



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:31 PM UTC

PDB ID : 5GTI / pdb_00005gti
Title : Native XFEL structure of photosystem II (two flash dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-08-20
Resolution : 2.50 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
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

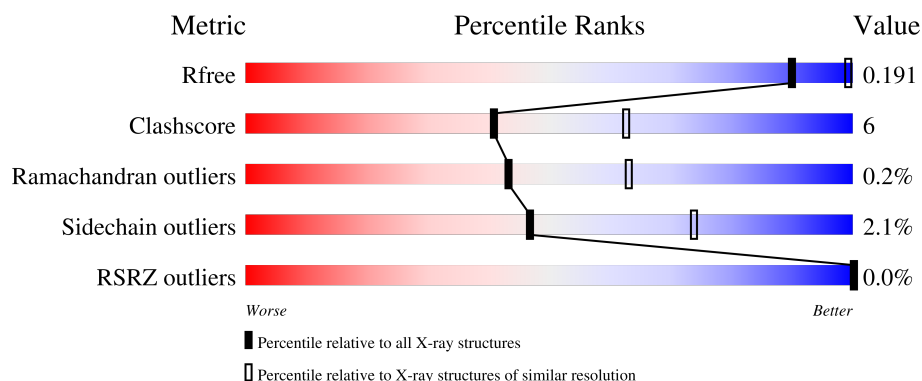
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



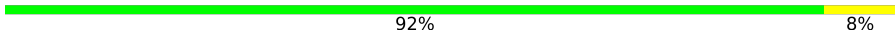
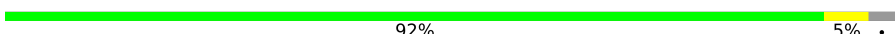
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	87% 10% .
1	a	344	87% 10% .
2	B	505	87% 13% .
2	b	505	88% 11% .
3	C	455	89% 9% .

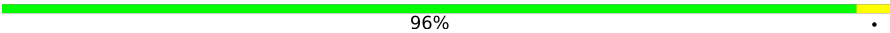
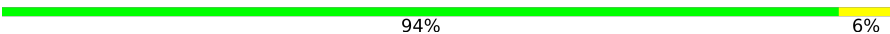
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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	 96% .
16	v	137	 94% 6%
17	X	40	 85% 10% 5%
17	x	40	 82% 12% 5%
18	Y	30	 73% 23% .
18	y	30	 77% 17% . .
19	Z	62	 85% 15%
19	z	62	 89% 11%
20	R	34	 79% 21%

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
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	d	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
27	GOL	B	628	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52752 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 D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

- 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	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

- Molecule 10 is a protein called Photosystem II PsbK protein.

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

- Molecule 12 is a protein called Photosystem II PsbM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	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
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
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 X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

- 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
			479	328	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
			273	186	47	40			

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		

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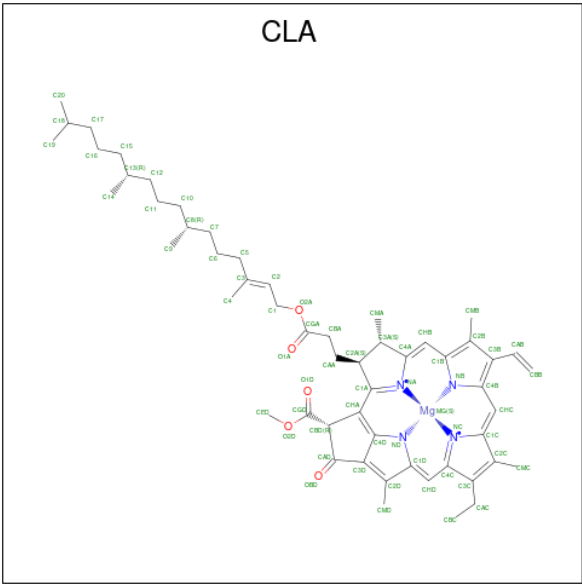
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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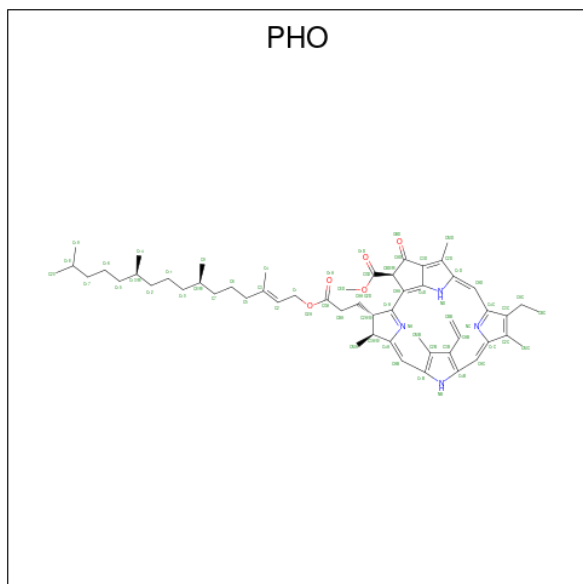
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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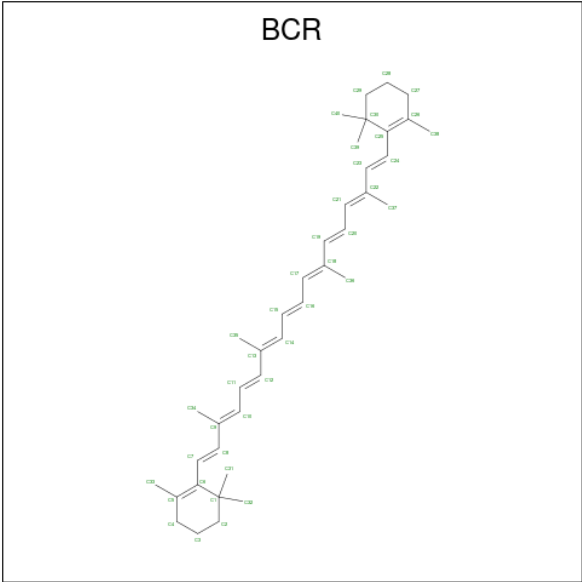
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



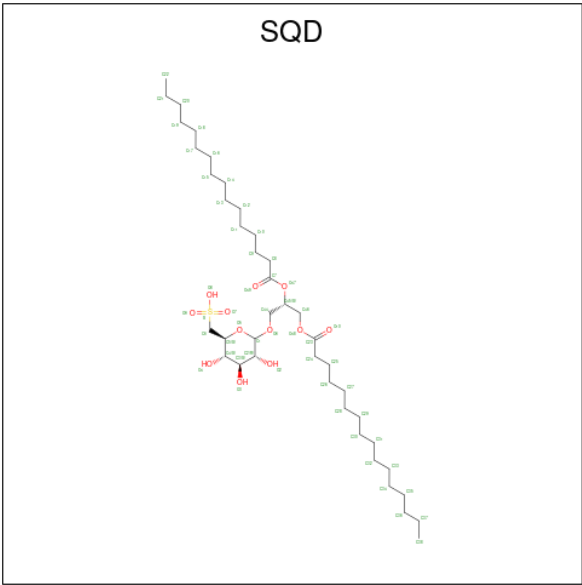
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



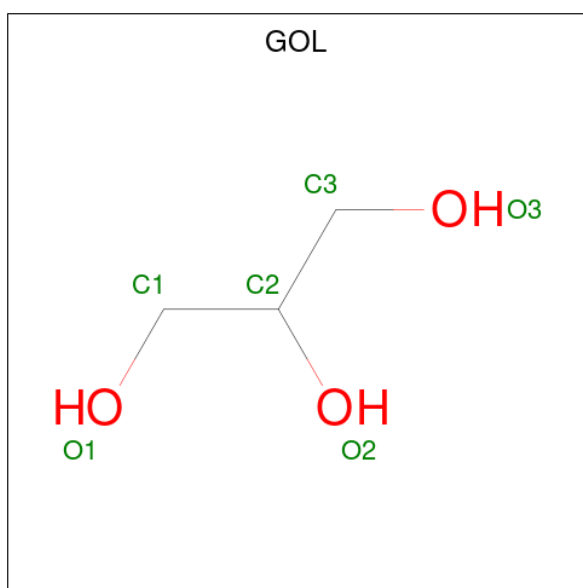
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



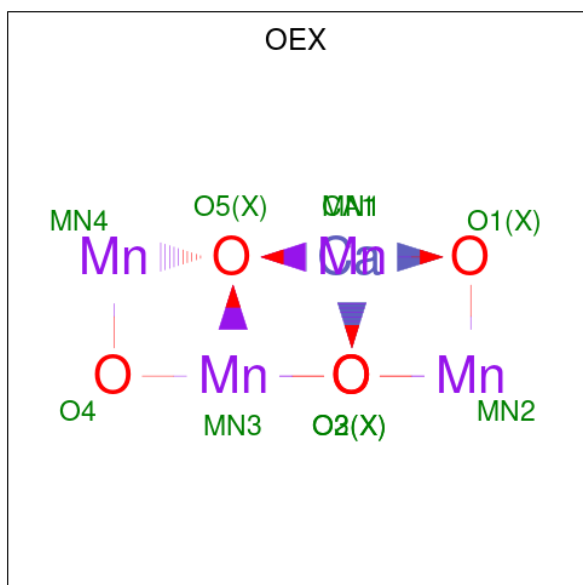
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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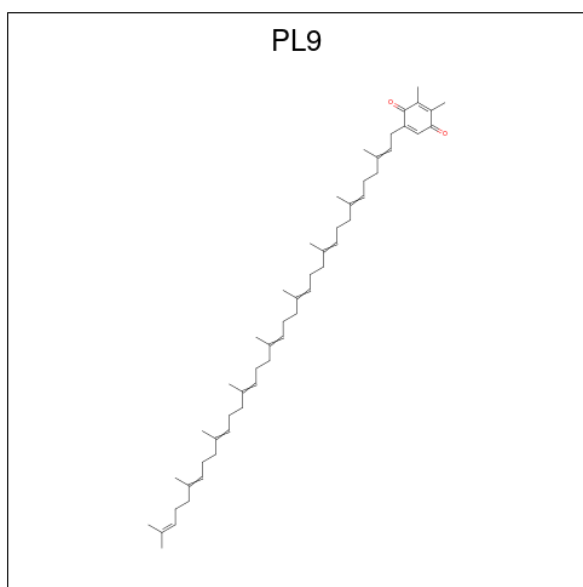
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	b	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 29 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

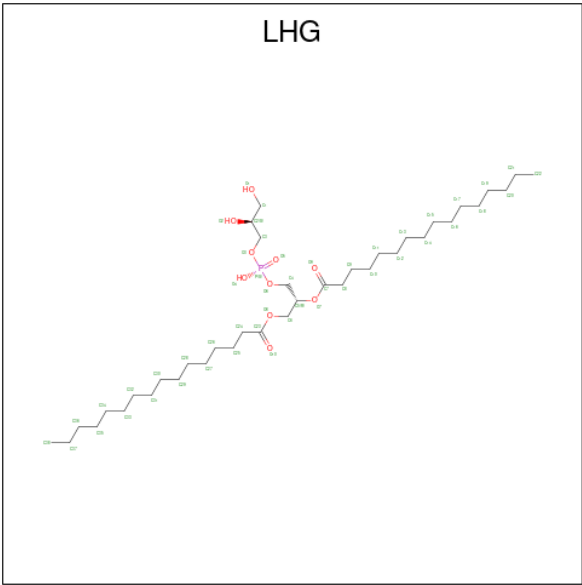
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	2	Total	C	O	0	0
			69	59	10		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	1	Total	C	O	0	0
			17	16	1		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

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



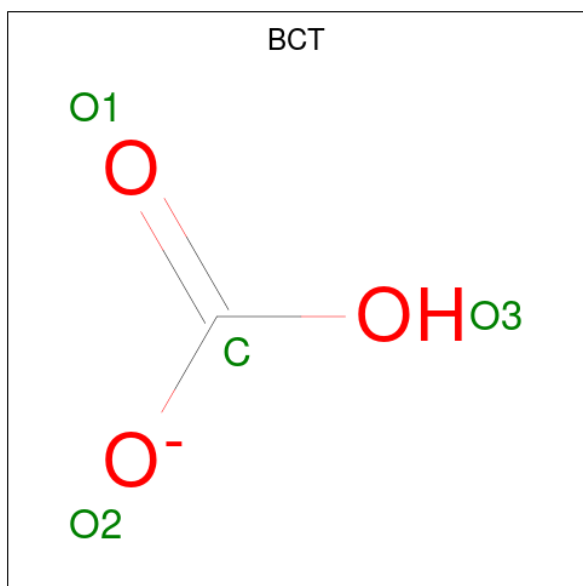
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	b	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).

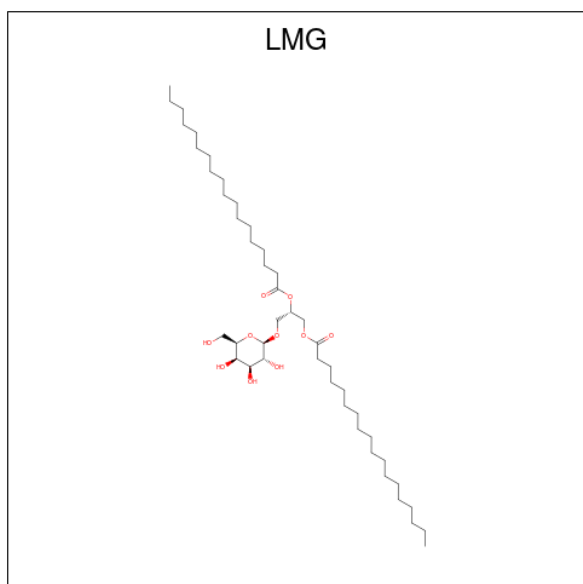


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		
33	C	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	V	1	Total	Ca	0	0
			1	1		
33	c	2	Total	Ca	0	0
			2	2		
33	o	1	Total	Ca	0	0
			1	1		

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



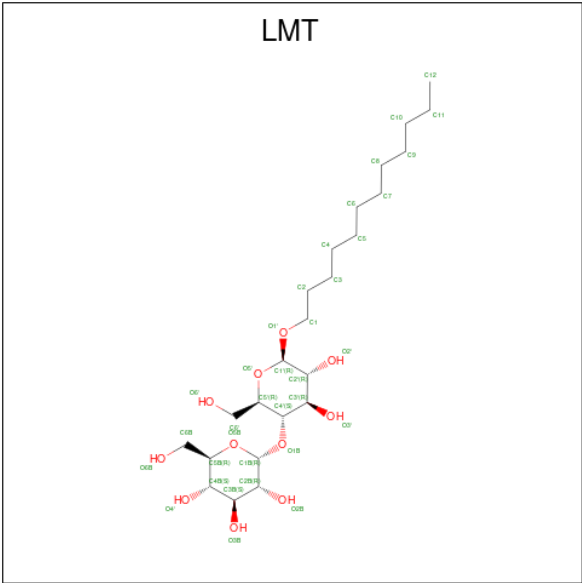
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



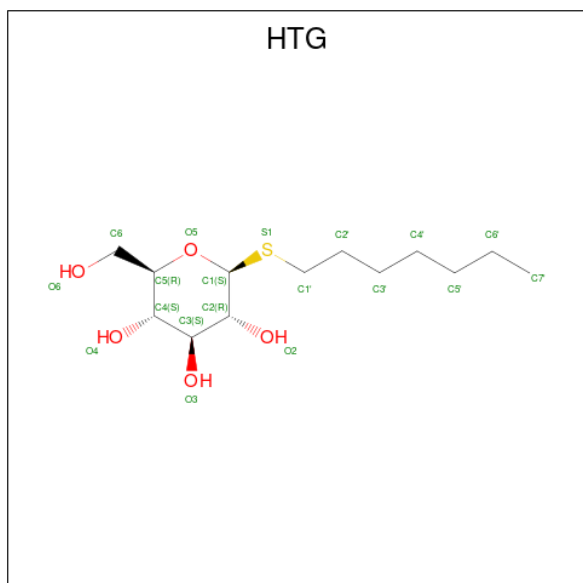
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			25	19	6		
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			26	19	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			35	24	11		
35	D	1	Total	C	O	0	0
			35	24	11		
35	E	1	Total	C	O	0	0
			35	24	11		
35	M	1	Total	C	O	0	0
			35	24	11		
35	M	1	Total	C	O	0	0
			35	24	11		
35	a	1	Total	C	O	0	0
			35	24	11		
35	b	1	Total	C	O	0	0
			25	19	6		
35	b	1	Total	C	O	0	0
			25	19	6		
35	e	1	Total	C	O	0	0
			35	24	11		
35	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



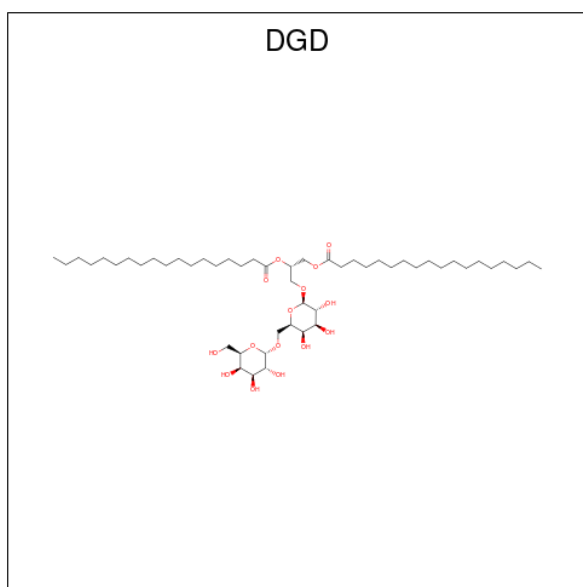
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		

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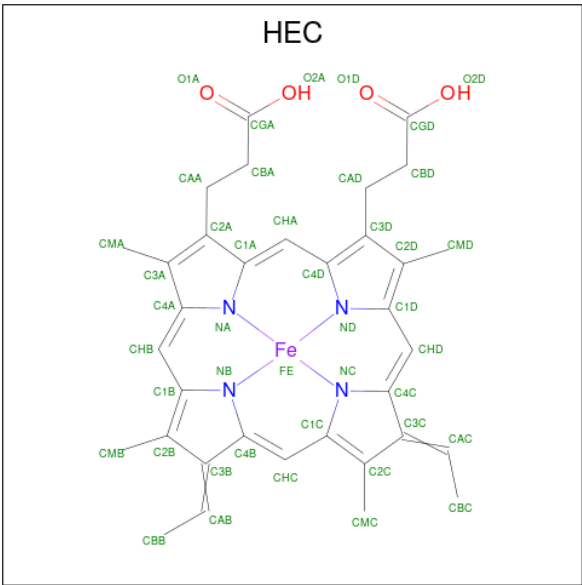
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	S		0	0
			9	8	1			
36	D	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O		0	0
			11	6	5			
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	135	Total	O	0	0
			135	135		
41	B	195	Total	O	0	0
			195	195		
41	C	151	Total	O	0	0
			151	151		
41	D	118	Total	O	0	0
			118	118		
41	E	25	Total	O	0	0
			25	25		
41	F	5	Total	O	0	0
			5	5		
41	H	22	Total	O	0	0
			22	22		
41	I	6	Total	O	0	0
			6	6		
41	J	4	Total	O	0	0
			4	4		
41	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	6	Total O 6 6	0	0
41	M	15	Total O 15 15	0	0
41	O	105	Total O 105 105	0	0
41	T	13	Total O 13 13	0	0
41	U	51	Total O 51 51	0	0
41	V	81	Total O 81 81	0	0
41	X	4	Total O 4 4	0	0
41	Y	1	Total O 1 1	0	0
41	Z	1	Total O 1 1	0	0
41	R	1	Total O 1 1	0	0
41	a	132	Total O 132 132	0	0
41	b	206	Total O 206 206	0	0
41	c	153	Total O 153 153	0	0
41	d	115	Total O 115 115	0	0
41	e	16	Total O 16 16	0	0
41	f	5	Total O 5 5	0	0
41	h	27	Total O 27 27	0	0
41	i	3	Total O 3 3	0	0
41	j	3	Total O 3 3	0	0
41	k	6	Total O 6 6	0	0
41	l	9	Total O 9 9	0	0

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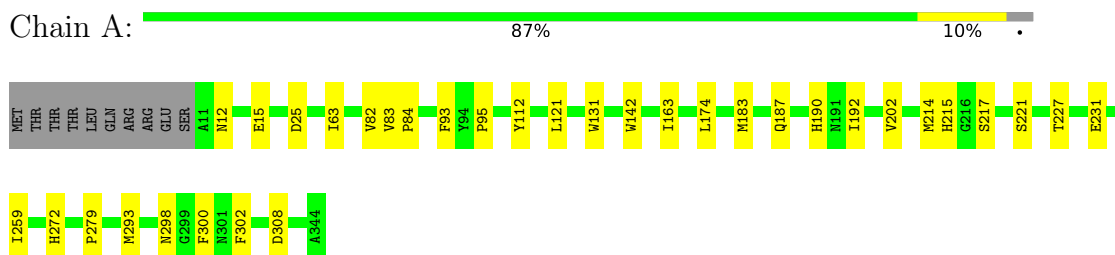
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	m	18	Total 18	O 18	0	0
41	o	115	Total 115	O 115	0	0
41	t	9	Total 9	O 9	0	0
41	u	62	Total 62	O 62	0	0
41	v	78	Total 78	O 78	0	0
41	x	8	Total 8	O 8	0	0
41	z	1	Total 1	O 1	0	0

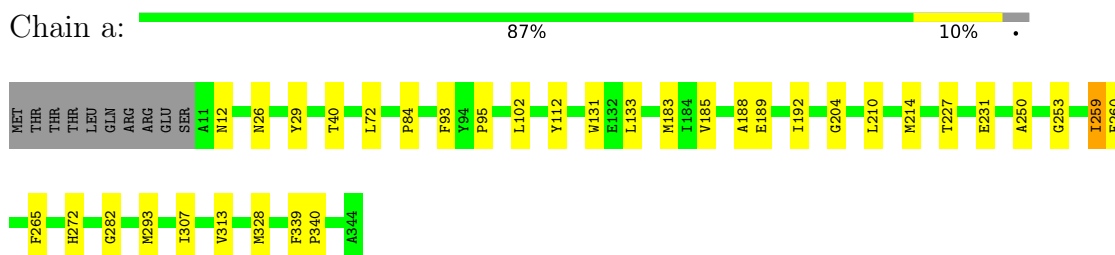
3 Residue-property plots

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

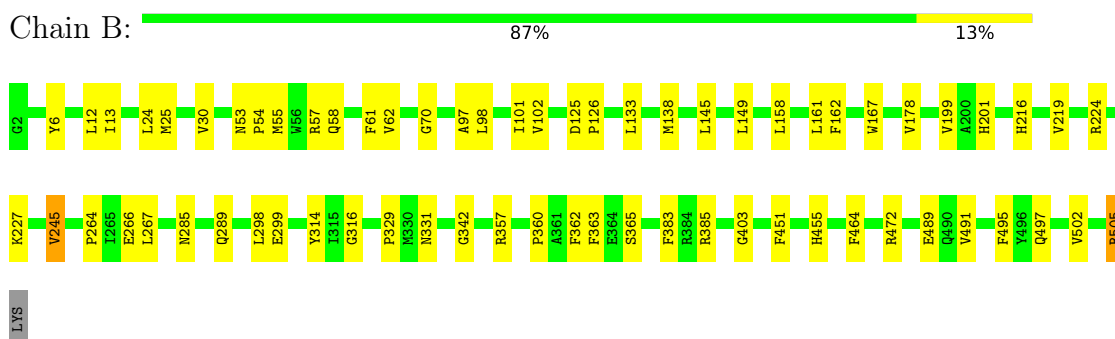
- Molecule 1: Photosystem II D1 protein



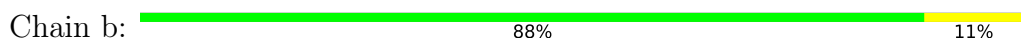
- Molecule 1: Photosystem II D1 protein

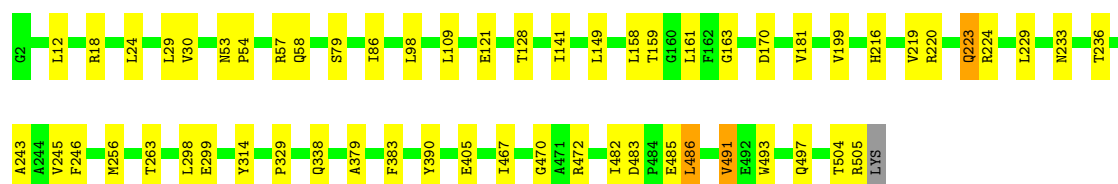


- Molecule 2: Photosystem II CP47 reaction center protein



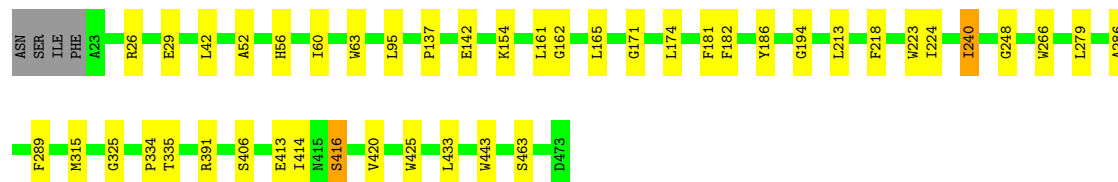
- Molecule 2: Photosystem II CP47 reaction center protein





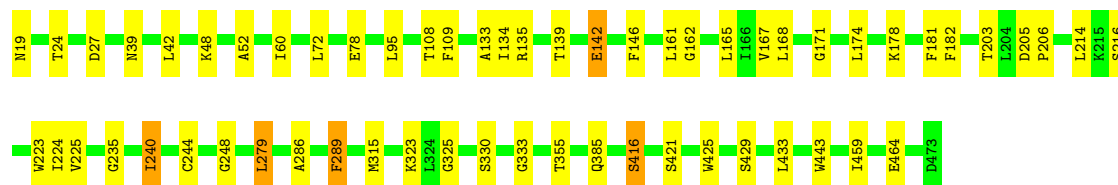
• Molecule 3: Photosystem II CP43 protein

Chain C: 89% 9% .



• Molecule 3: Photosystem II CP43 protein

Chain c: 87% 12% .



• Molecule 4: Photosystem II D2 protein

Chain D: 91% 9% .



• Molecule 4: Photosystem II D2 protein

Chain d: 92% 8% .



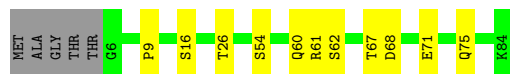
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 81% 15% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  81% 13% 6%



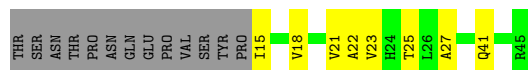
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  61% 16% 23%

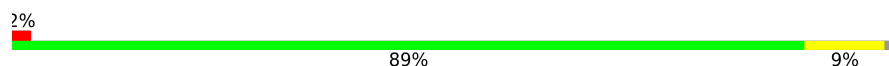


- Molecule 6: Cytochrome b559 subunit beta

Chain f:  52% 18% 30%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  2% 89% 9%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  2% 85% 15%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  79% 18%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  76% 21%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  79% 18% .



- Molecule 9: Photosystem II reaction center protein J

Chain j:  82% 18%



- Molecule 10: Photosystem II PsbK protein

Chain K:  81% 19%



- Molecule 10: Photosystem II PsbK protein

Chain k:  78% 19% .



- Molecule 11: Photosystem II reaction center protein L

Chain L:  89% 8% .



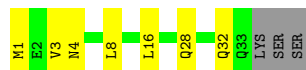
- Molecule 11: Photosystem II reaction center protein L

Chain l:  92% 5% .



- Molecule 12: Photosystem II PsbM protein

Chain M:  72% 19% 8%



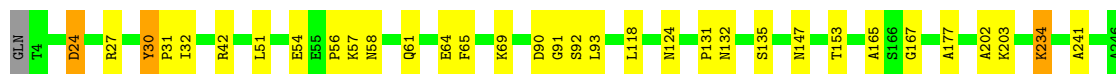
- Molecule 12: Photosystem II PsbM protein

Chain m:  67% 25% 6%



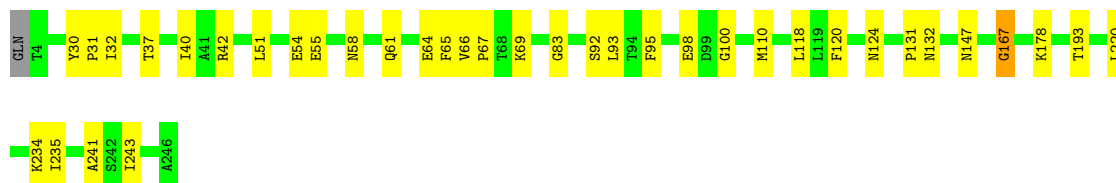
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  86% 12%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  84% 15%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 6% 6% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  78% 12% 6% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  82% 11% 8%

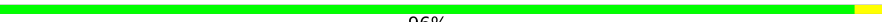


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  85% 9% 7%



• Molecule 16: Cytochrome c-550

Chain V:  96% .

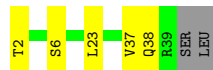
• Molecule 16: Cytochrome c-550

Chain v:  94% 6%

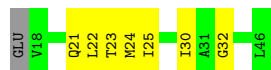
• Molecule 17: Photosystem II reaction center protein X

Chain X:  85% 10% 5%

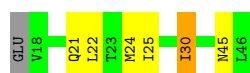
• Molecule 17: Photosystem II reaction center protein X

Chain x:  82% 12% 5%

• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  73% 23% .

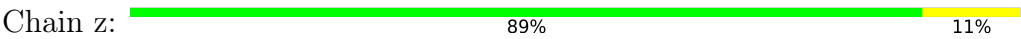
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  77% 17% . .

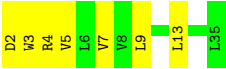
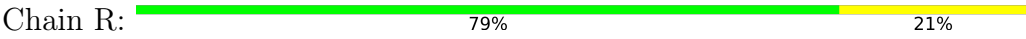
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:  85% 15%

• Molecule 19: Photosystem II reaction center protein Z



● 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	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 99.7 (19.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.187 0.145 , 0.191	Depositor DCC
R_{free} test set	14615 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	52752	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.55	0/2705	0.85	1/3689 (0.0%)
1	a	0.55	0/2705	0.83	0/3689
2	B	0.52	0/4109	0.82	0/5600
2	b	0.51	0/4109	0.82	4/5600 (0.1%)
3	C	0.48	0/3599	0.83	0/4900
3	c	0.49	0/3633	0.84	4/4946 (0.1%)
4	D	0.54	0/2821	0.84	4/3844 (0.1%)
4	d	0.53	0/2812	0.83	4/3832 (0.1%)
5	E	0.46	0/681	0.81	0/928
5	e	0.46	0/667	0.78	0/908
6	F	0.52	0/284	0.75	0/387
6	f	0.50	0/257	0.74	0/349
7	H	0.45	0/519	0.82	0/708
7	h	0.44	0/524	0.77	0/713
8	I	0.43	0/311	0.88	2/419 (0.5%)
8	i	0.45	0/311	0.84	0/419
9	J	0.43	0/278	0.84	0/376
9	j	0.45	0/283	0.77	0/383
10	K	0.48	0/303	0.85	0/416
10	k	0.48	0/303	0.88	0/416
11	L	0.51	0/303	0.73	0/412
11	l	0.45	0/303	0.79	0/412
12	M	0.59	0/253	0.84	0/346
12	m	0.56	0/262	0.93	2/357 (0.6%)
13	O	0.46	0/1896	0.83	2/2571 (0.1%)
13	o	0.48	0/1896	0.86	3/2571 (0.1%)
14	T	0.61	0/257	0.77	0/349
14	t	0.56	0/257	0.77	0/349
15	U	0.50	0/776	0.80	0/1052
15	u	0.51	0/785	0.79	0/1064
16	V	0.53	0/1085	0.81	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.49	0/1085	0.83	0/1473
17	X	0.42	0/284	0.79	0/384
17	x	0.42	0/284	0.77	0/384
18	Y	0.45	0/216	0.80	0/289
18	y	0.42	0/216	0.87	0/289
19	Z	0.43	0/490	0.86	1/669 (0.1%)
19	z	0.42	0/490	0.84	0/669
20	R	0.42	0/279	0.75	0/383
All	All	0.50	0/42631	0.83	27/58018 (0.0%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	30	TYR	CA-C-N	7.12	126.88	119.76
13	O	30	TYR	C-N-CA	7.12	126.88	119.76
4	D	170	ALA	CA-C-N	-6.73	113.05	119.85
4	D	170	ALA	C-N-CA	-6.73	113.05	119.85
13	o	55	GLU	CA-C-N	6.36	126.31	119.76
13	o	55	GLU	C-N-CA	6.36	126.31	119.76
4	d	170	ALA	CA-C-N	-6.18	113.60	119.85
4	d	170	ALA	C-N-CA	-6.18	113.60	119.85
3	c	333	GLY	CA-C-N	6.10	125.99	119.28
3	c	333	GLY	C-N-CA	6.10	125.99	119.28
19	Z	61	VAL	N-CA-C	-6.01	107.27	113.10
4	D	94	GLY	CA-C-N	5.65	125.74	119.87
4	D	94	GLY	C-N-CA	5.65	125.74	119.87
13	o	167	GLY	N-CA-C	5.63	118.90	111.70
1	A	142	TRP	N-CA-C	5.60	119.74	113.02
8	I	31	ASN	CA-C-N	-5.48	114.10	119.64
8	I	31	ASN	C-N-CA	-5.48	114.10	119.64
2	b	163	GLY	CA-C-N	5.27	124.97	119.64
2	b	163	GLY	C-N-CA	5.27	124.97	119.64
2	b	483	ASP	CA-C-N	5.19	124.81	119.05
2	b	483	ASP	C-N-CA	5.19	124.81	119.05
3	c	421	SER	CA-C-N	5.16	125.21	119.32
3	c	421	SER	C-N-CA	5.16	125.21	119.32
4	d	160	TYR	CA-C-N	-5.03	113.74	119.28
4	d	160	TYR	C-N-CA	-5.03	113.74	119.28
12	m	17	VAL	CA-C-N	-5.03	113.85	119.19
12	m	17	VAL	C-N-CA	-5.03	113.85	119.19

There are no chirality outliers.

There are no planarity outliers.

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	2620	0	2517	28	0
1	a	2620	0	2517	25	0
2	B	3969	0	3828	54	0
2	b	3969	0	3828	44	0
3	C	3486	0	3407	39	0
3	c	3519	0	3437	46	0
4	D	2726	0	2627	28	0
4	d	2717	0	2621	17	0
5	E	662	0	648	10	0
5	e	648	0	634	10	0
6	F	275	0	282	6	0
6	f	250	0	261	7	0
7	H	506	0	529	4	0
7	h	511	0	532	12	0
8	I	314	0	328	4	0
8	i	314	0	328	4	0
9	J	272	0	279	4	0
9	j	277	0	284	4	0
10	K	293	0	305	3	0
10	k	293	0	305	4	0
11	L	296	0	304	2	0
11	l	296	0	304	3	0
12	M	260	0	275	4	0
12	m	269	0	288	5	0
13	O	1865	0	1838	21	0
13	o	1865	0	1838	24	0
14	T	258	0	261	6	0
14	t	258	0	261	4	0
15	U	765	0	767	6	0
15	u	774	0	773	4	0
16	V	1064	0	1073	3	0
16	v	1064	0	1073	4	0
17	X	281	0	312	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	x	281	0	312	5	0
18	Y	215	0	246	4	0
18	y	215	0	246	4	0
19	Z	479	0	516	2	0
19	z	479	0	516	1	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	195	0	216	14	0
23	B	1040	0	1152	49	0
23	C	845	0	936	38	0
23	D	195	0	216	9	0
23	a	260	0	288	12	0
23	b	1040	0	1152	48	0
23	c	845	0	936	61	0
23	d	130	0	144	9	0
24	A	64	0	74	1	0
24	D	64	0	74	3	0
24	a	128	0	148	5	0
25	A	40	0	56	2	0
25	B	120	0	168	10	0
25	C	120	0	168	6	0
25	D	40	0	56	2	0
25	H	40	0	56	5	0
25	T	40	0	56	4	0
25	Y	40	0	56	3	0
25	a	40	0	56	1	0
25	b	120	0	168	5	0
25	c	80	0	112	4	0
25	d	40	0	56	1	0
25	h	40	0	56	4	0
25	k	40	0	56	5	0
25	t	40	0	56	4	0
25	y	40	0	56	1	0
26	A	108	0	156	3	0
26	B	54	0	78	2	0
26	D	43	0	53	2	0
26	L	54	0	78	4	0
26	a	108	0	156	5	0
26	f	43	0	53	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	6	0	8	0	0
27	B	12	0	16	5	0
27	C	6	0	8	0	0
27	O	6	0	8	0	0
27	a	6	0	8	1	0
27	b	6	0	8	0	0
27	d	6	0	8	0	0
28	A	10	0	0	0	0
28	a	10	0	0	1	0
29	A	55	0	80	5	0
29	D	55	0	80	1	0
29	a	55	0	80	8	0
29	d	55	0	80	2	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	1	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	69	0	0	0	0
30	c	32	0	0	0	0
30	d	17	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	49	0	74	4	0
31	D	98	0	148	7	0
31	E	42	0	57	0	0
31	L	49	0	74	0	0
31	b	49	0	74	0	0
31	d	147	0	222	8	0
31	e	42	0	57	3	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	O	1	0	0	0	0
33	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	c	2	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	4	0
34	J	51	0	72	2	0
34	Z	37	0	44	2	0
34	a	51	0	72	3	0
34	c	102	0	144	5	0
34	j	51	0	71	5	0
34	m	51	0	72	2	0
34	z	39	0	48	1	0
35	B	121	0	162	9	0
35	C	35	0	46	1	0
35	D	35	0	46	2	0
35	E	35	0	46	1	0
35	M	70	0	92	2	0
35	a	35	0	46	0	0
35	b	50	0	70	2	0
35	e	35	0	46	0	0
35	m	35	0	46	2	0
36	B	95	0	130	6	0
36	C	28	0	41	2	0
36	D	16	0	17	1	0
36	V	11	0	10	0	0
36	b	95	0	130	5	0
36	c	38	0	52	2	0
36	h	16	0	17	1	0
37	C	186	0	246	6	0
37	H	62	0	82	0	0
37	c	186	0	246	8	0
37	h	62	0	82	0	0
38	E	43	0	30	4	0
38	e	43	0	30	3	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	135	0	0	2	0
41	B	195	0	0	11	0
41	C	151	0	0	6	0
41	D	118	0	0	7	0
41	E	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	F	5	0	0	0	0
41	H	22	0	0	3	0
41	I	6	0	0	1	0
41	J	4	0	0	0	0
41	K	6	0	0	0	0
41	L	6	0	0	0	0
41	M	15	0	0	1	0
41	O	105	0	0	0	0
41	R	1	0	0	0	0
41	T	13	0	0	0	0
41	U	51	0	0	0	0
41	V	81	0	0	1	0
41	X	4	0	0	0	0
41	Y	1	0	0	0	0
41	Z	1	0	0	1	0
41	a	132	0	0	1	0
41	b	206	0	0	7	0
41	c	153	0	0	5	0
41	d	115	0	0	1	0
41	e	16	0	0	1	0
41	f	5	0	0	0	0
41	h	27	0	0	0	0
41	i	3	0	0	0	0
41	j	3	0	0	0	0
41	k	6	0	0	0	0
41	l	9	0	0	0	0
41	m	18	0	0	3	0
41	o	115	0	0	0	0
41	t	9	0	0	0	0
41	u	62	0	0	0	0
41	v	78	0	0	2	0
41	x	8	0	0	0	0
41	z	1	0	0	0	0
All	All	52752	0	51821	667	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (667) 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)
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.48	0.94
23:B:605:CLA:H42	23:B:606:CLA:H2	1.48	0.93
4:D:199:MET:O	41:D:501:HOH:O	1.96	0.83
13:o:124:ASN:HD22	13:o:147:ASN:HD22	1.28	0.81
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.62	0.80
25:H:101:BCR:HC8	25:H:101:BCR:H331	1.65	0.79
5:e:67:THR:H	5:e:75:GLN:HE22	1.30	0.78
25:t:101:BCR:H321	25:t:101:BCR:HC8	1.67	0.76
31:d:408:LHG:H382	31:d:408:LHG:H122	1.68	0.76
4:d:24:ARG:HD3	17:x:37:VAL:HG22	1.68	0.76
7:H:37:LEU:O	41:H:201:HOH:O	2.03	0.75
4:D:202:ALA:HB3	41:D:501:HOH:O	1.86	0.75
25:B:619:BCR:H363	25:t:101:BCR:H19C	1.67	0.75
3:C:63:TRP:HB3	41:C:604:HOH:O	1.88	0.74
2:b:497:GLN:HB2	2:b:504:THR:HB	1.70	0.73
23:A:405:CLA:H152	29:A:413:PL9:H252	1.71	0.73
13:O:54:GLU:HG2	13:O:64:GLU:H	1.54	0.72
23:c:512:CLA:HHC	23:c:512:CLA:HBB1	1.71	0.72
5:e:9:PRO:HA	31:e:101:LHG:HC31	1.70	0.72
23:c:503:CLA:HBB1	34:c:520:LMG:H231	1.70	0.72
2:b:224:ARG:HH11	35:b:620:LMT:H12	1.55	0.71
1:A:25:ASP:OD1	41:A:501:HOH:O	2.07	0.71
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.73	0.70
23:b:604:CLA:H42	23:b:605:CLA:H2	1.71	0.70
3:c:279:LEU:HD22	23:c:509:CLA:HED2	1.73	0.70
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.72	0.70
23:c:502:CLA:H61	23:c:512:CLA:H42	1.73	0.70
3:c:165:LEU:HD23	23:c:507:CLA:HED1	1.73	0.70
29:a:415:PL9:H262	31:e:101:LHG:H222	1.73	0.69
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.73	0.69
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.38	0.69
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.74	0.69
3:c:168:LEU:HD21	23:c:509:CLA:H61	1.73	0.69
26:A:409:SQD:H251	31:D:409:LHG:H131	1.76	0.68
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.27	0.68
23:C:506:CLA:HMD3	23:C:508:CLA:HAB	1.74	0.68
3:c:182:PHE:HA	36:c:521:HTG:H61	1.76	0.68
26:a:411:SQD:H301	23:c:508:CLA:H71	1.77	0.67
8:i:35:LYS:O	8:i:37:LEU:N	2.27	0.67
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.75	0.67
23:B:610:CLA:HHC	23:B:610:CLA:HBB1	1.75	0.67
1:A:214:MET:HG2	29:A:413:PL9:H103	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:THR:HB	20:R:4:ARG:HD2	1.77	0.67
23:B:615:CLA:H92	35:m:103:LMT:H92	1.76	0.67
2:B:227:LYS:NZ	41:B:704:HOH:O	2.28	0.66
23:c:506:CLA:H143	37:c:516:DGD:HAN1	1.77	0.66
8:I:37:LEU:O	41:I:201:HOH:O	2.13	0.66
3:C:279:LEU:HD22	23:C:510:CLA:HED2	1.77	0.66
2:b:405:GLU:OE1	41:b:701:HOH:O	2.12	0.66
23:c:513:CLA:HBB1	25:c:514:BCR:H371	1.79	0.65
31:d:408:LHG:H372	31:d:408:LHG:H142	1.78	0.65
23:b:615:CLA:H2	23:b:616:CLA:HBB2	1.78	0.65
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.78	0.65
2:B:61:PHE:O	41:B:701:HOH:O	2.14	0.65
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.79	0.65
13:o:66:VAL:HG21	13:o:110:MET:HE3	1.79	0.65
23:b:607:CLA:H122	34:m:101:LMG:H242	1.77	0.65
29:D:407:PL9:H28	41:D:501:HOH:O	1.96	0.64
18:Y:23:THR:HB	18:Y:24:MET:HE2	1.79	0.64
3:c:174:LEU:HD22	23:c:502:CLA:H203	1.79	0.64
23:B:607:CLA:HHC	23:B:607:CLA:HBB1	1.79	0.64
23:C:507:CLA:H71	35:C:522:LMT:H111	1.79	0.64
2:b:314:TYR:O	41:b:702:HOH:O	2.14	0.64
23:B:602:CLA:H12	23:B:602:CLA:H71	1.78	0.63
5:E:27:ILE:HD11	38:E:103:HEM:HBC2	1.79	0.63
1:a:40:THR:HG23	23:a:409:CLA:HBB1	1.79	0.63
35:B:633:LMT:H52	1:a:72:LEU:HD11	1.80	0.63
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.81	0.63
23:c:508:CLA:HBC3	23:c:510:CLA:H71	1.81	0.63
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.32	0.62
38:e:103:HEM:HAC	6:f:27:ALA:HB1	1.80	0.62
2:B:167:TRP:NE1	41:B:706:HOH:O	2.32	0.62
1:a:214:MET:HG2	29:a:415:PL9:H103	1.81	0.62
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.64	0.62
29:a:415:PL9:H512	26:f:101:SQD:H311	1.81	0.62
36:B:624:HTG:H1	35:B:633:LMT:H21	1.82	0.62
3:c:325:GLY:O	15:u:51:LYS:NZ	2.28	0.62
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.81	0.61
3:c:95:LEU:HD13	23:c:502:CLA:H142	1.81	0.61
3:c:165:LEU:HD22	41:c:704:HOH:O	2.00	0.61
31:d:407:LHG:HC62	11:l:15:THR:HG23	1.84	0.60
2:B:54:PRO:HB3	27:B:628:GOL:H11	1.84	0.60
26:L:102:SQD:O9	2:b:18:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.82	0.60
5:e:60:GLN:HE21	5:e:62:SER:H	1.48	0.60
34:C:501:LMG:H211	37:C:517:DGD:HA82	1.83	0.60
34:m:101:LMG:O2	41:m:201:HOH:O	2.17	0.60
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.85	0.59
2:B:497:GLN:NE2	17:X:38:GLN:O	2.34	0.59
31:D:409:LHG:H132	31:D:409:LHG:H372	1.85	0.59
37:c:517:DGD:HB41	34:c:519:LMG:H331	1.84	0.59
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.85	0.58
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.02	0.58
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.83	0.58
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.85	0.58
4:D:46:GLY:HA2	41:D:526:HOH:O	2.02	0.58
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.33	0.58
23:a:409:CLA:H152	23:c:506:CLA:H142	1.84	0.58
7:h:56:ASP:OD1	17:x:2:THR:OG1	2.20	0.58
23:B:615:CLA:H43	26:B:621:SQD:H111	1.85	0.57
23:C:502:CLA:H151	23:C:508:CLA:HMB3	1.87	0.57
23:c:511:CLA:H72	25:k:101:BCR:H282	1.86	0.57
26:A:409:SQD:H171	31:D:409:LHG:H182	1.86	0.57
3:C:60:ILE:HG22	23:C:504:CLA:HHD	1.86	0.57
23:c:505:CLA:CMD	23:c:507:CLA:HAB	2.35	0.57
36:B:624:HTG:H61	35:B:633:LMT:H6E	1.86	0.57
23:A:407:CLA:H152	37:C:517:DGD:HAW1	1.86	0.57
13:O:92:SER:HB3	13:O:131:PRO:HA	1.87	0.57
23:B:615:CLA:H191	35:B:634:LMT:H102	1.85	0.56
3:C:286:ALA:HB2	23:C:503:CLA:HMD1	1.86	0.56
2:b:30:VAL:HG12	23:b:605:CLA:HHD	1.87	0.56
5:E:27:ILE:CD1	38:E:103:HEM:HBC2	2.35	0.56
34:Z:101:LMG:O4	34:Z:101:LMG:O5	2.23	0.56
5:e:60:GLN:HE21	5:e:62:SER:N	2.03	0.56
23:A:407:CLA:H151	23:C:507:CLA:H13	1.86	0.56
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.88	0.56
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.87	0.56
2:B:264:PRO:HB2	41:B:706:HOH:O	2.06	0.56
1:a:227:THR:HB	1:a:231:GLU:HG3	1.86	0.56
2:B:216:HIS:HE1	23:B:610:CLA:C1A	2.19	0.56
2:B:98:LEU:HD13	36:B:624:HTG:H7'1	1.88	0.56
3:C:223:TRP:CG	3:C:224:ILE:H	2.24	0.56
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.88	0.55
11:L:20:GLY:O	11:L:24:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:413:SQD:H241	6:F:18:VAL:HG22	1.87	0.55
23:D:401:CLA:HHC	23:D:401:CLA:HBB1	1.88	0.55
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.38	0.55
34:a:417:LMG:H222	37:c:516:DGD:HAT2	1.88	0.55
3:C:26:ARG:HE	10:K:46:ARG:NH1	2.05	0.54
5:e:60:GLN:HG3	5:e:62:SER:H	1.73	0.54
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.20	0.54
23:b:608:CLA:HAB	4:d:123:ILE:HG12	1.90	0.54
3:c:167:VAL:HG11	23:c:512:CLA:HBA2	1.88	0.54
4:D:49:LEU:HD12	41:D:526:HOH:O	2.06	0.54
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.40	0.54
3:C:161:LEU:HD11	23:C:507:CLA:HBB1	1.90	0.54
23:a:406:CLA:H141	34:j:101:LMG:H361	1.90	0.54
3:c:27:ASP:HB3	10:k:46:ARG:HG3	1.89	0.54
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.73	0.54
12:M:8:LEU:HD11	35:M:103:LMT:H91	1.90	0.54
13:O:56:PRO:HB3	13:O:61:GLN:HG2	1.89	0.53
23:b:607:CLA:H18	31:d:406:LHG:H151	1.91	0.53
23:B:614:CLA:HBB1	23:B:614:CLA:HMB1	1.90	0.53
3:C:181:PHE:HE2	36:C:524:HTG:H7'3	1.73	0.53
23:a:409:CLA:H172	23:c:506:CLA:H91	1.90	0.53
25:H:101:BCR:H363	41:H:201:HOH:O	2.08	0.53
29:a:415:PL9:H401	6:f:18:VAL:HG13	1.90	0.53
19:z:32:ASP:O	19:z:36:SER:OG	2.24	0.53
35:B:634:LMT:H123	12:m:12:ALA:HA	1.91	0.53
2:b:219:VAL:O	41:b:703:HOH:O	2.19	0.53
2:b:299:GLU:HG3	41:b:862:HOH:O	2.09	0.53
3:c:286:ALA:HB2	23:c:502:CLA:HMD1	1.90	0.53
2:B:24:LEU:HD21	23:B:617:CLA:HAB	1.89	0.53
2:B:267:LEU:HG	41:B:706:HOH:O	2.08	0.53
23:d:402:CLA:H191	34:j:101:LMG:H222	1.91	0.53
16:v:12:LEU:HD12	16:v:69:ILE:HB	1.90	0.53
24:A:406:PHO:HAB	4:D:205:LEU:HD13	1.90	0.52
23:c:513:CLA:H152	34:c:520:LMG:H422	1.90	0.52
23:c:504:CLA:H151	23:c:508:CLA:H143	1.90	0.52
3:c:223:TRP:CG	3:c:224:ILE:H	2.28	0.52
31:A:415:LHG:H142	23:B:608:CLA:H201	1.91	0.52
2:B:285:ASN:O	2:B:289:GLN:HG2	2.09	0.52
41:E:203:HOH:O	9:J:2:SER:N	2.42	0.52
13:o:92:SER:HB3	13:o:131:PRO:HA	1.91	0.52
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:607:CLA:H192	23:B:617:CLA:H101	1.92	0.52
13:O:32:ILE:HG13	13:O:93:LEU:HD11	1.91	0.52
2:b:223:GLN:HA	2:b:223:GLN:HE21	1.75	0.52
31:A:415:LHG:H252	2:B:464:PHE:CZ	2.44	0.52
23:B:616:CLA:HHC	23:B:616:CLA:HBB1	1.92	0.52
2:B:55:MET:HE3	27:B:628:GOL:H32	1.91	0.52
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.92	0.52
6:F:30:THR:HG21	34:J:101:LMG:H412	1.91	0.51
1:a:183:MET:HA	23:a:404:CLA:HMD1	1.92	0.51
3:C:182:PHE:HA	36:C:523:HTG:H61	1.92	0.51
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.91	0.51
2:b:482:ILE:HD12	2:b:486:LEU:HD12	1.91	0.51
12:m:5:GLN:H	12:m:5:GLN:NE2	2.08	0.51
23:A:404:CLA:H191	31:D:408:LHG:H332	1.93	0.51
23:b:602:CLA:H101	23:b:609:CLA:H193	1.91	0.51
3:C:218:PHE:HE2	34:C:501:LMG:H111	1.75	0.51
41:M:203:HOH:O	14:T:1:FME:SD	2.59	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.51
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.46	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.10	0.51
1:A:183:MET:HA	23:A:404:CLA:HMD1	1.93	0.51
26:A:411:SQD:H261	2:b:109:LEU:HD13	1.93	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.11	0.51
3:c:244:CYS:HA	41:c:704:HOH:O	2.09	0.51
7:H:41:PHE:N	41:H:201:HOH:O	2.43	0.51
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.92	0.51
3:C:413:GLU:OE2	41:C:601:HOH:O	2.19	0.51
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.40	0.51
13:O:27:ARG:NH1	13:O:202:ALA:O	2.43	0.51
36:B:629:HTG:H61	1:a:102:LEU:HD12	1.93	0.50
2:b:224:ARG:NH1	4:d:16:ASP:OD2	2.42	0.50
38:E:103:HEM:HMC2	6:F:31:ILE:HG13	1.93	0.50
23:c:512:CLA:H143	23:c:513:CLA:H142	1.93	0.50
10:k:21:LEU:HD13	18:y:24:MET:HE2	1.93	0.50
23:B:613:CLA:CMB	23:B:615:CLA:HBB1	2.41	0.50
18:Y:22:LEU:HA	18:Y:25:ILE:HG22	1.92	0.50
24:a:408:PHO:HBA2	23:d:402:CLA:H142	1.94	0.50
2:b:149:LEU:HG	23:b:606:CLA:HBB2	1.93	0.50
23:c:501:CLA:C4D	23:c:503:CLA:H2	2.41	0.50
14:T:14:ILE:HG22	25:T:101:BCR:H10C	1.93	0.50
1:A:63:ILE:HB	3:C:335:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:407:CLA:H171	23:C:507:CLA:H112	1.92	0.50
23:B:604:CLA:HBB2	23:B:606:CLA:H193	1.93	0.50
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.92	0.50
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.50
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.27	0.50
4:d:332:GLN:OE1	4:d:332:GLN:N	2.44	0.50
26:a:413:SQD:H162	31:d:407:LHG:H382	1.92	0.50
2:b:141:ILE:HD11	7:h:14:LEU:HD22	1.93	0.50
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.47	0.50
23:c:510:CLA:H51	31:d:408:LHG:H371	1.93	0.50
2:B:54:PRO:HB2	27:B:628:GOL:H31	1.94	0.49
8:i:36:ASP:OD1	8:i:36:ASP:N	2.43	0.49
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.93	0.49
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.95	0.49
2:b:58:GLN:C	2:b:329:PRO:HB3	2.37	0.49
7:h:25:TRP:NE1	36:h:101:HTG:H5	2.26	0.49
25:B:618:BCR:H291	41:B:861:HOH:O	2.11	0.49
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.93	0.49
2:B:57:ARG:HH21	2:B:331:ASN:HD22	1.60	0.49
3:C:174:LEU:HB3	23:C:503:CLA:H151	1.94	0.49
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.47	0.49
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.94	0.49
2:B:266:GLU:HB2	41:B:706:HOH:O	2.11	0.49
23:a:406:CLA:HAB	23:d:402:CLA:H72	1.94	0.49
8:i:2:GLU:O	8:i:6:ILE:HG12	2.13	0.49
26:L:102:SQD:H1	26:L:102:SQD:H462	1.95	0.49
13:O:51:LEU:HD12	13:O:234:LYS:HG2	1.95	0.49
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.48	0.49
2:B:219:VAL:O	41:B:702:HOH:O	2.19	0.49
37:C:517:DGD:HG11	41:C:616:HOH:O	2.12	0.49
23:b:601:CLA:H72	23:b:601:CLA:H2	1.93	0.49
41:d:556:HOH:O	17:x:6:SER:HA	2.13	0.49
5:e:60:GLN:HB3	41:e:207:HOH:O	2.13	0.49
25:h:102:BCR:H331	25:h:102:BCR:C8	2.42	0.49
1:A:227:THR:HB	1:A:231:GLU:HG3	1.94	0.48
23:C:514:CLA:HAB	25:C:515:BCR:H24C	1.95	0.48
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.95	0.48
37:c:518:DGD:HAH1	34:j:101:LMG:H201	1.94	0.48
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.95	0.48
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.95	0.48
23:c:505:CLA:HBD	23:c:505:CLA:HAA1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:4:ARG:HH11	7:h:9:ASP:CG	2.21	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
1:A:221:SER:HA	4:D:139:ARG:HB2	1.96	0.48
26:B:621:SQD:H381	35:m:103:LMT:H123	1.94	0.48
13:o:124:ASN:HD22	13:o:147:ASN:ND2	2.05	0.48
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.94	0.48
13:O:124:ASN:HD22	13:O:147:ASN:ND2	2.07	0.48
14:T:2:GLU:CD	14:T:2:GLU:H	2.22	0.48
23:b:615:CLA:H152	23:b:615:CLA:H111	1.57	0.48
3:C:391:ARG:HD3	41:C:742:HOH:O	2.14	0.48
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.49	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.49	0.47
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.14	0.47
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.94	0.47
23:B:602:CLA:C4D	23:B:602:CLA:H72	2.44	0.47
19:Z:34:ASP:HB3	41:Z:201:HOH:O	2.14	0.47
5:e:26:THR:HB	38:e:103:HEM:HAB	1.97	0.47
3:C:60:ILE:HA	41:C:604:HOH:O	2.13	0.47
3:C:406:SER:HA	3:C:420:VAL:HG23	1.97	0.47
25:D:406:BCR:H381	34:J:101:LMG:H231	1.97	0.47
16:v:30:LYS:NZ	41:v:302:HOH:O	2.40	0.47
23:B:615:CLA:H62	23:B:615:CLA:H41	1.57	0.47
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.48	0.47
23:A:407:CLA:H171	23:C:507:CLA:H142	1.95	0.47
8:I:17:LEU:HD22	8:I:21:PHE:HE2	1.79	0.47
1:a:265:PHE:HE2	29:a:415:PL9:H111	1.80	0.47
24:a:408:PHO:HBC3	4:d:279:LEU:HD22	1.96	0.47
3:c:429:SER:HA	37:c:517:DGD:HBW1	1.97	0.47
23:c:513:CLA:HBA1	23:c:513:CLA:C4A	2.44	0.47
23:B:611:CLA:H122	23:B:616:CLA:HAA1	1.97	0.47
24:D:402:PHO:H3A	23:D:404:CLA:H142	1.95	0.47
35:D:403:LMT:H21	36:b:621:HTG:H1	1.96	0.47
4:d:85:MET:HE2	4:d:90:LEU:HD21	1.96	0.47
23:b:615:CLA:H61	23:b:615:CLA:H92	1.76	0.47
3:c:165:LEU:CD2	23:c:507:CLA:HED1	2.43	0.47
34:j:101:LMG:H292	34:j:101:LMG:H151	1.96	0.47
23:C:509:CLA:H142	23:C:509:CLA:H111	1.74	0.47
1:a:307:ILE:HD13	1:a:313:VAL:HA	1.97	0.47
31:d:408:LHG:H122	31:d:408:LHG:C38	2.42	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.51	0.46
23:B:605:CLA:HAB	23:B:612:CLA:H191	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:497:GLN:HE22	17:x:38:GLN:HB2	1.80	0.46
23:b:601:CLA:H91	25:h:102:BCR:H21C	1.97	0.46
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.97	0.46
13:o:132:ASN:O	13:o:132:ASN:ND2	2.46	0.46
1:A:217:SER:HA	4:D:272:LEU:HD12	1.97	0.46
25:A:408:BCR:H371	25:A:408:BCR:H24C	1.72	0.46
16:V:103:LYS:HB3	41:V:324:HOH:O	2.16	0.46
23:b:606:CLA:H162	23:b:606:CLA:H122	1.58	0.46
23:c:505:CLA:HMD3	23:c:507:CLA:HAB	1.96	0.46
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.96	0.46
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.97	0.46
2:B:357:ARG:NE	41:B:708:HOH:O	2.37	0.46
23:c:507:CLA:HAA2	23:c:507:CLA:HBD	1.97	0.46
23:c:509:CLA:H192	23:c:512:CLA:HHD	1.98	0.46
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.50	0.46
3:C:325:GLY:O	15:U:51:LYS:NZ	2.39	0.46
1:A:163:ILE:HD11	37:C:517:DGD:HA22	1.98	0.46
4:D:230:SER:HB2	41:D:577:HOH:O	2.16	0.46
26:L:102:SQD:H201	2:b:29:LEU:HD23	1.98	0.46
3:c:323:LYS:NZ	41:c:608:HOH:O	2.48	0.46
23:c:512:CLA:O2D	23:c:513:CLA:HBB2	2.16	0.46
1:a:26:ASN:HB3	26:a:413:SQD:H81	1.98	0.46
25:B:620:BCR:H331	25:B:620:BCR:C8	2.45	0.46
4:D:49:LEU:HB2	41:D:526:HOH:O	2.16	0.46
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.45	0.46
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	1.97	0.46
3:c:214:LEU:HD23	3:c:214:LEU:HA	1.80	0.46
6:f:18:VAL:HG23	26:f:101:SQD:O9	2.15	0.46
1:A:12:ASN:ND2	1:A:15:GLU:HB2	2.31	0.46
23:B:615:CLA:H203	34:B:622:LMG:H421	1.97	0.46
3:C:186:TYR:OH	3:C:194:GLY:HA3	2.16	0.46
23:D:401:CLA:C4A	23:D:401:CLA:HBA1	2.46	0.46
36:b:625:HTG:O2	36:b:626:HTG:S1	2.71	0.46
3:C:334:PRO:HA	13:O:153:THR:OG1	2.16	0.46
29:a:415:PL9:H322	29:a:415:PL9:H301	1.69	0.46
2:b:170:ASP:HA	7:h:66:GLY:HA2	1.98	0.46
23:b:605:CLA:H91	23:b:605:CLA:H111	1.72	0.46
2:B:133:LEU:HB3	2:B:138:MET:SD	2.56	0.45
23:B:603:CLA:H101	23:B:610:CLA:H193	1.99	0.45
35:E:102:LMT:O3'	35:E:102:LMT:O2B	2.27	0.45
23:b:603:CLA:H143	23:b:608:CLA:HAC1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:68:ASP:HB3	5:e:71:GLU:HB3	1.97	0.45
13:o:124:ASN:ND2	13:o:147:ASN:HD22	2.04	0.45
23:B:603:CLA:H141	23:B:603:CLA:H161	1.81	0.45
23:a:406:CLA:H112	34:j:101:LMG:H231	1.99	0.45
2:b:229:LEU:HD22	23:b:608:CLA:HED2	1.98	0.45
1:A:308:ASP:O	6:F:45:ARG:HD2	2.16	0.45
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.45
31:D:409:LHG:H141	31:D:409:LHG:H352	1.99	0.45
23:B:606:CLA:HAA1	23:B:606:CLA:HBD	1.99	0.45
1:a:183:MET:HB3	23:a:404:CLA:HBC2	1.97	0.45
34:a:417:LMG:H211	34:a:417:LMG:H241	1.72	0.45
23:b:605:CLA:H41	23:b:605:CLA:H62	1.60	0.45
29:A:413:PL9:H253	23:D:404:CLA:H141	1.99	0.45
2:B:360:PRO:HB3	27:B:627:GOL:H32	1.98	0.45
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.47	0.45
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	1.99	0.45
7:H:43:LEU:HD12	7:H:43:LEU:HA	1.87	0.45
2:b:24:LEU:HD21	23:b:616:CLA:CAB	2.45	0.45
3:c:78:GLU:HB3	41:v:325:HOH:O	2.15	0.45
13:o:40:ILE:HG12	13:o:243:ILE:HD13	1.97	0.45
2:B:54:PRO:CB	27:B:628:GOL:H11	2.47	0.45
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.52	0.45
23:c:507:CLA:H41	23:c:507:CLA:H62	1.70	0.45
3:C:52:ALA:HB2	23:C:512:CLA:HMA2	1.97	0.45
5:E:33:ALA:HB3	41:E:219:HOH:O	2.16	0.45
23:b:601:CLA:H93	23:b:601:CLA:H111	1.74	0.45
23:b:611:CLA:H172	23:b:613:CLA:ND	2.32	0.45
25:c:514:BCR:H351	25:c:514:BCR:H15C	1.66	0.45
13:o:30:TYR:HA	13:o:31:PRO:HD3	1.76	0.45
5:E:15:THR:HB	9:J:7:ILE:O	2.17	0.45
28:a:414:OEX:O4	41:a:501:HOH:O	2.21	0.45
2:b:79:SER:HA	41:b:713:HOH:O	2.17	0.45
23:d:403:CLA:H41	23:d:403:CLA:H61	1.50	0.45
9:j:20:VAL:HA	9:j:23:ILE:HG22	1.99	0.45
1:A:121:LEU:HD13	34:C:501:LMG:H182	1.99	0.44
23:A:404:CLA:CB	23:D:401:CLA:HAC2	2.47	0.44
23:B:606:CLA:H141	23:B:606:CLA:H161	1.78	0.44
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.63	0.44
23:a:405:CLA:H52	29:d:405:PL9:H151	1.99	0.44
23:b:614:CLA:H62	23:b:614:CLA:H41	1.45	0.44
3:c:109:PHE:CE2	34:c:520:LMG:HC72	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:501:CLA:C3D	23:c:503:CLA:H2	2.46	0.44
23:c:506:CLA:H162	23:c:506:CLA:H122	1.49	0.44
2:B:363:PHE:HB3	2:B:365:SER:O	2.17	0.44
23:B:605:CLA:H41	23:B:605:CLA:H62	1.76	0.44
29:a:415:PL9:H151	29:a:415:PL9:H171	1.57	0.44
23:b:610:CLA:OBD	23:b:610:CLA:H152	2.17	0.44
12:m:34:LYS:O	41:m:202:HOH:O	2.20	0.44
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.99	0.44
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.47	0.44
31:D:408:LHG:H192	14:T:17:PHE:HZ	1.82	0.44
12:M:28:GLN:O	12:M:32:GLN:HG3	2.17	0.44
35:M:101:LMT:H6D	11:l:9:PRO:HA	1.98	0.44
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.99	0.44
2:b:12:LEU:HB2	23:b:612:CLA:HMC2	1.99	0.44
3:c:146:PHE:HZ	23:c:512:CLA:HBB2	1.82	0.44
10:k:16:ALA:O	10:k:19:ASP:HB2	2.17	0.44
2:B:145:LEU:HD11	23:B:616:CLA:HMB1	1.99	0.44
23:C:508:CLA:H61	23:C:508:CLA:H92	1.71	0.44
20:R:9:LEU:O	20:R:13:LEU:HG	2.17	0.44
1:a:131:TRP:CH2	23:c:505:CLA:HAA2	2.52	0.44
25:a:410:BCR:H24C	25:a:410:BCR:H371	1.73	0.44
29:a:415:PL9:H403	6:f:22:ALA:HB2	1.99	0.44
23:c:507:CLA:H142	23:c:507:CLA:H112	1.75	0.44
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.98	0.44
34:B:622:LMG:O10	12:M:4:ASN:ND2	2.51	0.44
2:b:470:GLY:HA2	41:b:707:HOH:O	2.17	0.44
23:c:508:CLA:HMB3	23:c:508:CLA:HBB1	2.00	0.44
2:B:245:VAL:HG22	23:B:613:CLA:H202	2.00	0.44
23:B:610:CLA:HBA1	23:B:610:CLA:H3A	1.82	0.44
3:C:171:GLY:O	3:C:174:LEU:HB2	2.18	0.44
3:C:213:LEU:HD21	25:C:516:BCR:C20	2.47	0.44
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.72	0.44
23:c:511:CLA:H191	34:z:101:LMG:H242	2.00	0.44
13:o:193:THR:HG21	13:o:220:LEU:HD12	2.00	0.44
25:A:408:BCR:H15C	25:A:408:BCR:H351	1.80	0.43
2:B:13:ILE:HG12	23:B:613:CLA:HAC2	1.99	0.43
25:B:620:BCR:H15C	25:B:620:BCR:H351	1.86	0.43
23:C:507:CLA:HBA1	23:C:507:CLA:H3A	1.69	0.43
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.38	0.43
26:L:102:SQD:H211	25:T:101:BCR:H351	1.99	0.43
2:b:256:MET:HA	2:b:263:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:604:CLA:H62	23:b:604:CLA:H41	1.55	0.43
23:b:614:CLA:H162	23:b:614:CLA:H122	1.73	0.43
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.99	0.43
6:f:21:VAL:O	6:f:25:THR:HG23	2.18	0.43
13:o:51:LEU:HD23	13:o:67:PRO:HA	1.99	0.43
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.00	0.43
23:C:507:CLA:H91	23:C:507:CLA:H111	1.85	0.43
23:C:514:CLA:H161	34:C:521:LMG:H421	2.00	0.43
23:a:404:CLA:H193	23:a:404:CLA:H161	1.73	0.43
3:c:443:TRP:CZ2	23:c:508:CLA:HMD1	2.53	0.43
2:B:24:LEU:HD21	23:B:617:CLA:CAB	2.48	0.43
23:C:507:CLA:H41	23:C:507:CLA:H62	1.70	0.43
23:C:511:CLA:H112	23:C:511:CLA:H152	1.75	0.43
23:D:401:CLA:H203	23:D:401:CLA:H162	1.68	0.43
25:H:101:BCR:H331	25:H:101:BCR:C8	2.38	0.43
24:a:408:PHO:HBA2	24:a:408:PHO:H3A	1.83	0.43
2:b:159:THR:HA	2:b:181:VAL:O	2.18	0.43
3:c:48:LYS:HG2	3:c:133:ALA:O	2.17	0.43
9:j:3:GLU:O	9:j:6:ARG:HG2	2.18	0.43
37:C:518:DGD:HAE2	37:C:518:DGD:HA81	1.59	0.43
3:c:52:ALA:HB2	23:c:511:CLA:HMA2	2.01	0.43
3:c:60:ILE:HG22	23:c:503:CLA:HHD	2.01	0.43
3:c:171:GLY:O	3:c:174:LEU:HB2	2.17	0.43
23:c:512:CLA:HBB1	23:c:512:CLA:CHC	2.44	0.43
1:A:190:HIS:O	1:A:298:ASN:HB3	2.17	0.43
1:A:231:GLU:HB3	41:B:849:HOH:O	2.18	0.43
25:B:619:BCR:H15C	25:B:619:BCR:H351	1.76	0.43
38:E:103:HEM:HAC	6:F:27:ALA:HB1	2.01	0.43
23:b:611:CLA:HBB1	23:b:611:CLA:HMB1	1.98	0.43
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.84	0.43
23:B:615:CLA:H92	23:B:615:CLA:H61	1.75	0.43
3:C:56:HIS:HB2	23:C:510:CLA:HMB2	2.01	0.43
3:C:443:TRP:CE2	23:C:509:CLA:HMD2	2.53	0.43
3:C:463:SER:OG	8:I:33:LYS:NZ	2.49	0.43
25:H:101:BCR:H393	17:X:7:LEU:HD21	2.00	0.43
13:O:124:ASN:ND2	13:O:147:ASN:HD22	2.13	0.43
3:c:385:GLN:HG3	41:c:709:HOH:O	2.18	0.43
31:e:101:LHG:H241	31:e:101:LHG:HC61	1.87	0.43
2:B:299:GLU:HG3	41:B:821:HOH:O	2.17	0.43
31:d:407:LHG:H192	14:t:17:PHE:HZ	1.84	0.43
31:A:415:LHG:H151	11:L:23:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:PHE:O	23:B:607:CLA:HHD	2.19	0.43
26:a:413:SQD:H223	26:a:413:SQD:H191	1.90	0.43
35:D:403:LMT:O2B	35:D:403:LMT:O3'	2.28	0.43
13:O:30:TYR:HA	13:O:31:PRO:HD3	1.68	0.43
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.80	0.43
41:b:875:HOH:O	13:o:178:LYS:HD2	2.18	0.43
25:C:527:BCR:H24C	25:C:527:BCR:H371	1.70	0.43
13:O:90:ASP:O	13:O:132:ASN:N	2.45	0.43
34:a:417:LMG:HC71	3:c:216:SER:HB2	2.01	0.43
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.00	0.43
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.93	0.43
3:c:181:PHE:HE2	36:c:522:HTG:H7'3	1.84	0.43
13:o:234:LYS:HB2	13:o:234:LYS:HE2	1.85	0.43
1:A:131:TRP:CH2	23:C:506:CLA:HAA2	2.54	0.42
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.84	0.42
25:C:516:BCR:H24C	25:C:516:BCR:H371	1.80	0.42
23:D:405:CLA:HHC	23:D:405:CLA:HBB1	2.01	0.42
5:E:25:ILE:O	5:E:28:PRO:HD2	2.19	0.42
23:B:606:CLA:H92	23:B:606:CLA:H61	1.75	0.42
23:B:612:CLA:H112	23:B:612:CLA:H72	1.78	0.42
4:D:120:PHE:HA	4:D:123:ILE:HD12	2.00	0.42
23:b:612:CLA:H192	23:b:612:CLA:H162	1.85	0.42
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	2.01	0.42
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.93	0.42
36:B:625:HTG:O6	13:O:177:ALA:O	2.24	0.42
5:E:60:GLN:HE21	5:E:62:SER:HB3	1.83	0.42
1:a:29:TYR:CG	1:a:133:LEU:HD13	2.55	0.42
2:b:467:ILE:HD13	2:b:467:ILE:HA	1.79	0.42
23:b:602:CLA:H41	7:h:46:LEU:HA	2.01	0.42
23:c:506:CLA:HMC2	23:c:507:CLA:H102	2.01	0.42
1:A:187:GLN:HB2	23:A:404:CLA:HAC2	2.01	0.42
3:C:154:LYS:NZ	41:C:617:HOH:O	2.52	0.42
37:C:519:DGD:HBH1	37:C:519:DGD:HBT2	1.77	0.42
2:b:220:ARG:HG3	7:h:20:LYS:HG2	2.01	0.42
23:b:602:CLA:H111	23:b:602:CLA:H91	1.84	0.42
25:b:618:BCR:H371	25:b:618:BCR:H24C	1.80	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.42
3:c:425:TRP:CD1	23:c:504:CLA:HMA3	2.54	0.42
4:d:148:ALA:HB2	4:d:276:VAL:HG13	2.02	0.42
23:B:607:CLA:H122	23:B:607:CLA:H161	1.84	0.42
23:b:612:CLA:H61	23:b:612:CLA:H102	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:504:CLA:H43	37:c:518:DGD:HB32	2.02	0.42
23:c:513:CLA:H203	23:c:513:CLA:H161	1.72	0.42
1:A:221:SER:HB2	4:D:139:ARG:O	2.20	0.42
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.54	0.42
3:C:165:LEU:HD21	23:C:507:CLA:CBB	2.50	0.42
3:C:433:LEU:HD13	23:C:503:CLA:CHC	2.49	0.42
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.55	0.42
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.55	0.42
23:B:607:CLA:H192	23:B:607:CLA:H162	1.94	0.42
35:B:623:LMT:H91	35:B:623:LMT:H62	1.65	0.42
3:C:137:PRO:HG3	23:C:514:CLA:HED3	2.02	0.42
23:C:505:CLA:H62	23:C:505:CLA:H41	1.76	0.42
4:D:13:GLY:HA3	36:D:412:HTG:H62	2.01	0.42
4:D:135:LEU:HD23	4:D:135:LEU:HA	1.82	0.42
26:D:413:SQD:H342	17:X:24:THR:OG1	2.20	0.42
23:c:509:CLA:H92	23:c:509:CLA:H62	1.82	0.42
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.91	0.42
23:B:604:CLA:H2	23:B:606:CLA:H91	2.01	0.42
23:D:404:CLA:HBC3	23:D:404:CLA:HHD	2.02	0.42
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.00	0.42
7:h:43:LEU:HD12	7:h:43:LEU:HA	1.92	0.42
17:x:23:LEU:HD23	17:x:23:LEU:HA	1.90	0.42
2:B:102:VAL:HA	25:B:619:BCR:C40	2.50	0.42
2:B:149:LEU:HD12	2:B:149:LEU:HA	1.85	0.42
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.20	0.42
23:a:404:CLA:CBD	23:a:405:CLA:HAC2	2.50	0.42
23:b:613:CLA:H72	23:b:613:CLA:H111	1.81	0.42
23:b:616:CLA:H2	25:b:619:BCR:H362	2.02	0.42
36:b:622:HTG:H3	13:o:178:LYS:HE3	2.02	0.42
3:c:240:ILE:HG13	23:c:501:CLA:HBB1	2.01	0.42
23:c:506:CLA:H162	23:c:506:CLA:H203	1.93	0.42
23:c:513:CLA:H8	25:c:514:BCR:H23C	2.01	0.42
18:y:30:ILE:HA	18:y:30:ILE:HD12	1.80	0.42
2:B:385:ARG:HG2	13:O:165:ALA:O	2.19	0.42
23:B:617:CLA:H91	23:B:617:CLA:H112	1.82	0.42
23:b:606:CLA:H161	23:b:606:CLA:H192	1.76	0.42
4:d:236:ASN:HA	4:d:237:PRO:HD3	1.92	0.42
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.55	0.42
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.89	0.41
35:B:623:LMT:H5'	30:D:411:UNL:O9	2.20	0.41
4:d:348:ARG:HH21	4:d:352:LEU:C	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:k:101:BCR:H371	25:k:101:BCR:H24C	1.65	0.41
13:o:110:MET:HE2	13:o:110:MET:HB3	1.87	0.41
2:B:201:HIS:HB2	23:B:603:CLA:CHB	2.50	0.41
2:B:342:GLY:HA3	2:B:403:GLY:O	2.19	0.41
1:a:259:ILE:HG22	1:a:260:PHE:CD1	2.55	0.41
23:a:406:CLA:H143	23:a:406:CLA:H161	1.88	0.41
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.85	0.41
3:c:161:LEU:O	3:c:165:LEU:HG	2.20	0.41
3:c:433:LEU:HD13	23:c:502:CLA:CHC	2.50	0.41
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.54	0.41
38:e:103:HEM:CAC	6:f:27:ALA:HB1	2.49	0.41
3:C:425:TRP:CD1	23:C:505:CLA:HMA3	2.55	0.41
2:b:54:PRO:HD2	2:b:57:ARG:HG3	2.03	0.41
3:c:178:LYS:HB2	23:c:502:CLA:H161	2.02	0.41
15:u:42:TYR:HA	15:u:43:PRO:HA	1.82	0.41
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.56	0.41
15:U:64:ILE:HB	15:U:67:LEU:HD11	2.02	0.41
3:c:42:LEU:HD23	23:c:511:CLA:HED3	2.03	0.41
12:m:28:GLN:O	12:m:32:GLN:HG3	2.21	0.41
13:o:120:PHE:CD1	13:o:235:ILE:HD13	2.55	0.41
36:B:624:HTG:O5	27:a:412:GOL:H11	2.19	0.41
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.92	0.41
1:a:185:VAL:O	1:a:189:GLU:HG3	2.20	0.41
23:b:601:CLA:HAC1	25:h:102:BCR:H383	2.02	0.41
3:c:39:ASN:HD21	23:c:511:CLA:C1C	2.34	0.41
37:c:516:DGD:HG11	41:c:603:HOH:O	2.19	0.41
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.02	0.41
25:k:101:BCR:H11C	25:k:101:BCR:H341	1.92	0.41
1:A:202:VAL:HG11	23:A:405:CLA:C3D	2.51	0.41
23:B:614:CLA:OBD	23:B:615:CLA:HHC	2.20	0.41
25:B:618:BCR:H24C	25:B:618:BCR:H371	1.92	0.41
35:B:632:LMT:H122	14:t:7:VAL:HG12	2.03	0.41
23:C:510:CLA:HBD	23:C:510:CLA:HAA2	2.02	0.41
8:I:2:GLU:O	8:I:6:ILE:HG12	2.21	0.41
23:b:603:CLA:HBB2	23:b:605:CLA:H193	2.01	0.41
23:b:609:CLA:HMD1	7:h:27:THR:HB	2.03	0.41
25:t:101:BCR:H11C	25:t:101:BCR:H341	1.85	0.41
23:A:407:CLA:H3A	23:A:407:CLA:HBA1	1.81	0.41
31:A:415:LHG:HC2	2:B:6:TYR:OH	2.21	0.41
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.55	0.41
13:O:57:LYS:HE3	2:b:338:GLN:HA	2.03	0.41
13:O:91:GLY:HA3	13:O:132:ASN:HA	2.03	0.41
24:a:408:PHO:H61	23:d:402:CLA:H111	2.02	0.41
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.41
23:A:404:CLA:HBD	23:D:401:CLA:HAC2	2.02	0.41
41:A:622:HOH:O	3:C:414:ILE:HD13	2.21	0.41
2:B:489:GLU:HG2	2:B:495:PHE:CE2	2.55	0.41
2:B:502:VAL:O	2:B:505:ARG:HG3	2.20	0.41
25:B:618:BCR:H11C	25:B:618:BCR:H341	1.90	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.55	0.41
4:D:12:ARG:HA	4:D:12:ARG:HD3	1.91	0.41
15:U:45:LEU:HD23	15:U:45:LEU:HA	1.88	0.41
34:Z:101:LMG:H141	34:Z:101:LMG:H111	1.81	0.41
2:b:233:ASN:O	2:b:236:THR:HG22	2.21	0.41
23:b:602:CLA:HBD	23:b:602:CLA:HAA2	2.03	0.41
23:b:604:CLA:C2D	23:b:612:CLA:H172	2.51	0.41
3:c:205:ASP:HA	3:c:206:PRO:HD2	1.92	0.41
1:A:187:GLN:HB2	23:A:404:CLA:CAC	2.51	0.41
23:A:405:CLA:H61	23:A:405:CLA:H102	1.92	0.41
29:A:413:PL9:H503	17:X:24:THR:OG1	2.21	0.41
2:B:62:VAL:HB	23:B:606:CLA:HED3	2.02	0.41
2:B:97:ALA:O	2:B:101:ILE:HG12	2.21	0.41
23:B:608:CLA:C4A	23:B:608:CLA:HBA2	2.51	0.41
23:B:616:CLA:H112	23:B:616:CLA:H152	1.47	0.41
25:C:516:BCR:H11C	25:C:516:BCR:H341	1.79	0.41
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.90	0.41
31:D:408:LHG:H112	31:D:408:LHG:HC82	1.88	0.41
14:T:1:FME:HCN	35:b:628:LMT:H22	2.02	0.41
1:a:204:GLY:HA3	1:a:282:GLY:HA3	2.03	0.41
1:a:253:GLY:HA2	2:b:493:TRP:CH2	2.55	0.41
1:a:339:PHE:HB3	1:a:340:PRO:HD2	2.03	0.41
23:b:610:CLA:H122	23:b:615:CLA:HAA1	2.03	0.41
36:b:622:HTG:H7'2	36:b:622:HTG:H4'2	1.82	0.41
3:c:72:LEU:HD11	3:c:108:THR:HB	2.02	0.41
3:c:330:SER:HB3	13:o:100:GLY:O	2.21	0.41
34:c:519:LMG:H222	9:j:21:ILE:HD13	2.03	0.41
4:d:185:PHE:HB2	23:d:402:CLA:HMD3	2.03	0.41
29:d:405:PL9:H452	29:d:405:PL9:H421	1.89	0.41
14:t:14:ILE:HG22	25:t:101:BCR:H10C	2.02	0.41
15:u:57:SER:O	15:u:60:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:HA	29:A:413:PL9:O1	2.21	0.41
2:B:25:MET:HG2	25:B:618:BCR:H23C	2.03	0.41
2:b:86:ILE:H	2:b:86:ILE:HG13	1.63	0.41
23:b:612:CLA:HBD	23:b:612:CLA:HAA1	2.03	0.41
23:c:510:CLA:C1D	23:c:510:CLA:H171	2.51	0.41
5:e:60:GLN:NE2	5:e:61:ARG:H	2.18	0.41
3:C:433:LEU:HD22	23:C:503:CLA:HMC3	2.03	0.40
4:D:127:LEU:HD23	4:D:127:LEU:HA	1.95	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.86	0.40
25:Y:101:BCR:H11C	25:Y:101:BCR:H341	1.93	0.40
23:b:611:CLA:H193	23:b:611:CLA:H162	1.87	0.40
25:c:515:BCR:H371	25:c:515:BCR:H24C	1.85	0.40
23:d:402:CLA:HBD	23:d:402:CLA:HAA2	2.03	0.40
25:h:102:BCR:H20C	25:h:102:BCR:H361	1.96	0.40
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.09	0.40
3:C:223:TRP:CG	3:C:224:ILE:N	2.87	0.40
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.56	0.40
9:J:18:MET:O	9:J:22:VAL:HG23	2.21	0.40
18:Y:32:GLY:HA3	25:Y:101:BCR:C15	2.51	0.40
26:a:411:SQD:H341	23:c:508:CLA:H192	2.03	0.40
23:c:508:CLA:H162	23:c:508:CLA:H122	1.71	0.40
23:c:509:CLA:H142	23:c:509:CLA:H112	1.87	0.40
13:o:54:GLU:HG2	13:o:64:GLU:H	1.86	0.40
23:B:613:CLA:H61	23:B:613:CLA:H102	1.82	0.40
23:B:617:CLA:H11	23:B:617:CLA:H51	1.86	0.40
35:B:623:LMT:H6E	4:D:16:ASP:OD2	2.20	0.40
24:D:402:PHO:HHD	24:D:402:PHO:HBC2	2.04	0.40
1:a:210:LEU:HG	24:a:408:PHO:NC	2.36	0.40
3:c:135:ARG:HA	3:c:135:ARG:HD2	1.97	0.40
4:d:49:LEU:HD13	25:d:404:BCR:C15	2.52	0.40
5:e:60:GLN:NE2	5:e:62:SER:HB3	2.36	0.40
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.96	0.40
23:C:509:CLA:O2D	23:C:509:CLA:H2A	2.22	0.40
4:D:49:LEU:HD13	25:D:406:BCR:C15	2.51	0.40
24:D:402:PHO:NC	24:D:402:PHO:ND	2.70	0.40
16:V:94:SER:HA	16:V:104:MET:HE2	2.02	0.40
20:R:3:TRP:CE2	20:R:4:ARG:HG2	2.57	0.40
2:b:98:LEU:HD13	36:b:621:HTG:H7'1	2.02	0.40
23:b:615:CLA:H3A	23:b:615:CLA:HBA1	1.89	0.40
3:c:134:ILE:HD13	23:c:511:CLA:H92	2.03	0.40
3:c:459:ILE:HG21	3:c:464:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:511:CLA:HMB1	25:k:101:BCR:H382	2.03	0.40
23:d:403:CLA:H142	23:d:403:CLA:H112	1.73	0.40
2:B:12:LEU:HB2	23:B:613:CLA:HMC2	2.04	0.40
2:B:30:VAL:HG12	23:B:606:CLA:HHD	2.02	0.40
23:B:604:CLA:H143	23:B:609:CLA:HAC1	2.03	0.40
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.03	0.40
23:b:605:CLA:H61	23:b:605:CLA:H92	1.86	0.40
37:c:517:DGD:HB31	37:c:517:DGD:HB61	1.99	0.40
11:l:9:PRO:HB2	41:m:203:HOH:O	2.21	0.40
18:y:22:LEU:HA	18:y:25:ILE:HG22	2.04	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	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	55
1	a	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	36	55
2	B	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
2	b	502/505 (99%)	494 (98%)	8 (2%)	0	100	100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	43	63
3	c	453/455 (100%)	442 (98%)	10 (2%)	1 (0%)	43	63
4	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	6
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (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	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
13	o	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	89 (95%)	5 (5%)	0	100	100
15	u	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	2	3
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	7	13
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	13
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5212/5384 (97%)	5097 (98%)	107 (2%)	8 (0%)	43	63

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP

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Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
19	Z	30	PRO
1	a	259	ILE
19	z	30	PRO
18	y	45	ASN
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	269/279 (96%)	269 (100%)	0	100	100
1	a	269/279 (96%)	268 (100%)	1 (0%)	84	93
2	B	402/403 (100%)	396 (98%)	6 (2%)	57	80
2	b	402/403 (100%)	392 (98%)	10 (2%)	42	69
3	C	352/356 (99%)	346 (98%)	6 (2%)	53	78
3	c	356/356 (100%)	347 (98%)	9 (2%)	42	69
4	D	277/277 (100%)	276 (100%)	1 (0%)	84	93
4	d	276/277 (100%)	275 (100%)	1 (0%)	84	93
5	E	72/73 (99%)	71 (99%)	1 (1%)	59	81
5	e	70/73 (96%)	68 (97%)	2 (3%)	37	65
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	58
6	f	25/38 (66%)	23 (92%)	2 (8%)	11	24
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	57
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	65
8	i	34/34 (100%)	32 (94%)	2 (6%)	18	37
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	25
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	8
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	8
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	28 (97%)	1 (3%)	32	60
12	m	30/32 (94%)	27 (90%)	3 (10%)	7	15
13	O	206/207 (100%)	201 (98%)	5 (2%)	43	70
13	o	206/207 (100%)	203 (98%)	3 (2%)	57	80
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	56
14	t	26/28 (93%)	25 (96%)	1 (4%)	29	56
15	U	83/89 (93%)	81 (98%)	2 (2%)	43	70
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	70
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	87
16	v	117/117 (100%)	116 (99%)	1 (1%)	70	87
17	X	31/33 (94%)	30 (97%)	1 (3%)	34	62
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	24	49
18	y	22/23 (96%)	21 (96%)	1 (4%)	24	49
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	17
19	z	52/52 (100%)	48 (92%)	4 (8%)	12	25
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	60
All	All	4317/4403 (98%)	4228 (98%)	89 (2%)	47	74

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	161	LEU
2	B	245	VAL
2	B	362	PHE
2	B	472	ARG
2	B	505	ARG
3	C	29	GLU
3	C	142	GLU
3	C	240	ILE

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Mol	Chain	Res	Type
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	259	ILE
5	E	54	SER
6	F	23	VAL
7	H	12	ARG
7	H	56	ASP
8	I	33	LYS
9	J	3	GLU
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	16	LEU
13	O	24	ASP
13	O	69	LYS
13	O	118	LEU
13	O	135	SER
13	O	234	LYS
14	T	2	GLU
15	U	15	GLU
15	U	70	ARG
16	V	45	ILE
17	X	2	THR
18	Y	30	ILE
19	Z	3	ILE
19	Z	4	LEU
19	Z	6	GLN
19	Z	7	LEU
19	Z	62	VAL
20	R	7	VAL
1	a	12	ASN
2	b	53	ASN
2	b	128	THR
2	b	161	LEU
2	b	223	GLN
2	b	245	VAL
2	b	472	ARG
2	b	485	GLU
2	b	486	LEU

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Mol	Chain	Res	Type
2	b	491	VAL
2	b	505	ARG
3	c	19	ASN
3	c	24	THR
3	c	142	GLU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	416	SER
4	d	259	ILE
5	e	16	SER
5	e	54	SER
6	f	15	ILE
6	f	23	VAL
8	i	33	LYS
8	i	36	ASP
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
10	k	27	VAL
12	m	2	GLU
12	m	5	GLN
12	m	20	VAL
13	o	37	THR
13	o	69	LYS
13	o	118	LEU
14	t	2	GLU
15	u	15	GLU
15	u	61	VAL
16	v	45	ILE
18	y	30	ILE
19	z	4	LEU
19	z	6	GLN
19	z	7	LEU
19	z	62	VAL

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

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
2	B	53	ASN
2	B	289	GLN
2	B	331	ASN
3	C	28	GLN
3	C	201	ASN
3	C	415	ASN
4	D	61	HIS
5	E	60	GLN
6	F	44	GLN
13	O	124	ASN
13	O	130	GLN
13	O	155	ASN
15	U	73	GLN
19	Z	58	ASN
1	a	165	GLN
2	b	53	ASN
2	b	223	GLN
2	b	289	GLN
2	b	331	ASN
2	b	374	ASN
3	c	28	GLN
3	c	201	ASN
4	d	186	GLN
5	e	60	GLN
5	e	75	GLN
6	f	44	GLN
12	m	5	GLN
13	o	124	ASN
19	z	58	ASN

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	0.71	0	8,9,11	1.61	2 (25%)
8	FME	i	1	8	8,9,10	0.66	0	8,9,11	1.23	1 (12%)
8	FME	I	1	8	8,9,10	0.67	0	8,9,11	0.96	1 (12%)
14	FME	T	1	14	8,9,10	0.65	0	8,9,11	1.52	1 (12%)
12	FME	M	1	12	8,9,10	0.58	0	8,9,11	1.27	1 (12%)
12	FME	m	1	12	8,9,10	0.65	0	8,9,11	1.63	3 (37%)

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	-	0/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	-2.88	105.27	110.52
14	t	1	FME	CA-N-CN	-2.74	118.61	122.82
14	t	1	FME	O-C-CA	-2.73	117.76	124.77
12	M	1	FME	O-C-CA	-2.57	118.17	124.77
12	m	1	FME	CA-N-CN	-2.39	119.15	122.82
8	i	1	FME	O-C-CA	-2.34	118.75	124.77
12	m	1	FME	O1-CN-N	-2.32	119.33	125.32
12	m	1	FME	C-CA-N	2.18	113.70	109.50
8	I	1	FME	O-C-CA	-2.04	119.51	124.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	O1-CN-N-CA
14	T	1	FME	C-CA-CB-CG
12	m	1	FME	O1-CN-N-CA
12	m	1	FME	CB-CA-N-CN
14	T	1	FME	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
8	i	1	FME	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 218 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
27	GOL	a	412	-	5,5,5	0.44	0	5,5,5	0.30	0
23	CLA	b	611	2	69,73,73	1.99	18 (26%)	82,113,113	2.71	29 (35%)
23	CLA	c	503	3	69,73,73	2.05	20 (28%)	82,113,113	2.67	31 (37%)
23	CLA	c	506	3	69,73,73	2.01	18 (26%)	82,113,113	2.58	32 (39%)
26	SQD	A	409	-	52,54,54	0.93	2 (3%)	62,65,65	1.82	12 (19%)
36	HTG	b	625	-	19,19,19	0.90	1 (5%)	23,24,24	1.39	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	606	2	69,73,73	1.98	20 (28%)	82,113,113	2.72	32 (39%)
36	HTG	D	412	-	16,16,19	0.94	2 (12%)	20,21,24	1.20	1 (5%)
23	CLA	b	612	2	69,73,73	2.01	20 (28%)	82,113,113	2.66	29 (35%)
23	CLA	d	403	4	69,73,73	2.04	19 (27%)	82,113,113	2.74	31 (37%)
25	BCR	B	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.51	12 (21%)
25	BCR	c	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.68	14 (25%)
23	CLA	A	404	1	69,73,73	2.04	20 (28%)	82,113,113	2.70	33 (40%)
23	CLA	b	602	2	69,73,73	2.02	20 (28%)	82,113,113	2.75	35 (42%)
34	LMG	c	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.21	7 (11%)
36	HTG	c	521	-	19,19,19	0.86	1 (5%)	23,24,24	1.29	1 (4%)
36	HTG	b	622	-	19,19,19	0.93	1 (5%)	23,24,24	1.26	2 (8%)
25	BCR	H	101	-	41,41,41	1.11	1 (2%)	56,56,56	1.61	12 (21%)
23	CLA	c	504	41	69,73,73	2.03	21 (30%)	82,113,113	2.69	32 (39%)
36	HTG	B	625	-	19,19,19	0.77	1 (5%)	23,24,24	1.43	1 (4%)
23	CLA	C	509	3	69,73,73	2.01	20 (28%)	82,113,113	2.67	29 (35%)
23	CLA	B	614	2	69,73,73	1.99	19 (27%)	82,113,113	2.57	30 (36%)
23	CLA	B	609	2	69,73,73	1.95	19 (27%)	82,113,113	2.65	30 (36%)
23	CLA	B	615	2	69,73,73	1.99	19 (27%)	82,113,113	2.77	30 (36%)
23	CLA	C	511	3	69,73,73	2.02	18 (26%)	82,113,113	2.69	30 (36%)
25	BCR	a	410	-	41,41,41	0.99	1 (2%)	56,56,56	1.57	14 (25%)
25	BCR	y	101	-	41,41,41	1.10	1 (2%)	56,56,56	1.69	13 (23%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.84	15 (26%)
23	CLA	B	602	41	69,73,73	2.02	20 (28%)	82,113,113	2.68	33 (40%)
26	SQD	A	411	-	52,54,54	0.98	2 (3%)	62,65,65	1.06	5 (8%)
26	SQD	D	413	-	41,43,54	1.08	2 (4%)	51,54,65	1.61	11 (21%)
34	LMG	a	417	-	51,51,55	0.96	3 (5%)	59,59,63	1.11	4 (6%)
36	HTG	B	630	-	19,19,19	0.93	1 (5%)	23,24,24	1.17	1 (4%)
34	LMG	J	101	39	51,51,55	0.91	3 (5%)	59,59,63	1.08	5 (8%)
34	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.26	7 (11%)
23	CLA	a	406	41	69,73,73	1.97	19 (27%)	82,113,113	2.73	30 (36%)
23	CLA	C	507	3	69,73,73	2.03	21 (30%)	82,113,113	2.65	33 (40%)
23	CLA	C	503	3	69,73,73	2.04	19 (27%)	82,113,113	2.59	29 (35%)
23	CLA	B	605	2	69,73,73	1.99	19 (27%)	82,113,113	2.68	29 (35%)
23	CLA	C	506	3	69,73,73	2.02	20 (28%)	82,113,113	2.66	31 (37%)
25	BCR	C	527	-	41,41,41	1.02	1 (2%)	56,56,56	1.58	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PL9	D	407	-	55,55,55	0.69	2 (3%)	68,69,69	1.65	18 (26%)
23	CLA	d	402	4	69,73,73	1.98	19 (27%)	82,113,113	2.64	31 (37%)
26	SQD	a	413	-	52,54,54	1.04	3 (5%)	62,65,65	1.20	7 (11%)
23	CLA	c	510	3	69,73,73	1.99	20 (28%)	82,113,113	2.70	35 (42%)
23	CLA	c	507	41	69,73,73	2.06	20 (28%)	82,113,113	2.71	33 (40%)
27	GOL	B	628	-	5,5,5	0.56	0	5,5,5	0.51	0
23	CLA	c	511	3	69,73,73	2.05	19 (27%)	82,113,113	2.65	29 (35%)
25	BCR	D	406	-	41,41,41	1.05	1 (2%)	56,56,56	1.80	13 (23%)
23	CLA	b	603	2	69,73,73	2.02	19 (27%)	82,113,113	2.78	31 (37%)
23	CLA	B	608	41	69,73,73	2.05	20 (28%)	82,113,113	2.64	32 (39%)
31	LHG	b	630	-	48,48,48	0.94	2 (4%)	51,54,54	1.07	2 (3%)
34	LMG	Z	101	-	37,37,55	1.00	3 (8%)	45,45,63	1.54	8 (17%)
23	CLA	b	615	2	69,73,73	1.99	18 (26%)	82,113,113	2.66	31 (37%)
37	DGD	c	517	-	63,63,67	0.91	3 (4%)	77,77,81	0.99	4 (5%)
25	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	7 (12%)
23	CLA	B	604	2	69,73,73	2.01	20 (28%)	82,113,113	2.72	32 (39%)
31	LHG	D	409	-	48,48,48	0.94	2 (4%)	51,54,54	1.07	3 (5%)
31	LHG	A	415	-	48,48,48	0.86	2 (4%)	51,54,54	1.20	6 (11%)
25	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	9 (16%)
36	HTG	h	101	-	16,16,19	1.00	1 (6%)	20,21,24	1.17	1 (5%)
37	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.19	7 (9%)
25	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	11 (19%)
23	CLA	C	504	3	69,73,73	2.02	18 (26%)	82,113,113	2.67	27 (32%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.40	6 (10%)
26	SQD	a	411	-	52,54,54	0.92	2 (3%)	62,65,65	1.58	12 (19%)
37	DGD	C	519	-	63,63,67	0.84	2 (3%)	77,77,81	0.99	4 (5%)
23	CLA	c	501	3	69,73,73	2.03	21 (30%)	82,113,113	2.62	30 (36%)
27	GOL	A	410	-	5,5,5	0.38	0	5,5,5	0.28	0
36	HTG	B	626	-	19,19,19	0.88	1 (5%)	23,24,24	1.41	2 (8%)
35	LMT	b	620	-	25,25,36	0.47	0	30,30,47	0.66	0
29	PL9	A	413	-	55,55,55	0.65	2 (3%)	68,69,69	1.98	21 (30%)
35	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.87	0
35	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.86	3 (6%)
35	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.76	1 (2%)
40	HEC	V	202	16	46,50,50	1.75	9 (19%)	58,82,82	1.62	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	609	2	69,73,73	2.04	21 (30%)	82,113,113	2.70	31 (37%)
23	CLA	c	509	3	69,73,73	2.07	20 (28%)	82,113,113	2.70	31 (37%)
29	PL9	a	415	-	55,55,55	0.67	2 (3%)	68,69,69	2.02	19 (27%)
23	CLA	c	505	3	69,73,73	2.03	19 (27%)	82,113,113	2.61	29 (35%)
26	SQD	L	102	-	52,54,54	0.97	2 (3%)	62,65,65	1.50	9 (14%)
36	HTG	C	524	-	8,8,19	0.41	0	7,7,24	0.83	0
23	CLA	A	405	41	69,73,73	2.05	19 (27%)	82,113,113	2.69	33 (40%)
23	CLA	c	508	3	69,73,73	2.05	20 (28%)	82,113,113	2.64	27 (32%)
24	PHO	A	406	-	58,69,69	2.76	14 (24%)	55,99,99	2.95	20 (36%)
24	PHO	D	402	-	58,69,69	2.82	13 (22%)	55,99,99	3.00	16 (29%)
25	BCR	c	514	-	41,41,41	1.02	1 (2%)	56,56,56	1.85	15 (26%)
37	DGD	h	103	-	63,63,67	0.90	3 (4%)	77,77,81	0.97	3 (3%)
23	CLA	c	512	3	69,73,73	2.02	19 (27%)	82,113,113	2.71	32 (39%)
27	GOL	C	525	-	5,5,5	0.40	0	5,5,5	0.22	0
34	LMG	j	101	39	51,51,55	0.92	2 (3%)	59,59,63	1.08	5 (8%)
31	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	0.96	2 (4%)
23	CLA	B	617	2	69,73,73	2.01	20 (28%)	82,113,113	2.72	31 (37%)
26	SQD	f	101	-	41,43,54	1.12	2 (4%)	51,54,65	1.49	8 (15%)
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	13 (23%)
23	CLA	B	610	2	69,73,73	2.01	19 (27%)	82,113,113	2.64	27 (32%)
23	CLA	C	513	3	69,73,73	2.02	19 (27%)	82,113,113	2.64	33 (40%)
25	BCR	B	619	-	41,41,41	0.99	1 (2%)	56,56,56	1.56	11 (19%)
28	OEX	A	412	3,1,41	0,15,15	-	-	-	-	-
23	CLA	C	508	41	69,73,73	2.03	19 (27%)	82,113,113	2.61	31 (37%)
27	GOL	b	624	-	5,5,5	0.37	0	5,5,5	0.44	0
35	LMT	b	628	-	25,25,36	0.54	1 (4%)	30,30,47	1.22	4 (13%)
27	GOL	O	302	-	5,5,5	0.34	0	5,5,5	0.37	0
31	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.11	3 (6%)
23	CLA	D	405	4	69,73,73	2.06	18 (26%)	82,113,113	2.75	31 (37%)
36	HTG	B	629	-	19,19,19	0.88	2 (10%)	23,24,24	1.26	3 (13%)
23	CLA	B	603	2	69,73,73	2.08	21 (30%)	82,113,113	2.67	29 (35%)
36	HTG	c	522	-	19,19,19	0.91	2 (10%)	23,24,24	1.36	3 (13%)
25	BCR	b	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.54	14 (25%)
23	CLA	a	405	41	69,73,73	2.06	19 (27%)	82,113,113	2.72	33 (40%)
34	LMG	B	622	-	51,51,55	0.90	2 (3%)	59,59,63	1.16	5 (8%)
23	CLA	b	616	2	69,73,73	2.03	19 (27%)	82,113,113	2.61	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	505	41	69,73,73	2.04	20 (28%)	82,113,113	2.63	33 (40%)
34	LMG	c	519	-	51,51,55	0.96	3 (5%)	59,59,63	1.06	5 (8%)
23	CLA	c	513	3	69,73,73	2.05	21 (30%)	82,113,113	2.74	32 (39%)
25	BCR	T	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.87	13 (23%)
31	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.18	4 (7%)
35	LMT	m	103	-	36,36,36	0.50	1 (2%)	47,47,47	0.94	1 (2%)
25	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.84	13 (23%)
23	CLA	B	606	2	69,73,73	2.04	20 (28%)	82,113,113	2.70	32 (39%)
23	CLA	B	613	2	69,73,73	1.98	19 (27%)	82,113,113	2.63	30 (36%)
36	HTG	B	624	-	19,19,19	0.89	1 (5%)	23,24,24	1.32	4 (17%)
24	PHO	a	408	-	58,69,69	2.82	14 (24%)	55,99,99	2.82	17 (30%)
35	LMT	M	101	-	36,36,36	0.56	0	47,47,47	1.11	3 (6%)
40	HEC	v	201	16	46,50,50	1.73	8 (17%)	58,82,82	1.67	12 (20%)
34	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.09	3 (5%)
35	LMT	B	623	-	36,36,36	0.42	0	47,47,47	1.15	4 (8%)
23	CLA	B	607	2	69,73,73	1.98	18 (26%)	82,113,113	2.71	32 (39%)
34	LMG	C	521	-	51,51,55	0.99	3 (5%)	59,59,63	1.21	4 (6%)
26	SQD	B	621	-	52,54,54	0.99	2 (3%)	62,65,65	1.43	8 (12%)
23	CLA	b	601	41	69,73,73	2.08	20 (28%)	82,113,113	2.60	30 (36%)
35	LMT	C	522	-	36,36,36	0.53	1 (2%)	47,47,47	1.04	4 (8%)
25	BCR	d	404	-	41,41,41	1.13	1 (2%)	56,56,56	1.70	13 (23%)
35	LMT	D	403	-	36,36,36	0.58	1 (2%)	47,47,47	1.22	4 (8%)
31	LHG	d	408	-	48,48,48	0.96	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	C	502	3	69,73,73	1.99	20 (28%)	82,113,113	2.68	31 (37%)
37	DGD	c	518	-	63,63,67	0.87	3 (4%)	77,77,81	1.09	4 (5%)
25	BCR	A	408	-	41,41,41	1.00	1 (2%)	56,56,56	1.66	15 (26%)
35	LMT	B	634	-	26,26,36	0.50	0	31,31,47	0.92	1 (3%)
24	PHO	a	407	-	58,69,69	2.77	11 (18%)	55,99,99	3.05	19 (34%)
23	CLA	C	512	3	69,73,73	2.03	21 (30%)	82,113,113	2.60	29 (35%)
23	CLA	c	502	3	69,73,73	2.00	19 (27%)	82,113,113	2.67	27 (32%)
38	HEM	E	103	5,6	50,50,50	1.56	7 (14%)	67,82,82	1.63	16 (23%)
23	CLA	a	409	1	69,73,73	2.06	20 (28%)	82,113,113	2.65	35 (42%)
38	HEM	e	103	5,6	50,50,50	1.56	8 (16%)	67,82,82	1.61	12 (17%)
23	CLA	C	510	3	69,73,73	2.04	20 (28%)	82,113,113	2.73	30 (36%)
23	CLA	b	614	2	69,73,73	2.01	20 (28%)	82,113,113	2.68	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	613	2	69,73,73	2.04	20 (28%)	82,113,113	2.62	30 (36%)
29	PL9	d	405	-	55,55,55	0.66	2 (3%)	68,69,69	1.81	19 (27%)
23	CLA	C	514	3	69,73,73	2.03	21 (30%)	82,113,113	2.73	31 (37%)
23	CLA	D	404	4	69,73,73	2.00	19 (27%)	82,113,113	2.75	32 (39%)
25	BCR	h	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	9 (16%)
23	CLA	a	404	1	69,73,73	1.99	18 (26%)	82,113,113	2.65	34 (41%)
23	CLA	b	607	41	69,73,73	1.96	19 (27%)	82,113,113	2.64	30 (36%)
23	CLA	b	605	2	69,73,73	2.01	20 (28%)	82,113,113	2.72	32 (39%)
27	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.41	0
27	GOL	d	401	-	5,5,5	0.36	0	5,5,5	0.54	0
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.13	4 (8%)
23	CLA	B	616	2	69,73,73	2.00	18 (26%)	82,113,113	2.60	33 (40%)
36	HTG	C	523	-	19,19,19	0.88	1 (5%)	23,24,24	1.35	3 (13%)
23	CLA	b	610	41	69,73,73	2.07	20 (28%)	82,113,113	2.71	33 (40%)
35	LMT	B	632	-	25,25,36	0.45	0	30,30,47	0.71	0
35	LMT	B	633	-	36,36,36	0.56	1 (2%)	47,47,47	0.99	1 (2%)
31	LHG	d	406	-	48,48,48	0.88	3 (6%)	51,54,54	1.11	5 (9%)
37	DGD	c	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.08	6 (7%)
23	CLA	D	401	41	69,73,73	2.05	20 (28%)	82,113,113	2.74	34 (41%)
23	CLA	b	604	2	69,73,73	1.98	19 (27%)	82,113,113	2.68	31 (37%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.98	4 (5%)
36	HTG	b	621	-	19,19,19	1.14	2 (10%)	23,24,24	1.61	5 (21%)
23	CLA	A	407	1	69,73,73	2.03	20 (28%)	82,113,113	2.72	28 (34%)
31	LHG	d	407	-	48,48,48	0.92	2 (4%)	51,54,54	0.95	4 (7%)
32	BCT	A	416	21	3,3,3	0.53	0	2,3,3	0.34	0
23	CLA	B	611	41	69,73,73	2.04	20 (28%)	82,113,113	2.73	32 (39%)
23	CLA	b	608	2	69,73,73	2.01	20 (28%)	82,113,113	2.65	30 (36%)
28	OEX	a	414	3,1,41	0,15,15	-	-	-	-	-
37	DGD	H	102	-	63,63,67	0.89	2 (3%)	77,77,81	0.98	3 (3%)
35	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.80	1 (2%)
36	HTG	b	626	-	19,19,19	0.99	2 (10%)	23,24,24	1.18	2 (8%)
32	BCT	a	419	21	3,3,3	0.52	0	2,3,3	0.45	0
23	CLA	B	612	2	69,73,73	2.00	18 (26%)	82,113,113	2.73	32 (39%)
25	BCR	t	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.87	14 (25%)
36	HTG	V	203	-	11,11,19	0.27	0	15,15,24	1.17	1 (6%)
31	LHG	D	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.17	6 (10%)
36	HTG	b	623	-	19,19,19	0.99	2 (10%)	23,24,24	1.46	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	a	412	-	-	2/4/4/4	-
23	CLA	b	611	2	1/1/15/20	9/39/115/115	-
23	CLA	c	503	3	1/1/15/20	4/39/115/115	-
23	CLA	c	506	3	1/1/15/20	12/39/115/115	-
26	SQD	A	409	-	-	13/49/69/69	0/1/1/1
36	HTG	b	625	-	-	5/10/30/30	0/1/1/1
23	CLA	b	606	2	1/1/15/20	7/39/115/115	-
36	HTG	D	412	-	-	1/7/27/30	0/1/1/1
23	CLA	b	612	2	1/1/15/20	4/39/115/115	-
23	CLA	d	403	4	1/1/15/20	8/39/115/115	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
23	CLA	A	404	1	1/1/15/20	2/39/115/115	-
23	CLA	b	602	2	1/1/15/20	4/39/115/115	-
34	LMG	c	520	-	-	8/46/66/70	0/1/1/1
36	HTG	c	521	-	-	1/10/30/30	0/1/1/1
36	HTG	b	622	-	-	0/10/30/30	0/1/1/1
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
23	CLA	c	504	41	1/1/15/20	11/39/115/115	-
36	HTG	B	625	-	-	5/10/30/30	0/1/1/1
23	CLA	C	509	3	1/1/15/20	3/39/115/115	-
23	CLA	B	614	2	1/1/15/20	5/39/115/115	-
23	CLA	B	609	2	1/1/15/20	5/39/115/115	-
23	CLA	B	615	2	1/1/15/20	12/39/115/115	-
23	CLA	C	511	3	1/1/15/20	12/39/115/115	-
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	602	41	1/1/15/20	11/39/115/115	-
26	SQD	A	411	-	-	14/49/69/69	0/1/1/1
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
34	LMG	a	417	-	-	14/46/66/70	0/1/1/1
36	HTG	B	630	-	-	1/10/30/30	0/1/1/1
34	LMG	J	101	39	-	10/46/66/70	0/1/1/1
34	LMG	C	501	-	-	11/46/66/70	0/1/1/1
23	CLA	a	406	41	-	8/39/115/115	-
23	CLA	C	507	3	1/1/15/20	15/39/115/115	-
23	CLA	C	503	3	1/1/15/20	11/39/115/115	-
23	CLA	B	605	2	1/1/15/20	12/39/115/115	-
23	CLA	C	506	3	1/1/15/20	7/39/115/115	-
25	BCR	C	527	-	-	1/29/63/63	0/2/2/2
29	PL9	D	407	-	-	7/53/73/73	0/1/1/1
23	CLA	d	402	4	1/1/15/20	3/39/115/115	-
26	SQD	a	413	-	-	16/49/69/69	0/1/1/1
23	CLA	c	510	3	1/1/15/20	8/39/115/115	-
23	CLA	c	507	41	1/1/15/20	10/39/115/115	-
27	GOL	B	628	-	-	4/4/4/4	-
23	CLA	c	511	3	1/1/15/20	4/39/115/115	-
25	BCR	D	406	-	-	6/29/63/63	0/2/2/2
23	CLA	b	603	2	1/1/15/20	5/39/115/115	-
23	CLA	B	608	41	1/1/15/20	3/39/115/115	-
31	LHG	b	630	-	-	19/53/53/53	-
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
23	CLA	b	615	2	1/1/15/20	7/39/115/115	-
37	DGD	c	517	-	-	13/51/91/95	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	B	604	2	1/1/15/20	8/39/115/115	-
31	LHG	D	409	-	-	15/53/53/53	-
31	LHG	A	415	-	-	11/53/53/53	-
25	BCR	B	618	-	-	1/29/63/63	0/2/2/2
36	HTG	h	101	-	-	3/7/27/30	0/1/1/1
37	DGD	C	517	-	-	16/51/91/95	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	504	3	1/1/15/20	5/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
26	SQD	a	411	-	-	14/49/69/69	0/1/1/1
37	DGD	C	519	-	-	8/51/91/95	0/2/2/2
23	CLA	c	501	3	1/1/15/20	9/39/115/115	-
27	GOL	A	410	-	-	4/4/4/4	-
36	HTG	B	626	-	-	4/10/30/30	0/1/1/1
35	LMT	b	620	-	-	5/17/37/61	0/1/1/2
29	PL9	A	413	-	-	11/53/73/73	0/1/1/1
35	LMT	E	102	-	-	10/21/61/61	0/2/2/2
35	LMT	e	102	-	-	8/21/61/61	0/2/2/2
35	LMT	a	418	-	-	3/21/61/61	0/2/2/2
40	HEC	V	202	16	-	6/14/54/54	-
23	CLA	b	609	2	1/1/15/20	7/39/115/115	-
23	CLA	c	509	3	1/1/15/20	15/39/115/115	-
29	PL9	a	415	-	-	16/53/73/73	0/1/1/1
23	CLA	c	505	3	1/1/15/20	6/39/115/115	-
26	SQD	L	102	-	-	22/49/69/69	0/1/1/1
36	HTG	C	524	-	-	1/6/6/30	-
23	CLA	A	405	41	-	10/39/115/115	-
23	CLA	c	508	3	1/1/15/20	3/39/115/115	-
24	PHO	A	406	-	-	4/37/103/103	0/5/6/6
24	PHO	D	402	-	-	5/37/103/103	0/5/6/6
25	BCR	c	514	-	-	1/29/63/63	0/2/2/2
37	DGD	h	103	-	-	12/51/91/95	0/2/2/2
23	CLA	c	512	3	1/1/15/20	9/39/115/115	-
27	GOL	C	525	-	-	2/4/4/4	-
34	LMG	j	101	39	-	9/46/66/70	0/1/1/1
31	LHG	e	101	-	-	13/46/46/53	-
23	CLA	B	617	2	1/1/15/20	9/39/115/115	-
26	SQD	f	101	-	-	16/38/58/69	0/1/1/1
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	610	2	1/1/15/20	8/39/115/115	-
23	CLA	C	513	3	1/1/15/20	8/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	b	628	-	-	8/17/37/61	0/1/1/2
23	CLA	C	508	41	1/1/15/20	9/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
27	GOL	O	302	-	-	2/4/4/4	-
31	LHG	E	101	-	-	16/46/46/53	-
23	CLA	D	405	4	1/1/15/20	7/39/115/115	-
36	HTG	B	629	-	-	1/10/30/30	0/1/1/1
23	CLA	B	603	2	1/1/15/20	10/39/115/115	-
36	HTG	c	522	-	-	2/10/30/30	0/1/1/1
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	a	405	41	1/1/15/20	2/39/115/115	-
34	LMG	B	622	-	-	12/46/66/70	0/1/1/1
23	CLA	b	616	2	1/1/15/20	12/39/115/115	-
23	CLA	C	505	41	1/1/15/20	5/39/115/115	-
34	LMG	c	519	-	-	13/46/66/70	0/1/1/1
23	CLA	c	513	3	-	6/39/115/115	-
25	BCR	T	101	-	-	5/29/63/63	0/2/2/2
31	LHG	L	101	-	-	15/53/53/53	-
35	LMT	m	103	-	-	8/21/61/61	0/2/2/2
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
23	CLA	B	606	2	1/1/15/20	10/39/115/115	-
23	CLA	B	613	2	1/1/15/20	3/39/115/115	-
36	HTG	B	624	-	-	4/10/30/30	0/1/1/1
24	PHO	a	408	-	-	2/37/103/103	0/5/6/6
35	LMT	M	101	-	-	2/21/61/61	0/2/2/2
40	HEC	v	201	16	-	6/14/54/54	-
34	LMG	C	520	-	-	16/46/66/70	0/1/1/1
35	LMT	B	623	-	-	8/21/61/61	0/2/2/2
23	CLA	B	607	2	1/1/15/20	3/39/115/115	-
34	LMG	C	521	-	-	9/46/66/70	0/1/1/1
26	SQD	B	621	-	-	21/49/69/69	0/1/1/1
23	CLA	b	601	41	1/1/15/20	19/39/115/115	-
35	LMT	C	522	-	-	9/21/61/61	0/2/2/2
25	BCR	d	404	-	-	7/29/63/63	0/2/2/2
35	LMT	D	403	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	d	408	-	-	15/53/53/53	-
23	CLA	C	502	3	1/1/15/20	7/39/115/115	-
37	DGD	c	518	-	-	6/51/91/95	0/2/2/2
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
35	LMT	B	634	-	-	6/17/38/61	0/1/1/2
24	PHO	a	407	-	-	3/37/103/103	0/5/6/6
23	CLA	C	512	3	1/1/15/20	7/39/115/115	-
23	CLA	c	502	3	1/1/15/20	11/39/115/115	-
38	HEM	E	103	5,6	-	6/14/54/54	-
23	CLA	a	409	1	1/1/15/20	9/39/115/115	-
38	HEM	e	103	5,6	-	8/14/54/54	-
23	CLA	C	510	3	1/1/15/20	16/39/115/115	-
23	CLA	b	614	2	1/1/15/20	11/39/115/115	-
23	CLA	b	613	2	1/1/15/20	5/39/115/115	-
29	PL9	d	405	-	-	6/53/73/73	0/1/1/1
23	CLA	C	514	3	-	10/39/115/115	-
23	CLA	D	404	4	1/1/15/20	4/39/115/115	-
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
23	CLA	a	404	1	1/1/15/20	5/39/115/115	-
23	CLA	b	607	41	1/1/15/20	9/39/115/115	-
23	CLA	b	605	2	1/1/15/20	12/39/115/115	-
27	GOL	B	627	-	-	4/4/4/4	-
27	GOL	d	401	-	-	2/4/4/4	-
34	LMG	z	101	-	-	15/34/54/70	0/1/1/1
23	CLA	B	616	2	1/1/15/20	10/39/115/115	-
36	HTG	C	523	-	-	0/10/30/30	0/1/1/1
23	CLA	b	610	41	1/1/15/20	6/39/115/115	-
35	LMT	B	632	-	-	7/17/37/61	0/1/1/2
35	LMT	B	633	-	-	5/21/61/61	0/2/2/2
31	LHG	d	406	-	-	12/53/53/53	-
37	DGD	c	516	-	-	15/51/91/95	0/2/2/2
23	CLA	D	401	41	1/1/15/20	6/39/115/115	-
23	CLA	b	604	2	1/1/15/20	10/39/115/115	-
37	DGD	C	518	-	-	13/51/91/95	0/2/2/2
36	HTG	b	621	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	407	1	1/1/15/20	10/39/115/115	-
31	LHG	d	407	-	-	23/53/53/53	-
23	CLA	B	611	41	1/1/15/20	8/39/115/115	-
23	CLA	b	608	2	-	5/39/115/115	-
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2
35	LMT	M	103	-	-	14/21/61/61	0/2/2/2
36	HTG	b	626	-	-	0/10/30/30	0/1/1/1
23	CLA	B	612	2	1/1/15/20	4/39/115/115	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
36	HTG	V	203	-	-	0/2/19/30	0/1/1/1
31	LHG	D	408	-	-	17/53/53/53	-
34	LMG	m	101	-	-	15/46/66/70	0/1/1/1
36	HTG	b	623	-	-	2/10/30/30	0/1/1/1

