



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:54 AM UTC

PDB ID : 5GTH / pdb_00005gth
Title : Native XFEL structure of photosystem II (dark 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

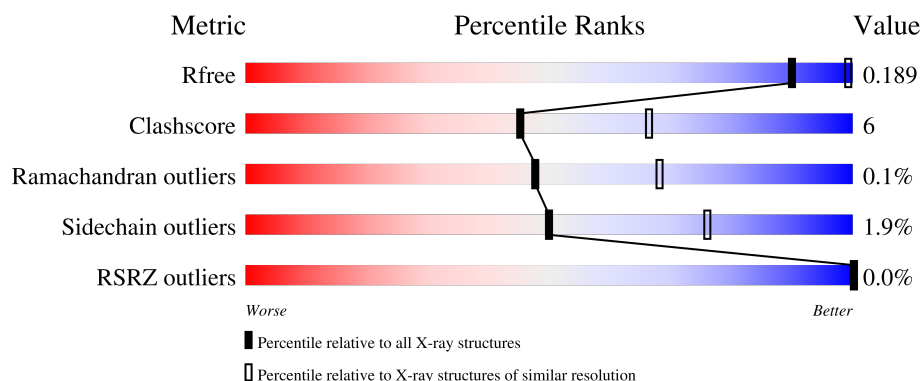
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

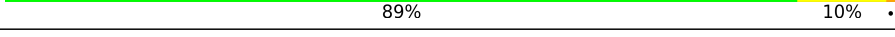
The reported resolution of this entry is 2.50 Å.

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	
1	a	344	
2	B	505	
2	b	505	
3	C	455	

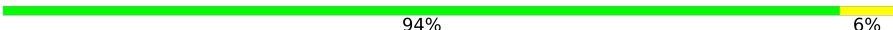
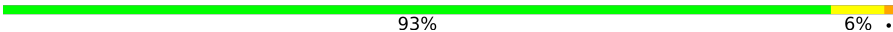
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Mol	Chain	Length	Quality of chain
3	c	455	90% 10% .
4	D	342	93% 7%
4	d	342	93% 7%
5	E	84	80% 17% .
5	e	84	79% 13% . 6%
6	F	44	61% 16% 23%
6	f	44	64% 7% 30%
7	H	65	2% 92% 6% .
7	h	65	85% 15%
8	I	38	82% 18%
8	i	38	76% 21% .
9	J	39	85% 10% . .
9	j	39	85% 15%
10	K	37	84% 14% .
10	k	37	70% 22% 8%
11	L	37	86% 11% .
11	l	37	92% 5% .
12	M	36	72% 19% 8%
12	m	36	69% 22% . 6%
13	O	244	85% 14%
13	o	244	86% 13%
14	T	32	81% 6% 6% 6%
14	t	32	81% 9% . 6%
15	U	104	78% 14% 8%
15	u	104	90% . 7%

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Mol	Chain	Length	Quality of chain
16	V	137	 94% 6%
16	v	137	 93% 6% .
17	X	40	 90% 5% 5%
17	x	40	 82% 12% 5%
18	Y	30	 73% 20% . .
18	y	30	 70% 27% .
19	Z	62	 85% 13% .
19	z	62	 85% 13% .
20	R	34	 85% 15%

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	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	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	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	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	C	513	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	408	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	c	513	X	-	-	-
23	CLA	d	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 52773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	5	0
			2639	1732	431	461	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	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	5	0
			3537	2317	589	618	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	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	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	1	0
			665	434	107	124			
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	1	0
			514	344	84	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 reaction center protein K.

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	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	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

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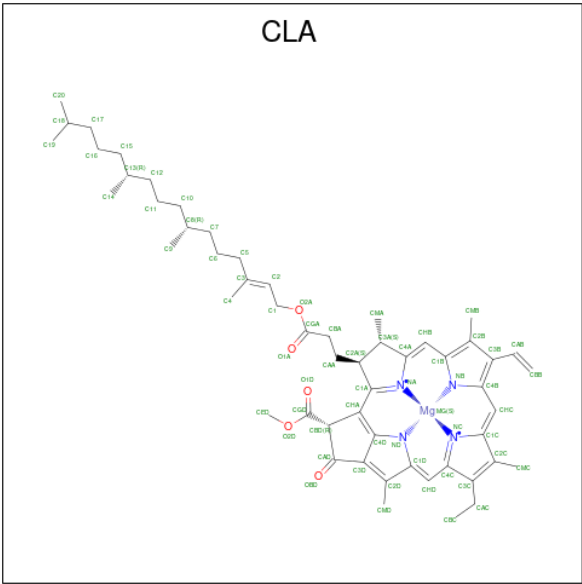
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- 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	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

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

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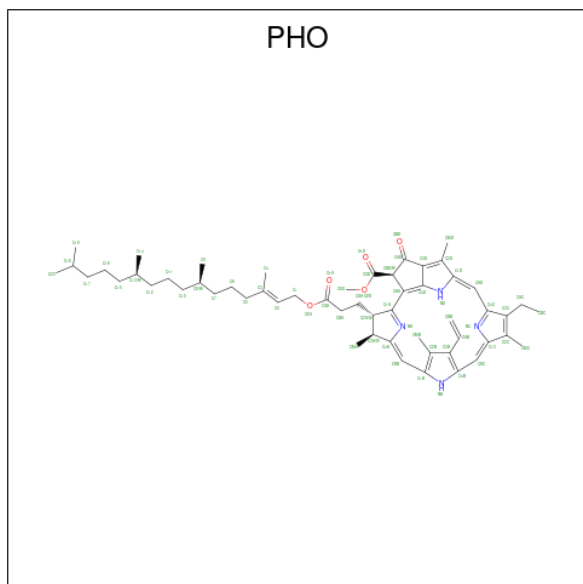
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

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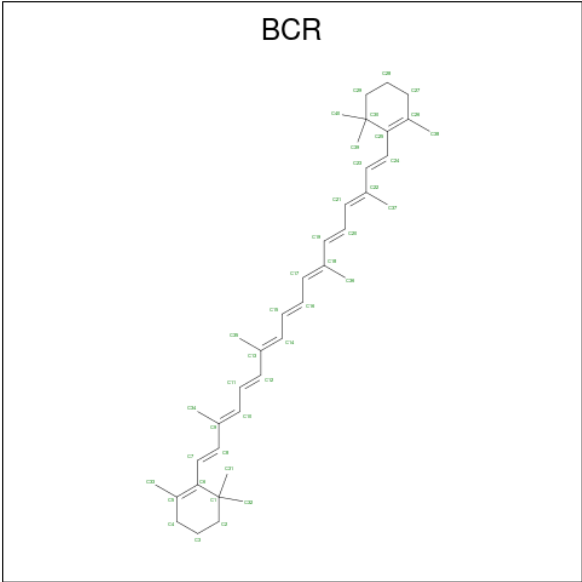
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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: $C_{40}H_{56}$).



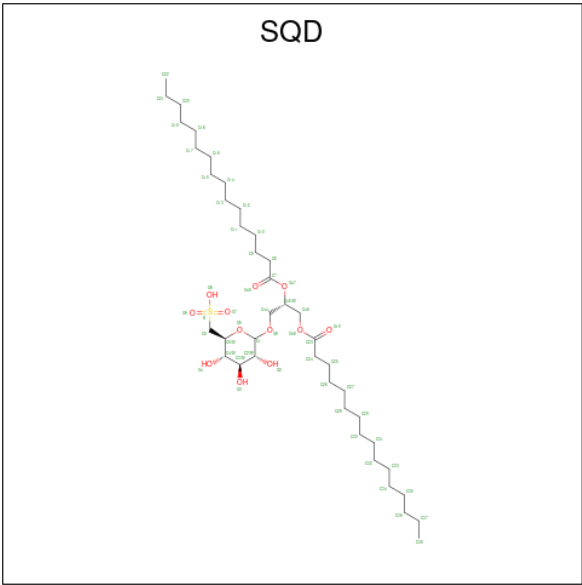
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
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-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



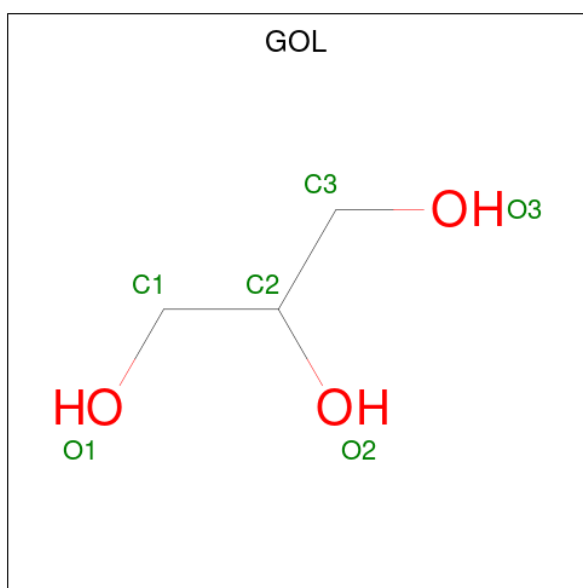
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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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: C₃H₈O₃).



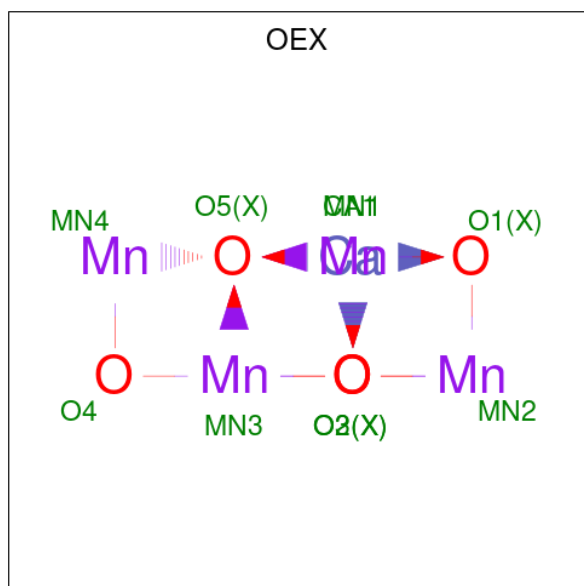
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

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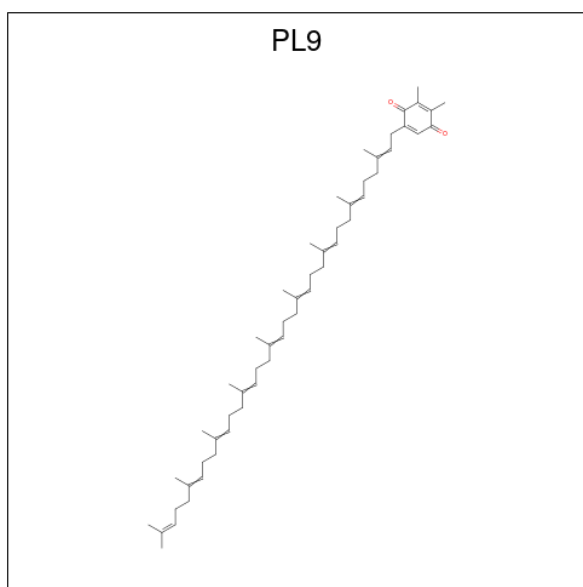
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	d	1	Total	C	O	0	0
			6	3	3		

- 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:).

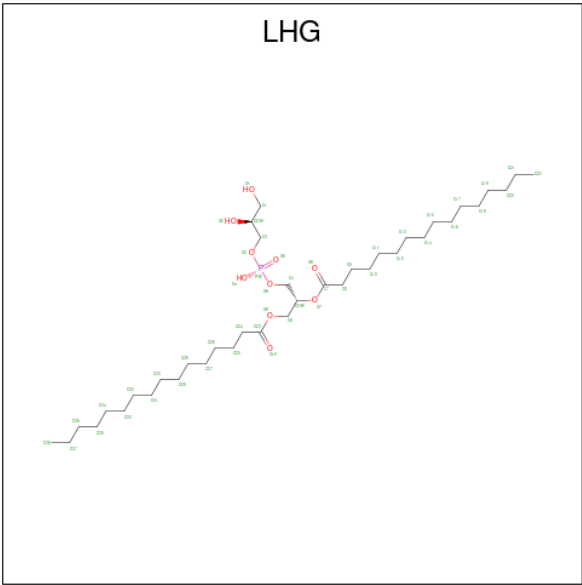
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
		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



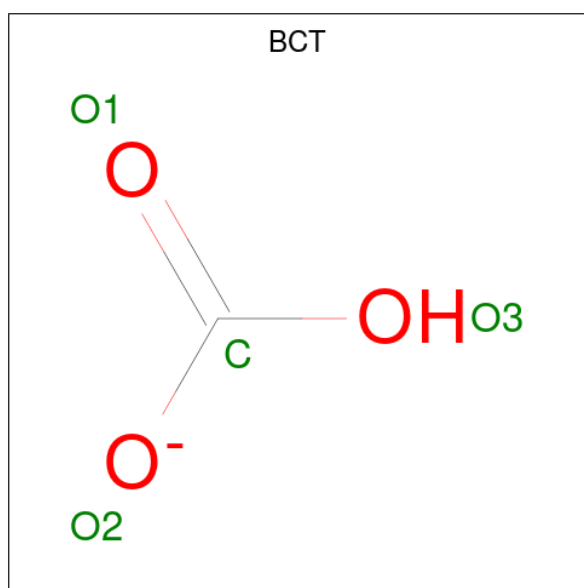
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		

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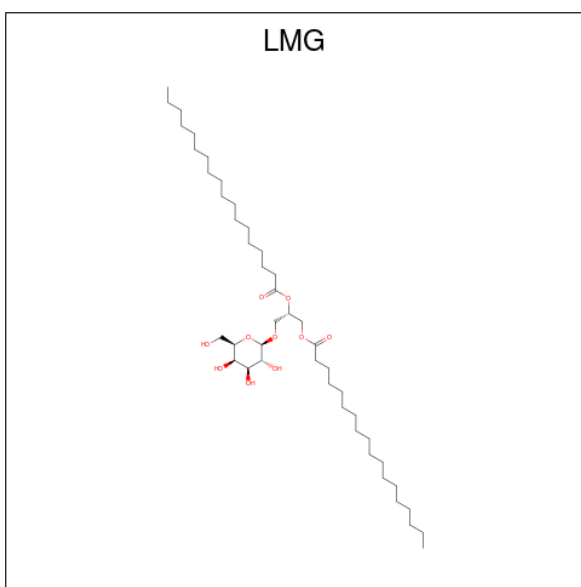
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0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

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



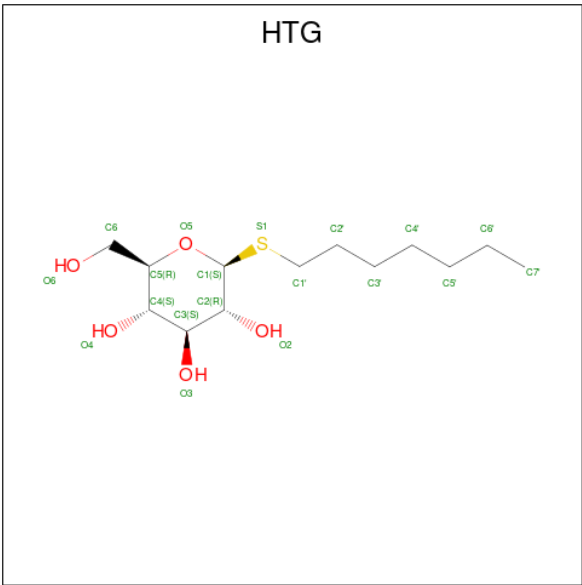
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



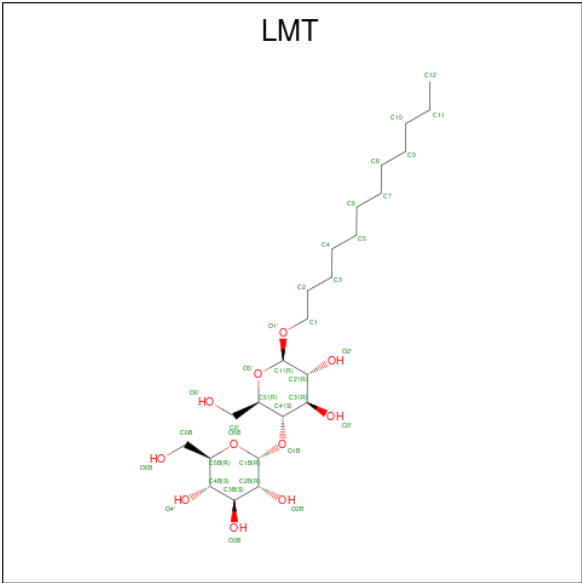
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	d	1	Total	C	O	S	0	0
			16	10	5	1		

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



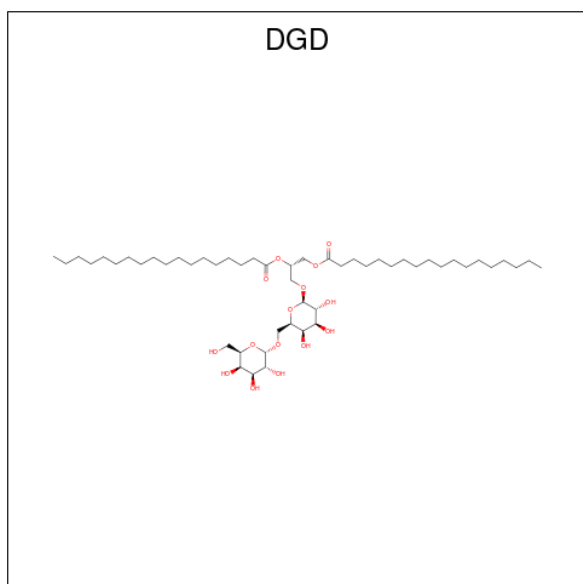
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O		0	0
			25	19	6			
35	B	1	Total	C	O		0	0
			35	24	11			
35	B	1	Total	C	O		0	0
			26	19	7			
35	D	1	Total	C	O		0	0
			35	24	11			
35	D	1	Total	C	O		0	0
			35	24	11			
35	E	1	Total	C	O		0	0
			35	24	11			
35	I	1	Total	C	O		0	0
			35	24	11			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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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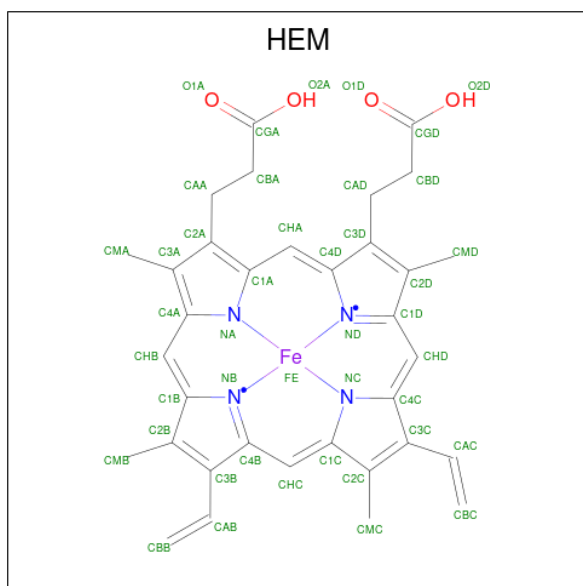
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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



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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 39 | J | 1 | Total Mg
1 1 | 0 | 0 |
| 39 | j | 1 | Total Mg
1 1 | 0 | 0 |

- [illegible]

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41 | A | 127 | Total O
127 127 | 0 | 0 |
| 41 | B | 175 | Total O
175 175 | 0 | 0 |
| 41 | C | 148 | Total O
148 148 | 0 | 0 |
| 41 | D | 111 | Total O
111 111 | 0 | 0 |
| 41 | E | 18 | Total O
18 18 | 0 | 0 |



WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	F	5	Total O 5 5	0	0
41	H	19	Total O 19 19	0	0
41	I	6	Total O 6 6	0	0
41	J	5	Total O 5 5	0	0
41	K	6	Total O 6 6	0	0
41	L	9	Total O 9 9	0	0
41	M	14	Total O 14 14	0	0
41	O	100	Total O 100 100	0	0
41	T	10	Total O 10 10	0	0
41	U	46	Total O 46 46	0	0
41	V	78	Total O 79 79	0	1
41	X	3	Total O 3 3	0	0
41	Y	1	Total O 1 1	0	0
41	a	130	Total O 130 130	0	0
41	b	192	Total O 192 192	0	0
41	c	136	Total O 136 136	0	0
41	d	108	Total O 108 108	0	0
41	e	15	Total O 15 15	0	0
41	f	5	Total O 5 5	0	0
41	h	28	Total O 28 28	0	0
41	i	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	j	3	Total 3	O 3	0	0
41	k	4	Total 4	O 4	0	0
41	l	7	Total 7	O 7	0	0
41	m	11	Total 11	O 11	0	0
41	o	109	Total 109	O 109	0	0
41	t	7	Total 7	O 7	0	0
41	u	64	Total 64	O 64	0	0
41	v	71	Total 71	O 71	0	0
41	x	4	Total 4	O 4	0	0
41	y	2	Total 2	O 2	0	0



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 89% 9% ..



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 90% 10% .



- Molecule 4: Photosystem II D2 protein

Chain D: 93% 7%



- Molecule 4: Photosystem II D2 protein

Chain d: 93% 7%



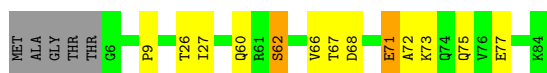
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 80% 17% .



- Molecule 5: Cytochrome b559 subunit alpha

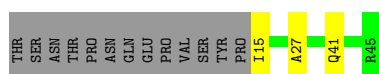
Chain e: 79% 13% 6%



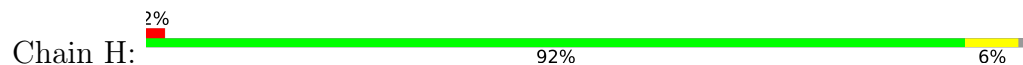
- Molecule 6: Cytochrome b559 subunit beta



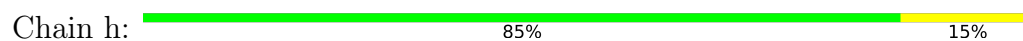
- Molecule 6: Cytochrome b559 subunit beta



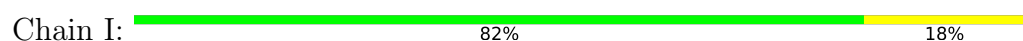
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



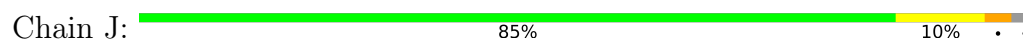
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





- Molecule 9: Photosystem II reaction center protein J

Chain j: 85% 15%



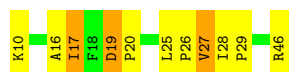
- Molecule 10: Photosystem II reaction center protein K

Chain K: 84% 14% .



- Molecule 10: Photosystem II reaction center protein K

Chain k: 70% 22% 8%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 86% 11% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 92% 5% .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 72% 19% 8%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 69% 22% . 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 85% 14%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 86% 13%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 6% 6% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 81% 9% 6%



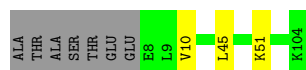
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 78% 14% 8%

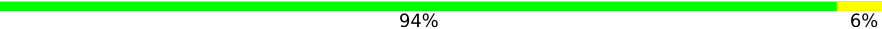


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 90% 7%



- Molecule 16: Cytochrome c-550

Chain V:  94% 6%



- Molecule 16: Cytochrome c-550

Chain v:  93% 6%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  90% 5% 5%



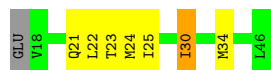
- Molecule 17: Photosystem II reaction center protein X

Chain x:  82% 12% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  73% 20% 7%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  70% 27% 3%

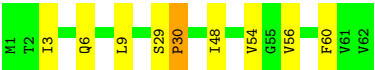
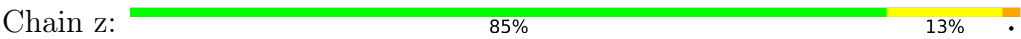


- Molecule 19: Photosystem II reaction center protein Z

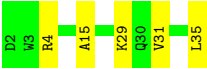
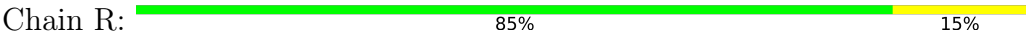
Chain Z:  85% 13% 2%



- 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	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.186 0.145 , 0.189	Depositor DCC
R_{free} test set	14615 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	52773	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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: CL, GOL, HEM, PHO, DGD, LMT, PL9, MG, CA, CLA, HEC, OEX, FME, UNL, FE2, BCT, LMG, SQD, HTG, LHG, BCR

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	0.57	0/2728	0.86	2/3719 (0.1%)
1	a	0.57	0/2739	0.84	1/3735 (0.0%)
2	B	0.52	0/4171	0.82	0/5683
2	b	0.52	0/4138	0.82	0/5640
3	C	0.50	1/3626 (0.0%)	0.84	1/4936 (0.0%)
3	c	0.51	0/3670	0.83	4/4996 (0.1%)
4	D	0.56	0/2827	0.84	4/3852 (0.1%)
4	d	0.56	0/2818	0.82	2/3840 (0.1%)
5	E	0.46	0/687	0.84	0/936
5	e	0.43	0/667	0.80	0/908
6	F	0.51	0/284	0.75	0/387
6	f	0.45	0/257	0.77	0/349
7	H	0.47	0/530	0.80	0/723
7	h	0.42	0/524	0.78	0/713
8	I	0.46	0/311	0.79	0/419
8	i	0.47	0/311	0.80	0/419
9	J	0.43	0/278	0.74	0/376
9	j	0.48	0/283	0.78	0/383
10	K	0.49	0/303	0.85	0/416
10	k	0.47	0/303	0.91	0/416
11	L	0.50	0/311	0.71	0/423
11	l	0.46	0/311	0.73	0/423
12	M	0.59	0/261	0.85	0/357
12	m	0.56	0/262	0.99	2/357 (0.6%)
13	O	0.46	0/1935	0.82	2/2623 (0.1%)
13	o	0.45	0/1910	0.82	2/2589 (0.1%)
14	T	0.58	0/257	0.75	0/349
14	t	0.58	0/257	0.80	0/349
15	U	0.48	0/776	0.81	0/1052
15	u	0.50	0/785	0.78	0/1064
16	V	0.51	0/1085	0.80	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.48	0/1085	0.81	0/1473
17	X	0.45	0/284	0.80	0/384
17	x	0.40	0/284	0.82	0/384
18	Y	0.42	0/216	0.78	0/289
18	y	0.44	0/216	0.83	0/289
19	Z	0.45	0/490	0.84	1/669 (0.1%)
19	z	0.42	0/490	0.85	0/669
20	R	0.44	0/279	0.75	0/383
All	All	0.51	1/42949 (0.0%)	0.82	21/58445 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	ILE	CA-CB	5.02	1.56	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	17	VAL	CA-C-N	-6.40	112.41	119.19
12	m	17	VAL	C-N-CA	-6.40	112.41	119.19
1	A	142	TRP	N-CA-C	6.33	120.62	113.02
3	C	193	GLY	N-CA-C	-6.25	104.77	112.33
3	c	333	GLY	CA-C-N	6.25	126.72	119.47
3	c	333	GLY	C-N-CA	6.25	126.72	119.47
4	D	170	ALA	CA-C-N	-6.23	113.56	119.85
4	D	170	ALA	C-N-CA	-6.23	113.56	119.85
4	D	94	GLY	CA-C-N	6.01	126.12	119.87
4	D	94	GLY	C-N-CA	6.01	126.12	119.87
13	o	55	GLU	CA-C-N	5.69	125.62	119.76
13	o	55	GLU	C-N-CA	5.69	125.62	119.76
19	Z	61	VAL	N-CA-C	-5.57	107.85	113.20
1	A	176	ILE	N-CA-C	5.50	115.64	110.30
3	c	76	ILE	CA-C-N	5.47	125.81	119.47
3	c	76	ILE	C-N-CA	5.47	125.81	119.47
4	d	170	ALA	CA-C-N	-5.11	114.69	119.85
4	d	170	ALA	C-N-CA	-5.11	114.69	119.85
1	a	142	TRP	N-CA-C	5.09	119.12	113.02
13	O	55	GLU	CA-C-N	5.08	125.01	119.78
13	O	55	GLU	C-N-CA	5.08	125.01	119.78

