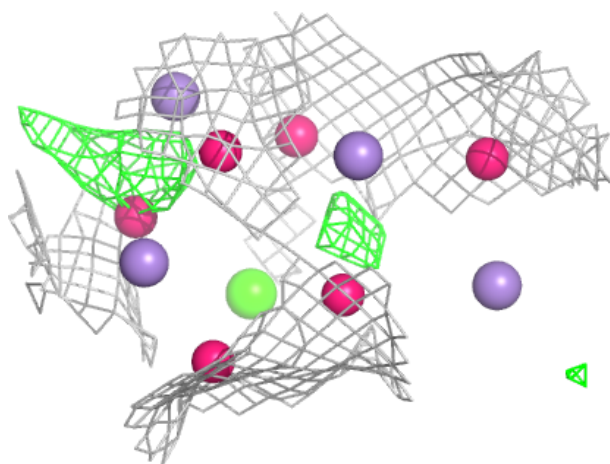
Electron density around OEX a 601 (B):

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



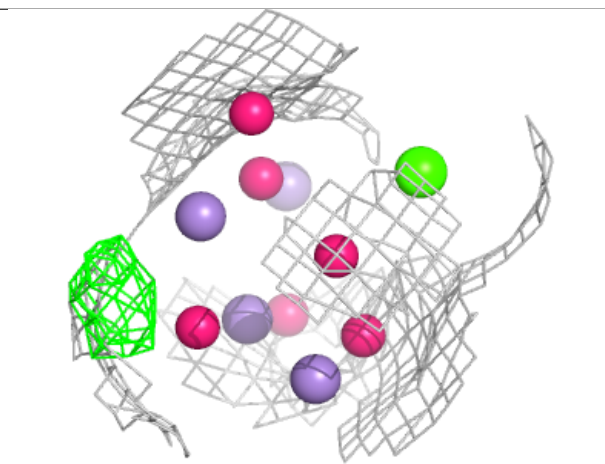
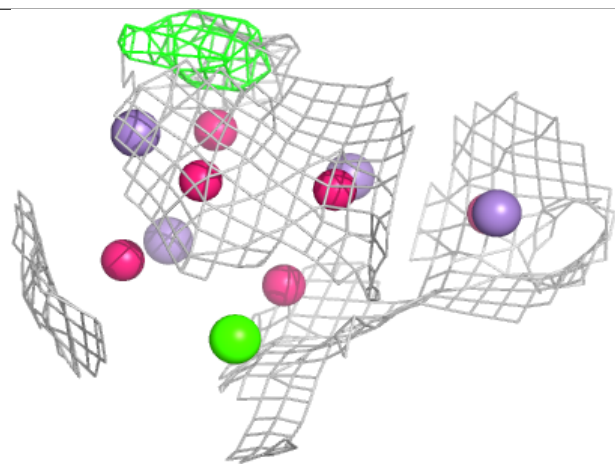
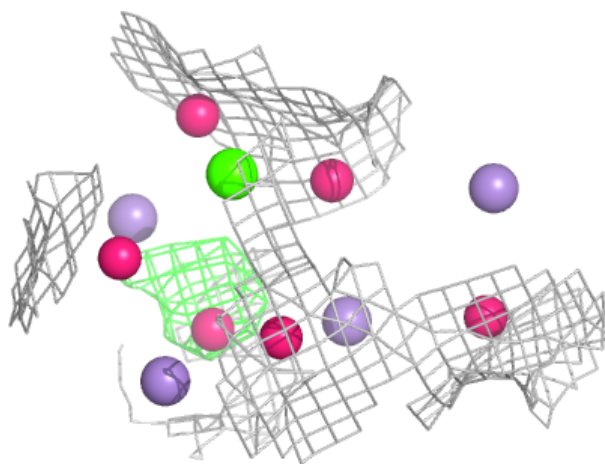
Electron density around OEY A 602 (A):

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



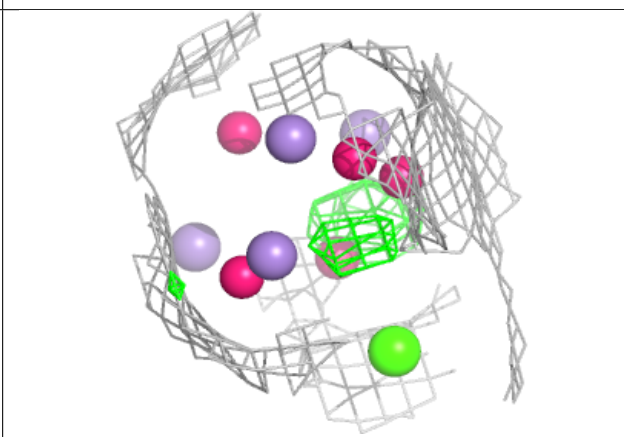
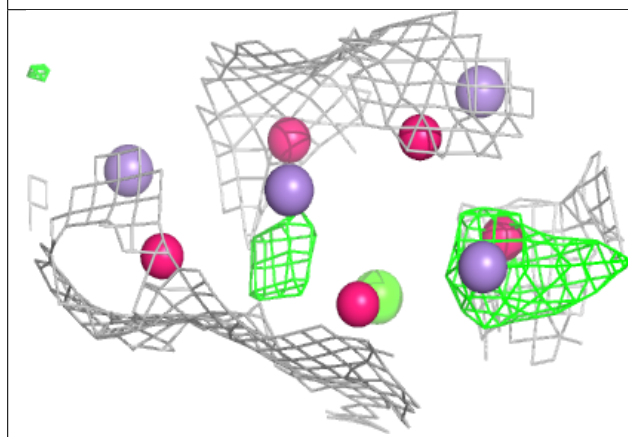
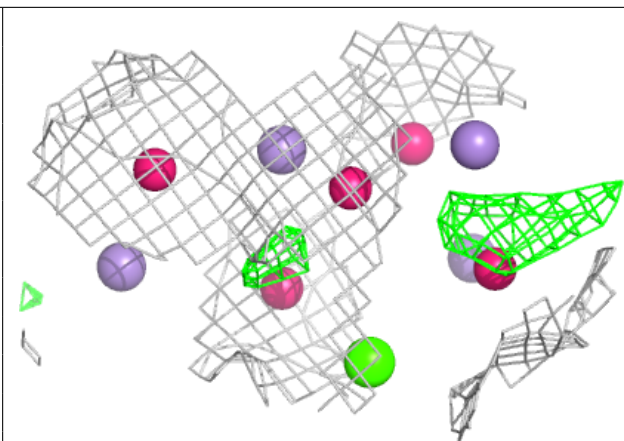
Electron density around OEY a 602 (A):

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



Electron density around OEX A 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.