All (1594) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	C1D-C2D	9.63	1.50	1.39
24	a	407	PHO	C1B-C2B	9.43	1.49	1.39
24	A	406	PHO	C1D-C2D	9.35	1.49	1.39
24	a	408	PHO	C1D-C2D	8.91	1.49	1.39
24	a	407	PHO	C1D-C2D	8.81	1.49	1.39
24	a	408	PHO	C1B-C2B	8.77	1.49	1.39
24	A	406	PHO	C1B-C2B	8.61	1.49	1.39
24	D	402	PHO	C3B-C4B	8.37	1.50	1.41
24	D	402	PHO	C1B-C2B	8.10	1.48	1.39
24	a	408	PHO	C3B-C4B	8.04	1.49	1.41
24	a	407	PHO	C3B-C4B	7.11	1.48	1.41
24	a	407	PHO	C4D-CHA	7.04	1.50	1.39
24	A	406	PHO	C4D-CHA	6.96	1.49	1.39
24	a	407	PHO	C3B-C2B	6.87	1.49	1.40
24	A	406	PHO	C3B-C2B	6.84	1.49	1.40
24	a	408	PHO	C3B-C2B	6.79	1.49	1.40
24	D	402	PHO	C4D-CHA	6.74	1.49	1.39
24	A	406	PHO	C3B-C4B	6.64	1.48	1.41
24	a	408	PHO	C4D-CHA	6.28	1.48	1.39
24	D	402	PHO	C3B-C2B	6.00	1.48	1.40
23	A	404	CLA	C1D-ND	5.82	1.45	1.37
24	A	406	PHO	C3D-C2D	5.71	1.49	1.39
24	a	407	PHO	C3D-C2D	5.70	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C3C-C2C	5.70	1.49	1.36
24	a	408	PHO	C3D-C2D	5.69	1.49	1.39
24	D	402	PHO	C3D-C2D	5.65	1.49	1.39
23	D	404	CLA	C3C-C2C	5.59	1.48	1.36
23	b	610	CLA	C3C-C2C	5.55	1.48	1.36
25	d	404	BCR	C23-C22	-5.54	1.34	1.46
24	D	402	PHO	OBD-CAD	5.52	1.29	1.22
23	B	617	CLA	C3C-C2C	5.50	1.48	1.36
23	A	405	CLA	CHC-C1C	5.48	1.49	1.38
23	B	602	CLA	C3C-C2C	5.48	1.48	1.36
23	C	508	CLA	C3C-C2C	5.44	1.48	1.36
23	b	613	CLA	C3C-C2C	5.44	1.48	1.36
23	b	615	CLA	C3C-C2C	5.43	1.48	1.36
23	c	508	CLA	C3C-C2C	5.43	1.48	1.36
23	B	603	CLA	C3C-C2C	5.43	1.48	1.36
23	c	512	CLA	C3C-C2C	5.41	1.48	1.36
23	A	407	CLA	C3C-C2C	5.40	1.48	1.36
24	a	408	PHO	OBD-CAD	5.40	1.29	1.22
23	a	406	CLA	C3C-C2C	5.39	1.48	1.36
23	a	405	CLA	C3C-C2C	5.38	1.48	1.36
38	e	103	HEM	FE-NB	5.36	2.11	1.94
23	B	611	CLA	C3C-C2C	5.34	1.48	1.36
23	c	511	CLA	C3C-C2C	5.34	1.48	1.36
23	D	405	CLA	C3C-C2C	5.33	1.48	1.36
23	b	616	CLA	C3C-C2C	5.33	1.48	1.36
23	C	504	CLA	C3C-C2C	5.33	1.48	1.36
23	b	612	CLA	C3C-C2C	5.31	1.48	1.36
23	c	501	CLA	C3C-C2C	5.31	1.48	1.36
23	b	611	CLA	C3C-C2C	5.30	1.48	1.36
23	b	603	CLA	C3C-C2C	5.29	1.48	1.36
23	b	606	CLA	C3C-C2C	5.29	1.48	1.36
23	c	505	CLA	C3C-C2C	5.27	1.48	1.36
23	C	505	CLA	C3C-C2C	5.27	1.48	1.36
23	c	513	CLA	C3C-C2C	5.27	1.48	1.36
25	y	101	BCR	C23-C22	-5.26	1.34	1.46
38	E	103	HEM	FE-NB	5.26	2.11	1.94
23	B	612	CLA	O2D-CGD	5.26	1.46	1.33
23	c	502	CLA	C3C-C2C	5.25	1.48	1.36
23	d	403	CLA	CHC-C1C	5.23	1.49	1.38
23	c	510	CLA	O2D-CGD	5.23	1.46	1.33
23	B	604	CLA	C3C-C2C	5.21	1.48	1.36
23	A	404	CLA	CHC-C1C	5.21	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C3C-C2C	5.21	1.48	1.36
24	a	408	PHO	O2D-CGD	5.20	1.46	1.33
23	d	403	CLA	C3C-C2C	5.20	1.48	1.36
23	B	608	CLA	C3C-C2C	5.19	1.48	1.36
25	b	619	BCR	C23-C22	-5.19	1.34	1.46
23	b	614	CLA	C3C-C2C	5.19	1.48	1.36
23	C	513	CLA	C3C-C2C	5.19	1.48	1.36
23	b	601	CLA	C3C-C2C	5.19	1.48	1.36
25	k	101	BCR	C23-C22	-5.18	1.34	1.46
23	B	609	CLA	C3C-C2C	5.18	1.47	1.36
23	C	513	CLA	CHC-C1C	5.17	1.48	1.38
23	C	511	CLA	C3C-C2C	5.17	1.47	1.36
23	D	401	CLA	C3C-C2C	5.16	1.47	1.36
23	c	504	CLA	O2D-CGD	5.16	1.45	1.33
23	C	507	CLA	O2D-CGD	5.15	1.45	1.33
23	b	605	CLA	C3C-C2C	5.15	1.47	1.36
23	D	405	CLA	CHC-C1C	5.15	1.48	1.38
23	a	409	CLA	C3C-C2C	5.14	1.47	1.36
23	c	509	CLA	C3C-C2C	5.14	1.47	1.36
23	b	602	CLA	C3C-C2C	5.14	1.47	1.36
23	B	615	CLA	C3C-C2C	5.13	1.47	1.36
23	B	606	CLA	C3C-C2C	5.13	1.47	1.36
23	b	608	CLA	C3C-C2C	5.13	1.47	1.36
23	c	507	CLA	C3C-C2C	5.12	1.47	1.36
23	b	609	CLA	CHC-C1C	5.10	1.48	1.38
23	C	502	CLA	C3C-C2C	5.10	1.47	1.36
23	A	404	CLA	C3C-C2C	5.10	1.47	1.36
23	c	507	CLA	CHC-C1C	5.10	1.48	1.38
23	b	602	CLA	O2D-CGD	5.09	1.45	1.33
23	B	605	CLA	CHC-C1C	5.09	1.48	1.38
23	A	405	CLA	C3C-C2C	5.09	1.47	1.36
23	c	509	CLA	O2D-CGD	5.09	1.45	1.33
23	c	506	CLA	O2D-CGD	5.09	1.45	1.33
23	C	506	CLA	C3C-C2C	5.09	1.47	1.36
23	C	514	CLA	CHC-C1C	5.08	1.48	1.38
23	D	401	CLA	O2D-CGD	5.08	1.45	1.33
23	b	601	CLA	O2D-CGD	5.08	1.45	1.33
23	B	614	CLA	O2D-CGD	5.07	1.45	1.33
23	C	507	CLA	C3C-C2C	5.07	1.47	1.36
23	B	610	CLA	O2D-CGD	5.07	1.45	1.33
23	B	616	CLA	C1D-ND	5.07	1.44	1.37
25	B	620	BCR	C23-C22	-5.06	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	OBD-CAD	5.06	1.28	1.22
23	A	407	CLA	CHC-C1C	5.06	1.48	1.38
23	B	611	CLA	CHC-C1C	5.06	1.48	1.38
25	T	101	BCR	C23-C22	-5.06	1.35	1.46
23	C	510	CLA	C3C-C2C	5.06	1.47	1.36
23	C	512	CLA	O2D-CGD	5.05	1.45	1.33
23	a	404	CLA	C3C-C2C	5.05	1.47	1.36
25	H	101	BCR	C23-C22	-5.05	1.35	1.46
23	a	409	CLA	CHC-C1C	5.05	1.48	1.38
23	B	613	CLA	C3C-C2C	5.04	1.47	1.36
23	B	616	CLA	O2D-CGD	5.04	1.45	1.33
23	B	610	CLA	C3C-C2C	5.04	1.47	1.36
23	B	606	CLA	C1D-ND	5.04	1.44	1.37
23	C	512	CLA	CHC-C1C	5.04	1.48	1.38
23	D	401	CLA	CHC-C1C	5.04	1.48	1.38
25	C	527	BCR	C23-C22	-5.03	1.35	1.46
23	b	616	CLA	O2D-CGD	5.02	1.45	1.33
23	A	407	CLA	O2D-CGD	5.02	1.45	1.33
23	C	503	CLA	C3C-C2C	5.02	1.47	1.36
23	C	514	CLA	C3C-C2C	5.02	1.47	1.36
25	C	516	BCR	C23-C22	-5.02	1.35	1.46
23	B	605	CLA	C3C-C2C	5.00	1.47	1.36
23	b	604	CLA	C3C-C2C	4.99	1.47	1.36
23	b	601	CLA	C1D-ND	4.99	1.44	1.37
23	C	503	CLA	CHC-C1C	4.98	1.48	1.38
23	c	503	CLA	C3C-C2C	4.98	1.47	1.36
23	B	608	CLA	CHC-C1C	4.98	1.48	1.38
23	C	514	CLA	C1D-ND	4.98	1.44	1.37
23	b	614	CLA	O2D-CGD	4.97	1.45	1.33
23	B	606	CLA	CHC-C1C	4.97	1.48	1.38
23	B	612	CLA	C1D-ND	4.97	1.44	1.37
23	C	504	CLA	C1D-ND	4.97	1.44	1.37
23	B	602	CLA	O2D-CGD	4.97	1.45	1.33
23	c	504	CLA	C3C-C2C	4.96	1.47	1.36
23	B	614	CLA	C3C-C2C	4.96	1.47	1.36
23	b	609	CLA	O2D-CGD	4.96	1.45	1.33
23	D	404	CLA	O2D-CGD	4.96	1.45	1.33
23	b	602	CLA	CHC-C1C	4.96	1.48	1.38
23	B	606	CLA	O2D-CGD	4.95	1.45	1.33
23	B	603	CLA	CHC-C1C	4.95	1.48	1.38
23	b	603	CLA	O2D-CGD	4.95	1.45	1.33
23	B	608	CLA	O2D-CGD	4.94	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C3C-C2C	4.94	1.47	1.36
23	c	505	CLA	CHC-C1C	4.94	1.48	1.38
23	D	405	CLA	O2D-CGD	4.94	1.45	1.33
23	C	505	CLA	O2D-CGD	4.94	1.45	1.33
23	C	510	CLA	O2D-CGD	4.92	1.45	1.33
23	c	510	CLA	C3C-C2C	4.92	1.47	1.36
25	C	515	BCR	C23-C22	-4.91	1.35	1.46
23	c	502	CLA	O2D-CGD	4.91	1.45	1.33
23	a	405	CLA	C1D-ND	4.90	1.44	1.37
23	b	601	CLA	CHC-C1C	4.90	1.48	1.38
23	b	610	CLA	CHC-C1C	4.90	1.48	1.38
23	b	609	CLA	C3C-C2C	4.90	1.47	1.36
23	B	603	CLA	O2D-CGD	4.90	1.45	1.33
23	c	509	CLA	C1D-ND	4.90	1.44	1.37
23	c	512	CLA	CHC-C1C	4.89	1.48	1.38
23	c	508	CLA	CHC-C1C	4.89	1.48	1.38
23	B	604	CLA	CHC-C1C	4.89	1.48	1.38
23	C	506	CLA	CHC-C1C	4.89	1.48	1.38
23	c	513	CLA	C1D-ND	4.89	1.44	1.37
25	D	406	BCR	C23-C22	-4.88	1.35	1.46
23	a	405	CLA	O2D-CGD	4.88	1.45	1.33
24	A	406	PHO	O2D-CGD	4.87	1.45	1.33
23	b	605	CLA	C1D-ND	4.87	1.44	1.37
23	c	505	CLA	O2D-CGD	4.87	1.45	1.33
23	c	511	CLA	C1D-ND	4.86	1.44	1.37
23	B	605	CLA	O2D-CGD	4.86	1.45	1.33
23	b	613	CLA	O2D-CGD	4.86	1.45	1.33
23	B	613	CLA	O2D-CGD	4.85	1.45	1.33
23	B	615	CLA	O2D-CGD	4.85	1.45	1.33
25	c	514	BCR	C23-C22	-4.85	1.35	1.46
23	c	506	CLA	C3C-C2C	4.85	1.47	1.36
23	b	612	CLA	CHC-C1C	4.85	1.48	1.38
25	B	618	BCR	C23-C22	-4.84	1.35	1.46
23	a	409	CLA	O2D-CGD	4.84	1.45	1.33
23	b	612	CLA	O2D-CGD	4.84	1.45	1.33
23	b	606	CLA	C1D-ND	4.84	1.44	1.37
23	d	403	CLA	C1D-ND	4.84	1.44	1.37
23	b	604	CLA	CHC-C1C	4.83	1.48	1.38
23	b	616	CLA	C1D-ND	4.83	1.44	1.37
23	c	507	CLA	C1D-ND	4.83	1.44	1.37
23	b	604	CLA	O2D-CGD	4.82	1.45	1.33
23	C	503	CLA	O2D-CGD	4.82	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	O2D-CGD	4.82	1.45	1.33
23	c	501	CLA	C1D-ND	4.82	1.44	1.37
23	b	615	CLA	O2D-CGD	4.82	1.45	1.33
23	b	614	CLA	CHC-C1C	4.81	1.48	1.38
23	C	502	CLA	CHC-C1C	4.81	1.48	1.38
25	A	408	BCR	C23-C22	-4.81	1.35	1.46
25	h	102	BCR	C23-C22	-4.81	1.35	1.46
23	C	508	CLA	CHC-C1C	4.81	1.48	1.38
23	c	511	CLA	CHC-C1C	4.81	1.48	1.38
23	b	605	CLA	O2D-CGD	4.80	1.45	1.33
23	C	512	CLA	C3C-C2C	4.80	1.47	1.36
24	a	407	PHO	O2D-CGD	4.80	1.45	1.33
23	c	503	CLA	C1D-ND	4.79	1.44	1.37
23	c	502	CLA	CHC-C1C	4.79	1.48	1.38
23	b	610	CLA	O2D-CGD	4.79	1.45	1.33
25	t	101	BCR	C23-C22	-4.79	1.35	1.46
23	B	612	CLA	C3C-C2C	4.79	1.47	1.36
23	c	513	CLA	O2D-CGD	4.78	1.45	1.33
23	A	405	CLA	O2D-CGD	4.78	1.45	1.33
23	B	609	CLA	O2D-CGD	4.78	1.45	1.33
23	D	405	CLA	C1D-ND	4.78	1.44	1.37
23	C	509	CLA	O2D-CGD	4.78	1.45	1.33
23	b	608	CLA	O2D-CGD	4.77	1.45	1.33
23	b	609	CLA	C1D-ND	4.77	1.44	1.37
23	d	402	CLA	CHC-C1C	4.77	1.48	1.38
23	B	617	CLA	O2D-CGD	4.77	1.45	1.33
23	c	513	CLA	CHC-C1C	4.76	1.48	1.38
23	c	512	CLA	O2D-CGD	4.76	1.44	1.33
23	B	611	CLA	O2D-CGD	4.76	1.44	1.33
23	B	610	CLA	CHC-C1C	4.76	1.48	1.38
23	B	604	CLA	O2D-CGD	4.76	1.44	1.33
24	D	402	PHO	O2D-CGD	4.76	1.44	1.33
23	a	404	CLA	O2D-CGD	4.76	1.44	1.33
23	B	603	CLA	C1D-ND	4.76	1.44	1.37
23	b	607	CLA	C3C-C2C	4.75	1.47	1.36
23	C	504	CLA	CHC-C1C	4.75	1.48	1.38
23	a	404	CLA	CHC-C1C	4.75	1.48	1.38
23	b	603	CLA	CHC-C1C	4.75	1.48	1.38
23	C	513	CLA	C1D-ND	4.75	1.44	1.37
25	b	617	BCR	C23-C22	-4.74	1.35	1.46
23	c	508	CLA	C1D-ND	4.74	1.44	1.37
23	c	503	CLA	CHC-C1C	4.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	C3C-C2C	4.73	1.47	1.36
23	C	511	CLA	O2D-CGD	4.73	1.44	1.33
23	B	617	CLA	CHC-C1C	4.73	1.48	1.38
23	c	507	CLA	O2D-CGD	4.72	1.44	1.33
23	C	502	CLA	C1D-ND	4.72	1.44	1.37
23	C	510	CLA	C1D-ND	4.72	1.44	1.37
23	C	503	CLA	C1D-ND	4.72	1.44	1.37
23	c	503	CLA	CHD-C1D	4.72	1.47	1.38
23	C	506	CLA	C1D-ND	4.71	1.44	1.37
23	a	406	CLA	O2D-CGD	4.71	1.44	1.33
23	c	501	CLA	O2D-CGD	4.70	1.44	1.33
23	b	604	CLA	C1D-ND	4.69	1.44	1.37
23	C	507	CLA	CHC-C1C	4.69	1.47	1.38
25	a	410	BCR	C23-C22	-4.69	1.35	1.46
23	b	603	CLA	C1D-ND	4.69	1.44	1.37
23	C	510	CLA	CHC-C1C	4.69	1.47	1.38
23	c	501	CLA	CHD-C1D	4.69	1.47	1.38
23	c	501	CLA	CHC-C1C	4.68	1.47	1.38
23	a	406	CLA	CHC-C1C	4.67	1.47	1.38
23	C	506	CLA	O2D-CGD	4.67	1.44	1.33
23	C	508	CLA	O2D-CGD	4.67	1.44	1.33
23	c	508	CLA	O2D-CGD	4.67	1.44	1.33
23	b	613	CLA	CHC-C1C	4.66	1.47	1.38
23	B	602	CLA	CHC-C1C	4.66	1.47	1.38
23	c	509	CLA	CHC-C1C	4.65	1.47	1.38
26	a	413	SQD	O48-C23	4.65	1.46	1.33
23	b	610	CLA	C1D-ND	4.64	1.44	1.37
23	C	513	CLA	O2D-CGD	4.64	1.44	1.33
23	b	608	CLA	CHC-C1C	4.64	1.47	1.38
25	b	618	BCR	C23-C22	-4.63	1.36	1.46
23	B	607	CLA	CHC-C1C	4.63	1.47	1.38
24	A	406	PHO	OBD-CAD	4.63	1.28	1.22
23	b	601	CLA	CHD-C1D	4.63	1.47	1.38
23	b	613	CLA	C1D-ND	4.62	1.43	1.37
23	a	405	CLA	CHC-C1C	4.62	1.47	1.38
23	b	606	CLA	CHC-C1C	4.62	1.47	1.38
23	d	402	CLA	O2D-CGD	4.62	1.44	1.33
23	a	404	CLA	C1D-ND	4.62	1.43	1.37
23	c	505	CLA	C1D-ND	4.61	1.43	1.37
23	B	612	CLA	CHC-C1C	4.60	1.47	1.38
23	c	502	CLA	C1D-ND	4.60	1.43	1.37
23	C	511	CLA	CHC-C1C	4.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C1D-ND	4.59	1.43	1.37
23	B	611	CLA	C1D-ND	4.59	1.43	1.37
23	b	611	CLA	O2D-CGD	4.59	1.44	1.33
23	a	409	CLA	C1D-ND	4.58	1.43	1.37
23	a	406	CLA	C1D-ND	4.58	1.43	1.37
23	A	407	CLA	C1D-ND	4.58	1.43	1.37
25	c	515	BCR	C23-C22	-4.57	1.36	1.46
23	B	607	CLA	O2D-CGD	4.57	1.44	1.33
23	A	404	CLA	O2D-CGD	4.56	1.44	1.33
23	C	502	CLA	O2D-CGD	4.56	1.44	1.33
23	B	615	CLA	CHC-C1C	4.55	1.47	1.38
23	B	613	CLA	CHC-C1C	4.55	1.47	1.38
23	a	409	CLA	CHD-C1D	4.55	1.47	1.38
34	z	101	LMG	O8-C28	4.54	1.46	1.33
23	B	616	CLA	CHC-C1C	4.54	1.47	1.38
23	B	603	CLA	CHD-C1D	4.54	1.47	1.38
23	c	504	CLA	C1D-ND	4.53	1.43	1.37
23	B	602	CLA	C1D-ND	4.53	1.43	1.37
23	D	404	CLA	CHC-C1C	4.53	1.47	1.38
23	c	506	CLA	C1D-ND	4.53	1.43	1.37
23	c	507	CLA	CHD-C1D	4.52	1.47	1.38
23	b	616	CLA	CHC-C1C	4.52	1.47	1.38
23	C	507	CLA	C1D-ND	4.52	1.43	1.37
23	b	601	CLA	O2A-CGA	4.51	1.46	1.33
23	B	615	CLA	C1D-ND	4.50	1.43	1.37
23	C	505	CLA	CHC-C1C	4.50	1.47	1.38
23	C	514	CLA	O2D-CGD	4.50	1.44	1.33
23	C	503	CLA	CHD-C1D	4.50	1.47	1.38
23	c	503	CLA	O2D-CGD	4.49	1.44	1.33
23	B	607	CLA	C1D-ND	4.49	1.43	1.37
23	c	511	CLA	O2D-CGD	4.49	1.44	1.33
23	B	602	CLA	O2A-CGA	4.49	1.46	1.33
23	C	507	CLA	CHD-C1D	4.49	1.47	1.38
23	b	615	CLA	CHC-C1C	4.49	1.47	1.38
23	c	510	CLA	C1D-ND	4.48	1.43	1.37
23	b	608	CLA	O2A-CGA	4.48	1.46	1.33
23	c	511	CLA	CHD-C1D	4.47	1.47	1.38
23	C	509	CLA	CHC-C1C	4.47	1.47	1.38
23	C	508	CLA	CHD-C1D	4.47	1.47	1.38
23	c	510	CLA	CHC-C1C	4.46	1.47	1.38
23	b	611	CLA	C1D-ND	4.46	1.43	1.37
23	c	512	CLA	C1D-ND	4.46	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	O2A-CGA	4.45	1.46	1.33
23	B	608	CLA	O2A-CGA	4.45	1.46	1.33
26	D	413	SQD	O47-C7	4.45	1.46	1.34
23	C	512	CLA	C1D-ND	4.44	1.43	1.37
23	C	511	CLA	CHD-C1D	4.43	1.47	1.38
23	a	409	CLA	CHD-C4C	4.42	1.49	1.39
23	C	508	CLA	C1D-ND	4.42	1.43	1.37
23	b	607	CLA	CHC-C1C	4.42	1.47	1.38
23	d	403	CLA	O2D-CGD	4.41	1.44	1.33
23	b	611	CLA	O2A-CGA	4.41	1.46	1.33
23	c	505	CLA	CHB-C1B	4.41	1.49	1.39
23	C	504	CLA	O2D-CGD	4.41	1.44	1.33
26	f	101	SQD	O47-C7	4.40	1.46	1.34
23	c	509	CLA	CHD-C1D	4.40	1.47	1.38
26	A	411	SQD	O48-C23	4.40	1.46	1.33
23	C	513	CLA	CHD-C1D	4.40	1.47	1.38
23	D	401	CLA	C1D-ND	4.40	1.43	1.37
23	C	505	CLA	C1D-ND	4.40	1.43	1.37
23	b	606	CLA	O2D-CGD	4.39	1.44	1.33
23	b	610	CLA	CHD-C1D	4.39	1.47	1.38
31	d	408	LHG	O7-C7	4.39	1.46	1.34
23	c	507	CLA	O2A-CGA	4.39	1.46	1.33
23	C	503	CLA	O2A-CGA	4.39	1.46	1.33
23	B	617	CLA	C1D-ND	4.39	1.43	1.37
23	B	604	CLA	C1D-ND	4.39	1.43	1.37
25	Y	101	BCR	C23-C22	-4.39	1.36	1.46
23	C	508	CLA	O2A-CGA	4.38	1.46	1.33
26	B	621	SQD	O47-C7	4.38	1.46	1.34
23	a	405	CLA	O2A-CGA	4.38	1.46	1.33
23	B	610	CLA	O2A-CGA	4.37	1.46	1.33
34	C	521	LMG	O8-C28	4.37	1.46	1.33
23	D	404	CLA	C1D-ND	4.37	1.43	1.37
23	c	513	CLA	O2A-CGA	4.36	1.46	1.33
26	a	413	SQD	O47-C7	4.36	1.46	1.34
23	c	512	CLA	O2A-CGA	4.36	1.46	1.33
23	b	609	CLA	CHD-C1D	4.36	1.46	1.38
23	b	615	CLA	O2A-CGA	4.36	1.46	1.33
40	V	202	HEC	CAC-C3C	4.36	1.49	1.35
23	C	510	CLA	CHD-C1D	4.36	1.46	1.38
23	b	615	CLA	C1D-ND	4.36	1.43	1.37
23	A	405	CLA	O2A-CGA	4.35	1.46	1.33
24	a	408	PHO	O2A-CGA	4.35	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	O2A-CGA	4.35	1.46	1.33
23	B	616	CLA	CHD-C1D	4.35	1.46	1.38
23	c	506	CLA	CHD-C1D	4.35	1.46	1.38
34	c	520	LMG	O7-C10	4.34	1.46	1.34
31	E	101	LHG	O8-C23	4.34	1.46	1.33
37	H	102	DGD	O1G-C1A	4.34	1.46	1.33
23	c	504	CLA	CHD-C1D	4.34	1.46	1.38
23	c	508	CLA	O2A-CGA	4.33	1.46	1.33
23	D	401	CLA	CHD-C1D	4.33	1.46	1.38
23	b	605	CLA	CHD-C1D	4.33	1.46	1.38
34	C	521	LMG	O7-C10	4.33	1.46	1.34
31	e	101	LHG	O8-C23	4.33	1.46	1.33
23	C	504	CLA	O2A-CGA	4.33	1.46	1.33
23	b	602	CLA	C1D-ND	4.33	1.43	1.37
23	B	607	CLA	O2A-CGA	4.33	1.46	1.33
26	B	621	SQD	O48-C23	4.33	1.46	1.33
23	c	513	CLA	CHD-C4C	4.32	1.49	1.39
23	c	513	CLA	CHD-C1D	4.32	1.46	1.38
34	c	519	LMG	O8-C28	4.31	1.45	1.33
23	c	506	CLA	CHC-C1C	4.31	1.47	1.38
23	C	514	CLA	CHD-C1D	4.31	1.46	1.38
26	L	102	SQD	O47-C7	4.31	1.46	1.34
23	C	512	CLA	O2A-CGA	4.31	1.45	1.33
23	b	605	CLA	CHC-C1C	4.31	1.47	1.38
23	B	614	CLA	CHC-C1C	4.31	1.47	1.38
23	C	511	CLA	C1D-ND	4.31	1.43	1.37
23	d	403	CLA	O2A-CGA	4.31	1.45	1.33
23	A	405	CLA	CHD-C1D	4.30	1.46	1.38
23	C	505	CLA	O2A-CGA	4.30	1.45	1.33
23	B	609	CLA	CHC-C1C	4.30	1.47	1.38
37	c	517	DGD	O1G-C1A	4.30	1.45	1.33
23	C	514	CLA	O2A-CGA	4.30	1.45	1.33
23	C	502	CLA	CHD-C1D	4.30	1.46	1.38
23	b	611	CLA	CHD-C1D	4.29	1.46	1.38
23	B	603	CLA	O2A-CGA	4.29	1.45	1.33
23	B	616	CLA	C3D-C2D	4.29	1.50	1.39
23	b	612	CLA	C1D-ND	4.29	1.43	1.37
23	c	504	CLA	CHC-C1C	4.28	1.47	1.38
23	b	612	CLA	O2A-CGA	4.27	1.45	1.33
23	B	614	CLA	O2A-CGA	4.27	1.45	1.33
34	j	101	LMG	O8-C28	4.27	1.45	1.33
40	V	202	HEC	CBB-CAB	-4.27	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CHD-C1D	4.27	1.46	1.38
40	V	202	HEC	CBC-CAC	-4.27	1.33	1.49
31	L	101	LHG	O8-C23	4.27	1.45	1.33
23	c	511	CLA	CHB-C1B	4.26	1.49	1.39
23	D	401	CLA	O2A-CGA	4.26	1.45	1.33
23	b	611	CLA	CHB-C1B	4.26	1.49	1.39
34	C	501	LMG	O7-C10	4.26	1.46	1.34
34	C	501	LMG	O8-C28	4.26	1.45	1.33
23	b	608	CLA	C1D-ND	4.26	1.43	1.37
26	L	102	SQD	O48-C23	4.26	1.45	1.33
23	c	502	CLA	O2A-CGA	4.25	1.45	1.33
26	f	101	SQD	O48-C23	4.25	1.45	1.33
23	a	404	CLA	CHD-C1D	4.25	1.46	1.38
34	c	520	LMG	O8-C28	4.25	1.45	1.33
40	v	201	HEC	CBC-CAC	-4.25	1.33	1.49
23	C	513	CLA	O2A-CGA	4.24	1.45	1.33
23	a	405	CLA	C3D-C2D	4.24	1.50	1.39
23	b	606	CLA	CHD-C1D	4.24	1.46	1.38
23	d	403	CLA	CHD-C1D	4.23	1.46	1.38
26	A	409	SQD	O48-C23	4.23	1.45	1.33
23	C	511	CLA	CHD-C4C	4.23	1.48	1.39
23	c	511	CLA	O2A-CGA	4.23	1.45	1.33
34	C	520	LMG	O8-C28	4.23	1.45	1.33
37	C	517	DGD	O2G-C1B	4.23	1.46	1.34
23	b	609	CLA	CHD-C4C	4.23	1.48	1.39
34	a	417	LMG	O7-C10	4.23	1.46	1.34
40	v	201	HEC	CAC-C3C	4.22	1.48	1.35
23	a	405	CLA	CHD-C1D	4.22	1.46	1.38
23	c	506	CLA	O2A-CGA	4.22	1.45	1.33
23	C	512	CLA	CHD-C1D	4.22	1.46	1.38
26	A	411	SQD	O47-C7	4.22	1.46	1.34
23	D	405	CLA	CHC-C4B	4.22	1.48	1.39
40	v	201	HEC	CBB-CAB	-4.22	1.33	1.49
38	e	103	HEM	FE-NC	4.21	2.09	1.95
34	m	101	LMG	O8-C28	4.21	1.45	1.33
23	b	616	CLA	C3D-C2D	4.21	1.50	1.39
34	B	622	LMG	O8-C28	4.21	1.45	1.33
23	C	507	CLA	O2A-CGA	4.20	1.45	1.33
23	b	601	CLA	CHD-C4C	4.20	1.48	1.39
23	c	507	CLA	CHD-C4C	4.20	1.48	1.39
23	c	510	CLA	CHD-C1D	4.20	1.46	1.38
23	c	503	CLA	O2A-CGA	4.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHD-C1D	4.20	1.46	1.38
25	B	619	BCR	C23-C22	-4.20	1.37	1.46
23	b	614	CLA	O2A-CGA	4.20	1.45	1.33
23	B	604	CLA	CHD-C1D	4.20	1.46	1.38
23	B	605	CLA	O2A-CGA	4.19	1.45	1.33
23	a	409	CLA	O2A-CGA	4.19	1.45	1.33
23	b	604	CLA	CHD-C1D	4.19	1.46	1.38
23	C	511	CLA	O2A-CGA	4.19	1.45	1.33
23	C	506	CLA	CHD-C1D	4.19	1.46	1.38
23	c	510	CLA	CHD-C4C	4.19	1.48	1.39
37	c	516	DGD	O1G-C1A	4.19	1.45	1.33
31	b	630	LHG	O8-C23	4.19	1.45	1.33
23	A	405	CLA	C1D-ND	4.18	1.43	1.37
23	B	610	CLA	CHD-C1D	4.18	1.46	1.38
23	B	613	CLA	CHD-C1D	4.17	1.46	1.38
23	b	613	CLA	CHD-C1D	4.17	1.46	1.38
23	D	401	CLA	CHC-C4B	4.17	1.48	1.39
23	B	606	CLA	CHD-C1D	4.17	1.46	1.38
23	b	614	CLA	CHD-C1D	4.17	1.46	1.38
31	e	101	LHG	O7-C7	4.17	1.46	1.34
23	B	616	CLA	O2A-CGA	4.17	1.45	1.33
34	J	101	LMG	O8-C28	4.17	1.45	1.33
23	b	615	CLA	CHD-C1D	4.16	1.46	1.38
34	a	417	LMG	O8-C28	4.16	1.45	1.33
31	D	409	LHG	O7-C7	4.16	1.46	1.34
23	C	508	CLA	CHD-C4C	4.16	1.48	1.39
26	a	411	SQD	O48-C23	4.16	1.45	1.33
23	d	403	CLA	CHC-C4B	4.15	1.48	1.39
36	b	621	HTG	C1'-S1	-4.15	1.75	1.81
23	b	613	CLA	CHC-C4B	4.14	1.48	1.39
23	C	502	CLA	O2A-CGA	4.14	1.45	1.33
23	B	608	CLA	CHC-C4B	4.14	1.48	1.39
23	B	606	CLA	O2A-CGA	4.14	1.45	1.33
23	B	612	CLA	O2A-CGA	4.14	1.45	1.33
24	A	406	PHO	O2A-CGA	4.14	1.45	1.33
23	D	405	CLA	O2A-CGA	4.14	1.45	1.33
23	b	613	CLA	C3D-C2D	4.14	1.50	1.39
23	B	609	CLA	C1D-ND	4.14	1.43	1.37
23	b	609	CLA	O2A-CGA	4.14	1.45	1.33
34	Z	101	LMG	O7-C10	4.13	1.46	1.34
23	b	613	CLA	O2A-CGA	4.13	1.45	1.33
31	d	408	LHG	O8-C23	4.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	617	CLA	O2A-CGA	4.13	1.45	1.33
23	c	512	CLA	CHD-C1D	4.13	1.46	1.38
31	E	101	LHG	O7-C7	4.12	1.45	1.34
23	c	505	CLA	O2A-CGA	4.12	1.45	1.33
23	B	603	CLA	CHD-C4C	4.12	1.48	1.39
31	D	409	LHG	O8-C23	4.12	1.45	1.33
23	b	602	CLA	O2A-CGA	4.12	1.45	1.33
23	B	615	CLA	CHD-C4C	4.11	1.48	1.39
23	C	510	CLA	CHD-C4C	4.11	1.48	1.39
23	B	602	CLA	CHD-C1D	4.11	1.46	1.38
23	B	607	CLA	CHD-C1D	4.11	1.46	1.38
23	b	610	CLA	CHC-C4B	4.11	1.48	1.39
34	C	520	LMG	O7-C10	4.10	1.45	1.34
31	b	630	LHG	O7-C7	4.09	1.45	1.34
23	c	512	CLA	C3D-C2D	4.09	1.50	1.39
23	B	605	CLA	CHD-C1D	4.09	1.46	1.38
23	b	606	CLA	O2A-CGA	4.09	1.45	1.33
23	D	405	CLA	CHD-C1D	4.09	1.46	1.38
23	A	404	CLA	CHC-C4B	4.09	1.48	1.39
23	B	616	CLA	OBD-CAD	4.09	1.29	1.22
23	c	508	CLA	C3D-C2D	4.08	1.50	1.39
34	c	519	LMG	O7-C10	4.08	1.45	1.34
23	C	504	CLA	CHD-C4C	4.08	1.48	1.39
23	A	407	CLA	CHD-C1D	4.08	1.46	1.38
23	c	501	CLA	CHD-C4C	4.08	1.48	1.39
37	C	518	DGD	O1G-C1A	4.08	1.45	1.33
23	b	602	CLA	CHD-C1D	4.08	1.46	1.38
26	a	411	SQD	O47-C7	4.07	1.45	1.34
23	A	407	CLA	O2A-CGA	4.07	1.45	1.33
23	B	608	CLA	CHD-C1D	4.07	1.46	1.38
23	B	608	CLA	C1D-ND	4.07	1.43	1.37
23	B	603	CLA	C3D-C2D	4.07	1.50	1.39
23	B	611	CLA	CHC-C4B	4.07	1.48	1.39
23	b	603	CLA	CHD-C1D	4.07	1.46	1.38
23	B	615	CLA	O2A-CGA	4.07	1.45	1.33
37	H	102	DGD	O2G-C1B	4.06	1.45	1.34
23	c	503	CLA	CHD-C4C	4.06	1.48	1.39
40	v	201	HEC	CAB-C3B	4.06	1.48	1.35
23	b	607	CLA	O2A-CGA	4.06	1.45	1.33
23	B	611	CLA	O2A-CGA	4.06	1.45	1.33
23	C	506	CLA	O2A-CGA	4.06	1.45	1.33
23	b	614	CLA	C1D-ND	4.06	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406	CLA	CHD-C1D	4.05	1.46	1.38
23	B	613	CLA	C3D-C2D	4.05	1.50	1.39
23	B	605	CLA	C1D-ND	4.05	1.43	1.37
31	D	408	LHG	O7-C7	4.05	1.45	1.34
23	B	617	CLA	C3D-C2D	4.05	1.50	1.39
31	d	407	LHG	O7-C7	4.05	1.45	1.34
37	c	518	DGD	O1G-C1A	4.05	1.45	1.33
23	b	616	CLA	O2A-CGA	4.05	1.45	1.33
23	C	507	CLA	CHD-C4C	4.04	1.48	1.39
23	B	609	CLA	O2A-CGA	4.04	1.45	1.33
23	C	510	CLA	O2A-CGA	4.04	1.45	1.33
23	C	509	CLA	C3D-C2D	4.04	1.50	1.39
23	c	505	CLA	CHD-C1D	4.04	1.46	1.38
23	c	502	CLA	CHD-C1D	4.04	1.46	1.38
23	C	509	CLA	O2A-CGA	4.04	1.45	1.33
23	B	611	CLA	OBD-CAD	4.03	1.29	1.22
23	d	403	CLA	C3D-C2D	4.03	1.50	1.39
23	C	508	CLA	C3D-C2D	4.03	1.50	1.39
23	B	606	CLA	C3D-C2D	4.03	1.50	1.39
23	c	504	CLA	O2A-CGA	4.03	1.45	1.33
23	a	406	CLA	C3D-C2D	4.02	1.50	1.39
23	B	610	CLA	C3D-C2D	4.02	1.50	1.39
37	h	103	DGD	O2G-C1B	4.02	1.45	1.34
23	c	501	CLA	C3D-C2D	4.02	1.50	1.39
23	C	512	CLA	C3D-C2D	4.02	1.50	1.39
34	z	101	LMG	O7-C10	4.02	1.45	1.34
23	C	514	CLA	C3D-C2D	4.02	1.50	1.39
23	C	503	CLA	CHD-C4C	4.02	1.48	1.39
23	b	608	CLA	CHD-C1D	4.02	1.46	1.38
23	b	612	CLA	CHD-C1D	4.01	1.46	1.38
23	b	605	CLA	O2A-CGA	4.01	1.45	1.33
38	E	103	HEM	FE-NC	4.01	2.08	1.95
23	C	505	CLA	CHB-C1B	4.01	1.48	1.39
23	c	508	CLA	CHD-C1D	4.01	1.46	1.38
37	C	519	DGD	O1G-C1A	4.00	1.45	1.33
23	c	512	CLA	CHC-C4B	4.00	1.48	1.39
23	A	404	CLA	CHD-C4C	4.00	1.48	1.39
23	B	613	CLA	O2A-CGA	4.00	1.45	1.33
23	c	506	CLA	CHD-C4C	4.00	1.48	1.39
23	C	512	CLA	CHD-C4C	4.00	1.48	1.39
23	C	506	CLA	CHB-C1B	3.99	1.48	1.39
23	A	407	CLA	CHD-C4C	3.99	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	CHD-C4C	3.98	1.48	1.39
23	C	514	CLA	CHD-C4C	3.98	1.48	1.39
23	a	406	CLA	O2A-CGA	3.98	1.45	1.33
23	b	601	CLA	C3D-C2D	3.98	1.49	1.39
23	B	614	CLA	C3D-C2D	3.98	1.49	1.39
23	c	504	CLA	C3D-C2D	3.97	1.49	1.39
23	B	611	CLA	C3D-C2D	3.97	1.49	1.39
23	b	602	CLA	CHD-C4C	3.97	1.48	1.39
23	a	404	CLA	CHD-C4C	3.97	1.48	1.39
23	C	506	CLA	CHD-C4C	3.97	1.48	1.39
23	b	610	CLA	CHD-C4C	3.97	1.48	1.39
40	V	202	HEC	CAB-C3B	3.96	1.47	1.35
23	B	607	CLA	C3D-C2D	3.96	1.49	1.39
26	D	413	SQD	O48-C23	3.96	1.44	1.33
23	c	511	CLA	OBD-CAD	3.95	1.29	1.22
23	C	509	CLA	OBD-CAD	3.95	1.29	1.22
23	c	510	CLA	O2A-CGA	3.95	1.44	1.33
23	C	509	CLA	CHD-C1D	3.95	1.46	1.38
23	B	614	CLA	CHD-C1D	3.95	1.46	1.38
23	B	615	CLA	C3D-C2D	3.94	1.49	1.39
23	B	605	CLA	OBD-CAD	3.94	1.29	1.22
23	B	608	CLA	CHD-C4C	3.94	1.48	1.39
23	C	504	CLA	CHD-C1D	3.94	1.46	1.38
23	C	505	CLA	CHD-C4C	3.94	1.48	1.39
23	C	509	CLA	CHB-C1B	3.94	1.48	1.39
23	b	605	CLA	C3D-C2D	3.94	1.49	1.39
23	c	501	CLA	O2A-CGA	3.94	1.44	1.33
23	B	607	CLA	CHD-C4C	3.93	1.48	1.39
23	d	402	CLA	C1D-ND	3.93	1.43	1.37
23	B	612	CLA	CHB-C1B	3.93	1.48	1.39
37	c	516	DGD	O2G-C1B	3.93	1.45	1.34
23	C	502	CLA	CHD-C4C	3.93	1.48	1.39
23	B	602	CLA	C3D-C2D	3.93	1.49	1.39
23	C	513	CLA	CHD-C4C	3.93	1.48	1.39
23	C	511	CLA	OBD-CAD	3.93	1.29	1.22
23	b	611	CLA	C3D-C2D	3.92	1.49	1.39
23	B	610	CLA	C1D-ND	3.92	1.43	1.37
23	b	611	CLA	CHC-C1C	3.92	1.46	1.38
23	d	403	CLA	CHD-C4C	3.92	1.48	1.39
23	B	609	CLA	CHD-C1D	3.92	1.46	1.38
23	B	604	CLA	O2A-CGA	3.92	1.44	1.33
23	B	611	CLA	CHD-C1D	3.92	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C3D-C2D	3.91	1.49	1.39
23	C	513	CLA	CHC-C4B	3.91	1.48	1.39
23	b	615	CLA	CHD-C4C	3.91	1.48	1.39
37	C	519	DGD	O2G-C1B	3.91	1.45	1.34
23	B	604	CLA	C3D-C2D	3.90	1.49	1.39
23	C	511	CLA	C3D-C2D	3.90	1.49	1.39
23	c	503	CLA	C3D-C2D	3.90	1.49	1.39
23	c	509	CLA	CHB-C1B	3.90	1.48	1.39
23	c	506	CLA	C3D-C2D	3.90	1.49	1.39
23	b	613	CLA	CHB-C1B	3.90	1.48	1.39
23	B	617	CLA	CHD-C1D	3.89	1.46	1.38
23	c	510	CLA	CHB-C1B	3.89	1.48	1.39
23	b	609	CLA	CHB-C1B	3.89	1.48	1.39
34	B	622	LMG	O7-C10	3.89	1.45	1.34
23	B	608	CLA	C1B-NB	-3.89	1.32	1.37
23	A	404	CLA	C3D-C2D	3.89	1.49	1.39
23	B	615	CLA	CHD-C1D	3.89	1.46	1.38
23	C	509	CLA	C1D-ND	3.89	1.43	1.37
23	C	507	CLA	C3D-C2D	3.89	1.49	1.39
23	d	402	CLA	CHD-C1D	3.89	1.46	1.38
23	b	603	CLA	OBD-CAD	3.89	1.29	1.22
23	b	608	CLA	C3D-C2D	3.89	1.49	1.39
23	b	606	CLA	CHD-C4C	3.88	1.48	1.39
23	b	601	CLA	OBD-CAD	3.88	1.29	1.22
23	c	509	CLA	CHD-C4C	3.88	1.48	1.39
23	C	503	CLA	CHB-C1B	3.88	1.48	1.39
23	c	507	CLA	CHC-C4B	3.88	1.48	1.39
23	c	511	CLA	CHD-C4C	3.88	1.48	1.39
23	D	404	CLA	O2A-CGA	3.88	1.44	1.33
23	c	507	CLA	C3D-C2D	3.88	1.49	1.39
23	b	614	CLA	OBD-CAD	3.88	1.29	1.22
23	b	610	CLA	CHB-C1B	3.87	1.48	1.39
23	b	607	CLA	CHB-C1B	3.87	1.48	1.39
23	c	513	CLA	C3D-C2D	3.87	1.49	1.39
23	b	608	CLA	CHD-C4C	3.87	1.48	1.39
23	c	512	CLA	CHD-C4C	3.87	1.48	1.39
23	b	609	CLA	C3D-C2D	3.87	1.49	1.39
23	A	405	CLA	C3D-C2D	3.87	1.49	1.39
23	a	409	CLA	C3D-C2D	3.86	1.49	1.39
23	b	604	CLA	O2A-CGA	3.86	1.44	1.33
23	A	405	CLA	CHD-C4C	3.86	1.48	1.39
34	m	101	LMG	O7-C10	3.86	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406	CLA	CHD-C4C	3.86	1.48	1.39
23	c	508	CLA	CHB-C1B	3.86	1.48	1.39
23	D	401	CLA	C3D-C2D	3.86	1.49	1.39
23	b	602	CLA	CHC-C4B	3.86	1.48	1.39
37	h	103	DGD	O1G-C1A	3.86	1.44	1.33
37	c	518	DGD	O2G-C1B	3.86	1.45	1.34
37	C	518	DGD	O2G-C1B	3.85	1.45	1.34
23	C	505	CLA	C3D-C2D	3.85	1.49	1.39
23	b	610	CLA	C3D-C2D	3.85	1.49	1.39
23	b	603	CLA	CHD-C4C	3.85	1.48	1.39
23	A	407	CLA	C3D-C2D	3.85	1.49	1.39
23	D	404	CLA	CHB-C1B	3.85	1.48	1.39
23	B	610	CLA	CHD-C4C	3.85	1.48	1.39
23	B	612	CLA	OBD-CAD	3.85	1.29	1.22
23	a	404	CLA	C3D-C2D	3.84	1.49	1.39
23	B	606	CLA	CHB-C1B	3.84	1.48	1.39
23	a	405	CLA	CHD-C4C	3.84	1.47	1.39
23	C	502	CLA	C3D-C2D	3.84	1.49	1.39
23	b	607	CLA	CHD-C1D	3.84	1.45	1.38
23	c	502	CLA	CHB-C1B	3.84	1.48	1.39
37	c	517	DGD	O2G-C1B	3.84	1.45	1.34
23	C	513	CLA	C3D-C2D	3.83	1.49	1.39
23	c	504	CLA	CHD-C4C	3.83	1.47	1.39
23	B	604	CLA	CHC-C4B	3.83	1.48	1.39
23	B	604	CLA	CHD-C4C	3.83	1.47	1.39
31	d	407	LHG	O8-C23	3.83	1.44	1.33
23	B	612	CLA	C3D-C2D	3.83	1.49	1.39
23	B	613	CLA	C1D-ND	3.83	1.42	1.37
23	A	404	CLA	CHD-C1D	3.83	1.45	1.38
23	b	605	CLA	CHD-C4C	3.83	1.47	1.39
23	b	612	CLA	C3D-C2D	3.82	1.49	1.39
23	B	611	CLA	CHB-C1B	3.82	1.48	1.39
23	c	505	CLA	CHD-C4C	3.82	1.47	1.39
23	C	503	CLA	C3D-C2D	3.82	1.49	1.39
23	B	602	CLA	OBD-CAD	3.82	1.29	1.22
23	d	402	CLA	C3D-C2D	3.82	1.49	1.39
23	D	401	CLA	CHD-C4C	3.82	1.47	1.39
23	C	510	CLA	C3D-C2D	3.81	1.49	1.39
23	b	607	CLA	C3D-C2D	3.81	1.49	1.39
23	b	605	CLA	CHB-C1B	3.81	1.48	1.39
23	b	614	CLA	CHD-C4C	3.81	1.47	1.39
23	B	603	CLA	OBD-CAD	3.81	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	CLA	CHC-C4B	3.81	1.48	1.39
23	c	505	CLA	CHC-C4B	3.80	1.47	1.39
23	b	603	CLA	O2A-CGA	3.80	1.44	1.33
23	b	609	CLA	OBD-CAD	3.80	1.29	1.22
23	b	611	CLA	CHD-C4C	3.79	1.47	1.39
23	B	609	CLA	CHB-C1B	3.79	1.47	1.39
23	D	405	CLA	OBD-CAD	3.79	1.29	1.22
23	b	605	CLA	OBD-CAD	3.79	1.29	1.22
23	B	609	CLA	C3D-C2D	3.79	1.49	1.39
23	c	502	CLA	CHD-C4C	3.79	1.47	1.39
23	d	402	CLA	CHD-C4C	3.79	1.47	1.39
23	D	405	CLA	CHB-C1B	3.79	1.47	1.39
26	A	409	SQD	O47-C7	3.78	1.45	1.34
23	C	512	CLA	OBD-CAD	3.78	1.29	1.22
23	B	610	CLA	CHC-C4B	3.78	1.47	1.39
23	b	614	CLA	CHB-C1B	3.78	1.47	1.39
23	C	510	CLA	OBD-CAD	3.78	1.29	1.22
23	b	613	CLA	CHD-C4C	3.78	1.47	1.39
23	c	503	CLA	CHC-C4B	3.78	1.47	1.39
23	c	502	CLA	C3D-C2D	3.77	1.49	1.39
23	B	606	CLA	CHC-C4B	3.77	1.47	1.39
23	b	615	CLA	C3D-C2D	3.77	1.49	1.39
23	B	613	CLA	C1B-NB	-3.77	1.32	1.37
23	D	405	CLA	CHD-C4C	3.77	1.47	1.39
23	B	608	CLA	C3D-C2D	3.76	1.49	1.39
23	b	608	CLA	OBD-CAD	3.76	1.29	1.22
23	C	503	CLA	CHC-C4B	3.76	1.47	1.39
23	B	606	CLA	CHD-C4C	3.76	1.47	1.39
23	B	602	CLA	CHD-C4C	3.75	1.47	1.39
23	c	509	CLA	C3D-C2D	3.75	1.49	1.39
23	b	612	CLA	CHD-C4C	3.75	1.47	1.39
23	b	607	CLA	CHD-C4C	3.75	1.47	1.39
23	b	616	CLA	CHD-C4C	3.75	1.47	1.39
23	C	514	CLA	CHB-C1B	3.74	1.47	1.39
31	L	101	LHG	O7-C7	3.74	1.44	1.34
23	c	501	CLA	CHB-C1B	3.73	1.47	1.39
31	d	406	LHG	O8-C23	3.73	1.44	1.33
23	c	509	CLA	OBD-CAD	3.73	1.28	1.22
23	B	617	CLA	CHC-C4B	3.73	1.47	1.39
23	C	504	CLA	C3D-C2D	3.73	1.49	1.39
23	B	615	CLA	CHB-C1B	3.73	1.47	1.39
23	b	615	CLA	CHB-C1B	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	CHC-C4B	3.72	1.47	1.39
23	B	616	CLA	CHD-C4C	3.72	1.47	1.39
23	B	617	CLA	CHB-C1B	3.72	1.47	1.39
23	b	609	CLA	CHC-C4B	3.72	1.47	1.39
23	C	502	CLA	CHC-C4B	3.71	1.47	1.39
23	C	508	CLA	CHC-C4B	3.71	1.47	1.39
23	D	404	CLA	CHD-C1D	3.71	1.45	1.38
23	C	507	CLA	CHC-C4B	3.71	1.47	1.39
23	B	614	CLA	OBD-CAD	3.71	1.28	1.22
23	B	605	CLA	CHB-C1B	3.71	1.47	1.39
23	a	405	CLA	OBD-CAD	3.70	1.28	1.22
23	c	508	CLA	CHD-C4C	3.70	1.47	1.39
23	b	610	CLA	OBD-CAD	3.70	1.28	1.22
23	D	404	CLA	C3D-C2D	3.70	1.49	1.39
23	b	612	CLA	CHC-C4B	3.70	1.47	1.39
34	j	101	LMG	O7-C10	3.69	1.44	1.34
23	b	614	CLA	CHC-C4B	3.69	1.47	1.39
23	c	503	CLA	OBD-CAD	3.69	1.28	1.22
23	b	604	CLA	CHD-C4C	3.69	1.47	1.39
23	C	506	CLA	OBD-CAD	3.69	1.28	1.22
31	A	415	LHG	O7-C7	3.69	1.44	1.34
23	b	603	CLA	C3D-C2D	3.69	1.49	1.39
23	c	504	CLA	OBD-CAD	3.68	1.28	1.22
23	B	604	CLA	CHB-C1B	3.68	1.47	1.39
23	B	612	CLA	CHD-C4C	3.68	1.47	1.39
23	C	512	CLA	CHB-C1B	3.68	1.47	1.39
23	B	615	CLA	CHC-C4B	3.68	1.47	1.39
23	B	613	CLA	CHB-C1B	3.68	1.47	1.39
23	C	503	CLA	OBD-CAD	3.68	1.28	1.22
23	c	513	CLA	CHC-C4B	3.68	1.47	1.39
23	C	502	CLA	CHB-C1B	3.68	1.47	1.39
23	B	614	CLA	CHD-C4C	3.68	1.47	1.39
23	a	404	CLA	CHB-C1B	3.68	1.47	1.39
37	C	517	DGD	O1G-C1A	3.67	1.44	1.33
23	b	606	CLA	CHB-C1B	3.67	1.47	1.39
23	b	610	CLA	O2A-CGA	3.67	1.44	1.33
23	a	409	CLA	CHC-C4B	3.67	1.47	1.39
23	b	606	CLA	C3D-C2D	3.66	1.49	1.39
23	c	507	CLA	OBD-CAD	3.66	1.28	1.22
23	b	601	CLA	CHC-C4B	3.66	1.47	1.39
23	C	510	CLA	CHB-C1B	3.66	1.47	1.39
23	b	616	CLA	CHB-C1B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	CLA	OBD-CAD	3.66	1.28	1.22
23	b	614	CLA	C3D-C2D	3.66	1.49	1.39
23	B	611	CLA	CHD-C4C	3.66	1.47	1.39
24	a	407	PHO	O2A-CGA	3.65	1.44	1.33
23	b	608	CLA	CHC-C4B	3.65	1.47	1.39
23	B	612	CLA	CHC-C4B	3.65	1.47	1.39
23	C	505	CLA	OBD-CAD	3.65	1.28	1.22
23	c	506	CLA	C1B-NB	-3.64	1.33	1.37
23	c	506	CLA	OBD-CAD	3.64	1.28	1.22
23	B	610	CLA	CHB-C1B	3.64	1.47	1.39
23	A	405	CLA	OBD-CAD	3.64	1.28	1.22
23	b	616	CLA	OBD-CAD	3.64	1.28	1.22
23	D	401	CLA	OBD-CAD	3.64	1.28	1.22
23	d	402	CLA	CHC-C4B	3.64	1.47	1.39
23	c	503	CLA	CHB-C1B	3.63	1.47	1.39
23	d	402	CLA	CHB-C1B	3.63	1.47	1.39
23	D	405	CLA	C3D-C2D	3.63	1.48	1.39
23	c	504	CLA	C4B-NB	-3.63	1.33	1.37
23	b	606	CLA	CHC-C4B	3.63	1.47	1.39
23	B	617	CLA	CHD-C4C	3.63	1.47	1.39
23	B	613	CLA	CHD-C4C	3.63	1.47	1.39
23	C	513	CLA	OBD-CAD	3.62	1.28	1.22
23	d	402	CLA	OBD-CAD	3.62	1.28	1.22
31	D	408	LHG	O8-C23	3.62	1.43	1.33
23	c	513	CLA	OBD-CAD	3.62	1.28	1.22
23	A	407	CLA	OBD-CAD	3.62	1.28	1.22
23	c	510	CLA	CHC-C4B	3.62	1.47	1.39
23	c	511	CLA	CHC-C4B	3.61	1.47	1.39
23	C	514	CLA	CHC-C4B	3.61	1.47	1.39
23	C	511	CLA	CHB-C1B	3.61	1.47	1.39
23	c	508	CLA	CHC-C4B	3.60	1.47	1.39
23	B	605	CLA	CHC-C4B	3.60	1.47	1.39
23	B	602	CLA	CHC-C4B	3.59	1.47	1.39
23	c	504	CLA	CHB-C1B	3.59	1.47	1.39
23	c	511	CLA	C3D-C2D	3.59	1.48	1.39
23	D	404	CLA	OBD-CAD	3.59	1.28	1.22
23	B	603	CLA	CHB-C1B	3.59	1.47	1.39
23	B	607	CLA	CHC-C4B	3.59	1.47	1.39
23	c	508	CLA	OBD-CAD	3.59	1.28	1.22
23	c	501	CLA	CHC-C4B	3.58	1.47	1.39
31	A	415	LHG	O8-C23	3.58	1.43	1.33
23	C	505	CLA	CHC-C4B	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	CHC-C4B	3.58	1.47	1.39
23	c	513	CLA	CHB-C1B	3.58	1.47	1.39
23	A	405	CLA	CHC-C4B	3.58	1.47	1.39
23	A	405	CLA	C1B-NB	-3.57	1.33	1.37
24	D	402	PHO	O2A-CGA	3.57	1.43	1.33
23	B	617	CLA	OBD-CAD	3.57	1.28	1.22
23	C	504	CLA	CHB-C1B	3.57	1.47	1.39
23	a	405	CLA	C1B-NB	-3.57	1.33	1.37
23	c	510	CLA	OBD-CAD	3.57	1.28	1.22
23	a	404	CLA	CHC-C4B	3.56	1.47	1.39
23	b	607	CLA	C1D-ND	3.56	1.42	1.37
23	b	603	CLA	CHC-C4B	3.56	1.47	1.39
23	b	602	CLA	CHB-C1B	3.56	1.47	1.39
23	c	512	CLA	OBD-CAD	3.56	1.28	1.22
23	B	603	CLA	CHC-C4B	3.55	1.47	1.39
23	D	401	CLA	CHB-C1B	3.55	1.47	1.39
23	c	506	CLA	CHB-C1B	3.55	1.47	1.39
23	A	405	CLA	CHB-C1B	3.54	1.47	1.39
23	b	613	CLA	OBD-CAD	3.54	1.28	1.22
23	b	607	CLA	C1B-NB	-3.54	1.33	1.37
23	b	602	CLA	OBD-CAD	3.53	1.28	1.22
23	a	404	CLA	O2A-CGA	3.53	1.43	1.33
23	a	406	CLA	OBD-CAD	3.53	1.28	1.22
23	A	404	CLA	OBD-CAD	3.52	1.28	1.22
23	B	608	CLA	OBD-CAD	3.52	1.28	1.22
23	b	601	CLA	CHB-C1B	3.52	1.47	1.39
23	b	604	CLA	CHC-C4B	3.52	1.47	1.39
23	B	614	CLA	CHB-C1B	3.52	1.47	1.39
23	B	614	CLA	CHC-C4B	3.52	1.47	1.39
23	b	604	CLA	OBD-CAD	3.51	1.28	1.22
23	d	403	CLA	CHB-C1B	3.51	1.47	1.39
23	c	505	CLA	C3D-C2D	3.51	1.48	1.39
23	b	604	CLA	CHB-C1B	3.51	1.47	1.39
23	A	407	CLA	C1B-NB	-3.51	1.33	1.37
23	c	509	CLA	C4B-NB	-3.51	1.33	1.37
23	b	605	CLA	CHC-C4B	3.50	1.47	1.39
23	c	512	CLA	CHB-C1B	3.50	1.47	1.39
23	c	505	CLA	OBD-CAD	3.49	1.28	1.22
23	d	402	CLA	C1B-NB	-3.49	1.33	1.37
34	J	101	LMG	O7-C10	3.49	1.44	1.34
23	B	605	CLA	CHD-C4C	3.49	1.47	1.39
23	D	404	CLA	CHC-C4B	3.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	OBD-CAD	3.49	1.28	1.22
23	B	613	CLA	OBD-CAD	3.49	1.28	1.22
23	c	509	CLA	CHC-C4B	3.49	1.47	1.39
23	c	502	CLA	OBD-CAD	3.48	1.28	1.22
23	b	615	CLA	OBD-CAD	3.48	1.28	1.22
23	B	608	CLA	CHB-C1B	3.48	1.47	1.39
36	b	623	HTG	C1'-S1	-3.47	1.76	1.81
23	C	507	CLA	OBD-CAD	3.47	1.28	1.22
31	d	406	LHG	O7-C7	3.47	1.44	1.34
23	C	509	CLA	CHC-C4B	3.47	1.47	1.39
23	C	504	CLA	OBD-CAD	3.47	1.28	1.22
23	B	613	CLA	CHC-C4B	3.47	1.47	1.39
23	a	409	CLA	CHB-C1B	3.47	1.47	1.39
23	B	602	CLA	CHB-C1B	3.47	1.47	1.39
23	B	604	CLA	OBD-CAD	3.45	1.28	1.22
23	c	502	CLA	CHC-C4B	3.45	1.47	1.39
23	b	612	CLA	CHB-C1B	3.45	1.47	1.39
23	c	510	CLA	C3D-C2D	3.44	1.48	1.39
36	b	626	HTG	C1'-S1	-3.44	1.76	1.81
23	a	409	CLA	C1B-NB	-3.44	1.33	1.37
23	b	612	CLA	OBD-CAD	3.44	1.28	1.22
23	b	604	CLA	C3D-C2D	3.43	1.48	1.39
38	e	103	HEM	C4D-ND	-3.42	1.34	1.40
23	B	612	CLA	CHD-C1D	3.42	1.45	1.38
36	B	624	HTG	C1'-S1	-3.42	1.76	1.81
23	B	605	CLA	C3D-C2D	3.41	1.48	1.39
23	c	504	CLA	CHC-C4B	3.41	1.47	1.39
23	b	608	CLA	CHB-C1B	3.41	1.47	1.39
23	b	611	CLA	OBD-CAD	3.41	1.28	1.22
23	b	616	CLA	CHC-C4B	3.40	1.47	1.39
38	E	103	HEM	C1B-NB	-3.40	1.34	1.40
23	B	610	CLA	C1B-NB	-3.40	1.33	1.37
23	A	407	CLA	CHB-C1B	3.39	1.47	1.39
23	B	609	CLA	CHD-C4C	3.39	1.46	1.39
23	C	508	CLA	OBD-CAD	3.37	1.28	1.22
23	b	607	CLA	CHC-C4B	3.37	1.47	1.39
23	B	617	CLA	C1B-NB	-3.36	1.33	1.37
23	C	507	CLA	CHB-C1B	3.36	1.47	1.39
23	d	403	CLA	OBD-CAD	3.36	1.28	1.22
23	C	513	CLA	CHB-C1B	3.36	1.47	1.39
23	c	507	CLA	CHB-C1B	3.36	1.46	1.39
23	A	404	CLA	O2A-CGA	3.35	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C1B-NB	-3.35	1.33	1.37
38	E	103	HEM	C4D-ND	-3.35	1.34	1.40
23	B	607	CLA	CHB-C1B	3.35	1.46	1.39
23	a	405	CLA	C4B-NB	-3.35	1.33	1.37
23	a	409	CLA	OBD-CAD	3.34	1.28	1.22
23	B	612	CLA	C1B-NB	-3.34	1.33	1.37
23	B	605	CLA	C1B-NB	-3.34	1.33	1.37
23	C	506	CLA	CHC-C4B	3.33	1.46	1.39
23	c	506	CLA	CHC-C4B	3.33	1.46	1.39
23	B	616	CLA	CHB-C1B	3.33	1.46	1.39
23	C	512	CLA	CHC-C4B	3.33	1.46	1.39
23	C	509	CLA	CHD-C4C	3.33	1.46	1.39
23	B	609	CLA	OBD-CAD	3.32	1.28	1.22
23	b	607	CLA	OBD-CAD	3.32	1.28	1.22
23	C	514	CLA	OBD-CAD	3.28	1.28	1.22
23	c	509	CLA	C1B-NB	-3.28	1.33	1.37
23	b	606	CLA	OBD-CAD	3.27	1.28	1.22
23	b	615	CLA	CHC-C4B	3.27	1.46	1.39
23	B	606	CLA	OBD-CAD	3.26	1.28	1.22
23	d	402	CLA	C4B-NB	-3.26	1.33	1.37
23	a	405	CLA	CHC-C4B	3.25	1.46	1.39
36	b	622	HTG	C1'-S1	-3.25	1.76	1.81
23	C	506	CLA	C3D-C2D	3.25	1.47	1.39
23	C	507	CLA	C1B-NB	-3.25	1.33	1.37
23	B	609	CLA	CHC-C4B	3.25	1.46	1.39
38	e	103	HEM	C1B-NB	-3.24	1.34	1.40
23	B	615	CLA	OBD-CAD	3.24	1.28	1.22
23	B	607	CLA	OBD-CAD	3.24	1.28	1.22
23	B	614	CLA	C4B-NB	-3.24	1.33	1.37
23	C	511	CLA	C4B-NB	-3.23	1.33	1.37
23	b	608	CLA	C1B-NB	-3.23	1.33	1.37
23	C	502	CLA	OBD-CAD	3.22	1.28	1.22
23	c	508	CLA	C4B-NB	-3.22	1.33	1.37
23	b	611	CLA	CHC-C4B	3.22	1.46	1.39
23	D	401	CLA	C1B-NB	-3.21	1.33	1.37
23	b	603	CLA	C1B-NB	-3.21	1.33	1.37
24	D	402	PHO	C3A-C2A	-3.21	1.51	1.54
36	B	630	HTG	C1'-S1	-3.21	1.76	1.81
23	C	504	CLA	C1B-NB	-3.21	1.33	1.37
23	c	513	CLA	C1B-NB	-3.20	1.33	1.37
23	C	509	CLA	C4B-NB	-3.20	1.33	1.37
23	C	508	CLA	C1B-NB	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C1B-C2B	3.20	1.50	1.43
23	c	512	CLA	C1B-NB	-3.19	1.33	1.37
23	C	510	CLA	C4B-NB	-3.19	1.33	1.37
23	b	615	CLA	C1B-NB	-3.19	1.33	1.37
23	a	406	CLA	CHC-C4B	3.18	1.46	1.39
36	h	101	HTG	C1'-S1	-3.17	1.77	1.81
23	C	508	CLA	CHB-C1B	3.17	1.46	1.39
23	B	615	CLA	C4B-NB	-3.17	1.33	1.37
23	a	405	CLA	CHB-C1B	3.17	1.46	1.39
23	c	501	CLA	OBD-CAD	3.16	1.27	1.22
23	d	403	CLA	C1B-NB	-3.16	1.33	1.37
36	c	522	HTG	C1'-S1	-3.16	1.77	1.81
23	b	612	CLA	C4B-NB	-3.16	1.33	1.37
23	b	613	CLA	C4B-NB	-3.16	1.33	1.37
23	B	609	CLA	C4B-NB	-3.16	1.33	1.37
23	c	508	CLA	C1B-NB	-3.15	1.33	1.37
23	B	606	CLA	C4B-NB	-3.15	1.33	1.37
23	b	603	CLA	CHB-C1B	3.15	1.46	1.39
23	B	616	CLA	CHC-C4B	3.14	1.46	1.39
23	b	606	CLA	C1B-NB	-3.14	1.33	1.37
23	B	604	CLA	C1B-NB	-3.13	1.33	1.37
36	b	625	HTG	C1'-S1	-3.12	1.77	1.81
23	b	616	CLA	C1B-NB	-3.12	1.33	1.37
40	V	202	HEC	C1B-NB	-3.12	1.33	1.39
23	c	506	CLA	C4B-NB	-3.10	1.33	1.37
23	C	505	CLA	C4B-NB	-3.09	1.33	1.37
23	D	401	CLA	C1C-C2C	3.08	1.50	1.44
23	c	503	CLA	C4B-NB	-3.08	1.33	1.37
23	c	504	CLA	C1B-NB	-3.08	1.33	1.37
23	b	611	CLA	C1B-C2B	3.07	1.50	1.43
23	a	405	CLA	C1B-C2B	3.06	1.50	1.43
40	V	202	HEC	C4D-ND	-3.05	1.33	1.39
23	c	507	CLA	C1B-NB	-3.05	1.33	1.37
23	B	614	CLA	C1B-NB	-3.05	1.33	1.37
23	C	511	CLA	CHC-C4B	3.05	1.46	1.39
40	V	202	HEC	C4B-NB	-3.04	1.33	1.39
23	A	404	CLA	CHB-C1B	3.03	1.46	1.39
23	C	510	CLA	C1C-C2C	3.03	1.50	1.44
36	C	523	HTG	C1'-S1	-3.03	1.77	1.81
23	b	607	CLA	C4B-NB	-3.02	1.33	1.37
23	a	406	CLA	CHB-C1B	3.02	1.46	1.39
36	B	626	HTG	C1'-S1	-3.02	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C4B-NB	-3.02	1.33	1.37
23	B	611	CLA	C1B-NB	-3.01	1.33	1.37
23	b	604	CLA	C1B-C2B	3.01	1.50	1.43
23	C	511	CLA	C4C-C3C	3.01	1.50	1.45
23	b	610	CLA	C4B-NB	-3.01	1.33	1.37
29	a	415	PL9	C6-C5	3.00	1.50	1.35
23	C	512	CLA	C1B-C2B	2.99	1.50	1.43
23	A	405	CLA	C4B-NB	-2.99	1.33	1.37
36	B	629	HTG	C1'-S1	-2.99	1.77	1.81
23	c	502	CLA	C1B-NB	-2.98	1.34	1.37
23	C	505	CLA	C1B-NB	-2.97	1.34	1.37
23	C	509	CLA	C1B-NB	-2.97	1.34	1.37
23	c	511	CLA	C1B-C2B	2.97	1.50	1.43
23	a	404	CLA	C4B-NB	-2.97	1.34	1.37
23	b	605	CLA	C1B-NB	-2.96	1.34	1.37
23	b	609	CLA	C1B-NB	-2.96	1.34	1.37
23	A	407	CLA	C4B-NB	-2.95	1.34	1.37
23	B	616	CLA	C1B-C2B	2.95	1.50	1.43
23	C	511	CLA	C1B-NB	-2.95	1.34	1.37
23	c	501	CLA	C4B-NB	-2.94	1.34	1.37
23	D	405	CLA	C1B-C2B	2.94	1.50	1.43
23	C	514	CLA	C4B-NB	-2.94	1.34	1.37
23	B	617	CLA	C4B-NB	-2.93	1.34	1.37
23	b	616	CLA	C4B-NB	-2.93	1.34	1.37
23	D	404	CLA	C1C-C2C	2.93	1.50	1.44
23	B	603	CLA	C4B-NB	-2.93	1.34	1.37
23	B	602	CLA	C1B-NB	-2.93	1.34	1.37
23	c	501	CLA	C4D-CHA	2.93	1.48	1.38
23	B	608	CLA	C1C-C2C	2.92	1.50	1.44
23	c	505	CLA	C1B-C2B	2.92	1.50	1.43
29	A	413	PL9	C6-C5	2.92	1.49	1.35
23	b	601	CLA	C1B-NB	-2.92	1.34	1.37
23	c	509	CLA	C1B-C2B	2.91	1.50	1.43
23	B	609	CLA	C1B-C2B	2.91	1.50	1.43
23	C	513	CLA	C1B-NB	-2.91	1.34	1.37
40	v	201	HEC	C1B-NB	-2.90	1.34	1.39
23	B	607	CLA	C1B-NB	-2.89	1.34	1.37
23	c	503	CLA	C4C-C3C	2.89	1.49	1.45
23	a	406	CLA	C4B-NB	-2.89	1.34	1.37
23	C	503	CLA	C1B-C2B	2.88	1.49	1.43
23	B	611	CLA	C4B-NB	-2.88	1.34	1.37
23	C	510	CLA	C1B-NB	-2.87	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C1B-C2B	2.87	1.49	1.43
23	C	511	CLA	C1B-C2B	2.87	1.49	1.43
23	C	503	CLA	C4B-NB	-2.86	1.34	1.37
23	D	405	CLA	C1C-C2C	2.86	1.50	1.44
23	C	514	CLA	C1B-NB	-2.85	1.34	1.37
23	C	514	CLA	C1C-C2C	2.85	1.50	1.44
23	B	608	CLA	C4D-CHA	2.84	1.48	1.38
23	C	511	CLA	C4D-CHA	2.84	1.48	1.38
24	A	406	PHO	CHA-CBD	-2.84	1.48	1.51
23	b	606	CLA	C1B-C2B	2.84	1.49	1.43
23	a	404	CLA	C1B-NB	-2.84	1.34	1.37
23	c	504	CLA	C4C-C3C	2.84	1.49	1.45
23	b	604	CLA	C4D-CHA	2.84	1.48	1.38
36	D	412	HTG	C1'-S1	-2.83	1.77	1.81
23	b	616	CLA	C4D-CHA	2.83	1.48	1.38
23	B	609	CLA	C1B-NB	-2.83	1.34	1.37
23	C	508	CLA	C1B-C2B	2.83	1.49	1.43
23	c	511	CLA	C4B-NB	-2.83	1.34	1.37
23	D	405	CLA	C3B-C4B	2.83	1.51	1.42
23	b	602	CLA	C4B-NB	-2.83	1.34	1.37
23	B	612	CLA	C1B-C2B	2.83	1.49	1.43
23	B	603	CLA	C1B-NB	-2.82	1.34	1.37
23	c	512	CLA	C4D-CHA	2.82	1.48	1.38
23	B	613	CLA	C1B-C2B	2.82	1.49	1.43
40	v	201	HEC	C4D-ND	-2.82	1.34	1.39
23	b	604	CLA	C1B-NB	-2.82	1.34	1.37
23	C	504	CLA	C4D-CHA	2.82	1.48	1.38
23	B	615	CLA	C4C-C3C	2.82	1.49	1.45
23	b	607	CLA	C1B-C2B	2.82	1.49	1.43
36	c	521	HTG	C1'-S1	-2.81	1.77	1.81
23	C	512	CLA	C4B-NB	-2.81	1.34	1.37
23	C	502	CLA	C1B-NB	-2.81	1.34	1.37
23	D	404	CLA	C4C-C3C	2.81	1.49	1.45
23	b	605	CLA	C1B-C2B	2.81	1.49	1.43
23	A	404	CLA	C1B-NB	-2.80	1.34	1.37
23	a	409	CLA	C4C-C3C	2.80	1.49	1.45
23	b	611	CLA	C1B-NB	-2.79	1.34	1.37
23	C	508	CLA	C4D-CHA	2.79	1.48	1.38
23	C	512	CLA	C1B-NB	-2.79	1.34	1.37
23	b	613	CLA	C4D-CHA	2.79	1.48	1.38
23	B	605	CLA	C1B-C2B	2.79	1.49	1.43
23	D	401	CLA	C3B-C4B	2.78	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C1B-C2B	2.78	1.49	1.43
23	b	615	CLA	C4D-CHA	2.78	1.47	1.38
23	d	402	CLA	C1B-C2B	2.78	1.49	1.43
23	b	607	CLA	C4D-CHA	2.77	1.47	1.38
23	c	508	CLA	C1C-C2C	2.77	1.50	1.44
23	c	507	CLA	C4D-CHA	2.77	1.47	1.38
23	B	605	CLA	C4D-CHA	2.77	1.47	1.38
23	B	610	CLA	C3B-C4B	2.77	1.50	1.42
23	b	610	CLA	C4C-C3C	2.77	1.49	1.45
23	b	616	CLA	C1B-C2B	2.77	1.49	1.43
23	C	506	CLA	C4B-NB	-2.77	1.34	1.37
23	b	613	CLA	C1B-NB	-2.77	1.34	1.37
23	C	502	CLA	C4D-CHA	2.76	1.47	1.38
23	b	611	CLA	C4D-CHA	2.76	1.47	1.38
23	b	615	CLA	C1B-C2B	2.76	1.49	1.43
23	b	612	CLA	C1B-NB	-2.76	1.34	1.37
23	C	504	CLA	C4C-C3C	2.76	1.49	1.45
23	b	605	CLA	C4B-NB	-2.76	1.34	1.37
23	b	603	CLA	C1B-C2B	2.75	1.49	1.43
23	b	601	CLA	C4B-NB	-2.75	1.34	1.37
23	D	405	CLA	C1B-NB	-2.75	1.34	1.37
40	v	201	HEC	C1D-ND	-2.74	1.34	1.39
23	b	610	CLA	C1B-NB	-2.74	1.34	1.37
23	C	502	CLA	C4B-NB	-2.74	1.34	1.37
23	b	603	CLA	C4B-NB	-2.74	1.34	1.37
23	c	510	CLA	C4B-NB	-2.73	1.34	1.37
23	a	409	CLA	C4D-CHA	2.73	1.47	1.38
23	b	613	CLA	C1C-C2C	2.73	1.50	1.44
23	C	503	CLA	C1B-NB	-2.73	1.34	1.37
23	B	615	CLA	C1B-C2B	2.73	1.49	1.43
23	B	617	CLA	C4D-CHA	2.72	1.47	1.38
23	c	511	CLA	C4D-CHA	2.72	1.47	1.38
23	D	404	CLA	C4B-NB	-2.72	1.34	1.37
23	c	503	CLA	C1B-NB	-2.72	1.34	1.37
23	B	616	CLA	C1B-NB	-2.72	1.34	1.37
23	C	513	CLA	C1C-C2C	2.72	1.50	1.44
23	C	505	CLA	C4D-CHA	2.71	1.47	1.38
23	D	401	CLA	C4D-CHA	2.71	1.47	1.38
23	b	610	CLA	C4D-CHA	2.71	1.47	1.38
23	c	503	CLA	C1B-C2B	2.71	1.49	1.43
23	C	514	CLA	C1B-C2B	2.70	1.49	1.43
23	C	504	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	C1B-NB	-2.70	1.34	1.37
23	c	502	CLA	C4B-NB	-2.70	1.34	1.37
29	D	407	PL9	C6-C5	2.70	1.48	1.35
23	c	502	CLA	C1B-C2B	2.70	1.49	1.43
36	B	625	HTG	C1'-S1	-2.70	1.77	1.81
23	c	501	CLA	C1B-NB	-2.69	1.34	1.37
23	b	604	CLA	C1C-C2C	2.69	1.50	1.44
23	b	603	CLA	C3B-C4B	2.69	1.50	1.42
23	A	407	CLA	C4D-CHA	2.69	1.47	1.38
23	b	603	CLA	C1C-C2C	2.69	1.50	1.44
23	B	602	CLA	C1B-C2B	2.69	1.49	1.43
23	c	505	CLA	C1B-NB	-2.68	1.34	1.37
23	B	613	CLA	C1C-C2C	2.68	1.50	1.44
23	C	504	CLA	C4B-NB	-2.68	1.34	1.37
23	c	504	CLA	C4D-CHA	2.68	1.47	1.38
23	c	511	CLA	C1B-NB	-2.68	1.34	1.37
40	V	202	HEC	C1D-ND	-2.68	1.34	1.39
23	D	404	CLA	C1B-C2B	2.68	1.49	1.43
38	E	103	HEM	C1C-C2C	-2.68	1.40	1.45
23	B	613	CLA	C4D-CHA	2.68	1.47	1.38
23	c	507	CLA	C4B-NB	-2.68	1.34	1.37
23	B	612	CLA	C1C-C2C	2.67	1.49	1.44
29	d	405	PL9	C6-C5	2.67	1.48	1.35
23	B	604	CLA	C1B-C2B	2.67	1.49	1.43
23	D	404	CLA	C3D-C4D	-2.67	1.38	1.44
23	a	409	CLA	C4B-NB	-2.67	1.34	1.37
23	B	606	CLA	C4D-CHA	2.67	1.47	1.38
23	c	508	CLA	C1B-C2B	2.67	1.49	1.43
23	B	603	CLA	C4C-C3C	2.67	1.49	1.45
23	c	507	CLA	C1C-C2C	2.66	1.49	1.44
23	C	509	CLA	C1B-C2B	2.66	1.49	1.43
23	B	616	CLA	C4D-CHA	2.66	1.47	1.38
24	D	402	PHO	CHA-CBD	-2.66	1.48	1.51
23	B	604	CLA	C4D-CHA	2.65	1.47	1.38
23	B	609	CLA	C4D-CHA	2.65	1.47	1.38
34	Z	101	LMG	O8-C28	2.65	1.46	1.33
23	B	606	CLA	C1B-C2B	2.65	1.49	1.43
23	B	613	CLA	C4B-NB	-2.65	1.34	1.37
23	c	506	CLA	C1B-C2B	2.65	1.49	1.43
23	b	612	CLA	C1B-C2B	2.65	1.49	1.43
23	a	406	CLA	C1B-NB	-2.65	1.34	1.37
23	c	505	CLA	C1C-C2C	2.65	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C4D-CHA	2.64	1.47	1.38
23	B	617	CLA	C1B-C2B	2.64	1.49	1.43
23	B	612	CLA	C4B-NB	-2.64	1.34	1.37
23	b	611	CLA	C4B-NB	-2.64	1.34	1.37
23	B	607	CLA	C4B-NB	-2.64	1.34	1.37
23	b	602	CLA	C4D-CHA	2.64	1.47	1.38
23	C	512	CLA	C4D-CHA	2.64	1.47	1.38
23	C	510	CLA	C4D-CHA	2.64	1.47	1.38
23	a	404	CLA	C4D-CHA	2.63	1.47	1.38
23	B	607	CLA	C3B-C4B	2.63	1.50	1.42
23	C	512	CLA	C1C-C2C	2.63	1.49	1.44
23	a	409	CLA	C1B-C2B	2.63	1.49	1.43
23	B	603	CLA	C4D-CHA	2.63	1.47	1.38
23	c	502	CLA	C3B-C2B	2.63	1.50	1.41
23	A	404	CLA	C1C-C2C	2.63	1.49	1.44
23	c	510	CLA	C1B-NB	-2.62	1.34	1.37
23	B	608	CLA	C4C-C3C	2.62	1.49	1.45
23	C	506	CLA	C3D-C4D	-2.62	1.38	1.44
23	C	513	CLA	C4D-CHA	2.62	1.47	1.38
23	a	406	CLA	C4D-CHA	2.62	1.47	1.38
23	b	606	CLA	C4B-NB	-2.62	1.34	1.37
23	b	601	CLA	C4D-CHA	2.62	1.47	1.38
23	c	504	CLA	C1B-C2B	2.62	1.49	1.43
23	c	510	CLA	C1B-C2B	2.62	1.49	1.43
23	c	510	CLA	C4D-CHA	2.62	1.47	1.38
23	c	503	CLA	C4D-CHA	2.62	1.47	1.38
35	D	403	LMT	O1'-C1'	2.62	1.44	1.40
23	B	605	CLA	C1C-C2C	2.61	1.49	1.44
23	b	607	CLA	C1C-C2C	2.61	1.49	1.44
23	B	606	CLA	C1C-C2C	2.61	1.49	1.44
23	b	608	CLA	C4D-CHA	2.61	1.47	1.38
23	B	615	CLA	C4D-CHA	2.60	1.47	1.38
23	C	506	CLA	C1C-C2C	2.60	1.49	1.44
23	A	405	CLA	C3B-C4B	2.60	1.50	1.42
23	D	405	CLA	C4D-CHA	2.60	1.47	1.38
23	b	608	CLA	C3D-C4D	-2.60	1.38	1.44
23	B	614	CLA	C4C-C3C	2.60	1.49	1.45
23	b	605	CLA	C4D-CHA	2.60	1.47	1.38
23	c	501	CLA	C4C-C3C	2.59	1.49	1.45
37	c	518	DGD	O2G-C2G	-2.59	1.40	1.46
23	C	508	CLA	C1C-C2C	2.59	1.49	1.44
23	B	604	CLA	C4C-C3C	2.59	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	C4D-CHA	2.59	1.47	1.38
23	B	612	CLA	C4D-CHA	2.59	1.47	1.38
23	B	603	CLA	C1B-C2B	2.59	1.49	1.43
23	B	602	CLA	C4D-CHA	2.58	1.47	1.38
23	b	614	CLA	C4D-CHA	2.58	1.47	1.38
23	b	609	CLA	C4D-CHA	2.58	1.47	1.38
23	B	605	CLA	C4B-NB	-2.58	1.34	1.37
23	B	615	CLA	C1B-NB	-2.58	1.34	1.37
23	c	513	CLA	C4B-NB	-2.58	1.34	1.37
23	c	505	CLA	C4B-NB	-2.57	1.34	1.37
23	b	601	CLA	C1B-C2B	2.57	1.49	1.43
23	C	502	CLA	C1B-C2B	2.57	1.49	1.43
23	c	502	CLA	C4D-CHA	2.56	1.47	1.38
23	c	505	CLA	C4D-CHA	2.56	1.47	1.38
23	c	506	CLA	C4D-CHA	2.56	1.47	1.38
23	C	509	CLA	C4D-CHA	2.56	1.47	1.38
23	C	514	CLA	C4D-CHA	2.56	1.47	1.38
23	C	503	CLA	C4D-CHA	2.55	1.47	1.38
23	B	607	CLA	C1B-C2B	2.55	1.49	1.43
23	C	505	CLA	C1C-C2C	2.55	1.49	1.44
23	a	405	CLA	C4D-CHA	2.55	1.47	1.38
23	b	610	CLA	C1B-C2B	2.55	1.49	1.43
23	B	616	CLA	C4B-NB	-2.55	1.34	1.37
23	b	614	CLA	C1B-NB	-2.55	1.34	1.37
23	B	610	CLA	C4D-CHA	2.54	1.47	1.38
23	c	512	CLA	C3B-C4B	2.54	1.50	1.42
23	C	502	CLA	C3D-C4D	-2.54	1.38	1.44
23	b	603	CLA	C4D-CHA	2.54	1.47	1.38
23	a	404	CLA	C1C-C2C	2.54	1.49	1.44
23	B	607	CLA	C4D-CHA	2.54	1.47	1.38
23	B	614	CLA	C3B-C2B	2.54	1.49	1.41
38	e	103	HEM	C1D-ND	-2.54	1.33	1.38
23	b	611	CLA	C4C-C3C	2.54	1.49	1.45
23	C	509	CLA	C4C-C3C	2.54	1.49	1.45
23	C	510	CLA	C1B-C2B	2.54	1.49	1.43
23	B	611	CLA	C4D-CHA	2.53	1.47	1.38
23	d	403	CLA	C4B-NB	-2.53	1.34	1.37
23	c	507	CLA	C1B-C2B	2.53	1.49	1.43
24	a	408	PHO	CHA-CBD	-2.53	1.48	1.51
23	B	602	CLA	C4B-NB	-2.53	1.34	1.37
23	c	512	CLA	C4B-NB	-2.53	1.34	1.37
23	b	615	CLA	C4B-NB	-2.53	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	C4D-CHA	2.53	1.47	1.38
23	A	404	CLA	C4C-C3C	2.52	1.49	1.45
23	B	614	CLA	C1C-C2C	2.52	1.49	1.44
23	b	602	CLA	C1C-C2C	2.52	1.49	1.44
23	B	603	CLA	C3D-C4D	-2.52	1.38	1.44
23	c	513	CLA	C1C-C2C	2.51	1.49	1.44
23	c	506	CLA	C3D-C4D	-2.51	1.38	1.44
38	e	103	HEM	C1C-C2C	-2.51	1.40	1.45
23	A	404	CLA	C1B-C2B	2.51	1.49	1.43
23	b	612	CLA	C4D-CHA	2.50	1.47	1.38
23	a	409	CLA	C1C-C2C	2.50	1.49	1.44
23	b	602	CLA	C1B-C2B	2.50	1.49	1.43
23	C	507	CLA	C4B-NB	-2.50	1.34	1.37
23	A	404	CLA	C3B-C2B	2.50	1.49	1.41
23	d	402	CLA	C3D-C4D	-2.50	1.38	1.44
23	C	508	CLA	C3B-C4B	2.49	1.50	1.42
23	b	616	CLA	C3D-C4D	-2.49	1.38	1.44
23	B	614	CLA	C4D-CHA	2.49	1.47	1.38
23	c	508	CLA	C4D-CHA	2.49	1.46	1.38
23	b	610	CLA	C1C-C2C	2.48	1.49	1.44
23	b	602	CLA	C1B-NB	-2.48	1.34	1.37
23	c	509	CLA	C1C-C2C	2.48	1.49	1.44
23	B	602	CLA	C1C-C2C	2.48	1.49	1.44
23	a	404	CLA	C1B-C2B	2.48	1.48	1.43
23	A	405	CLA	C4D-CHA	2.48	1.46	1.38
40	v	201	HEC	C4B-NB	-2.48	1.34	1.39
23	B	612	CLA	C3D-C4D	-2.48	1.38	1.44
23	b	612	CLA	C3B-C4B	2.48	1.49	1.42
23	c	513	CLA	C4D-CHA	2.47	1.46	1.38
23	b	606	CLA	C3B-C4B	2.47	1.49	1.42
23	D	405	CLA	C4B-NB	-2.47	1.34	1.37
23	b	616	CLA	C4C-C3C	2.47	1.49	1.45
23	c	512	CLA	C1B-C2B	2.46	1.48	1.43
23	C	509	CLA	C3B-C2B	2.46	1.49	1.41
23	C	508	CLA	C4B-NB	-2.46	1.34	1.37
23	b	613	CLA	C3B-C2B	2.46	1.49	1.41
23	C	507	CLA	C3D-C4D	-2.45	1.38	1.44
23	A	405	CLA	C1B-C2B	2.45	1.48	1.43
23	a	409	CLA	C3B-C4B	2.45	1.49	1.42
23	b	606	CLA	C4D-CHA	2.45	1.46	1.38
23	C	513	CLA	C3B-C4B	2.44	1.49	1.42
23	A	405	CLA	C3D-C4D	-2.44	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	615	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	604	CLA	C4B-NB	-2.44	1.34	1.37
23	C	508	CLA	C3D-C4D	-2.44	1.38	1.44
23	d	402	CLA	C4C-C3C	2.44	1.49	1.45
23	B	610	CLA	C1B-C2B	2.44	1.48	1.43
23	c	511	CLA	C1C-C2C	2.44	1.49	1.44
23	A	405	CLA	C4C-C3C	2.43	1.49	1.45
23	C	506	CLA	C4D-CHA	2.43	1.46	1.38
23	b	602	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	610	CLA	C1C-C2C	2.43	1.49	1.44
23	D	404	CLA	C3B-C2B	2.43	1.49	1.41
35	B	633	LMT	O1'-C1'	2.43	1.44	1.40
23	b	612	CLA	C4C-C3C	2.43	1.49	1.45
23	c	504	CLA	C3B-C2B	2.43	1.49	1.41
23	b	612	CLA	C1C-C2C	2.42	1.49	1.44
23	C	506	CLA	C4C-C3C	2.42	1.49	1.45
23	c	510	CLA	C4C-C3C	2.42	1.49	1.45
24	a	408	PHO	C3A-C2A	-2.42	1.52	1.54
23	c	513	CLA	C1B-C2B	2.42	1.48	1.43
23	C	503	CLA	C3D-C4D	-2.42	1.38	1.44
23	a	409	CLA	C3D-C4D	-2.42	1.38	1.44
23	c	513	CLA	C3B-C4B	2.42	1.49	1.42
23	C	513	CLA	C1B-C2B	2.42	1.48	1.43
23	b	602	CLA	C3B-C4B	2.42	1.49	1.42
23	b	606	CLA	C1C-C2C	2.42	1.49	1.44
23	c	505	CLA	C3B-C4B	2.42	1.49	1.42
23	c	509	CLA	C3D-C4D	-2.42	1.38	1.44
23	D	401	CLA	C1B-C2B	2.42	1.48	1.43
23	c	501	CLA	C1B-C2B	2.42	1.48	1.43
23	b	612	CLA	C3B-C2B	2.42	1.49	1.41
23	b	611	CLA	C3B-C2B	2.41	1.49	1.41
23	d	402	CLA	C1C-C2C	2.41	1.49	1.44
23	C	509	CLA	C1C-C2C	2.41	1.49	1.44
23	c	503	CLA	C3D-C4D	-2.41	1.38	1.44
23	C	505	CLA	C3D-C4D	-2.41	1.38	1.44
23	B	606	CLA	C3B-C4B	2.41	1.49	1.42
23	b	610	CLA	C3D-C4D	-2.40	1.38	1.44
23	d	403	CLA	C1C-C2C	2.40	1.49	1.44
23	a	404	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	505	CLA	C3B-C2B	2.40	1.49	1.41
23	B	608	CLA	C4B-NB	-2.40	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C4C-C3C	2.39	1.49	1.45
23	b	605	CLA	C3B-C4B	2.39	1.49	1.42
23	C	512	CLA	C4C-C3C	2.39	1.49	1.45
23	b	601	CLA	C3B-C4B	2.39	1.49	1.42
23	b	614	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	613	CLA	C4C-C3C	2.39	1.49	1.45
23	B	608	CLA	C1B-C2B	2.39	1.48	1.43
23	C	502	CLA	C1C-C2C	2.39	1.49	1.44
23	b	603	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	614	CLA	C3B-C2B	2.38	1.49	1.41
23	b	607	CLA	C4C-C3C	2.38	1.49	1.45
23	c	509	CLA	C4C-C3C	2.38	1.49	1.45
23	C	512	CLA	C3B-C2B	2.38	1.49	1.41
23	B	607	CLA	C1C-C2C	2.38	1.49	1.44
23	b	614	CLA	C1C-C2C	2.38	1.49	1.44
23	c	510	CLA	C3D-C4D	-2.38	1.38	1.44
35	C	522	LMT	O1'-C1'	2.38	1.44	1.40
23	d	403	CLA	C1B-C2B	2.37	1.48	1.43
23	A	404	CLA	C3B-C4B	2.37	1.49	1.42
23	d	403	CLA	C4D-CHA	2.37	1.46	1.38
23	A	404	CLA	C4B-NB	-2.37	1.34	1.37
23	b	609	CLA	C1C-C2C	2.37	1.49	1.44
23	b	608	CLA	C3B-C4B	2.37	1.49	1.42
23	C	505	CLA	C4C-C3C	2.37	1.49	1.45
23	B	617	CLA	C3D-C4D	-2.36	1.38	1.44
23	C	511	CLA	C3D-C4D	-2.36	1.38	1.44
23	B	611	CLA	C3B-C4B	2.36	1.49	1.42
23	b	609	CLA	C3B-C4B	2.36	1.49	1.42
23	B	606	CLA	C3D-C4D	-2.36	1.38	1.44
23	D	401	CLA	C4B-NB	-2.36	1.34	1.37
23	B	613	CLA	C3B-C2B	2.36	1.49	1.41
23	C	502	CLA	C3B-C2B	2.36	1.49	1.41
23	C	502	CLA	C4C-C3C	2.35	1.49	1.45
23	c	512	CLA	C1C-C2C	2.35	1.49	1.44
23	b	602	CLA	C3B-C2B	2.35	1.49	1.41
23	C	510	CLA	C3D-C4D	-2.35	1.38	1.44
23	b	612	CLA	C3D-C4D	-2.35	1.38	1.44
23	C	507	CLA	C1C-C2C	2.35	1.49	1.44
23	B	609	CLA	C1C-NC	-2.35	1.34	1.37
23	c	505	CLA	C3D-C4D	-2.35	1.38	1.44
23	c	504	CLA	C1C-C2C	2.35	1.49	1.44
23	a	404	CLA	C3B-C2B	2.35	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	C3B-C4B	2.35	1.49	1.42
23	A	407	CLA	C1B-C2B	2.35	1.48	1.43
23	A	404	CLA	C4D-CHA	2.34	1.46	1.38
23	d	403	CLA	C3D-C4D	-2.34	1.38	1.44
23	c	502	CLA	C3D-C4D	-2.34	1.38	1.44
23	a	406	CLA	C3B-C4B	2.34	1.49	1.42
23	b	608	CLA	C3B-C2B	2.34	1.49	1.41
23	C	506	CLA	C3B-C4B	2.34	1.49	1.42
23	b	614	CLA	C4B-NB	-2.34	1.34	1.37
23	b	604	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	608	CLA	C1B-C2B	2.33	1.48	1.43
23	C	507	CLA	C3B-C4B	2.33	1.49	1.42
23	b	610	CLA	C3B-C2B	2.33	1.49	1.41
23	b	608	CLA	C1C-C2C	2.33	1.49	1.44
23	b	606	CLA	C3D-C4D	-2.33	1.39	1.44
23	C	507	CLA	C4C-C3C	2.33	1.49	1.45
23	B	612	CLA	C3B-C2B	2.32	1.49	1.41
23	c	505	CLA	C4C-C3C	2.32	1.49	1.45
23	c	508	CLA	C3B-C2B	2.32	1.49	1.41
23	c	508	CLA	C3D-C4D	-2.32	1.39	1.44
23	C	504	CLA	C3B-C4B	2.32	1.49	1.42
23	b	609	CLA	C1B-C2B	2.32	1.48	1.43
24	a	407	PHO	C1D-ND	-2.32	1.34	1.38
23	C	510	CLA	C3B-C4B	2.32	1.49	1.42
23	B	613	CLA	C3D-C4D	-2.31	1.39	1.44
23	B	602	CLA	C3B-C4B	2.31	1.49	1.42
23	B	603	CLA	C1C-C2C	2.31	1.49	1.44
23	B	611	CLA	C1B-C2B	2.31	1.48	1.43
23	B	617	CLA	C1C-C2C	2.31	1.49	1.44
23	b	605	CLA	C4C-C3C	2.31	1.49	1.45
23	B	611	CLA	C1C-C2C	2.31	1.49	1.44
23	D	401	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	611	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	614	CLA	C4C-C3C	2.31	1.49	1.45
23	a	405	CLA	C3D-C4D	-2.31	1.39	1.44
23	B	604	CLA	C1C-C2C	2.30	1.49	1.44
23	b	615	CLA	C4C-C3C	2.30	1.48	1.45
23	a	405	CLA	C3B-C2B	2.29	1.48	1.41
23	b	604	CLA	C3B-C4B	2.29	1.49	1.42
23	b	613	CLA	C1B-C2B	2.29	1.48	1.43
23	b	614	CLA	C3B-C4B	2.29	1.49	1.42
23	C	510	CLA	C3B-C2B	2.29	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C4B-NB	-2.29	1.34	1.37
23	c	513	CLA	C4C-C3C	2.29	1.48	1.45
23	c	506	CLA	C4C-C3C	2.29	1.48	1.45
23	B	604	CLA	C3D-C4D	-2.29	1.39	1.44
23	b	607	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	604	CLA	C4B-NB	-2.28	1.34	1.37
23	B	606	CLA	C1C-NC	-2.28	1.34	1.37
23	c	511	CLA	C3B-C2B	2.28	1.48	1.41
24	D	402	PHO	C4B-NB	-2.28	1.34	1.38
23	B	616	CLA	C3D-C4D	-2.28	1.39	1.44
23	B	607	CLA	C3D-C4D	-2.27	1.39	1.44
23	c	510	CLA	C1C-C2C	2.27	1.49	1.44
23	A	404	CLA	C3D-C4D	-2.27	1.39	1.44
37	h	103	DGD	O5D-C1E	2.27	1.44	1.40
23	B	604	CLA	C3B-C2B	2.27	1.48	1.41
23	c	503	CLA	C3B-C4B	2.27	1.49	1.42
23	B	605	CLA	C3D-C4D	-2.27	1.39	1.44
24	A	406	PHO	C1B-NB	-2.26	1.34	1.38
23	a	406	CLA	C3B-C2B	2.26	1.48	1.41
23	c	507	CLA	C1D-C2D	2.26	1.49	1.45
23	C	503	CLA	C3B-C4B	2.26	1.49	1.42
23	B	617	CLA	C3B-C2B	2.26	1.48	1.41
23	B	616	CLA	C1C-C2C	2.25	1.49	1.44
23	c	509	CLA	C3B-C2B	2.25	1.48	1.41
23	B	602	CLA	C4C-C3C	2.25	1.48	1.45
38	E	103	HEM	C3B-C4B	2.25	1.49	1.44
23	a	406	CLA	C1B-C2B	2.25	1.48	1.43
23	D	404	CLA	C4D-CHA	2.25	1.46	1.38
23	A	405	CLA	C1C-C2C	2.25	1.49	1.44
23	B	610	CLA	C3D-C4D	-2.25	1.39	1.44
23	B	606	CLA	C1B-NB	-2.25	1.34	1.37
23	b	616	CLA	C3B-C2B	2.25	1.48	1.41
23	c	507	CLA	C4C-C3C	2.24	1.48	1.45
23	c	503	CLA	C1C-C2C	2.24	1.49	1.44
23	B	608	CLA	C3D-C4D	-2.24	1.39	1.44
23	a	406	CLA	C1C-NC	-2.24	1.34	1.37
23	b	610	CLA	C3B-C4B	2.24	1.49	1.42
23	B	615	CLA	C3B-C4B	2.24	1.49	1.42
23	C	512	CLA	C3B-C4B	2.24	1.49	1.42
23	c	501	CLA	C3D-C4D	-2.24	1.39	1.44
23	c	508	CLA	C4C-C3C	2.23	1.48	1.45
23	c	513	CLA	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C4B-NB	-2.23	1.34	1.37
23	c	504	CLA	C3D-C4D	-2.23	1.39	1.44
23	C	514	CLA	C3B-C4B	2.23	1.49	1.42
24	D	402	PHO	C1D-ND	-2.23	1.34	1.38
34	Z	101	LMG	O1-C1	2.22	1.43	1.40
23	B	611	CLA	C3D-C4D	-2.22	1.39	1.44
23	C	509	CLA	C3D-C4D	-2.22	1.39	1.44
24	a	408	PHO	C4B-NB	-2.22	1.34	1.38
23	b	613	CLA	C3B-C4B	2.22	1.49	1.42
23	c	507	CLA	C3D-C4D	-2.22	1.39	1.44
23	c	501	CLA	C3B-C4B	2.22	1.49	1.42
23	B	609	CLA	C1C-C2C	2.22	1.49	1.44
23	D	405	CLA	C3D-C4D	-2.22	1.39	1.44
23	c	511	CLA	C4C-C3C	2.22	1.48	1.45
23	B	603	CLA	C3B-C4B	2.21	1.49	1.42
23	B	609	CLA	C3B-C4B	2.21	1.49	1.42
23	b	605	CLA	C1C-C2C	2.21	1.49	1.44
23	c	502	CLA	C1C-C2C	2.21	1.49	1.44
23	C	512	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	609	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	602	CLA	C3B-C2B	2.21	1.48	1.41
25	b	619	BCR	C30-C25	-2.21	1.51	1.53
23	A	407	CLA	C3D-C4D	-2.21	1.39	1.44
23	b	601	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	601	CLA	C3B-C2B	2.20	1.48	1.41
23	c	501	CLA	C3B-C2B	2.20	1.48	1.41
23	B	616	CLA	C3B-C4B	2.20	1.49	1.42
24	a	407	PHO	C4B-NB	-2.20	1.34	1.38
23	A	407	CLA	C3B-C4B	2.20	1.49	1.42
23	C	513	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	605	CLA	C3D-C4D	-2.20	1.39	1.44
23	C	502	CLA	C3B-C4B	2.19	1.49	1.42
23	A	407	CLA	C1C-C2C	2.19	1.49	1.44
23	b	601	CLA	C1C-C2C	2.19	1.49	1.44
23	B	611	CLA	C3B-C2B	2.19	1.48	1.41
23	d	403	CLA	C3B-C2B	2.19	1.48	1.41
23	C	504	CLA	C3D-C4D	-2.19	1.39	1.44
38	e	103	HEM	C4B-NB	-2.19	1.34	1.38
23	C	513	CLA	C3B-C2B	2.18	1.48	1.41
23	c	512	CLA	C4C-C3C	2.18	1.48	1.45
23	c	501	CLA	C1C-C2C	2.18	1.49	1.44
34	a	417	LMG	O1-C1	2.18	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C3B-C2B	2.18	1.48	1.41
23	C	507	CLA	C1B-C2B	2.18	1.48	1.43
23	B	608	CLA	C3B-C4B	2.17	1.49	1.42
24	a	408	PHO	C1B-NB	-2.17	1.34	1.38
23	c	507	CLA	C3B-C4B	2.17	1.49	1.42
23	C	503	CLA	C1C-C2C	2.17	1.48	1.44
23	B	603	CLA	C3B-C2B	2.17	1.48	1.41
23	B	605	CLA	C3B-C4B	2.17	1.49	1.42
23	b	602	CLA	C4C-C3C	2.16	1.48	1.45
38	E	103	HEM	C1D-ND	-2.16	1.34	1.38
23	B	614	CLA	C1B-C2B	2.16	1.48	1.43
36	b	621	HTG	C1-S1	-2.16	1.77	1.80
23	B	602	CLA	C3D-C4D	-2.16	1.39	1.44
23	C	507	CLA	C1D-C2D	2.16	1.49	1.45
23	A	407	CLA	C3B-C2B	2.16	1.48	1.41
23	c	512	CLA	C3D-C4D	-2.16	1.39	1.44
23	b	609	CLA	C3D-C4D	-2.15	1.39	1.44
37	c	517	DGD	O3G-C1D	2.15	1.43	1.40
31	d	406	LHG	O7-C5	-2.15	1.41	1.46
29	A	413	PL9	C2-C3	2.15	1.40	1.34
23	B	604	CLA	C3B-C4B	2.14	1.49	1.42
23	C	514	CLA	C3D-C4D	-2.14	1.39	1.44
23	c	510	CLA	C3B-C2B	2.14	1.48	1.41
23	C	514	CLA	C3B-C2B	2.14	1.48	1.41
23	b	615	CLA	C3B-C4B	2.14	1.49	1.42
23	b	605	CLA	C3B-C2B	2.14	1.48	1.41
29	D	407	PL9	C2-C1	-2.13	1.39	1.44
23	C	508	CLA	C4C-C3C	2.13	1.48	1.45
23	a	405	CLA	C1C-C2C	2.13	1.48	1.44
23	c	513	CLA	C3B-C2B	2.13	1.48	1.41
23	C	509	CLA	C1C-NC	-2.13	1.34	1.37
24	a	408	PHO	C1D-ND	-2.13	1.34	1.38
23	C	510	CLA	C4C-C3C	2.13	1.48	1.45
26	a	413	SQD	O6-C1	2.13	1.43	1.40
34	c	519	LMG	O1-C1	2.13	1.43	1.40
23	B	605	CLA	C3B-C2B	2.12	1.48	1.41
29	d	405	PL9	C2-C3	2.12	1.40	1.34
23	B	606	CLA	C4C-C3C	2.12	1.48	1.45
36	B	629	HTG	C1-S1	-2.12	1.77	1.80
23	B	610	CLA	C4B-NB	-2.12	1.35	1.37
23	c	509	CLA	C3B-C4B	2.12	1.48	1.42
36	b	626	HTG	C1-S1	-2.12	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C3B-C4B	2.11	1.48	1.42
35	E	102	LMT	O1'-C1'	2.11	1.43	1.40
23	c	502	CLA	C3B-C4B	2.10	1.48	1.42
36	D	412	HTG	C1-S1	-2.10	1.77	1.80
23	C	506	CLA	C3B-C2B	2.10	1.48	1.41
23	d	402	CLA	C3B-C2B	2.10	1.48	1.41
23	c	511	CLA	C3B-C4B	2.10	1.48	1.42
23	B	615	CLA	C3D-C4D	-2.09	1.39	1.44
40	V	202	HEC	C4A-C3A	-2.09	1.41	1.45
34	C	521	LMG	O1-C1	2.09	1.43	1.40
23	b	613	CLA	C3D-C4D	-2.09	1.39	1.44
23	B	611	CLA	C4C-C3C	2.09	1.48	1.45
23	b	604	CLA	C3B-C2B	2.09	1.48	1.41
23	C	514	CLA	C1D-C2D	2.09	1.49	1.45
35	b	628	LMT	O1'-C1'	2.09	1.43	1.40
23	B	617	CLA	C1C-NC	-2.09	1.34	1.37
23	c	504	CLA	C3B-C4B	2.07	1.48	1.42
23	B	615	CLA	C1C-C2C	2.07	1.48	1.44
23	C	505	CLA	C3B-C4B	2.07	1.48	1.42
23	b	609	CLA	C4C-C3C	2.07	1.48	1.45
23	c	510	CLA	C3B-C4B	2.07	1.48	1.42
38	e	103	HEM	C3C-C4C	-2.07	1.42	1.46
23	c	503	CLA	C3B-C2B	2.06	1.48	1.41
24	A	406	PHO	CBD-CGD	-2.06	1.49	1.52
34	J	101	LMG	O1-C1	2.06	1.43	1.40
23	C	507	CLA	C3B-C2B	2.06	1.48	1.41
35	a	418	LMT	O1'-C1'	2.06	1.43	1.40
23	b	601	CLA	C1D-C2D	2.06	1.49	1.45
23	b	608	CLA	C1C-NC	-2.06	1.34	1.37
23	B	610	CLA	C1D-C2D	2.06	1.49	1.45
23	c	506	CLA	C1C-NC	-2.05	1.34	1.37
23	b	609	CLA	C1D-C2D	2.05	1.49	1.45
23	c	513	CLA	C1D-C2D	2.05	1.49	1.45
23	A	407	CLA	C1D-C2D	2.05	1.49	1.45
23	b	616	CLA	C3B-C4B	2.05	1.48	1.42
23	b	613	CLA	C4C-C3C	2.05	1.48	1.45
23	c	504	CLA	C1D-C2D	2.05	1.49	1.45
23	b	606	CLA	C4C-C3C	2.04	1.48	1.45
24	A	406	PHO	C3D-C4D	-2.04	1.38	1.41
23	B	608	CLA	C3B-C2B	2.04	1.48	1.41
23	C	511	CLA	C3B-C2B	2.04	1.48	1.41
36	c	522	HTG	C1-S1	-2.04	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	C4C-C3C	2.03	1.48	1.45
24	A	406	PHO	C4B-NB	-2.03	1.34	1.38
23	C	503	CLA	C4C-C3C	2.03	1.48	1.45
23	B	614	CLA	C3D-C4D	-2.03	1.39	1.44
29	a	415	PL9	C2-C3	2.03	1.39	1.34
23	b	606	CLA	C3B-C2B	2.03	1.48	1.41
23	C	512	CLA	C1C-NC	-2.03	1.34	1.37
23	D	401	CLA	C4C-C3C	2.02	1.48	1.45
23	B	617	CLA	C3B-C4B	2.02	1.48	1.42
23	D	401	CLA	C1D-C2D	2.02	1.49	1.45
23	c	501	CLA	C1D-C2D	2.02	1.49	1.45
36	b	623	HTG	C1-S1	-2.01	1.77	1.80
23	B	603	CLA	C1D-C2D	2.01	1.49	1.45
35	m	103	LMT	O1'-C1'	2.01	1.43	1.40
23	a	409	CLA	C3B-C2B	2.01	1.47	1.41
23	a	405	CLA	C3B-C4B	2.01	1.48	1.42
23	b	607	CLA	C1A-CHA	2.01	1.51	1.43