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	2634	0	2546	24	0
1	a	2639	0	2554	26	0
2	B	4007	0	3879	42	0
2	b	3986	0	3855	44	0
3	C	3501	0	3428	31	0
3	c	3537	0	3471	31	0
4	D	2729	0	2632	18	0
4	d	2720	0	2626	17	0
5	E	665	0	653	11	0
5	e	648	0	634	14	0
6	F	275	0	282	6	0
6	f	250	0	261	2	0
7	H	514	0	542	4	0
7	h	511	0	532	11	0
8	I	314	0	328	3	0
8	i	314	0	328	4	0
9	J	272	0	279	3	0
9	j	277	0	284	4	0
10	K	293	0	305	4	0
10	k	293	0	305	8	0
11	L	301	0	315	3	0
11	l	301	0	315	2	0
12	M	265	0	286	4	0
12	m	269	0	288	7	0
13	O	1889	0	1871	22	0
13	o	1873	0	1852	18	0
14	T	258	0	261	5	0
14	t	258	0	261	3	0
15	U	765	0	767	7	0
15	u	774	0	773	2	0
16	V	1064	0	1073	5	0
16	v	1064	0	1073	5	0
17	X	281	0	312	2	0
17	x	281	0	312	6	0
18	Y	215	0	246	5	0
18	y	215	0	246	4	0
19	Z	479	0	516	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	479	0	516	4	0
20	R	273	0	305	5	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	260	0	288	12	0
23	B	1040	0	1152	40	0
23	C	845	0	936	42	0
23	D	130	0	144	3	0
23	a	195	0	216	9	0
23	b	1040	0	1152	37	0
23	c	845	0	936	45	0
23	d	195	0	216	12	0
24	A	64	0	74	2	0
24	D	64	0	74	1	0
24	a	128	0	148	4	0
25	A	40	0	56	1	0
25	B	120	0	168	8	0
25	C	80	0	112	5	0
25	D	40	0	56	2	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0
25	T	40	0	56	5	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	7	0
25	c	80	0	112	10	0
25	d	40	0	56	5	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
25	t	40	0	56	3	0
25	y	40	0	56	1	0
26	A	108	0	156	6	0
26	B	54	0	78	2	0
26	D	43	0	53	1	0
26	L	54	0	78	5	0
26	a	108	0	156	4	0
26	f	43	0	53	0	0
27	A	6	0	8	0	0
27	B	12	0	16	2	0
27	C	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
29	A	55	0	80	6	0
29	D	55	0	80	3	0
29	a	55	0	80	4	0
29	d	55	0	80	0	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	98	0	148	5	0
31	D	98	0	148	6	0
31	E	42	0	57	1	0
31	d	147	0	222	10	0
31	e	42	0	57	2	0
31	l	49	0	74	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	51	0	72	1	0
33	C	102	0	144	7	0
33	J	51	0	72	3	0
33	Z	88	0	116	3	0
33	a	51	0	72	4	0
33	b	51	0	72	1	0
33	c	102	0	144	2	0
33	j	51	0	72	2	0
33	z	39	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	76	0	104	6	0
34	C	38	0	52	1	0
34	D	16	0	17	0	0
34	V	11	0	10	0	0
34	b	76	0	104	4	0
34	c	38	0	52	2	0
34	d	16	0	17	1	0
35	B	86	0	116	4	0
35	D	70	0	92	4	0
35	E	35	0	46	1	0
35	I	35	0	46	1	0
35	M	70	0	92	3	0
35	a	35	0	46	0	0
35	b	50	0	70	1	0
35	e	35	0	46	0	0
35	m	35	0	46	0	0
36	C	186	0	246	8	0
36	H	62	0	82	1	0
36	c	186	0	246	8	0
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0
37	V	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
38	E	43	0	30	3	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	127	0	0	2	0
41	B	175	0	0	1	0
41	C	148	0	0	1	0
41	D	111	0	0	0	0
41	E	18	0	0	1	0
41	F	5	0	0	0	0
41	H	19	0	0	0	0
41	I	6	0	0	1	0
41	J	5	0	0	1	0
41	K	6	0	0	0	0
41	L	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	M	14	0	0	1	0
41	O	100	0	0	1	0
41	T	10	0	0	0	0
41	U	46	0	0	0	0
41	V	79	0	0	1	0
41	X	3	0	0	0	0
41	Y	1	0	0	0	0
41	a	130	0	0	2	0
41	b	192	0	0	5	0
41	c	136	0	0	1	0
41	d	108	0	0	1	0
41	e	15	0	0	0	0
41	f	5	0	0	0	0
41	h	28	0	0	0	0
41	i	4	0	0	0	0
41	j	3	0	0	0	0
41	k	4	0	0	0	0
41	l	7	0	0	0	0
41	m	11	0	0	1	0
41	o	109	0	0	0	0
41	t	7	0	0	1	0
41	u	64	0	0	0	0
41	v	71	0	0	2	0
41	x	4	0	0	0	0
41	y	2	0	0	0	0
All	All	52773	0	52080	604	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 (604) 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)
23:B:604:CLA:H42	23:B:605:CLA:H2	1.46	0.95
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.52	0.91
2:b:224:ARG:HH11	35:b:621:LMT:H12	1.41	0.84
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.27	0.81
34:B:622:HTG:H1	35:B:630:LMT:H21	1.60	0.81
4:d:192:THR:HG23	23:d:403:CLA:HBC2	1.66	0.76
26:A:410:SQD:H251	31:D:409:LHG:H131	1.66	0.75
5:e:67:THR:H	5:e:75:GLN:HE22	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:OD1	41:A:501:HOH:O	2.05	0.75
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.69	0.75
5:e:9:PRO:HA	31:e:101:LHG:HC31	1.70	0.74
41:M:205:HOH:O	14:T:1:FME:SD	2.45	0.74
13:O:54:GLU:HG2	13:O:64:GLU:H	1.53	0.73
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.70	0.72
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.71	0.72
13:o:124:ASN:HD22	13:o:147:ASN:HD22	1.35	0.72
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.20	0.72
23:c:503:CLA:HBB1	23:c:512:CLA:H41	1.71	0.71
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.71	0.71
23:c:508:CLA:HBC3	23:c:510:CLA:H71	1.73	0.70
23:c:513:CLA:HBB1	25:c:514:BCR:H371	1.73	0.70
5:E:40:THR:HB	20:R:4:ARG:HG2	1.72	0.70
3:c:279:LEU:HD22	23:c:509:CLA:HED2	1.74	0.70
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.73	0.69
16:v:30:LYS:NZ	41:v:301:HOH:O	2.25	0.69
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.26	0.69
6:F:30:THR:HG21	33:J:101:LMG:H412	1.74	0.69
3:c:168:LEU:HD21	23:c:509:CLA:H61	1.75	0.68
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.75	0.67
25:B:618:BCR:H363	25:t:101:BCR:H19C	1.76	0.67
3:C:279:LEU:HD22	23:C:510:CLA:HED2	1.77	0.66
8:I:37:LEU:O	41:I:201:HOH:O	2.14	0.66
12:m:5:GLN:H	12:m:5:GLN:HE21	1.42	0.66
29:A:414:PL9:H253	23:D:404:CLA:H141	1.78	0.66
31:D:409:LHG:H132	31:D:409:LHG:H372	1.78	0.66
23:c:510:CLA:HBC3	23:c:510:CLA:H192	1.79	0.65
8:i:36:ASP:OD1	8:i:36:ASP:N	2.29	0.65
2:b:497:GLN:HB2	2:b:504:THR:HB	1.79	0.65
4:D:205:LEU:HD13	24:D:401:PHO:HAB	1.79	0.65
23:B:601:CLA:H12	23:B:601:CLA:H71	1.79	0.64
24:A:407:PHO:H3A	23:D:404:CLA:H142	1.80	0.63
23:A:408:CLA:H172	36:C:517:DGD:HAF1	1.79	0.63
13:o:124:ASN:ND2	13:o:147:ASN:HD22	1.96	0.63
23:A:408:CLA:H171	23:C:507:CLA:H142	1.81	0.63
8:i:35:LYS:O	8:i:37:LEU:N	2.32	0.63
3:C:286:ALA:HB2	23:C:503:CLA:HMD1	1.81	0.63
31:d:409:LHG:H372	31:d:409:LHG:H142	1.80	0.63
13:O:27:ARG:NH1	13:O:202:ALA:O	2.32	0.62
33:C:501:LMG:H211	36:C:517:DGD:HA82	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:513:CLA:HBB1	25:c:514:BCR:H24C	1.82	0.62
23:c:501:CLA:C4D	23:c:503:CLA:H2	2.30	0.62
23:C:506:CLA:HMD3	23:C:508:CLA:HAB	1.81	0.62
23:b:604:CLA:H42	23:b:605:CLA:H2	1.81	0.62
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.82	0.61
1:a:40:THR:HG23	23:a:408:CLA:HBB1	1.81	0.61
2:B:24:LEU:HD21	23:B:616:CLA:HAB	1.82	0.61
23:c:505:CLA:CMD	23:c:507:CLA:HAB	2.31	0.61
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.82	0.61
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.83	0.61
3:c:182:PHE:HA	34:c:521:HTG:H61	1.83	0.61
16:V:118:HIS:ND1	41:V:301:HOH:O	2.31	0.61
23:A:406:CLA:H152	29:A:414:PL9:H252	1.82	0.60
3:C:218:PHE:HE2	33:C:501:LMG:H111	1.67	0.60
2:B:285:ASN:O	2:B:289:GLN:HG2	2.01	0.60
23:d:404:CLA:H162	7:h:37:LEU:HD21	1.84	0.59
31:D:408:LHG:HC62	11:L:15:THR:HG23	1.85	0.59
13:O:124:ASN:ND2	13:O:147:ASN:HD22	1.97	0.59
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.38	0.59
34:B:623:HTG:O6	13:O:177:ALA:O	2.21	0.59
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.84	0.59
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.15	0.58
5:e:60:GLN:HG3	5:e:62:SER:H	1.68	0.58
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.32	0.58
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.69	0.58
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.86	0.57
5:e:27:ILE:HD11	38:e:103:HEM:HBC2	1.85	0.57
25:t:101:BCR:H321	25:t:101:BCR:HC8	1.84	0.57
33:Z:102:LMG:O5	33:Z:102:LMG:O4	2.23	0.57
12:M:8:LEU:HD11	35:M:103:LMT:H91	1.85	0.57
3:c:438:LEU:HD11	23:c:505:CLA:HBB1	1.86	0.57
26:L:101:SQD:O9	2:b:18:ARG:NH2	2.28	0.57
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.85	0.57
31:A:417:LHG:H201	11:L:26:VAL:HG11	1.87	0.56
13:O:92:SER:HB3	13:O:131:PRO:HA	1.88	0.56
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.70	0.56
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.88	0.56
2:b:24:LEU:HD21	23:b:616:CLA:HAB	1.86	0.56
3:c:286:ALA:HB2	23:c:502:CLA:HMD1	1.87	0.56
26:a:410:SQD:H301	23:c:508:CLA:H71	1.88	0.56
3:c:213[B]:LEU:HD11	25:c:515:BCR:H373	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.87	0.56
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.88	0.56
7:h:56:ASP:OD1	17:x:2:THR:OG1	2.23	0.56
23:c:501:CLA:HHC	23:c:501:CLA:HBB1	1.87	0.55
5:E:27:ILE:HD11	38:E:103:HEM:HBC2	1.88	0.55
31:A:417:LHG:H191	29:D:407:PL9:H201	1.88	0.55
8:i:2:GLU:O	8:i:6:ILE:HG12	2.06	0.55
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.89	0.55
3:C:182:PHE:HA	34:C:521:HTG:H61	1.87	0.55
1:a:310:LYS:NZ	41:a:507:HOH:O	2.40	0.55
1:a:45:THR:HG23	23:d:401:CLA:H201	1.89	0.55
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.20	0.55
23:c:509:CLA:H192	23:c:512:CLA:HHD	1.89	0.55
1:A:187:GLN:HB2	23:A:404:CLA:HAC2	1.88	0.55
23:b:601:CLA:HAC1	25:h:101:BCR:H383	1.89	0.55
4:d:24:ARG:HD3	17:x:37:VAL:HG22	1.89	0.55
25:d:405:BCR:H383	33:j:101:LMG:H171	1.90	0.54
18:Y:23:THR:HB	18:Y:24:MET:HE2	1.89	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.54
16:V:6:GLU:N	16:V:6:GLU:OE2	2.40	0.54
1:a:160:ILE:HD11	36:c:516:DGD:HBT2	1.89	0.54
23:B:604:CLA:HBB1	23:B:604:CLA:HMB1	1.89	0.54
23:C:513:CLA:O2D	23:C:514:CLA:HBB2	2.08	0.54
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.70	0.54
23:b:602:CLA:H101	23:b:609:CLA:H193	1.90	0.54
2:B:57:ARG:HH21	2:B:331:ASN:HD22	1.56	0.54
5:e:60:GLN:NE2	5:e:62:SER:HB3	2.22	0.54
3:c:174:LEU:HB3	23:c:502:CLA:H152	1.90	0.53
23:C:507:CLA:H71	35:I:101:LMT:H111	1.89	0.53
2:b:171:PRO:HD3	7:h:66:GLY:HA2	1.89	0.53
23:c:506:CLA:H71	25:c:515:BCR:H10C	1.90	0.53
23:b:612:CLA:H171	23:b:613:CLA:HBB2	1.90	0.53
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.39	0.53
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.91	0.53
13:O:32:ILE:HG13	13:O:93:LEU:HD11	1.91	0.53
23:A:408:CLA:H152	36:C:517:DGD:HAW2	1.91	0.52
25:D:406:BCR:H383	33:J:101:LMG:H171	1.90	0.52
14:T:2:GLU:H	14:T:2:GLU:CD	2.17	0.52
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.44	0.52
2:B:489:GLU:HG2	2:B:495:PHE:CE2	2.43	0.52
3:c:181:PHE:HE2	34:c:522:HTG:H7'3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:17:LEU:HD22	8:I:21:PHE:HE2	1.75	0.52
23:c:501:CLA:C3D	23:c:503:CLA:H2	2.40	0.52
25:d:405:BCR:H391	9:j:20:VAL:HG13	1.91	0.52
23:B:614:CLA:H43	26:B:620:SQD:H111	1.91	0.52
33:b:620:LMG:O2	41:b:701:HOH:O	2.19	0.52
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.09	0.52
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.45	0.52
3:C:223:TRP:CG	3:C:224:ILE:H	2.28	0.52
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.91	0.52
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.92	0.52
3:c:223:TRP:CG	3:c:224:ILE:H	2.28	0.52
4:d:103:ARG:HH21	5:e:77:GLU:HG3	1.74	0.52
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.92	0.52
2:b:299:GLU:HG3	41:b:879:HOH:O	2.09	0.52
5:E:27:ILE:CD1	38:E:103:HEM:HBC2	2.40	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.09	0.51
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.92	0.51
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.10	0.51
23:c:504:CLA:H42	36:c:517:DGD:HB42	1.91	0.51
26:A:410:SQD:H192	31:D:409:LHG:H201	1.92	0.51
1:a:227:THR:HB	1:a:231:GLU:HG3	1.91	0.51
23:c:512:CLA:H143	23:c:513:CLA:H142	1.92	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.51
4:D:49:LEU:HD13	25:D:406:BCR:C15	2.41	0.51
12:m:5:GLN:H	12:m:5:GLN:NE2	2.08	0.51
23:c:505:CLA:HMD3	23:c:507:CLA:HAB	1.93	0.51
23:b:601:CLA:H72	23:b:601:CLA:H2	1.93	0.51
33:c:519:LMG:H181	10:k:27:VAL:HG11	1.93	0.51
13:o:42:ARG:O	13:o:241:ALA:HA	2.11	0.51
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.76	0.51
23:A:406:CLA:HED1	36:C:519:DGD:HAE2	1.92	0.51
3:c:429:SER:HA	36:c:517:DGD:HBW1	1.92	0.51
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.91	0.51
2:b:341:LYS:HE2	2:b:431:GLU:HG3	1.93	0.51
23:c:508:CLA:HMB3	23:c:508:CLA:HBB1	1.93	0.51
31:d:409:LHG:H122	31:d:409:LHG:C38	2.41	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.11	0.50
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.45	0.50
3:c:363:GLY:O	3:c:367:GLU:HG2	2.11	0.50
23:c:512:CLA:O2D	23:c:513:CLA:HBB2	2.11	0.50
13:O:81:ILE:HA	13:O:100:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:408:CLA:H151	23:C:507:CLA:H13	1.93	0.50
18:Y:22:LEU:HA	18:Y:25:ILE:HG22	1.93	0.50
5:e:60:GLN:HE21	5:e:62:SER:HB3	1.77	0.50
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	1.93	0.50
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.93	0.50
3:c:325:GLY:O	15:u:51:LYS:NZ	2.39	0.50
9:J:18:MET:O	9:J:22:VAL:HG23	2.12	0.49
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.93	0.49
1:a:226:GLU:OE2	41:a:501:HOH:O	2.18	0.49
3:C:186:TYR:OH	3:C:194:GLY:HA3	2.13	0.49
35:D:402:LMT:H21	34:b:628:HTG:H1	1.93	0.49
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.47	0.49
10:k:17:ILE:HD13	10:k:17:ILE:H	1.77	0.49
23:B:614:CLA:H62	23:B:614:CLA:H41	1.56	0.49
29:a:414:PL9:H262	31:e:101:LHG:H201	1.94	0.49
23:b:614:CLA:H162	23:b:614:CLA:H122	1.53	0.49
3:c:443:TRP:CE2	23:c:508:CLA:HMD2	2.47	0.49
26:D:413:SQD:H241	6:F:18:VAL:HG22	1.94	0.49
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.95	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.13	0.48
31:d:409:LHG:H122	31:d:409:LHG:H382	1.95	0.48
33:B:621:LMG:O10	12:M:4:ASN:ND2	2.45	0.48
10:K:17:ILE:H	10:K:17:ILE:HD13	1.77	0.48
2:b:423:LYS:NZ	41:b:709:HOH:O	2.45	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.48	0.48
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.14	0.48
33:a:416:LMG:H222	36:c:516:DGD:HAT2	1.95	0.48
23:b:604:CLA:H143	23:b:615:CLA:HMA3	1.95	0.48
25:d:405:BCR:H391	9:j:20:VAL:CG1	2.43	0.48
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.42	0.48
23:b:605:CLA:H41	23:b:605:CLA:H62	1.62	0.48
3:c:78:GLU:HB3	41:v:321:HOH:O	2.12	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
3:C:406:SER:HA	3:C:420:VAL:HG23	1.95	0.48
23:c:504:CLA:H151	23:c:508:CLA:H143	1.94	0.48
23:d:404:CLA:H142	23:d:404:CLA:H112	1.75	0.48
23:B:602:CLA:H101	23:B:609:CLA:H193	1.95	0.48
23:b:610:CLA:HHC	23:b:610:CLA:HBB1	1.96	0.48
23:c:511:CLA:H72	25:k:101:BCR:H282	1.96	0.48
2:B:245:VAL:HG22	23:B:612:CLA:H202	1.95	0.48
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:497:GLN:HE22	17:x:38:GLN:HB2	1.79	0.48
13:o:210:GLU:OE2	13:o:240:TYR:OH	2.22	0.48
23:A:408:CLA:H171	23:C:507:CLA:H112	1.95	0.48
34:B:622:HTG:H61	35:B:630:LMT:H6E	1.95	0.48
25:c:514:BCR:H341	25:c:514:BCR:H11C	1.73	0.48
33:c:520:LMG:H232	33:c:520:LMG:H391	1.96	0.48
1:A:227:THR:HB	1:A:231:GLU:HG3	1.96	0.47
2:B:299:GLU:HG2	2:B:402:TYR:HD1	1.79	0.47
23:c:512:CLA:HHC	23:c:512:CLA:HBB1	1.96	0.47
23:c:513:CLA:H8	25:c:514:BCR:H23C	1.96	0.47
26:L:101:SQD:H462	26:L:101:SQD:H1	1.97	0.47
1:a:183:MET:HA	23:a:404:CLA:HMD1	1.96	0.47
3:c:174:LEU:HD22	23:c:502:CLA:H203	1.96	0.47
5:e:26:THR:HB	38:e:103:HEM:HAB	1.96	0.47
4:D:12:ARG:HH12	17:X:39:ARG:NH1	2.13	0.47
1:a:214:MET:HG2	29:a:414:PL9:H103	1.96	0.47
2:b:58:GLN:C	2:b:329:PRO:HB3	2.39	0.47
5:e:67:THR:N	5:e:75:GLN:HE22	2.09	0.47
12:m:5:GLN:HE21	12:m:5:GLN:N	2.11	0.47
1:A:217:SER:HA	4:D:272:LEU:HD12	1.97	0.47
23:C:507:CLA:H2	25:C:516:BCR:H10C	1.95	0.47
5:e:68:ASP:OD1	5:e:71:GLU:HB2	2.15	0.47
31:A:416:LHG:H361	23:B:613:CLA:H51	1.96	0.47
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.95	0.47
3:C:391:ARG:HD3	41:C:715:HOH:O	2.14	0.47
31:D:408:LHG:H192	14:T:17:PHE:HZ	1.80	0.47
25:T:101:BCR:HC7	25:T:101:BCR:H331	1.49	0.47
33:a:416:LMG:HC71	3:c:216:SER:HB2	1.96	0.47
2:b:283:GLU:OE2	2:b:287:ARG:NH1	2.45	0.47
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.97	0.47
1:A:238[A]:LYS:NZ	41:A:504:HOH:O	2.47	0.47
29:A:414:PL9:H151	29:A:414:PL9:H171	1.57	0.47
26:a:410:SQD:H271	31:d:409:LHG:H141	1.96	0.47
3:c:213[A]:LEU:HG	23:c:506:CLA:H193	1.97	0.47
4:d:85:MET:HE2	4:d:90:LEU:HD21	1.96	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.51	0.46
3:c:146:PHE:HZ	23:c:512:CLA:HBB2	1.80	0.46
23:c:505:CLA:HBD	23:c:505:CLA:HAA1	1.96	0.46
2:B:58:GLN:C	2:B:329:PRO:HB3	2.39	0.46
2:B:216:HIS:CE1	23:B:609:CLA:NA	2.82	0.46
3:C:325:GLY:O	15:U:51:LYS:NZ	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:341:LYS:NZ	34:b:622:HTG:S1	2.75	0.46
2:b:357:ARG:HB3	41:b:746:HOH:O	2.15	0.46
25:c:515:BCR:H15C	25:c:515:BCR:H351	1.81	0.46
23:B:608:CLA:H191	4:D:89:LEU:HD13	1.98	0.46
6:F:21:VAL:O	6:F:25:THR:HG23	2.16	0.46
35:M:101:LMT:H6D	11:l:9:PRO:HA	1.97	0.46
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.97	0.46
23:d:404:CLA:H61	23:d:404:CLA:H41	1.59	0.46
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.97	0.46
23:B:615:CLA:H152	23:B:615:CLA:H112	1.56	0.46
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.96	0.46
23:b:608:CLA:H102	4:d:120:PHE:CE1	2.51	0.46
23:C:514:CLA:H152	33:Z:101:LMG:H412	1.96	0.46
23:C:505:CLA:H62	23:C:505:CLA:H41	1.68	0.46
2:B:36[A]:SER:OG	25:B:618:BCR:H362	2.16	0.46
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	1.97	0.46
25:B:619:BCR:H331	25:B:619:BCR:C8	2.46	0.46
7:H:25:TRP:O	7:H:28:THR:OG1	2.28	0.46
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.97	0.46
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.50	0.46
24:a:407:PHO:HBC3	4:d:279:LEU:HD22	1.97	0.46
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.49	0.46
23:C:507:CLA:H91	23:C:507:CLA:H111	1.80	0.46
12:M:28:GLN:O	12:M:32:GLN:HG3	2.16	0.46
23:a:408:CLA:H152	23:c:506:CLA:H101	1.98	0.46
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.51	0.46
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.80	0.45
13:O:32:ILE:HG21	13:O:93:LEU:HD21	1.99	0.45
26:a:410:SQD:H141	31:d:409:LHG:H152	1.97	0.45
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.78	0.45
3:c:27:ASP:HB3	10:k:46:ARG:HG3	1.96	0.45
36:c:518:DGD:HBH2	31:d:409:LHG:H211	1.98	0.45
1:a:92:HIS:HE2	3:c:360:ASP:CG	2.24	0.45
2:B:363:PHE:HB3	2:B:365:SER:O	2.16	0.45
2:B:489:GLU:HB3	2:B:495:PHE:CG	2.51	0.45
35:M:101:LMT:H101	23:b:614:CLA:H92	1.98	0.45
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.97	0.45
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.75	0.45
11:L:20:GLY:O	11:L:24[A]:ILE:HG12	2.16	0.45
2:b:30:VAL:HG12	23:b:605:CLA:HHD	1.99	0.45
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.99	0.45
1:A:163:ILE:HD11	36:C:517:DGD:HA22	1.99	0.45
23:B:603:CLA:C4D	23:B:605:CLA:H43	2.47	0.45
33:C:501:LMG:H152	36:C:517:DGD:HA91	1.99	0.45
23:C:514:CLA:H172	33:Z:101:LMG:H402	1.98	0.45
2:b:86:ILE:HD12	2:b:88:PRO:HD3	1.98	0.45
25:d:405:BCR:H15C	25:d:405:BCR:H351	1.82	0.45
13:o:39:ARG:NH2	13:o:98:GLU:OE1	2.50	0.45
1:A:12:ASN:O	1:A:16:ARG:HG3	2.17	0.45
2:B:54:PRO:HB3	27:B:626:GOL:H11	1.99	0.45
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	1.99	0.45
26:L:101:SQD:H302	26:L:101:SQD:H332	1.80	0.45
2:b:490:GLN:HG3	2:b:496:TYR:HE2	1.80	0.45
41:d:576:HOH:O	17:x:6:SER:HA	2.16	0.45
26:B:620:SQD:H351	26:B:620:SQD:H383	1.84	0.45
4:D:186:GLN:HB2	23:D:404:CLA:HBC1	1.99	0.45
25:H:101:BCR:H331	25:H:101:BCR:C8	2.47	0.45
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.68	0.45
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.99	0.45
23:b:616:CLA:H92	23:b:616:CLA:H62	1.68	0.45
13:o:54:GLU:HG2	13:o:64:GLU:H	1.82	0.45
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.44
23:A:408:CLA:H143	23:C:506:CLA:H192	2.00	0.44
2:B:299:GLU:HG3	41:B:800:HOH:O	2.17	0.44
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.78	0.44
38:E:103:HEM:HAC	6:F:27:ALA:HB1	1.98	0.44
2:b:497:GLN:NE2	17:x:38:GLN:O	2.51	0.44
23:c:508:CLA:H93	31:d:409:LHG:H162	2.00	0.44
26:A:412:SQD:H292	26:A:412:SQD:H262	1.72	0.44
31:A:416:LHG:H312	31:A:416:LHG:H282	1.74	0.44
23:b:614:CLA:H101	25:b:617:BCR:H362	1.98	0.44
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.99	0.44
13:O:39:ARG:HB2	13:O:246:ALA:HB2	1.99	0.44
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.99	0.44
23:c:509:CLA:H92	23:c:509:CLA:H62	1.75	0.44
31:d:408:LHG:H192	14:t:17:PHE:HZ	1.83	0.44
5:e:66:VAL:HA	5:e:75:GLN:NE2	2.32	0.44
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.99	0.44
34:B:622:HTG:O5	27:a:411:GOL:H11	2.18	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
23:C:507:CLA:HMC2	23:C:508:CLA:H102	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:121[B]:LEU:HD23	33:a:416:LMG:H212	2.00	0.44
23:a:404:CLA:H191	31:d:408:LHG:H321	2.00	0.44
23:c:510:CLA:H61	23:c:510:CLA:H102	1.69	0.44
2:B:497:GLN:NE2	17:X:38:GLN:O	2.46	0.44
23:a:408:CLA:H152	23:c:506:CLA:H142	2.00	0.44
23:b:615:CLA:H92	23:b:615:CLA:H61	1.76	0.44
25:c:514:BCR:H371	25:c:514:BCR:H24C	1.74	0.44
31:d:408:LHG:HC62	11:l:15:THR:HG23	2.00	0.44
23:B:604:CLA:H62	23:B:604:CLA:H41	1.74	0.44
23:B:616:CLA:H11	23:B:616:CLA:H51	1.81	0.44
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.99	0.44
3:C:154:LYS:HG2	3:C:266:TRP:CE3	2.53	0.44
23:C:504:CLA:HBB2	23:C:513:CLA:H92	2.00	0.44
23:C:508:CLA:H62	23:C:508:CLA:H41	1.75	0.44
23:b:603:CLA:H141	23:b:603:CLA:H161	1.84	0.44
35:B:630:LMT:H52	1:a:72:LEU:HD11	1.99	0.44
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.99	0.44
23:C:514:CLA:HAB	25:C:515:BCR:H24C	1.99	0.44
35:E:102:LMT:O6'	41:E:201:HOH:O	2.21	0.44
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.99	0.44
1:A:214:MET:HG2	29:A:414:PL9:C10	2.48	0.44
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.88	0.44
9:J:6:ARG:HG3	41:J:201:HOH:O	2.17	0.44
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	2.00	0.44
1:a:307[A]:ILE:CG2	1:a:311:GLY:HA2	2.48	0.44
3:c:38:GLY:HA3	23:c:511:CLA:HMD2	2.00	0.44
23:c:509:CLA:HMB1	23:c:511:CLA:HBB1	1.99	0.44
12:m:34:LYS:O	41:m:201:HOH:O	2.21	0.44
13:O:124:ASN:HD22	13:O:147:ASN:ND2	2.05	0.44
15:U:48:LEU:O	15:U:52:ASN:ND2	2.41	0.44
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.99	0.44
23:b:604:CLA:H62	23:b:604:CLA:H41	1.71	0.44
3:c:171:GLY:O	3:c:174:LEU:HB2	2.17	0.44
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.53	0.43
1:A:183:MET:HA	23:A:404:CLA:HMD1	2.00	0.43
23:C:507:CLA:H41	23:C:507:CLA:H62	1.83	0.43
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.88	0.43
29:a:414:PL9:H503	17:x:24:THR:OG1	2.17	0.43
12:m:28:GLN:O	12:m:32:GLN:HG3	2.18	0.43
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.00	0.43
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:PRO:HB3	27:B:625:GOL:H32	1.99	0.43
33:C:501:LMG:H161	33:C:501:LMG:H191	1.80	0.43
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.43
13:O:110[B]:MET:HE2	13:O:116:ILE:HD11	2.00	0.43
23:a:405:CLA:HED1	36:c:518:DGD:HAE2	1.99	0.43
25:a:409:BCR:H11C	25:a:409:BCR:H341	1.88	0.43
23:c:513:CLA:H203	23:c:513:CLA:H161	1.75	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	2.00	0.43
3:C:142:GLU:CD	3:C:142:GLU:H	2.25	0.43
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.48	0.43
1:A:341:LEU:HD13	27:C:523:GOL:H31	1.99	0.43
7:H:43:LEU:HD12	7:H:43:LEU:HA	1.85	0.43
5:E:26:THR:HA	20:R:15:ALA:HB1	2.00	0.43
13:O:18:LYS:HD3	41:O:460:HOH:O	2.17	0.43
2:b:219:VAL:O	41:b:702:HOH:O	2.21	0.43
38:e:103:HEM:CAC	6:f:27:ALA:HB1	2.49	0.43
13:o:92:SER:HB3	13:o:131:PRO:HA	1.99	0.43
34:B:622:HTG:H6'2	34:B:622:HTG:H3'1	1.94	0.43
25:H:101:BCR:H11C	25:H:101:BCR:H341	1.79	0.43
26:L:101:SQD:H211	25:T:101:BCR:H351	1.99	0.43
23:C:514:CLA:H141	23:C:514:CLA:H162	1.82	0.43
33:C:501:LMG:H232	23:C:506:CLA:H92	2.00	0.43
23:C:509:CLA:H142	23:C:509:CLA:H111	1.71	0.43
35:D:402:LMT:H51	2:b:39:LEU:HD22	2.00	0.43
25:H:101:BCR:H331	25:H:101:BCR:HC8	2.00	0.43
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.54	0.43
1:a:217:SER:HA	4:d:272:LEU:HD12	2.00	0.43
23:a:405:CLA:HAB	23:d:403:CLA:H72	2.01	0.43
13:o:32:ILE:HG21	13:o:93:LEU:HD21	2.00	0.43
1:A:214:MET:HG2	29:A:414:PL9:H103	2.00	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.19	0.43
24:a:407:PHO:H112	24:a:407:PHO:H72	1.75	0.43
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.43
2:B:102:VAL:HA	25:B:618:BCR:C40	2.49	0.43
3:C:60:ILE:HG22	23:C:504:CLA:HHD	1.99	0.43
36:C:518:DGD:HAF2	36:C:518:DGD:HAE2	1.86	0.43
25:Y:101:BCR:H15C	25:Y:101:BCR:H351	1.88	0.43
3:c:294:ASN:HA	3:c:297:TYR:O	2.18	0.43
23:c:508:CLA:H162	23:c:508:CLA:H122	1.74	0.43
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.53	0.43
33:j:101:LMG:H341	33:j:101:LMG:H242	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:404:CLA:CBD	23:d:401:CLA:HAC2	2.48	0.42
2:b:101:ILE:O	2:b:104:SER:HB3	2.19	0.42
2:B:61:PHE:CZ	23:B:607:CLA:HBB1	2.54	0.42
23:B:606:CLA:H192	23:B:616:CLA:H101	2.01	0.42
3:C:443:TRP:CZ2	23:C:509:CLA:HMD1	2.54	0.42
8:I:2:GLU:O	8:I:6:ILE:HG12	2.19	0.42
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.00	0.42
23:b:609:CLA:C3B	25:h:101:BCR:H323	2.49	0.42
23:c:505:CLA:H112	23:c:505:CLA:H72	1.75	0.42
34:d:411:HTG:H5	7:h:25:TRP:NE1	2.33	0.42
19:z:29:SER:HA	19:z:30:PRO:HD3	1.91	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.62	0.42
23:B:602:CLA:H203	23:B:602:CLA:H162	1.75	0.42
13:O:57:LYS:HE3	2:b:338:GLN:HA	2.02	0.42
20:R:29:LYS:HB3	20:R:29:LYS:HE2	1.79	0.42
3:c:48:LYS:HG2	3:c:133:ALA:O	2.20	0.42
36:c:516:DGD:HAW2	36:c:516:DGD:HAN1	1.88	0.42
35:B:629:LMT:H2'	41:t:203:HOH:O	2.19	0.42
3:C:363:GLY:O	3:C:367:GLU:HG2	2.18	0.42
31:E:101:LHG:H261	31:E:101:LHG:H291	1.71	0.42
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.54	0.42
23:b:603:CLA:HBB2	23:b:605:CLA:H193	2.01	0.42
23:A:405:CLA:HED1	29:D:407:PL9:H362	2.01	0.42
2:B:133:LEU:HB3	2:B:138:MET:SD	2.59	0.42
35:D:403:LMT:O2B	30:D:411:UNL:O6	2.37	0.42
23:a:404:CLA:H161	23:a:404:CLA:H193	1.65	0.42
2:b:124:ARG:HD2	2:b:129:GLY:O	2.19	0.42
23:B:616:CLA:H152	23:B:616:CLA:H111	1.68	0.42
3:c:205:ASP:HA	3:c:206:PRO:HD2	1.89	0.42
23:c:506:CLA:H162	23:c:506:CLA:H122	1.64	0.42
2:B:341:LYS:NZ	34:B:623:HTG:O2	2.37	0.42
23:B:602:CLA:H92	36:H:102:DGD:HB71	2.00	0.42
23:B:614:CLA:H92	23:B:614:CLA:H61	1.67	0.42
35:D:403:LMT:H91	35:D:403:LMT:H62	1.81	0.42
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.84	0.42
25:b:619:BCR:H331	25:b:619:BCR:C8	2.49	0.42
25:h:101:BCR:C8	25:h:101:BCR:H331	2.50	0.42
18:y:38:LEU:O	18:y:42:ARG:HG2	2.19	0.42
19:z:56:VAL:HG12	19:z:60:PHE:HE1	1.84	0.42
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.89	0.42
23:B:610:CLA:H122	23:B:615:CLA:HAA1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:30:ILE:HD12	18:Y:30:ILE:HA	1.86	0.42
10:k:16:ALA:O	10:k:19:ASP:HB2	2.20	0.42
25:k:101:BCR:H11C	25:k:101:BCR:H341	1.94	0.42
1:A:274:PHE:HD1	26:A:410:SQD:H101	1.85	0.42
31:A:416:LHG:O4	4:D:141:TYR:OH	2.28	0.42
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.42
23:B:602:CLA:H91	23:B:602:CLA:H111	1.84	0.42
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.02	0.42
2:b:224:ARG:NH1	4:d:16:ASP:OD2	2.51	0.42
25:b:618:BCR:H20C	25:b:618:BCR:H361	1.92	0.42
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.82	0.42
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.85	0.41
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.88	0.41
3:C:161:LEU:HD11	23:C:507:CLA:HBB1	2.02	0.41
23:C:508:CLA:H92	23:C:508:CLA:H61	1.88	0.41
6:F:34:LEU:HD23	6:F:34:LEU:HA	1.93	0.41
25:c:515:BCR:H24C	25:c:515:BCR:H371	1.83	0.41
2:B:502:VAL:O	2:B:505:ARG:HG3	2.20	0.41
25:B:619:BCR:H15C	25:B:619:BCR:H351	1.88	0.41
26:L:101:SQD:H212	26:L:101:SQD:H181	1.86	0.41
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.41
36:c:517:DGD:HA91	36:c:518:DGD:HBF2	2.02	0.41
4:d:43:LEU:HD22	25:d:405:BCR:H323	2.02	0.41
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.01	0.41
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.90	0.41
10:k:20:PRO:HB3	18:y:21:GLN:HG3	2.03	0.41
13:o:51:LEU:HD23	13:o:67:PRO:HA	2.03	0.41
15:u:45:LEU:HD23	15:u:45:LEU:HA	1.81	0.41
2:B:149:LEU:HG	23:B:606:CLA:HBB2	2.02	0.41
23:B:601:CLA:H42	23:B:601:CLA:OBD	2.20	0.41
23:B:605:CLA:H92	23:B:605:CLA:H61	1.75	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.55	0.41
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.02	0.41
3:C:433:LEU:HD13	23:C:503:CLA:CHC	2.51	0.41
1:a:281:VAL:HG12	26:a:410:SQD:H201	2.02	0.41
23:c:513:CLA:C4A	23:c:513:CLA:HBA1	2.49	0.41
23:B:614:CLA:HAA1	23:B:614:CLA:HBD	2.01	0.41
23:C:509:CLA:H91	23:C:509:CLA:H112	1.82	0.41
31:D:409:LHG:H372	31:D:409:LHG:C13	2.50	0.41
1:a:265:PHE:HE2	29:a:414:PL9:H111	1.84	0.41
18:y:22:LEU:HA	18:y:25:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:506:CLA:H101	23:C:506:CLA:H61	1.79	0.41
25:C:515:BCR:H20C	25:C:515:BCR:H361	1.85	0.41
15:U:24:LYS:HB3	15:U:81:HIS:O	2.21	0.41
23:b:604:CLA:H91	23:b:604:CLA:H111	1.81	0.41
23:B:604:CLA:HAB	23:B:611:CLA:H191	2.02	0.41
23:B:611:CLA:H92	23:B:611:CLA:H62	1.91	0.41
33:C:501:LMG:H121	23:C:506:CLA:H201	2.02	0.41
15:U:64:ILE:HA	15:U:65:PRO:HD3	1.85	0.41
20:R:31:VAL:O	20:R:35:LEU:HG	2.21	0.41
9:j:3:GLU:O	9:j:6:ARG:HG2	2.20	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.90	0.41
5:E:25:ILE:O	5:E:28:PRO:HD2	2.21	0.41
5:E:42:LEU:HA	20:R:4:ARG:HH21	1.85	0.41
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.56	0.41
1:a:182:PHE:O	1:a:186:PHE:HB2	2.20	0.41
2:b:305:ILE:HA	2:b:306:PRO:HD3	1.84	0.41
23:d:401:CLA:C4A	23:d:401:CLA:HBA1	2.50	0.41
10:k:26:PRO:O	10:k:29:PRO:HD2	2.20	0.41
25:C:516:BCR:H24C	25:C:516:BCR:H371	1.82	0.41
2:b:16:PRO:HG2	2:b:123:PHE:HB3	2.03	0.41
23:b:608:CLA:H3A	23:b:608:CLA:HBA2	1.88	0.41
23:c:507:CLA:H142	23:c:507:CLA:H112	1.89	0.41
13:o:140:THR:O	13:o:201:VAL:HB	2.20	0.41
1:A:121[A]:LEU:HG	33:C:501:LMG:H182	2.02	0.41
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.56	0.41
23:B:616:CLA:H91	23:B:616:CLA:H112	1.80	0.41
25:B:619:BCR:H24C	25:B:619:BCR:H371	1.80	0.41
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.21	0.41
23:C:506:CLA:H111	23:C:506:CLA:H93	1.87	0.41
13:O:56:PRO:HB3	13:O:61:GLN:CD	2.45	0.41
25:T:101:BCR:H11C	25:T:101:BCR:H341	1.86	0.41
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.97	0.41
1:a:267:ASN:HB3	1:a:270[B]:SER:OG	2.21	0.41
33:a:416:LMG:H211	33:a:416:LMG:H241	1.68	0.41
23:b:605:CLA:H111	23:b:605:CLA:H91	1.87	0.41
23:b:611:CLA:H172	23:b:613:CLA:ND	2.36	0.41
23:b:613:CLA:H203	23:b:613:CLA:H161	1.86	0.41
41:c:609:HOH:O	10:k:25:LEU:HB2	2.20	0.41
23:d:403:CLA:HBD	23:d:403:CLA:HAA2	2.02	0.41
25:h:101:BCR:H371	25:h:101:BCR:H24C	1.86	0.41
13:o:30:TYR:HA	13:o:31:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:80:THR:HA	16:v:86:GLN:O	2.21	0.41
1:A:45:THR:HG21	26:A:412:SQD:H202	2.03	0.41
2:B:157:HIS:HE1	23:B:606:CLA:NA	2.19	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.55	0.41
4:D:223:PHE:CZ	4:D:245:SER:HB2	2.56	0.41
33:J:101:LMG:H191	33:J:101:LMG:H231	2.03	0.41
10:K:15:TYR:CE1	19:Z:5:PHE:HZ	2.39	0.41
2:b:12:LEU:HB2	23:b:612:CLA:HMC2	2.03	0.41
2:b:223:GLN:HA	2:b:223:GLN:HE21	1.86	0.41
23:b:615:CLA:HBA1	23:b:615:CLA:H3A	1.88	0.41
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.94	0.41
23:d:401:CLA:H162	23:d:401:CLA:H203	1.85	0.41
12:m:6:LEU:HD23	12:m:6:LEU:HA	1.91	0.41
1:A:102:LEU:HD12	34:b:625:HTG:H61	2.03	0.40
2:B:191:ASN:HA	2:B:192:PRO:HD2	1.96	0.40
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.03	0.40
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.03	0.40
1:a:210:LEU:HG	24:a:407:PHO:NC	2.35	0.40
24:a:406:PHO:HAB	4:d:205:LEU:HD13	2.03	0.40
23:b:609:CLA:C2B	25:h:101:BCR:H323	2.50	0.40
23:d:404:CLA:H62	23:d:404:CLA:H92	1.75	0.40
5:e:66:VAL:HA	5:e:75:GLN:HE22	1.86	0.40
7:h:62:TRP:C	7:h:64:ALA:H	2.28	0.40
14:t:14:ILE:HG22	25:t:101:BCR:H10C	2.02	0.40
24:A:407:PHO:HHD	24:A:407:PHO:HBC2	2.04	0.40
3:C:137:PRO:HG3	23:C:514:CLA:HED3	2.02	0.40
2:b:159:THR:HA	2:b:181:VAL:O	2.21	0.40
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.83	0.40
23:b:604:CLA:HBD	23:b:604:CLA:HAA1	2.04	0.40
3:c:135:ARG:HA	3:c:135:ARG:HD2	1.96	0.40
3:c:334:PRO:HA	13:o:153:THR:OG1	2.21	0.40
4:d:186:GLN:HB2	23:d:403:CLA:HBC1	2.03	0.40
13:o:39:ARG:HH22	13:o:98:GLU:CD	2.29	0.40
23:A:405:CLA:H92	23:A:405:CLA:H62	1.89	0.40
2:B:201:HIS:HB2	23:B:602:CLA:CHB	2.51	0.40
3:C:38:GLY:HA3	23:C:512:CLA:HMD2	2.02	0.40
36:C:518:DGD:HAE2	36:C:518:DGD:HA81	1.80	0.40
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.57	0.40
16:V:57:GLU:H	16:V:57:GLU:CD	2.30	0.40
2:b:63:LEU:N	2:b:64:PRO:HD2	2.36	0.40
7:h:4:ARG:HH11	7:h:9:ASP:CG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:28:ILE:HD11	18:y:28:ILE:HD13	2.03	0.40
19:z:48:ILE:HD11	33:z:101:LMG:H192	2.02	0.40
26:A:412:SQD:H261	2:b:109:LEU:HD13	2.02	0.40
29:A:414:PL9:H272	29:A:414:PL9:H251	1.91	0.40
23:C:513:CLA:HMB2	23:C:513:CLA:H202	2.02	0.40
4:D:202:ALA:HB2	29:D:407:PL9:H353	2.04	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.87	0.40
18:Y:34:MET:HE2	18:Y:34:MET:HB2	1.99	0.40
2:b:24:LEU:HD21	23:b:616:CLA:CAB	2.50	0.40
2:b:432:PHE:H	34:b:622:HTG:HO3	1.65	0.40
23:b:612:CLA:H122	23:b:612:CLA:H162	1.86	0.40
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.25	0.40
5:e:68:ASP:O	5:e:72:ALA:HB2	2.21	0.40
16:v:41:HIS:HA	16:v:45:ILE:O	2.22	0.40
2:B:482:ILE:HD12	2:B:486:LEU:HD22	2.04	0.40
3:C:25:ASN:O	3:C:41:ARG:HD3	2.20	0.40
23:C:513:CLA:H101	23:C:514:CLA:H141	2.02	0.40
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.84	0.40
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.03	0.40
23:b:612:CLA:HBD	23:b:612:CLA:HAA1	2.04	0.40
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.92	0.40
23:c:507:CLA:H62	23:c:507:CLA:H41	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	36	55
1	a	337/344 (98%)	330 (98%)	6 (2%)	1 (0%)	36	55
2	B	510/505 (101%)	504 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	506/505 (100%)	499 (99%)	7 (1%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	30	49
3	c	458/455 (101%)	445 (97%)	11 (2%)	2 (0%)	30	49
4	D	341/342 (100%)	332 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	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
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	60 (95%)	3 (5%)	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	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	238 (97%)	8 (3%)	0	100	100
13	o	243/244 (100%)	234 (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%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
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	5255/5384 (98%)	5126 (98%)	120 (2%)	9 (0%)	48	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
19	Z	30	PRO
19	z	30	PRO
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	270 (99%)	2 (1%)	76	89
1	a	274/279 (98%)	272 (99%)	2 (1%)	76	89
2	B	410/403 (102%)	401 (98%)	9 (2%)	45	73
2	b	406/403 (101%)	398 (98%)	8 (2%)	48	75
3	C	356/356 (100%)	350 (98%)	6 (2%)	53	78
3	c	361/356 (101%)	351 (97%)	10 (3%)	38	66
4	D	278/277 (100%)	277 (100%)	1 (0%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	277/277 (100%)	274 (99%)	3 (1%)	65	84
5	E	73/73 (100%)	71 (97%)	2 (3%)	39	67
5	e	70/73 (96%)	68 (97%)	2 (3%)	37	65
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	28	54
7	H	55/54 (102%)	53 (96%)	2 (4%)	31	58
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%)	24 (92%)	2 (8%)	12	25
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	8
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	8
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	29 (97%)	1 (3%)	33	61
12	m	30/32 (94%)	28 (93%)	2 (7%)	15	31
13	O	211/207 (102%)	208 (99%)	3 (1%)	59	81
13	o	208/207 (100%)	205 (99%)	3 (1%)	59	81
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%)	83 (99%)	1 (1%)	63	83
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%)	31 (100%)	0	100	100
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%)	20 (91%)	2 (9%)	9	19
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	56
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4360/4403 (99%)	4274 (98%)	86 (2%)	50	75

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	35	VAL
2	B	53	ASN
2	B	86	ILE
2	B	223	GLN
2	B	236	THR
2	B	362	PHE
2	B	472	ARG
2	B	489	GLU
2	B	492	GLU
2	B	505	ARG
3	C	25	ASN
3	C	142	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	136	VAL
5	E	54	SER
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
8	I	33	LYS
9	J	6	ARG
9	J	9	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	33	GLN
13	O	24	ASP
13	O	69	LYS
13	O	234	LYS
14	T	2	GLU
15	U	10	VAL
15	U	70	ARG

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Mol	Chain	Res	Type
16	V	30	LYS
18	Y	30	ILE
19	Z	3	ILE
19	Z	6	GLN
1	a	12	ASN
1	a	35	VAL
2	b	36	SER
2	b	53	ASN
2	b	121	GLU
2	b	223	GLN
2	b	245	VAL
2	b	431	GLU
2	b	472	ARG
2	b	485	GLU
3	c	19	ASN
3	c	21	ILE
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	462[A]	GLU
3	c	462[B]	GLU
4	d	136	VAL
4	d	259	ILE
4	d	329	MET
5	e	62	SER
5	e	71	GLU
6	f	15	ILE
8	i	33	LYS
8	i	36	ASP
9	j	2	SER
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
10	k	27	VAL
12	m	5	GLN
12	m	20	VAL
13	o	69	LYS
13	o	118	LEU

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Mol	Chain	Res	Type
13	o	132	ASN
14	t	2	GLU
15	u	10	VAL
16	v	30	LYS
18	y	30	ILE
18	y	45	ASN
19	z	3	ILE
19	z	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	53	ASN
2	B	331	ASN
2	B	338	GLN
3	C	28	GLN
3	C	415	ASN
4	D	61	HIS
4	D	186	GLN
4	D	255	GLN
5	E	60	GLN
6	F	44	GLN
12	M	5	GLN
12	M	28	GLN
13	O	124	ASN
13	O	130	GLN
15	U	73	GLN
15	U	81	HIS
19	Z	58	ASN
1	a	12	ASN
1	a	165	GLN
1	a	234	ASN
2	b	53	ASN
2	b	223	GLN
2	b	289	GLN
2	b	331	ASN
2	b	374	ASN
3	c	19	ASN
3	c	28	GLN
3	c	201	ASN
5	e	60	GLN

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Mol	Chain	Res	Type
5	e	75	GLN
6	f	44	GLN
12	m	5	GLN
13	o	124	ASN
15	u	78	ASN
15	u	81	HIS
16	v	25	GLN
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	0.68	0	8,9,11	1.75	3 (37%)
8	FME	i	1	8	8,9,10	0.67	0	8,9,11	1.26	1 (12%)
12	FME	m	1	12	8,9,10	0.62	0	8,9,11	1.31	2 (25%)
14	FME	T	1	14	8,9,10	0.65	0	8,9,11	1.44	2 (25%)
12	FME	M	1	12	8,9,10	0.62	0	8,9,11	1.44	2 (25%)
8	FME	I	1	8	8,9,10	0.62	0	8,9,11	1.07	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	4/7/9/11	-
12	FME	M	1	12	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.78	117.62	124.77
14	t	1	FME	CA-N-CN	-2.63	118.77	122.82
8	I	1	FME	O-C-CA	-2.33	118.77	124.77
12	M	1	FME	CA-N-CN	-2.31	119.27	122.82
14	T	1	FME	O-C-CA	-2.29	118.88	124.77
12	M	1	FME	O-C-CA	-2.26	118.95	124.77
14	T	1	FME	CB-CA-N	-2.23	106.45	110.52
12	m	1	FME	CA-N-CN	-2.19	119.45	122.82
8	i	1	FME	O-C-CA	-2.17	119.18	124.77
12	m	1	FME	O1-CN-N	-2.15	119.77	125.32
14	t	1	FME	O1-CN-N	-2.13	119.81	125.32

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 214 ligands modelled in this entry, 14 are monoatomic and 18 are unknown - leaving 182 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	405	41	69,73,73	2.01	20 (28%)	82,113,113	2.69	33 (40%)
29	PL9	D	407	-	55,55,55	0.67	1 (1%)	68,69,69	1.74	22 (32%)
33	LMG	c	520	-	51,51,55	0.97	3 (5%)	59,59,63	1.24	6 (10%)
23	CLA	B	605	2	69,73,73	2.05	19 (27%)	82,113,113	2.74	30 (36%)
31	LHG	D	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.11	5 (9%)
23	CLA	B	612	2	69,73,73	1.98	19 (27%)	82,113,113	2.62	30 (36%)
23	CLA	b	602	2	69,73,73	2.06	20 (28%)	82,113,113	2.69	35 (42%)
23	CLA	B	616	2	69,73,73	2.04	20 (28%)	82,113,113	2.69	29 (35%)
23	CLA	C	502	3	69,73,73	1.96	19 (27%)	82,113,113	2.73	32 (39%)
23	CLA	b	613	2	69,73,73	2.03	20 (28%)	82,113,113	2.60	31 (37%)
33	LMG	j	101	39	51,51,55	0.89	2 (3%)	59,59,63	1.07	5 (8%)
34	HTG	C	521	-	19,19,19	0.85	1 (5%)	23,24,24	1.31	3 (13%)
23	CLA	C	511	3	69,73,73	2.02	19 (27%)	82,113,113	2.72	34 (41%)
33	LMG	Z	101	-	51,51,55	0.99	3 (5%)	59,59,63	1.28	5 (8%)
26	SQD	A	412	-	52,54,54	0.98	2 (3%)	62,65,65	1.07	5 (8%)
27	GOL	d	402	-	5,5,5	0.34	0	5,5,5	0.57	0
33	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.13	4 (6%)
23	CLA	c	511	3	69,73,73	2.07	21 (30%)	82,113,113	2.74	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.18	5 (8%)
34	HTG	D	412	-	16,16,19	0.95	2 (12%)	20,21,24	1.27	1 (5%)
27	GOL	a	411	-	5,5,5	0.39	0	5,5,5	0.45	0
36	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.16	7 (9%)
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	5 (6%)
33	LMG	c	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.03	4 (6%)
23	CLA	c	501	3	69,73,73	2.03	20 (28%)	82,113,113	2.64	30 (36%)
33	LMG	J	101	39	51,51,55	0.92	2 (3%)	59,59,63	0.99	5 (8%)
23	CLA	C	512	3	69,73,73	2.03	20 (28%)	82,113,113	2.70	31 (37%)
23	CLA	c	504	41	69,73,73	2.03	20 (28%)	82,113,113	2.72	33 (40%)
23	CLA	C	509	3	69,73,73	2.05	20 (28%)	82,113,113	2.64	28 (34%)
33	LMG	Z	102	-	37,37,55	1.02	3 (8%)	45,45,63	1.64	8 (17%)
23	CLA	d	403	4	69,73,73	2.02	19 (27%)	82,113,113	2.64	32 (39%)
36	DGD	c	518	-	63,63,67	0.87	3 (4%)	77,77,81	1.09	6 (7%)
23	CLA	c	512	3	69,73,73	2.02	19 (27%)	82,113,113	2.75	30 (36%)
35	LMT	e	102	-	36,36,36	0.50	0	47,47,47	0.83	2 (4%)
23	CLA	c	508	3	69,73,73	2.05	20 (28%)	82,113,113	2.67	29 (35%)
34	HTG	c	521	-	19,19,19	0.84	1 (5%)	23,24,24	1.34	1 (4%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
25	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.40	11 (19%)
23	CLA	b	601	41	69,73,73	2.07	20 (28%)	82,113,113	2.61	30 (36%)
23	CLA	c	509	3	69,73,73	2.08	20 (28%)	82,113,113	2.65	30 (36%)
23	CLA	b	603	2	69,73,73	2.06	20 (28%)	82,113,113	2.76	31 (37%)
23	CLA	C	505	41	69,73,73	2.03	20 (28%)	82,113,113	2.65	32 (39%)
35	LMT	b	627	-	25,25,36	0.57	1 (4%)	30,30,47	1.07	3 (10%)
36	DGD	h	102	-	63,63,67	0.90	4 (6%)	77,77,81	1.03	5 (6%)
23	CLA	B	611	2	69,73,73	2.02	19 (27%)	82,113,113	2.63	31 (37%)
23	CLA	c	503	3	69,73,73	2.03	20 (28%)	82,113,113	2.72	30 (36%)
23	CLA	B	608	2	69,73,73	1.97	19 (27%)	82,113,113	2.70	31 (37%)
25	BCR	K	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.43	10 (17%)
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.58	10 (17%)
34	HTG	b	625	-	19,19,19	0.84	2 (10%)	23,24,24	1.60	3 (13%)
34	HTG	b	628	-	19,19,19	0.93	1 (5%)	23,24,24	1.73	4 (17%)
26	SQD	D	413	-	41,43,54	1.09	2 (4%)	51,54,65	1.76	11 (21%)
24	PHO	a	407	-	58,69,69	2.82	12 (20%)	55,99,99	2.92	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	608	2	69,73,73	2.04	20 (28%)	82,113,113	2.64	28 (34%)
23	CLA	B	615	2	69,73,73	1.98	17 (24%)	82,113,113	2.63	30 (36%)
27	GOL	A	411	-	5,5,5	0.40	0	5,5,5	0.32	0
23	CLA	A	404	1	69,73,73	2.07	20 (28%)	82,113,113	2.69	34 (41%)
24	PHO	D	401	-	58,69,69	2.75	13 (22%)	55,99,99	3.13	18 (32%)
33	LMG	a	416	-	51,51,55	0.95	2 (3%)	59,59,63	1.08	3 (5%)
23	CLA	C	506	3	69,73,73	1.99	20 (28%)	82,113,113	2.71	33 (40%)
35	LMT	m	102	-	36,36,36	0.51	0	47,47,47	0.93	2 (4%)
32	BCT	a	418	21	3,3,3	0.49	0	2,3,3	1.02	0
27	GOL	B	626	-	5,5,5	0.53	0	5,5,5	0.40	0
26	SQD	A	410	-	52,54,54	0.92	2 (3%)	62,65,65	1.84	12 (19%)
38	HEM	e	103	6,5	50,50,50	1.52	7 (14%)	67,82,82	1.63	12 (17%)
25	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.65	13 (23%)
36	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	1.00	6 (7%)
23	CLA	b	616	2	69,73,73	2.05	20 (28%)	82,113,113	2.73	33 (40%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	12 (21%)
35	LMT	D	403	-	36,36,36	0.44	0	47,47,47	1.33	7 (14%)
31	LHG	A	416	-	48,48,48	0.90	3 (6%)	51,54,54	1.12	5 (9%)
34	HTG	c	522	-	19,19,19	0.88	1 (5%)	23,24,24	1.37	3 (13%)
35	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.03	2 (4%)
25	BCR	C	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.59	10 (17%)
32	BCT	A	418	21	3,3,3	0.49	0	2,3,3	1.00	0
23	CLA	b	604	2	69,73,73	1.99	18 (26%)	82,113,113	2.70	30 (36%)
25	BCR	d	405	-	41,41,41	1.11	2 (4%)	56,56,56	1.89	13 (23%)
25	BCR	c	514	-	41,41,41	1.06	1 (2%)	56,56,56	1.79	13 (23%)
23	CLA	a	408	1	69,73,73	2.03	20 (28%)	82,113,113	2.69	35 (42%)
35	LMT	B	630	-	36,36,36	0.53	1 (2%)	47,47,47	0.97	2 (4%)
34	HTG	d	411	-	16,16,19	1.02	1 (6%)	20,21,24	1.32	1 (5%)
23	CLA	A	405	41	69,73,73	2.04	20 (28%)	82,113,113	2.77	33 (40%)
27	GOL	C	523	-	5,5,5	0.41	0	5,5,5	0.27	0
23	CLA	B	604	2	69,73,73	1.99	18 (26%)	82,113,113	2.64	31 (37%)
25	BCR	B	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.53	8 (14%)
25	BCR	H	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.74	12 (21%)
23	CLA	B	614	2	69,73,73	2.01	21 (30%)	82,113,113	2.75	33 (40%)
23	CLA	a	404	1	69,73,73	2.00	18 (26%)	82,113,113	2.68	33 (40%)
23	CLA	C	513	3	69,73,73	2.02	20 (28%)	82,113,113	2.64	35 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	A	407	-	58,69,69	2.84	13 (22%)	55,99,99	3.05	17 (30%)
23	CLA	c	506	3	69,73,73	2.03	20 (28%)	82,113,113	2.62	33 (40%)
27	GOL	B	625	-	5,5,5	0.38	0	5,5,5	0.40	0
34	HTG	b	622	-	19,19,19	0.89	1 (5%)	23,24,24	1.37	3 (13%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.77	16 (28%)
23	CLA	B	613	2	69,73,73	2.03	19 (27%)	82,113,113	2.64	33 (40%)
26	SQD	L	101	-	52,54,54	0.97	2 (3%)	62,65,65	1.50	9 (14%)
25	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.75	16 (28%)
23	CLA	B	602	2	69,73,73	2.07	21 (30%)	82,113,113	2.67	33 (40%)
23	CLA	D	404	4	69,73,73	1.99	19 (27%)	82,113,113	2.75	31 (37%)
23	CLA	c	507	41	69,73,73	2.03	19 (27%)	82,113,113	2.60	30 (36%)
23	CLA	b	611	2	69,73,73	2.04	19 (27%)	82,113,113	2.66	30 (36%)
26	SQD	B	620	-	52,54,54	1.01	3 (5%)	62,65,65	1.46	9 (14%)
31	LHG	A	417	-	48,48,48	0.94	2 (4%)	51,54,54	1.10	2 (3%)
35	LMT	a	417	-	36,36,36	0.46	0	47,47,47	0.78	1 (2%)
23	CLA	B	609	2	69,73,73	2.01	17 (24%)	82,113,113	2.65	29 (35%)
23	CLA	c	510	3	69,73,73	1.97	20 (28%)	82,113,113	2.75	34 (41%)
23	CLA	C	508	41	69,73,73	2.04	19 (27%)	82,113,113	2.64	30 (36%)
23	CLA	b	614	2	69,73,73	1.98	20 (28%)	82,113,113	2.71	31 (37%)
35	LMT	b	621	-	25,25,36	0.46	0	30,30,47	0.66	0
34	HTG	C	522	-	19,19,19	0.97	1 (5%)	23,24,24	1.80	5 (21%)
40	HEC	V	202	16	46,50,50	1.74	9 (19%)	58,82,82	1.61	13 (22%)
34	HTG	B	627	-	19,19,19	0.89	2 (10%)	23,24,24	1.28	2 (8%)
35	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.09	4 (8%)
23	CLA	D	405	4	69,73,73	2.03	18 (26%)	82,113,113	2.81	31 (37%)
35	LMT	M	103	-	36,36,36	0.47	0	47,47,47	0.79	1 (2%)
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.00	6 (7%)
25	BCR	b	618	-	41,41,41	1.06	1 (2%)	56,56,56	1.40	9 (16%)
34	HTG	b	623	-	19,19,19	0.99	1 (5%)	23,24,24	1.62	3 (13%)
38	HEM	E	103	6,5	50,50,50	1.55	7 (14%)	67,82,82	1.67	16 (23%)
23	CLA	B	606	2	69,73,73	2.03	18 (26%)	82,113,113	2.73	30 (36%)
34	HTG	B	622	-	19,19,19	0.93	1 (5%)	23,24,24	1.38	4 (17%)
35	LMT	E	102	-	36,36,36	0.53	1 (2%)	47,47,47	0.86	0
36	DGD	c	517	-	63,63,67	0.91	3 (4%)	77,77,81	1.00	6 (7%)
23	CLA	C	504	3	69,73,73	2.00	18 (26%)	82,113,113	2.69	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	B	624	-	19,19,19	0.92	1 (5%)	23,24,24	1.54	3 (13%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.51	11 (19%)
23	CLA	b	615	2	69,73,73	1.98	18 (26%)	82,113,113	2.67	28 (34%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	10 (17%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.13	5 (11%)
23	CLA	b	610	41	69,73,73	2.10	20 (28%)	82,113,113	2.69	32 (39%)
23	CLA	A	406	41	69,73,73	2.03	20 (28%)	82,113,113	2.75	32 (39%)
23	CLA	b	605	2	69,73,73	2.03	21 (30%)	82,113,113	2.69	29 (35%)
31	LHG	e	101	-	41,41,48	1.03	2 (4%)	44,47,54	0.96	2 (4%)
31	LHG	d	409	-	48,48,48	0.97	2 (4%)	51,54,54	1.01	3 (5%)
24	PHO	a	406	-	58,69,69	2.73	13 (22%)	55,99,99	2.99	17 (30%)
28	OEX	A	413	41,1,3	0,15,15	-	-	-	-	-
40	HEC	v	201	16	46,50,50	1.75	9 (19%)	58,82,82	1.66	13 (22%)
25	BCR	A	409	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	12 (21%)
23	CLA	B	603	2	69,73,73	2.02	19 (27%)	82,113,113	2.67	31 (37%)
23	CLA	b	609	2	69,73,73	2.03	19 (27%)	82,113,113	2.69	30 (36%)
23	CLA	c	505	3	69,73,73	2.02	19 (27%)	82,113,113	2.63	30 (36%)
23	CLA	C	507	3	69,73,73	2.04	21 (30%)	82,113,113	2.66	34 (41%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
28	OEX	a	413	41,1,3	0,15,15	-	-	-	-	-
25	BCR	D	406	-	41,41,41	1.06	1 (2%)	56,56,56	1.84	14 (25%)
25	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.70	13 (23%)
27	GOL	b	624	-	5,5,5	0.34	0	5,5,5	0.48	0
29	PL9	A	414	-	55,55,55	0.67	2 (3%)	68,69,69	1.97	22 (32%)
35	LMT	B	631	-	26,26,36	0.50	0	31,31,47	0.82	1 (3%)
23	CLA	B	607	41	69,73,73	2.02	20 (28%)	82,113,113	2.69	31 (37%)
31	LHG	l	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.07	3 (5%)
23	CLA	C	503	3	69,73,73	2.03	19 (27%)	82,113,113	2.57	29 (35%)
23	CLA	C	510	3	69,73,73	2.06	20 (28%)	82,113,113	2.68	31 (37%)
23	CLA	d	404	4	69,73,73	2.06	21 (30%)	82,113,113	2.71	36 (43%)
25	BCR	B	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.66	12 (21%)
35	LMT	D	402	-	36,36,36	0.65	1 (2%)	47,47,47	1.28	4 (8%)
23	CLA	b	612	2	69,73,73	2.04	20 (28%)	82,113,113	2.59	28 (34%)
34	HTG	B	623	-	19,19,19	0.77	1 (5%)	23,24,24	1.49	1 (4%)
25	BCR	c	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.71	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	D	408	-	48,48,48	0.88	3 (6%)	51,54,54	0.98	3 (5%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.08	5 (6%)
26	SQD	a	410	-	52,54,54	0.90	2 (3%)	62,65,65	1.70	12 (19%)
23	CLA	d	401	41	69,73,73	2.04	20 (28%)	82,113,113	2.78	33 (40%)
23	CLA	B	610	41	69,73,73	2.06	20 (28%)	82,113,113	2.69	32 (39%)
23	CLA	c	513	3	69,73,73	2.06	20 (28%)	82,113,113	2.73	30 (36%)
31	LHG	d	408	-	48,48,48	0.89	2 (4%)	51,54,54	0.92	3 (5%)
23	CLA	c	502	3	69,73,73	2.01	20 (28%)	82,113,113	2.61	30 (36%)
23	CLA	b	607	41	69,73,73	1.95	18 (26%)	82,113,113	2.67	30 (36%)
29	PL9	d	406	-	55,55,55	0.64	1 (1%)	68,69,69	1.77	18 (26%)
34	HTG	V	203	-	11,11,19	0.25	0	15,15,24	1.00	2 (13%)
31	LHG	d	407	-	48,48,48	0.89	3 (6%)	51,54,54	1.06	5 (9%)
35	LMT	B	629	-	25,25,36	0.46	0	30,30,47	0.69	0
33	LMG	b	620	-	51,51,55	0.87	2 (3%)	59,59,63	1.26	8 (13%)
23	CLA	B	601	41	69,73,73	2.07	20 (28%)	82,113,113	2.65	31 (37%)
23	CLA	A	408	1	69,73,73	2.04	21 (30%)	82,113,113	2.74	30 (36%)
23	CLA	C	514	3	69,73,73	2.05	21 (30%)	82,113,113	2.73	30 (36%)
25	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.71	13 (23%)
26	SQD	f	101	-	41,43,54	1.12	3 (7%)	51,54,65	1.36	7 (13%)
25	BCR	a	409	-	41,41,41	0.95	1 (2%)	56,56,56	1.51	12 (21%)
26	SQD	a	412	-	52,54,54	1.00	2 (3%)	62,65,65	1.21	8 (12%)
29	PL9	a	414	-	55,55,55	0.67	2 (3%)	68,69,69	2.02	21 (30%)
23	CLA	b	606	2	69,73,73	1.99	19 (27%)	82,113,113	2.70	33 (40%)