All (2909) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	PHO	C2D-C1D-ND	11.76	117.93	109.43
24	a	407	PHO	C2D-C1D-ND	11.72	117.90	109.43
24	A	406	PHO	C2D-C1D-ND	10.60	117.09	109.43
23	D	405	CLA	C1D-ND-C4D	-10.40	99.02	106.31
23	D	401	CLA	C1D-ND-C4D	-10.33	99.06	106.31
24	a	408	PHO	C2D-C1D-ND	10.33	116.90	109.43
23	C	514	CLA	C1D-ND-C4D	-10.13	99.20	106.31
23	d	403	CLA	C1D-ND-C4D	-10.01	99.29	106.31
23	A	407	CLA	C1D-ND-C4D	-9.95	99.33	106.31
23	c	511	CLA	C1D-ND-C4D	-9.91	99.36	106.31
23	c	513	CLA	C1D-ND-C4D	-9.89	99.37	106.31
23	C	510	CLA	C1D-ND-C4D	-9.85	99.40	106.31
24	a	407	PHO	O2D-CGD-CBD	9.85	121.77	110.95
23	D	404	CLA	C1D-ND-C4D	-9.85	99.40	106.31
23	B	615	CLA	C1D-ND-C4D	-9.79	99.44	106.31
23	B	606	CLA	C1D-ND-C4D	-9.78	99.45	106.31
23	B	609	CLA	C1D-ND-C4D	-9.75	99.47	106.31
23	c	502	CLA	C1D-ND-C4D	-9.73	99.49	106.31
23	a	406	CLA	C1D-ND-C4D	-9.72	99.49	106.31
23	A	405	CLA	C1D-ND-C4D	-9.71	99.50	106.31
23	c	505	CLA	C1D-ND-C4D	-9.70	99.51	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C1D-ND-C4D	-9.66	99.53	106.31
23	b	606	CLA	C1D-ND-C4D	-9.64	99.55	106.31
23	b	605	CLA	C1D-ND-C4D	-9.64	99.55	106.31
23	B	604	CLA	C1D-ND-C4D	-9.62	99.56	106.31
23	b	603	CLA	C1D-ND-C4D	-9.61	99.57	106.31
23	b	609	CLA	C1D-ND-C4D	-9.58	99.59	106.31
23	c	504	CLA	C1D-ND-C4D	-9.57	99.60	106.31
23	C	512	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	B	607	CLA	C1D-ND-C4D	-9.50	99.65	106.31
23	C	504	CLA	C1D-ND-C4D	-9.43	99.69	106.31
23	B	612	CLA	C1D-ND-C4D	-9.42	99.70	106.31
23	b	608	CLA	C1D-ND-C4D	-9.38	99.73	106.31
23	C	509	CLA	C1D-ND-C4D	-9.38	99.73	106.31
23	b	610	CLA	C1D-ND-C4D	-9.37	99.74	106.31
23	B	611	CLA	C1D-ND-C4D	-9.33	99.76	106.31
23	B	610	CLA	C1D-ND-C4D	-9.29	99.79	106.31
23	b	613	CLA	C1D-ND-C4D	-9.29	99.79	106.31
23	c	509	CLA	C1D-ND-C4D	-9.25	99.82	106.31
24	A	406	PHO	O2D-CGD-CBD	9.24	121.10	110.95
23	a	405	CLA	C1D-ND-C4D	-9.23	99.83	106.31
23	b	614	CLA	C1D-ND-C4D	-9.19	99.87	106.31
23	b	602	CLA	C1D-ND-C4D	-9.18	99.87	106.31
23	C	503	CLA	C1D-ND-C4D	-9.17	99.88	106.31
23	B	617	CLA	C1D-ND-C4D	-9.15	99.89	106.31
23	d	402	CLA	C1D-ND-C4D	-9.13	99.91	106.31
23	B	605	CLA	C1D-ND-C4D	-9.01	99.99	106.31
23	c	503	CLA	C1D-ND-C4D	-9.00	100.00	106.31
23	b	612	CLA	C1D-ND-C4D	-8.99	100.01	106.31
23	c	512	CLA	C1D-ND-C4D	-8.97	100.02	106.31
23	B	608	CLA	C1D-ND-C4D	-8.95	100.03	106.31
23	b	615	CLA	C1D-ND-C4D	-8.93	100.05	106.31
23	b	607	CLA	C1D-ND-C4D	-8.91	100.06	106.31
23	B	613	CLA	C1D-ND-C4D	-8.90	100.07	106.31
23	C	502	CLA	C1D-ND-C4D	-8.85	100.11	106.31
23	C	511	CLA	C1D-ND-C4D	-8.84	100.11	106.31
23	c	508	CLA	C1D-ND-C4D	-8.81	100.13	106.31
23	C	505	CLA	C1D-ND-C4D	-8.79	100.15	106.31
23	c	501	CLA	C1D-ND-C4D	-8.77	100.16	106.31
23	C	513	CLA	C1D-ND-C4D	-8.77	100.16	106.31
23	C	506	CLA	C1D-ND-C4D	-8.74	100.18	106.31
23	b	601	CLA	C1D-ND-C4D	-8.73	100.19	106.31
23	a	409	CLA	C1D-ND-C4D	-8.70	100.21	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	C1D-ND-C4D	-8.70	100.21	106.31
23	c	510	CLA	C1D-ND-C4D	-8.68	100.22	106.31
23	c	506	CLA	C1D-ND-C4D	-8.68	100.22	106.31
23	c	507	CLA	C1D-ND-C4D	-8.66	100.23	106.31
23	B	616	CLA	C1D-ND-C4D	-8.62	100.26	106.31
23	B	603	CLA	C1D-ND-C4D	-8.61	100.27	106.31
23	A	404	CLA	C1D-ND-C4D	-8.61	100.27	106.31
23	B	614	CLA	C1D-ND-C4D	-8.59	100.29	106.31
23	b	604	CLA	C1D-ND-C4D	-8.58	100.29	106.31
23	b	611	CLA	C1D-ND-C4D	-8.50	100.35	106.31
23	C	507	CLA	C1D-ND-C4D	-8.38	100.43	106.31
23	C	508	CLA	C1D-ND-C4D	-8.34	100.46	106.31
24	a	408	PHO	O2D-CGD-CBD	8.28	120.04	110.95
24	D	402	PHO	O2D-CGD-CBD	7.87	119.59	110.95
24	A	406	PHO	C3B-C4B-NB	7.82	112.56	107.46
24	a	407	PHO	C3B-C4B-NB	7.70	112.48	107.46
23	b	616	CLA	C1D-ND-C4D	-7.66	100.94	106.31
23	C	506	CLA	CMD-C2D-C1D	7.58	138.07	124.73
23	c	507	CLA	CMD-C2D-C1D	7.48	137.91	124.73
23	A	404	CLA	CMD-C2D-C1D	7.21	137.43	124.73
23	B	608	CLA	C4A-NA-C1A	-7.16	103.41	106.68
23	c	510	CLA	CMD-C2D-C1D	7.14	137.30	124.73
23	C	507	CLA	CMD-C2D-C1D	7.13	137.28	124.73
23	b	615	CLA	CMD-C2D-C1D	7.12	137.27	124.73
23	B	612	CLA	CHD-C4C-C3C	-6.99	114.58	124.77
23	B	609	CLA	CHD-C4C-C3C	-6.94	114.66	124.77
23	C	504	CLA	CMD-C2D-C1D	6.93	136.92	124.73
24	D	402	PHO	C2B-C1B-NB	6.91	114.43	109.43
23	c	507	CLA	O2D-CGD-CBD	6.89	123.27	111.23
23	b	614	CLA	CMD-C2D-C1D	6.84	136.78	124.73
23	c	509	CLA	CMD-C2D-C1D	6.79	136.69	124.73
23	b	603	CLA	CMD-C2D-C1D	6.77	136.66	124.73
24	D	402	PHO	C3B-C4B-NB	6.70	111.83	107.46
23	B	617	CLA	CHD-C4C-C3C	-6.68	115.03	124.77
23	B	611	CLA	CHD-C4C-C3C	-6.68	115.04	124.77
23	c	513	CLA	CMD-C2D-C1D	6.66	136.46	124.73
23	B	617	CLA	O2D-CGD-CBD	6.65	122.85	111.23
23	D	404	CLA	CMD-C2D-C1D	6.64	136.43	124.73
23	A	407	CLA	CMD-C2D-C1D	6.64	136.42	124.73
23	A	407	CLA	C2D-C1D-ND	6.64	116.69	110.13
23	D	405	CLA	CHD-C4C-C3C	-6.63	115.11	124.77
23	C	507	CLA	C4A-NA-C1A	-6.62	103.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CMD-C2D-C1D	6.61	136.37	124.73
23	b	609	CLA	C4A-NA-C1A	-6.61	103.66	106.68
23	C	509	CLA	C2D-C1D-ND	6.60	116.66	110.13
23	b	604	CLA	CMD-C2D-C1D	6.60	136.35	124.73
23	B	609	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	b	613	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	b	601	CLA	CMD-C2D-C1D	6.57	136.30	124.73
23	B	612	CLA	CMD-C2D-C1D	6.57	136.30	124.73
23	b	602	CLA	CMD-C2D-C1D	6.54	136.25	124.73
23	b	607	CLA	C2D-C1D-ND	6.54	116.60	110.13
23	b	613	CLA	CHD-C4C-C3C	-6.49	115.31	124.77
25	D	406	BCR	C7-C8-C9	-6.47	116.66	126.23
23	C	510	CLA	CMD-C2D-C1D	6.46	136.11	124.73
23	B	612	CLA	C2D-C1D-ND	6.46	116.52	110.13
23	B	606	CLA	CHD-C4C-C3C	-6.44	115.39	124.77
23	B	611	CLA	C2D-C1D-ND	6.44	116.50	110.13
23	B	615	CLA	C2D-C1D-ND	6.43	116.49	110.13
23	c	512	CLA	O2D-CGD-CBD	6.43	122.47	111.23
24	a	408	PHO	C3B-C4B-NB	6.40	111.64	107.46
23	c	503	CLA	CMD-C2D-C1D	6.39	135.99	124.73
23	D	401	CLA	CHD-C4C-C3C	-6.38	115.47	124.77
23	D	405	CLA	CMD-C2D-C1D	6.38	135.97	124.73
23	b	602	CLA	C4A-NA-C1A	-6.38	103.77	106.68
23	b	604	CLA	O2D-CGD-CBD	6.37	122.37	111.23
23	D	405	CLA	C2D-C1D-ND	6.36	116.42	110.13
23	b	616	CLA	C4A-NA-C1A	-6.36	103.78	106.68
23	b	609	CLA	CMD-C2D-C1D	6.35	135.91	124.73
23	B	605	CLA	CMD-C2D-C1D	6.34	135.89	124.73
23	B	613	CLA	O2D-CGD-CBD	6.34	122.31	111.23
23	B	602	CLA	CMD-C2D-C1D	6.33	135.88	124.73
23	B	608	CLA	CMD-C2D-C1D	6.33	135.88	124.73
23	C	514	CLA	C2D-C1D-ND	6.32	116.38	110.13
23	B	603	CLA	CMD-C2D-C1D	6.32	135.85	124.73
23	c	513	CLA	C4A-NA-C1A	-6.32	103.80	106.68
23	a	404	CLA	CMD-C2D-C1D	6.32	135.85	124.73
23	D	404	CLA	C2D-C1D-ND	6.31	116.37	110.13
23	c	507	CLA	C4A-NA-C1A	-6.31	103.80	106.68
23	D	401	CLA	C2D-C1D-ND	6.30	116.36	110.13
23	C	508	CLA	O2D-CGD-CBD	6.30	122.24	111.23
23	a	406	CLA	C2D-C1D-ND	6.28	116.34	110.13
23	B	610	CLA	CHD-C4C-C3C	-6.28	115.62	124.77
23	c	505	CLA	CMD-C2D-C1D	6.26	135.76	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	O2D-CGD-CBD	6.26	122.17	111.23
23	C	510	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
23	B	607	CLA	CMD-C2D-C1D	6.24	135.72	124.73
23	b	611	CLA	CMD-C2D-C1D	6.24	135.72	124.73
23	b	606	CLA	CMD-C2D-C1D	6.24	135.71	124.73
23	B	603	CLA	O2D-CGD-CBD	6.23	122.13	111.23
23	A	404	CLA	C4A-NA-C1A	-6.23	103.84	106.68
23	B	606	CLA	CMD-C2D-C1D	6.23	135.69	124.73
23	C	514	CLA	CMD-C2D-C1D	6.23	135.69	124.73
23	c	502	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
23	c	505	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	b	611	CLA	O2D-CGD-CBD	6.22	122.11	111.23
24	a	407	PHO	C2B-C1B-NB	6.22	113.92	109.43
23	b	610	CLA	CMD-C2D-C1D	6.22	135.67	124.73
24	D	402	PHO	C4D-ND-C1D	-6.22	101.42	108.87
23	C	513	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
23	A	405	CLA	CMD-C2D-C1D	6.20	135.65	124.73
23	d	403	CLA	CMD-C2D-C1D	6.20	135.65	124.73
23	a	406	CLA	CMD-C2D-C1D	6.20	135.64	124.73
23	d	403	CLA	CHD-C4C-C3C	-6.19	115.74	124.77
23	B	606	CLA	C2D-C1D-ND	6.19	116.25	110.13
29	a	415	PL9	C7-C3-C4	6.19	122.01	116.91
23	B	615	CLA	O2D-CGD-CBD	6.19	122.05	111.23
23	C	504	CLA	C2D-C1D-ND	6.18	116.24	110.13
23	c	504	CLA	C2D-C1D-ND	6.17	116.23	110.13
23	c	501	CLA	CMD-C2D-C1D	6.17	135.59	124.73
23	b	606	CLA	C2D-C1D-ND	6.17	116.23	110.13
23	c	511	CLA	C2D-C1D-ND	6.17	116.23	110.13
23	B	603	CLA	C4A-NA-C1A	-6.16	103.87	106.68
23	B	617	CLA	C2D-C1D-ND	6.16	116.22	110.13
23	c	506	CLA	CMD-C2D-C1D	6.16	135.57	124.73
23	a	406	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
23	b	608	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
23	c	512	CLA	C2D-C1D-ND	6.15	116.21	110.13
23	B	614	CLA	C2D-C1D-ND	6.13	116.20	110.13
23	B	610	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	C	511	CLA	CMD-C2D-C1D	6.12	135.50	124.73
23	B	607	CLA	C2D-C1D-ND	6.11	116.18	110.13
23	C	509	CLA	CHD-C4C-C3C	-6.10	115.87	124.77
23	a	409	CLA	C4A-NA-C1A	-6.10	103.90	106.68
23	C	503	CLA	CMD-C2D-C1D	6.10	135.46	124.73
23	B	611	CLA	CMD-C2D-C1D	6.09	135.46	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C2D-C1D-ND	6.09	116.16	110.13
23	B	615	CLA	CMD-C2D-C1D	6.09	135.45	124.73
23	b	614	CLA	O2D-CGD-CBD	6.09	121.87	111.23
23	c	512	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
23	B	604	CLA	C2D-C1D-ND	6.08	116.14	110.13
23	b	606	CLA	CHD-C4C-C3C	-6.08	115.92	124.77
23	A	407	CLA	CHD-C4C-C3C	-6.07	115.92	124.77
23	C	506	CLA	CHD-C4C-C3C	-6.07	115.92	124.77
23	C	510	CLA	C2D-C1D-ND	6.07	116.13	110.13
23	D	401	CLA	CMD-C2D-C1D	6.07	135.42	124.73
23	b	605	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	B	610	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	c	508	CLA	CHD-C4C-C3C	-6.07	115.93	124.77
23	B	617	CLA	C4A-NA-C1A	-6.06	103.91	106.68
23	c	511	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
23	C	514	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
23	b	604	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
23	b	602	CLA	CHD-C4C-C3C	-6.04	115.96	124.77
23	d	403	CLA	C2D-C1D-ND	6.04	116.10	110.13
23	B	605	CLA	CHD-C4C-C3C	-6.03	115.98	124.77
23	b	614	CLA	C2D-C1D-ND	6.03	116.09	110.13
23	C	508	CLA	CMD-C2D-C1D	6.02	135.34	124.73
23	b	605	CLA	CHD-C4C-C3C	-6.01	116.01	124.77
23	C	512	CLA	C2D-C1D-ND	6.00	116.07	110.13
23	C	513	CLA	C4A-NA-C1A	-6.00	103.94	106.68
23	B	605	CLA	C2D-C1D-ND	6.00	116.06	110.13
23	B	613	CLA	CHD-C4C-C3C	-5.99	116.03	124.77
23	C	505	CLA	CMD-C2D-C1D	5.99	135.28	124.73
23	a	405	CLA	CMD-C2D-C1D	5.98	135.26	124.73
23	c	504	CLA	CMD-C2D-C1D	5.98	135.25	124.73
23	c	503	CLA	C4A-NA-C1A	-5.96	103.96	106.68
23	c	508	CLA	O2D-CGD-CBD	5.96	121.65	111.23
23	B	602	CLA	C2D-C1D-ND	5.96	116.02	110.13
23	b	606	CLA	C4A-NA-C1A	-5.96	103.96	106.68
23	b	611	CLA	C2C-C1C-NC	5.95	116.23	109.98
23	c	513	CLA	C2D-C1D-ND	5.94	116.01	110.13
23	c	510	CLA	C1-C2-C3	-5.94	116.46	126.20
23	B	604	CLA	O2D-CGD-CBD	5.94	121.61	111.23
23	B	607	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
26	A	409	SQD	O6-C1-C2	5.94	117.29	108.27
23	C	513	CLA	CMD-C2D-C1D	5.92	135.16	124.73
23	a	409	CLA	CMD-C2D-C1D	5.91	135.14	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CHD-C4C-C3C	-5.91	116.15	124.77
23	B	614	CLA	CMD-C2D-C1D	5.91	135.13	124.73
23	b	608	CLA	C2D-C1D-ND	5.90	115.97	110.13
23	B	611	CLA	O2D-CGD-CBD	5.89	121.52	111.23
23	B	616	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
23	b	601	CLA	O2D-CGD-CBD	5.88	121.50	111.23
24	a	408	PHO	C2B-C1B-NB	5.88	113.68	109.43
23	C	508	CLA	CHD-C4C-C3C	-5.88	116.21	124.77
23	b	603	CLA	CHD-C4C-C3C	-5.87	116.21	124.77
23	b	610	CLA	C4A-NA-C1A	-5.86	104.00	106.68
23	B	613	CLA	C2D-C1D-ND	5.86	115.92	110.13
23	c	502	CLA	CMD-C2D-C1D	5.85	135.02	124.73
23	B	602	CLA	CHD-C4C-C3C	-5.84	116.25	124.77
23	c	502	CLA	C2D-C1D-ND	5.84	115.91	110.13
23	C	502	CLA	O2D-CGD-CBD	5.84	121.43	111.23
23	A	405	CLA	C2D-C1D-ND	5.84	115.90	110.13
23	a	405	CLA	C2D-C1D-ND	5.83	115.90	110.13
23	B	604	CLA	CHD-C4C-C3C	-5.83	116.28	124.77
23	b	612	CLA	CMD-C2D-C1D	5.83	134.99	124.73
23	C	502	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
23	B	608	CLA	C2D-C1D-ND	5.82	115.89	110.13
23	b	609	CLA	CHD-C4C-C3C	-5.82	116.29	124.77
23	b	601	CLA	CHD-C4C-C3C	-5.81	116.30	124.77
23	a	404	CLA	C4A-NA-C1A	-5.81	104.03	106.68
23	D	404	CLA	CHD-C4C-C3C	-5.81	116.30	124.77
23	B	602	CLA	O2D-CGD-CBD	5.80	121.37	111.23
23	b	615	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	c	501	CLA	O2D-CGD-CBD	5.79	121.35	111.23
23	b	616	CLA	O2D-CGD-CBD	5.79	121.34	111.23
23	b	607	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
23	d	402	CLA	CMD-C2D-C1D	5.78	134.90	124.73
24	D	402	PHO	C3D-C4D-ND	5.77	115.11	107.71
23	C	511	CLA	O2D-CGD-CBD	5.77	121.31	111.23
23	C	502	CLA	CMD-C2D-C1D	5.76	134.87	124.73
23	C	506	CLA	O2D-CGD-CBD	5.75	121.29	111.23
25	T	101	BCR	C15-C16-C17	-5.75	111.75	123.52
23	C	505	CLA	C2D-C1D-ND	5.74	115.81	110.13
26	D	413	SQD	O47-C7-C8	5.73	123.88	111.48
23	B	617	CLA	CMD-C2D-C1D	5.72	134.81	124.73
23	b	605	CLA	C2D-C1D-ND	5.72	115.79	110.13
23	b	612	CLA	CHD-C4C-C3C	-5.72	116.44	124.77
23	b	614	CLA	CHD-C4C-C3C	-5.72	116.44	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413	PL9	C7-C3-C4	5.72	121.62	116.91
23	b	609	CLA	C2D-C1D-ND	5.71	115.78	110.13
23	b	616	CLA	CHD-C4C-C3C	-5.71	116.44	124.77
24	a	407	PHO	C4D-ND-C1D	-5.71	102.03	108.87
23	c	509	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	c	510	CLA	C4A-NA-C1A	-5.71	104.08	106.68
23	C	512	CLA	CMD-C2D-C1D	5.71	134.78	124.73
23	b	611	CLA	C2D-C1D-ND	5.70	115.77	110.13
24	a	408	PHO	C3D-C4D-ND	5.68	114.99	107.71
23	A	404	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
23	B	616	CLA	CMD-C2D-C1D	5.68	134.73	124.73
23	b	602	CLA	C2D-C1D-ND	5.67	115.74	110.13
23	B	607	CLA	C4A-NA-C1A	-5.67	104.09	106.68
23	B	608	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
23	b	616	CLA	CMD-C2D-C1D	5.67	134.71	124.73
25	Y	101	BCR	C33-C5-C6	-5.66	118.30	124.48
23	C	509	CLA	O2D-CGD-CBD	5.66	121.13	111.23
23	c	501	CLA	C4A-NA-C1A	-5.66	104.10	106.68
23	b	603	CLA	O2D-CGD-CBD	5.65	121.11	111.23
23	b	608	CLA	CMD-C2D-C1D	5.65	134.68	124.73
23	C	503	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
23	a	405	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
23	c	505	CLA	C2D-C1D-ND	5.64	115.71	110.13
23	b	607	CLA	CMD-C2D-C1D	5.64	134.66	124.73
23	b	603	CLA	C2D-C1D-ND	5.63	115.70	110.13
23	c	508	CLA	CMD-C2D-C1D	5.63	134.65	124.73
23	C	513	CLA	C2D-C1D-ND	5.63	115.70	110.13
23	c	505	CLA	O2D-CGD-CBD	5.63	121.07	111.23
23	C	504	CLA	C4A-NA-C1A	-5.62	104.11	106.68
23	C	503	CLA	O2D-CGD-CBD	5.62	121.05	111.23
23	C	505	CLA	C2C-C1C-NC	5.62	115.88	109.98
23	b	604	CLA	C2D-C1D-ND	5.62	115.68	110.13
23	c	509	CLA	C2D-C1D-ND	5.61	115.68	110.13
23	a	404	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
24	a	408	PHO	C4D-ND-C1D	-5.58	102.19	108.87
23	c	506	CLA	C2D-C1D-ND	5.58	115.65	110.13
23	c	503	CLA	O2D-CGD-CBD	5.58	120.98	111.23
23	b	605	CLA	O2D-CGD-CBD	5.57	120.97	111.23
23	b	601	CLA	C4A-NA-C1A	-5.57	104.14	106.68
23	B	614	CLA	CHD-C4C-C3C	-5.57	116.66	124.77
23	b	611	CLA	CHD-C4C-C3C	-5.56	116.66	124.77
23	b	610	CLA	O2D-CGD-CBD	5.56	120.95	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	CMD-C2D-C1D	5.55	134.51	124.73
23	d	402	CLA	C2C-C1C-NC	5.55	115.81	109.98
23	B	604	CLA	C4A-NA-C1A	-5.55	104.15	106.68
23	d	403	CLA	C4A-NA-C1A	-5.54	104.15	106.68
23	C	502	CLA	C2D-C1D-ND	5.54	115.61	110.13
23	C	512	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
23	B	616	CLA	C2D-C1D-ND	5.53	115.60	110.13
23	b	610	CLA	C2D-C1D-ND	5.53	115.60	110.13
23	c	507	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
23	b	606	CLA	O2D-CGD-CBD	5.53	120.89	111.23
23	c	501	CLA	C2D-C1D-ND	5.52	115.59	110.13
23	d	402	CLA	C2D-C1D-ND	5.52	115.59	110.13
23	b	613	CLA	CMD-C2D-C1D	5.51	134.44	124.73
23	B	611	CLA	C4A-NA-C1A	-5.50	104.17	106.68
23	C	504	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
23	C	503	CLA	C2D-C1D-ND	5.50	115.57	110.13
23	c	512	CLA	CMD-C2D-C1D	5.50	134.41	124.73
23	b	612	CLA	C2D-C1D-ND	5.50	115.56	110.13
23	c	503	CLA	C2D-C1D-ND	5.49	115.56	110.13
23	c	506	CLA	CHD-C4C-C3C	-5.49	116.76	124.77
23	c	502	CLA	O2D-CGD-CBD	5.49	120.83	111.23
23	B	607	CLA	O2D-CGD-CBD	5.49	120.82	111.23
23	c	513	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
25	y	101	BCR	C33-C5-C6	-5.46	118.52	124.48
23	b	612	CLA	C4A-NA-C1A	-5.46	104.19	106.68
23	C	507	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
26	a	411	SQD	O6-C1-C2	5.46	116.56	108.27
23	C	508	CLA	C2D-C1D-ND	5.42	115.49	110.13
23	B	610	CLA	C4A-NA-C1A	-5.41	104.21	106.68
23	a	405	CLA	C2C-C1C-NC	5.41	115.67	109.98
23	C	505	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
23	a	409	CLA	C2D-C1D-ND	5.39	115.46	110.13
23	b	615	CLA	C4A-NA-C1A	-5.39	104.22	106.68
23	b	615	CLA	C2C-C1C-NC	5.38	115.63	109.98
23	c	504	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
23	A	405	CLA	C4A-NA-C1A	-5.37	104.23	106.68
23	C	514	CLA	C4A-NA-C1A	-5.37	104.23	106.68
24	A	406	PHO	C2B-C1B-NB	5.37	113.31	109.43
23	b	612	CLA	O2D-CGD-CBD	5.35	120.59	111.23
25	c	514	BCR	C15-C14-C13	-5.35	119.77	127.28
23	C	506	CLA	C4A-NA-C1A	-5.35	104.24	106.68
23	c	504	CLA	CHD-C4C-C3C	-5.35	116.97	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CHD-C4C-C3C	-5.34	116.98	124.77
23	d	403	CLA	O2D-CGD-CBD	5.33	120.55	111.23
23	A	407	CLA	C2B-C1B-NB	5.32	115.84	110.33
23	b	616	CLA	C2D-C1D-ND	5.32	115.39	110.13
23	C	505	CLA	O2D-CGD-CBD	5.31	120.52	111.23
23	b	604	CLA	C4A-NA-C1A	-5.31	104.26	106.68
23	d	402	CLA	C4A-NA-C1A	-5.30	104.26	106.68
24	A	406	PHO	C4D-ND-C1D	-5.30	102.53	108.87
26	B	621	SQD	O6-C1-C2	5.29	116.31	108.27
23	c	507	CLA	C2D-C1D-ND	5.29	115.36	110.13
23	b	607	CLA	C2C-C1C-NC	5.28	115.53	109.98
23	b	603	CLA	C4A-NA-C1A	-5.28	104.27	106.68
23	C	513	CLA	O2D-CGD-CBD	5.28	120.46	111.23
23	b	602	CLA	O2D-CGD-CBD	5.28	120.45	111.23
23	D	404	CLA	C2C-C1C-NC	5.27	115.52	109.98
23	D	404	CLA	C4A-NA-C1A	-5.27	104.27	106.68
23	D	405	CLA	O2D-CGD-CBD	5.27	120.44	111.23
23	c	510	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
23	C	510	CLA	O2D-CGD-CBD	5.26	120.43	111.23
23	C	511	CLA	C2C-C1C-NC	5.26	115.50	109.98
23	B	612	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
24	a	408	PHO	C1-C2-C3	-5.25	117.59	126.20
36	B	625	HTG	C1'-S1-C1	5.25	111.79	100.45
23	b	608	CLA	C4A-NA-C1A	-5.25	104.29	106.68
23	b	610	CLA	C3B-C2B-C1B	-5.24	101.00	107.17
23	C	511	CLA	C2D-C1D-ND	5.24	115.31	110.13
29	d	405	PL9	C42-C43-C44	-5.23	115.66	127.62
26	f	101	SQD	O47-C7-C8	5.22	122.78	111.48
23	b	613	CLA	C4A-NA-C1A	-5.22	104.30	106.68
23	c	504	CLA	C2C-C1C-NC	5.21	115.46	109.98
23	A	407	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
23	c	504	CLA	C2B-C1B-NB	5.21	115.73	110.33
23	C	502	CLA	C4A-NA-C1A	-5.21	104.30	106.68
23	B	603	CLA	CHD-C4C-C3C	-5.20	117.18	124.77
36	B	626	HTG	C1'-S1-C1	5.20	111.68	100.45
23	A	405	CLA	C2B-C1B-NB	5.18	115.70	110.33
23	d	402	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
23	b	601	CLA	C2D-C1D-ND	5.18	115.25	110.13
23	a	405	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
23	b	609	CLA	O2D-CGD-CBD	5.17	120.28	111.23
23	a	404	CLA	C2D-C1D-ND	5.17	115.24	110.13
23	a	406	CLA	C4A-NA-C1A	-5.17	104.32	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	C2D-C1D-ND	5.16	115.23	110.13
23	B	616	CLA	C4A-NA-C1A	-5.15	104.33	106.68
23	c	512	CLA	C2B-C1B-NB	5.15	115.67	110.33
23	c	501	CLA	CHD-C4C-C3C	-5.14	117.28	124.77
23	c	503	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
23	b	603	CLA	C2B-C1B-NB	5.13	115.65	110.33
23	B	615	CLA	C2C-C1C-NC	5.13	115.37	109.98
23	C	514	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
23	B	614	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	a	404	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
23	b	607	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	c	513	CLA	O2D-CGD-CBD	5.12	120.18	111.23
23	C	511	CLA	C4A-NA-C1A	-5.12	104.34	106.68
23	a	409	CLA	CHD-C4C-C3C	-5.11	117.32	124.77
36	b	623	HTG	C1'-S1-C1	5.10	111.47	100.45
25	b	619	BCR	C3-C4-C5	-5.09	104.97	114.06
24	A	406	PHO	C3D-C4D-ND	5.09	114.23	107.71
23	c	510	CLA	C2D-C1D-ND	5.08	115.16	110.13
25	B	618	BCR	C33-C5-C6	-5.08	118.94	124.48
23	B	611	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	b	615	CLA	CHD-C4C-C3C	-5.08	117.37	124.77
23	C	512	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
23	C	509	CLA	C2C-C1C-NC	5.07	115.31	109.98
23	C	511	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
23	c	503	CLA	CHD-C4C-C3C	-5.07	117.38	124.77
23	C	507	CLA	C2D-C1D-ND	5.07	115.14	110.13
23	A	407	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
23	A	405	CLA	CHD-C4C-C3C	-5.06	117.40	124.77
23	c	508	CLA	C2C-C1C-NC	5.06	115.29	109.98
23	D	401	CLA	C3D-C4D-ND	5.05	118.20	109.99
23	a	406	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	C	508	CLA	C4A-NA-C1A	-5.05	104.38	106.68
23	c	503	CLA	C2C-C1C-NC	5.05	115.28	109.98
23	a	405	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
23	c	509	CLA	O2D-CGD-CBD	5.03	120.03	111.23
24	a	407	PHO	C3D-C4D-ND	5.03	114.16	107.71
23	A	405	CLA	C3D-C4D-ND	5.03	118.17	109.99
23	a	409	CLA	O2D-CGD-CBD	5.03	120.02	111.23
23	d	403	CLA	C3D-C4D-ND	5.02	118.15	109.99
23	d	402	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
23	C	504	CLA	C2B-C1B-NB	5.01	115.52	110.33
23	B	614	CLA	C3B-C2B-C1B	-5.01	101.26	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
23	B	603	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
23	c	508	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
23	b	613	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	c	509	CLA	C4A-NA-C1A	-5.00	104.40	106.68
23	b	616	CLA	C2C-C1C-NC	5.00	115.23	109.98
26	L	102	SQD	O47-C7-C8	5.00	122.29	111.48
23	B	609	CLA	CMD-C2D-C1D	4.99	133.52	124.73
23	a	406	CLA	O2D-CGD-CBD	4.98	119.94	111.23
23	B	606	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
23	c	508	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
23	b	613	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
23	D	404	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	c	506	CLA	C2C-C1C-NC	4.97	115.20	109.98
23	C	502	CLA	C2C-C1C-NC	4.96	115.19	109.98
23	a	409	CLA	C2B-C1B-NB	4.96	115.47	110.33
23	c	507	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
23	A	407	CLA	C4A-NA-C1A	-4.96	104.42	106.68
36	c	521	HTG	C1'-S1-C1	4.96	111.16	100.45
23	c	504	CLA	O2D-CGD-CBD	4.96	119.89	111.23
23	B	617	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
23	C	504	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
23	B	615	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
23	A	405	CLA	O2D-CGD-CBD	4.93	119.86	111.23
23	a	404	CLA	C2B-C1B-NB	4.93	115.44	110.33
23	b	614	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
23	b	605	CLA	C2C-C1C-NC	4.93	115.16	109.98
23	B	614	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
36	b	621	HTG	C1'-S1-C1	4.92	111.08	100.45
23	C	506	CLA	C2D-C1D-ND	4.92	114.99	110.13
29	a	415	PL9	C7-C3-C2	-4.91	117.60	123.39
23	b	612	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
23	b	611	CLA	C4A-NA-C1A	-4.91	104.44	106.68
34	C	501	LMG	O7-C10-C11	4.91	122.11	111.48
23	D	405	CLA	C2B-C1B-NB	4.91	115.42	110.33
23	C	510	CLA	C1-C2-C3	-4.91	118.15	126.20
23	d	403	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	B	612	CLA	O2D-CGD-CBD	4.90	119.80	111.23
25	T	101	BCR	C7-C8-C9	-4.90	118.98	126.23
23	b	602	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	C	511	CLA	C1-C2-C3	-4.90	118.17	126.20
23	C	513	CLA	C2B-C1B-NB	4.89	115.40	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	O2D-CGD-CBD	4.89	119.78	111.23
23	d	403	CLA	C2B-C1B-NB	4.89	115.40	110.33
26	A	409	SQD	O47-C7-C8	4.89	122.06	111.48
23	B	607	CLA	C2B-C1B-NB	4.89	115.40	110.33
23	B	606	CLA	O2D-CGD-CBD	4.89	119.78	111.23
29	A	413	PL9	C7-C3-C2	-4.89	117.63	123.39
23	c	504	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	C	510	CLA	C4A-NA-C1A	-4.89	104.45	106.68
23	C	506	CLA	C2C-C1C-NC	4.88	115.11	109.98
23	c	502	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
23	C	504	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	C	509	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
23	C	504	CLA	C2C-C1C-NC	4.88	115.10	109.98
36	D	412	HTG	C1'-S1-C1	4.88	110.98	100.45
23	B	605	CLA	C1-C2-C3	-4.87	118.22	126.20
23	B	603	CLA	C2D-C1D-ND	4.87	114.95	110.13
23	b	605	CLA	C3D-C4D-ND	4.87	117.90	109.99
23	c	512	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
40	V	202	HEC	CHC-C4B-NB	4.86	129.75	124.45
23	B	606	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	a	405	CLA	C2B-C1B-NB	4.86	115.36	110.33
23	c	509	CLA	C1-C2-C3	-4.84	118.27	126.20
23	C	513	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
23	a	404	CLA	C2C-C1C-NC	4.84	115.06	109.98
23	c	503	CLA	C2B-C1B-NB	4.84	115.34	110.33
23	C	505	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
23	b	608	CLA	C2B-C1B-NB	4.83	115.34	110.33
23	b	601	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
23	C	514	CLA	C3D-C4D-ND	4.83	117.84	109.99
23	c	513	CLA	CHD-C1D-ND	-4.83	118.01	124.80
23	c	513	CLA	C3D-C4D-ND	4.82	117.83	109.99
23	c	502	CLA	C2C-C1C-NC	4.82	115.05	109.98
26	L	102	SQD	O6-C1-C2	4.82	115.59	108.27
23	c	510	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	B	615	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
23	c	512	CLA	C4A-NA-C1A	-4.82	104.48	106.68
23	C	510	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
23	C	512	CLA	C4A-NA-C1A	-4.81	104.48	106.68
23	B	603	CLA	C2C-C1C-NC	4.81	115.03	109.98
23	b	608	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
23	B	602	CLA	C3D-C4D-ND	4.80	117.80	109.99
23	C	514	CLA	C3D-C2D-C1D	-4.80	99.28	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	O2D-CGD-CBD	4.80	119.63	111.23
25	c	515	BCR	C7-C8-C9	-4.80	119.14	126.23
23	B	606	CLA	C4A-NA-C1A	-4.79	104.49	106.68
23	b	606	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	c	502	CLA	C3D-C4D-ND	4.78	117.76	109.99
23	C	503	CLA	C4A-NA-C1A	-4.77	104.50	106.68
23	A	404	CLA	C2C-C1C-NC	4.77	114.99	109.98
23	B	610	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	b	612	CLA	C2B-C1B-NB	4.77	115.27	110.33
23	b	602	CLA	C2B-C1B-NB	4.77	115.27	110.33
23	B	603	CLA	C2B-C1B-NB	4.76	115.27	110.33
23	B	616	CLA	C2C-C1C-NC	4.76	114.98	109.98
23	b	616	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	b	610	CLA	C3D-C4D-ND	4.75	117.72	109.99
23	c	513	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	D	405	CLA	C3D-C4D-ND	4.75	117.71	109.99
23	C	508	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
23	B	617	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	c	507	CLA	CHD-C1D-ND	-4.75	118.12	124.80
23	b	608	CLA	O2D-CGD-CBD	4.74	119.52	111.23
23	b	611	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	C	512	CLA	C2B-C1B-NB	4.74	115.24	110.33
23	a	406	CLA	C3D-C4D-ND	4.73	117.68	109.99
23	C	511	CLA	CHD-C4C-C3C	-4.73	117.88	124.77
23	c	501	CLA	C2C-C1C-NC	4.73	114.95	109.98
23	b	616	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
23	C	511	CLA	C2B-C1B-NB	4.73	115.23	110.33
23	B	609	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	b	609	CLA	C3D-C4D-ND	4.72	117.66	109.99
23	B	615	CLA	C2B-C1B-NB	4.72	115.22	110.33
25	Y	101	BCR	C16-C17-C18	-4.72	120.66	127.28
23	c	509	CLA	C2C-C1C-NC	4.72	114.94	109.98
23	A	407	CLA	CHD-C1D-ND	-4.72	118.16	124.80
23	b	615	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	B	604	CLA	C3D-C4D-ND	4.71	117.65	109.99
23	c	511	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
23	C	512	CLA	C3D-C4D-ND	4.71	117.64	109.99
23	B	602	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
23	C	502	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
23	d	402	CLA	C3D-C4D-ND	4.71	117.64	109.99
23	B	608	CLA	C2C-C1C-NC	4.71	114.92	109.98
23	A	404	CLA	C3B-C2B-C1B	-4.71	101.62	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C2B-C1B-NB	4.70	115.20	110.33
23	D	405	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
23	C	509	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	B	607	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	A	405	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	D	401	CLA	CHD-C1D-ND	-4.70	118.19	124.80
23	b	606	CLA	C2B-C1B-NB	4.70	115.19	110.33
23	b	606	CLA	C3B-C2B-C1B	-4.70	101.64	107.17
23	c	504	CLA	C3D-C4D-ND	4.69	117.62	109.99
25	t	101	BCR	C33-C5-C6	-4.69	119.36	124.48
23	B	610	CLA	C3D-C4D-ND	4.69	117.62	109.99
23	D	405	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	b	604	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	d	402	CLA	O2D-CGD-CBD	4.68	119.42	111.23
23	C	507	CLA	O2D-CGD-CBD	4.68	119.41	111.23
23	b	604	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	B	605	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
23	D	401	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
23	b	611	CLA	C3B-C4B-NB	4.67	114.70	110.53
23	b	613	CLA	C2B-C1B-NB	4.67	115.17	110.33
23	b	614	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
38	e	103	HEM	CHC-C4B-NB	4.67	129.44	124.42
25	C	515	BCR	C15-C14-C13	-4.67	120.73	127.28
23	C	509	CLA	C3C-C4C-NC	4.66	116.40	110.43
23	c	506	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	b	602	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	b	603	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
23	a	406	CLA	C2B-C1B-NB	4.66	115.15	110.33
23	d	403	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	b	603	CLA	C2C-C1C-NC	4.65	114.86	109.98
23	B	603	CLA	C3D-C4D-ND	4.64	117.54	109.99
23	C	510	CLA	C3D-C4D-ND	4.64	117.52	109.99
23	B	614	CLA	C2B-C1B-NB	4.64	115.13	110.33
23	C	511	CLA	C3D-C4D-ND	4.63	117.52	109.99
23	b	603	CLA	C3D-C4D-ND	4.63	117.51	109.99
23	B	607	CLA	CHD-C1D-ND	-4.63	118.29	124.80
23	b	610	CLA	C2B-C1B-NB	4.62	115.12	110.33
23	A	404	CLA	C2B-C1B-NB	4.62	115.12	110.33
23	B	615	CLA	C3D-C4D-ND	4.62	117.50	109.99
23	C	510	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	B	615	CLA	C4A-NA-C1A	-4.62	104.57	106.68
23	C	505	CLA	C2B-C1B-NB	4.62	115.11	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	CLA	O2D-CGD-CBD	4.62	119.30	111.23
23	c	513	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
23	B	610	CLA	C2C-C1C-NC	4.61	114.83	109.98
23	C	507	CLA	C2C-C1C-NC	4.61	114.82	109.98
23	a	405	CLA	C3D-C4D-ND	4.61	117.48	109.99
23	a	405	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	B	606	CLA	C3D-C4D-ND	4.60	117.47	109.99
23	C	503	CLA	C3B-C2B-C1B	-4.60	101.74	107.17
23	c	508	CLA	C4A-NA-C1A	-4.60	104.58	106.68
23	B	613	CLA	C2C-C1C-NC	4.60	114.81	109.98
40	v	201	HEC	CHC-C4B-NB	4.60	129.46	124.45
23	D	401	CLA	O2D-CGD-CBD	4.59	119.26	111.23
23	c	505	CLA	C2C-C1C-NC	4.59	114.81	109.98
23	B	602	CLA	C2B-C1B-NB	4.59	115.09	110.33
23	B	606	CLA	CMB-C2B-C1B	4.59	132.41	125.42
23	b	604	CLA	C2C-C1C-NC	4.58	114.80	109.98
23	B	609	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	C	514	CLA	CHD-C1D-ND	-4.58	118.35	124.80
23	b	611	CLA	O2D-CGD-O1D	-4.58	114.93	123.85
23	C	507	CLA	CHD-C1D-ND	-4.58	118.36	124.80
23	D	401	CLA	C4A-NA-C1A	-4.58	104.59	106.68
23	c	510	CLA	C2C-C1C-NC	4.58	114.79	109.98
23	c	513	CLA	C2C-C1C-NC	4.58	114.79	109.98
23	B	613	CLA	C4A-NA-C1A	-4.58	104.59	106.68
23	c	513	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	D	404	CLA	C3D-C4D-ND	4.57	117.42	109.99
36	B	630	HTG	C1'-S1-C1	4.57	110.32	100.45
23	B	604	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
37	C	517	DGD	O2G-C1B-C2B	4.57	121.37	111.48
23	c	508	CLA	C2B-C1B-NB	4.57	115.06	110.33
36	C	523	HTG	C1'-S1-C1	4.57	110.31	100.45
23	c	501	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	B	609	CLA	C2C-C1C-NC	4.56	114.78	109.98
23	c	512	CLA	C2C-C1C-NC	4.56	114.77	109.98
23	C	505	CLA	C1C-C2C-C3C	-4.56	102.18	106.98
23	B	607	CLA	C3B-C2B-C1B	-4.56	101.79	107.17
23	B	613	CLA	C3B-C2B-C1B	-4.56	101.80	107.17
23	C	508	CLA	C2C-C1C-NC	4.56	114.77	109.98
23	a	409	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	C	505	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	B	605	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.55	99.62	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C3D-C4D-ND	4.55	117.38	109.99
23	b	610	CLA	C2C-C1C-NC	4.55	114.76	109.98
23	B	609	CLA	O2D-CGD-CBD	4.55	119.18	111.23
23	C	503	CLA	C3D-C4D-ND	4.55	117.38	109.99
23	B	605	CLA	C2C-C1C-NC	4.54	114.75	109.98
23	B	612	CLA	C2C-C1C-NC	4.54	114.75	109.98
23	B	616	CLA	CMB-C2B-C1B	4.54	132.33	125.42
23	b	608	CLA	C3D-C4D-ND	4.54	117.36	109.99
23	C	503	CLA	C2C-C1C-NC	4.53	114.75	109.98
23	C	509	CLA	C2B-C1B-NB	4.53	115.02	110.33
23	c	512	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	a	409	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	B	617	CLA	C2B-C1B-NB	4.52	115.02	110.33
23	D	401	CLA	C2B-C1B-NB	4.52	115.02	110.33
23	b	608	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	B	606	CLA	C2B-C1B-NB	4.52	115.01	110.33
23	C	513	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
25	T	101	BCR	C33-C5-C6	-4.51	119.56	124.48
23	C	514	CLA	C2B-C1B-NB	4.51	115.01	110.33
23	a	406	CLA	CHD-C1D-ND	-4.51	118.45	124.80
23	B	611	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
26	a	411	SQD	O47-C7-C8	4.51	121.23	111.48
23	b	601	CLA	C3D-C4D-ND	4.50	117.31	109.99
25	c	514	BCR	C20-C21-C22	-4.50	120.96	127.28
23	c	507	CLA	C2B-C1B-NB	4.50	115.00	110.33
23	a	405	CLA	C3B-C4B-NB	4.50	114.55	110.53
23	A	407	CLA	C3D-C4D-ND	4.50	117.30	109.99
40	V	202	HEC	CBB-CAB-C3B	-4.49	118.45	127.43
23	B	609	CLA	C3D-C4D-ND	4.49	117.29	109.99
23	a	404	CLA	C1C-C2C-C3C	-4.49	102.26	106.98
23	c	501	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	b	602	CLA	C2C-C1C-NC	4.49	114.70	109.98
23	D	404	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	B	602	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
23	b	601	CLA	C2C-C1C-NC	4.49	114.69	109.98
23	c	505	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	C	509	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	C	502	CLA	C2B-C1B-NB	4.48	114.98	110.33
25	b	617	BCR	C7-C8-C9	-4.48	119.60	126.23
23	c	510	CLA	C2B-C1B-NB	4.48	114.97	110.33
23	c	509	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	b	615	CLA	CHD-C1D-ND	-4.48	118.50	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C2B-C1B-NB	4.48	114.97	110.33
23	b	605	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
23	C	502	CLA	C1D-CHD-C4C	-4.48	116.51	126.02
23	b	602	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	b	613	CLA	C2C-C1C-NC	4.47	114.68	109.98
23	c	511	CLA	C3D-C4D-ND	4.47	117.25	109.99
23	d	402	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
23	B	604	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	c	507	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	c	503	CLA	C3D-C4D-ND	4.47	117.25	109.99
23	B	613	CLA	C3D-C4D-ND	4.46	117.24	109.99
23	B	607	CLA	C2C-C1C-NC	4.46	114.67	109.98
23	C	502	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
23	B	610	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	a	409	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	b	615	CLA	O2D-CGD-CBD	4.45	119.00	111.23
23	B	616	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	b	606	CLA	C2C-C1C-NC	4.44	114.65	109.98
23	B	608	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	b	612	CLA	C2C-C1C-NC	4.43	114.64	109.98
23	a	406	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
23	B	605	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	c	501	CLA	C3D-C4D-ND	4.43	117.18	109.99
23	B	616	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
23	c	511	CLA	O2D-CGD-CBD	4.42	118.97	111.23
23	B	605	CLA	C3C-C4C-NC	4.42	116.09	110.43
23	b	612	CLA	C3D-C4D-ND	4.42	117.17	109.99
25	d	404	BCR	C7-C8-C9	-4.42	119.70	126.23
23	c	503	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
26	B	621	SQD	O47-C7-C8	4.41	121.03	111.48
23	B	602	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	C	508	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	b	603	CLA	C1D-CHD-C4C	-4.41	116.65	126.02
23	B	612	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
23	b	606	CLA	C3D-C4D-ND	4.41	117.15	109.99
23	d	403	CLA	CHD-C1D-ND	-4.41	118.60	124.80
23	B	613	CLA	C3C-C4C-NC	4.41	116.07	110.43
23	D	405	CLA	C4A-NA-C1A	-4.41	104.67	106.68
23	C	512	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
23	b	616	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	c	502	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	B	615	CLA	CHD-C1D-ND	-4.40	118.61	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C2C-C1C-NC	4.40	114.60	109.98
23	C	505	CLA	C3B-C4B-NB	4.40	114.45	110.53
23	b	605	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	A	404	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
23	B	614	CLA	C4A-NA-C1A	-4.39	104.68	106.68
23	a	404	CLA	C3D-C4D-ND	4.39	117.12	109.99
23	a	409	CLA	C2C-C1C-NC	4.39	114.59	109.98
23	C	503	CLA	C3D-C2D-C1D	-4.39	99.85	105.83
23	c	502	CLA	C3D-C2D-C1D	-4.39	99.85	105.83
23	c	509	CLA	C3D-C4D-ND	4.38	117.11	109.99
23	A	405	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
23	c	505	CLA	C3C-C4C-NC	4.38	116.04	110.43
23	B	604	CLA	C2C-C1C-NC	4.38	114.58	109.98
23	b	605	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	B	612	CLA	C4A-NA-C1A	-4.37	104.69	106.68
23	b	614	CLA	C2B-C1B-NB	4.37	114.86	110.33
25	B	618	BCR	C7-C8-C9	-4.36	119.78	126.23
23	B	608	CLA	C3D-C4D-ND	4.36	117.07	109.99
23	C	507	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
23	b	609	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
23	C	514	CLA	O2D-CGD-CBD	4.35	118.84	111.23
38	E	103	HEM	CHC-C4B-NB	4.35	129.11	124.42
24	D	402	PHO	C1-C2-C3	-4.35	119.06	126.20
25	B	619	BCR	C15-C14-C13	-4.35	121.17	127.28
23	B	616	CLA	C1D-CHD-C4C	-4.35	116.78	126.02
23	c	502	CLA	C1C-C2C-C3C	-4.35	102.41	106.98
23	b	607	CLA	C3C-C4C-NC	4.34	115.99	110.43
23	C	506	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
23	c	507	CLA	C3D-C4D-ND	4.34	117.04	109.99
23	C	510	CLA	CHD-C1D-ND	-4.34	118.70	124.80
23	b	609	CLA	CHD-C1D-ND	-4.34	118.70	124.80
23	c	508	CLA	C3D-C4D-ND	4.33	117.03	109.99
23	B	611	CLA	C3D-C4D-ND	4.33	117.03	109.99
23	C	512	CLA	C2C-C1C-NC	4.33	114.53	109.98
23	b	602	CLA	CHD-C1D-ND	-4.33	118.71	124.80
23	c	504	CLA	CHD-C1D-ND	-4.33	118.71	124.80
23	b	608	CLA	C2C-C1C-NC	4.32	114.52	109.98
29	a	415	PL9	C32-C33-C34	-4.32	117.73	127.62
23	B	613	CLA	C1-C2-C3	-4.32	119.12	126.20
23	C	507	CLA	C3D-C4D-ND	4.32	117.01	109.99
23	c	511	CLA	CHD-C1D-ND	-4.32	118.72	124.80
25	t	101	BCR	C15-C16-C17	-4.32	114.69	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	CLA	C3D-C4D-ND	4.31	117.00	109.99
23	b	616	CLA	C1D-CHD-C4C	-4.31	116.86	126.02
23	A	407	CLA	C2C-C1C-NC	4.31	114.51	109.98
23	c	510	CLA	C3D-C4D-ND	4.31	116.99	109.99
29	d	405	PL9	C10-C9-C11	4.31	122.71	115.23
26	f	101	SQD	C1-O5-C5	4.31	122.13	113.72
23	B	606	CLA	C1D-CHD-C4C	-4.31	116.86	126.02
23	B	616	CLA	O2D-CGD-CBD	4.31	118.76	111.23
23	D	404	CLA	C1-C2-C3	-4.30	119.15	126.20
23	B	616	CLA	C3D-C4D-ND	4.30	116.97	109.99
23	B	610	CLA	CHD-C1D-ND	-4.30	118.75	124.80
23	b	614	CLA	C3D-C4D-ND	4.29	116.97	109.99
23	a	404	CLA	C1D-CHD-C4C	-4.29	116.90	126.02
23	C	510	CLA	C2B-C1B-NB	4.29	114.77	110.33
23	b	613	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	B	611	CLA	C2B-C1B-NB	4.29	114.77	110.33
23	C	506	CLA	C2B-C1B-NB	4.28	114.77	110.33
23	B	610	CLA	C3C-C4C-NC	4.28	115.92	110.43
23	b	615	CLA	C2B-C1B-NB	4.28	114.77	110.33
23	b	610	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
23	A	405	CLA	C2C-C1C-NC	4.28	114.48	109.98
23	b	606	CLA	O2D-CGD-O1D	-4.28	115.52	123.85
23	B	608	CLA	CHD-C1D-ND	-4.27	118.79	124.80
23	c	502	CLA	CHD-C1D-ND	-4.27	118.79	124.80
23	B	613	CLA	C2B-C1B-NB	4.27	114.76	110.33
23	c	505	CLA	C4A-NA-C1A	-4.27	104.73	106.68
23	D	404	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
23	D	401	CLA	C3B-C2B-C1B	-4.26	102.14	107.17
23	C	507	CLA	C2B-C1B-NB	4.26	114.75	110.33
23	b	601	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	B	602	CLA	CHD-C1D-ND	-4.26	118.81	124.80
31	E	101	LHG	O7-C7-C8	4.26	120.70	111.48
26	A	409	SQD	C1-O5-C5	-4.26	105.41	113.72
23	a	405	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	b	603	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	a	406	CLA	C2C-C1C-NC	4.25	114.45	109.98
23	c	506	CLA	C3D-C4D-ND	4.25	116.90	109.99
23	c	511	CLA	C1-C2-C3	-4.25	119.24	126.20
23	C	504	CLA	CHD-C1D-ND	-4.24	118.83	124.80
23	C	511	CLA	C3B-C4B-NB	4.24	114.32	110.53
23	B	613	CLA	CMD-C2D-C1D	4.24	132.19	124.73
23	c	508	CLA	C1C-C2C-C3C	-4.23	102.53	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C4A-NA-C1A	-4.23	104.75	106.68
23	c	502	CLA	C4A-NA-C1A	-4.23	104.75	106.68
23	C	513	CLA	C3D-C4D-ND	4.23	116.87	109.99
23	c	505	CLA	C3B-C2B-C1B	-4.23	102.18	107.17
23	b	611	CLA	C1C-C2C-C3C	-4.23	102.53	106.98
23	b	615	CLA	C3B-C2B-C1B	-4.23	102.18	107.17
23	b	614	CLA	C2C-C1C-NC	4.23	114.42	109.98
23	B	606	CLA	C2C-C1C-NC	4.23	114.42	109.98
23	C	505	CLA	C3D-C4D-ND	4.23	116.86	109.99
23	B	614	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
23	b	607	CLA	C3B-C4B-NB	4.22	114.30	110.53
23	d	402	CLA	C2B-C1B-NB	4.22	114.70	110.33
23	b	615	CLA	C3D-C4D-ND	4.22	116.84	109.99
23	A	405	CLA	CHD-C1D-ND	-4.22	118.87	124.80
23	b	611	CLA	C3B-C2B-C1B	-4.22	102.20	107.17
23	c	501	CLA	CHD-C1D-ND	-4.21	118.87	124.80
23	C	509	CLA	CMD-C2D-C1D	4.21	132.15	124.73
26	A	409	SQD	C1-C2-C3	-4.21	101.15	110.01
23	C	504	CLA	C3D-C4D-ND	4.21	116.83	109.99
23	b	607	CLA	C3D-C4D-ND	4.21	116.83	109.99
34	J	101	LMG	O7-C10-C11	4.20	120.58	111.48
23	C	512	CLA	CHD-C1D-ND	-4.20	118.89	124.80
34	Z	101	LMG	O7-C10-C11	4.20	120.57	111.48
23	B	611	CLA	C3C-C4C-NC	4.20	115.81	110.43
23	B	609	CLA	C1D-CHD-C4C	-4.19	117.10	126.02
23	b	609	CLA	C1-C2-C3	-4.19	119.33	126.20
23	B	603	CLA	CHD-C1D-ND	-4.19	118.90	124.80
40	v	201	HEC	CBB-CAB-C3B	-4.19	119.06	127.43
23	C	502	CLA	C3D-C4D-ND	4.19	116.80	109.99
23	b	604	CLA	C2B-C1B-NB	4.19	114.67	110.33
23	B	612	CLA	C1C-C2C-C3C	-4.19	102.58	106.98
26	D	413	SQD	O6-C1-C2	4.19	114.63	108.27
23	C	506	CLA	C3D-C4D-ND	4.18	116.78	109.99
23	B	610	CLA	O2D-CGD-CBD	4.18	118.53	111.23
23	c	504	CLA	C3B-C4B-NB	4.18	114.26	110.53
23	C	511	CLA	CHD-C1D-ND	-4.18	118.93	124.80
23	c	501	CLA	C2B-C1B-NB	4.18	114.66	110.33
23	c	509	CLA	C2B-C1B-NB	4.17	114.66	110.33
23	B	609	CLA	C3C-C4C-NC	4.17	115.78	110.43
23	C	509	CLA	C3B-C4B-NB	4.17	114.26	110.53
25	b	619	BCR	C7-C8-C9	-4.17	120.07	126.23
23	b	612	CLA	C1-C2-C3	-4.17	119.37	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C3C-C4C-NC	4.16	115.76	110.43
23	b	611	CLA	C1-C2-C3	-4.16	119.38	126.20
25	T	101	BCR	C11-C10-C9	-4.16	121.44	127.28
23	b	608	CLA	CHD-C1D-ND	-4.16	118.95	124.80
23	c	503	CLA	CHD-C1D-ND	-4.15	118.96	124.80
37	c	516	DGD	O2G-C1B-C2B	4.15	120.47	111.48
23	c	507	CLA	C2C-C1C-NC	4.15	114.34	109.98
23	A	404	CLA	C3D-C4D-ND	4.15	116.74	109.99
23	D	401	CLA	C1C-C2C-C3C	-4.15	102.62	106.98
23	b	606	CLA	CHD-C1D-ND	-4.15	118.96	124.80
31	D	409	LHG	O7-C7-C8	4.15	120.45	111.48
23	b	607	CLA	C4A-NA-C1A	-4.14	104.79	106.68
23	B	611	CLA	C2C-C1C-NC	4.14	114.33	109.98
23	C	508	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	D	404	CLA	C3C-C4C-NC	4.14	115.74	110.43
23	c	506	CLA	CHD-C1D-ND	-4.14	118.97	124.80
23	B	617	CLA	C1D-CHD-C4C	-4.14	117.22	126.02
23	b	610	CLA	C1-C2-C3	-4.14	119.42	126.20
23	C	507	CLA	C3B-C2B-C1B	-4.14	102.30	107.17
23	b	601	CLA	CHD-C1D-ND	-4.13	118.98	124.80
23	b	609	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
23	A	404	CLA	O2A-CGA-CBA	4.13	124.43	111.83
23	C	502	CLA	O2D-CGD-O1D	-4.13	115.81	123.85
23	B	613	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
23	c	512	CLA	C3D-C4D-ND	4.13	116.69	109.99
23	b	614	CLA	CHD-C1D-ND	-4.12	119.00	124.80
23	b	613	CLA	C3C-C4C-NC	4.12	115.71	110.43
23	C	506	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
23	B	604	CLA	C2B-C1B-NB	4.12	114.60	110.33
23	b	611	CLA	C3D-C4D-ND	4.12	116.68	109.99
23	B	608	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
23	C	503	CLA	C2B-C1B-NB	4.12	114.59	110.33
23	b	607	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
23	C	505	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
23	B	602	CLA	C4A-NA-C1A	-4.10	104.81	106.68
23	c	506	CLA	C4A-NA-C1A	-4.10	104.81	106.68
23	c	503	CLA	C1D-CHD-C4C	-4.10	117.31	126.02
23	B	616	CLA	C2B-C1B-NB	4.10	114.58	110.33
23	A	404	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
23	B	608	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
23	a	405	CLA	O2D-CGD-CBD	4.09	118.38	111.23
23	B	615	CLA	C1C-C2C-C3C	-4.09	102.68	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
23	b	606	CLA	C1D-CHD-C4C	-4.08	117.34	126.02
23	b	609	CLA	C2B-C1B-NB	4.08	114.56	110.33
23	C	512	CLA	O2D-CGD-CBD	4.08	118.37	111.23
23	B	606	CLA	CHD-C1D-ND	-4.08	119.06	124.80
23	B	605	CLA	C4A-NA-C1A	-4.08	104.82	106.68
23	B	612	CLA	C3D-C4D-ND	4.08	116.61	109.99
23	b	609	CLA	C2C-C1C-NC	4.08	114.26	109.98
23	c	506	CLA	O2D-CGD-CBD	4.07	118.35	111.23
29	D	407	PL9	C42-C43-C44	-4.07	118.30	127.62
23	b	612	CLA	C3D-C2D-C1D	-4.07	100.27	105.83
23	C	514	CLA	C2C-C1C-NC	4.07	114.25	109.98
23	c	510	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
23	c	510	CLA	CHD-C1D-ND	-4.06	119.08	124.80
29	a	415	PL9	C27-C28-C29	-4.06	118.32	127.62
23	C	513	CLA	C1D-CHD-C4C	-4.06	117.38	126.02
23	D	405	CLA	CMB-C2B-C1B	4.06	131.60	125.42
23	a	406	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
23	B	605	CLA	C3D-C4D-ND	4.05	116.58	109.99
23	d	402	CLA	C3D-C2D-C1D	-4.05	100.30	105.83
23	D	405	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	D	404	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	C	511	CLA	C3D-C2D-C1D	-4.05	100.31	105.83
23	b	605	CLA	C1D-CHD-C4C	-4.04	117.42	126.02
23	B	614	CLA	C3D-C4D-ND	4.04	116.56	109.99
23	C	510	CLA	C2C-C1C-NC	4.04	114.23	109.98
23	B	604	CLA	C1D-CHD-C4C	-4.04	117.43	126.02
23	c	510	CLA	O2D-CGD-CBD	4.04	118.29	111.23
23	B	611	CLA	C1-C2-C3	-4.04	119.58	126.20
23	C	504	CLA	O2D-CGD-CBD	4.04	118.29	111.23
23	c	511	CLA	C2B-C1B-NB	4.04	114.51	110.33
23	C	508	CLA	CHD-C1D-ND	-4.04	119.12	124.80
23	C	513	CLA	C2C-C1C-NC	4.04	114.22	109.98
23	B	609	CLA	C2B-C1B-NB	4.03	114.51	110.33
23	b	603	CLA	CHD-C1D-ND	-4.03	119.13	124.80
23	b	604	CLA	C3C-C4C-NC	4.03	115.59	110.43
23	B	617	CLA	C3C-C4C-NC	4.03	115.59	110.43
23	D	405	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
23	B	603	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
23	B	614	CLA	C1-C2-C3	-4.02	119.61	126.20
23	d	403	CLA	O2D-CGD-O1D	-4.02	116.03	123.85
23	C	506	CLA	C3C-C4C-NC	4.01	115.57	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	C3C-C4C-NC	4.01	115.57	110.43
23	B	617	CLA	C2C-C1C-NC	4.00	114.19	109.98
34	c	519	LMG	O7-C10-C11	3.99	120.12	111.48
23	b	603	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
23	b	602	CLA	C1D-CHD-C4C	-3.99	117.53	126.02
23	b	615	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
23	B	612	CLA	C3C-C4C-NC	3.99	115.54	110.43
25	b	619	BCR	C15-C14-C13	-3.99	121.69	127.28
25	C	515	BCR	C16-C17-C18	-3.98	121.70	127.28
23	c	505	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
25	d	404	BCR	C38-C26-C25	-3.98	120.14	124.48
23	B	606	CLA	C3C-C4C-NC	3.97	115.52	110.43
23	B	604	CLA	CHD-C1D-ND	-3.97	119.22	124.80
23	c	512	CLA	C1D-CHD-C4C	-3.97	117.59	126.02
25	k	101	BCR	C24-C23-C22	-3.97	120.37	126.23
23	A	407	CLA	O2D-CGD-CBD	3.97	118.16	111.23
23	C	502	CLA	C1-C2-C3	-3.96	119.70	126.20
23	C	508	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
23	C	502	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
34	c	520	LMG	O6-C5-C4	3.96	116.84	109.70
23	C	512	CLA	CAC-C3C-C4C	3.96	129.94	124.79
23	C	504	CLA	C1D-CHD-C4C	-3.95	117.61	126.02
23	B	612	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
23	C	510	CLA	C3C-C4C-NC	3.95	115.49	110.43
25	t	101	BCR	C35-C13-C12	3.95	124.12	118.09
23	A	405	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
23	C	506	CLA	C1D-CHD-C4C	-3.95	117.63	126.02
23	C	508	CLA	C3C-C4C-NC	3.95	115.49	110.43
25	c	514	BCR	C16-C17-C18	-3.95	121.74	127.28
23	c	512	CLA	C1-C2-C3	-3.95	119.73	126.20
25	C	527	BCR	C7-C8-C9	-3.94	120.40	126.23
23	b	610	CLA	C1D-CHD-C4C	-3.94	117.64	126.02
25	H	101	BCR	C7-C8-C9	-3.94	120.40	126.23
23	b	607	CLA	CHD-C1D-ND	-3.94	119.26	124.80
25	k	101	BCR	C11-C10-C9	-3.94	121.75	127.28
23	c	506	CLA	C3B-C4B-NB	3.94	114.04	110.53
23	B	611	CLA	C1D-CHD-C4C	-3.94	117.65	126.02
23	c	509	CLA	CHD-C1D-ND	-3.93	119.27	124.80
23	B	616	CLA	C1C-C2C-C3C	-3.93	102.84	106.98
23	C	509	CLA	C4C-C3C-C2C	-3.93	101.17	106.89
34	C	521	LMG	O7-C10-C11	3.93	119.98	111.48
23	c	506	CLA	C3B-C2B-C1B	-3.93	102.54	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	201	HEC	CBC-CAC-C3C	-3.93	119.59	127.43
23	b	605	CLA	C4A-NA-C1A	-3.92	104.89	106.68
23	b	605	CLA	CHD-C1D-ND	-3.92	119.29	124.80
31	L	101	LHG	O7-C7-C8	3.91	119.95	111.48
23	b	615	CLA	C3B-C4B-NB	3.91	114.02	110.53
23	B	608	CLA	C2B-C1B-NB	3.91	114.38	110.33
23	b	604	CLA	CMB-C2B-C1B	3.91	131.37	125.42
23	a	405	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
23	b	614	CLA	C1-C2-C3	-3.90	119.80	126.20
23	A	404	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	b	610	CLA	CHD-C1D-ND	-3.90	119.31	124.80
31	b	630	LHG	O7-C7-C8	3.90	119.92	111.48
23	b	614	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
23	c	510	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
23	b	615	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
36	c	522	HTG	C1'-S1-C1	3.89	108.85	100.45
23	C	513	CLA	CHD-C1D-ND	-3.88	119.34	124.80
36	b	622	HTG	C1'-S1-C1	3.88	108.83	100.45
25	d	404	BCR	C33-C5-C6	-3.88	120.25	124.48
23	a	404	CLA	CHD-C1D-ND	-3.88	119.35	124.80
23	B	612	CLA	CHD-C1D-ND	-3.87	119.35	124.80
23	c	504	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
23	b	616	CLA	C3D-C4D-ND	3.87	116.28	109.99
23	b	601	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
25	D	406	BCR	C38-C26-C25	-3.87	120.27	124.48
23	c	505	CLA	CMB-C2B-C1B	3.86	131.30	125.42
23	B	612	CLA	C2B-C1B-NB	3.86	114.33	110.33
25	H	101	BCR	C16-C17-C18	-3.86	121.86	127.28
23	B	609	CLA	CHD-C1D-ND	-3.86	119.37	124.80
35	D	403	LMT	O5'-C5'-C4'	3.86	117.70	109.72
23	C	503	CLA	CHD-C1D-ND	-3.86	119.38	124.80
23	C	509	CLA	O2D-CGD-O1D	-3.85	116.35	123.85
36	h	101	HTG	C1'-S1-C1	3.85	108.76	100.45
23	B	611	CLA	CHD-C1D-ND	-3.85	119.39	124.80
23	C	507	CLA	C1-C2-C3	-3.85	119.90	126.20
23	b	604	CLA	C3D-C4D-ND	3.84	116.24	109.99
38	E	103	HEM	CAD-CBD-CGD	3.84	123.86	113.67
23	b	611	CLA	C3C-C4C-NC	3.84	115.35	110.43
25	b	617	BCR	C33-C5-C6	-3.84	120.29	124.48
23	b	602	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
23	C	507	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
23	B	615	CLA	O2D-CGD-O1D	-3.84	116.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CHD-C1D-ND	-3.84	119.40	124.80
23	B	613	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	C	514	CLA	C3C-C4C-NC	3.84	115.34	110.43
23	b	607	CLA	C1C-C2C-C3C	-3.84	102.95	106.98
23	c	505	CLA	C2B-C1B-NB	3.83	114.30	110.33
23	b	607	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
25	k	101	BCR	C15-C14-C13	-3.83	121.91	127.28
23	b	612	CLA	C1D-CHD-C4C	-3.82	117.89	126.02
23	c	502	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
23	b	604	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
23	c	509	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
23	b	616	CLA	C3C-C4C-NC	3.82	115.32	110.43
23	c	510	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
25	H	101	BCR	C24-C23-C22	-3.81	120.60	126.23
23	b	611	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
23	b	612	CLA	CHD-C1D-ND	-3.81	119.44	124.80
23	a	405	CLA	CBC-CAC-C3C	-3.81	102.10	112.42
23	d	403	CLA	C2C-C1C-NC	3.81	113.98	109.98
23	C	511	CLA	C1C-C2C-C3C	-3.81	102.98	106.98
23	B	607	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
23	d	402	CLA	CHD-C1D-ND	-3.80	119.45	124.80
23	b	613	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
23	C	508	CLA	CMB-C2B-C1B	3.80	131.20	125.42
23	B	613	CLA	C3B-C4B-NB	3.80	113.92	110.53
25	A	408	BCR	C15-C14-C13	-3.80	121.95	127.28
23	A	404	CLA	C1C-C2C-C3C	-3.80	102.99	106.98
23	b	611	CLA	CHD-C1D-ND	-3.79	119.47	124.80
25	B	619	BCR	C29-C30-C25	3.79	115.94	110.44
23	a	409	CLA	CHD-C1D-ND	-3.79	119.47	124.80
23	d	402	CLA	C3C-C4C-NC	3.79	115.28	110.43
23	a	409	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
25	C	516	BCR	C11-C10-C9	-3.78	121.98	127.28
23	c	513	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
23	b	605	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
23	C	503	CLA	CMB-C2B-C1B	3.78	131.17	125.42
23	B	617	CLA	CHD-C1D-ND	-3.77	119.49	124.80
23	b	604	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
23	D	401	CLA	C2C-C1C-NC	3.77	113.94	109.98
34	a	417	LMG	O7-C10-C11	3.77	119.63	111.48
23	c	509	CLA	C3C-C4C-NC	3.77	115.26	110.43
23	B	615	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
35	M	101	LMT	O1'-C1'-C2'	3.77	113.99	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	C3B-C4B-NB	3.76	113.89	110.53
23	C	505	CLA	CHD-C1D-ND	-3.76	119.51	124.80
23	b	616	CLA	C3B-C4B-NB	3.76	113.89	110.53
23	C	514	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
23	c	511	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
23	B	603	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
23	B	610	CLA	C3B-C2B-C1B	-3.75	102.74	107.17
23	c	502	CLA	C1-C2-C3	-3.75	120.05	126.20
23	c	501	CLA	O2D-CGD-O1D	-3.75	116.54	123.85
23	A	407	CLA	C4-C3-C5	3.75	121.74	115.23
23	B	605	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
23	c	512	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
23	C	511	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
23	c	513	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
23	D	401	CLA	CHD-C4C-NC	3.74	130.03	124.23
23	c	502	CLA	C1D-CHD-C4C	-3.74	118.07	126.02
23	c	503	CLA	CAC-C3C-C4C	3.74	129.66	124.79
23	B	607	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
23	b	614	CLA	C3C-C4C-NC	3.74	115.22	110.43
23	a	406	CLA	C1-C2-C3	-3.74	120.07	126.20
23	b	608	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
23	B	616	CLA	CHD-C1D-ND	-3.73	119.55	124.80
23	C	512	CLA	C3B-C4B-NB	3.73	113.86	110.53
25	t	101	BCR	C11-C10-C9	-3.73	122.04	127.28
25	b	619	BCR	C10-C11-C12	-3.73	112.39	123.20
23	C	505	CLA	C3C-C4C-NC	3.73	115.21	110.43
23	C	509	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
23	c	501	CLA	CAC-C3C-C4C	3.72	129.64	124.79
25	D	406	BCR	C33-C5-C6	-3.72	120.42	124.48
23	B	606	CLA	O2D-CGD-O1D	-3.72	116.60	123.85
23	D	401	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
23	C	502	CLA	CHD-C1D-ND	-3.72	119.57	124.80
23	c	505	CLA	CHD-C1D-ND	-3.72	119.57	124.80
35	B	623	LMT	O5'-C5'-C4'	3.71	117.40	109.72
31	A	415	LHG	O7-C7-C8	3.71	119.51	111.48
23	B	610	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
23	A	407	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
23	D	404	CLA	C2B-C1B-NB	3.71	114.17	110.33
23	b	613	CLA	CHD-C1D-ND	-3.71	119.58	124.80
23	A	404	CLA	CAA-C2A-C3A	-3.71	102.98	113.00
23	a	404	CLA	CAA-C2A-C3A	-3.70	102.99	113.00
23	c	512	CLA	C3C-C4C-NC	3.70	115.17	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	C3C-C4C-NC	3.70	115.17	110.43
23	a	409	CLA	C3B-C4B-NB	3.70	113.83	110.53
38	E	103	HEM	CHD-C4C-NC	3.70	128.48	124.45
23	C	508	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
23	d	402	CLA	C1-C2-C3	-3.70	120.14	126.20
23	C	503	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
34	B	622	LMG	O7-C10-C11	3.70	119.48	111.48
23	b	607	CLA	C2B-C1B-NB	3.69	114.16	110.33
23	C	502	CLA	C3C-C4C-NC	3.69	115.16	110.43
23	C	513	CLA	C3C-C4C-NC	3.69	115.16	110.43
23	d	403	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
23	b	603	CLA	CMB-C2B-C1B	3.69	131.03	125.42
23	c	506	CLA	C1D-CHD-C4C	-3.69	118.19	126.02
23	b	609	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
23	B	607	CLA	C3C-C4C-NC	3.68	115.15	110.43
23	c	501	CLA	C1D-CHD-C4C	-3.68	118.19	126.02
23	B	603	CLA	CAA-C2A-C3A	-3.68	103.05	113.00
29	A	413	PL9	C37-C38-C39	-3.68	119.21	127.62
23	C	508	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
23	b	612	CLA	C3C-C4C-NC	3.67	115.14	110.43
23	b	609	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	B	614	CLA	C3C-C4C-NC	3.67	115.13	110.43
23	c	505	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	b	611	CLA	C2B-C1B-NB	3.67	114.13	110.33
23	c	512	CLA	CHD-C1D-ND	-3.66	119.65	124.80
23	b	608	CLA	C1D-CHD-C4C	-3.66	118.24	126.02
34	c	520	LMG	O7-C10-C11	3.65	119.38	111.48
23	B	609	CLA	C4A-NA-C1A	-3.65	105.01	106.68
25	C	515	BCR	C33-C5-C6	-3.65	120.50	124.48
36	b	625	HTG	C1'-S1-C1	3.65	108.33	100.45
23	C	510	CLA	C1D-CHD-C4C	-3.65	118.27	126.02
24	A	406	PHO	C1A-C2A-C3A	-3.65	99.37	102.84
23	d	402	CLA	CMB-C2B-C1B	3.65	130.97	125.42
23	b	601	CLA	C1C-C2C-C3C	-3.65	103.15	106.98
37	C	518	DGD	O2G-C1B-C2B	3.64	119.36	111.48
23	B	608	CLA	C3C-C4C-NC	3.64	115.09	110.43
23	b	606	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
23	c	504	CLA	C1D-CHD-C4C	-3.63	118.29	126.02
23	B	602	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	a	408	PHO	C4-C3-C5	3.63	121.54	115.23
29	A	413	PL9	C32-C33-C34	-3.63	119.31	127.62
23	B	605	CLA	CHD-C1D-ND	-3.63	119.69	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C3B-C4B-NB	3.63	113.77	110.53
23	C	506	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
23	b	610	CLA	C3C-C4C-NC	3.63	115.08	110.43
25	c	514	BCR	C11-C10-C9	-3.63	122.19	127.28
23	B	612	CLA	CHD-C4C-NC	3.63	129.85	124.23
24	A	406	PHO	CBC-CAC-C3C	-3.63	107.68	112.87
23	B	609	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
29	a	415	PL9	C42-C43-C44	-3.62	119.33	127.62
35	C	522	LMT	C1'-O5'-C5'	3.62	120.80	113.72
25	Y	101	BCR	C15-C14-C13	-3.62	122.20	127.28
23	B	602	CLA	C1D-CHD-C4C	-3.62	118.33	126.02
23	B	615	CLA	C3B-C4B-NB	3.62	113.76	110.53
23	C	510	CLA	CMC-C2C-C1C	3.62	130.69	125.03
26	A	411	SQD	O47-C7-C8	3.62	119.30	111.48
26	f	101	SQD	O7-S-C6	3.61	112.15	106.76
23	c	506	CLA	C2B-C1B-NB	3.61	114.07	110.33
29	D	407	PL9	C10-C9-C11	3.61	121.50	115.23
23	D	405	CLA	C2C-C1C-NC	3.61	113.77	109.98
25	b	619	BCR	C24-C23-C22	-3.60	120.90	126.23
31	d	408	LHG	O7-C7-C8	3.60	119.28	111.48
37	H	102	DGD	O2G-C1B-C2B	3.60	119.28	111.48
23	c	511	CLA	C3C-C4C-NC	3.60	115.04	110.43
29	d	405	PL9	C22-C23-C24	-3.60	119.39	127.62
23	B	612	CLA	C3B-C4B-NB	3.59	113.74	110.53
23	b	604	CLA	CHD-C1D-ND	-3.59	119.75	124.80
23	b	613	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
23	c	501	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
23	B	617	CLA	C4C-C3C-C2C	-3.59	101.67	106.89
23	B	613	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
23	b	614	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
23	c	504	CLA	C3C-C4C-NC	3.59	115.02	110.43
23	c	508	CLA	C1D-CHD-C4C	-3.58	118.40	126.02
23	C	511	CLA	C4-C3-C5	3.58	121.45	115.23
23	C	506	CLA	C1-C2-C3	-3.58	120.33	126.20
36	c	522	HTG	C1-O5-C5	3.58	118.99	112.56
23	c	507	CLA	C3C-C4C-NC	3.58	115.02	110.43
23	b	606	CLA	C3C-C4C-NC	3.58	115.01	110.43
23	d	403	CLA	C3C-C4C-NC	3.58	115.01	110.43
23	b	604	CLA	C1-C2-C3	-3.58	120.34	126.20
23	c	507	CLA	C1C-C2C-C3C	-3.58	103.22	106.98
26	a	411	SQD	C1-C2-C3	-3.58	102.49	110.01
23	B	614	CLA	CHD-C1D-ND	-3.58	119.77	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	h	103	DGD	O1G-C1A-C2A	3.57	122.73	111.83
23	c	509	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
23	b	605	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
23	c	508	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
23	b	612	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
25	B	618	BCR	C16-C17-C18	-3.57	122.27	127.28
23	C	503	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
29	d	405	PL9	C25-C24-C26	3.56	121.42	115.23
23	C	506	CLA	C3B-C4B-NB	3.56	113.71	110.53
23	a	405	CLA	CAA-C2A-C3A	-3.56	103.38	113.00
25	T	101	BCR	C15-C14-C13	3.56	132.27	127.28
23	c	506	CLA	C1-C2-C3	-3.55	120.37	126.20
23	B	607	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
34	Z	101	LMG	C1-C2-C3	3.55	117.48	110.01
23	c	508	CLA	CHD-C1D-ND	-3.55	119.81	124.80
23	C	503	CLA	C3C-C4C-NC	3.55	114.97	110.43
23	b	603	CLA	C3B-C4B-NB	3.54	113.69	110.53
23	b	608	CLA	C3C-C4C-NC	3.54	114.97	110.43
23	c	501	CLA	C1-C2-C3	-3.54	120.40	126.20
23	b	603	CLA	CAA-C2A-C3A	-3.53	103.45	113.00
23	C	509	CLA	C4A-NA-C1A	-3.53	105.07	106.68
23	D	401	CLA	CMC-C2C-C1C	3.53	130.56	125.03
29	a	415	PL9	C22-C23-C24	-3.53	119.54	127.62
25	D	406	BCR	C24-C23-C22	-3.53	121.01	126.23
23	D	405	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
23	C	513	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
29	a	415	PL9	C15-C14-C16	3.53	121.35	115.23
25	b	618	BCR	C7-C8-C9	-3.53	121.02	126.23
23	C	512	CLA	C3C-C4C-NC	3.53	114.95	110.43
23	c	506	CLA	C3C-C4C-NC	3.53	114.95	110.43
23	c	513	CLA	C3C-C4C-NC	3.52	114.94	110.43
24	a	407	PHO	O2A-CGA-CBA	3.52	122.58	111.83
35	D	403	LMT	C1'-O5'-C5'	3.52	120.60	113.72
23	C	512	CLA	C1D-CHD-C4C	-3.52	118.53	126.02
23	c	509	CLA	C1-O2A-CGA	3.52	125.18	116.65
23	B	612	CLA	CMC-C2C-C1C	3.52	130.53	125.03
23	b	602	CLA	C3C-C4C-NC	3.52	114.94	110.43
23	a	406	CLA	C3B-C4B-NB	3.52	113.67	110.53
24	a	407	PHO	O2D-CGD-O1D	-3.52	117.01	123.85
25	t	101	BCR	C37-C22-C23	3.51	123.46	118.09
31	d	406	LHG	O7-C7-C8	3.51	119.08	111.48
23	c	504	CLA	C4A-NA-C1A	-3.51	105.08	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	CAC-C3C-C4C	3.51	129.36	124.79
23	b	613	CLA	O2D-CGD-CBD	3.51	117.36	111.23
23	c	503	CLA	C1-C2-C3	-3.51	120.45	126.20
23	B	614	CLA	O2D-CGD-CBD	3.50	117.36	111.23
23	b	605	CLA	C3C-C4C-NC	3.50	114.92	110.43
23	c	503	CLA	C3C-C4C-NC	3.50	114.92	110.43
23	B	602	CLA	C1-C2-C3	-3.50	120.46	126.20
23	B	611	CLA	C4C-C3C-C2C	-3.50	101.79	106.89
23	b	605	CLA	C3B-C4B-NB	3.50	113.66	110.53
23	B	602	CLA	C3C-C4C-NC	3.50	114.92	110.43
23	c	507	CLA	CMB-C2B-C1B	3.50	130.75	125.42
23	c	511	CLA	C3B-C4B-NB	3.50	113.65	110.53
23	B	605	CLA	C1D-CHD-C4C	-3.49	118.59	126.02
25	b	619	BCR	C38-C26-C25	-3.49	120.67	124.48
34	C	521	LMG	C3-C4-C5	3.49	116.57	110.23
23	C	514	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
23	c	502	CLA	C3C-C4C-NC	3.49	114.90	110.43
23	C	504	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
23	c	511	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
34	z	101	LMG	O7-C10-C11	3.49	119.03	111.48
23	B	614	CLA	C1D-CHD-C4C	-3.49	118.61	126.02
23	c	506	CLA	C4B-C3B-C2B	-3.49	102.97	107.30
23	B	615	CLA	CMB-C2B-C1B	3.48	130.72	125.42
25	a	410	BCR	C15-C14-C13	-3.48	122.39	127.28
34	C	521	LMG	O6-C5-C4	3.48	115.97	109.70
23	B	609	CLA	C1-C2-C3	-3.48	120.50	126.20
37	c	517	DGD	O2G-C1B-C2B	3.48	119.00	111.48
24	A	406	PHO	O1D-CGD-CBD	-3.48	119.45	124.72
23	b	611	CLA	CHC-C1C-C2C	-3.48	117.07	126.95
25	h	102	BCR	C16-C17-C18	-3.48	122.40	127.28
23	B	616	CLA	C3B-C4B-NB	3.47	113.63	110.53
23	b	603	CLA	C3C-C4C-NC	3.47	114.88	110.43
23	C	504	CLA	C3C-C4C-NC	3.47	114.88	110.43
23	b	612	CLA	O2A-CGA-CBA	3.47	122.42	111.83
25	T	101	BCR	C12-C13-C14	-3.47	113.55	119.01
23	b	615	CLA	CHC-C1C-C2C	-3.47	117.09	126.95
23	b	610	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
23	c	503	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
23	A	405	CLA	C1D-CHD-C4C	-3.47	118.66	126.02
23	b	611	CLA	C4B-C3B-C2B	-3.46	102.99	107.30
23	a	409	CLA	C4-C3-C5	3.46	121.24	115.23
23	c	506	CLA	C1C-C2C-C3C	-3.46	103.34	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	C3C-C4C-NC	3.46	114.86	110.43
25	t	101	BCR	C12-C13-C14	-3.45	113.58	119.01
26	a	413	SQD	O48-C23-C24	3.45	122.36	111.83
40	v	201	HEC	CHD-C4C-NC	3.45	128.21	124.45
23	B	609	CLA	C3B-C4B-NB	3.45	113.61	110.53
23	B	614	CLA	C3B-C4B-NB	3.45	113.61	110.53
23	c	505	CLA	C4C-C3C-C2C	-3.45	101.87	106.89
23	B	603	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
23	B	614	CLA	CMC-C2C-C1C	3.45	130.42	125.03
23	B	608	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
23	d	402	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
25	y	101	BCR	C15-C14-C13	-3.44	122.45	127.28
23	B	609	CLA	CHD-C4C-NC	3.44	129.56	124.23
34	j	101	LMG	O7-C10-C11	3.44	118.92	111.48
23	B	604	CLA	C3C-C4C-NC	3.44	114.83	110.43
23	a	406	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
25	B	618	BCR	C28-C27-C26	-3.44	107.93	114.06
36	b	626	HTG	C1'-S1-C1	3.44	107.87	100.45
23	b	609	CLA	C3C-C4C-NC	3.43	114.83	110.43
23	C	512	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
23	A	407	CLA	C1D-CHD-C4C	-3.43	118.72	126.02
23	b	615	CLA	CMB-C2B-C1B	3.43	130.64	125.42
26	A	409	SQD	C45-O47-C7	-3.43	109.60	117.80
23	c	511	CLA	C4A-NA-C1A	-3.42	105.12	106.68
23	B	606	CLA	C4C-C3C-C2C	-3.42	101.91	106.89
23	c	508	CLA	C3B-C4B-NB	3.42	113.58	110.53
25	C	527	BCR	C11-C10-C9	-3.42	122.48	127.28
25	a	410	BCR	C20-C21-C22	-3.42	122.48	127.28
23	B	604	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
23	a	409	CLA	C1C-C2C-C3C	-3.42	103.39	106.98
23	B	603	CLA	C3C-C4C-NC	3.42	114.81	110.43
23	b	607	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
23	B	604	CLA	O2A-CGA-O1A	-3.41	115.09	123.63
23	C	511	CLA	CMB-C2B-C1B	3.41	130.61	125.42
38	e	103	HEM	CHD-C1D-ND	3.41	128.09	124.42
23	A	404	CLA	O2D-CGD-CBD	3.41	117.19	111.23
26	A	409	SQD	C44-O6-C1	-3.41	106.49	113.80
23	B	610	CLA	C4B-C3B-C2B	-3.41	103.06	107.30
23	b	609	CLA	O2A-CGA-CBA	3.41	122.22	111.83
23	b	609	CLA	C1C-C2C-C3C	-3.41	103.40	106.98
23	A	404	CLA	O2A-CGA-O1A	-3.40	115.11	123.63
26	A	411	SQD	O8-S-C6	3.40	112.54	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C3C-C4C-NC	3.40	114.78	110.43
23	c	504	CLA	CAC-C3C-C4C	3.40	129.21	124.79
23	a	406	CLA	CHD-C4C-NC	3.39	129.50	124.23
23	b	614	CLA	C3B-C4B-NB	3.39	113.56	110.53
23	C	503	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
23	C	511	CLA	CHC-C1C-C2C	-3.39	117.32	126.95
23	B	613	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
23	A	404	CLA	CMC-C2C-C1C	3.38	130.32	125.03
23	c	510	CLA	CBC-CAC-C3C	-3.38	103.25	112.42
25	h	102	BCR	C38-C26-C25	-3.38	120.79	124.48
23	b	616	CLA	C4C-C3C-C2C	-3.38	101.97	106.89
36	B	629	HTG	C1'-S1-C1	3.38	107.74	100.45
34	C	520	LMG	O7-C10-C11	3.38	118.78	111.48
23	C	507	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
23	b	612	CLA	C3B-C4B-NB	3.38	113.54	110.53
38	E	103	HEM	C1B-NB-C4B	3.37	109.20	105.21
25	A	408	BCR	C38-C26-C25	-3.37	120.80	124.48
23	A	407	CLA	C3B-C4B-NB	3.37	113.54	110.53
25	k	101	BCR	C29-C30-C25	3.37	115.33	110.44
23	c	501	CLA	C3C-C4C-NC	3.37	114.74	110.43
23	B	615	CLA	CHC-C1C-C2C	-3.36	117.39	126.95
29	a	415	PL9	C30-C29-C31	3.36	121.06	115.23
34	m	101	LMG	O7-C10-C11	3.36	118.75	111.48
36	b	625	HTG	C1-O5-C5	3.36	118.59	112.56
38	e	103	HEM	CHD-C4C-NC	3.36	128.11	124.45
23	C	514	CLA	C1-C2-C3	-3.36	120.70	126.20
29	d	405	PL9	C20-C19-C21	3.35	121.05	115.23
23	B	610	CLA	CMB-C2B-C1B	3.35	130.52	125.42
23	b	605	CLA	CMB-C2B-C1B	3.35	130.51	125.42
23	C	513	CLA	O2A-CGA-CBA	3.35	122.03	111.83
29	A	413	PL9	C27-C28-C29	-3.34	119.97	127.62
23	b	607	CLA	C4B-C3B-C2B	-3.34	103.14	107.30
23	B	616	CLA	CED-O2D-CGD	3.34	123.49	115.92
23	c	502	CLA	CHD-C4C-NC	3.34	129.41	124.23
23	a	406	CLA	C3C-C4C-NC	3.34	114.70	110.43
23	C	509	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
23	B	610	CLA	C1D-CHD-C4C	-3.33	118.94	126.02
23	B	611	CLA	O2A-CGA-CBA	3.33	122.00	111.83
23	B	615	CLA	CBC-CAC-C3C	-3.33	103.39	112.42
29	A	413	PL9	C22-C23-C24	-3.33	120.01	127.62
23	c	503	CLA	CMB-C2B-C1B	3.33	130.49	125.42
23	B	605	CLA	O2A-CGA-CBA	3.33	121.98	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	O2A-CGA-CBA	3.32	121.97	111.83
23	D	404	CLA	O2A-CGA-CBA	3.32	121.96	111.83
23	B	617	CLA	CHD-C4C-NC	3.32	129.38	124.23
23	b	610	CLA	O2A-CGA-CBA	3.32	121.95	111.83
23	C	514	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
23	C	502	CLA	C3B-C4B-NB	3.32	113.49	110.53
23	c	512	CLA	CMA-C3A-C4A	-3.32	102.86	111.77
25	A	408	BCR	C24-C23-C22	-3.31	121.33	126.23
29	a	415	PL9	C37-C38-C39	-3.31	120.04	127.62
23	c	502	CLA	C3B-C4B-NB	3.31	113.49	110.53
34	C	501	LMG	C7-O1-C1	-3.31	106.69	113.80
23	b	615	CLA	C3C-C4C-NC	3.31	114.67	110.43
25	b	618	BCR	C38-C26-C25	-3.31	120.87	124.48
23	b	615	CLA	C11-C10-C8	-3.31	104.97	115.97
23	C	509	CLA	CHD-C1D-ND	-3.31	120.15	124.80
23	b	614	CLA	O2A-CGA-CBA	3.30	121.91	111.83
23	C	502	CLA	CBC-CAC-C3C	-3.30	103.47	112.42
25	B	620	BCR	C38-C26-C25	-3.30	120.88	124.48
23	c	512	CLA	CMB-C2B-C1B	3.30	130.44	125.42
23	B	609	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
23	B	612	CLA	C1-C2-C3	-3.29	120.80	126.20
23	C	503	CLA	C1-C2-C3	-3.29	120.81	126.20
23	b	601	CLA	C3C-C4C-NC	3.29	114.64	110.43
23	C	510	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
23	D	401	CLA	CAA-C2A-C3A	-3.29	104.12	113.00
23	D	405	CLA	CHD-C4C-NC	3.29	129.33	124.23
35	b	628	LMT	O5'-C1'-C2'	3.28	117.12	110.37
23	c	510	CLA	C3B-C4B-NB	3.28	113.46	110.53
23	b	604	CLA	CMC-C2C-C1C	3.28	130.16	125.03
23	B	603	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
23	c	509	CLA	C3B-C4B-NB	3.28	113.45	110.53
23	B	613	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
23	D	405	CLA	C4C-C3C-C2C	-3.28	102.12	106.89
23	B	608	CLA	CMC-C2C-C1C	3.28	130.15	125.03
23	a	405	CLA	C1-C2-C3	-3.27	120.83	126.20
23	C	507	CLA	C3C-C4C-NC	3.27	114.62	110.43
38	e	103	HEM	CHA-C4D-ND	3.27	128.41	124.37
23	B	604	CLA	O2A-CGA-CBA	3.27	121.80	111.83
23	C	512	CLA	C4-C3-C5	3.26	120.89	115.23
23	b	616	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
38	e	103	HEM	CAD-CBD-CGD	3.26	122.32	113.67
23	c	505	CLA	C1C-C2C-C3C	-3.26	103.55	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
23	C	504	CLA	C3B-C4B-NB	3.26	113.44	110.53
23	C	505	CLA	C4A-NA-C1A	-3.25	105.19	106.68
23	B	613	CLA	CHD-C1D-ND	-3.25	120.22	124.80
26	A	409	SQD	O48-C23-C24	3.25	121.75	111.83
23	a	404	CLA	C3C-C4C-NC	3.25	114.59	110.43
23	c	512	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
23	B	605	CLA	C3B-C4B-NB	3.25	113.43	110.53
23	b	606	CLA	C3B-C4B-NB	3.24	113.42	110.53
23	C	504	CLA	C4-C3-C5	3.24	120.85	115.23
23	c	503	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
23	c	507	CLA	C1D-CHD-C4C	-3.24	119.14	126.02
23	B	615	CLA	O2A-CGA-CBA	3.24	121.71	111.83
23	a	409	CLA	CAA-C2A-C3A	-3.24	104.25	113.00
23	b	612	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
23	C	511	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
23	c	507	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
29	A	413	PL9	C30-C29-C31	3.23	120.84	115.23
23	d	403	CLA	CHD-C4C-NC	3.23	129.24	124.23
24	A	406	PHO	C1-O2A-CGA	3.23	124.47	116.65
23	a	409	CLA	CAC-C3C-C4C	3.23	128.99	124.79
23	c	513	CLA	CAA-C2A-C3A	-3.23	104.27	113.00
34	m	101	LMG	O8-C28-C29	3.23	121.68	111.83
26	B	621	SQD	O7-S-C6	3.22	111.57	106.76
23	b	608	CLA	CHD-C4C-NC	3.22	129.23	124.23
23	C	504	CLA	CHC-C1C-C2C	-3.22	117.79	126.95
23	C	505	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
23	d	403	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
23	B	615	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
23	a	409	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
23	a	409	CLA	C3C-C4C-NC	3.22	114.55	110.43
23	a	409	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
23	c	505	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
23	A	405	CLA	C3B-C4B-NB	3.21	113.40	110.53
31	d	407	LHG	O7-C7-C8	3.21	118.43	111.48
31	e	101	LHG	O7-C7-C8	3.21	118.43	111.48
23	C	506	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
23	c	502	CLA	CBC-CAC-C3C	-3.21	103.71	112.42
23	c	510	CLA	CAC-C3C-C4C	3.21	128.97	124.79
35	b	628	LMT	C1'-O5'-C5'	3.21	119.99	113.72
26	a	411	SQD	C45-O47-C7	-3.21	110.11	117.80
23	B	617	CLA	C3B-C4B-NB	3.21	113.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CAC-C3C-C4C	3.21	128.96	124.79
23	b	603	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
23	b	613	CLA	O2A-CGA-CBA	3.21	121.61	111.83
24	D	402	PHO	C1A-C2A-C3A	-3.20	99.79	102.84
29	A	413	PL9	C42-C43-C44	-3.20	120.30	127.62
29	A	413	PL9	C15-C14-C16	3.20	120.78	115.23
23	C	514	CLA	CMB-C2B-C1B	3.20	130.29	125.42
23	a	405	CLA	CHC-C1C-C2C	-3.20	117.86	126.95
23	d	403	CLA	CMB-C2B-C1B	3.20	130.28	125.42
24	D	402	PHO	C6-C5-C3	-3.19	105.69	113.47
40	V	202	HEC	CHA-C1A-NA	3.19	127.93	124.45
23	B	617	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
23	b	615	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
23	A	405	CLA	C3C-C4C-NC	3.19	114.51	110.43
23	b	602	CLA	C1-C2-C3	-3.19	120.98	126.20
23	b	603	CLA	O2A-CGA-CBA	3.19	121.55	111.83
25	y	101	BCR	C40-C30-C25	-3.19	105.25	110.24
23	d	402	CLA	O2A-CGA-CBA	3.19	121.55	111.83
23	b	616	CLA	CHC-C1C-C2C	-3.19	117.90	126.95
23	C	506	CLA	CMB-C2B-C1B	3.18	130.27	125.42
23	a	404	CLA	O2D-CGD-CBD	3.18	116.79	111.23
23	c	509	CLA	O2A-CGA-CBA	3.18	121.53	111.83
25	t	101	BCR	C3-C4-C5	-3.18	108.39	114.06
23	b	605	CLA	CAC-C3C-C4C	3.18	128.92	124.79
23	c	510	CLA	CMC-C2C-C1C	3.18	130.00	125.03
23	C	514	CLA	C2A-C1A-CHA	-3.18	118.36	123.87
23	D	401	CLA	C3C-C4C-NC	3.18	114.50	110.43
23	d	403	CLA	CMC-C2C-C1C	3.18	130.00	125.03
23	b	609	CLA	CBC-CAC-C3C	-3.17	103.82	112.42
23	B	611	CLA	CHD-C4C-NC	3.17	129.15	124.23
23	b	608	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
23	D	404	CLA	C1D-CHD-C4C	-3.17	119.29	126.02
23	b	614	CLA	C1C-C2C-C3C	-3.17	103.65	106.98
23	b	607	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
23	B	610	CLA	C4C-C3C-C2C	-3.16	102.28	106.89
25	H	101	BCR	C38-C26-C25	-3.16	121.03	124.48
25	C	527	BCR	C24-C23-C22	-3.16	121.55	126.23
23	c	507	CLA	C1-C2-C3	-3.16	121.01	126.20
23	a	406	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
23	c	503	CLA	C3B-C4B-NB	3.16	113.35	110.53
25	Y	101	BCR	C16-C15-C14	-3.16	117.06	123.52
25	c	515	BCR	C2-C1-C6	3.16	115.02	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	CAA-C2A-C3A	-3.15	104.47	113.00
23	C	510	CLA	C4C-C3C-C2C	-3.15	102.30	106.89
23	B	602	CLA	C3B-C4B-NB	3.15	113.34	110.53
23	B	603	CLA	C3B-C4B-NB	3.15	113.34	110.53
23	D	404	CLA	C3B-C4B-NB	3.15	113.34	110.53
25	Y	101	BCR	C37-C22-C23	3.15	122.90	118.09
23	B	614	CLA	CAC-C3C-C4C	3.15	128.89	124.79
23	C	513	CLA	CHD-C4C-NC	3.15	129.11	124.23
23	C	507	CLA	CAC-C3C-C4C	3.15	128.88	124.79
34	C	520	LMG	O8-C28-C29	3.14	121.42	111.83
34	Z	101	LMG	C4-C3-C2	3.14	116.35	110.83
23	C	503	CLA	C3B-C4B-NB	3.14	113.34	110.53
23	b	601	CLA	C4-C3-C5	3.14	120.68	115.23
23	a	404	CLA	O2A-CGA-CBA	3.14	121.41	111.83
23	b	616	CLA	O2A-CGA-CBA	3.14	121.41	111.83
36	b	621	HTG	C1-O5-C5	3.14	118.19	112.56
23	D	401	CLA	C1-C2-C3	-3.14	121.06	126.20
23	b	602	CLA	CHD-C4C-NC	3.14	129.10	124.23
23	a	406	CLA	C4C-C3C-C2C	-3.14	102.33	106.89
23	c	512	CLA	C4-C3-C5	3.14	120.67	115.23
23	B	611	CLA	C1C-C2C-C3C	-3.13	103.68	106.98
31	A	415	LHG	O8-C23-O10	-3.13	115.79	123.63
23	B	606	CLA	CHD-C4C-NC	3.13	129.09	124.23
23	a	405	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	c	501	CLA	CHC-C1C-C2C	-3.13	118.05	126.95
23	B	615	CLA	C3C-C4C-NC	3.13	114.44	110.43
23	C	509	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	B	608	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
23	C	506	CLA	C4C-C3C-C2C	-3.12	102.34	106.89
23	C	511	CLA	O2A-CGA-CBA	3.12	121.36	111.83
23	B	615	CLA	C4-C3-C5	3.12	120.64	115.23
23	b	606	CLA	CHD-C4C-NC	3.12	129.07	124.23
23	b	613	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
25	a	410	BCR	C24-C23-C22	-3.12	121.62	126.23
23	C	508	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
26	a	413	SQD	O47-C7-C8	3.12	118.23	111.48
23	B	604	CLA	CAA-C2A-C3A	-3.12	104.57	113.00
23	B	613	CLA	CAC-C3C-C4C	3.12	128.84	124.79
23	b	605	CLA	CHD-C4C-NC	3.12	129.06	124.23
23	b	601	CLA	CHD-C4C-NC	3.11	129.06	124.23
34	c	519	LMG	O8-C28-C29	3.11	121.32	111.83
23	b	610	CLA	C4C-C3C-C2C	-3.11	102.36	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C11-C10-C9	-3.11	122.92	127.28
23	a	405	CLA	CHD-C4C-NC	3.11	129.05	124.23
23	D	405	CLA	CMC-C2C-C1C	3.10	129.89	125.03
25	T	101	BCR	C35-C13-C12	3.10	122.83	118.09
23	C	507	CLA	CBC-CAC-C3C	-3.10	104.00	112.42
23	B	612	CLA	C4B-C3B-C2B	-3.10	103.44	107.30
23	B	611	CLA	CAA-C2A-C3A	-3.10	104.62	113.00
23	a	405	CLA	C3C-C4C-NC	3.10	114.40	110.43
23	C	507	CLA	C4-C3-C5	3.10	120.61	115.23
25	c	515	BCR	C38-C26-C25	-3.10	121.10	124.48
23	b	616	CLA	CAC-C3C-C4C	3.10	128.82	124.79
23	b	605	CLA	O2A-CGA-CBA	3.10	121.27	111.83
23	C	509	CLA	C1-C2-C3	-3.10	121.12	126.20
23	D	404	CLA	C2A-C1A-CHA	-3.09	118.50	123.87
38	e	103	HEM	C1B-NB-C4B	3.09	108.87	105.21
23	B	607	CLA	O2A-CGA-CBA	3.09	121.26	111.83
23	B	616	CLA	CHD-C4C-NC	3.09	129.02	124.23
23	c	506	CLA	CHC-C1C-C2C	-3.09	118.17	126.95
23	B	606	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
23	B	605	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
23	c	505	CLA	C1-C2-C3	-3.08	121.14	126.20
23	B	605	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
23	c	511	CLA	CHD-C4C-NC	3.08	129.01	124.23
23	b	614	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
23	C	502	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
23	B	615	CLA	CAC-C3C-C4C	3.08	128.80	124.79
23	C	510	CLA	CAC-C3C-C4C	3.08	128.80	124.79
38	E	103	HEM	CHB-C1B-NB	3.08	128.17	124.37
23	C	508	CLA	C1-C2-C3	-3.08	121.16	126.20
23	c	511	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
29	D	407	PL9	C53-C6-C1	3.07	121.57	115.28
23	b	603	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
34	Z	101	LMG	C3-C4-C5	3.07	115.80	110.23
23	d	403	CLA	O2A-CGA-CBA	3.07	121.19	111.83
23	a	406	CLA	CAA-C2A-C3A	-3.07	104.71	113.00
23	b	605	CLA	C1-C2-C3	-3.07	121.17	126.20
23	b	610	CLA	CAA-C2A-C3A	-3.06	104.72	113.00
23	B	604	CLA	C4-C3-C5	3.06	120.54	115.23
25	B	620	BCR	C7-C8-C9	-3.06	121.70	126.23
23	b	613	CLA	CHD-C4C-NC	3.06	128.98	124.23
23	C	505	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	C	504	CLA	C4C-C3C-C2C	-3.06	102.44	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	O2A-CGA-CBA	3.06	121.16	111.83
23	c	513	CLA	CAC-C3C-C4C	3.06	128.77	124.79
23	a	404	CLA	O2A-CGA-O1A	-3.05	115.99	123.63
38	e	103	HEM	CHB-C1B-NB	3.05	128.14	124.37
23	c	506	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
23	c	509	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
23	A	405	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
40	v	201	HEC	CHA-C1A-NA	3.05	127.77	124.45
23	c	510	CLA	O2A-CGA-CBA	3.05	121.13	111.83
23	c	511	CLA	C4-C3-C5	3.05	120.52	115.23
23	b	612	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
23	B	604	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
23	B	603	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
25	d	404	BCR	C15-C14-C13	-3.05	123.01	127.28
23	C	511	CLA	C3C-C4C-NC	3.05	114.33	110.43
23	b	608	CLA	C1-C2-C3	-3.05	121.21	126.20
23	b	605	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
25	t	101	BCR	C21-C20-C19	-3.04	114.38	123.20
23	d	402	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
25	b	618	BCR	C20-C21-C22	-3.04	123.01	127.28
31	D	409	LHG	O8-C23-C24	3.04	121.10	111.83
23	a	405	CLA	C4A-NA-C1A	-3.04	105.29	106.68
23	B	616	CLA	CMC-C2C-C1C	3.04	129.78	125.03
29	A	413	PL9	C20-C19-C21	3.04	120.50	115.23
25	B	620	BCR	C15-C14-C13	-3.03	123.02	127.28
23	B	610	CLA	O2A-CGA-CBA	3.03	121.09	111.83
23	b	616	CLA	CHD-C1D-ND	-3.03	120.53	124.80
23	c	509	CLA	CMB-C2B-C1B	3.03	130.04	125.42
23	C	514	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
23	A	404	CLA	CAA-C2A-C1A	-3.03	102.05	111.97
23	B	610	CLA	C1-C2-C3	-3.03	121.24	126.20
23	C	512	CLA	CMC-C2C-C1C	3.02	129.76	125.03
23	c	512	CLA	CHD-C4C-NC	3.02	128.92	124.23
26	L	102	SQD	C3-C4-C5	3.02	115.72	110.23
29	D	407	PL9	C12-C13-C14	-3.02	120.70	127.62
23	B	608	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
23	C	504	CLA	O2A-CGA-CBA	3.02	121.05	111.83
31	D	408	LHG	O8-C23-O10	-3.02	116.07	123.63
25	h	102	BCR	C7-C8-C9	-3.02	121.77	126.23
23	B	607	CLA	C3B-C4B-NB	3.02	113.23	110.53
23	b	603	CLA	CHD-C4C-NC	3.02	128.91	124.23
23	D	405	CLA	C3B-C4B-NB	3.02	113.22	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	O2A-CGA-CBA	3.02	121.04	111.83
23	B	602	CLA	O2A-CGA-CBA	3.02	121.03	111.83
34	z	101	LMG	O8-C28-C29	3.02	121.03	111.83
23	c	504	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
37	C	517	DGD	O6D-C1D-O3G	-3.02	102.92	110.04
26	L	102	SQD	O7-S-C6	3.01	111.26	106.76
23	A	407	CLA	CHD-C4C-NC	3.01	128.91	124.23
26	a	413	SQD	C3-C4-C5	3.01	115.69	110.23
23	c	501	CLA	C3B-C4B-NB	3.01	113.22	110.53
23	C	509	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
23	B	605	CLA	O2A-CGA-O1A	-3.01	116.10	123.63
23	c	507	CLA	CMC-C2C-C1C	3.01	129.74	125.03
31	b	630	LHG	O8-C23-C24	3.01	121.01	111.83
23	c	505	CLA	C3B-C4B-NB	3.01	113.22	110.53
23	B	604	CLA	CHD-C4C-NC	3.01	128.89	124.23
23	b	608	CLA	C3B-C4B-NB	3.00	113.21	110.53
23	A	405	CLA	O2A-CGA-CBA	3.00	120.99	111.83
25	A	408	BCR	C11-C10-C9	-3.00	123.07	127.28
23	b	616	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	c	506	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	a	406	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
38	e	103	HEM	C4D-ND-C1D	3.00	108.76	105.21
23	C	507	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
23	C	509	CLA	C4-C3-C5	3.00	120.43	115.23
24	D	402	PHO	O2D-CGD-O1D	-3.00	118.02	123.85
23	b	609	CLA	CHD-C4C-NC	2.99	128.87	124.23
23	C	507	CLA	CMC-C2C-C1C	2.99	129.71	125.03
23	b	602	CLA	C3B-C4B-NB	2.99	113.20	110.53
23	D	404	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
25	t	101	BCR	C1-C6-C7	2.99	123.76	115.65
23	C	514	CLA	CMC-C2C-C1C	2.99	129.70	125.03
34	J	101	LMG	O8-C28-C29	2.99	120.94	111.83
23	D	405	CLA	C1C-C2C-C3C	-2.99	103.84	106.98
23	A	404	CLA	C3B-C4B-NB	2.99	113.19	110.53
23	B	616	CLA	CBC-CAC-C3C	-2.98	104.33	112.42
23	b	601	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
29	A	413	PL9	C17-C18-C19	-2.98	120.80	127.62
36	V	203	HTG	C1-C2-C3	2.98	113.99	109.64
23	a	409	CLA	C1-C2-C3	-2.98	121.31	126.20
23	B	616	CLA	CAC-C3C-C4C	2.98	128.67	124.79
29	d	405	PL9	C35-C34-C36	2.98	120.40	115.23
23	b	606	CLA	C4-C3-C5	2.98	120.40	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	O2A-CGA-O1A	-2.98	116.18	123.63
23	B	617	CLA	CMB-C2B-C1B	2.98	129.95	125.42
23	b	611	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
23	B	602	CLA	CMB-C2B-C1B	2.98	129.95	125.42
23	B	616	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
25	b	618	BCR	C29-C30-C25	2.98	114.76	110.44
23	b	606	CLA	CMB-C2B-C1B	2.98	129.95	125.42
23	c	513	CLA	CMC-C2C-C1C	2.98	129.68	125.03
23	b	616	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
23	C	507	CLA	O2A-CGA-CBA	2.98	120.91	111.83
23	A	405	CLA	O2A-CGA-O1A	-2.97	116.19	123.63
23	C	510	CLA	CHD-C4C-NC	2.97	128.84	124.23
25	c	515	BCR	C3-C4-C5	-2.97	108.75	114.06
23	D	404	CLA	O2A-CGA-O1A	-2.97	116.20	123.63
23	D	401	CLA	C4-C3-C5	2.97	120.39	115.23
25	y	101	BCR	C23-C24-C25	-2.97	119.06	127.00
35	C	522	LMT	O1B-C4'-C3'	2.97	114.78	107.23
23	B	603	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
23	B	602	CLA	CHD-C4C-NC	2.97	128.83	124.23
29	D	407	PL9	C37-C38-C39	-2.97	120.83	127.62
25	C	527	BCR	C20-C21-C22	-2.96	123.12	127.28
37	c	516	DGD	C2G-O2G-C1B	-2.96	110.70	117.80
23	D	404	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
23	c	504	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
23	d	403	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	B	610	CLA	C3B-C4B-NB	2.96	113.17	110.53
23	A	405	CLA	CMB-C2B-C1B	2.96	129.93	125.42
37	h	103	DGD	O1G-C1A-O1A	-2.96	116.22	123.63
23	c	503	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
26	A	409	SQD	O7-S-C6	2.96	111.17	106.76
25	C	516	BCR	C33-C5-C6	-2.96	121.26	124.48
25	B	618	BCR	C29-C30-C25	2.96	114.73	110.44
23	c	511	CLA	O2A-CGA-CBA	2.95	120.84	111.83
23	c	501	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
23	b	605	CLA	C2A-C1A-CHA	-2.95	118.75	123.87
31	A	415	LHG	C5-O7-C7	-2.95	110.73	117.80
23	c	508	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
34	B	622	LMG	O8-C28-C29	2.95	120.83	111.83
23	C	512	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
23	c	504	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
25	T	101	BCR	C16-C15-C14	2.95	129.54	123.52
23	b	605	CLA	CHC-C1C-C2C	-2.94	118.58	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CMB-C2B-C1B	2.94	129.90	125.42
26	A	411	SQD	O48-C23-C24	2.94	120.81	111.83
23	B	602	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	b	614	CLA	O2A-CGA-O1A	-2.94	116.27	123.63
23	b	612	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
34	c	520	LMG	O8-C28-C29	2.94	120.80	111.83
23	b	608	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
23	C	514	CLA	CAC-C3C-C4C	2.94	128.61	124.79
23	b	607	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
23	c	510	CLA	C3C-C4C-NC	2.94	114.19	110.43
23	A	407	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
23	b	615	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
38	E	103	HEM	CBD-CAD-C3D	-2.94	104.42	112.53
23	A	404	CLA	CAA-CBA-CGA	-2.93	104.88	113.21
23	C	503	CLA	CBC-CAC-C3C	-2.93	104.47	112.42
23	c	506	CLA	C4-C3-C5	2.93	120.32	115.23
23	b	602	CLA	CMC-C2C-C1C	2.93	129.62	125.03
25	b	619	BCR	C4-C5-C6	-2.93	118.74	122.70
23	C	505	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
24	A	406	PHO	C1-C2-C3	-2.93	121.40	126.20
23	a	404	CLA	CHD-C4C-NC	2.93	128.77	124.23
24	A	406	PHO	CMB-C2B-C3B	2.93	130.53	124.68
23	d	403	CLA	CAC-C3C-C4C	2.93	128.60	124.79
23	b	610	CLA	CHD-C4C-NC	2.93	128.77	124.23
23	B	607	CLA	C4C-C3C-C2C	-2.92	102.63	106.89
38	E	103	HEM	CHD-C1D-ND	2.92	127.57	124.42
23	C	513	CLA	CMC-C2C-C1C	2.92	129.60	125.03
25	b	619	BCR	C39-C30-C25	-2.92	105.66	110.24
23	b	613	CLA	C3B-C4B-NB	2.92	113.14	110.53
23	A	405	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
23	B	604	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
23	b	609	CLA	CAC-C3C-C4C	2.91	128.58	124.79
23	C	505	CLA	C1-C2-C3	-2.91	121.42	126.20
23	B	603	CLA	CAC-C3C-C4C	2.91	128.58	124.79
25	c	514	BCR	C2-C1-C6	2.91	114.67	110.44
23	c	510	CLA	CHC-C1C-C2C	-2.91	118.68	126.95
23	c	512	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
25	D	406	BCR	C40-C30-C25	-2.91	105.68	110.24
23	b	609	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
23	B	607	CLA	CHD-C4C-NC	2.91	128.74	124.23
23	C	502	CLA	C4-C3-C5	2.91	120.27	115.23
23	C	507	CLA	C2A-C1A-CHA	-2.90	118.83	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	PHO	CMA-C3A-C4A	-2.90	108.35	114.61
23	b	604	CLA	C4C-C3C-C2C	-2.90	102.66	106.89
23	b	608	CLA	C4C-C3C-C2C	-2.90	102.66	106.89
23	c	511	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
23	b	610	CLA	C4-C3-C5	2.90	120.27	115.23
23	c	503	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
23	c	507	CLA	CAC-C3C-C4C	2.90	128.57	124.79
23	b	605	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
29	a	415	PL9	C25-C24-C26	2.90	120.26	115.23
23	B	609	CLA	O2A-CGA-CBA	2.90	120.68	111.83
23	D	404	CLA	CMC-C2C-C1C	2.90	129.56	125.03
23	c	506	CLA	O2A-CGA-CBA	2.90	120.67	111.83
23	A	405	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
23	A	404	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
23	B	617	CLA	O2A-CGA-CBA	2.90	120.67	111.83
23	c	502	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
23	B	616	CLA	C1-C2-C3	-2.89	121.46	126.20
23	b	612	CLA	C2A-C1A-CHA	-2.89	118.85	123.87
23	b	601	CLA	C3B-C4B-NB	2.89	113.11	110.53
23	C	514	CLA	CHD-C4C-NC	2.89	128.71	124.23
23	c	510	CLA	CHD-C4C-NC	2.89	128.71	124.23
23	B	609	CLA	CMB-C2B-C1B	2.89	129.82	125.42
23	B	604	CLA	CBC-CAC-C3C	-2.89	104.59	112.42
23	c	513	CLA	C1-C2-C3	-2.89	121.47	126.20
23	D	404	CLA	C4-C3-C5	2.89	120.24	115.23
23	B	613	CLA	C4-C3-C5	2.88	120.23	115.23
26	B	621	SQD	O48-C23-C24	2.88	120.62	111.83
23	B	614	CLA	C4-C3-C5	2.88	120.23	115.23
23	b	604	CLA	CAC-C3C-C4C	2.88	128.54	124.79
23	b	614	CLA	CAC-C3C-C4C	2.88	128.54	124.79
23	D	401	CLA	CMB-C2B-C1B	2.88	129.80	125.42
25	C	527	BCR	C3-C4-C5	-2.88	108.93	114.06
36	B	629	HTG	C1-O5-C5	2.88	117.72	112.56
23	A	405	CLA	CBC-CAC-C3C	-2.88	104.62	112.42
25	B	620	BCR	C20-C21-C22	-2.87	123.25	127.28
23	C	502	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
23	B	617	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
23	B	613	CLA	O2A-CGA-CBA	2.87	120.59	111.83
25	H	101	BCR	C29-C30-C25	2.87	114.61	110.44
23	C	512	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
23	B	604	CLA	CMB-C2B-C1B	2.87	129.79	125.42
25	t	101	BCR	C7-C6-C5	-2.87	114.95	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C11-C10-C9	-2.87	123.26	127.28
23	B	612	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
23	b	607	CLA	CMB-C2B-C1B	2.87	129.78	125.42
26	D	413	SQD	O47-C7-O49	-2.87	117.01	123.70
25	y	101	BCR	C10-C11-C12	-2.86	114.90	123.20
23	C	502	CLA	CAC-C3C-C4C	2.86	128.52	124.79
23	b	604	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	A	408	BCR	C20-C21-C22	-2.86	123.26	127.28
23	b	605	CLA	CMC-C2C-C1C	2.86	129.51	125.03
23	c	510	CLA	C4-C3-C5	2.86	120.19	115.23
23	b	604	CLA	C3B-C4B-NB	2.86	113.08	110.53
23	B	604	CLA	C3B-C4B-NB	2.86	113.08	110.53
23	c	506	CLA	CGD-CBD-CAD	-2.85	101.60	110.85
23	c	512	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
25	c	514	BCR	C38-C26-C25	-2.85	121.37	124.48
23	B	602	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
25	A	408	BCR	C7-C8-C9	-2.85	122.02	126.23
23	B	614	CLA	C4B-C3B-C2B	-2.85	103.75	107.30
23	B	609	CLA	O2A-CGA-O1A	-2.85	116.50	123.63
37	c	518	DGD	O2G-C1B-C2B	2.85	117.65	111.48
25	A	408	BCR	C8-C7-C6	-2.85	119.39	127.00
24	a	407	PHO	OBD-CAD-C3D	-2.85	123.45	127.89
29	d	405	PL9	C37-C38-C39	-2.85	121.11	127.62
23	A	404	CLA	CHD-C4C-NC	2.85	128.64	124.23
23	a	404	CLA	CHC-C1C-C2C	-2.84	118.86	126.95
36	b	625	HTG	O5-C5-C4	2.84	114.82	109.70
34	a	417	LMG	O6-C5-C4	2.84	114.82	109.70
23	d	403	CLA	O2A-CGA-O1A	-2.84	116.52	123.63
31	A	415	LHG	O8-C23-C24	2.84	120.49	111.83
23	A	407	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
31	E	101	LHG	O8-C23-C24	2.84	120.49	111.83
23	b	605	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
25	C	515	BCR	C7-C8-C9	-2.84	122.04	126.23
23	b	613	CLA	CMC-C2C-C1C	2.84	129.47	125.03
23	a	409	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
23	c	513	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
23	c	512	CLA	O2A-CGA-CBA	2.83	120.48	111.83
23	b	605	CLA	C4-C3-C5	2.83	120.15	115.23
23	b	603	CLA	CMC-C2C-C1C	2.83	129.46	125.03
23	c	513	CLA	C3B-C4B-NB	2.83	113.06	110.53
23	c	512	CLA	CHB-C4A-NA	2.83	128.49	124.40
31	d	408	LHG	O8-C23-C24	2.83	120.46	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C4-C3-C5	2.83	120.14	115.23
23	C	511	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
23	b	601	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
23	c	513	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
29	D	407	PL9	C7-C3-C2	-2.82	120.06	123.39
23	b	606	CLA	C4B-C3B-C2B	-2.82	103.79	107.30
23	C	507	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
31	d	406	LHG	O8-C23-O10	-2.82	116.56	123.63
23	b	612	CLA	O2A-CGA-O1A	-2.82	116.56	123.63
25	b	618	BCR	C37-C22-C21	-2.82	118.24	122.82
23	b	605	CLA	CED-O2D-CGD	2.82	122.32	115.92
23	A	404	CLA	CAC-C3C-C4C	2.82	128.46	124.79
23	b	606	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
23	D	404	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
23	C	503	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
23	a	405	CLA	CMB-C2B-C1B	2.81	129.71	125.42
25	D	406	BCR	C28-C27-C26	-2.81	109.04	114.06
23	A	405	CLA	CAA-C2A-C3A	-2.81	105.39	113.00
23	c	502	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
23	c	501	CLA	C4B-C3B-C2B	-2.81	103.80	107.30
23	c	506	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
23	B	614	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
23	B	605	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
23	c	508	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
23	C	504	CLA	C1-C2-C3	-2.80	121.61	126.20
23	A	407	CLA	CAA-C2A-C3A	-2.80	105.43	113.00
29	D	407	PL9	C7-C3-C4	2.80	119.22	116.91
23	B	607	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
23	b	609	CLA	CMC-C2C-C1C	2.80	129.41	125.03
23	c	502	CLA	O2A-CGA-CBA	2.80	120.37	111.83
23	C	507	CLA	CHD-C4C-NC	2.80	128.57	124.23
23	B	615	CLA	CHD-C4C-NC	2.80	128.57	124.23
23	C	507	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
35	B	633	LMT	O5'-C5'-C4'	2.80	115.51	109.72
25	t	101	BCR	C20-C21-C22	-2.80	123.36	127.28
23	c	507	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
36	b	622	HTG	O5-C1-C2	2.80	114.17	110.32
23	D	405	CLA	C2A-C1A-CHA	-2.79	119.02	123.87
23	B	607	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
23	b	604	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
40	V	202	HEC	CHA-C4D-ND	2.79	128.92	123.86
23	B	603	CLA	O2A-CGA-CBA	2.79	120.35	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	C1-C2-C3	-2.79	121.62	126.20
23	C	502	CLA	CHD-C4C-NC	2.79	128.56	124.23
25	k	101	BCR	C3-C4-C5	-2.79	109.08	114.06
25	y	101	BCR	C28-C27-C26	-2.79	109.08	114.06
23	b	608	CLA	O2A-CGA-CBA	2.79	120.34	111.83
25	d	404	BCR	C23-C24-C25	-2.79	119.55	127.00
23	C	508	CLA	CMC-C2C-C1C	2.79	129.39	125.03
35	M	101	LMT	C1-O1'-C1'	-2.79	108.92	113.68
23	c	513	CLA	O2A-CGA-CBA	2.79	120.33	111.83
23	D	401	CLA	CMA-C3A-C2A	-2.79	103.21	113.98
31	L	101	LHG	O8-C23-C24	2.78	120.33	111.83
23	B	606	CLA	C2A-C1A-CHA	-2.78	119.04	123.87
23	C	511	CLA	CAC-C3C-C4C	2.78	128.41	124.79
25	B	619	BCR	C36-C18-C19	2.78	122.33	118.09
23	B	608	CLA	CED-O2D-CGD	2.78	122.22	115.92
23	C	512	CLA	C4B-C3B-C2B	-2.78	103.85	107.30
23	B	605	CLA	CMB-C2B-C1B	2.78	129.65	125.42
23	c	505	CLA	C4B-C3B-C2B	-2.78	103.85	107.30
29	d	405	PL9	C17-C18-C19	-2.77	121.27	127.62
23	C	513	CLA	C4C-C3C-C2C	-2.77	102.85	106.89
23	B	605	CLA	C4-C3-C5	2.77	120.04	115.23
23	d	402	CLA	CHC-C1C-C2C	-2.77	119.06	126.95
31	D	408	LHG	O7-C7-C8	2.77	117.48	111.48
24	a	408	PHO	CMB-C2B-C3B	2.77	130.22	124.68
23	a	409	CLA	CMA-C3A-C2A	-2.77	103.26	113.98
23	C	503	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
23	c	510	CLA	CMB-C2B-C1B	2.77	129.64	125.42
25	c	514	BCR	C28-C27-C26	-2.77	109.11	114.06
23	C	510	CLA	C1-O2A-CGA	2.77	123.36	116.65
23	d	403	CLA	C2A-C1A-CHA	-2.77	119.06	123.87
23	B	609	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
37	C	519	DGD	O1G-C1A-C2A	2.77	120.28	111.83
37	c	518	DGD	O1G-C1A-C2A	2.77	120.28	111.83
23	B	604	CLA	CHC-C1C-C2C	-2.77	119.09	126.95
23	b	616	CLA	C4-C3-C5	2.77	120.03	115.23
23	B	602	CLA	C4B-C3B-C2B	-2.76	103.86	107.30
23	D	401	CLA	C4B-C3B-C2B	-2.76	103.86	107.30
23	B	606	CLA	C1-C2-C3	-2.76	121.67	126.20
23	D	401	CLA	CBC-CAC-C3C	-2.76	104.93	112.42
37	c	516	DGD	O3G-C3G-C2G	-2.76	104.10	110.82
23	c	501	CLA	C4-C3-C5	2.76	120.02	115.23
23	C	503	CLA	CAC-C3C-C4C	2.76	128.38	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	BCR	C33-C5-C6	-2.76	121.47	124.48
23	B	606	CLA	O2A-CGA-CBA	2.76	120.25	111.83
31	d	407	LHG	O8-C23-C24	2.76	120.25	111.83
23	b	611	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
23	c	504	CLA	C4-C3-C5	2.76	120.02	115.23
23	C	506	CLA	CHD-C4C-NC	2.76	128.51	124.23
23	C	511	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
23	B	605	CLA	CMC-C2C-C1C	2.76	129.34	125.03
23	A	405	CLA	CAC-C3C-C4C	2.76	128.38	124.79
23	b	610	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
23	d	402	CLA	CBC-CAC-C3C	-2.76	104.95	112.42
23	b	608	CLA	CMC-C2C-C1C	2.75	129.34	125.03
23	B	608	CLA	CBC-CAC-C3C	-2.75	104.96	112.42
23	D	405	CLA	CAA-C2A-C3A	-2.75	105.56	113.00
23	b	609	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
23	B	609	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
23	b	607	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
25	B	619	BCR	C37-C22-C21	-2.75	118.36	122.82
23	B	611	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
23	B	606	CLA	O2A-CGA-O1A	-2.75	116.76	123.63
23	b	616	CLA	C1-C2-C3	-2.75	121.70	126.20
25	b	618	BCR	C37-C22-C23	2.75	122.28	118.09
25	C	527	BCR	C10-C11-C12	-2.75	115.25	123.20
25	a	410	BCR	C38-C26-C25	-2.74	121.49	124.48
23	c	511	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
23	a	404	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
23	c	511	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
23	C	503	CLA	CHD-C4C-NC	2.74	128.49	124.23
23	B	612	CLA	OBD-CAD-C3D	-2.74	122.00	128.42
23	b	602	CLA	O2A-CGA-CBA	2.74	120.19	111.83
23	B	604	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
23	b	603	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
23	b	602	CLA	C11-C10-C8	-2.74	106.86	115.97
24	A	406	PHO	C4A-C3A-C2A	-2.74	100.23	102.84
26	f	101	SQD	C4-C3-C2	-2.73	106.03	110.83
25	B	620	BCR	C21-C20-C19	-2.73	115.28	123.20
23	B	617	CLA	CBC-CAC-C3C	-2.73	105.01	112.42
23	C	506	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
23	C	508	CLA	O2A-CGA-CBA	2.73	120.16	111.83
23	b	604	CLA	CHD-C4C-NC	2.73	128.46	124.23
34	m	101	LMG	C7-O1-C1	-2.73	107.95	113.80
23	b	610	CLA	O2A-CGA-O1A	-2.73	116.81	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C2A-C1A-CHA	-2.73	119.14	123.87
23	b	611	CLA	CAC-C3C-C4C	2.73	128.34	124.79
23	a	409	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
23	B	616	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
23	B	610	CLA	CHD-C4C-NC	2.73	128.46	124.23
26	L	102	SQD	O48-C23-C24	2.72	120.14	111.83
23	c	507	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
25	B	620	BCR	C24-C23-C22	-2.72	122.21	126.23
23	c	503	CLA	O2A-CGA-CBA	2.72	120.14	111.83
23	b	608	CLA	CBC-CAC-C3C	-2.72	105.04	112.42
23	c	509	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
23	b	610	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
26	D	413	SQD	O5-C5-C4	2.72	114.59	109.70
23	B	607	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
23	D	404	CLA	CHC-C1C-C2C	-2.71	119.23	126.95
26	D	413	SQD	O48-C23-C24	2.71	120.11	111.83
23	C	514	CLA	O2A-CGA-CBA	2.71	120.11	111.83
23	B	607	CLA	CMB-C2B-C1B	2.71	129.55	125.42
23	a	404	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
23	B	602	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
23	C	510	CLA	C3B-C4B-NB	2.71	112.95	110.53
23	a	409	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
23	b	602	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
23	b	606	CLA	CMC-C2C-C1C	2.71	129.27	125.03
23	b	606	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
24	D	402	PHO	C4D-CHA-CBD	2.71	109.75	108.45
23	b	601	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
23	B	604	CLA	C2A-C1A-CHA	-2.71	119.17	123.87
23	C	509	CLA	O2A-CGA-CBA	2.71	120.08	111.83
23	b	613	CLA	O2A-CGA-O1A	-2.70	116.86	123.63
25	k	101	BCR	C10-C11-C12	-2.70	115.36	123.20
23	b	612	CLA	CHD-C4C-NC	2.70	128.42	124.23
24	a	408	PHO	CMA-C3A-C4A	-2.70	108.79	114.61
23	C	506	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
23	B	617	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
23	b	613	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
36	C	523	HTG	C1-O5-C5	2.70	117.41	112.56
23	a	404	CLA	C1-C2-C3	-2.70	121.77	126.20
23	D	405	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
26	a	411	SQD	O8-S-C6	2.70	111.19	105.97
23	C	505	CLA	CMB-C2B-C1B	2.70	129.53	125.42
34	j	101	LMG	O8-C28-C29	2.70	120.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C4C-C3C-C2C	-2.70	102.97	106.89
23	a	404	CLA	C2A-C1A-CHA	-2.70	119.19	123.87
29	d	405	PL9	C40-C39-C41	2.69	119.90	115.23
37	C	517	DGD	C4E-C3E-C2E	-2.69	106.10	110.83
29	A	413	PL9	C12-C13-C14	-2.69	121.46	127.62
26	a	411	SQD	C1-O5-C5	-2.69	108.46	113.72
23	D	405	CLA	CAC-C3C-C4C	2.69	128.29	124.79
23	C	514	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
23	D	401	CLA	C2A-C1A-CHA	-2.69	119.20	123.87
37	C	518	DGD	C2G-O2G-C1B	-2.69	111.36	117.80
23	B	608	CLA	CHD-C4C-NC	2.69	128.40	124.23
23	C	506	CLA	C4-C3-C5	2.69	119.89	115.23
23	D	401	CLA	O2A-CGA-O1A	-2.68	116.91	123.63
23	C	502	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
23	B	610	CLA	CMC-C2C-C1C	2.68	129.22	125.03
26	A	409	SQD	O47-C7-O49	-2.68	117.44	123.70
23	b	614	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
29	D	407	PL9	C22-C23-C24	-2.68	121.49	127.62
23	B	610	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
23	b	603	CLA	C4-C3-C5	2.68	119.88	115.23
23	B	611	CLA	CAC-C3C-C4C	2.68	128.27	124.79
38	E	103	HEM	CHA-C4D-ND	2.67	127.67	124.37
23	c	512	CLA	CBC-CAC-C3C	-2.67	105.17	112.42
23	b	604	CLA	O1D-CGD-CBD	-2.67	119.25	124.52
23	B	602	CLA	C2A-C1A-CHA	-2.67	119.23	123.87
23	B	616	CLA	O2A-CGA-CBA	2.67	119.98	111.83
23	C	505	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
23	C	513	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
23	b	608	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
23	C	504	CLA	CHD-C4C-NC	2.67	128.37	124.23
23	b	612	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
23	B	608	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
25	C	516	BCR	C15-C14-C13	-2.67	123.54	127.28
23	b	609	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
40	V	202	HEC	C4B-NB-C1B	2.66	110.16	105.82
23	A	404	CLA	C4C-C3C-C2C	-2.66	103.01	106.89
29	d	405	PL9	C7-C8-C9	-2.66	122.24	126.83
23	c	513	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
23	b	601	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
31	d	406	LHG	O8-C23-C24	2.66	119.95	111.83
23	B	617	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
23	B	614	CLA	O2A-CGA-CBA	2.66	119.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	CMB-C2B-C1B	2.66	129.47	125.42
23	c	510	CLA	O1D-CGD-CBD	-2.66	119.27	124.52
23	a	406	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
29	a	415	PL9	C35-C34-C36	2.66	119.84	115.23
23	C	510	CLA	CMB-C2B-C1B	2.66	129.47	125.42
23	C	512	CLA	CHD-C4C-NC	2.66	128.35	124.23
23	b	615	CLA	CBC-CAC-C3C	-2.66	105.22	112.42
23	b	602	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
23	b	610	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
23	C	511	CLA	CBC-CAC-C3C	-2.66	105.22	112.42
23	C	507	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
23	B	606	CLA	CAC-C3C-C4C	2.65	128.24	124.79
23	C	510	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
23	C	510	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
23	b	614	CLA	CHD-C4C-NC	2.65	128.34	124.23
29	A	413	PL9	C35-C34-C36	2.65	119.83	115.23
34	Z	101	LMG	O6-C1-C2	2.65	115.81	110.37
29	a	415	PL9	C20-C19-C21	2.65	119.83	115.23
23	D	401	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
25	A	408	BCR	C16-C17-C18	-2.65	123.56	127.28
34	J	101	LMG	C8-O7-C10	-2.65	111.46	117.80
37	h	103	DGD	O2G-C1B-C2B	2.65	117.21	111.48
23	b	602	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
23	B	611	CLA	CMB-C2B-C1B	2.65	129.45	125.42
23	C	507	CLA	C4C-C3C-C2C	-2.65	103.04	106.89
23	b	614	CLA	CMB-C2B-C1B	2.65	129.45	125.42
23	C	504	CLA	C4B-C3B-C2B	-2.64	104.01	107.30
23	b	602	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
40	v	201	HEC	C4B-NB-C1B	2.64	110.13	105.82
29	A	413	PL9	C25-C24-C26	2.64	119.81	115.23
23	c	504	CLA	CMC-C2C-C1C	2.64	129.16	125.03
23	C	513	CLA	CBC-CAC-C3C	-2.64	105.26	112.42
40	V	202	HEC	CHB-C1B-NB	2.64	128.65	123.86
23	A	404	CLA	C4-C3-C5	2.64	119.81	115.23
25	b	618	BCR	C28-C27-C26	-2.64	109.35	114.06
23	C	504	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
23	C	506	CLA	CMC-C2C-C1C	2.64	129.16	125.03
23	c	505	CLA	CAC-C3C-C4C	2.64	128.22	124.79
25	y	101	BCR	C21-C20-C19	-2.64	115.56	123.20
23	a	406	CLA	C4-C3-C5	2.64	119.80	115.23
23	C	507	CLA	C3B-C4B-NB	2.64	112.88	110.53
23	b	604	CLA	CHC-C1C-C2C	-2.63	119.46	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C4-C3-C5	2.63	119.80	115.23
29	a	415	PL9	C10-C9-C11	2.63	119.80	115.23
29	a	415	PL9	C17-C18-C19	-2.63	121.60	127.62
25	B	619	BCR	C38-C26-C25	-2.63	121.61	124.48
37	c	517	DGD	O1G-C1A-C2A	2.63	119.86	111.83
23	C	504	CLA	CAC-C3C-C4C	2.63	128.21	124.79
29	D	407	PL9	C15-C14-C16	2.63	119.79	115.23
23	c	508	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
31	d	408	LHG	O8-C23-O10	-2.63	117.05	123.63
23	B	613	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
29	D	407	PL9	C51-C49-C50	2.63	120.64	114.59
23	c	508	CLA	CHD-C4C-NC	2.63	128.31	124.23
23	b	615	CLA	CAC-C3C-C4C	2.63	128.21	124.79
23	c	509	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
23	B	603	CLA	C2A-C1A-CHA	-2.63	119.31	123.87
36	b	621	HTG	O5-C1-C2	2.63	113.94	110.32
23	a	406	CLA	CMB-C2B-C1B	2.62	129.41	125.42
23	C	506	CLA	CAC-C3C-C4C	2.62	128.20	124.79
29	d	405	PL9	C12-C13-C14	-2.62	121.62	127.62
23	c	501	CLA	O2A-CGA-CBA	2.62	119.83	111.83
23	c	505	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
23	B	604	CLA	CAC-C3C-C4C	2.62	128.20	124.79
23	B	615	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
23	A	405	CLA	C2A-C1A-CHA	-2.62	119.32	123.87
23	c	510	CLA	O2A-CGA-O1A	-2.62	117.08	123.63
26	A	409	SQD	O9-S-O7	-2.62	105.30	113.82
36	b	626	HTG	C1-O5-C5	2.62	117.26	112.56
23	b	614	CLA	C4B-C3B-C2B	-2.62	104.05	107.30
36	B	626	HTG	O5-C1-C2	2.62	113.92	110.32
24	D	402	PHO	CMB-C2B-C3B	2.62	129.91	124.68
23	A	407	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
23	c	506	CLA	CHD-C4C-NC	2.61	128.29	124.23
23	b	605	CLA	CBC-CAC-C3C	-2.61	105.34	112.42
25	a	410	BCR	C2-C1-C6	2.61	114.23	110.44
23	C	508	CLA	CHD-C4C-NC	2.61	128.28	124.23
23	c	509	CLA	CHD-C4C-NC	2.61	128.28	124.23
23	a	405	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
23	D	404	CLA	CMB-C2B-C1B	2.61	129.40	125.42
23	b	609	CLA	CMB-C2B-C1B	2.61	129.39	125.42
23	d	402	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
23	B	613	CLA	CMC-C2C-C1C	2.61	129.11	125.03
23	C	513	CLA	CHC-C1C-C2C	-2.61	119.54	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C24-C23-C22	-2.61	122.38	126.23
23	a	409	CLA	O2A-CGA-CBA	2.61	119.78	111.83
23	C	506	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
25	c	515	BCR	C33-C5-C6	-2.60	121.64	124.48
25	d	404	BCR	C28-C27-C26	-2.60	109.41	114.06
23	c	513	CLA	C4-C3-C5	2.60	119.75	115.23
23	c	512	CLA	C3B-C4B-NB	2.60	112.85	110.53
26	a	413	SQD	O5-C5-C4	2.60	114.39	109.70
23	a	406	CLA	O2A-CGA-CBA	2.60	119.77	111.83
25	d	404	BCR	C37-C22-C23	2.60	122.06	118.09
29	A	413	PL9	C10-C9-C11	2.60	119.74	115.23
23	c	505	CLA	CHD-C4C-NC	2.60	128.26	124.23
23	c	507	CLA	CHD-C4C-NC	2.60	128.26	124.23
25	T	101	BCR	C16-C17-C18	-2.60	123.63	127.28
23	A	404	CLA	C2A-C1A-CHA	-2.60	119.36	123.87
23	B	603	CLA	CMB-C2B-C1B	2.60	129.37	125.42
23	c	501	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
23	C	509	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
23	B	612	CLA	C2A-C1A-CHA	-2.59	119.37	123.87
23	A	405	CLA	C4C-C3C-C2C	-2.59	103.12	106.89
25	C	516	BCR	C21-C20-C19	-2.59	115.69	123.20
23	C	510	CLA	O2A-CGA-CBA	2.59	119.74	111.83
34	c	520	LMG	C3-C4-C5	2.59	114.93	110.23
23	D	401	CLA	O2A-CGA-CBA	2.59	119.74	111.83
25	C	527	BCR	C38-C26-C25	-2.59	121.66	124.48
23	c	504	CLA	C1-O2A-CGA	2.59	122.92	116.65
23	b	615	CLA	C4-C3-C5	2.59	119.72	115.23
35	D	403	LMT	O5B-C5B-C4B	2.59	114.36	109.70
23	c	513	CLA	CHD-C4C-NC	2.58	128.24	124.23
23	B	611	CLA	CHC-C1C-C2C	-2.58	119.60	126.95
24	A	406	PHO	CMA-C3A-C4A	-2.58	109.04	114.61
23	a	409	CLA	CMB-C2B-C1B	2.58	129.35	125.42
23	b	616	CLA	CHD-C4C-NC	2.58	128.24	124.23
23	c	507	CLA	O2A-CGA-CBA	2.58	119.70	111.83
26	a	411	SQD	O47-C7-O49	-2.58	117.68	123.70
23	B	608	CLA	C4C-C3C-C2C	-2.58	103.14	106.89
23	b	601	CLA	C2A-C1A-CHA	-2.58	119.39	123.87
23	C	505	CLA	C1-O2A-CGA	2.58	122.89	116.65
23	C	513	CLA	CMB-C2B-C1B	2.58	129.34	125.42
23	C	503	CLA	C4B-C3B-C2B	-2.57	104.10	107.30
24	a	408	PHO	C1A-C2A-C3A	-2.57	100.39	102.84
25	C	516	BCR	C7-C8-C9	-2.57	122.43	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	C2A-C1A-CHA	-2.57	119.40	123.87
24	a	407	PHO	O2A-CGA-O1A	-2.57	117.19	123.63
23	B	617	CLA	C4-C3-C5	2.57	119.69	115.23
24	a	408	PHO	O1D-CGD-CBD	-2.57	120.82	124.72
23	c	513	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
23	b	611	CLA	CBC-CAC-C3C	-2.57	105.45	112.42
25	H	101	BCR	C7-C6-C5	2.57	127.48	121.56
23	C	505	CLA	CMC-C2C-C1C	2.57	129.05	125.03
23	B	615	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
34	j	101	LMG	C8-O7-C10	-2.57	111.65	117.80
23	B	607	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
34	J	101	LMG	O7-C10-O9	-2.57	117.70	123.70
23	C	506	CLA	O2A-CGA-CBA	2.57	119.67	111.83
23	C	503	CLA	CMC-C2C-C1C	2.57	129.05	125.03
23	B	611	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
23	c	502	CLA	C4C-C3C-C2C	-2.57	103.16	106.89
23	B	614	CLA	CHD-C4C-NC	2.57	128.21	124.23
26	D	413	SQD	C3-C4-C5	2.57	114.89	110.23
23	B	616	CLA	C4C-C3C-C2C	-2.57	103.16	106.89
31	e	101	LHG	O8-C23-C24	2.57	119.66	111.83
25	D	406	BCR	C3-C4-C5	-2.56	109.48	114.06
23	c	509	CLA	CAC-C3C-C4C	2.56	128.13	124.79
23	c	513	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
23	B	606	CLA	C3B-C4B-NB	2.56	112.82	110.53
23	c	506	CLA	CMB-C2B-C1B	2.56	129.32	125.42
23	c	510	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
23	B	605	CLA	CHC-C1C-C2C	-2.56	119.68	126.95
23	B	603	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
37	C	518	DGD	O1G-C1A-C2A	2.56	119.63	111.83
26	f	101	SQD	O48-C23-C24	2.56	119.63	111.83
23	C	508	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
29	D	407	PL9	C20-C19-C21	2.55	119.66	115.23
25	h	102	BCR	C29-C30-C25	2.55	114.14	110.44
25	B	619	BCR	C2-C1-C6	2.55	114.14	110.44
29	A	413	PL9	C40-C39-C41	2.55	119.65	115.23
25	B	620	BCR	C10-C11-C12	-2.55	115.82	123.20
23	d	403	CLA	CBC-CAC-C3C	-2.55	105.51	112.42
23	B	611	CLA	CMC-C2C-C1C	2.54	129.01	125.03
23	b	616	CLA	O2A-CGA-O1A	-2.54	117.26	123.63
25	c	515	BCR	C36-C18-C19	2.54	121.97	118.09
25	y	101	BCR	C16-C17-C18	-2.54	123.71	127.28
23	c	502	CLA	C2A-C1A-CHA	-2.54	119.45	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	520	LMG	C1-O6-C5	2.54	118.69	113.72
23	c	505	CLA	O2A-CGA-CBA	2.54	119.59	111.83
23	C	514	CLA	C3B-C4B-NB	2.54	112.80	110.53
23	b	601	CLA	O2A-CGA-CBA	2.54	119.59	111.83
25	B	618	BCR	C15-C14-C13	-2.54	123.72	127.28
23	B	614	CLA	C4C-C3C-C2C	-2.54	103.19	106.89
23	B	617	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
23	b	608	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
23	B	606	CLA	CMC-C2C-C1C	2.54	129.00	125.03
37	c	517	DGD	O5D-C1E-C2E	2.54	112.12	108.27
26	f	101	SQD	O47-C7-O49	-2.54	117.78	123.70
25	b	619	BCR	C21-C20-C19	-2.53	115.86	123.20
29	d	405	PL9	C53-C6-C1	2.53	120.47	115.28
36	b	623	HTG	O5-C1-C2	2.53	113.81	110.32
26	a	413	SQD	O9-S-C6	2.53	110.54	106.76
23	b	603	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
23	a	405	CLA	CAA-CBA-CGA	2.53	120.40	113.21
25	b	618	BCR	C3-C4-C5	-2.53	109.54	114.06
31	d	406	LHG	C5-O7-C7	-2.53	111.74	117.80
23	a	409	CLA	CMC-C2C-C1C	2.53	128.99	125.03
26	B	621	SQD	C1-C2-C3	-2.53	104.69	110.01
25	C	527	BCR	C15-C14-C13	-2.53	123.73	127.28
25	D	406	BCR	C21-C20-C19	-2.53	115.88	123.20
36	B	624	HTG	C1-O5-C5	2.52	117.09	112.56
23	b	609	CLA	C3B-C4B-NB	2.52	112.78	110.53
25	d	404	BCR	C16-C17-C18	-2.52	123.74	127.28
23	C	505	CLA	CAC-C3C-C4C	2.52	128.07	124.79
23	b	602	CLA	C11-C12-C13	-2.52	107.58	115.97
23	c	507	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
23	d	403	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
26	f	101	SQD	O5-C5-C4	2.52	114.24	109.70
25	C	527	BCR	C2-C1-C6	2.52	114.10	110.44
23	B	608	CLA	C1-O2A-CGA	2.52	122.75	116.65
23	c	507	CLA	C4-C3-C5	2.52	119.60	115.23
23	c	512	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
23	B	613	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
23	D	401	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
25	B	618	BCR	C11-C10-C9	-2.52	123.75	127.28
23	a	409	CLA	CHD-C4C-NC	2.52	128.13	124.23
23	b	614	CLA	CMC-C2C-C1C	2.51	128.96	125.03
23	B	602	CLA	CAC-C3C-C4C	2.51	128.06	124.79
23	B	612	CLA	C4C-C3C-C2C	-2.51	103.23	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
23	C	505	CLA	C4-C3-C5	2.51	119.59	115.23
23	A	404	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
23	c	508	CLA	CAA-C2A-C3A	-2.51	106.21	113.00
23	B	607	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
23	c	504	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
23	B	608	CLA	C3B-C4B-NB	2.51	112.77	110.53
25	h	102	BCR	C10-C11-C12	-2.51	115.94	123.20
23	b	610	CLA	CAC-C3C-C4C	2.51	128.05	124.79
23	c	502	CLA	CMC-C2C-C1C	2.51	128.95	125.03
24	D	402	PHO	C4-C3-C5	2.51	119.58	115.23
25	a	410	BCR	C33-C5-C6	-2.50	121.75	124.48
23	A	407	CLA	CMA-C3A-C2A	-2.50	104.30	113.98
34	B	622	LMG	O1-C1-C2	-2.50	104.47	108.27
23	B	612	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
25	C	515	BCR	C38-C26-C25	-2.50	121.76	124.48
37	C	519	DGD	C3G-C2G-C1G	-2.50	105.96	111.78
23	C	513	CLA	C4-C3-C5	2.50	119.56	115.23
23	b	602	CLA	C4-C3-C5	2.50	119.56	115.23
24	a	408	PHO	CBA-CAA-C2A	-2.49	106.43	113.78
40	v	201	HEC	CHB-C1B-NB	2.49	128.38	123.86
23	a	405	CLA	O2A-CGA-CBA	2.49	119.44	111.83
26	a	411	SQD	O48-C23-C24	2.49	119.44	111.83
40	V	202	HEC	CHD-C4C-NC	2.49	127.17	124.45
26	a	413	SQD	C1-O5-C5	2.49	118.59	113.72
23	b	615	CLA	C11-C12-C13	-2.49	107.68	115.97
23	C	512	CLA	O2A-CGA-CBA	2.49	119.44	111.83
23	B	615	CLA	CMC-C2C-C1C	2.49	128.93	125.03
23	B	611	CLA	C3B-C4B-NB	2.49	112.75	110.53
29	A	413	PL9	C53-C6-C1	2.49	120.38	115.28
23	b	614	CLA	CAA-C2A-C3A	-2.49	106.27	113.00
36	b	623	HTG	C1-O5-C5	2.49	117.02	112.56
25	Y	101	BCR	C36-C18-C19	2.49	121.89	118.09
23	B	608	CLA	CMB-C2B-C1B	2.49	129.21	125.42
34	m	101	LMG	C8-O7-C10	-2.49	111.84	117.80
25	Y	101	BCR	C21-C20-C19	-2.49	116.00	123.20
23	C	513	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
23	d	403	CLA	C3B-C4B-NB	2.48	112.75	110.53
23	c	508	CLA	CMC-C2C-C1C	2.48	128.92	125.03
23	a	406	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
23	b	606	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
29	d	405	PL9	C27-C28-C29	-2.48	121.94	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	O2A-CGA-CBA	2.48	119.40	111.83
25	a	410	BCR	C37-C22-C21	-2.48	118.80	122.82
37	C	517	DGD	C3G-C2G-C1G	-2.48	106.00	111.78
23	B	611	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
25	c	515	BCR	C15-C14-C13	-2.48	123.80	127.28
25	k	101	BCR	C2-C1-C6	2.48	114.04	110.44
23	B	606	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
25	b	618	BCR	C15-C14-C13	-2.48	123.80	127.28
23	A	405	CLA	CHD-C4C-NC	2.48	128.07	124.23
34	a	417	LMG	O8-C28-C29	2.48	119.38	111.83
23	a	405	CLA	CHB-C1B-NB	-2.47	120.34	124.05
31	D	408	LHG	O8-C23-C24	2.47	119.37	111.83
23	d	402	CLA	C4C-C3C-C2C	-2.47	103.29	106.89
23	b	604	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
40	V	202	HEC	CBC-CAC-C3C	-2.47	122.50	127.43
23	c	506	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
23	c	503	CLA	C4-C3-C5	2.47	119.51	115.23
23	c	511	CLA	CMC-C2C-C1C	2.46	128.88	125.03
23	c	507	CLA	C6-C7-C8	-2.46	107.78	115.97
25	b	618	BCR	C21-C20-C19	-2.46	116.07	123.20
23	C	513	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
34	C	521	LMG	O8-C28-C29	2.46	119.33	111.83
23	C	507	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
25	h	102	BCR	C16-C15-C14	-2.46	118.49	123.52
23	d	402	CLA	C4-C3-C5	2.45	119.49	115.23
23	c	511	CLA	CAC-C3C-C4C	2.45	127.98	124.79
23	d	403	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
35	B	623	LMT	C1'-O5'-C5'	2.45	118.51	113.72
35	B	634	LMT	O1'-C1'-C2'	2.45	112.00	108.27
23	B	616	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
23	d	403	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
23	c	505	CLA	C4-C3-C5	2.45	119.48	115.23
23	C	502	CLA	CMC-C2C-C1C	2.45	128.86	125.03
26	a	411	SQD	C44-O6-C1	-2.45	108.55	113.80
25	Y	101	BCR	C10-C11-C12	-2.45	116.11	123.20
23	d	402	CLA	CAA-C2A-C3A	-2.45	106.39	113.00
23	B	602	CLA	C4-C3-C5	2.44	119.47	115.23
23	c	509	CLA	CMC-C2C-C1C	2.44	128.85	125.03
35	B	623	LMT	C3'-C4'-C5'	2.44	116.34	110.93
23	B	613	CLA	C2A-C1A-CHA	-2.44	119.63	123.87
29	D	407	PL9	C7-C8-C9	-2.44	122.63	126.83
23	C	511	CLA	C4-C3-C2	-2.44	117.36	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
23	b	603	CLA	CBC-CAC-C3C	-2.44	105.81	112.42
25	H	101	BCR	C15-C14-C13	-2.44	123.86	127.28
23	B	603	CLA	CHD-C4C-NC	2.44	128.01	124.23
23	b	604	CLA	C4-C3-C5	2.44	119.46	115.23
29	D	407	PL9	C30-C29-C31	2.44	119.46	115.23
23	b	602	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
23	b	606	CLA	CBC-CAC-C3C	-2.43	105.82	112.42
23	c	504	CLA	CHD-C4C-NC	2.43	128.00	124.23
23	a	404	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	b	603	CLA	CAC-C3C-C4C	2.43	127.95	124.79
23	C	513	CLA	CMA-C3A-C4A	-2.43	105.24	111.77
37	c	516	DGD	O2G-C1B-O1B	-2.43	118.02	123.70
25	Y	101	BCR	C29-C28-C27	-2.43	105.93	111.28
23	d	402	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
23	c	509	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
23	B	607	CLA	C4-C3-C5	2.43	119.44	115.23
25	k	101	BCR	C34-C9-C8	2.43	121.80	118.09
23	d	402	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
23	D	405	CLA	C4-C3-C5	2.43	119.44	115.23
25	a	410	BCR	C11-C10-C9	-2.43	123.88	127.28
34	z	101	LMG	C8-O7-C10	-2.43	111.99	117.80
23	c	509	CLA	C2A-C1A-CHA	-2.43	119.66	123.87
25	C	515	BCR	C23-C24-C25	-2.42	120.53	127.00
24	a	408	PHO	O2D-CGD-O1D	-2.42	119.14	123.85
23	b	611	CLA	CHD-C4C-NC	2.42	127.98	124.23
23	b	606	CLA	O2A-CGA-CBA	2.42	119.21	111.83
23	b	610	CLA	CMC-C2C-C1C	2.42	128.81	125.03
24	A	406	PHO	CMC-C2C-C1C	2.42	129.09	124.73
23	c	501	CLA	CHD-C4C-NC	2.42	127.98	124.23
25	A	408	BCR	C3-C4-C5	-2.41	109.75	114.06
25	C	516	BCR	C2-C1-C6	2.41	113.95	110.44
23	C	513	CLA	C1-C2-C3	-2.41	122.24	126.20
23	b	613	CLA	CED-O2D-CGD	2.41	121.39	115.92
29	a	415	PL9	C51-C49-C50	2.41	120.14	114.59
36	B	624	HTG	C1'-S1-C1	2.41	105.66	100.45
34	J	101	LMG	O8-C28-O10	-2.41	117.60	123.63
23	b	610	CLA	CMB-C2B-C1B	2.41	129.09	125.42
23	b	610	CLA	C3B-C4B-NB	2.41	112.68	110.53
23	c	509	CLA	CED-O2D-CGD	2.41	121.38	115.92
23	D	404	CLA	CHD-C4C-NC	2.41	127.96	124.23
23	B	617	CLA	C1-C2-C3	-2.41	122.25	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C2A-C1A-CHA	-2.41	119.69	123.87
23	B	607	CLA	CMC-C2C-C1C	2.40	128.79	125.03
29	a	415	PL9	C40-C39-C41	2.40	119.40	115.23
25	Y	101	BCR	C34-C9-C8	2.40	121.76	118.09
23	b	607	CLA	O2A-CGA-CBA	2.40	119.17	111.83
23	a	405	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
23	b	615	CLA	CHD-C4C-NC	2.40	127.96	124.23
31	A	415	LHG	O7-C7-O9	-2.40	118.09	123.70
23	C	513	CLA	CBA-CAA-C2A	-2.40	106.65	113.79
23	b	614	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
31	d	406	LHG	O7-C7-O9	-2.40	118.09	123.70
25	A	408	BCR	C31-C1-C6	-2.40	106.48	110.24
23	c	503	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
34	m	101	LMG	O8-C28-O10	-2.40	117.63	123.63
37	C	517	DGD	C2G-O2G-C1B	-2.40	112.05	117.80
25	b	617	BCR	C3-C4-C5	-2.40	109.78	114.06
23	a	406	CLA	CBC-CAC-C3C	-2.40	105.92	112.42
23	D	405	CLA	C1-C2-C3	-2.40	122.27	126.20
23	C	510	CLA	CHC-C1C-C2C	-2.39	120.14	126.95
34	C	501	LMG	O1-C1-C2	2.39	111.90	108.27
23	B	607	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
26	D	413	SQD	C1-C2-C3	-2.39	104.99	110.01
23	B	612	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
26	a	411	SQD	O5-C1-C2	-2.38	105.47	110.37
26	f	101	SQD	O5-C1-C2	2.38	115.27	110.37
23	C	513	CLA	C3B-C4B-NB	2.38	112.66	110.53
25	c	514	BCR	C37-C22-C21	-2.38	118.96	122.82
23	a	404	CLA	CAA-C2A-C1A	-2.38	104.18	111.97
23	b	616	CLA	OBD-CAD-C3D	-2.38	122.86	128.42
29	a	415	PL9	C53-C6-C1	2.38	120.15	115.28
25	H	101	BCR	C2-C1-C6	2.38	113.89	110.44
37	c	518	DGD	C3G-C2G-C1G	-2.38	106.25	111.78
36	B	629	HTG	O5-C5-C4	2.37	113.98	109.70
29	D	407	PL9	C25-C24-C26	2.37	119.35	115.23
29	d	405	PL9	C51-C49-C50	2.37	120.05	114.59
25	y	101	BCR	C1-C6-C7	2.37	122.09	115.65
23	B	605	CLA	CHD-C4C-NC	2.37	127.91	124.23
36	c	522	HTG	O5-C5-C4	2.37	113.97	109.70
26	A	409	SQD	O9-S-C6	2.37	110.30	106.76
23	b	602	CLA	CAC-C3C-C4C	2.37	127.87	124.79
23	C	505	CLA	CHD-C4C-NC	2.37	127.90	124.23
23	B	612	CLA	CMB-C2B-C1B	2.37	129.02	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C11-C10-C8	-2.37	108.10	115.97
37	H	102	DGD	O1G-C1A-C2A	2.36	119.04	111.83
23	b	607	CLA	C1-O2A-CGA	2.36	122.37	116.65
25	d	404	BCR	C23-C22-C21	-2.36	115.29	119.01
23	b	602	CLA	CMB-C2B-C1B	2.36	129.02	125.42
23	d	403	CLA	C1-C2-C3	-2.36	122.33	126.20
23	C	508	CLA	C3B-C4B-NB	2.36	112.64	110.53
23	C	502	CLA	CMB-C2B-C1B	2.36	129.01	125.42
23	B	613	CLA	CHD-C4C-NC	2.36	127.89	124.23
23	b	607	CLA	CMC-C2C-C1C	2.36	128.72	125.03
25	a	410	BCR	C32-C1-C6	-2.36	106.54	110.24
37	c	516	DGD	C3G-C2G-C1G	-2.36	106.29	111.78
24	a	407	PHO	CMB-C2B-C3B	2.36	129.39	124.68
23	C	511	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
34	j	101	LMG	O8-C28-O10	-2.36	117.73	123.63
23	D	404	CLA	CAC-C3C-C4C	2.36	127.85	124.79
25	D	406	BCR	C29-C30-C25	2.35	113.86	110.44
23	d	402	CLA	CMC-C2C-C1C	2.35	128.71	125.03
29	D	407	PL9	C40-C39-C41	2.35	119.31	115.23
23	C	508	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
23	b	601	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
23	A	405	CLA	C4-C3-C5	2.35	119.31	115.23
23	C	502	CLA	O2A-CGA-CBA	2.35	119.01	111.83
23	B	612	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
34	Z	101	LMG	C9-C8-C7	-2.35	106.30	111.78
25	D	406	BCR	C16-C17-C18	-2.35	123.98	127.28
23	c	506	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
23	c	504	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
23	D	405	CLA	CHC-C1C-C2C	-2.35	120.28	126.95
23	C	514	CLA	C4-C3-C5	2.35	119.30	115.23
23	c	509	CLA	C4-C3-C5	2.35	119.30	115.23
23	C	514	CLA	CHC-C1C-C2C	-2.35	120.28	126.95
35	C	522	LMT	O1'-C1'-C2'	2.35	111.83	108.27
23	B	604	CLA	CMC-C2C-C1C	2.34	128.70	125.03
23	B	605	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
25	A	408	BCR	C35-C13-C12	2.34	121.66	118.09
23	c	504	CLA	O2A-CGA-CBA	2.34	118.96	111.83
23	c	508	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
23	b	610	CLA	CMA-C3A-C2A	-2.34	104.95	113.98
34	C	520	LMG	O8-C28-O10	-2.34	117.78	123.63
23	c	504	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
23	a	409	CLA	O2A-CGA-O1A	-2.33	117.79	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	519	DGD	O2G-C1B-C2B	2.33	116.52	111.48
23	C	514	CLA	CBC-CAC-C3C	-2.33	106.10	112.42
23	C	503	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
23	b	615	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
25	y	101	BCR	C37-C22-C23	2.33	121.65	118.09
25	c	515	BCR	C21-C20-C19	-2.33	116.45	123.20
23	B	610	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
23	C	503	CLA	O2A-CGA-CBA	2.33	118.93	111.83
25	B	620	BCR	C29-C30-C25	2.33	113.82	110.44
29	A	413	PL9	C45-C44-C46	2.33	119.27	115.23
23	B	602	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	c	507	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
23	C	511	CLA	C2A-C1A-CHA	-2.32	119.83	123.87
23	c	507	CLA	C3B-C4B-NB	2.32	112.60	110.53
25	d	404	BCR	C21-C20-C19	-2.32	116.47	123.20
38	E	103	HEM	C4B-C3B-C2B	-2.32	105.15	107.28
35	b	628	LMT	C1'-C2'-C3'	2.32	114.89	110.01
23	C	510	CLA	CBC-CAC-C3C	-2.32	106.13	112.42
23	C	508	CLA	CAC-C3C-C4C	2.32	127.81	124.79
24	a	407	PHO	C1-C2-C3	-2.32	122.40	126.20
23	b	605	CLA	C1-O2A-CGA	2.32	122.26	116.65
23	c	507	CLA	C2A-C1A-CHA	-2.32	119.84	123.87
23	C	506	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
26	A	409	SQD	O48-C23-O10	-2.31	117.84	123.63
23	C	505	CLA	CHB-C4A-NA	2.31	127.74	124.40
23	b	613	CLA	C1-C2-C3	-2.31	122.41	126.20
23	B	604	CLA	C1-C2-C3	-2.31	122.41	126.20
25	c	514	BCR	C7-C8-C9	-2.31	122.82	126.23
31	L	101	LHG	O4-P-O5	2.31	123.19	112.44
23	C	506	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
24	a	407	PHO	O1D-CGD-CBD	-2.31	121.22	124.72
23	B	602	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
40	v	201	HEC	O2D-CGD-CBD	2.31	121.30	114.00
29	a	415	PL9	C45-C44-C46	2.31	119.24	115.23
23	A	407	CLA	O2A-CGA-CBA	2.31	118.87	111.83
23	b	613	CLA	C4-C3-C5	2.31	119.23	115.23
25	B	620	BCR	C37-C22-C23	2.31	121.61	118.09
35	m	103	LMT	O5B-C5B-C4B	2.31	113.85	109.70
25	c	514	BCR	C35-C13-C14	-2.31	119.08	122.82
23	b	612	CLA	CMC-C2C-C1C	2.31	128.64	125.03
34	C	501	LMG	O7-C10-O9	-2.30	118.32	123.70
25	A	408	BCR	C37-C22-C21	-2.30	119.08	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	CAC-C3C-C4C	2.30	127.79	124.79
23	b	601	CLA	CMB-C2B-C1B	2.30	128.92	125.42
23	d	403	CLA	C4-C3-C5	2.30	119.22	115.23
26	L	102	SQD	C1-C2-C3	-2.30	105.17	110.01
23	C	503	CLA	C4-C3-C5	2.30	119.22	115.23
23	c	510	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
24	a	408	PHO	C4-C3-C2	-2.30	117.72	123.63
23	C	511	CLA	CHD-C4C-NC	2.30	127.79	124.23
23	A	404	CLA	C16-C15-C13	-2.30	108.33	115.97
25	b	619	BCR	C37-C22-C23	2.30	121.59	118.09
23	C	512	CLA	C11-C10-C8	-2.29	108.34	115.97
23	b	609	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
25	b	619	BCR	C16-C17-C18	-2.29	124.06	127.28
31	A	415	LHG	O8-C6-C5	-2.29	101.79	108.40
23	B	617	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
38	e	103	HEM	C4C-NC-C1C	2.29	109.55	105.82
23	C	510	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
23	b	606	CLA	CAC-C3C-C4C	2.29	127.77	124.79
23	B	608	CLA	CAC-C3C-C4C	2.29	127.77	124.79
23	c	512	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
23	C	508	CLA	C11-C10-C8	-2.29	108.36	115.97
23	b	613	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
23	b	611	CLA	CMB-C2B-C1B	2.29	128.90	125.42
25	B	620	BCR	C3-C4-C5	-2.29	109.98	114.06
23	D	405	CLA	CBC-CAC-C3C	-2.28	106.23	112.42
26	L	102	SQD	C1-O5-C5	-2.28	109.26	113.72
23	b	602	CLA	CBC-CAC-C3C	-2.28	106.23	112.42
23	c	510	CLA	C4-C3-C2	-2.28	117.76	123.63
23	B	608	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
37	c	517	DGD	O1G-C1A-O1A	-2.28	117.92	123.63
23	B	612	CLA	O2A-CGA-CBA	2.28	118.79	111.83
23	B	609	CLA	CBC-CAC-C3C	-2.28	106.24	112.42
23	c	511	CLA	CAA-CBA-CGA	-2.28	106.74	113.21
23	c	510	CLA	C4C-C3C-C2C	-2.28	103.58	106.89
23	C	509	CLA	CHB-C4A-NA	2.27	127.68	124.40
23	A	405	CLA	CMA-C3A-C4A	-2.27	105.66	111.77
25	c	514	BCR	C3-C4-C5	-2.27	110.00	114.06
25	Y	101	BCR	C28-C27-C26	-2.27	110.00	114.06
36	b	621	HTG	O5-C5-C4	2.27	113.79	109.70
34	j	101	LMG	O7-C10-O9	-2.27	118.40	123.70
25	B	620	BCR	C2-C3-C4	-2.27	106.29	111.28
25	k	101	BCR	C20-C21-C22	-2.27	124.10	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	Z	101	LMG	O6-C5-C4	2.27	113.78	109.70
25	B	619	BCR	C33-C5-C6	-2.27	122.01	124.48
24	a	407	PHO	CMC-C2C-C1C	2.27	128.81	124.73
26	B	621	SQD	C3-C4-C5	2.26	114.33	110.23
23	B	602	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
25	c	515	BCR	C37-C22-C23	2.26	121.54	118.09
34	Z	101	LMG	C1-O6-C5	2.26	118.13	113.72
23	c	504	CLA	CHB-C4A-NA	2.26	127.66	124.40
24	A	406	PHO	O2D-CGD-O1D	-2.26	119.45	123.85
23	b	601	CLA	CMC-C2C-C1C	2.26	128.56	125.03
25	Y	101	BCR	C40-C30-C25	-2.26	106.70	110.24
23	b	601	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
23	C	505	CLA	CBC-CAC-C3C	-2.25	106.31	112.42
23	B	616	CLA	C6-C7-C8	-2.25	108.47	115.97
23	c	503	CLA	CBC-CAC-C3C	-2.25	106.31	112.42
23	C	509	CLA	CHD-C4C-NC	2.25	127.73	124.23
25	B	619	BCR	C16-C17-C18	-2.25	124.12	127.28
26	D	413	SQD	O48-C23-O10	-2.25	117.99	123.63
23	C	508	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
23	B	611	CLA	C6-C7-C8	-2.25	108.49	115.97
25	t	101	BCR	C37-C22-C21	-2.25	119.17	122.82
23	A	407	CLA	CBC-CAC-C3C	-2.25	106.32	112.42
26	D	413	SQD	C44-O6-C1	-2.25	108.97	113.80
25	t	101	BCR	C16-C17-C18	-2.25	124.13	127.28
24	D	402	PHO	O2A-CGA-CBA	2.24	118.68	111.83
23	b	615	CLA	O2A-CGA-CBA	2.24	118.68	111.83
23	C	509	CLA	C2A-C1A-CHA	-2.24	119.97	123.87
26	L	102	SQD	O47-C7-O49	-2.24	118.46	123.70
23	c	506	CLA	CMC-C2C-C1C	2.24	128.54	125.03
25	c	515	BCR	C29-C30-C25	2.24	113.69	110.44
29	A	413	PL9	C47-C48-C49	-2.24	120.17	127.64
23	A	407	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
23	a	404	CLA	CMC-C2C-C1C	2.23	128.53	125.03
23	c	505	CLA	C2A-C1A-CHA	-2.23	119.99	123.87
23	c	503	CLA	CHD-C4C-NC	2.23	127.70	124.23
25	B	620	BCR	C37-C22-C21	-2.23	119.20	122.82
25	d	404	BCR	C11-C10-C9	-2.23	124.15	127.28
31	D	409	LHG	O8-C23-O10	-2.23	118.05	123.63
23	B	609	CLA	C4-C3-C5	2.23	119.10	115.23
23	a	404	CLA	C4-C3-C5	2.23	119.10	115.23
23	D	401	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
25	B	618	BCR	C31-C1-C6	-2.23	106.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413	PL9	C37-C36-C34	-2.23	105.80	113.19
23	B	609	CLA	CHB-C4A-NA	2.23	127.62	124.40
23	C	512	CLA	C1-C2-C3	-2.23	122.55	126.20
23	B	607	CLA	CAC-C3C-C4C	2.23	127.69	124.79
26	L	102	SQD	C44-O6-C1	-2.23	109.02	113.80
23	C	502	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
23	a	405	CLA	CHB-C4A-NA	2.23	127.61	124.40
23	C	505	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
25	T	101	BCR	C7-C6-C5	-2.23	116.43	121.56
23	b	609	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
23	c	501	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
38	E	103	HEM	CBA-CAA-C2A	-2.22	106.39	112.53
25	C	527	BCR	C36-C18-C19	2.22	121.48	118.09
23	B	609	CLA	CMC-C2C-C1C	2.22	128.51	125.03
23	B	602	CLA	CMA-C3A-C4A	-2.22	105.80	111.77
25	a	410	BCR	C36-C18-C19	2.22	121.48	118.09
24	a	407	PHO	C4A-C3A-C2A	-2.22	100.72	102.84
24	A	406	PHO	CAC-C3C-C4C	2.22	129.74	124.03
38	E	103	HEM	O2D-CGD-CBD	2.22	121.02	114.00
24	a	407	PHO	CBA-CAA-C2A	-2.22	107.24	113.78
25	h	102	BCR	C35-C13-C12	2.22	121.48	118.09
23	b	604	CLA	CHA-C1A-NA	-2.22	121.37	126.39
29	a	415	PL9	C47-C48-C49	-2.22	120.25	127.64
23	b	606	CLA	C1-C2-C3	-2.21	122.57	126.20
36	B	624	HTG	O2-C2-C3	-2.21	105.16	110.38
23	C	508	CLA	C4-C3-C5	2.21	119.07	115.23
23	b	607	CLA	CHD-C4C-NC	2.21	127.66	124.23
25	y	101	BCR	C7-C6-C5	-2.21	116.46	121.56
25	C	516	BCR	C24-C23-C22	-2.21	122.96	126.23
23	c	505	CLA	CMC-C2C-C1C	2.21	128.49	125.03
25	k	101	BCR	C7-C8-C9	-2.21	122.97	126.23
31	L	101	LHG	C5-O7-C7	-2.21	112.51	117.80
23	c	513	CLA	CMB-C2B-C1B	2.21	128.78	125.42
23	C	506	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
23	C	514	CLA	C4B-C3B-C2B	-2.21	104.56	107.30
25	c	515	BCR	C15-C16-C17	-2.20	119.01	123.52
29	d	405	PL9	C25-C24-C23	-2.20	117.97	123.63
25	k	101	BCR	C28-C27-C26	-2.20	110.13	114.06
23	b	610	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
23	c	503	CLA	CMC-C2C-C1C	2.20	128.48	125.03
29	d	405	PL9	C45-C44-C43	-2.20	117.97	123.63
23	B	611	CLA	CAA-CBA-CGA	-2.20	106.95	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	102	LMT	O1B-C1B-C2B	2.20	113.51	108.09
25	A	408	BCR	C36-C18-C19	2.20	121.45	118.09
23	b	613	CLA	CHB-C4A-NA	2.20	127.58	124.40
25	a	410	BCR	C10-C11-C12	-2.20	116.82	123.20
23	D	401	CLA	CAA-CBA-CGA	2.20	119.46	113.21
23	c	511	CLA	CBC-CAC-C3C	-2.20	106.45	112.42
23	A	405	CLA	C1-C2-C3	-2.20	122.59	126.20
23	a	406	CLA	CHB-C4A-NA	2.20	127.57	124.40
23	C	507	CLA	CHB-C1B-C2B	-2.20	121.04	127.43
23	b	607	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
25	d	404	BCR	C40-C30-C25	-2.19	106.80	110.24
36	C	523	HTG	O5-C1-C2	2.19	113.34	110.32
25	D	406	BCR	C10-C11-C12	-2.19	116.84	123.20
25	B	619	BCR	C37-C22-C23	2.19	121.44	118.09
23	a	404	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
38	e	103	HEM	CBD-CAD-C3D	-2.19	106.47	112.53
37	C	518	DGD	O1G-C1A-O1A	-2.19	118.14	123.63
35	M	101	LMT	O1B-C1B-C2B	2.19	113.48	108.09
23	c	513	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
34	c	519	LMG	O7-C10-O9	-2.19	118.58	123.70
23	b	615	CLA	C1-O2A-CGA	2.19	121.95	116.65
29	A	413	PL9	C51-C49-C50	2.19	119.63	114.59
23	c	511	CLA	CMB-C2B-C1B	2.19	128.75	125.42
23	b	607	CLA	CBC-CAC-C3C	-2.19	106.49	112.42
29	d	405	PL9	C42-C41-C39	-2.19	105.94	113.19
38	e	103	HEM	CHA-C1A-NA	2.19	127.82	123.86
23	C	513	CLA	CHB-C4A-NA	2.18	127.55	124.40
23	C	509	CLA	CAC-C3C-C4C	2.18	127.63	124.79
23	B	606	CLA	CHB-C4A-NA	2.18	127.55	124.40
23	b	613	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
25	d	404	BCR	C29-C30-C25	2.18	113.61	110.44
23	C	513	CLA	CAC-C3C-C4C	2.18	127.63	124.79
23	c	513	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
25	H	101	BCR	C31-C1-C6	-2.18	106.82	110.24
23	C	502	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
23	B	612	CLA	C1-O2A-CGA	2.18	121.93	116.65
38	E	103	HEM	C4D-ND-C1D	2.18	107.79	105.21
35	b	628	LMT	C3'-C4'-C5'	-2.18	106.10	110.93
23	b	616	CLA	C2A-C1A-CHA	-2.18	120.09	123.87
23	a	409	CLA	CBC-CAC-C3C	-2.18	106.52	112.42
25	B	619	BCR	C10-C11-C12	-2.18	116.89	123.20
40	v	201	HEC	CHA-C4D-ND	2.18	127.81	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C2A-C1A-CHA	-2.18	120.09	123.87
23	a	404	CLA	CED-O2D-CGD	2.17	120.85	115.92
23	C	505	CLA	O2A-CGA-CBA	2.17	118.47	111.83
23	C	504	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
40	V	202	HEC	CHD-C1D-ND	2.17	127.80	123.86
23	c	507	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
23	B	614	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
38	E	103	HEM	CHA-C1A-NA	2.17	127.80	123.86
23	B	614	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
25	k	101	BCR	C36-C18-C19	2.17	121.40	118.09
23	b	602	CLA	CMA-C3A-C2A	-2.17	105.60	113.98
23	b	614	CLA	CBC-CAC-C3C	-2.17	106.55	112.42
37	C	517	DGD	O2G-C1B-O1B	-2.17	118.64	123.70
23	B	613	CLA	C6-C5-C3	-2.17	108.19	113.47
38	E	103	HEM	C4C-NC-C1C	2.16	109.35	105.82
23	c	504	CLA	CED-O2D-CGD	2.16	120.82	115.92
31	E	101	LHG	O8-C23-O10	-2.16	118.22	123.63
23	c	504	CLA	CMB-C2B-C1B	2.16	128.71	125.42
24	a	407	PHO	C1A-C2A-C3A	-2.16	100.78	102.84
23	C	505	CLA	C2A-C1A-CHA	-2.16	120.12	123.87
23	A	404	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
23	C	509	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
23	b	611	CLA	C2A-C1A-CHA	-2.16	120.12	123.87
23	C	514	CLA	CMA-C3A-C2A	-2.16	105.64	113.98
25	A	408	BCR	C37-C22-C23	2.16	121.38	118.09
23	c	502	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
23	b	603	CLA	CHB-C4A-NA	2.16	127.51	124.40
25	C	515	BCR	C21-C20-C19	-2.15	116.96	123.20
23	B	603	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
23	B	603	CLA	CBC-CAC-C3C	-2.15	106.59	112.42
25	b	617	BCR	C16-C17-C18	-2.15	124.26	127.28
24	a	408	PHO	O2A-CGA-CBA	2.15	118.39	111.83
23	B	609	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
23	A	404	CLA	C1-C2-C3	-2.15	122.68	126.20
23	B	611	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
23	c	503	CLA	C1-O2A-CGA	2.15	121.85	116.65
23	c	505	CLA	C1-O2A-CGA	2.15	121.85	116.65
23	a	405	CLA	CMA-C3A-C2A	-2.15	105.68	113.98
23	B	606	CLA	OBD-CAD-C3D	-2.15	123.40	128.42
23	b	602	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
23	B	605	CLA	CHB-C4A-NA	2.15	127.50	124.40
40	V	202	HEC	CHB-C1B-C2B	-2.14	121.21	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
23	A	405	CLA	CMA-C3A-C2A	-2.14	105.71	113.98
23	B	614	CLA	C7-C6-C5	-2.14	107.56	113.26
23	D	401	CLA	C3B-C4B-NB	2.14	112.44	110.53
23	B	613	CLA	C11-C12-C13	-2.14	108.86	115.97
23	c	501	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
23	a	404	CLA	CMB-C2B-C3B	2.14	131.58	126.55
35	D	403	LMT	O1B-C1B-C2B	2.14	113.34	108.09
35	a	418	LMT	C1B-O1B-C4'	-2.14	112.92	117.98
23	a	405	CLA	C4-C3-C5	2.13	118.93	115.23
25	T	101	BCR	C10-C11-C12	-2.13	117.02	123.20
23	b	606	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
23	D	405	CLA	CHB-C4A-NA	2.13	127.48	124.40
23	a	405	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
25	c	514	BCR	C15-C16-C17	-2.13	119.16	123.52
25	T	101	BCR	C21-C20-C19	-2.13	117.03	123.20
34	c	519	LMG	O8-C28-O10	-2.13	118.30	123.63
31	d	407	LHG	O8-C23-O10	-2.13	118.31	123.63
25	b	618	BCR	C10-C11-C12	-2.13	117.04	123.20
35	B	623	LMT	O1B-C4'-C3'	2.13	112.64	107.23
23	B	616	CLA	C2A-C1A-CHA	-2.13	120.18	123.87
24	a	408	PHO	C4A-C3A-C2A	-2.12	100.82	102.84
26	A	411	SQD	O48-C23-O10	-2.12	118.31	123.63
34	m	101	LMG	C1-C2-C3	-2.12	105.54	110.01
34	c	520	LMG	C9-C8-C7	-2.12	106.83	111.78
29	D	407	PL9	C42-C41-C39	-2.12	106.15	113.19
23	B	617	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	y	101	BCR	C29-C30-C25	2.12	113.52	110.44
23	B	612	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	C	512	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
23	a	404	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
24	a	407	PHO	C4-C3-C5	2.12	118.91	115.23
25	Y	101	BCR	C38-C26-C25	-2.12	122.17	124.48
34	B	622	LMG	C8-O7-C10	-2.12	112.72	117.80
23	c	501	CLA	CMC-C2C-C1C	2.12	128.34	125.03
25	t	101	BCR	C2-C1-C6	2.12	113.52	110.44
25	D	406	BCR	C37-C22-C23	2.12	121.32	118.09
34	c	520	LMG	O8-C28-O10	-2.12	118.33	123.63
23	C	508	CLA	C6-C7-C8	-2.12	108.93	115.97
23	C	507	CLA	CMD-C2D-C3D	-2.12	122.84	127.69
23	c	510	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
26	D	413	SQD	C46-C45-C44	-2.11	106.85	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C2A-C1A-CHA	-2.11	120.20	123.87
23	b	604	CLA	CBC-CAC-C3C	-2.11	106.69	112.42
23	B	606	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
26	B	621	SQD	O48-C23-O10	-2.11	118.35	123.63
23	d	402	CLA	CHD-C4C-NC	2.11	127.50	124.23
25	Y	101	BCR	C11-C10-C9	-2.11	124.32	127.28
29	d	405	PL9	C7-C3-C2	-2.11	120.90	123.39
38	E	103	HEM	O2A-CGA-CBA	2.11	120.66	114.00
23	C	508	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	B	610	CLA	C1-O2A-CGA	2.11	121.75	116.65
34	C	501	LMG	O8-C28-C29	2.11	118.25	111.83
38	E	103	HEM	C3B-C4B-NB	-2.11	107.96	109.47
23	B	608	CLA	C4-C3-C5	2.10	118.88	115.23
25	D	406	BCR	C32-C1-C6	-2.10	106.95	110.24
23	c	512	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
35	C	522	LMT	O5'-C5'-C4'	2.10	114.06	109.72
23	C	512	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
23	B	614	CLA	CED-O2D-CGD	2.10	120.67	115.92
25	c	515	BCR	C16-C17-C18	-2.10	124.34	127.28
25	h	102	BCR	C20-C21-C22	-2.10	124.34	127.28
23	D	404	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
23	b	611	CLA	C7-C6-C5	-2.10	107.67	113.26
35	M	103	LMT	O5'-C5'-C4'	2.10	114.06	109.72
29	D	407	PL9	C17-C18-C19	-2.10	122.82	127.62
40	V	202	HEC	C2A-C1A-NA	-2.10	108.30	110.32
23	c	508	CLA	C1-O2A-CGA	2.10	121.72	116.65
23	a	404	CLA	CMA-C3A-C4A	-2.10	106.14	111.77
34	c	519	LMG	C8-O7-C10	-2.10	112.78	117.80
40	V	202	HEC	CBA-CAA-C2A	-2.09	106.74	112.53
34	a	417	LMG	O1-C1-C2	2.09	111.45	108.27
23	b	608	CLA	C11-C10-C8	-2.09	109.01	115.97
23	b	615	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
23	a	405	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
25	C	516	BCR	C34-C9-C10	-2.09	119.43	122.82
35	e	102	LMT	O5'-C5'-C4'	2.09	114.04	109.72
23	b	612	CLA	C6-C5-C3	-2.09	108.38	113.47
25	C	516	BCR	C15-C16-C17	-2.09	119.25	123.52
23	B	603	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
37	C	517	DGD	O1G-C1A-O1A	-2.08	118.42	123.63
25	a	410	BCR	C15-C16-C17	-2.08	119.26	123.52
24	A	406	PHO	CBA-CAA-C2A	-2.08	107.64	113.78
40	v	201	HEC	O2A-CGA-CBA	2.08	120.58	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
23	a	406	CLA	C2A-C1A-CHA	-2.08	120.26	123.87
23	A	407	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
26	D	413	SQD	O7-S-C6	2.08	109.86	106.76
23	c	507	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	b	619	BCR	C33-C5-C4	2.08	118.02	113.60
40	v	201	HEC	C2A-C1A-NA	-2.07	108.32	110.32
23	b	608	CLA	C4-C3-C5	2.07	118.83	115.23
23	c	501	CLA	CMB-C2B-C1B	2.07	128.58	125.42
23	b	613	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
23	B	606	CLA	C4-C3-C5	2.07	118.83	115.23
23	B	604	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
25	b	617	BCR	C29-C30-C25	2.07	113.45	110.44
23	b	615	CLA	C6-C7-C8	-2.07	109.08	115.97
24	D	402	PHO	C4A-C3A-C2A	-2.07	100.87	102.84
25	C	516	BCR	C38-C26-C25	-2.07	122.22	124.48
25	c	514	BCR	C34-C9-C10	-2.07	119.46	122.82
24	A	406	PHO	C7-C6-C5	-2.07	107.75	113.26
25	C	516	BCR	C37-C22-C23	2.07	121.25	118.09
23	a	409	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
23	b	602	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
23	d	402	CLA	CAC-C3C-C4C	2.07	127.48	124.79
36	B	624	HTG	O5-C1-C2	2.07	113.17	110.32
23	b	606	CLA	C1-O2A-CGA	2.07	121.65	116.65
23	D	401	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
23	B	615	CLA	CAA-C2A-C3A	-2.07	107.42	113.00
23	C	512	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
23	c	507	CLA	CHB-C1B-C2B	-2.06	121.43	127.43
23	b	601	CLA	CAC-C3C-C4C	2.06	127.48	124.79
23	b	609	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
23	B	611	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
23	c	510	CLA	C6-C7-C8	-2.06	109.11	115.97
23	D	405	CLA	O2A-CGA-CBA	2.06	118.12	111.83
25	B	618	BCR	C21-C20-C19	-2.06	117.23	123.20
23	B	608	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
38	e	103	HEM	O2D-CGD-CBD	2.06	120.51	114.00
25	c	514	BCR	C37-C22-C23	2.06	121.23	118.09
40	v	201	HEC	C4C-NC-C1C	2.06	109.18	105.82
37	C	519	DGD	O1G-C1A-O1A	-2.06	118.48	123.63
23	b	601	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
37	c	516	DGD	C6D-O5D-C1E	-2.06	109.38	113.80
23	D	404	CLA	OBD-CAD-C3D	-2.06	123.61	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	e	102	LMT	C1B-C2B-C3B	2.06	114.34	110.01
23	c	509	CLA	C6-C5-C3	-2.06	108.46	113.47
23	b	616	CLA	CBC-CAC-C3C	-2.05	106.85	112.42
23	c	510	CLA	CED-O2D-CGD	2.05	120.58	115.92
23	B	612	CLA	CED-O2D-CGD	2.05	120.57	115.92
25	b	619	BCR	C2-C1-C6	2.05	113.42	110.44
23	c	512	CLA	CMC-C2C-C1C	2.05	128.24	125.03
37	c	518	DGD	O6E-C1E-O5D	-2.05	105.19	110.04
25	a	410	BCR	C3-C4-C5	-2.05	110.40	114.06
23	B	614	CLA	CMB-C2B-C3B	2.05	131.37	126.55
23	B	606	CLA	C4B-C3B-C2B	-2.05	104.75	107.30
23	c	503	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	H	101	BCR	C39-C30-C25	-2.05	107.03	110.24
24	D	402	PHO	CAA-CBA-CGA	-2.05	107.40	113.21
23	B	602	CLA	CMC-C2C-C1C	2.05	128.23	125.03
23	c	513	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
23	A	405	CLA	CMC-C2C-C1C	2.04	128.22	125.03
23	b	608	CLA	CAC-C3C-C4C	2.04	127.45	124.79
23	c	504	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
23	b	616	CLA	CED-O2D-CGD	2.04	120.55	115.92
23	b	610	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
23	D	404	CLA	C11-C12-C13	-2.04	109.19	115.97
25	y	101	BCR	C16-C15-C14	-2.04	119.35	123.52
25	b	617	BCR	C38-C26-C25	-2.03	122.27	124.48
23	B	616	CLA	CHB-C4A-NA	2.03	127.33	124.40
34	B	622	LMG	C12-C11-C10	-2.03	106.25	113.69
26	B	621	SQD	O47-C7-O49	-2.03	118.95	123.70
23	A	404	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
25	b	618	BCR	C8-C7-C6	-2.03	121.57	127.00
23	B	610	CLA	C2A-C1A-CHA	-2.03	120.34	123.87
29	D	407	PL9	C47-C48-C49	-2.03	120.88	127.64
31	d	407	LHG	C5-O7-C7	-2.03	112.94	117.80
23	b	616	CLA	CHA-C1A-NA	-2.03	121.80	126.39
23	B	617	CLA	CAC-C3C-C4C	2.03	127.43	124.79
23	C	502	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
25	C	527	BCR	C33-C5-C6	-2.03	122.27	124.48
23	B	617	CLA	CAA-C2A-C3A	-2.03	107.53	113.00
26	a	411	SQD	O48-C23-O10	-2.02	118.56	123.63
23	b	608	CLA	CMB-C2B-C1B	2.02	128.50	125.42
23	c	503	CLA	C2A-C1A-CHA	-2.02	120.35	123.87
25	b	618	BCR	C15-C16-C17	-2.02	119.38	123.52
23	a	409	CLA	CMA-C3A-C4A	-2.02	106.33	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
23	C	513	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
25	c	514	BCR	C10-C11-C12	-2.02	117.34	123.20
34	C	501	LMG	C30-C29-C28	-2.02	106.29	113.69
25	c	515	BCR	C31-C1-C6	-2.02	107.08	110.24
37	H	102	DGD	C2G-O2G-C1B	-2.02	112.97	117.80
25	B	619	BCR	C28-C27-C26	-2.02	110.46	114.06
25	a	410	BCR	C34-C9-C8	2.02	121.17	118.09
34	C	501	LMG	C9-C8-C7	-2.02	107.09	111.78
23	B	602	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
23	C	510	CLA	C16-C15-C13	-2.01	109.27	115.97
25	k	101	BCR	C16-C15-C14	-2.01	119.40	123.52
25	T	101	BCR	C37-C22-C23	2.01	121.17	118.09
23	b	609	CLA	C7-C6-C5	-2.01	107.89	113.26
23	a	409	CLA	CHB-C4A-NA	2.01	127.31	124.40
25	Y	101	BCR	C8-C7-C6	-2.01	121.62	127.00
34	z	101	LMG	C7-O1-C1	-2.01	109.48	113.80
36	b	621	HTG	C3-C4-C5	2.01	113.88	110.23
23	c	512	CLA	CHA-C1A-NA	-2.01	121.83	126.39
25	h	102	BCR	C11-C10-C9	-2.01	124.46	127.28
29	d	405	PL9	C36-C34-C33	-2.01	116.66	121.17
23	B	616	CLA	CHA-C1A-NA	-2.01	121.84	126.39
23	D	401	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
23	b	610	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
26	a	411	SQD	O9-S-C6	2.01	109.75	106.76
23	C	507	CLA	CMB-C2B-C1B	2.01	128.47	125.42
23	b	614	CLA	CMA-C3A-C2A	-2.01	106.23	113.98
24	A	406	PHO	C4D-CHA-CBD	2.01	109.42	108.45
25	H	101	BCR	C16-C15-C14	-2.00	119.42	123.52
23	C	505	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
26	A	411	SQD	C46-C45-C44	-2.00	107.12	111.78
26	a	413	SQD	O48-C23-O10	-2.00	118.62	123.63