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
23	CLA	a	405	41	-	7/39/115/115	-
29	PL9	D	407	-	-	11/53/73/73	0/1/1/1
33	LMG	c	520	-	-	7/46/66/70	0/1/1/1
23	CLA	B	605	2	1/1/15/20	9/39/115/115	-
31	LHG	D	409	-	-	14/53/53/53	-
23	CLA	B	612	2	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	602	2	1/1/15/20	5/39/115/115	-
23	CLA	B	616	2	1/1/15/20	13/39/115/115	-
23	CLA	C	502	3	1/1/15/20	6/39/115/115	-
23	CLA	b	613	2	1/1/15/20	8/39/115/115	-
33	LMG	j	101	39	-	12/46/66/70	0/1/1/1
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
23	CLA	C	511	3	1/1/15/20	14/39/115/115	-
33	LMG	Z	101	-	-	9/46/66/70	0/1/1/1
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
27	GOL	d	402	-	-	2/4/4/4	-
33	LMG	B	621	-	-	12/46/66/70	0/1/1/1
23	CLA	c	511	3	1/1/15/20	3/39/115/115	-
33	LMG	C	501	-	-	9/46/66/70	0/1/1/1
34	HTG	D	412	-	-	0/7/27/30	0/1/1/1
27	GOL	a	411	-	-	2/4/4/4	-
36	DGD	c	516	-	-	13/51/91/95	0/2/2/2
36	DGD	C	518	-	-	13/51/91/95	0/2/2/2
33	LMG	c	519	-	-	13/46/66/70	0/1/1/1
23	CLA	c	501	3	1/1/15/20	5/39/115/115	-
33	LMG	J	101	39	-	9/46/66/70	0/1/1/1
23	CLA	C	512	3	1/1/15/20	4/39/115/115	-
23	CLA	c	504	41	1/1/15/20	5/39/115/115	-
23	CLA	C	509	3	1/1/15/20	2/39/115/115	-
33	LMG	Z	102	-	-	15/31/51/70	0/1/1/1
23	CLA	d	403	4	1/1/15/20	5/39/115/115	-
36	DGD	c	518	-	-	5/51/91/95	0/2/2/2
23	CLA	c	512	3	1/1/15/20	12/39/115/115	-
35	LMT	e	102	-	-	9/21/61/61	0/2/2/2
23	CLA	c	508	3	1/1/15/20	4/39/115/115	-
34	HTG	c	521	-	-	5/10/30/30	0/1/1/1
33	LMG	C	520	-	-	15/46/66/70	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	b	601	41	1/1/15/20	16/39/115/115	-
23	CLA	c	509	3	1/1/15/20	13/39/115/115	-
23	CLA	b	603	2	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	505	41	1/1/15/20	7/39/115/115	-
35	LMT	b	627	-	-	6/17/37/61	0/1/1/2
36	DGD	h	102	-	-	14/51/91/95	0/2/2/2
23	CLA	B	611	2	1/1/15/20	3/39/115/115	-
23	CLA	c	503	3	1/1/15/20	1/39/115/115	-
23	CLA	B	608	2	1/1/15/20	4/39/115/115	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
25	BCR	C	516	-	-	1/29/63/63	0/2/2/2
34	HTG	b	625	-	-	6/10/30/30	0/1/1/1
34	HTG	b	628	-	-	6/10/30/30	0/1/1/1
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
24	PHO	a	407	-	-	2/37/103/103	0/5/6/6
23	CLA	b	608	2	-	4/39/115/115	-
23	CLA	B	615	2	1/1/15/20	12/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	A	404	1	1/1/15/20	4/39/115/115	-
24	PHO	D	401	-	-	5/37/103/103	0/5/6/6
33	LMG	a	416	-	-	15/46/66/70	0/1/1/1
23	CLA	C	506	3	1/1/15/20	9/39/115/115	-
35	LMT	m	102	-	-	7/21/61/61	0/2/2/2
27	GOL	B	626	-	-	2/4/4/4	-
26	SQD	A	410	-	-	12/49/69/69	0/1/1/1
38	HEM	e	103	6,5	-	8/14/54/54	-
25	BCR	y	101	-	-	7/29/63/63	0/2/2/2
36	DGD	C	519	-	-	15/51/91/95	0/2/2/2
23	CLA	b	616	2	1/1/15/20	13/39/115/115	-
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
35	LMT	D	403	-	-	10/21/61/61	0/2/2/2
31	LHG	A	416	-	-	11/53/53/53	-
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
35	LMT	M	101	-	-	2/21/61/61	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	14/39/115/115	-
25	BCR	d	405	-	-	4/29/63/63	0/2/2/2
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	408	1	1/1/15/20	10/39/115/115	-
35	LMT	B	630	-	-	7/21/61/61	0/2/2/2
34	HTG	d	411	-	-	3/7/27/30	0/1/1/1
23	CLA	A	405	41	1/1/15/20	5/39/115/115	-
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	B	604	2	1/1/15/20	10/39/115/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	614	2	1/1/15/20	11/39/115/115	-
23	CLA	a	404	1	1/1/15/20	8/39/115/115	-
23	CLA	C	513	3	1/1/15/20	7/39/115/115	-
24	PHO	A	407	-	-	3/37/103/103	0/5/6/6
23	CLA	c	506	3	1/1/15/20	9/39/115/115	-
27	GOL	B	625	-	-	4/4/4/4	-
34	HTG	b	622	-	-	2/10/30/30	0/1/1/1
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	613	2	1/1/15/20	5/39/115/115	-
26	SQD	L	101	-	-	22/49/69/69	0/1/1/1
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	602	2	1/1/15/20	8/39/115/115	-
23	CLA	D	404	4	1/1/15/20	2/39/115/115	-
23	CLA	c	507	41	1/1/15/20	9/39/115/115	-
23	CLA	b	611	2	1/1/15/20	6/39/115/115	-
26	SQD	B	620	-	-	14/49/69/69	0/1/1/1
31	LHG	A	417	-	-	20/53/53/53	-
35	LMT	a	417	-	-	4/21/61/61	0/2/2/2
23	CLA	B	609	2	1/1/15/20	4/39/115/115	-
23	CLA	c	510	3	1/1/15/20	8/39/115/115	-
23	CLA	C	508	41	1/1/15/20	9/39/115/115	-
23	CLA	b	614	2	1/1/15/20	12/39/115/115	-
35	LMT	b	621	-	-	7/17/37/61	0/1/1/2
34	HTG	C	522	-	-	2/10/30/30	0/1/1/1
40	HEC	V	202	16	-	6/14/54/54	-
34	HTG	B	627	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	I	101	-	-	10/21/61/61	0/2/2/2
23	CLA	D	405	4	1/1/15/20	8/39/115/115	-
35	LMT	M	103	-	-	11/21/61/61	0/2/2/2
36	DGD	H	102	-	-	14/51/91/95	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
34	HTG	b	623	-	-	3/10/30/30	0/1/1/1
38	HEM	E	103	6,5	-	6/14/54/54	-
23	CLA	B	606	2	1/1/15/20	4/39/115/115	-
34	HTG	B	622	-	-	3/10/30/30	0/1/1/1
35	LMT	E	102	-	-	11/21/61/61	0/2/2/2
36	DGD	c	517	-	-	13/51/91/95	0/2/2/2
23	CLA	C	504	3	-	2/39/115/115	-
34	HTG	B	624	-	-	4/10/30/30	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	b	615	2	1/1/15/20	6/39/115/115	-
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
31	LHG	E	101	-	-	20/46/46/53	-
23	CLA	b	610	41	1/1/15/20	4/39/115/115	-
23	CLA	A	406	41	1/1/15/20	12/39/115/115	-
23	CLA	b	605	2	1/1/15/20	9/39/115/115	-
31	LHG	e	101	-	-	13/46/46/53	-
31	LHG	d	409	-	-	15/53/53/53	-
24	PHO	a	406	-	-	0/37/103/103	0/5/6/6
40	HEC	v	201	16	-	6/14/54/54	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	B	603	2	1/1/15/20	6/39/115/115	-
23	CLA	b	609	2	1/1/15/20	5/39/115/115	-
23	CLA	c	505	3	1/1/15/20	6/39/115/115	-
23	CLA	C	507	3	1/1/15/20	13/39/115/115	-
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
35	LMT	B	631	-	-	7/17/38/61	0/1/1/2
25	BCR	D	406	-	-	6/29/63/63	0/2/2/2
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
27	GOL	b	624	-	-	1/4/4/4	-
29	PL9	A	414	-	-	11/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	607	41	1/1/15/20	4/39/115/115	-
31	LHG	l	101	-	-	19/53/53/53	-
23	CLA	C	503	3	1/1/15/20	7/39/115/115	-
23	CLA	C	510	3	1/1/15/20	8/39/115/115	-
23	CLA	d	404	4	1/1/15/20	14/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
35	LMT	D	402	-	-	6/21/61/61	0/2/2/2
23	CLA	b	612	2	1/1/15/20	5/39/115/115	-
34	HTG	B	623	-	-	6/10/30/30	0/1/1/1
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
31	LHG	D	408	-	-	15/53/53/53	-
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
26	SQD	a	410	-	-	12/49/69/69	0/1/1/1
23	CLA	d	401	41	1/1/15/20	6/39/115/115	-
23	CLA	B	610	41	1/1/15/20	7/39/115/115	-
23	CLA	c	513	3	1/1/15/20	2/39/115/115	-
31	LHG	d	408	-	-	20/53/53/53	-
23	CLA	c	502	3	1/1/15/20	7/39/115/115	-
23	CLA	b	607	41	1/1/15/20	5/39/115/115	-
29	PL9	d	406	-	-	6/53/73/73	0/1/1/1
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
31	LHG	d	407	-	-	13/53/53/53	-
35	LMT	B	629	-	-	10/17/37/61	0/1/1/2
33	LMG	b	620	-	-	12/46/66/70	0/1/1/1
23	CLA	B	601	41	1/1/15/20	12/39/115/115	-
23	CLA	A	408	1	1/1/15/20	13/39/115/115	-
23	CLA	C	514	3	-	13/39/115/115	-
25	BCR	b	619	-	-	2/29/63/63	0/2/2/2
26	SQD	f	101	-	-	16/38/58/69	0/1/1/1
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
26	SQD	a	412	-	-	11/49/69/69	0/1/1/1
29	PL9	a	414	-	-	14/53/73/73	0/1/1/1
23	CLA	b	606	2	1/1/15/20	8/39/115/115	-