All (65) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	608	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	B	617	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	401	CLA	ND
23	D	404	CLA	ND
23	D	405	CLA	ND
23	a	404	CLA	ND
23	a	405	CLA	ND
23	a	409	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	501	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (1345) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2B-C3B-CAB-CBB
23	B	603	CLA	C4B-C3B-CAB-CBB
23	B	604	CLA	C2B-C3B-CAB-CBB
23	B	604	CLA	C4B-C3B-CAB-CBB
23	B	604	CLA	C2-C3-C5-C6
23	B	604	CLA	C4-C3-C5-C6
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	B	617	CLA	C2B-C3B-CAB-CBB
23	B	617	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	506	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	C2-C1-O2A-CGA
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	514	CLA	C2B-C3B-CAB-CBB
23	C	514	CLA	C4B-C3B-CAB-CBB
23	a	406	CLA	C2B-C3B-CAB-CBB
23	a	406	CLA	C4B-C3B-CAB-CBB
23	a	409	CLA	C2B-C3B-CAB-CBB
23	a	409	CLA	C4B-C3B-CAB-CBB
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C11-C12-C13-C14
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	C2B-C3B-CAB-CBB
23	c	501	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C14-C13-C15-C16
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C2-C1-O2A-CGA
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	d	403	CLA	C2B-C3B-CAB-CBB
23	d	403	CLA	C4B-C3B-CAB-CBB
25	D	406	BCR	C7-C8-C9-C10
25	D	406	BCR	C21-C22-C23-C24
25	H	101	BCR	C5-C6-C7-C8
25	H	101	BCR	C7-C8-C9-C34
25	T	101	BCR	C7-C8-C9-C10
25	T	101	BCR	C13-C14-C15-C16
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	d	404	BCR	C7-C8-C9-C10
25	d	404	BCR	C7-C8-C9-C34
25	d	404	BCR	C21-C22-C23-C24
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	411	SQD	C5-C6-S-O7
26	A	411	SQD	C5-C6-S-O8
26	A	411	SQD	C5-C6-S-O9
26	B	621	SQD	O49-C7-O47-C45
26	B	621	SQD	C8-C7-O47-C45
26	B	621	SQD	C5-C6-S-O7
26	B	621	SQD	C5-C6-S-O9
26	D	413	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
26	D	413	SQD	C8-C7-O47-C45
26	D	413	SQD	C5-C6-S-O7
26	D	413	SQD	C5-C6-S-O8
26	D	413	SQD	C5-C6-S-O9
26	L	102	SQD	O49-C7-O47-C45
26	L	102	SQD	C8-C7-O47-C45
26	L	102	SQD	C5-C6-S-O7
26	L	102	SQD	C5-C6-S-O8
26	L	102	SQD	C5-C6-S-O9
26	a	413	SQD	C5-C6-S-O7
26	a	413	SQD	C5-C6-S-O8
26	a	413	SQD	C5-C6-S-O9
26	f	101	SQD	O49-C7-O47-C45
26	f	101	SQD	C8-C7-O47-C45
26	f	101	SQD	C5-C6-S-O7
26	f	101	SQD	C5-C6-S-O8
26	f	101	SQD	C5-C6-S-O9
27	B	627	GOL	O1-C1-C2-C3
27	B	628	GOL	C1-C2-C3-O3
27	B	628	GOL	O2-C2-C3-O3
27	C	525	GOL	O1-C1-C2-O2
27	C	525	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	a	412	GOL	O1-C1-C2-O2
27	a	412	GOL	O1-C1-C2-C3
27	b	624	GOL	O1-C1-C2-C3
27	d	401	GOL	O1-C1-C2-O2
27	d	401	GOL	O1-C1-C2-C3
29	A	413	PL9	C15-C14-C16-C17
29	a	415	PL9	C14-C16-C17-C18
31	D	408	LHG	C3-O3-P-O4
31	D	408	LHG	C4-O6-P-O3
31	D	408	LHG	C4-O6-P-O4
31	D	408	LHG	C4-O6-P-O5
31	E	101	LHG	C3-O3-P-O4
31	E	101	LHG	C3-O3-P-O5
31	E	101	LHG	C3-O3-P-O6
31	E	101	LHG	O10-C23-O8-C6
31	E	101	LHG	C24-C23-O8-C6
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	b	630	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
31	b	630	LHG	C4-O6-P-O4
31	b	630	LHG	C4-O6-P-O5
31	d	406	LHG	C3-O3-P-O4
31	d	406	LHG	C3-O3-P-O6
31	d	407	LHG	O2-C2-C3-O3
31	d	407	LHG	C3-O3-P-O5
31	d	407	LHG	C3-O3-P-O6
31	d	407	LHG	C4-O6-P-O3
31	d	407	LHG	C4-O6-P-O4
31	d	407	LHG	C4-O6-P-O5
31	d	408	LHG	C4-O6-P-O4
31	e	101	LHG	C3-O3-P-O5
31	e	101	LHG	O10-C23-O8-C6
31	e	101	LHG	C24-C23-O8-C6
34	C	501	LMG	O9-C10-O7-C8
34	Z	101	LMG	C2-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
34	c	520	LMG	O9-C10-O7-C8
34	c	520	LMG	C11-C10-O7-C8
34	z	101	LMG	O6-C1-O1-C7
34	z	101	LMG	O9-C10-O7-C8
34	z	101	LMG	C11-C10-O7-C8
35	B	632	LMT	O5'-C1'-O1'-C1
35	B	633	LMT	O5'-C1'-O1'-C1
35	B	634	LMT	O5'-C1'-O1'-C1
35	C	522	LMT	O5'-C1'-O1'-C1
35	D	403	LMT	C2'-C1'-O1'-C1
35	D	403	LMT	O5'-C1'-O1'-C1
35	b	620	LMT	C2'-C1'-O1'-C1
35	b	620	LMT	O5'-C1'-O1'-C1
35	b	628	LMT	O5'-C1'-O1'-C1
35	m	103	LMT	C2'-C1'-O1'-C1
36	B	625	HTG	C2'-C1'-S1-C1
36	B	626	HTG	O5-C1-S1-C1'
38	E	103	HEM	C2C-C3C-CAC-CBC
38	e	103	HEM	C2B-C3B-CAB-CBB
38	e	103	HEM	C2C-C3C-CAC-CBC
38	e	103	HEM	C4C-C3C-CAC-CBC
40	V	202	HEC	C2B-C3B-CAB-CBB
40	V	202	HEC	C4B-C3B-CAB-CBB
40	V	202	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
40	V	202	HEC	C4C-C3C-CAC-CBC
40	v	201	HEC	C2B-C3B-CAB-CBB
40	v	201	HEC	C4B-C3B-CAB-CBB
40	v	201	HEC	C2C-C3C-CAC-CBC
40	v	201	HEC	C4C-C3C-CAC-CBC
23	b	608	CLA	O1D-CGD-O2D-CED
35	C	522	LMT	C3'-C4'-O1B-C1B
23	B	615	CLA	C3-C5-C6-C7
23	b	614	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
34	C	501	LMG	C11-C10-O7-C8
23	C	504	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	C4-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
29	A	413	PL9	C25-C24-C26-C27
29	a	415	PL9	C30-C29-C31-C32
23	B	615	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	C	507	CLA	C2-C3-C5-C6
23	b	604	CLA	C2-C3-C5-C6
29	A	413	PL9	C13-C14-C16-C17
29	A	413	PL9	C23-C24-C26-C27
29	a	415	PL9	C28-C29-C31-C32
23	c	507	CLA	C2A-CAA-CBA-CGA
23	A	407	CLA	C3-C5-C6-C7
23	c	506	CLA	C3-C5-C6-C7
23	B	617	CLA	C3-C5-C6-C7
23	C	513	CLA	C3-C5-C6-C7
23	c	501	CLA	CBD-CGD-O2D-CED
31	A	415	LHG	O2-C2-C3-O3
34	C	521	LMG	O6-C5-C6-O5
35	M	103	LMT	C4B-C5B-C6B-O6B
23	c	509	CLA	CBD-CGD-O2D-CED
35	C	522	LMT	O5B-C5B-C6B-O6B
35	B	623	LMT	O5B-C5B-C6B-O6B
35	M	103	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
34	c	519	LMG	C4-C5-C6-O5
23	C	508	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	c	504	CLA	C4-C3-C5-C6
29	a	415	PL9	C25-C24-C26-C27
23	C	508	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	c	504	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
36	B	626	HTG	O5-C5-C6-O6
29	A	413	PL9	C14-C16-C17-C18
29	D	407	PL9	C39-C41-C42-C43
29	d	405	PL9	C39-C41-C42-C43
36	h	101	HTG	C4-C5-C6-O6
23	A	405	CLA	CBD-CGD-O2D-CED
23	C	514	CLA	CBD-CGD-O2D-CED
36	b	625	HTG	O5-C5-C6-O6
35	E	102	LMT	O5'-C1'-O1'-C1
35	M	103	LMT	O5'-C1'-O1'-C1
35	a	418	LMT	O5'-C1'-O1'-C1
35	e	102	LMT	O5'-C1'-O1'-C1
35	m	103	LMT	O5'-C1'-O1'-C1
34	c	520	LMG	O6-C5-C6-O5
34	c	519	LMG	O6-C5-C6-O5
35	E	102	LMT	O5'-C5'-C6'-O6'
23	c	509	CLA	C3-C5-C6-C7
25	t	101	BCR	C13-C14-C15-C16
31	A	415	LHG	C1-C2-C3-O3
31	d	407	LHG	C1-C2-C3-O3
23	A	407	CLA	CBA-CGA-O2A-C1
23	B	602	CLA	CBA-CGA-O2A-C1
23	C	510	CLA	CBA-CGA-O2A-C1
36	h	101	HTG	O5-C5-C6-O6
29	a	415	PL9	C15-C14-C16-C17
23	b	614	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
29	a	415	PL9	C13-C14-C16-C17
23	b	614	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	C6-C7-C8-C9
23	B	606	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C11-C10-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	504	CLA	C11-C12-C13-C14
23	c	506	CLA	C6-C7-C8-C9
23	c	512	CLA	C6-C7-C8-C9
35	B	623	LMT	C4B-C5B-C6B-O6B
35	B	632	LMT	C2'-C1'-O1'-C1
35	B	633	LMT	C2'-C1'-O1'-C1
35	E	102	LMT	C2'-C1'-O1'-C1
35	M	103	LMT	C2'-C1'-O1'-C1
35	a	418	LMT	C2'-C1'-O1'-C1
35	e	102	LMT	C2'-C1'-O1'-C1
31	D	408	LHG	O2-C2-C3-O3
25	D	406	BCR	C7-C8-C9-C34
25	D	406	BCR	C37-C22-C23-C24
25	T	101	BCR	C7-C8-C9-C34
25	d	404	BCR	C37-C22-C23-C24
35	M	103	LMT	O5B-C5B-C6B-O6B
25	H	101	BCR	C7-C8-C9-C10
35	E	102	LMT	C4'-C5'-C6'-O6'
26	A	409	SQD	C8-C7-O47-C45
26	A	411	SQD	O6-C44-C45-O47
26	a	413	SQD	O6-C44-C45-O47
23	C	511	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	C5-C6-C7-C8
34	Z	101	LMG	C10-C11-C12-C13
23	b	601	CLA	C2-C1-O2A-CGA
31	d	408	LHG	C33-C34-C35-C36
34	z	101	LMG	O6-C5-C6-O5
23	c	511	CLA	C3-C5-C6-C7
23	C	510	CLA	O1A-CGA-O2A-C1
23	a	404	CLA	C15-C16-C17-C18
23	B	616	CLA	C11-C12-C13-C15
23	a	409	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
31	d	408	LHG	C24-C23-O8-C6
36	c	522	HTG	O5-C5-C6-O6
23	B	617	CLA	C10-C11-C12-C13
35	B	623	LMT	C3'-C4'-O1B-C1B
29	a	415	PL9	C24-C26-C27-C28
23	b	611	CLA	C15-C16-C17-C18
23	b	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
37	C	518	DGD	C1A-C2A-C3A-C4A
23	B	602	CLA	C5-C6-C7-C8
23	B	602	CLA	C15-C16-C17-C18
23	B	615	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
23	C	514	CLA	C13-C15-C16-C17
23	b	607	CLA	C13-C15-C16-C17
23	c	507	CLA	C8-C10-C11-C12
23	c	509	CLA	C5-C6-C7-C8
23	B	606	CLA	C5-C6-C7-C8
36	b	623	HTG	O5-C5-C6-O6
37	c	517	DGD	C1B-C2B-C3B-C4B
23	A	407	CLA	O1A-CGA-O2A-C1
26	B	621	SQD	O5-C1-O6-C44
23	C	506	CLA	C8-C10-C11-C12
23	b	605	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
23	b	614	CLA	C13-C15-C16-C17
23	c	502	CLA	C13-C15-C16-C17
23	c	502	CLA	C15-C16-C17-C18
23	c	513	CLA	C15-C16-C17-C18
35	B	623	LMT	C5'-C4'-O1B-C1B
23	B	602	CLA	O1A-CGA-O2A-C1
34	c	520	LMG	C4-C5-C6-O5
26	A	409	SQD	O49-C7-O47-C45
35	M	103	LMT	C4'-C5'-C6'-O6'
23	b	616	CLA	C3-C5-C6-C7
23	B	607	CLA	C13-C15-C16-C17
23	b	602	CLA	C15-C16-C17-C18
23	c	504	CLA	C5-C6-C7-C8
23	d	403	CLA	O1A-CGA-O2A-C1
37	c	516	DGD	O6D-C5D-C6D-O5D
34	c	519	LMG	C28-C29-C30-C31
23	C	509	CLA	C10-C11-C12-C13
23	b	601	CLA	C8-C10-C11-C12
23	b	604	CLA	C15-C16-C17-C18
23	b	605	CLA	C8-C10-C11-C12
23	B	606	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CBA-CGA-O2A-C1
35	B	634	LMT	O1'-C1-C2-C3
23	C	511	CLA	O1A-CGA-O2A-C1
23	a	409	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	C13-C15-C16-C17
23	b	604	CLA	C3-C5-C6-C7
34	a	417	LMG	O9-C10-O7-C8
23	B	607	CLA	C2A-CAA-CBA-CGA
35	b	628	LMT	O1'-C1-C2-C3
23	C	502	CLA	C15-C16-C17-C18
23	b	606	CLA	C15-C16-C17-C18
23	C	503	CLA	CBD-CGD-O2D-CED
37	C	517	DGD	O6D-C5D-C6D-O5D
23	C	507	CLA	C8-C10-C11-C12
23	b	606	CLA	C10-C11-C12-C13
23	B	616	CLA	C8-C10-C11-C12
23	c	510	CLA	C10-C11-C12-C13
23	B	605	CLA	C4-C3-C5-C6
34	a	417	LMG	C11-C10-O7-C8
31	D	408	LHG	C32-C33-C34-C35
35	B	634	LMT	C2'-C1'-O1'-C1
37	C	518	DGD	C2E-C1E-O5D-C6D
37	c	516	DGD	C2E-C1E-O5D-C6D
23	c	509	CLA	O1D-CGD-O2D-CED
29	a	415	PL9	C39-C41-C42-C43
23	b	604	CLA	C8-C10-C11-C12
23	b	611	CLA	C8-C10-C11-C12
31	d	408	LHG	O10-C23-O8-C6
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
37	C	517	DGD	C4D-C5D-C6D-O5D
37	c	516	DGD	C4D-C5D-C6D-O5D
23	B	603	CLA	C15-C16-C17-C18
27	A	410	GOL	O1-C1-C2-C3
27	A	410	GOL	C1-C2-C3-O3
27	B	627	GOL	C1-C2-C3-O3
31	A	415	LHG	O1-C1-C2-C3
31	D	409	LHG	O1-C1-C2-C3
35	C	522	LMT	C4B-C5B-C6B-O6B
26	B	621	SQD	C30-C31-C32-C33
23	B	616	CLA	C16-C17-C18-C20
26	L	102	SQD	C18-C19-C20-C21
31	e	101	LHG	C11-C12-C13-C14
34	Z	101	LMG	O6-C1-O1-C7
37	c	516	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
34	j	101	LMG	C10-C11-C12-C13
36	B	624	HTG	C1'-C2'-C3'-C4'
23	c	501	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	C16-C17-C18-C19
23	B	606	CLA	O1A-CGA-O2A-C1
26	A	409	SQD	C9-C10-C11-C12
26	a	411	SQD	C9-C10-C11-C12
34	j	101	LMG	C21-C22-C23-C24
31	d	408	LHG	C32-C33-C34-C35
34	m	101	LMG	C35-C36-C37-C38
37	H	102	DGD	C6A-C7A-C8A-C9A
23	c	506	CLA	C10-C11-C12-C13
23	c	508	CLA	C5-C6-C7-C8
26	L	102	SQD	C27-C28-C29-C30
26	a	411	SQD	C11-C12-C13-C14
26	a	411	SQD	C15-C16-C17-C18
31	L	101	LHG	C25-C26-C27-C28
34	m	101	LMG	C38-C39-C40-C41
27	B	627	GOL	O2-C2-C3-O3
27	O	302	GOL	O1-C1-C2-O2
27	b	624	GOL	O1-C1-C2-O2
35	B	634	LMT	C2-C1-O1'-C1'
23	C	508	CLA	CBD-CGD-O2D-CED
34	a	417	LMG	C31-C32-C33-C34
35	m	103	LMT	C7-C8-C9-C10
23	C	514	CLA	O1D-CGD-O2D-CED
23	A	405	CLA	C4B-C3B-CAB-CBB
23	B	608	CLA	C4B-C3B-CAB-CBB
23	D	404	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	B	609	CLA	C16-C17-C18-C20
23	B	611	CLA	C2A-CAA-CBA-CGA
34	m	101	LMG	C11-C10-O7-C8
34	C	521	LMG	C16-C17-C18-C19
31	E	101	LHG	C24-C25-C26-C27
36	B	629	HTG	O5-C5-C6-O6
34	C	520	LMG	C16-C17-C18-C19
34	a	417	LMG	C30-C31-C32-C33
23	B	605	CLA	C3-C5-C6-C7
34	C	501	LMG	C14-C15-C16-C17
26	A	409	SQD	C11-C10-C9-C8
23	B	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C5-C6-C7-C8
23	a	404	CLA	C13-C15-C16-C17
23	b	603	CLA	C13-C15-C16-C17
23	c	506	CLA	C13-C15-C16-C17
23	B	611	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
23	c	502	CLA	C16-C17-C18-C20
34	B	622	LMG	C36-C37-C38-C39
34	J	101	LMG	C19-C20-C21-C22
23	b	615	CLA	C13-C15-C16-C17
34	C	521	LMG	C37-C38-C39-C40
37	C	519	DGD	CBA-CCA-CDA-CEA
31	D	409	LHG	C24-C23-O8-C6
26	a	413	SQD	C24-C25-C26-C27
23	D	401	CLA	C15-C16-C17-C18
35	b	628	LMT	C4'-C5'-C6'-O6'
36	B	626	HTG	C4-C5-C6-O6
26	D	413	SQD	C30-C31-C32-C33
37	H	102	DGD	CBA-CCA-CDA-CEA
36	h	101	HTG	S1-C1'-C2'-C3'
31	D	408	LHG	C13-C14-C15-C16
34	B	622	LMG	C28-C29-C30-C31
23	A	405	CLA	C2B-C3B-CAB-CBB
23	C	506	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C2B-C3B-CAB-CBB
25	D	406	BCR	C23-C24-C25-C30
25	H	101	BCR	C1-C6-C7-C8
25	T	101	BCR	C1-C6-C7-C8
25	T	101	BCR	C5-C6-C7-C8
34	Z	101	LMG	C17-C18-C19-C20
26	L	102	SQD	C24-C25-C26-C27
34	J	101	LMG	C30-C31-C32-C33
36	B	626	HTG	C3'-C4'-C5'-C6'
35	b	620	LMT	C1-C2-C3-C4
23	a	404	CLA	C2A-CAA-CBA-CGA
31	A	415	LHG	C32-C33-C34-C35
37	C	517	DGD	C9A-CAA-CBA-CCA
31	D	409	LHG	O10-C23-O8-C6
29	a	415	PL9	C4-C3-C7-C8
26	A	411	SQD	C16-C17-C18-C19
34	c	519	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
37	c	517	DGD	C4B-C5B-C6B-C7B
34	m	101	LMG	O9-C10-O7-C8
23	A	405	CLA	O1D-CGD-O2D-CED
31	e	101	LHG	C26-C27-C28-C29
37	C	517	DGD	C5B-C6B-C7B-C8B
23	C	511	CLA	C5-C6-C7-C8
29	a	415	PL9	C23-C24-C26-C27
26	A	409	SQD	C12-C13-C14-C15
23	B	617	CLA	C6-C7-C8-C9
26	A	411	SQD	C18-C19-C20-C21
37	c	516	DGD	C5A-C6A-C7A-C8A
37	C	518	DGD	O6E-C1E-O5D-C6D
37	c	517	DGD	O6E-C1E-O5D-C6D
26	A	409	SQD	C15-C16-C17-C18
37	C	517	DGD	C8A-C9A-CAA-CBA
37	H	102	DGD	C5B-C6B-C7B-C8B
34	m	101	LMG	C39-C40-C41-C42
34	C	520	LMG	C12-C13-C14-C15
35	B	634	LMT	C6-C7-C8-C9
35	M	103	LMT	O1'-C1-C2-C3
26	A	411	SQD	C8-C7-O47-C45
26	a	413	SQD	C8-C7-O47-C45
31	E	101	LHG	C8-C7-O7-C5
26	D	413	SQD	C7-C8-C9-C10
26	B	621	SQD	C24-C25-C26-C27
31	D	408	LHG	C14-C15-C16-C17
37	h	103	DGD	CAA-CBA-CCA-CDA
23	b	605	CLA	C3-C5-C6-C7
23	B	611	CLA	C16-C17-C18-C20
23	b	607	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	c	502	CLA	C16-C17-C18-C19
31	D	409	LHG	C13-C14-C15-C16
31	b	630	LHG	C12-C13-C14-C15
23	C	506	CLA	C4-C3-C5-C6
31	D	408	LHG	C16-C17-C18-C19
34	C	521	LMG	C17-C18-C19-C20
34	m	101	LMG	C14-C15-C16-C17
35	b	628	LMT	C4-C5-C6-C7
23	B	605	CLA	C2C-C3C-CAC-CBC
35	m	103	LMT	C11-C10-C9-C8
36	B	625	HTG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
35	M	101	LMT	C2-C3-C4-C5
23	b	601	CLA	C3-C5-C6-C7
23	b	601	CLA	C10-C11-C12-C13
26	a	413	SQD	C25-C26-C27-C28
34	B	622	LMG	C17-C18-C19-C20
26	D	413	SQD	C23-C24-C25-C26
26	L	102	SQD	C14-C15-C16-C17
35	B	633	LMT	C2-C3-C4-C5
29	d	405	PL9	C34-C36-C37-C38
23	C	512	CLA	CBD-CGD-O2D-CED
34	B	622	LMG	C11-C10-O7-C8
23	B	611	CLA	C13-C15-C16-C17
23	b	608	CLA	C13-C15-C16-C17
38	E	103	HEM	C4C-C3C-CAC-CBC
38	e	103	HEM	C4B-C3B-CAB-CBB
37	C	517	DGD	C7B-C8B-C9B-CAB
37	C	518	DGD	CAB-CBB-CCB-CDB
31	D	409	LHG	C26-C27-C28-C29
23	B	612	CLA	C8-C10-C11-C12
23	C	507	CLA	C13-C15-C16-C17
23	D	405	CLA	C10-C11-C12-C13
37	C	519	DGD	C8B-C9B-CAB-CBB
34	Z	101	LMG	O6-C5-C6-O5
35	B	623	LMT	O5'-C5'-C6'-O6'
26	A	409	SQD	O6-C44-C45-O47
26	a	411	SQD	C27-C28-C29-C30
26	f	101	SQD	C29-C30-C31-C32
37	C	518	DGD	C7B-C8B-C9B-CAB
37	c	517	DGD	C5A-C6A-C7A-C8A
37	c	517	DGD	C9A-CAA-CBA-CCA
37	c	517	DGD	C3B-C4B-C5B-C6B
31	L	101	LHG	C34-C35-C36-C37
35	C	522	LMT	O5'-C5'-C6'-O6'
23	B	609	CLA	C16-C17-C18-C19
23	C	510	CLA	C8-C10-C11-C12
35	D	403	LMT	O1'-C1-C2-C3
31	d	406	LHG	C25-C26-C27-C28
34	C	521	LMG	C15-C16-C17-C18
34	J	101	LMG	C35-C36-C37-C38
23	c	510	CLA	C3-C5-C6-C7
26	a	413	SQD	C7-C8-C9-C10
23	C	506	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	505	CLA	C2-C3-C5-C6
23	B	610	CLA	CBD-CGD-O2D-CED
26	D	413	SQD	C24-C25-C26-C27
24	D	402	PHO	C2C-C3C-CAC-CBC
37	H	102	DGD	CDB-CEB-CFB-CGB
31	E	101	LHG	C27-C28-C29-C30
23	B	612	CLA	C16-C17-C18-C20
37	c	516	DGD	O6E-C5E-C6E-O5E
27	A	410	GOL	O1-C1-C2-O2
27	B	627	GOL	O1-C1-C2-O2
23	B	610	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	a	406	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
26	L	102	SQD	C13-C14-C15-C16
26	D	413	SQD	C32-C33-C34-C35
26	L	102	SQD	C10-C11-C12-C13
36	b	625	HTG	C3'-C4'-C5'-C6'
31	b	630	LHG	O6-C4-C5-C6
26	A	411	SQD	O49-C7-O47-C45
26	a	413	SQD	O49-C7-O47-C45
23	B	605	CLA	C6-C7-C8-C10
23	b	601	CLA	C6-C7-C8-C10
36	b	621	HTG	S1-C1'-C2'-C3'
23	a	409	CLA	C16-C17-C18-C20
23	b	615	CLA	C5-C6-C7-C8
31	L	101	LHG	C17-C18-C19-C20
35	b	628	LMT	O5'-C5'-C6'-O6'
23	B	616	CLA	C4-C3-C5-C6
29	D	407	PL9	C30-C29-C31-C32
35	e	102	LMT	C4'-C5'-C6'-O6'
23	b	609	CLA	C2-C3-C5-C6
29	D	407	PL9	C13-C14-C16-C17
29	D	407	PL9	C28-C29-C31-C32
34	C	521	LMG	C4-C5-C6-O5
23	B	615	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C9
26	A	411	SQD	C15-C16-C17-C18
35	e	102	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
34	C	520	LMG	C37-C38-C39-C40
34	J	101	LMG	C12-C13-C14-C15
23	b	601	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
37	c	516	DGD	C2A-C1A-O1G-C1G
23	B	606	CLA	C8-C10-C11-C12
31	E	101	LHG	O9-C7-O7-C5
34	B	622	LMG	O9-C10-O7-C8
35	C	522	LMT	C2'-C1'-O1'-C1
23	b	612	CLA	C10-C11-C12-C13
36	b	623	HTG	S1-C1'-C2'-C3'
26	a	413	SQD	C27-C28-C29-C30
26	B	621	SQD	C44-C45-C46-O48
26	L	102	SQD	C44-C45-C46-O48
31	e	101	LHG	C9-C10-C11-C12
23	b	611	CLA	CBA-CGA-O2A-C1
34	J	101	LMG	O6-C5-C6-O5
23	B	612	CLA	C16-C17-C18-C19
26	a	413	SQD	C33-C34-C35-C36
35	e	102	LMT	C3-C4-C5-C6
37	C	517	DGD	O6E-C5E-C6E-O5E
34	j	101	LMG	C38-C39-C40-C41
31	L	101	LHG	C12-C13-C14-C15
23	b	611	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
23	B	616	CLA	C2-C3-C5-C6
23	b	611	CLA	C2-C3-C5-C6
23	B	603	CLA	C13-C15-C16-C17
23	a	405	CLA	C15-C16-C17-C18
23	b	609	CLA	C13-C15-C16-C17
31	d	407	LHG	C34-C35-C36-C37
34	j	101	LMG	O6-C5-C6-O5
23	b	611	CLA	O1A-CGA-O2A-C1
23	b	610	CLA	C15-C16-C17-C18
34	j	101	LMG	C29-C30-C31-C32
35	C	522	LMT	C1-C2-C3-C4
31	D	408	LHG	C7-C8-C9-C10
26	B	621	SQD	C24-C23-O48-C46
37	c	518	DGD	C2A-C1A-O1G-C1G
26	L	102	SQD	C46-C45-O47-C7
37	H	102	DGD	C4A-C5A-C6A-C7A
35	b	628	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
34	C	501	LMG	C10-C11-C12-C13
37	c	516	DGD	O1A-C1A-O1G-C1G
37	c	517	DGD	CBA-CCA-CDA-CEA
26	L	102	SQD	C24-C23-O48-C46
31	d	408	LHG	C27-C28-C29-C30
34	c	519	LMG	C35-C36-C37-C38
37	C	518	DGD	C9B-CAB-CBB-CCB
37	c	518	DGD	CAB-CBB-CCB-CDB
31	A	415	LHG	C25-C26-C27-C28
31	D	408	LHG	C28-C29-C30-C31
34	a	417	LMG	C35-C36-C37-C38
31	L	101	LHG	C30-C31-C32-C33
37	h	103	DGD	C5B-C6B-C7B-C8B
26	f	101	SQD	O6-C44-C45-O47
36	b	625	HTG	C4'-C5'-C6'-C7'
31	A	415	LHG	C9-C10-C11-C12
31	L	101	LHG	C24-C25-C26-C27
23	C	502	CLA	C2A-CAA-CBA-CGA
35	m	103	LMT	C9-C10-C11-C12
35	E	102	LMT	C2B-C1B-O1B-C4'
23	b	601	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
37	C	518	DGD	CDA-CEA-CFA-CGA
34	C	520	LMG	C11-C10-O7-C8
23	C	503	CLA	O1D-CGD-O2D-CED
26	A	409	SQD	C16-C17-C18-C19
37	C	518	DGD	CCB-CDB-CEB-CFB
37	c	516	DGD	CDA-CEA-CFA-CGA
26	f	101	SQD	C26-C27-C28-C29
23	C	511	CLA	C4-C3-C5-C6
23	b	601	CLA	C4-C3-C5-C6
29	d	405	PL9	C15-C14-C16-C17
23	b	605	CLA	CBA-CGA-O2A-C1
37	c	518	DGD	CBA-CCA-CDA-CEA
31	A	415	LHG	C11-C10-C9-C8
31	D	409	LHG	O1-C1-C2-O2
23	B	605	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	b	601	CLA	C11-C10-C8-C9
34	C	520	LMG	C17-C18-C19-C20
23	B	613	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C10-C11-C12-C13
23	B	615	CLA	C4B-C3B-CAB-CBB
23	b	607	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
26	f	101	SQD	C31-C32-C33-C34
34	Z	101	LMG	C15-C16-C17-C18
23	c	502	CLA	C10-C11-C12-C13
35	E	102	LMT	C5-C6-C7-C8
35	E	102	LMT	O5B-C1B-O1B-C4'
34	m	101	LMG	C2-C1-O1-C7
35	b	628	LMT	C2'-C1'-O1'-C1
37	C	517	DGD	C2E-C1E-O5D-C6D
37	c	517	DGD	C2E-C1E-O5D-C6D
34	C	501	LMG	C37-C38-C39-C40
37	h	103	DGD	C9B-CAB-CBB-CCB
23	B	604	CLA	C3-C5-C6-C7
23	c	512	CLA	C3-C5-C6-C7
23	b	605	CLA	CBD-CGD-O2D-CED
36	B	624	HTG	C4'-C5'-C6'-C7'
23	b	601	CLA	CAA-CBA-CGA-O2A
37	h	103	DGD	O2G-C1B-C2B-C3B
31	d	407	LHG	C13-C14-C15-C16
23	A	405	CLA	C12-C13-C15-C16
23	B	615	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C10
23	C	514	CLA	C11-C10-C8-C7
23	b	604	CLA	C11-C10-C8-C7
23	b	611	CLA	C6-C7-C8-C10
23	b	615	CLA	C12-C13-C15-C16
23	c	502	CLA	C12-C13-C15-C16
23	c	506	CLA	C6-C7-C8-C10
23	a	409	CLA	C16-C17-C18-C19
31	b	630	LHG	C32-C33-C34-C35
35	a	418	LMT	C4-C5-C6-C7
37	c	518	DGD	O1A-C1A-O1G-C1G
34	z	101	LMG	C16-C17-C18-C19
23	B	610	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
23	b	609	CLA	C4-C3-C5-C6
23	c	512	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	D	407	PL9	C15-C14-C16-C17
37	H	102	DGD	O2G-C1B-C2B-C3B
23	b	605	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
26	B	621	SQD	O10-C23-O48-C46
35	m	103	LMT	C3-C4-C5-C6
23	B	605	CLA	CBA-CGA-O2A-C1
31	D	409	LHG	C17-C18-C19-C20
35	m	103	LMT	C6-C7-C8-C9
23	b	616	CLA	C8-C10-C11-C12
31	b	630	LHG	C14-C15-C16-C17
31	e	101	LHG	C24-C25-C26-C27
23	C	502	CLA	CBD-CGD-O2D-CED
26	A	409	SQD	O6-C44-C45-C46
26	A	411	SQD	O6-C44-C45-C46
26	a	413	SQD	O6-C44-C45-C46
31	E	101	LHG	C4-C5-C6-O8
31	e	101	LHG	C4-C5-C6-O8
34	a	417	LMG	C7-C8-C9-O8
26	A	411	SQD	C19-C20-C21-C22
23	B	610	CLA	O1D-CGD-O2D-CED
34	c	520	LMG	C21-C22-C23-C24
24	a	407	PHO	C4-C3-C5-C6
34	c	519	LMG	C10-C11-C12-C13
24	a	407	PHO	C2-C3-C5-C6
31	d	407	LHG	C26-C27-C28-C29
31	d	406	LHG	C32-C33-C34-C35
23	C	508	CLA	C2B-C3B-CAB-CBB
23	b	603	CLA	C2B-C3B-CAB-CBB
25	b	617	BCR	C1-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C30
35	B	632	LMT	C7-C8-C9-C10
36	B	625	HTG	C2'-C3'-C4'-C5'
26	f	101	SQD	C27-C28-C29-C30
34	C	520	LMG	C36-C37-C38-C39
23	D	401	CLA	C13-C15-C16-C17
23	b	610	CLA	C13-C15-C16-C17
31	d	407	LHG	C32-C33-C34-C35
37	C	518	DGD	C9A-CAA-CBA-CCA
37	c	517	DGD	CAA-CBA-CCA-CDA
23	c	506	CLA	C15-C16-C17-C18
23	c	509	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	a	411	SQD	O6-C44-C45-O47
31	e	101	LHG	O7-C5-C6-O8
34	c	520	LMG	O1-C7-C8-O7
29	A	413	PL9	C4-C3-C7-C8
26	a	411	SQD	C30-C31-C32-C33
37	C	517	DGD	CAB-CBB-CCB-CDB
34	a	417	LMG	C10-C11-C12-C13
23	c	511	CLA	O1A-CGA-O2A-C1
34	c	519	LMG	C29-C30-C31-C32
23	C	511	CLA	C2-C3-C5-C6
23	b	601	CLA	C2-C3-C5-C6
29	d	405	PL9	C13-C14-C16-C17
37	C	517	DGD	C6B-C7B-C8B-C9B
23	D	405	CLA	C3-C5-C6-C7
23	C	513	CLA	C14-C13-C15-C16
23	b	609	CLA	C6-C7-C8-C9
23	b	611	CLA	C6-C7-C8-C9
26	A	411	SQD	C30-C31-C32-C33
36	C	524	HTG	S1-C1'-C2'-C3'
31	d	406	LHG	C33-C34-C35-C36
31	b	630	LHG	C35-C36-C37-C38
23	b	614	CLA	O1D-CGD-O2D-CED
31	E	101	LHG	C25-C26-C27-C28
37	C	517	DGD	C3B-C4B-C5B-C6B
23	A	404	CLA	C13-C15-C16-C17
31	d	407	LHG	C14-C15-C16-C17
31	A	415	LHG	O1-C1-C2-O2
31	d	407	LHG	C24-C23-O8-C6
23	D	401	CLA	C16-C17-C18-C20
23	C	513	CLA	C10-C11-C12-C13
26	L	102	SQD	O10-C23-O48-C46
31	d	408	LHG	C9-C10-C11-C12
35	C	522	LMT	O1'-C1-C2-C3
31	D	408	LHG	C1-C2-C3-O3
35	b	620	LMT	C6-C7-C8-C9
23	C	512	CLA	CBA-CGA-O2A-C1
34	J	101	LMG	C34-C35-C36-C37
23	b	607	CLA	C16-C17-C18-C20
23	B	607	CLA	C10-C11-C12-C13
23	c	501	CLA	C10-C11-C12-C13
23	A	405	CLA	C11-C10-C8-C7
23	B	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	B	617	CLA	C12-C13-C15-C16
23	C	513	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	d	402	CLA	C11-C12-C13-C15
34	C	520	LMG	C28-C29-C30-C31
34	Z	101	LMG	C19-C20-C21-C22
37	c	516	DGD	C4B-C5B-C6B-C7B
31	b	630	LHG	C34-C35-C36-C37
26	B	621	SQD	C5-C6-S-O8
37	C	518	DGD	C5D-C6D-O5D-C1E
37	c	517	DGD	C5D-C6D-O5D-C1E
37	C	517	DGD	C7A-C8A-C9A-CAA
23	B	606	CLA	C13-C15-C16-C17
36	b	625	HTG	C4-C5-C6-O6
34	C	520	LMG	O9-C10-O7-C8
26	D	413	SQD	C29-C30-C31-C32
23	B	605	CLA	O1A-CGA-O2A-C1
23	C	512	CLA	O1A-CGA-O2A-C1
31	d	407	LHG	O10-C23-O8-C6
23	C	507	CLA	C3-C5-C6-C7
23	b	614	CLA	C15-C16-C17-C18
23	B	603	CLA	O2A-C1-C2-C3
34	c	519	LMG	C21-C22-C23-C24
23	b	615	CLA	C15-C16-C17-C18
23	C	514	CLA	C3-C5-C6-C7
37	C	519	DGD	C2A-C1A-O1G-C1G
34	m	101	LMG	O6-C1-O1-C7
37	C	517	DGD	O6E-C1E-O5D-C6D
34	m	101	LMG	O1-C7-C8-C9
34	z	101	LMG	O1-C7-C8-C9
37	h	103	DGD	O1G-C1G-C2G-C3G
34	c	520	LMG	C28-C29-C30-C31
23	C	507	CLA	C16-C17-C18-C20
34	B	622	LMG	C32-C33-C34-C35
34	B	622	LMG	C18-C19-C20-C21
23	B	605	CLA	C2-C3-C5-C6
26	D	413	SQD	C27-C28-C29-C30
26	f	101	SQD	O47-C45-C46-O48
31	E	101	LHG	O7-C5-C6-O8
34	a	417	LMG	O7-C8-C9-O8
34	m	101	LMG	O1-C7-C8-O7
34	z	101	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
37	h	103	DGD	O1G-C1G-C2G-O2G
23	c	512	CLA	C13-C15-C16-C17
23	B	617	CLA	C14-C13-C15-C16
31	d	407	LHG	C29-C30-C31-C32
31	b	630	LHG	C27-C28-C29-C30
36	B	630	HTG	S1-C1'-C2'-C3'
26	a	411	SQD	C35-C36-C37-C38
34	m	101	LMG	C22-C23-C24-C25
23	b	609	CLA	O1A-CGA-O2A-C1
37	C	519	DGD	O1A-C1A-O1G-C1G
35	B	623	LMT	C6-C7-C8-C9
31	D	408	LHG	C17-C18-C19-C20
23	b	609	CLA	CBA-CGA-O2A-C1
24	D	402	PHO	C16-C17-C18-C19
23	b	605	CLA	O1D-CGD-O2D-CED
29	d	405	PL9	C45-C44-C46-C47
36	B	625	HTG	O5-C5-C6-O6
23	B	605	CLA	C4C-C3C-CAC-CBC
35	M	103	LMT	C2B-C1B-O1B-C4'
34	B	622	LMG	C33-C34-C35-C36
31	D	409	LHG	C15-C16-C17-C18
27	B	628	GOL	O1-C1-C2-O2
23	B	608	CLA	C3-C5-C6-C7
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	513	CLA	C4B-C3B-CAB-CBB
23	b	601	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB
34	C	501	LMG	C29-C28-O8-C9
35	E	102	LMT	C3-C4-C5-C6
23	B	605	CLA	C13-C15-C16-C17
23	C	503	CLA	C10-C11-C12-C13
23	B	602	CLA	CAA-CBA-CGA-O2A
26	A	411	SQD	C29-C30-C31-C32
34	C	520	LMG	C40-C41-C42-C43
37	H	102	DGD	CCA-CDA-CEA-CFA
31	b	630	LHG	C13-C14-C15-C16
34	c	519	LMG	C31-C32-C33-C34
34	m	101	LMG	C30-C31-C32-C33
31	d	407	LHG	O6-C4-C5-C6
31	D	409	LHG	C29-C30-C31-C32
34	J	101	LMG	C36-C37-C38-C39
35	e	102	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	C11-C12-C13-C15
23	B	606	CLA	C6-C7-C8-C10
23	B	611	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C7
23	b	607	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	b	616	CLA	C11-C12-C13-C15
23	c	501	CLA	C11-C12-C13-C15
23	c	504	CLA	C11-C10-C8-C7
23	C	508	CLA	O1D-CGD-O2D-CED
23	B	610	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	O1A-CGA-O2A-C1
23	C	512	CLA	C3-C5-C6-C7
31	L	101	LHG	C13-C14-C15-C16
35	M	103	LMT	C6-C7-C8-C9
35	B	632	LMT	C4-C5-C6-C7
35	B	632	LMT	C5-C6-C7-C8
34	C	501	LMG	O10-C28-O8-C9
31	b	630	LHG	O6-C4-C5-O7
26	a	411	SQD	C26-C27-C28-C29
23	B	602	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	d	402	CLA	C11-C12-C13-C14
23	b	602	CLA	C10-C11-C12-C13
31	D	408	LHG	C26-C27-C28-C29
34	C	520	LMG	C32-C33-C34-C35
25	k	101	BCR	C9-C10-C11-C12
23	D	401	CLA	C16-C17-C18-C19
23	B	609	CLA	C13-C15-C16-C17
23	C	503	CLA	C3-C5-C6-C7
26	B	621	SQD	O47-C45-C46-O48
26	L	102	SQD	O47-C45-C46-O48
23	a	406	CLA	C10-C11-C12-C13
26	a	411	SQD	O6-C44-C45-C46
26	f	101	SQD	C44-C45-C46-O48
34	c	520	LMG	O1-C7-C8-C9
35	M	103	LMT	C9-C10-C11-C12
24	a	408	PHO	C8-C10-C11-C12
23	B	602	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	CAD-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C5-C6-C7-C8
37	h	103	DGD	C9A-CAA-CBA-CCA
23	c	510	CLA	C16-C17-C18-C20
31	d	406	LHG	O10-C23-O8-C6
35	M	103	LMT	O5B-C1B-O1B-C4'
35	M	103	LMT	C1-C2-C3-C4
34	C	501	LMG	C13-C14-C15-C16
35	B	634	LMT	C4-C5-C6-C7
26	B	621	SQD	C33-C34-C35-C36
31	b	630	LHG	C16-C17-C18-C19
37	C	518	DGD	C8A-C9A-CAA-CBA
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
31	E	101	LHG	C4-O6-P-O5
31	L	101	LHG	C4-O6-P-O5
31	d	406	LHG	C3-O3-P-O5
31	d	407	LHG	C3-O3-P-O4
31	d	408	LHG	C4-O6-P-O3
31	d	407	LHG	C9-C10-C11-C12
31	b	630	LHG	C25-C26-C27-C28
31	d	407	LHG	C16-C17-C18-C19
23	B	608	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	D	404	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	b	607	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
25	B	618	BCR	C1-C6-C7-C8
29	d	405	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
34	z	101	LMG	C10-C11-C12-C13
31	D	409	LHG	C2-C3-O3-P
31	d	408	LHG	C2-C3-O3-P
34	C	520	LMG	C11-C12-C13-C14
23	b	616	CLA	O1A-CGA-O2A-C1
35	E	102	LMT	O1'-C1-C2-C3
26	a	411	SQD	C16-C17-C18-C19
31	D	409	LHG	C14-C15-C16-C17
31	D	408	LHG	C11-C10-C9-C8
34	C	520	LMG	C35-C36-C37-C38
31	E	101	LHG	C23-C24-C25-C26
35	D	403	LMT	O5B-C5B-C6B-O6B
31	d	406	LHG	C24-C23-O8-C6
26	B	621	SQD	C46-C45-O47-C7
29	D	407	PL9	C29-C31-C32-C33
34	C	520	LMG	C34-C35-C36-C37
37	h	103	DGD	CBB-CCB-CDB-CEB
37	c	517	DGD	C7B-C8B-C9B-CAB
35	B	623	LMT	C5-C6-C7-C8
23	A	405	CLA	C14-C13-C15-C16
23	B	616	CLA	C11-C12-C13-C14
23	b	606	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C12-C13-C14
26	L	102	SQD	C31-C32-C33-C34
23	C	510	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
23	c	506	CLA	C12-C13-C15-C16
31	d	407	LHG	O6-C4-C5-O7
31	d	406	LHG	C24-C25-C26-C27
34	B	622	LMG	C13-C14-C15-C16
34	C	501	LMG	C17-C18-C19-C20
34	a	417	LMG	C20-C21-C22-C23
35	D	403	LMT	C5-C6-C7-C8
26	a	413	SQD	O5-C1-O6-C44
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C11-C12-C13-C14
23	A	407	CLA	C4-C3-C5-C6
26	L	102	SQD	C26-C27-C28-C29
31	d	408	LHG	C29-C30-C31-C32
34	c	519	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
26	a	413	SQD	C24-C23-O48-C46
23	C	507	CLA	C16-C17-C18-C19
31	d	406	LHG	C34-C35-C36-C37
34	m	101	LMG	C37-C38-C39-C40
26	a	413	SQD	O10-C23-O48-C46
26	f	101	SQD	O6-C44-C45-C46
34	z	101	LMG	C4-C5-C6-O5
34	a	417	LMG	C29-C30-C31-C32
26	L	102	SQD	C11-C10-C9-C8
26	a	413	SQD	C18-C19-C20-C21
26	B	621	SQD	C45-C44-O6-C1
34	J	101	LMG	C8-C7-O1-C1
23	c	501	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C2A-CAA-CBA-CGA
25	y	101	BCR	C9-C10-C11-C12
34	B	622	LMG	O6-C5-C6-O5
35	e	102	LMT	O5B-C1B-O1B-C4'
26	B	621	SQD	C9-C10-C11-C12
29	a	415	PL9	C20-C19-C21-C22
23	B	610	CLA	CBA-CGA-O2A-C1
26	A	411	SQD	C7-C8-C9-C10
34	B	622	LMG	C10-C11-C12-C13
23	A	405	CLA	C11-C10-C8-C9
23	D	405	CLA	C11-C10-C8-C9
23	a	406	CLA	C6-C7-C8-C9
23	a	409	CLA	C11-C10-C8-C9
23	b	607	CLA	C14-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C14
23	B	604	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	CBA-CGA-O2A-C1
23	C	510	CLA	C4B-C3B-CAB-CBB
23	a	404	CLA	C16-C17-C18-C19
31	E	101	LHG	C15-C16-C17-C18
29	a	415	PL9	C18-C19-C21-C22
34	m	101	LMG	C21-C22-C23-C24
24	D	402	PHO	C16-C17-C18-C20
35	M	103	LMT	C11-C10-C9-C8
31	D	408	LHG	C34-C35-C36-C37
23	B	603	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C6-C7-C8-C10
23	b	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C13-C15-C16-C17
37	c	517	DGD	CCB-CDB-CEB-CFB
34	c	519	LMG	C29-C28-O8-C9
34	z	101	LMG	C18-C19-C20-C21
35	C	522	LMT	C4-C5-C6-C7
23	b	609	CLA	C3A-C2A-CAA-CBA
23	d	403	CLA	C3A-C2A-CAA-CBA
29	A	413	PL9	C30-C29-C31-C32
23	D	401	CLA	C2C-C3C-CAC-CBC
34	z	101	LMG	C28-C29-C30-C31
34	z	101	LMG	C12-C13-C14-C15
23	d	402	CLA	C2-C1-O2A-CGA
31	d	407	LHG	C31-C32-C33-C34
23	C	509	CLA	C13-C15-C16-C17
23	c	513	CLA	C10-C11-C12-C13
23	C	509	CLA	C5-C6-C7-C8
29	a	415	PL9	C2-C3-C7-C8
23	C	504	CLA	C15-C16-C17-C18
35	B	633	LMT	C4-C5-C6-C7
23	B	603	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C12-C13-C14
23	B	611	CLA	C14-C13-C15-C16
23	B	612	CLA	C11-C12-C13-C14
23	C	503	CLA	C14-C13-C15-C16
23	C	511	CLA	C6-C7-C8-C9
23	C	514	CLA	C14-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C9
23	b	607	CLA	C11-C12-C13-C14
23	c	509	CLA	C11-C12-C13-C14
23	A	407	CLA	C8-C10-C11-C12
23	B	604	CLA	O1A-CGA-O2A-C1
31	d	406	LHG	C7-C8-C9-C10
23	C	505	CLA	C8-C10-C11-C12
23	B	610	CLA	C2-C3-C5-C6
29	A	413	PL9	C28-C29-C31-C32
35	D	403	LMT	C4'-C5'-C6'-O6'
23	c	511	CLA	C1A-C2A-CAA-CBA
34	a	417	LMG	C36-C37-C38-C39
34	j	101	LMG	C36-C37-C38-C39
23	b	601	CLA	C16-C17-C18-C19
40	V	202	HEC	CAD-CBD-CGD-O1D
40	V	202	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
37	c	516	DGD	CDB-CEB-CFB-CGB
35	B	623	LMT	O5B-C1B-O1B-C4'
31	L	101	LHG	C28-C29-C30-C31
23	C	510	CLA	C2B-C3B-CAB-CBB
23	b	601	CLA	C2B-C3B-CAB-CBB
25	D	406	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	d	404	BCR	C1-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C26
23	b	601	CLA	CAA-CBA-CGA-O1A
31	d	408	LHG	C34-C35-C36-C37
36	B	624	HTG	C3'-C4'-C5'-C6'
23	C	510	CLA	CBD-CGD-O2D-CED
34	Z	101	LMG	C29-C28-O8-C9
38	e	103	HEM	CAD-CBD-CGD-O1D
37	H	102	DGD	C9B-CAB-CBB-CCB
23	C	510	CLA	C11-C10-C8-C7
23	D	405	CLA	C11-C10-C8-C7
23	D	405	CLA	C12-C13-C15-C16
23	a	405	CLA	C11-C10-C8-C7
23	a	406	CLA	C6-C7-C8-C10
23	b	610	CLA	C11-C12-C13-C15
23	c	504	CLA	C11-C12-C13-C15
31	b	630	LHG	C18-C19-C20-C21
23	B	602	CLA	C13-C15-C16-C17
31	d	407	LHG	O7-C5-C6-O8
31	d	408	LHG	O7-C5-C6-O8
34	C	521	LMG	O7-C8-C9-O8
37	h	103	DGD	CDA-CEA-CFA-CGA
35	b	620	LMT	C2-C3-C4-C5
38	E	103	HEM	CAD-CBD-CGD-O1D
40	v	201	HEC	CAD-CBD-CGD-O2D
23	C	503	CLA	C16-C17-C18-C20
26	B	621	SQD	C11-C10-C9-C8
26	L	102	SQD	C16-C17-C18-C19
34	C	521	LMG	C18-C19-C20-C21
23	c	513	CLA	C4-C3-C5-C6
23	c	507	CLA	C5-C6-C7-C8
23	b	616	CLA	C2-C3-C5-C6
29	A	413	PL9	C2-C3-C7-C8
37	c	516	DGD	CCB-CDB-CEB-CFB
40	v	201	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C6-C7-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	c	504	CLA	C14-C13-C15-C16
23	c	509	CLA	C14-C13-C15-C16
31	L	101	LHG	C11-C10-C9-C8
31	A	415	LHG	C29-C30-C31-C32
23	b	611	CLA	C13-C15-C16-C17
23	b	616	CLA	C4-C3-C5-C6
29	a	415	PL9	C45-C44-C46-C47
29	a	415	PL9	C43-C44-C46-C47
23	c	509	CLA	C10-C11-C12-C13
34	a	417	LMG	C34-C35-C36-C37
35	b	628	LMT	C6-C7-C8-C9
26	A	409	SQD	C14-C15-C16-C17
37	h	103	DGD	O1B-C1B-C2B-C3B
23	B	603	CLA	C2A-CAA-CBA-CGA
36	D	412	HTG	C1'-C2'-C3'-C4'
38	e	103	HEM	CAA-CBA-CGA-O2A
23	c	503	CLA	C8-C10-C11-C12
27	A	410	GOL	O2-C2-C3-O3
31	d	408	LHG	O6-C4-C5-O7
36	c	521	HTG	C4-C5-C6-O6
31	e	101	LHG	C14-C15-C16-C17
23	A	407	CLA	C4B-C3B-CAB-CBB
23	B	609	CLA	C4B-C3B-CAB-CBB
23	C	502	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
26	D	413	SQD	O10-C23-O48-C46
38	E	103	HEM	CAD-CBD-CGD-O2D
31	D	409	LHG	C10-C11-C12-C13
31	e	101	LHG	C25-C26-C27-C28
23	C	502	CLA	O1D-CGD-O2D-CED
24	A	406	PHO	CHA-CBD-CGD-O1D
24	D	402	PHO	CHA-CBD-CGD-O1D
37	c	517	DGD	C8A-C9A-CAA-CBA
35	m	103	LMT	O5'-C5'-C6'-O6'
35	M	101	LMT	C9-C10-C11-C12
29	A	413	PL9	C45-C44-C46-C47
38	e	103	HEM	CAD-CBD-CGD-O2D
31	L	101	LHG	C33-C34-C35-C36
34	Z	101	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	A	407	CLA	C11-C10-C8-C9
23	a	406	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C12-C13-C14
23	c	505	CLA	C11-C12-C13-C14
37	c	516	DGD	C5D-C6D-O5D-C1E
37	h	103	DGD	C2G-C3G-O3G-C1D
23	C	511	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	A	405	CLA	C3-C5-C6-C7
37	C	519	DGD	C6B-C7B-C8B-C9B
26	D	413	SQD	C24-C23-O48-C46
34	C	521	LMG	C10-C11-C12-C13
23	B	602	CLA	C3A-C2A-CAA-CBA
23	b	608	CLA	C3A-C2A-CAA-CBA
29	D	407	PL9	C45-C44-C46-C47
23	c	513	CLA	C2-C3-C5-C6
34	C	501	LMG	C18-C19-C20-C21
27	B	628	GOL	O1-C1-C2-C3
26	B	621	SQD	C34-C35-C36-C37
26	a	411	SQD	C19-C20-C21-C22
35	D	403	LMT	C2B-C1B-O1B-C4'
31	d	407	LHG	C11-C10-C9-C8
37	c	518	DGD	CCB-CDB-CEB-CFB
34	Z	101	LMG	C18-C19-C20-C21
24	D	402	PHO	C5-C6-C7-C8
23	a	409	CLA	C15-C16-C17-C18
31	d	406	LHG	C11-C10-C9-C8
37	c	516	DGD	CCA-CDA-CEA-CFA
31	D	409	LHG	C9-C10-C11-C12
23	c	508	CLA	C4-C3-C5-C6
23	b	613	CLA	CAA-CBA-CGA-O2A
26	L	102	SQD	O48-C23-C24-C25
31	A	415	LHG	O8-C23-C24-C25
37	C	517	DGD	CCB-CDB-CEB-CFB
35	e	102	LMT	C5-C6-C7-C8
23	b	601	CLA	C13-C15-C16-C17
37	h	103	DGD	C8A-C9A-CAA-CBA
23	B	605	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	510	CLA	C11-C12-C13-C14
23	c	504	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
34	Z	101	LMG	O7-C10-C11-C12
34	j	101	LMG	C19-C20-C21-C22
37	H	102	DGD	O1B-C1B-C2B-C3B
38	e	103	HEM	CAA-CBA-CGA-O1A
34	j	101	LMG	C28-C29-C30-C31
23	B	616	CLA	C13-C15-C16-C17
35	E	102	LMT	C4B-C5B-C6B-O6B
23	B	610	CLA	C4-C3-C5-C6
35	B	633	LMT	C5-C6-C7-C8
26	f	101	SQD	O47-C7-C8-C9
31	b	630	LHG	O7-C7-C8-C9
37	C	519	DGD	C1B-C2B-C3B-C4B
23	A	407	CLA	C11-C10-C8-C7
23	B	617	CLA	C11-C12-C13-C15
23	C	507	CLA	C12-C13-C15-C16
23	C	511	CLA	C12-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C10
23	b	614	CLA	C12-C13-C15-C16
23	c	504	CLA	C12-C13-C15-C16
23	c	505	CLA	C11-C12-C13-C15
23	c	509	CLA	C12-C13-C15-C16
23	A	405	CLA	C2C-C3C-CAC-CBC
23	A	407	CLA	C2B-C3B-CAB-CBB
23	B	615	CLA	C2B-C3B-CAB-CBB
23	C	502	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
25	c	514	BCR	C23-C24-C25-C30
36	B	625	HTG	C4'-C5'-C6'-C7'
23	b	602	CLA	CAA-CBA-CGA-O2A
31	D	409	LHG	C28-C29-C30-C31
23	B	609	CLA	C2-C1-O2A-CGA
23	B	614	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
34	B	622	LMG	C22-C23-C24-C25
29	a	415	PL9	C9-C11-C12-C13
26	B	621	SQD	O48-C23-C24-C25
23	B	614	CLA	CAA-CBA-CGA-O2A
36	B	624	HTG	C2'-C1'-S1-C1
34	z	101	LMG	C22-C23-C24-C25
34	C	520	LMG	O8-C28-C29-C30
23	a	404	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	CAA-CBA-CGA-O2A
34	c	519	LMG	O7-C10-C11-C12
31	L	101	LHG	O7-C7-C8-C9
23	A	407	CLA	C2-C3-C5-C6
23	B	604	CLA	CBD-CGD-O2D-CED
26	A	409	SQD	C30-C31-C32-C33
36	c	522	HTG	C4-C5-C6-O6
34	z	101	LMG	C13-C14-C15-C16
38	E	103	HEM	CAA-CBA-CGA-O2A
23	C	510	CLA	C11-C10-C8-C9
23	D	405	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C10-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C12-C13-C14
23	c	512	CLA	C15-C16-C17-C18
34	J	101	LMG	O7-C10-C11-C12
37	c	518	DGD	CDB-CEB-CFB-CGB
23	B	611	CLA	C4B-C3B-CAB-CBB
23	b	616	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	B	606	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
23	B	613	CLA	CAA-CBA-CGA-O2A
29	A	413	PL9	C43-C44-C46-C47
25	C	527	BCR	C7-C8-C9-C10
38	E	103	HEM	CAA-CBA-CGA-O1A
37	H	102	DGD	C7B-C8B-C9B-CAB
23	c	510	CLA	CAA-CBA-CGA-O2A
37	C	518	DGD	O2G-C1B-C2B-C3B
23	B	614	CLA	C15-C16-C17-C18
35	B	632	LMT	C11-C10-C9-C8
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	a	406	CLA	C11-C10-C8-C7
23	c	510	CLA	C12-C13-C15-C16
31	b	630	LHG	C19-C20-C21-C22
26	a	411	SQD	C11-C10-C9-C8
24	A	406	PHO	O2A-C1-C2-C3
23	c	503	CLA	C15-C16-C17-C18
23	b	612	CLA	CAA-CBA-CGA-O2A
31	b	630	LHG	C11-C12-C13-C14
23	A	404	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
37	C	517	DGD	CDB-CEB-CFB-CGB
23	c	513	CLA	C16-C17-C18-C20
34	z	101	LMG	C15-C16-C17-C18
34	a	417	LMG	C37-C38-C39-C40
34	m	101	LMG	O7-C10-C11-C12
34	a	417	LMG	C21-C22-C23-C24
23	D	405	CLA	C8-C10-C11-C12
23	D	404	CLA	C2C-C3C-CAC-CBC
37	C	519	DGD	C9B-CAB-CBB-CCB
31	e	101	LHG	O8-C23-C24-C25
24	A	406	PHO	C2-C3-C5-C6
35	M	103	LMT	C4-C5-C6-C7
26	f	101	SQD	C24-C25-C26-C27
26	f	101	SQD	O49-C7-C8-C9
31	b	630	LHG	O9-C7-C8-C9
34	C	520	LMG	O10-C28-C29-C30
34	c	519	LMG	O9-C10-C11-C12
31	d	408	LHG	C28-C29-C30-C31
23	C	507	CLA	C14-C13-C15-C16
36	b	621	HTG	C2'-C3'-C4'-C5'
23	b	612	CLA	C8-C10-C11-C12
24	a	408	PHO	C2C-C3C-CAC-CBC
31	A	415	LHG	O10-C23-C24-C25
26	B	621	SQD	C35-C36-C37-C38
26	B	621	SQD	O10-C23-C24-C25
37	C	518	DGD	CBB-CCB-CDB-CEB
23	b	604	CLA	C13-C15-C16-C17
25	y	101	BCR	C21-C22-C23-C24
23	D	401	CLA	C4C-C3C-CAC-CBC
26	A	409	SQD	C13-C14-C15-C16
23	B	614	CLA	CAA-CBA-CGA-O1A
26	L	102	SQD	O10-C23-C24-C25
36	b	625	HTG	C1'-C2'-C3'-C4'
34	j	101	LMG	C8-C7-O1-C1
37	C	517	DGD	C5D-C6D-O5D-C1E
26	a	411	SQD	C10-C11-C12-C13
23	C	511	CLA	CAA-CBA-CGA-O1A
34	Z	101	LMG	O9-C10-C11-C12
23	B	613	CLA	C13-C15-C16-C17
23	b	613	CLA	CAA-CBA-CGA-O1A
35	D	403	LMT	O5B-C1B-O1B-C4'
26	A	409	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	O7-C7-C8-C9
34	J	101	LMG	O9-C10-C11-C12
31	d	408	LHG	C25-C26-C27-C28
23	C	512	CLA	C16-C17-C18-C19
23	B	617	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
23	c	505	CLA	CAA-CBA-CGA-O2A
37	c	516	DGD	O2G-C1B-C2B-C3B
35	B	632	LMT	C3'-C4'-O1B-C1B
23	b	612	CLA	CAA-CBA-CGA-O1A
23	c	510	CLA	CAA-CBA-CGA-O1A
31	e	101	LHG	O10-C23-C24-C25
37	C	519	DGD	O6D-C5D-C6D-O5D
23	b	610	CLA	C2-C1-O2A-CGA
31	L	101	LHG	O9-C7-C8-C9
26	a	411	SQD	O47-C7-C8-C9
34	C	501	LMG	O8-C28-C29-C30
23	C	503	CLA	C16-C17-C18-C19
34	C	520	LMG	C31-C32-C33-C34
23	c	505	CLA	CAA-CBA-CGA-O1A
31	D	409	LHG	C32-C33-C34-C35

There are no ring outliers.

162 monomers are involved in 390 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	412	GOL	1	0
23	b	611	CLA	3	0
23	c	503	CLA	4	0
23	c	506	CLA	6	0
26	A	409	SQD	2	0
36	b	625	HTG	1	0
23	b	606	CLA	3	0
36	D	412	HTG	1	0
23	b	612	CLA	5	0
23	d	403	CLA	2	0
25	B	620	BCR	2	0
25	c	515	BCR	1	0
23	A	404	CLA	6	0
23	b	602	CLA	4	0
34	c	520	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	c	521	HTG	1	0
36	b	622	HTG	2	0
25	H	101	BCR	5	0
23	c	504	CLA	3	0
36	B	625	HTG	1	0
23	C	509	CLA	3	0
23	B	614	CLA	2	0
23	B	609	CLA	1	0
23	B	615	CLA	8	0
23	C	511	CLA	1	0
25	a	410	BCR	1	0
25	y	101	BCR	1	0
25	Y	101	BCR	3	0
23	B	602	CLA	2	0
26	A	411	SQD	1	0
26	D	413	SQD	2	0
34	a	417	LMG	3	0
34	J	101	LMG	2	0
34	C	501	LMG	3	0
23	a	406	CLA	4	0
23	C	507	CLA	9	0
23	C	503	CLA	4	0
23	B	605	CLA	3	0
23	C	506	CLA	4	0
25	C	527	BCR	1	0
29	D	407	PL9	1	0
23	d	402	CLA	7	0
26	a	413	SQD	3	0
23	c	510	CLA	3	0
23	c	507	CLA	8	0
27	B	628	GOL	4	0
23	c	511	CLA	8	0
25	D	406	BCR	2	0
23	b	603	CLA	3	0
23	B	608	CLA	2	0
34	Z	101	LMG	2	0
23	b	615	CLA	6	0
37	c	517	DGD	3	0
25	C	515	BCR	1	0
23	B	604	CLA	4	0
31	D	409	LHG	4	0
31	A	415	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	618	BCR	5	0
36	h	101	HTG	1	0
37	C	517	DGD	4	0
25	C	516	BCR	4	0
23	C	504	CLA	4	0
25	b	617	BCR	1	0
26	a	411	SQD	2	0
37	C	519	DGD	1	0
23	c	501	CLA	3	0
35	b	620	LMT	1	0
29	A	413	PL9	5	0
35	E	102	LMT	1	0
23	b	609	CLA	3	0
23	c	509	CLA	5	0
29	a	415	PL9	8	0
23	c	505	CLA	4	0
26	L	102	SQD	4	0
36	C	524	HTG	1	0
23	A	405	CLA	3	0
23	c	508	CLA	7	0
24	A	406	PHO	1	0
24	D	402	PHO	3	0
25	c	514	BCR	3	0
23	c	512	CLA	8	0
34	j	101	LMG	5	0
31	e	101	LHG	3	0
23	B	617	CLA	5	0
26	f	101	SQD	2	0
25	k	101	BCR	5	0
23	B	610	CLA	4	0
23	C	513	CLA	1	0
25	B	619	BCR	3	0
23	C	508	CLA	4	0
35	b	628	LMT	1	0
23	D	405	CLA	1	0
36	B	629	HTG	1	0
23	B	603	CLA	3	0
36	c	522	HTG	1	0
25	b	618	BCR	3	0
23	a	405	CLA	2	0
34	B	622	LMG	2	0
23	b	616	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	505	CLA	2	0
34	c	519	LMG	2	0
23	c	513	CLA	7	0
25	T	101	BCR	4	0
35	m	103	LMT	2	0
25	b	619	BCR	1	0
23	B	606	CLA	9	0
23	B	613	CLA	5	0
36	B	624	HTG	4	0
24	a	408	PHO	5	0
35	M	101	LMT	1	0
35	B	623	LMT	3	0
23	B	607	CLA	5	0
34	C	521	LMG	1	0
26	B	621	SQD	2	0
23	b	601	CLA	4	0
35	C	522	LMT	1	0
25	d	404	BCR	1	0
35	D	403	LMT	2	0
31	d	408	LHG	4	0
23	C	502	CLA	4	0
37	c	518	DGD	2	0
25	A	408	BCR	2	0
35	B	634	LMT	2	0
23	C	512	CLA	2	0
23	c	502	CLA	6	0
38	E	103	HEM	4	0
23	a	409	CLA	3	0
38	e	103	HEM	3	0
23	C	510	CLA	3	0
23	b	614	CLA	2	0
23	b	613	CLA	2	0
29	d	405	PL9	2	0
23	C	514	CLA	3	0
23	D	404	CLA	3	0
25	h	102	BCR	4	0
23	a	404	CLA	4	0
23	b	607	CLA	2	0
23	b	605	CLA	8	0
27	B	627	GOL	1	0
34	z	101	LMG	1	0
23	B	616	CLA	4	0

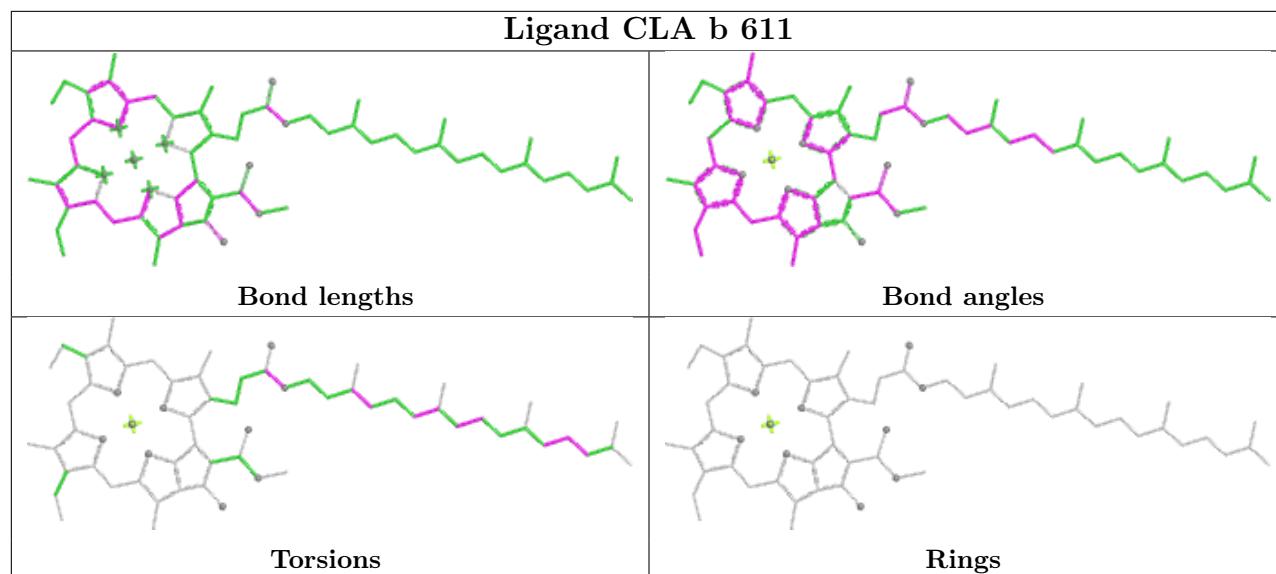
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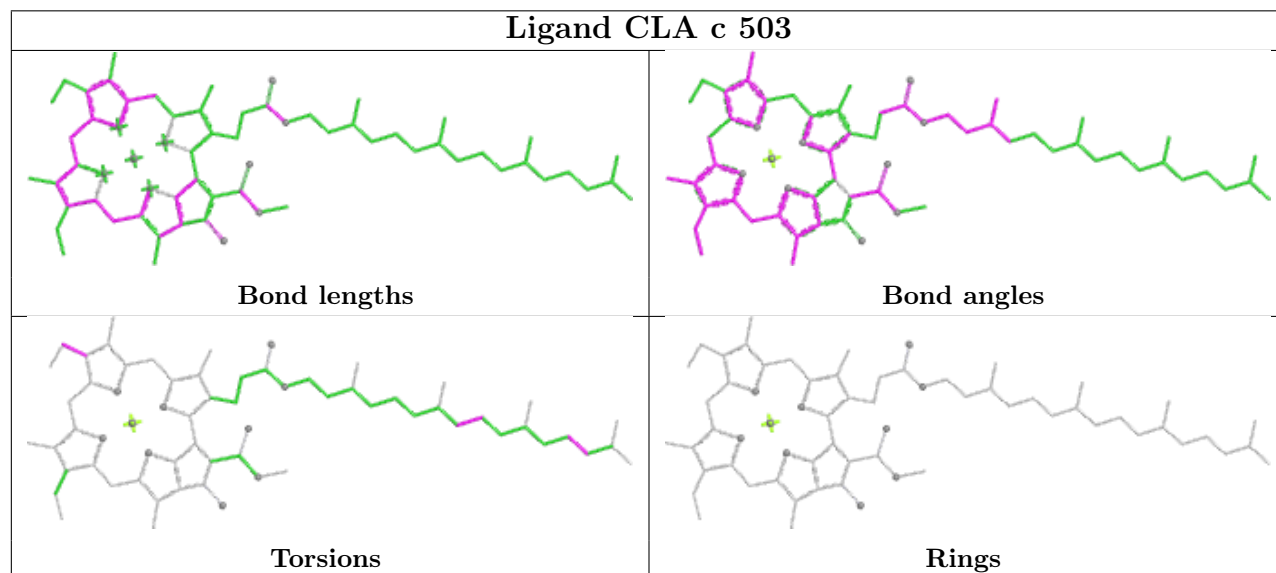
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	C	523	HTG	1	0
23	b	610	CLA	2	0
35	B	632	LMT	1	0
35	B	633	LMT	3	0
31	d	406	LHG	1	0
37	c	516	DGD	3	0
23	D	401	CLA	5	0
23	b	604	CLA	3	0
37	C	518	DGD	1	0
36	b	621	HTG	2	0
23	A	407	CLA	5	0
31	d	407	LHG	3	0
23	B	611	CLA	1	0
23	b	608	CLA	3	0
28	a	414	OEX	1	0
35	M	103	LMT	1	0
36	b	626	HTG	1	0
23	B	612	CLA	2	0
25	t	101	BCR	4	0
31	D	408	LHG	3	0
34	m	101	LMG	2	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.

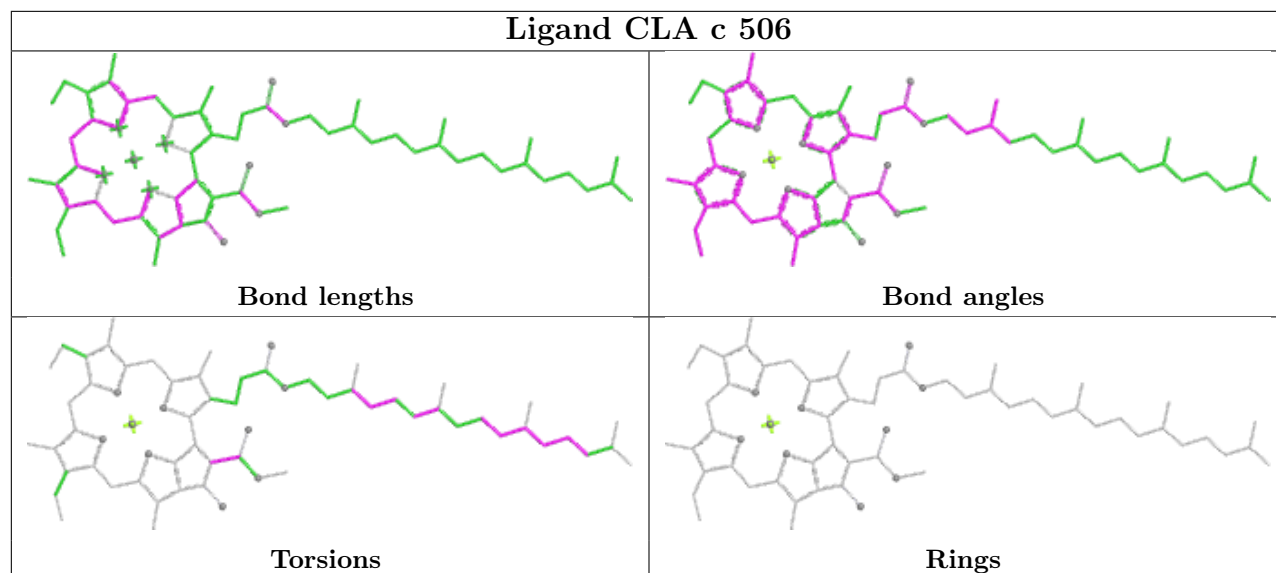
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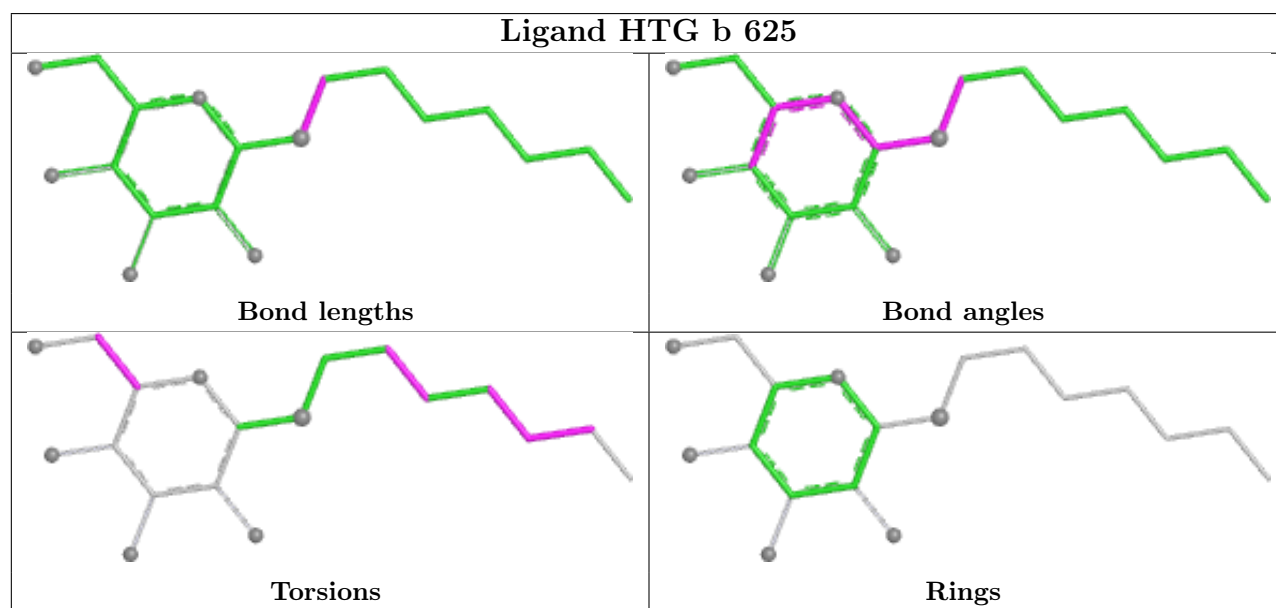
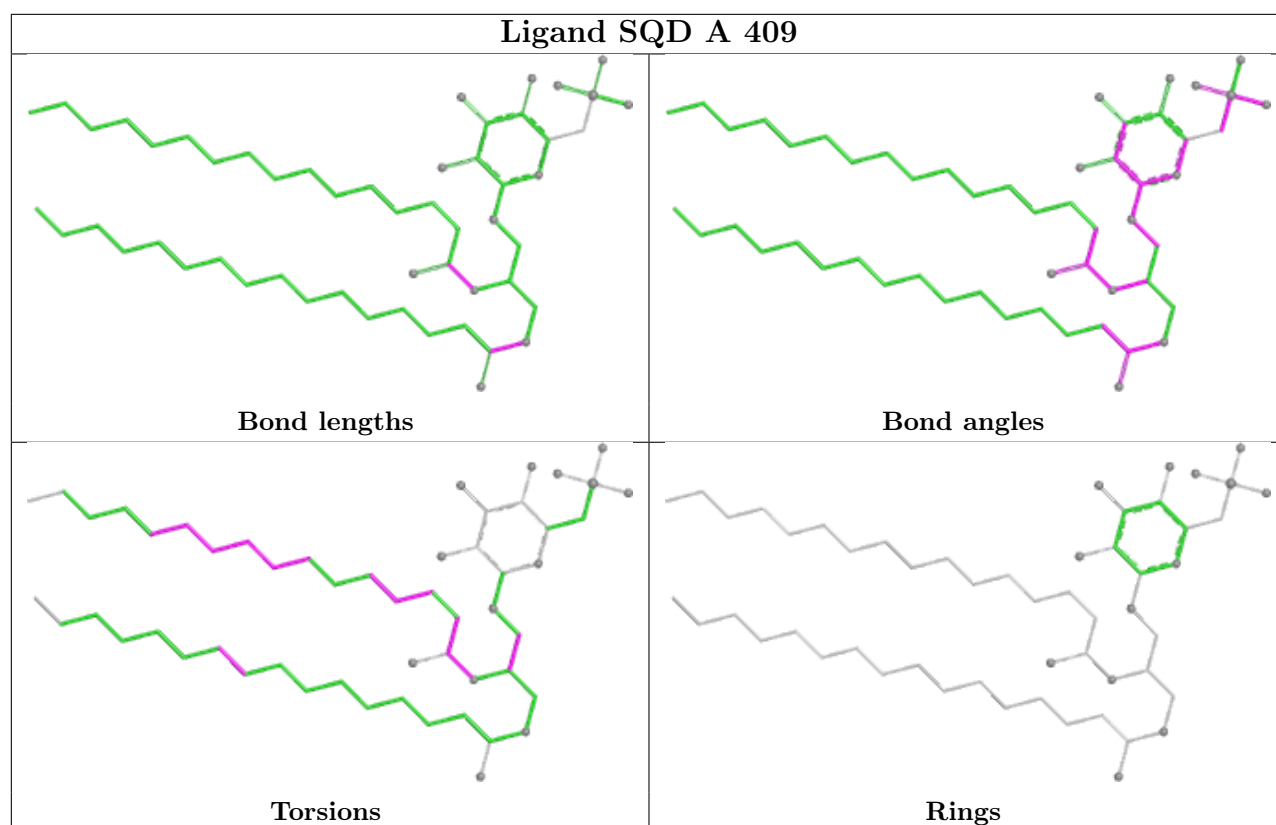


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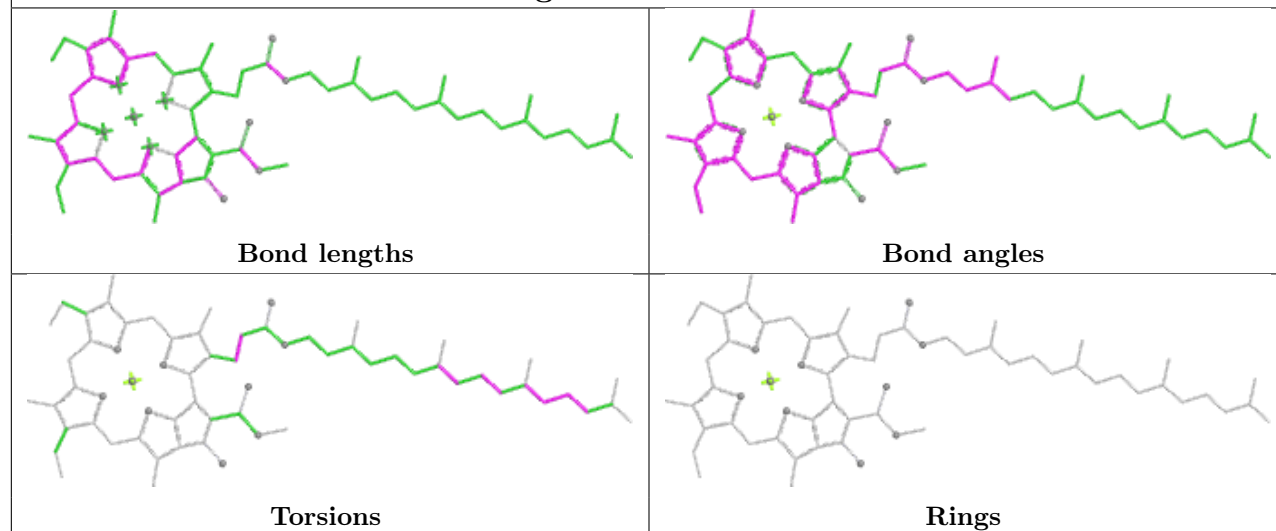


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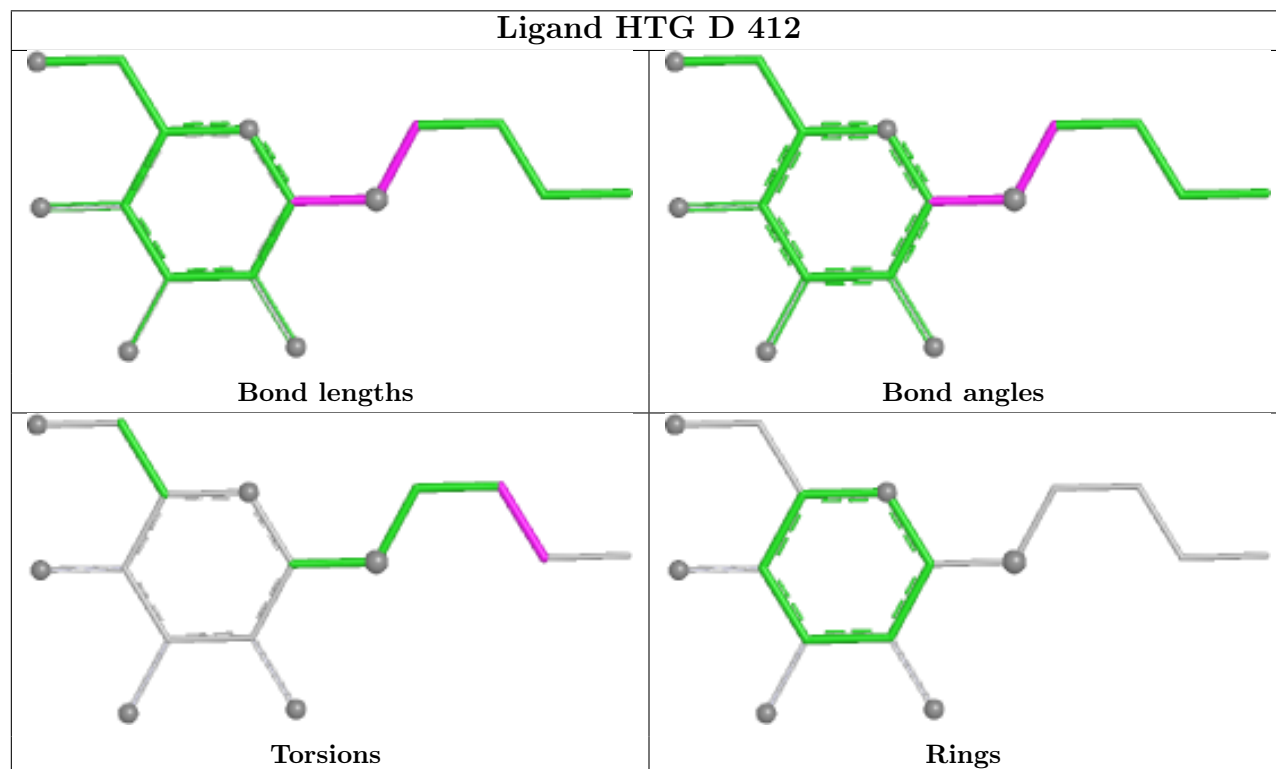




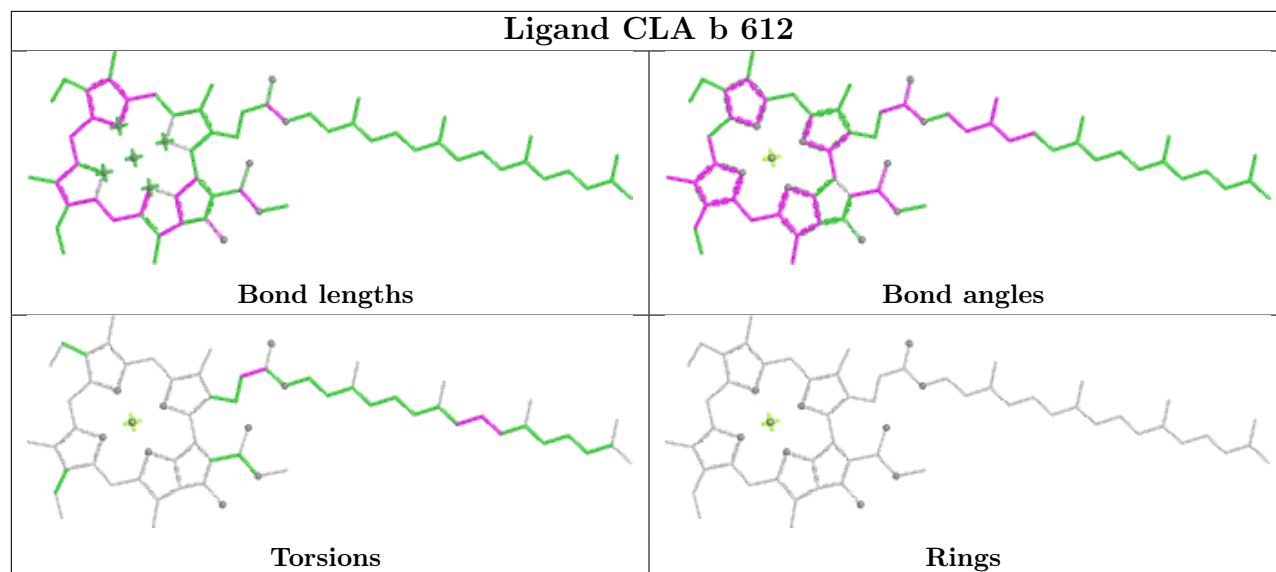
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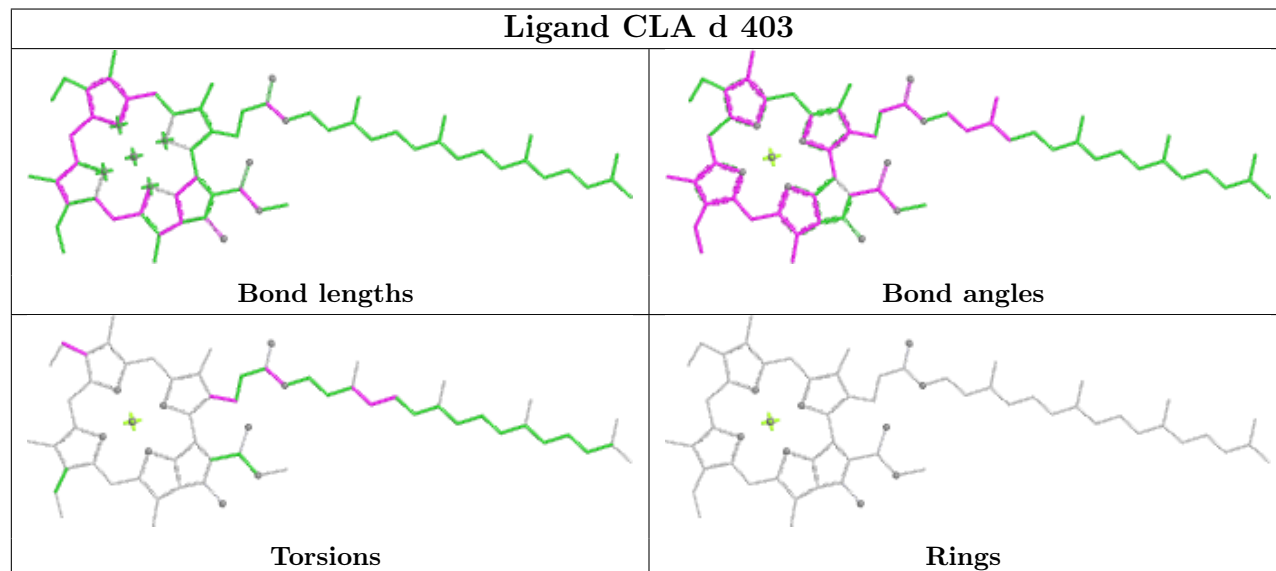
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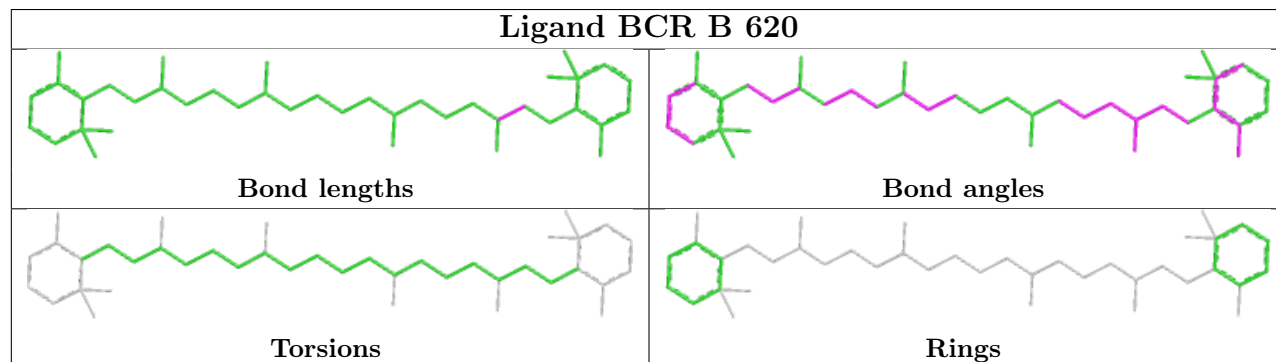
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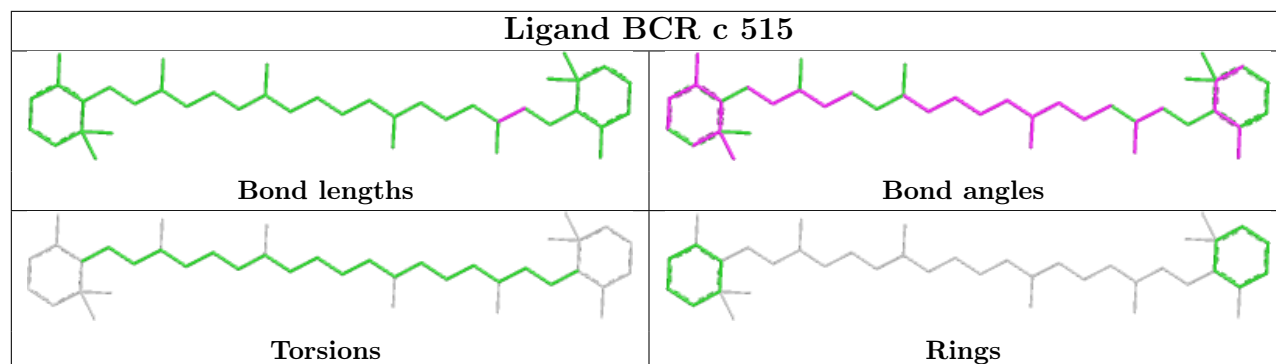
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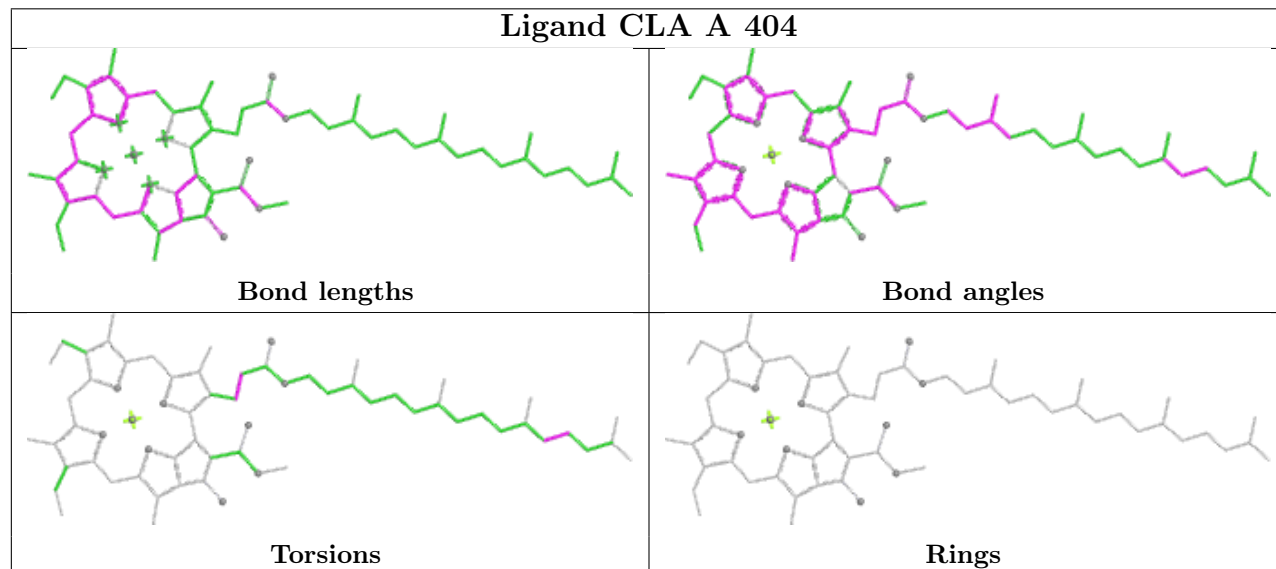
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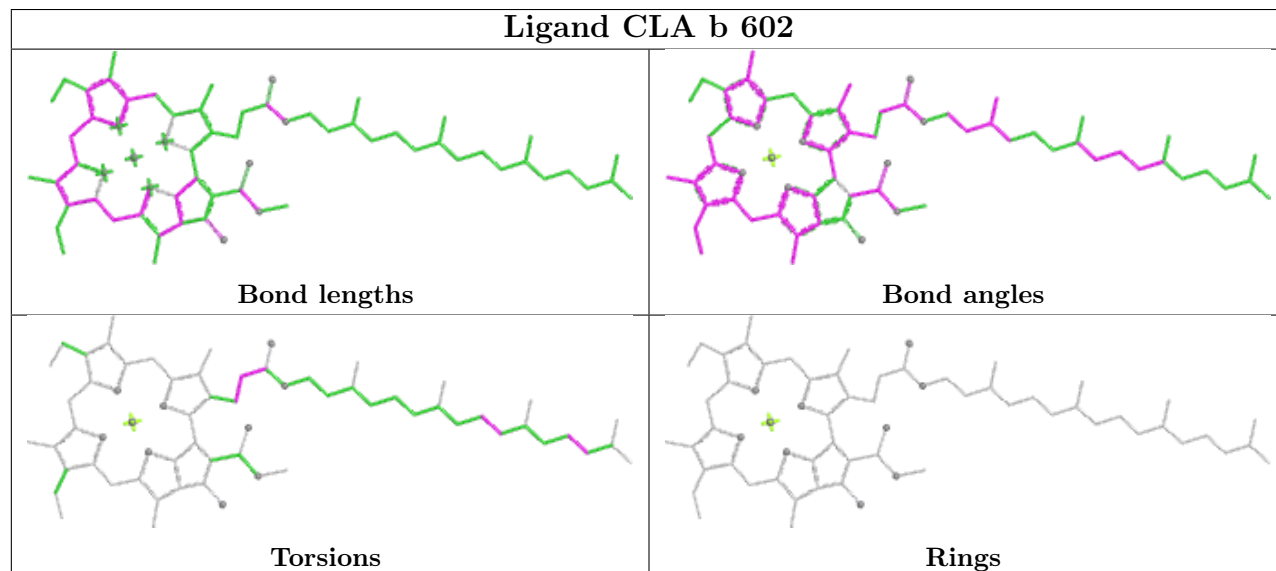
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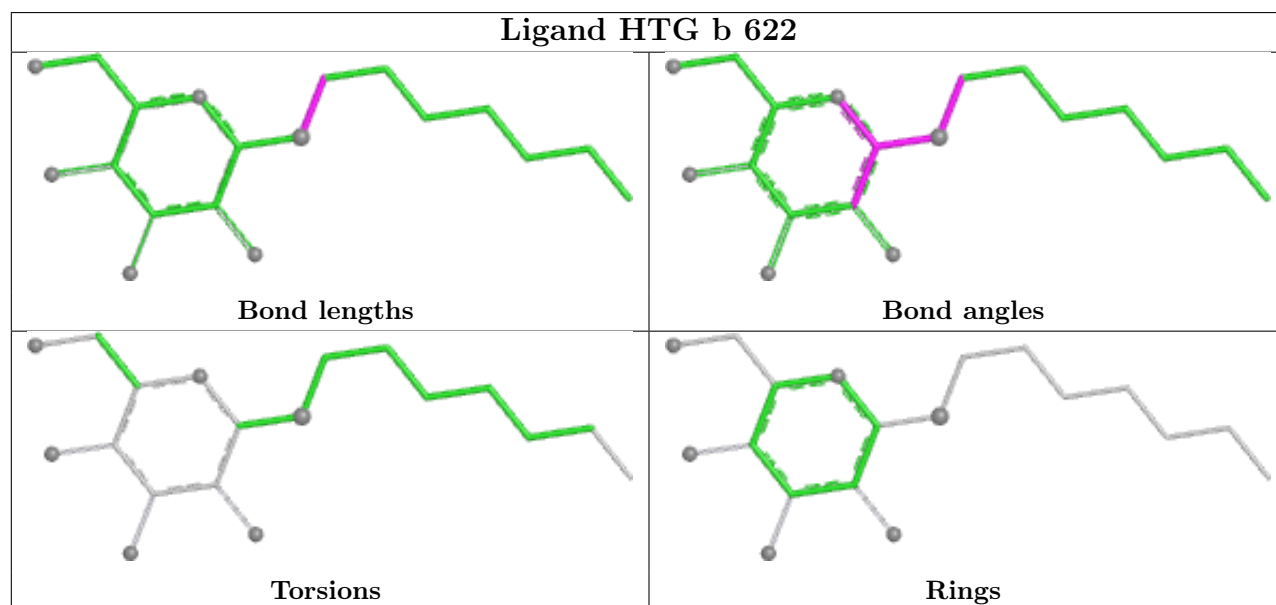
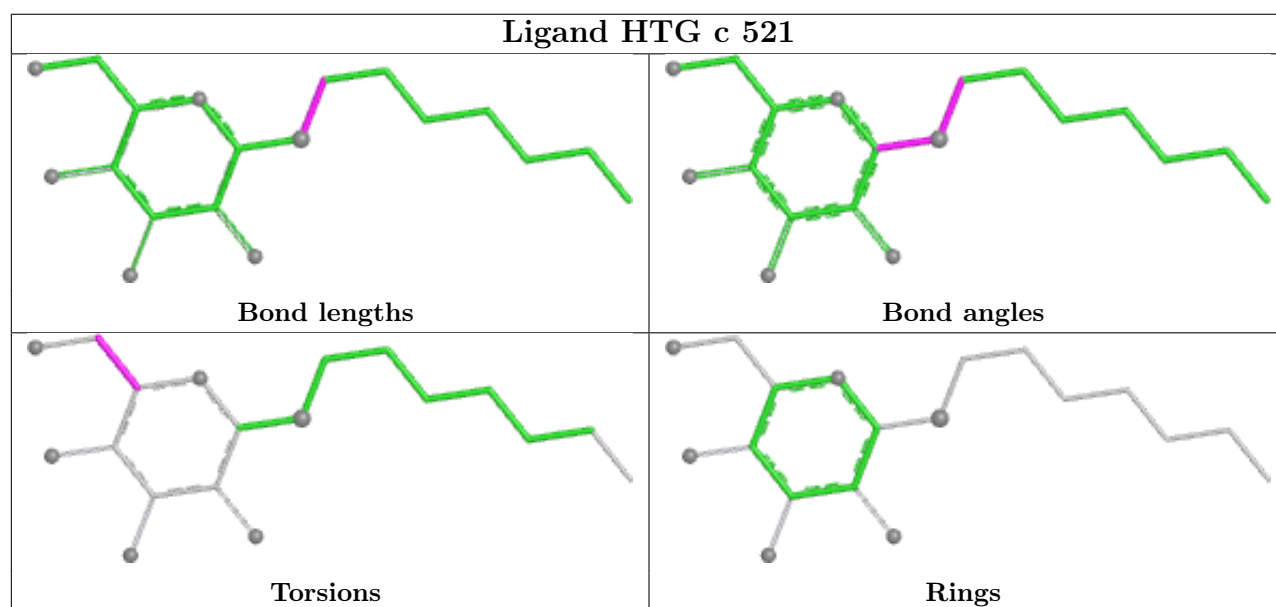
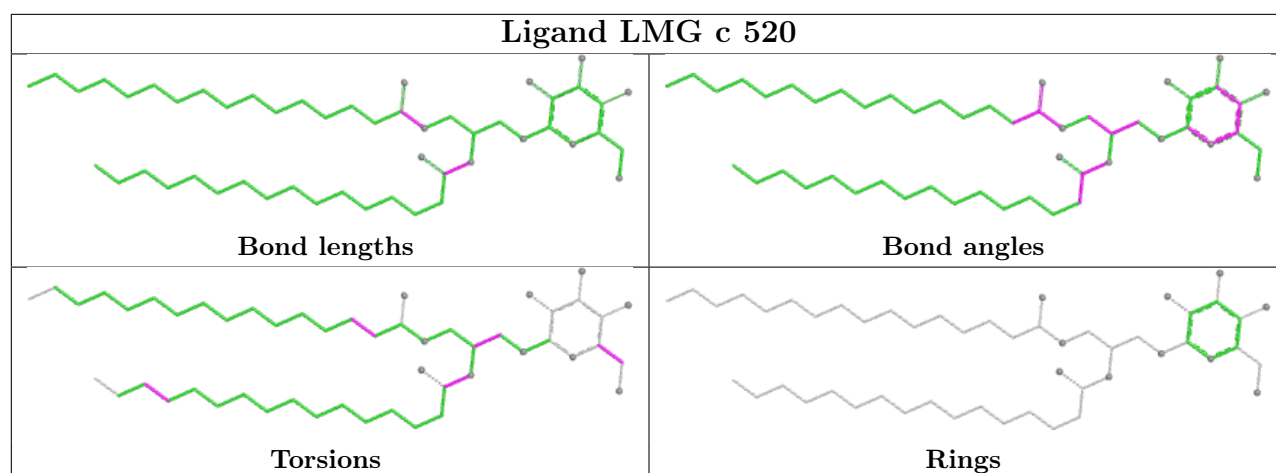


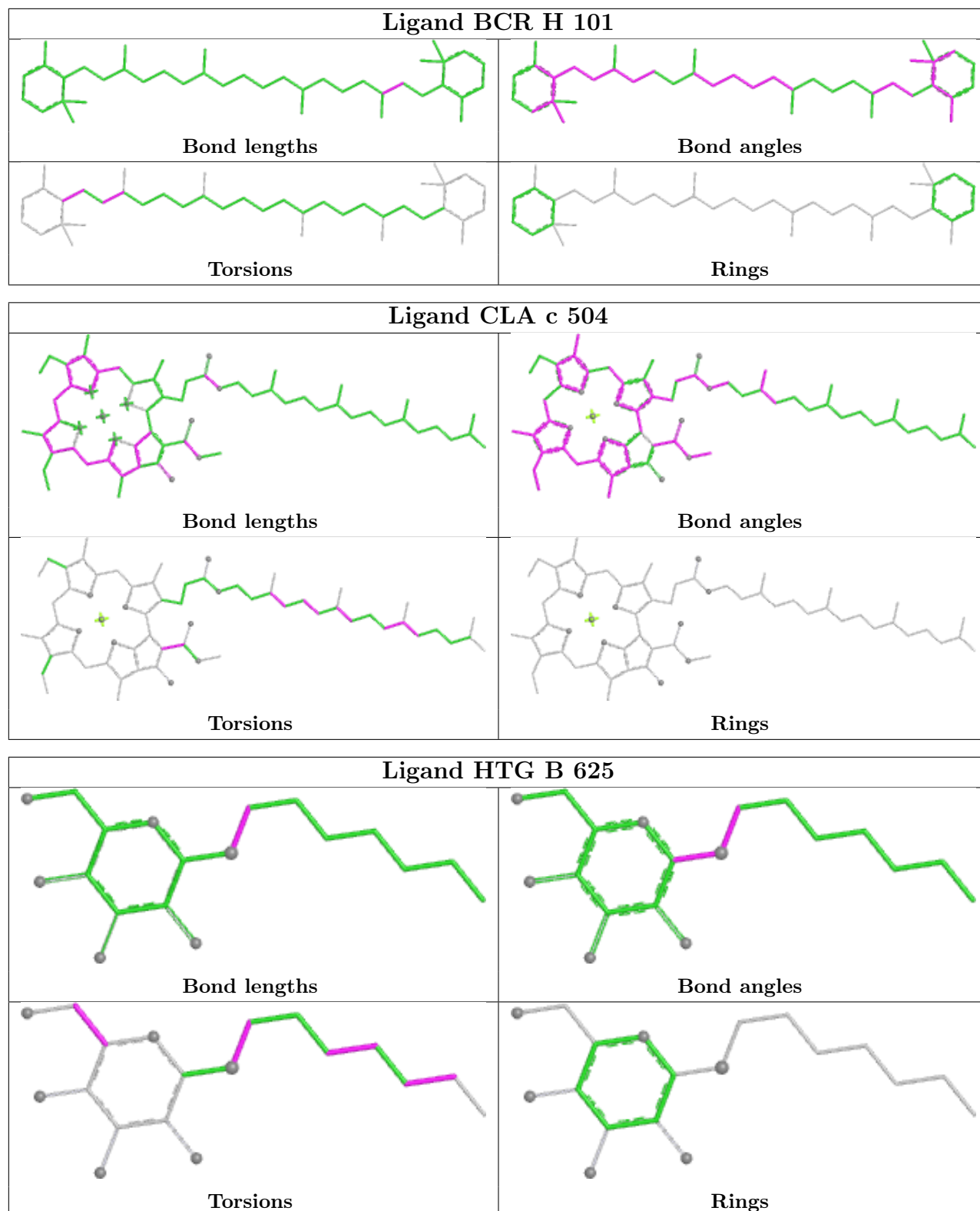
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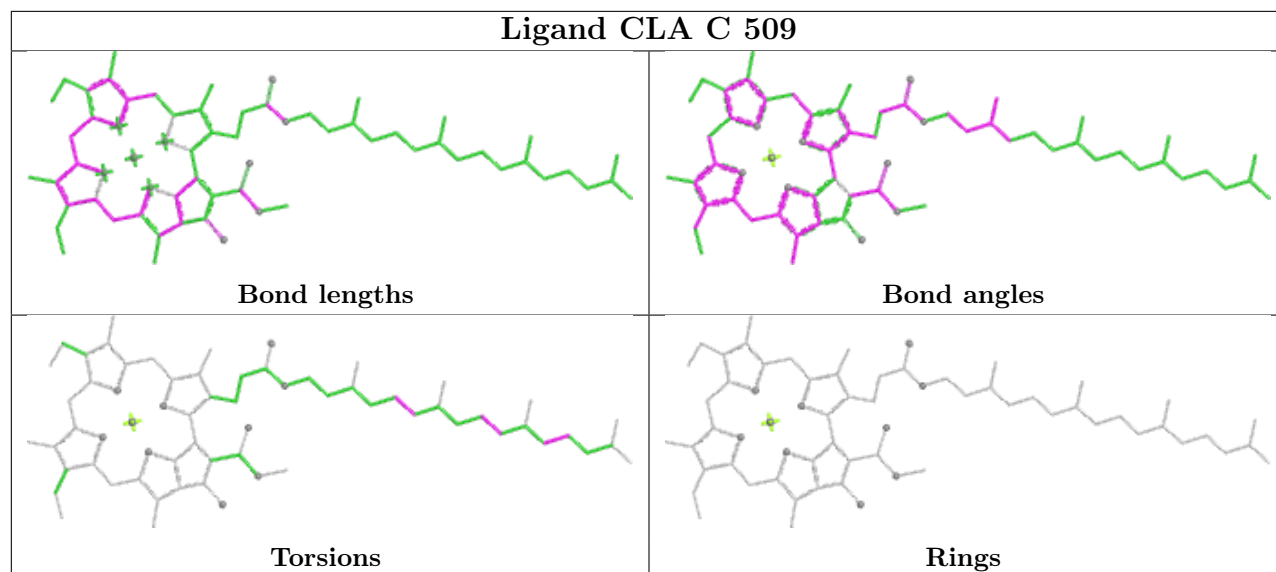
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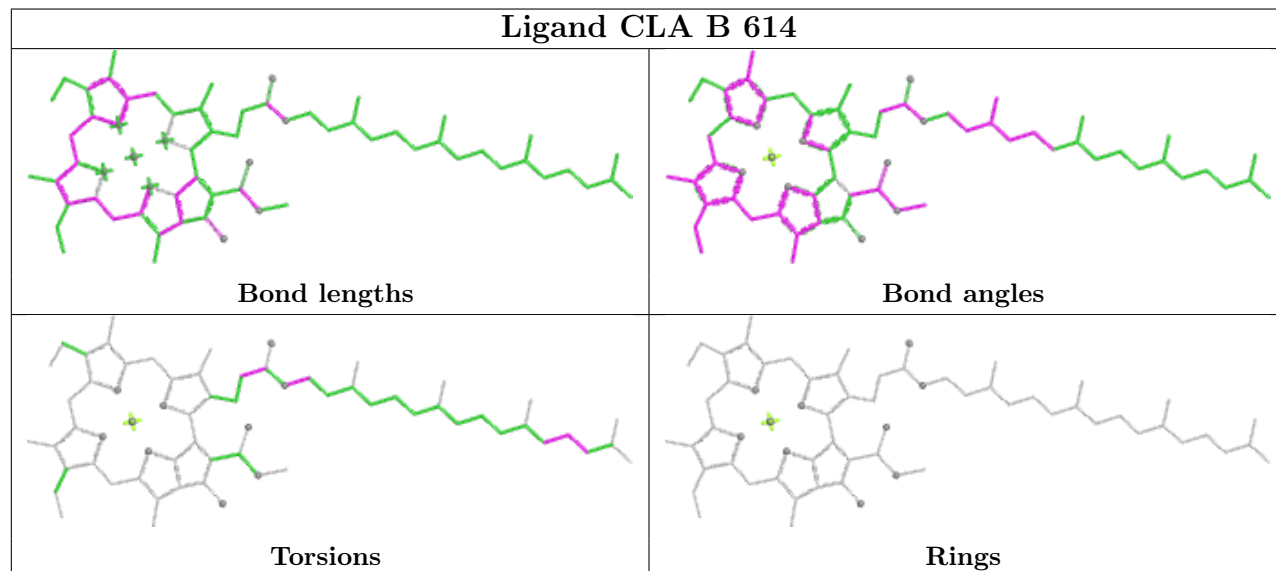




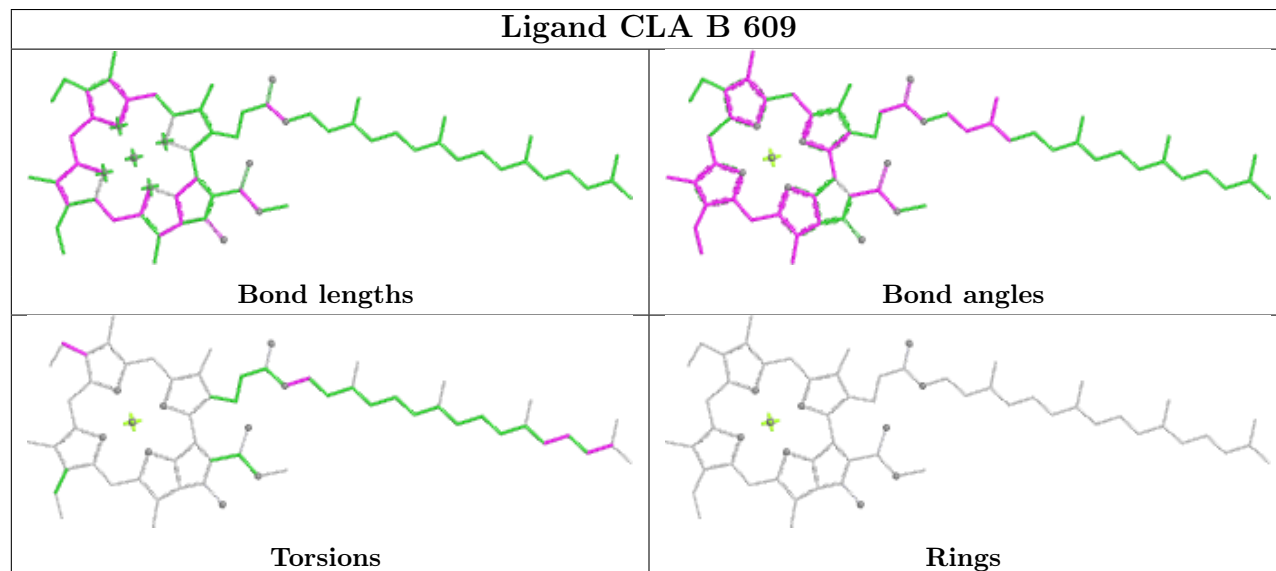
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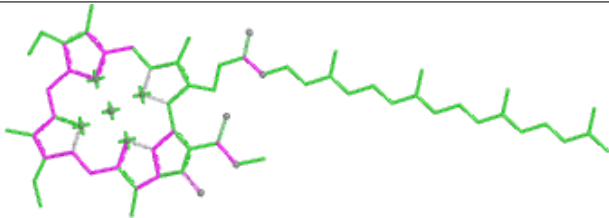
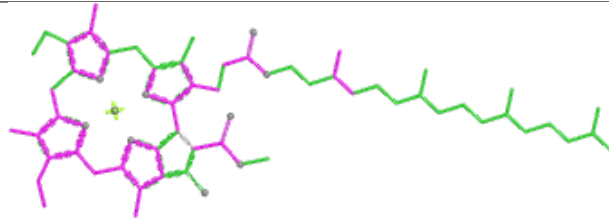
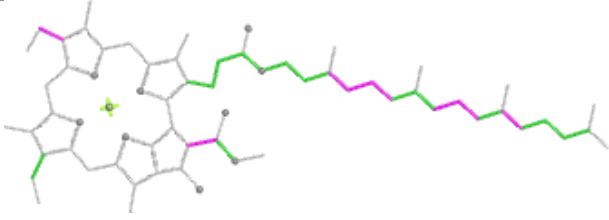
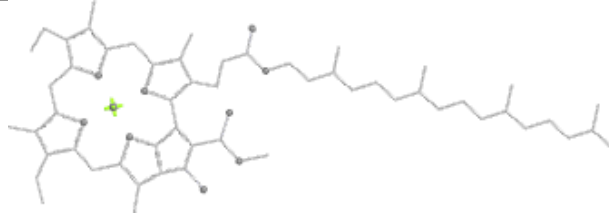


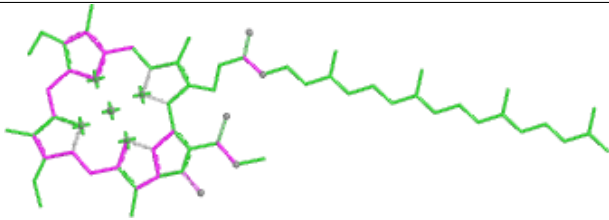
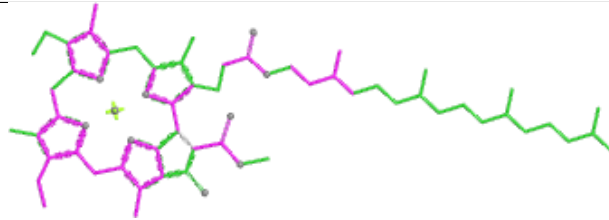
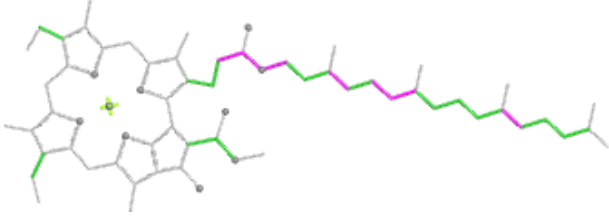
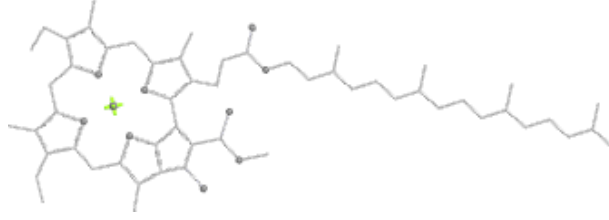
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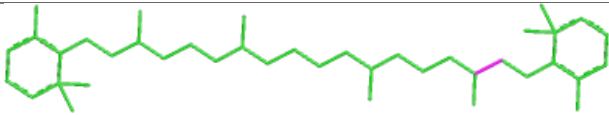
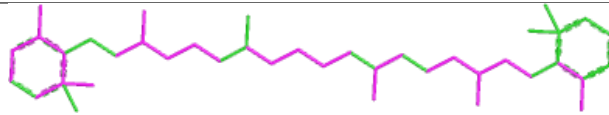
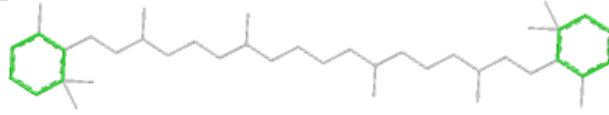


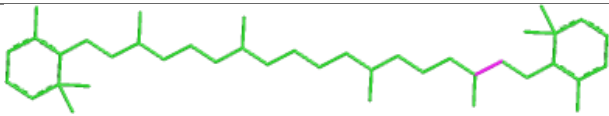
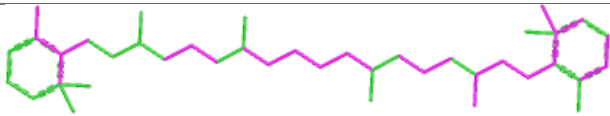
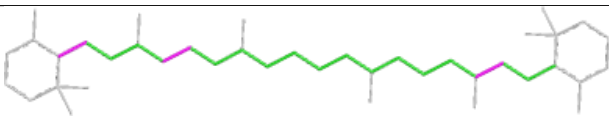
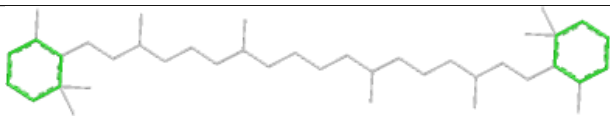
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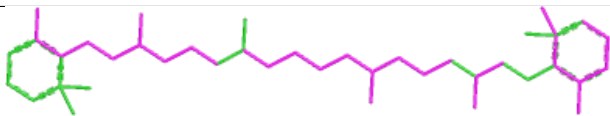
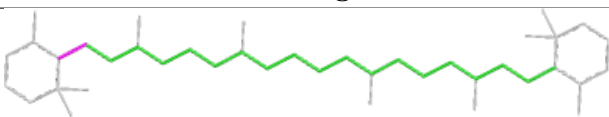
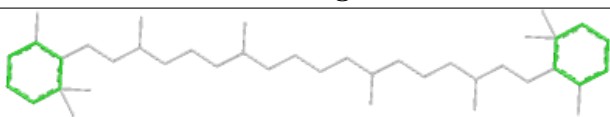


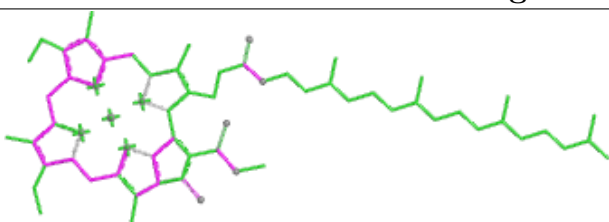
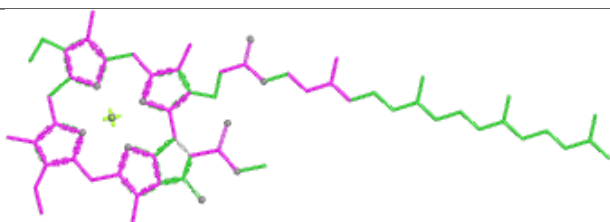
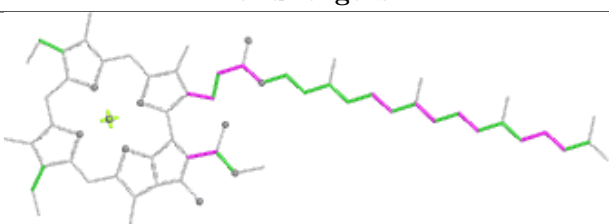
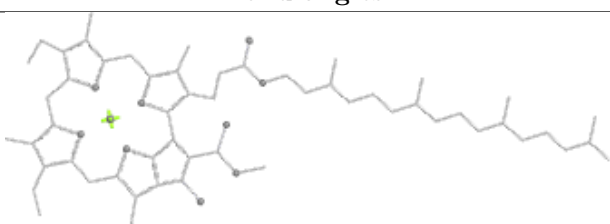
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

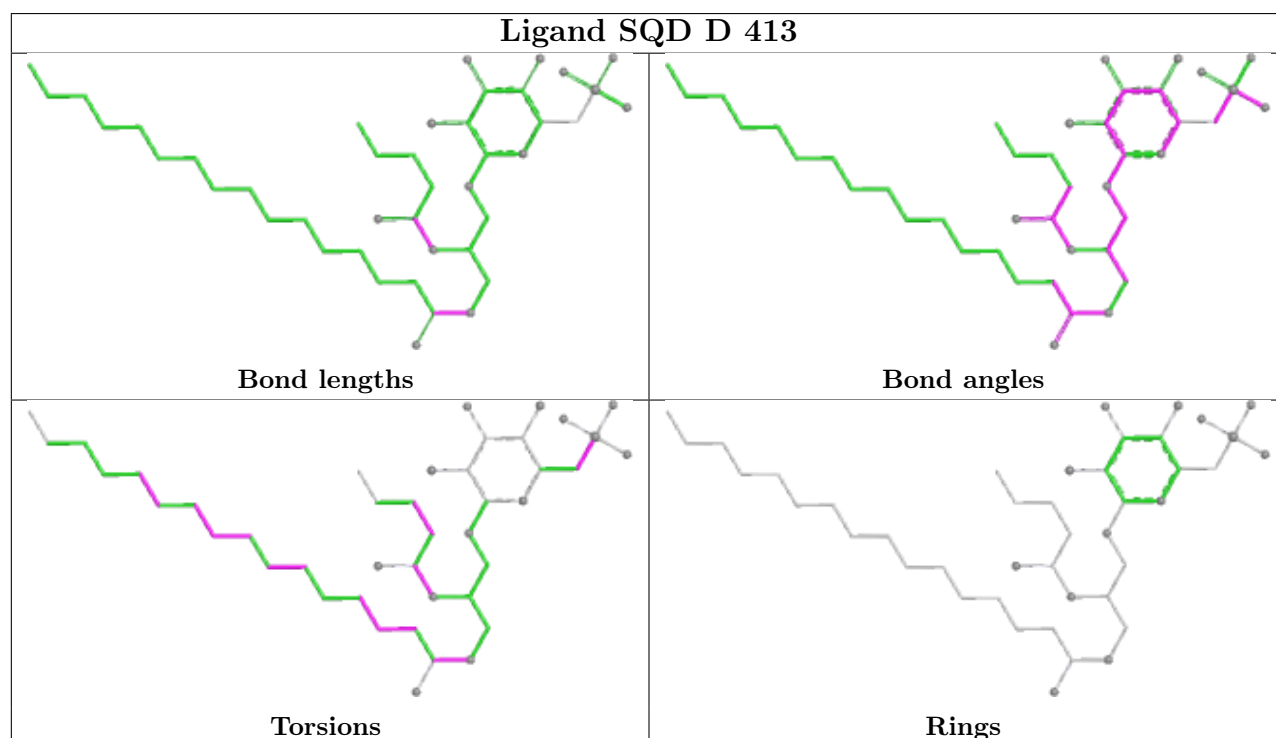
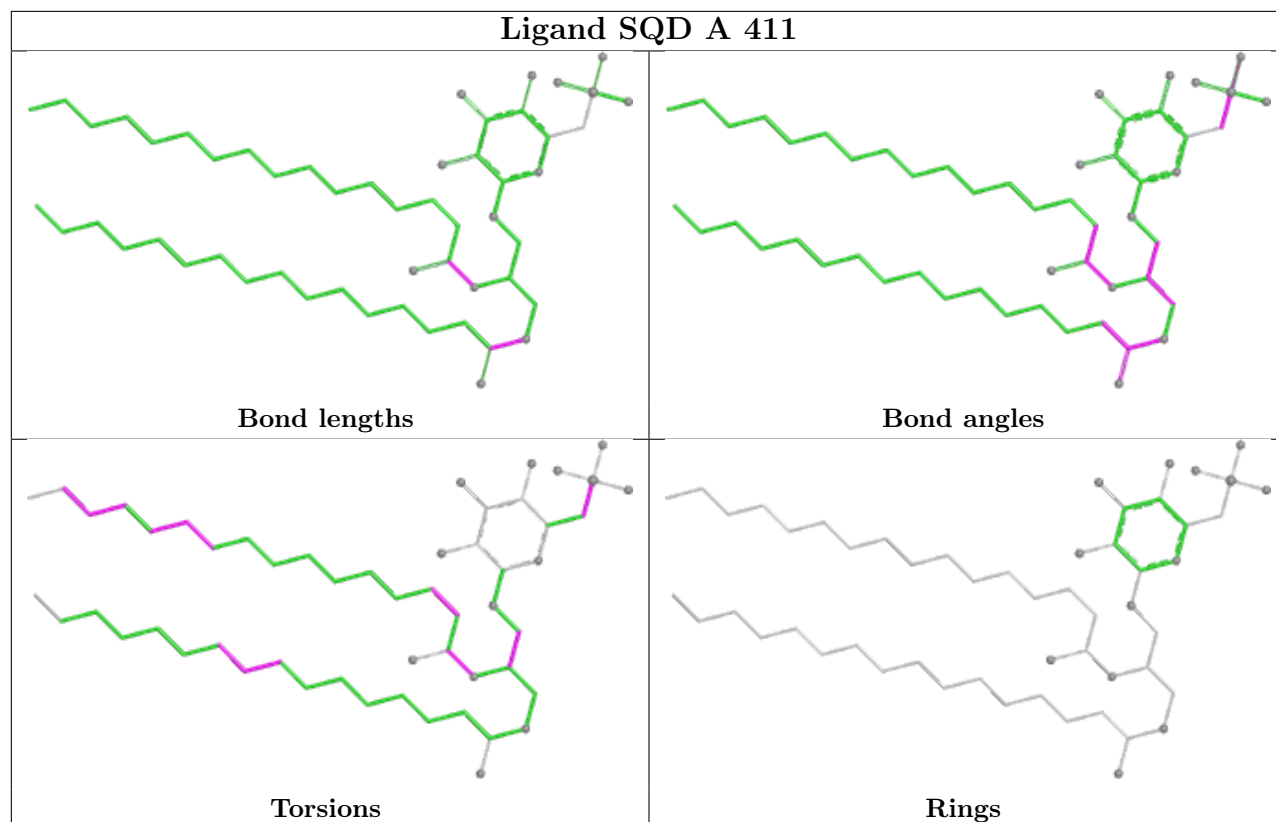
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

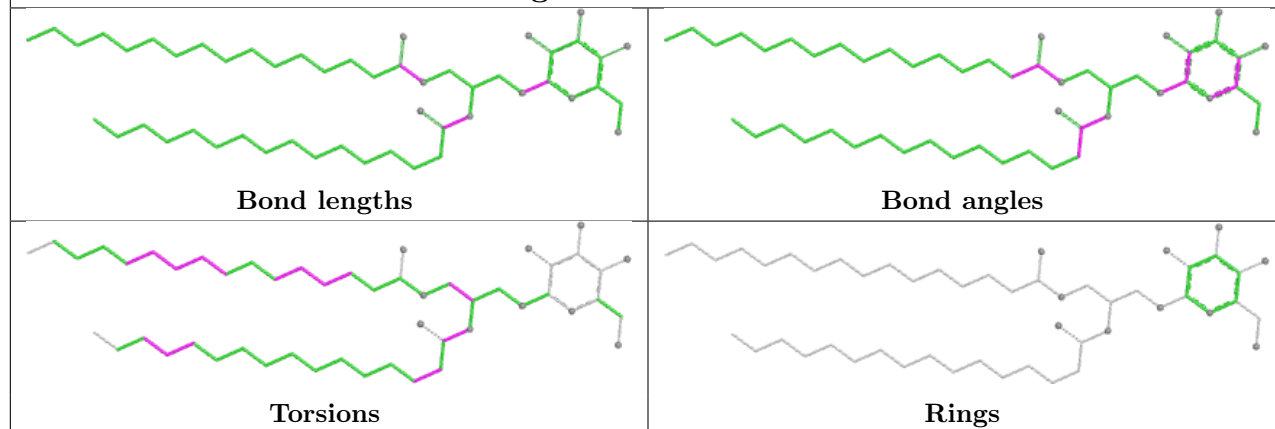
Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

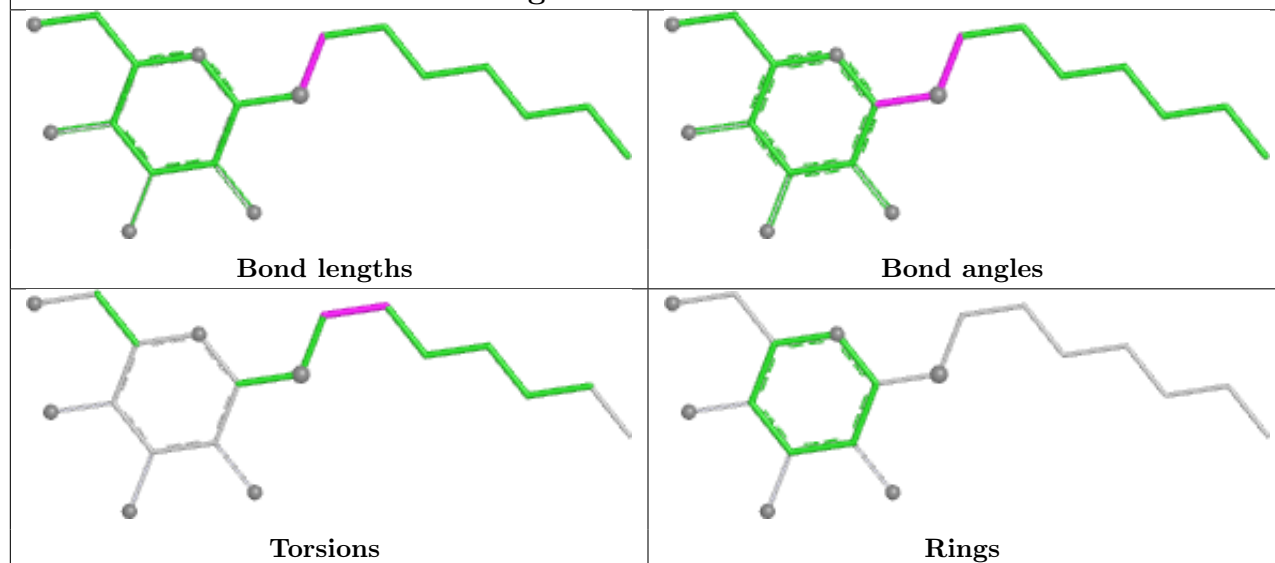
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings



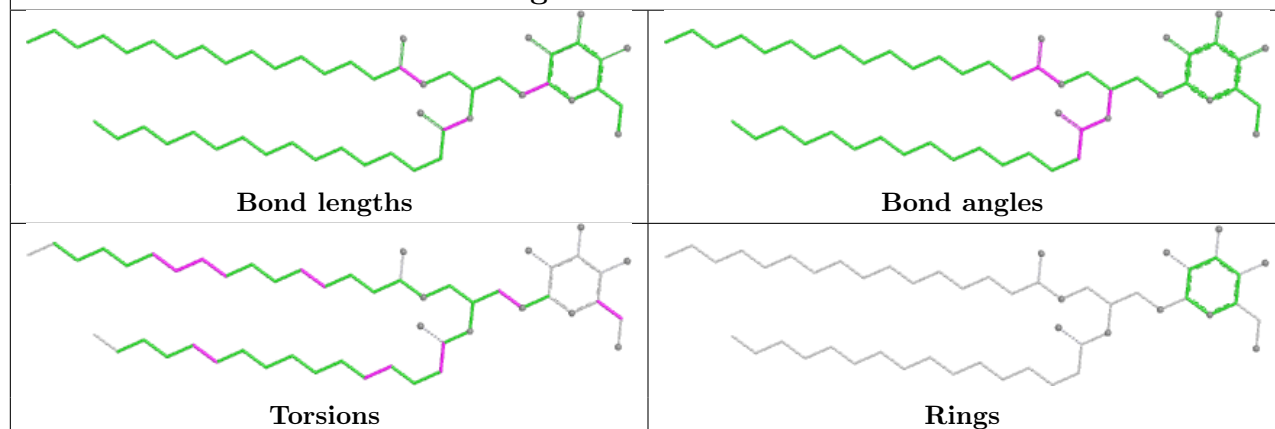
Ligand LMG a 417

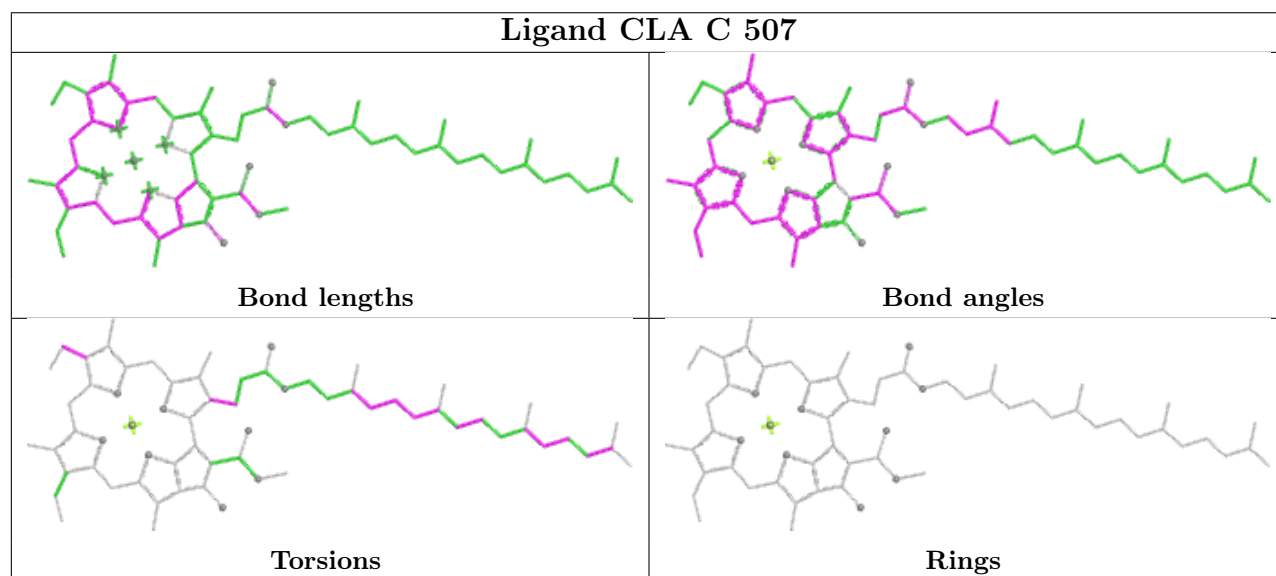
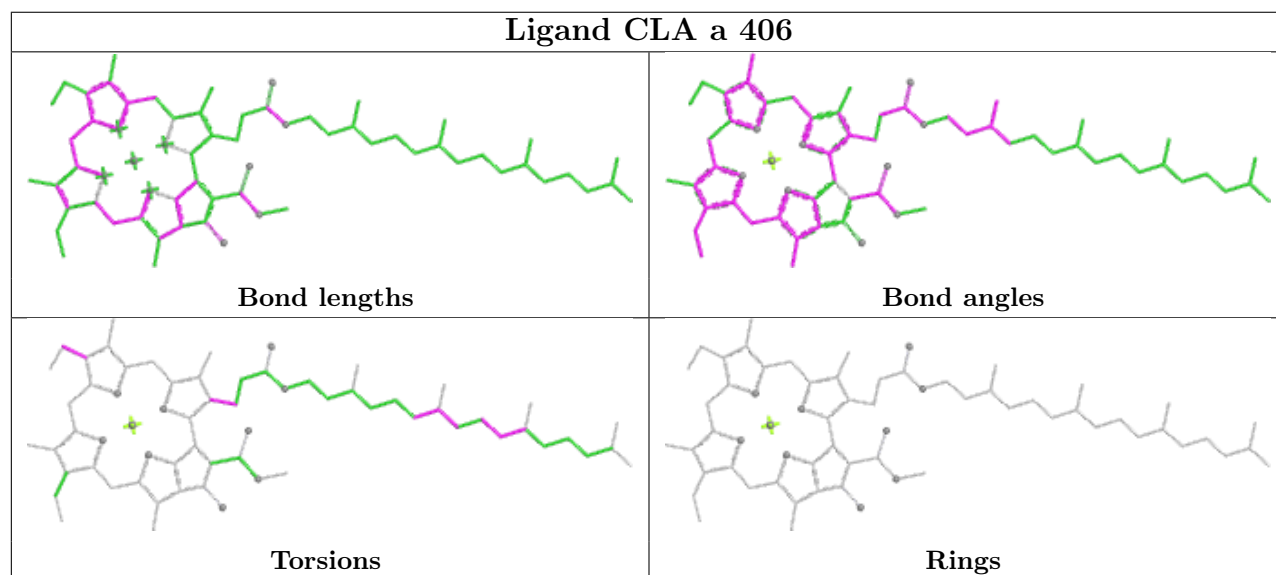
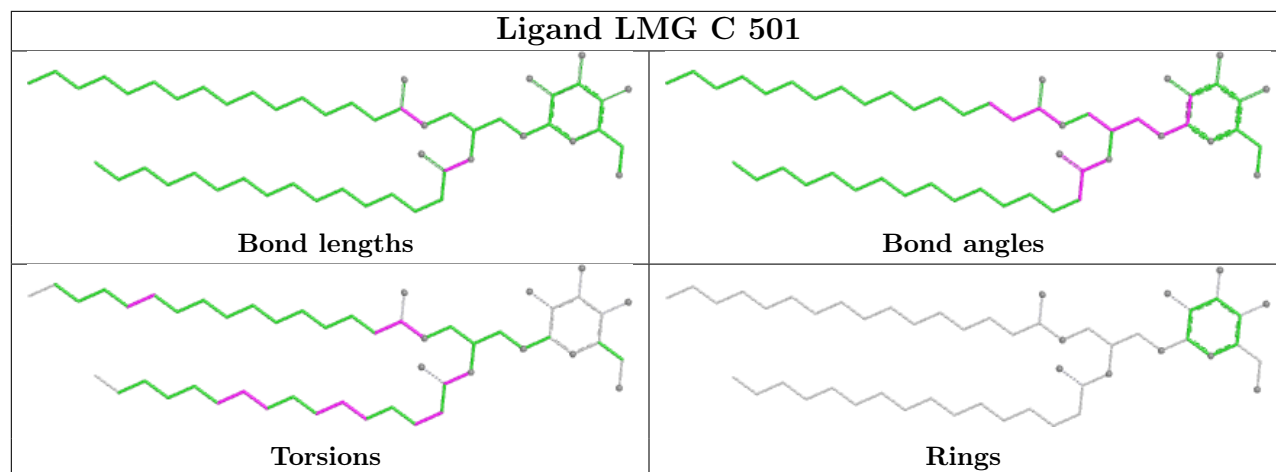


Ligand HTG B 630

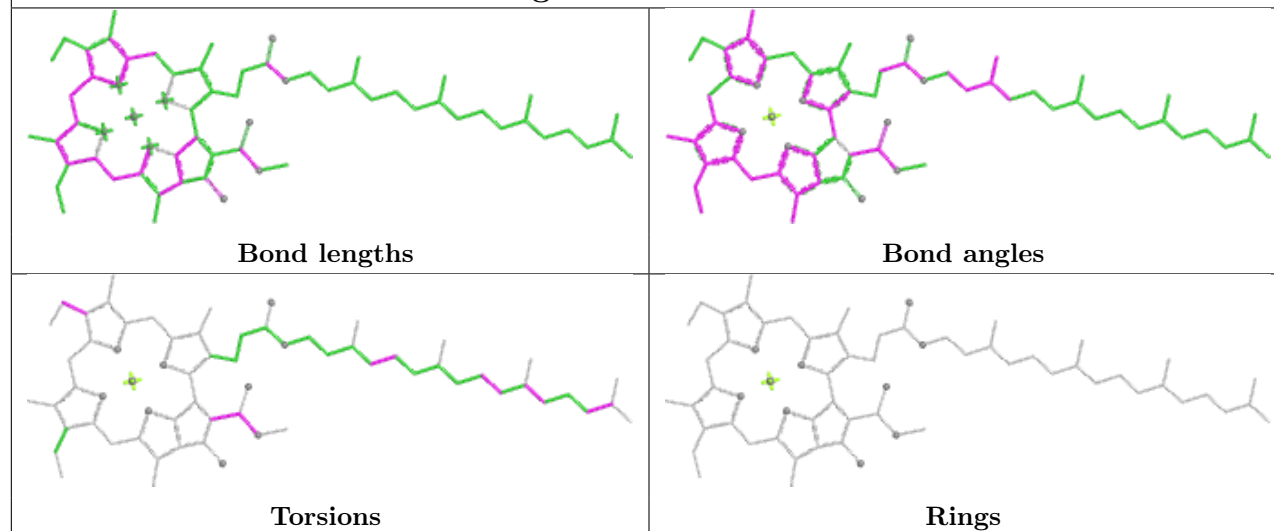


Ligand LMG J 101

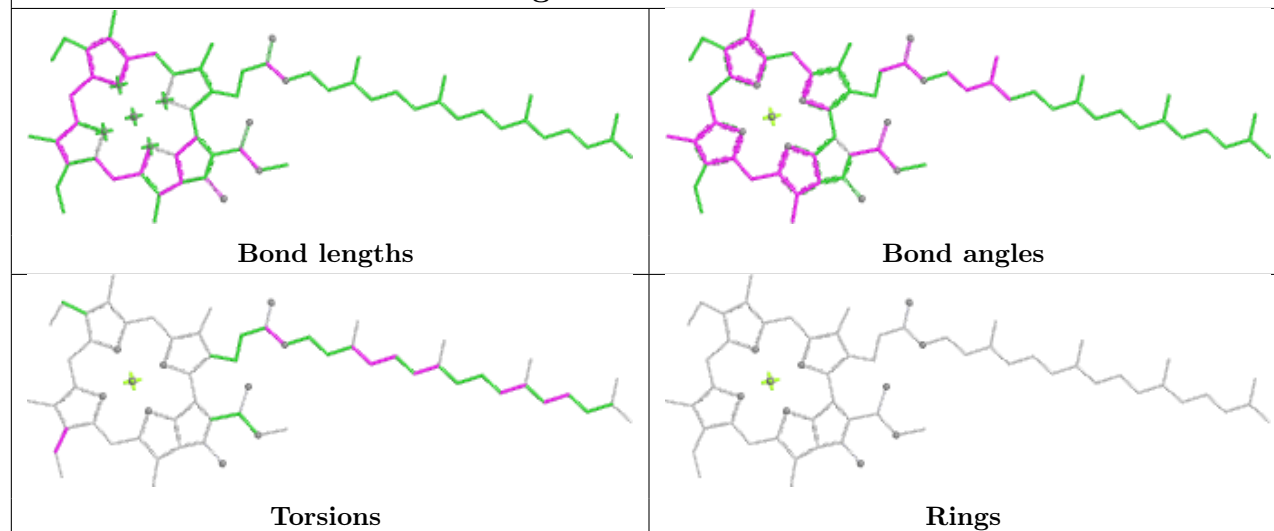




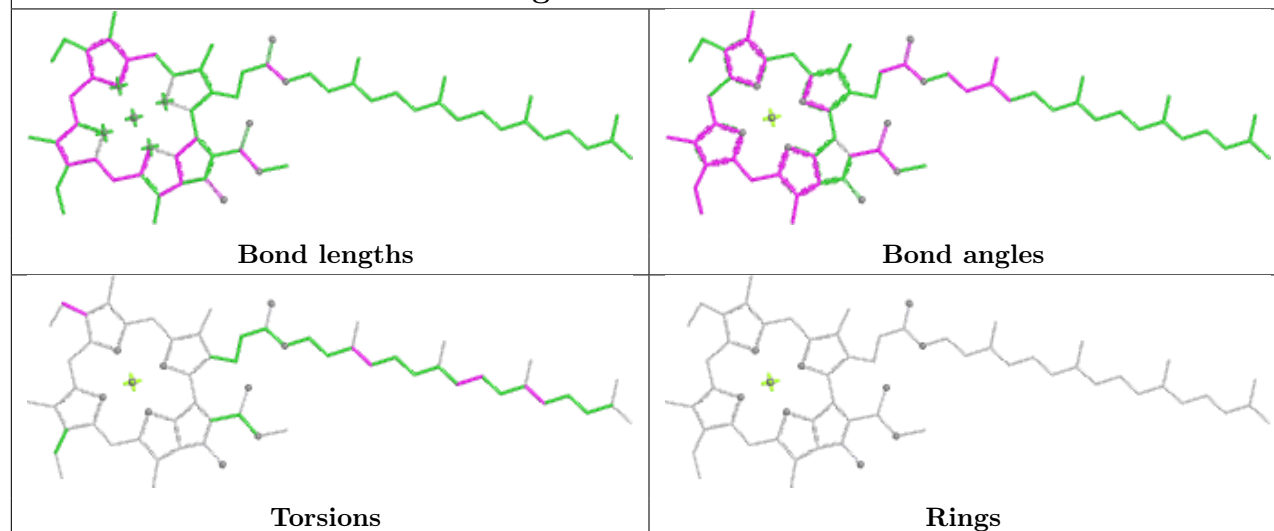
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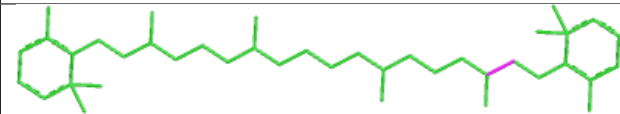
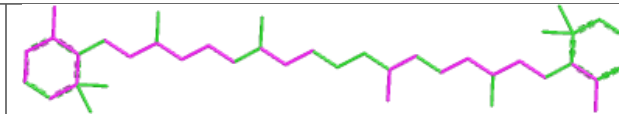
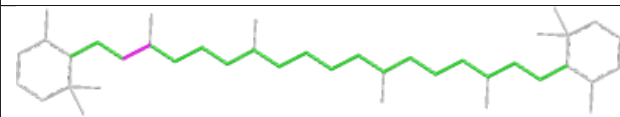
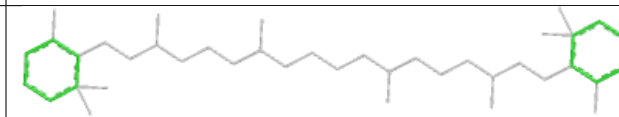


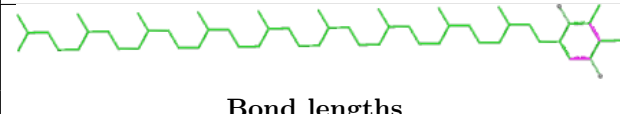
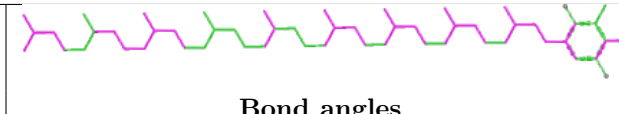
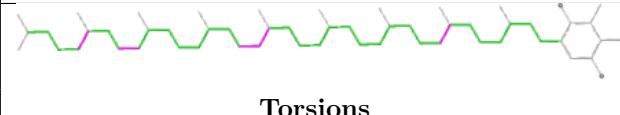
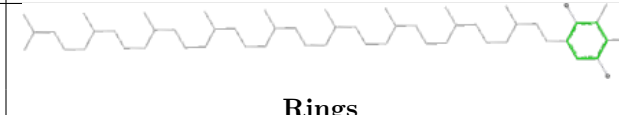
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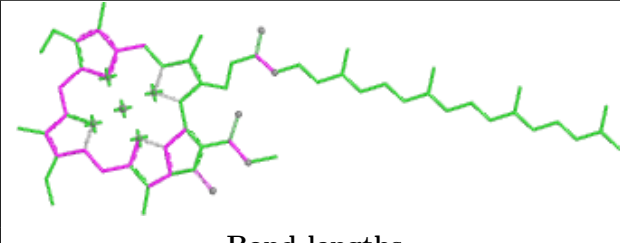
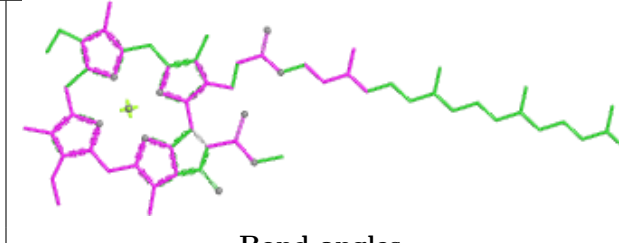
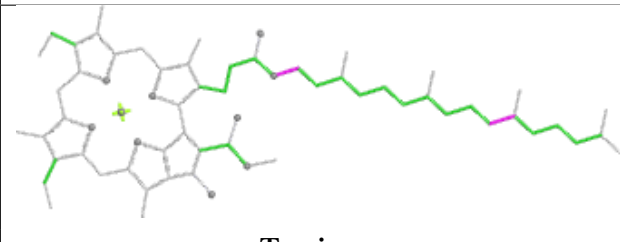
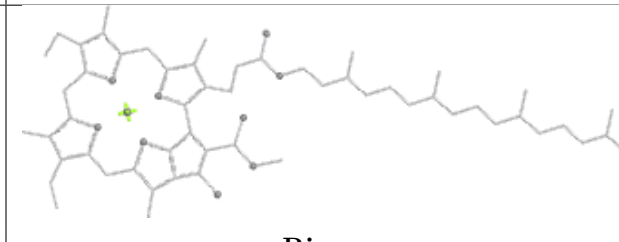


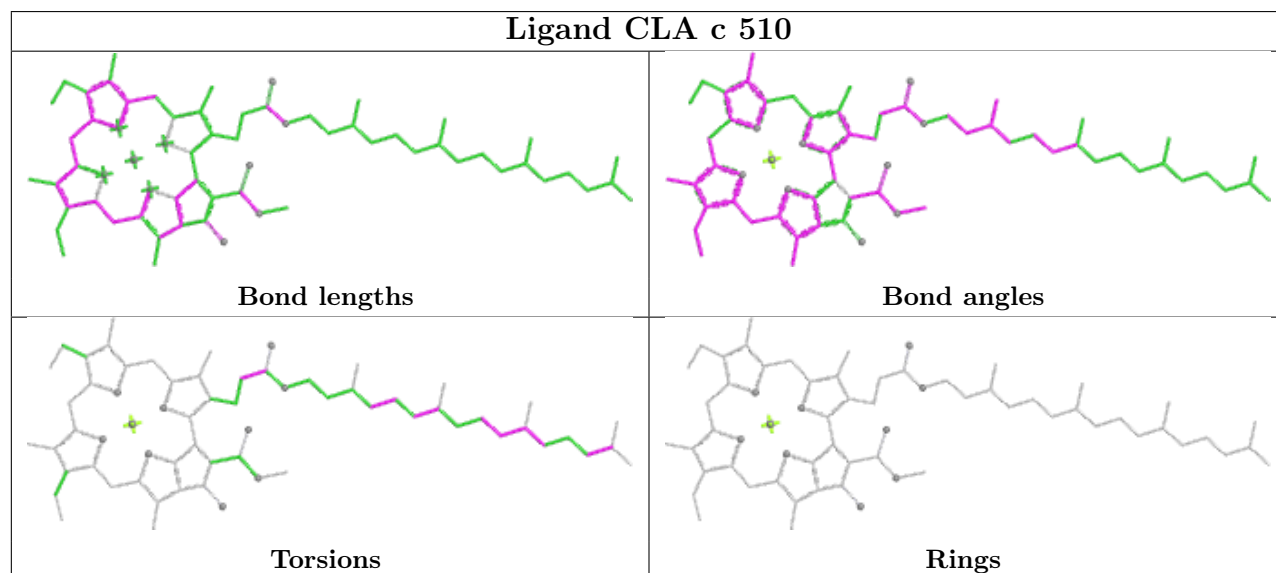
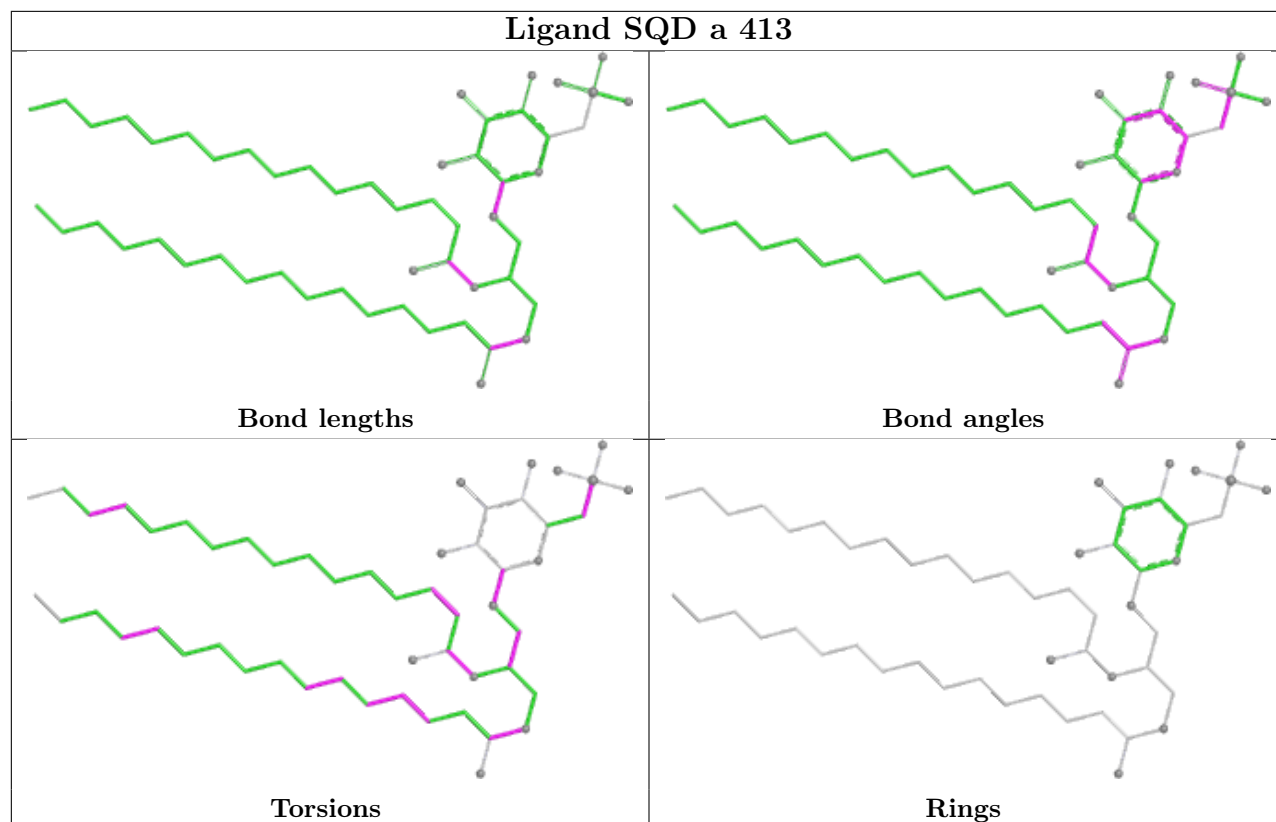
Ligand CLA C 506



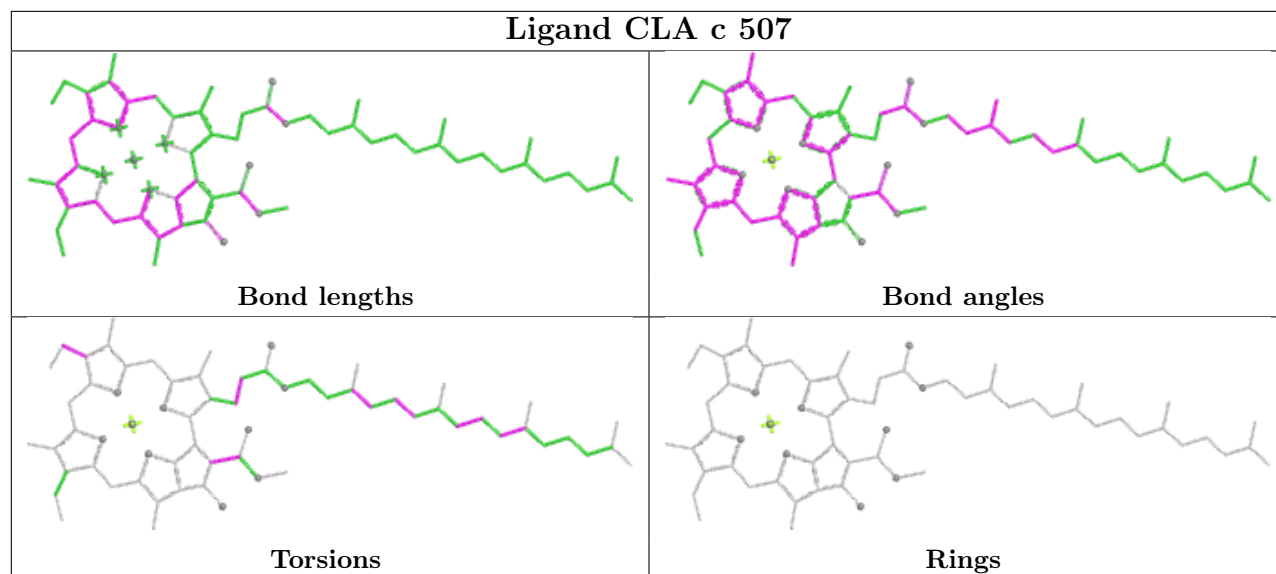
Ligand BCR C 527	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

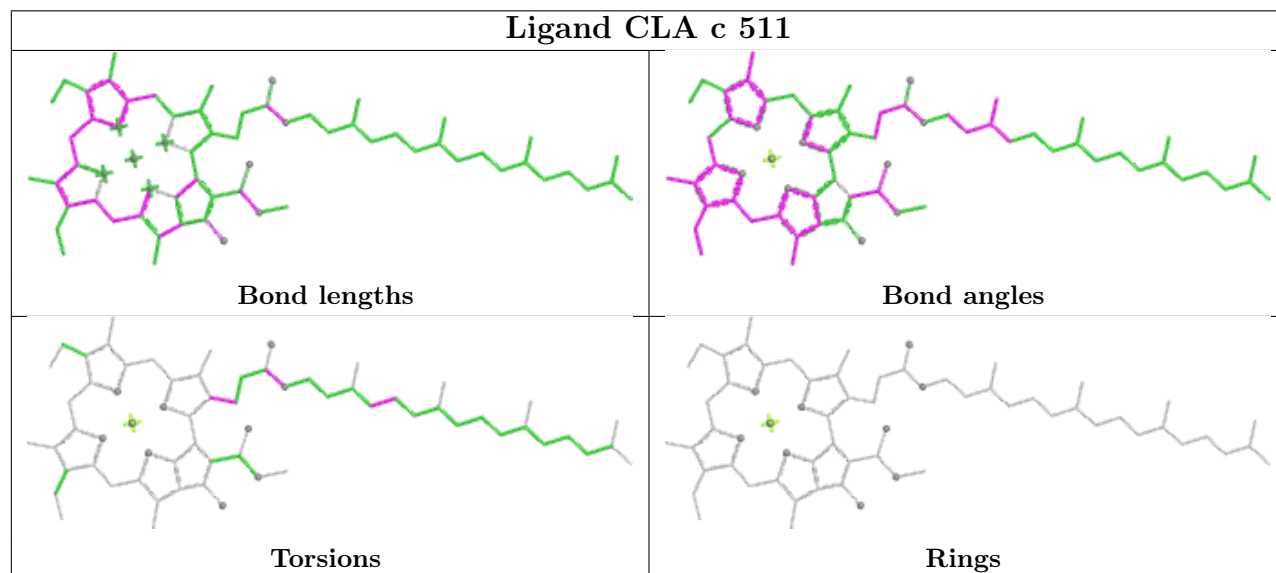
Ligand CLA d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings



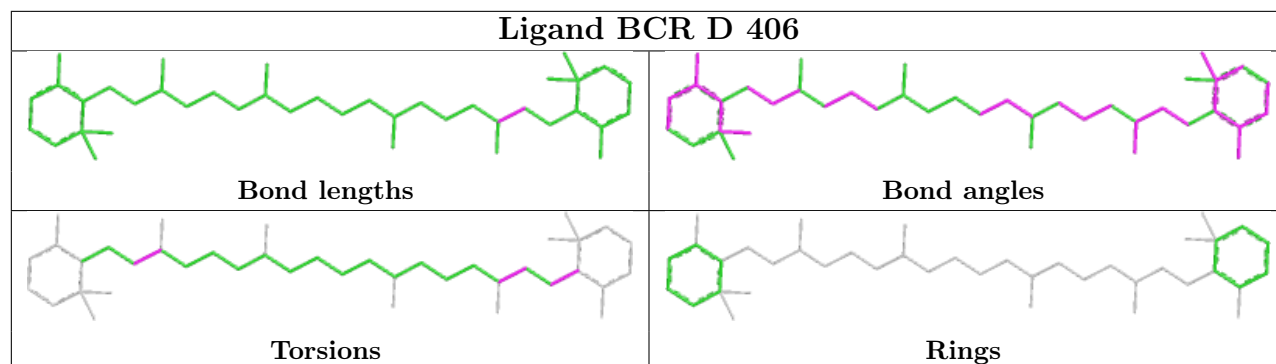
Ligand CLA c 507

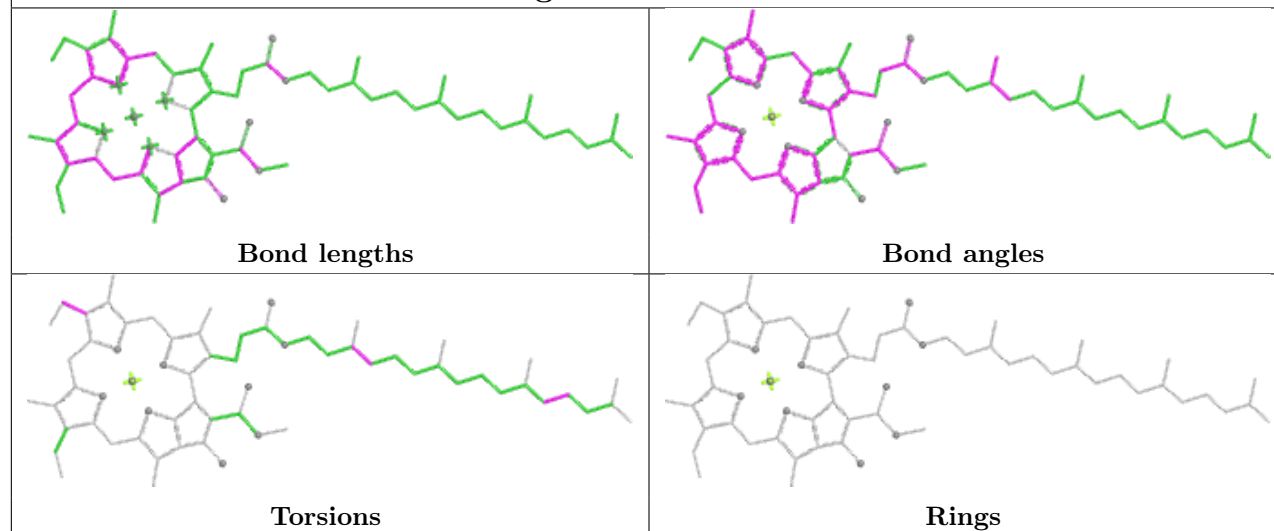
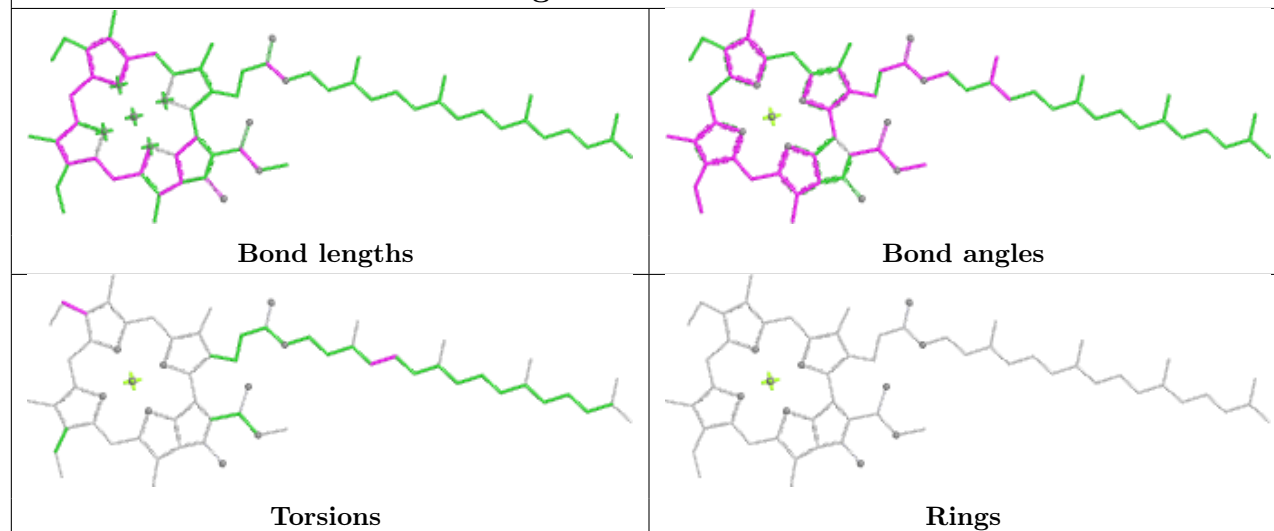


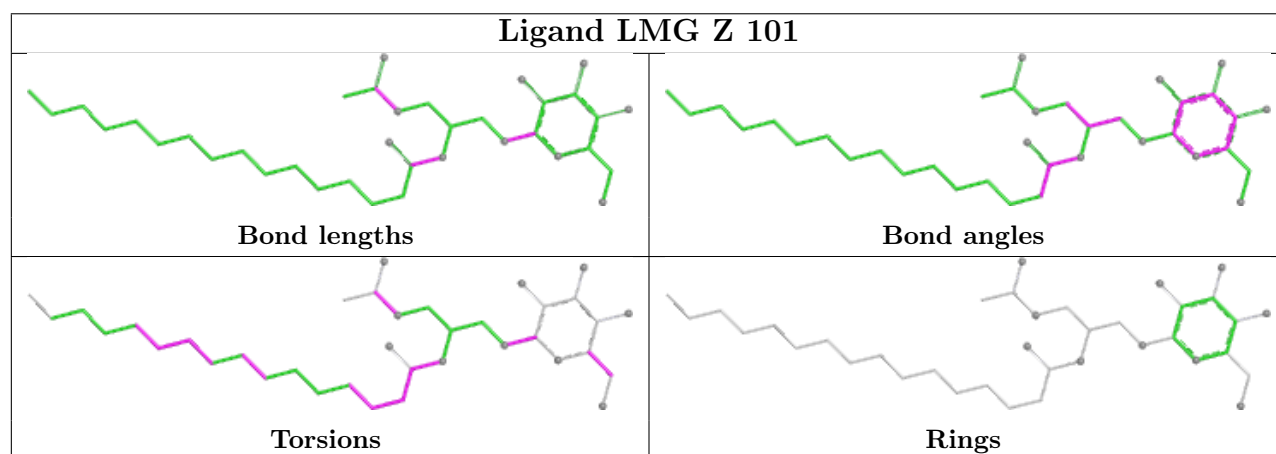
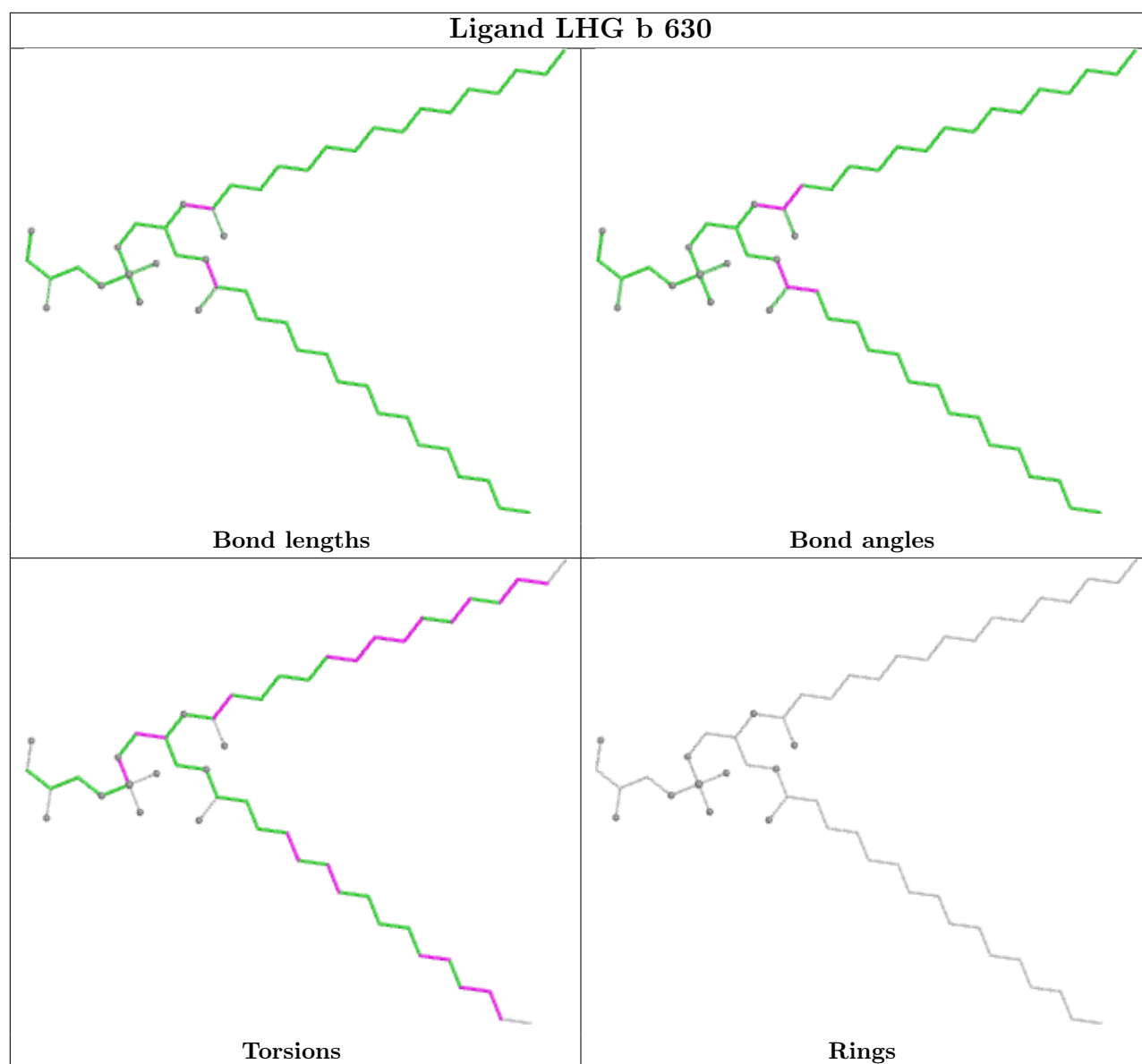
Ligand CLA c 511

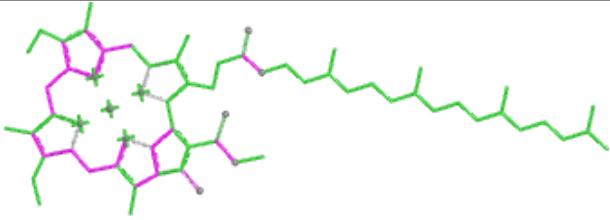
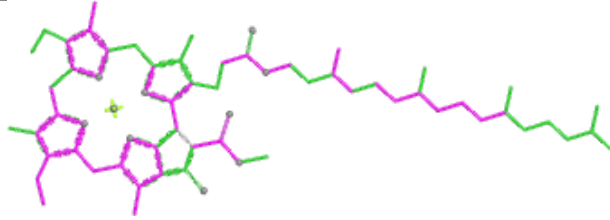
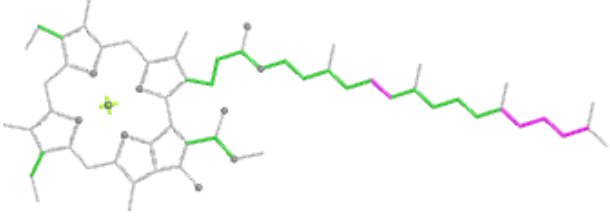
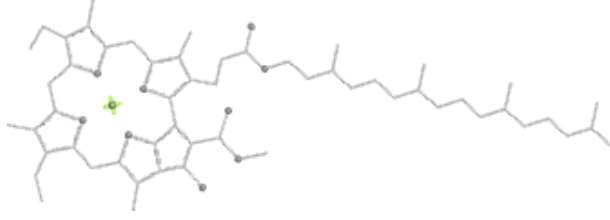
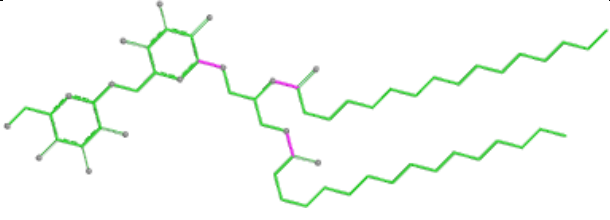
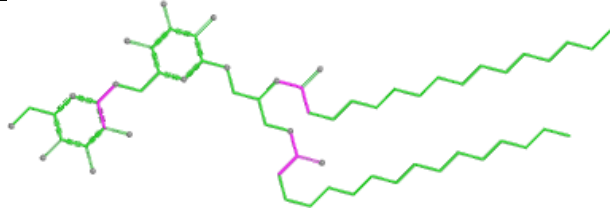
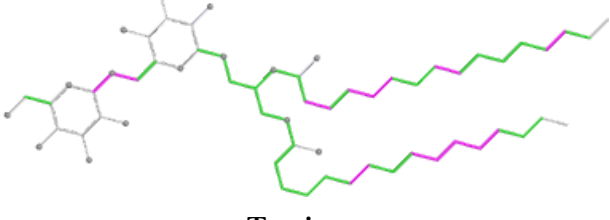
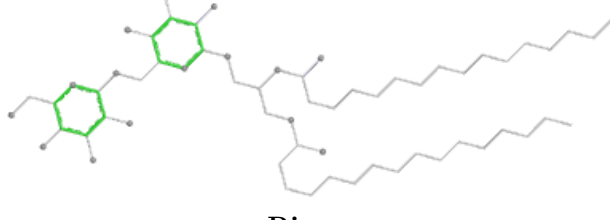
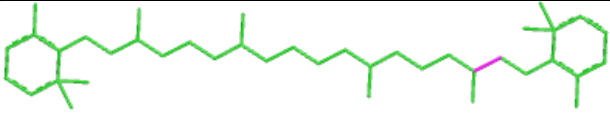
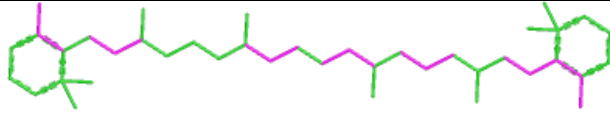
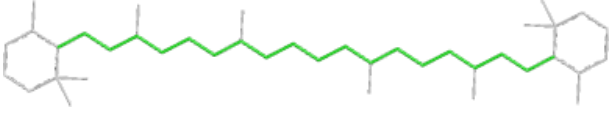
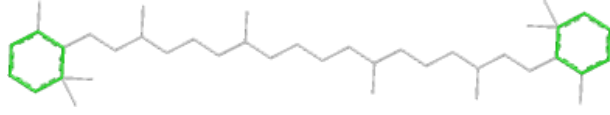


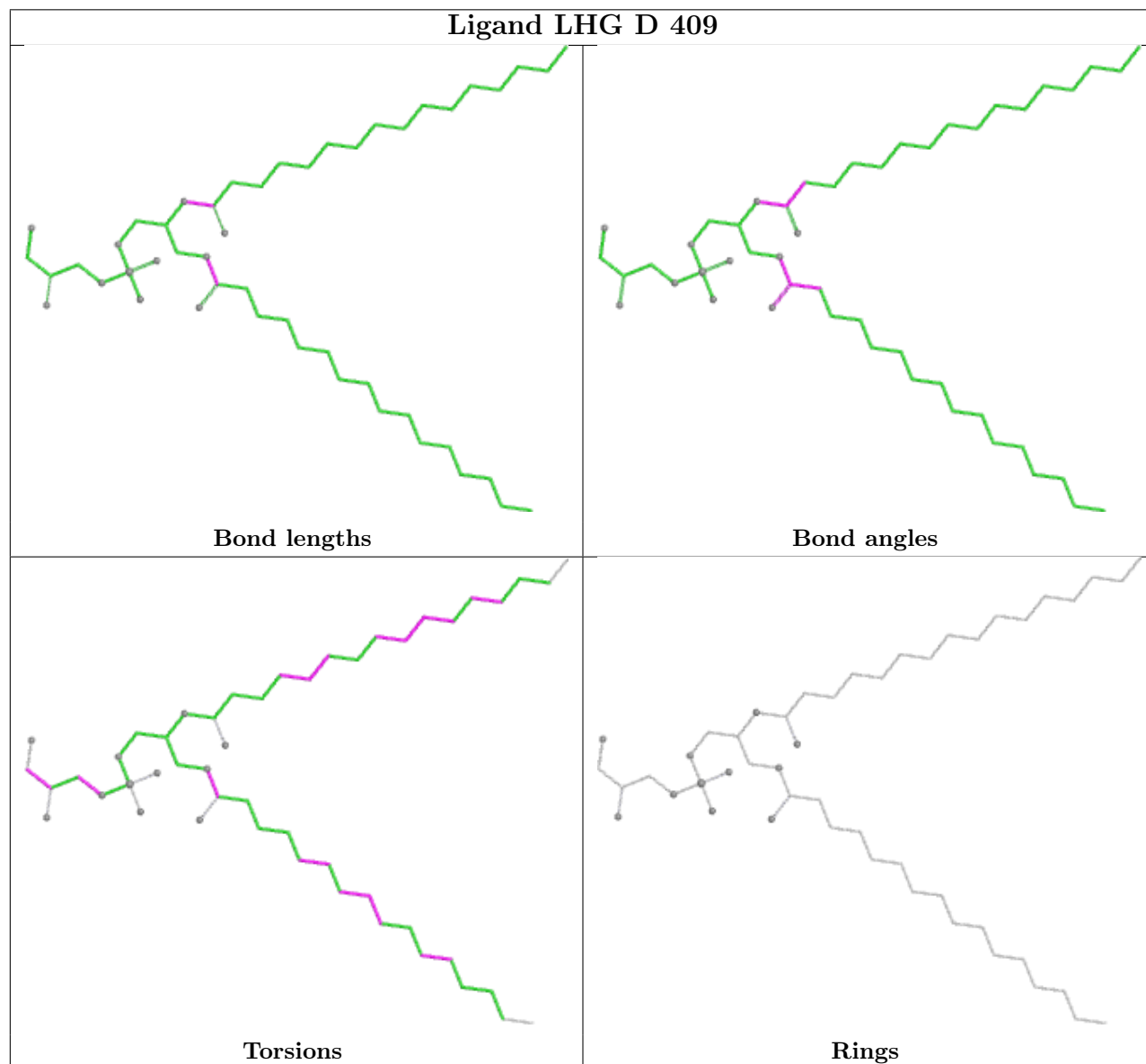
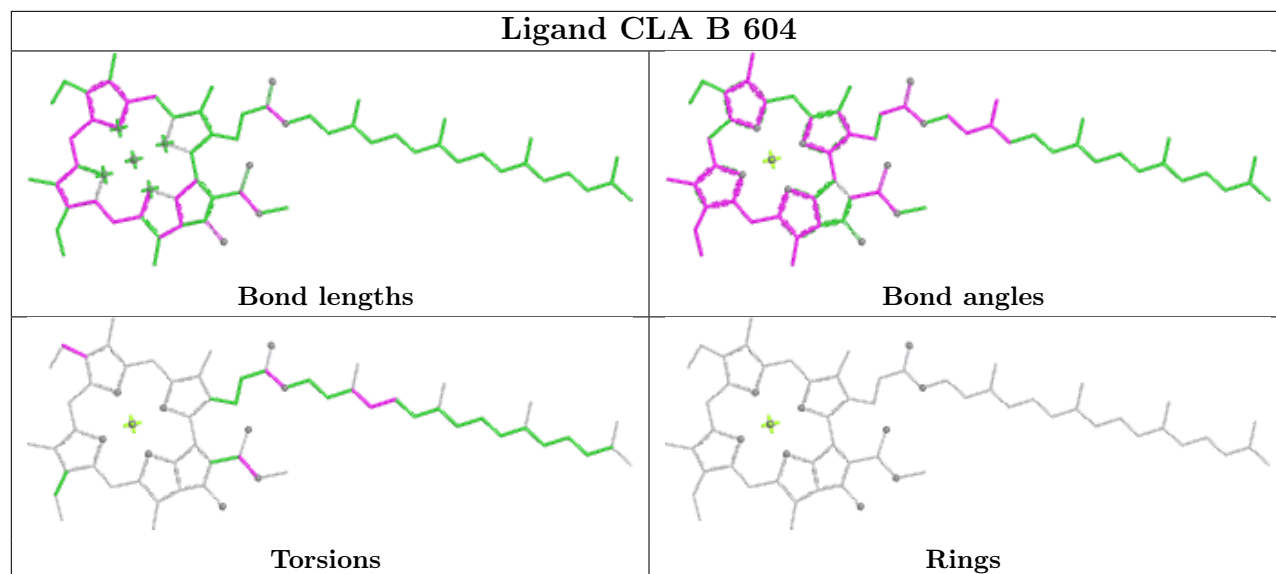
Ligand BCR D 406

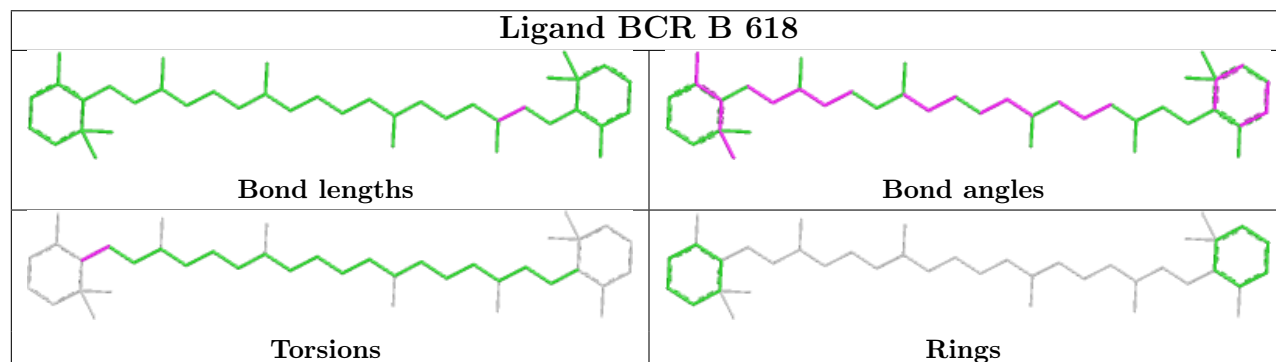
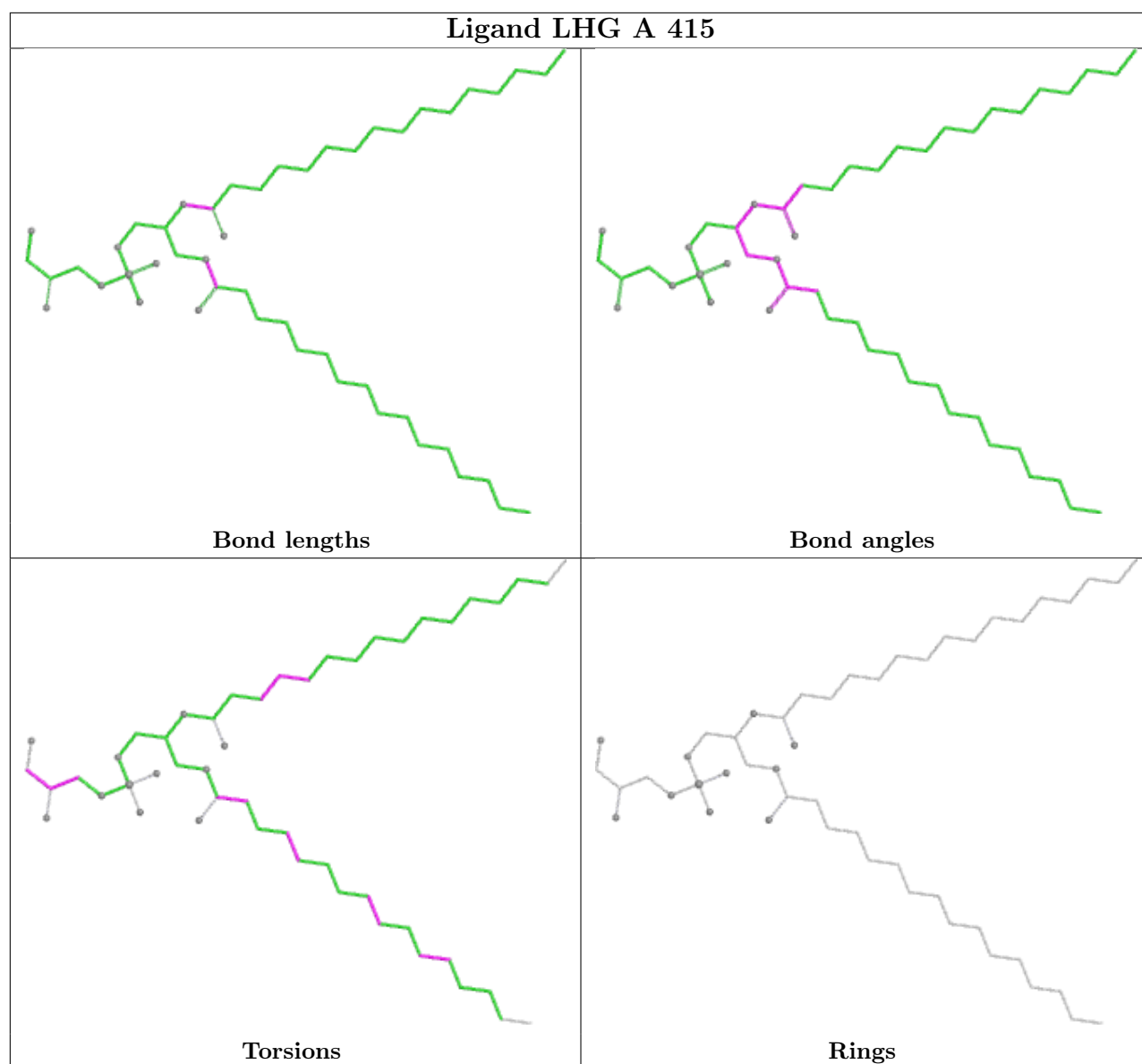


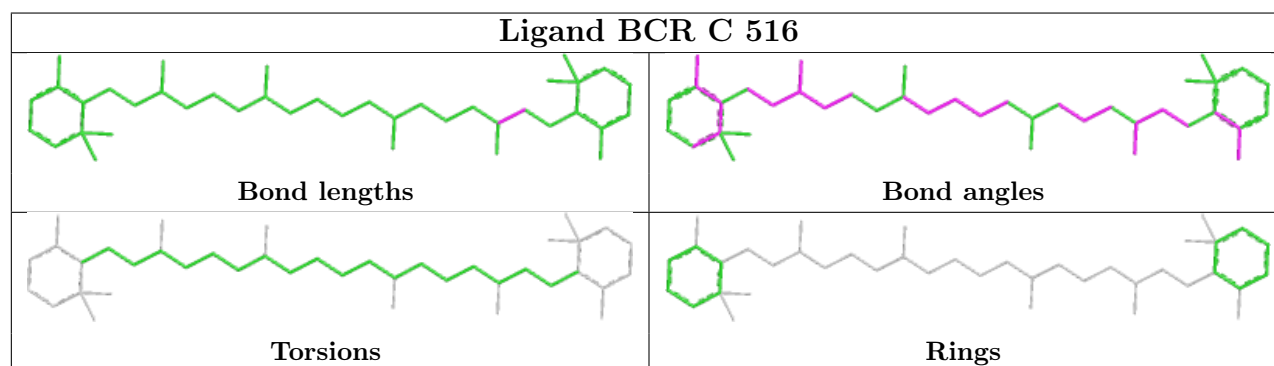
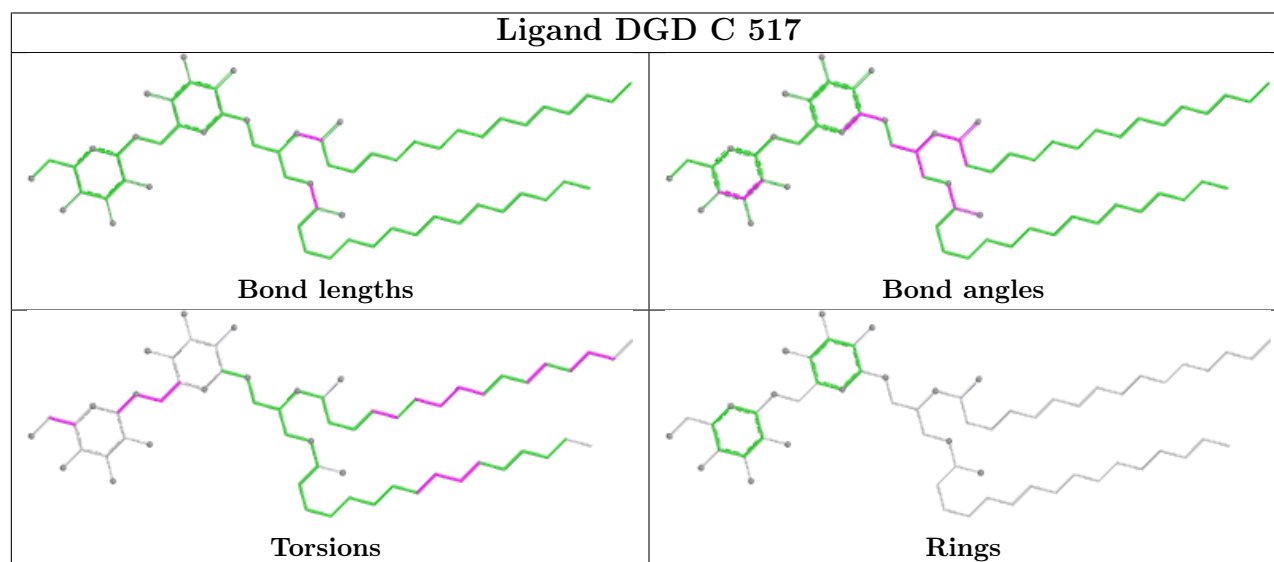
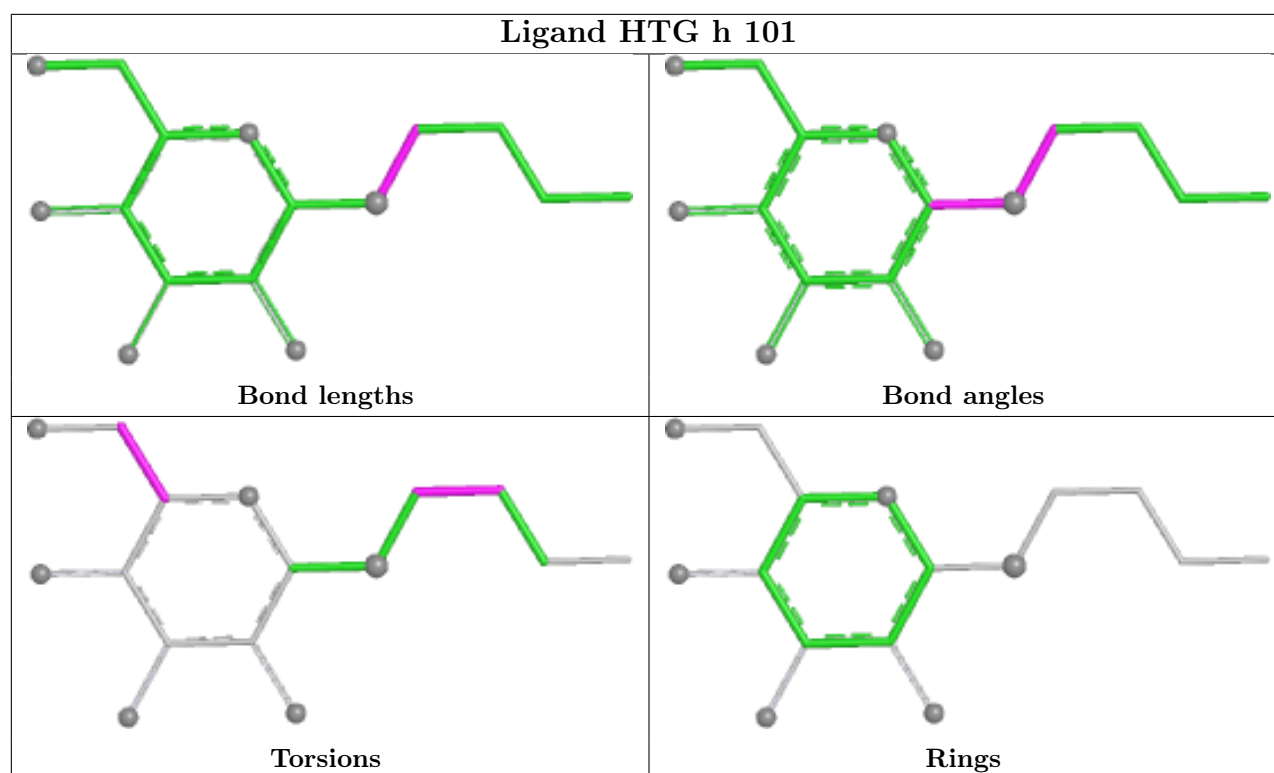
Ligand CLA b 603**Ligand CLA B 608**

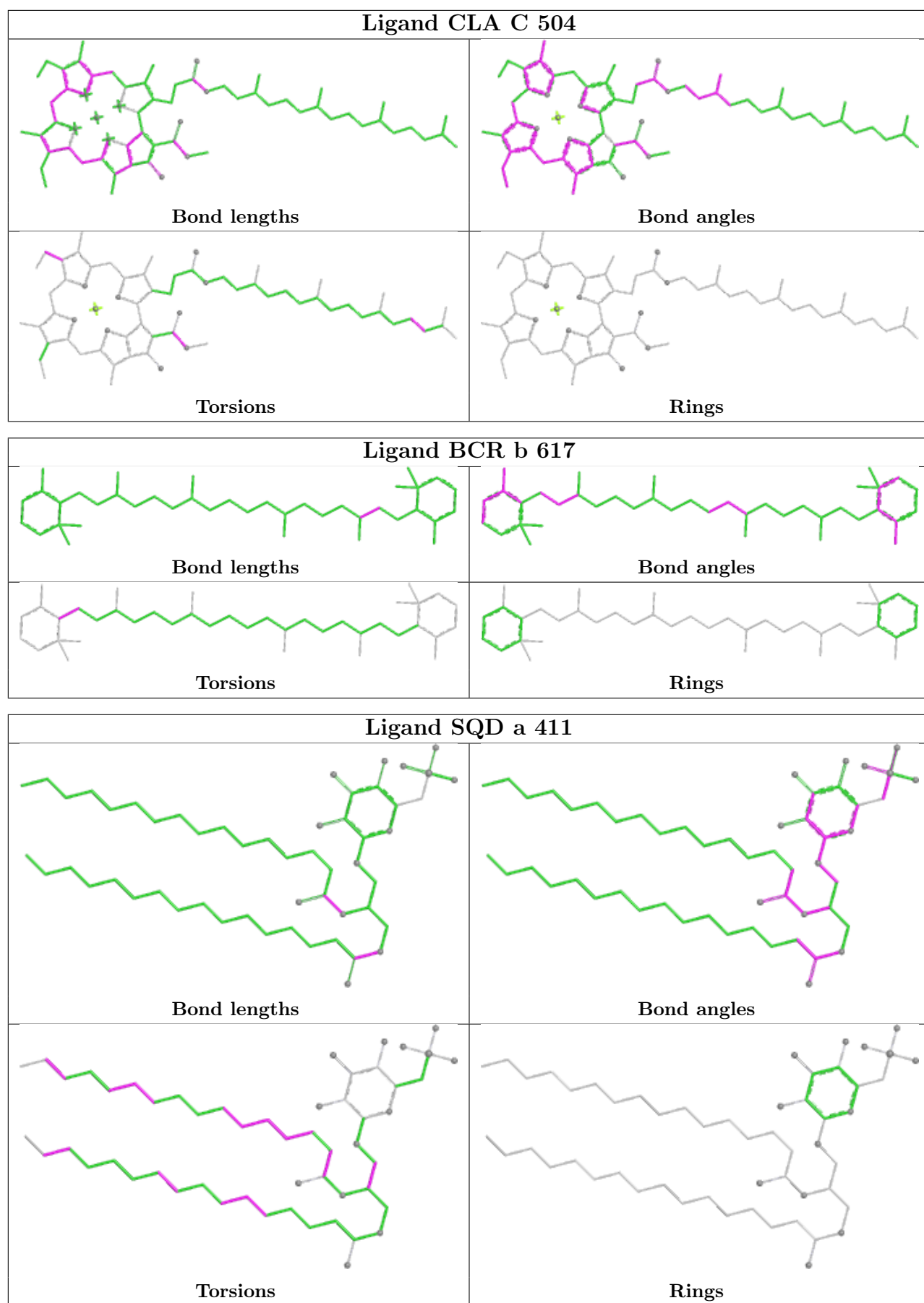


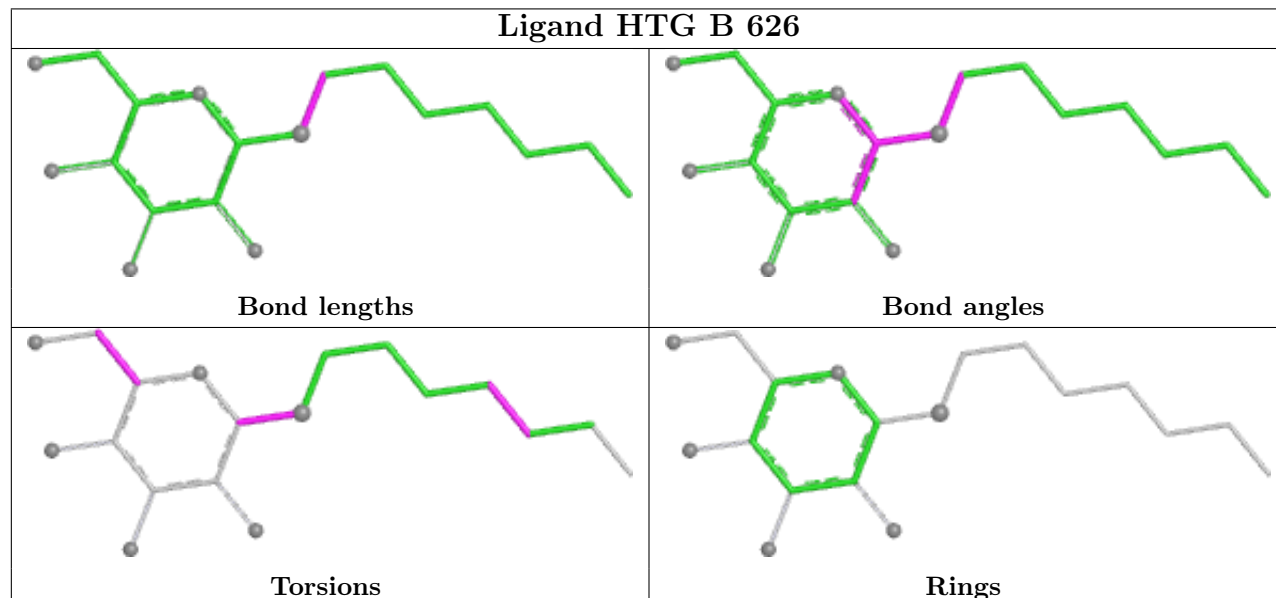
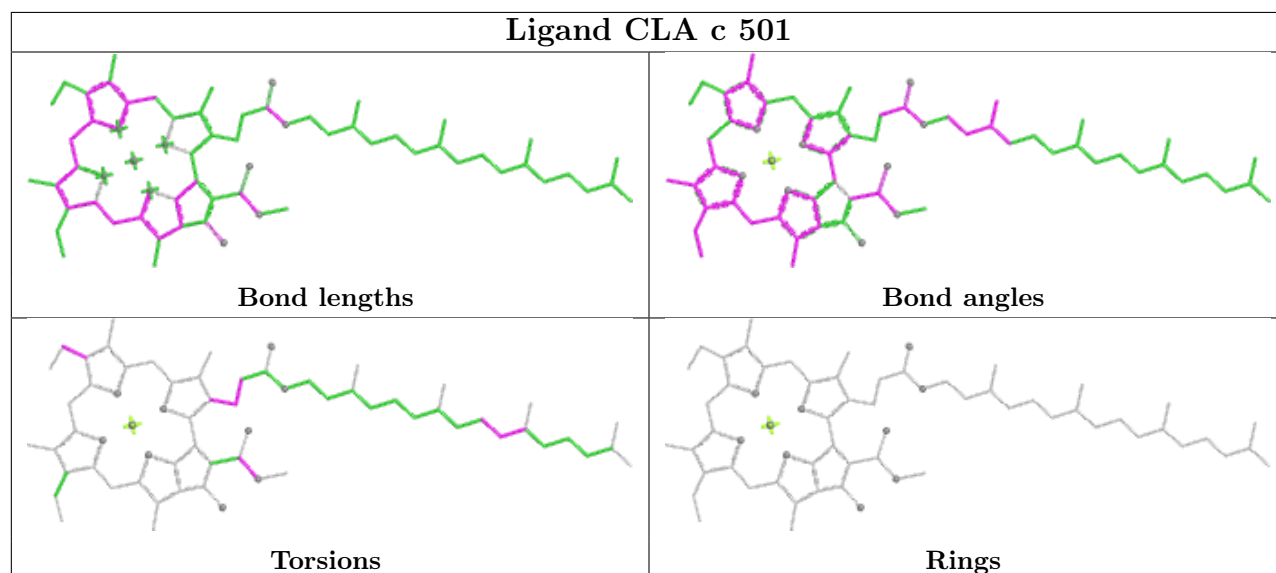
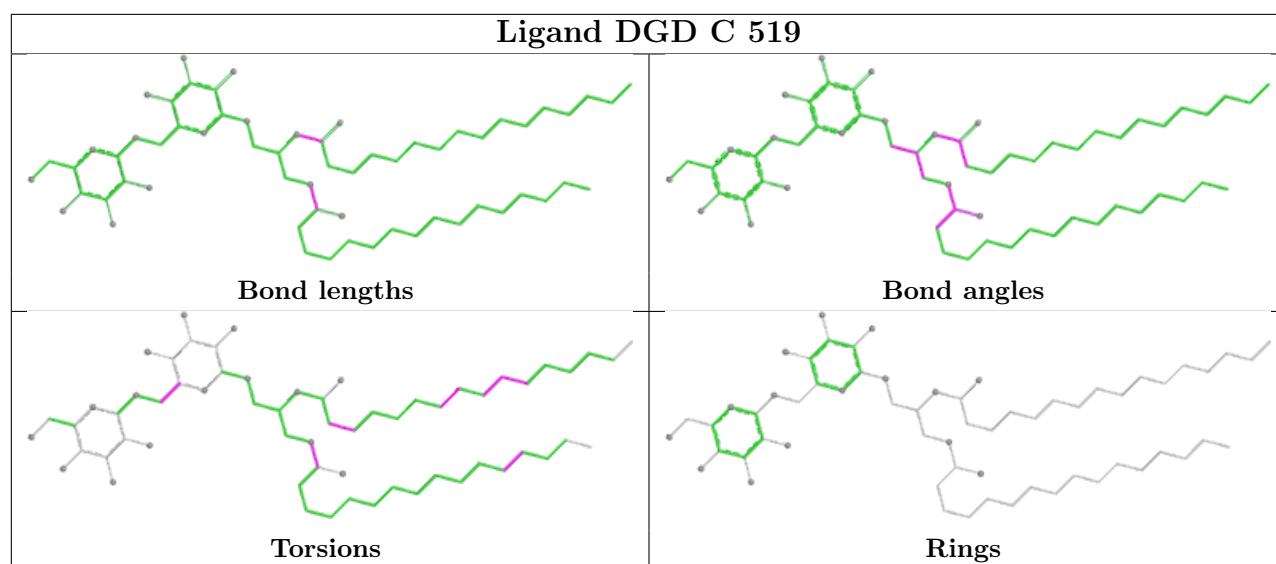
Ligand CLA b 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 517	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

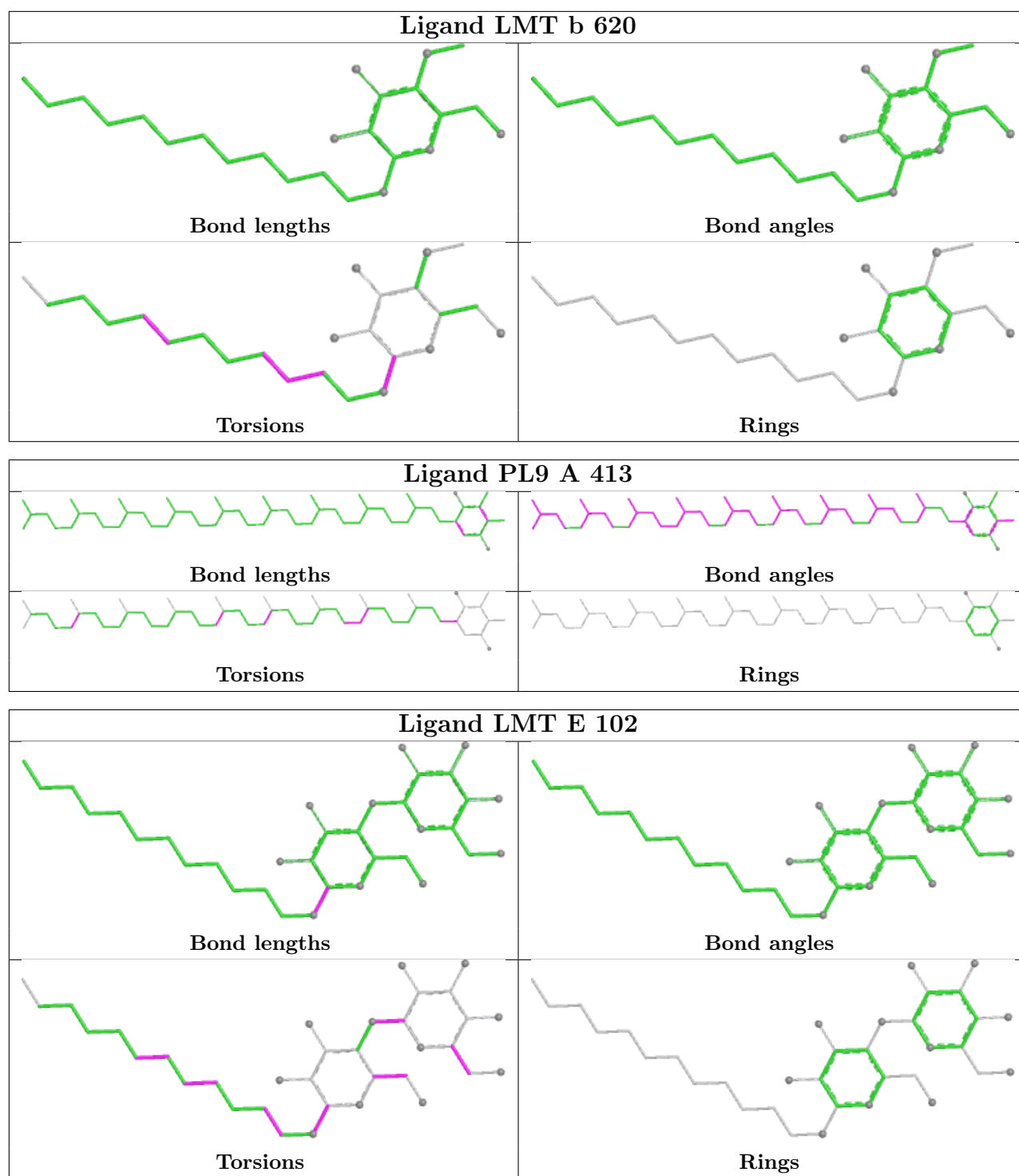


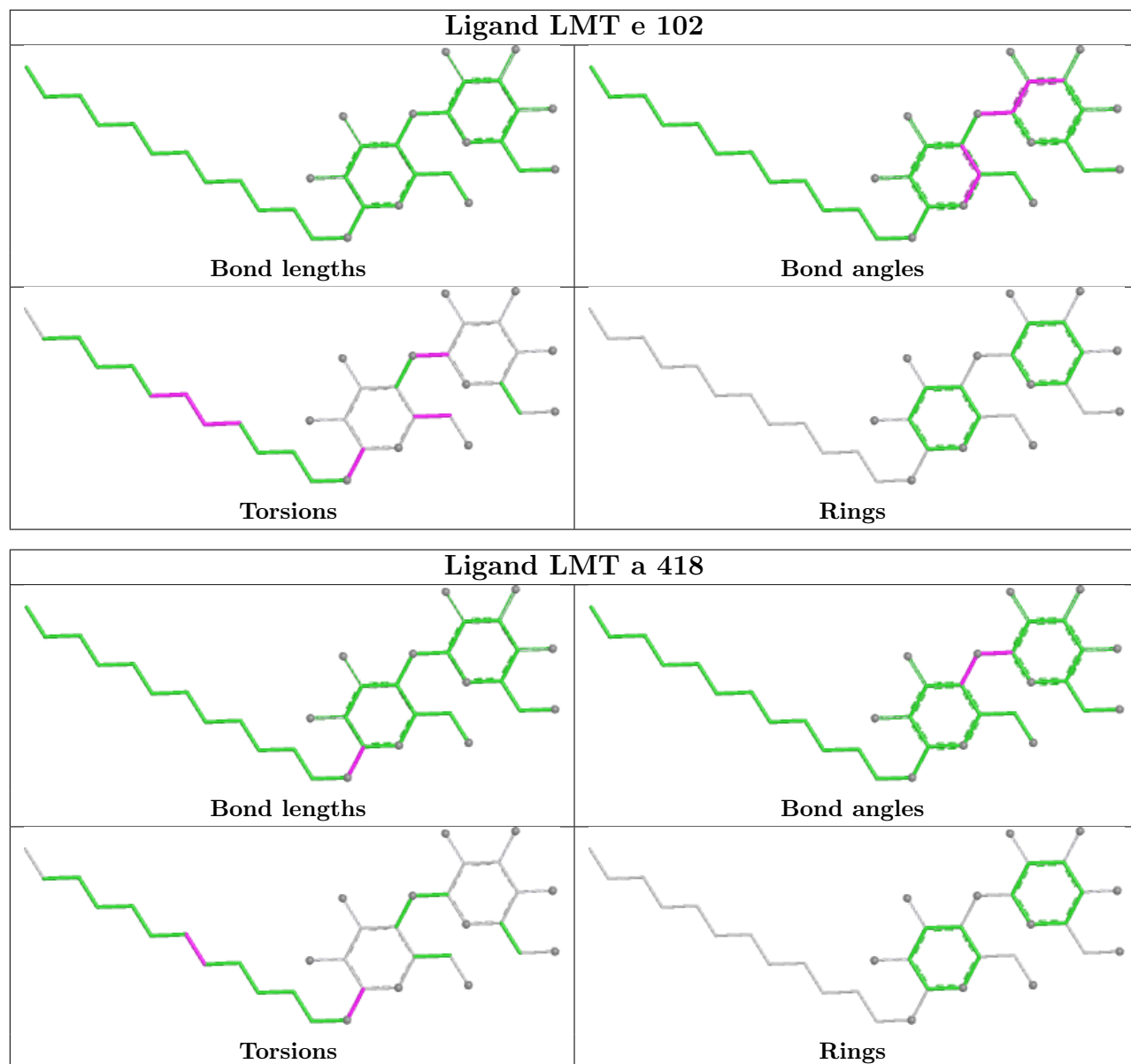




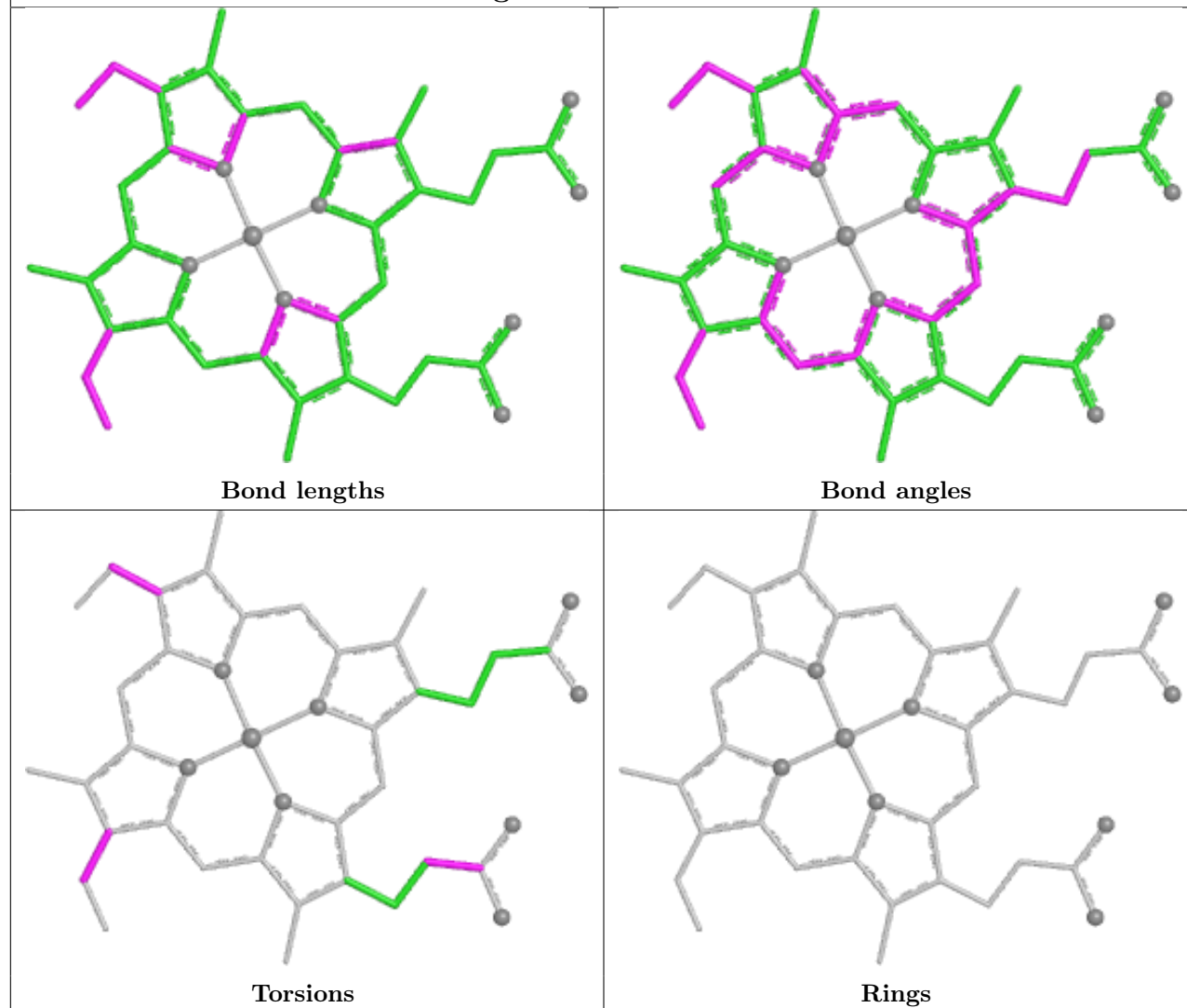




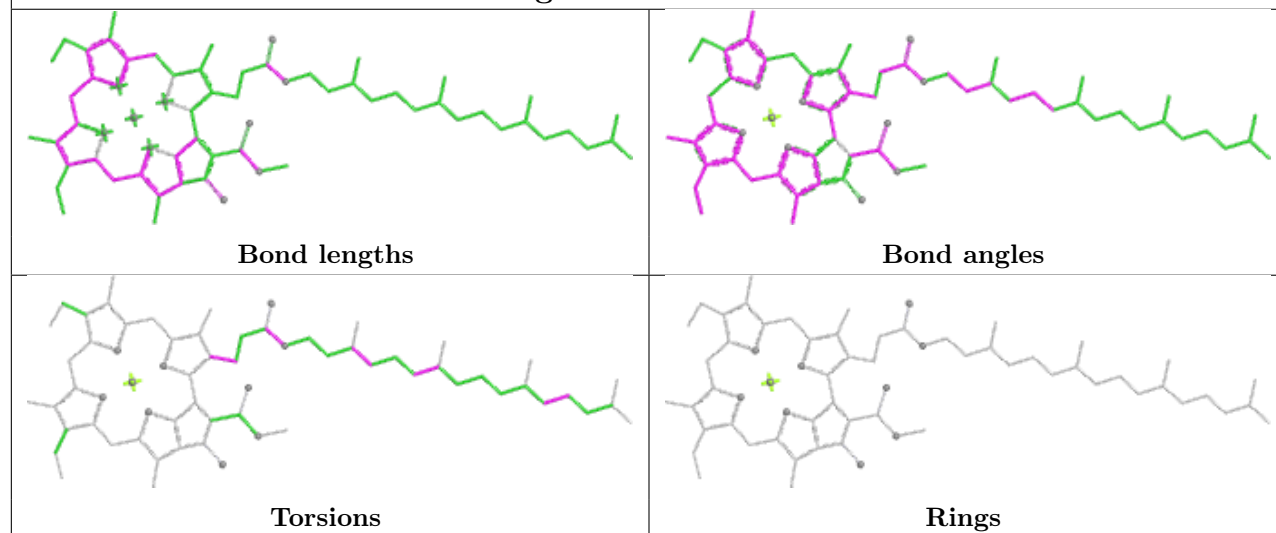


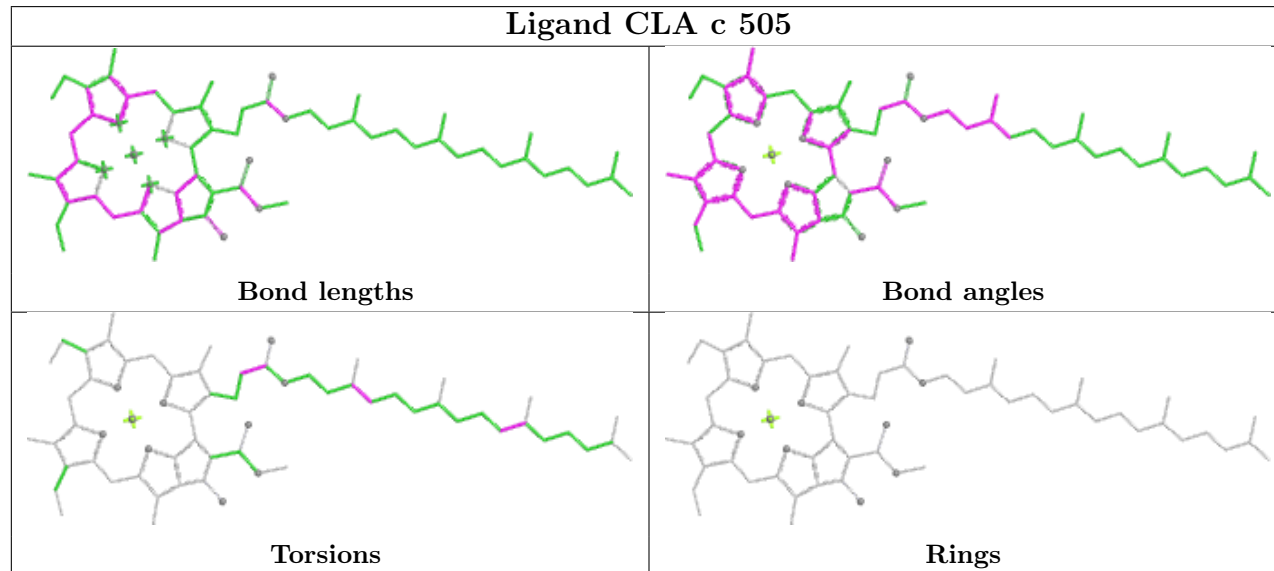
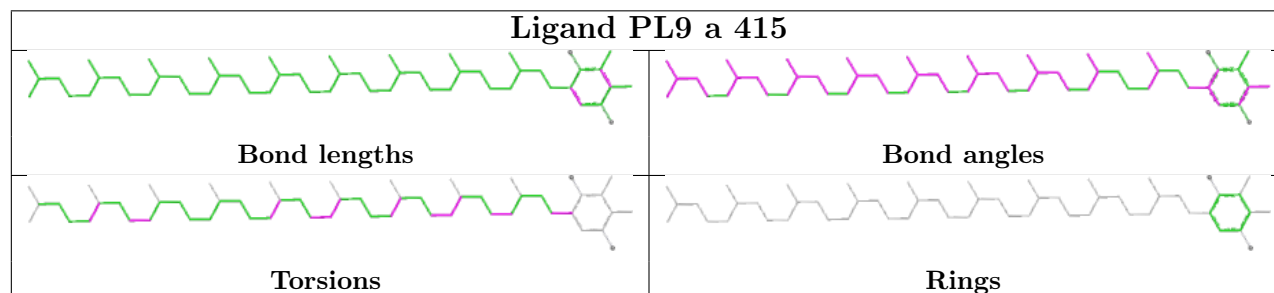
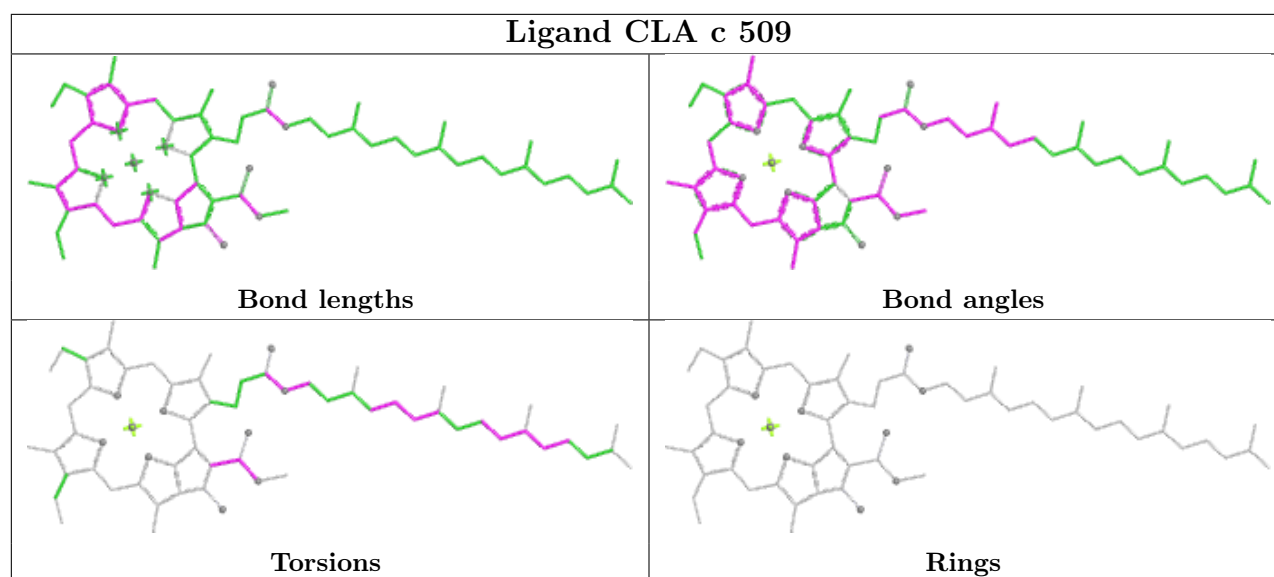


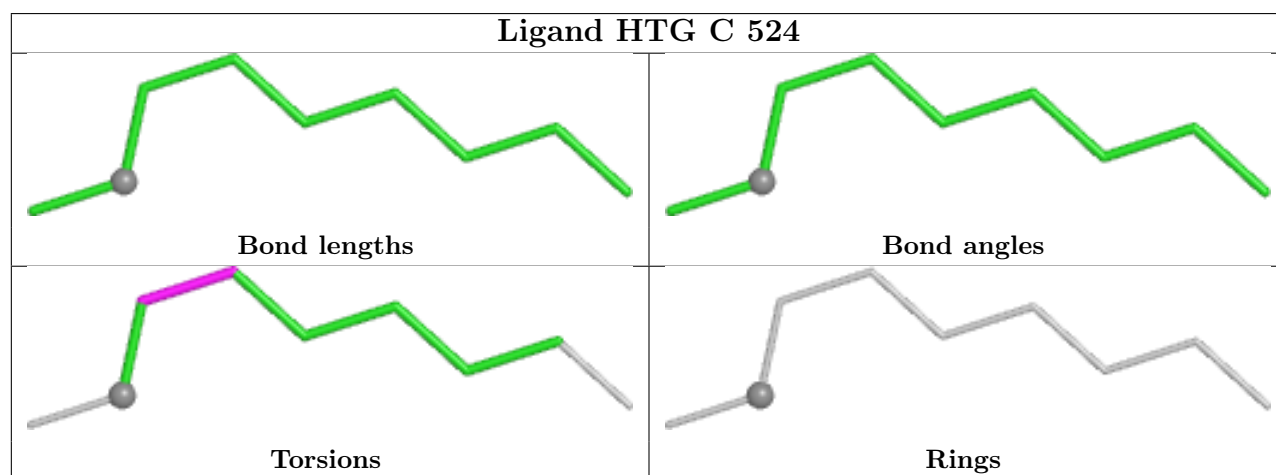
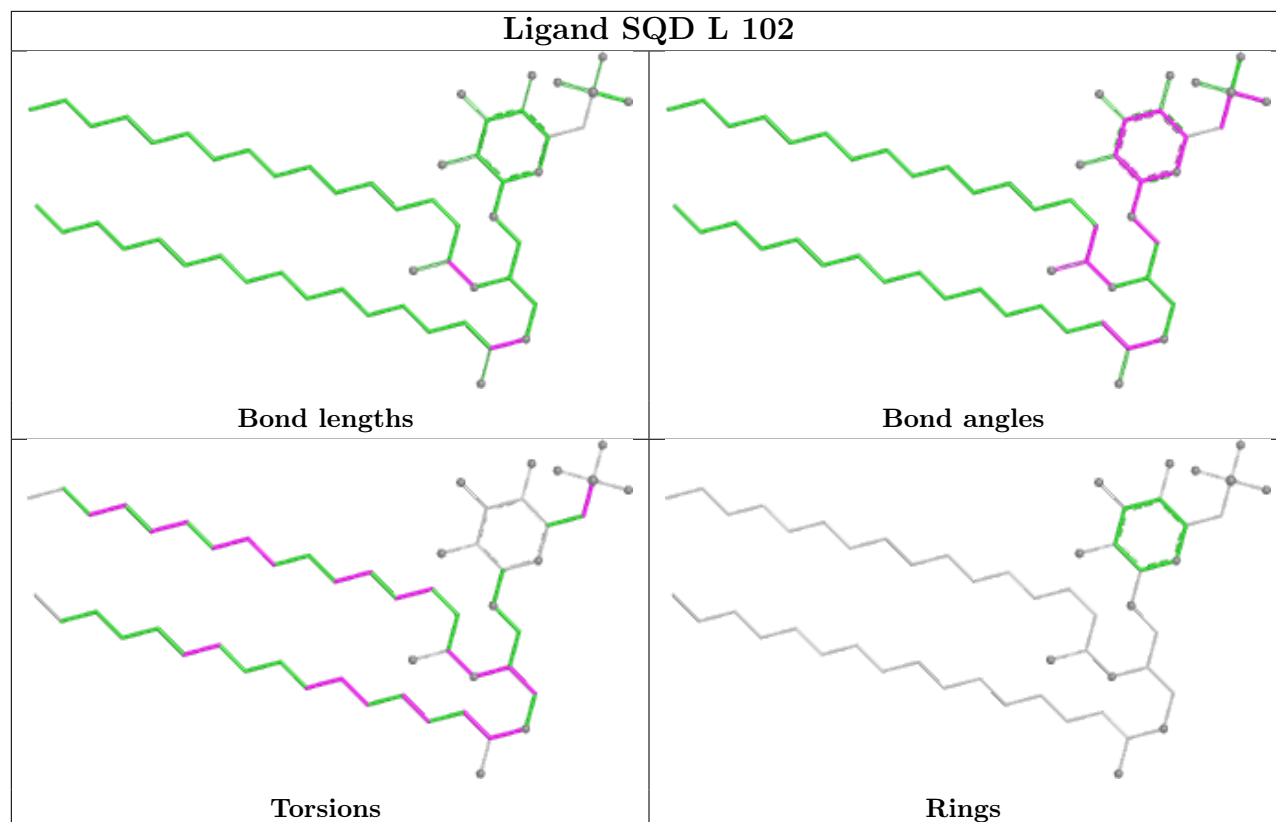
Ligand HEC V 202



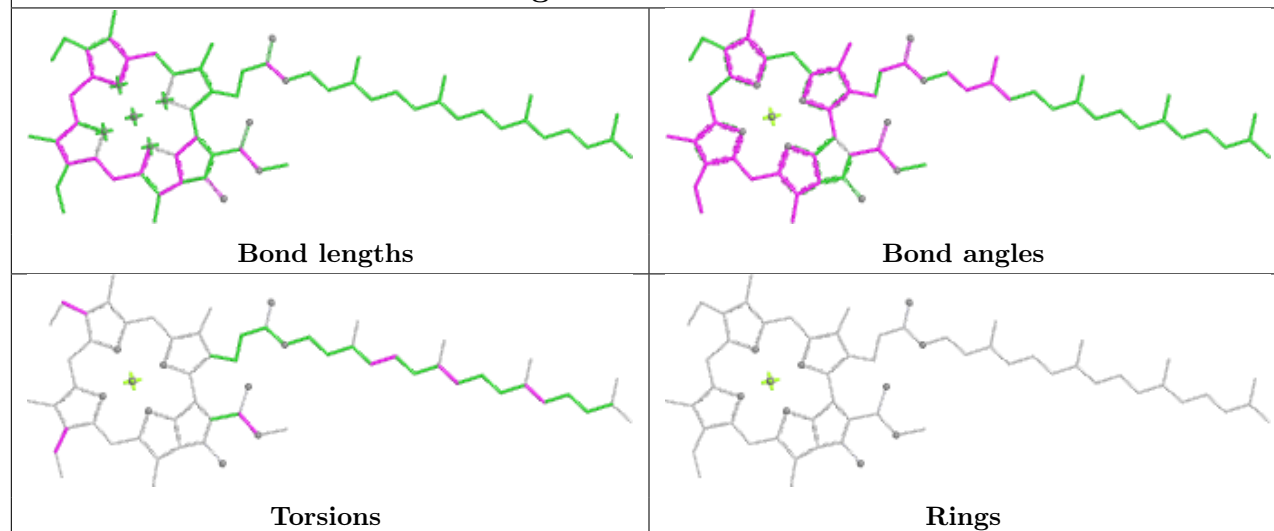
Ligand CLA b 609



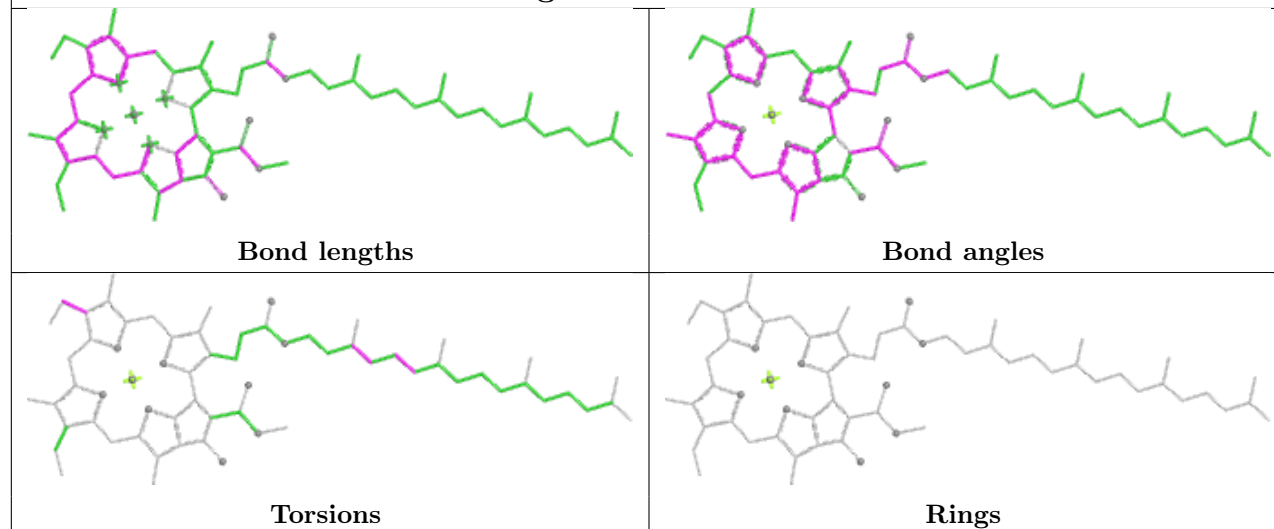




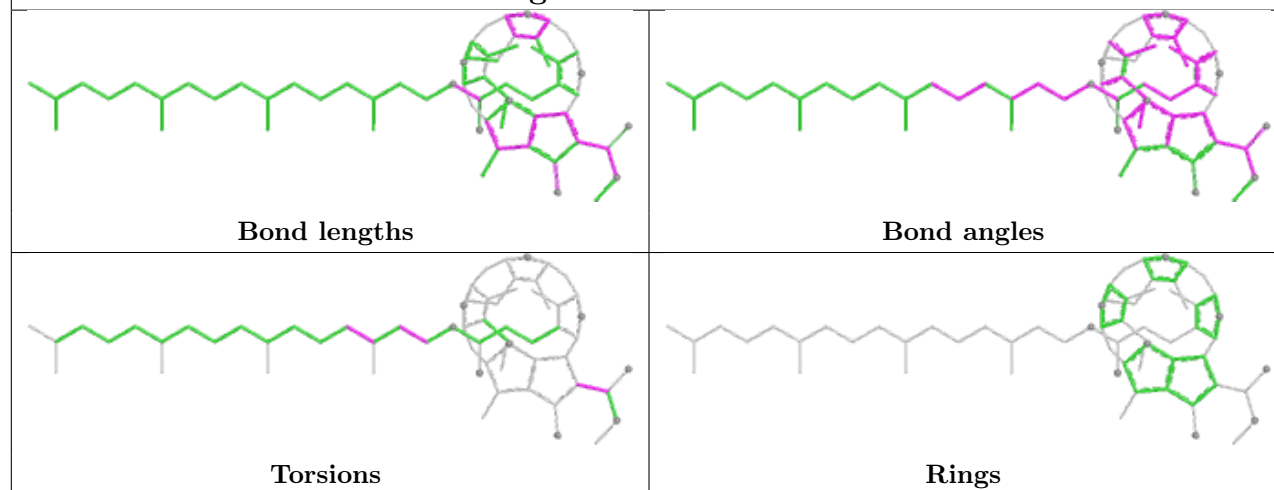
Ligand CLA A 405

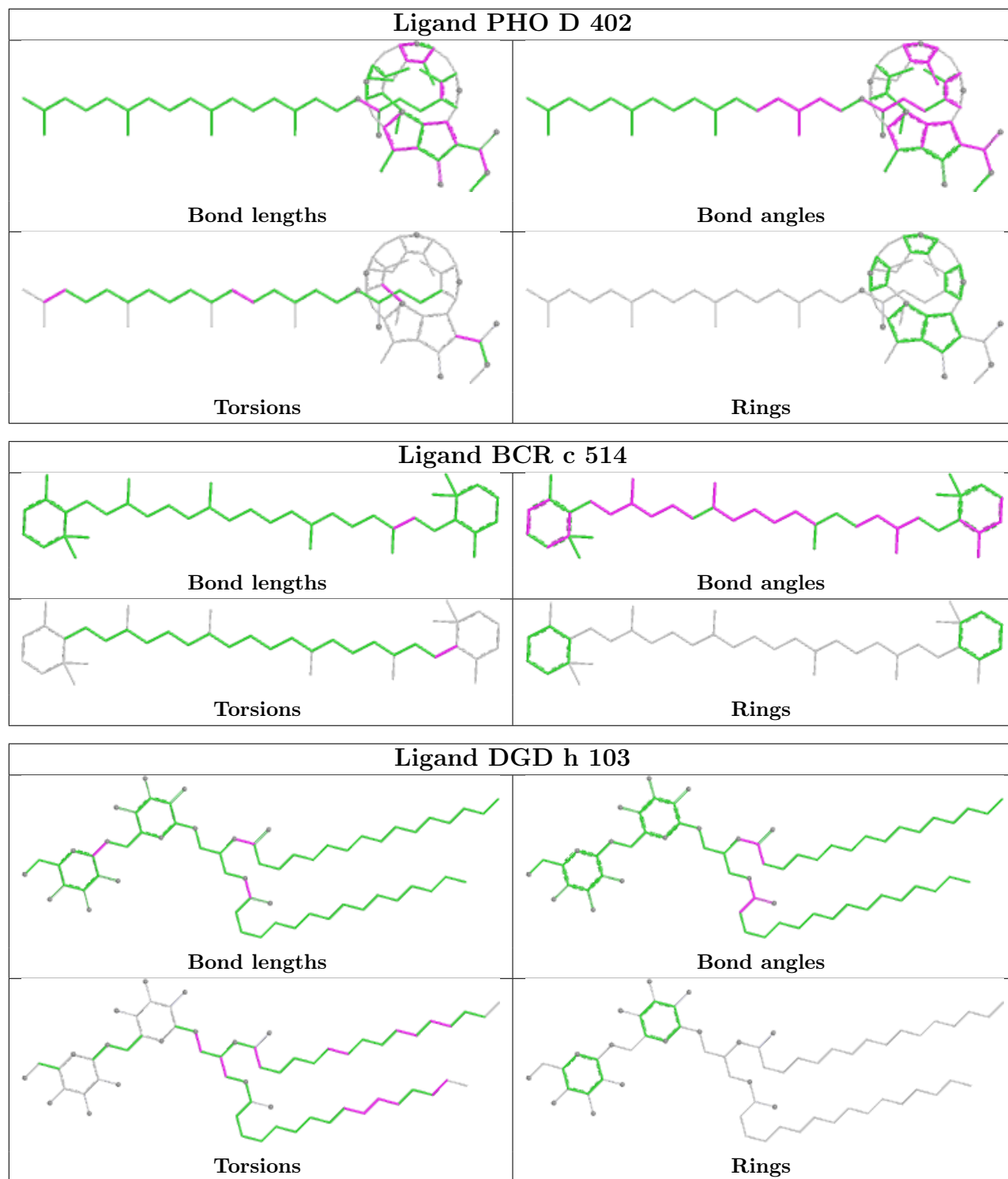


Ligand CLA c 508

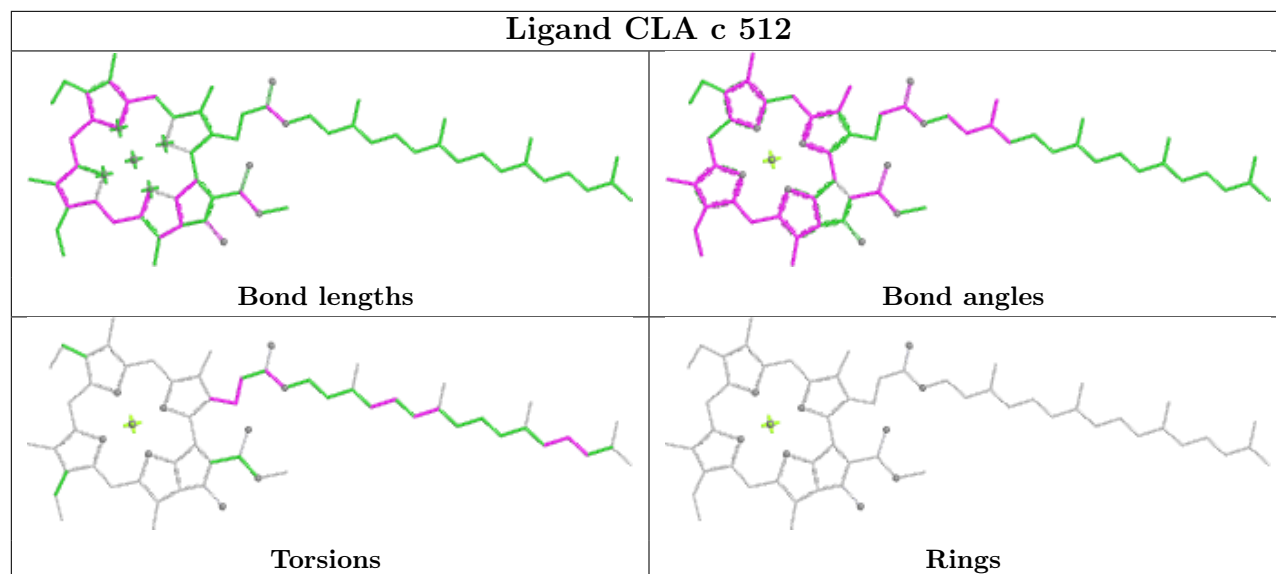


Ligand PHO A 406

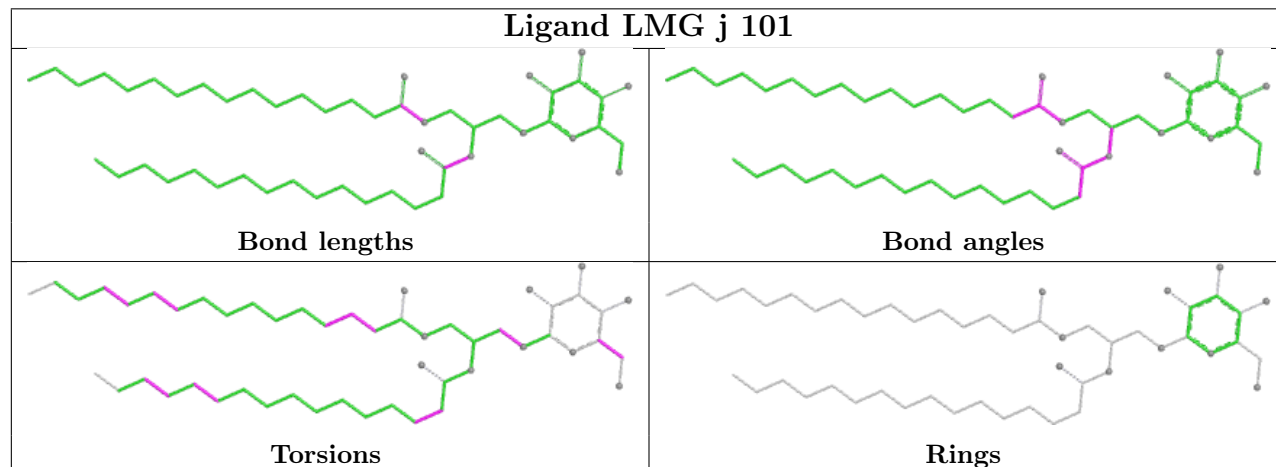


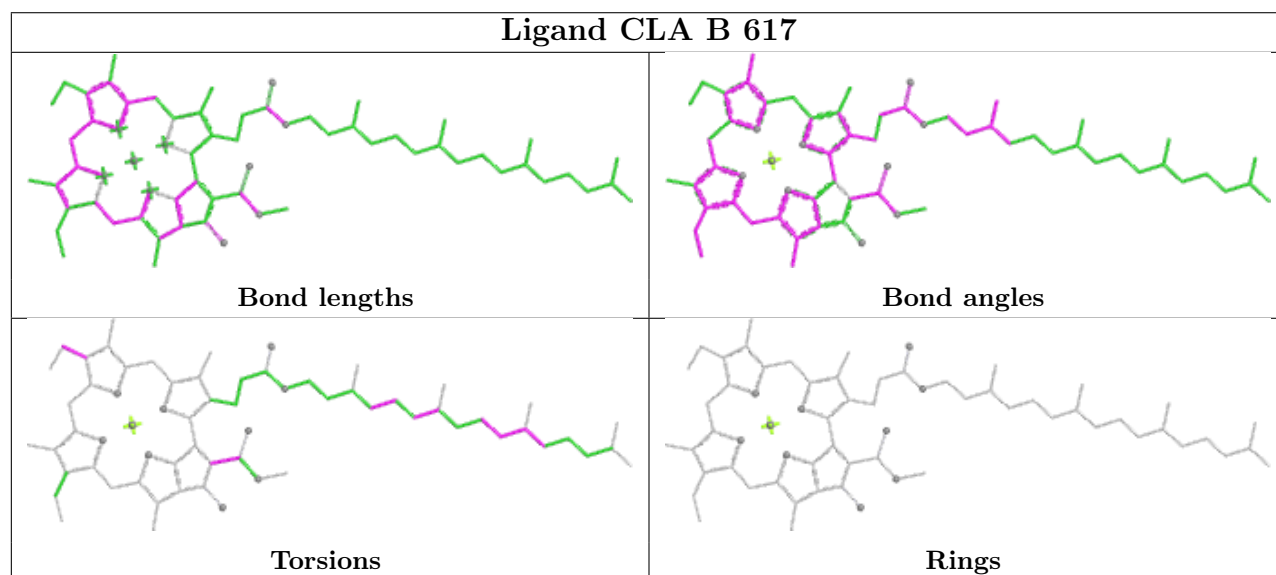
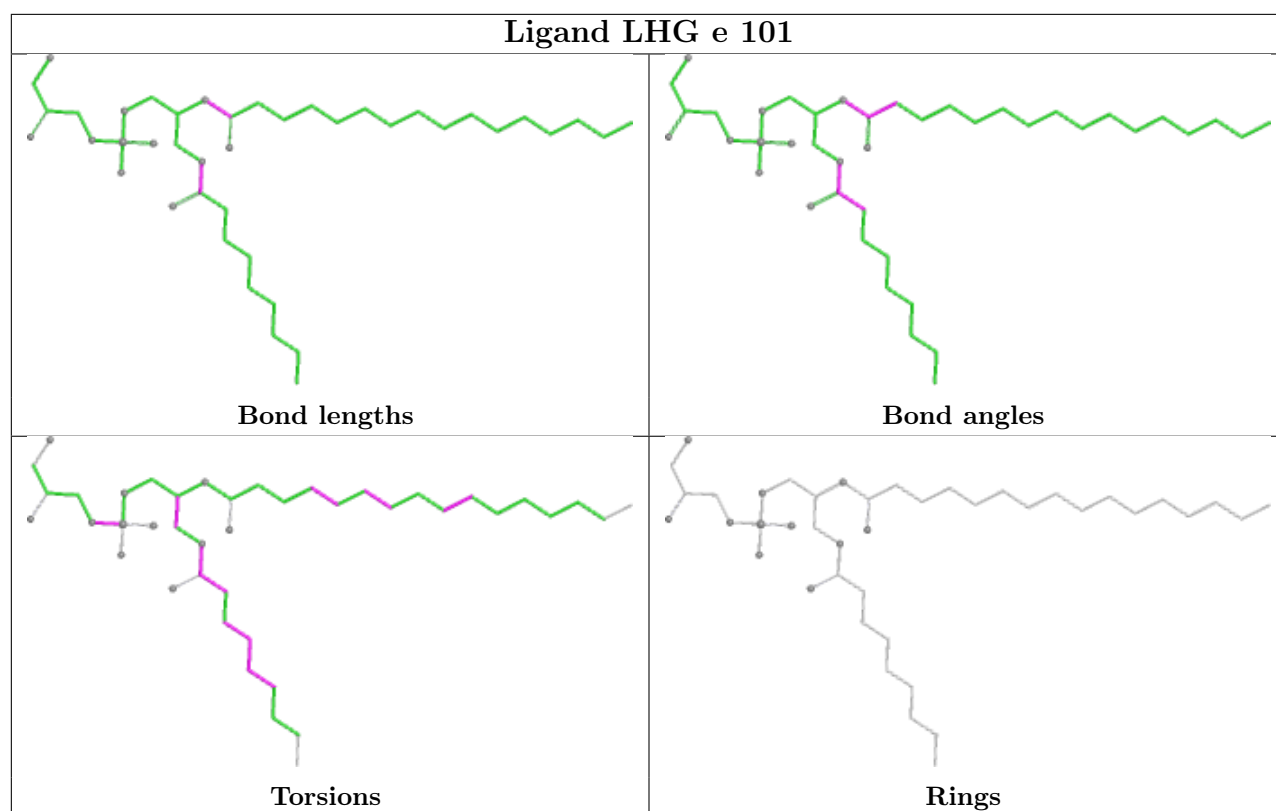


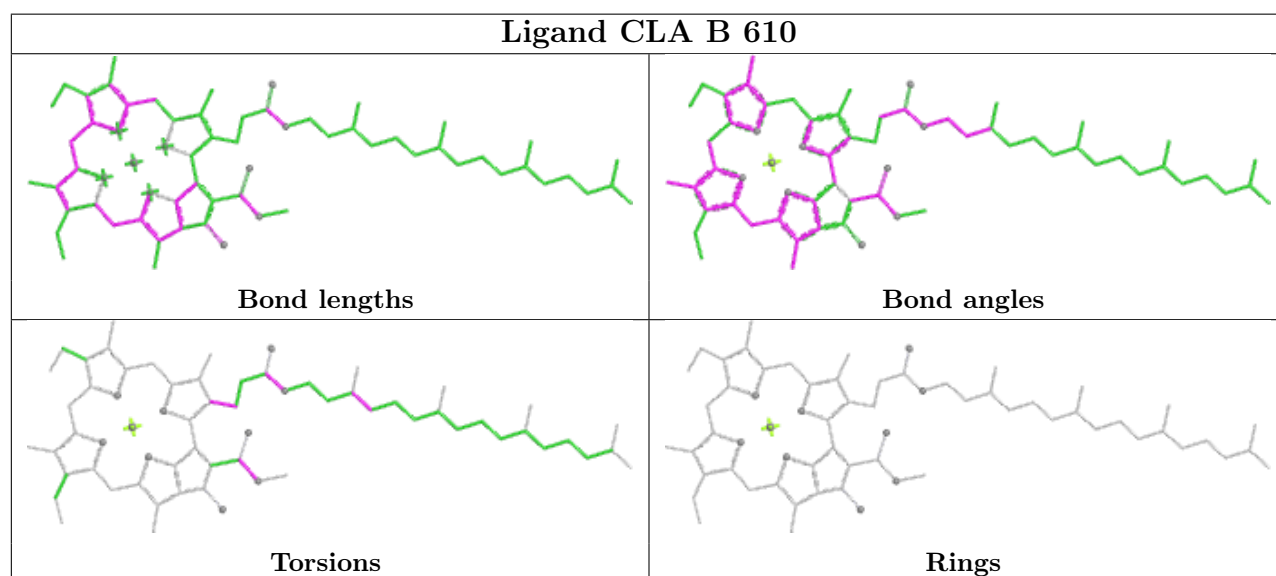
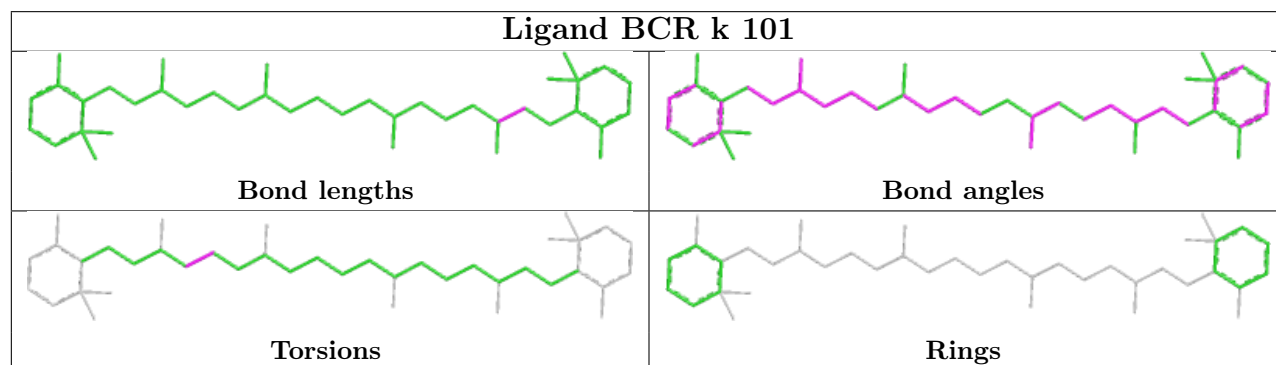
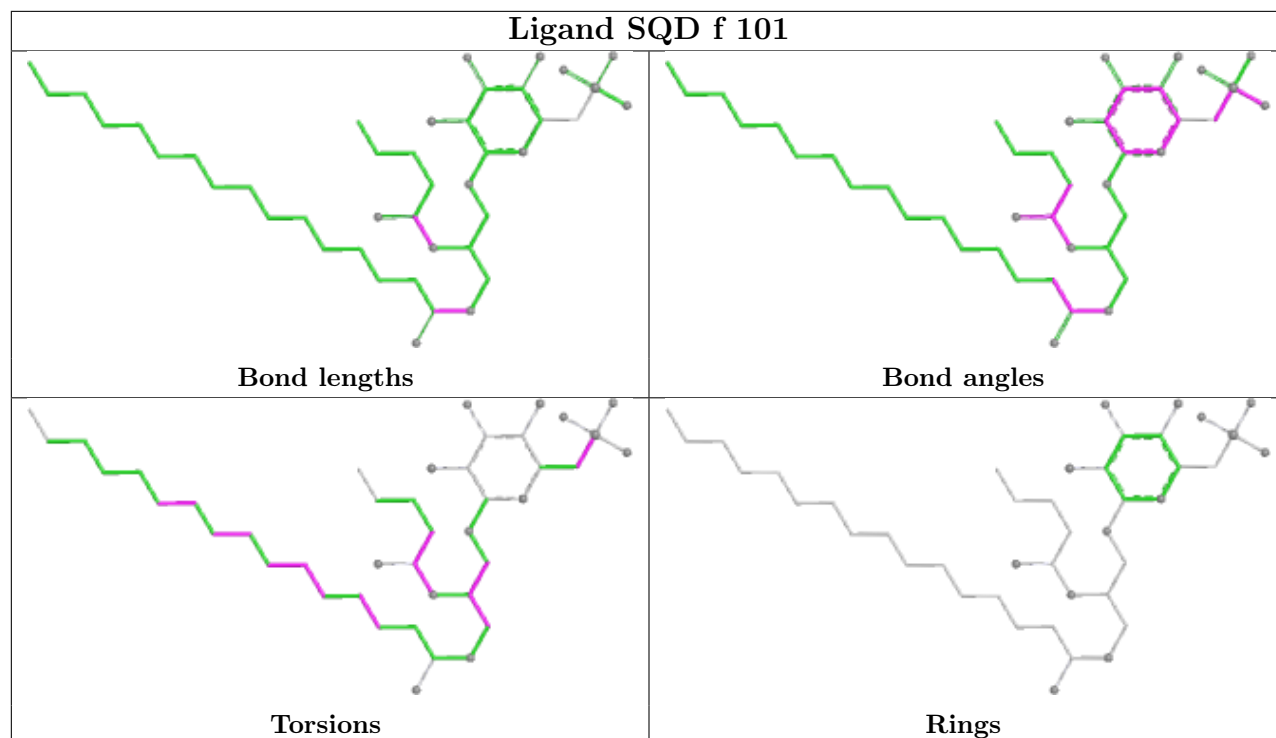
Ligand CLA c 512

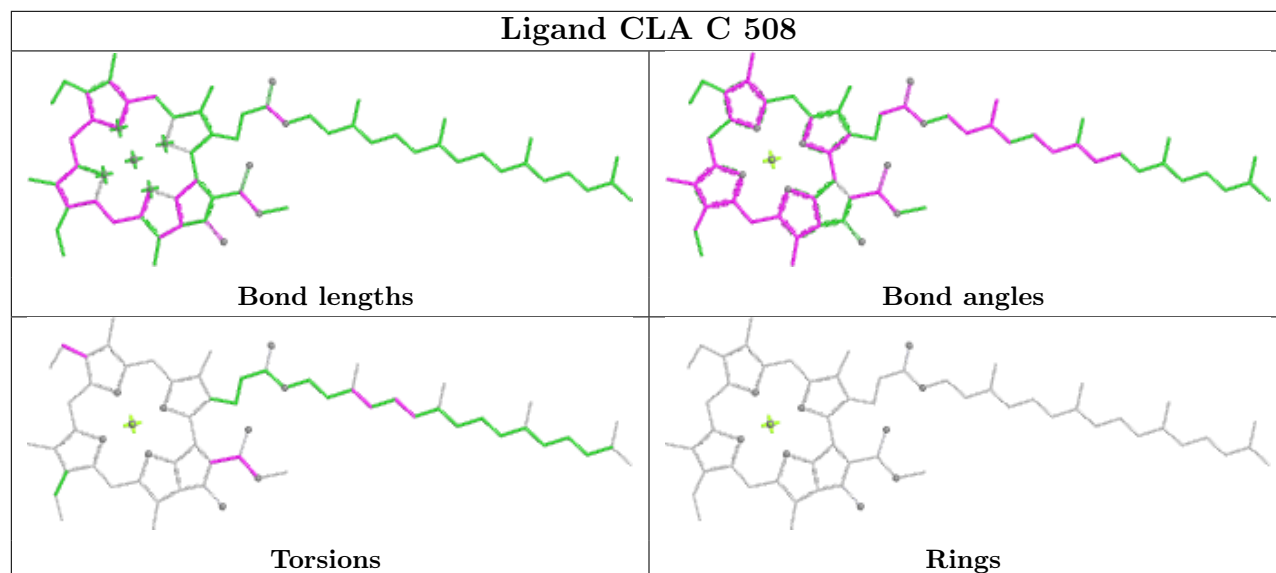
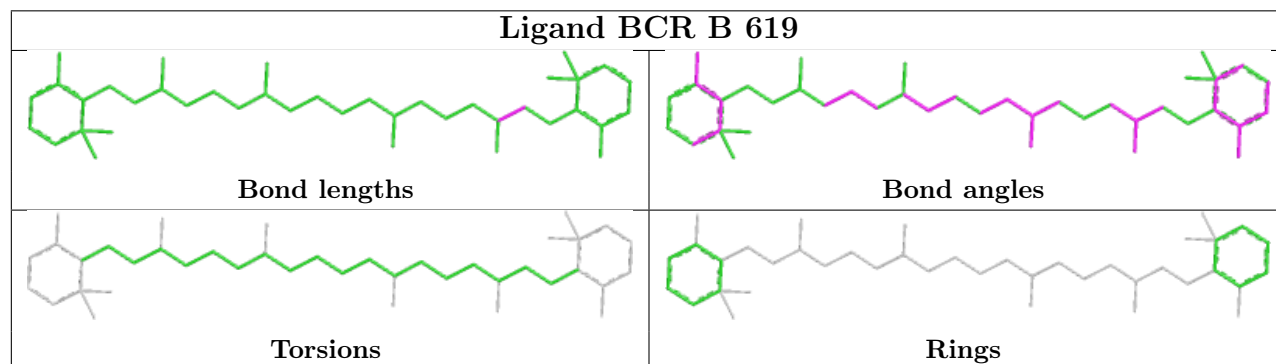
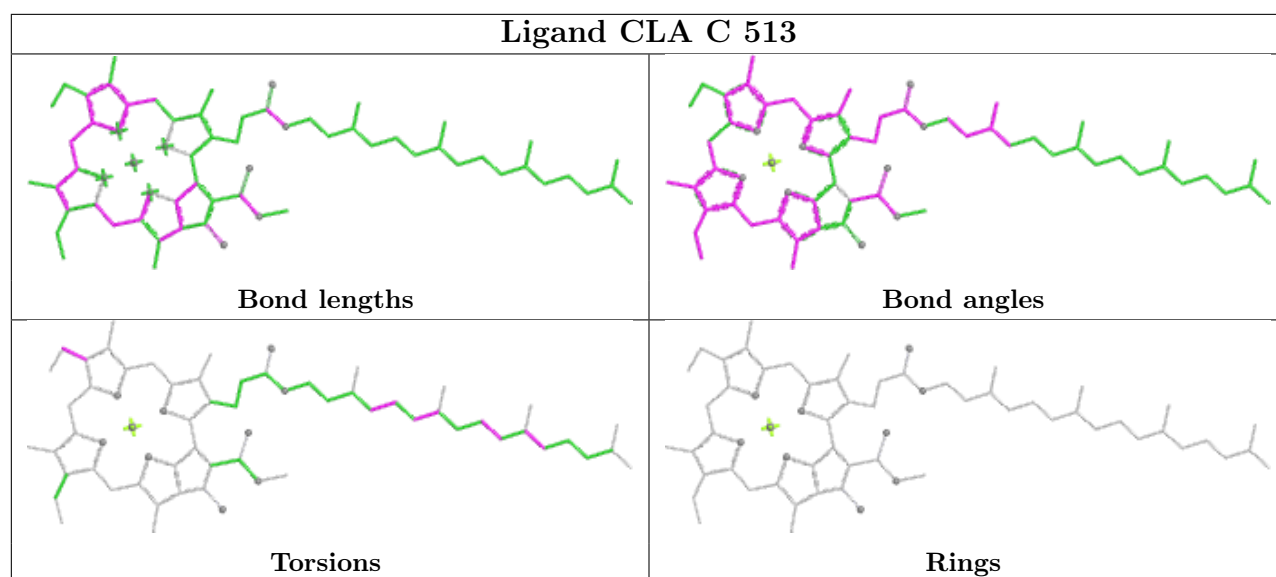


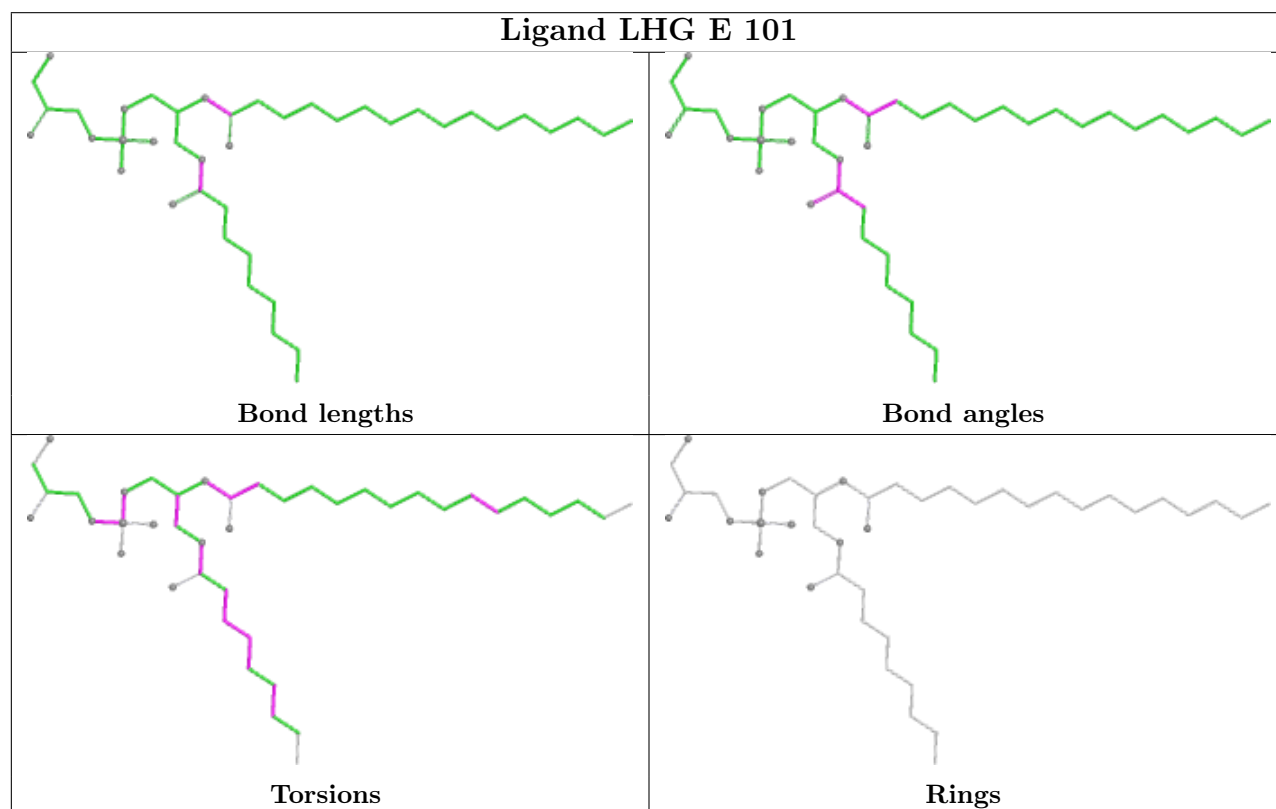
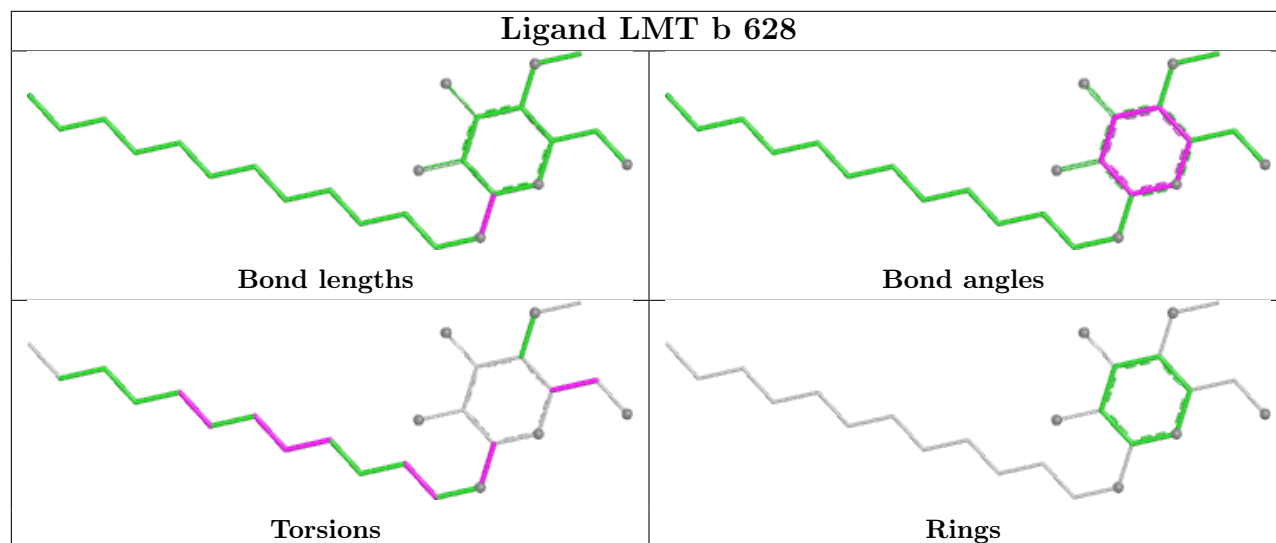
Ligand LMG j 101