All (1594) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	PHO	C1D-C2D	9.75	1.50	1.39
24	a	407	PHO	C1D-C2D	9.34	1.49	1.39
24	A	407	PHO	C1D-C2D	9.30	1.49	1.39
24	A	407	PHO	C1B-C2B	9.12	1.49	1.39
24	a	406	PHO	C1D-C2D	8.90	1.49	1.39
24	a	406	PHO	C1B-C2B	8.82	1.49	1.39
24	D	401	PHO	C1B-C2B	8.72	1.49	1.39
24	a	407	PHO	C1B-C2B	8.64	1.49	1.39
24	a	407	PHO	C3B-C4B	8.38	1.50	1.41
24	A	407	PHO	C3B-C4B	8.34	1.49	1.41
24	a	406	PHO	C4D-CHA	7.11	1.50	1.39
24	a	406	PHO	C3B-C4B	6.97	1.48	1.41
24	D	401	PHO	C3B-C2B	6.82	1.49	1.40
24	A	407	PHO	C4D-CHA	6.74	1.49	1.39
24	a	406	PHO	C3B-C2B	6.71	1.49	1.40
24	D	401	PHO	C4D-CHA	6.67	1.49	1.39
24	a	407	PHO	C3B-C2B	6.61	1.49	1.40
24	A	407	PHO	C3B-C2B	6.31	1.48	1.40
24	D	401	PHO	C3B-C4B	6.21	1.47	1.41
24	a	407	PHO	C4D-CHA	6.13	1.48	1.39
23	b	610	CLA	C3C-C2C	5.67	1.49	1.36
23	c	512	CLA	C3C-C2C	5.67	1.49	1.36
24	a	406	PHO	C3D-C2D	5.63	1.49	1.39
24	D	401	PHO	C3D-C2D	5.61	1.49	1.39
23	b	603	CLA	C3C-C2C	5.59	1.48	1.36
24	a	407	PHO	C3D-C2D	5.55	1.49	1.39
23	C	509	CLA	C3C-C2C	5.54	1.48	1.36
23	C	508	CLA	C3C-C2C	5.53	1.48	1.36
23	A	408	CLA	C3C-C2C	5.49	1.48	1.36
23	B	601	CLA	C3C-C2C	5.49	1.48	1.36
24	A	407	PHO	C3D-C2D	5.48	1.49	1.39
23	B	602	CLA	C3C-C2C	5.44	1.48	1.36
23	b	613	CLA	C3C-C2C	5.43	1.48	1.36
23	C	513	CLA	C3C-C2C	5.42	1.48	1.36
23	B	616	CLA	C3C-C2C	5.41	1.48	1.36
23	c	508	CLA	C3C-C2C	5.41	1.48	1.36
23	B	610	CLA	C3C-C2C	5.41	1.48	1.36
23	B	608	CLA	C3C-C2C	5.41	1.48	1.36
23	b	605	CLA	C3C-C2C	5.39	1.48	1.36
24	a	407	PHO	OBD-CAD	5.38	1.29	1.22
23	d	401	CLA	C1D-ND	5.38	1.44	1.37
23	C	507	CLA	O2D-CGD	5.37	1.46	1.33
23	B	603	CLA	C3C-C2C	5.37	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C3C-C2C	5.36	1.48	1.36
23	b	616	CLA	CHC-C1C	5.36	1.49	1.38
23	A	406	CLA	CHC-C1C	5.36	1.49	1.38
23	C	504	CLA	C3C-C2C	5.34	1.48	1.36
23	b	615	CLA	C3C-C2C	5.34	1.48	1.36
23	b	606	CLA	C3C-C2C	5.30	1.48	1.36
23	B	607	CLA	C3C-C2C	5.29	1.48	1.36
23	a	405	CLA	C3C-C2C	5.29	1.48	1.36
23	D	405	CLA	CHC-C1C	5.29	1.49	1.38
25	K	102	BCR	C23-C22	-5.28	1.34	1.46
23	b	612	CLA	C3C-C2C	5.27	1.48	1.36
23	c	501	CLA	C3C-C2C	5.26	1.48	1.36
25	C	515	BCR	C23-C22	-5.26	1.34	1.46
23	D	404	CLA	C3C-C2C	5.26	1.48	1.36
23	B	614	CLA	C3C-C2C	5.25	1.48	1.36
23	d	404	CLA	C3C-C2C	5.25	1.48	1.36
23	d	401	CLA	C3C-C2C	5.25	1.48	1.36
23	c	509	CLA	C3C-C2C	5.24	1.48	1.36
23	b	616	CLA	C3C-C2C	5.24	1.48	1.36
23	A	405	CLA	C3C-C2C	5.24	1.48	1.36
23	b	602	CLA	C3C-C2C	5.24	1.48	1.36
23	C	503	CLA	C3C-C2C	5.23	1.48	1.36
23	C	511	CLA	C3C-C2C	5.23	1.48	1.36
23	b	601	CLA	O2D-CGD	5.23	1.46	1.33
23	C	512	CLA	O2D-CGD	5.21	1.46	1.33
23	B	606	CLA	C3C-C2C	5.20	1.48	1.36
23	b	603	CLA	O2D-CGD	5.20	1.46	1.33
23	C	505	CLA	C3C-C2C	5.19	1.48	1.36
23	c	511	CLA	C1D-ND	5.19	1.44	1.37
23	D	405	CLA	C3C-C2C	5.19	1.48	1.36
23	C	505	CLA	O2D-CGD	5.18	1.46	1.33
23	c	505	CLA	C3C-C2C	5.18	1.47	1.36
23	b	601	CLA	C3C-C2C	5.18	1.47	1.36
38	e	103	HEM	FE-NB	5.18	2.10	1.94
23	a	408	CLA	C3C-C2C	5.18	1.47	1.36
23	b	603	CLA	CHC-C1C	5.17	1.48	1.38
23	c	506	CLA	O2D-CGD	5.17	1.45	1.33
23	B	616	CLA	CHC-C1C	5.17	1.48	1.38
25	k	101	BCR	C23-C22	-5.17	1.34	1.46
23	b	604	CLA	C3C-C2C	5.16	1.47	1.36
23	b	602	CLA	O2D-CGD	5.16	1.45	1.33
25	b	619	BCR	C23-C22	-5.16	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C3C-C2C	5.16	1.47	1.36
23	A	404	CLA	C1D-ND	5.14	1.44	1.37
23	d	404	CLA	CHC-C1C	5.14	1.48	1.38
24	a	407	PHO	O2D-CGD	5.14	1.45	1.33
23	A	404	CLA	C3C-C2C	5.14	1.47	1.36
23	B	612	CLA	C3C-C2C	5.13	1.47	1.36
38	E	103	HEM	FE-NB	5.13	2.10	1.94
23	C	514	CLA	C3C-C2C	5.12	1.47	1.36
23	B	609	CLA	CHC-C1C	5.12	1.48	1.38
23	b	608	CLA	C3C-C2C	5.12	1.47	1.36
23	b	611	CLA	C3C-C2C	5.12	1.47	1.36
23	c	513	CLA	C3C-C2C	5.11	1.47	1.36
23	B	611	CLA	C1D-ND	5.10	1.44	1.37
23	c	511	CLA	C3C-C2C	5.10	1.47	1.36
23	B	605	CLA	C1D-ND	5.10	1.44	1.37
23	C	502	CLA	C3C-C2C	5.10	1.47	1.36
23	b	611	CLA	O2D-CGD	5.10	1.45	1.33
23	c	509	CLA	O2D-CGD	5.09	1.45	1.33
23	c	503	CLA	C3C-C2C	5.09	1.47	1.36
23	B	601	CLA	O2D-CGD	5.09	1.45	1.33
23	B	605	CLA	C3C-C2C	5.09	1.47	1.36
23	c	507	CLA	C3C-C2C	5.09	1.47	1.36
23	B	615	CLA	O2D-CGD	5.09	1.45	1.33
23	C	506	CLA	CHC-C1C	5.08	1.48	1.38
23	c	502	CLA	C3C-C2C	5.08	1.47	1.36
25	d	405	BCR	C23-C22	-5.08	1.35	1.46
23	A	408	CLA	O2D-CGD	5.07	1.45	1.33
23	B	602	CLA	O2D-CGD	5.07	1.45	1.33
23	C	514	CLA	CHC-C1C	5.07	1.48	1.38
23	c	513	CLA	O2D-CGD	5.07	1.45	1.33
23	B	609	CLA	O2D-CGD	5.07	1.45	1.33
23	B	602	CLA	C1D-ND	5.06	1.44	1.37
23	B	611	CLA	O2D-CGD	5.06	1.45	1.33
23	c	504	CLA	O2D-CGD	5.06	1.45	1.33
23	c	506	CLA	C3C-C2C	5.05	1.47	1.36
25	D	406	BCR	C23-C22	-5.05	1.35	1.46
23	b	613	CLA	O2D-CGD	5.03	1.45	1.33
23	d	403	CLA	C3C-C2C	5.03	1.47	1.36
23	A	406	CLA	O2D-CGD	5.03	1.45	1.33
23	b	609	CLA	O2D-CGD	5.02	1.45	1.33
23	c	510	CLA	O2D-CGD	5.02	1.45	1.33
23	B	614	CLA	O2D-CGD	5.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CHC-C1C	5.00	1.48	1.38
23	A	405	CLA	CHC-C1C	5.00	1.48	1.38
23	c	505	CLA	CHC-C1C	5.00	1.48	1.38
23	B	615	CLA	C3C-C2C	5.00	1.47	1.36
23	b	610	CLA	CHC-C1C	4.99	1.48	1.38
25	c	514	BCR	C23-C22	-4.99	1.35	1.46
23	b	616	CLA	C1D-ND	4.98	1.44	1.37
23	C	514	CLA	C1D-ND	4.98	1.44	1.37
23	B	608	CLA	O2D-CGD	4.98	1.45	1.33
24	A	407	PHO	O2D-CGD	4.97	1.45	1.33
23	B	613	CLA	O2D-CGD	4.97	1.45	1.33
23	c	513	CLA	CHC-C1C	4.97	1.48	1.38
23	C	510	CLA	O2D-CGD	4.97	1.45	1.33
23	B	604	CLA	CHC-C1C	4.96	1.48	1.38
23	C	513	CLA	CHC-C1C	4.96	1.48	1.38
25	t	101	BCR	C23-C22	-4.96	1.35	1.46
23	c	502	CLA	O2D-CGD	4.95	1.45	1.33
23	A	404	CLA	CHC-C1C	4.95	1.48	1.38
23	c	507	CLA	CHC-C1C	4.95	1.48	1.38
24	A	407	PHO	OBD-CAD	4.95	1.28	1.22
23	B	613	CLA	C3C-C2C	4.95	1.47	1.36
23	c	507	CLA	C1D-ND	4.95	1.44	1.37
23	C	506	CLA	C3C-C2C	4.94	1.47	1.36
23	b	607	CLA	C3C-C2C	4.94	1.47	1.36
25	C	516	BCR	C23-C22	-4.94	1.35	1.46
23	b	608	CLA	O2D-CGD	4.94	1.45	1.33
23	b	614	CLA	O2D-CGD	4.94	1.45	1.33
23	a	404	CLA	C3C-C2C	4.93	1.47	1.36
23	C	512	CLA	C3C-C2C	4.93	1.47	1.36
23	B	604	CLA	C3C-C2C	4.93	1.47	1.36
23	b	612	CLA	CHC-C1C	4.93	1.48	1.38
23	d	403	CLA	O2D-CGD	4.92	1.45	1.33
23	a	404	CLA	C1D-ND	4.92	1.44	1.37
23	c	501	CLA	C1D-ND	4.92	1.44	1.37
23	B	606	CLA	CHC-C1C	4.91	1.48	1.38
23	b	616	CLA	O2D-CGD	4.91	1.45	1.33
23	b	609	CLA	CHC-C1C	4.91	1.48	1.38
25	b	618	BCR	C23-C22	-4.90	1.35	1.46
23	a	408	CLA	CHC-C1C	4.90	1.48	1.38
23	c	512	CLA	O2D-CGD	4.89	1.45	1.33
23	b	607	CLA	O2D-CGD	4.89	1.45	1.33
25	B	619	BCR	C23-C22	-4.89	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	409	BCR	C23-C22	-4.89	1.35	1.46
23	B	605	CLA	O2D-CGD	4.88	1.45	1.33
23	d	404	CLA	C1D-ND	4.88	1.44	1.37
23	c	510	CLA	C3C-C2C	4.88	1.47	1.36
23	D	404	CLA	O2D-CGD	4.87	1.45	1.33
23	b	604	CLA	CHC-C1C	4.87	1.48	1.38
23	b	612	CLA	O2D-CGD	4.87	1.45	1.33
24	D	401	PHO	O2D-CGD	4.87	1.45	1.33
23	c	504	CLA	C3C-C2C	4.86	1.47	1.36
25	H	101	BCR	C23-C22	-4.86	1.35	1.46
23	C	503	CLA	CHC-C1C	4.86	1.48	1.38
23	B	605	CLA	CHC-C1C	4.86	1.48	1.38
23	C	511	CLA	CHC-C1C	4.86	1.48	1.38
23	c	511	CLA	CHC-C1C	4.86	1.48	1.38
23	c	508	CLA	CHC-C1C	4.86	1.48	1.38
23	C	506	CLA	O2D-CGD	4.85	1.45	1.33
23	B	611	CLA	C3C-C2C	4.85	1.47	1.36
23	b	601	CLA	C1D-ND	4.84	1.44	1.37
23	B	606	CLA	C1D-ND	4.84	1.44	1.37
23	C	507	CLA	C3C-C2C	4.84	1.47	1.36
23	c	509	CLA	C1D-ND	4.84	1.44	1.37
23	B	609	CLA	C3C-C2C	4.84	1.47	1.36
23	c	507	CLA	O2D-CGD	4.83	1.45	1.33
25	y	101	BCR	C23-C22	-4.83	1.35	1.46
23	C	508	CLA	O2D-CGD	4.83	1.45	1.33
25	b	617	BCR	C23-C22	-4.83	1.35	1.46
23	c	503	CLA	CHC-C1C	4.83	1.48	1.38
25	T	101	BCR	C23-C22	-4.82	1.35	1.46
23	B	604	CLA	O2D-CGD	4.82	1.45	1.33
23	D	405	CLA	O2D-CGD	4.82	1.45	1.33
23	c	504	CLA	C1D-ND	4.82	1.44	1.37
23	B	610	CLA	C1D-ND	4.81	1.44	1.37
23	b	604	CLA	O2D-CGD	4.81	1.45	1.33
23	a	408	CLA	O2D-CGD	4.81	1.45	1.33
24	D	401	PHO	OBD-CAD	4.81	1.28	1.22
23	B	610	CLA	O2D-CGD	4.81	1.45	1.33
23	c	503	CLA	C1D-ND	4.80	1.44	1.37
23	A	408	CLA	CHC-C1C	4.80	1.48	1.38
23	B	606	CLA	O2D-CGD	4.80	1.45	1.33
23	b	605	CLA	O2D-CGD	4.80	1.45	1.33
23	C	509	CLA	O2D-CGD	4.79	1.45	1.33
23	b	602	CLA	CHC-C1C	4.79	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C1D-ND	4.78	1.44	1.37
23	d	403	CLA	CHC-C1C	4.78	1.48	1.38
23	b	602	CLA	C1D-ND	4.78	1.44	1.37
23	b	601	CLA	CHC-C1C	4.78	1.48	1.38
23	C	507	CLA	C1D-ND	4.78	1.44	1.37
24	a	406	PHO	OBD-CAD	4.78	1.28	1.22
23	d	401	CLA	CHC-C1C	4.77	1.48	1.38
23	c	513	CLA	C1D-ND	4.77	1.44	1.37
23	C	504	CLA	CHC-C1C	4.77	1.48	1.38
23	b	614	CLA	C3C-C2C	4.76	1.47	1.36
23	a	404	CLA	O2D-CGD	4.76	1.44	1.33
23	A	408	CLA	CHD-C1D	4.76	1.47	1.38
23	b	605	CLA	C1D-ND	4.75	1.44	1.37
23	B	609	CLA	O2A-CGA	4.75	1.47	1.33
23	d	401	CLA	O2D-CGD	4.75	1.44	1.33
23	a	405	CLA	CHC-C1C	4.75	1.48	1.38
23	B	602	CLA	CHD-C1D	4.75	1.47	1.38
23	c	512	CLA	CHC-C1C	4.75	1.48	1.38
23	b	615	CLA	O2D-CGD	4.75	1.44	1.33
23	c	503	CLA	O2D-CGD	4.74	1.44	1.33
23	C	503	CLA	CHD-C1D	4.74	1.47	1.38
25	c	515	BCR	C23-C22	-4.74	1.35	1.46
23	b	609	CLA	C1D-ND	4.73	1.44	1.37
23	B	607	CLA	CHC-C1C	4.73	1.48	1.38
23	A	404	CLA	O2D-CGD	4.73	1.44	1.33
23	B	603	CLA	C1D-ND	4.72	1.44	1.37
23	B	615	CLA	C1D-ND	4.72	1.44	1.37
23	a	405	CLA	O2D-CGD	4.71	1.44	1.33
23	C	511	CLA	O2D-CGD	4.71	1.44	1.33
23	b	609	CLA	C3C-C2C	4.71	1.46	1.36
25	h	101	BCR	C23-C22	-4.71	1.35	1.46
23	c	509	CLA	CHC-C1C	4.70	1.47	1.38
23	c	501	CLA	CHC-C1C	4.70	1.47	1.38
23	b	608	CLA	CHC-C1C	4.70	1.47	1.38
23	C	514	CLA	O2D-CGD	4.70	1.44	1.33
23	b	606	CLA	C1D-ND	4.69	1.44	1.37
23	D	405	CLA	C1D-ND	4.69	1.44	1.37
23	b	607	CLA	CHC-C1C	4.69	1.47	1.38
23	B	616	CLA	O2D-CGD	4.69	1.44	1.33
23	b	612	CLA	C1D-ND	4.68	1.44	1.37
23	c	506	CLA	C1D-ND	4.68	1.44	1.37
23	B	613	CLA	C1D-ND	4.68	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	O2D-CGD	4.68	1.44	1.33
23	c	505	CLA	O2D-CGD	4.68	1.44	1.33
23	b	611	CLA	C1D-ND	4.67	1.44	1.37
23	C	503	CLA	C1D-ND	4.67	1.44	1.37
23	c	502	CLA	C1D-ND	4.66	1.44	1.37
23	A	405	CLA	CHC-C4B	4.66	1.49	1.39
23	c	508	CLA	O2D-CGD	4.66	1.44	1.33
23	b	603	CLA	C1D-ND	4.66	1.44	1.37
23	C	507	CLA	CHC-C1C	4.66	1.47	1.38
23	A	408	CLA	C1D-ND	4.66	1.44	1.37
23	B	616	CLA	C1D-ND	4.65	1.44	1.37
23	c	511	CLA	O2D-CGD	4.65	1.44	1.33
23	B	601	CLA	CHC-C1C	4.65	1.47	1.38
23	c	501	CLA	CHD-C1D	4.64	1.47	1.38
23	C	507	CLA	CHD-C1D	4.63	1.47	1.38
23	B	602	CLA	CHC-C1C	4.63	1.47	1.38
23	B	603	CLA	O2D-CGD	4.63	1.44	1.33
23	C	510	CLA	CHC-C1C	4.62	1.47	1.38
23	C	513	CLA	O2D-CGD	4.62	1.44	1.33
23	b	610	CLA	CHD-C1D	4.62	1.47	1.38
23	C	512	CLA	CHC-C1C	4.62	1.47	1.38
23	b	615	CLA	CHC-C1C	4.62	1.47	1.38
23	A	405	CLA	O2D-CGD	4.62	1.44	1.33
23	B	613	CLA	CHC-C1C	4.61	1.47	1.38
23	B	608	CLA	CHC-C1C	4.61	1.47	1.38
25	Y	101	BCR	C23-C22	-4.61	1.36	1.46
23	C	510	CLA	C1D-ND	4.60	1.43	1.37
23	B	601	CLA	C1D-ND	4.60	1.43	1.37
23	b	606	CLA	O2D-CGD	4.60	1.44	1.33
23	C	502	CLA	C1D-ND	4.59	1.43	1.37
23	C	508	CLA	CHC-C1C	4.59	1.47	1.38
23	b	610	CLA	O2D-CGD	4.58	1.44	1.33
23	C	508	CLA	C1D-ND	4.58	1.43	1.37
23	C	502	CLA	CHC-C1C	4.58	1.47	1.38
23	A	405	CLA	C1D-ND	4.57	1.43	1.37
23	C	513	CLA	C1D-ND	4.57	1.43	1.37
23	d	404	CLA	O2D-CGD	4.57	1.44	1.33
23	b	606	CLA	CHC-C1C	4.57	1.47	1.38
33	z	101	LMG	O8-C28	4.57	1.46	1.33
23	B	607	CLA	O2D-CGD	4.57	1.44	1.33
23	c	505	CLA	C1D-ND	4.56	1.43	1.37
23	c	504	CLA	CHC-C1C	4.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	CHC-C1C	4.56	1.47	1.38
23	C	504	CLA	C1D-ND	4.56	1.43	1.37
23	B	601	CLA	O2A-CGA	4.56	1.46	1.33
25	B	617	BCR	C23-C22	-4.55	1.36	1.46
23	b	608	CLA	C1D-ND	4.55	1.43	1.37
23	b	604	CLA	C1D-ND	4.55	1.43	1.37
24	a	406	PHO	O2D-CGD	4.55	1.44	1.33
23	B	611	CLA	CHC-C1C	4.54	1.47	1.38
23	a	405	CLA	C1D-ND	4.54	1.43	1.37
23	b	613	CLA	CHC-C1C	4.53	1.47	1.38
23	D	404	CLA	C1D-ND	4.53	1.43	1.37
23	c	512	CLA	C1D-ND	4.53	1.43	1.37
23	b	610	CLA	C1D-ND	4.52	1.43	1.37
23	b	601	CLA	CHD-C1D	4.52	1.47	1.38
23	b	615	CLA	C1D-ND	4.52	1.43	1.37
23	c	508	CLA	C1D-ND	4.52	1.43	1.37
23	C	502	CLA	O2D-CGD	4.52	1.44	1.33
23	b	613	CLA	C1D-ND	4.51	1.43	1.37
26	D	413	SQD	O47-C7	4.51	1.47	1.34
23	C	503	CLA	O2A-CGA	4.51	1.46	1.33
23	b	611	CLA	CHC-C1C	4.50	1.47	1.38
23	b	602	CLA	CHD-C1D	4.50	1.47	1.38
23	c	510	CLA	C1D-ND	4.50	1.43	1.37
26	a	412	SQD	O48-C23	4.50	1.46	1.33
31	E	101	LHG	O8-C23	4.49	1.46	1.33
23	C	508	CLA	CHD-C1D	4.49	1.47	1.38
23	C	512	CLA	C1D-ND	4.49	1.43	1.37
23	C	503	CLA	O2D-CGD	4.48	1.44	1.33
23	C	511	CLA	C1D-ND	4.48	1.43	1.37
23	a	404	CLA	CHC-C1C	4.48	1.47	1.38
23	C	510	CLA	CHD-C1D	4.48	1.47	1.38
23	c	508	CLA	O2A-CGA	4.47	1.46	1.33
26	f	101	SQD	O47-C7	4.47	1.46	1.34
23	C	513	CLA	CHD-C1D	4.47	1.47	1.38
23	B	603	CLA	CHD-C1D	4.47	1.47	1.38
23	d	401	CLA	O2A-CGA	4.46	1.46	1.33
23	C	514	CLA	CHD-C1D	4.45	1.47	1.38
26	B	620	SQD	O47-C7	4.44	1.46	1.34
23	B	612	CLA	CHC-C1C	4.44	1.47	1.38
23	b	601	CLA	O2A-CGA	4.44	1.46	1.33
23	d	404	CLA	CHD-C1D	4.44	1.47	1.38
23	c	506	CLA	CHC-C1C	4.43	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404	CLA	O2A-CGA	4.42	1.46	1.33
23	C	508	CLA	O2A-CGA	4.42	1.46	1.33
23	b	611	CLA	O2A-CGA	4.42	1.46	1.33
25	a	409	BCR	C23-C22	-4.42	1.36	1.46
23	c	510	CLA	CHC-C1C	4.41	1.47	1.38
36	c	517	DGD	O1G-C1A	4.41	1.46	1.33
23	B	615	CLA	CHC-C1C	4.41	1.47	1.38
23	d	403	CLA	O2A-CGA	4.41	1.46	1.33
23	b	614	CLA	CHC-C1C	4.41	1.47	1.38
23	b	605	CLA	CHD-C1D	4.40	1.47	1.38
23	b	612	CLA	O2A-CGA	4.40	1.46	1.33
23	C	505	CLA	CHC-C1C	4.40	1.47	1.38
23	D	404	CLA	CHC-C1C	4.39	1.47	1.38
26	A	412	SQD	O47-C7	4.39	1.46	1.34
23	b	609	CLA	CHD-C1D	4.39	1.47	1.38
33	Z	101	LMG	O7-C10	4.39	1.46	1.34
23	c	501	CLA	O2D-CGD	4.39	1.44	1.33
23	C	504	CLA	O2D-CGD	4.39	1.44	1.33
31	d	409	LHG	O7-C7	4.38	1.46	1.34
23	d	401	CLA	CHD-C1D	4.38	1.47	1.38
23	B	610	CLA	OBD-CAD	4.38	1.30	1.22
23	B	609	CLA	C1D-ND	4.38	1.43	1.37
23	B	607	CLA	CHD-C1D	4.37	1.46	1.38
23	c	507	CLA	CHD-C1D	4.36	1.46	1.38
23	B	607	CLA	C1D-ND	4.36	1.43	1.37
23	c	507	CLA	O2A-CGA	4.36	1.46	1.33
23	C	512	CLA	O2A-CGA	4.36	1.46	1.33
23	C	505	CLA	O2A-CGA	4.36	1.46	1.33
23	b	608	CLA	O2A-CGA	4.36	1.46	1.33
23	c	512	CLA	O2A-CGA	4.35	1.46	1.33
26	B	620	SQD	O48-C23	4.35	1.46	1.33
33	C	501	LMG	O8-C28	4.35	1.46	1.33
23	B	601	CLA	CHD-C1D	4.35	1.46	1.38
23	C	512	CLA	CHD-C1D	4.35	1.46	1.38
33	Z	101	LMG	O8-C28	4.35	1.46	1.33
26	A	412	SQD	O48-C23	4.35	1.46	1.33
23	a	408	CLA	CHD-C1D	4.34	1.46	1.38
23	B	614	CLA	CHD-C1D	4.34	1.46	1.38
23	c	503	CLA	CHD-C1D	4.33	1.46	1.38
23	C	511	CLA	CHD-C1D	4.32	1.46	1.38
23	B	608	CLA	C1D-ND	4.32	1.43	1.37
31	l	101	LHG	O8-C23	4.32	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	CLA	CHD-C1D	4.32	1.46	1.38
23	d	403	CLA	C1B-NB	-4.32	1.32	1.37
40	V	202	HEC	CBC-CAC	-4.32	1.33	1.49
23	c	513	CLA	CHD-C1D	4.32	1.46	1.38
23	b	616	CLA	CHD-C1D	4.31	1.46	1.38
23	C	506	CLA	O2A-CGA	4.31	1.45	1.33
23	c	506	CLA	CHD-C1D	4.31	1.46	1.38
31	e	101	LHG	O8-C23	4.31	1.45	1.33
23	A	405	CLA	O2A-CGA	4.31	1.45	1.33
23	C	514	CLA	O2A-CGA	4.31	1.45	1.33
26	L	101	SQD	O48-C23	4.30	1.45	1.33
23	B	607	CLA	O2A-CGA	4.30	1.45	1.33
23	B	612	CLA	CHD-C1D	4.30	1.46	1.38
23	c	509	CLA	O2A-CGA	4.29	1.45	1.33
23	C	509	CLA	CHD-C1D	4.29	1.46	1.38
23	C	505	CLA	C1D-ND	4.29	1.43	1.37
23	c	502	CLA	CHC-C1C	4.29	1.47	1.38
23	B	615	CLA	O2A-CGA	4.28	1.45	1.33
23	C	509	CLA	CHC-C1C	4.28	1.47	1.38
33	c	520	LMG	O8-C28	4.28	1.45	1.33
33	c	520	LMG	O7-C10	4.28	1.46	1.34
26	A	410	SQD	O48-C23	4.28	1.45	1.33
23	c	502	CLA	O2A-CGA	4.28	1.45	1.33
31	A	417	LHG	O8-C23	4.27	1.45	1.33
23	C	509	CLA	C1D-ND	4.27	1.43	1.37
23	c	502	CLA	CHD-C1D	4.27	1.46	1.38
23	c	504	CLA	O2A-CGA	4.26	1.45	1.33
23	c	513	CLA	O2A-CGA	4.26	1.45	1.33
23	C	504	CLA	CHD-C4C	4.26	1.48	1.39
23	B	612	CLA	C1B-NB	-4.26	1.32	1.37
33	B	621	LMG	O8-C28	4.25	1.45	1.33
23	b	615	CLA	O2A-CGA	4.25	1.45	1.33
33	Z	102	LMG	O7-C10	4.25	1.46	1.34
23	b	613	CLA	CHD-C1D	4.25	1.46	1.38
33	c	519	LMG	O8-C28	4.25	1.45	1.33
26	L	101	SQD	O47-C7	4.25	1.46	1.34
23	C	511	CLA	O2A-CGA	4.25	1.45	1.33
23	C	506	CLA	C1D-ND	4.25	1.43	1.37
40	V	202	HEC	CAC-C3C	4.25	1.48	1.35
40	v	201	HEC	CBC-CAC	-4.25	1.33	1.49
23	b	614	CLA	C1D-ND	4.24	1.43	1.37
23	B	602	CLA	CHD-C4C	4.24	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	CHD-C4C	4.24	1.48	1.39
23	b	605	CLA	CHC-C1C	4.24	1.47	1.38
23	B	606	CLA	O2A-CGA	4.24	1.45	1.33
23	d	401	CLA	C3D-C2D	4.24	1.50	1.39
26	f	101	SQD	O48-C23	4.24	1.45	1.33
33	a	416	LMG	O7-C10	4.23	1.46	1.34
23	B	615	CLA	CHD-C1D	4.23	1.46	1.38
23	C	504	CLA	CHD-C1D	4.23	1.46	1.38
23	c	511	CLA	CHD-C4C	4.22	1.48	1.39
23	C	502	CLA	O2A-CGA	4.22	1.45	1.33
33	C	501	LMG	O7-C10	4.22	1.46	1.34
23	b	606	CLA	CHD-C1D	4.22	1.46	1.38
23	b	611	CLA	CHB-C1B	4.22	1.48	1.39
23	A	406	CLA	C1D-ND	4.22	1.43	1.37
40	v	201	HEC	CBB-CAB	-4.21	1.33	1.49
23	b	608	CLA	CHD-C1D	4.21	1.46	1.38
23	b	604	CLA	CHD-C1D	4.21	1.46	1.38
23	C	513	CLA	O2A-CGA	4.21	1.45	1.33
40	V	202	HEC	CBB-CAB	-4.20	1.33	1.49
23	b	616	CLA	CHC-C4B	4.19	1.48	1.39
23	c	510	CLA	CHD-C1D	4.19	1.46	1.38
40	v	201	HEC	CAC-C3C	4.19	1.48	1.35
23	A	406	CLA	O2A-CGA	4.19	1.45	1.33
23	C	508	CLA	C3D-C2D	4.19	1.50	1.39
31	e	101	LHG	O7-C7	4.19	1.46	1.34
23	c	511	CLA	CHB-C1B	4.18	1.48	1.39
23	c	512	CLA	CHD-C1D	4.18	1.46	1.38
24	a	407	PHO	O2A-CGA	4.18	1.45	1.33
23	c	505	CLA	CHB-C1B	4.17	1.48	1.39
23	C	511	CLA	CHD-C4C	4.17	1.48	1.39
23	a	405	CLA	O2A-CGA	4.17	1.45	1.33
38	e	103	HEM	FE-NC	4.17	2.08	1.95
23	C	507	CLA	CHD-C4C	4.17	1.48	1.39
23	a	405	CLA	CHD-C1D	4.16	1.46	1.38
23	c	511	CLA	CHD-C1D	4.16	1.46	1.38
23	c	508	CLA	C3D-C2D	4.16	1.50	1.39
23	c	509	CLA	CHD-C1D	4.16	1.46	1.38
23	c	506	CLA	O2A-CGA	4.16	1.45	1.33
23	b	611	CLA	CHD-C1D	4.16	1.46	1.38
23	B	611	CLA	CHD-C1D	4.16	1.46	1.38
23	C	502	CLA	CHD-C1D	4.16	1.46	1.38
23	b	614	CLA	CHD-C1D	4.16	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	O2A-CGA	4.16	1.45	1.33
23	c	511	CLA	O2A-CGA	4.15	1.45	1.33
23	B	607	CLA	CHD-C4C	4.15	1.48	1.39
33	C	520	LMG	O8-C28	4.15	1.45	1.33
31	d	409	LHG	O8-C23	4.15	1.45	1.33
23	c	505	CLA	O2A-CGA	4.15	1.45	1.33
23	B	616	CLA	O2A-CGA	4.15	1.45	1.33
23	C	509	CLA	C3D-C2D	4.15	1.50	1.39
33	J	101	LMG	O8-C28	4.15	1.45	1.33
23	B	605	CLA	CHC-C4B	4.15	1.48	1.39
23	A	404	CLA	CHD-C1D	4.14	1.46	1.38
31	D	409	LHG	O7-C7	4.14	1.46	1.34
23	B	615	CLA	C3D-C2D	4.14	1.50	1.39
24	D	401	PHO	O2A-CGA	4.14	1.45	1.33
23	c	503	CLA	CHC-C4B	4.14	1.48	1.39
23	C	513	CLA	CHD-C4C	4.14	1.48	1.39
23	B	604	CLA	O2A-CGA	4.13	1.45	1.33
23	B	613	CLA	C3D-C2D	4.13	1.50	1.39
23	b	608	CLA	C3D-C2D	4.13	1.50	1.39
23	B	609	CLA	CHD-C1D	4.13	1.46	1.38
40	V	202	HEC	CAB-C3B	4.13	1.48	1.35
23	c	504	CLA	CHD-C1D	4.13	1.46	1.38
23	C	510	CLA	O2A-CGA	4.13	1.45	1.33
23	B	614	CLA	CHC-C1C	4.13	1.46	1.38
23	b	601	CLA	C3D-C2D	4.12	1.50	1.39
23	c	503	CLA	O2A-CGA	4.12	1.45	1.33
23	b	602	CLA	CHD-C4C	4.12	1.48	1.39
23	D	404	CLA	CHD-C1D	4.12	1.46	1.38
23	c	508	CLA	CHD-C1D	4.12	1.46	1.38
33	a	416	LMG	O8-C28	4.12	1.45	1.33
33	c	519	LMG	O7-C10	4.12	1.45	1.34
23	d	404	CLA	C3D-C2D	4.12	1.50	1.39
23	b	613	CLA	C3D-C2D	4.11	1.50	1.39
23	b	610	CLA	CHC-C4B	4.11	1.48	1.39
23	B	606	CLA	CHD-C1D	4.11	1.46	1.38
23	B	602	CLA	C3D-C2D	4.11	1.50	1.39
23	c	502	CLA	C3D-C2D	4.10	1.50	1.39
36	h	102	DGD	O2G-C1B	4.10	1.45	1.34
33	C	520	LMG	O7-C10	4.10	1.45	1.34
26	a	412	SQD	O47-C7	4.10	1.45	1.34
23	b	605	CLA	C3D-C2D	4.10	1.50	1.39
38	E	103	HEM	FE-NC	4.10	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	410	SQD	O48-C23	4.10	1.45	1.33
40	v	201	HEC	CAB-C3B	4.10	1.48	1.35
23	a	408	CLA	O2A-CGA	4.09	1.45	1.33
23	B	601	CLA	C3D-C2D	4.09	1.50	1.39
36	H	102	DGD	O2G-C1B	4.09	1.45	1.34
36	H	102	DGD	O1G-C1A	4.09	1.45	1.33
23	c	513	CLA	CHD-C4C	4.09	1.48	1.39
23	b	612	CLA	CHD-C1D	4.09	1.46	1.38
33	j	101	LMG	O8-C28	4.09	1.45	1.33
23	A	404	CLA	CHD-C4C	4.09	1.48	1.39
23	C	504	CLA	O2A-CGA	4.09	1.45	1.33
23	B	604	CLA	CHD-C1D	4.08	1.46	1.38
23	C	510	CLA	CHD-C4C	4.08	1.48	1.39
31	l	101	LHG	O7-C7	4.07	1.45	1.34
23	c	509	CLA	CHD-C4C	4.07	1.48	1.39
23	c	501	CLA	CHB-C1B	4.07	1.48	1.39
23	c	510	CLA	CHD-C4C	4.07	1.48	1.39
23	d	403	CLA	CHD-C1D	4.07	1.46	1.38
23	D	404	CLA	O2A-CGA	4.07	1.45	1.33
23	c	501	CLA	CHD-C4C	4.06	1.48	1.39
26	D	413	SQD	O48-C23	4.06	1.45	1.33
23	D	405	CLA	CHD-C1D	4.06	1.46	1.38
33	b	620	LMG	O8-C28	4.06	1.45	1.33
23	b	614	CLA	CHD-C4C	4.05	1.48	1.39
33	z	101	LMG	O7-C10	4.05	1.45	1.34
23	B	611	CLA	CHB-C1B	4.05	1.48	1.39
23	C	514	CLA	CHD-C4C	4.05	1.48	1.39
23	D	404	CLA	CHD-C4C	4.05	1.48	1.39
23	b	613	CLA	O2A-CGA	4.05	1.45	1.33
36	c	518	DGD	O1G-C1A	4.05	1.45	1.33
23	B	615	CLA	OBD-CAD	4.05	1.29	1.22
23	b	603	CLA	CHD-C1D	4.05	1.46	1.38
23	B	612	CLA	O2A-CGA	4.04	1.45	1.33
36	h	102	DGD	O1G-C1A	4.04	1.45	1.33
25	B	618	BCR	C23-C22	-4.04	1.37	1.46
36	c	516	DGD	O1G-C1A	4.04	1.45	1.33
23	C	509	CLA	O2A-CGA	4.04	1.45	1.33
23	b	603	CLA	CHD-C4C	4.03	1.48	1.39
23	b	615	CLA	CHD-C1D	4.03	1.46	1.38
23	A	405	CLA	C3D-C2D	4.03	1.50	1.39
23	B	616	CLA	C3D-C2D	4.03	1.50	1.39
23	B	603	CLA	CHD-C4C	4.03	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	O2A-CGA	4.03	1.45	1.33
23	a	408	CLA	CHD-C4C	4.03	1.48	1.39
23	b	616	CLA	C3D-C2D	4.02	1.50	1.39
23	c	510	CLA	O2A-CGA	4.02	1.45	1.33
23	b	607	CLA	C3D-C2D	4.02	1.49	1.39
23	A	406	CLA	CHD-C1D	4.01	1.46	1.38
23	b	609	CLA	CHD-C4C	4.01	1.48	1.39
23	C	508	CLA	CHD-C4C	4.01	1.48	1.39
23	C	503	CLA	CHD-C4C	4.01	1.48	1.39
23	B	615	CLA	CHD-C4C	4.01	1.48	1.39
23	b	611	CLA	C3D-C2D	4.01	1.49	1.39
23	B	610	CLA	C3D-C2D	4.00	1.49	1.39
23	B	608	CLA	CHD-C1D	4.00	1.46	1.38
23	B	613	CLA	O2A-CGA	4.00	1.45	1.33
23	b	605	CLA	CHD-C4C	4.00	1.48	1.39
23	c	509	CLA	C3D-C2D	4.00	1.49	1.39
23	A	408	CLA	CHD-C4C	4.00	1.48	1.39
23	c	511	CLA	OBD-CAD	4.00	1.29	1.22
23	B	610	CLA	CHD-C1D	4.00	1.46	1.38
23	C	506	CLA	CHD-C1D	4.00	1.46	1.38
23	B	604	CLA	C1D-ND	4.00	1.43	1.37
23	d	404	CLA	CHD-C4C	4.00	1.48	1.39
31	E	101	LHG	O7-C7	4.00	1.45	1.34
23	c	505	CLA	CHD-C1D	4.00	1.46	1.38
23	c	501	CLA	CHC-C4B	3.99	1.48	1.39
23	B	601	CLA	CHD-C4C	3.99	1.48	1.39
23	B	605	CLA	CHD-C4C	3.99	1.48	1.39
23	C	509	CLA	CHB-C1B	3.99	1.48	1.39
26	a	410	SQD	O47-C7	3.99	1.45	1.34
23	c	503	CLA	CHD-C4C	3.99	1.48	1.39
23	B	613	CLA	CHD-C1D	3.99	1.46	1.38
23	C	509	CLA	OBD-CAD	3.99	1.29	1.22
23	c	501	CLA	O2A-CGA	3.99	1.45	1.33
23	B	614	CLA	CHD-C4C	3.99	1.48	1.39
23	b	610	CLA	CHD-C4C	3.98	1.48	1.39
23	b	602	CLA	O2A-CGA	3.98	1.45	1.33
23	B	610	CLA	CHC-C4B	3.98	1.48	1.39
23	C	513	CLA	C3D-C2D	3.98	1.49	1.39
23	B	616	CLA	CHD-C4C	3.98	1.48	1.39
23	b	608	CLA	CHC-C4B	3.98	1.48	1.39
23	c	502	CLA	CHD-C4C	3.97	1.48	1.39
23	b	606	CLA	CHD-C4C	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C3D-C2D	3.96	1.49	1.39
23	D	405	CLA	OBD-CAD	3.96	1.29	1.22
23	b	612	CLA	CHD-C4C	3.96	1.48	1.39
31	A	417	LHG	O7-C7	3.96	1.45	1.34
23	b	606	CLA	O2A-CGA	3.95	1.44	1.33
23	c	507	CLA	CHD-C4C	3.95	1.48	1.39
23	B	609	CLA	C3D-C2D	3.95	1.49	1.39
36	C	518	DGD	O2G-C1B	3.95	1.45	1.34
23	b	611	CLA	CHD-C4C	3.95	1.48	1.39
23	b	605	CLA	O2A-CGA	3.95	1.44	1.33
23	b	609	CLA	OBD-CAD	3.95	1.29	1.22
23	B	602	CLA	O2A-CGA	3.95	1.44	1.33
23	B	616	CLA	CHD-C1D	3.94	1.46	1.38
31	d	408	LHG	O7-C7	3.94	1.45	1.34
23	d	404	CLA	CHC-C4B	3.94	1.48	1.39
23	B	614	CLA	O2A-CGA	3.94	1.44	1.33
23	b	609	CLA	O2A-CGA	3.94	1.44	1.33
31	D	408	LHG	O7-C7	3.94	1.45	1.34
23	c	505	CLA	CHD-C4C	3.94	1.48	1.39
36	c	516	DGD	O2G-C1B	3.94	1.45	1.34
23	B	605	CLA	CHB-C1B	3.94	1.48	1.39
23	C	505	CLA	C3D-C2D	3.94	1.49	1.39
23	c	507	CLA	C3D-C2D	3.94	1.49	1.39
23	B	605	CLA	CHD-C1D	3.93	1.46	1.38
23	a	405	CLA	CHD-C4C	3.93	1.48	1.39
23	b	613	CLA	CHD-C4C	3.93	1.48	1.39
23	b	605	CLA	CHB-C1B	3.93	1.48	1.39
23	b	614	CLA	O2A-CGA	3.93	1.44	1.33
23	b	612	CLA	CHC-C4B	3.93	1.48	1.39
23	B	604	CLA	CHB-C1B	3.92	1.48	1.39
23	C	510	CLA	OBD-CAD	3.92	1.29	1.22
23	c	508	CLA	OBD-CAD	3.92	1.29	1.22
23	c	504	CLA	C3D-C2D	3.92	1.49	1.39
23	b	604	CLA	O2A-CGA	3.91	1.44	1.33
36	C	517	DGD	O2G-C1B	3.91	1.45	1.34
23	B	606	CLA	CHD-C4C	3.91	1.48	1.39
23	a	405	CLA	C3D-C2D	3.91	1.49	1.39
23	b	616	CLA	O2A-CGA	3.91	1.44	1.33
23	D	405	CLA	CHC-C4B	3.91	1.48	1.39
23	a	408	CLA	C1D-ND	3.91	1.43	1.37
23	B	603	CLA	C3D-C2D	3.91	1.49	1.39
23	B	614	CLA	C3D-C2D	3.90	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C3D-C2D	3.90	1.49	1.39
23	A	404	CLA	C3D-C2D	3.90	1.49	1.39
23	b	608	CLA	CHD-C4C	3.90	1.48	1.39
33	B	621	LMG	O7-C10	3.90	1.45	1.34
23	B	604	CLA	OBD-CAD	3.90	1.29	1.22
23	c	506	CLA	C3D-C2D	3.90	1.49	1.39
23	B	605	CLA	O2A-CGA	3.89	1.44	1.33
23	C	514	CLA	C3D-C2D	3.89	1.49	1.39
23	b	616	CLA	CHD-C4C	3.89	1.48	1.39
23	b	604	CLA	OBD-CAD	3.89	1.29	1.22
23	c	507	CLA	OBD-CAD	3.89	1.29	1.22
23	C	503	CLA	C3D-C2D	3.89	1.49	1.39
23	c	505	CLA	CHC-C4B	3.89	1.48	1.39
23	b	603	CLA	O2A-CGA	3.89	1.44	1.33
23	a	404	CLA	OBD-CAD	3.88	1.29	1.22
23	D	405	CLA	CHD-C4C	3.88	1.48	1.39
23	c	506	CLA	CHD-C4C	3.88	1.48	1.39
23	c	512	CLA	CHD-C4C	3.87	1.48	1.39
23	C	505	CLA	CHD-C1D	3.87	1.46	1.38
23	a	404	CLA	C3D-C2D	3.87	1.49	1.39
23	A	408	CLA	O2A-CGA	3.87	1.44	1.33
23	b	603	CLA	OBD-CAD	3.87	1.29	1.22
23	b	610	CLA	OBD-CAD	3.87	1.29	1.22
23	b	609	CLA	C3D-C2D	3.87	1.49	1.39
36	C	519	DGD	O1G-C1A	3.86	1.44	1.33
23	b	610	CLA	C3D-C2D	3.86	1.49	1.39
23	B	613	CLA	CHB-C1B	3.86	1.48	1.39
31	D	409	LHG	O8-C23	3.86	1.44	1.33
23	B	611	CLA	CHD-C4C	3.86	1.48	1.39
23	C	512	CLA	CHD-C4C	3.86	1.48	1.39
23	B	610	CLA	O2A-CGA	3.86	1.44	1.33
23	d	403	CLA	CHD-C4C	3.85	1.48	1.39
23	c	508	CLA	CHD-C4C	3.85	1.48	1.39
23	B	611	CLA	C3D-C2D	3.85	1.49	1.39
23	d	401	CLA	CHD-C4C	3.85	1.48	1.39
23	a	404	CLA	CHD-C4C	3.85	1.48	1.39
23	B	608	CLA	O2A-CGA	3.85	1.44	1.33
23	b	614	CLA	OBD-CAD	3.85	1.29	1.22
23	B	609	CLA	CHD-C4C	3.85	1.48	1.39
23	B	609	CLA	CHC-C4B	3.85	1.48	1.39
24	a	406	PHO	O2A-CGA	3.85	1.44	1.33
23	B	612	CLA	C3D-C2D	3.85	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	CHC-C4B	3.85	1.48	1.39
23	B	606	CLA	CHC-C4B	3.85	1.48	1.39
23	A	406	CLA	C3D-C2D	3.84	1.49	1.39
23	b	612	CLA	C3D-C2D	3.84	1.49	1.39
36	C	518	DGD	O1G-C1A	3.84	1.44	1.33
23	c	512	CLA	C3D-C2D	3.83	1.49	1.39
23	b	610	CLA	CHB-C1B	3.83	1.48	1.39
23	C	510	CLA	C3D-C2D	3.83	1.49	1.39
23	b	610	CLA	O2A-CGA	3.83	1.44	1.33
36	C	519	DGD	O2G-C1B	3.83	1.45	1.34
23	c	501	CLA	C3D-C2D	3.83	1.49	1.39
23	c	506	CLA	OBD-CAD	3.83	1.29	1.22
23	b	602	CLA	CHC-C4B	3.83	1.48	1.39
23	C	506	CLA	CHB-C1B	3.82	1.48	1.39
23	b	606	CLA	C3D-C2D	3.82	1.49	1.39
23	B	606	CLA	C3D-C2D	3.82	1.49	1.39
23	B	613	CLA	CHC-C4B	3.82	1.48	1.39
36	c	518	DGD	O2G-C1B	3.82	1.45	1.34
23	b	611	CLA	CHC-C4B	3.82	1.48	1.39
23	c	510	CLA	CHB-C1B	3.82	1.48	1.39
36	c	517	DGD	O2G-C1B	3.82	1.45	1.34
23	a	408	CLA	C3D-C2D	3.82	1.49	1.39
23	B	614	CLA	CHB-C1B	3.82	1.48	1.39
23	B	610	CLA	CHB-C1B	3.82	1.48	1.39
31	d	407	LHG	O8-C23	3.81	1.44	1.33
23	C	505	CLA	CHC-C4B	3.81	1.48	1.39
23	C	511	CLA	OBD-CAD	3.81	1.29	1.22
23	c	504	CLA	CHD-C4C	3.81	1.47	1.39
23	C	506	CLA	CHD-C4C	3.81	1.47	1.39
23	b	615	CLA	CHD-C4C	3.80	1.47	1.39
23	b	601	CLA	CHC-C4B	3.80	1.47	1.39
23	A	405	CLA	CHB-C1B	3.80	1.47	1.39
23	b	605	CLA	OBD-CAD	3.79	1.29	1.22
23	c	502	CLA	CHB-C1B	3.79	1.47	1.39
23	B	607	CLA	C3D-C2D	3.79	1.49	1.39
23	a	405	CLA	OBD-CAD	3.79	1.29	1.22
23	B	605	CLA	C3D-C2D	3.79	1.49	1.39
23	b	609	CLA	CHB-C1B	3.79	1.47	1.39
31	A	416	LHG	O7-C7	3.79	1.45	1.34
23	B	612	CLA	C1D-ND	3.79	1.42	1.37
23	b	601	CLA	OBD-CAD	3.79	1.29	1.22
23	b	607	CLA	CHD-C1D	3.78	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	OBD-CAD	3.78	1.29	1.22
33	J	101	LMG	O7-C10	3.78	1.45	1.34
23	C	512	CLA	CHB-C1B	3.78	1.47	1.39
23	B	608	CLA	C3D-C2D	3.77	1.49	1.39
23	b	613	CLA	CHB-C1B	3.77	1.47	1.39
23	B	613	CLA	OBD-CAD	3.77	1.29	1.22
23	B	609	CLA	CHB-C1B	3.76	1.47	1.39
23	b	608	CLA	OBD-CAD	3.76	1.29	1.22
23	C	505	CLA	CHB-C1B	3.76	1.47	1.39
23	c	512	CLA	OBD-CAD	3.76	1.29	1.22
23	C	505	CLA	CHD-C4C	3.76	1.47	1.39
23	d	403	CLA	CHB-C1B	3.76	1.47	1.39
23	A	404	CLA	C1B-NB	-3.75	1.32	1.37
23	b	614	CLA	CHB-C1B	3.75	1.47	1.39
23	b	604	CLA	CHB-C1B	3.75	1.47	1.39
23	C	512	CLA	C3D-C2D	3.75	1.49	1.39
26	A	410	SQD	O47-C7	3.75	1.44	1.34
23	D	405	CLA	C3D-C2D	3.75	1.49	1.39
23	b	614	CLA	C3D-C2D	3.75	1.49	1.39
23	C	504	CLA	C3D-C2D	3.75	1.49	1.39
23	D	404	CLA	C3D-C2D	3.74	1.49	1.39
23	C	507	CLA	C3D-C2D	3.74	1.49	1.39
31	A	416	LHG	O8-C23	3.74	1.44	1.33
23	A	404	CLA	CHC-C4B	3.74	1.47	1.39
23	c	509	CLA	CHB-C1B	3.73	1.47	1.39
23	A	404	CLA	O2A-CGA	3.73	1.44	1.33
23	B	616	CLA	OBD-CAD	3.73	1.28	1.22
23	c	508	CLA	CHB-C1B	3.72	1.47	1.39
23	B	603	CLA	O2A-CGA	3.72	1.44	1.33
23	A	406	CLA	OBD-CAD	3.72	1.28	1.22
23	C	513	CLA	OBD-CAD	3.72	1.28	1.22
23	d	404	CLA	OBD-CAD	3.72	1.28	1.22
23	B	605	CLA	OBD-CAD	3.72	1.28	1.22
23	B	610	CLA	CHD-C4C	3.72	1.47	1.39
23	C	510	CLA	CHC-C4B	3.72	1.47	1.39
23	c	513	CLA	CHC-C4B	3.72	1.47	1.39
23	b	604	CLA	CHC-C4B	3.71	1.47	1.39
23	C	503	CLA	CHC-C4B	3.71	1.47	1.39
23	A	405	CLA	CHD-C1D	3.71	1.45	1.38
23	B	606	CLA	CHB-C1B	3.71	1.47	1.39
23	d	403	CLA	CHC-C4B	3.71	1.47	1.39
23	b	612	CLA	CHB-C1B	3.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	405	CLA	O2A-CGA	3.70	1.44	1.33
23	d	403	CLA	C3D-C2D	3.70	1.49	1.39
23	b	615	CLA	CHB-C1B	3.69	1.47	1.39
23	C	507	CLA	CHC-C4B	3.69	1.47	1.39
23	d	403	CLA	C1D-ND	3.69	1.42	1.37
23	C	502	CLA	C3D-C2D	3.69	1.49	1.39
23	A	404	CLA	OBD-CAD	3.69	1.28	1.22
23	C	507	CLA	OBD-CAD	3.69	1.28	1.22
23	c	509	CLA	OBD-CAD	3.69	1.28	1.22
23	C	511	CLA	CHB-C1B	3.69	1.47	1.39
23	C	513	CLA	CHC-C4B	3.69	1.47	1.39
31	d	408	LHG	O8-C23	3.68	1.44	1.33
23	B	608	CLA	CHD-C4C	3.68	1.47	1.39
23	B	616	CLA	CHB-C1B	3.68	1.47	1.39
23	B	608	CLA	CHB-C1B	3.68	1.47	1.39
23	B	601	CLA	CHC-C4B	3.67	1.47	1.39
23	c	504	CLA	CHB-C1B	3.67	1.47	1.39
23	b	602	CLA	CHB-C1B	3.67	1.47	1.39
36	C	517	DGD	O1G-C1A	3.67	1.44	1.33
23	D	404	CLA	CHB-C1B	3.67	1.47	1.39
23	c	512	CLA	CHC-C4B	3.67	1.47	1.39
23	B	604	CLA	CHD-C4C	3.66	1.47	1.39
23	C	508	CLA	CHC-C4B	3.66	1.47	1.39
33	b	620	LMG	O7-C10	3.66	1.44	1.34
23	A	408	CLA	C3D-C2D	3.66	1.49	1.39
23	c	511	CLA	CHC-C4B	3.66	1.47	1.39
23	C	502	CLA	CHD-C4C	3.66	1.47	1.39
23	c	509	CLA	CHC-C4B	3.66	1.47	1.39
23	c	505	CLA	OBD-CAD	3.66	1.28	1.22
23	b	603	CLA	C3D-C2D	3.66	1.49	1.39
23	c	503	CLA	C3D-C2D	3.65	1.48	1.39
23	a	404	CLA	CHB-C1B	3.65	1.47	1.39
23	B	613	CLA	CHD-C4C	3.64	1.47	1.39
23	C	502	CLA	CHB-C1B	3.64	1.47	1.39
23	b	615	CLA	C3D-C2D	3.64	1.48	1.39
23	B	611	CLA	OBD-CAD	3.64	1.28	1.22
23	B	616	CLA	CHC-C4B	3.63	1.47	1.39
23	A	405	CLA	CHD-C4C	3.63	1.47	1.39
23	a	408	CLA	OBD-CAD	3.63	1.28	1.22
23	c	504	CLA	OBD-CAD	3.62	1.28	1.22
23	b	607	CLA	OBD-CAD	3.62	1.28	1.22
23	b	609	CLA	CHC-C4B	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	OBD-CAD	3.62	1.28	1.22
23	B	604	CLA	C1B-NB	-3.62	1.33	1.37
23	C	514	CLA	OBD-CAD	3.61	1.28	1.22
23	c	502	CLA	OBD-CAD	3.61	1.28	1.22
23	C	514	CLA	CHB-C1B	3.61	1.47	1.39
23	b	613	CLA	CHC-C4B	3.61	1.47	1.39
23	C	511	CLA	C3D-C2D	3.61	1.48	1.39
23	C	505	CLA	OBD-CAD	3.60	1.28	1.22
23	d	403	CLA	OBD-CAD	3.60	1.28	1.22
23	c	511	CLA	C3D-C2D	3.60	1.48	1.39
23	B	612	CLA	CHB-C1B	3.59	1.47	1.39
23	a	408	CLA	C1B-NB	-3.59	1.33	1.37
23	b	607	CLA	C1B-NB	-3.59	1.33	1.37
23	A	408	CLA	CHC-C4B	3.59	1.47	1.39
23	b	607	CLA	O2A-CGA	3.59	1.43	1.33
23	c	513	CLA	OBD-CAD	3.59	1.28	1.22
24	A	407	PHO	O2A-CGA	3.59	1.43	1.33
23	b	616	CLA	OBD-CAD	3.58	1.28	1.22
23	c	507	CLA	CHC-C4B	3.58	1.47	1.39
23	B	612	CLA	OBD-CAD	3.58	1.28	1.22
23	b	606	CLA	CHB-C1B	3.58	1.47	1.39
23	C	512	CLA	CHC-C4B	3.58	1.47	1.39
23	D	405	CLA	CHB-C1B	3.57	1.47	1.39
23	C	506	CLA	CHC-C4B	3.57	1.47	1.39
23	b	604	CLA	CHD-C4C	3.56	1.47	1.39
23	C	510	CLA	CHB-C1B	3.56	1.47	1.39
23	b	607	CLA	CHB-C1B	3.56	1.47	1.39
23	b	607	CLA	CHD-C4C	3.56	1.47	1.39
23	c	504	CLA	CHC-C4B	3.56	1.47	1.39
23	C	506	CLA	OBD-CAD	3.56	1.28	1.22
23	c	513	CLA	CHB-C1B	3.56	1.47	1.39
33	j	101	LMG	O7-C10	3.56	1.44	1.34
23	c	503	CLA	CHB-C1B	3.56	1.47	1.39
23	B	602	CLA	OBD-CAD	3.55	1.28	1.22
31	d	407	LHG	O7-C7	3.55	1.44	1.34
23	C	509	CLA	CHD-C4C	3.55	1.47	1.39
23	B	602	CLA	CHB-C1B	3.55	1.47	1.39
23	B	612	CLA	CHC-C4B	3.55	1.47	1.39
23	b	608	CLA	CHB-C1B	3.54	1.47	1.39
23	a	408	CLA	CHB-C1B	3.53	1.47	1.39
23	C	504	CLA	CHB-C1B	3.53	1.47	1.39
23	A	406	CLA	CHD-C4C	3.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C4B-NB	-3.53	1.33	1.37
23	C	504	CLA	CHC-C4B	3.53	1.47	1.39
23	b	606	CLA	CHC-C4B	3.52	1.47	1.39
34	B	622	HTG	C1'-S1	-3.52	1.76	1.81
23	a	404	CLA	CHC-C4B	3.52	1.47	1.39
23	c	512	CLA	CHB-C1B	3.51	1.47	1.39
23	c	505	CLA	C3D-C2D	3.50	1.48	1.39
23	B	607	CLA	CHC-C4B	3.50	1.47	1.39
23	b	602	CLA	OBD-CAD	3.50	1.28	1.22
23	a	408	CLA	CHC-C4B	3.50	1.47	1.39
23	C	503	CLA	OBD-CAD	3.50	1.28	1.22
23	C	504	CLA	OBD-CAD	3.49	1.28	1.22
23	c	506	CLA	C1B-NB	-3.49	1.33	1.37
23	B	604	CLA	CHC-C4B	3.49	1.47	1.39
23	B	614	CLA	C4B-NB	-3.49	1.33	1.37
23	c	508	CLA	CHC-C4B	3.48	1.47	1.39
23	C	508	CLA	OBD-CAD	3.48	1.28	1.22
23	B	611	CLA	CHC-C4B	3.47	1.47	1.39
23	b	616	CLA	CHB-C1B	3.47	1.47	1.39
23	b	614	CLA	CHC-C4B	3.47	1.47	1.39
23	c	507	CLA	CHB-C1B	3.47	1.47	1.39
34	b	628	HTG	C1'-S1	-3.47	1.76	1.81
23	B	603	CLA	C1B-NB	-3.47	1.33	1.37
23	b	612	CLA	OBD-CAD	3.46	1.28	1.22
23	a	405	CLA	CHB-C1B	3.46	1.47	1.39
23	B	603	CLA	CHC-C4B	3.46	1.47	1.39
23	C	514	CLA	CHC-C4B	3.45	1.47	1.39
23	B	601	CLA	CHB-C1B	3.45	1.47	1.39
23	b	608	CLA	C1B-NB	-3.45	1.33	1.37
23	b	615	CLA	CHC-C4B	3.45	1.47	1.39
34	b	623	HTG	C1'-S1	-3.45	1.76	1.81
23	B	608	CLA	CHC-C4B	3.45	1.47	1.39
23	B	608	CLA	OBD-CAD	3.45	1.28	1.22
23	c	506	CLA	CHC-C4B	3.44	1.47	1.39
23	B	607	CLA	CHB-C1B	3.44	1.47	1.39
23	C	503	CLA	CHB-C1B	3.44	1.47	1.39
23	b	601	CLA	CHB-C1B	3.44	1.47	1.39
23	d	401	CLA	CHB-C1B	3.43	1.47	1.39
23	A	405	CLA	OBD-CAD	3.43	1.28	1.22
23	a	405	CLA	CHC-C4B	3.43	1.47	1.39
23	c	506	CLA	CHB-C1B	3.43	1.47	1.39
23	b	604	CLA	C3D-C2D	3.42	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	CLA	OBD-CAD	3.42	1.28	1.22
23	C	511	CLA	CHC-C4B	3.41	1.47	1.39
23	B	615	CLA	CHB-C1B	3.41	1.47	1.39
23	c	501	CLA	OBD-CAD	3.40	1.28	1.22
23	C	507	CLA	CHB-C1B	3.40	1.47	1.39
23	B	603	CLA	OBD-CAD	3.39	1.28	1.22
31	D	408	LHG	O8-C23	3.39	1.43	1.33
23	d	401	CLA	CHC-C4B	3.39	1.47	1.39
23	B	607	CLA	OBD-CAD	3.39	1.28	1.22
23	b	603	CLA	C1B-NB	-3.38	1.33	1.37
23	C	502	CLA	CHC-C4B	3.38	1.47	1.39
23	c	510	CLA	CHC-C4B	3.38	1.47	1.39
23	b	615	CLA	OBD-CAD	3.37	1.28	1.22
23	c	509	CLA	C1B-NB	-3.37	1.33	1.37
23	b	606	CLA	C1B-NB	-3.37	1.33	1.37
23	B	614	CLA	OBD-CAD	3.37	1.28	1.22
23	c	510	CLA	C3D-C2D	3.36	1.48	1.39
23	b	605	CLA	CHC-C4B	3.36	1.46	1.39
23	b	607	CLA	CHC-C4B	3.35	1.46	1.39
23	c	504	CLA	C4B-NB	-3.35	1.33	1.37
23	c	503	CLA	OBD-CAD	3.34	1.28	1.22
23	b	607	CLA	C1D-ND	3.34	1.42	1.37
23	a	404	CLA	O2A-CGA	3.33	1.43	1.33
23	A	406	CLA	CHC-C4B	3.33	1.46	1.39
23	A	408	CLA	C1B-NB	-3.32	1.33	1.37
23	c	513	CLA	C1B-NB	-3.32	1.33	1.37
23	c	510	CLA	OBD-CAD	3.32	1.28	1.22
23	B	604	CLA	C3D-C2D	3.32	1.48	1.39
23	B	612	CLA	CHD-C4C	3.31	1.46	1.39
23	b	613	CLA	C4B-NB	-3.31	1.33	1.37
23	A	408	CLA	CHB-C1B	3.30	1.46	1.39
23	C	509	CLA	CHC-C4B	3.29	1.46	1.39
23	C	506	CLA	C3D-C2D	3.29	1.48	1.39
23	C	509	CLA	C4B-NB	-3.29	1.33	1.37
23	A	406	CLA	CHB-C1B	3.29	1.46	1.39
23	d	401	CLA	C1B-NB	-3.28	1.33	1.37
23	c	509	CLA	C4B-NB	-3.28	1.33	1.37
23	B	603	CLA	CHB-C1B	3.28	1.46	1.39
34	C	522	HTG	C1'-S1	-3.28	1.76	1.81
23	b	615	CLA	C1B-NB	-3.28	1.33	1.37
23	B	602	CLA	CHC-C4B	3.28	1.46	1.39
34	d	411	HTG	C1'-S1	-3.27	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404	CLA	C1B-NB	-3.27	1.33	1.37
23	B	613	CLA	C1B-NB	-3.26	1.33	1.37
38	E	103	HEM	C1B-NB	-3.26	1.34	1.40
38	e	103	HEM	C1B-NB	-3.26	1.34	1.40
23	C	513	CLA	CHB-C1B	3.26	1.46	1.39
23	A	404	CLA	CHB-C1B	3.23	1.46	1.39
34	B	624	HTG	C1'-S1	-3.23	1.76	1.81
38	E	103	HEM	C4D-ND	-3.23	1.34	1.40
23	B	609	CLA	C1B-NB	-3.23	1.33	1.37
23	b	611	CLA	OBD-CAD	3.23	1.28	1.22
23	b	613	CLA	OBD-CAD	3.22	1.28	1.22
23	A	406	CLA	C4B-NB	-3.21	1.33	1.37
23	B	606	CLA	C1B-NB	-3.20	1.33	1.37
23	A	406	CLA	C1B-NB	-3.20	1.33	1.37
23	d	404	CLA	CHB-C1B	3.19	1.46	1.39
23	b	603	CLA	CHB-C1B	3.18	1.46	1.39
23	B	606	CLA	OBD-CAD	3.18	1.28	1.22
23	c	506	CLA	C4B-NB	-3.18	1.33	1.37
23	A	408	CLA	C4B-NB	-3.18	1.33	1.37
23	B	613	CLA	C4B-NB	-3.18	1.33	1.37
23	a	404	CLA	C1B-NB	-3.17	1.33	1.37
23	B	601	CLA	C1B-NB	-3.17	1.33	1.37
40	V	202	HEC	C4D-ND	-3.16	1.33	1.39
23	C	508	CLA	CHB-C1B	3.16	1.46	1.39
23	c	502	CLA	CHC-C4B	3.16	1.46	1.39
23	C	512	CLA	C1B-C2B	3.16	1.50	1.43
23	C	506	CLA	C1B-NB	-3.14	1.33	1.37
40	v	201	HEC	C1B-NB	-3.14	1.33	1.39
23	b	611	CLA	C1B-NB	-3.12	1.33	1.37
23	a	404	CLA	C4B-NB	-3.12	1.33	1.37
23	A	405	CLA	C1B-NB	-3.12	1.33	1.37
23	b	610	CLA	C4B-NB	-3.11	1.33	1.37
23	D	404	CLA	OBD-CAD	3.11	1.27	1.22
23	C	511	CLA	C1B-NB	-3.11	1.33	1.37
23	B	609	CLA	OBD-CAD	3.11	1.27	1.22
23	C	514	CLA	C4B-NB	-3.11	1.33	1.37
23	b	610	CLA	C4C-C3C	3.10	1.50	1.45
23	B	615	CLA	CHC-C4B	3.10	1.46	1.39
23	d	403	CLA	C4B-NB	-3.10	1.33	1.37
23	C	505	CLA	C1B-NB	-3.10	1.33	1.37
23	b	606	CLA	OBD-CAD	3.10	1.27	1.22
23	C	502	CLA	C1B-NB	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1B-NB	-3.09	1.33	1.37
23	b	614	CLA	C1B-C2B	3.09	1.50	1.43
38	e	103	HEM	C4D-ND	-3.08	1.34	1.40
23	C	508	CLA	C1B-NB	-3.08	1.33	1.37
23	c	503	CLA	C1B-NB	-3.07	1.33	1.37
23	c	502	CLA	C1B-C2B	3.07	1.50	1.43
23	D	404	CLA	C4C-C3C	3.07	1.50	1.45
23	b	614	CLA	C1B-NB	-3.06	1.33	1.37
23	B	614	CLA	CHC-C4B	3.06	1.46	1.39
23	c	502	CLA	C1B-NB	-3.05	1.33	1.37
34	B	627	HTG	C1'-S1	-3.04	1.77	1.81
34	b	622	HTG	C1'-S1	-3.04	1.77	1.81
23	B	610	CLA	C1B-NB	-3.03	1.33	1.37
23	c	505	CLA	C1B-C2B	3.02	1.50	1.43
23	B	611	CLA	C1B-NB	-3.02	1.33	1.37
23	D	404	CLA	C4B-NB	-3.02	1.33	1.37
23	B	608	CLA	C1B-NB	-3.02	1.33	1.37
23	A	404	CLA	C4C-C3C	3.02	1.50	1.45
23	B	602	CLA	C4B-NB	-3.00	1.33	1.37
34	c	522	HTG	C1'-S1	-2.99	1.77	1.81
23	A	405	CLA	C1C-C2C	2.99	1.50	1.44
23	B	607	CLA	C4D-CHA	2.99	1.48	1.38
23	B	607	CLA	C1B-NB	-2.99	1.33	1.37
24	A	407	PHO	C3A-C2A	-2.99	1.52	1.54
40	V	202	HEC	C1B-NB	-2.99	1.34	1.39
23	c	504	CLA	C1B-NB	-2.98	1.33	1.37
23	B	614	CLA	C1B-C2B	2.98	1.50	1.43
23	B	612	CLA	C4B-NB	-2.98	1.33	1.37
23	d	401	CLA	C4B-NB	-2.98	1.33	1.37
23	c	512	CLA	C1B-NB	-2.96	1.34	1.37
35	D	402	LMT	O1'-C1'	2.96	1.45	1.40
23	c	509	CLA	C4C-C3C	2.96	1.50	1.45
29	a	414	PL9	C6-C5	2.96	1.49	1.35
23	C	510	CLA	C4B-NB	-2.95	1.34	1.37
23	C	502	CLA	OBD-CAD	2.95	1.27	1.22
23	b	601	CLA	C4B-NB	-2.95	1.34	1.37
23	c	507	CLA	C4D-CHA	2.95	1.48	1.38
23	b	612	CLA	C4B-NB	-2.95	1.34	1.37
23	B	615	CLA	C1B-NB	-2.94	1.34	1.37
23	b	605	CLA	C1B-C2B	2.94	1.50	1.43
23	C	513	CLA	C1B-NB	-2.94	1.34	1.37
23	C	505	CLA	C4B-NB	-2.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	CLA	C1B-C2B	2.93	1.50	1.43
23	C	512	CLA	C4B-NB	-2.93	1.34	1.37
23	B	616	CLA	C1B-NB	-2.93	1.34	1.37
23	c	507	CLA	C1B-NB	-2.92	1.34	1.37
23	C	505	CLA	C1B-C2B	2.92	1.50	1.43
23	b	604	CLA	C1B-C2B	2.91	1.50	1.43
23	D	404	CLA	CHC-C4B	2.91	1.45	1.39
24	a	407	PHO	C3A-C2A	-2.91	1.52	1.54
23	C	508	CLA	C1B-C2B	2.91	1.50	1.43
29	A	414	PL9	C6-C5	2.91	1.49	1.35
23	B	603	CLA	C1B-C2B	2.91	1.49	1.43
23	D	405	CLA	C3B-C4B	2.90	1.51	1.42
23	A	408	CLA	OBD-CAD	2.90	1.27	1.22
23	b	611	CLA	C1B-C2B	2.90	1.49	1.43
23	A	404	CLA	C4B-NB	-2.90	1.34	1.37
23	C	511	CLA	C4B-NB	-2.90	1.34	1.37
23	b	610	CLA	C1B-NB	-2.90	1.34	1.37
23	C	509	CLA	C1B-C2B	2.89	1.49	1.43
34	C	521	HTG	C1'-S1	-2.89	1.77	1.81
23	B	616	CLA	C1B-C2B	2.88	1.49	1.43
23	c	511	CLA	C1B-C2B	2.88	1.49	1.43
23	b	602	CLA	C4B-NB	-2.87	1.34	1.37
23	B	608	CLA	C4B-NB	-2.87	1.34	1.37
23	B	603	CLA	C4D-CHA	2.85	1.48	1.38
23	b	615	CLA	C4D-CHA	2.85	1.48	1.38
23	C	510	CLA	C1C-C2C	2.84	1.50	1.44
40	v	201	HEC	C4D-ND	-2.84	1.34	1.39
23	B	604	CLA	C4B-NB	-2.84	1.34	1.37
23	c	502	CLA	C4B-NB	-2.84	1.34	1.37
38	E	103	HEM	C1C-C2C	-2.84	1.39	1.45
23	b	613	CLA	C4D-CHA	2.84	1.48	1.38
23	C	505	CLA	C4D-CHA	2.84	1.48	1.38
23	b	601	CLA	C1B-NB	-2.84	1.34	1.37
23	b	613	CLA	C1B-NB	-2.84	1.34	1.37
23	C	508	CLA	C4D-CHA	2.84	1.48	1.38
23	c	501	CLA	C1B-NB	-2.83	1.34	1.37
23	C	502	CLA	C1B-C2B	2.83	1.49	1.43
23	A	404	CLA	C1B-C2B	2.83	1.49	1.43
23	B	602	CLA	C1B-C2B	2.83	1.49	1.43
23	A	408	CLA	C4D-CHA	2.83	1.48	1.38
34	D	412	HTG	C1'-S1	-2.83	1.77	1.81
23	D	405	CLA	C1B-C2B	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C1C-C2C	2.83	1.50	1.44
23	c	505	CLA	C1C-C2C	2.83	1.50	1.44
23	b	611	CLA	C4C-C3C	2.82	1.49	1.45
23	C	508	CLA	C4B-NB	-2.82	1.34	1.37
23	c	513	CLA	C1C-C2C	2.82	1.50	1.44
23	C	509	CLA	C4D-CHA	2.81	1.48	1.38
23	c	508	CLA	C1B-NB	-2.81	1.34	1.37
23	c	508	CLA	C1B-C2B	2.80	1.49	1.43
23	B	604	CLA	C1B-C2B	2.80	1.49	1.43
23	c	508	CLA	C4B-NB	-2.80	1.34	1.37
23	b	602	CLA	C1B-NB	-2.79	1.34	1.37
23	b	603	CLA	C1C-C2C	2.79	1.50	1.44
23	C	509	CLA	C4C-C3C	2.79	1.49	1.45
40	V	202	HEC	C4B-NB	-2.79	1.34	1.39
23	b	605	CLA	C4D-CHA	2.79	1.48	1.38
23	C	503	CLA	C4B-NB	-2.78	1.34	1.37
23	b	607	CLA	C4D-CHA	2.78	1.47	1.38
23	c	509	CLA	C1B-C2B	2.78	1.49	1.43
23	b	605	CLA	C1B-NB	-2.78	1.34	1.37
23	D	404	CLA	C1C-C2C	2.77	1.50	1.44
23	b	613	CLA	C1B-C2B	2.77	1.49	1.43
23	c	506	CLA	C1B-C2B	2.77	1.49	1.43
23	C	510	CLA	C4D-CHA	2.77	1.47	1.38
23	c	510	CLA	C1B-C2B	2.77	1.49	1.43
23	B	608	CLA	C1B-C2B	2.77	1.49	1.43
23	a	405	CLA	C4B-NB	-2.77	1.34	1.37
34	c	521	HTG	C1'-S1	-2.77	1.77	1.81
23	C	503	CLA	C1B-NB	-2.76	1.34	1.37
23	B	606	CLA	C4B-NB	-2.76	1.34	1.37
23	b	609	CLA	C1B-NB	-2.76	1.34	1.37
23	C	511	CLA	C4C-C3C	2.76	1.49	1.45
23	b	610	CLA	C1C-C2C	2.76	1.50	1.44
23	b	604	CLA	C1C-C2C	2.76	1.50	1.44
23	b	609	CLA	C4B-NB	-2.76	1.34	1.37
23	a	408	CLA	C4D-CHA	2.76	1.47	1.38
23	C	510	CLA	C1B-NB	-2.76	1.34	1.37
23	B	615	CLA	C4D-CHA	2.76	1.47	1.38
23	C	512	CLA	C4D-CHA	2.75	1.47	1.38
23	C	504	CLA	C4B-NB	-2.75	1.34	1.37
23	C	502	CLA	C4D-CHA	2.75	1.47	1.38
23	b	607	CLA	C1B-C2B	2.75	1.49	1.43
23	B	604	CLA	C4D-CHA	2.74	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C4D-CHA	2.74	1.47	1.38
23	b	616	CLA	C3B-C4B	2.74	1.50	1.42
23	C	511	CLA	C4D-CHA	2.74	1.47	1.38
23	D	404	CLA	C1B-C2B	2.74	1.49	1.43
23	B	615	CLA	C1B-C2B	2.74	1.49	1.43
23	c	510	CLA	C4B-NB	-2.74	1.34	1.37
23	C	512	CLA	C1C-C2C	2.74	1.50	1.44
23	B	612	CLA	C1B-C2B	2.74	1.49	1.43
23	B	613	CLA	C4D-CHA	2.74	1.47	1.38
23	C	514	CLA	C1C-C2C	2.73	1.50	1.44
23	b	615	CLA	C1B-C2B	2.73	1.49	1.43
23	A	406	CLA	C3B-C4B	2.73	1.50	1.42
23	c	501	CLA	C4D-CHA	2.73	1.47	1.38
23	c	511	CLA	C4B-NB	-2.73	1.34	1.37
23	c	511	CLA	C1B-NB	-2.73	1.34	1.37
23	C	504	CLA	C1B-NB	-2.73	1.34	1.37
23	C	507	CLA	C4D-CHA	2.73	1.47	1.38
23	B	602	CLA	C4C-C3C	2.73	1.49	1.45
23	b	604	CLA	C4D-CHA	2.73	1.47	1.38
23	C	503	CLA	C4D-CHA	2.72	1.47	1.38
23	c	507	CLA	C1B-C2B	2.72	1.49	1.43
23	C	502	CLA	C4B-NB	-2.72	1.34	1.37
23	c	505	CLA	C1B-NB	-2.72	1.34	1.37
40	v	201	HEC	C1D-ND	-2.72	1.34	1.39
23	b	603	CLA	C3B-C4B	2.72	1.50	1.42
23	B	614	CLA	C4D-CHA	2.72	1.47	1.38
23	C	505	CLA	C1C-C2C	2.72	1.50	1.44
23	d	403	CLA	C4C-C3C	2.72	1.49	1.45
23	C	514	CLA	C1B-NB	-2.71	1.34	1.37
23	B	603	CLA	C4B-NB	-2.71	1.34	1.37
23	c	505	CLA	C4B-NB	-2.71	1.34	1.37
23	b	606	CLA	C4B-NB	-2.71	1.34	1.37
23	C	504	CLA	C4D-CHA	2.71	1.47	1.38
23	b	605	CLA	C4B-NB	-2.70	1.34	1.37
23	B	601	CLA	C4D-CHA	2.70	1.47	1.38
23	b	608	CLA	C4B-NB	-2.70	1.34	1.37
23	c	509	CLA	C4D-CHA	2.70	1.47	1.38
29	d	406	PL9	C6-C5	2.70	1.48	1.35
23	B	611	CLA	C1B-C2B	2.70	1.49	1.43
23	b	609	CLA	C1B-C2B	2.70	1.49	1.43
23	b	610	CLA	C4D-CHA	2.70	1.47	1.38
24	A	407	PHO	CHA-CBD	-2.70	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	CLA	C4C-C3C	2.70	1.49	1.45
23	D	405	CLA	C1C-C2C	2.70	1.50	1.44
23	B	601	CLA	C1B-C2B	2.69	1.49	1.43
23	B	603	CLA	C4C-C3C	2.69	1.49	1.45
23	c	508	CLA	C4D-CHA	2.69	1.47	1.38
23	b	602	CLA	C4D-CHA	2.69	1.47	1.38
23	c	504	CLA	C4D-CHA	2.69	1.47	1.38
23	c	513	CLA	C4B-NB	-2.69	1.34	1.37
23	c	510	CLA	C1B-NB	-2.69	1.34	1.37
23	b	616	CLA	C4D-CHA	2.69	1.47	1.38
23	c	512	CLA	C4B-NB	-2.69	1.34	1.37
23	c	504	CLA	C1C-C2C	2.69	1.50	1.44
23	b	612	CLA	C1B-NB	-2.69	1.34	1.37
23	A	405	CLA	C3B-C4B	2.68	1.50	1.42
23	c	503	CLA	C4D-CHA	2.68	1.47	1.38
23	A	405	CLA	C4D-CHA	2.68	1.47	1.38
23	b	604	CLA	C1B-NB	-2.68	1.34	1.37
23	D	404	CLA	C1B-NB	-2.68	1.34	1.37
23	C	513	CLA	C4D-CHA	2.68	1.47	1.38
23	B	610	CLA	C4B-NB	-2.68	1.34	1.37
23	c	512	CLA	C1B-C2B	2.68	1.49	1.43
33	Z	102	LMG	O8-C28	2.68	1.46	1.33
23	B	611	CLA	C1C-C2C	2.68	1.50	1.44
23	B	606	CLA	C4D-CHA	2.67	1.47	1.38
24	D	401	PHO	CHA-CBD	-2.67	1.48	1.51
23	b	609	CLA	C4D-CHA	2.67	1.47	1.38
34	B	623	HTG	C1'-S1	-2.67	1.77	1.81
23	b	612	CLA	C4D-CHA	2.67	1.47	1.38
23	B	611	CLA	C4D-CHA	2.67	1.47	1.38
40	V	202	HEC	C1D-ND	-2.67	1.34	1.39
23	c	511	CLA	C4D-CHA	2.66	1.47	1.38
23	c	502	CLA	C4D-CHA	2.66	1.47	1.38
23	c	508	CLA	C1C-C2C	2.65	1.49	1.44
23	B	604	CLA	C3D-C4D	-2.65	1.38	1.44
23	D	405	CLA	C1B-NB	-2.65	1.34	1.37
23	b	601	CLA	C4D-CHA	2.64	1.47	1.38
23	d	401	CLA	C1B-C2B	2.64	1.49	1.43
23	b	616	CLA	C1B-NB	-2.64	1.34	1.37
23	B	608	CLA	C4D-CHA	2.64	1.47	1.38
23	c	512	CLA	C4D-CHA	2.64	1.47	1.38
23	C	514	CLA	C1B-C2B	2.64	1.49	1.43
23	b	611	CLA	C4B-NB	-2.64	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	201	HEC	C4B-NB	-2.64	1.34	1.39
23	C	509	CLA	C1B-NB	-2.63	1.34	1.37
34	b	625	HTG	C1'-S1	-2.63	1.77	1.81
23	B	616	CLA	C4D-CHA	2.63	1.47	1.38
23	c	505	CLA	C4D-CHA	2.63	1.47	1.38
23	B	611	CLA	C4B-NB	-2.63	1.34	1.37
29	D	407	PL9	C6-C5	2.63	1.48	1.35
23	b	614	CLA	C4D-CHA	2.63	1.47	1.38
23	B	607	CLA	C1C-C2C	2.62	1.49	1.44
23	B	609	CLA	C3B-C4B	2.62	1.50	1.42
23	B	613	CLA	C4C-C3C	2.62	1.49	1.45
23	C	506	CLA	C4B-NB	-2.62	1.34	1.37
23	a	404	CLA	C1B-C2B	2.62	1.49	1.43
23	c	504	CLA	C4C-C3C	2.62	1.49	1.45
23	c	510	CLA	C4D-CHA	2.62	1.47	1.38
23	d	401	CLA	C4D-CHA	2.61	1.47	1.38
23	b	615	CLA	C4B-NB	-2.61	1.34	1.37
23	b	602	CLA	C1B-C2B	2.61	1.49	1.43
23	d	404	CLA	C4B-NB	-2.61	1.34	1.37
23	b	602	CLA	C1C-C2C	2.61	1.49	1.44
23	C	503	CLA	C3D-C4D	-2.60	1.38	1.44
23	B	602	CLA	C1B-NB	-2.60	1.34	1.37
23	b	606	CLA	C1B-C2B	2.60	1.49	1.43
23	B	602	CLA	C4D-CHA	2.60	1.47	1.38
23	a	405	CLA	C1B-NB	-2.60	1.34	1.37
23	B	613	CLA	C1C-C2C	2.60	1.49	1.44
23	c	503	CLA	C1B-C2B	2.60	1.49	1.43
23	D	405	CLA	C4D-CHA	2.59	1.47	1.38
23	d	403	CLA	C4D-CHA	2.59	1.47	1.38
23	B	607	CLA	C4B-NB	-2.59	1.34	1.37
23	C	510	CLA	C1B-C2B	2.59	1.49	1.43
23	C	503	CLA	C1B-C2B	2.59	1.49	1.43
23	B	606	CLA	C3B-C4B	2.59	1.50	1.42
23	d	403	CLA	C3D-C4D	-2.59	1.38	1.44
23	c	513	CLA	C3B-C4B	2.59	1.50	1.42
23	c	504	CLA	C1B-C2B	2.59	1.49	1.43
23	C	504	CLA	C3B-C4B	2.58	1.50	1.42
23	b	611	CLA	C4D-CHA	2.58	1.47	1.38
23	c	503	CLA	C1C-C2C	2.58	1.49	1.44
23	C	507	CLA	C4C-C3C	2.58	1.49	1.45
23	b	616	CLA	C1C-C2C	2.57	1.49	1.44
23	b	607	CLA	C4B-NB	-2.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	C4D-CHA	2.57	1.47	1.38
23	b	606	CLA	C4D-CHA	2.57	1.47	1.38
23	C	506	CLA	C3D-C4D	-2.57	1.38	1.44
23	C	504	CLA	C4C-C3C	2.57	1.49	1.45
23	C	505	CLA	C3B-C2B	2.57	1.49	1.41
23	C	504	CLA	C1B-C2B	2.57	1.49	1.43
23	B	605	CLA	C1B-C2B	2.57	1.49	1.43
23	a	408	CLA	C4B-NB	-2.56	1.34	1.37
23	A	406	CLA	C1C-C2C	2.56	1.49	1.44
23	B	607	CLA	C4C-C3C	2.56	1.49	1.45
23	b	612	CLA	C4C-C3C	2.56	1.49	1.45
23	d	403	CLA	C1B-C2B	2.56	1.49	1.43
23	C	512	CLA	C4C-C3C	2.56	1.49	1.45
23	B	607	CLA	C1B-C2B	2.55	1.49	1.43
23	c	507	CLA	C1C-C2C	2.55	1.49	1.44
23	B	610	CLA	C4D-CHA	2.54	1.47	1.38
23	B	612	CLA	C1C-C2C	2.54	1.49	1.44
23	c	501	CLA	C1B-C2B	2.54	1.49	1.43
23	b	603	CLA	C1B-C2B	2.54	1.49	1.43
23	a	405	CLA	C1B-C2B	2.54	1.49	1.43
23	c	506	CLA	C4D-CHA	2.53	1.47	1.38
23	B	605	CLA	C3B-C4B	2.53	1.50	1.42
23	c	513	CLA	C4D-CHA	2.53	1.47	1.38
23	b	603	CLA	C4D-CHA	2.53	1.47	1.38
23	a	404	CLA	C4D-CHA	2.53	1.47	1.38
23	C	509	CLA	C3B-C2B	2.53	1.49	1.41
23	A	404	CLA	C4D-CHA	2.53	1.47	1.38
23	D	404	CLA	C3D-C4D	-2.53	1.38	1.44
23	B	606	CLA	C1B-C2B	2.53	1.49	1.43
23	C	507	CLA	C4B-NB	-2.53	1.34	1.37
23	b	612	CLA	C1B-C2B	2.52	1.49	1.43
23	B	609	CLA	C4D-CHA	2.52	1.47	1.38
23	C	507	CLA	C3D-C4D	-2.52	1.38	1.44
23	C	511	CLA	C1B-C2B	2.52	1.49	1.43
23	b	607	CLA	C1C-C2C	2.51	1.49	1.44
23	c	509	CLA	C1C-C2C	2.51	1.49	1.44
23	C	510	CLA	C4C-C3C	2.51	1.49	1.45
23	a	405	CLA	C4D-CHA	2.51	1.47	1.38
23	B	616	CLA	C3D-C4D	-2.51	1.38	1.44
23	B	605	CLA	C4C-C3C	2.51	1.49	1.45
23	A	406	CLA	C1B-C2B	2.51	1.49	1.43
23	C	513	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C1B-C2B	2.50	1.49	1.43
23	C	510	CLA	C3B-C2B	2.50	1.49	1.41
23	C	505	CLA	C3D-C4D	-2.50	1.38	1.44
23	c	501	CLA	C4C-C3C	2.49	1.49	1.45
23	a	405	CLA	C3D-C4D	-2.49	1.38	1.44
23	b	608	CLA	C4D-CHA	2.49	1.46	1.38
23	A	404	CLA	C3D-C4D	-2.49	1.38	1.44
23	a	408	CLA	C1C-C2C	2.49	1.49	1.44
23	B	602	CLA	C3D-C4D	-2.49	1.38	1.44
23	c	501	CLA	C4B-NB	-2.49	1.34	1.37
36	c	518	DGD	O2G-C2G	-2.48	1.40	1.46
23	d	404	CLA	C4D-CHA	2.48	1.46	1.38
23	B	609	CLA	C1B-C2B	2.48	1.48	1.43
23	A	408	CLA	C3D-C4D	-2.48	1.38	1.44
23	B	609	CLA	C1C-C2C	2.47	1.49	1.44
23	c	512	CLA	C3B-C4B	2.47	1.49	1.42
23	B	605	CLA	C1C-C2C	2.47	1.49	1.44
23	B	611	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	507	CLA	C1B-C2B	2.46	1.48	1.43
23	C	513	CLA	C3B-C4B	2.46	1.49	1.42
23	c	505	CLA	C3B-C4B	2.46	1.49	1.42
23	C	513	CLA	C1C-C2C	2.46	1.49	1.44
23	C	506	CLA	C1B-C2B	2.46	1.48	1.43
23	c	510	CLA	C4C-C3C	2.46	1.49	1.45
23	B	605	CLA	C4D-CHA	2.46	1.46	1.38
23	B	601	CLA	C4C-C3C	2.46	1.49	1.45
23	C	502	CLA	C4C-C3C	2.46	1.49	1.45
23	B	601	CLA	C4B-NB	-2.46	1.34	1.37
23	C	502	CLA	C3B-C2B	2.45	1.49	1.41
23	b	612	CLA	C3B-C2B	2.45	1.49	1.41
23	C	506	CLA	C4D-CHA	2.45	1.46	1.38
23	c	501	CLA	C3B-C4B	2.45	1.49	1.42
23	b	607	CLA	C4C-C3C	2.45	1.49	1.45
23	B	616	CLA	C1C-C2C	2.45	1.49	1.44
23	b	603	CLA	C4B-NB	-2.45	1.34	1.37
23	c	510	CLA	C3D-C4D	-2.44	1.38	1.44
23	c	503	CLA	C3B-C4B	2.44	1.49	1.42
23	b	606	CLA	C3B-C4B	2.44	1.49	1.42
23	A	405	CLA	C4B-NB	-2.44	1.34	1.37
23	a	404	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	610	CLA	C1B-C2B	2.44	1.48	1.43
23	b	616	CLA	C3D-C4D	-2.44	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C4C-C3C	2.43	1.49	1.45
23	C	511	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	606	CLA	C1C-C2C	2.43	1.49	1.44
23	C	508	CLA	C4C-C3C	2.42	1.49	1.45
23	b	602	CLA	C3D-C4D	-2.42	1.38	1.44
23	b	609	CLA	C3B-C4B	2.42	1.49	1.42
23	c	506	CLA	C3D-C4D	-2.42	1.38	1.44
23	a	408	CLA	C3B-C4B	2.42	1.49	1.42
23	C	502	CLA	C3D-C4D	-2.42	1.38	1.44
23	A	406	CLA	C3D-C4D	-2.41	1.38	1.44
24	D	401	PHO	C1B-NB	-2.41	1.34	1.38
23	b	608	CLA	C3D-C4D	-2.41	1.38	1.44
23	D	404	CLA	C3B-C2B	2.41	1.49	1.41
24	a	406	PHO	C4B-NB	-2.41	1.34	1.38
24	a	407	PHO	CHA-CBD	-2.41	1.48	1.51
23	b	616	CLA	C1B-C2B	2.40	1.48	1.43
23	b	612	CLA	C1C-C2C	2.40	1.49	1.44
23	B	615	CLA	C1C-C2C	2.40	1.49	1.44
23	B	610	CLA	C4C-C3C	2.40	1.49	1.45
23	d	404	CLA	C3B-C4B	2.40	1.49	1.42
23	C	509	CLA	C1C-C2C	2.40	1.49	1.44
23	b	606	CLA	C1C-C2C	2.39	1.49	1.44
23	c	507	CLA	C4B-NB	-2.39	1.34	1.37
23	b	613	CLA	C3B-C2B	2.39	1.49	1.41
23	a	405	CLA	C3B-C2B	2.39	1.49	1.41
23	B	614	CLA	C1B-NB	-2.39	1.34	1.37
23	b	614	CLA	C3B-C2B	2.39	1.49	1.41
23	C	512	CLA	C3B-C4B	2.39	1.49	1.42
23	b	605	CLA	C3B-C4B	2.39	1.49	1.42
23	B	613	CLA	C3B-C2B	2.39	1.49	1.41
23	c	504	CLA	C3B-C2B	2.39	1.49	1.41
23	D	404	CLA	C4D-CHA	2.39	1.46	1.38
23	A	408	CLA	C1B-C2B	2.39	1.48	1.43
38	e	103	HEM	C1D-ND	-2.38	1.34	1.38
23	b	611	CLA	C3B-C2B	2.38	1.49	1.41
23	b	614	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	613	CLA	C1C-C2C	2.38	1.49	1.44
23	D	405	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	615	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	608	CLA	C1C-C2C	2.38	1.49	1.44
23	c	512	CLA	C4C-C3C	2.38	1.49	1.45
23	c	511	CLA	C1C-C2C	2.38	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C4C-C3C	2.37	1.49	1.45
23	B	601	CLA	C3B-C4B	2.37	1.49	1.42
23	b	616	CLA	C4B-NB	-2.37	1.34	1.37
23	B	607	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	612	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	605	CLA	C4C-C3C	2.37	1.49	1.45
23	b	610	CLA	C3B-C2B	2.37	1.49	1.41
23	B	601	CLA	C3D-C4D	-2.36	1.38	1.44
23	C	508	CLA	C1C-C2C	2.36	1.49	1.44
23	A	405	CLA	C1B-C2B	2.36	1.48	1.43
23	b	606	CLA	C3D-C4D	-2.36	1.38	1.44
23	D	405	CLA	C4B-NB	-2.36	1.34	1.37
23	c	511	CLA	C3B-C2B	2.36	1.49	1.41
23	a	405	CLA	C4C-C3C	2.35	1.49	1.45
23	c	508	CLA	C3B-C2B	2.35	1.49	1.41
23	b	609	CLA	C4C-C3C	2.35	1.49	1.45
23	A	404	CLA	C3B-C2B	2.35	1.49	1.41
23	b	610	CLA	C1B-C2B	2.35	1.48	1.43
23	c	502	CLA	C3B-C2B	2.35	1.49	1.41
23	b	612	CLA	C3B-C4B	2.35	1.49	1.42
23	d	404	CLA	C1B-C2B	2.35	1.48	1.43
23	C	510	CLA	C3B-C4B	2.35	1.49	1.42
23	C	508	CLA	C3D-C4D	-2.35	1.38	1.44
23	C	514	CLA	C3B-C4B	2.35	1.49	1.42
23	b	614	CLA	C4B-NB	-2.34	1.34	1.37
33	Z	102	LMG	O1-C1	2.34	1.44	1.40
23	C	512	CLA	C1B-NB	-2.34	1.34	1.37
23	b	602	CLA	C3B-C2B	2.34	1.49	1.41
23	A	406	CLA	C4D-CHA	2.34	1.46	1.38
23	B	611	CLA	C3B-C2B	2.34	1.49	1.41
23	b	607	CLA	C3D-C4D	-2.34	1.38	1.44
23	B	616	CLA	C3B-C4B	2.34	1.49	1.42
23	C	510	CLA	C3D-C4D	-2.34	1.38	1.44
23	c	509	CLA	C3D-C4D	-2.34	1.38	1.44
23	B	614	CLA	C4C-C3C	2.33	1.49	1.45
23	c	503	CLA	C4B-NB	-2.33	1.34	1.37
23	b	608	CLA	C3B-C2B	2.33	1.49	1.41
23	b	601	CLA	C3B-C4B	2.33	1.49	1.42
23	B	615	CLA	C3B-C4B	2.33	1.49	1.42
23	B	604	CLA	C1C-C2C	2.33	1.49	1.44
23	A	408	CLA	C1C-C2C	2.32	1.49	1.44
23	c	511	CLA	C4C-C3C	2.32	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	501	CLA	C3D-C4D	-2.32	1.39	1.44
23	b	609	CLA	C1C-C2C	2.32	1.49	1.44
23	c	513	CLA	C1B-C2B	2.32	1.48	1.43
23	c	509	CLA	C3B-C4B	2.32	1.49	1.42
23	B	609	CLA	C3D-C4D	-2.32	1.39	1.44
23	B	602	CLA	C1C-C2C	2.31	1.49	1.44
23	a	404	CLA	C3B-C2B	2.31	1.49	1.41
23	b	610	CLA	C3D-C4D	-2.31	1.39	1.44
23	B	616	CLA	C4C-C3C	2.31	1.49	1.45
23	C	511	CLA	C1C-C2C	2.31	1.49	1.44
23	b	603	CLA	C4C-C3C	2.30	1.48	1.45
23	C	506	CLA	C4C-C3C	2.30	1.48	1.45
23	b	604	CLA	C3B-C2B	2.30	1.48	1.41
23	B	613	CLA	C1B-C2B	2.30	1.48	1.43
23	c	502	CLA	C3D-C4D	-2.30	1.39	1.44
23	B	601	CLA	C1C-C2C	2.30	1.49	1.44
23	a	405	CLA	C3B-C4B	2.30	1.49	1.42
23	b	602	CLA	C3B-C4B	2.30	1.49	1.42
24	D	401	PHO	C4B-NB	-2.29	1.34	1.38
23	d	404	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	605	CLA	C1B-NB	-2.29	1.34	1.37
23	d	404	CLA	C1C-C2C	2.29	1.49	1.44
23	b	608	CLA	C1B-C2B	2.29	1.48	1.43
23	c	505	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	610	CLA	C3B-C4B	2.28	1.49	1.42
23	A	408	CLA	C3B-C4B	2.28	1.49	1.42
23	b	604	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	608	CLA	C3B-C4B	2.28	1.49	1.42
23	B	603	CLA	C3B-C2B	2.28	1.48	1.41
24	A	407	PHO	C4B-NB	-2.28	1.34	1.38
23	b	610	CLA	C3B-C4B	2.28	1.49	1.42
23	B	610	CLA	C3D-C4D	-2.28	1.39	1.44
38	e	103	HEM	C1C-C2C	-2.28	1.40	1.45
23	C	502	CLA	C1C-C2C	2.28	1.49	1.44
23	d	401	CLA	C3B-C2B	2.27	1.48	1.41
40	v	201	HEC	C4A-C3A	-2.27	1.40	1.45
23	B	616	CLA	C3B-C2B	2.27	1.48	1.41
23	c	513	CLA	C3D-C4D	-2.27	1.39	1.44
23	C	508	CLA	C3B-C4B	2.27	1.49	1.42
23	C	512	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	510	CLA	C3B-C4B	2.26	1.49	1.42
23	c	503	CLA	C3D-C4D	-2.26	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C3D-C4D	-2.26	1.39	1.44
23	a	408	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	501	CLA	C1C-C2C	2.26	1.49	1.44
23	B	608	CLA	C3B-C4B	2.26	1.49	1.42
23	C	514	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	611	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	603	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	513	CLA	C4C-C3C	2.25	1.48	1.45
35	b	627	LMT	O1'-C1'	2.25	1.44	1.40
23	C	512	CLA	C3B-C2B	2.25	1.48	1.41
23	b	609	CLA	C3D-C4D	-2.25	1.39	1.44
23	b	602	CLA	C4C-C3C	2.25	1.48	1.45
23	b	603	CLA	C3D-C4D	-2.25	1.39	1.44
24	a	406	PHO	C1D-ND	-2.24	1.34	1.38
23	B	606	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	601	CLA	C1C-C2C	2.24	1.49	1.44
23	d	401	CLA	C3B-C4B	2.24	1.49	1.42
23	c	509	CLA	C3B-C2B	2.24	1.48	1.41
26	B	620	SQD	O6-C1	2.24	1.43	1.40
23	B	616	CLA	C4B-NB	-2.24	1.34	1.37
23	A	404	CLA	C1C-C2C	2.23	1.49	1.44
23	c	502	CLA	C4C-C3C	2.23	1.48	1.45
23	A	405	CLA	C3B-C2B	2.23	1.48	1.41
23	C	506	CLA	C3B-C4B	2.23	1.49	1.42
23	A	405	CLA	C3D-C4D	-2.23	1.39	1.44
23	c	511	CLA	C1D-C2D	2.23	1.49	1.45
23	B	614	CLA	C1C-NC	-2.23	1.34	1.37
23	d	401	CLA	C1D-C2D	2.22	1.49	1.45
23	c	506	CLA	C4C-C3C	2.22	1.48	1.45
35	E	102	LMT	O1'-C1'	2.22	1.43	1.40
23	B	612	CLA	C4C-C3C	2.22	1.48	1.45
35	B	630	LMT	O1'-C1'	2.22	1.43	1.40
23	B	607	CLA	C3B-C4B	2.22	1.49	1.42
23	C	507	CLA	C3B-C4B	2.22	1.49	1.42
23	c	508	CLA	C3D-C4D	-2.22	1.39	1.44
23	C	503	CLA	C3B-C4B	2.22	1.49	1.42
23	b	615	CLA	C4C-C3C	2.21	1.48	1.45
23	C	503	CLA	C3B-C2B	2.21	1.48	1.41
23	B	601	CLA	C3B-C2B	2.21	1.48	1.41
23	b	605	CLA	C1C-C2C	2.21	1.49	1.44
36	c	517	DGD	O3G-C1D	2.21	1.43	1.40
23	C	513	CLA	C4B-NB	-2.21	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1C-C2C	2.20	1.49	1.44
23	c	508	CLA	C3B-C4B	2.20	1.49	1.42
23	c	512	CLA	C3D-C4D	-2.20	1.39	1.44
23	B	612	CLA	C3B-C2B	2.20	1.48	1.41
23	B	614	CLA	C3D-C4D	-2.19	1.39	1.44
23	a	408	CLA	C1D-C2D	2.19	1.49	1.45
23	C	507	CLA	C1D-C2D	2.19	1.49	1.45
23	b	601	CLA	C3B-C2B	2.19	1.48	1.41
23	c	511	CLA	C3B-C4B	2.19	1.49	1.42
23	C	513	CLA	C3B-C2B	2.18	1.48	1.41
23	B	607	CLA	C3B-C2B	2.18	1.48	1.41
23	C	505	CLA	C3B-C4B	2.18	1.49	1.42
23	A	404	CLA	C1D-C2D	2.18	1.49	1.45
23	B	602	CLA	C3B-C2B	2.18	1.48	1.41
36	h	102	DGD	O5D-C1E	2.18	1.43	1.40
38	E	103	HEM	C1D-ND	-2.18	1.34	1.38
31	A	416	LHG	O7-C5	-2.18	1.41	1.46
23	c	511	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	615	CLA	C3B-C4B	2.17	1.49	1.42
23	b	604	CLA	C3B-C4B	2.17	1.49	1.42
23	C	506	CLA	C3B-C2B	2.17	1.48	1.41
23	B	608	CLA	C3D-C4D	-2.17	1.39	1.44
23	a	405	CLA	C1C-C2C	2.16	1.48	1.44
23	d	404	CLA	C3B-C2B	2.16	1.48	1.41
23	b	601	CLA	C4C-C3C	2.16	1.48	1.45
24	A	407	PHO	C1B-NB	-2.16	1.34	1.38
23	C	514	CLA	C4C-C3C	2.16	1.48	1.45
23	c	503	CLA	C3B-C2B	2.16	1.48	1.41
23	C	507	CLA	C3B-C2B	2.16	1.48	1.41
23	B	608	CLA	C1C-C2C	2.16	1.48	1.44
23	B	610	CLA	C1C-C2C	2.16	1.48	1.44
29	A	414	PL9	C2-C3	2.16	1.40	1.34
23	C	503	CLA	C1C-C2C	2.15	1.48	1.44
23	d	403	CLA	C1C-C2C	2.15	1.48	1.44
23	b	613	CLA	C4C-C3C	2.15	1.48	1.45
23	b	605	CLA	C3B-C2B	2.14	1.48	1.41
23	A	406	CLA	C4C-C3C	2.14	1.48	1.45
23	A	408	CLA	C4C-C3C	2.14	1.48	1.45
23	A	406	CLA	C1D-C2D	2.14	1.49	1.45
29	a	414	PL9	C2-C3	2.13	1.40	1.34
38	E	103	HEM	C4B-NB	-2.13	1.34	1.38
23	C	504	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	625	HTG	C1-S1	-2.13	1.77	1.80
23	c	512	CLA	C1C-C2C	2.12	1.48	1.44
25	b	619	BCR	C30-C25	-2.12	1.51	1.53
35	I	101	LMT	O1'-C1'	2.12	1.43	1.40
23	b	605	CLA	C1C-NC	-2.12	1.34	1.37
23	C	511	CLA	C3B-C2B	2.12	1.48	1.41
23	c	504	CLA	C3D-C4D	-2.12	1.39	1.44
23	b	614	CLA	C3B-C4B	2.12	1.48	1.42
23	b	605	CLA	C3D-C4D	-2.12	1.39	1.44
23	a	404	CLA	C1C-C2C	2.12	1.48	1.44
23	b	613	CLA	C3D-C4D	-2.11	1.39	1.44
23	c	507	CLA	C3B-C4B	2.11	1.48	1.42
23	A	408	CLA	C3B-C2B	2.11	1.48	1.41
23	b	606	CLA	C3B-C2B	2.11	1.48	1.41
23	c	502	CLA	C1C-C2C	2.11	1.48	1.44
23	c	510	CLA	C1C-C2C	2.11	1.48	1.44
23	b	614	CLA	C4C-C3C	2.11	1.48	1.45
23	B	614	CLA	C3B-C4B	2.11	1.48	1.42
23	C	505	CLA	C4C-C3C	2.11	1.48	1.45
23	b	614	CLA	C1C-C2C	2.11	1.48	1.44
23	c	513	CLA	C3B-C2B	2.11	1.48	1.41
23	B	610	CLA	C3B-C2B	2.10	1.48	1.41
23	c	506	CLA	C3B-C2B	2.10	1.48	1.41
23	c	506	CLA	C1C-NC	-2.10	1.34	1.37
34	B	627	HTG	C1-S1	-2.10	1.77	1.80
24	a	406	PHO	CBD-CGD	-2.10	1.49	1.52
23	c	510	CLA	C3B-C2B	2.09	1.48	1.41
23	B	602	CLA	C3B-C4B	2.09	1.48	1.42
23	C	514	CLA	C3B-C2B	2.09	1.48	1.41
36	H	102	DGD	O5D-C1E	2.09	1.43	1.40
23	B	602	CLA	C1D-C2D	2.09	1.49	1.45
23	A	408	CLA	C1C-NC	-2.09	1.34	1.37
23	b	601	CLA	C3D-C4D	-2.09	1.39	1.44
23	B	615	CLA	C3D-C4D	-2.08	1.39	1.44
23	b	608	CLA	C4C-C3C	2.08	1.48	1.45
23	B	612	CLA	C3D-C4D	-2.08	1.39	1.44
23	b	611	CLA	C1C-C2C	2.08	1.48	1.44
23	B	613	CLA	C3D-C4D	-2.08	1.39	1.44
23	B	604	CLA	C3B-C2B	2.08	1.48	1.41
31	d	407	LHG	O7-C5	-2.07	1.41	1.46
23	c	502	CLA	C3B-C4B	2.07	1.48	1.42
23	C	513	CLA	C4C-C3C	2.07	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3D-C4D	-2.07	1.39	1.44
34	D	412	HTG	C1-S1	-2.07	1.77	1.80
23	c	504	CLA	C3B-C4B	2.07	1.48	1.42
23	C	509	CLA	C1C-NC	-2.07	1.34	1.37
23	d	404	CLA	C1D-C2D	2.07	1.49	1.45
23	d	401	CLA	C3D-C4D	-2.06	1.39	1.44
23	c	506	CLA	C3B-C4B	2.06	1.48	1.42
23	c	505	CLA	C4C-C3C	2.06	1.48	1.45
23	B	608	CLA	C3B-C2B	2.06	1.48	1.41
25	B	617	BCR	C1-C6	-2.06	1.51	1.53
33	c	520	LMG	O1-C1	2.06	1.43	1.40
23	c	507	CLA	C4C-C3C	2.06	1.48	1.45
25	d	405	BCR	C30-C25	-2.06	1.51	1.53
23	B	614	CLA	C1C-C2C	2.06	1.48	1.44
24	D	401	PHO	CBD-CGD	-2.06	1.49	1.52
36	C	519	DGD	O2G-C2G	-2.05	1.41	1.46
23	A	405	CLA	C1D-C2D	2.05	1.49	1.45
36	h	102	DGD	O2G-C2G	-2.05	1.41	1.46
23	C	509	CLA	C3D-C4D	-2.05	1.39	1.44
23	B	614	CLA	C3B-C2B	2.05	1.48	1.41
23	c	501	CLA	C1D-C2D	2.05	1.49	1.45
23	C	514	CLA	C1D-C2D	2.04	1.49	1.45
23	b	616	CLA	C3B-C2B	2.04	1.48	1.41
23	b	613	CLA	C3B-C4B	2.04	1.48	1.42
23	d	403	CLA	C3B-C2B	2.04	1.48	1.41
23	B	611	CLA	C4C-C3C	2.03	1.48	1.45
23	B	603	CLA	C3B-C4B	2.03	1.48	1.42
31	D	408	LHG	O7-C5	-2.03	1.41	1.46
24	a	406	PHO	C1B-NB	-2.03	1.34	1.38
26	f	101	SQD	O6-C1	2.02	1.43	1.40
33	Z	101	LMG	O1-C1	2.02	1.43	1.40
23	d	404	CLA	C4C-C3C	2.02	1.48	1.45
24	a	407	PHO	C1D-ND	-2.02	1.35	1.38
23	c	507	CLA	C3D-C4D	-2.02	1.39	1.44
23	b	616	CLA	C4C-C3C	2.02	1.48	1.45
40	V	202	HEC	C4A-C3A	-2.02	1.41	1.45
38	e	103	HEM	C3C-C4C	-2.01	1.42	1.46
23	d	401	CLA	C1C-C2C	2.01	1.48	1.44
23	b	603	CLA	C1D-C2D	2.00	1.49	1.45