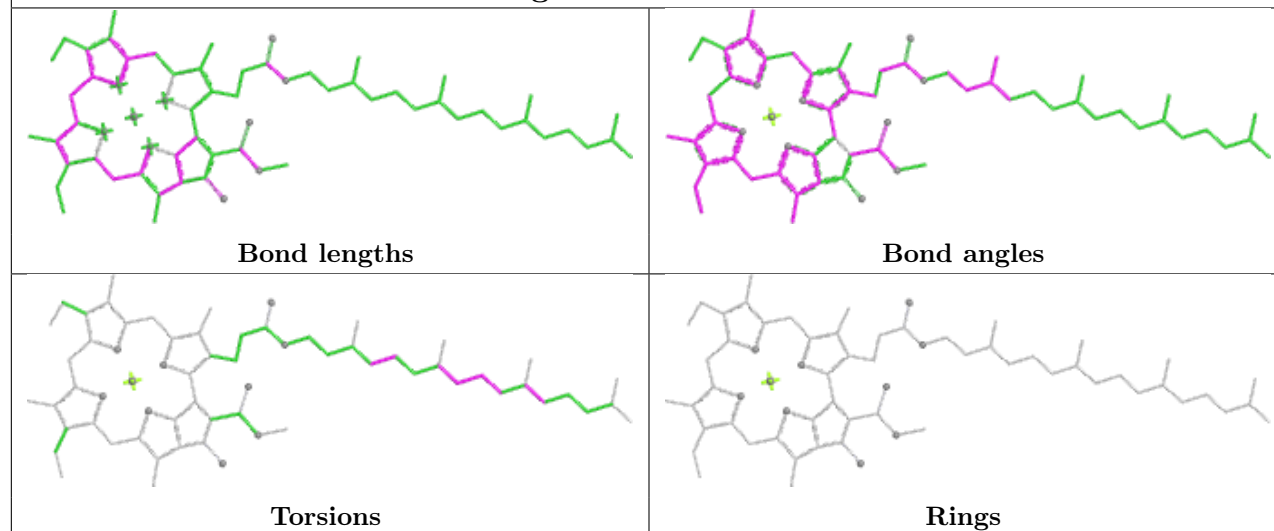




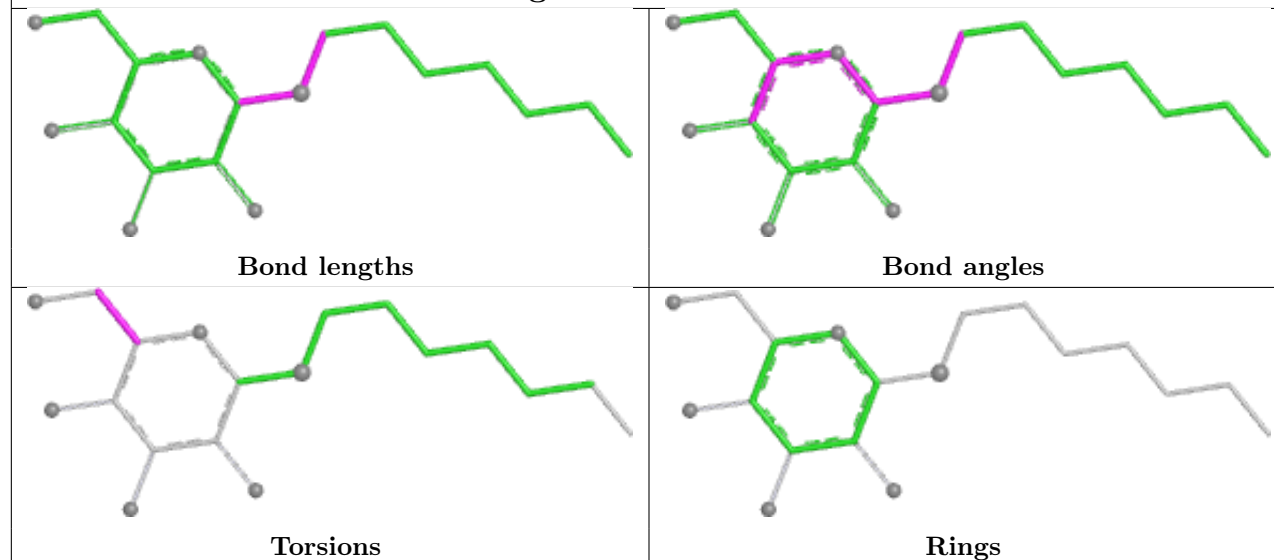




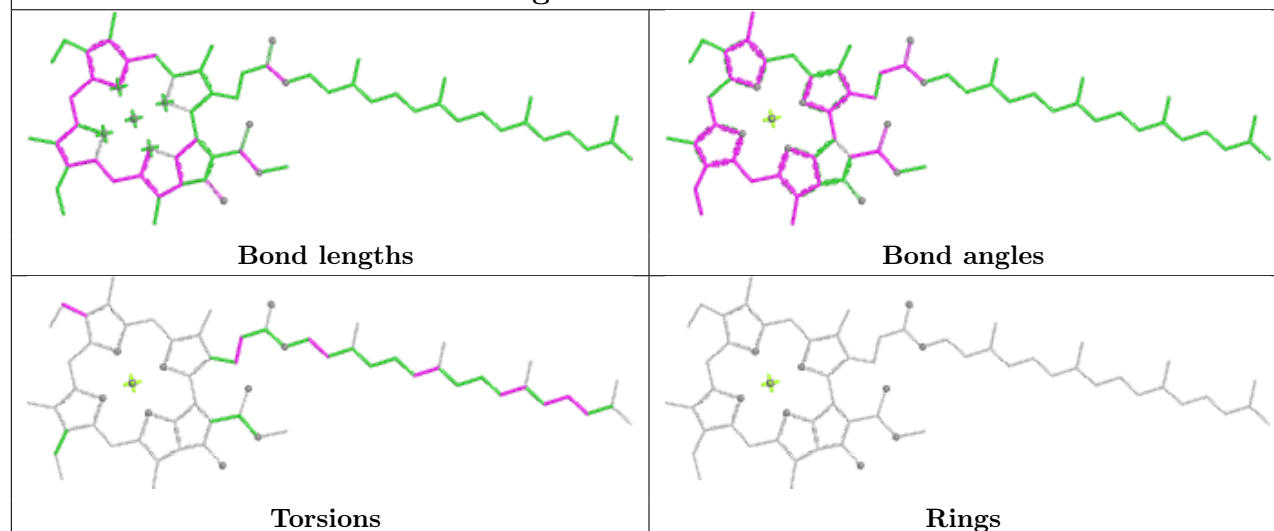
Ligand CLA D 405

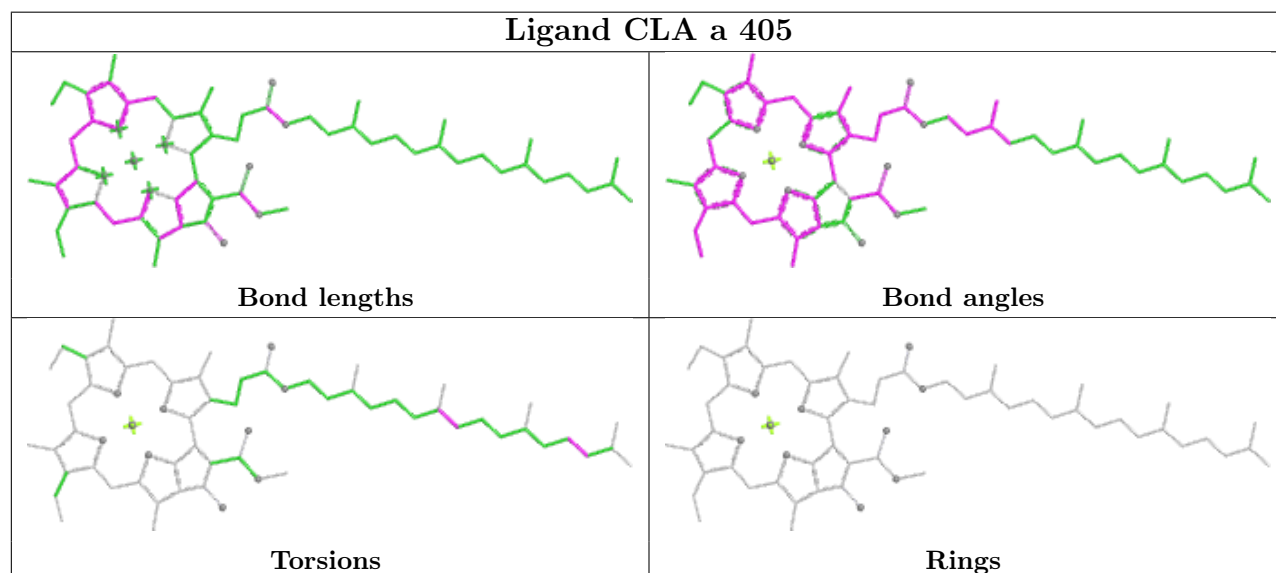
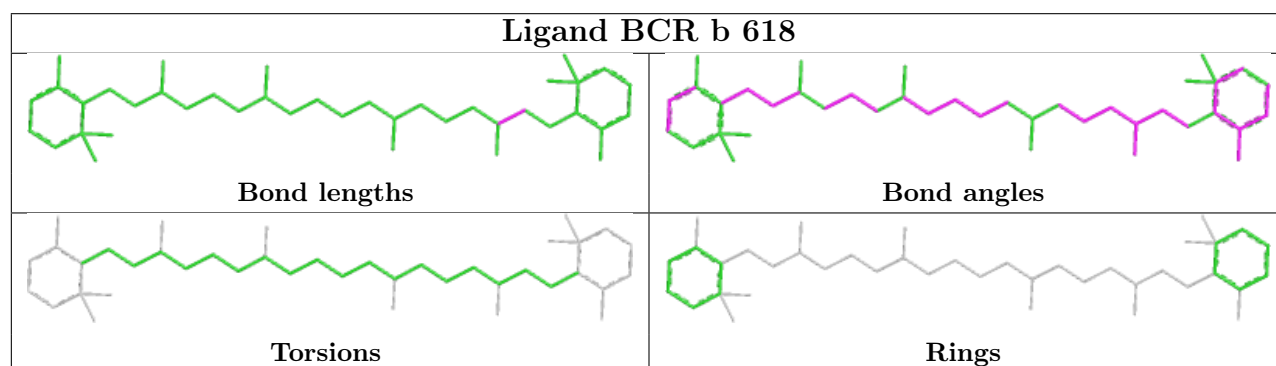
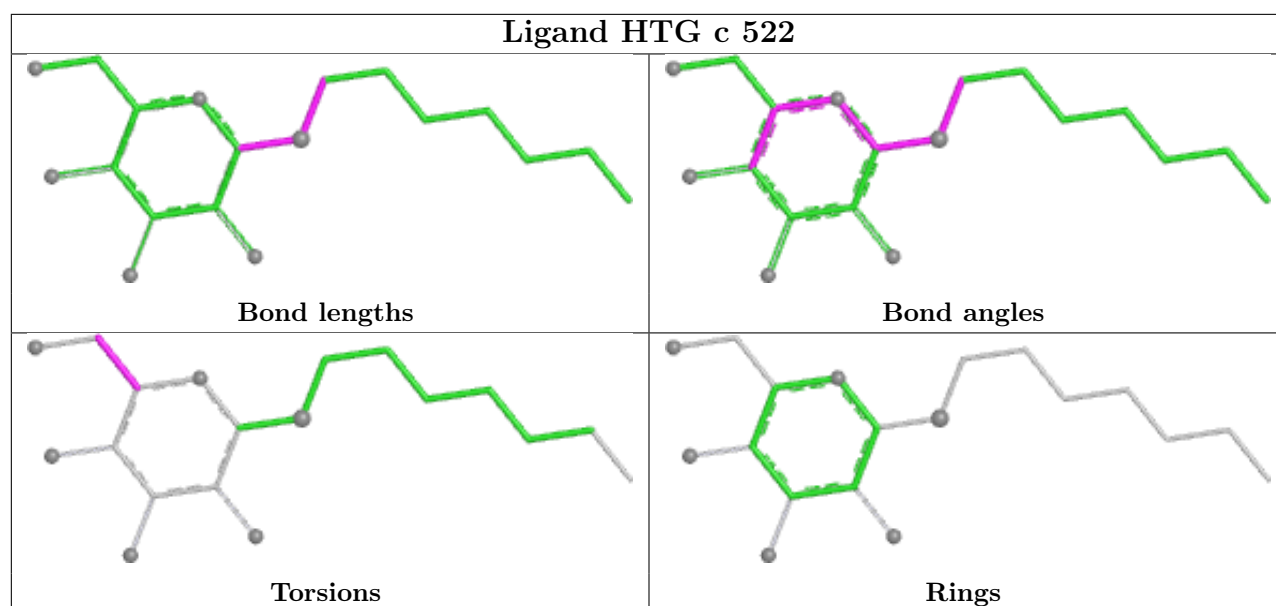


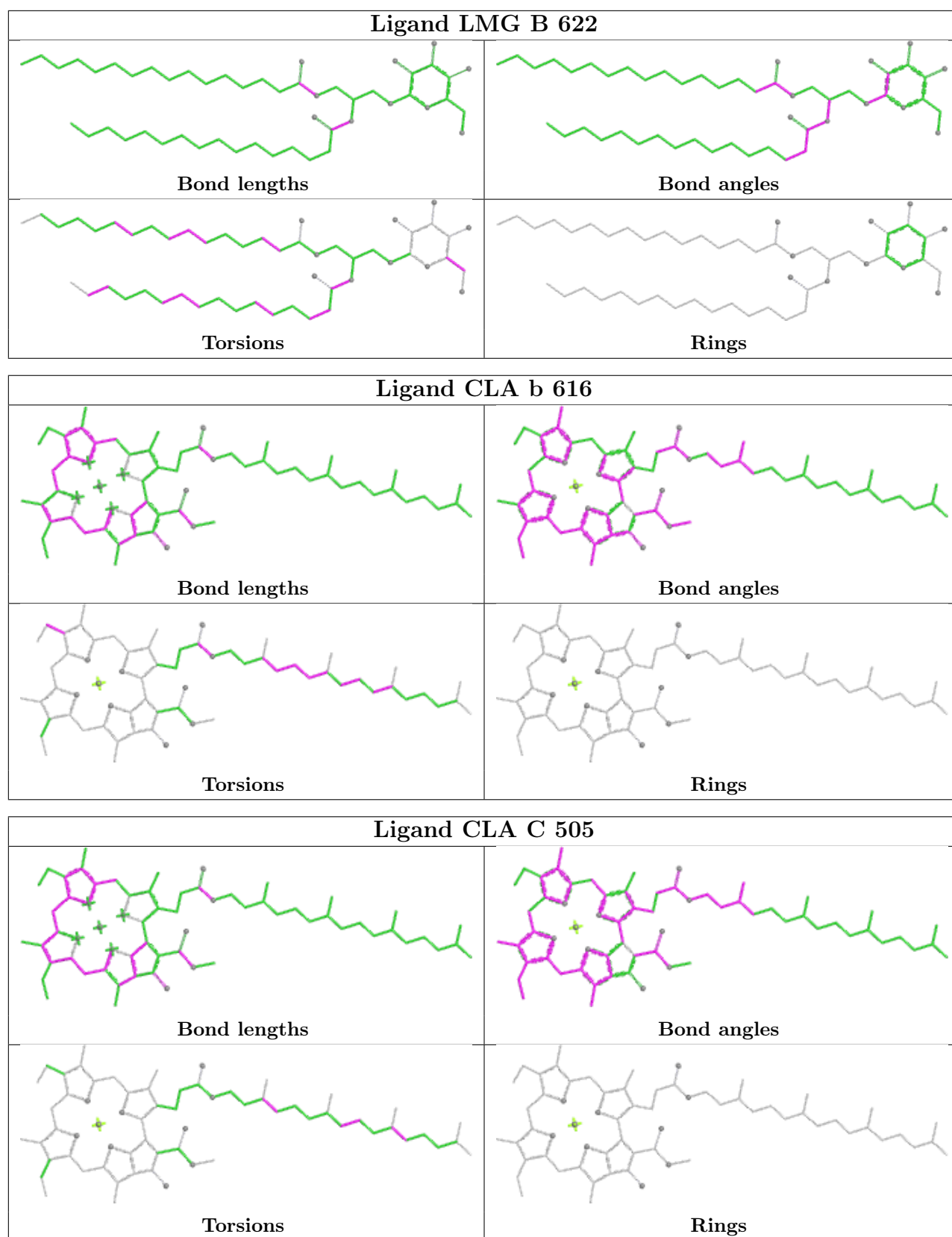
Ligand HTG B 629

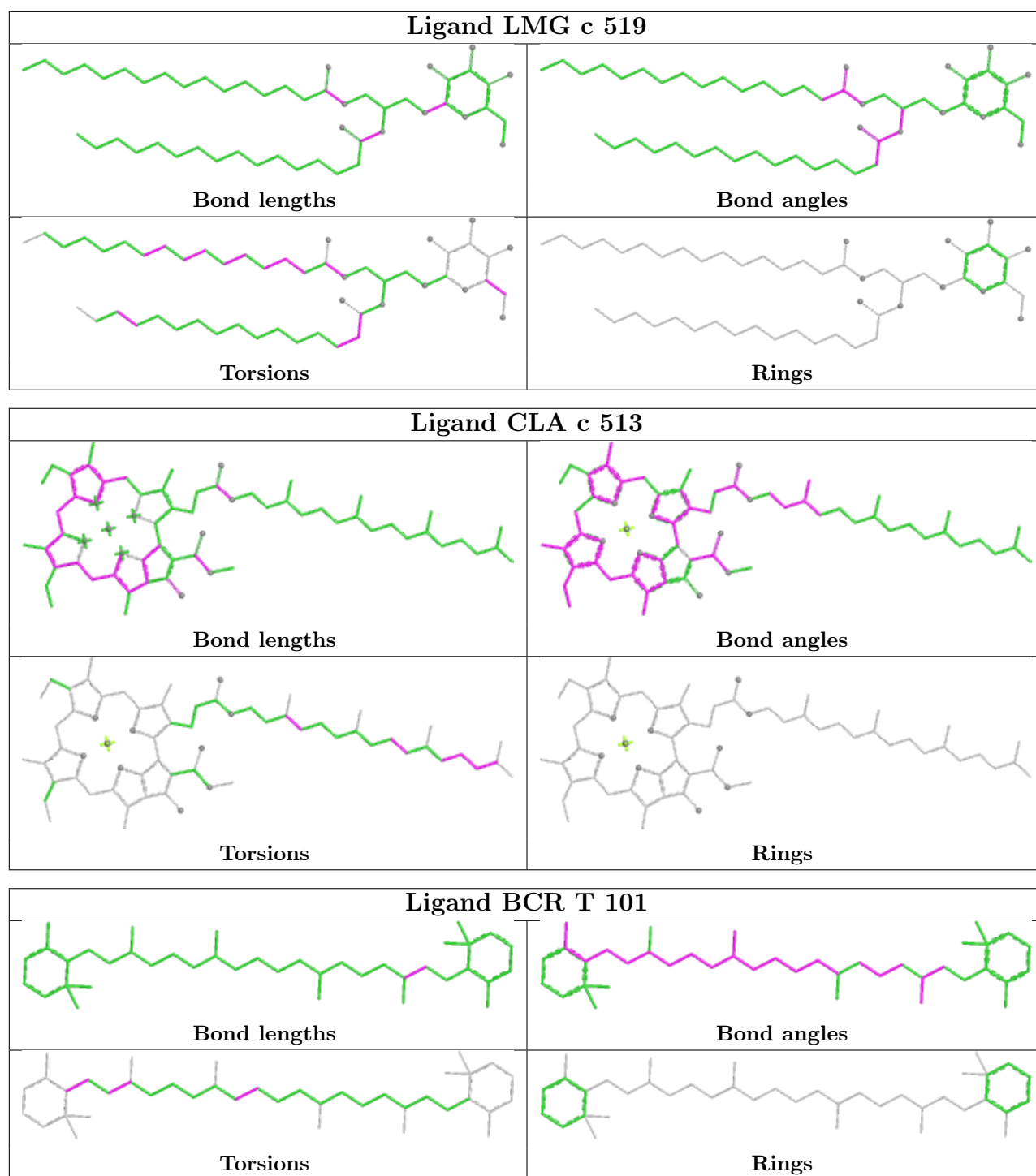


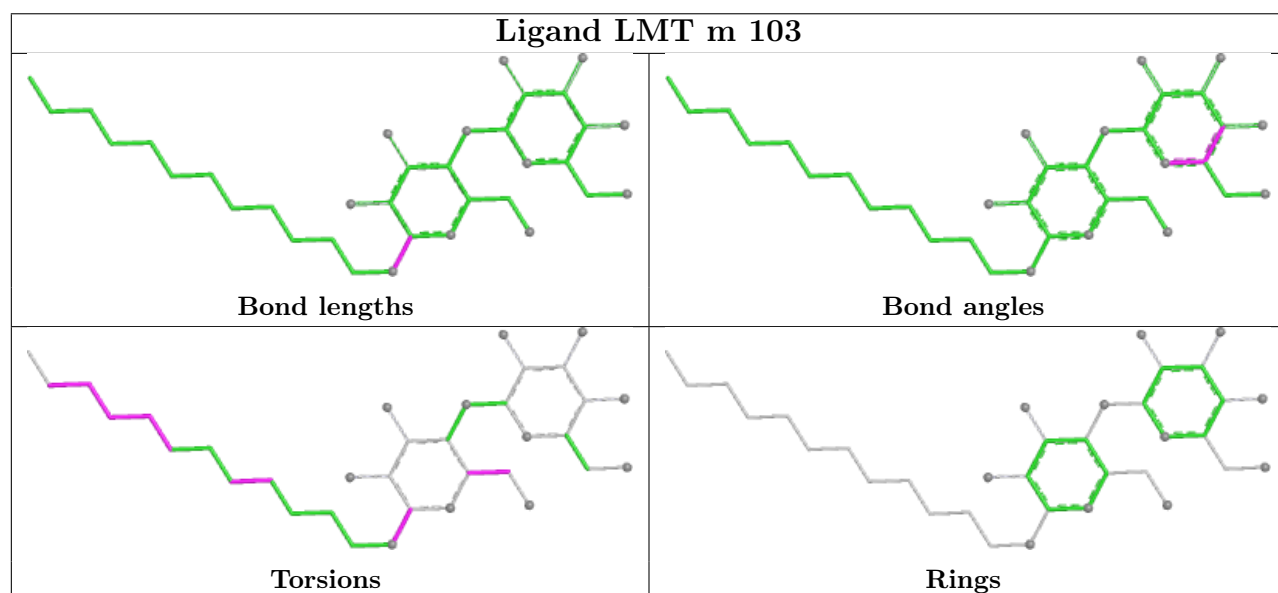
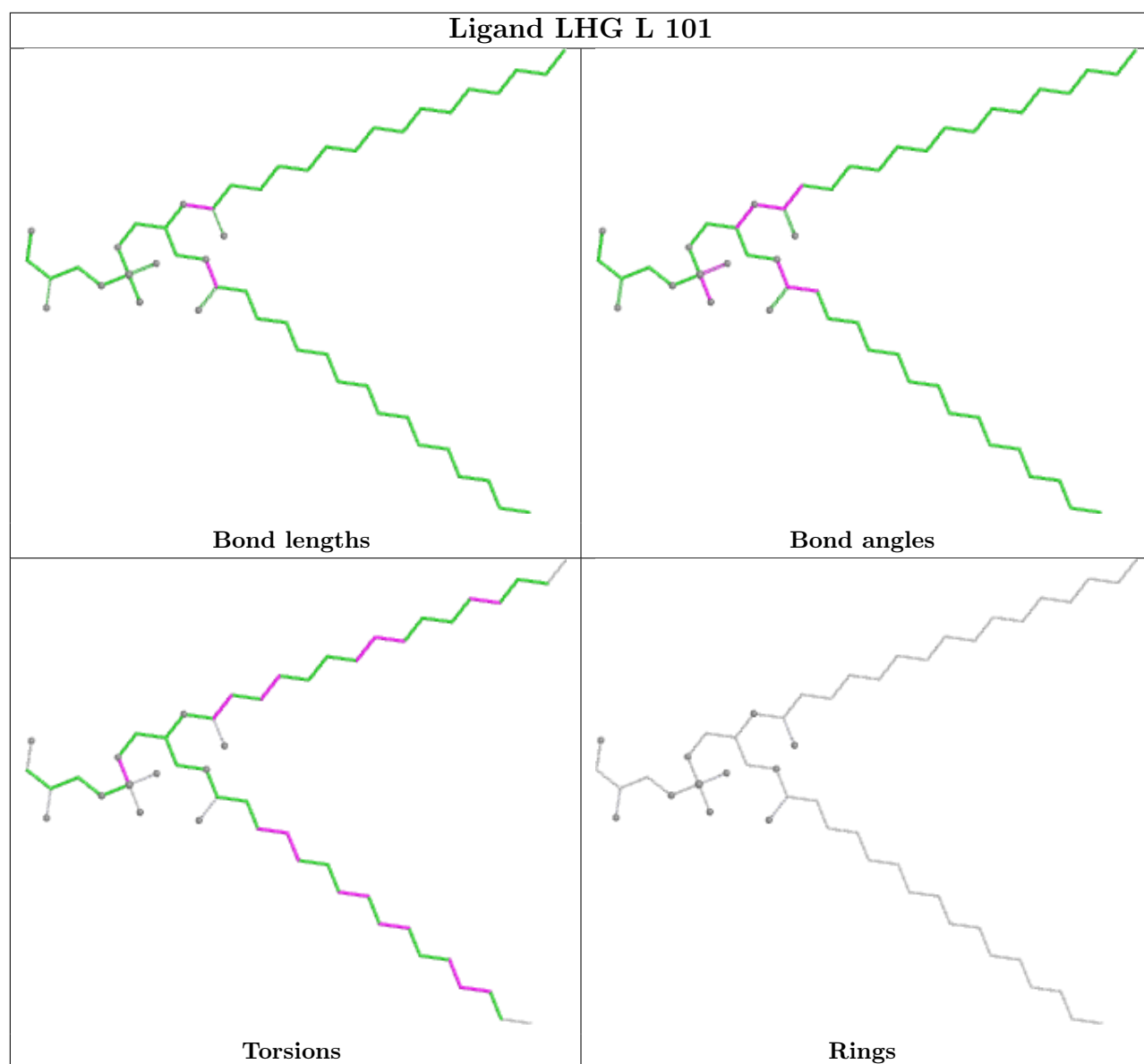
Ligand CLA B 603

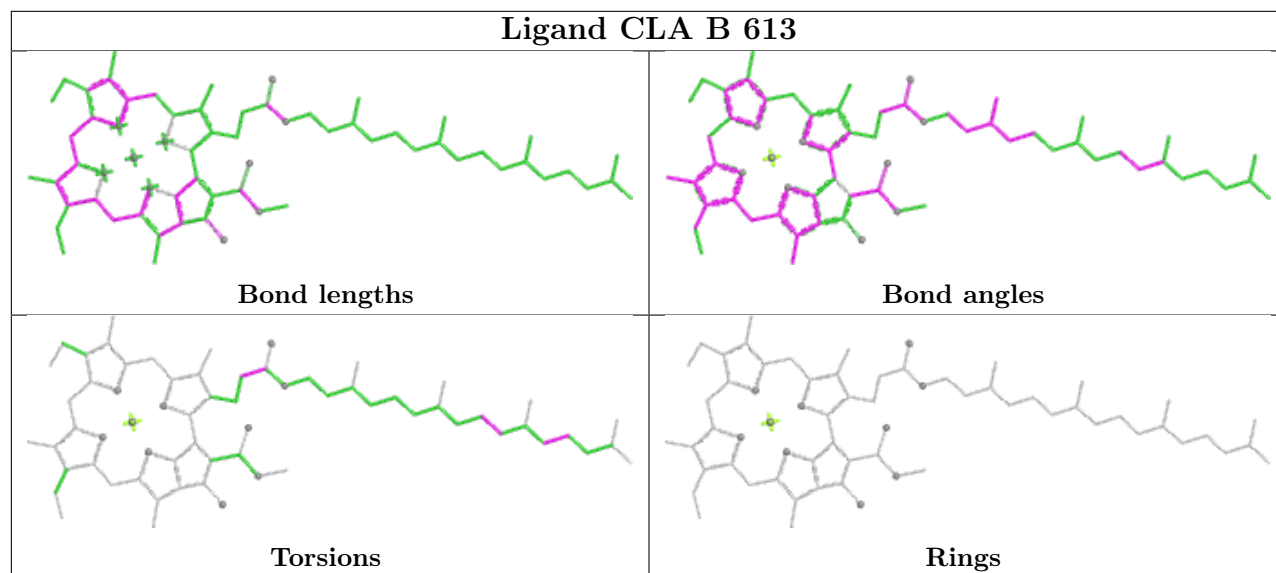
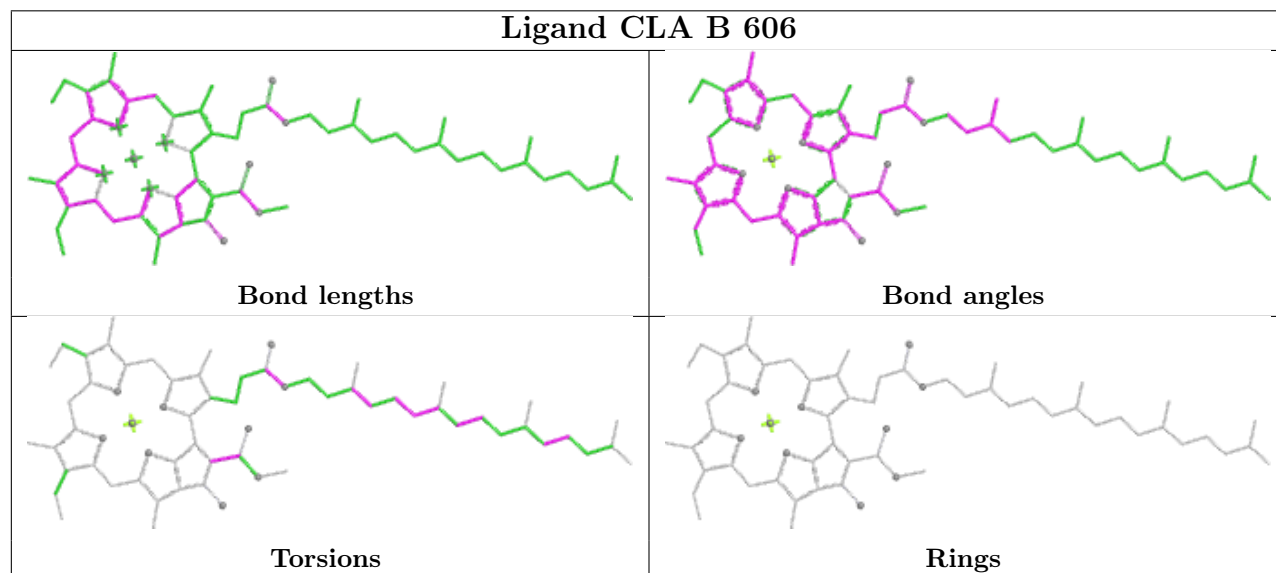
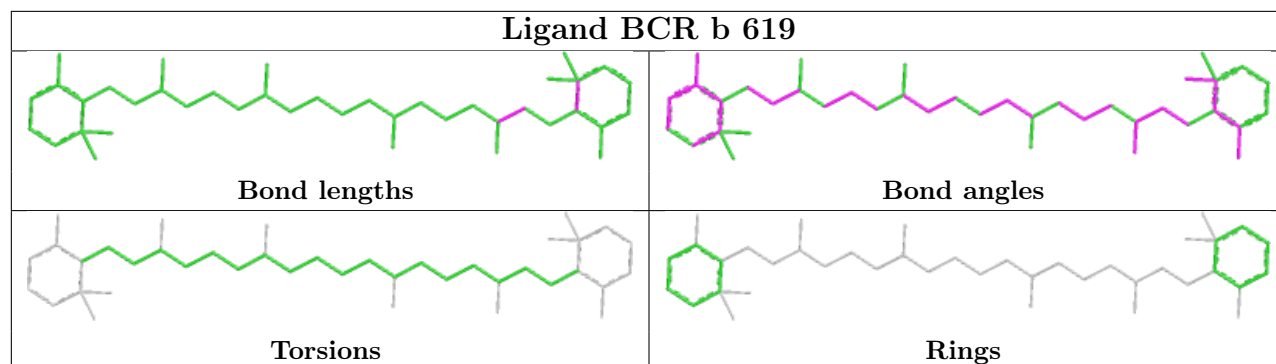


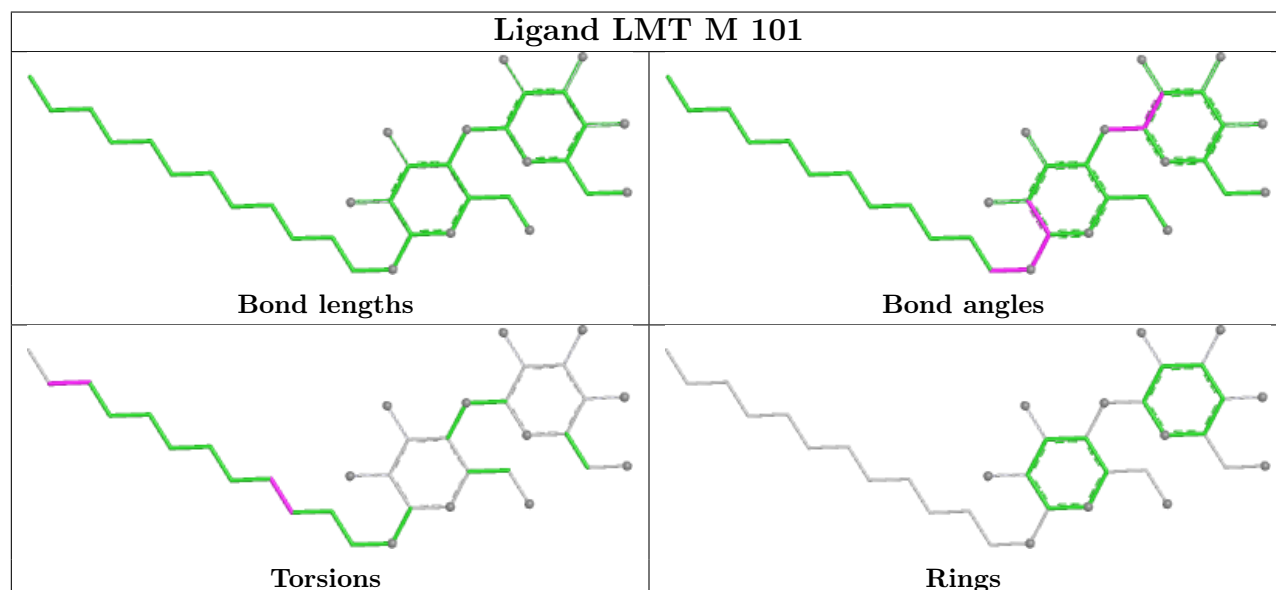
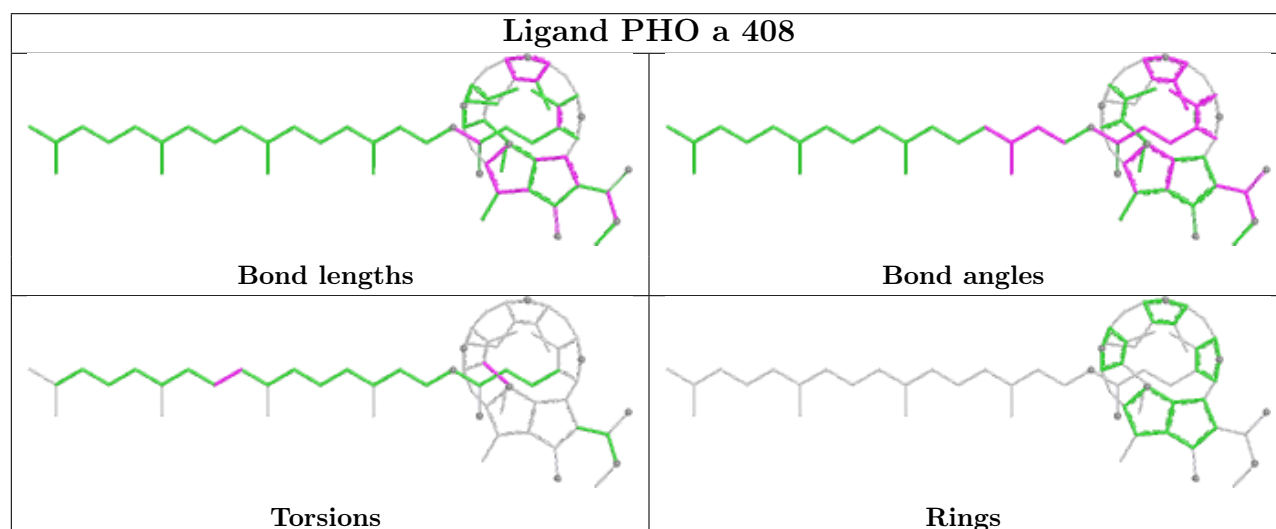
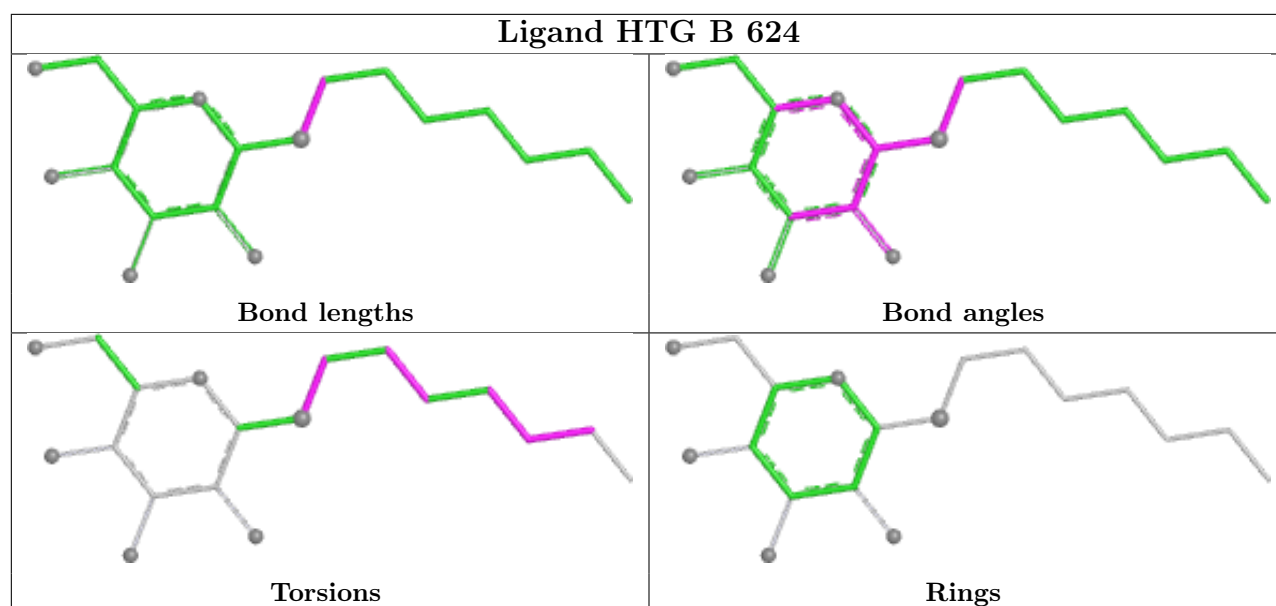




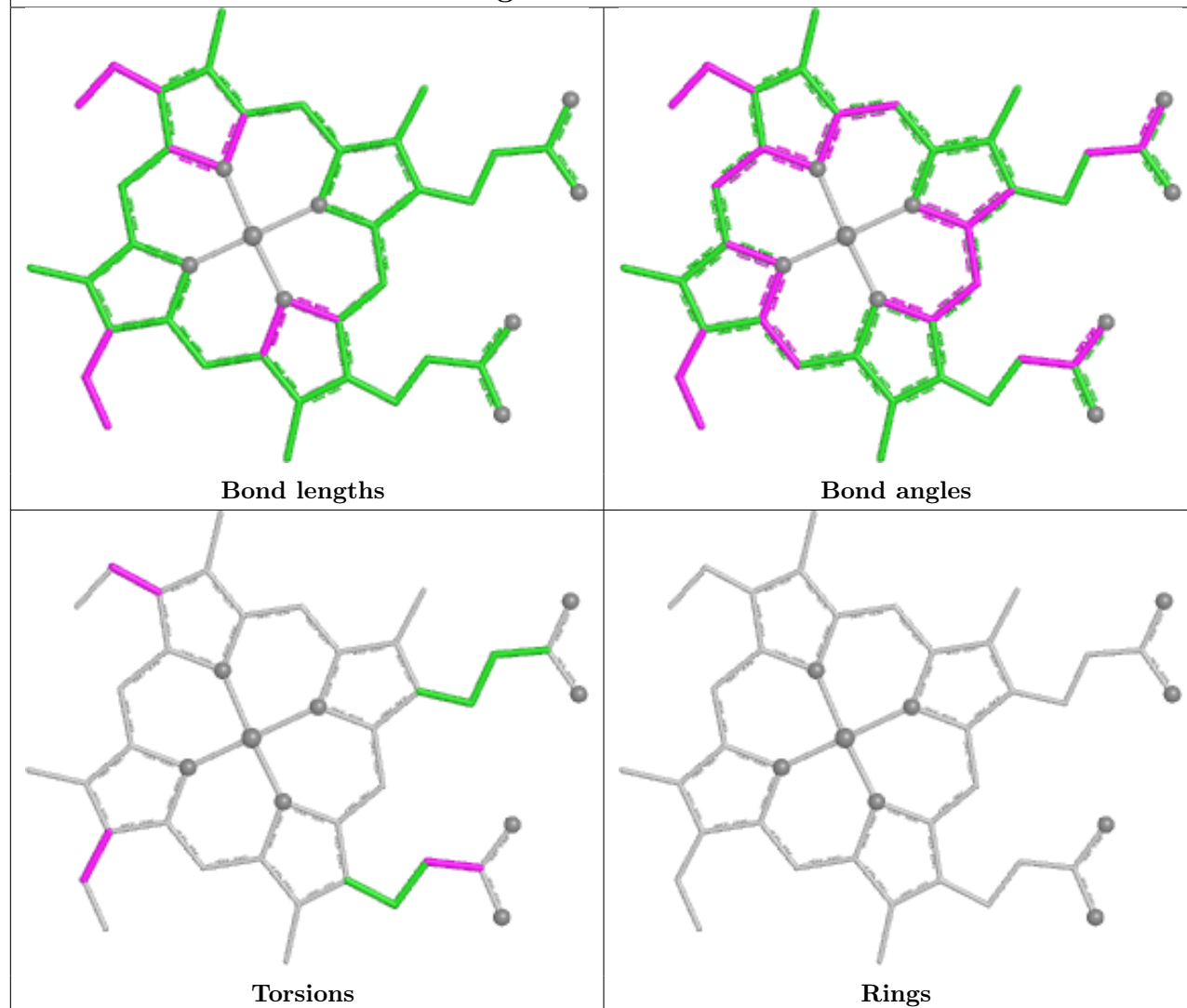




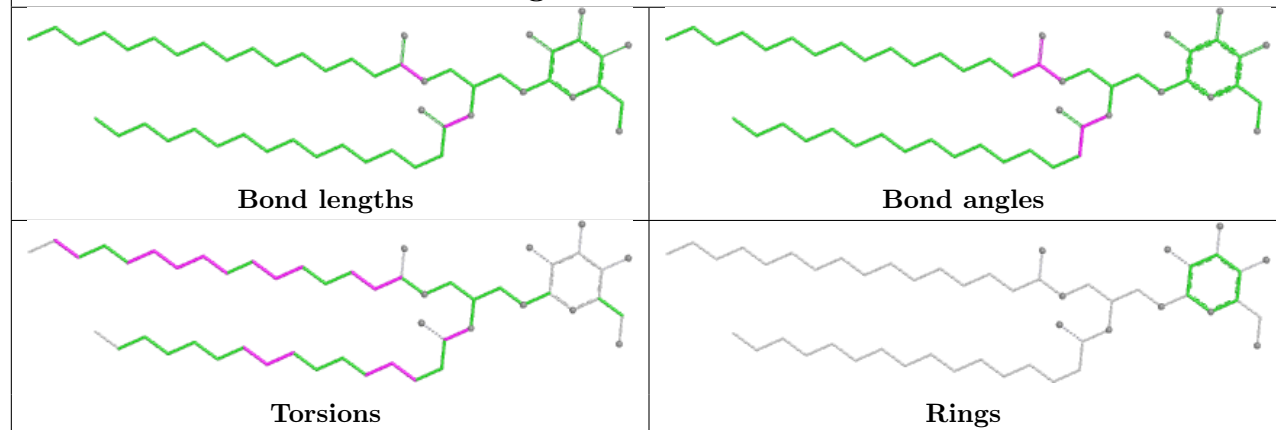


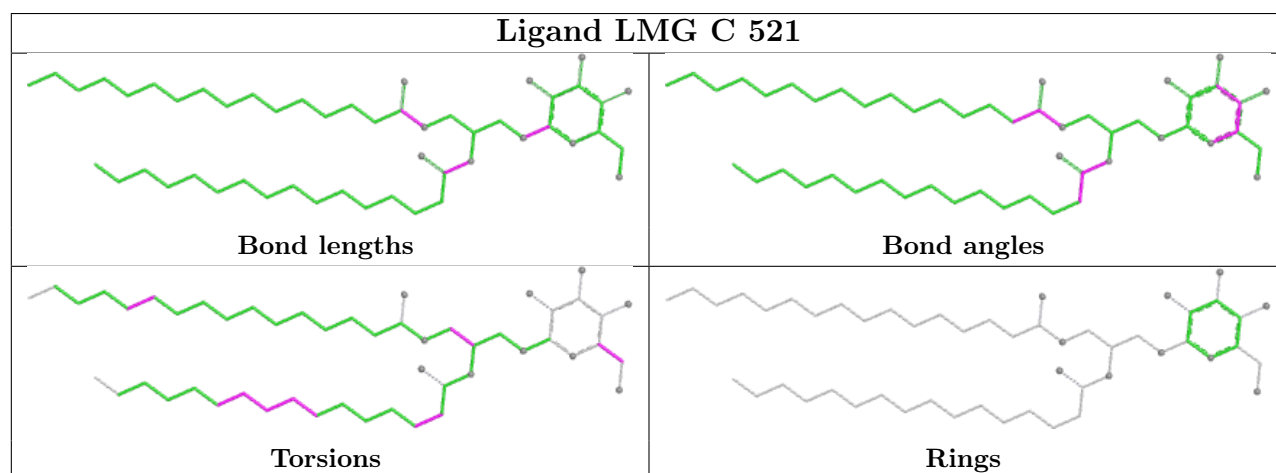
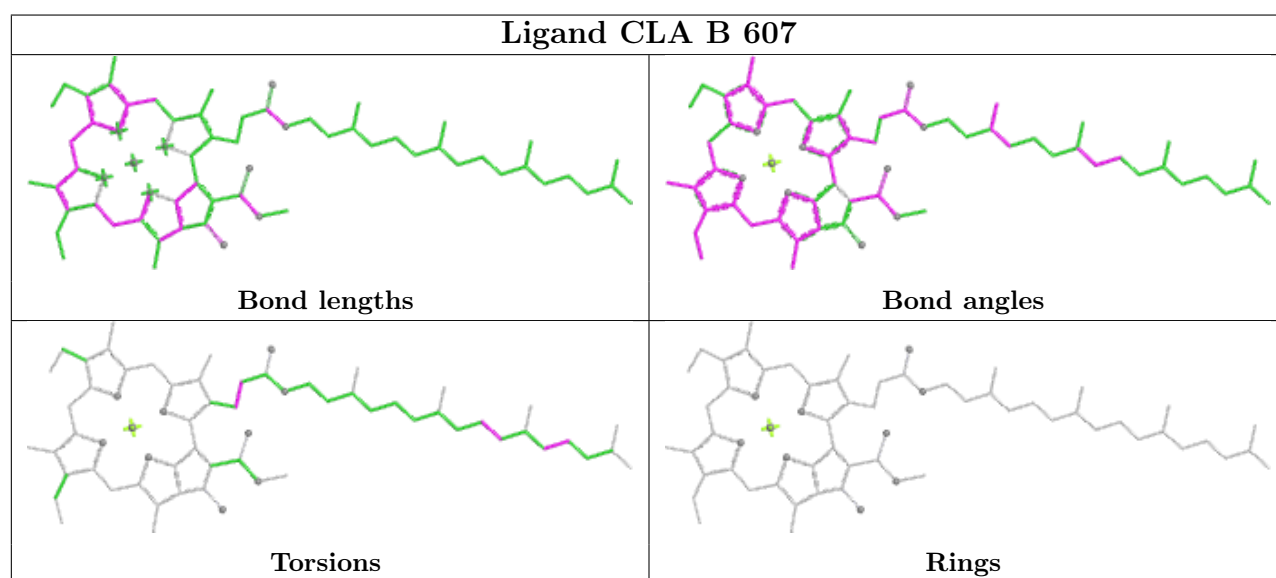
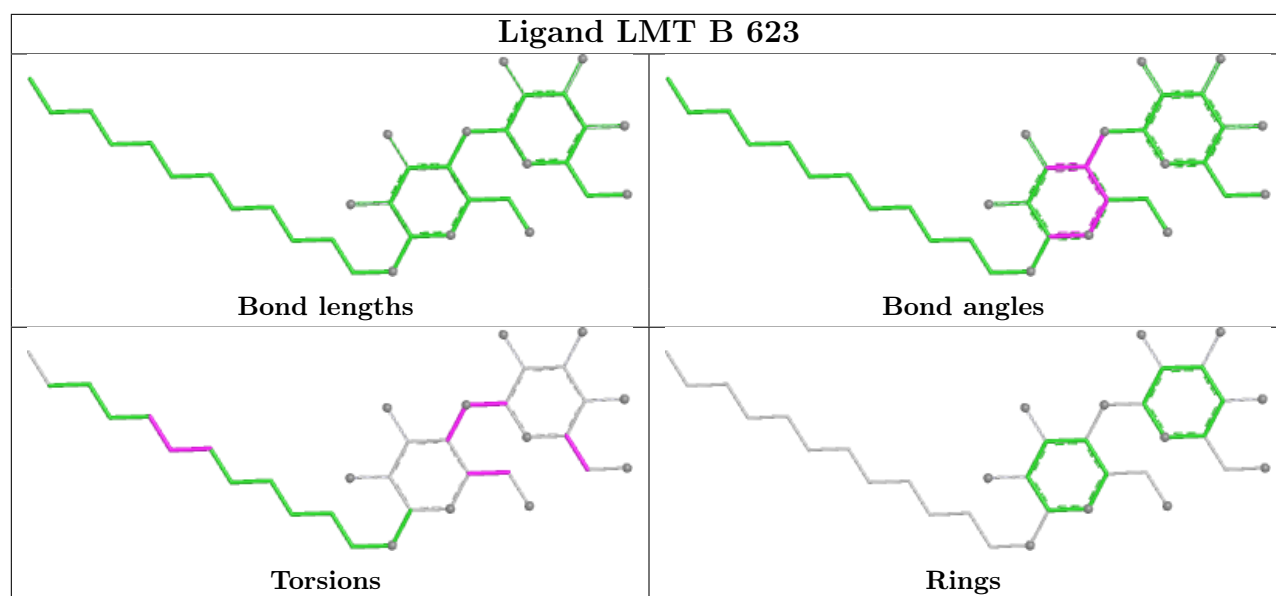


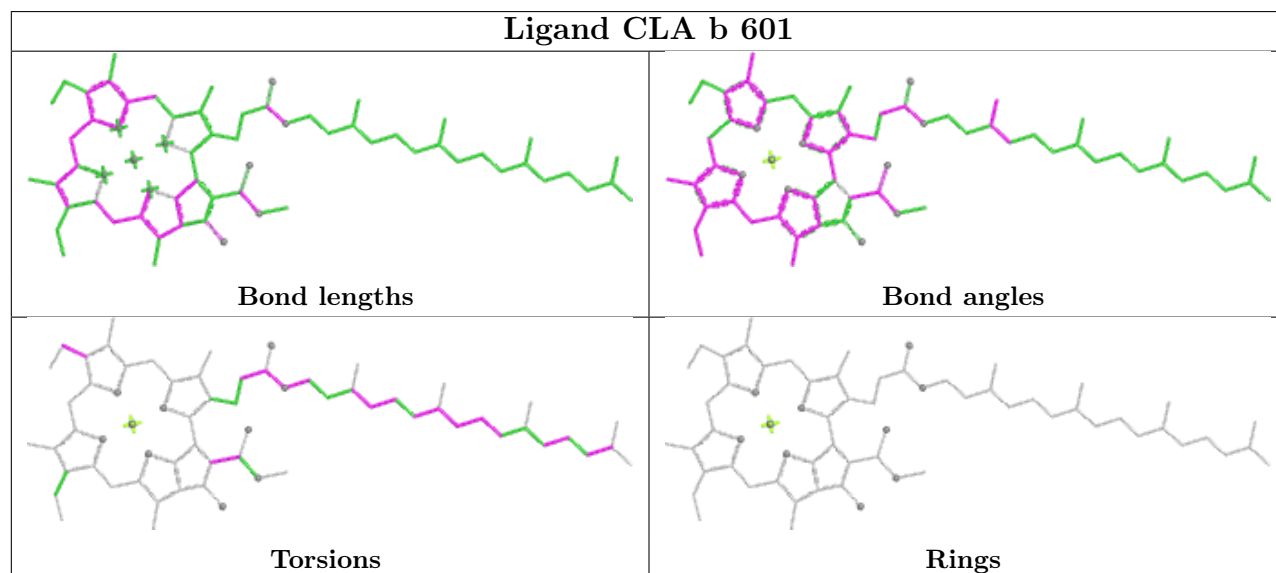
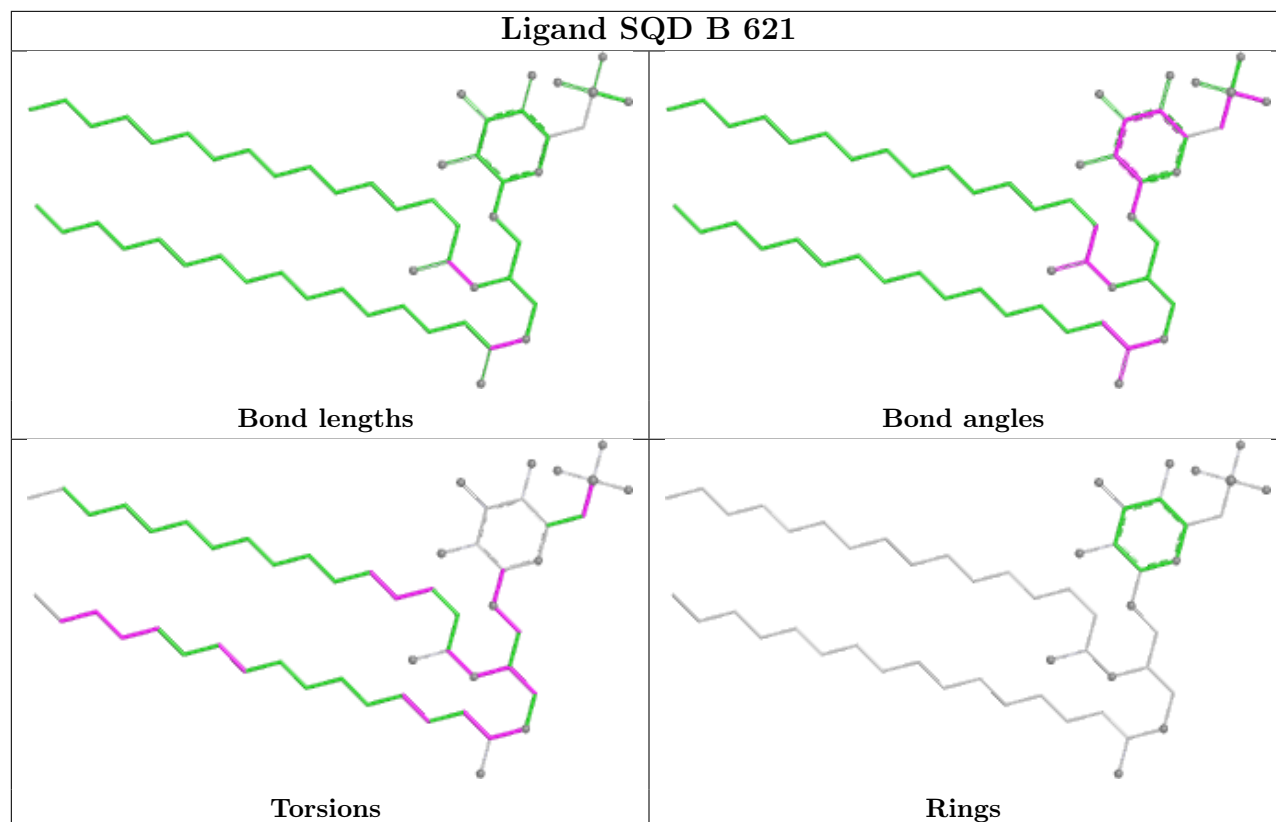
Ligand HEC v 201

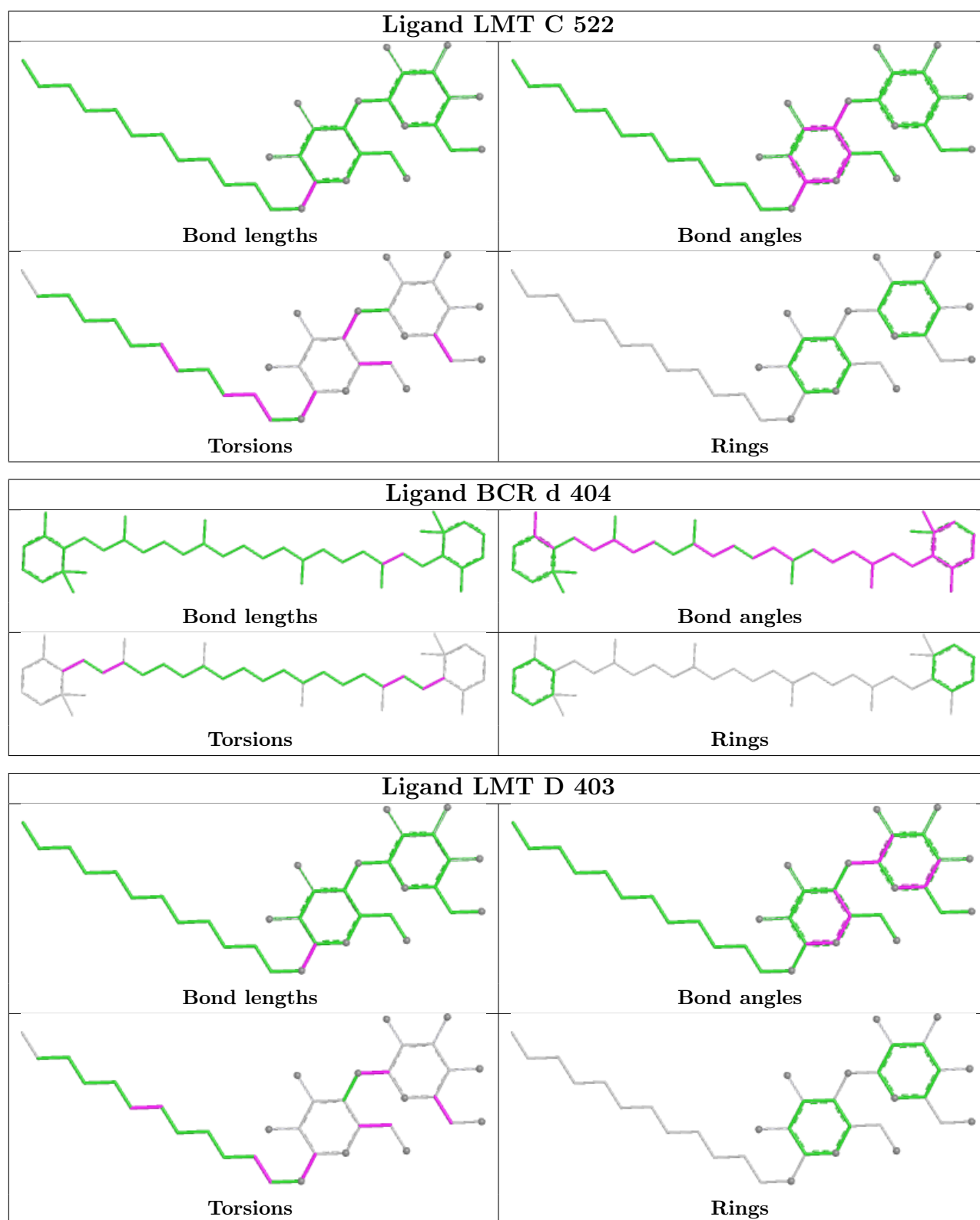


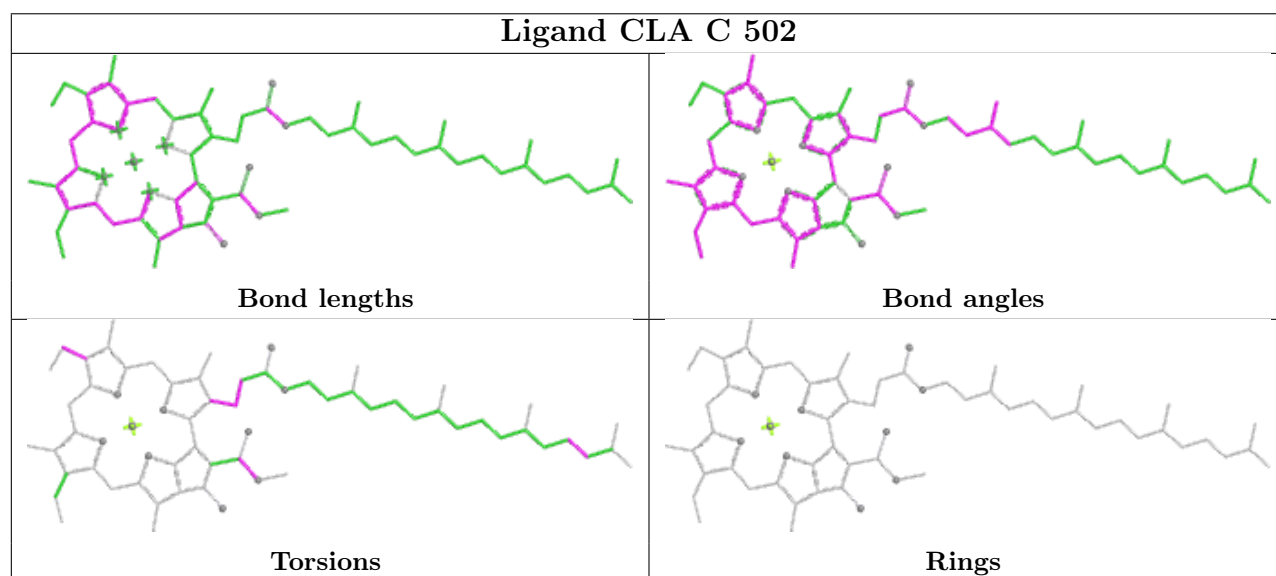
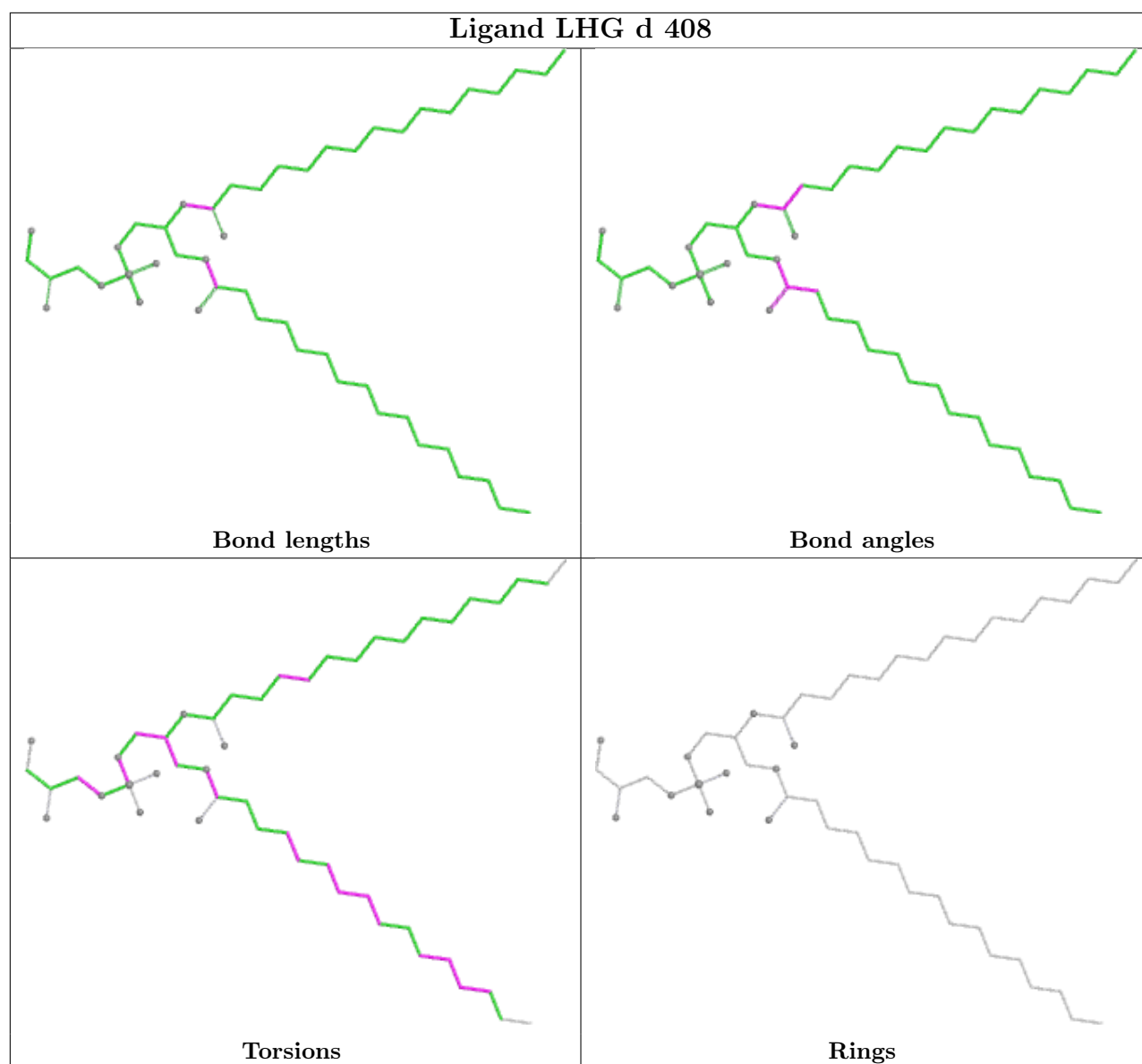
Ligand LMG C 520

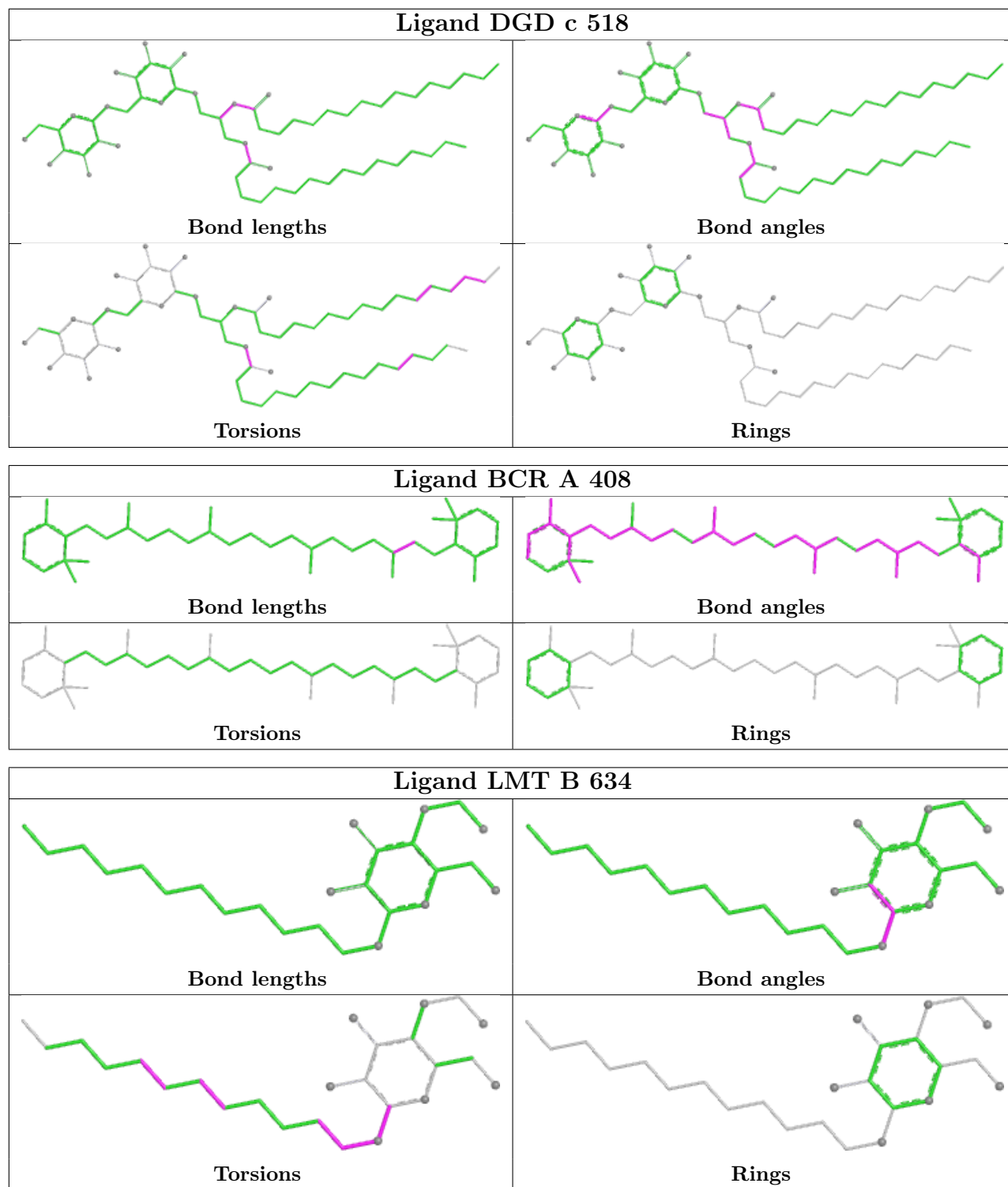


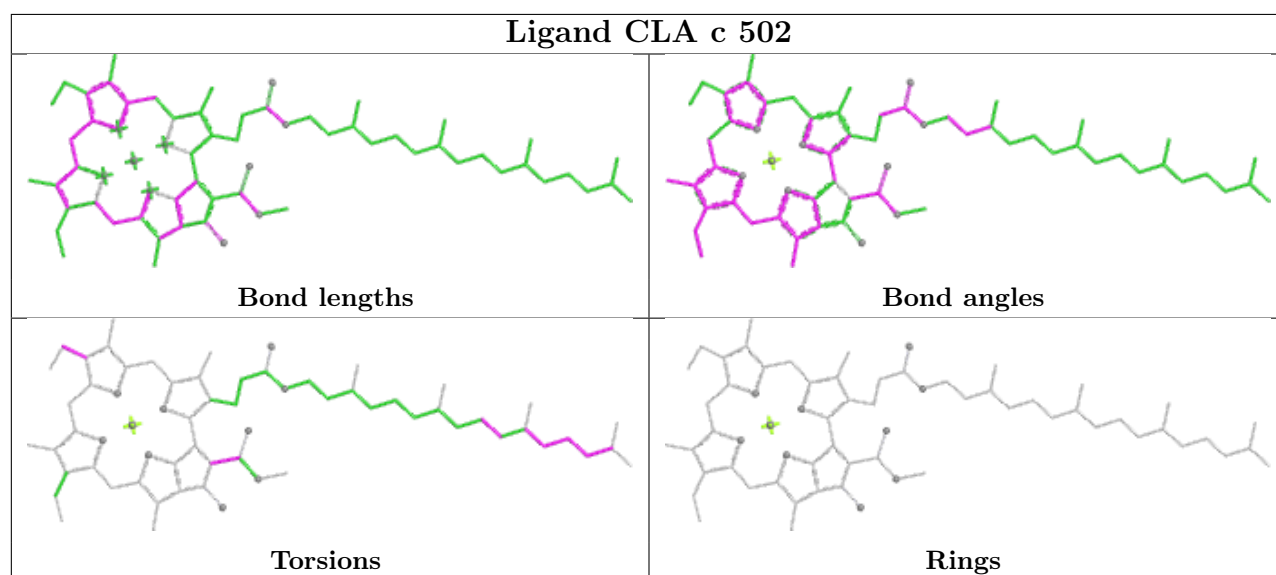
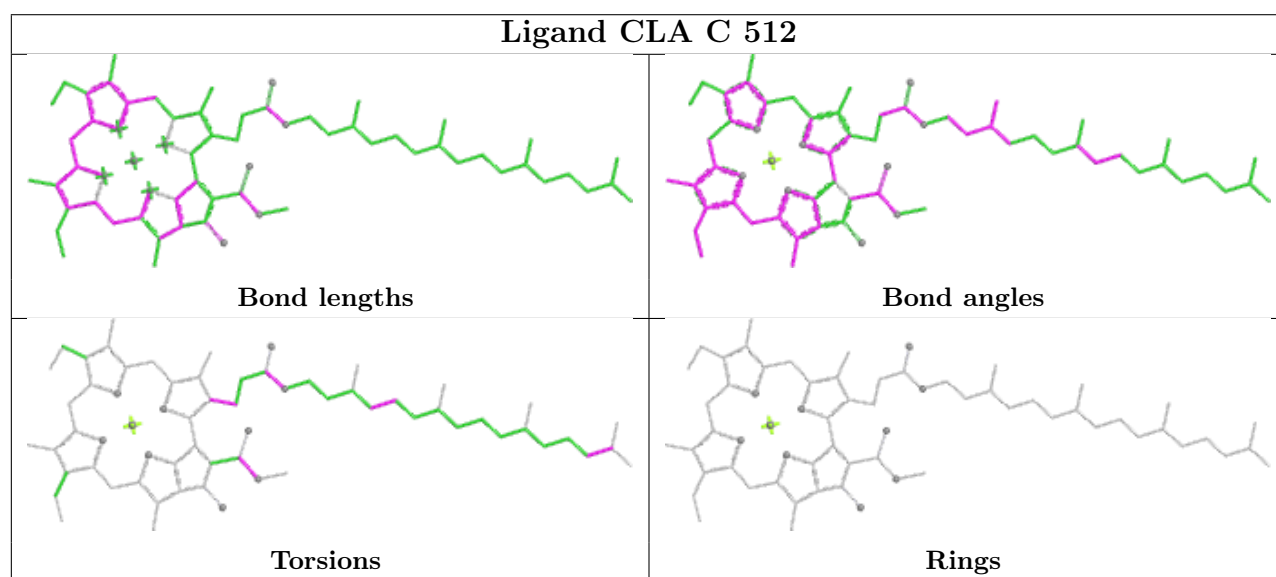
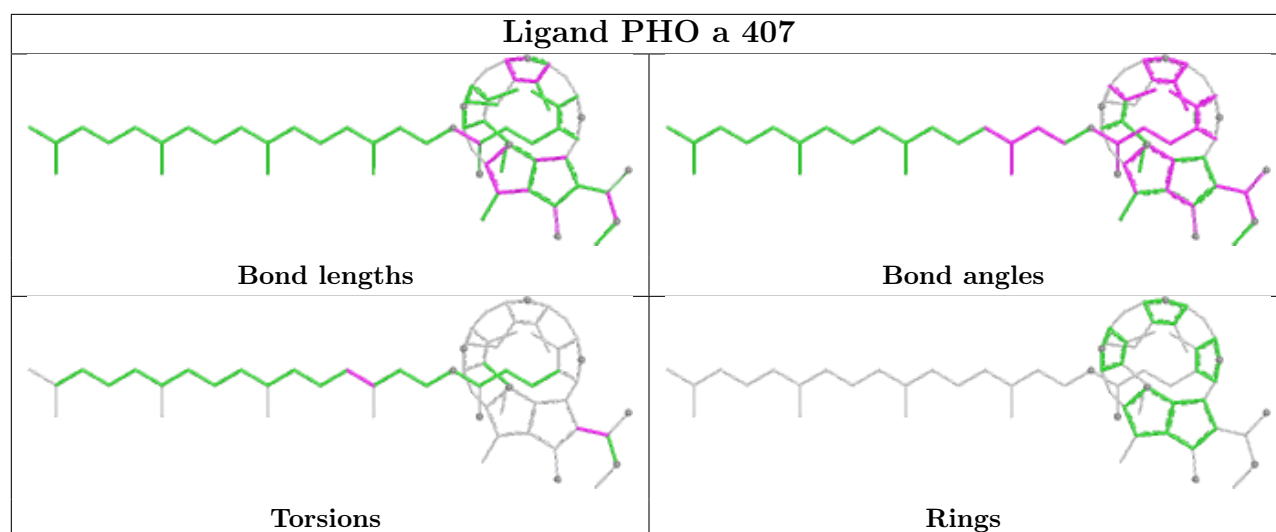


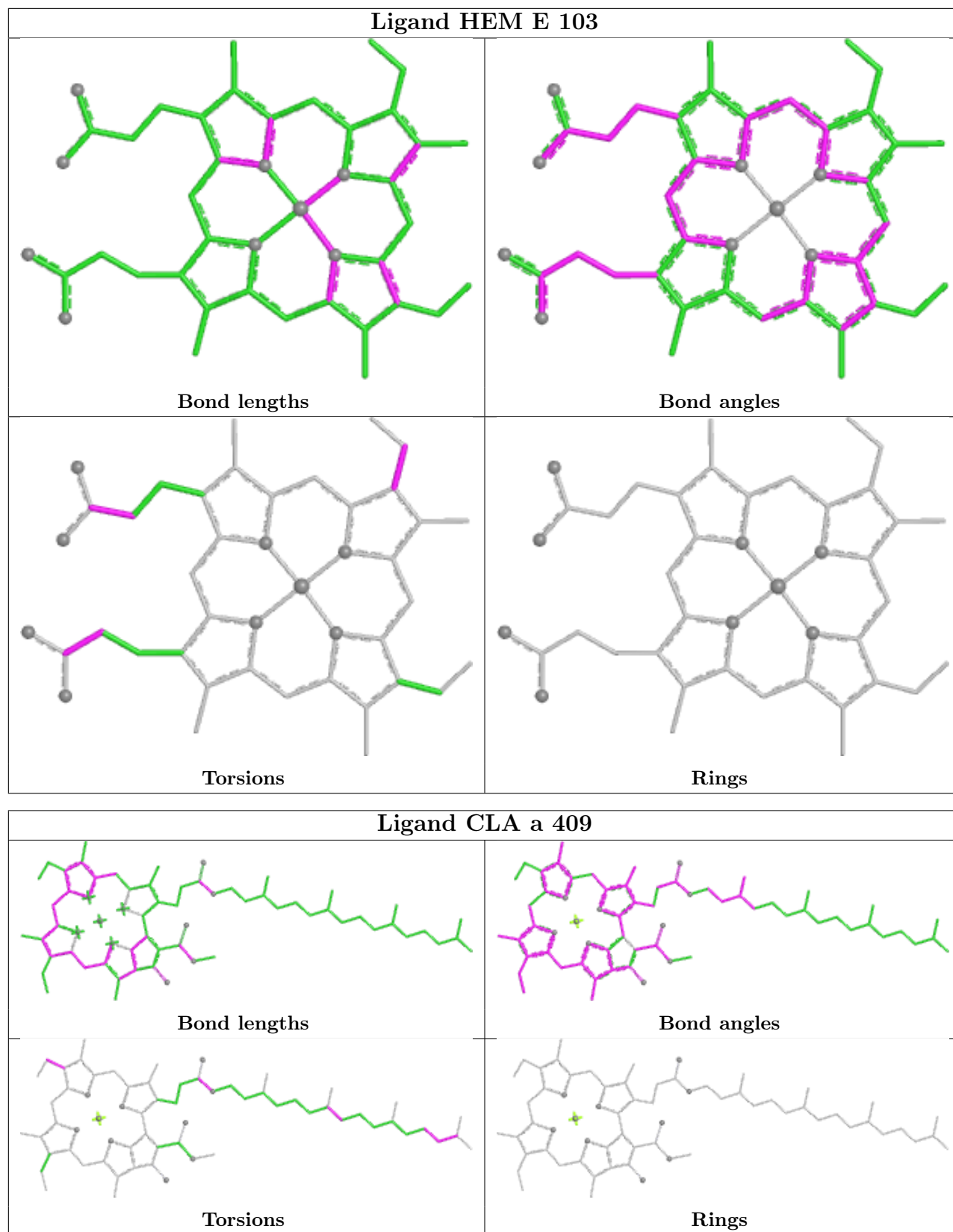




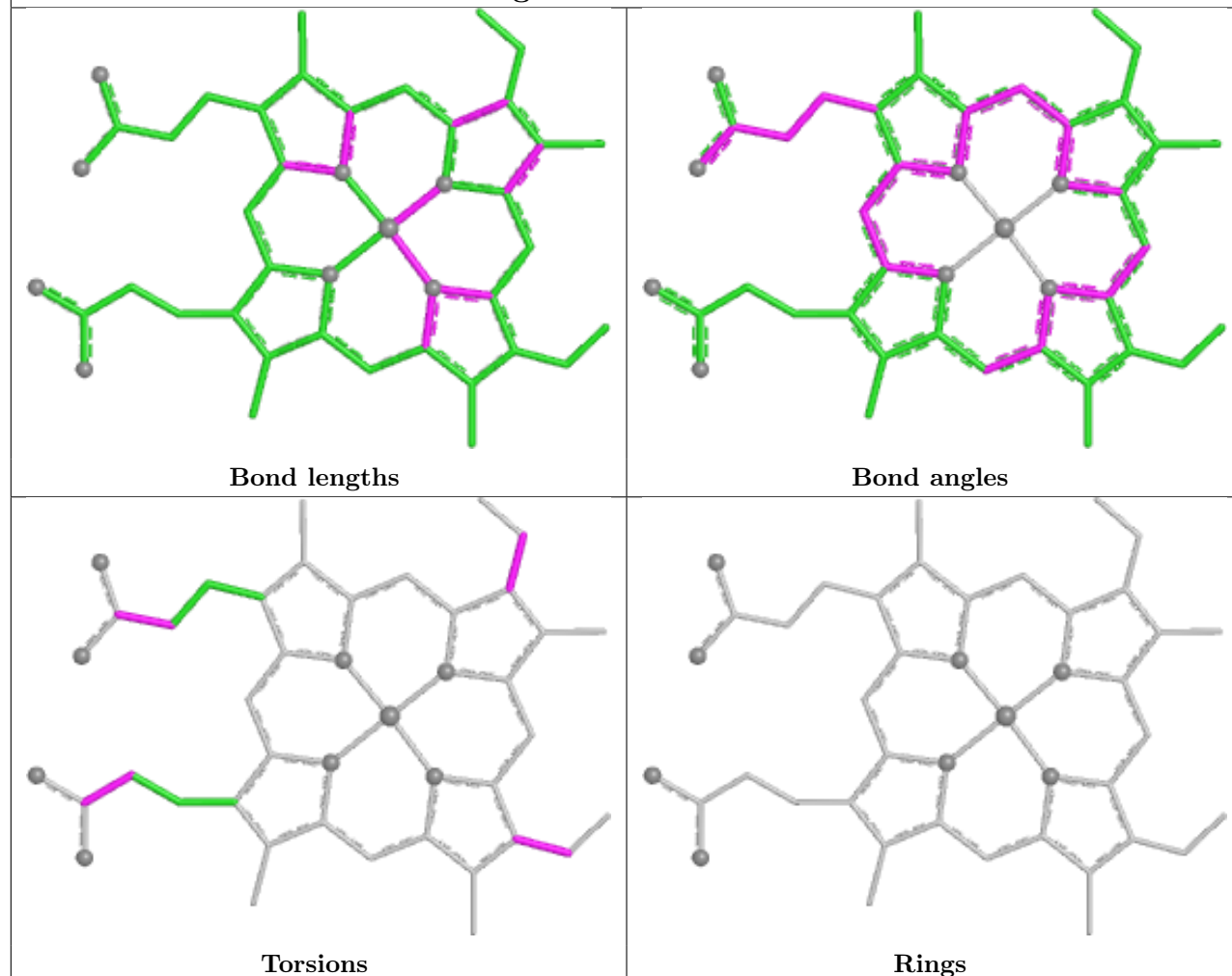




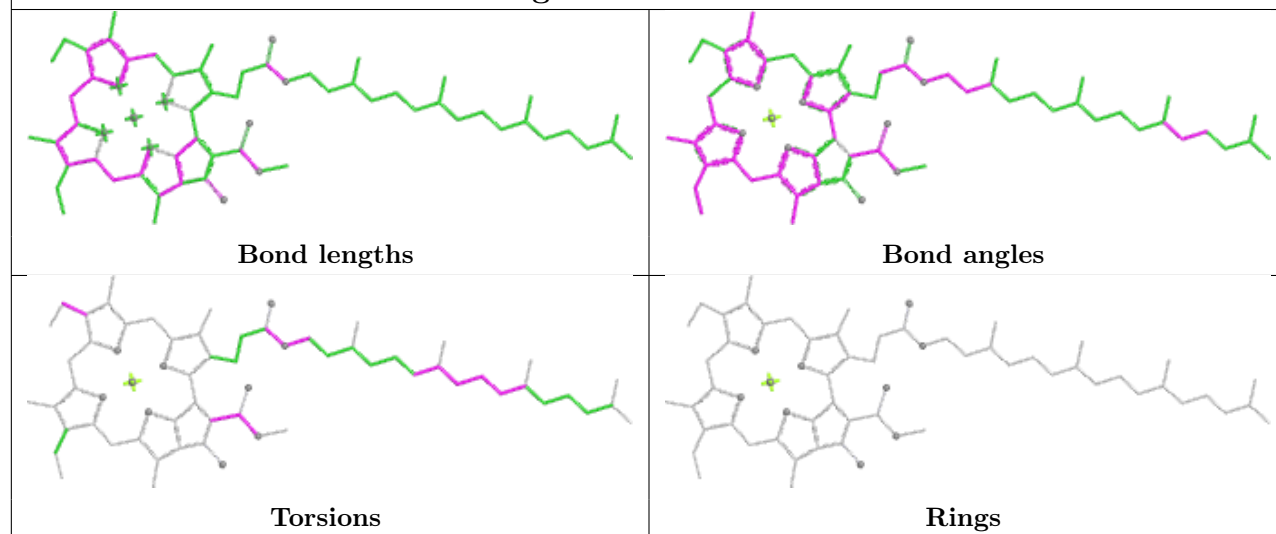


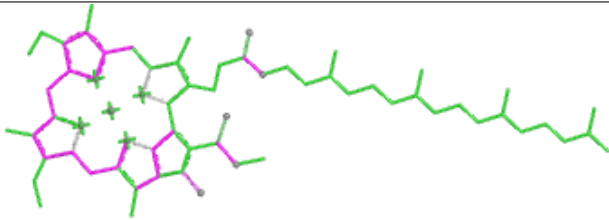
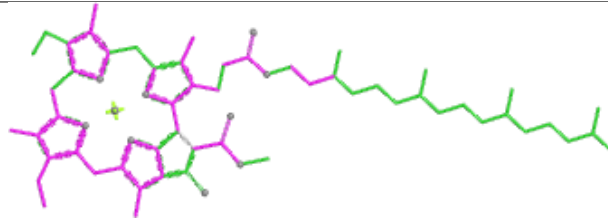
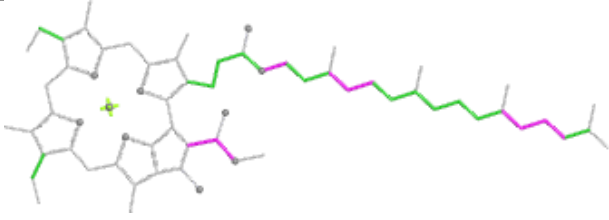
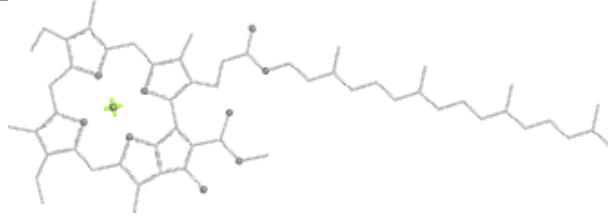


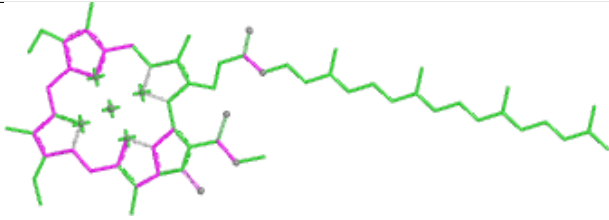
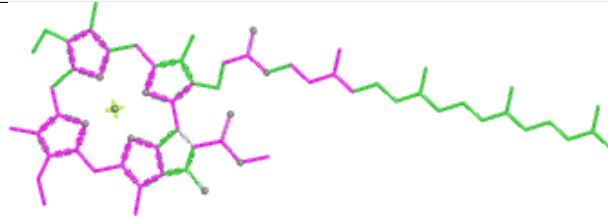
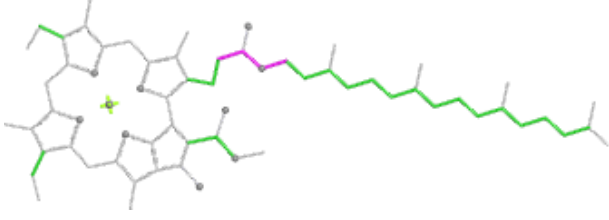
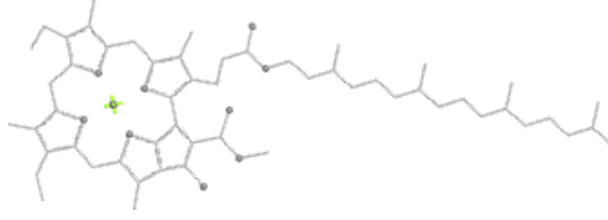
Ligand HEM e 103

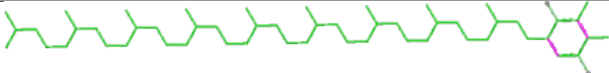
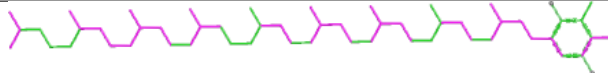


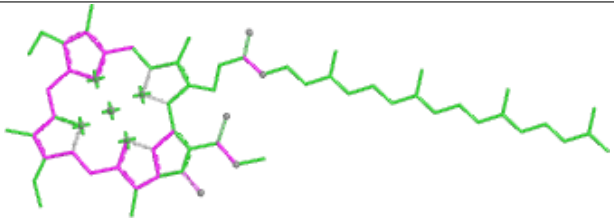
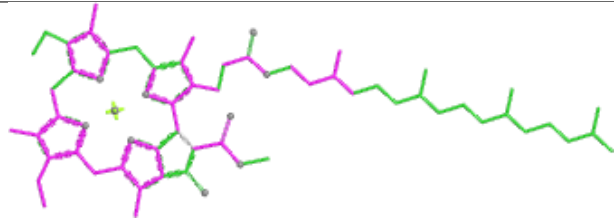
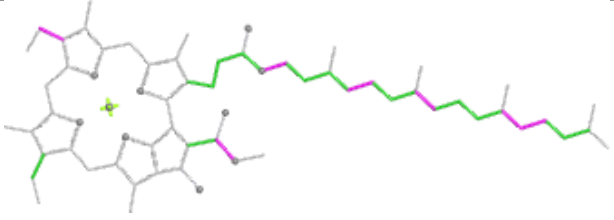
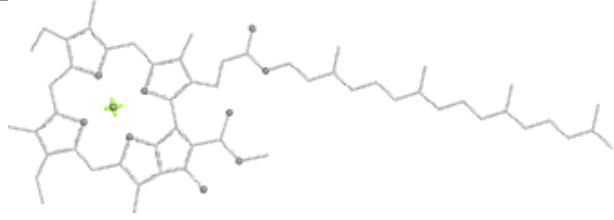
Ligand CLA C 510

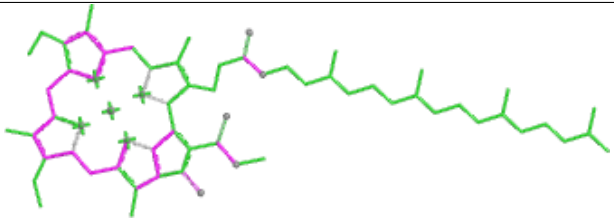
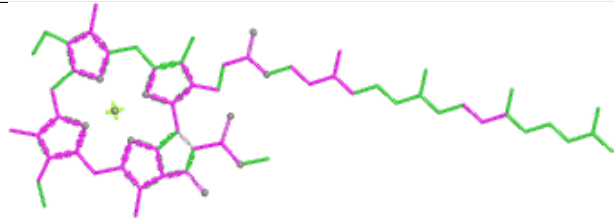
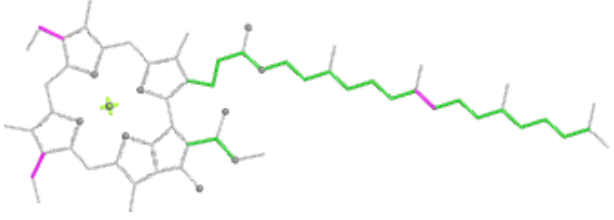
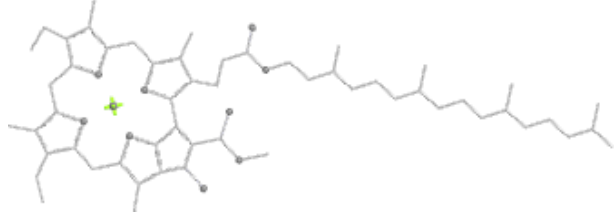


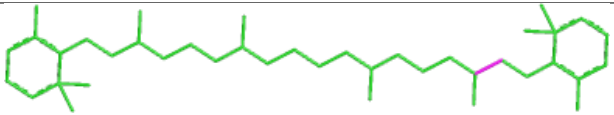
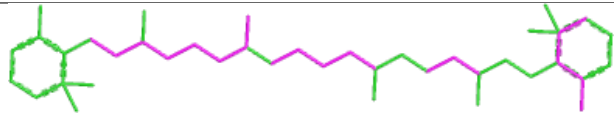
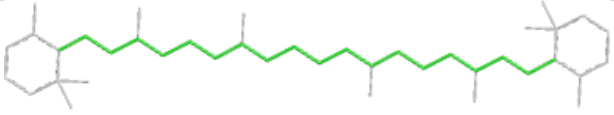
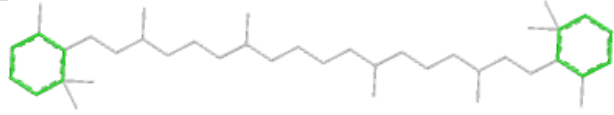
Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

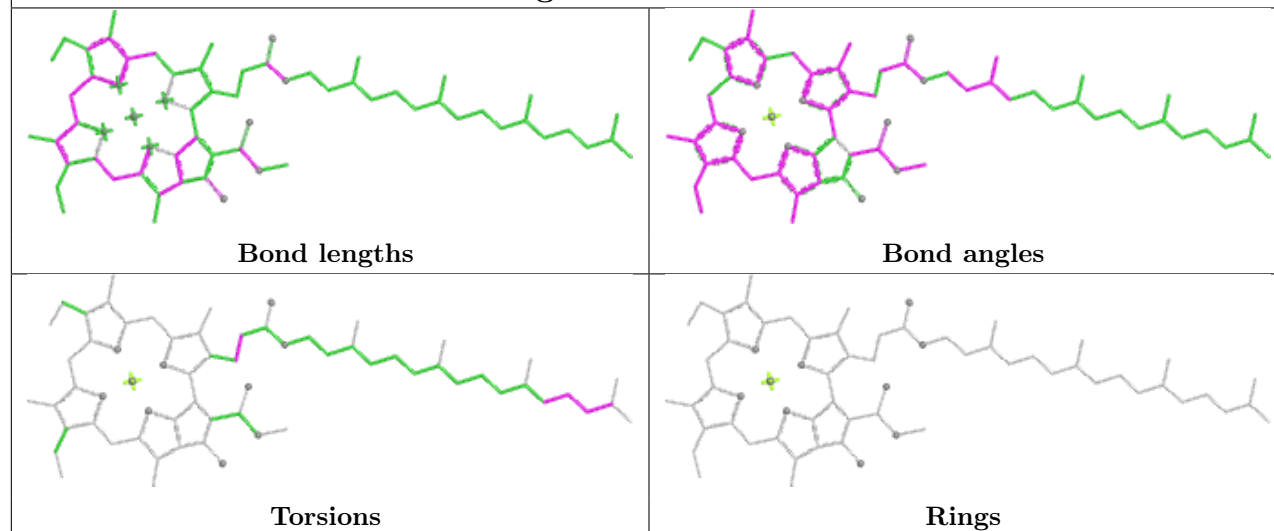
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

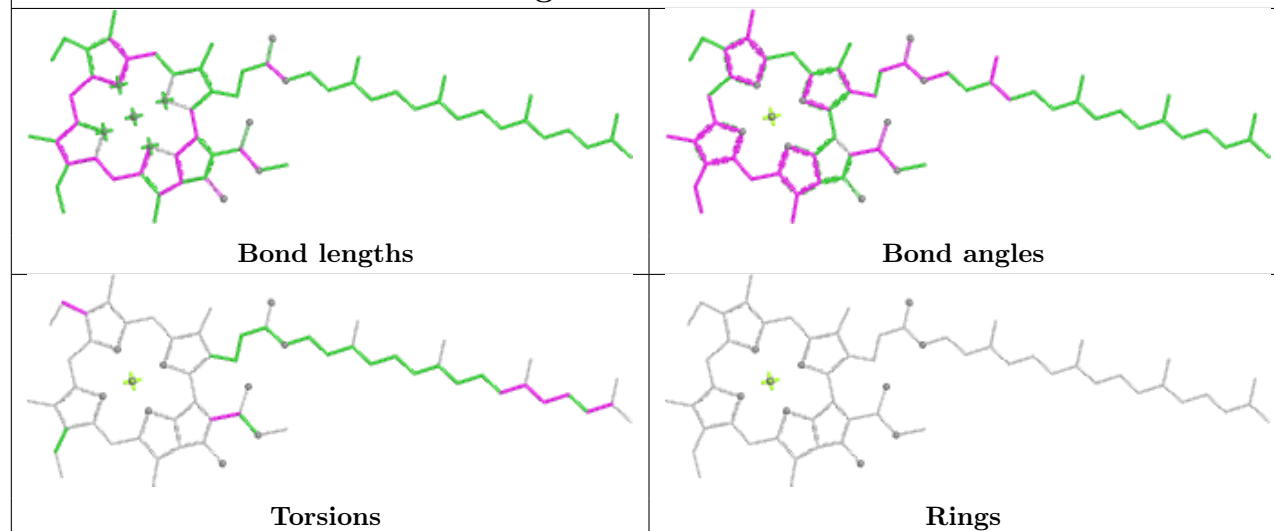
Ligand CLA D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

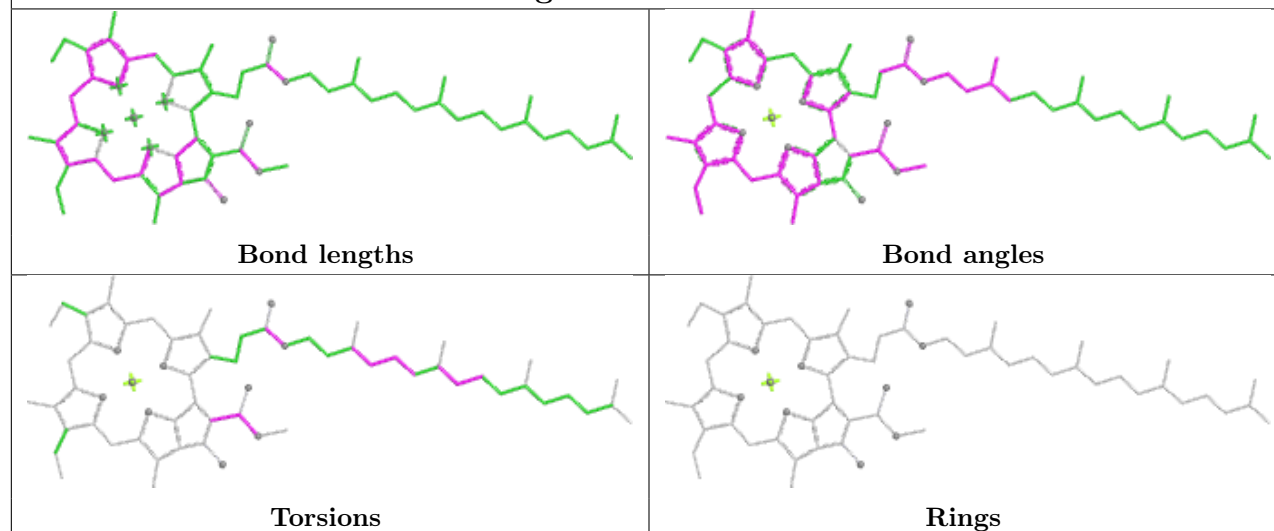
Ligand CLA a 404

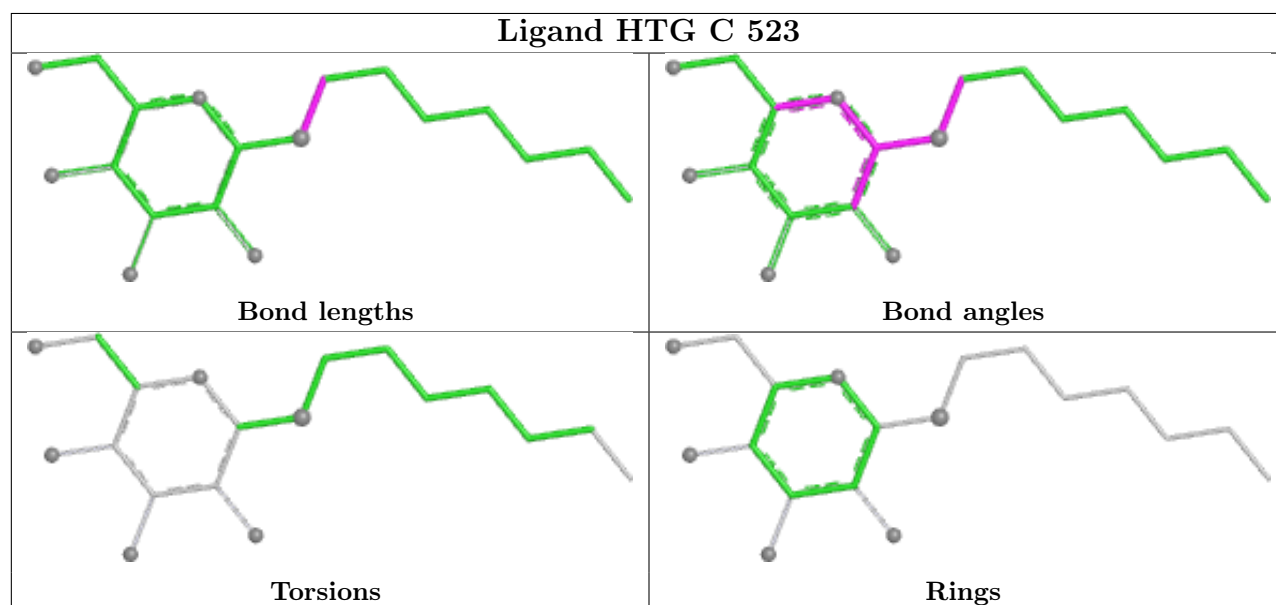
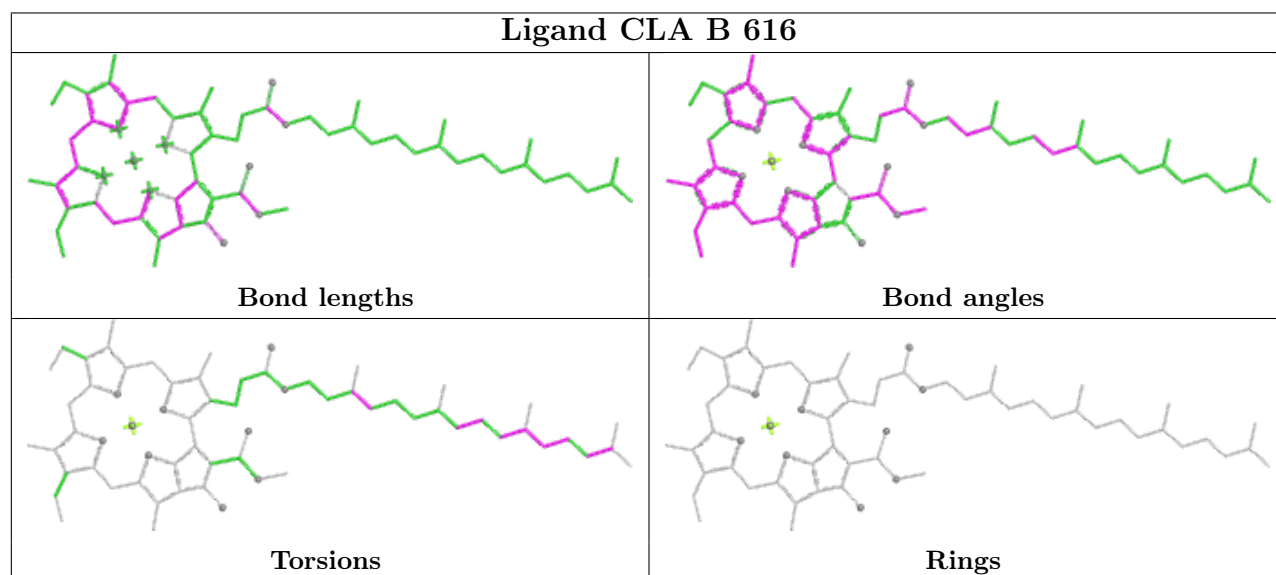
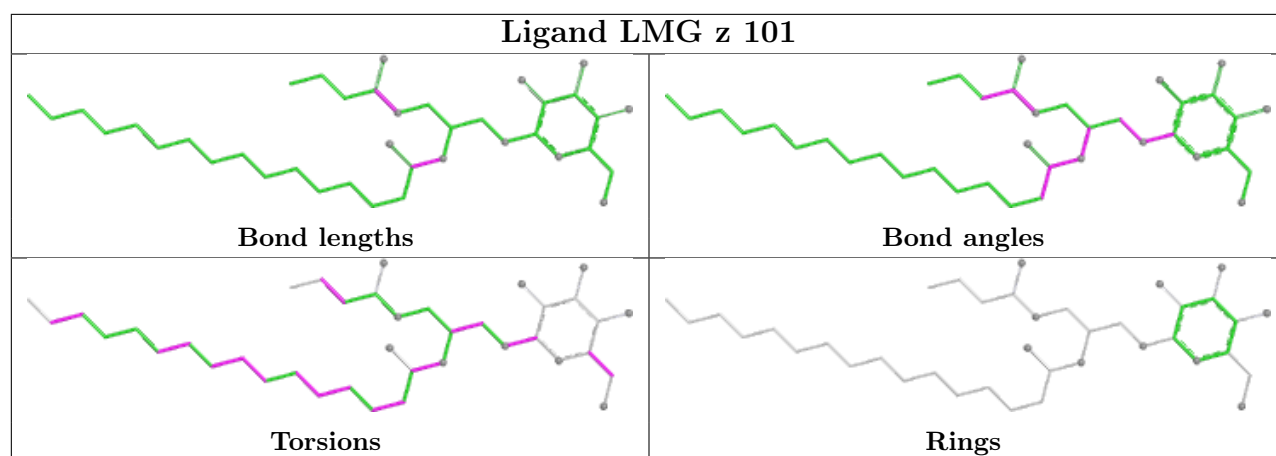


Ligand CLA b 607

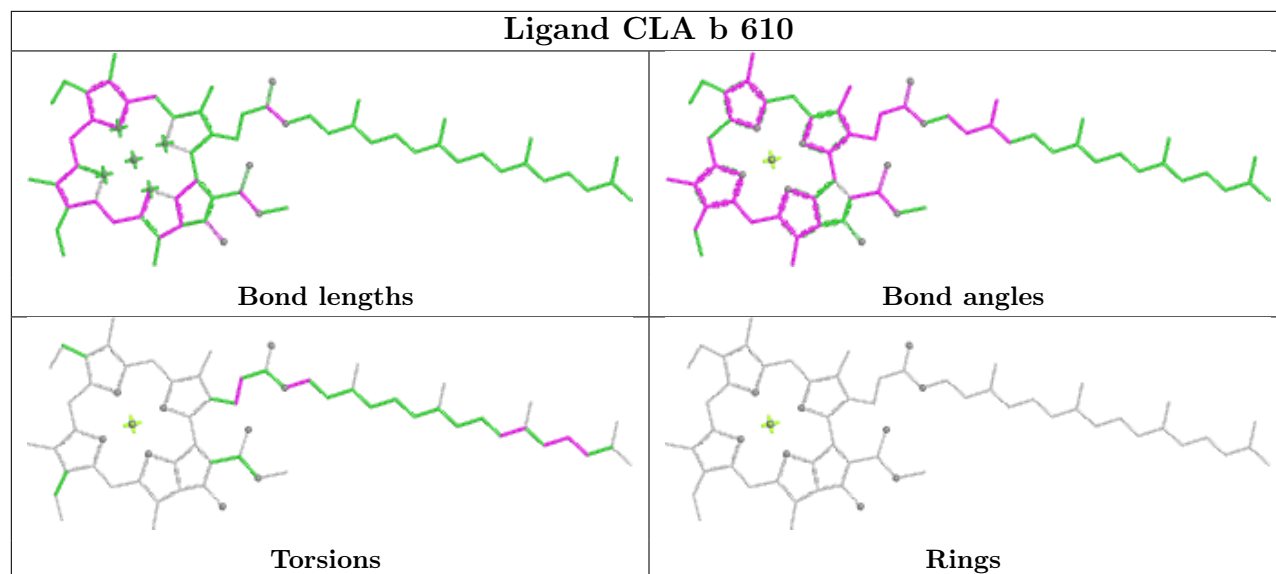


Ligand CLA b 605

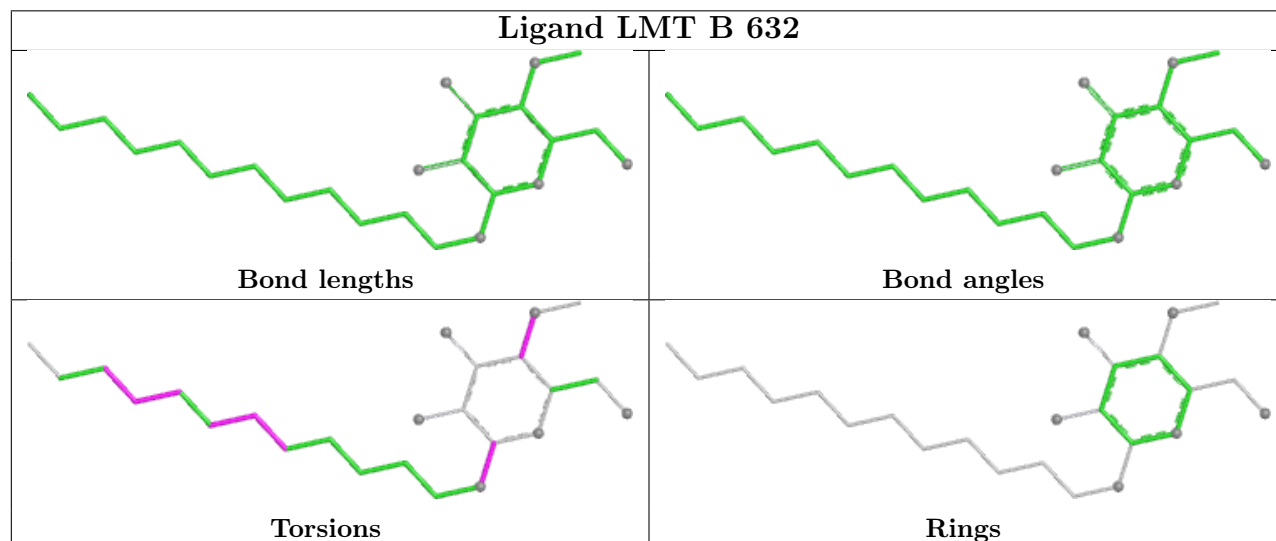




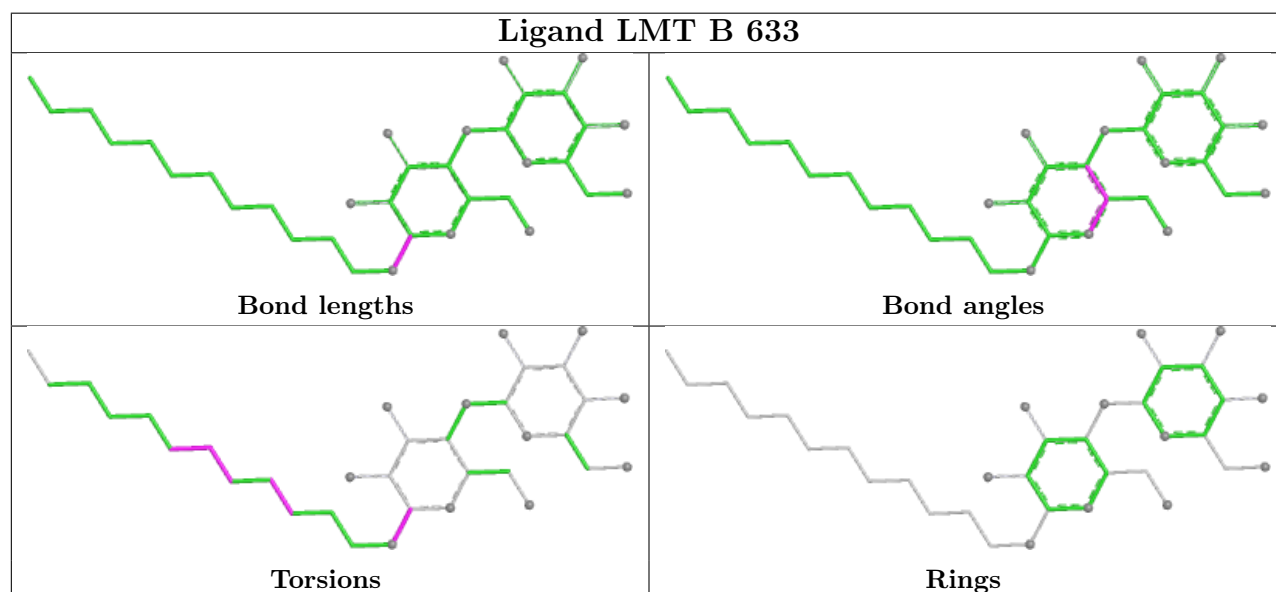
Ligand CLA b 610

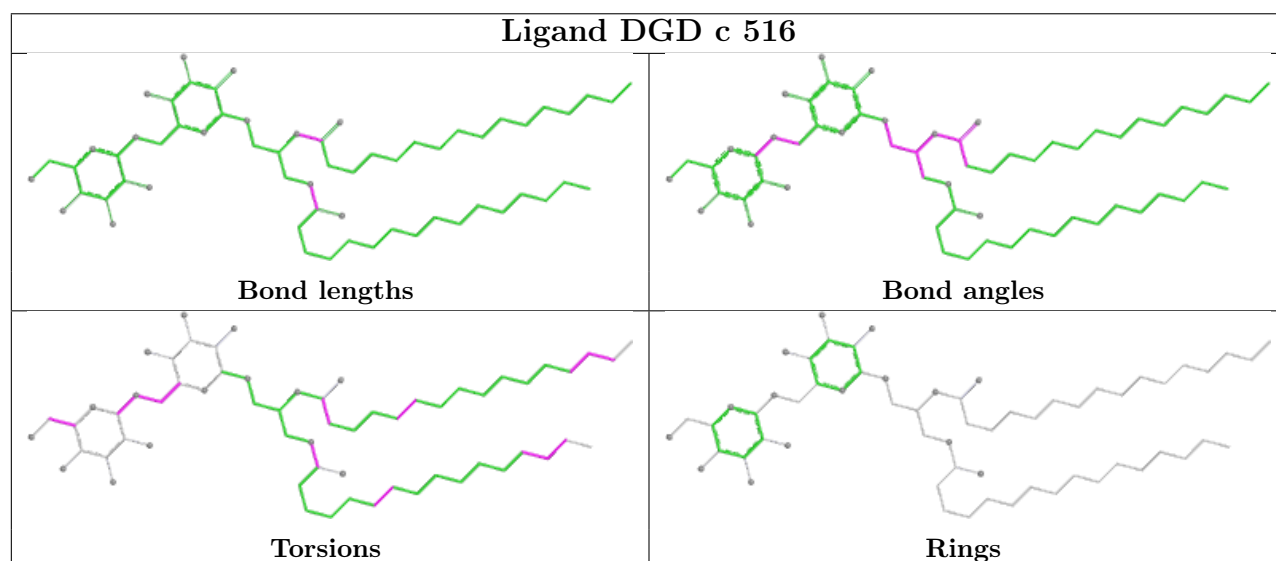
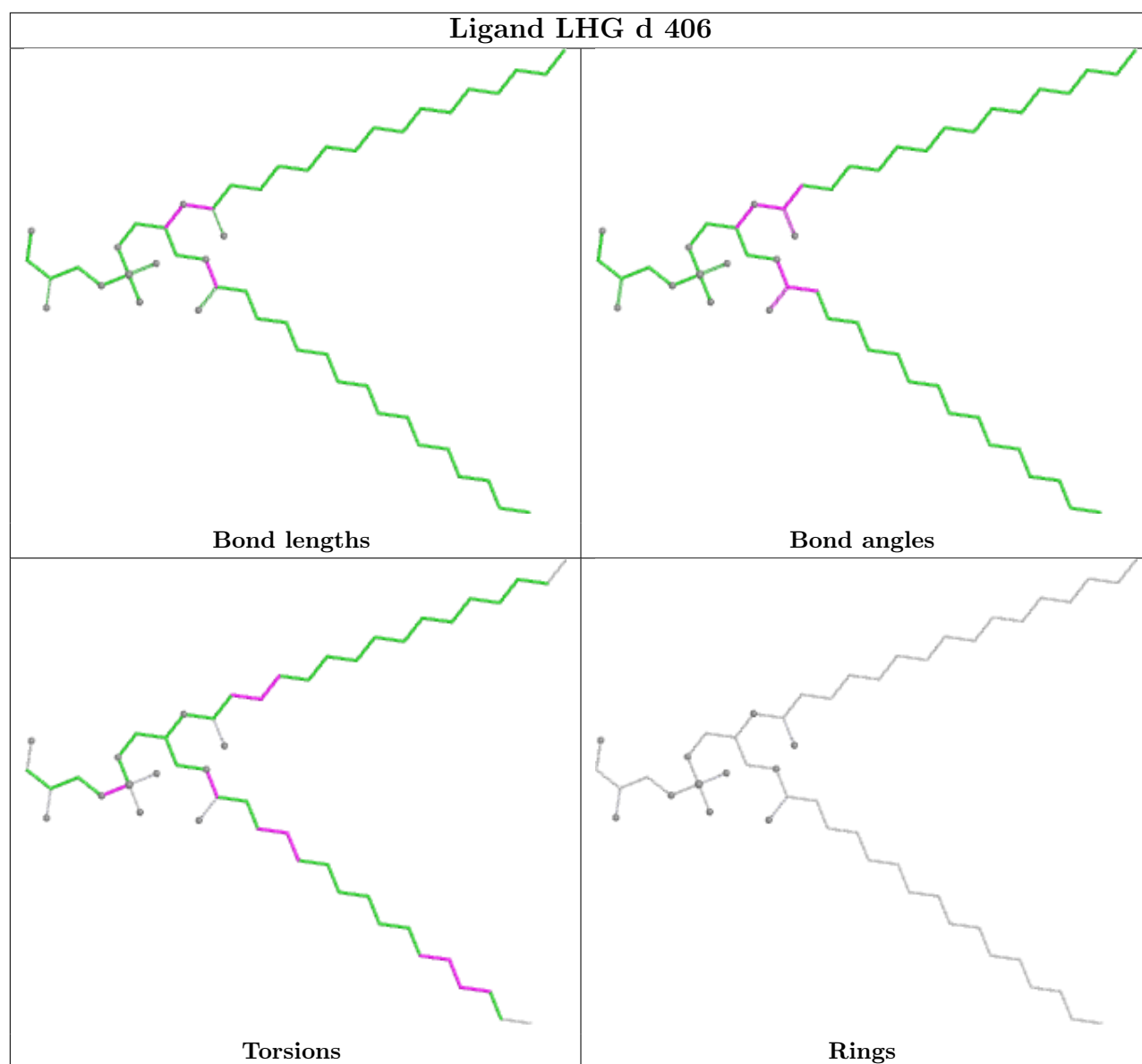


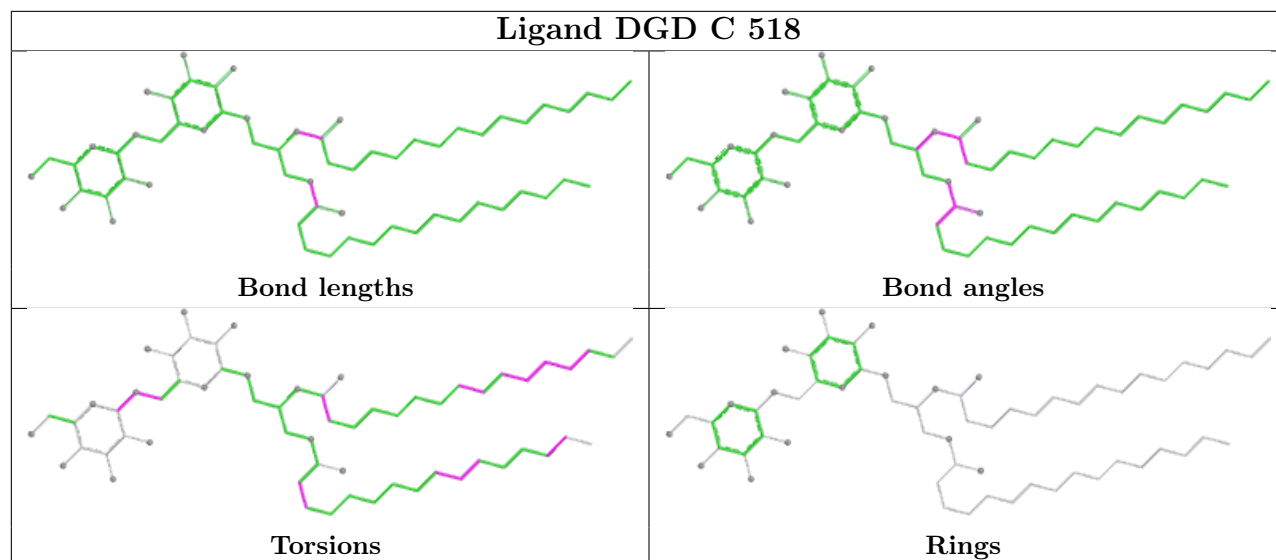
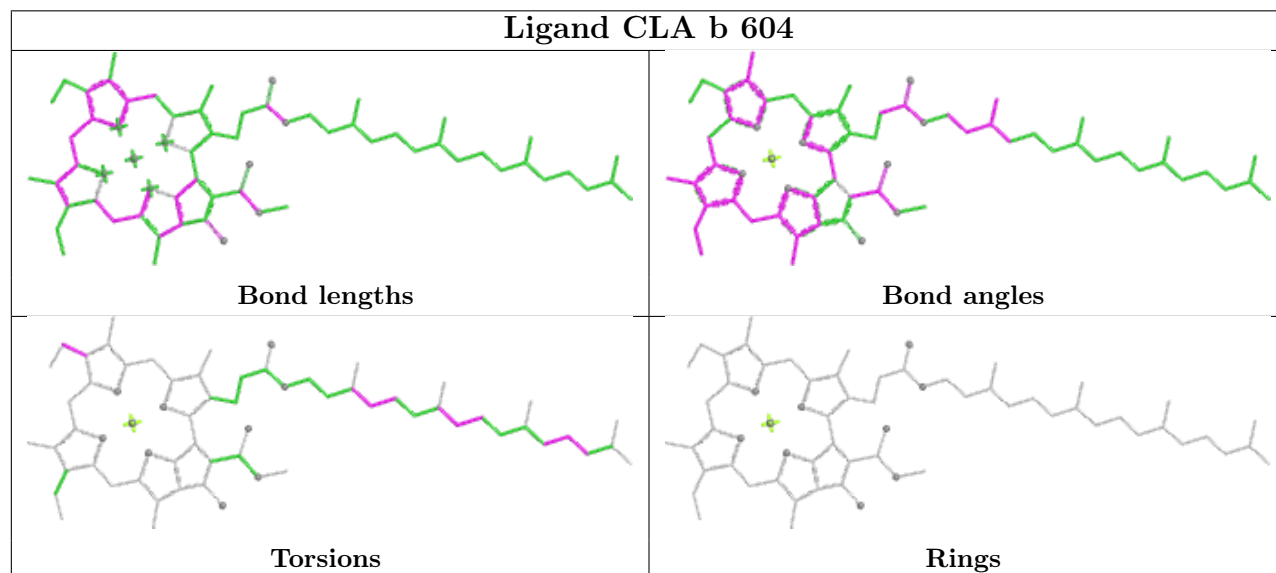
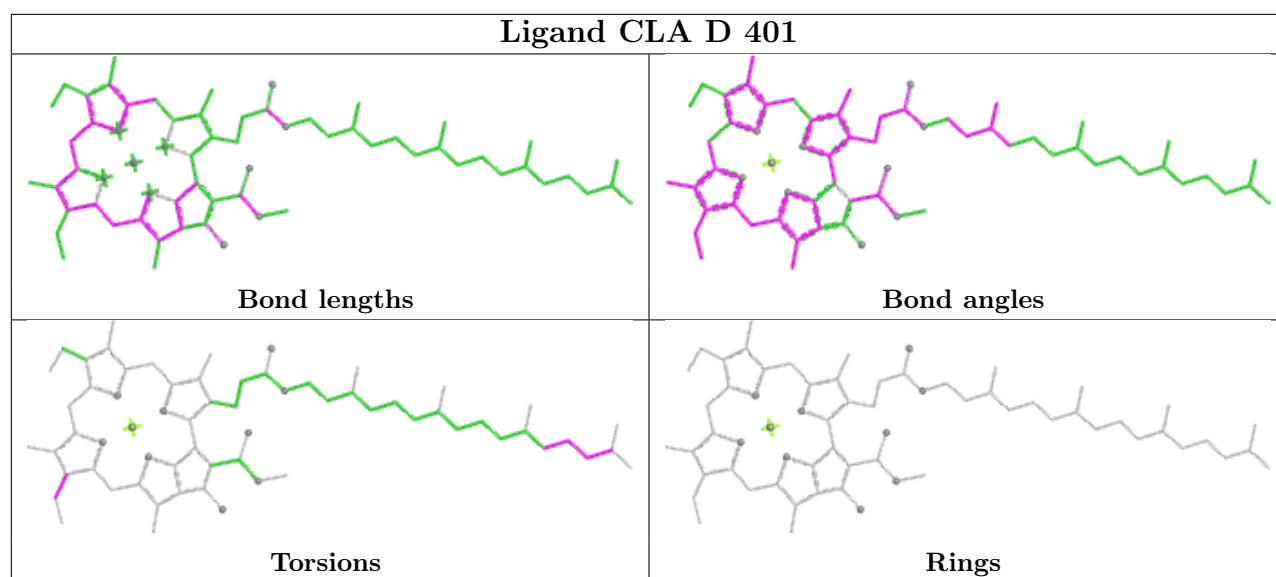
Ligand LMT B 632

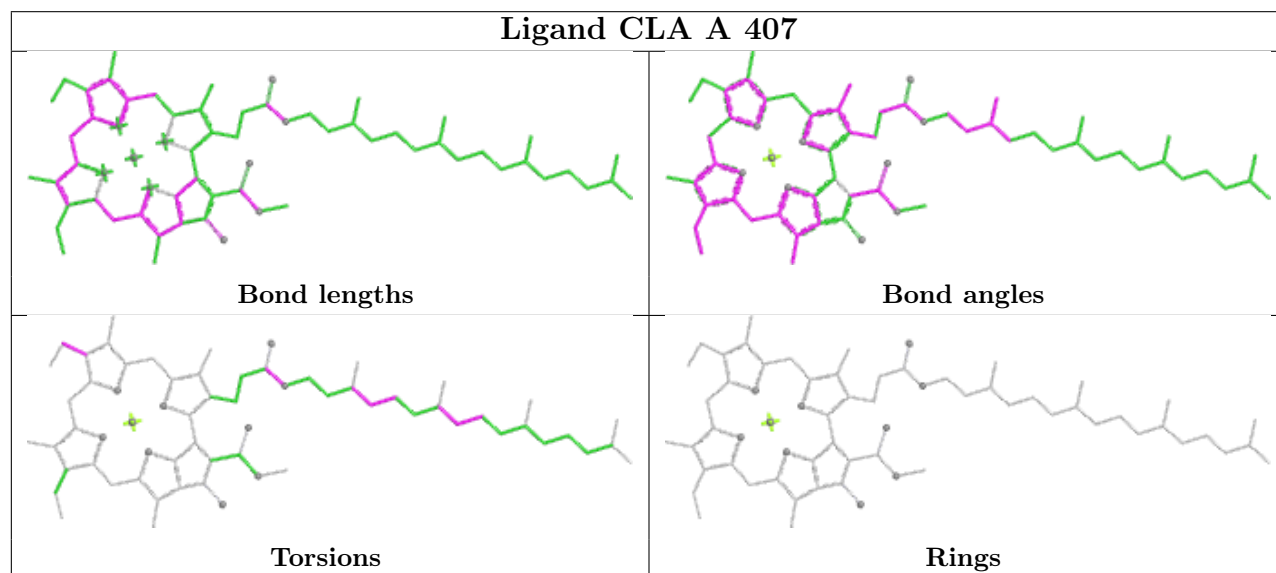
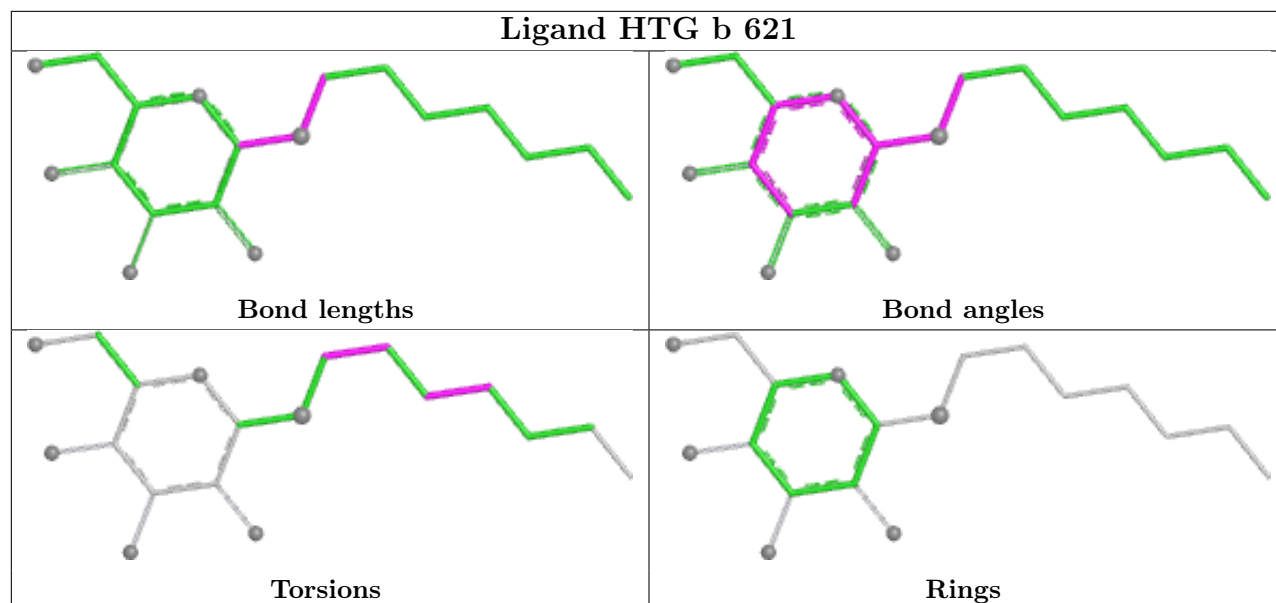


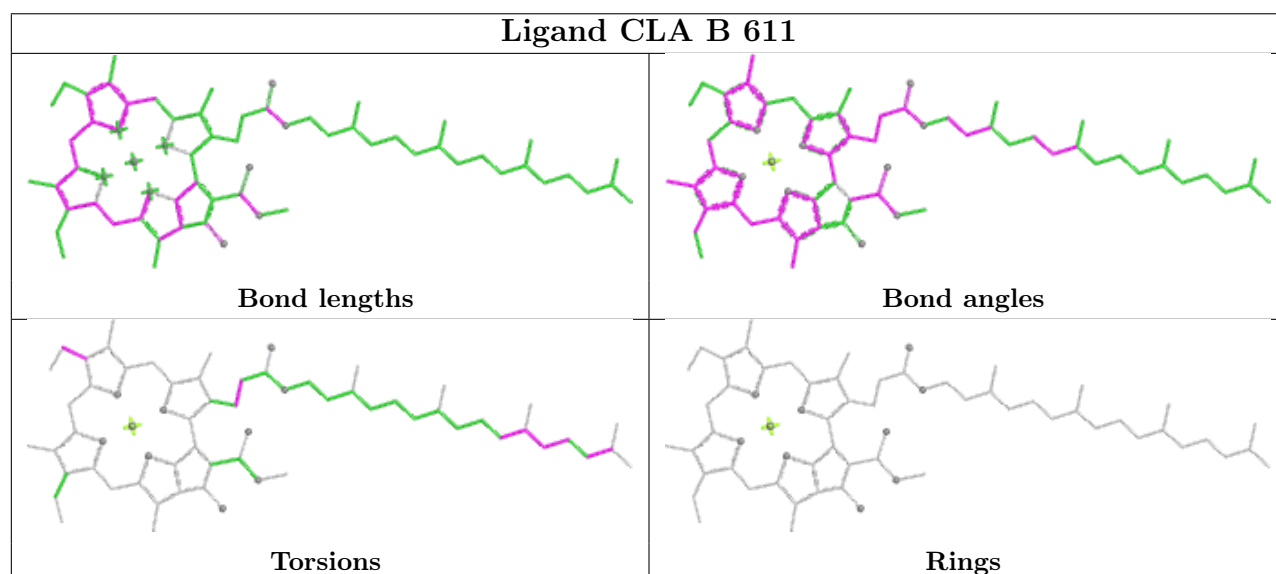
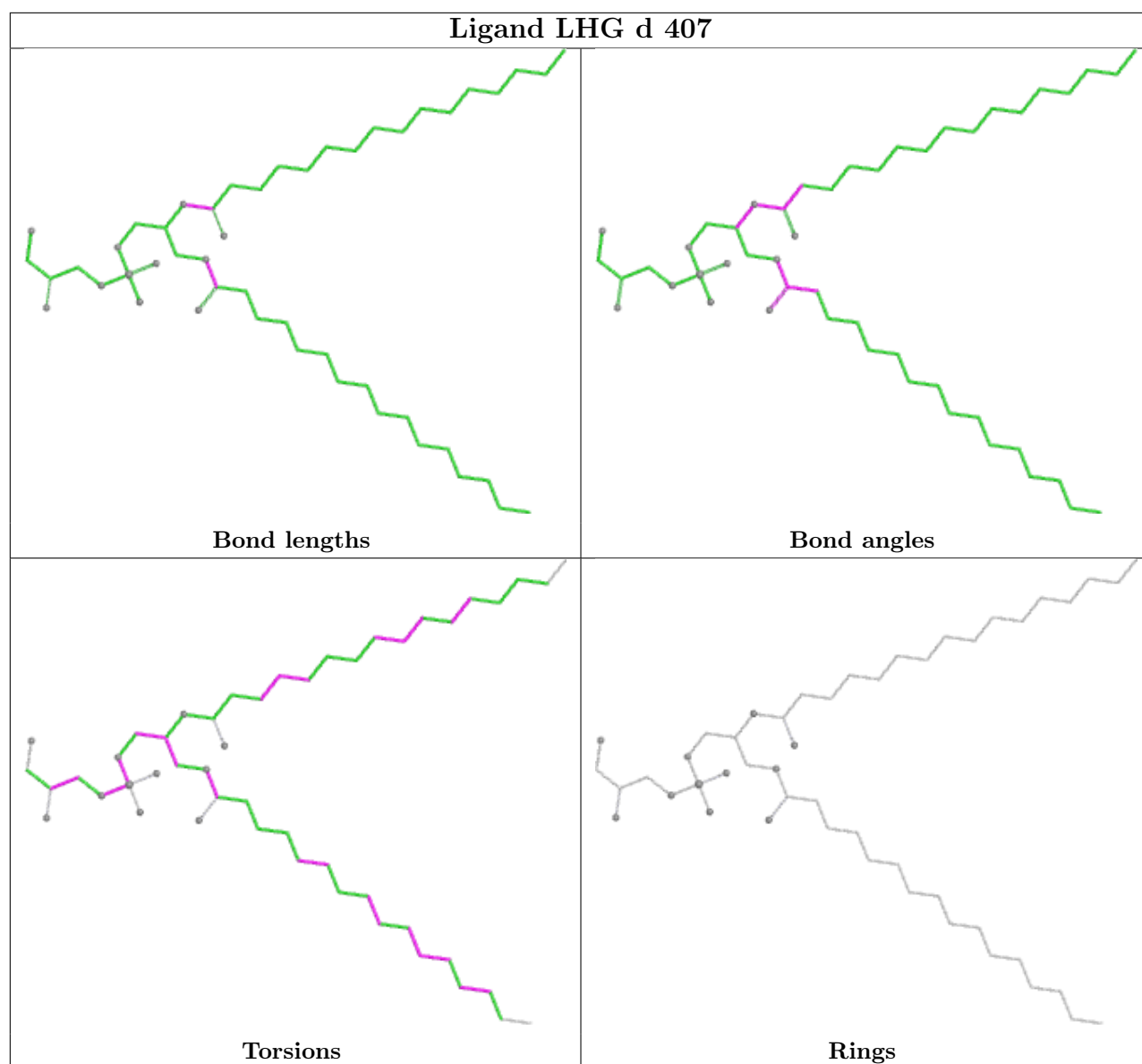
Ligand LMT B 633

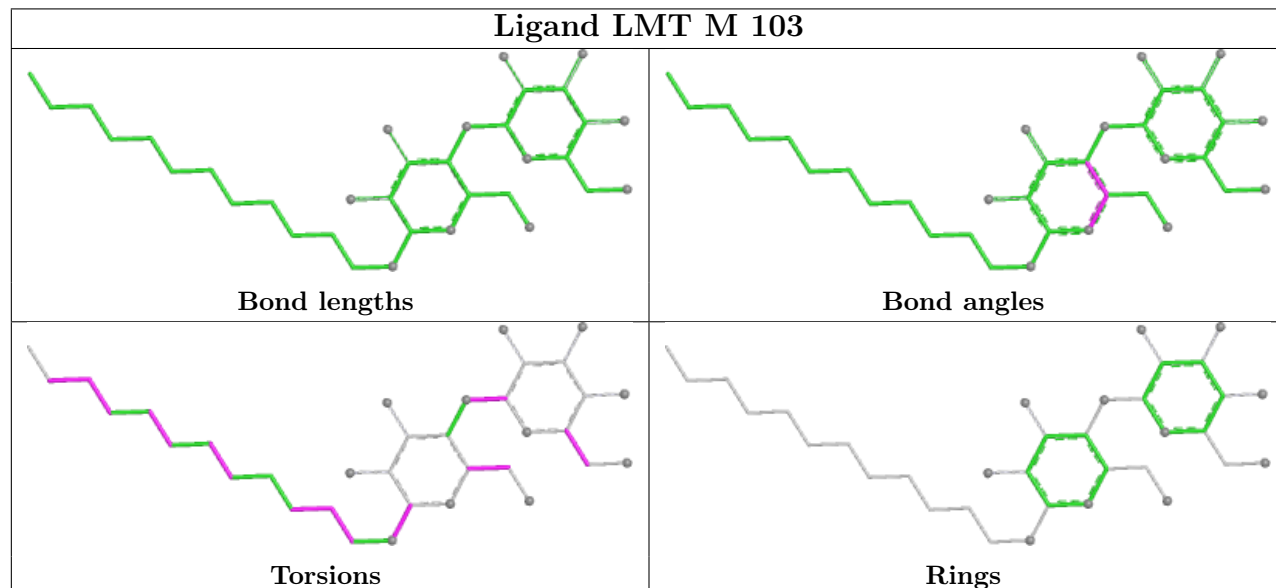
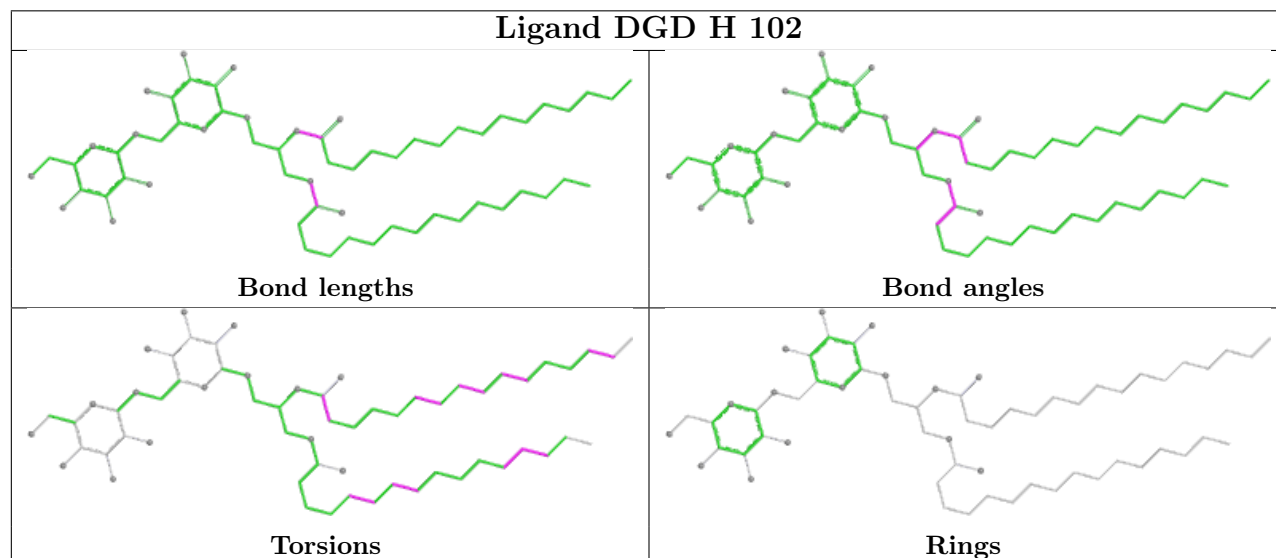
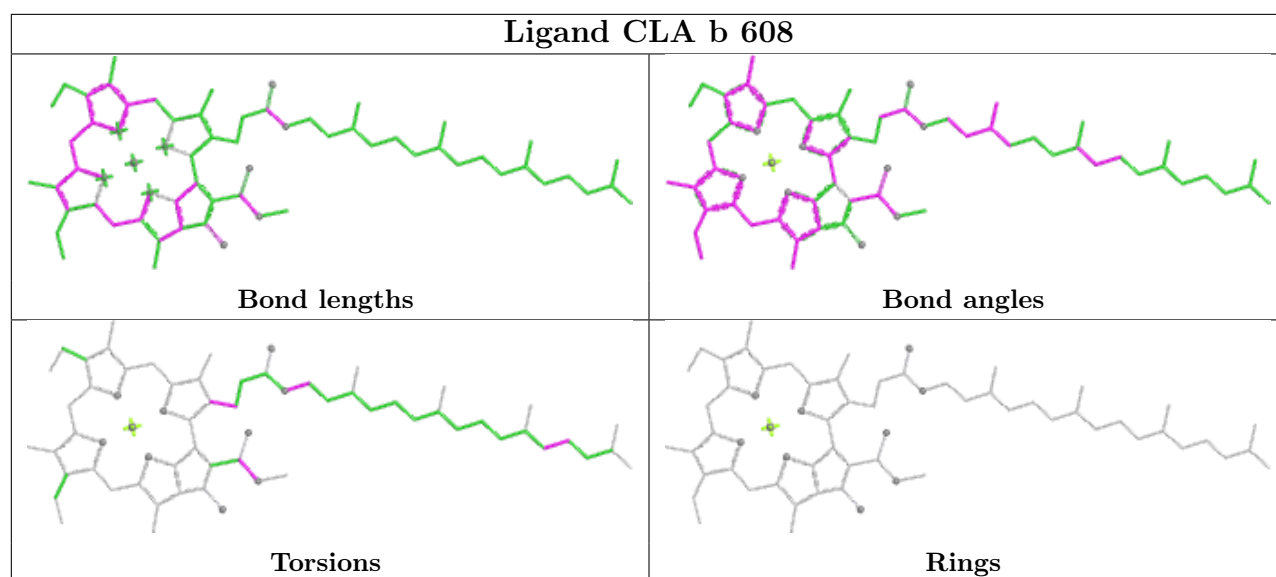