All (2936) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	PHO	C2D-C1D-ND	11.80	117.96	109.43
24	a	406	PHO	C2D-C1D-ND	11.75	117.92	109.43
24	A	407	PHO	C2D-C1D-ND	11.24	117.56	109.43
23	B	605	CLA	C1D-ND-C4D	-10.65	98.84	106.31
23	A	405	CLA	C1D-ND-C4D	-10.58	98.89	106.31
23	A	406	CLA	C1D-ND-C4D	-10.49	98.95	106.31
23	C	514	CLA	C1D-ND-C4D	-10.33	99.06	106.31
24	a	407	PHO	C2D-C1D-ND	10.29	116.87	109.43
23	B	608	CLA	C1D-ND-C4D	-10.02	99.28	106.31
23	D	405	CLA	C1D-ND-C4D	-10.00	99.29	106.31
23	C	504	CLA	C1D-ND-C4D	-9.94	99.33	106.31
23	d	401	CLA	C1D-ND-C4D	-9.92	99.35	106.31
23	a	405	CLA	C1D-ND-C4D	-9.92	99.35	106.31
23	b	603	CLA	C1D-ND-C4D	-9.92	99.35	106.31
23	c	503	CLA	C1D-ND-C4D	-9.90	99.37	106.31
23	c	511	CLA	C1D-ND-C4D	-9.89	99.38	106.31
23	c	504	CLA	C1D-ND-C4D	-9.64	99.55	106.31
23	C	512	CLA	C1D-ND-C4D	-9.62	99.56	106.31
23	C	510	CLA	C1D-ND-C4D	-9.59	99.59	106.31
23	c	513	CLA	C1D-ND-C4D	-9.56	99.61	106.31
23	c	512	CLA	C1D-ND-C4D	-9.53	99.62	106.31
23	d	404	CLA	C1D-ND-C4D	-9.52	99.63	106.31
23	B	609	CLA	C1D-ND-C4D	-9.51	99.64	106.31
23	c	505	CLA	C1D-ND-C4D	-9.43	99.70	106.31
23	b	605	CLA	C1D-ND-C4D	-9.42	99.70	106.31
23	b	607	CLA	C1D-ND-C4D	-9.34	99.76	106.31
23	a	408	CLA	C1D-ND-C4D	-9.32	99.77	106.31
23	B	606	CLA	C1D-ND-C4D	-9.26	99.81	106.31
24	D	401	PHO	O2D-CGD-CBD	9.24	121.10	110.95
23	b	615	CLA	C1D-ND-C4D	-9.20	99.86	106.31
23	C	511	CLA	C1D-ND-C4D	-9.20	99.86	106.31
23	B	610	CLA	C1D-ND-C4D	-9.19	99.86	106.31
23	b	608	CLA	C1D-ND-C4D	-9.18	99.87	106.31
23	c	510	CLA	C1D-ND-C4D	-9.18	99.87	106.31
23	b	606	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	B	615	CLA	C1D-ND-C4D	-9.10	99.93	106.31
23	c	501	CLA	C1D-ND-C4D	-9.10	99.93	106.31
23	B	612	CLA	C1D-ND-C4D	-9.08	99.94	106.31
23	c	506	CLA	C1D-ND-C4D	-9.05	99.96	106.31
23	b	611	CLA	C1D-ND-C4D	-9.04	99.97	106.31
23	B	601	CLA	C1D-ND-C4D	-9.04	99.97	106.31
23	b	610	CLA	C1D-ND-C4D	-9.01	99.99	106.31
23	c	509	CLA	C1D-ND-C4D	-9.01	99.99	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C1D-ND-C4D	-9.00	100.00	106.31
23	B	607	CLA	C1D-ND-C4D	-8.98	100.01	106.31
23	B	614	CLA	C1D-ND-C4D	-8.96	100.03	106.31
23	C	506	CLA	C1D-ND-C4D	-8.96	100.03	106.31
23	b	609	CLA	C1D-ND-C4D	-8.94	100.04	106.31
23	A	408	CLA	C1D-ND-C4D	-8.92	100.06	106.31
23	b	604	CLA	C1D-ND-C4D	-8.90	100.06	106.31
23	c	508	CLA	C1D-ND-C4D	-8.88	100.08	106.31
23	b	616	CLA	C1D-ND-C4D	-8.87	100.09	106.31
23	b	612	CLA	C1D-ND-C4D	-8.84	100.11	106.31
23	d	403	CLA	C1D-ND-C4D	-8.84	100.11	106.31
24	a	407	PHO	O2D-CGD-CBD	8.82	120.64	110.95
24	a	406	PHO	O2D-CGD-CBD	8.81	120.63	110.95
23	b	614	CLA	C1D-ND-C4D	-8.81	100.13	106.31
23	C	502	CLA	C1D-ND-C4D	-8.78	100.15	106.31
23	B	611	CLA	C1D-ND-C4D	-8.75	100.18	106.31
23	b	613	CLA	C1D-ND-C4D	-8.74	100.18	106.31
23	C	509	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	c	507	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	b	601	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	B	603	CLA	C1D-ND-C4D	-8.71	100.20	106.31
23	C	503	CLA	C1D-ND-C4D	-8.69	100.21	106.31
23	B	602	CLA	C1D-ND-C4D	-8.69	100.22	106.31
23	C	505	CLA	C1D-ND-C4D	-8.68	100.22	106.31
23	c	502	CLA	C1D-ND-C4D	-8.66	100.24	106.31
23	C	513	CLA	C1D-ND-C4D	-8.60	100.28	106.31
23	B	613	CLA	C1D-ND-C4D	-8.56	100.31	106.31
23	b	602	CLA	C1D-ND-C4D	-8.52	100.34	106.31
23	D	404	CLA	C1D-ND-C4D	-8.49	100.36	106.31
24	D	401	PHO	C3B-C4B-NB	8.42	112.95	107.46
23	C	508	CLA	C1D-ND-C4D	-8.42	100.41	106.31
23	C	507	CLA	C1D-ND-C4D	-8.36	100.45	106.31
23	a	404	CLA	C1D-ND-C4D	-8.35	100.45	106.31
23	B	604	CLA	C1D-ND-C4D	-8.26	100.51	106.31
23	A	404	CLA	C1D-ND-C4D	-8.21	100.55	106.31
24	A	407	PHO	C3B-C4B-NB	7.95	112.64	107.46
24	a	406	PHO	C3B-C4B-NB	7.89	112.60	107.46
23	A	404	CLA	CMD-C2D-C1D	7.82	138.49	124.73
24	A	407	PHO	O2D-CGD-CBD	7.70	119.41	110.95
23	c	511	CLA	CMD-C2D-C1D	7.51	137.94	124.73
23	C	506	CLA	CMD-C2D-C1D	7.43	137.81	124.73
23	c	510	CLA	CMD-C2D-C1D	7.39	137.75	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CMD-C2D-C1D	7.33	137.64	124.73
23	C	511	CLA	CMD-C2D-C1D	7.30	137.58	124.73
23	B	606	CLA	C4A-NA-C1A	-7.23	103.38	106.68
24	A	407	PHO	C2B-C1B-NB	7.20	114.64	109.43
23	b	604	CLA	CMD-C2D-C1D	7.17	137.35	124.73
24	a	407	PHO	C3B-C4B-NB	7.15	112.12	107.46
23	B	611	CLA	CMD-C2D-C1D	7.13	137.29	124.73
23	b	615	CLA	CMD-C2D-C1D	7.12	137.27	124.73
23	C	504	CLA	C4A-NA-C1A	-7.01	103.48	106.68
23	b	603	CLA	CMD-C2D-C1D	6.99	137.04	124.73
23	A	408	CLA	C4A-NA-C1A	-6.94	103.51	106.68
23	b	616	CLA	C4A-NA-C1A	-6.89	103.54	106.68
23	B	604	CLA	CMD-C2D-C1D	6.88	136.85	124.73
23	b	607	CLA	C2D-C1D-ND	6.88	116.93	110.13
23	A	405	CLA	CHD-C4C-C3C	-6.86	114.77	124.77
23	B	607	CLA	C4A-NA-C1A	-6.83	103.56	106.68
23	D	404	CLA	C4A-NA-C1A	-6.80	103.58	106.68
23	B	602	CLA	CMD-C2D-C1D	6.78	136.67	124.73
23	c	501	CLA	CMD-C2D-C1D	6.72	136.56	124.73
23	A	405	CLA	C2D-C1D-ND	6.70	116.76	110.13
23	D	405	CLA	CMD-C2D-C1D	6.68	136.49	124.73
23	b	614	CLA	CMD-C2D-C1D	6.67	136.47	124.73
26	A	410	SQD	O6-C1-C2	6.66	118.38	108.27
23	C	512	CLA	CMD-C2D-C1D	6.65	136.44	124.73
23	B	607	CLA	CMD-C2D-C1D	6.64	136.43	124.73
23	B	608	CLA	C2D-C1D-ND	6.64	116.70	110.13
23	A	408	CLA	CMD-C2D-C1D	6.64	136.43	124.73
23	B	606	CLA	CMD-C2D-C1D	6.62	136.39	124.73
23	c	513	CLA	C4A-NA-C1A	-6.62	103.66	106.68
23	B	609	CLA	CHD-C4C-C3C	-6.59	115.16	124.77
24	a	407	PHO	C2B-C1B-NB	6.57	114.18	109.43
23	C	514	CLA	CMD-C2D-C1D	6.57	136.29	124.73
23	C	504	CLA	CMD-C2D-C1D	6.52	136.22	124.73
23	a	404	CLA	CMD-C2D-C1D	6.52	136.21	124.73
23	b	616	CLA	CHD-C4C-C3C	-6.49	115.31	124.77
23	c	505	CLA	CHD-C4C-C3C	-6.49	115.31	124.77
23	D	405	CLA	CHD-C4C-C3C	-6.49	115.32	124.77
23	a	405	CLA	CMD-C2D-C1D	6.48	136.15	124.73
23	B	605	CLA	C2D-C1D-ND	6.48	116.54	110.13
23	c	504	CLA	CMD-C2D-C1D	6.47	136.12	124.73
23	B	608	CLA	CHD-C4C-C3C	-6.47	115.34	124.77
23	C	502	CLA	CMD-C2D-C1D	6.46	136.11	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	CLA	CMD-C2D-C1D	6.45	136.09	124.73
23	c	508	CLA	O2D-CGD-CBD	6.44	122.48	111.23
23	C	508	CLA	O2D-CGD-CBD	6.42	122.45	111.23
23	A	406	CLA	CMD-C2D-C1D	6.40	136.00	124.73
23	B	616	CLA	O2D-CGD-CBD	6.40	122.41	111.23
23	C	511	CLA	C4A-NA-C1A	-6.39	103.76	106.68
23	b	616	CLA	CMD-C2D-C1D	6.39	135.98	124.73
23	c	513	CLA	CMD-C2D-C1D	6.38	135.97	124.73
23	c	507	CLA	CMD-C2D-C1D	6.38	135.96	124.73
23	C	506	CLA	CHD-C4C-C3C	-6.38	115.47	124.77
23	B	616	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
23	C	506	CLA	O2D-CGD-CBD	6.35	122.33	111.23
23	b	609	CLA	CMD-C2D-C1D	6.34	135.90	124.73
23	c	503	CLA	CMD-C2D-C1D	6.34	135.89	124.73
24	a	406	PHO	C2B-C1B-NB	6.32	114.00	109.43
23	B	614	CLA	CMD-C2D-C1D	6.30	135.82	124.73
23	C	509	CLA	C2D-C1D-ND	6.29	116.35	110.13
23	B	612	CLA	CHD-C4C-C3C	-6.29	115.60	124.77
23	b	604	CLA	O2D-CGD-CBD	6.29	122.22	111.23
23	B	616	CLA	C4A-NA-C1A	-6.29	103.81	106.68
23	b	604	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
23	C	507	CLA	C4A-NA-C1A	-6.28	103.81	106.68
23	c	504	CLA	C2D-C1D-ND	6.27	116.33	110.13
23	d	401	CLA	C2D-C1D-ND	6.27	116.33	110.13
23	b	602	CLA	CMD-C2D-C1D	6.27	135.77	124.73
23	d	403	CLA	C4A-NA-C1A	-6.25	103.83	106.68
23	b	610	CLA	CMD-C2D-C1D	6.25	135.74	124.73
23	B	613	CLA	C2D-C1D-ND	6.25	116.31	110.13
23	A	406	CLA	C2D-C1D-ND	6.24	116.31	110.13
23	B	615	CLA	CHD-C4C-C3C	-6.24	115.68	124.77
23	C	504	CLA	C2D-C1D-ND	6.23	116.30	110.13
23	B	606	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
23	B	611	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
23	B	609	CLA	CMD-C2D-C1D	6.23	135.69	124.73
23	B	604	CLA	CHD-C4C-C3C	-6.23	115.70	124.77
23	B	610	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	b	602	CLA	O2D-CGD-CBD	6.21	122.09	111.23
23	d	401	CLA	CMD-C2D-C1D	6.21	135.66	124.73
23	c	505	CLA	CMD-C2D-C1D	6.21	135.66	124.73
23	B	601	CLA	CMD-C2D-C1D	6.19	135.63	124.73
23	D	405	CLA	O2D-CGD-CBD	6.18	122.04	111.23
23	B	610	CLA	C2D-C1D-ND	6.18	116.24	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	CMD-C2D-C1D	6.17	135.59	124.73
23	B	605	CLA	CMD-C2D-C1D	6.17	135.59	124.73
23	B	616	CLA	CMD-C2D-C1D	6.16	135.58	124.73
23	c	503	CLA	C2D-C1D-ND	6.15	116.21	110.13
23	b	608	CLA	CHD-C4C-C3C	-6.15	115.81	124.77
23	b	612	CLA	CMD-C2D-C1D	6.15	135.55	124.73
24	A	407	PHO	C4D-ND-C1D	-6.14	101.52	108.87
23	C	505	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	c	512	CLA	O2D-CGD-CBD	6.14	121.96	111.23
23	b	606	CLA	CHD-C4C-C3C	-6.14	115.83	124.77
23	C	514	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	d	401	CLA	CHD-C4C-C3C	-6.13	115.84	124.77
23	a	405	CLA	C2D-C1D-ND	6.12	116.19	110.13
23	B	609	CLA	C2D-C1D-ND	6.10	116.16	110.13
23	b	606	CLA	C2D-C1D-ND	6.10	116.16	110.13
23	b	601	CLA	O2D-CGD-CBD	6.10	121.89	111.23
23	c	507	CLA	O2D-CGD-CBD	6.09	121.88	111.23
23	C	513	CLA	C4A-NA-C1A	-6.09	103.90	106.68
23	B	615	CLA	C2D-C1D-ND	6.09	116.15	110.13
23	b	613	CLA	CHD-C4C-C3C	-6.09	115.90	124.77
23	c	503	CLA	CHD-C4C-C3C	-6.09	115.90	124.77
23	c	512	CLA	C2D-C1D-ND	6.08	116.15	110.13
23	b	613	CLA	C2D-C1D-ND	6.08	116.14	110.13
23	C	510	CLA	CMD-C2D-C1D	6.08	135.43	124.73
23	D	405	CLA	C2D-C1D-ND	6.08	116.14	110.13
23	d	403	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	b	602	CLA	C4A-NA-C1A	-6.06	103.91	106.68
23	b	605	CLA	CHD-C4C-C3C	-6.06	115.93	124.77
23	d	404	CLA	CMD-C2D-C1D	6.06	135.40	124.73
23	c	506	CLA	CMD-C2D-C1D	6.06	135.40	124.73
23	b	601	CLA	CMD-C2D-C1D	6.05	135.39	124.73
23	b	614	CLA	O2D-CGD-CBD	6.05	121.81	111.23
23	C	512	CLA	CHD-C4C-C3C	-6.04	115.96	124.77
23	B	614	CLA	C2D-C1D-ND	6.04	116.10	110.13
23	b	605	CLA	CMD-C2D-C1D	6.04	135.36	124.73
23	B	612	CLA	C2D-C1D-ND	6.03	116.10	110.13
23	B	601	CLA	O2D-CGD-CBD	6.03	121.77	111.23
24	D	401	PHO	C2B-C1B-NB	6.02	113.78	109.43
23	C	512	CLA	C2D-C1D-ND	6.02	116.08	110.13
23	A	408	CLA	C2D-C1D-ND	6.01	116.08	110.13
23	b	615	CLA	C2D-C1D-ND	6.01	116.08	110.13
23	C	503	CLA	CMD-C2D-C1D	6.01	135.32	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405	CLA	CHD-C4C-C3C	-6.01	116.02	124.77
23	B	614	CLA	O2D-CGD-CBD	6.00	121.73	111.23
23	B	607	CLA	C2D-C1D-ND	5.99	116.05	110.13
23	b	608	CLA	C2D-C1D-ND	5.99	116.05	110.13
25	D	406	BCR	C7-C8-C9	-5.99	117.38	126.23
23	D	404	CLA	C2C-C1C-NC	5.98	116.26	109.98
23	c	503	CLA	C4A-NA-C1A	-5.98	103.95	106.68
23	B	606	CLA	C2D-C1D-ND	5.97	116.04	110.13
23	b	601	CLA	C4A-NA-C1A	-5.96	103.96	106.68
23	B	605	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
23	C	510	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
23	b	603	CLA	C4A-NA-C1A	-5.95	103.97	106.68
23	c	511	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
23	b	610	CLA	C4A-NA-C1A	-5.94	103.97	106.68
23	B	610	CLA	CMD-C2D-C1D	5.94	135.19	124.73
23	B	612	CLA	O2D-CGD-CBD	5.94	121.61	111.23
24	D	401	PHO	C4D-ND-C1D	-5.93	101.76	108.87
23	b	616	CLA	O2D-CGD-CBD	5.93	121.59	111.23
23	c	511	CLA	C2D-C1D-ND	5.92	115.99	110.13
23	b	606	CLA	CMD-C2D-C1D	5.92	135.15	124.73
23	C	513	CLA	O2D-CGD-CBD	5.91	121.57	111.23
23	C	506	CLA	C4A-NA-C1A	-5.91	103.98	106.68
23	b	606	CLA	C4A-NA-C1A	-5.91	103.98	106.68
23	B	604	CLA	O2D-CGD-CBD	5.91	121.56	111.23
23	b	611	CLA	C2D-C1D-ND	5.90	115.96	110.13
23	c	508	CLA	C2D-C1D-ND	5.90	115.96	110.13
23	C	510	CLA	C2D-C1D-ND	5.89	115.96	110.13
23	A	406	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
23	B	615	CLA	CMD-C2D-C1D	5.89	135.09	124.73
23	b	605	CLA	C2D-C1D-ND	5.88	115.95	110.13
23	B	602	CLA	C4A-NA-C1A	-5.88	104.00	106.68
23	B	616	CLA	C2D-C1D-ND	5.87	115.94	110.13
23	c	513	CLA	C2D-C1D-ND	5.87	115.94	110.13
23	A	405	CLA	CMD-C2D-C1D	5.87	135.07	124.73
23	b	611	CLA	O2D-CGD-CBD	5.87	121.49	111.23
23	C	514	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
23	C	505	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
26	D	413	SQD	O47-C7-C8	5.86	124.15	111.48
23	d	404	CLA	C2D-C1D-ND	5.85	115.91	110.13
23	b	603	CLA	C2D-C1D-ND	5.85	115.91	110.13
23	b	611	CLA	CMD-C2D-C1D	5.84	135.02	124.73
23	b	603	CLA	CHD-C4C-C3C	-5.84	116.26	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
23	c	507	CLA	CHD-C4C-C3C	-5.82	116.29	124.77
23	A	408	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
23	B	613	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
23	c	512	CLA	CHD-C4C-C3C	-5.79	116.34	124.77
23	b	603	CLA	O2D-CGD-CBD	5.78	121.34	111.23
23	d	404	CLA	C4A-NA-C1A	-5.78	104.04	106.68
23	c	512	CLA	CMD-C2D-C1D	5.78	134.91	124.73
23	C	513	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
23	B	611	CLA	C2D-C1D-ND	5.78	115.84	110.13
23	B	614	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
23	b	614	CLA	C2D-C1D-ND	5.77	115.84	110.13
23	a	408	CLA	C2D-C1D-ND	5.77	115.84	110.13
34	B	624	HTG	C1'-S1-C1	5.77	112.91	100.45
23	c	507	CLA	C2D-C1D-ND	5.77	115.84	110.13
23	b	602	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
23	c	506	CLA	C2D-C1D-ND	5.76	115.83	110.13
24	a	406	PHO	C4D-ND-C1D	-5.76	101.97	108.87
23	c	501	CLA	O2D-CGD-CBD	5.76	121.29	111.23
23	C	502	CLA	O2D-CGD-CBD	5.76	121.29	111.23
23	b	601	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
25	Y	101	BCR	C33-C5-C6	-5.74	118.22	124.48
23	B	606	CLA	O2D-CGD-CBD	5.73	121.25	111.23
23	b	616	CLA	C2D-C1D-ND	5.72	115.79	110.13
23	c	508	CLA	CHD-C4C-C3C	-5.72	116.44	124.77
23	C	508	CLA	CMD-C2D-C1D	5.72	134.80	124.73
23	c	510	CLA	C1-C2-C3	-5.71	116.84	126.20
23	c	506	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	B	601	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
26	D	413	SQD	O6-C1-C2	5.71	116.94	108.27
23	b	615	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	b	614	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
34	b	623	HTG	C1'-S1-C1	5.69	112.73	100.45
23	B	603	CLA	CMD-C2D-C1D	5.68	134.74	124.73
23	B	610	CLA	O2D-CGD-CBD	5.68	121.17	111.23
23	b	612	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
24	a	407	PHO	C3D-C4D-ND	5.67	114.98	107.71
23	C	505	CLA	CMD-C2D-C1D	5.67	134.72	124.73
23	c	513	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
23	C	503	CLA	CHD-C4C-C3C	-5.66	116.51	124.77
23	C	502	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
23	C	503	CLA	O2D-CGD-CBD	5.65	121.10	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C4A-NA-C1A	-5.64	104.10	106.68
23	b	607	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
23	c	508	CLA	C4A-NA-C1A	-5.64	104.11	106.68
23	a	408	CLA	CMD-C2D-C1D	5.63	134.65	124.73
23	C	502	CLA	C2D-C1D-ND	5.63	115.70	110.13
23	C	508	CLA	C2D-C1D-ND	5.62	115.69	110.13
24	A	407	PHO	C3D-C4D-ND	5.61	114.90	107.71
23	c	504	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
23	a	404	CLA	C2C-C1C-NC	5.61	115.88	109.98
24	a	407	PHO	C4D-ND-C1D	-5.59	102.17	108.87
23	b	610	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
23	C	509	CLA	C2C-C1C-NC	5.59	115.85	109.98
23	c	501	CLA	C4A-NA-C1A	-5.58	104.13	106.68
23	c	502	CLA	CHD-C4C-C3C	-5.58	116.63	124.77
23	c	502	CLA	C2C-C1C-NC	5.58	115.84	109.98
34	B	623	HTG	C1'-S1-C1	5.58	112.50	100.45
23	c	502	CLA	C2D-C1D-ND	5.58	115.65	110.13
23	b	604	CLA	C2D-C1D-ND	5.57	115.64	110.13
23	B	609	CLA	C4A-NA-C1A	-5.57	104.14	106.68
23	b	609	CLA	C4A-NA-C1A	-5.55	104.14	106.68
23	b	605	CLA	O2D-CGD-CBD	5.55	120.94	111.23
23	B	607	CLA	CHD-C4C-C3C	-5.55	116.68	124.77
23	C	513	CLA	CMD-C2D-C1D	5.55	134.50	124.73
23	b	607	CLA	CMD-C2D-C1D	5.52	134.45	124.73
23	c	501	CLA	C2D-C1D-ND	5.52	115.59	110.13
23	C	508	CLA	CHD-C4C-C3C	-5.52	116.73	124.77
23	D	404	CLA	C2D-C1D-ND	5.51	115.58	110.13
23	d	404	CLA	C2B-C1B-NB	5.51	116.04	110.33
23	B	601	CLA	C2D-C1D-ND	5.51	115.58	110.13
23	C	511	CLA	O2D-CGD-CBD	5.51	120.86	111.23
23	c	509	CLA	C2D-C1D-ND	5.50	115.57	110.13
23	B	608	CLA	CMD-C2D-C1D	5.49	134.40	124.73
23	b	610	CLA	O2D-CGD-CBD	5.49	120.82	111.23
23	B	605	CLA	O2D-CGD-CBD	5.48	120.82	111.23
23	c	512	CLA	C2B-C1B-NB	5.47	116.00	110.33
23	B	603	CLA	C2D-C1D-ND	5.47	115.54	110.13
23	c	505	CLA	C2D-C1D-ND	5.47	115.54	110.13
23	A	406	CLA	C2B-C1B-NB	5.47	116.00	110.33
24	D	401	PHO	C3D-C4D-ND	5.47	114.72	107.71
23	c	503	CLA	O2D-CGD-CBD	5.47	120.79	111.23
23	b	611	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
23	c	510	CLA	CHD-C4C-C3C	-5.46	116.81	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C2D-C1D-ND	5.46	115.53	110.13
23	C	509	CLA	CHD-C4C-C3C	-5.45	116.82	124.77
23	C	509	CLA	O2D-CGD-CBD	5.45	120.76	111.23
23	d	403	CLA	C2C-C1C-NC	5.45	115.71	109.98
23	C	502	CLA	C4A-NA-C1A	-5.44	104.20	106.68
23	C	505	CLA	C2C-C1C-NC	5.43	115.69	109.98
24	A	407	PHO	C1-C2-C3	-5.43	117.30	126.20
23	b	609	CLA	C2D-C1D-ND	5.43	115.50	110.13
24	a	407	PHO	C1-C2-C3	-5.43	117.31	126.20
23	b	606	CLA	O2D-CGD-CBD	5.41	120.69	111.23
23	C	503	CLA	C4A-NA-C1A	-5.41	104.21	106.68
23	C	505	CLA	O2D-CGD-CBD	5.39	120.66	111.23
23	C	513	CLA	C2D-C1D-ND	5.39	115.46	110.13
23	b	608	CLA	O2D-CGD-CBD	5.38	120.64	111.23
23	a	408	CLA	CHD-C4C-C3C	-5.38	116.93	124.77
23	B	614	CLA	C2C-C1C-NC	5.37	115.63	109.98
23	b	608	CLA	CMD-C2D-C1D	5.37	134.19	124.73
23	c	506	CLA	C2C-C1C-NC	5.37	115.62	109.98
23	c	502	CLA	O2D-CGD-CBD	5.36	120.60	111.23
23	B	604	CLA	C2D-C1D-ND	5.34	115.41	110.13
23	d	404	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
23	b	604	CLA	C4A-NA-C1A	-5.34	104.24	106.68
26	a	410	SQD	O47-C7-C8	5.32	122.99	111.48
23	B	607	CLA	O2D-CGD-CBD	5.32	120.53	111.23
23	b	602	CLA	C2D-C1D-ND	5.32	115.39	110.13
23	C	503	CLA	C2D-C1D-ND	5.31	115.39	110.13
23	b	613	CLA	CMD-C2D-C1D	5.31	134.09	124.73
23	b	609	CLA	CHD-C4C-C3C	-5.31	117.04	124.77
23	A	406	CLA	C3D-C4D-ND	5.30	118.61	109.99
23	c	504	CLA	C3B-C2B-C1B	-5.29	100.93	107.17
29	a	414	PL9	C7-C3-C4	5.29	121.27	116.91
23	C	504	CLA	C2B-C1B-NB	5.29	115.81	110.33
23	b	610	CLA	C2D-C1D-ND	5.28	115.35	110.13
23	C	511	CLA	C2D-C1D-ND	5.27	115.35	110.13
23	b	609	CLA	O2D-CGD-CBD	5.26	120.43	111.23
23	c	509	CLA	O2D-CGD-CBD	5.26	120.43	111.23
23	C	502	CLA	C2C-C1C-NC	5.26	115.51	109.98
23	c	501	CLA	CHD-C4C-C3C	-5.26	117.11	124.77
23	c	510	CLA	C2D-C1D-ND	5.25	115.32	110.13
23	c	508	CLA	CMD-C2D-C1D	5.25	133.97	124.73
23	B	613	CLA	C4A-NA-C1A	-5.25	104.28	106.68
23	A	408	CLA	C2B-C1B-NB	5.24	115.76	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	C4A-NA-C1A	-5.24	104.29	106.68
23	a	408	CLA	O2D-CGD-CBD	5.24	120.38	111.23
23	B	603	CLA	O2D-CGD-CBD	5.23	120.38	111.23
26	a	410	SQD	O6-C1-C2	5.23	116.22	108.27
23	C	506	CLA	C2D-C1D-ND	5.23	115.30	110.13
23	B	615	CLA	C4A-NA-C1A	-5.23	104.29	106.68
23	D	404	CLA	C1-C2-C3	-5.23	117.63	126.20
23	c	509	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
23	C	514	CLA	C4A-NA-C1A	-5.22	104.30	106.68
23	C	508	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
23	d	404	CLA	O2D-CGD-CBD	5.21	120.35	111.23
23	b	614	CLA	C3B-C2B-C1B	-5.21	101.02	107.17
23	B	613	CLA	C2C-C1C-NC	5.21	115.45	109.98
23	A	406	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
23	A	408	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
23	b	616	CLA	C2B-C1B-NB	5.21	115.73	110.33
23	b	613	CLA	C2C-C1C-NC	5.20	115.44	109.98
23	c	512	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
23	c	510	CLA	C4A-NA-C1A	-5.19	104.31	106.68
23	d	403	CLA	C2D-C1D-ND	5.19	115.26	110.13
23	C	511	CLA	CHD-C4C-C3C	-5.18	117.21	124.77
23	a	404	CLA	CHD-C4C-C3C	-5.18	117.23	124.77
23	a	404	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
24	a	406	PHO	C3D-C4D-ND	5.17	114.34	107.71
23	b	607	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
23	b	611	CLA	C2C-C1C-NC	5.14	115.38	109.98
23	B	613	CLA	CMD-C2D-C1D	5.14	133.78	124.73
25	t	101	BCR	C33-C5-C6	-5.13	118.88	124.48
23	c	509	CLA	C1-C2-C3	-5.13	117.78	126.20
23	C	512	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
23	b	606	CLA	C2B-C1B-NB	5.12	115.64	110.33
23	A	404	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	c	511	CLA	C4A-NA-C1A	-5.12	104.34	106.68
23	a	408	CLA	C4A-NA-C1A	-5.12	104.34	106.68
23	c	502	CLA	CMD-C2D-C1D	5.11	133.73	124.73
23	C	508	CLA	C4A-NA-C1A	-5.10	104.35	106.68
23	a	404	CLA	C4A-NA-C1A	-5.10	104.35	106.68
23	D	404	CLA	CHD-C4C-C3C	-5.10	117.34	124.77
26	B	620	SQD	O6-C1-C2	5.10	116.01	108.27
23	b	603	CLA	C2B-C1B-NB	5.09	115.61	110.33
23	B	602	CLA	C2C-C1C-NC	5.09	115.33	109.98
23	b	613	CLA	C3B-C2B-C1B	-5.09	101.17	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
34	C	522	HTG	C1-O5-C5	5.08	121.68	112.56
23	A	408	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
23	B	604	CLA	C2C-C1C-NC	5.07	115.31	109.98
23	c	505	CLA	O2D-CGD-CBD	5.06	120.08	111.23
23	C	511	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
23	B	602	CLA	CHD-C4C-C3C	-5.05	117.41	124.77
23	b	612	CLA	C2D-C1D-ND	5.05	115.13	110.13
23	B	614	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
23	C	510	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
23	C	513	CLA	C2B-C1B-NB	5.04	115.56	110.33
23	B	603	CLA	CHD-C4C-C3C	-5.04	117.42	124.77
23	B	602	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
25	c	515	BCR	C7-C8-C9	-5.03	118.79	126.23
23	b	612	CLA	O2D-CGD-CBD	5.03	120.03	111.23
23	b	611	CLA	C4A-NA-C1A	-5.03	104.38	106.68
23	A	405	CLA	C3D-C4D-ND	5.03	118.16	109.99
23	b	608	CLA	C4A-NA-C1A	-5.02	104.39	106.68
23	c	509	CLA	C4A-NA-C1A	-5.02	104.39	106.68
23	C	514	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
23	b	610	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
23	C	510	CLA	O2D-CGD-CBD	5.01	119.99	111.23
23	B	605	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
23	C	507	CLA	C2C-C1C-NC	5.00	115.24	109.98
23	B	613	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
23	b	615	CLA	C2C-C1C-NC	5.00	115.23	109.98
23	b	610	CLA	C1-C2-C3	-5.00	118.01	126.20
38	E	103	HEM	CHC-C4B-NB	5.00	129.80	124.42
23	C	504	CLA	CHD-C4C-C3C	-5.00	117.49	124.77
23	B	605	CLA	C3D-C4D-ND	5.00	118.11	109.99
23	C	514	CLA	C3D-C4D-ND	4.99	118.11	109.99
23	c	513	CLA	C2B-C1B-NB	4.99	115.50	110.33
23	c	513	CLA	O2D-CGD-CBD	4.99	119.95	111.23
26	L	101	SQD	O47-C7-C8	4.99	122.27	111.48
23	B	603	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
23	C	504	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
23	C	507	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
23	B	603	CLA	C2C-C1C-NC	4.98	115.21	109.98
26	f	101	SQD	O47-C7-C8	4.98	122.25	111.48
23	d	401	CLA	C2B-C1B-NB	4.98	115.49	110.33
23	d	401	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
23	b	609	CLA	C1-C2-C3	-4.97	118.05	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	521	HTG	C1'-S1-C1	4.97	111.18	100.45
23	B	611	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	C	505	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
23	B	607	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
23	A	405	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	B	602	CLA	C2D-C1D-ND	4.94	115.02	110.13
23	d	403	CLA	CHD-C4C-C3C	-4.93	117.58	124.77
23	d	401	CLA	C2C-C1C-NC	4.93	115.16	109.98
23	b	614	CLA	C2B-C1B-NB	4.93	115.44	110.33
23	B	607	CLA	C2C-C1C-NC	4.93	115.16	109.98
23	C	502	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
23	c	509	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
23	d	401	CLA	C1C-C2C-C3C	-4.92	101.80	106.98
23	D	405	CLA	C2B-C1B-NB	4.92	115.43	110.33
23	C	510	CLA	C4A-NA-C1A	-4.92	104.44	106.68
23	c	504	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
23	b	606	CLA	C3B-C2B-C1B	-4.91	101.39	107.17
23	a	405	CLA	C3D-C4D-ND	4.90	117.96	109.99
23	b	616	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	c	504	CLA	C2B-C1B-NB	4.90	115.41	110.33
23	B	601	CLA	C2B-C1B-NB	4.90	115.41	110.33
23	b	607	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	a	404	CLA	C2B-C1B-NB	4.90	115.40	110.33
23	B	613	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
23	b	602	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
23	A	405	CLA	C2B-C1B-NB	4.89	115.40	110.33
23	B	614	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	C	505	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	C	509	CLA	CMD-C2D-C1D	4.89	133.34	124.73
23	C	505	CLA	C2B-C1B-NB	4.89	115.39	110.33
23	B	608	CLA	C3D-C2D-C1D	-4.88	99.16	105.83
23	c	508	CLA	C2C-C1C-NC	4.88	115.10	109.98
23	B	616	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
23	C	509	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
23	D	404	CLA	O2D-CGD-CBD	4.87	119.75	111.23
25	T	101	BCR	C15-C16-C17	-4.87	113.55	123.52
23	C	512	CLA	C2B-C1B-NB	4.87	115.38	110.33
23	B	610	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	A	404	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
34	D	412	HTG	C1'-S1-C1	4.86	110.95	100.45
23	A	404	CLA	CHD-C4C-C3C	-4.86	117.69	124.77
23	C	513	CLA	C3B-C2B-C1B	-4.86	101.44	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	O2D-CGD-CBD	4.86	119.72	111.23
23	d	401	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
23	c	508	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
23	B	612	CLA	C3C-C4C-NC	4.85	116.65	110.43
33	C	501	LMG	O7-C10-C11	4.85	121.98	111.48
23	c	509	CLA	C2C-C1C-NC	4.85	115.07	109.98
23	c	505	CLA	C4A-NA-C1A	-4.85	104.47	106.68
23	a	405	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	A	405	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
23	D	404	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
23	a	405	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
23	d	401	CLA	C3D-C4D-ND	4.83	117.84	109.99
25	y	101	BCR	C33-C5-C6	-4.83	119.21	124.48
40	V	202	HEC	CHC-C4B-NB	4.83	129.71	124.45
23	c	504	CLA	O2D-CGD-CBD	4.82	119.65	111.23
23	b	601	CLA	C2B-C1B-NB	4.82	115.32	110.33
23	b	606	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
23	C	509	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
23	c	510	CLA	C2C-C1C-NC	4.81	115.04	109.98
23	a	404	CLA	C2D-C1D-ND	4.81	114.89	110.13
23	D	405	CLA	C4A-NA-C1A	-4.81	104.48	106.68
23	C	511	CLA	C2C-C1C-NC	4.80	115.03	109.98
23	b	610	CLA	C2C-C1C-NC	4.80	115.03	109.98
23	b	615	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	c	512	CLA	C4A-NA-C1A	-4.80	104.49	106.68
23	d	404	CLA	C3D-C4D-ND	4.80	117.78	109.99
23	B	606	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
34	d	411	HTG	C1'-S1-C1	4.79	110.80	100.45
23	B	609	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	B	605	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	B	601	CLA	C4A-NA-C1A	-4.79	104.49	106.68
23	b	615	CLA	C4A-NA-C1A	-4.79	104.49	106.68
23	C	503	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
23	B	613	CLA	C1-C2-C3	-4.79	118.35	126.20
23	B	612	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
34	b	625	HTG	C1'-S1-C1	4.78	110.78	100.45
23	B	601	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
23	b	612	CLA	C4A-NA-C1A	-4.78	104.50	106.68
23	b	614	CLA	C4A-NA-C1A	-4.78	104.50	106.68
23	c	512	CLA	C2C-C1C-NC	4.77	115.00	109.98
29	D	407	PL9	C42-C43-C44	-4.77	116.71	127.62
23	a	408	CLA	C3D-C4D-ND	4.76	117.73	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C3D-C4D-ND	4.76	117.73	109.99
23	C	507	CLA	C2D-C1D-ND	4.76	114.84	110.13
23	c	503	CLA	C2B-C1B-NB	4.76	115.26	110.33
23	B	611	CLA	C2C-C1C-NC	4.75	114.97	109.98
23	B	613	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	b	605	CLA	C2C-C1C-NC	4.75	114.97	109.98
23	A	405	CLA	CHD-C1D-ND	-4.74	118.13	124.80
23	d	403	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
23	b	616	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
23	B	615	CLA	O2D-CGD-CBD	4.74	119.51	111.23
23	B	602	CLA	O2D-CGD-CBD	4.73	119.50	111.23
23	C	510	CLA	C2B-C1B-NB	4.73	115.23	110.33
23	a	405	CLA	C2B-C1B-NB	4.73	115.23	110.33
23	A	405	CLA	C4A-NA-C1A	-4.73	104.52	106.68
23	c	503	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
23	C	504	CLA	CHD-C1D-ND	-4.72	118.15	124.80
23	C	514	CLA	CHD-C1D-ND	-4.72	118.15	124.80
23	b	612	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
23	c	507	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
23	b	603	CLA	C3D-C4D-ND	4.72	117.66	109.99
23	d	403	CLA	C3D-C4D-ND	4.72	117.66	109.99
23	C	504	CLA	C3D-C4D-ND	4.71	117.65	109.99
26	L	101	SQD	O6-C1-C2	4.71	115.43	108.27
23	B	616	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	D	404	CLA	C1C-C2C-C3C	-4.71	102.03	106.98
23	C	509	CLA	C3B-C4B-NB	4.71	114.73	110.53
23	c	511	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	C	508	CLA	C2C-C1C-NC	4.71	114.93	109.98
23	b	611	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	c	509	CLA	C2B-C1B-NB	4.70	115.20	110.33
38	e	103	HEM	CHC-C4B-NB	4.70	129.48	124.42
23	b	608	CLA	C2B-C1B-NB	4.70	115.19	110.33
23	b	604	CLA	C2C-C1C-NC	4.69	114.91	109.98
23	C	502	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	D	404	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	C	505	CLA	C1C-C2C-C3C	-4.69	102.05	106.98
23	c	502	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	a	404	CLA	C1C-C2C-C3C	-4.68	102.05	106.98
23	c	511	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	a	405	CLA	O2D-CGD-CBD	4.68	119.41	111.23
23	B	616	CLA	C2B-C1B-NB	4.68	115.18	110.33
23	A	406	CLA	O2D-CGD-CBD	4.67	119.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	410	SQD	C1-C2-C3	-4.67	100.18	110.01
23	b	607	CLA	C4A-NA-C1A	-4.67	104.55	106.68
23	a	408	CLA	C2B-C1B-NB	4.67	115.17	110.33
23	B	608	CLA	C3D-C4D-ND	4.66	117.57	109.99
23	D	405	CLA	C3D-C4D-ND	4.66	117.57	109.99
23	c	503	CLA	C2C-C1C-NC	4.66	114.88	109.98
23	A	406	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
26	A	410	SQD	O47-C7-C8	4.66	121.56	111.48
23	c	503	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	C	506	CLA	C2C-C1C-NC	4.66	114.87	109.98
23	b	610	CLA	C3D-C4D-ND	4.65	117.55	109.99
23	B	601	CLA	C3D-C4D-ND	4.65	117.55	109.99
23	c	506	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	b	608	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	c	513	CLA	C3D-C4D-ND	4.65	117.54	109.99
23	c	507	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	d	404	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
23	B	609	CLA	C3D-C4D-ND	4.64	117.54	109.99
23	B	612	CLA	C2C-C1C-NC	4.64	114.86	109.98
23	b	613	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	d	401	CLA	CHD-C1D-ND	-4.64	118.28	124.80
23	B	603	CLA	C2B-C1B-NB	4.63	115.13	110.33
23	A	404	CLA	C2D-C1D-ND	4.63	114.71	110.13
23	B	610	CLA	C2C-C1C-NC	4.63	114.84	109.98
23	A	404	CLA	C2B-C1B-NB	4.63	115.12	110.33
23	c	508	CLA	C2B-C1B-NB	4.63	115.12	110.33
23	B	602	CLA	C2B-C1B-NB	4.63	115.12	110.33
23	b	609	CLA	C2C-C1C-NC	4.62	114.84	109.98
23	C	514	CLA	C2B-C1B-NB	4.62	115.12	110.33
23	C	512	CLA	C2C-C1C-NC	4.62	114.84	109.98
23	c	510	CLA	O2D-CGD-CBD	4.61	119.30	111.23
23	B	601	CLA	C2C-C1C-NC	4.61	114.83	109.98
23	C	514	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
23	C	510	CLA	C3D-C4D-ND	4.61	117.48	109.99
23	C	511	CLA	C2B-C1B-NB	4.61	115.11	110.33
23	b	608	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
23	c	508	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
25	T	101	BCR	C33-C5-C6	-4.61	119.46	124.48
23	C	508	CLA	C2B-C1B-NB	4.60	115.10	110.33
23	B	606	CLA	C2B-C1B-NB	4.60	115.09	110.33
23	b	602	CLA	C2B-C1B-NB	4.60	115.09	110.33
23	c	510	CLA	C3B-C2B-C1B	-4.60	101.75	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C2C-C1C-NC	4.59	114.81	109.98
23	B	602	CLA	C3D-C4D-ND	4.59	117.45	109.99
23	b	602	CLA	C2C-C1C-NC	4.59	114.80	109.98
23	D	405	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	C	511	CLA	C3D-C4D-ND	4.59	117.44	109.99
23	c	513	CLA	CHD-C1D-ND	-4.58	118.35	124.80
23	B	608	CLA	O2D-CGD-CBD	4.58	119.24	111.23
23	B	608	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
31	D	409	LHG	O7-C7-C8	4.58	121.39	111.48
23	b	614	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	b	614	CLA	C2C-C1C-NC	4.58	114.79	109.98
25	H	101	BCR	C11-C10-C9	-4.58	120.86	127.28
23	D	405	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	c	505	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	B	615	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
23	B	614	CLA	C2B-C1B-NB	4.57	115.07	110.33
25	c	514	BCR	C11-C10-C9	-4.57	120.86	127.28
23	a	408	CLA	C2C-C1C-NC	4.57	114.78	109.98
23	b	610	CLA	C2B-C1B-NB	4.57	115.07	110.33
23	C	503	CLA	C2C-C1C-NC	4.57	114.78	109.98
23	b	608	CLA	C3D-C4D-ND	4.56	117.41	109.99
23	b	609	CLA	C3D-C4D-ND	4.56	117.40	109.99
23	c	508	CLA	O2D-CGD-O1D	-4.56	114.98	123.85
25	d	405	BCR	C15-C14-C13	-4.56	120.89	127.28
23	c	504	CLA	C2C-C1C-NC	4.55	114.76	109.98
23	C	504	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	c	502	CLA	C1C-C2C-C3C	-4.55	102.20	106.98
23	b	611	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
23	b	605	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	c	510	CLA	C2B-C1B-NB	4.54	115.03	110.33
23	B	605	CLA	C2B-C1B-NB	4.54	115.03	110.33
23	c	512	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
23	c	513	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	C	512	CLA	C3D-C4D-ND	4.53	117.35	109.99
23	C	512	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	c	504	CLA	C3D-C4D-ND	4.53	117.34	109.99
23	c	513	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
23	c	503	CLA	C3D-C4D-ND	4.52	117.34	109.99
23	c	511	CLA	CHD-C1D-ND	-4.52	118.44	124.80
23	c	508	CLA	C3D-C4D-ND	4.52	117.33	109.99
23	b	601	CLA	C2C-C1C-NC	4.51	114.71	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C3D-C4D-ND	4.50	117.31	109.99
23	B	611	CLA	C4A-NA-C1A	-4.50	104.63	106.68
23	C	502	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	b	603	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
23	c	511	CLA	C3D-C4D-ND	4.50	117.30	109.99
23	B	606	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
23	b	604	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
23	c	501	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	C	510	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
25	B	617	BCR	C33-C5-C6	-4.49	119.59	124.48
23	b	612	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	C	503	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
23	a	405	CLA	C2C-C1C-NC	4.49	114.69	109.98
23	b	613	CLA	C2B-C1B-NB	4.48	114.98	110.33
23	b	612	CLA	C2C-C1C-NC	4.48	114.69	109.98
23	c	504	CLA	CHD-C1D-ND	-4.48	118.50	124.80
23	c	510	CLA	C3D-C4D-ND	4.48	117.27	109.99
23	b	601	CLA	C3D-C4D-ND	4.48	117.27	109.99
23	b	602	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	b	609	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
23	c	505	CLA	C3C-C4C-NC	4.48	116.16	110.43
23	b	615	CLA	O2D-CGD-CBD	4.47	119.04	111.23
23	b	616	CLA	C1D-CHD-C4C	-4.47	116.52	126.02
23	B	604	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	b	604	CLA	C3C-C4C-NC	4.47	116.16	110.43
23	C	511	CLA	CHD-C1D-ND	-4.47	118.51	124.80
23	a	408	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	b	613	CLA	C4A-NA-C1A	-4.47	104.64	106.68
40	v	201	HEC	CHC-C4B-NB	4.47	129.31	124.45
23	C	509	CLA	C3C-C4C-NC	4.46	116.15	110.43
23	b	603	CLA	CHD-C1D-ND	-4.46	118.53	124.80
23	b	607	CLA	C3D-C4D-ND	4.46	117.23	109.99
23	C	505	CLA	C3B-C4B-NB	4.46	114.51	110.53
23	B	615	CLA	C2C-C1C-NC	4.46	114.66	109.98
23	B	604	CLA	C3B-C2B-C1B	-4.46	101.92	107.17
23	b	615	CLA	C2B-C1B-NB	4.45	114.94	110.33
34	b	628	HTG	C1-O5-C5	4.45	120.54	112.56
23	c	509	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	C	507	CLA	O2D-CGD-CBD	4.44	119.00	111.23
23	b	615	CLA	C3B-C2B-C1B	-4.44	101.93	107.17
23	c	501	CLA	C2C-C1C-NC	4.44	114.65	109.98
23	b	611	CLA	C3D-C4D-ND	4.44	117.21	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	C3B-C4B-NB	4.44	114.49	110.53
23	C	503	CLA	C3D-C4D-ND	4.44	117.20	109.99
23	b	609	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	a	408	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
23	b	613	CLA	O2D-CGD-CBD	4.43	118.97	111.23
23	b	612	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	b	605	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
23	C	514	CLA	O2D-CGD-CBD	4.43	118.97	111.23
23	B	606	CLA	CHD-C1D-ND	-4.42	118.58	124.80
23	B	609	CLA	O2D-CGD-CBD	4.42	118.95	111.23
23	c	502	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
29	a	414	PL9	C7-C3-C2	-4.41	118.19	123.39
23	c	506	CLA	C3D-C4D-ND	4.41	117.16	109.99
23	b	607	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
23	B	605	CLA	CHD-C1D-ND	-4.41	118.60	124.80
23	B	608	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	D	405	CLA	CHD-C1D-ND	-4.41	118.60	124.80
23	B	615	CLA	C2B-C1B-NB	4.41	114.90	110.33
23	d	403	CLA	O2D-CGD-CBD	4.40	118.93	111.23
23	c	510	CLA	CHD-C1D-ND	-4.40	118.60	124.80
23	B	610	CLA	C4A-NA-C1A	-4.40	104.67	106.68
26	A	410	SQD	C1-O5-C5	-4.40	105.12	113.72
23	c	502	CLA	C3D-C4D-ND	4.40	117.14	109.99
23	B	610	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
23	c	504	CLA	C4A-NA-C1A	-4.40	104.67	106.68
23	c	505	CLA	C3D-C4D-ND	4.39	117.13	109.99
23	B	605	CLA	C4A-NA-C1A	-4.39	104.67	106.68
23	C	512	CLA	CHD-C1D-ND	-4.39	118.62	124.80
23	c	501	CLA	C3D-C4D-ND	4.39	117.13	109.99
33	Z	102	LMG	O7-C10-C11	4.39	120.97	111.48
23	b	611	CLA	C1-C2-C3	-4.39	119.01	126.20
23	b	603	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
23	A	404	CLA	C3D-C4D-ND	4.39	117.12	109.99
23	d	404	CLA	CHD-C1D-ND	-4.38	118.63	124.80
23	C	503	CLA	C2B-C1B-NB	4.38	114.87	110.33