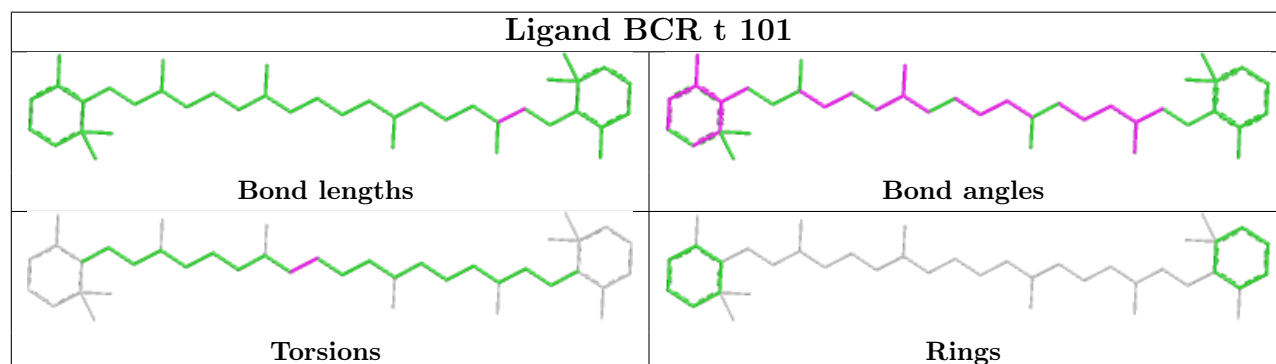
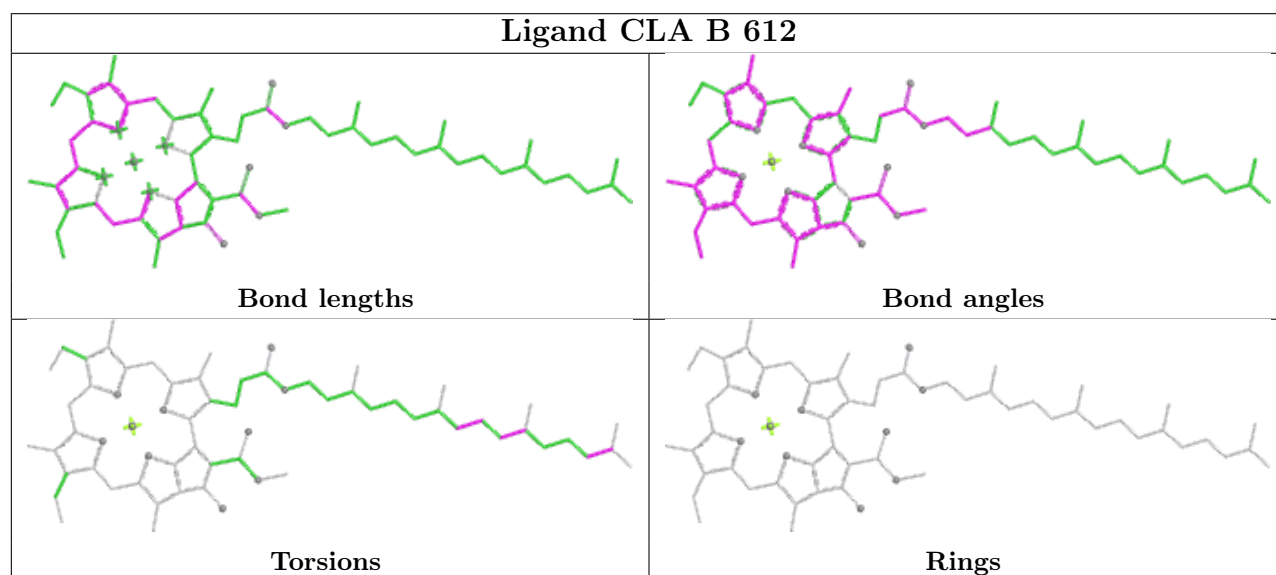
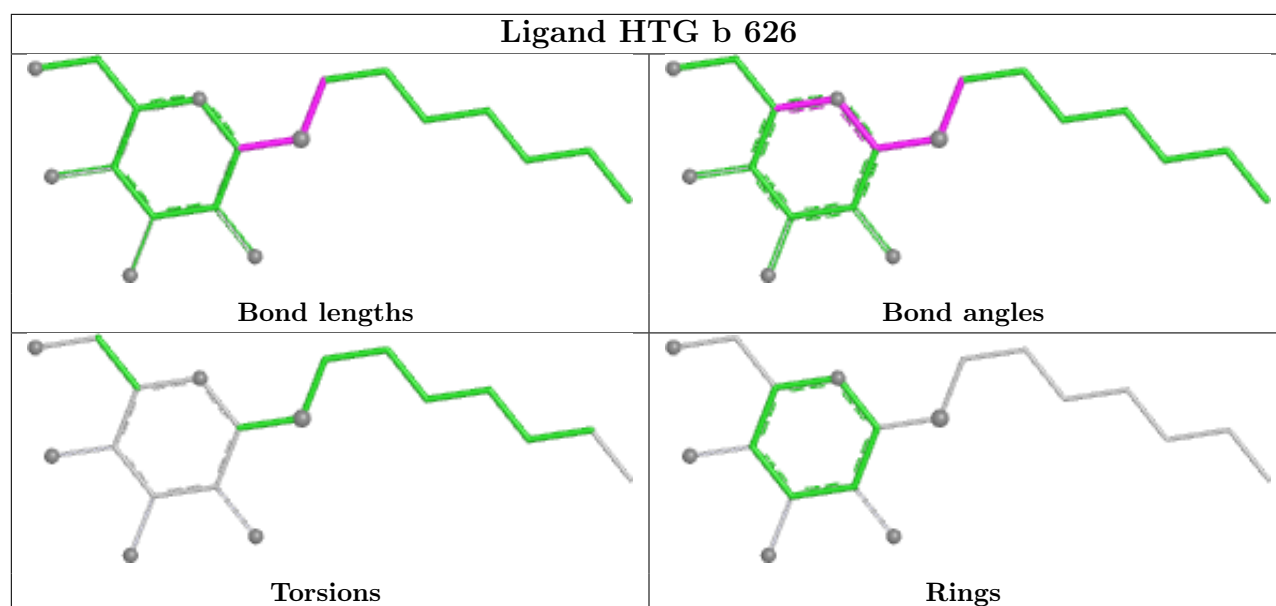


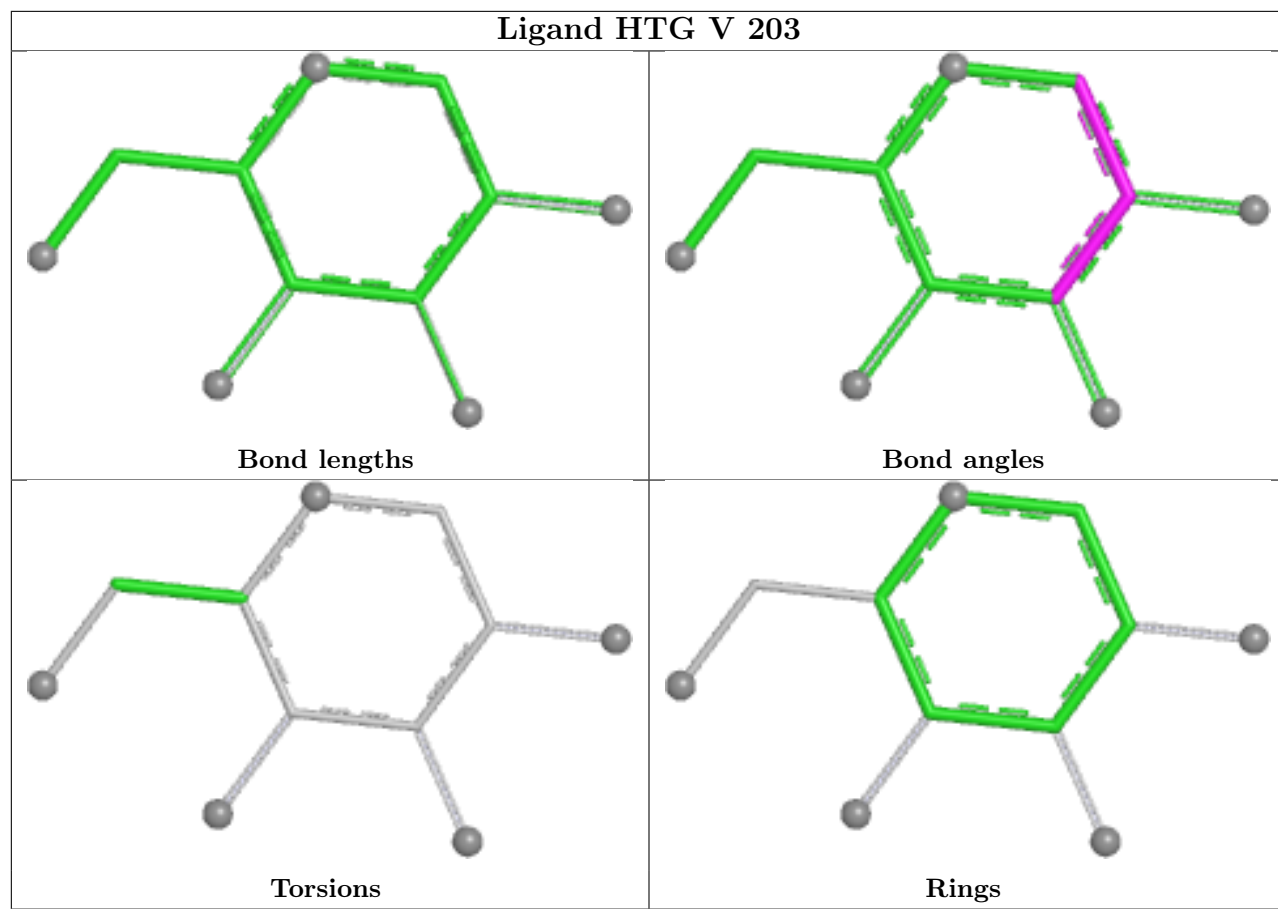


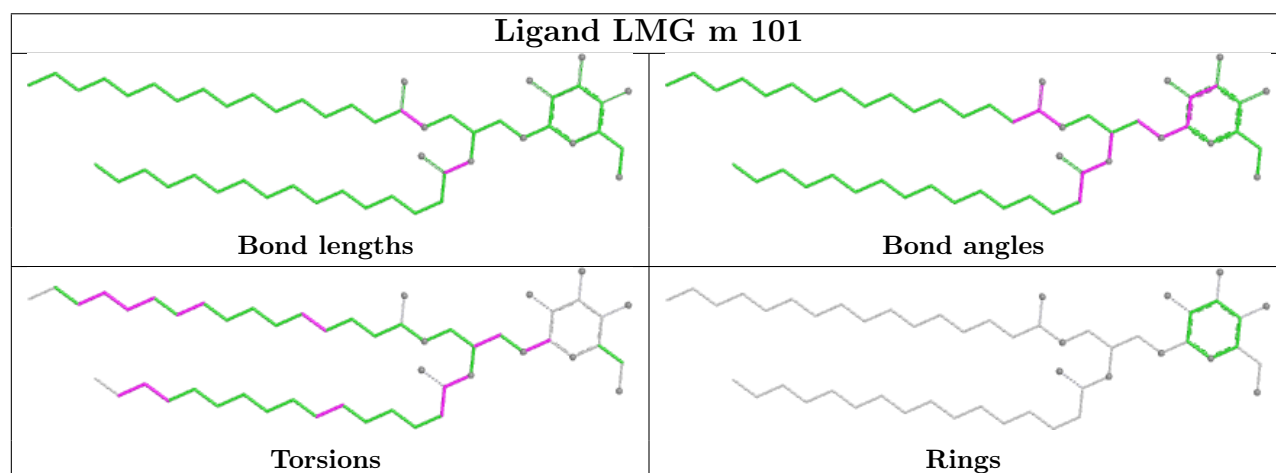
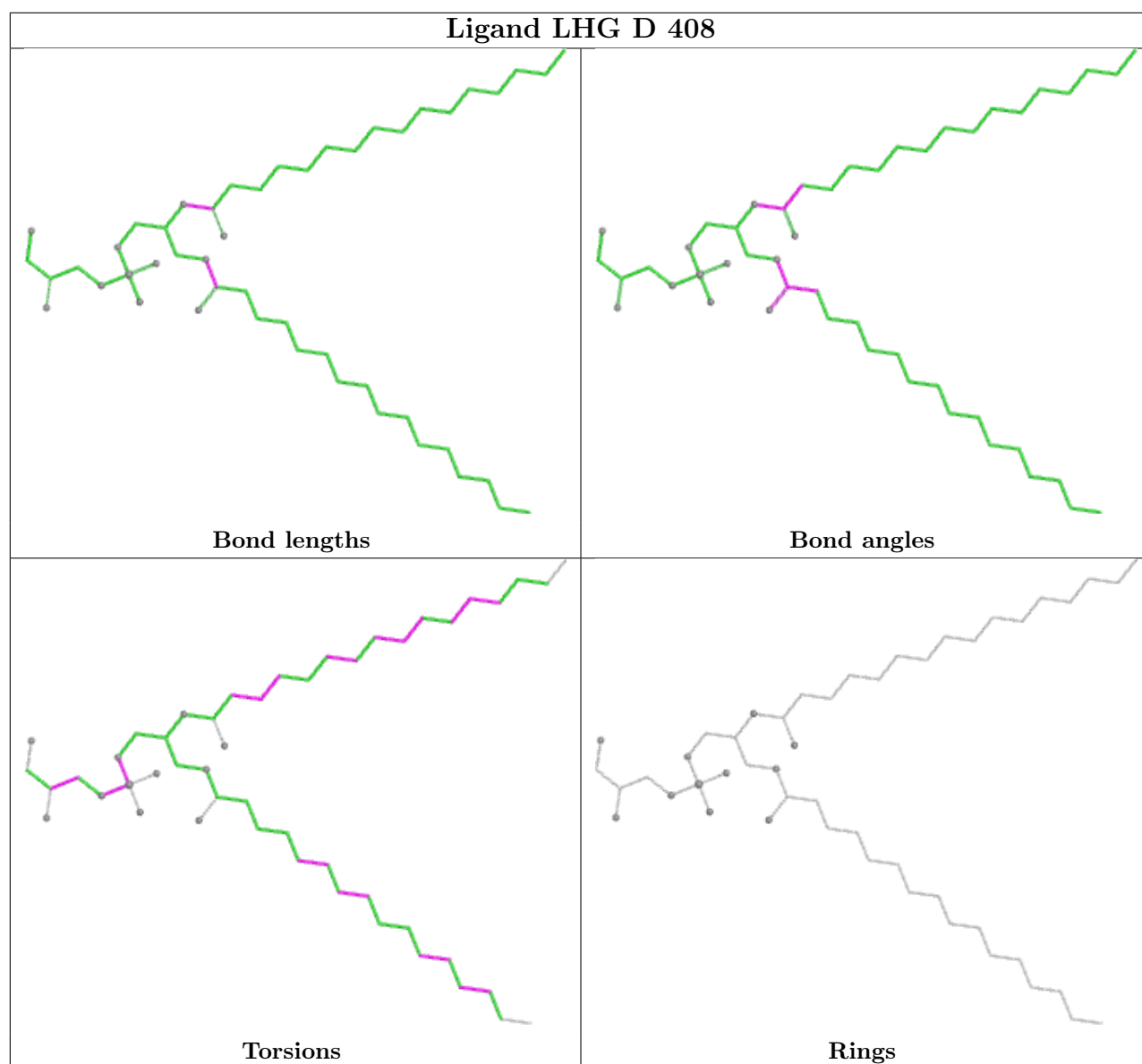


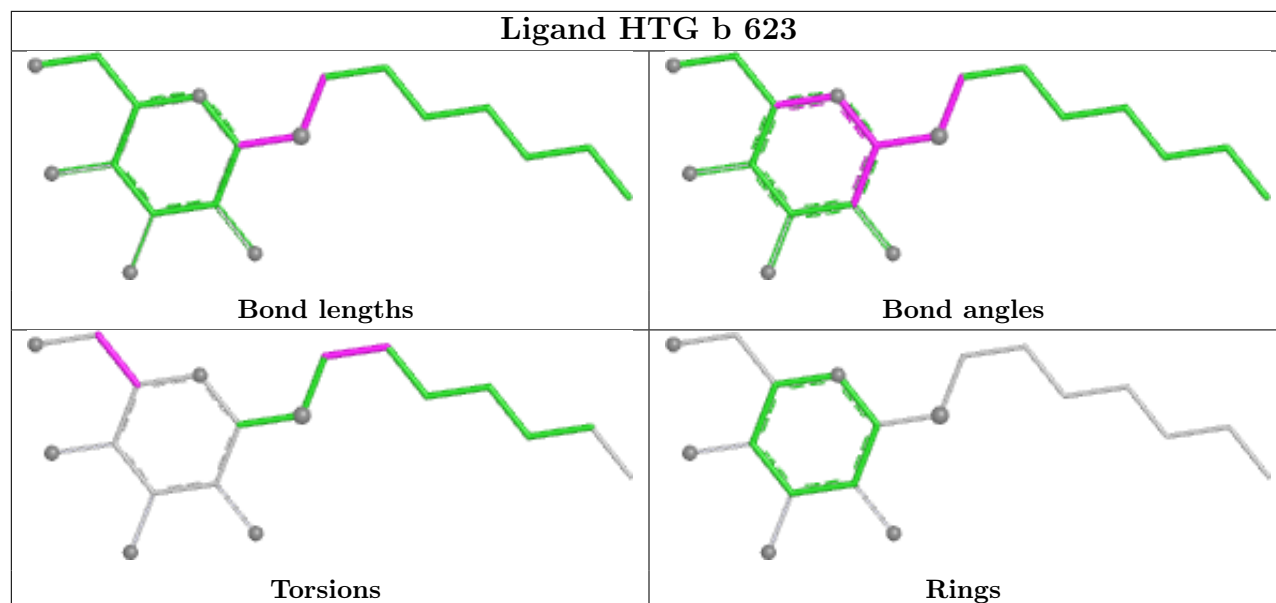












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	334/344 (97%)	-1.11	0	100	100	22, 33, 58, 97	0
1	a	334/344 (97%)	-1.11	0	100	100	24, 36, 65, 113	0
2	B	504/505 (99%)	-1.05	0	100	100	24, 38, 68, 118	0
2	b	504/505 (99%)	-1.02	0	100	100	25, 40, 77, 122	0
3	C	451/455 (99%)	-1.00	0	100	100	27, 48, 70, 108	0
3	c	455/455 (100%)	-0.99	0	100	100	32, 52, 72, 118	0
4	D	342/342 (100%)	-1.11	0	100	100	22, 35, 58, 113	0
4	d	341/342 (99%)	-1.11	0	100	100	24, 39, 59, 124	0
5	E	81/84 (96%)	-0.89	0	100	100	40, 59, 90, 125	0
5	e	79/84 (94%)	-0.87	0	100	100	45, 62, 100, 125	0
6	F	34/44 (77%)	-0.92	0	100	100	41, 51, 81, 96	0
6	f	31/44 (70%)	-0.82	0	100	100	48, 53, 84, 128	0
7	H	64/65 (98%)	-0.88	1 (1%)	70	67	37, 51, 72, 104	0
7	h	65/65 (100%)	-0.98	1 (1%)	72	68	40, 54, 79, 152	0
8	I	37/38 (97%)	-0.93	0	100	100	36, 48, 98, 129	0
8	i	37/38 (97%)	-0.78	0	100	100	38, 49, 107, 137	0
9	J	38/39 (97%)	-0.96	0	100	100	37, 55, 113, 156	0
9	j	39/39 (100%)	-0.86	0	100	100	46, 56, 109, 137	0
10	K	37/37 (100%)	-1.06	0	100	100	49, 58, 81, 98	0
10	k	37/37 (100%)	-1.04	0	100	100	52, 60, 82, 99	0
11	L	36/37 (97%)	-1.16	0	100	100	23, 30, 98, 143	0
11	l	36/37 (97%)	-1.15	0	100	100	24, 31, 97, 143	0
12	M	32/36 (88%)	-1.12	0	100	100	24, 31, 53, 125	0
12	m	33/36 (91%)	-1.10	0	100	100	24, 32, 66, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-1.01	0 100 100	22, 50, 103, 163	0
13	o	243/244 (99%)	-1.01	0 100 100	26, 50, 108, 151	0
14	T	29/32 (90%)	-1.11	0 100 100	26, 31, 68, 97	0
14	t	29/32 (90%)	-1.11	0 100 100	26, 31, 69, 98	0
15	U	96/104 (92%)	-1.07	0 100 100	32, 44, 72, 86	0
15	u	97/104 (93%)	-1.15	0 100 100	37, 47, 72, 105	0
16	V	137/137 (100%)	-1.03	0 100 100	30, 46, 74, 111	0
16	v	137/137 (100%)	-1.02	0 100 100	37, 54, 79, 112	0
17	X	38/40 (95%)	-0.77	0 100 100	49, 58, 80, 121	0
17	x	38/40 (95%)	-0.59	0 100 100	50, 60, 84, 123	0
18	Y	29/30 (96%)	-0.51	0 100 100	60, 76, 112, 120	0
18	y	29/30 (96%)	-0.74	0 100 100	63, 76, 107, 118	0
19	Z	62/62 (100%)	-0.83	0 100 100	57, 77, 127, 161	0
19	z	62/62 (100%)	-0.59	0 100 100	61, 79, 127, 161	0
20	R	34/34 (100%)	0.46	0 100 100	92, 116, 145, 149	0
All	All	5284/5384 (98%)	-1.01	2 (0%) 100 100	22, 45, 88, 163	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	2.2
7	h	65	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	m	1	10/11	0.96	0.06	26,43,69,74	0
14	FME	t	1	10/11	0.97	0.04	22,34,47,66	0
14	FME	T	1	10/11	0.97	0.05	19,37,45,52	0
8	FME	I	1	10/11	0.98	0.04	29,49,53,54	0
12	FME	M	1	10/11	0.98	0.06	33,41,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.98	0.04	38,50,63,74	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
30	UNL	m	102	10/-	0.70	0.13	36,47,64,66	0
36	HTG	D	412	16/19	0.72	0.11	43,118,136,138	0
35	LMT	E	102	35/35	0.73	0.13	91,129,157,163	0
36	HTG	B	626	19/19	0.73	0.11	51,135,163,189	0
30	UNL	J	102	10/-	0.73	0.17	59,66,85,90	0
36	HTG	b	622	19/19	0.73	0.15	77,105,127,134	0
34	LMG	C	521	51/55	0.74	0.11	50,107,149,153	0
36	HTG	B	630	19/19	0.74	0.09	67,116,145,154	0
36	HTG	C	524	9/19	0.74	0.18	70,90,106,139	0
35	LMT	D	403	35/35	0.74	0.11	40,112,125,126	0
30	UNL	A	414	28/-	0.74	0.13	66,93,121,126	0
27	GOL	O	302	6/6	0.75	0.09	63,68,72,78	0
30	UNL	i	101	40/-	0.76	0.12	56,91,147,151	0
35	LMT	B	633	35/35	0.76	0.12	39,117,133,139	0
30	UNL	a	416	30/-	0.76	0.11	86,102,121,129	0
35	LMT	a	418	35/35	0.77	0.11	97,118,139,139	0
35	LMT	e	102	35/35	0.77	0.11	75,139,161,171	0
36	HTG	C	523	19/19	0.77	0.10	95,107,121,133	0
30	UNL	j	102	10/-	0.78	0.11	57,81,94,94	0
30	UNL	K	101	34/-	0.78	0.10	62,102,116,137	0
36	HTG	b	626	19/19	0.78	0.09	66,114,151,181	0
36	HTG	B	625	19/19	0.79	0.15	43,101,109,111	0
35	LMT	C	522	35/35	0.79	0.10	83,119,141,151	0
30	UNL	M	102	10/-	0.81	0.09	38,51,60,60	0
36	HTG	c	521	19/19	0.81	0.08	71,125,137,163	0
26	SQD	f	101	43/54	0.82	0.10	86,117,154,157	0
30	UNL	B	631	33/-	0.83	0.12	36,92,134,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	b	629	36/-	0.83	0.09	46,85,130,141	0
35	LMT	M	103	35/35	0.83	0.09	37,128,152,157	0
34	LMG	c	520	51/55	0.83	0.09	62,104,135,147	0
35	LMT	B	623	35/35	0.83	0.09	50,95,120,122	0
36	HTG	b	623	19/19	0.83	0.10	73,116,140,180	0
30	UNL	D	411	40/-	0.83	0.10	49,76,125,128	0
30	UNL	I	101	40/-	0.83	0.10	39,89,141,148	0
36	HTG	c	522	19/19	0.83	0.10	83,139,149,158	0
31	LHG	e	101	42/49	0.84	0.09	63,119,140,150	0
30	UNL	b	627	33/-	0.85	0.09	53,80,145,147	0
35	LMT	b	620	25/35	0.85	0.09	55,88,143,147	0
35	LMT	M	101	35/35	0.85	0.08	40,85,105,107	0
35	LMT	m	103	35/35	0.85	0.10	40,85,113,117	0
30	UNL	c	525	32/-	0.85	0.10	74,104,124,132	0
36	HTG	h	101	16/19	0.85	0.09	71,110,125,143	0
27	GOL	a	412	6/6	0.86	0.12	56,70,85,86	0
31	LHG	E	101	42/49	0.86	0.09	47,95,114,121	0
36	HTG	b	621	19/19	0.86	0.10	33,91,127,144	0
34	LMG	Z	101	37/55	0.87	0.10	57,103,134,149	0
26	SQD	B	621	54/54	0.87	0.09	44,82,109,118	0
26	SQD	a	413	54/54	0.87	0.07	37,73,134,146	0
27	GOL	d	401	6/6	0.87	0.24	36,51,76,77	0
36	HTG	V	203	11/19	0.87	0.08	88,101,107,108	0
26	SQD	A	411	54/54	0.87	0.07	41,71,114,129	0
33	CA	B	601	1/1	0.88	0.07	144,144,144,144	0
35	LMT	B	632	25/35	0.88	0.10	41,68,135,136	0
30	UNL	D	410	17/-	0.89	0.09	46,64,94,102	0
27	GOL	B	628	6/6	0.89	0.12	47,58,65,72	0
29	PL9	a	415	55/55	0.89	0.10	56,82,108,115	0
26	SQD	D	413	43/54	0.90	0.10	58,106,117,124	0
35	LMT	b	628	25/35	0.90	0.08	37,63,135,142	0
36	HTG	B	629	19/19	0.90	0.07	47,59,78,83	0
26	SQD	L	102	54/54	0.90	0.07	39,73,114,123	0
34	LMG	z	101	39/55	0.90	0.10	69,117,144,151	0
29	PL9	A	413	55/55	0.91	0.10	44,83,100,110	0
27	GOL	b	624	6/6	0.91	0.10	75,92,97,104	0
34	LMG	C	501	51/55	0.91	0.09	40,81,110,113	0
30	UNL	x	101	18/-	0.91	0.09	47,66,104,105	0
25	BCR	D	406	40/40	0.91	0.07	35,46,78,84	0
35	LMT	B	634	26/35	0.92	0.08	48,90,109,115	0
34	LMG	C	520	51/55	0.92	0.08	43,75,125,134	0
23	CLA	b	601	65/65	0.92	0.07	46,70,107,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	X	101	18/-	0.92	0.10	39,66,83,87	0
34	LMG	a	417	51/55	0.92	0.07	42,79,99,115	0
36	HTG	B	624	19/19	0.92	0.07	33,71,128,130	0
34	LMG	c	519	51/55	0.92	0.08	47,78,122,143	0
27	GOL	C	525	6/6	0.93	0.12	45,56,66,73	0
23	CLA	C	507	65/65	0.93	0.07	42,57,106,115	0
23	CLA	B	602	65/65	0.93	0.08	39,61,93,123	0
36	HTG	b	625	19/19	0.93	0.06	40,60,90,94	0
23	CLA	c	513	65/65	0.93	0.07	58,74,112,119	0
27	GOL	A	410	6/6	0.93	0.08	45,57,60,90	0
25	BCR	C	515	40/40	0.93	0.07	49,60,74,82	0
34	LMG	J	101	51/55	0.93	0.07	33,54,96,105	0
23	CLA	C	505	65/65	0.94	0.07	32,46,91,111	0
25	BCR	C	527	40/40	0.94	0.07	43,55,71,72	0
23	CLA	C	514	65/65	0.94	0.07	50,65,100,107	0
25	BCR	Y	101	40/40	0.94	0.06	40,51,62,71	0
25	BCR	y	101	40/40	0.94	0.06	48,60,74,77	0
25	BCR	B	620	40/40	0.94	0.06	30,43,67,78	0
27	GOL	B	627	6/6	0.94	0.09	60,77,93,95	0
34	LMG	j	101	51/55	0.94	0.06	41,56,92,119	0
34	LMG	B	622	51/55	0.94	0.06	35,53,83,101	0
30	UNL	d	409	17/-	0.94	0.06	48,58,94,99	0
37	DGD	c	517	62/66	0.94	0.06	42,55,110,126	0
23	CLA	C	513	65/65	0.95	0.06	46,60,106,112	0
31	LHG	d	406	49/49	0.95	0.07	27,48,81,84	0
26	SQD	A	409	54/54	0.95	0.07	41,66,99,109	0
23	CLA	b	616	65/65	0.95	0.06	34,51,101,111	0
23	CLA	c	504	65/65	0.95	0.06	41,52,94,117	0
23	CLA	c	506	65/65	0.95	0.06	47,65,98,117	0
23	CLA	c	507	65/65	0.95	0.07	43,57,70,72	0
29	PL9	D	407	55/55	0.95	0.05	20,30,44,53	0
26	SQD	a	411	54/54	0.95	0.07	44,69,108,113	0
23	CLA	c	512	65/65	0.95	0.07	53,66,96,104	0
25	BCR	b	619	40/40	0.95	0.05	33,46,69,80	0
25	BCR	d	404	40/40	0.95	0.06	43,55,79,81	0
25	BCR	k	101	40/40	0.95	0.07	50,60,84,87	0
25	BCR	t	101	40/40	0.95	0.05	23,43,64,68	0
34	LMG	m	101	51/55	0.95	0.05	33,52,85,99	0
37	DGD	C	518	62/66	0.95	0.06	35,51,111,119	0
37	DGD	c	516	62/66	0.95	0.06	35,47,74,93	0
31	LHG	A	415	49/49	0.95	0.06	29,46,67,82	0
37	DGD	c	518	62/66	0.95	0.05	39,50,74,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	508	65/65	0.96	0.06	40,51,66,78	0
23	CLA	C	509	65/65	0.96	0.05	33,46,93,103	0
23	CLA	d	403	65/65	0.96	0.06	41,52,102,116	0
24	PHO	a	408	64/64	0.96	0.05	30,40,53,60	0
25	BCR	A	408	40/40	0.96	0.05	23,34,48,56	0
25	BCR	B	619	40/40	0.96	0.04	21,36,52,60	0
23	CLA	C	511	65/65	0.96	0.05	36,48,61,67	0
23	CLA	B	607	65/65	0.96	0.06	28,37,76,93	0
31	LHG	D	409	49/49	0.96	0.07	32,50,107,117	0
25	BCR	C	516	40/40	0.96	0.06	38,50,63,68	0
31	LHG	b	630	49/49	0.96	0.05	26,43,59,64	0
23	CLA	B	617	65/65	0.96	0.07	33,45,121,132	0
31	LHG	d	408	49/49	0.96	0.07	40,55,105,111	0
23	CLA	D	405	65/65	0.96	0.07	33,48,111,119	0
25	BCR	H	101	40/40	0.96	0.05	35,46,66,73	0
25	BCR	T	101	40/40	0.96	0.04	21,37,55,60	0
23	CLA	a	409	65/65	0.96	0.07	30,44,124,130	0
25	BCR	b	617	40/40	0.96	0.04	21,35,45,51	0
25	BCR	b	618	40/40	0.96	0.04	22,36,51,56	0
29	PL9	d	405	55/55	0.96	0.05	24,33,49,66	0
23	CLA	C	502	65/65	0.96	0.06	36,45,67,70	0
25	BCR	c	514	40/40	0.96	0.05	58,68,80,83	0
25	BCR	c	515	40/40	0.96	0.05	41,54,66,70	0
23	CLA	b	602	65/65	0.96	0.06	36,48,68,77	0
25	BCR	h	102	40/40	0.96	0.06	42,57,71,74	0
23	CLA	C	503	65/65	0.96	0.06	33,43,60,67	0
23	CLA	c	501	65/65	0.96	0.05	43,53,67,72	0
23	CLA	C	504	65/65	0.96	0.06	37,47,66,75	0
37	DGD	C	519	62/66	0.96	0.05	30,44,80,109	0
37	DGD	H	102	62/66	0.96	0.06	29,42,64,68	0
23	CLA	A	407	65/65	0.96	0.06	28,38,98,117	0
23	CLA	B	603	65/65	0.96	0.05	31,41,57,69	0
23	CLA	c	511	65/65	0.96	0.06	47,56,78,89	0
23	CLA	b	605	65/65	0.97	0.05	26,34,51,76	0
23	CLA	b	606	65/65	0.97	0.05	29,42,91,110	0
23	CLA	b	607	65/65	0.97	0.05	21,30,58,67	0
23	CLA	b	608	65/65	0.97	0.05	34,44,67,72	0
23	CLA	b	609	65/65	0.97	0.05	39,48,63,74	0
25	BCR	a	410	40/40	0.97	0.05	28,38,55,58	0
23	CLA	b	610	65/65	0.97	0.05	35,44,56,61	0
23	CLA	b	611	65/65	0.97	0.05	27,35,57,62	0
23	CLA	b	612	65/65	0.97	0.06	28,35,48,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	613	65/65	0.97	0.05	24,36,79,89	0
23	CLA	b	614	65/65	0.97	0.05	25,35,93,107	0
23	CLA	b	615	65/65	0.97	0.05	33,43,65,87	0
23	CLA	C	506	65/65	0.97	0.05	33,44,75,82	0
23	CLA	B	611	65/65	0.97	0.06	29,41,55,70	0
23	CLA	c	502	65/65	0.97	0.05	40,55,70,74	0
23	CLA	c	503	65/65	0.97	0.05	44,55,67,84	0
23	CLA	B	612	65/65	0.97	0.05	24,32,49,54	0
23	CLA	c	505	65/65	0.97	0.06	36,46,76,82	0
23	CLA	B	613	65/65	0.97	0.05	26,33,45,65	0
23	CLA	B	614	65/65	0.97	0.04	23,31,72,87	0
31	LHG	D	408	49/49	0.97	0.06	25,37,56,78	0
23	CLA	c	508	65/65	0.97	0.05	39,53,121,131	0
23	CLA	c	509	65/65	0.97	0.06	46,56,73,79	0
31	LHG	L	101	49/49	0.97	0.04	26,39,54,75	0
23	CLA	c	510	65/65	0.97	0.05	39,51,67,71	0
23	CLA	C	512	65/65	0.97	0.06	39,54,77,85	0
31	LHG	d	407	49/49	0.97	0.06	24,38,58,65	0
23	CLA	B	615	65/65	0.97	0.05	23,32,86,95	0
23	CLA	B	604	65/65	0.97	0.05	30,43,56,67	0
32	BCT	a	419	4/4	0.97	0.05	41,45,48,58	0
23	CLA	B	605	65/65	0.97	0.05	22,31,101,111	0
33	CA	O	301	1/1	0.97	0.06	101,101,101,101	0
33	CA	V	201	1/1	0.97	0.04	94,94,94,94	0
24	PHO	D	402	64/64	0.97	0.04	25,31,44,55	0
23	CLA	a	406	65/65	0.97	0.05	30,38,98,103	0
37	DGD	C	517	62/66	0.97	0.05	30,41,77,88	0
23	CLA	A	405	65/65	0.97	0.05	24,33,85,94	0
25	BCR	B	618	40/40	0.97	0.04	24,37,48,49	0
23	CLA	B	608	65/65	0.97	0.05	20,28,59,67	0
23	CLA	B	610	65/65	0.97	0.05	31,42,53,89	0
23	CLA	b	603	65/65	0.97	0.05	32,44,61,70	0
23	CLA	b	604	65/65	0.97	0.05	24,33,95,101	0
37	DGD	h	103	62/66	0.97	0.05	34,46,67,76	0
23	CLA	D	404	65/65	0.98	0.05	21,29,50,56	0
22	CL	a	403	1/1	0.98	0.04	41,41,41,41	0
23	CLA	a	404	65/65	0.98	0.05	27,33,52,66	0
32	BCT	A	416	4/4	0.98	0.05	32,45,46,51	0
23	CLA	a	405	65/65	0.98	0.04	23,29,52,60	0
23	CLA	C	510	65/65	0.98	0.06	39,53,71,79	0
23	CLA	d	402	65/65	0.98	0.05	27,32,58,72	0
23	CLA	B	616	65/65	0.98	0.04	29,38,60,67	0

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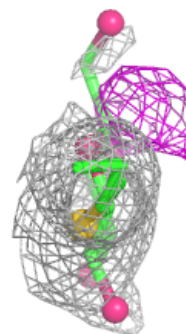
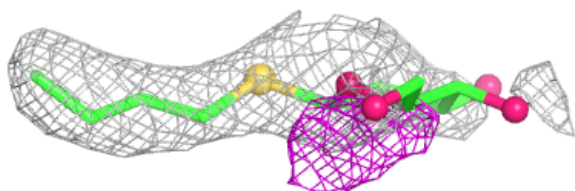
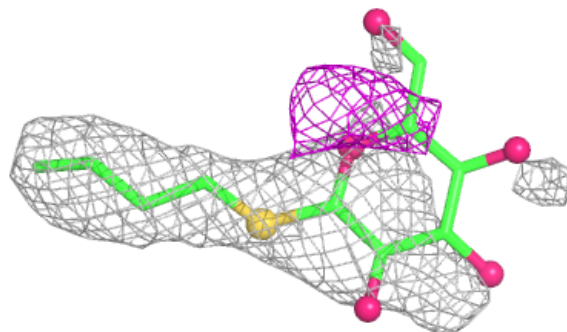
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	CA	c	523	1/1	0.98	0.10	68,68,68,68	0
24	PHO	A	406	64/64	0.98	0.04	22,29,39,46	0
23	CLA	A	404	65/65	0.98	0.04	22,25,39,58	0
24	PHO	a	407	64/64	0.98	0.04	24,31,45,50	0
23	CLA	B	609	65/65	0.98	0.04	30,42,56,66	0
23	CLA	B	606	65/65	0.98	0.05	24,33,46,51	0
23	CLA	D	401	65/65	0.98	0.04	21,28,43,47	0
38	HEM	E	103	43/43	0.98	0.06	43,56,69,83	0
38	HEM	e	103	43/43	0.98	0.06	52,78,106,116	0
39	MG	J	103	1/1	0.98	0.10	43,43,43,43	0
40	HEC	v	201	43/43	0.98	0.05	44,53,63,82	0
33	CA	o	301	1/1	0.99	0.02	89,89,89,89	0
21	FE2	a	401	1/1	0.99	0.03	47,47,47,47	0
22	CL	A	402	1/1	0.99	0.07	24,24,24,24	0
33	CA	C	526	1/1	0.99	0.10	59,59,59,59	0
22	CL	A	403	1/1	0.99	0.03	27,27,27,27	0
22	CL	a	402	1/1	0.99	0.06	28,28,28,28	0
21	FE2	A	401	1/1	0.99	0.03	46,46,46,46	0
39	MG	j	103	1/1	0.99	0.06	48,48,48,48	0
40	HEC	V	202	43/43	0.99	0.05	33,36,48,70	0
33	CA	c	524	1/1	0.99	0.03	66,66,66,66	0
28	OEX	A	412	10/10	1.00	0.03	23,32,46,47	0
28	OEX	a	414	10/10	1.00	0.02	29,36,46,48	0

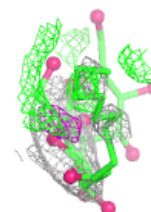
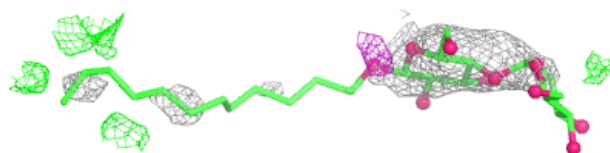
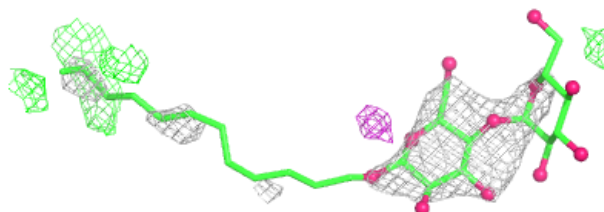
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG 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)

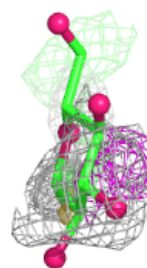
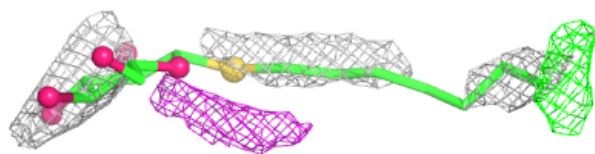
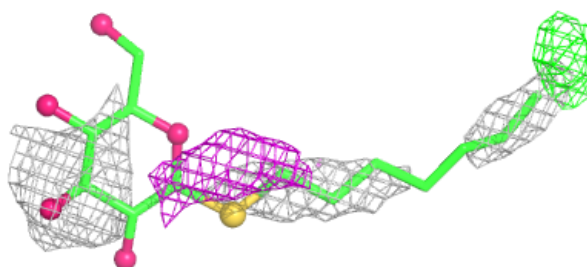
**Electron density around LMT E 102:**

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

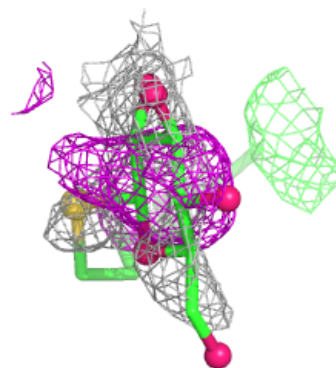
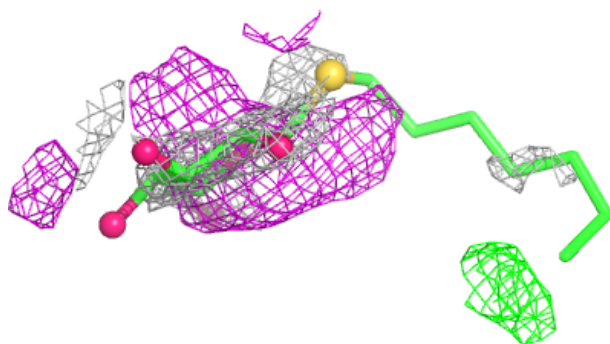
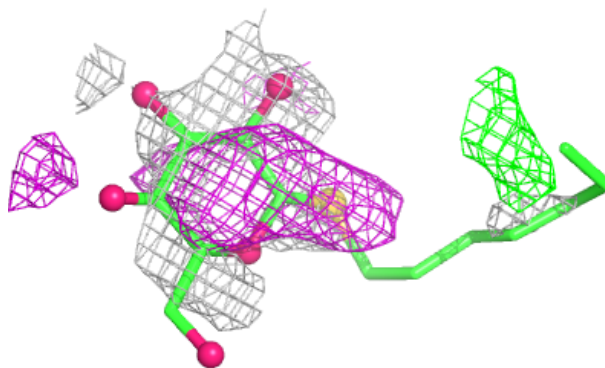


Electron density around HTG B 626:

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

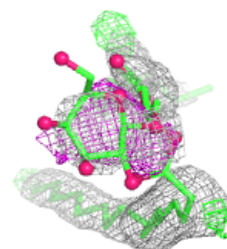
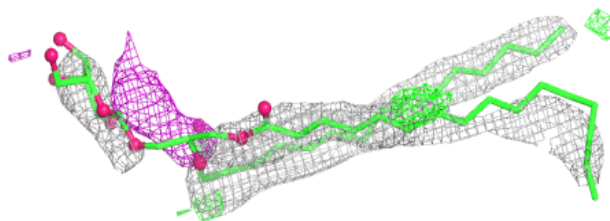
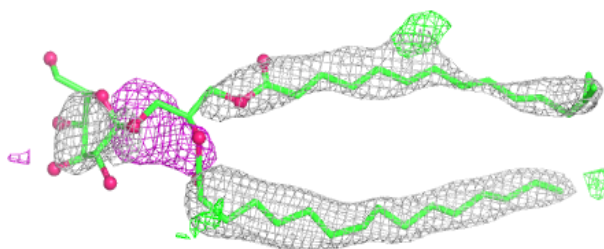
**Electron density around HTG b 622:**

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

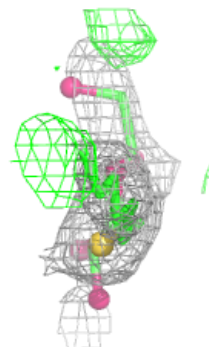
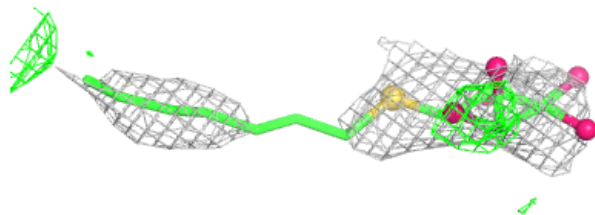
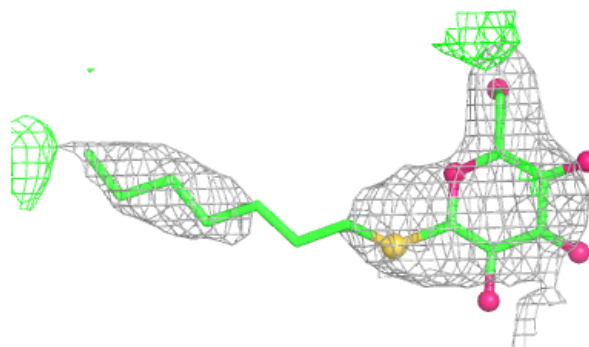


Electron density around LMG C 521:

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

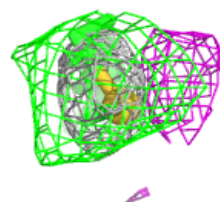
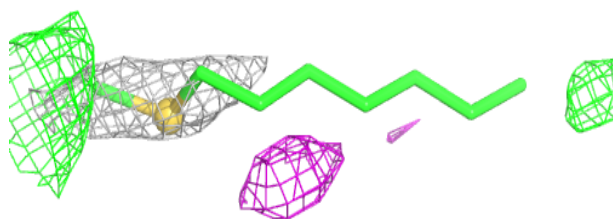
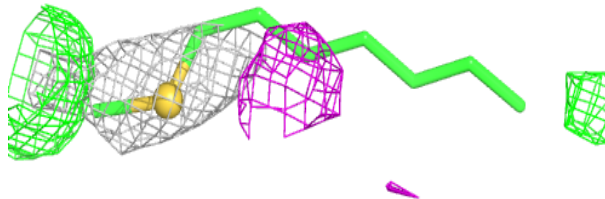
**Electron density around HTG B 630:**

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

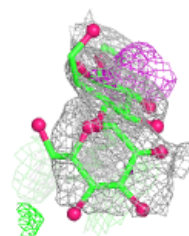
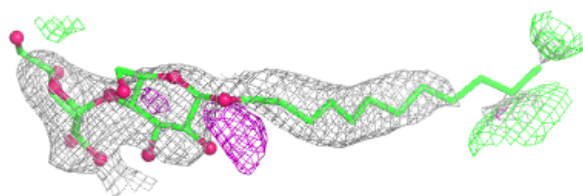
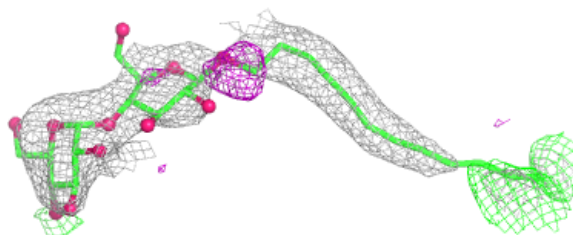


Electron density around HTG C 524:

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

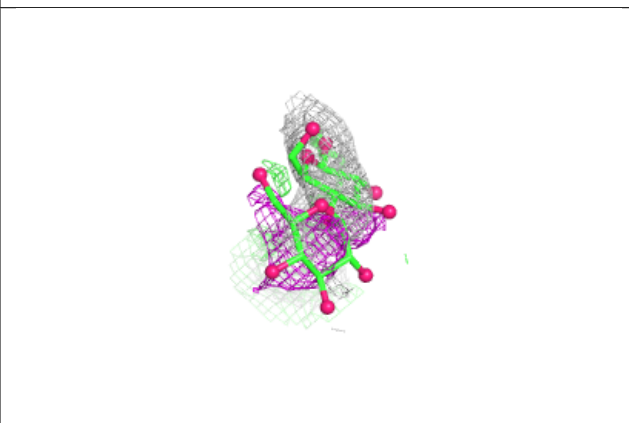
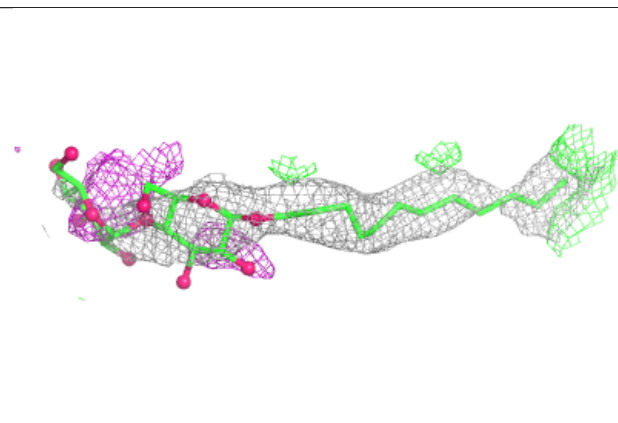
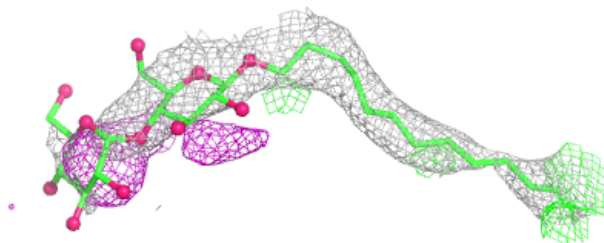
**Electron density around LMT D 403:**

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

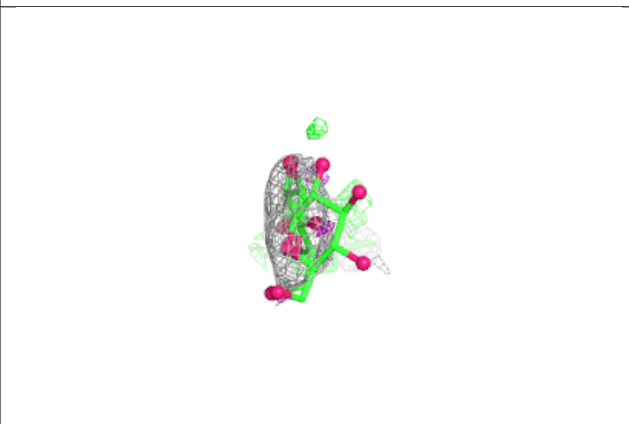
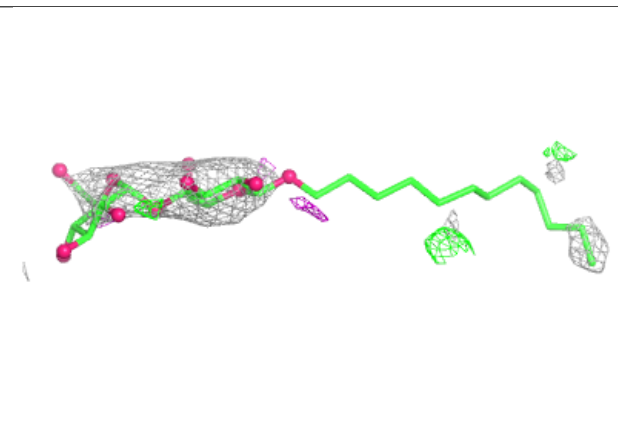
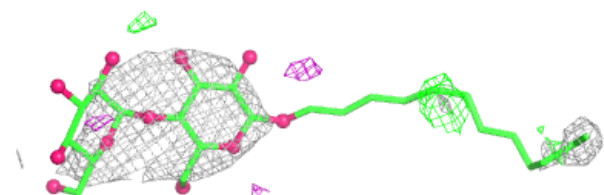


Electron density around LMT B 633:

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

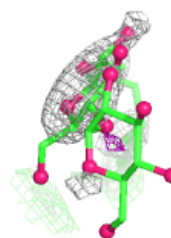
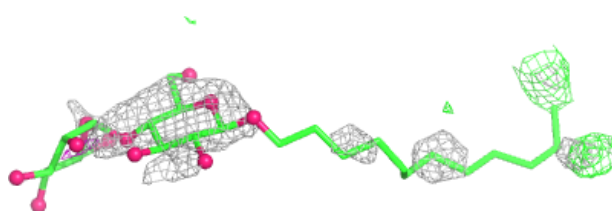
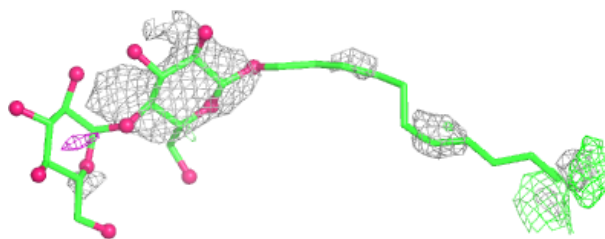
**Electron density around LMT a 418:**

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

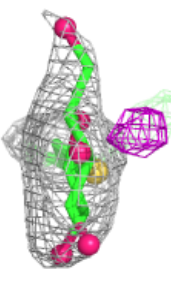
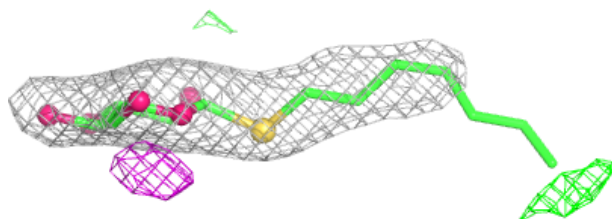
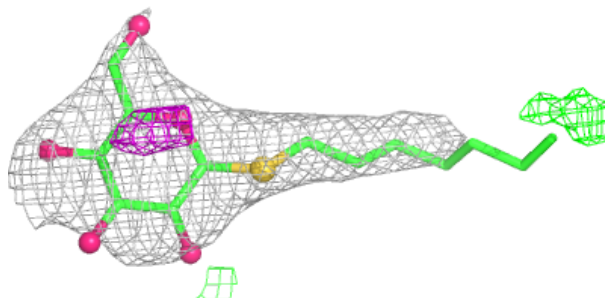


Electron density around LMT e 102:

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

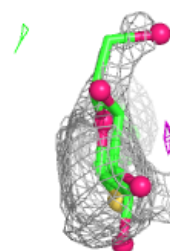
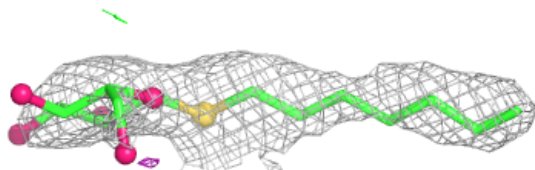
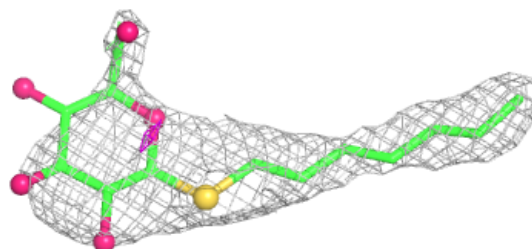
**Electron density around HTG C 523:**

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

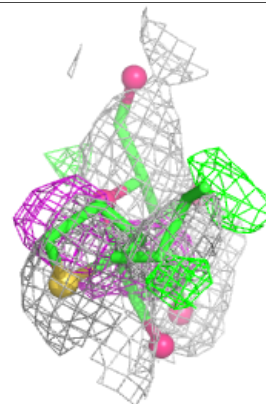
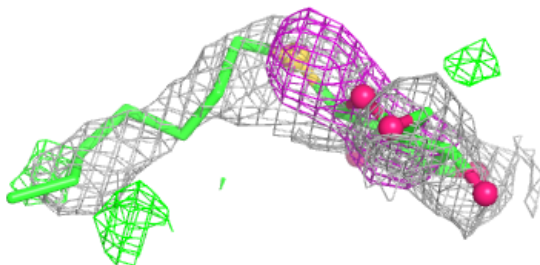
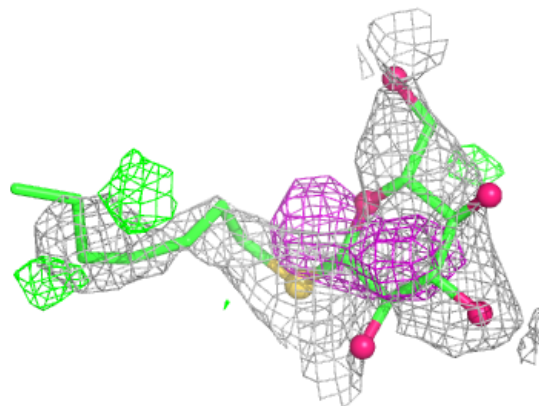


Electron density around HTG b 626:

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

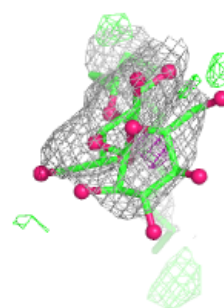
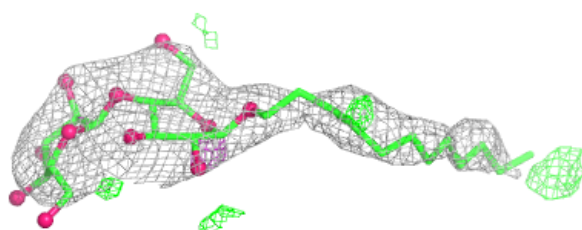
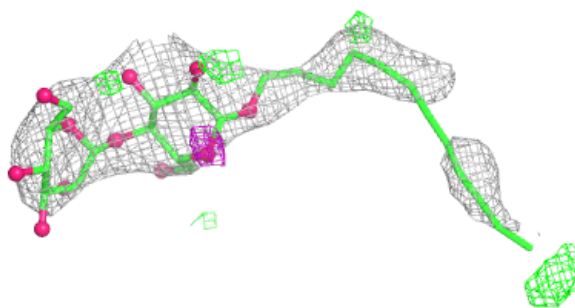
**Electron density around HTG B 625:**

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

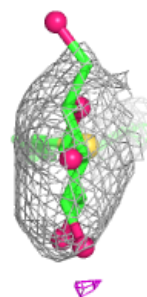
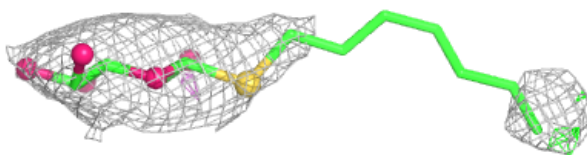
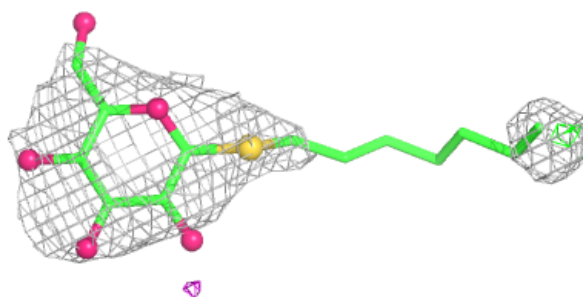


Electron density around LMT C 522:

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

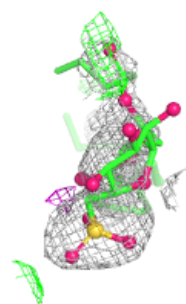
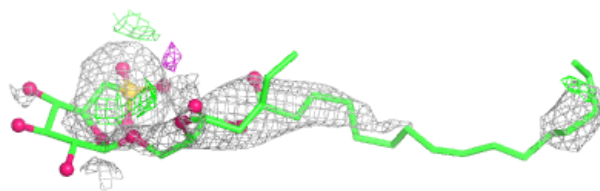
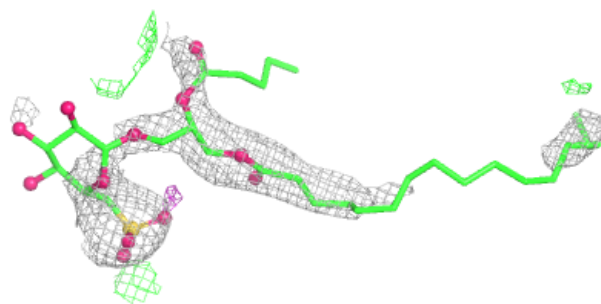
**Electron density around HTG c 521:**

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

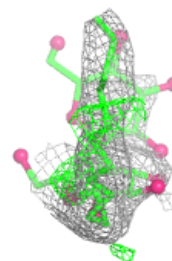
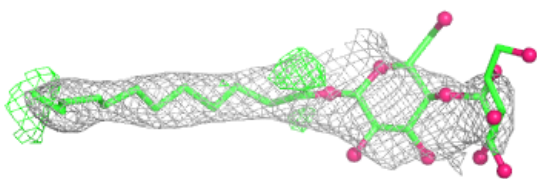
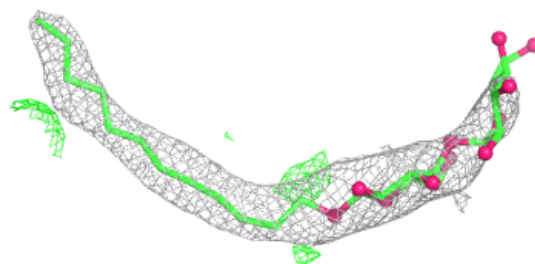


Electron density around SQD f 101:

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

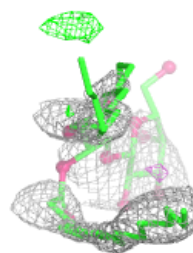
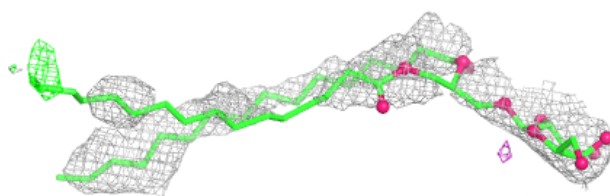
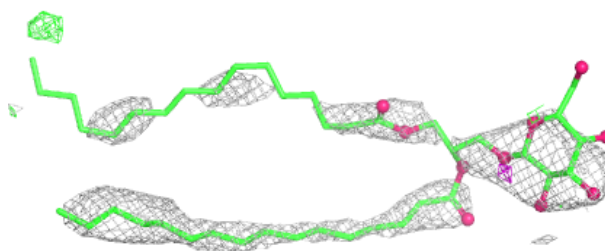
**Electron density around LMT M 103:**

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

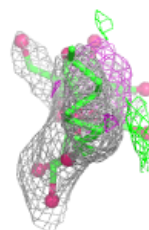
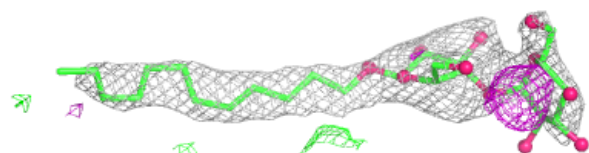
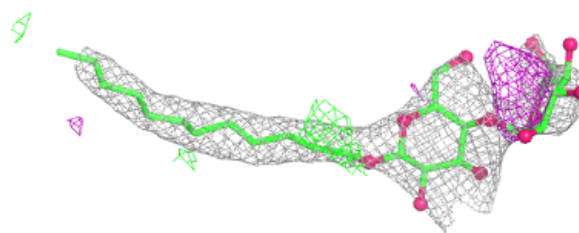


Electron density around LMG c 520:

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

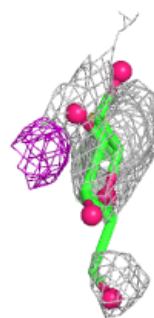
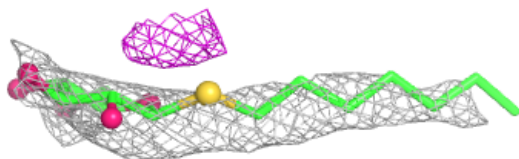
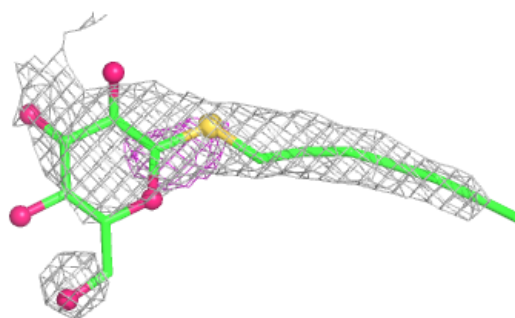
**Electron density around LMT B 623:**

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

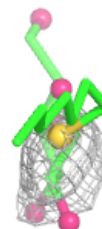
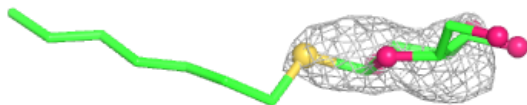
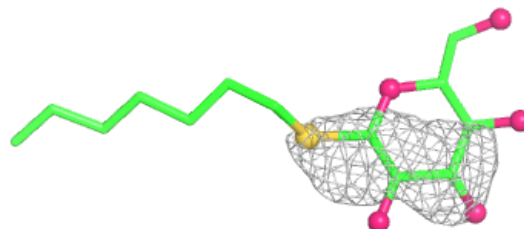


Electron density around HTG b 623:

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

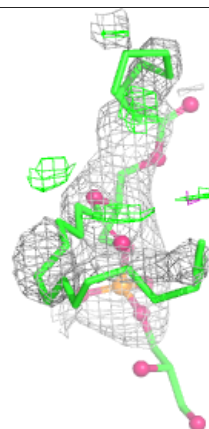
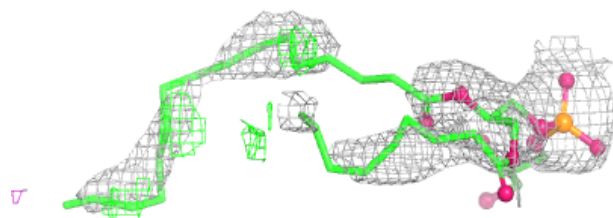
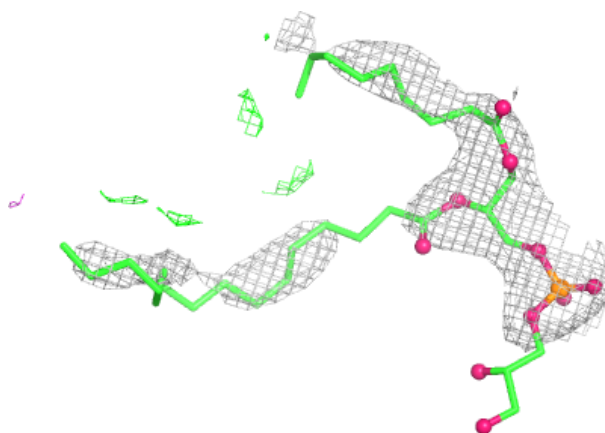
**Electron density around HTG c 522:**

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

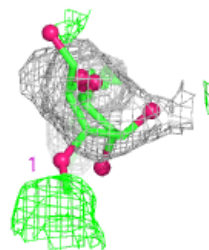
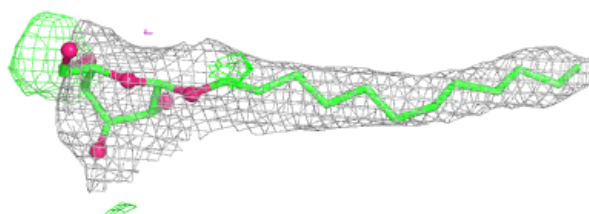
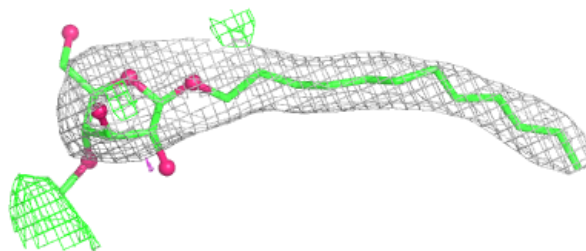


Electron density around LHG e 101:

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

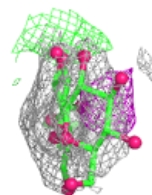
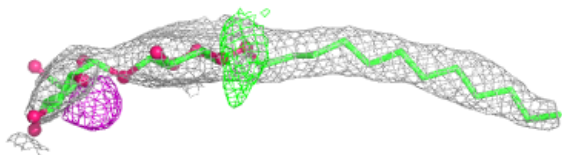
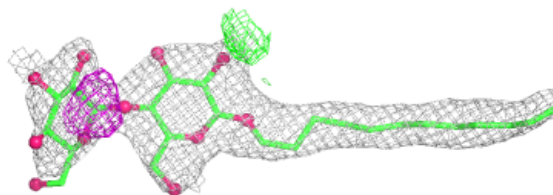
**Electron density around LMT b 620:**

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

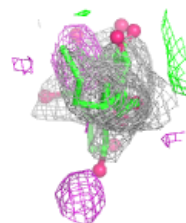
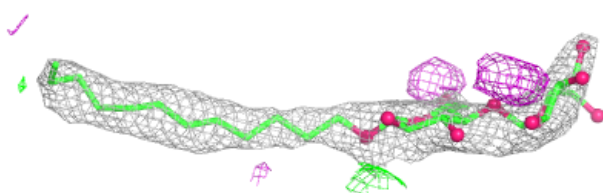
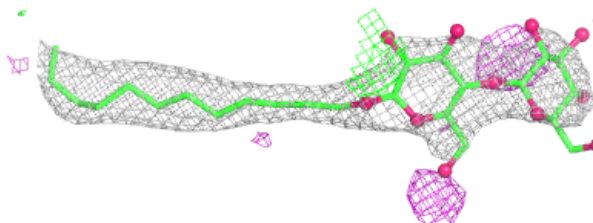


Electron density around LMT M 101:

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

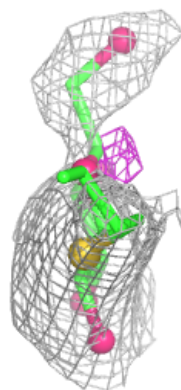
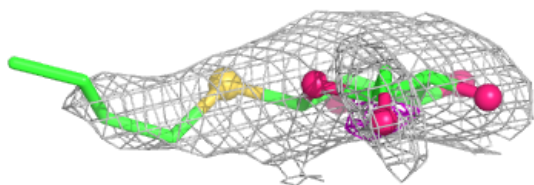
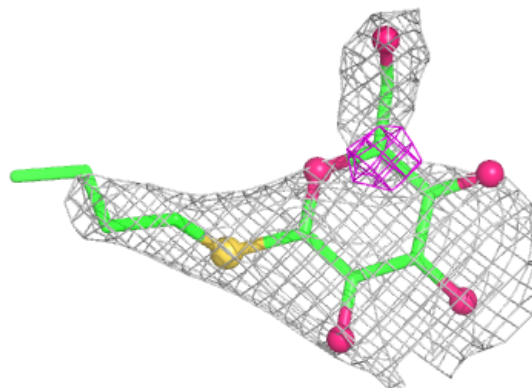
**Electron density around LMT m 103:**

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

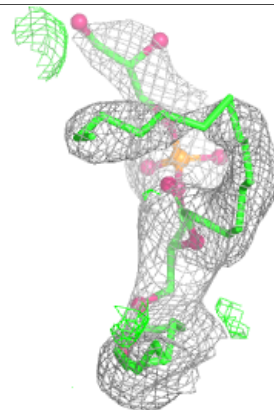
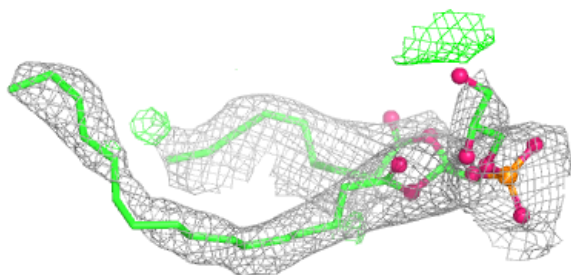
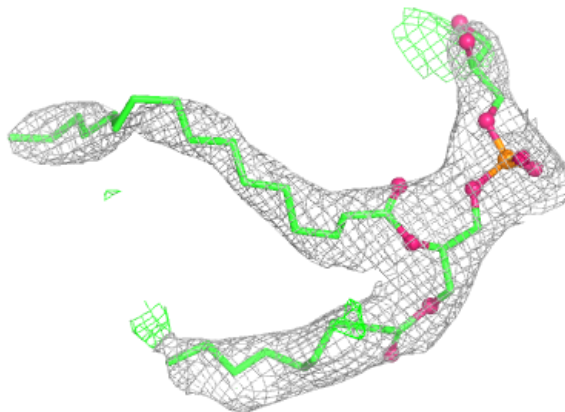


Electron density around HTG h 101:

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

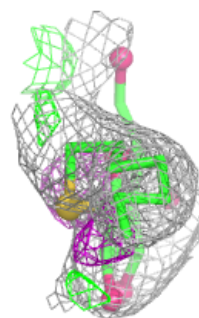
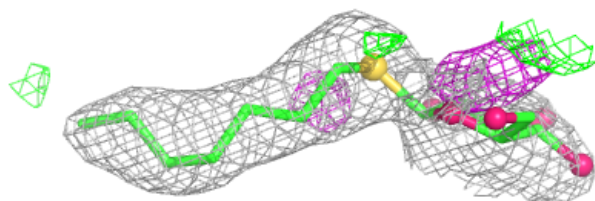
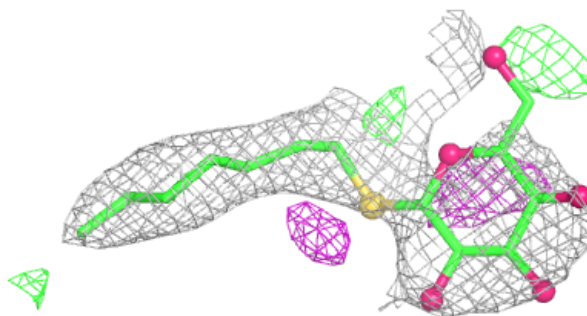
**Electron density around LHG E 101:**

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

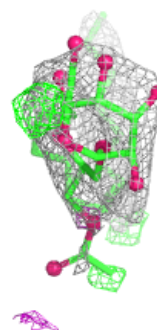
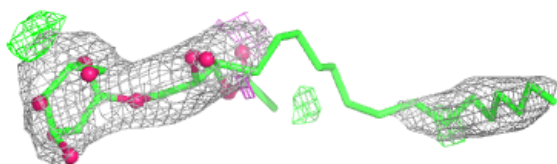
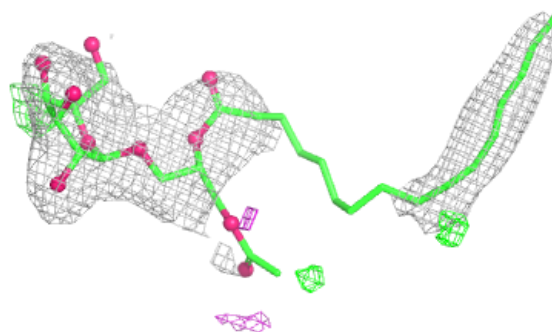


Electron density around HTG b 621:

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

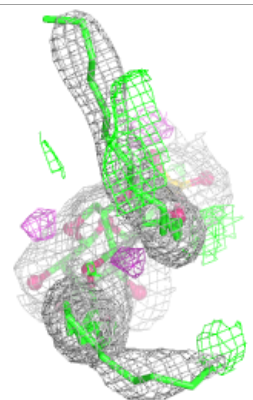
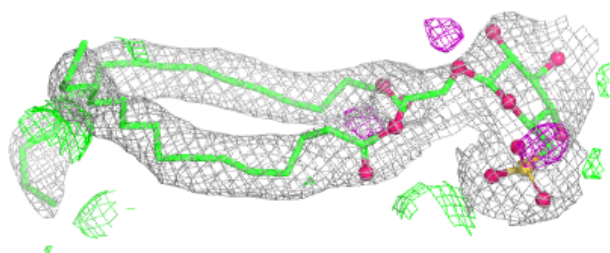
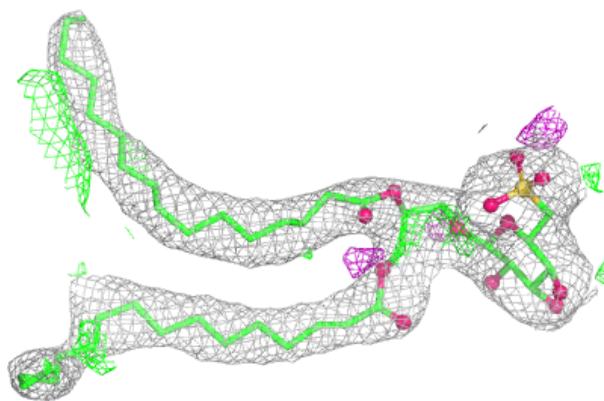
**Electron density around LMG Z 101:**

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

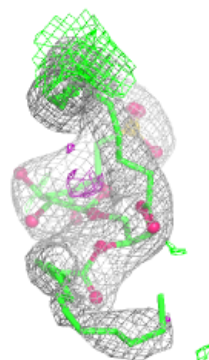
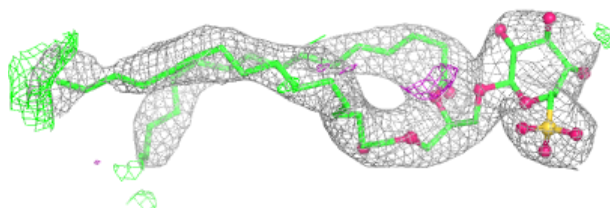
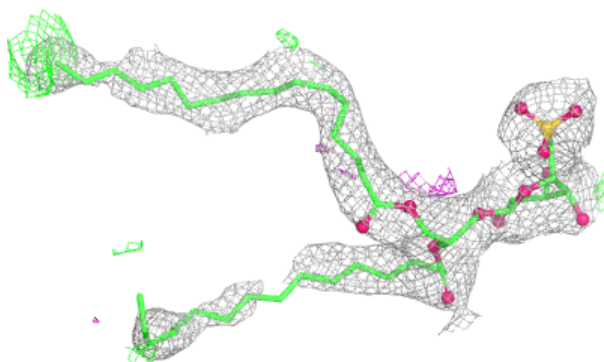


Electron density around SQD B 621:

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

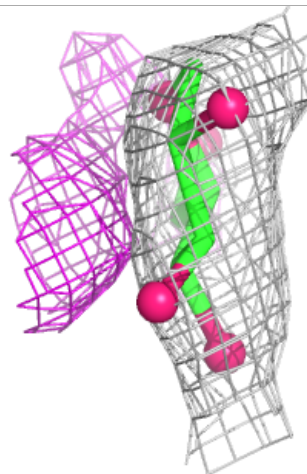
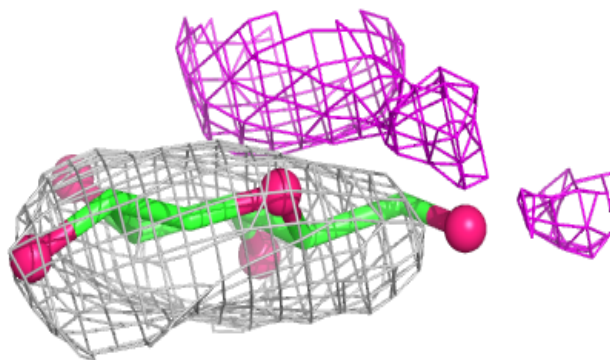
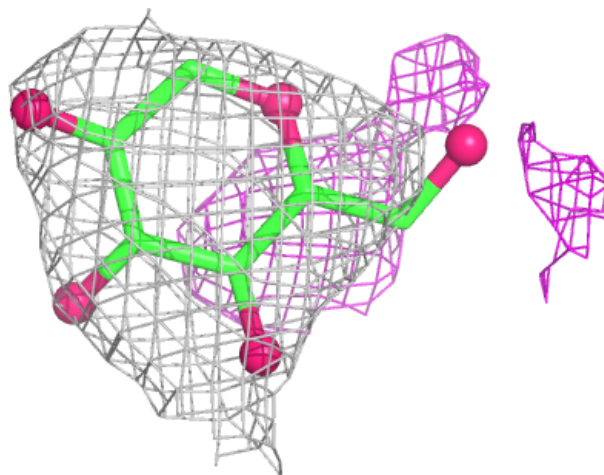
**Electron density around SQD a 413:**

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



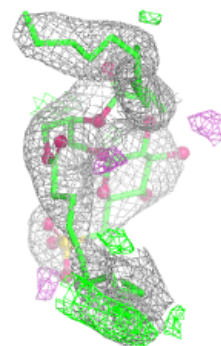
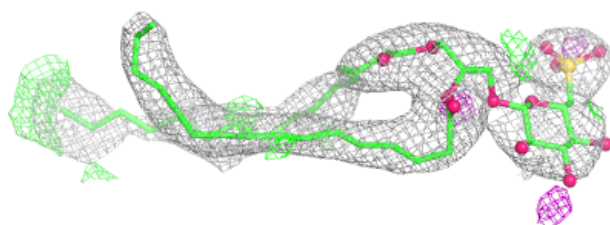
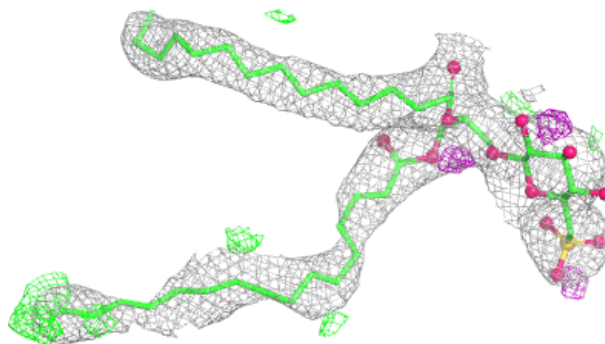
Electron density around HTG V 203:

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

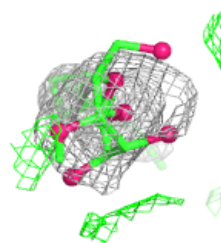
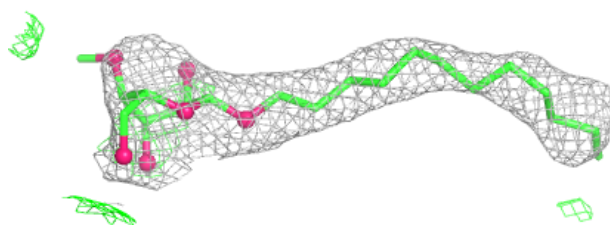
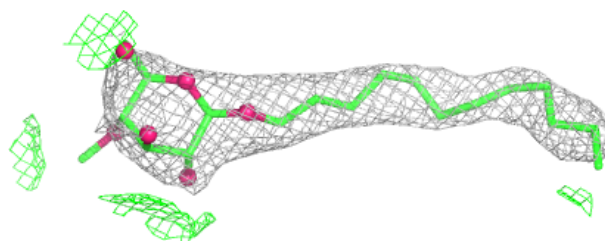


Electron density around SQD A 411:

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

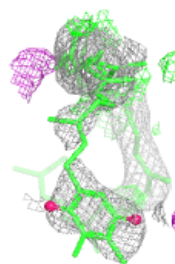
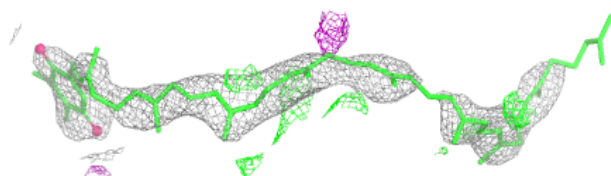
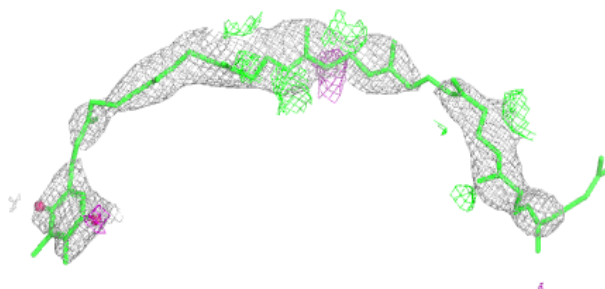
**Electron density around LMT B 632:**

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

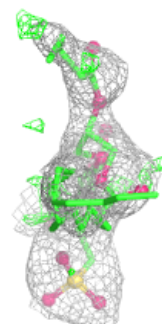
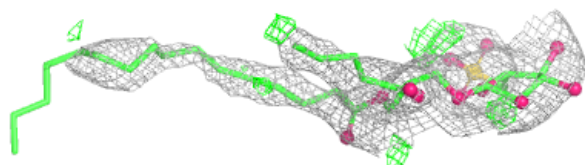
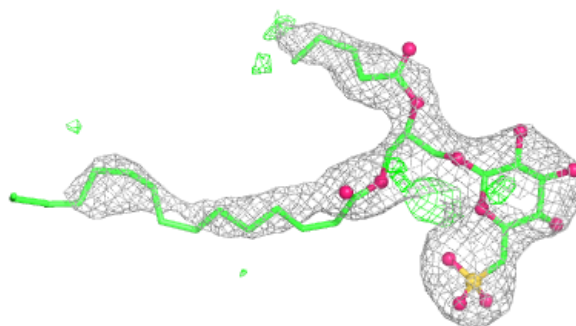


Electron density around PL9 a 415:

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

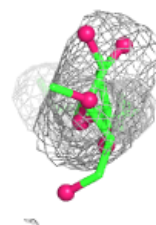
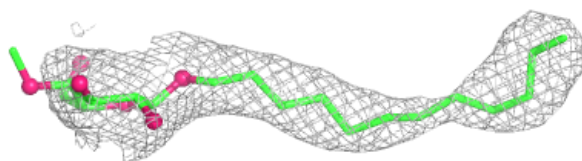
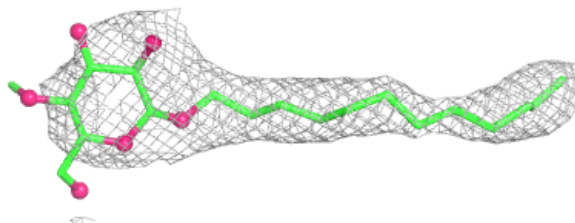
**Electron density around SQD D 413:**

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

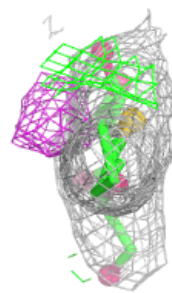
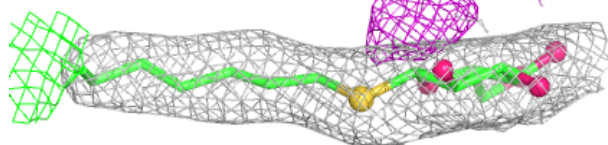
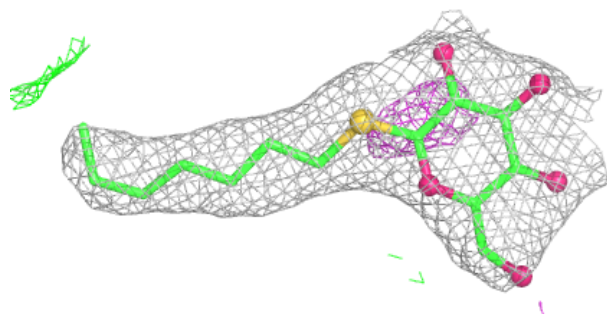


Electron density around LMT b 628:

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

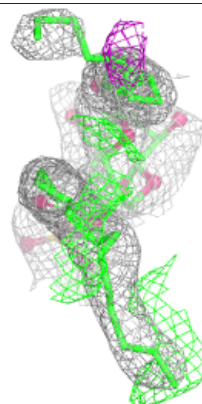
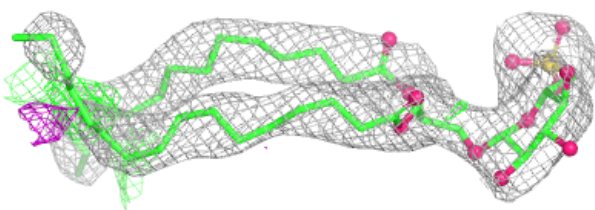
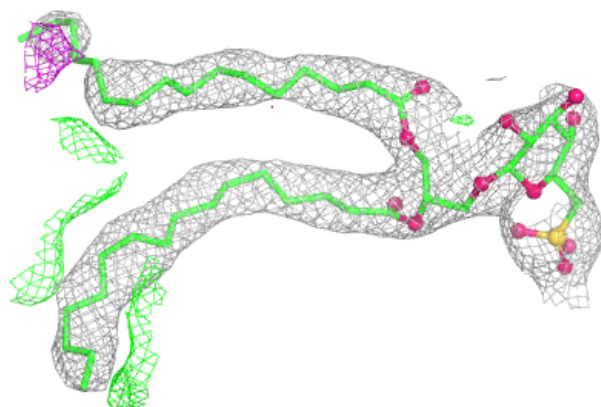
**Electron density around HTG B 629:**

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

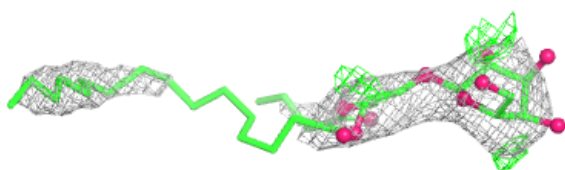
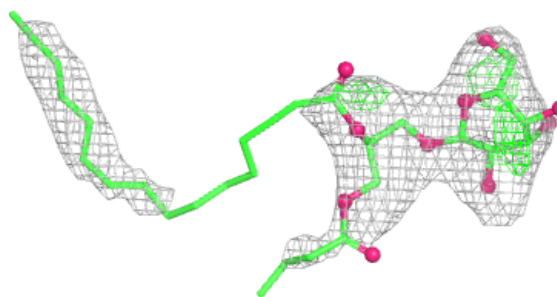


Electron density around SQD L 102:

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

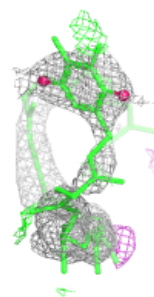
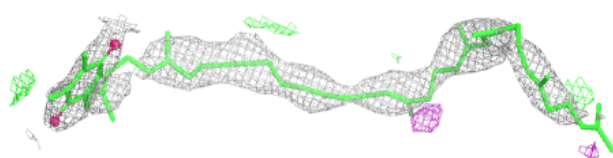
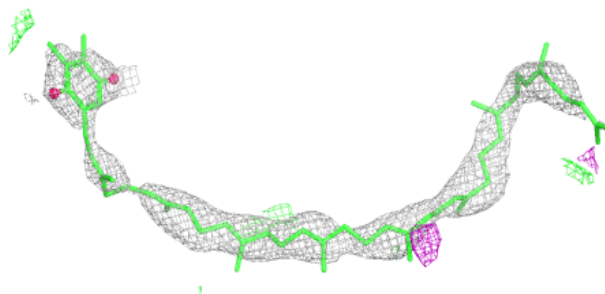
**Electron density around LMG z 101:**

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

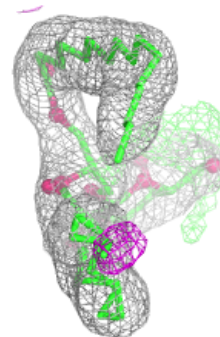
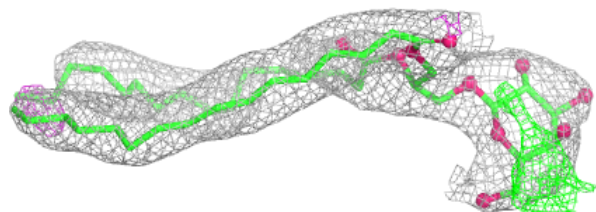
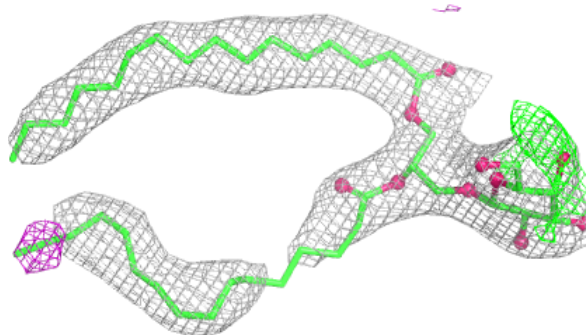


Electron density around PL9 A 413:

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

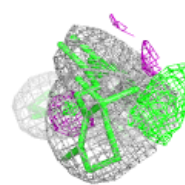
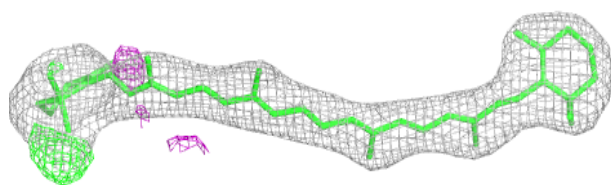
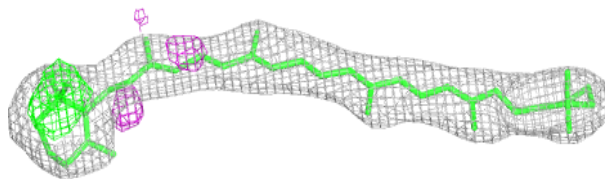
**Electron density around LMG C 501:**

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

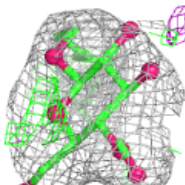
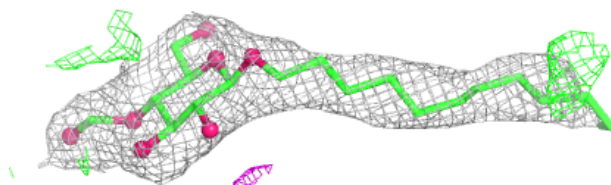
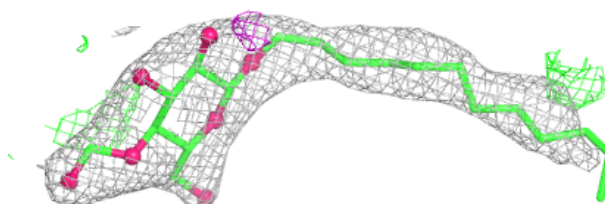


Electron density around BCR D 406:

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

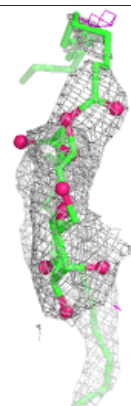
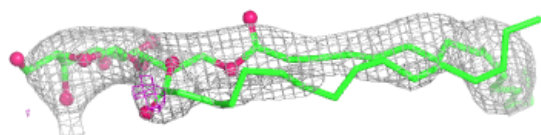
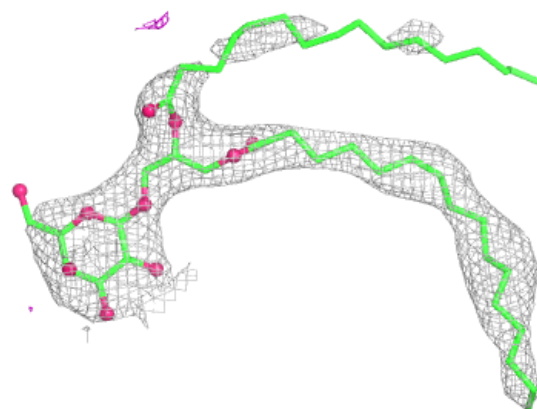
**Electron density around LMT B 634:**

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

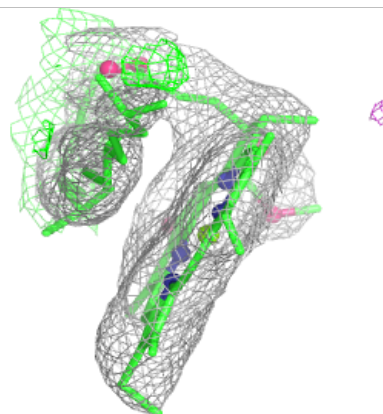
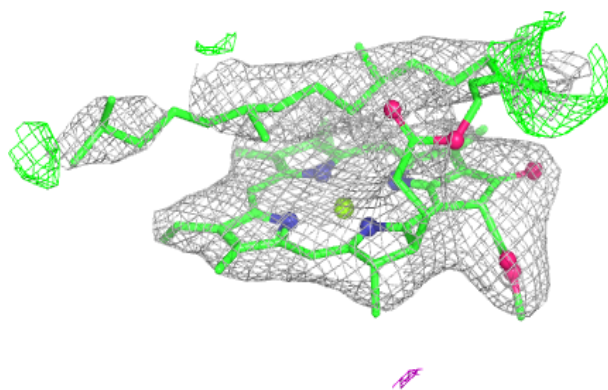
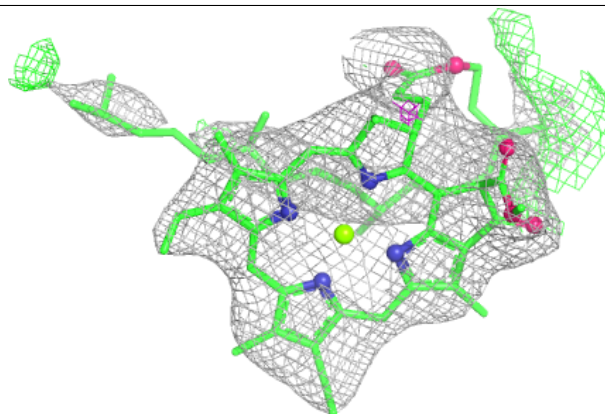


Electron density around LMG C 520:

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

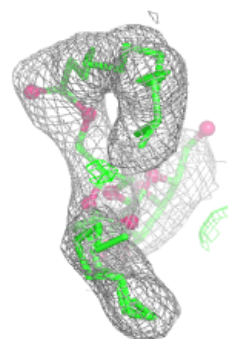
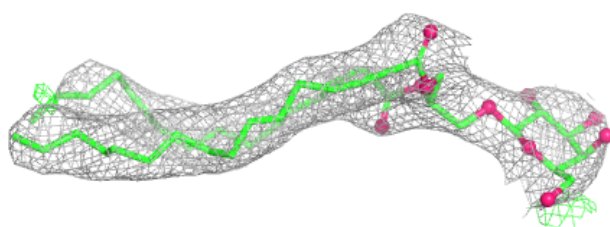
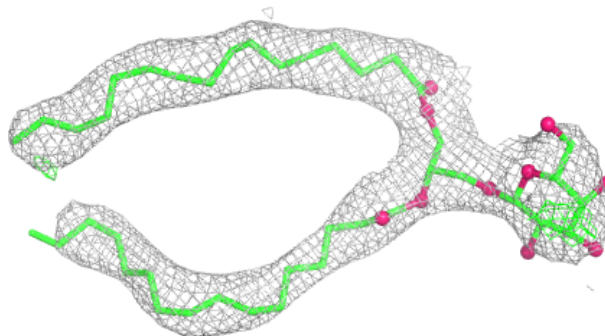
**Electron density around CLA b 601:**

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

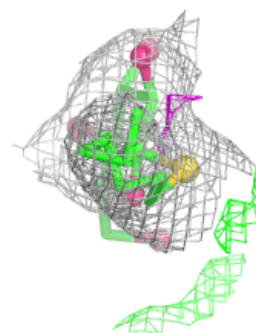
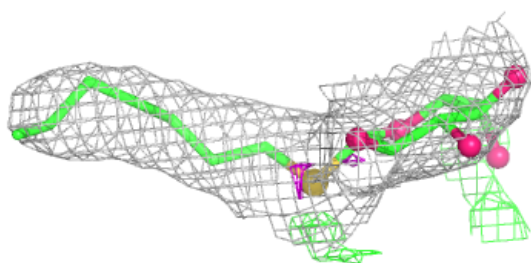
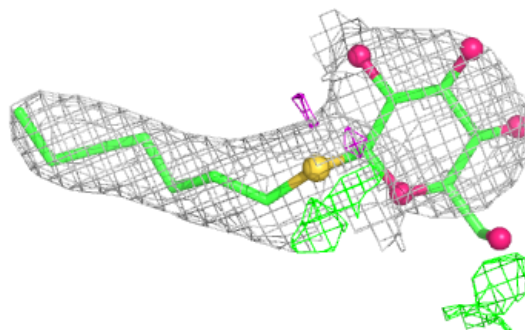


Electron density around LMG a 417:

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

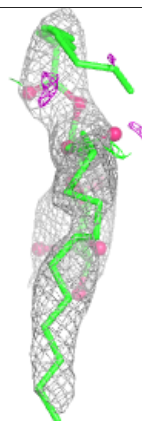
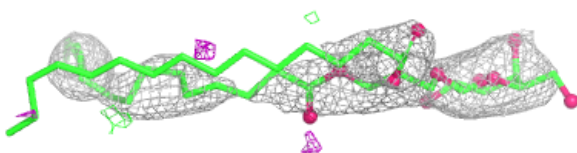
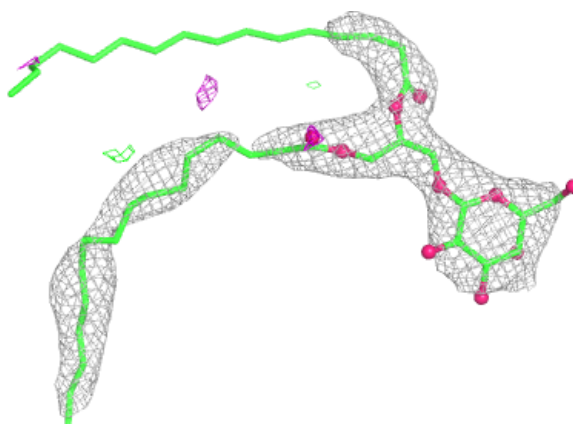
**Electron density around HTG B 624:**

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

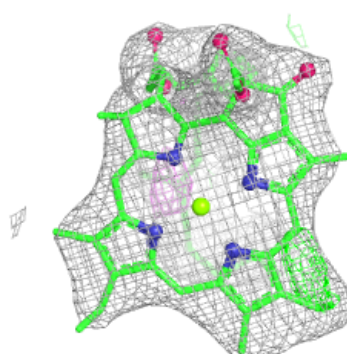
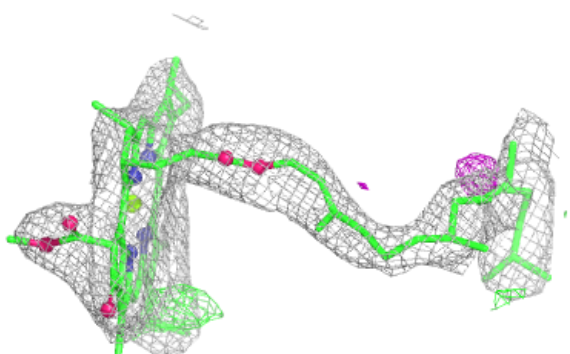
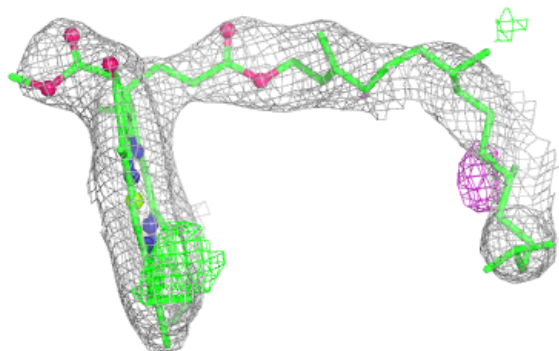


Electron density around LMG c 519:

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

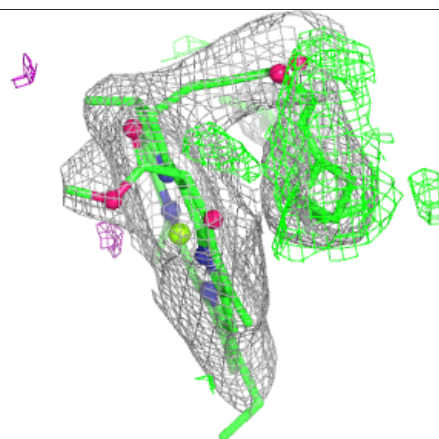
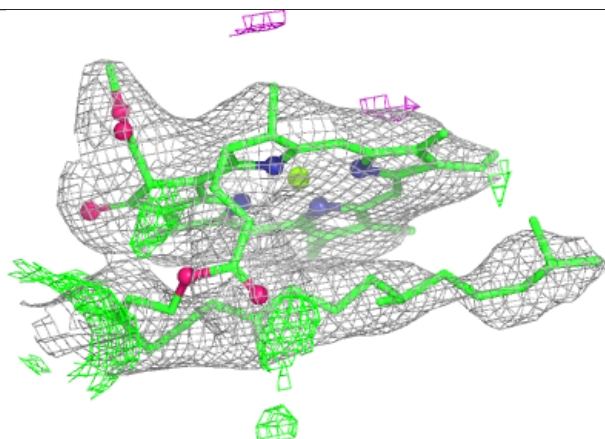
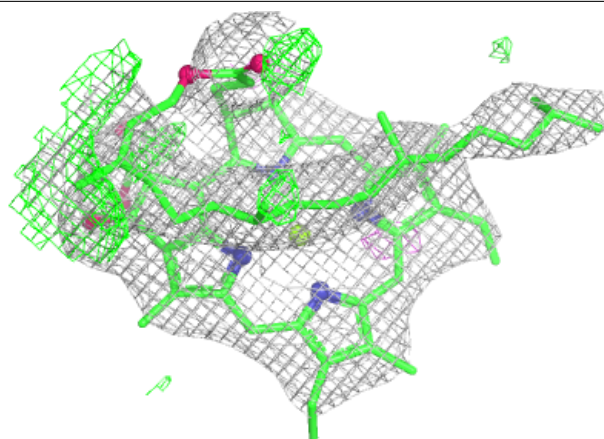
**Electron density around CLA C 507:**

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

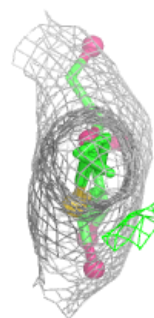
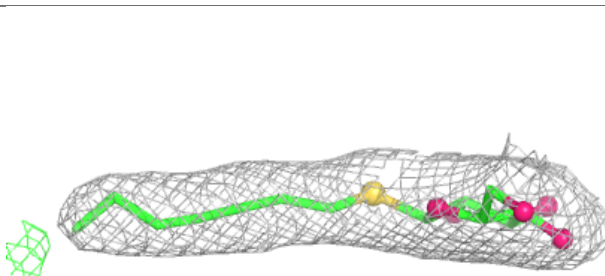
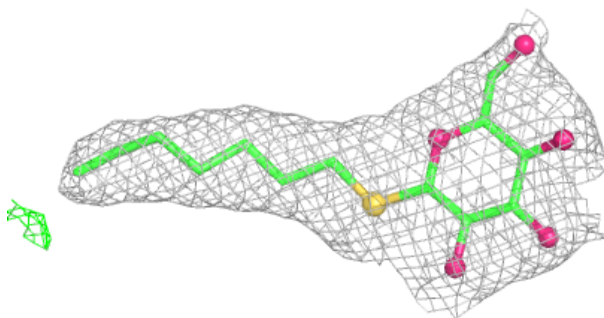


Electron density around CLA B 602:

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

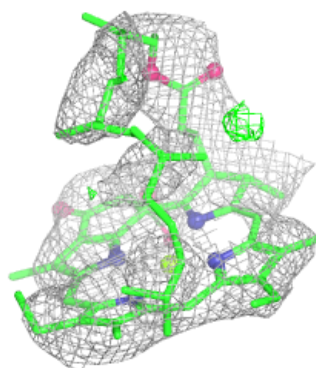
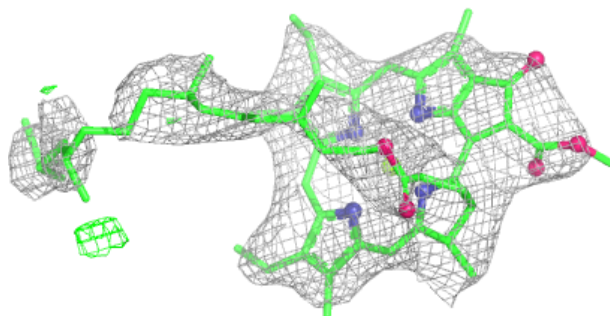
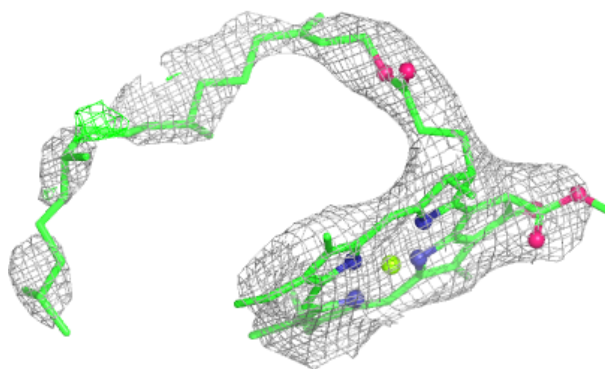
**Electron density around HTG b 625:**

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

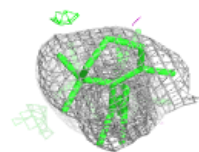
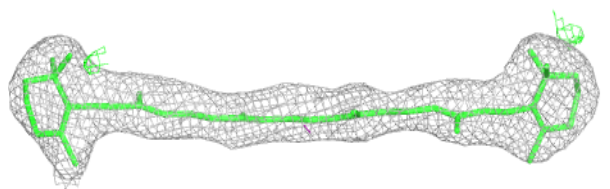
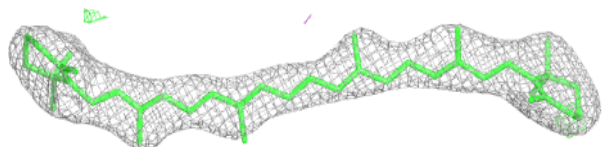


Electron density around CLA c 513:

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

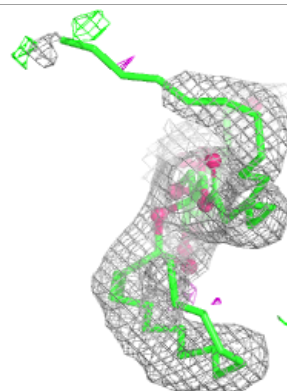
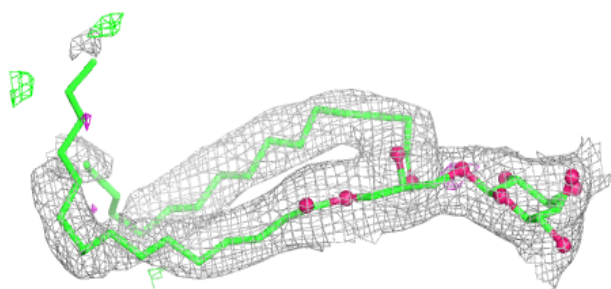
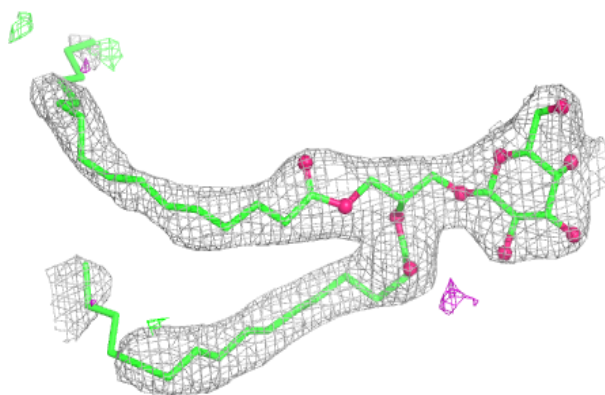
**Electron density around BCR C 515:**

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

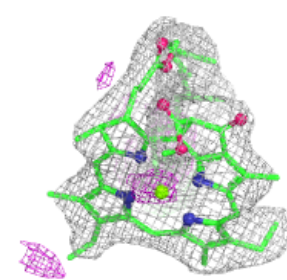
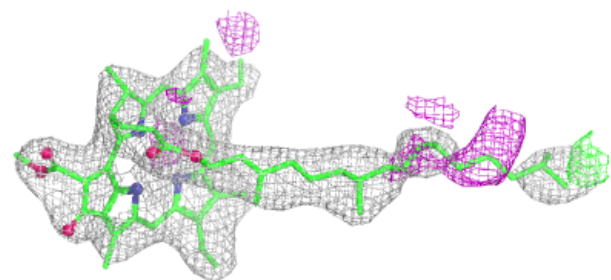
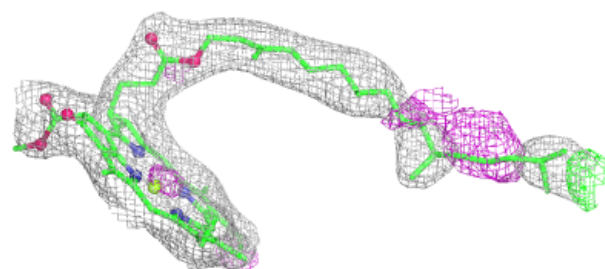


Electron density around LMG J 101:

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

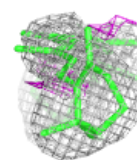
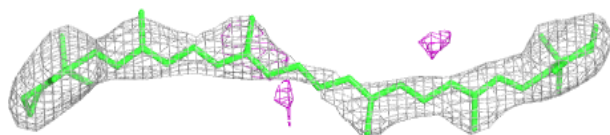
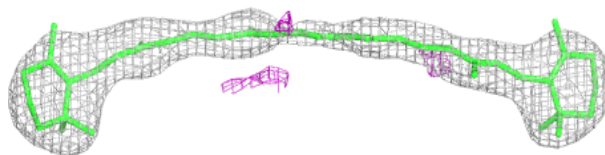
**Electron density around CLA C 505:**

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

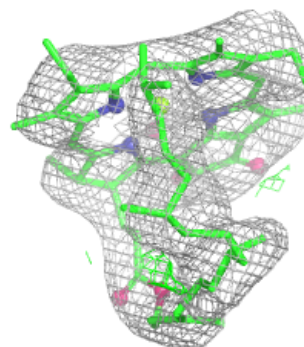
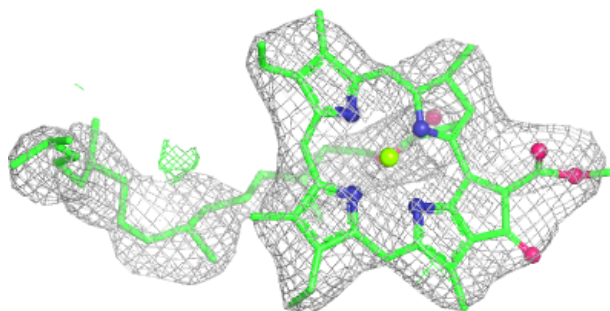
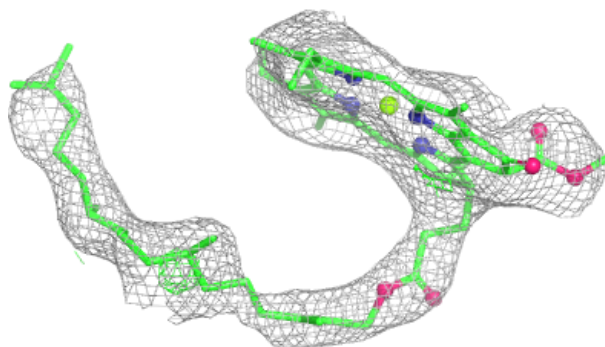


Electron density around BCR C 527:

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

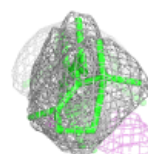
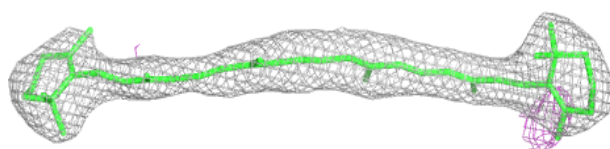
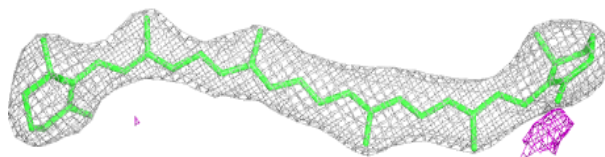
**Electron density around CLA C 514:**

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

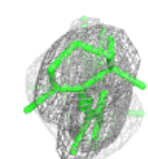
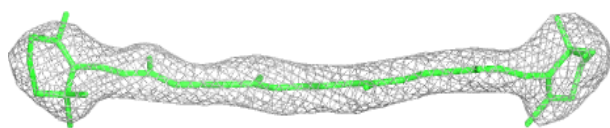
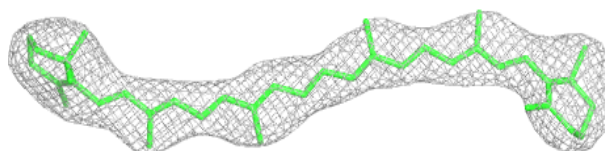


Electron density around BCR Y 101:

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

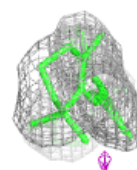
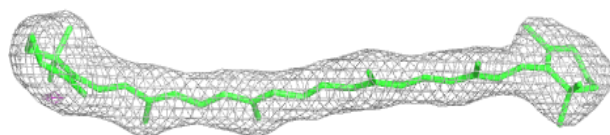
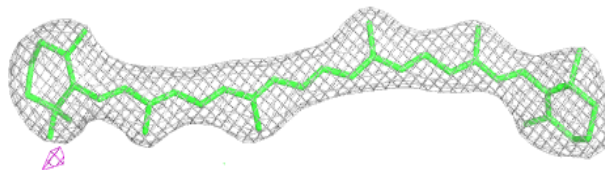
**Electron density around BCR y 101:**

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

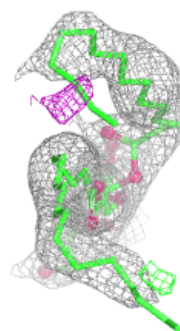
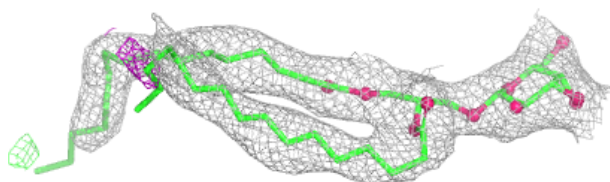
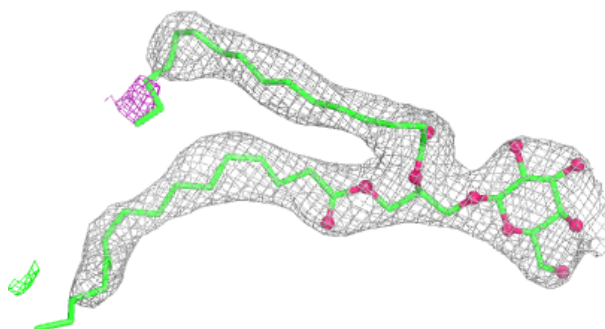


Electron density around BCR B 620:

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

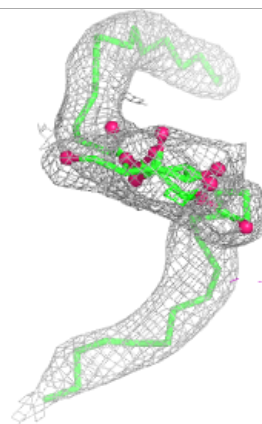
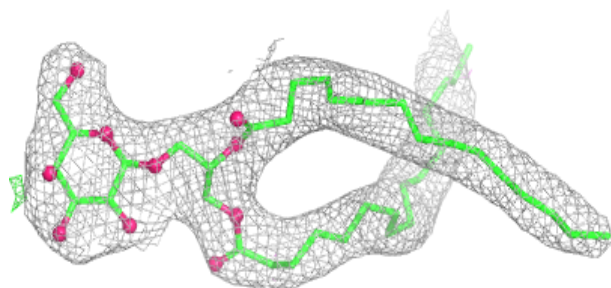
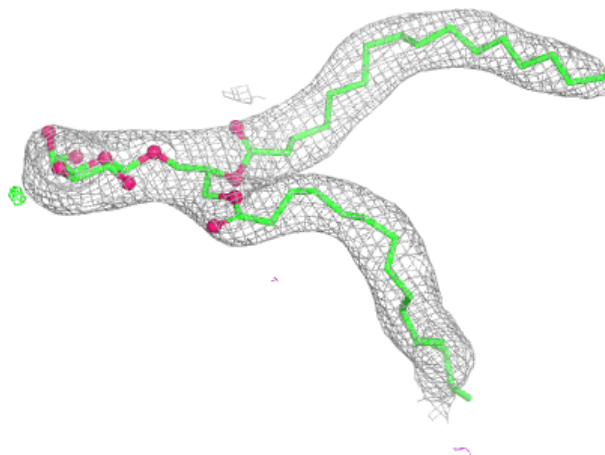
**Electron density around LMG j 101:**

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



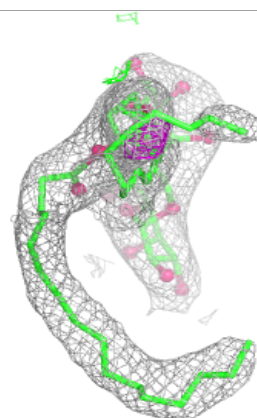
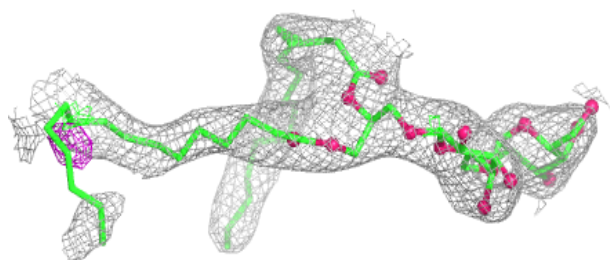
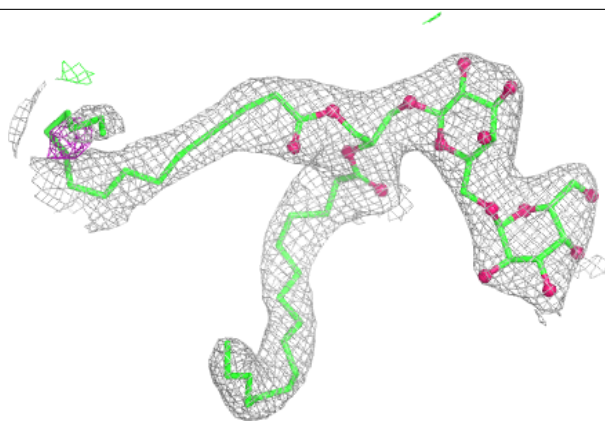
Electron density around LMG B 622:

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



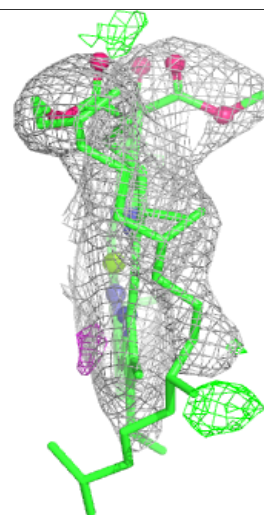
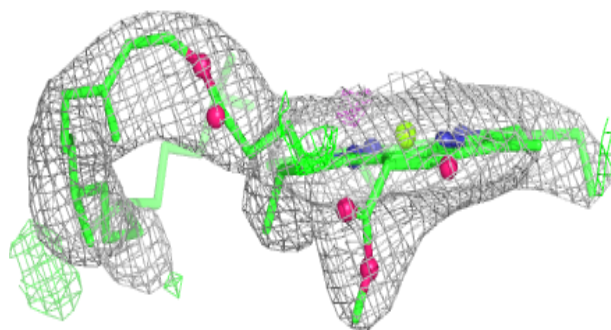
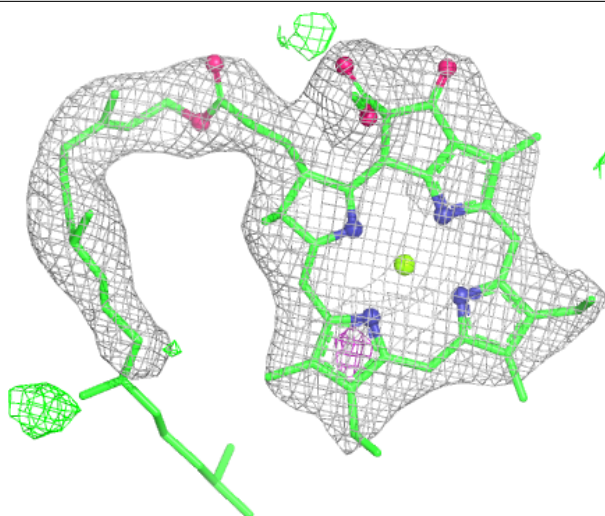
Electron density around DGD c 517:

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



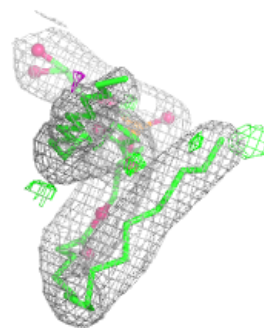
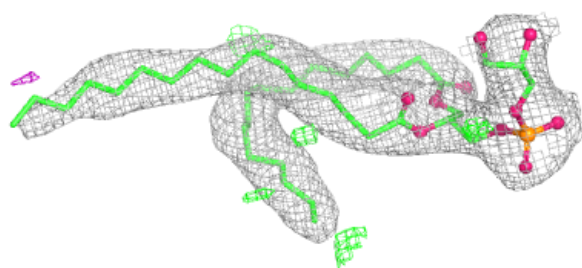
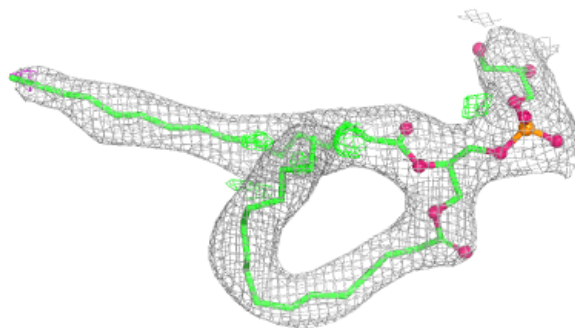
Electron density around CLA C 513:

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



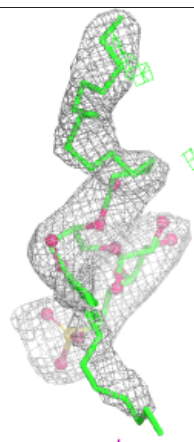
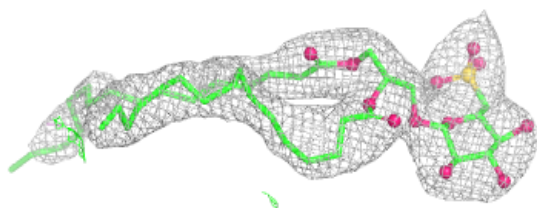
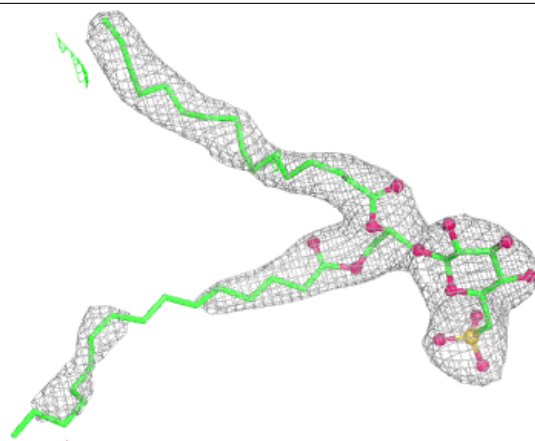
Electron density around LHG d 406:

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



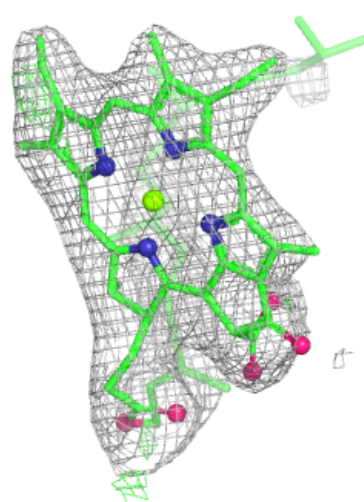
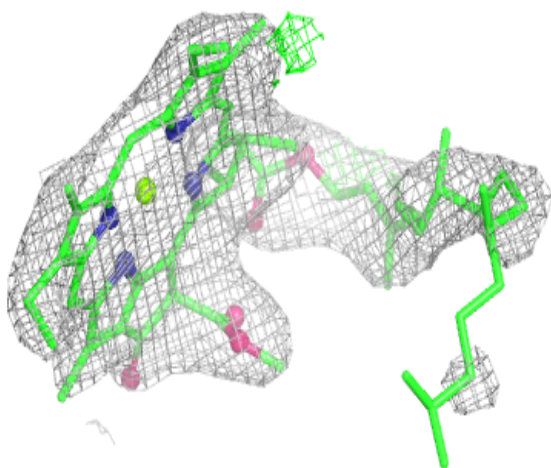
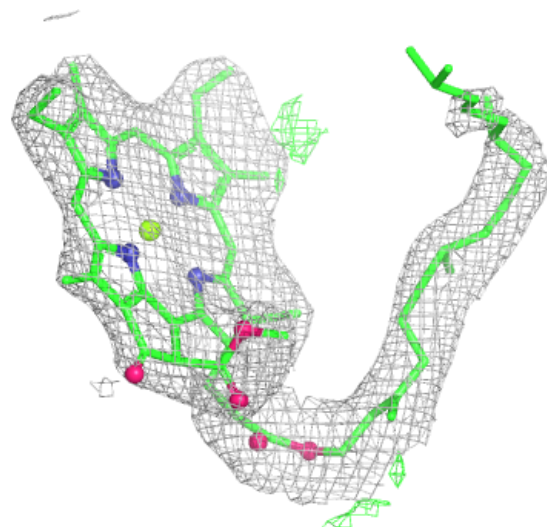
Electron density around SQD A 409:

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



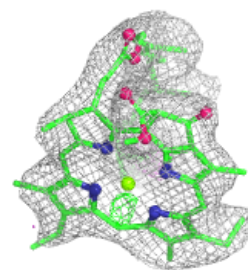
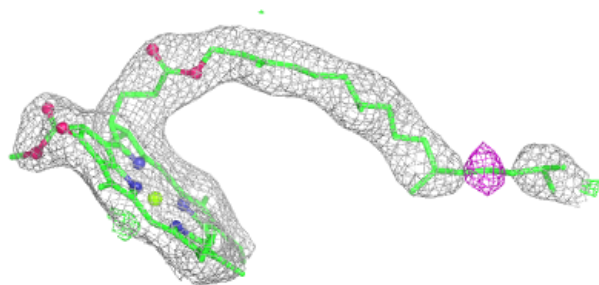
Electron density around CLA b 616:

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

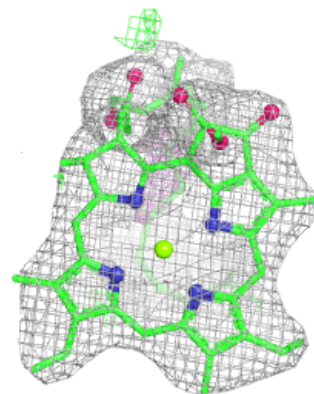
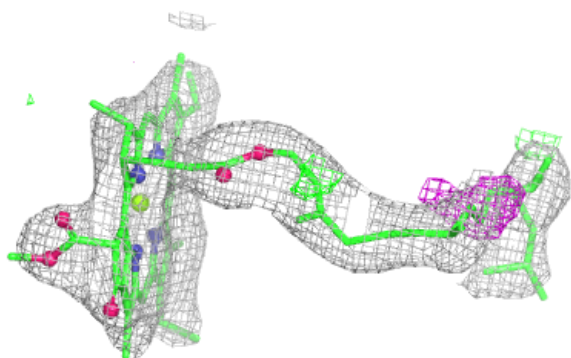
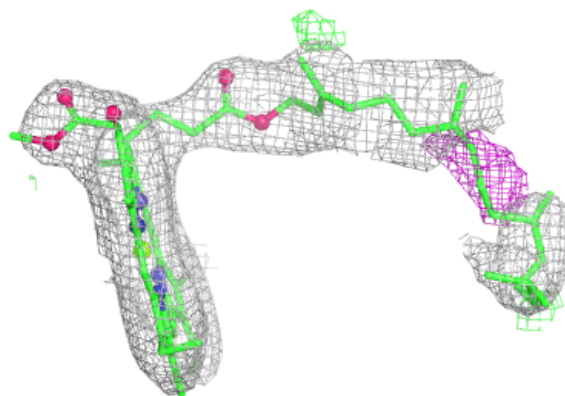


Electron density around CLA c 504:

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

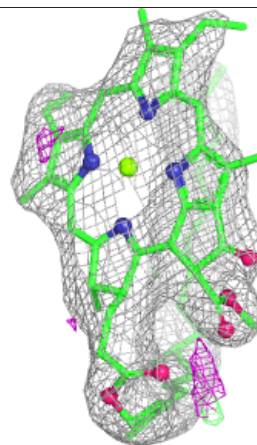
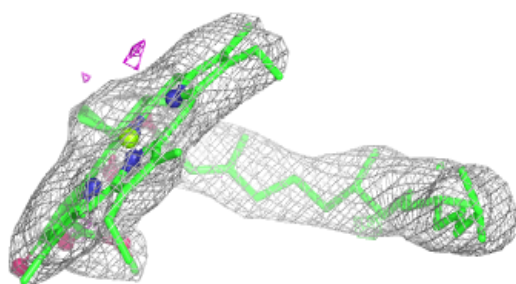
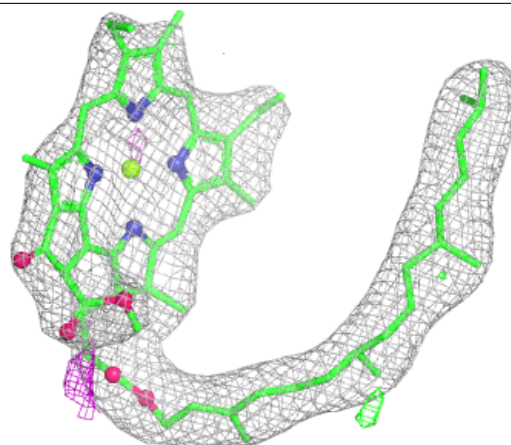
**Electron density around CLA c 506:**

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

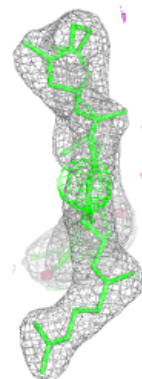
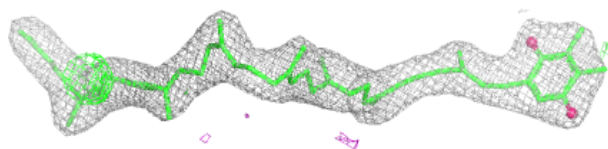
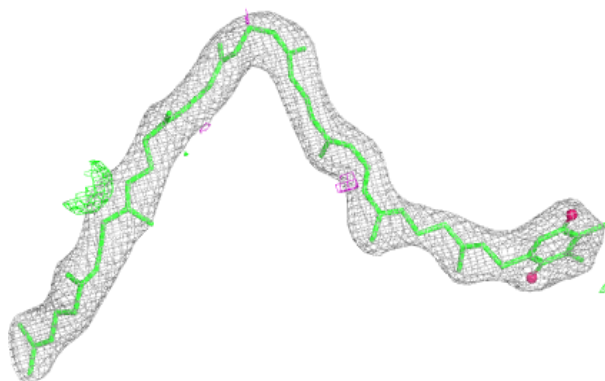


Electron density around CLA c 507:

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

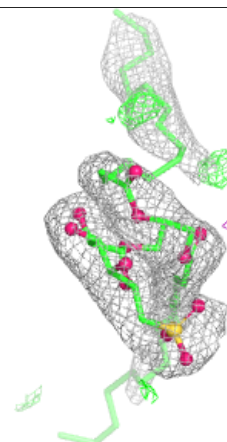
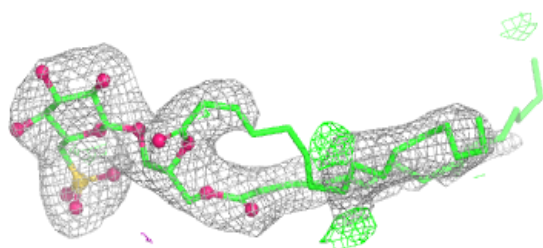
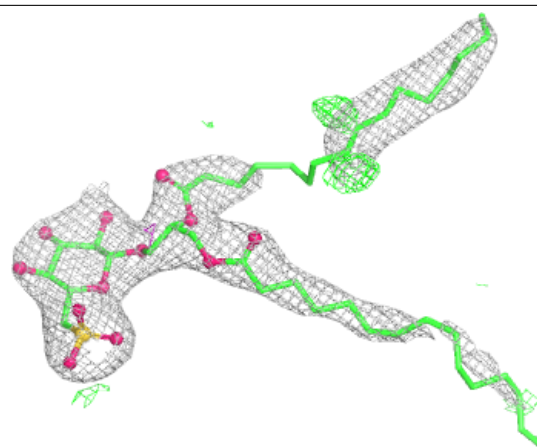
**Electron density around PL9 D 407:**

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



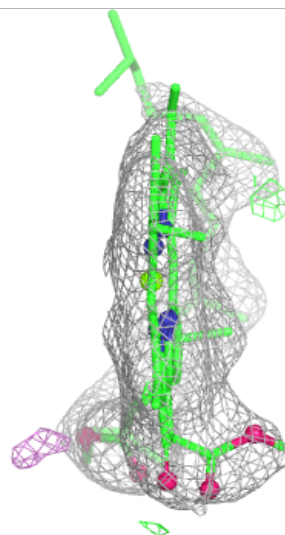
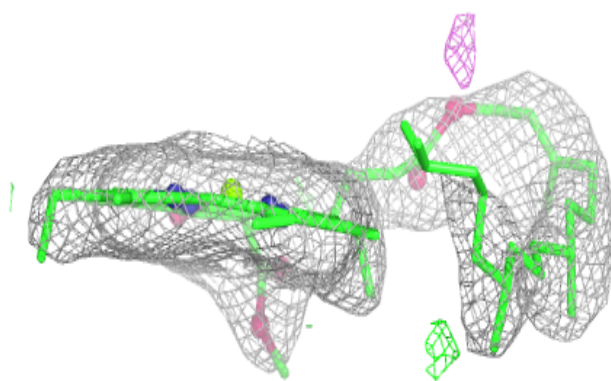
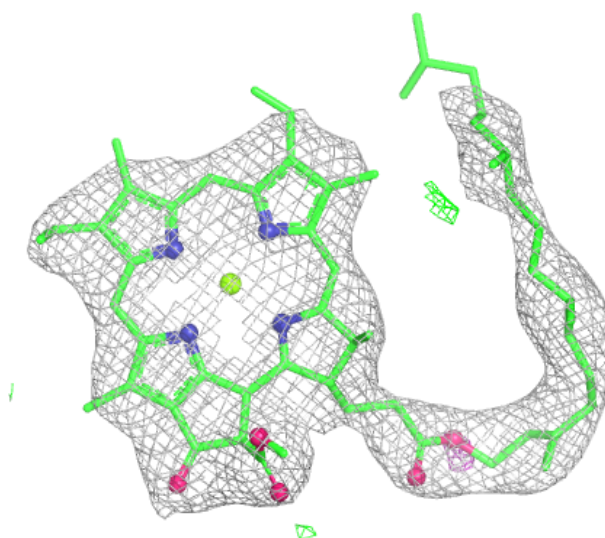
Electron density around SQD a 411:

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



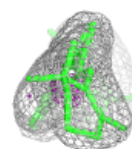
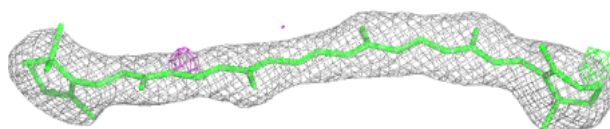
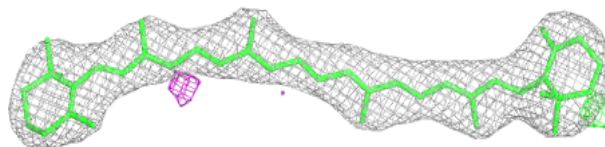
Electron density around CLA c 512:

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

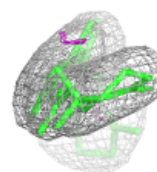
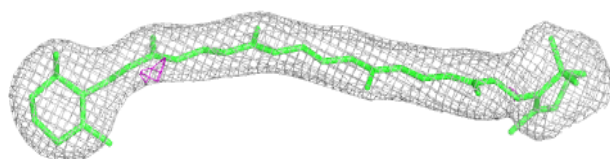
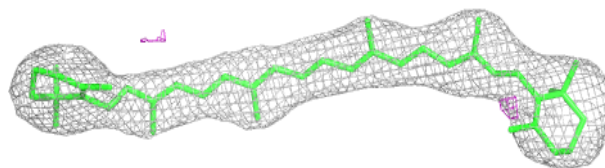


Electron density around BCR b 619:

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

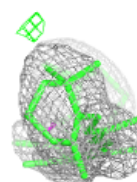
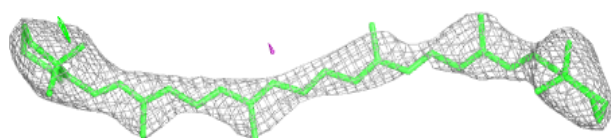
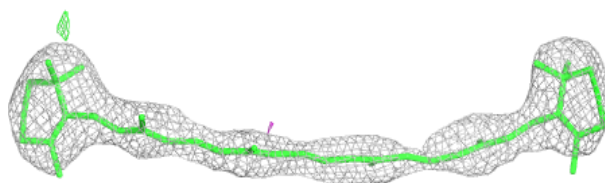
**Electron density around BCR d 404:**

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

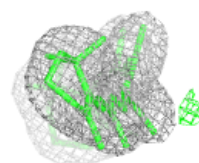
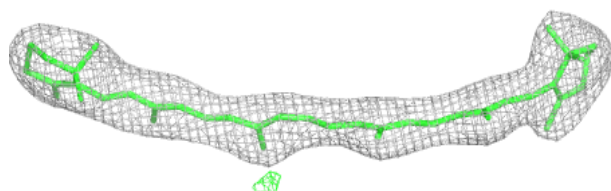
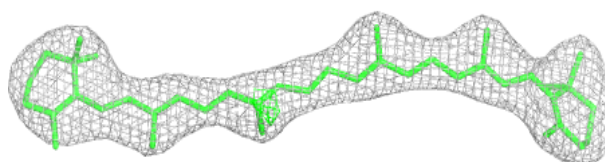


Electron density around BCR k 101:

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

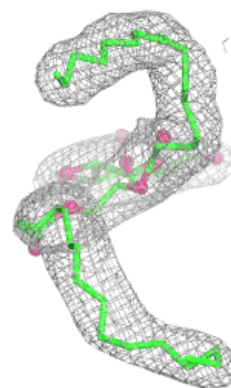
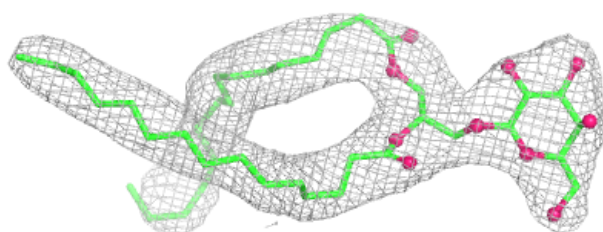
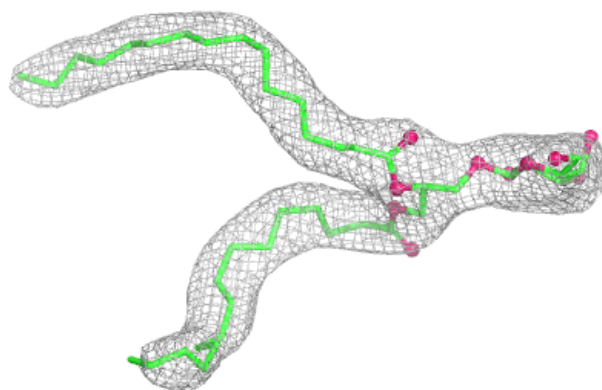
**Electron density around BCR t 101:**

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

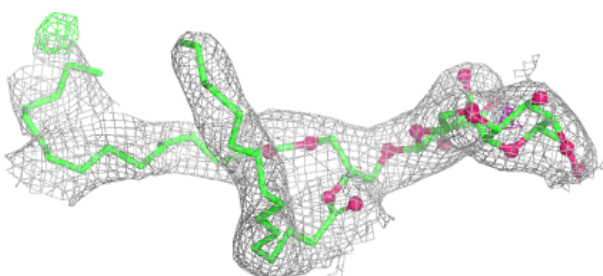
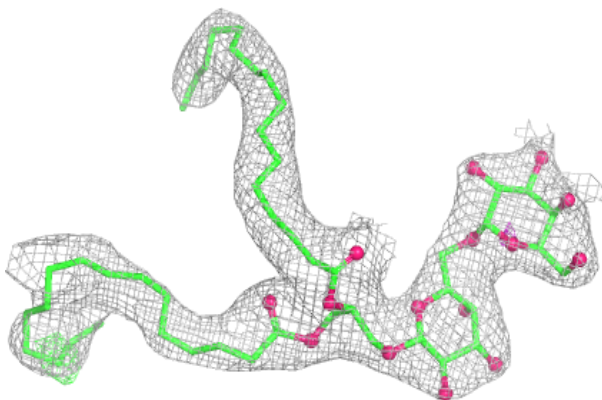


Electron density around LMG m 101:

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

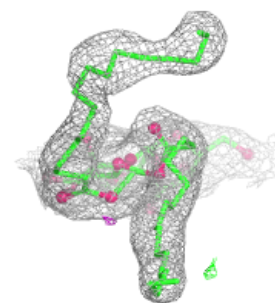
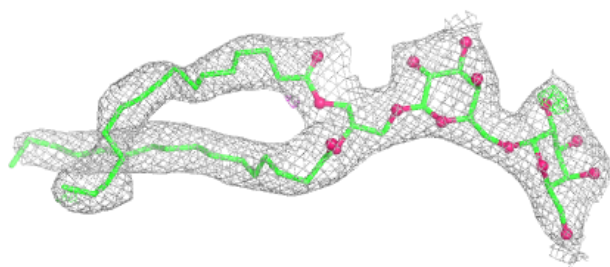
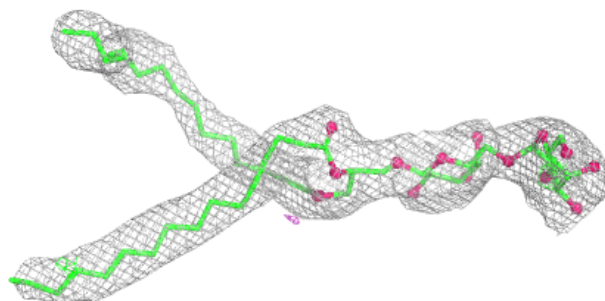
**Electron density around DGD C 518:**

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

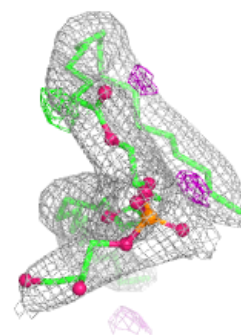
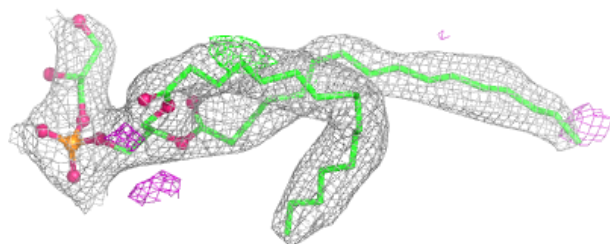
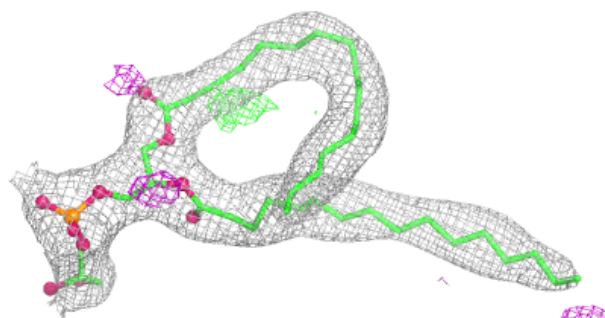


Electron density around DGD c 516:

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

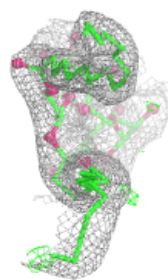
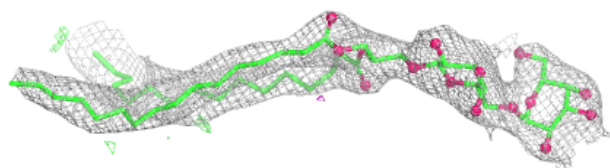
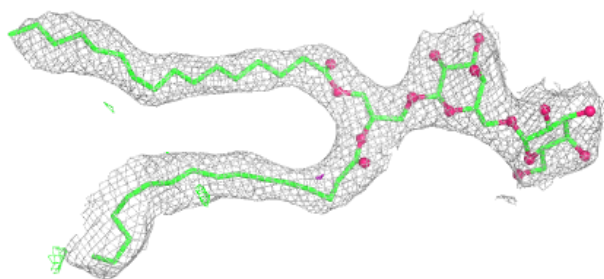
**Electron density around LHG A 415:**

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

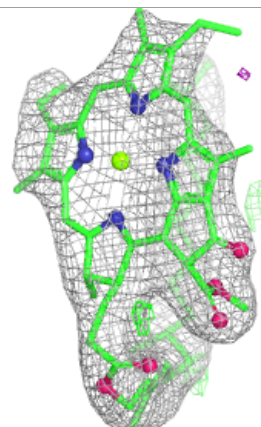
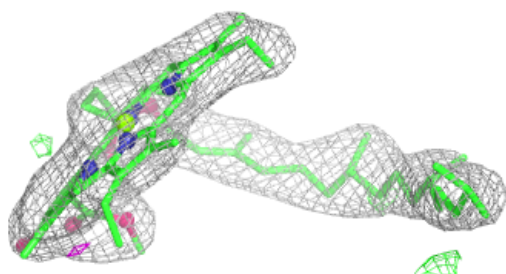
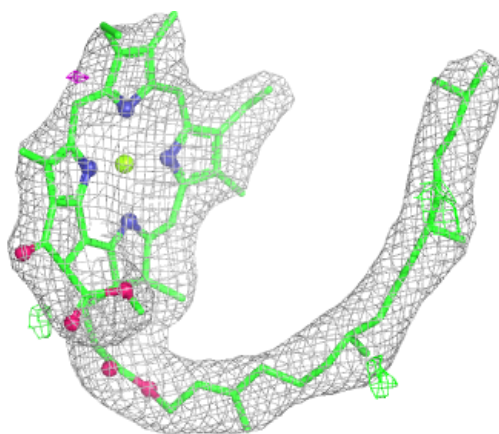


Electron density around DGD c 518:

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

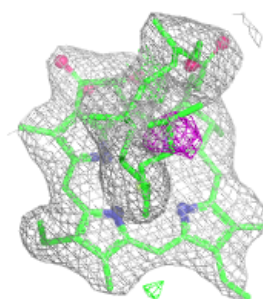
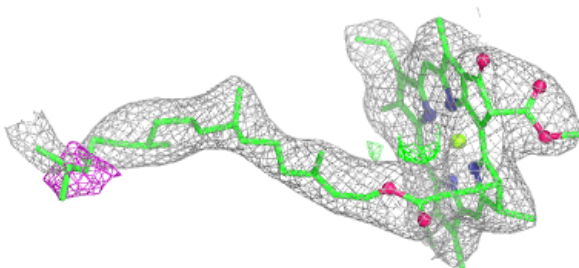
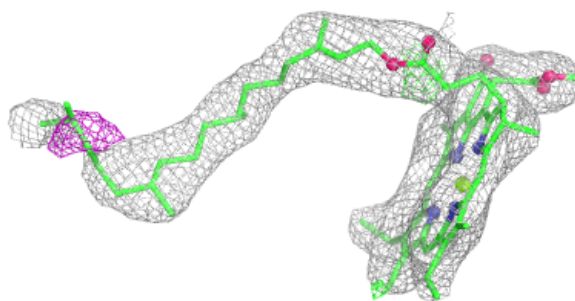
**Electron density around CLA C 508:**

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

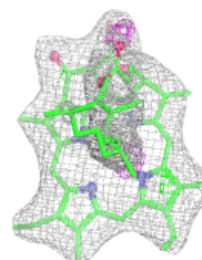
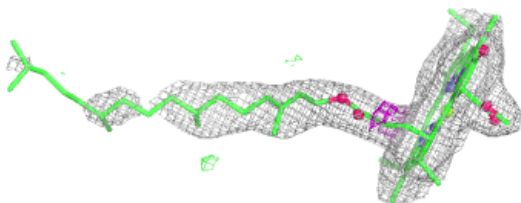
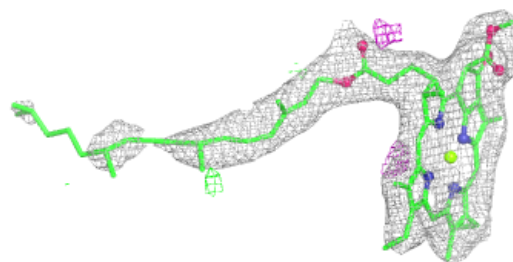


Electron density around CLA C 509:

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

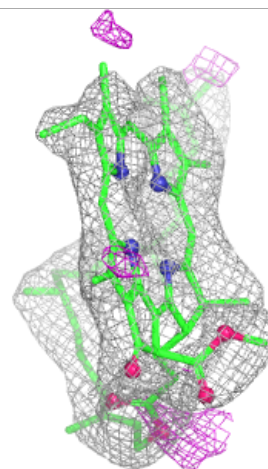
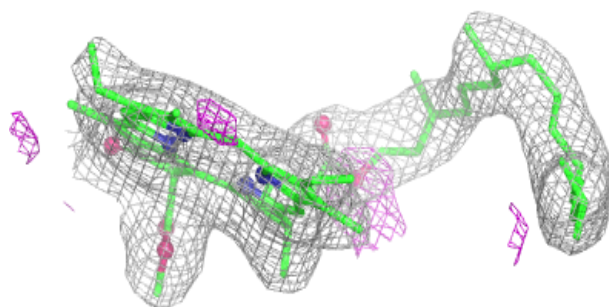
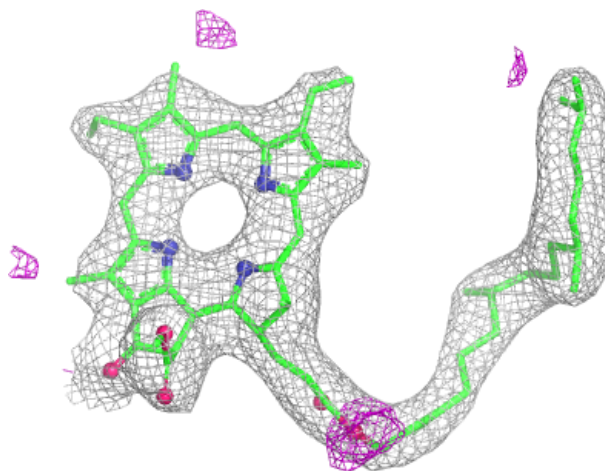
**Electron density around CLA d 403:**

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



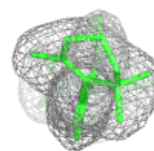
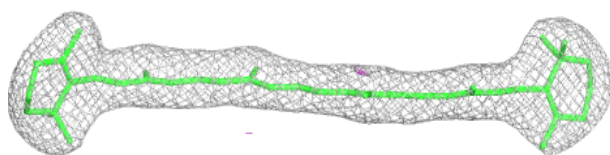
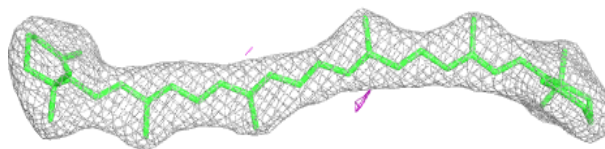
Electron density around PHO a 408:

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

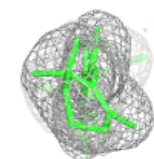
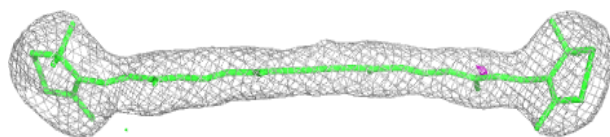
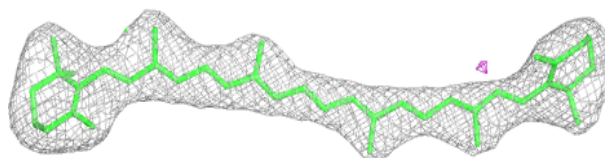


Electron density around BCR A 408:

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

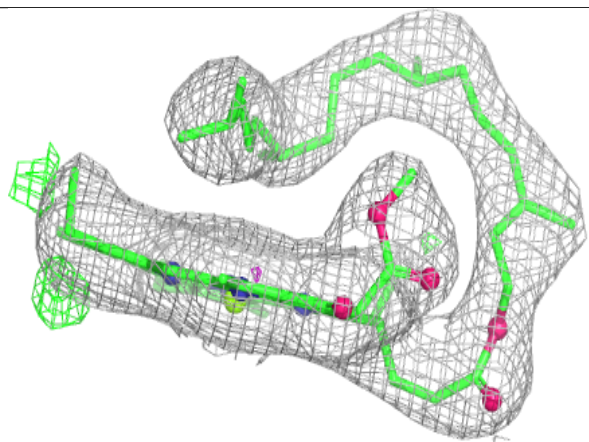
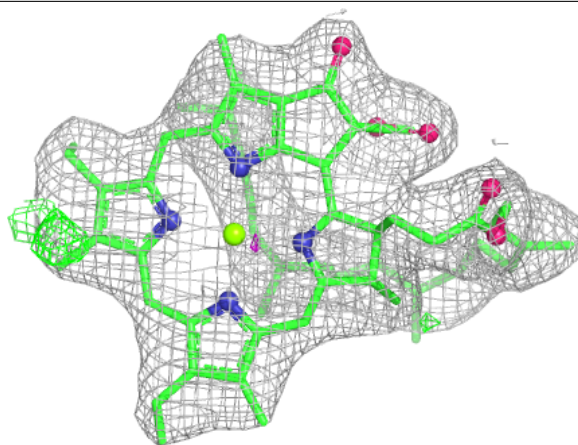
**Electron density around BCR B 619:**

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



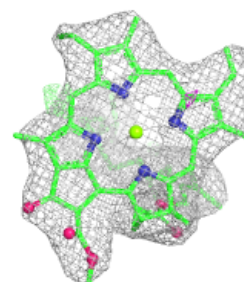
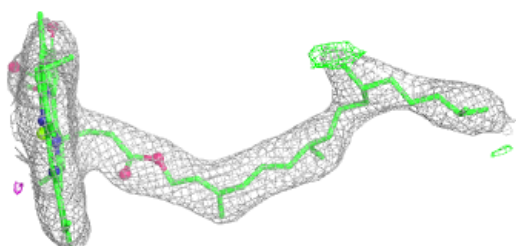
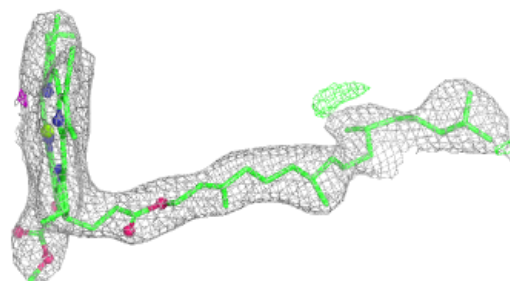
Electron density around CLA C 511:

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

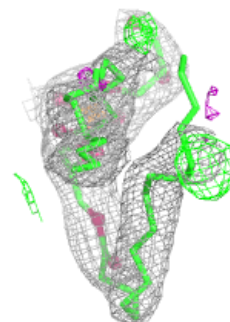
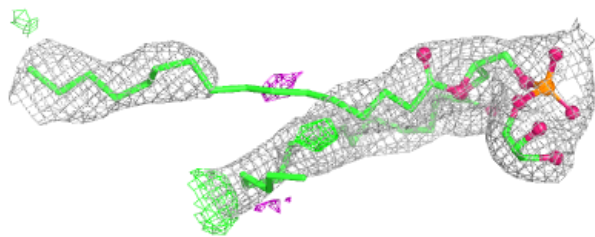
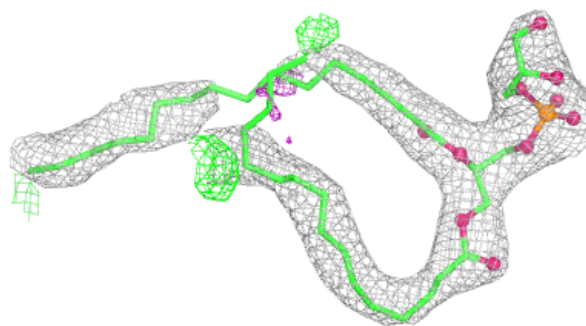


Electron density around CLA B 607:

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

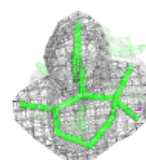
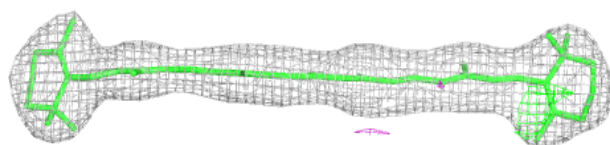
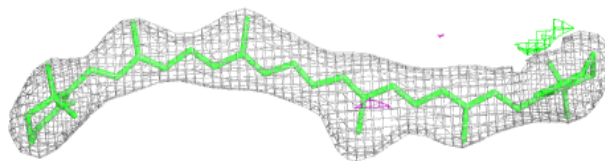
**Electron density around LHG D 409:**

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



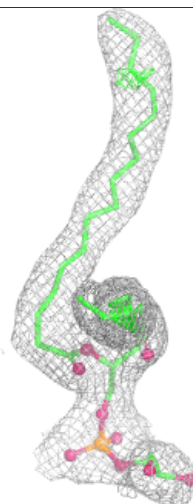
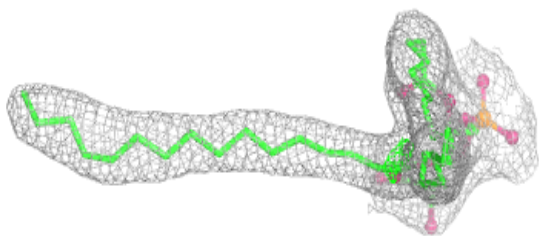
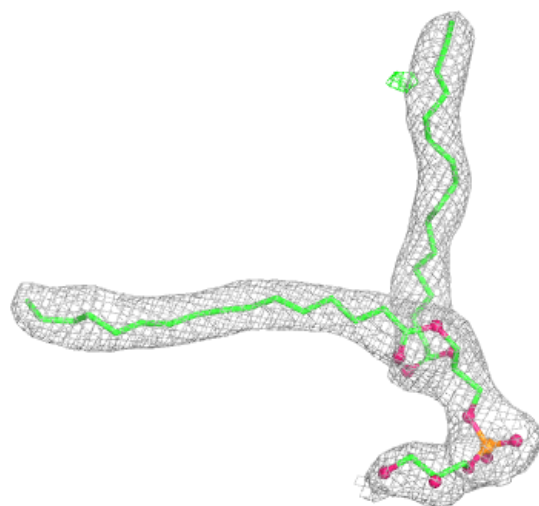
Electron density around BCR C 516:

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



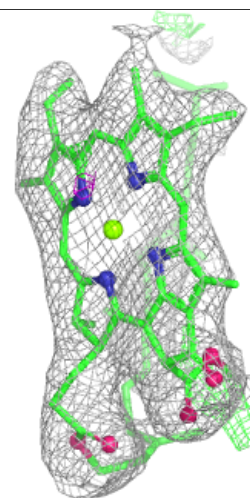
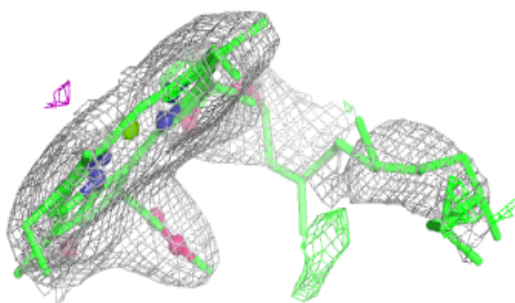
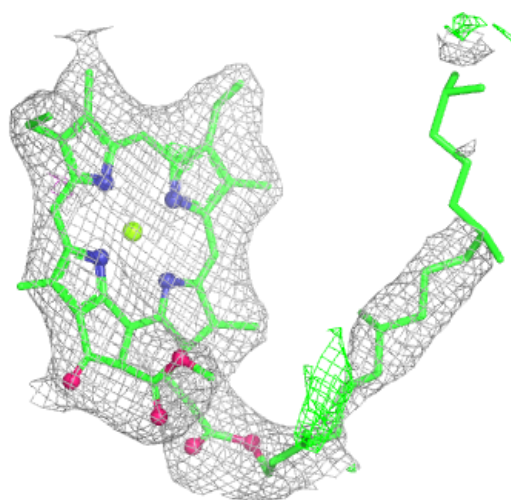
Electron density around LHG b 630:

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



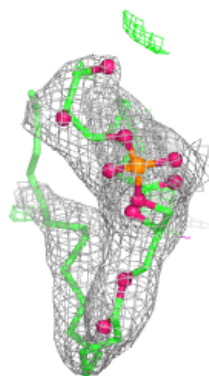
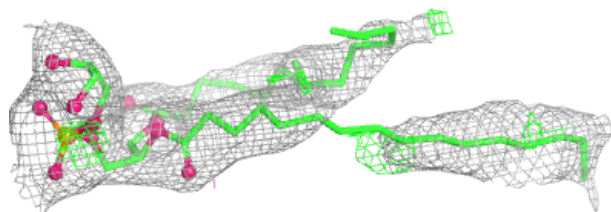
Electron density around CLA B 617:

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

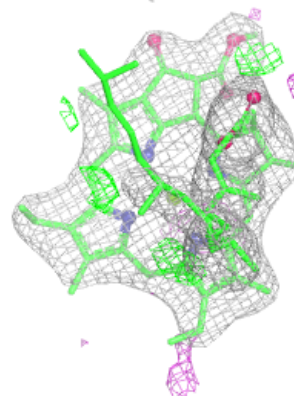
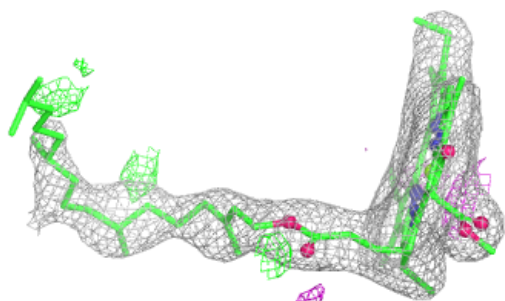
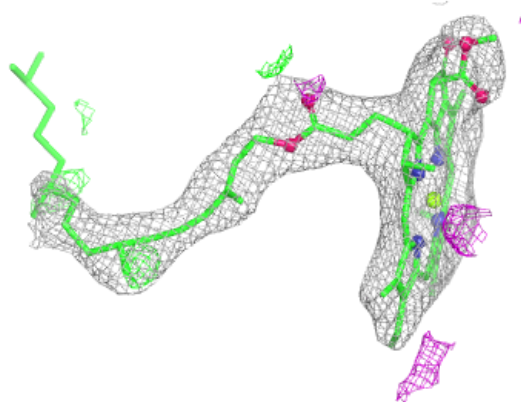


Electron density around LHG d 408:

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

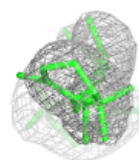
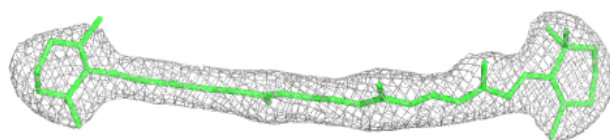
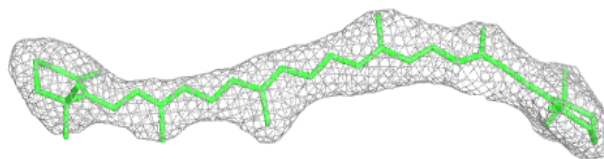
**Electron density around CLA D 405:**

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

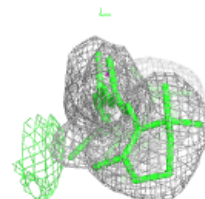
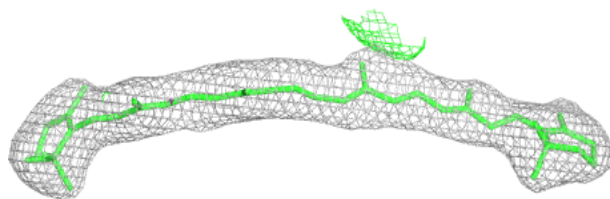
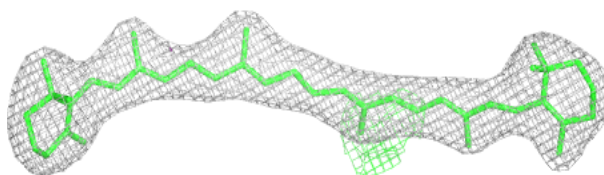


Electron density around BCR H 101:

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

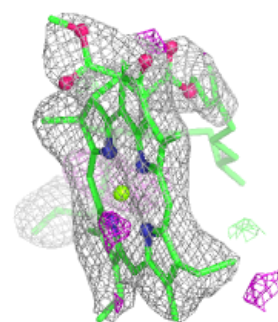
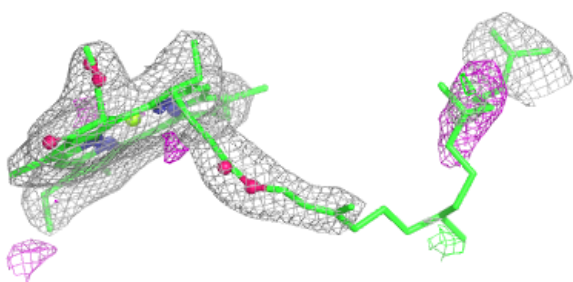
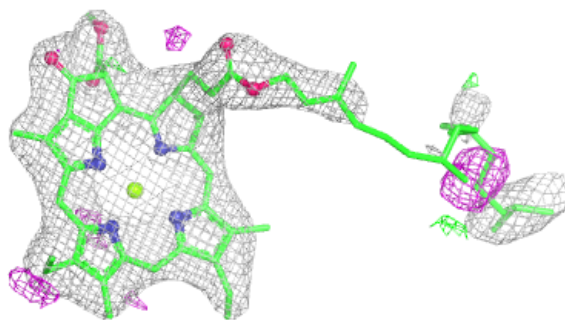
**Electron density around BCR T 101:**

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

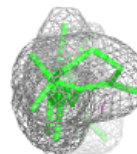
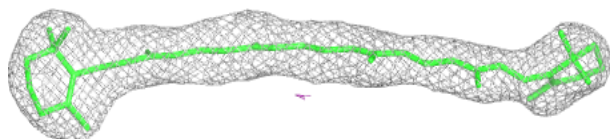
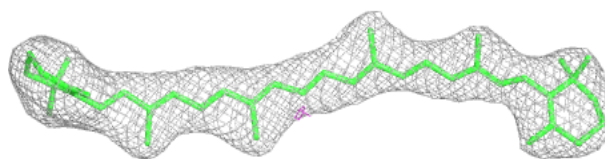


Electron density around CLA a 409:

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

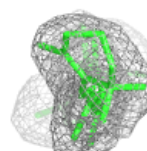
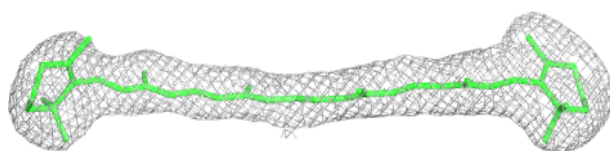
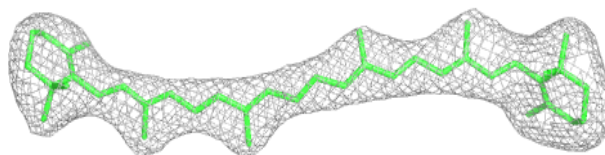
**Electron density around BCR b 617:**

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

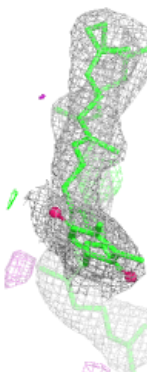
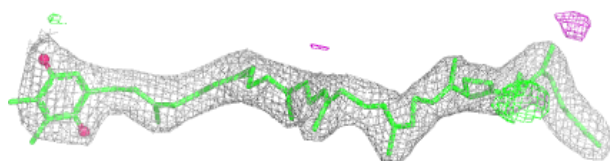
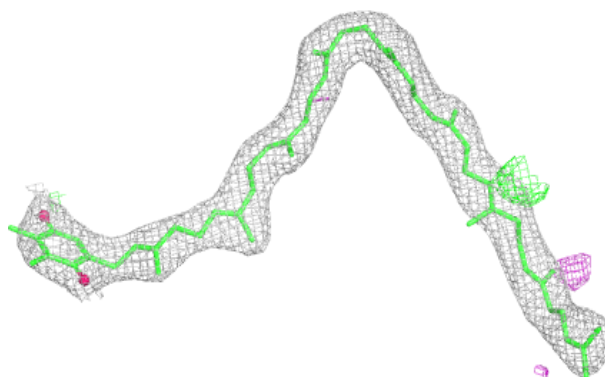


Electron density around BCR b 618:

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

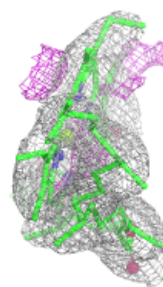
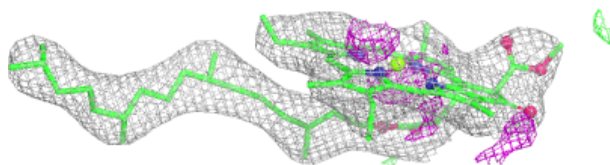
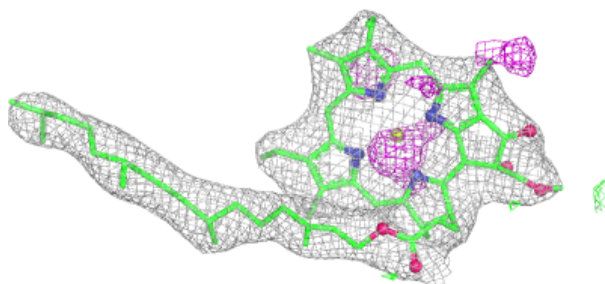
**Electron density around PL9 d 405:**

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

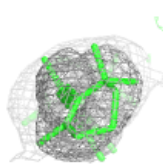
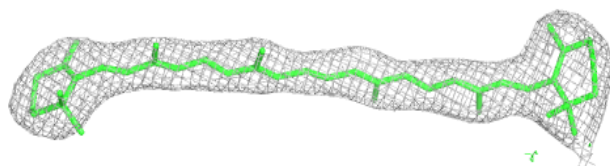
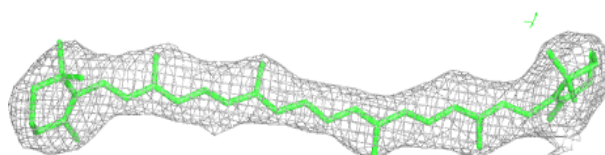


Electron density around CLA C 502:

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

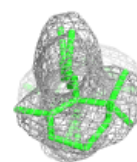
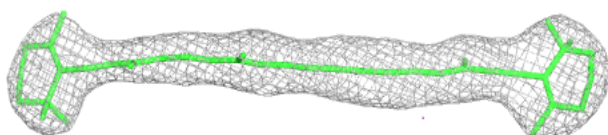
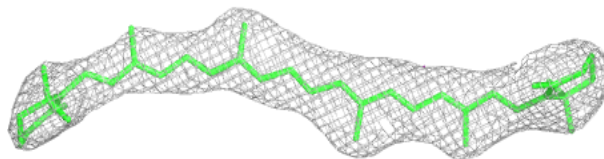
**Electron density around BCR c 514:**

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

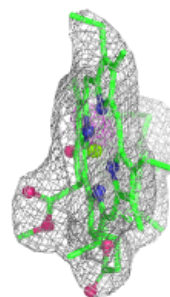
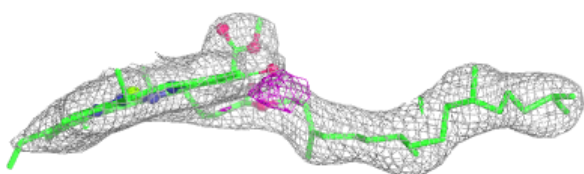
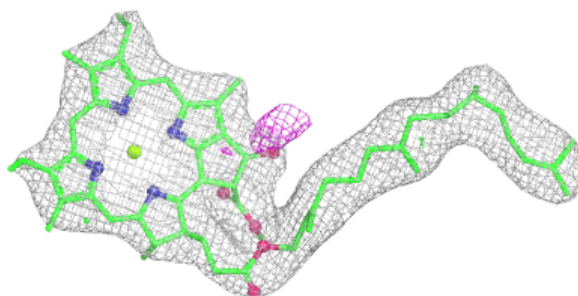


Electron density around BCR c 515:

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

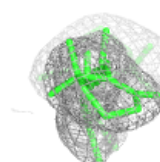
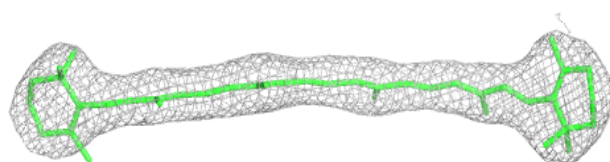
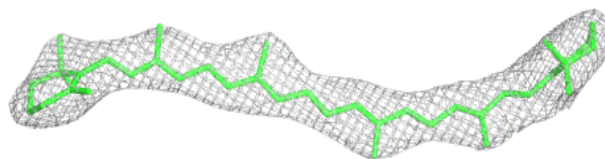
**Electron density around CLA b 602:**

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

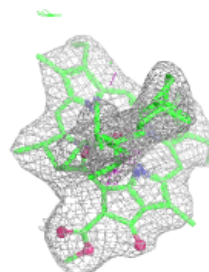
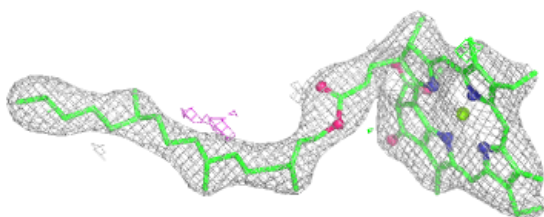
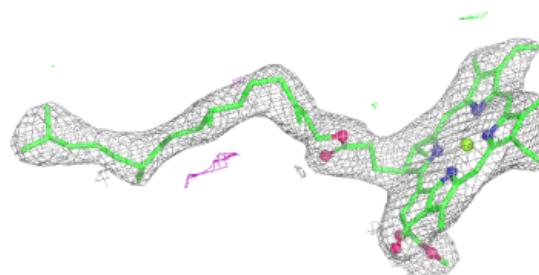


Electron density around BCR h 102:

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

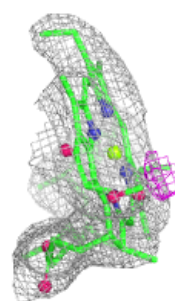
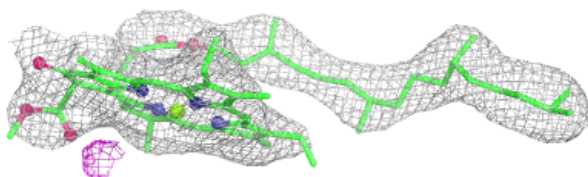
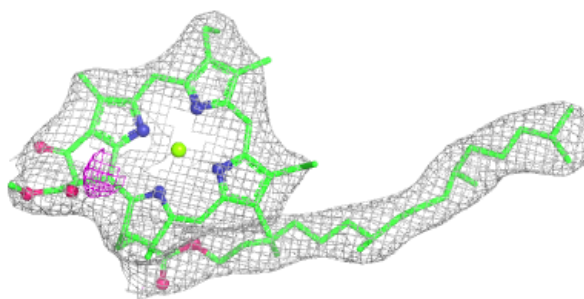
**Electron density around CLA C 503:**

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

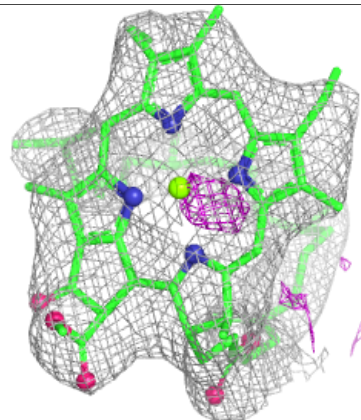
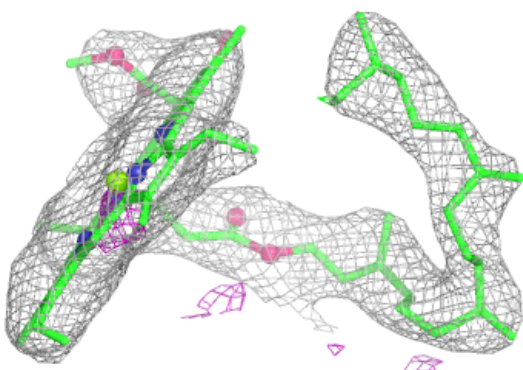
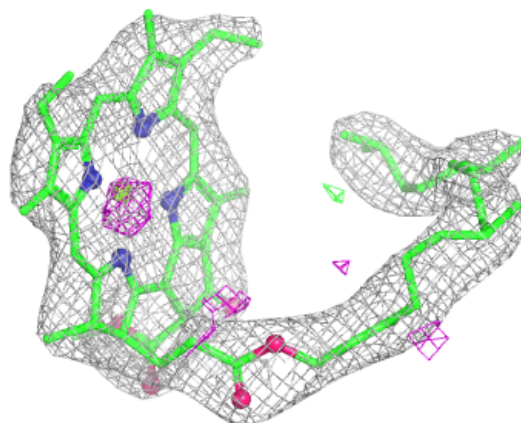


Electron density around CLA c 501:

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

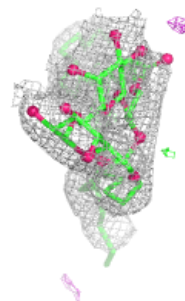
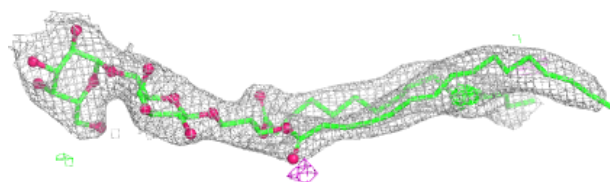
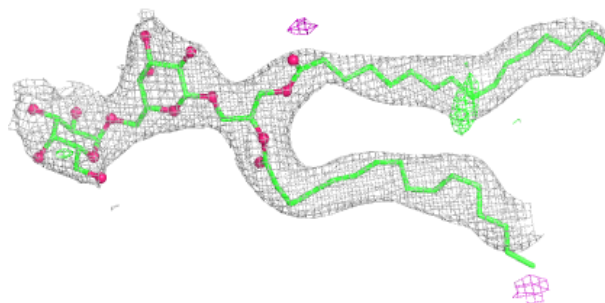
**Electron density around CLA C 504:**

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

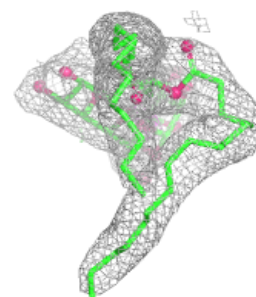
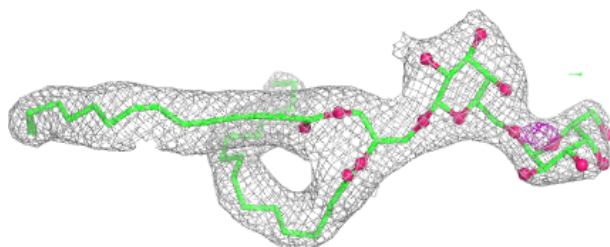
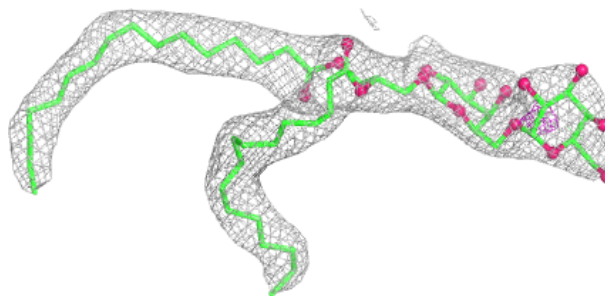


Electron density around DGD C 519:

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

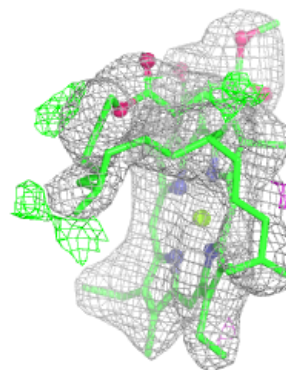
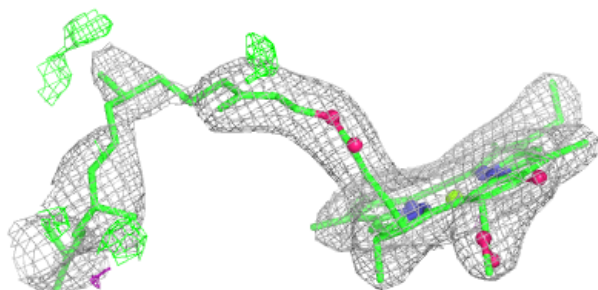
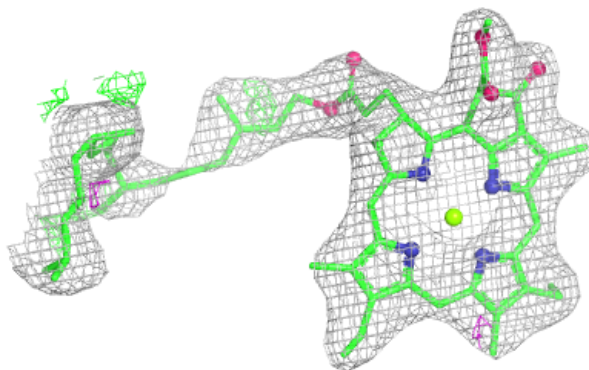
**Electron density around DGD H 102:**

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

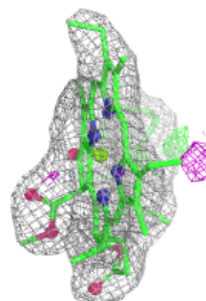
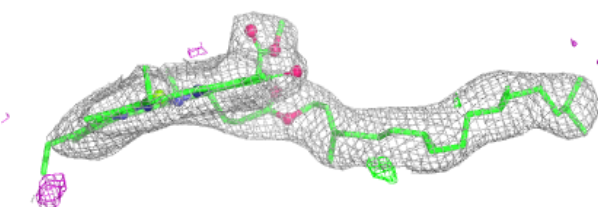
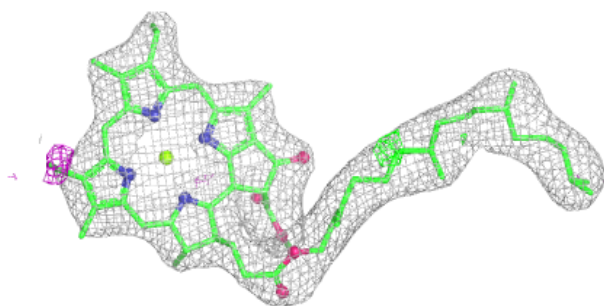


Electron density around CLA A 407:

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

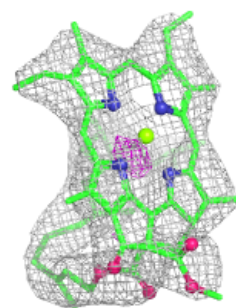
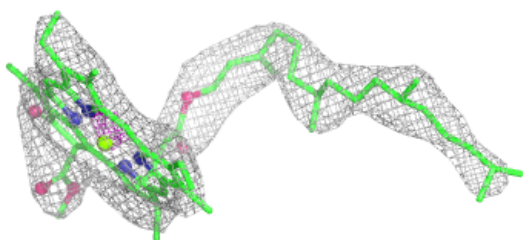
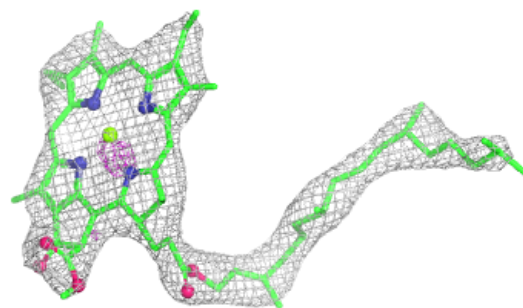
**Electron density around CLA B 603:**

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

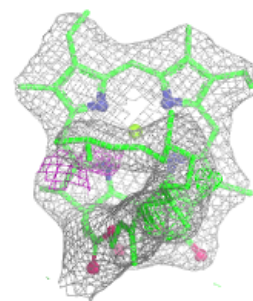
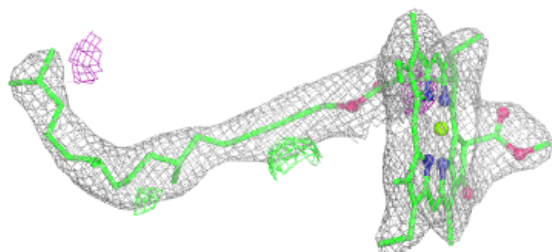
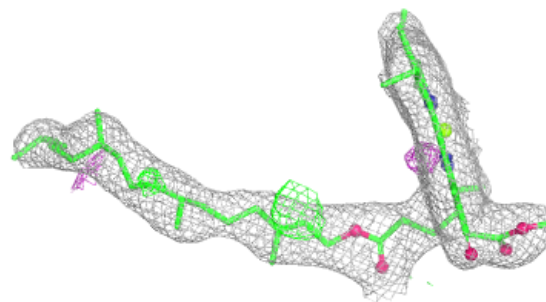


Electron density around CLA c 511:

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

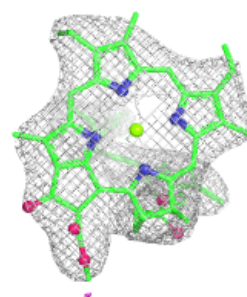
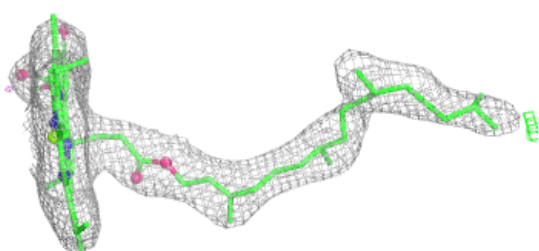
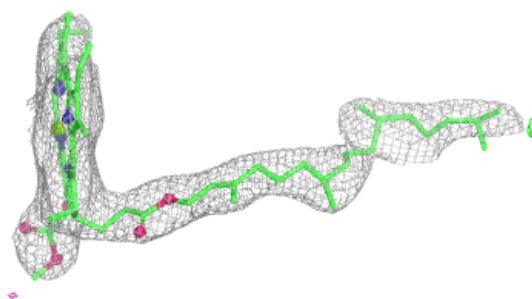
**Electron density around CLA b 605:**

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

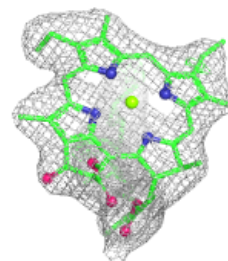
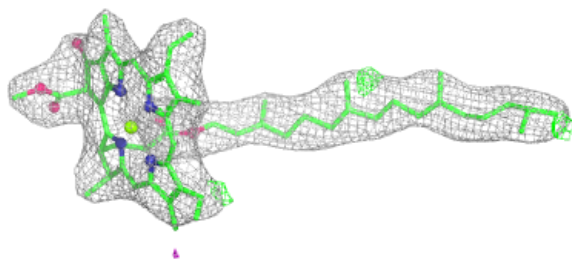
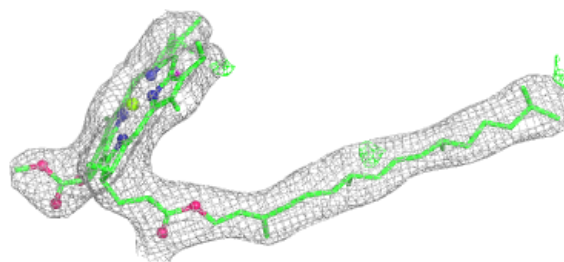


Electron density around CLA b 606:

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

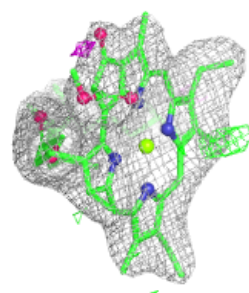
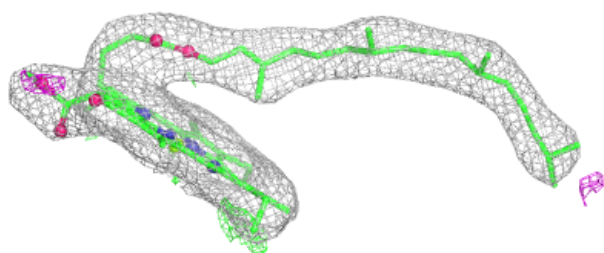
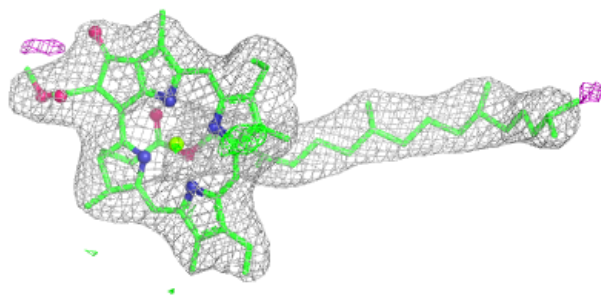
**Electron density around CLA b 607:**

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

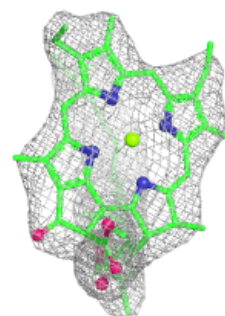
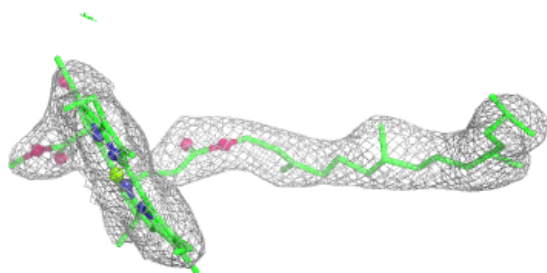
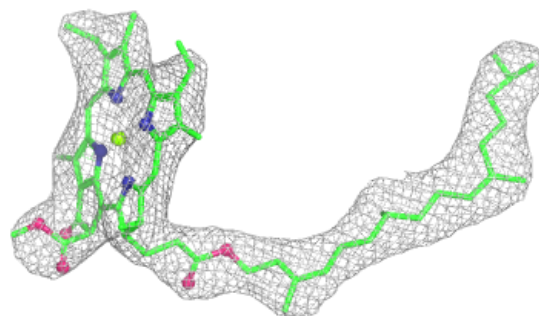


Electron density around CLA b 608:

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

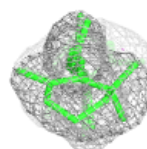
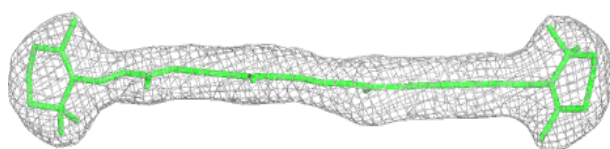
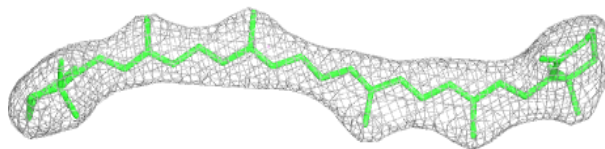
**Electron density around CLA b 609:**

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

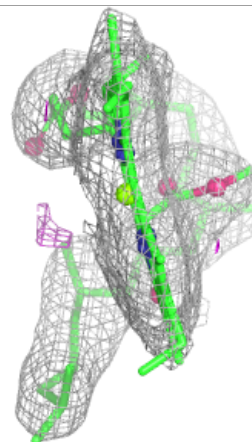
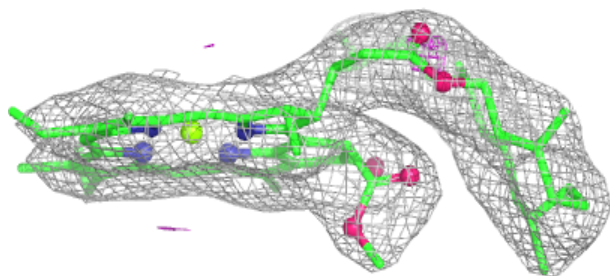
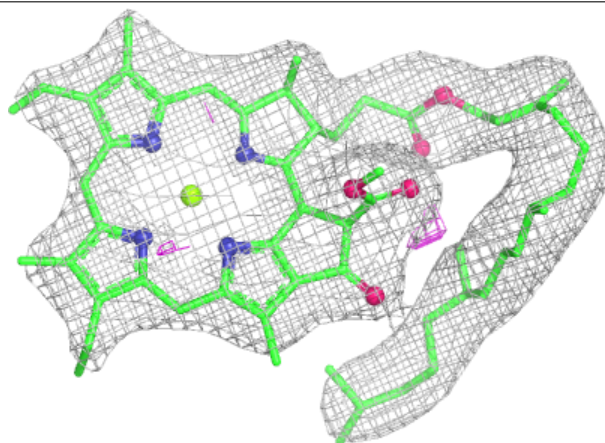


Electron density around BCR a 410:

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

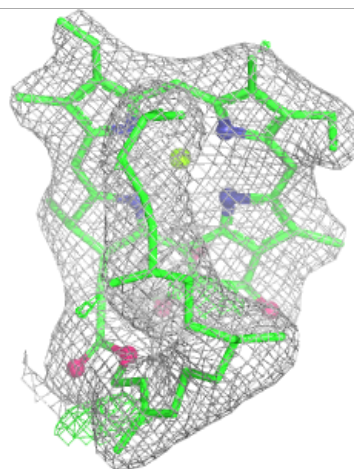
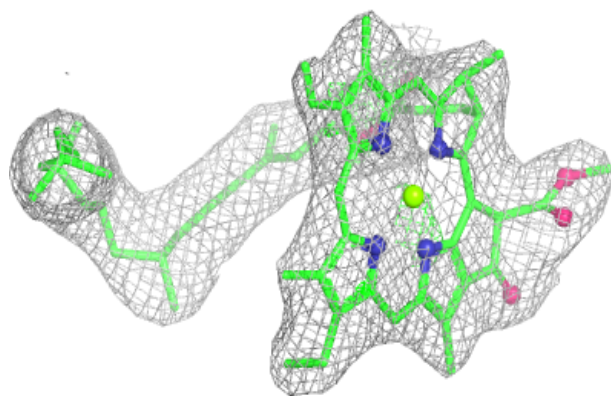
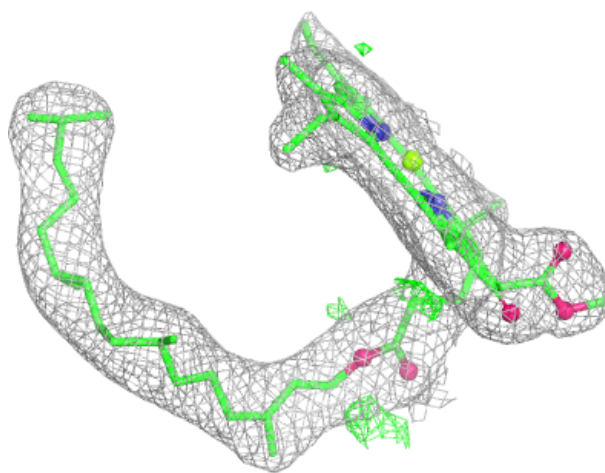
**Electron density around CLA b 610:**

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



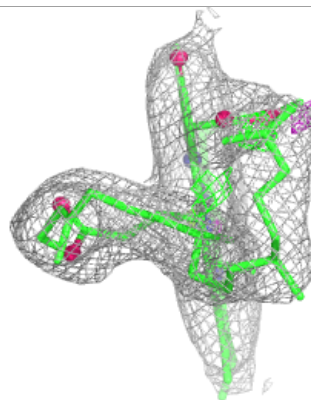
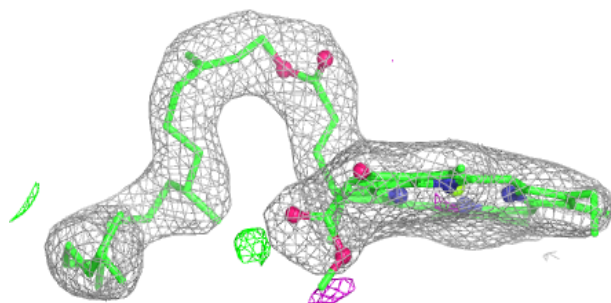
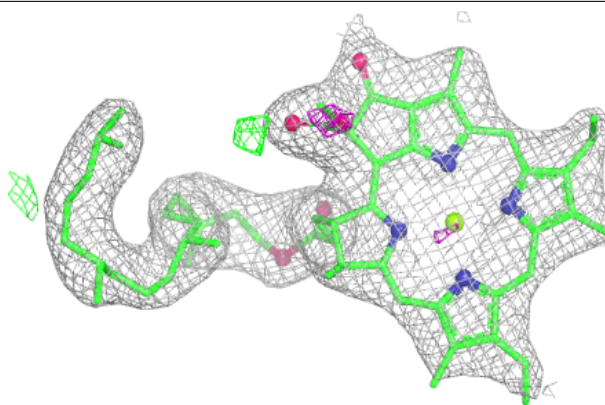
Electron density around CLA b 611:

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



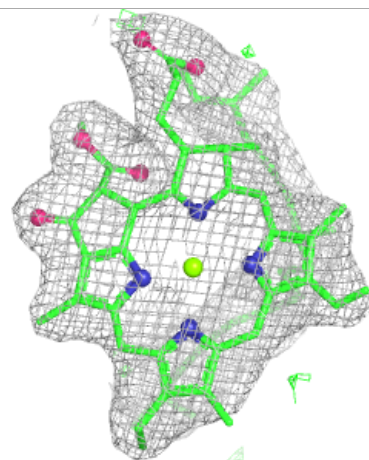
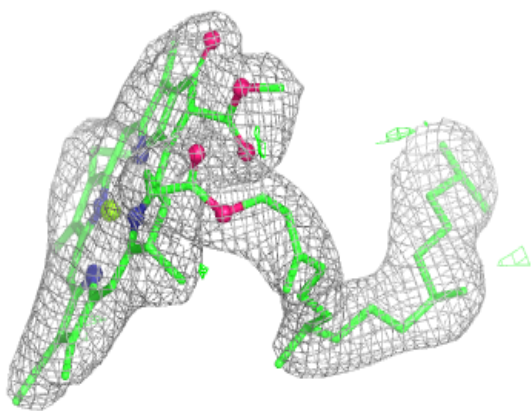
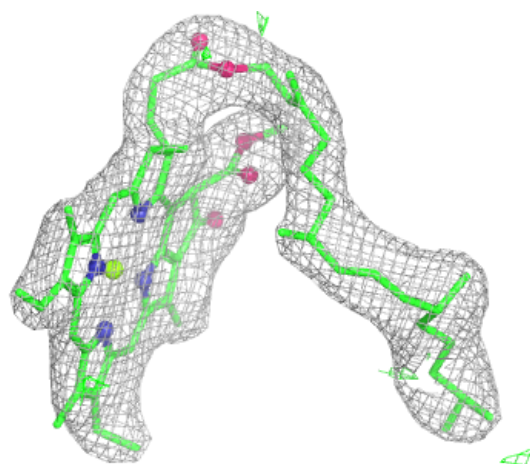
Electron density around CLA b 612:

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



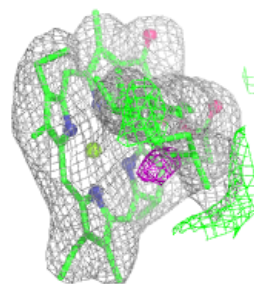
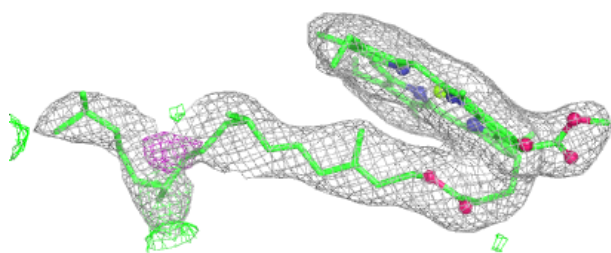
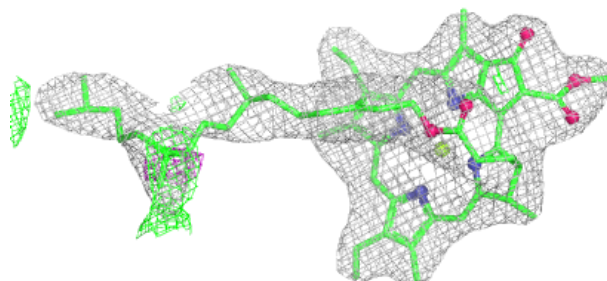
Electron density around CLA b 613:

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



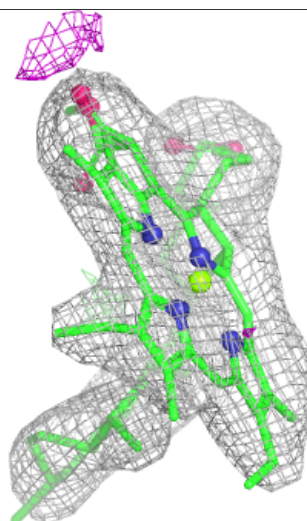
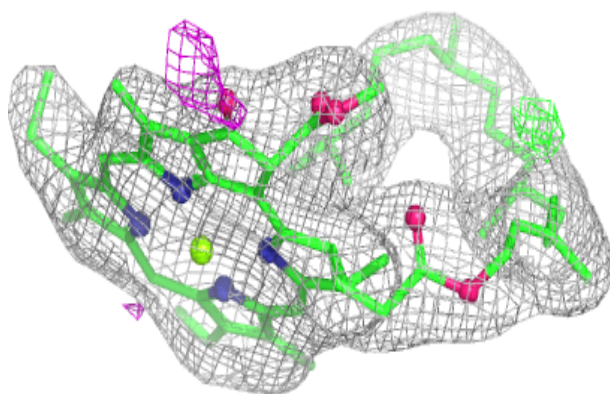
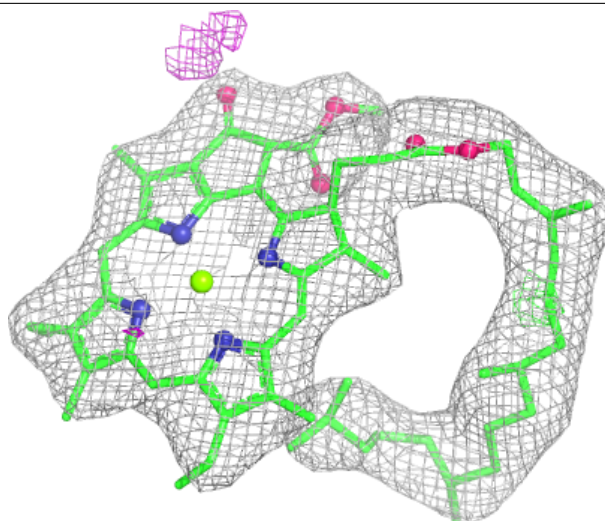
Electron density around CLA b 614:

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



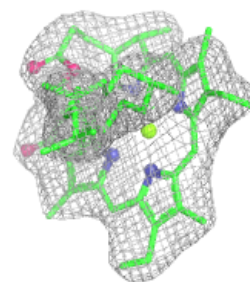
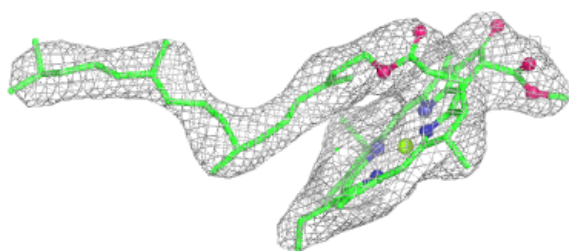
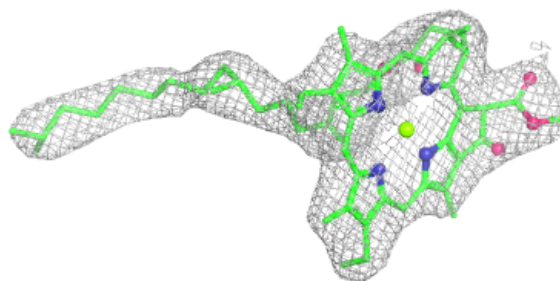
Electron density around CLA b 615:

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

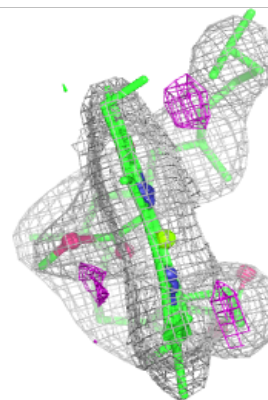
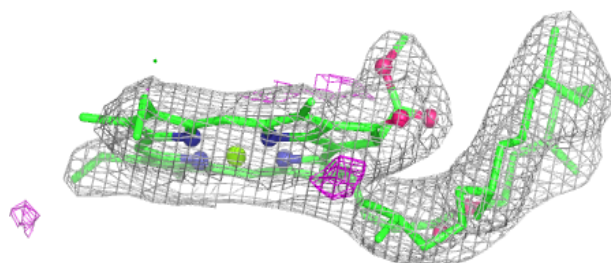
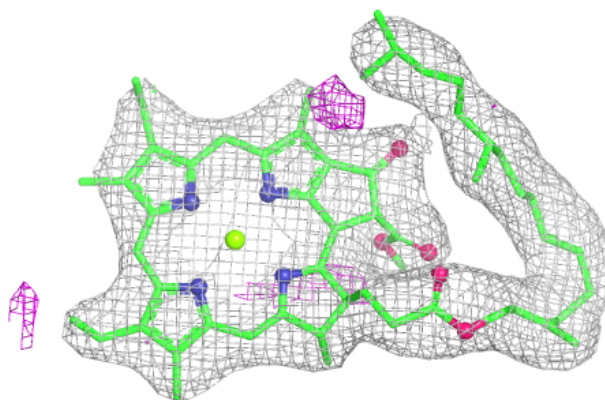


Electron density around CLA C 506:

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

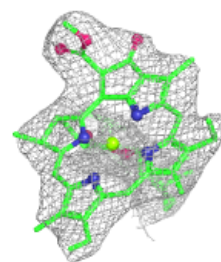
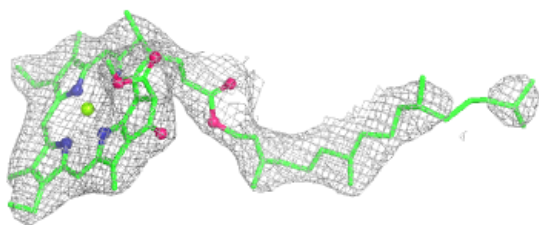
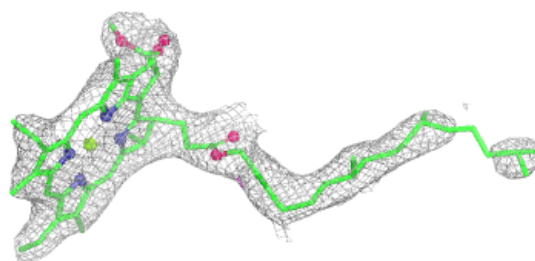
**Electron density around CLA B 611:**

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

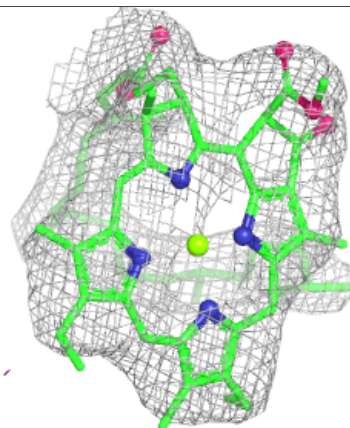
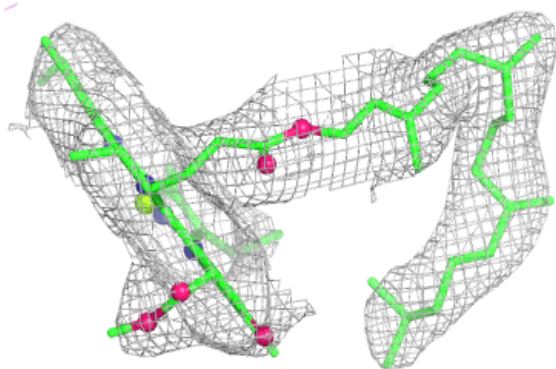
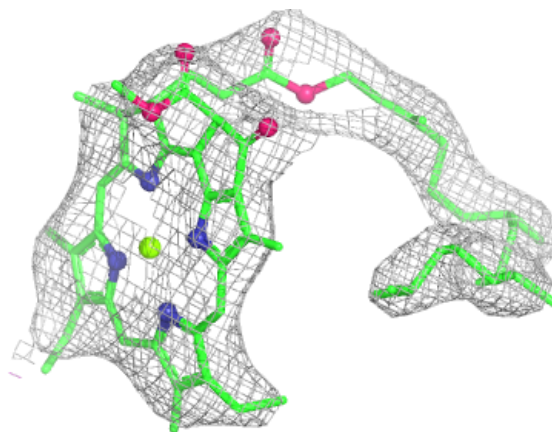


Electron density around CLA c 502:

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

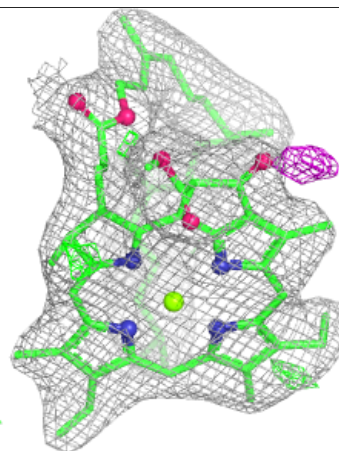
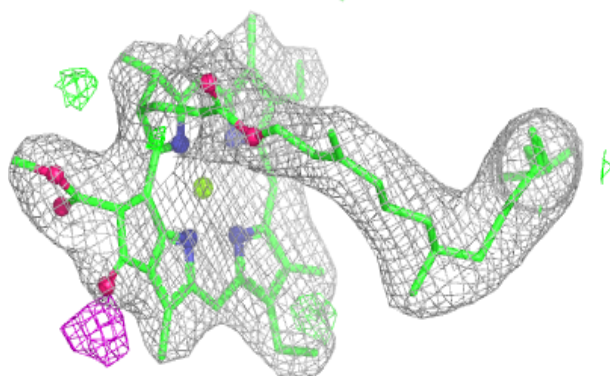
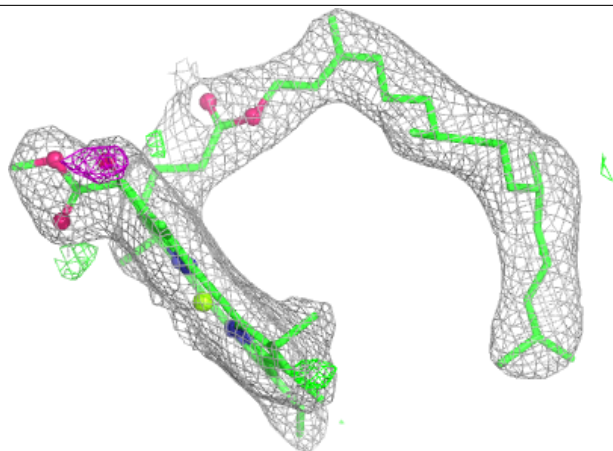
**Electron density around CLA c 503:**

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



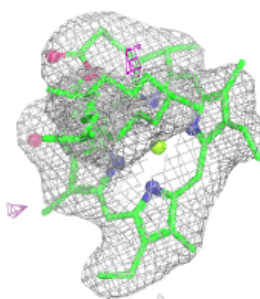
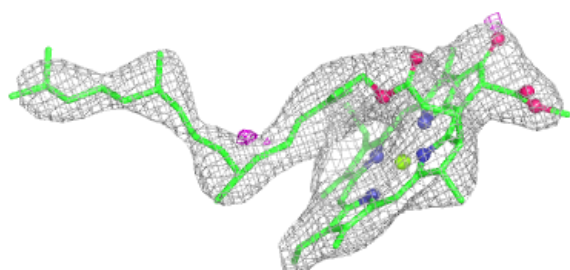
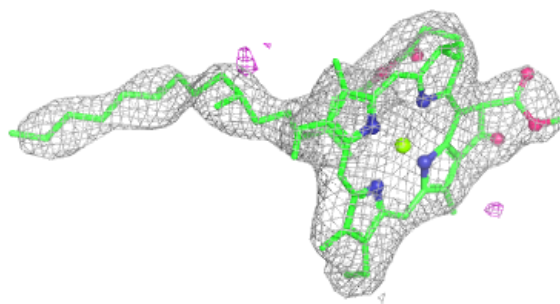
Electron density around CLA B 612:

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

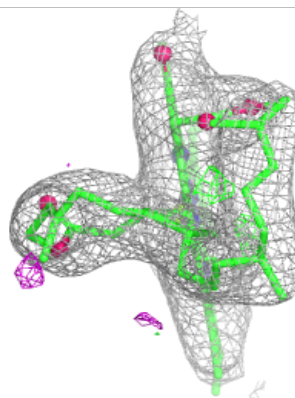
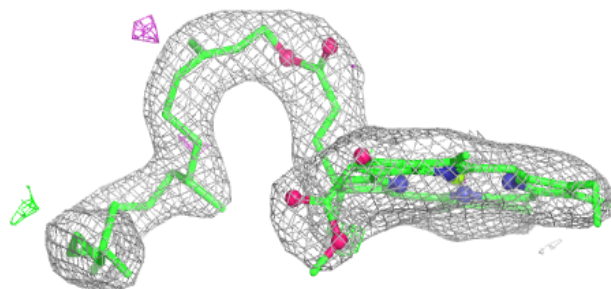
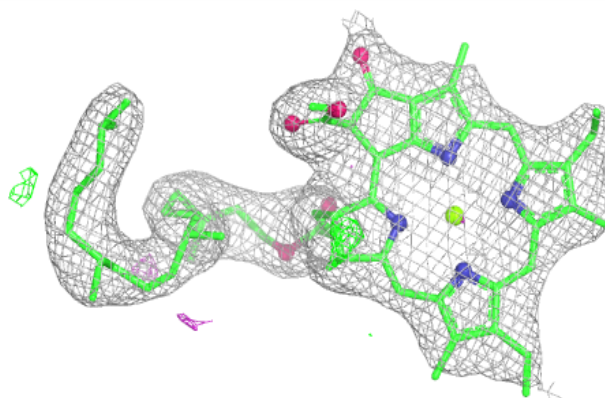


Electron density around CLA c 505:

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

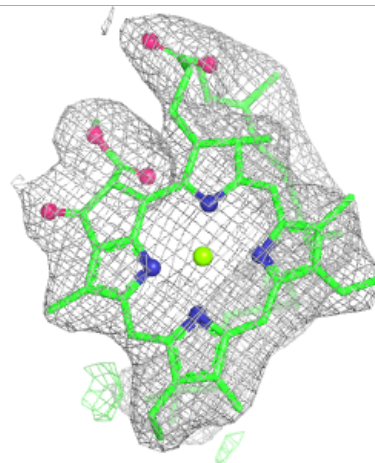
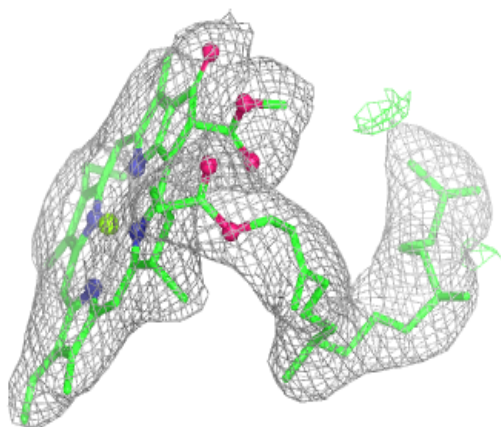
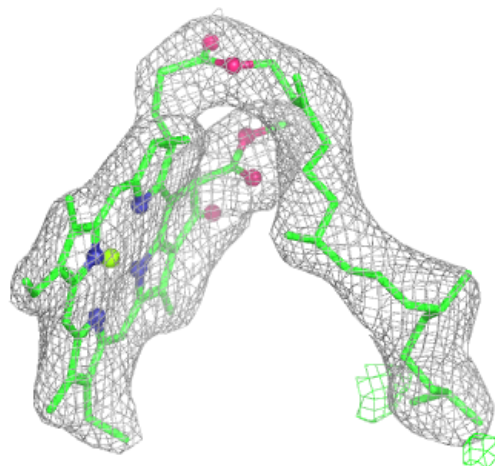
**Electron density around CLA B 613:**

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



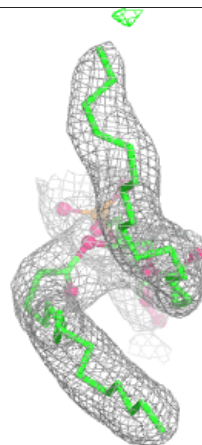
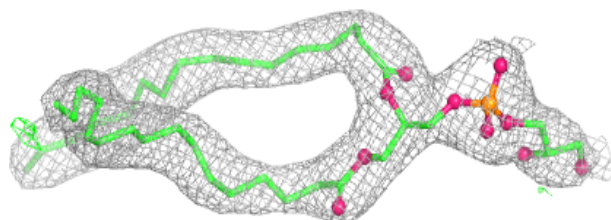
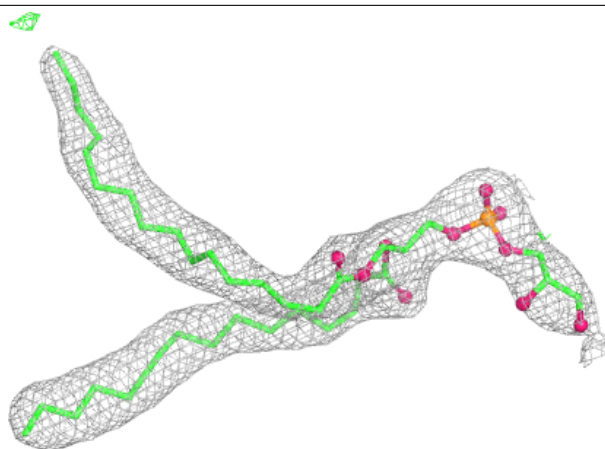
Electron density around CLA B 614:

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



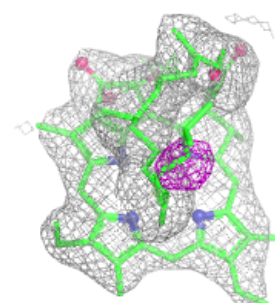
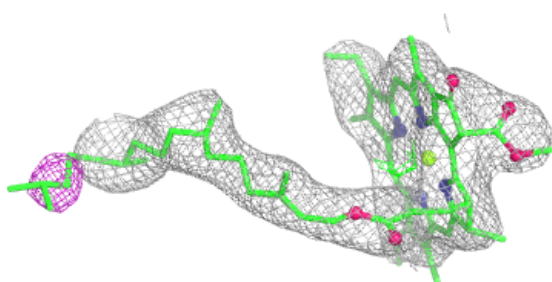
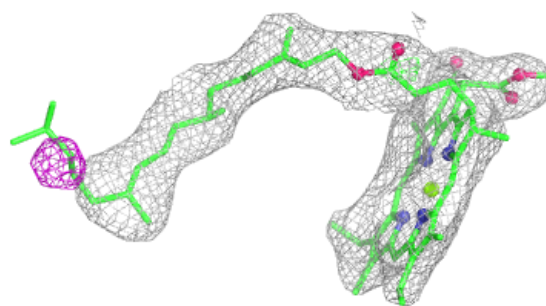
Electron density around LHG D 408:

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

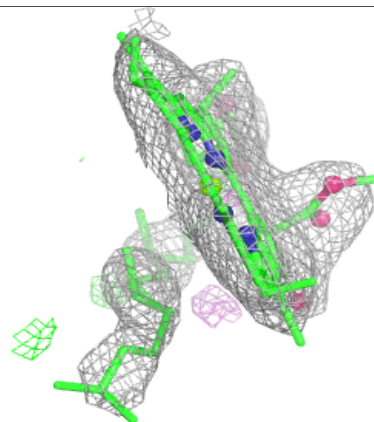
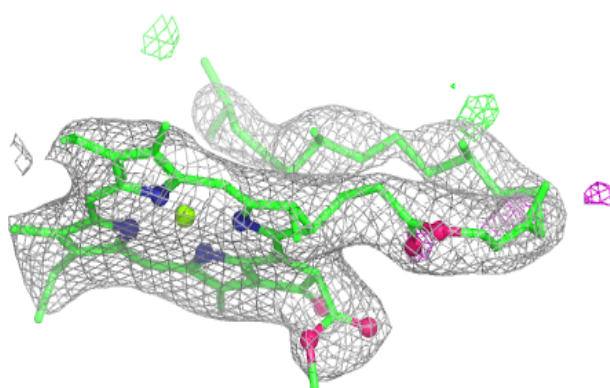
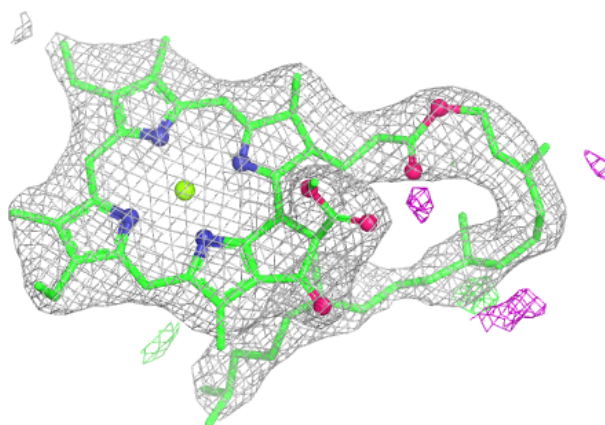


Electron density around CLA c 508:

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

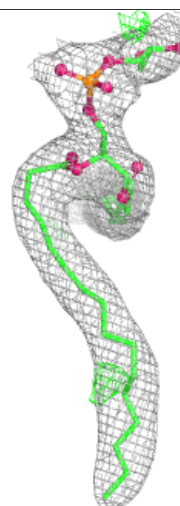
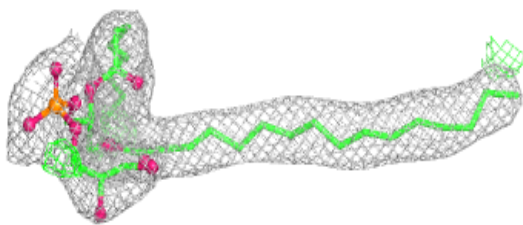
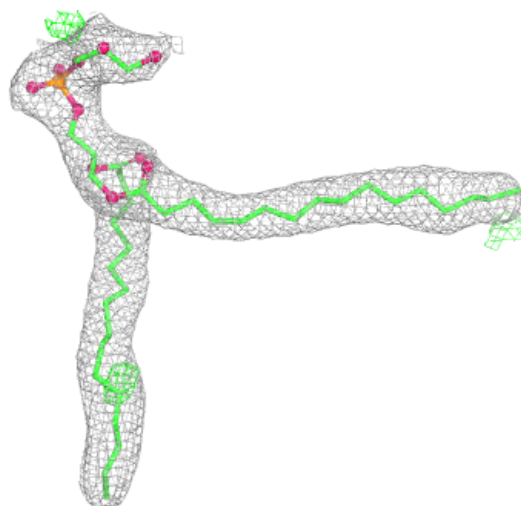
**Electron density around CLA c 509:**

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



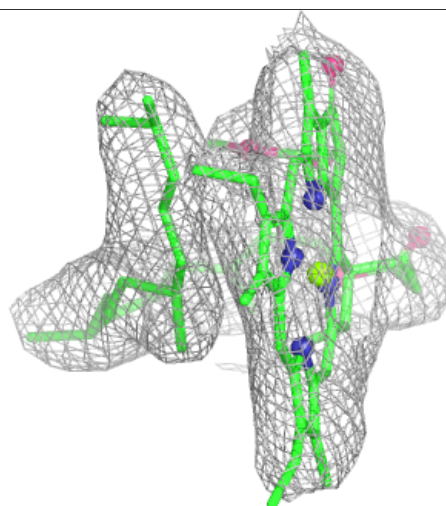
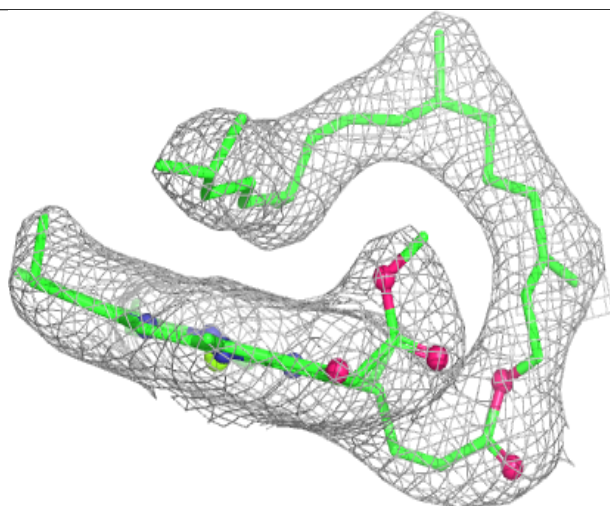
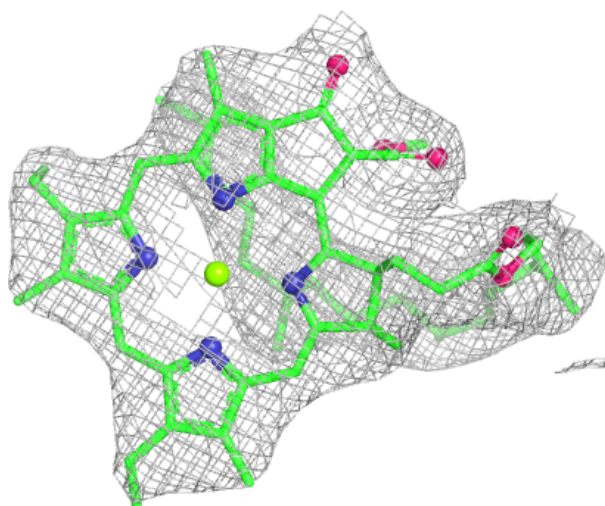
Electron density around LHG L 101:

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



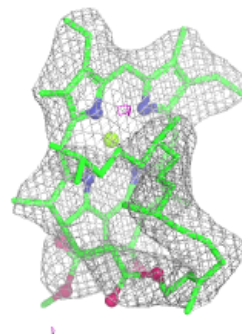
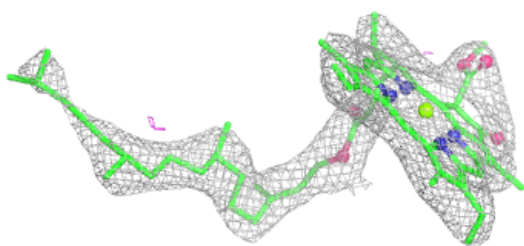
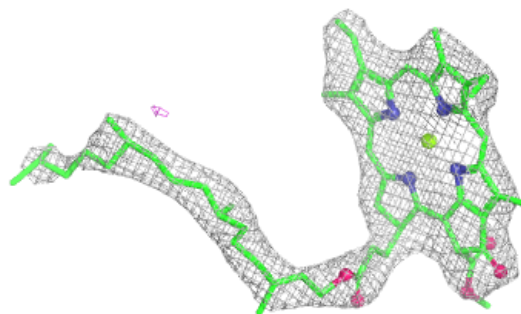
Electron density around CLA c 510:

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

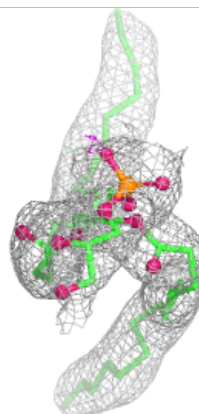
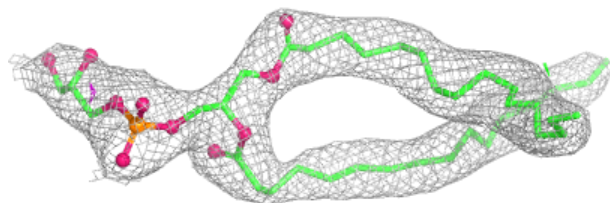
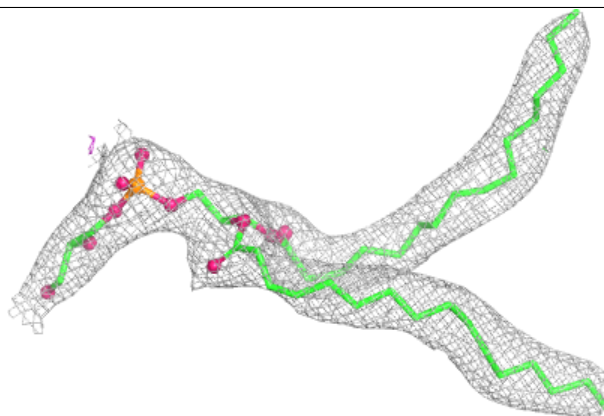


Electron density around CLA C 512:

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

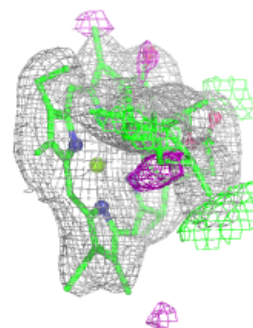
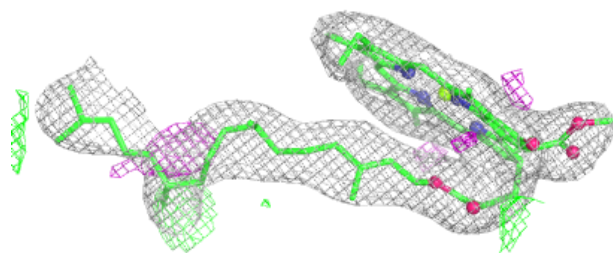
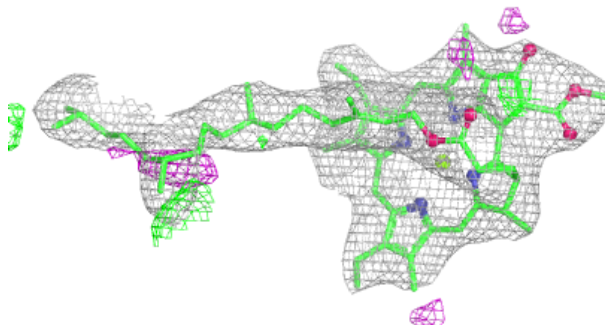
**Electron density around LHG d 407:**

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

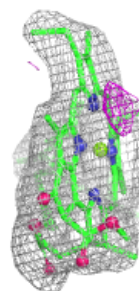
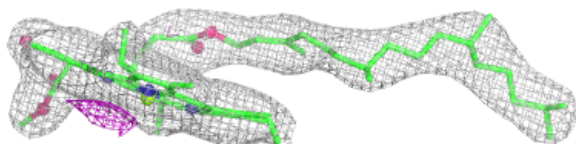
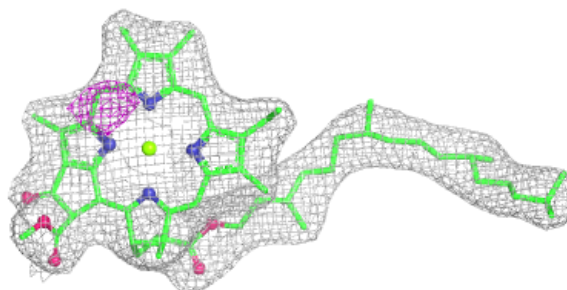


Electron density around CLA B 615:

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

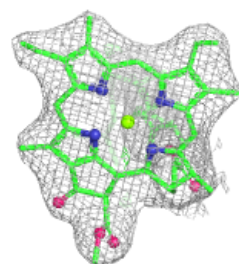
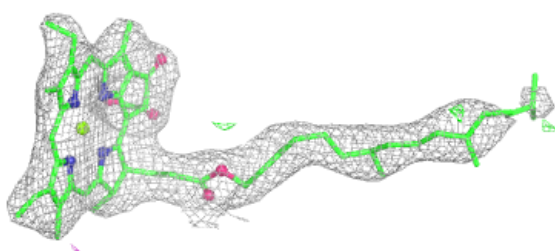
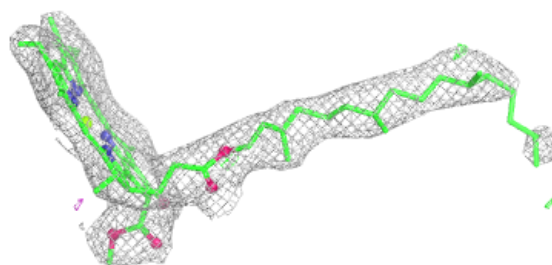
**Electron density around CLA B 604:**

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



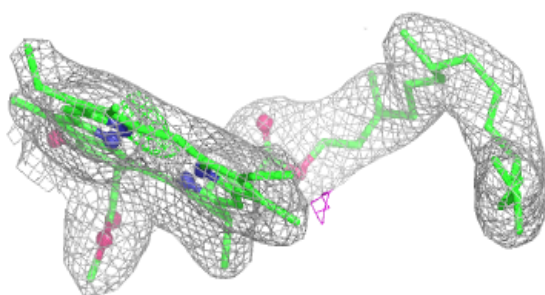
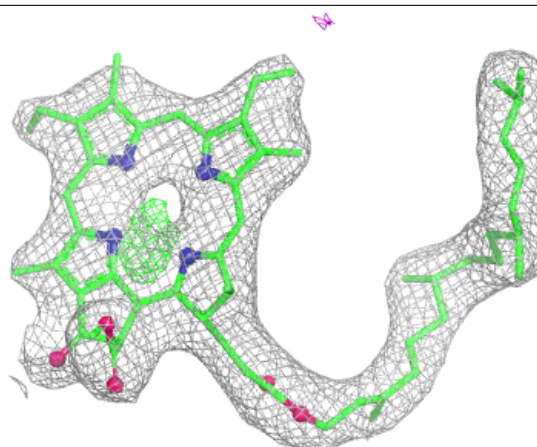
Electron density around CLA B 605:

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



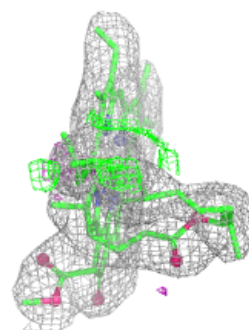
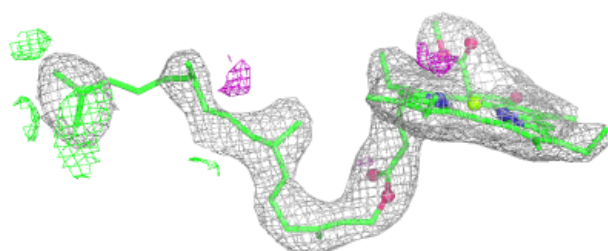
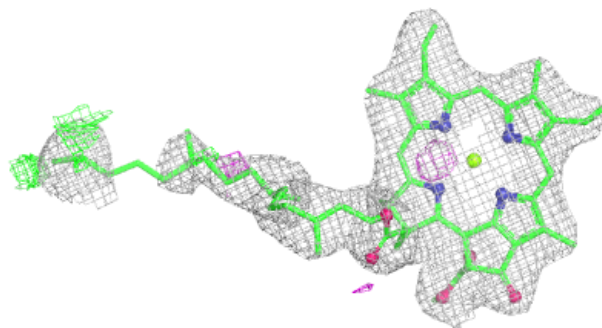
Electron density around PHO D 402:

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

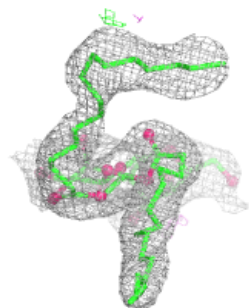
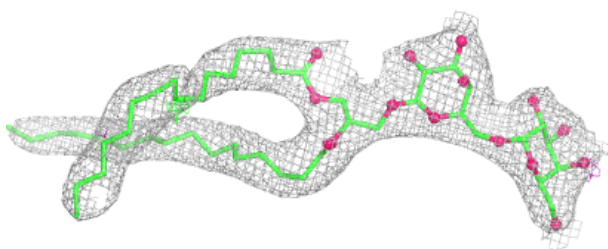
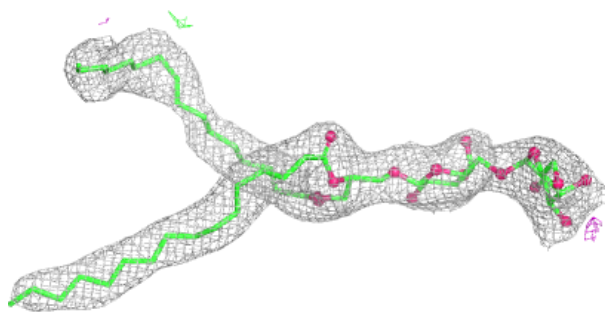


Electron density around CLA a 406:

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

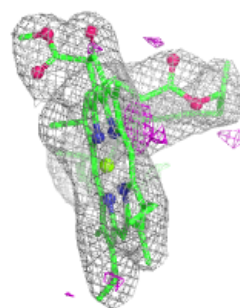
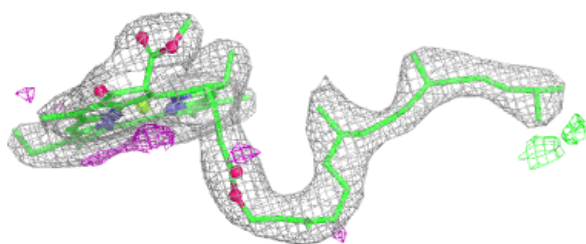
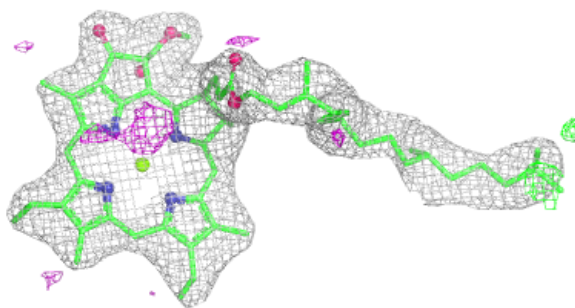
**Electron density around DGD C 517:**

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

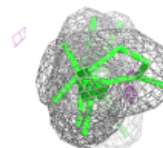
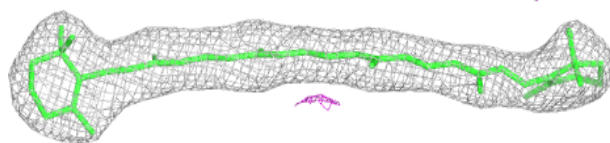
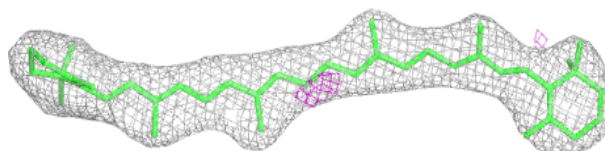


Electron density around CLA A 405:

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

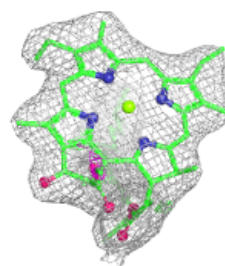
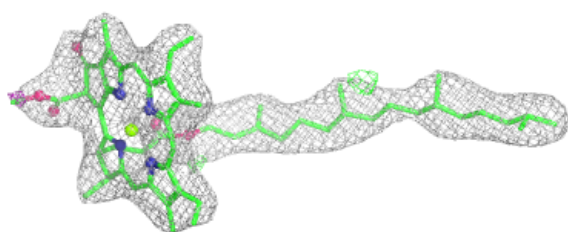
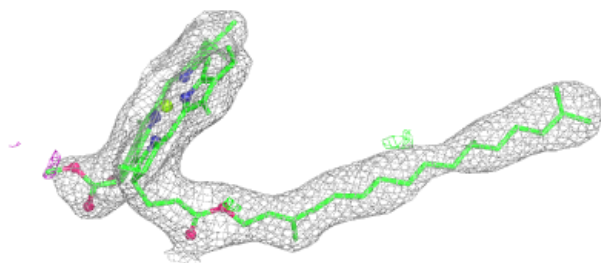
**Electron density around BCR B 618:**

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

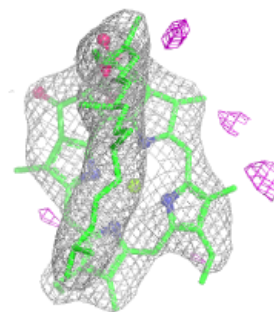
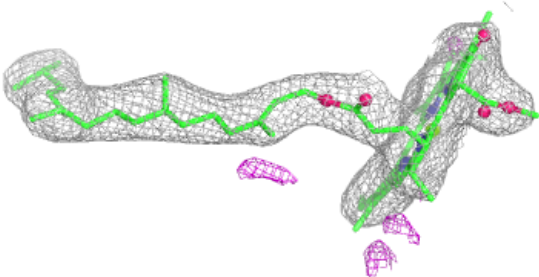
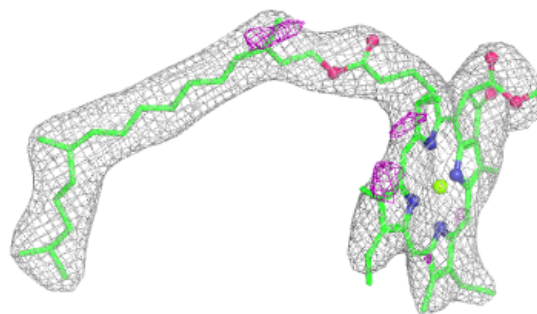


Electron density around CLA B 608:

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

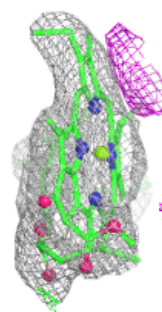
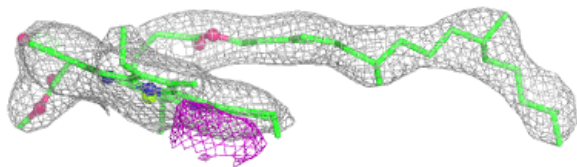
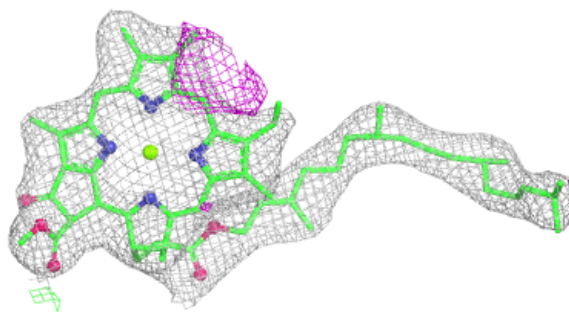
**Electron density around CLA B 610:**

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

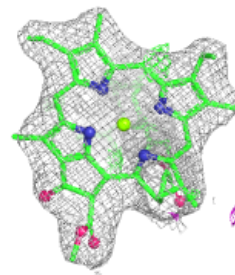
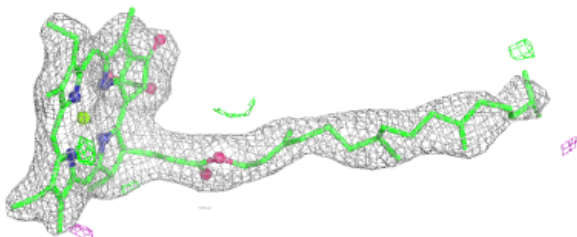
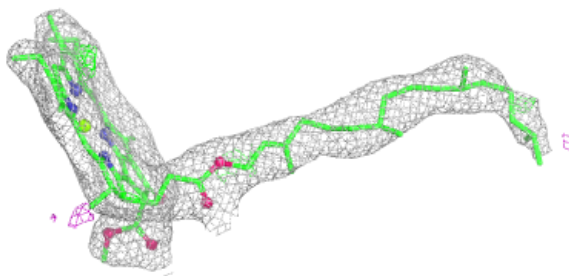


Electron density around CLA b 603:

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

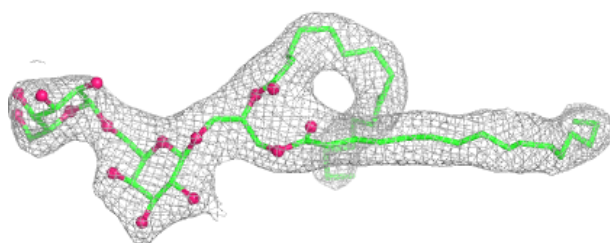
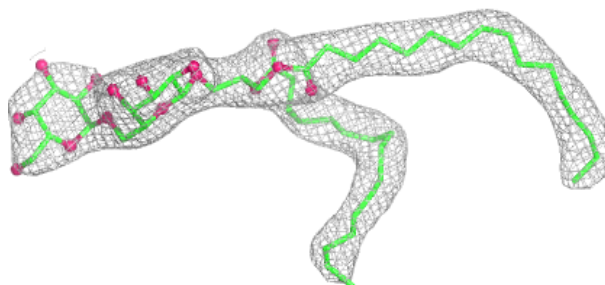
**Electron density around CLA b 604:**

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

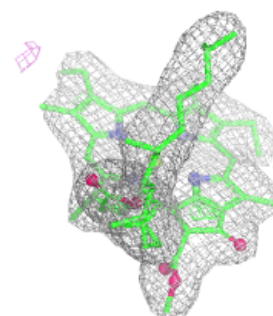
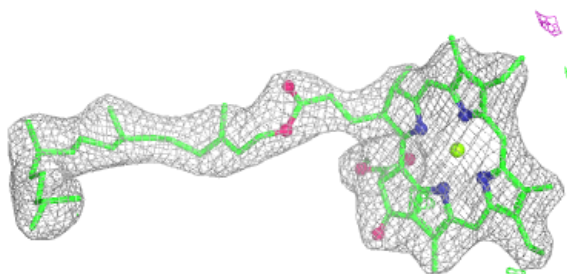
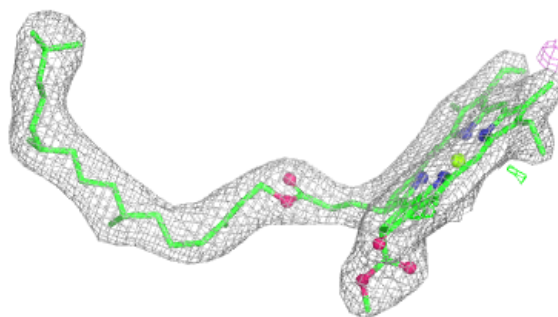


Electron density around DGD h 103:

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

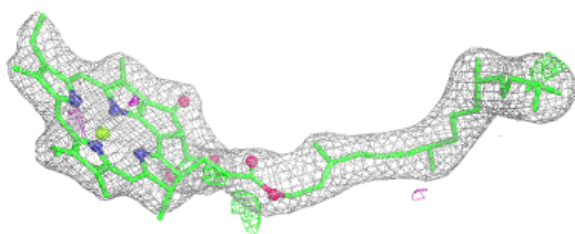
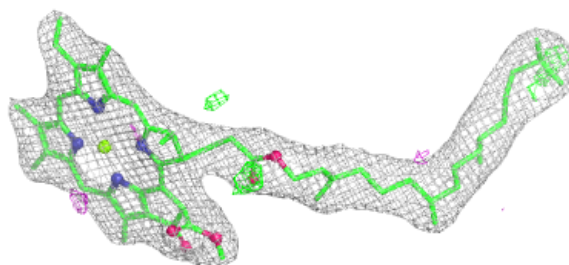
**Electron density around CLA D 404:**

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

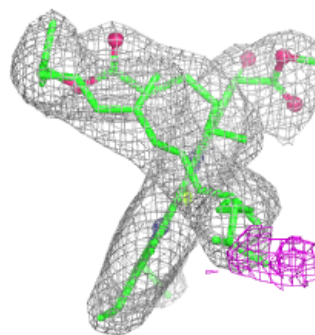
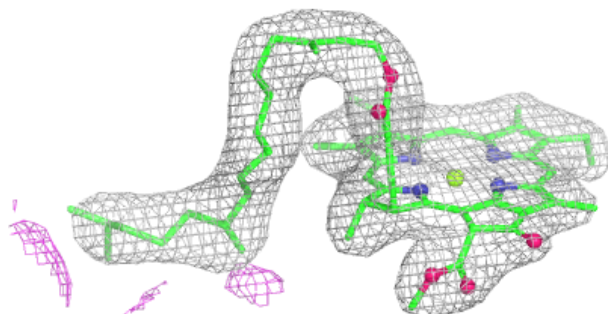
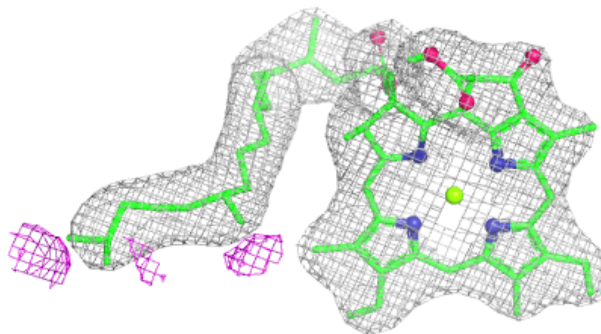


Electron density around CLA a 404:

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

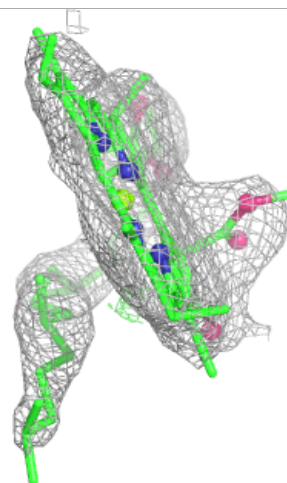
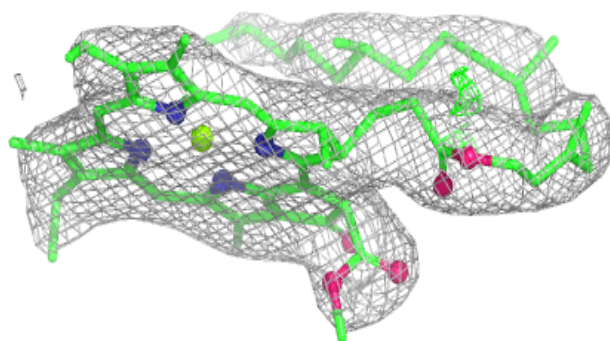
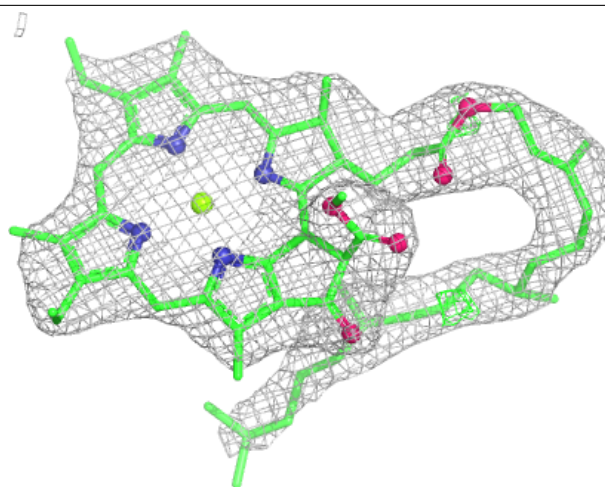
**Electron density around CLA a 405:**

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



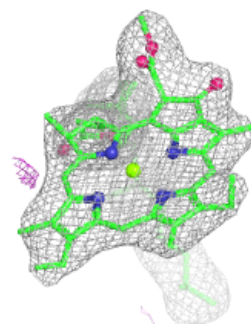
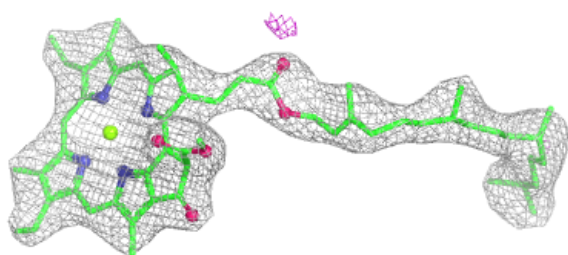
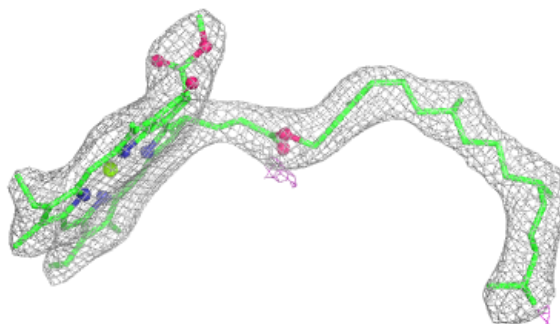
Electron density around CLA C 510:

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



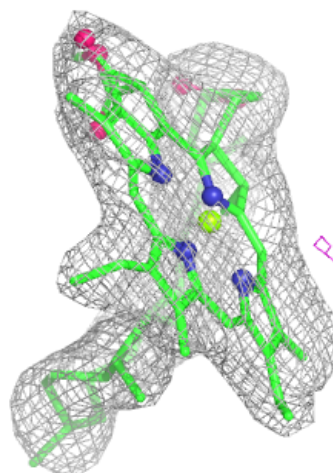
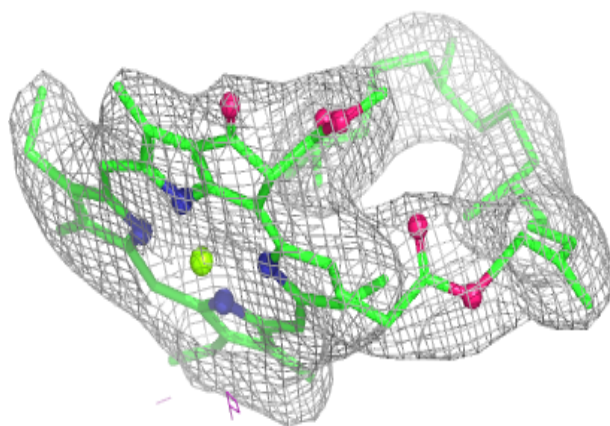
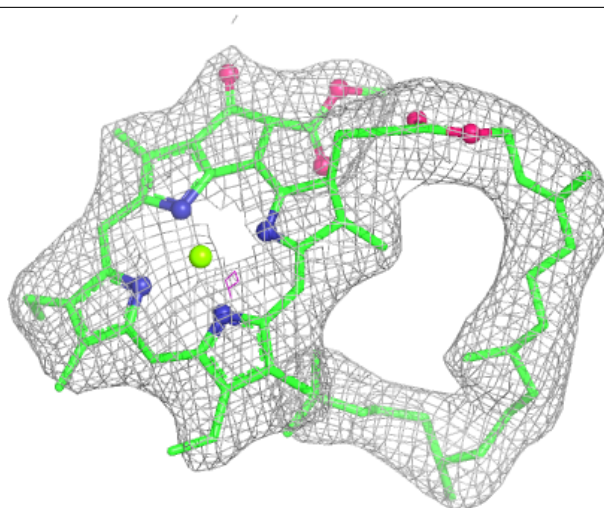
Electron density around CLA d 402:

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



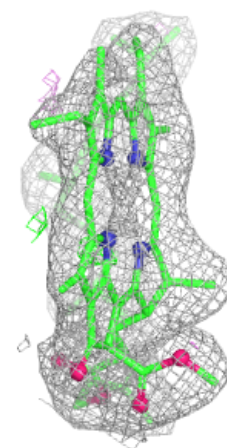
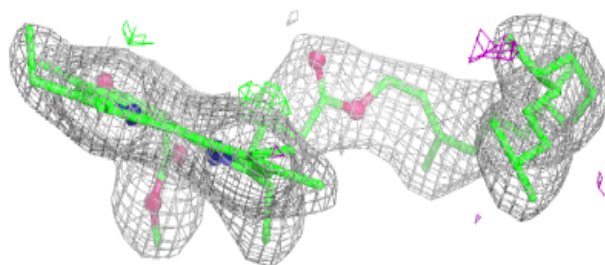
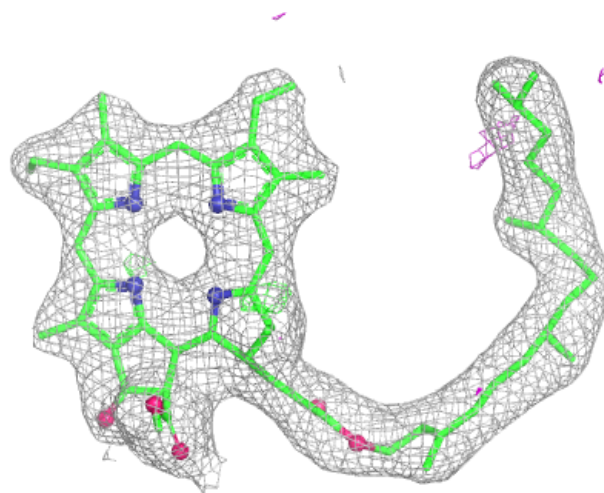
Electron density around CLA B 616:

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



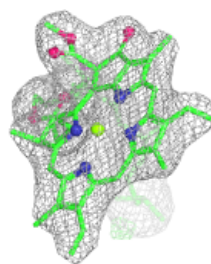
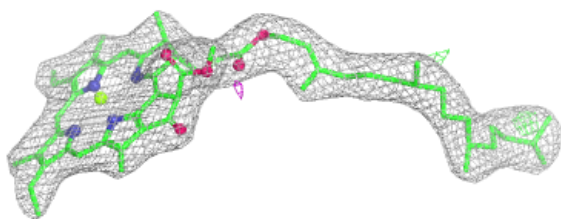
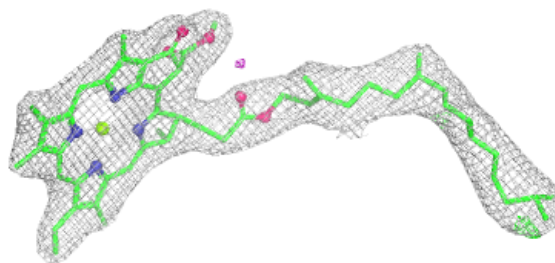
Electron density around PHO A 406:

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



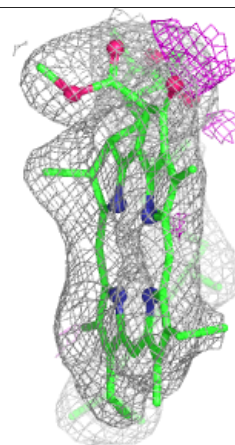
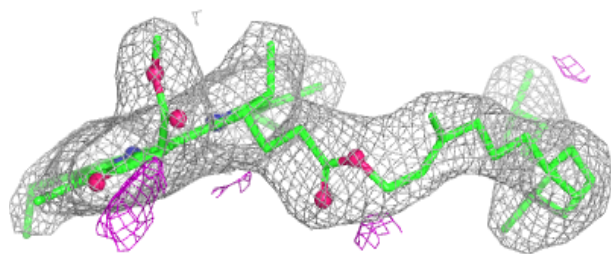
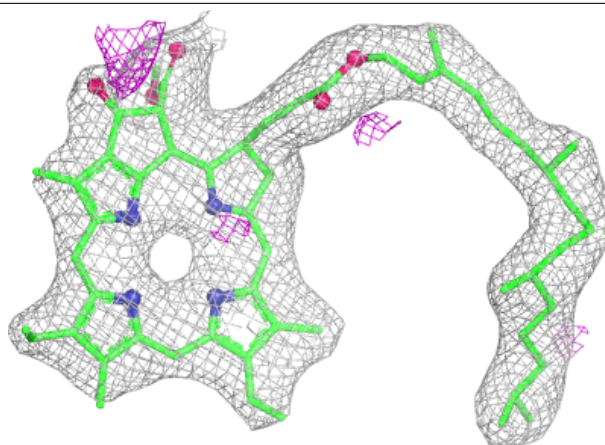
Electron density around CLA A 404:

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



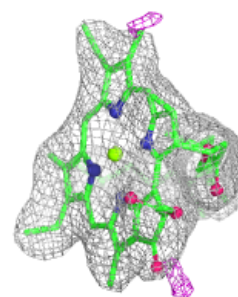
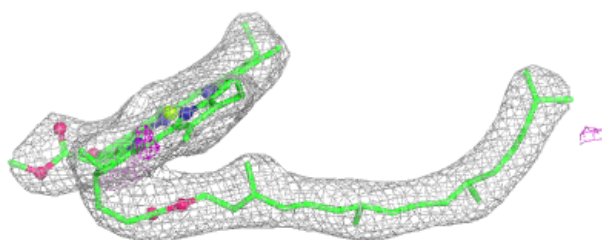
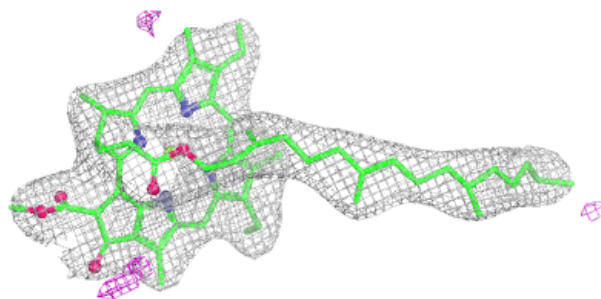
Electron density around PHO a 407:

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

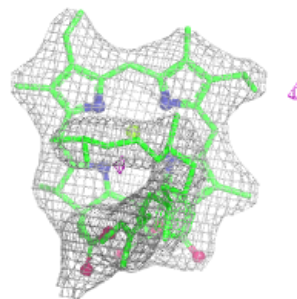
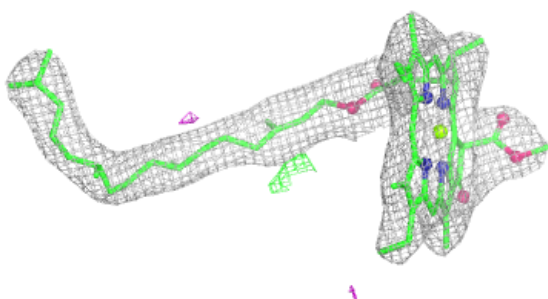
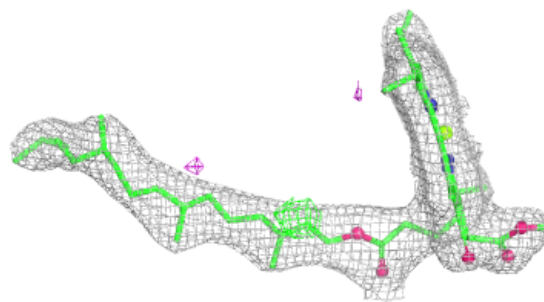


Electron density around CLA B 609:

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

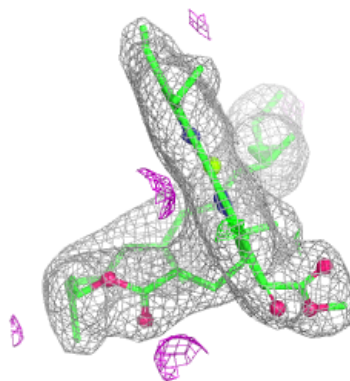
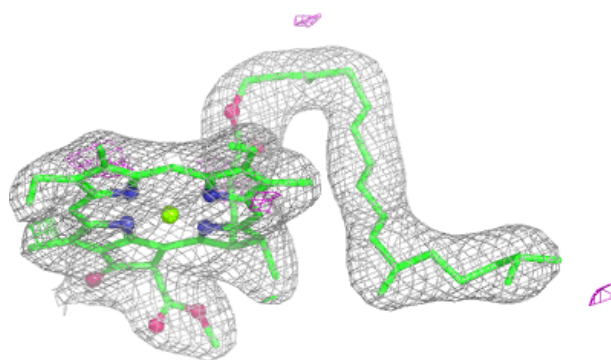
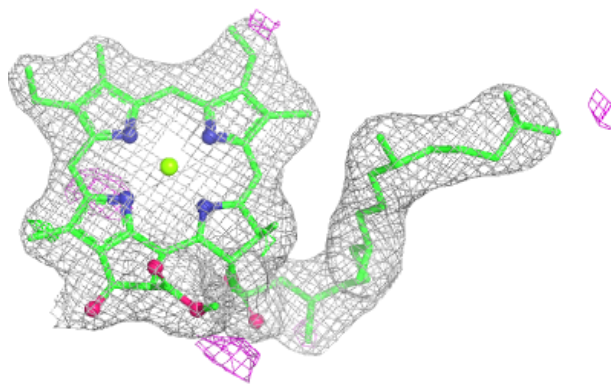
**Electron density around CLA B 606:**

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



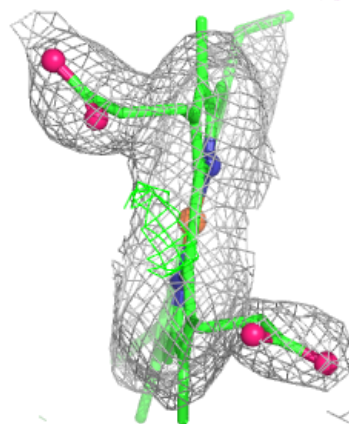
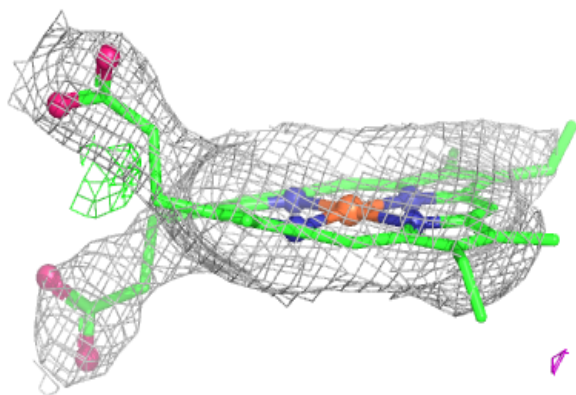
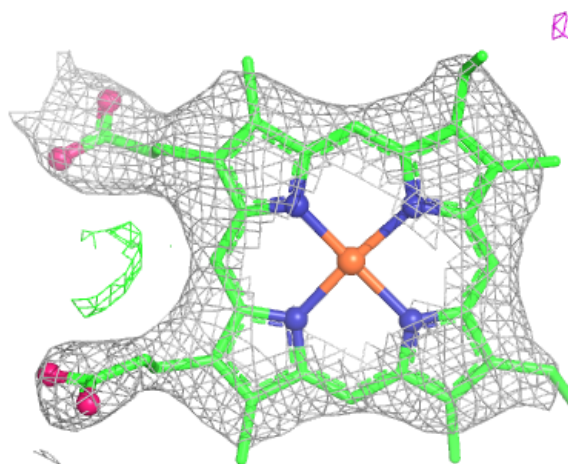
Electron density around CLA D 401:

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



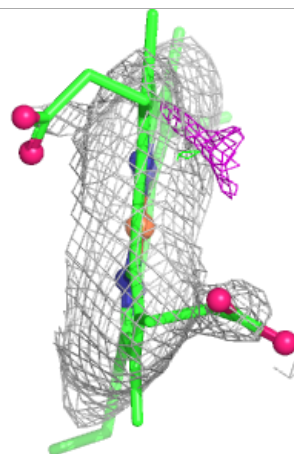
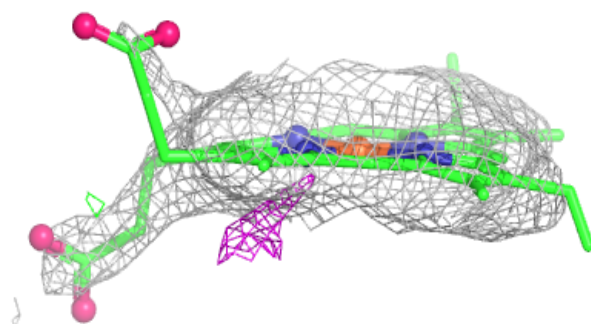
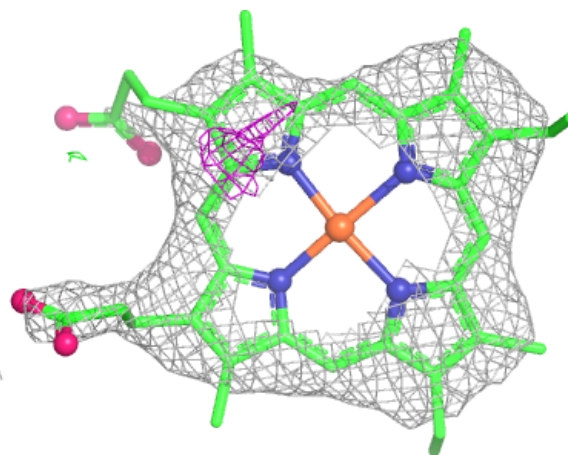
Electron density around HEM E 103:

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



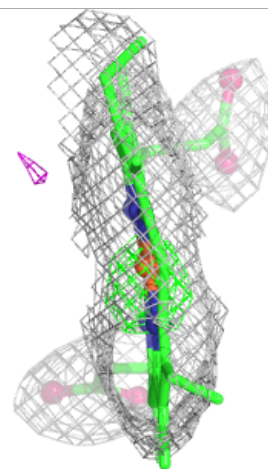
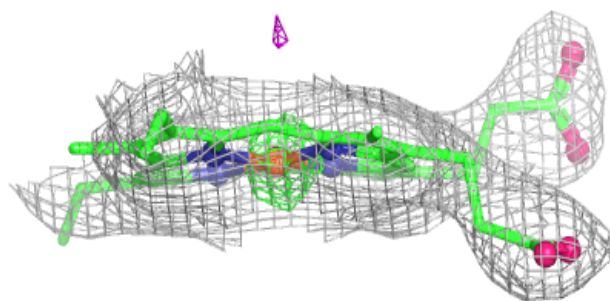
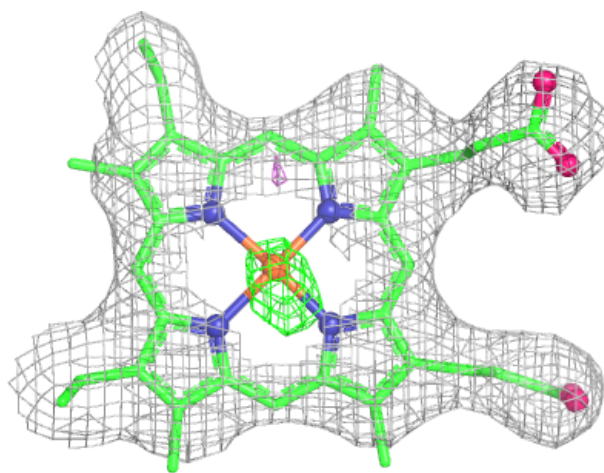
Electron density around HEM e 103:

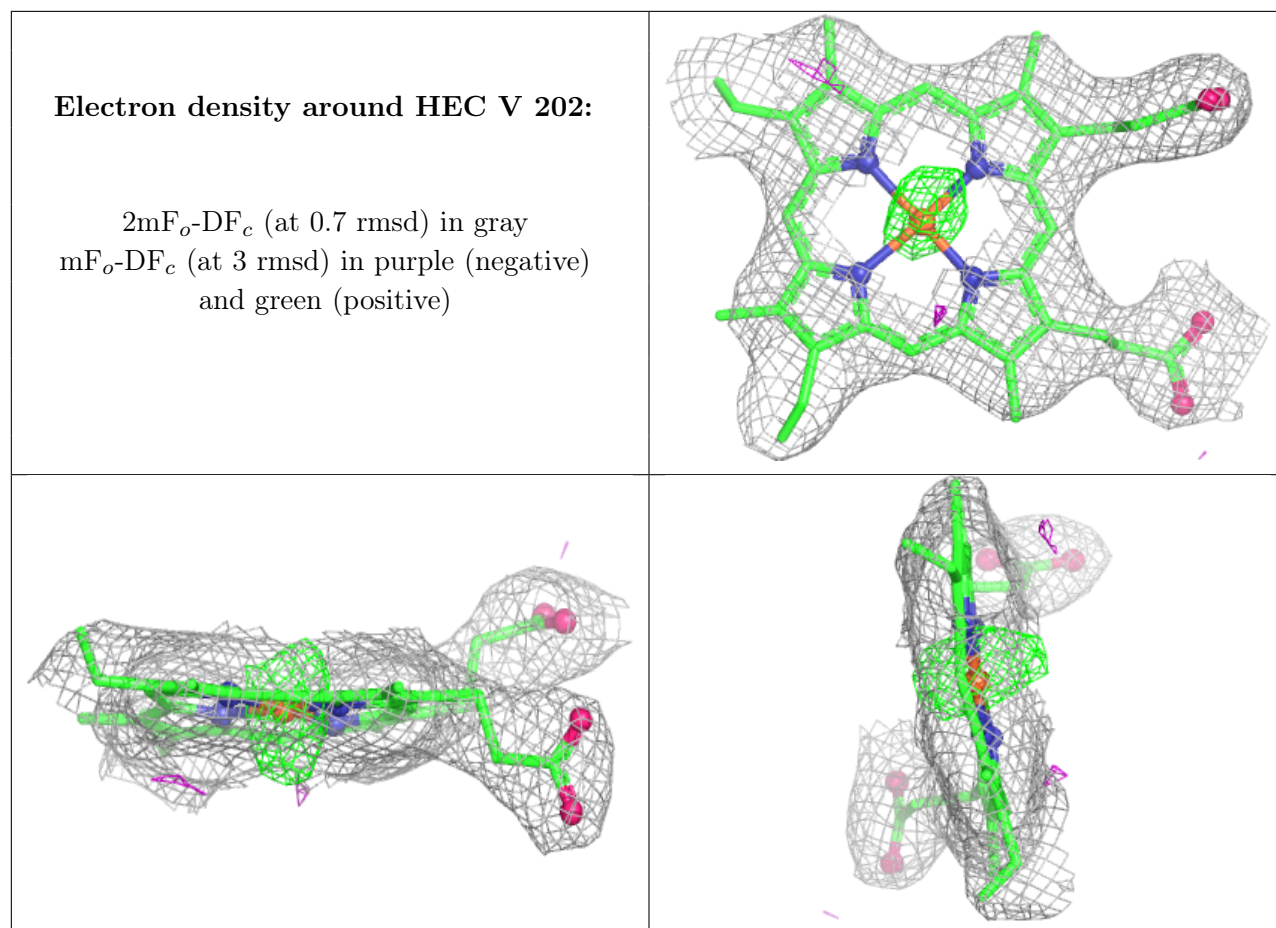
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC v 201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.