23	B	607	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
23	c	506	CLA	C3B-C4B-NB	4.38	114.44	110.53
23	d	403	CLA	C2B-C1B-NB	4.38	114.87	110.33
23	C	513	CLA	C3D-C4D-ND	4.37	117.10	109.99
23	c	505	CLA	C2C-C1C-NC	4.37	114.58	109.98
23	a	404	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	B	612	CLA	C3D-C4D-ND	4.37	117.09	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CHD-C1D-ND	-4.37	118.66	124.80
23	b	608	CLA	C2C-C1C-NC	4.37	114.57	109.98
23	C	509	CLA	C2B-C1B-NB	4.37	114.85	110.33
23	c	507	CLA	C2C-C1C-NC	4.36	114.56	109.98
23	B	611	CLA	O2D-CGD-CBD	4.36	118.85	111.23
23	A	408	CLA	C2C-C1C-NC	4.36	114.56	109.98
23	B	601	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
23	C	507	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
23	B	603	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	B	609	CLA	C2C-C1C-NC	4.35	114.55	109.98
23	C	506	CLA	C3C-C4C-NC	4.35	116.00	110.43
23	b	602	CLA	C3D-C4D-ND	4.35	117.06	109.99
29	a	414	PL9	C32-C33-C34	-4.35	117.67	127.62
23	C	502	CLA	C1C-C2C-C3C	-4.35	102.41	106.98
23	B	612	CLA	C1-C2-C3	-4.35	119.07	126.20
23	a	405	CLA	CHD-C1D-ND	-4.35	118.69	124.80
23	B	614	CLA	C1D-CHD-C4C	-4.34	116.79	126.02
23	c	502	CLA	C2B-C1B-NB	4.34	114.83	110.33
23	b	615	CLA	CHD-C1D-ND	-4.34	118.70	124.80
26	B	620	SQD	O47-C7-C8	4.34	120.86	111.48
23	c	503	CLA	CHD-C1D-ND	-4.34	118.70	124.80
23	B	604	CLA	C3C-C4C-NC	4.34	115.98	110.43
23	b	601	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
23	b	605	CLA	C2B-C1B-NB	4.33	114.82	110.33
23	c	502	CLA	C3B-C4B-NB	4.33	114.39	110.53
23	B	605	CLA	C2C-C1C-NC	4.33	114.53	109.98
23	a	405	CLA	C4A-NA-C1A	-4.33	104.70	106.68
23	B	611	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
23	C	506	CLA	C3B-C2B-C1B	-4.32	102.07	107.17
23	C	507	CLA	C3D-C4D-ND	4.32	117.02	109.99
23	A	404	CLA	CHD-C1D-ND	-4.32	118.72	124.80
23	b	605	CLA	CHD-C1D-ND	-4.32	118.72	124.80
23	b	609	CLA	C2B-C1B-NB	4.32	114.80	110.33
23	d	403	CLA	C1C-C2C-C3C	-4.32	102.44	106.98
23	c	501	CLA	C3B-C2B-C1B	-4.31	102.08	107.17
23	C	510	CLA	C2C-C1C-NC	4.31	114.51	109.98
23	c	506	CLA	O2D-CGD-CBD	4.31	118.77	111.23
23	b	604	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
23	B	608	CLA	C2B-C1B-NB	4.31	114.79	110.33
23	B	603	CLA	C3D-C2D-C1D	-4.31	99.96	105.83
23	B	610	CLA	C3D-C4D-ND	4.30	116.98	109.99
23	B	608	CLA	CHD-C1D-ND	-4.30	118.75	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	CLA	CHD-C1D-ND	-4.30	118.75	124.80
25	B	617	BCR	C7-C8-C9	-4.30	119.88	126.23
34	b	628	HTG	C1'-S1-C1	4.30	109.73	100.45
23	c	501	CLA	O2D-CGD-O1D	-4.29	115.49	123.85
23	B	607	CLA	CHD-C1D-ND	-4.29	118.76	124.80
23	B	602	CLA	CHD-C1D-ND	-4.29	118.76	124.80
23	C	505	CLA	C1D-CHD-C4C	-4.29	116.90	126.02
23	B	609	CLA	CHD-C1D-ND	-4.29	118.77	124.80
23	c	513	CLA	C2C-C1C-NC	4.29	114.49	109.98
23	A	406	CLA	CHD-C1D-ND	-4.29	118.77	124.80
23	a	404	CLA	C1D-CHD-C4C	-4.29	116.91	126.02
23	B	616	CLA	C3D-C4D-ND	4.28	116.95	109.99
23	b	616	CLA	C3D-C4D-ND	4.28	116.94	109.99
23	B	615	CLA	C3D-C4D-ND	4.28	116.94	109.99
23	B	612	CLA	C2B-C1B-NB	4.28	114.76	110.33
23	B	610	CLA	C2B-C1B-NB	4.28	114.76	110.33
25	b	619	BCR	C3-C4-C5	-4.28	106.43	114.06
23	b	607	CLA	CHD-C1D-ND	-4.28	118.78	124.80
23	a	408	CLA	C1-C2-C3	-4.28	119.19	126.20
23	A	404	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
23	B	606	CLA	C2C-C1C-NC	4.27	114.47	109.98
23	B	615	CLA	C3B-C2B-C1B	-4.27	102.14	107.17
23	c	512	CLA	C1-C2-C3	-4.27	119.20	126.20
23	A	406	CLA	C4A-NA-C1A	-4.27	104.73	106.68
25	C	515	BCR	C15-C14-C13	-4.27	121.29	127.28
23	c	507	CLA	C2B-C1B-NB	4.27	114.75	110.33
23	b	605	CLA	C4A-NA-C1A	-4.27	104.73	106.68
23	C	512	CLA	C4A-NA-C1A	-4.27	104.73	106.68
23	C	508	CLA	C1D-CHD-C4C	-4.27	116.95	126.02
23	c	509	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
23	b	607	CLA	C2B-C1B-NB	4.26	114.75	110.33
34	C	522	HTG	C1'-S1-C1	4.26	109.65	100.45
23	c	511	CLA	C2C-C1C-NC	4.25	114.44	109.98
23	c	510	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
23	C	507	CLA	C2B-C1B-NB	4.24	114.73	110.33
23	c	511	CLA	C2B-C1B-NB	4.24	114.73	110.33
23	b	606	CLA	C1D-CHD-C4C	-4.24	117.00	126.02
23	b	606	CLA	C3D-C4D-ND	4.24	116.88	109.99
23	C	506	CLA	C3D-C4D-ND	4.24	116.88	109.99
25	d	405	BCR	C28-C27-C26	-4.24	106.50	114.06
23	A	404	CLA	C3B-C4B-NB	4.24	114.31	110.53
24	D	401	PHO	C1-C2-C3	-4.24	119.26	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C2C-C1C-NC	4.23	114.43	109.98
23	B	614	CLA	C3B-C4B-NB	4.23	114.31	110.53
23	B	606	CLA	C3D-C4D-ND	4.23	116.87	109.99
23	D	405	CLA	C1-C2-C3	-4.23	119.26	126.20
35	D	402	LMT	C1'-O5'-C5'	4.23	121.98	113.72
34	b	622	HTG	C1'-S1-C1	4.22	109.57	100.45
23	A	405	CLA	O2D-CGD-CBD	4.22	118.61	111.23
23	C	507	CLA	C1-C2-C3	-4.22	119.28	126.20
23	C	507	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
23	B	603	CLA	C1D-CHD-C4C	-4.21	117.06	126.02
23	b	614	CLA	C3D-C4D-ND	4.21	116.84	109.99
23	c	503	CLA	C1D-CHD-C4C	-4.21	117.07	126.02
23	A	408	CLA	CHD-C1D-ND	-4.21	118.88	124.80
23	C	502	CLA	C1D-CHD-C4C	-4.21	117.07	126.02
23	B	607	CLA	C3D-C4D-ND	4.21	116.83	109.99
23	c	511	CLA	O2D-CGD-CBD	4.21	118.59	111.23
24	D	401	PHO	CBC-CAC-C3C	-4.20	106.85	112.87
23	B	614	CLA	C3D-C4D-ND	4.20	116.82	109.99
23	C	502	CLA	C1-C2-C3	-4.20	119.31	126.20
25	d	405	BCR	C29-C30-C25	4.20	116.54	110.44
23	D	405	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
23	C	508	CLA	C3D-C4D-ND	4.20	116.81	109.99
23	C	513	CLA	C3D-C2D-C1D	-4.20	100.11	105.83
23	B	615	CLA	CMB-C2B-C1B	4.19	131.80	125.42
23	C	509	CLA	C3D-C4D-ND	4.19	116.80	109.99
23	c	510	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
23	b	601	CLA	CHD-C1D-ND	-4.19	118.91	124.80
23	A	404	CLA	O2A-CGA-CBA	4.19	124.60	111.83
23	B	610	CLA	C3C-C4C-NC	4.18	115.79	110.43
29	A	414	PL9	C7-C3-C2	-4.18	118.46	123.39
35	D	402	LMT	O5'-C5'-C4'	4.18	118.36	109.72
23	C	510	CLA	CHD-C1D-ND	-4.17	118.93	124.80
23	b	613	CLA	C3D-C4D-ND	4.17	116.77	109.99
25	b	617	BCR	C33-C5-C6	-4.17	119.93	124.48
23	A	408	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	b	607	CLA	C3C-C4C-NC	4.16	115.76	110.43
23	A	408	CLA	C4-C3-C5	4.16	122.45	115.23
34	B	627	HTG	C1'-S1-C1	4.16	109.43	100.45
23	B	602	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
23	C	502	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	b	615	CLA	C3D-C4D-ND	4.15	116.74	109.99
23	B	605	CLA	CMB-C2B-C1B	4.15	131.74	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C7-C8-C9	-4.15	120.10	126.23
25	b	619	BCR	C7-C8-C9	-4.15	120.10	126.23
23	A	408	CLA	O2D-CGD-CBD	4.14	118.47	111.23
23	c	506	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
23	C	511	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
23	b	602	CLA	CHD-C1D-ND	-4.14	118.98	124.80
23	A	405	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
23	b	612	CLA	C1-C2-C3	-4.13	119.42	126.20
23	D	404	CLA	C3D-C4D-ND	4.13	116.70	109.99
34	b	625	HTG	C1-O5-C5	4.13	119.97	112.56
33	Z	101	LMG	C3-C4-C5	4.13	117.72	110.23
23	c	501	CLA	C2B-C1B-NB	4.12	114.60	110.33
23	C	508	CLA	CMB-C2B-C1B	4.12	131.69	125.42
23	C	506	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
23	b	610	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
23	B	614	CLA	C1C-C2C-C3C	-4.11	102.65	106.98
23	d	403	CLA	CHD-C1D-ND	-4.11	119.01	124.80
23	C	507	CLA	C1C-C2C-C3C	-4.11	102.65	106.98
23	C	514	CLA	C2C-C1C-NC	4.11	114.30	109.98
29	a	414	PL9	C27-C28-C29	-4.11	118.21	127.62
23	c	505	CLA	C2B-C1B-NB	4.11	114.59	110.33
36	c	516	DGD	O2G-C1B-C2B	4.11	120.37	111.48
23	b	613	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
23	b	606	CLA	C2C-C1C-NC	4.11	114.30	109.98
23	B	605	CLA	C1-C2-C3	-4.10	119.47	126.20
23	C	510	CLA	C1-C2-C3	-4.10	119.47	126.20
25	k	101	BCR	C11-C10-C9	-4.10	121.53	127.28
23	c	507	CLA	CHD-C1D-ND	-4.10	119.03	124.80
23	B	604	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
23	B	612	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
23	a	404	CLA	C3D-C2D-C1D	-4.09	100.26	105.83
23	C	506	CLA	C2B-C1B-NB	4.08	114.56	110.33
23	B	609	CLA	C3C-C4C-NC	4.08	115.66	110.43
23	B	612	CLA	CMD-C2D-C1D	4.08	131.91	124.73
23	B	612	CLA	O2D-CGD-O1D	-4.08	115.91	123.85
34	c	522	HTG	C1'-S1-C1	4.08	109.25	100.45
23	c	511	CLA	C1-C2-C3	-4.07	119.52	126.20
40	v	201	HEC	CBB-CAB-C3B	-4.07	119.30	127.43
23	C	512	CLA	O2D-CGD-CBD	4.07	118.34	111.23
23	b	604	CLA	C3D-C4D-ND	4.07	116.60	109.99
23	B	613	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
23	d	401	CLA	C1D-CHD-C4C	-4.06	117.40	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	CHD-C1D-ND	-4.06	119.09	124.80
34	C	521	HTG	C1'-S1-C1	4.05	109.21	100.45
23	B	604	CLA	C2B-C1B-NB	4.05	114.53	110.33
23	B	615	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	C	508	CLA	CHD-C1D-ND	-4.05	119.11	124.80
23	b	603	CLA	C1D-CHD-C4C	-4.05	117.42	126.02
25	c	514	BCR	C20-C21-C22	-4.04	121.61	127.28
23	c	507	CLA	C3D-C4D-ND	4.04	116.55	109.99
23	C	502	CLA	CHD-C1D-ND	-4.04	119.12	124.80
23	D	405	CLA	C1D-CHD-C4C	-4.04	117.44	126.02
29	a	414	PL9	C22-C23-C24	-4.03	118.39	127.62
23	B	607	CLA	C2B-C1B-NB	4.03	114.51	110.33
23	B	616	CLA	C1D-CHD-C4C	-4.03	117.45	126.02
23	B	611	CLA	CHD-C1D-ND	-4.03	119.13	124.80
23	B	606	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
23	A	404	CLA	CAA-C2A-C3A	-4.03	102.12	113.00
23	B	611	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
23	C	512	CLA	C3B-C4B-NB	4.02	114.12	110.53
25	b	618	BCR	C7-C8-C9	-4.02	120.28	126.23
23	B	608	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
33	c	520	LMG	O7-C10-C11	4.02	120.18	111.48
23	B	613	CLA	C3D-C4D-ND	4.02	116.52	109.99
23	B	607	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
23	C	513	CLA	C1D-CHD-C4C	-4.02	117.49	126.02
31	E	101	LHG	O7-C7-C8	4.00	120.14	111.48
23	B	613	CLA	C3C-C4C-NC	4.00	115.55	110.43
23	b	603	CLA	C2C-C1C-NC	3.99	114.18	109.98
29	A	414	PL9	C7-C3-C4	3.99	120.20	116.91
23	B	604	CLA	C4A-NA-C1A	-3.99	104.86	106.68
23	D	404	CLA	CHD-C1D-ND	-3.99	119.19	124.80
23	c	507	CLA	CMB-C2B-C1B	3.99	131.49	125.42
33	J	101	LMG	O7-C10-C11	3.99	120.11	111.48
23	c	502	CLA	C4A-NA-C1A	-3.99	104.86	106.68
23	c	506	CLA	C2B-C1B-NB	3.99	114.46	110.33
29	d	406	PL9	C42-C43-C44	-3.99	118.50	127.62
25	H	101	BCR	C16-C17-C18	-3.99	121.69	127.28
23	C	503	CLA	O2D-CGD-O1D	-3.99	116.09	123.85
23	a	404	CLA	O2D-CGD-CBD	3.99	118.20	111.23
23	c	508	CLA	C3C-C4C-NC	3.98	115.53	110.43
23	B	605	CLA	O2D-CGD-O1D	-3.98	116.09	123.85
23	c	506	CLA	CHD-C1D-ND	-3.98	119.20	124.80
23	A	404	CLA	CAC-C3C-C4C	3.98	129.97	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	CAA-C2A-C3A	-3.98	102.24	113.00
23	b	604	CLA	CHD-C1D-ND	-3.98	119.20	124.80
23	B	601	CLA	C1-C2-C3	-3.98	119.68	126.20
23	D	404	CLA	C2B-C1B-NB	3.98	114.45	110.33
26	a	410	SQD	C45-O47-C7	-3.98	108.28	117.80
23	b	613	CLA	C3C-C4C-NC	3.98	115.52	110.43
23	B	606	CLA	C3C-C4C-NC	3.98	115.52	110.43
23	A	406	CLA	CMB-C2B-C1B	3.97	131.47	125.42
23	B	615	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
23	B	604	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
23	C	506	CLA	CHD-C1D-ND	-3.97	119.22	124.80
23	C	505	CLA	C3D-C4D-ND	3.96	116.43	109.99
23	B	611	CLA	C3D-C4D-ND	3.96	116.43	109.99
23	C	511	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
29	a	414	PL9	C15-C14-C16	3.96	122.10	115.23
35	I	101	LMT	C1'-O5'-C5'	3.96	121.45	113.72
23	d	401	CLA	C3B-C4B-NB	3.95	114.06	110.53
23	b	606	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
23	b	613	CLA	C1D-CHD-C4C	-3.94	117.64	126.02
23	b	609	CLA	CHD-C1D-ND	-3.94	119.26	124.80
23	b	614	CLA	C1D-CHD-C4C	-3.94	117.64	126.02
23	c	512	CLA	CHD-C1D-ND	-3.94	119.26	124.80
23	c	503	CLA	C3C-C4C-NC	3.94	115.47	110.43
23	b	610	CLA	CHD-C1D-ND	-3.93	119.27	124.80
23	c	506	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
23	B	610	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
23	c	505	CLA	CMB-C2B-C1B	3.93	131.40	125.42
23	c	513	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
23	B	616	CLA	C3C-C4C-NC	3.93	115.46	110.43
23	c	511	CLA	C4-C3-C5	3.92	122.04	115.23
23	C	506	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
23	d	403	CLA	C3D-C2D-C1D	-3.92	100.49	105.83
25	B	618	BCR	C29-C30-C25	3.92	116.13	110.44
23	a	405	CLA	C1D-CHD-C4C	-3.92	117.70	126.02
23	B	604	CLA	C3D-C4D-ND	3.92	116.35	109.99
23	B	608	CLA	C1-C2-C3	-3.92	119.78	126.20
23	b	612	CLA	C1D-CHD-C4C	-3.91	117.70	126.02
23	A	405	CLA	CHD-C4C-NC	3.91	130.30	124.23
36	H	102	DGD	O2G-C1B-C2B	3.91	119.94	111.48
23	c	506	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	C	505	CLA	C3C-C4C-NC	3.90	115.43	110.43
23	A	408	CLA	C1-C2-C3	-3.90	119.80	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	C2B-C1B-NB	3.90	114.37	110.33
23	c	509	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	b	605	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
33	Z	101	LMG	O7-C10-C11	3.90	119.92	111.48
23	c	502	CLA	CHD-C1D-ND	-3.89	119.32	124.80
23	A	405	CLA	C2C-C1C-NC	3.89	114.07	109.98
25	C	515	BCR	C16-C17-C18	-3.89	121.82	127.28
25	d	405	BCR	C7-C8-C9	-3.89	120.48	126.23
23	B	612	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
23	c	511	CLA	C1D-CHD-C4C	-3.88	117.77	126.02
23	d	403	CLA	C3B-C4B-NB	3.88	114.00	110.53
23	b	615	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
23	b	604	CLA	C1-C2-C3	-3.88	119.84	126.20
23	B	605	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
23	b	602	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
23	b	615	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
23	a	408	CLA	C3B-C4B-NB	3.87	113.99	110.53
23	B	608	CLA	C4A-NA-C1A	-3.87	104.91	106.68
23	D	405	CLA	CMB-C2B-C1B	3.87	131.31	125.42
23	D	404	CLA	C3C-C4C-NC	3.87	115.39	110.43
23	B	614	CLA	CHD-C1D-ND	-3.87	119.36	124.80
25	B	618	BCR	C15-C14-C13	-3.87	121.85	127.28
23	c	507	CLA	C4A-NA-C1A	-3.86	104.92	106.68
23	C	507	CLA	CAC-C3C-C4C	3.86	129.81	124.79
23	c	507	CLA	C3C-C4C-NC	3.86	115.37	110.43
23	b	604	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	C	513	CLA	CHD-C1D-ND	-3.85	119.38	124.80
23	c	505	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
23	B	616	CLA	C2C-C1C-NC	3.85	114.03	109.98
23	b	605	CLA	C3B-C4B-NB	3.85	113.97	110.53
23	B	604	CLA	C1-C2-C3	-3.85	119.89	126.20
23	B	610	CLA	CAA-C2A-C3A	-3.84	102.61	113.00
23	b	608	CLA	CHD-C1D-ND	-3.84	119.39	124.80
23	B	602	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
23	B	608	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	c	505	CLA	C3D-C2D-C1D	-3.84	100.60	105.83
23	b	614	CLA	CHD-C1D-ND	-3.84	119.41	124.80
23	B	613	CLA	CMC-C2C-C1C	3.83	131.02	125.03
23	B	616	CLA	CHD-C1D-ND	-3.83	119.42	124.80
23	b	606	CLA	CHD-C1D-ND	-3.83	119.42	124.80
23	B	615	CLA	C3C-C4C-NC	3.82	115.33	110.43
25	c	514	BCR	C15-C14-C13	-3.82	121.92	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	PL9	C7-C8-C9	-3.82	120.25	126.83
23	C	502	CLA	C3B-C4B-NB	3.82	113.94	110.53
23	c	513	CLA	C3C-C4C-NC	3.82	115.32	110.43
29	a	414	PL9	C37-C38-C39	-3.82	118.88	127.62
38	e	103	HEM	CHD-C4C-NC	3.82	128.61	124.45
23	b	610	CLA	C3C-C4C-NC	3.82	115.32	110.43
23	b	616	CLA	C3C-C4C-NC	3.81	115.32	110.43
25	b	619	BCR	C38-C26-C25	-3.81	120.32	124.48
23	B	611	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
23	b	607	CLA	C3B-C4B-NB	3.81	113.93	110.53
33	B	621	LMG	O7-C10-C11	3.80	119.71	111.48
23	C	503	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
23	b	614	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
23	B	609	CLA	C2B-C1B-NB	3.80	114.27	110.33
23	b	611	CLA	CHD-C1D-ND	-3.80	119.46	124.80
23	B	601	CLA	C1D-CHD-C4C	-3.80	117.95	126.02
23	A	408	CLA	C1D-CHD-C4C	-3.80	117.95	126.02
23	C	508	CLA	O2D-CGD-O1D	-3.80	116.46	123.85
23	b	608	CLA	C1C-C2C-C3C	-3.80	102.99	106.98
33	c	519	LMG	O7-C10-C11	3.79	119.68	111.48
23	b	602	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
23	c	508	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
26	A	410	SQD	C44-O6-C1	-3.79	105.67	113.80
23	C	514	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
23	b	604	CLA	CMB-C2B-C1B	3.78	131.18	125.42
23	a	405	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
23	d	401	CLA	O2D-CGD-CBD	3.78	117.84	111.23
23	B	603	CLA	CHD-C1D-ND	-3.78	119.49	124.80
29	A	414	PL9	C27-C28-C29	-3.78	118.98	127.62
23	b	601	CLA	C1D-CHD-C4C	-3.78	118.00	126.02
23	c	509	CLA	C3C-C4C-NC	3.77	115.27	110.43
23	A	405	CLA	CMC-C2C-C1C	3.77	130.93	125.03
23	c	510	CLA	C3B-C4B-NB	3.77	113.90	110.53
23	c	510	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
23	C	508	CLA	C3C-C4C-NC	3.77	115.26	110.43
23	A	404	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
23	b	611	CLA	C3B-C4B-NB	3.77	113.89	110.53
23	B	611	CLA	C3C-C4C-NC	3.77	115.26	110.43
23	B	612	CLA	C4C-C3C-C2C	-3.77	101.41	106.89
23	b	609	CLA	C1D-CHD-C4C	-3.77	118.02	126.02
23	b	611	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
23	c	512	CLA	C1D-CHD-C4C	-3.76	118.02	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C3C-C4C-NC	3.76	115.25	110.43
23	b	605	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
23	A	405	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
25	c	514	BCR	C16-C17-C18	-3.76	122.01	127.28
33	c	520	LMG	O6-C5-C4	3.76	116.47	109.70
23	b	612	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
31	A	417	LHG	O7-C7-C8	3.75	119.59	111.48
23	A	404	CLA	C1D-CHD-C4C	-3.74	118.06	126.02
23	C	510	CLA	C3C-C4C-NC	3.74	115.22	110.43
23	C	503	CLA	CHD-C1D-ND	-3.74	119.54	124.80
33	j	101	LMG	O7-C10-C11	3.74	119.57	111.48
23	C	504	CLA	O2D-CGD-CBD	3.73	117.76	111.23
23	b	606	CLA	C3C-C4C-NC	3.73	115.21	110.43
23	c	508	CLA	C3B-C4B-NB	3.73	113.86	110.53
23	b	614	CLA	C3B-C4B-NB	3.73	113.86	110.53
38	E	103	HEM	CAD-CBD-CGD	3.73	123.55	113.67
23	A	408	CLA	C3C-C4C-NC	3.72	115.20	110.43
23	a	408	CLA	CHD-C1D-ND	-3.72	119.56	124.80
29	d	406	PL9	C10-C9-C11	3.72	121.68	115.23
34	C	522	HTG	O5-C5-C4	3.72	116.40	109.70
25	C	516	BCR	C7-C8-C9	-3.72	120.73	126.23
23	c	502	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
23	b	609	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
23	d	403	CLA	O2A-CGA-CBA	3.71	123.16	111.83
23	C	512	CLA	C3C-C4C-NC	3.71	115.19	110.43
23	b	616	CLA	CHD-C1D-ND	-3.71	119.58	124.80
23	d	404	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
23	b	604	CLA	C2B-C1B-NB	3.71	114.17	110.33
23	C	512	CLA	C1D-CHD-C4C	-3.71	118.14	126.02
23	D	405	CLA	C3C-C4C-NC	3.71	115.18	110.43
25	Y	101	BCR	C15-C14-C13	-3.71	122.08	127.28
25	k	101	BCR	C24-C23-C22	-3.70	120.75	126.23
23	b	612	CLA	C3C-C4C-NC	3.70	115.17	110.43
33	a	416	LMG	O7-C10-C11	3.70	119.49	111.48
23	C	509	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
25	h	101	BCR	C7-C8-C9	-3.69	120.77	126.23
23	B	609	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
29	d	406	PL9	C7-C8-C9	-3.69	120.48	126.83
23	d	401	CLA	CAA-C2A-C3A	-3.69	103.03	113.00
23	c	512	CLA	C3C-C4C-NC	3.69	115.15	110.43
23	B	609	CLA	CMB-C2B-C1B	3.69	131.03	125.42
33	Z	101	LMG	O6-C5-C4	3.68	116.33	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C4C-C3C-C2C	-3.68	101.53	106.89
23	B	610	CLA	CHD-C1D-ND	-3.68	119.63	124.80
23	b	612	CLA	CHD-C1D-ND	-3.68	119.63	124.80
23	B	607	CLA	C1D-CHD-C4C	-3.68	118.21	126.02
23	C	511	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
23	D	404	CLA	C3B-C4B-NB	3.67	113.81	110.53
23	B	602	CLA	C3B-C4B-NB	3.67	113.81	110.53
23	b	610	CLA	C1D-CHD-C4C	-3.67	118.23	126.02
23	C	514	CLA	C1-C2-C3	-3.67	120.19	126.20
23	C	505	CLA	CHD-C1D-ND	-3.66	119.65	124.80
25	H	101	BCR	C24-C23-C22	-3.66	120.83	126.23
23	B	603	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
23	C	511	CLA	C1-C2-C3	-3.65	120.21	126.20
23	C	509	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
23	C	502	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
23	d	404	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
23	B	611	CLA	C2B-C1B-NB	3.65	114.11	110.33
23	c	504	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
25	k	101	BCR	C29-C30-C25	3.65	115.74	110.44
23	B	613	CLA	CAC-C3C-C4C	3.64	129.53	124.79
24	A	407	PHO	C1A-C2A-C3A	-3.64	99.37	102.84
23	B	604	CLA	C3B-C4B-NB	3.64	113.78	110.53
25	K	102	BCR	C7-C8-C9	-3.64	120.85	126.23
23	c	504	CLA	CAC-C3C-C4C	3.64	129.53	124.79
23	c	506	CLA	C3C-C4C-NC	3.64	115.09	110.43
23	c	508	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
23	c	508	CLA	CHD-C1D-ND	-3.63	119.69	124.80
23	b	613	CLA	C3B-C4B-NB	3.63	113.77	110.53
23	B	603	CLA	O2A-CGA-O1A	-3.63	114.55	123.63
23	b	608	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
23	c	512	CLA	CMB-C2B-C1B	3.63	130.95	125.42
23	B	603	CLA	CAA-C2A-C3A	-3.63	103.19	113.00
38	E	103	HEM	C1B-NB-C4B	3.63	109.50	105.21
23	d	403	CLA	C1-C2-C3	-3.63	120.26	126.20
23	A	406	CLA	C2C-C1C-NC	3.62	113.79	109.98
23	C	510	CLA	C1D-CHD-C4C	-3.62	118.32	126.02
23	B	612	CLA	C4A-NA-C1A	-3.62	105.03	106.68
23	c	512	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
23	B	603	CLA	C3B-C4B-NB	3.62	113.76	110.53
23	B	614	CLA	CMB-C2B-C1B	3.62	130.93	125.42
26	a	410	SQD	C1-O5-C5	-3.62	106.66	113.72
23	B	601	CLA	C1C-C2C-C3C	-3.61	103.18	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	PL9	C22-C23-C24	-3.61	119.35	127.62
23	A	406	CLA	C3C-C4C-NC	3.61	115.06	110.43
23	d	401	CLA	CHD-C4C-NC	3.61	129.83	124.23
23	b	615	CLA	C3B-C4B-NB	3.61	113.75	110.53
23	b	607	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	c	506	CLA	C4B-C3B-C2B	-3.61	102.81	107.30
23	d	401	CLA	C4A-NA-C1A	-3.61	105.03	106.68
23	C	503	CLA	C1C-C2C-C3C	-3.61	103.19	106.98
23	B	610	CLA	C4C-C3C-C2C	-3.61	101.64	106.89
23	b	609	CLA	CMB-C2B-C1B	3.61	130.91	125.42
23	B	616	CLA	C4C-C3C-C2C	-3.61	101.64	106.89
33	Z	102	LMG	C3-C4-C5	3.61	116.77	110.23
23	c	504	CLA	C1D-CHD-C4C	-3.60	118.36	126.02
23	C	514	CLA	C3C-C4C-NC	3.60	115.05	110.43
23	b	605	CLA	C3C-C4C-NC	3.60	115.04	110.43
40	V	202	HEC	CBB-CAB-C3B	-3.60	120.24	127.43
23	d	404	CLA	C2C-C1C-NC	3.60	113.76	109.98
24	D	401	PHO	C1A-C2A-C3A	-3.60	99.42	102.84
23	C	509	CLA	C1-C2-C3	-3.60	120.30	126.20
26	L	101	SQD	O7-S-C6	3.60	112.12	106.76
23	b	609	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
23	b	604	CLA	C1D-CHD-C4C	-3.59	118.39	126.02
23	c	506	CLA	C4A-NA-C1A	-3.59	105.04	106.68
25	A	409	BCR	C33-C5-C6	-3.59	120.57	124.48
23	B	610	CLA	O2A-CGA-CBA	3.59	122.77	111.83
23	a	408	CLA	C3C-C4C-NC	3.59	115.02	110.43
23	C	505	CLA	C4A-NA-C1A	-3.59	105.04	106.68
23	b	611	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
23	b	614	CLA	C1-C2-C3	-3.58	120.33	126.20
23	B	614	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
23	C	504	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
23	B	613	CLA	C3B-C4B-NB	3.58	113.72	110.53
36	C	518	DGD	O2G-C1B-C2B	3.57	119.21	111.48
23	b	608	CLA	C3C-C4C-NC	3.57	115.01	110.43
23	a	404	CLA	CHD-C1D-ND	-3.57	119.78	124.80
33	z	101	LMG	O7-C10-C11	3.57	119.20	111.48
23	b	613	CLA	O2A-CGA-CBA	3.57	122.72	111.83
36	C	517	DGD	O2G-C1B-C2B	3.57	119.19	111.48
23	A	406	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
23	c	509	CLA	C3B-C4B-NB	3.56	113.71	110.53
25	h	101	BCR	C16-C17-C18	-3.56	122.28	127.28
23	D	405	CLA	C2C-C1C-NC	3.56	113.72	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C3C-C4C-NC	3.56	114.99	110.43
23	C	508	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
23	b	608	CLA	C1D-CHD-C4C	-3.56	118.46	126.02
23	a	408	CLA	C1D-CHD-C4C	-3.56	118.46	126.02
36	c	517	DGD	O2G-C1B-C2B	3.56	119.18	111.48
23	B	607	CLA	C3C-C4C-NC	3.56	114.98	110.43
23	c	511	CLA	C3B-C4B-NB	3.56	113.70	110.53
31	d	407	LHG	O7-C7-C8	3.55	119.17	111.48
23	c	505	CLA	CHD-C1D-ND	-3.55	119.80	124.80
23	b	603	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
23	B	608	CLA	C3C-C4C-NC	3.54	114.97	110.43
23	c	507	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
25	H	101	BCR	C38-C26-C25	-3.54	120.62	124.48
23	a	408	CLA	C1C-C2C-C3C	-3.54	103.26	106.98
31	l	101	LHG	O7-C7-C8	3.54	119.13	111.48
23	b	609	CLA	CAC-C3C-C4C	3.53	129.39	124.79
25	b	617	BCR	C7-C8-C9	-3.53	121.01	126.23
23	a	408	CLA	CAA-C2A-C3A	-3.53	103.46	113.00
38	e	103	HEM	C1B-NB-C4B	3.53	109.39	105.21
23	B	607	CLA	CAA-C2A-C3A	-3.53	103.47	113.00
23	C	507	CLA	CBC-CAC-C3C	-3.53	102.86	112.42
25	C	516	BCR	C11-C10-C9	-3.53	122.33	127.28
23	C	502	CLA	CBC-CAC-C3C	-3.53	102.86	112.42
23	C	513	CLA	C1C-C2C-C3C	-3.52	103.27	106.98
25	t	101	BCR	C37-C22-C23	3.52	123.47	118.09
23	b	601	CLA	C3C-C4C-NC	3.52	114.94	110.43
23	C	506	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
23	B	608	CLA	CHD-C4C-NC	3.52	129.69	124.23
23	c	504	CLA	C3C-C4C-NC	3.52	114.94	110.43
23	B	609	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
23	A	405	CLA	C3C-C4C-NC	3.51	114.93	110.43
23	c	501	CLA	C1D-CHD-C4C	-3.51	118.55	126.02
23	B	608	CLA	O2A-CGA-O1A	-3.51	114.84	123.63
23	B	602	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
23	c	506	CLA	C1-C2-C3	-3.51	120.45	126.20
31	d	409	LHG	O7-C7-C8	3.51	119.07	111.48
23	B	614	CLA	CHC-C1C-C2C	-3.51	116.98	126.95
23	c	501	CLA	CAC-C3C-C4C	3.51	129.35	124.79
23	c	513	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
25	K	102	BCR	C24-C23-C22	-3.50	121.05	126.23
23	c	503	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	C	510	CLA	CMC-C2C-C1C	3.50	130.50	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C1-C2-C3	-3.50	120.47	126.20
23	b	610	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	C	502	CLA	C3C-C4C-NC	3.50	114.91	110.43
23	b	615	CLA	C3C-C4C-NC	3.50	114.91	110.43
23	C	512	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
33	Z	102	LMG	C1-C2-C3	3.49	117.36	110.01
23	B	615	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
23	c	513	CLA	CMC-C2C-C1C	3.49	130.49	125.03
23	d	401	CLA	CBC-CAC-C3C	-3.49	102.95	112.42
23	C	513	CLA	C3C-C4C-NC	3.49	114.90	110.43
23	C	512	CLA	CAC-C3C-C4C	3.49	129.33	124.79
23	c	504	CLA	C3B-C4B-NB	3.49	113.64	110.53
23	d	403	CLA	C3C-C4C-NC	3.49	114.90	110.43
38	E	103	HEM	CHB-C1B-NB	3.48	128.68	124.37
25	t	101	BCR	C21-C20-C19	-3.48	113.11	123.20
23	c	509	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
23	c	502	CLA	C3C-C4C-NC	3.47	114.88	110.43
38	e	103	HEM	CHB-C1B-NB	3.47	128.66	124.37
23	B	610	CLA	C1-C2-C3	-3.47	120.51	126.20
23	b	601	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
31	A	416	LHG	O8-C23-C24	3.47	122.41	111.83
29	A	414	PL9	C32-C33-C34	-3.47	119.69	127.62
26	A	412	SQD	O48-C23-C24	3.47	122.40	111.83
23	b	602	CLA	C3C-C4C-NC	3.46	114.86	110.43
23	b	611	CLA	C3C-C4C-NC	3.46	114.86	110.43
23	b	616	CLA	C4C-C3C-C2C	-3.46	101.86	106.89
23	A	406	CLA	C1-C2-C3	-3.46	120.53	126.20
25	d	405	BCR	C33-C5-C6	-3.46	120.71	124.48
23	c	501	CLA	C3C-C4C-NC	3.45	114.85	110.43
23	c	505	CLA	C4C-C3C-C2C	-3.45	101.87	106.89
23	C	509	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
23	B	613	CLA	CHD-C1D-ND	-3.45	119.95	124.80
23	B	613	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
23	B	611	CLA	C3B-C4B-NB	3.44	113.60	110.53
23	b	603	CLA	C3C-C4C-NC	3.44	114.83	110.43
38	E	103	HEM	CHD-C4C-NC	3.44	128.20	124.45
23	b	614	CLA	CAC-C3C-C4C	3.44	129.26	124.79
23	c	501	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
29	D	407	PL9	C53-C6-C1	3.43	122.30	115.28
23	B	606	CLA	C1C-C2C-C3C	-3.43	103.38	106.98
23	b	605	CLA	CMB-C2B-C1B	3.42	130.63	125.42
25	A	409	BCR	C24-C23-C22	-3.42	121.17	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C2-C1-C6	3.42	115.41	110.44
23	B	605	CLA	C3C-C4C-NC	3.42	114.81	110.43
23	B	614	CLA	O2A-CGA-O1A	-3.41	115.09	123.63
25	t	101	BCR	C11-C10-C9	-3.41	122.49	127.28
23	C	510	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
23	C	504	CLA	C4-C3-C5	3.41	121.15	115.23
23	B	614	CLA	C3C-C4C-NC	3.41	114.80	110.43
23	C	512	CLA	CMC-C2C-C1C	3.41	130.36	125.03
23	b	605	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
23	C	504	CLA	C1C-C2C-C3C	-3.41	103.40	106.98
23	B	615	CLA	CED-O2D-CGD	3.40	123.64	115.92
25	D	406	BCR	C38-C26-C25	-3.40	120.77	124.48
23	B	611	CLA	C1-C2-C3	-3.40	120.62	126.20
23	D	405	CLA	CHD-C4C-NC	3.40	129.50	124.23
23	b	607	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
23	b	615	CLA	C11-C10-C8	-3.40	104.67	115.97
23	c	511	CLA	C3C-C4C-NC	3.39	114.78	110.43
23	c	509	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
23	b	607	CLA	CMB-C2B-C1B	3.39	130.59	125.42
25	D	406	BCR	C24-C23-C22	-3.39	121.22	126.23
23	C	507	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
23	C	514	CLA	C1C-C2C-C3C	-3.39	103.42	106.98
23	a	404	CLA	C1-C2-C3	-3.39	120.65	126.20
23	b	609	CLA	O2A-CGA-CBA	3.38	122.14	111.83
23	C	514	CLA	CMB-C2B-C1B	3.38	130.57	125.42
26	a	410	SQD	C1-C2-C3	-3.38	102.91	110.01
23	b	608	CLA	C1-C2-C3	-3.38	120.67	126.20
23	a	404	CLA	C3C-C4C-NC	3.37	114.75	110.43
25	T	101	BCR	C7-C8-C9	-3.37	121.25	126.23
23	c	502	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
23	C	512	CLA	C1-C2-C3	-3.37	120.68	126.20
23	C	507	CLA	CMC-C2C-C1C	3.37	130.30	125.03
25	h	101	BCR	C38-C26-C25	-3.37	120.81	124.48
29	A	414	PL9	C37-C38-C39	-3.37	119.92	127.62
25	y	101	BCR	C38-C26-C25	-3.36	120.81	124.48
23	b	605	CLA	C4-C3-C5	3.36	121.06	115.23
23	C	509	CLA	CHD-C1D-ND	-3.36	120.07	124.80
23	a	405	CLA	C3C-C4C-NC	3.36	114.73	110.43
23	B	609	CLA	C4B-C3B-C2B	-3.36	103.13	107.30
23	a	405	CLA	C3B-C4B-NB	3.36	113.53	110.53
40	v	201	HEC	CBC-CAC-C3C	-3.35	120.73	127.43
29	a	414	PL9	C42-C43-C44	-3.35	119.95	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	CMB-C2B-C1B	3.35	130.52	125.42
23	b	609	CLA	CBC-CAC-C3C	-3.35	103.34	112.42
23	a	408	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
23	c	504	CLA	CMC-C2C-C1C	3.35	130.26	125.03
23	B	601	CLA	C3C-C4C-NC	3.35	114.72	110.43
23	A	408	CLA	C3B-C4B-NB	3.34	113.52	110.53
23	B	608	CLA	C3B-C4B-NB	3.34	113.51	110.53
23	B	603	CLA	O2A-CGA-CBA	3.34	122.02	111.83
23	B	609	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
23	d	404	CLA	C3C-C4C-NC	3.34	114.71	110.43
23	C	506	CLA	CMC-C2C-C1C	3.34	130.25	125.03
23	d	401	CLA	C1-C2-C3	-3.34	120.73	126.20
23	b	610	CLA	O2A-CGA-CBA	3.34	122.01	111.83
23	b	615	CLA	CMB-C2B-C1B	3.34	130.50	125.42
23	C	505	CLA	C4B-C3B-C2B	-3.33	103.16	107.30
29	a	414	PL9	C10-C9-C11	3.33	121.00	115.23
38	e	103	HEM	CHA-C4D-ND	3.32	128.48	124.37
23	D	404	CLA	O2A-CGA-CBA	3.32	121.97	111.83
23	b	603	CLA	CAA-C2A-C3A	-3.32	104.02	113.00
25	c	515	BCR	C38-C26-C25	-3.32	120.86	124.48
23	b	616	CLA	CHD-C4C-NC	3.32	129.38	124.23
34	c	522	HTG	C1-O5-C5	3.32	118.52	112.56
23	b	606	CLA	C4-C3-C5	3.32	120.99	115.23
23	b	613	CLA	CHD-C1D-ND	-3.32	120.13	124.80
23	b	612	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
33	c	520	LMG	C3-C4-C5	3.31	116.24	110.23
23	B	601	CLA	C3B-C4B-NB	3.31	113.49	110.53
23	B	603	CLA	C4-C3-C5	3.31	120.97	115.23
23	A	408	CLA	C4C-C3C-C2C	-3.31	102.08	106.89
23	b	610	CLA	C4C-C3C-C2C	-3.31	102.08	106.89
26	f	101	SQD	C1-O5-C5	3.31	120.18	113.72
26	a	412	SQD	O47-C7-C8	3.31	118.63	111.48
33	Z	102	LMG	C4-C3-C2	3.30	116.63	110.83
25	T	101	BCR	C15-C14-C13	3.30	131.91	127.28
23	B	605	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
23	c	507	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
23	D	404	CLA	CAC-C3C-C4C	3.30	129.08	124.79
31	A	416	LHG	O8-C23-O10	-3.30	115.38	123.63
23	b	609	CLA	C3C-C4C-NC	3.30	114.65	110.43
23	B	614	CLA	CAC-C3C-C4C	3.29	129.07	124.79
35	D	403	LMT	O1B-C4'-C3'	3.29	115.60	107.23
23	a	408	CLA	C4B-C3B-C2B	-3.29	103.21	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	O2A-CGA-O1A	-3.29	115.41	123.63
25	A	409	BCR	C15-C14-C13	-3.28	122.67	127.28
25	C	515	BCR	C33-C5-C6	-3.28	120.90	124.48
23	A	408	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
25	d	405	BCR	C16-C17-C18	-3.28	122.68	127.28
23	c	513	CLA	CAC-C3C-C4C	3.28	129.05	124.79
29	d	406	PL9	C20-C19-C21	3.28	120.91	115.23
23	c	509	CLA	C4C-C3C-C2C	-3.27	102.13	106.89
23	d	403	CLA	C1D-CHD-C4C	-3.27	119.07	126.02
23	A	406	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
35	M	101	LMT	O1'-C1'-C2'	3.27	113.23	108.27
23	B	607	CLA	O2D-CGD-O1D	-3.26	117.49	123.85
25	D	406	BCR	C3-C4-C5	-3.26	108.24	114.06
23	A	404	CLA	O2D-CGD-CBD	3.26	116.93	111.23
23	c	510	CLA	CBC-CAC-C3C	-3.26	103.58	112.42
29	A	414	PL9	C15-C14-C16	3.26	120.89	115.23
23	B	602	CLA	C3C-C4C-NC	3.26	114.60	110.43
23	D	405	CLA	CAA-C2A-C3A	-3.26	104.20	113.00
23	a	404	CLA	O2A-CGA-CBA	3.26	121.76	111.83
25	b	617	BCR	C16-C17-C18	-3.25	122.71	127.28
23	A	404	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
23	c	501	CLA	C1-C2-C3	-3.25	120.87	126.20
40	v	201	HEC	CHD-C4C-NC	3.25	127.99	124.45
23	c	513	CLA	CAA-C2A-C3A	-3.25	104.23	113.00
23	c	502	CLA	CHC-C1C-C2C	-3.24	117.73	126.95
29	A	414	PL9	C30-C29-C31	3.24	120.86	115.23
23	b	603	CLA	O2A-CGA-CBA	3.24	121.72	111.83
34	B	622	HTG	C1-O5-C5	3.24	118.37	112.56
23	B	614	CLA	C4A-NA-C1A	-3.24	105.20	106.68
23	A	408	CLA	CAA-C2A-C3A	-3.24	104.25	113.00
23	b	615	CLA	CHC-C1C-C2C	-3.24	117.75	126.95
26	a	410	SQD	O47-C7-O49	-3.23	116.14	123.70
23	c	510	CLA	C4-C3-C5	3.23	120.84	115.23
23	b	602	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
23	b	605	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
24	D	401	PHO	O1D-CGD-CBD	-3.23	119.82	124.72
23	D	405	CLA	CMC-C2C-C1C	3.23	130.08	125.03
23	B	608	CLA	O2A-CGA-CBA	3.23	121.68	111.83
23	b	616	CLA	O2A-CGA-CBA	3.23	121.68	111.83
23	a	405	CLA	CHD-C4C-NC	3.23	129.24	124.23
29	D	407	PL9	C12-C13-C14	-3.23	120.24	127.62
23	C	509	CLA	C4B-C3B-C2B	-3.22	103.29	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	CMB-C2B-C1B	3.22	130.33	125.42
23	b	604	CLA	O2A-CGA-CBA	3.22	121.67	111.83
23	c	512	CLA	C3B-C4B-NB	3.22	113.41	110.53
26	B	620	SQD	O48-C23-C24	3.22	121.65	111.83
25	D	406	BCR	C28-C27-C26	-3.22	108.32	114.06
23	c	502	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
29	a	414	PL9	C30-C29-C31	3.22	120.81	115.23
23	b	603	CLA	CMB-C2B-C1B	3.21	130.31	125.42
23	B	610	CLA	C1C-C2C-C3C	-3.21	103.61	106.98
23	c	502	CLA	CBC-CAC-C3C	-3.21	103.73	112.42
23	C	512	CLA	C4-C3-C5	3.20	120.79	115.23
25	B	618	BCR	C37-C22-C21	-3.20	117.63	122.82
23	D	405	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
40	v	201	HEC	CHA-C1A-NA	3.20	127.94	124.45
38	e	103	HEM	CAD-CBD-CGD	3.20	122.15	113.67
23	B	604	CLA	CHD-C1D-ND	-3.20	120.30	124.80
23	C	510	CLA	CAC-C3C-C4C	3.20	128.95	124.79
23	C	504	CLA	CHC-C1C-C2C	-3.20	117.86	126.95
23	b	612	CLA	O2A-CGA-CBA	3.20	121.58	111.83
23	B	603	CLA	CMB-C2B-C1B	3.20	130.28	125.42
23	a	404	CLA	O2A-CGA-O1A	-3.19	115.64	123.63
29	A	414	PL9	C20-C19-C21	3.19	120.77	115.23
23	c	501	CLA	CMB-C2B-C1B	3.19	130.28	125.42
33	b	620	LMG	O8-C28-C29	3.19	121.56	111.83
23	b	608	CLA	CHD-C4C-NC	3.19	129.18	124.23
23	b	613	CLA	O2A-CGA-O1A	-3.19	115.65	123.63
23	c	509	CLA	CAC-C3C-C4C	3.19	128.94	124.79
23	b	616	CLA	C2C-C1C-NC	3.19	113.33	109.98
23	b	612	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	C	509	CLA	C4A-NA-C1A	-3.18	105.23	106.68
23	b	606	CLA	C1C-C2C-C3C	-3.18	103.64	106.98
23	b	606	CLA	C3B-C4B-NB	3.18	113.37	110.53
29	D	407	PL9	C22-C23-C24	-3.18	120.35	127.62
38	e	103	HEM	CHD-C1D-ND	3.18	127.84	124.42
23	C	509	CLA	O2A-CGA-O1A	-3.18	115.68	123.63
23	B	609	CLA	CHD-C4C-NC	3.18	129.16	124.23
23	C	509	CLA	CAC-C3C-C4C	3.18	128.92	124.79
25	T	101	BCR	C12-C13-C14	-3.18	114.01	119.01
23	C	502	CLA	CHC-C1C-C2C	-3.18	117.92	126.95
23	C	508	CLA	C4C-C3C-C2C	-3.18	102.27	106.89
23	c	510	CLA	CHD-C4C-NC	3.17	129.15	124.23
23	C	504	CLA	C3C-C4C-NC	3.17	114.50	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C3B-C4B-NB	3.17	113.36	110.53
23	c	503	CLA	CMB-C2B-C1B	3.17	130.25	125.42
23	B	616	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
23	A	406	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
23	c	512	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
23	b	612	CLA	C4-C3-C5	3.17	120.72	115.23
23	d	401	CLA	C4B-C3B-C2B	-3.17	103.37	107.30
23	b	604	CLA	CMC-C2C-C1C	3.17	129.98	125.03
23	b	607	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
23	b	616	CLA	CMB-C2B-C1B	3.16	130.24	125.42
25	c	515	BCR	C15-C14-C13	-3.16	122.84	127.28
31	A	416	LHG	O7-C7-C8	3.16	118.32	111.48
23	b	614	CLA	C1C-C2C-C3C	-3.16	103.66	106.98
23	B	609	CLA	C1-C2-C3	-3.16	121.03	126.20
23	C	506	CLA	C4C-C3C-C2C	-3.15	102.30	106.89
23	b	607	CLA	C1-O2A-CGA	3.15	124.28	116.65
23	c	505	CLA	C1C-C2C-C3C	-3.15	103.66	106.98
23	b	608	CLA	CMC-C2C-C1C	3.15	129.96	125.03
23	B	602	CLA	CHC-C1C-C2C	-3.15	118.00	126.95
23	d	404	CLA	CAC-C3C-C4C	3.15	128.89	124.79
23	c	511	CLA	CHD-C4C-NC	3.15	129.11	124.23
26	A	410	SQD	O48-C23-C24	3.14	121.42	111.83
23	B	603	CLA	C3C-C4C-NC	3.14	114.46	110.43
23	D	404	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
23	b	614	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
23	c	511	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
23	C	509	CLA	CHC-C1C-C2C	-3.14	118.03	126.95
23	C	511	CLA	O2A-CGA-CBA	3.14	121.40	111.83
23	B	615	CLA	C3B-C4B-NB	3.14	113.33	110.53
23	a	404	CLA	CHC-C1C-C2C	-3.14	118.03	126.95
23	b	605	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
23	A	404	CLA	C3C-C4C-NC	3.13	114.45	110.43
23	B	605	CLA	CHD-C4C-NC	3.13	129.09	124.23
23	B	613	CLA	O2A-CGA-CBA	3.13	121.39	111.83
23	B	613	CLA	C4-C3-C5	3.13	120.66	115.23
33	b	620	LMG	O7-C10-C11	3.13	118.25	111.48
23	C	511	CLA	CBC-CAC-C3C	-3.13	103.94	112.42
23	c	506	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
31	e	101	LHG	O7-C7-C8	3.13	118.25	111.48
23	B	601	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
23	c	508	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
23	B	609	CLA	O2A-CGA-CBA	3.12	121.36	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	V	202	HEC	CHA-C1A-NA	3.12	127.85	124.45
25	k	101	BCR	C15-C14-C13	-3.12	122.90	127.28
23	c	510	CLA	CHC-C1C-C2C	-3.12	118.07	126.95
24	a	407	PHO	CMA-C3A-C4A	-3.12	107.88	114.61
23	b	606	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
23	b	611	CLA	CHC-C1C-C2C	-3.12	118.08	126.95
23	b	611	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
25	T	101	BCR	C11-C10-C9	-3.12	122.91	127.28
23	D	404	CLA	C1D-CHD-C4C	-3.12	119.39	126.02
23	a	408	CLA	O2A-CGA-CBA	3.12	121.34	111.83
24	a	406	PHO	CMA-C3A-C4A	-3.11	107.90	114.61
23	B	616	CLA	CHD-C4C-NC	3.11	129.05	124.23
33	C	520	LMG	O8-C28-C29	3.11	121.32	111.83
23	b	611	CLA	CAC-C3C-C4C	3.11	128.84	124.79
23	c	507	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
23	a	408	CLA	CAC-C3C-C4C	3.11	128.83	124.79
33	C	520	LMG	O7-C10-C11	3.11	118.20	111.48
25	C	516	BCR	C33-C5-C6	-3.11	121.09	124.48
23	B	611	CLA	CHD-C4C-NC	3.11	129.05	124.23
29	d	406	PL9	C25-C24-C26	3.10	120.62	115.23
26	a	412	SQD	C3-C4-C5	3.10	115.86	110.23
25	C	516	BCR	C15-C14-C13	-3.10	122.92	127.28
23	D	404	CLA	CHC-C1C-C2C	-3.10	118.13	126.95
23	B	612	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
33	B	621	LMG	O8-C28-C29	3.10	121.29	111.83
23	C	506	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
34	b	622	HTG	O5-C1-C2	3.10	114.59	110.32
23	B	603	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
23	b	607	CLA	CAC-C3C-C4C	3.10	128.82	124.79
25	c	515	BCR	C2-C1-C6	3.10	114.94	110.44
23	B	606	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
23	b	610	CLA	C4-C3-C5	3.09	120.59	115.23
24	a	407	PHO	C4-C3-C5	3.09	120.59	115.23
26	a	412	SQD	O48-C23-C24	3.09	121.26	111.83
31	E	101	LHG	O8-C23-C24	3.09	121.25	111.83
23	b	602	CLA	C3B-C4B-NB	3.09	113.29	110.53
31	l	101	LHG	O8-C23-C24	3.09	121.25	111.83
25	B	618	BCR	C3-C4-C5	-3.09	108.55	114.06
23	d	404	CLA	CHD-C4C-NC	3.09	129.02	124.23
23	b	605	CLA	CHD-C4C-NC	3.09	129.02	124.23
23	b	609	CLA	C3B-C4B-NB	3.09	113.28	110.53
23	c	502	CLA	CMB-C2B-C1B	3.08	130.12	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
23	A	406	CLA	O2A-CGA-CBA	3.08	121.24	111.83
23	C	504	CLA	C3B-C4B-NB	3.08	113.28	110.53
23	B	614	CLA	O2A-CGA-CBA	3.08	121.23	111.83
23	b	607	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
23	c	513	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	b	612	CLA	C3B-C4B-NB	3.08	113.28	110.53
23	C	507	CLA	C4-C3-C5	3.08	120.57	115.23
26	B	620	SQD	O7-S-C6	3.07	111.34	106.76
23	b	603	CLA	C3B-C4B-NB	3.07	113.27	110.53
23	c	502	CLA	O2A-CGA-CBA	3.07	121.20	111.83
23	B	615	CLA	CHD-C4C-NC	3.07	128.99	124.23
23	B	614	CLA	CBC-CAC-C3C	-3.07	104.10	112.42
23	b	614	CLA	O2A-CGA-CBA	3.07	121.18	111.83
23	c	505	CLA	CMC-C2C-C1C	3.07	129.82	125.03
25	b	619	BCR	C15-C14-C13	-3.06	122.98	127.28
33	c	520	LMG	O8-C28-C29	3.06	121.17	111.83
23	c	511	CLA	CAC-C3C-C4C	3.06	128.78	124.79
23	d	401	CLA	CHC-C1C-C2C	-3.06	118.25	126.95
23	B	604	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	b	605	CLA	O2A-CGA-O1A	-3.06	115.98	123.63
35	I	101	LMT	O1B-C4'-C3'	3.06	115.00	107.23
23	b	612	CLA	CAC-C3C-C4C	3.06	128.77	124.79
26	a	410	SQD	O8-S-C6	3.06	111.87	105.97
25	t	101	BCR	C7-C6-C5	-3.06	114.52	121.56
25	a	409	BCR	C11-C10-C9	-3.05	122.99	127.28
23	b	607	CLA	CBC-CAC-C3C	-3.05	104.14	112.42
23	c	502	CLA	C1-C2-C3	-3.05	121.19	126.20
25	y	101	BCR	C21-C20-C19	-3.05	114.35	123.20
23	b	606	CLA	CHD-C4C-NC	3.05	128.97	124.23
23	d	404	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
25	Y	101	BCR	C16-C17-C18	-3.05	123.00	127.28
23	b	603	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
23	C	510	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
23	d	403	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
23	C	513	CLA	O2A-CGA-CBA	3.05	121.12	111.83
23	B	602	CLA	CMB-C2B-C1B	3.05	130.06	125.42
26	L	101	SQD	O48-C23-C24	3.04	121.12	111.83
23	d	401	CLA	C3C-C4C-NC	3.04	114.33	110.43
31	d	409	LHG	O8-C23-C24	3.04	121.12	111.83
23	b	611	CLA	O2A-CGA-CBA	3.04	121.11	111.83
23	B	602	CLA	CAA-C2A-C3A	-3.04	104.78	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
23	b	616	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
25	D	406	BCR	C16-C17-C18	-3.04	123.02	127.28
29	d	406	PL9	C40-C39-C41	3.04	120.50	115.23
23	C	510	CLA	C3B-C4B-NB	3.04	113.24	110.53
23	C	512	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
23	B	604	CLA	C4C-C3C-C2C	-3.03	102.47	106.89
25	t	101	BCR	C35-C13-C12	3.03	122.72	118.09
23	B	611	CLA	CMC-C2C-C1C	3.03	129.77	125.03
23	B	616	CLA	C3B-C4B-NB	3.03	113.24	110.53
23	B	609	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
23	c	506	CLA	CAC-C3C-C4C	3.03	128.73	124.79
24	A	407	PHO	C4D-CHA-CBD	3.03	109.91	108.45
23	B	616	CLA	CMB-C2B-C1B	3.03	130.03	125.42
23	B	601	CLA	O2A-CGA-CBA	3.03	121.06	111.83
23	a	408	CLA	O2A-CGA-O1A	-3.02	116.06	123.63
23	a	408	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
23	c	511	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
23	b	611	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
23	b	604	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
23	C	505	CLA	CMC-C2C-C1C	3.02	129.75	125.03
25	d	405	BCR	C37-C22-C23	3.02	122.70	118.09
23	a	405	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
23	b	607	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
23	C	507	CLA	C3B-C4B-NB	3.02	113.22	110.53
23	B	606	CLA	C4-C3-C5	3.02	120.46	115.23
33	z	101	LMG	O8-C28-C29	3.02	121.03	111.83
23	c	503	CLA	CMC-C2C-C1C	3.01	129.75	125.03
23	b	603	CLA	CHD-C4C-NC	3.01	128.91	124.23
23	b	603	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
23	C	507	CLA	C3C-C4C-NC	3.01	114.28	110.43
23	b	605	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
23	c	505	CLA	CAC-C3C-C4C	3.01	128.70	124.79
23	c	513	CLA	C3B-C4B-NB	3.01	113.21	110.53
23	B	605	CLA	C4C-C3C-C2C	-3.01	102.52	106.89
36	h	102	DGD	O1G-C1A-C2A	3.01	121.00	111.83
36	C	519	DGD	O1G-C1A-C2A	3.00	121.00	111.83
34	b	623	HTG	O5-C1-C2	3.00	114.46	110.32
23	c	509	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
23	c	512	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	B	613	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
25	c	514	BCR	C24-C23-C22	-3.00	121.80	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
23	c	507	CLA	C1-C2-C3	-3.00	121.29	126.20
25	H	101	BCR	C3-C4-C5	-2.99	108.72	114.06
23	C	514	CLA	C2A-C1A-CHA	-2.99	118.67	123.87
25	A	409	BCR	C38-C26-C25	-2.99	121.22	124.48
24	a	406	PHO	C1-C2-C3	-2.99	121.30	126.20
23	C	507	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
23	B	601	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
29	d	406	PL9	C22-C23-C24	-2.99	120.79	127.62
23	c	501	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
23	c	503	CLA	C1-C2-C3	-2.99	121.31	126.20
23	C	511	CLA	C3C-C4C-NC	2.99	114.25	110.43
29	A	414	PL9	C42-C43-C44	-2.98	120.79	127.62
23	C	514	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
23	b	616	CLA	C4-C3-C5	2.98	120.41	115.23
23	b	607	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
23	D	405	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
33	J	101	LMG	O8-C28-C29	2.98	120.93	111.83
23	b	613	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
23	C	512	CLA	CHD-C4C-NC	2.98	128.85	124.23
25	B	618	BCR	C38-C26-C25	-2.98	121.23	124.48
23	C	511	CLA	C3B-C4B-NB	2.98	113.19	110.53
23	A	404	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
31	A	417	LHG	O8-C23-C24	2.98	120.92	111.83
26	L	101	SQD	C3-C4-C5	2.98	115.63	110.23
23	c	501	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
23	c	503	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
23	c	506	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
25	A	409	BCR	C11-C10-C9	-2.97	123.11	127.28
23	B	614	CLA	CHD-C4C-NC	2.97	128.84	124.23
23	c	505	CLA	C3B-C4B-NB	2.97	113.18	110.53
23	c	513	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
23	B	601	CLA	CHD-C4C-NC	2.97	128.83	124.23
24	a	406	PHO	O2A-CGA-CBA	2.97	120.88	111.83
36	c	516	DGD	C2G-O2G-C1B	-2.97	110.69	117.80
23	b	608	CLA	C3B-C4B-NB	2.97	113.18	110.53
23	D	404	CLA	O2A-CGA-O1A	-2.97	116.21	123.63
25	B	619	BCR	C24-C23-C22	-2.97	121.85	126.23
26	A	412	SQD	O47-C7-C8	2.97	117.90	111.48
25	c	515	BCR	C21-C20-C19	-2.96	114.61	123.20
23	c	512	CLA	CHC-C1C-C2C	-2.96	118.53	126.95
23	b	601	CLA	C4C-C3C-C2C	-2.96	102.58	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
23	d	404	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
23	C	502	CLA	CAC-C3C-C4C	2.96	128.64	124.79
23	C	504	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	C	513	CLA	CBC-CAC-C3C	-2.96	104.40	112.42
23	b	613	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
23	d	403	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
23	a	408	CLA	CMA-C3A-C2A	-2.96	102.55	113.98
25	t	101	BCR	C1-C6-C7	2.96	123.67	115.65
23	C	505	CLA	C1-O2A-CGA	2.95	123.80	116.65
23	A	405	CLA	CAA-C2A-C3A	-2.95	105.02	113.00
23	B	612	CLA	CAC-C3C-C4C	2.95	128.63	124.79
24	a	407	PHO	C1A-C2A-C3A	-2.95	100.03	102.84
26	D	413	SQD	O7-S-C6	2.95	111.16	106.76
26	a	412	SQD	C1-O5-C5	2.95	119.48	113.72
23	B	606	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
23	b	616	CLA	CAC-C3C-C4C	2.95	128.63	124.79
23	B	601	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
23	c	504	CLA	CMB-C2B-C1B	2.94	129.90	125.42
25	c	514	BCR	C38-C26-C25	-2.94	121.28	124.48
23	c	513	CLA	C4-C3-C5	2.94	120.33	115.23
23	c	509	CLA	C1-O2A-CGA	2.94	123.77	116.65
23	c	510	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
23	C	511	CLA	CMB-C2B-C1B	2.94	129.89	125.42
23	B	606	CLA	CHD-C4C-NC	2.94	128.79	124.23
23	b	601	CLA	C4-C3-C5	2.94	120.33	115.23
23	B	612	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
23	c	505	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
23	C	507	CLA	C4B-C3B-C2B	-2.93	103.65	107.30
23	b	613	CLA	C1-C2-C3	-2.93	121.39	126.20
33	j	101	LMG	C8-O7-C10	-2.93	110.79	117.80
23	b	610	CLA	CAC-C3C-C4C	2.93	128.60	124.79
23	b	602	CLA	CMC-C2C-C1C	2.93	129.61	125.03
26	B	620	SQD	C3-C4-C5	2.93	115.54	110.23
23	c	503	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
23	C	511	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
23	b	602	CLA	CHD-C4C-NC	2.92	128.76	124.23
23	c	503	CLA	O2A-CGA-CBA	2.92	120.75	111.83
25	k	101	BCR	C2-C1-C6	2.92	114.69	110.44
23	D	405	CLA	C3B-C4B-NB	2.92	113.14	110.53
23	B	615	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
23	c	508	CLA	C4B-C3B-C2B	-2.92	103.67	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	O2A-CGA-CBA	2.92	120.73	111.83
23	A	406	CLA	CHD-C4C-NC	2.92	128.75	124.23
23	a	408	CLA	CMB-C2B-C1B	2.92	129.86	125.42
23	A	404	CLA	CAA-CBA-CGA	-2.92	104.93	113.21
23	C	502	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
23	C	513	CLA	CHD-C4C-NC	2.91	128.75	124.23
25	t	101	BCR	C7-C8-C9	-2.91	121.93	126.23
23	C	514	CLA	CAC-C3C-C4C	2.91	128.58	124.79
23	B	615	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
31	D	408	LHG	O7-C7-C8	2.91	117.78	111.48
23	c	506	CLA	C4-C3-C5	2.91	120.28	115.23
23	A	408	CLA	CMA-C3A-C2A	-2.91	102.74	113.98
23	b	615	CLA	C4-C3-C5	2.90	120.27	115.23
23	B	616	CLA	O2A-CGA-CBA	2.90	120.69	111.83
23	c	504	CLA	C1-C2-C3	-2.90	121.44	126.20
23	A	406	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
23	d	403	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
23	C	514	CLA	CHD-C4C-NC	2.90	128.73	124.23
23	C	506	CLA	C4B-C3B-C2B	-2.90	103.69	107.30
23	a	404	CLA	C4B-C3B-C2B	-2.90	103.69	107.30
31	d	409	LHG	O8-C23-O10	-2.90	116.37	123.63
23	a	405	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
23	B	613	CLA	O2D-CGD-CBD	2.90	116.29	111.23
23	c	511	CLA	C4B-C3B-C2B	-2.89	103.70	107.30
25	K	102	BCR	C3-C4-C5	-2.89	108.90	114.06
29	a	414	PL9	C20-C19-C21	2.89	120.25	115.23
35	D	402	LMT	O1'-C1'-C2'	2.89	112.66	108.27
36	h	102	DGD	O2G-C1B-C2B	2.89	117.73	111.48
23	c	509	CLA	O2A-CGA-CBA	2.89	120.64	111.83
25	t	101	BCR	C19-C18-C17	-2.89	114.47	119.01
23	C	504	CLA	C1-C2-C3	-2.89	121.47	126.20
25	Y	101	BCR	C16-C15-C14	-2.89	117.61	123.52
23	C	503	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
23	D	405	CLA	CBC-CAC-C3C	-2.89	104.60	112.42
23	B	610	CLA	C3B-C4B-NB	2.88	113.11	110.53
23	C	514	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
29	A	414	PL9	C10-C9-C11	2.88	120.23	115.23
23	c	506	CLA	CGD-CBD-CAD	-2.88	101.51	110.85
23	C	506	CLA	CMB-C2B-C1B	2.88	129.81	125.42
23	a	405	CLA	C1-C2-C3	-2.88	121.47	126.20
23	b	610	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
25	c	515	BCR	C16-C17-C18	-2.88	123.24	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CAC-C3C-C4C	2.88	128.54	124.79
23	B	601	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
23	b	612	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
31	D	409	LHG	O8-C23-C24	2.88	120.61	111.83
23	B	605	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
25	Y	101	BCR	C38-C26-C25	-2.88	121.34	124.48
23	b	604	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
26	D	413	SQD	O47-C7-O49	-2.87	116.99	123.70
23	B	607	CLA	C3B-C4B-NB	2.87	113.09	110.53
23	c	504	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
23	A	406	CLA	CAA-C2A-C3A	-2.87	105.24	113.00
23	b	614	CLA	O2A-CGA-O1A	-2.87	116.45	123.63
23	C	510	CLA	CHD-C4C-NC	2.87	128.68	124.23
24	D	401	PHO	CMA-C3A-C4A	-2.87	108.43	114.61
25	a	409	BCR	C15-C14-C13	-2.87	123.26	127.28
23	b	601	CLA	CHD-C4C-NC	2.86	128.67	124.23
23	b	615	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
23	c	507	CLA	CAC-C3C-C4C	2.86	128.51	124.79
33	c	519	LMG	O8-C28-C29	2.86	120.56	111.83
34	b	625	HTG	O5-C5-C4	2.86	114.86	109.70
23	C	511	CLA	CAC-C3C-C4C	2.86	128.51	124.79
23	C	503	CLA	C3B-C4B-NB	2.86	113.08	110.53
23	B	615	CLA	CMC-C2C-C1C	2.86	129.50	125.03
23	B	614	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
23	b	603	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
23	B	610	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
23	d	404	CLA	CMB-C2B-C1B	2.86	129.77	125.42
36	C	518	DGD	O1G-C1A-C2A	2.85	120.54	111.83
23	C	513	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
40	V	202	HEC	CBC-CAC-C3C	-2.85	121.74	127.43
26	a	410	SQD	C44-O6-C1	-2.85	107.69	113.80
23	C	508	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
23	A	404	CLA	C2A-C1A-CHA	-2.85	118.92	123.87
23	C	513	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
26	A	410	SQD	O7-S-C6	2.85	111.01	106.76
23	B	610	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
23	B	603	CLA	CAC-C3C-C4C	2.85	128.49	124.79
23	B	614	CLA	C1-C2-C3	-2.85	121.53	126.20
23	c	512	CLA	O2A-CGA-CBA	2.85	120.51	111.83
25	y	101	BCR	C15-C14-C13	-2.85	123.29	127.28
23	C	507	CLA	O2A-CGA-CBA	2.84	120.51	111.83
23	B	608	CLA	C4B-C3B-C2B	-2.84	103.77	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	C4-C3-C5	2.84	120.17	115.23
23	C	506	CLA	C1-C2-C3	-2.84	121.54	126.20
29	d	406	PL9	C35-C34-C36	2.84	120.16	115.23
25	B	617	BCR	C38-C26-C25	-2.84	121.38	124.48
23	B	603	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
23	b	615	CLA	CHD-C4C-NC	2.84	128.63	124.23
23	b	603	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
23	B	602	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
23	B	607	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
23	b	614	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
25	d	405	BCR	C40-C30-C25	-2.84	105.79	110.24
25	b	618	BCR	C38-C26-C25	-2.84	121.39	124.48
23	b	606	CLA	C1-C2-C3	-2.84	121.55	126.20
23	B	612	CLA	CHD-C1D-ND	-2.83	120.81	124.80
23	a	405	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
23	C	503	CLA	C1-C2-C3	-2.83	121.55	126.20
23	c	503	CLA	CHD-C4C-NC	2.83	128.62	124.23
23	b	611	CLA	CBC-CAC-C3C	-2.83	104.74	112.42
29	D	407	PL9	C7-C8-C9	-2.83	121.95	126.83
25	a	409	BCR	C20-C21-C22	-2.83	123.31	127.28
23	b	611	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
29	D	407	PL9	C40-C39-C41	2.83	120.14	115.23
23	a	405	CLA	CAA-C2A-C3A	-2.83	105.35	113.00
23	b	609	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
23	B	604	CLA	CMC-C2C-C1C	2.83	129.45	125.03
25	b	619	BCR	C10-C11-C12	-2.83	115.01	123.20
23	b	606	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
29	A	414	PL9	C12-C13-C14	-2.83	121.16	127.62
31	d	408	LHG	O7-C7-C8	2.83	117.59	111.48
23	b	610	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
23	b	614	CLA	CMC-C2C-C1C	2.82	129.45	125.03
29	D	407	PL9	C27-C28-C29	-2.82	121.16	127.62
23	b	608	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
23	b	602	CLA	C1-C2-C3	-2.82	121.57	126.20
23	B	604	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
23	B	606	CLA	C4B-C3B-C2B	-2.82	103.79	107.30
23	C	506	CLA	C3B-C4B-NB	2.82	113.05	110.53
25	b	619	BCR	C24-C23-C22	-2.82	122.06	126.23
23	c	511	CLA	CAA-CBA-CGA	-2.82	105.20	113.21
23	c	501	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
23	b	613	CLA	C4-C3-C5	2.82	120.12	115.23
23	C	506	CLA	O2A-CGA-CBA	2.82	120.42	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
25	B	619	BCR	C38-C26-C25	-2.81	121.42	124.48
26	f	101	SQD	O7-S-C6	2.81	110.95	106.76
23	B	602	CLA	CAC-C3C-C4C	2.81	128.45	124.79
25	C	515	BCR	C23-C24-C25	-2.81	119.49	127.00
23	c	510	CLA	C3C-C4C-NC	2.81	114.03	110.43
24	a	406	PHO	C4A-C3A-C2A	-2.81	100.17	102.84
23	B	603	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
23	C	507	CLA	C2A-C1A-CHA	-2.81	119.00	123.87
23	c	509	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
33	b	620	LMG	O6-C5-C4	2.81	114.76	109.70
25	B	619	BCR	C15-C14-C13	-2.81	123.34	127.28
25	d	405	BCR	C21-C20-C19	-2.80	115.08	123.20
25	B	619	BCR	C21-C20-C19	-2.80	115.08	123.20
23	B	609	CLA	C3B-C4B-NB	2.80	113.03	110.53
23	c	513	CLA	O2A-CGA-CBA	2.80	120.38	111.83
23	b	613	CLA	CHD-C4C-NC	2.80	128.57	124.23
23	d	404	CLA	O2A-CGA-CBA	2.80	120.37	111.83
23	B	603	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
25	K	102	BCR	C2-C1-C6	2.80	114.50	110.44
34	B	624	HTG	O5-C1-C2	2.80	114.17	110.32
23	B	612	CLA	O2A-CGA-CBA	2.80	120.37	111.83
23	A	405	CLA	CBC-CAC-C3C	-2.80	104.84	112.42
23	b	613	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
23	c	504	CLA	O2A-CGA-CBA	2.80	120.36	111.83
23	C	514	CLA	C3B-C4B-NB	2.80	113.03	110.53
23	C	503	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
23	A	408	CLA	C4B-C3B-C2B	-2.80	103.83	107.30
23	B	605	CLA	C2A-C1A-CHA	-2.80	119.02	123.87
29	D	407	PL9	C10-C9-C11	2.80	120.08	115.23
23	B	613	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
23	B	615	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
23	C	502	CLA	CHD-C4C-NC	2.79	128.56	124.23
23	C	504	CLA	CMB-C2B-C1B	2.79	129.67	125.42
40	V	202	HEC	CHA-C4D-ND	2.79	128.92	123.86
25	D	406	BCR	C29-C30-C25	2.79	114.49	110.44
25	d	405	BCR	C16-C15-C14	-2.79	117.81	123.52
23	c	501	CLA	C4-C3-C5	2.78	120.06	115.23
23	A	405	CLA	C2A-C1A-CHA	-2.78	119.04	123.87
23	c	511	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
25	Y	101	BCR	C10-C11-C12	-2.78	115.14	123.20
23	B	604	CLA	O2A-CGA-CBA	2.78	120.31	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
23	b	602	CLA	CAC-C3C-C4C	2.78	128.40	124.79
23	C	505	CLA	CHC-C1C-C2C	-2.78	119.06	126.95
23	c	504	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
35	B	630	LMT	O5'-C5'-C4'	2.78	115.46	109.72
26	a	410	SQD	O9-S-C6	2.78	110.90	106.76
23	c	506	CLA	O2A-CGA-CBA	2.77	120.29	111.83
26	D	413	SQD	C3-C4-C5	2.77	115.26	110.23
23	C	511	CLA	CHD-C4C-NC	2.77	128.53	124.23
23	B	615	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
33	b	620	LMG	C7-O1-C1	-2.77	107.85	113.80
23	c	501	CLA	O2A-CGA-CBA	2.77	120.29	111.83
23	c	505	CLA	CHD-C4C-NC	2.77	128.53	124.23
23	C	512	CLA	O2A-CGA-CBA	2.77	120.29	111.83
23	C	514	CLA	CMC-C2C-C1C	2.77	129.37	125.03
26	D	413	SQD	C44-O6-C1	-2.77	107.85	113.80
23	c	510	CLA	O2A-CGA-CBA	2.77	120.28	111.83
25	D	406	BCR	C33-C5-C6	-2.77	121.46	124.48
23	b	609	CLA	CMC-C2C-C1C	2.77	129.36	125.03
25	B	617	BCR	C11-C10-C9	-2.77	123.39	127.28
25	b	617	BCR	C15-C14-C13	-2.77	123.40	127.28
23	c	507	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
23	b	609	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
34	b	628	HTG	O5-C5-C4	2.77	114.69	109.70
23	C	506	CLA	CHD-C4C-NC	2.77	128.52	124.23
23	D	405	CLA	C4B-C3B-C2B	-2.76	103.86	107.30
23	c	511	CLA	CHC-C1C-C2C	-2.76	119.09	126.95
23	B	611	CLA	C2A-C1A-CHA	-2.76	119.07	123.87
23	c	508	CLA	O2A-CGA-CBA	2.76	120.25	111.83
23	C	504	CLA	O2A-CGA-CBA	2.76	120.25	111.83
23	c	512	CLA	CHD-C4C-NC	2.76	128.51	124.23
33	Z	102	LMG	O6-C5-C4	2.76	114.67	109.70
23	b	614	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
23	B	613	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
29	A	414	PL9	C17-C18-C19	-2.76	121.32	127.62
23	c	511	CLA	CMB-C2B-C1B	2.76	129.62	125.42
23	B	607	CLA	C4C-C3C-C2C	-2.75	102.88	106.89
23	b	601	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
23	C	508	CLA	C4-C3-C5	2.75	120.01	115.23
23	B	610	CLA	CHD-C4C-NC	2.75	128.50	124.23
24	A	407	PHO	C6-C5-C3	-2.75	106.76	113.47
23	b	612	CLA	C2A-C1A-CHA	-2.75	119.09	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	CLA	C2A-C1A-CHA	-2.75	119.09	123.87
23	a	408	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
23	C	512	CLA	CMB-C2B-C1B	2.75	129.61	125.42
25	A	409	BCR	C20-C21-C22	-2.75	123.42	127.28
23	a	405	CLA	CMB-C2B-C1B	2.75	129.60	125.42
23	B	613	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
23	c	509	CLA	CHC-C1C-C2C	-2.75	119.14	126.95
25	h	101	BCR	C10-C11-C12	-2.75	115.24	123.20
23	d	401	CLA	CMA-C3A-C2A	-2.75	103.36	113.98
23	C	503	CLA	CHD-C4C-NC	2.75	128.49	124.23
23	c	502	CLA	CHD-C4C-NC	2.75	128.49	124.23
23	c	505	CLA	C1-C2-C3	-2.75	121.70	126.20
23	b	613	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
25	k	101	BCR	C3-C4-C5	-2.75	109.16	114.06
34	C	521	HTG	C1-O5-C5	2.74	117.48	112.56
23	A	404	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
23	A	408	CLA	CHD-C4C-NC	2.74	128.49	124.23
23	C	508	CLA	C1-C2-C3	-2.74	121.70	126.20
23	D	404	CLA	CMB-C2B-C1B	2.74	129.59	125.42
31	e	101	LHG	O8-C23-C24	2.74	120.20	111.83
23	a	405	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
25	b	619	BCR	C2-C1-C6	2.74	114.42	110.44
23	b	602	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
23	c	504	CLA	CHD-C4C-NC	2.73	128.47	124.23
23	c	510	CLA	CMC-C2C-C1C	2.73	129.31	125.03
26	D	413	SQD	C1-C2-C3	-2.73	104.26	110.01
25	C	515	BCR	C7-C8-C9	-2.73	122.19	126.23
23	B	607	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
25	c	515	BCR	C33-C5-C6	-2.73	121.50	124.48
23	b	604	CLA	CAC-C3C-C4C	2.73	128.34	124.79
23	a	404	CLA	CAA-C2A-C1A	-2.73	103.03	111.97
23	C	505	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
23	B	607	CLA	CBC-CAC-C3C	-2.73	105.02	112.42
25	A	409	BCR	C8-C7-C6	-2.73	119.70	127.00
40	V	202	HEC	CHD-C4C-NC	2.73	127.42	124.45
23	c	506	CLA	CHD-C4C-NC	2.73	128.46	124.23
26	f	101	SQD	O48-C23-C24	2.73	120.15	111.83
33	Z	101	LMG	O8-C28-C29	2.72	120.14	111.83
23	d	404	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
23	C	509	CLA	O2A-CGA-CBA	2.72	120.14	111.83
23	B	604	CLA	C4-C3-C5	2.72	119.95	115.23
23	c	503	CLA	C4-C3-C5	2.72	119.95	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CHC-C1C-C2C	-2.72	119.21	126.95
23	c	508	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
25	b	618	BCR	C29-C30-C25	2.72	114.39	110.44
23	b	614	CLA	CMB-C2B-C1B	2.72	129.56	125.42
23	A	408	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
23	D	404	CLA	CMC-C2C-C1C	2.72	129.28	125.03
23	B	612	CLA	C4-C3-C5	2.72	119.95	115.23
23	B	604	CLA	C1-O2A-CGA	2.72	123.23	116.65
25	k	101	BCR	C20-C21-C22	-2.72	123.47	127.28
23	C	510	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
23	C	512	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
29	D	407	PL9	C7-C3-C4	2.72	119.15	116.91
23	B	606	CLA	C3B-C4B-NB	2.72	112.95	110.53
31	E	101	LHG	C5-O7-C7	-2.72	111.30	117.80
23	C	508	CLA	CAC-C3C-C4C	2.72	128.32	124.79
23	D	404	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
23	b	605	CLA	C2A-C1A-CHA	-2.72	119.16	123.87
24	a	406	PHO	O2D-CGD-O1D	-2.71	118.56	123.85
23	D	404	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
23	B	608	CLA	C4C-C3C-C2C	-2.71	102.94	106.89
23	c	503	CLA	C3B-C4B-NB	2.71	112.95	110.53
23	B	616	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
23	A	406	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
23	b	604	CLA	C3B-C4B-NB	2.71	112.95	110.53
25	a	409	BCR	C37-C22-C23	2.71	122.23	118.09
23	b	612	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
23	C	513	CLA	C3B-C4B-NB	2.71	112.95	110.53
23	b	602	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
24	D	401	PHO	CMB-C2B-C3B	2.71	130.09	124.68
25	d	405	BCR	C39-C30-C25	-2.71	106.00	110.24
23	B	614	CLA	C4B-C3B-C2B	-2.71	103.94	107.30
25	B	618	BCR	C37-C22-C23	2.71	122.22	118.09
23	c	506	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
23	B	612	CLA	CMC-C2C-C1C	2.71	129.26	125.03
23	c	504	CLA	CED-O2D-CGD	2.71	122.06	115.92
23	B	608	CLA	CHC-C1C-C2C	-2.71	119.26	126.95
35	D	403	LMT	O5'-C5'-C4'	2.71	115.32	109.72
23	B	603	CLA	CBC-CAC-C3C	-2.71	105.08	112.42
23	B	614	CLA	C4-C3-C5	2.71	119.92	115.23
25	a	409	BCR	C32-C1-C6	-2.71	106.00	110.24
36	C	519	DGD	O2G-C1B-C2B	2.70	117.33	111.48
25	b	619	BCR	C4-C5-C6	-2.70	119.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	O2A-CGA-CBA	2.70	120.08	111.83
31	D	409	LHG	O8-C23-O10	-2.70	116.87	123.63
23	b	602	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
23	c	512	CLA	CBA-CAA-C2A	-2.70	105.76	113.79
23	b	604	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
23	c	508	CLA	C1-C2-C3	-2.70	121.77	126.20
23	b	616	CLA	C1-C2-C3	-2.70	121.78	126.20
23	A	404	CLA	CMD-C2D-C3D	-2.70	121.50	127.69
23	B	604	CLA	CMB-C2B-C1B	2.70	129.53	125.42
23	C	513	CLA	C4-C3-C5	2.69	119.90	115.23
23	C	512	CLA	CHC-C1C-C2C	-2.69	119.30	126.95
23	c	512	CLA	C4-C3-C5	2.69	119.90	115.23
23	b	601	CLA	O2A-CGA-CBA	2.69	120.04	111.83
23	c	511	CLA	O2A-CGA-CBA	2.69	120.04	111.83
23	b	608	CLA	O2A-CGA-CBA	2.69	120.04	111.83
23	c	512	CLA	CHB-C4A-NA	2.69	128.28	124.40
23	B	610	CLA	CMB-C2B-C1B	2.69	129.51	125.42
25	b	617	BCR	C20-C21-C22	-2.69	123.51	127.28
23	c	508	CLA	C2A-C1A-CHA	-2.69	119.21	123.87
23	c	511	CLA	CBC-CAC-C3C	-2.69	105.14	112.42
23	C	502	CLA	O2A-CGA-CBA	2.68	120.02	111.83
24	a	407	PHO	O2D-CGD-O1D	-2.68	118.62	123.85
23	b	615	CLA	C11-C12-C13	-2.68	107.04	115.97
23	b	616	CLA	C2A-C1A-CHA	-2.68	119.21	123.87
23	c	504	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
24	A	407	PHO	CMB-C2B-C3B	2.68	130.04	124.68
26	L	101	SQD	C44-O6-C1	-2.68	108.06	113.80
23	c	503	CLA	O2A-CGA-O1A	-2.68	116.94	123.63
25	T	101	BCR	C7-C6-C5	-2.68	115.39	121.56
23	b	614	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
38	e	103	HEM	C3B-C4B-NB	-2.67	107.55	109.47
23	b	601	CLA	C3B-C4B-NB	2.67	112.92	110.53
35	D	403	LMT	C4B-C3B-C2B	2.67	115.52	110.83
29	d	406	PL9	C51-C49-C50	2.67	120.74	114.59
25	K	102	BCR	C15-C14-C13	-2.67	123.53	127.28
36	c	516	DGD	O3G-C3G-C2G	-2.67	104.32	110.82
23	B	602	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
31	D	408	LHG	O8-C23-O10	-2.67	116.95	123.63
23	b	608	CLA	C2A-C1A-CHA	-2.67	119.23	123.87
23	C	505	CLA	CBC-CAC-C3C	-2.67	105.18	112.42
23	A	408	CLA	CBC-CAC-C3C	-2.67	105.19	112.42
25	D	406	BCR	C40-C30-C25	-2.67	106.06	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C4-C3-C5	2.67	119.85	115.23
23	D	404	CLA	C4-C3-C5	2.66	119.85	115.23
23	B	616	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
23	b	610	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
23	B	610	CLA	CAC-C3C-C4C	2.66	128.25	124.79
33	b	620	LMG	C8-O7-C10	-2.66	111.43	117.80
25	A	409	BCR	C16-C17-C18	-2.66	123.55	127.28
29	a	414	PL9	C35-C34-C36	2.66	119.84	115.23
23	b	601	CLA	O1D-CGD-CBD	-2.66	119.27	124.52
23	b	605	CLA	CED-O2D-CGD	2.66	121.94	115.92
23	c	504	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
23	c	506	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
23	B	609	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
26	A	412	SQD	O48-C23-O10	-2.66	116.98	123.63
23	b	603	CLA	C2A-C1A-CHA	-2.66	119.26	123.87
23	d	404	CLA	C2A-C1A-CHA	-2.65	119.26	123.87
36	c	517	DGD	O1G-C1A-C2A	2.65	119.93	111.83
25	D	406	BCR	C37-C22-C23	2.65	122.14	118.09
23	d	403	CLA	C4-C3-C5	2.65	119.83	115.23
23	c	503	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
23	C	505	CLA	CHD-C4C-NC	2.65	128.34	124.23
29	D	407	PL9	C7-C3-C2	-2.65	120.27	123.39
38	e	103	HEM	C4D-ND-C1D	2.65	108.34	105.21
25	y	101	BCR	C10-C11-C12	-2.65	115.53	123.20
23	b	607	CLA	C4-C3-C5	2.65	119.83	115.23
23	c	507	CLA	C3B-C4B-NB	2.65	112.89	110.53
23	B	607	CLA	CHD-C4C-NC	2.65	128.34	124.23
23	c	507	CLA	CHD-C4C-NC	2.65	128.33	124.23
23	c	507	CLA	C4-C3-C5	2.64	119.82	115.23
33	b	620	LMG	C1-C2-C3	-2.64	104.45	110.01
23	c	510	CLA	CMB-C2B-C1B	2.64	129.44	125.42
24	a	406	PHO	CMB-C2B-C3B	2.64	129.97	124.68
23	c	501	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
23	B	606	CLA	O2A-CGA-CBA	2.64	119.89	111.83
23	b	611	CLA	CHD-C4C-NC	2.64	128.32	124.23
23	b	612	CLA	CHD-C4C-NC	2.64	128.32	124.23
23	B	606	CLA	CMB-C2B-C1B	2.64	129.44	125.42
23	C	514	CLA	C4-C3-C5	2.64	119.81	115.23
23	c	508	CLA	CAC-C3C-C4C	2.64	128.22	124.79
23	B	604	CLA	CHD-C4C-NC	2.64	128.32	124.23
26	A	410	SQD	C45-O47-C7	-2.64	111.49	117.80
23	B	615	CLA	CBC-CAC-C3C	-2.64	105.27	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C11-C10-C8	-2.64	107.21	115.97
23	c	507	CLA	C6-C7-C8	-2.63	107.21	115.97
25	H	101	BCR	C29-C30-C25	2.63	114.27	110.44
23	C	503	CLA	CAC-C3C-C4C	2.63	128.22	124.79
23	C	507	CLA	CAA-C2A-C3A	-2.63	105.88	113.00
23	b	604	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
23	d	404	CLA	CMC-C2C-C1C	2.63	129.15	125.03
23	B	608	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
23	C	502	CLA	CMC-C2C-C1C	2.63	129.15	125.03
23	b	604	CLA	CHC-C1C-C2C	-2.63	119.47	126.95
31	d	407	LHG	O8-C23-O10	-2.63	117.05	123.63
24	a	407	PHO	O1D-CGD-CBD	-2.63	120.73	124.72
23	b	612	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
23	b	609	CLA	CHD-C4C-NC	2.63	128.31	124.23
25	C	516	BCR	C15-C16-C17	-2.62	118.15	123.52
23	d	403	CLA	C4C-C3C-C2C	-2.62	103.08	106.89
29	a	414	PL9	C25-C24-C26	2.62	119.78	115.23
26	D	413	SQD	O48-C23-C24	2.62	119.83	111.83
25	b	618	BCR	C24-C23-C22	-2.62	122.36	126.23
24	a	407	PHO	CMB-C2B-C3B	2.62	129.92	124.68
23	B	602	CLA	C2A-C1A-CHA	-2.62	119.32	123.87
23	C	513	CLA	CBA-CAA-C2A	-2.62	106.00	113.79
23	b	614	CLA	CHD-C4C-NC	2.62	128.29	124.23
23	b	609	CLA	C4C-C3C-C2C	-2.62	103.08	106.89
23	A	406	CLA	C3B-C4B-NB	2.62	112.87	110.53
23	C	508	CLA	O2A-CGA-CBA	2.62	119.81	111.83
25	b	619	BCR	C39-C30-C25	-2.62	106.14	110.24
25	k	101	BCR	C7-C8-C9	-2.62	122.37	126.23
23	C	511	CLA	C4-C3-C5	2.61	119.77	115.23
25	c	515	BCR	C3-C4-C5	-2.61	109.40	114.06
23	b	603	CLA	CMC-C2C-C1C	2.61	129.12	125.03
23	c	510	CLA	O1D-CGD-CBD	-2.61	119.38	124.52
23	B	611	CLA	O2A-CGA-CBA	2.61	119.78	111.83
23	B	604	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
25	D	406	BCR	C15-C14-C13	-2.61	123.62	127.28
24	A	407	PHO	O2A-CGA-CBA	2.61	119.78	111.83
23	c	505	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
23	D	405	CLA	C4-C3-C5	2.61	119.75	115.23
31	d	407	LHG	O8-C23-C24	2.61	119.78	111.83
23	C	513	CLA	CMB-C2B-C1B	2.61	129.39	125.42
25	c	514	BCR	C28-C27-C26	-2.61	109.41	114.06
36	C	519	DGD	O1G-C1A-O1A	-2.60	117.11	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C4B-C3B-C2B	-2.60	104.06	107.30
25	B	617	BCR	C16-C17-C18	-2.60	123.63	127.28
26	A	412	SQD	O8-S-C6	2.60	111.00	105.97
25	A	409	BCR	C37-C22-C21	-2.60	118.60	122.82
23	B	611	CLA	OBD-CAD-C3D	-2.60	122.34	128.42
25	B	618	BCR	C36-C18-C19	2.60	122.06	118.09
29	D	407	PL9	C37-C38-C39	-2.60	121.67	127.62
23	b	615	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
29	A	414	PL9	C25-C24-C26	2.60	119.74	115.23
29	D	407	PL9	C20-C19-C21	2.60	119.74	115.23
23	D	405	CLA	CAC-C3C-C4C	2.60	128.17	124.79
23	b	602	CLA	C11-C12-C13	-2.60	107.33	115.97
23	B	611	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
26	a	410	SQD	O48-C23-C24	2.60	119.75	111.83
24	D	401	PHO	C4-C3-C5	2.60	119.73	115.23
24	a	406	PHO	O1D-CGD-CBD	-2.59	120.79	124.72
23	B	602	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
23	C	511	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
23	A	406	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
23	C	507	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
23	B	606	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
23	b	602	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
29	d	406	PL9	C37-C38-C39	-2.59	121.69	127.62
29	A	414	PL9	C35-C34-C36	2.59	119.72	115.23
23	C	510	CLA	O2A-CGA-CBA	2.59	119.72	111.83
23	A	405	CLA	CAA-CBA-CGA	2.59	120.55	113.21
23	d	404	CLA	CHC-C1C-C2C	-2.59	119.60	126.95
25	Y	101	BCR	C37-C22-C23	2.59	122.04	118.09
23	d	401	CLA	C4-C3-C5	2.58	119.72	115.23
34	C	521	HTG	O5-C1-C2	2.58	113.88	110.32
23	A	404	CLA	CMC-C2C-C1C	2.58	129.07	125.03
33	C	501	LMG	C7-O1-C1	-2.58	108.26	113.80
26	a	412	SQD	O5-C5-C4	2.58	114.35	109.70
25	b	618	BCR	C28-C27-C26	-2.58	109.45	114.06
25	B	617	BCR	C31-C1-C6	-2.58	106.20	110.24
29	d	406	PL9	C17-C18-C19	-2.58	121.72	127.62
23	b	604	CLA	CHD-C4C-NC	2.58	128.23	124.23
23	A	405	CLA	CMA-C3A-C2A	-2.58	104.01	113.98
36	C	518	DGD	O1G-C1A-O1A	-2.58	117.18	123.63
23	C	513	CLA	C4B-C3B-C2B	-2.58	104.10	107.30
25	y	101	BCR	C37-C22-C23	2.58	122.02	118.09
23	A	408	CLA	CMB-C2B-C1B	2.58	129.34	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	CHB-C4A-NA	2.57	128.12	124.40
23	d	403	CLA	CBC-CAC-C3C	-2.57	105.44	112.42
23	b	601	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
23	d	401	CLA	C1-O2A-CGA	2.57	122.87	116.65
38	E	103	HEM	CHA-C4D-ND	2.57	127.55	124.37
23	C	513	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
25	K	102	BCR	C36-C18-C19	2.57	122.01	118.09
23	c	502	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
23	c	511	CLA	CMC-C2C-C1C	2.57	129.05	125.03
23	C	507	CLA	CMB-C2B-C1B	2.57	129.33	125.42
29	d	406	PL9	C12-C13-C14	-2.57	121.75	127.62
25	t	101	BCR	C3-C4-C5	-2.57	109.48	114.06
23	B	606	CLA	CAA-C2A-C3A	-2.57	106.07	113.00
23	B	605	CLA	CMC-C2C-C1C	2.56	129.04	125.03
23	C	507	CLA	CHD-C4C-NC	2.56	128.21	124.23
23	c	509	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
25	y	101	BCR	C24-C23-C22	-2.56	122.44	126.23
23	C	504	CLA	CAC-C3C-C4C	2.56	128.12	124.79
23	a	404	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
23	d	403	CLA	CMB-C2B-C1B	2.56	129.32	125.42
25	B	618	BCR	C28-C27-C26	-2.56	109.49	114.06
23	b	604	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
23	b	608	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
33	C	501	LMG	C9-C8-C7	-2.56	105.82	111.78
23	C	506	CLA	CBC-CAC-C3C	-2.56	105.49	112.42
23	b	603	CLA	C4-C3-C5	2.56	119.67	115.23
24	A	407	PHO	O2D-CGD-O1D	-2.56	118.87	123.85
23	A	405	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
23	B	609	CLA	CMC-C2C-C1C	2.55	129.03	125.03
23	C	505	CLA	C1-C2-C3	-2.55	122.01	126.20
23	C	503	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
23	C	504	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
25	C	516	BCR	C38-C26-C25	-2.55	121.70	124.48
33	a	416	LMG	O6-C5-C4	2.55	114.29	109.70
26	a	412	SQD	O7-S-C6	2.55	110.56	106.76
23	B	610	CLA	CAA-CBA-CGA	-2.55	105.98	113.21
25	A	409	BCR	C36-C18-C19	2.55	121.98	118.09
23	b	610	CLA	C2A-C1A-CHA	-2.54	119.45	123.87
38	E	103	HEM	CBD-CAD-C3D	-2.54	105.50	112.53
23	c	513	CLA	C2A-C1A-CHA	-2.54	119.45	123.87
29	A	414	PL9	C40-C39-C41	2.54	119.64	115.23
23	C	506	CLA	C4-C3-C5	2.54	119.64	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	522	HTG	C3-C4-C5	2.54	114.84	110.23
23	B	612	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
36	H	102	DGD	O1G-C1A-C2A	2.54	119.58	111.83
23	C	506	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
23	b	611	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
29	d	406	PL9	C15-C14-C16	2.54	119.63	115.23
23	b	606	CLA	CAC-C3C-C4C	2.54	128.09	124.79
23	A	405	CLA	CMB-C2B-C1B	2.53	129.28	125.42
36	C	518	DGD	C2G-O2G-C1B	-2.53	111.73	117.80
34	B	622	HTG	O5-C1-C2	2.53	113.81	110.32
25	c	514	BCR	C33-C5-C6	-2.53	121.72	124.48
23	c	513	CLA	CHD-C4C-NC	2.53	128.15	124.23
29	A	414	PL9	C45-C44-C46	2.53	119.62	115.23
23	d	401	CLA	C11-C12-C13	-2.53	107.56	115.97
23	B	601	CLA	CMB-C2B-C1B	2.53	129.27	125.42
25	K	102	BCR	C33-C5-C6	-2.53	121.72	124.48
23	B	610	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
23	C	510	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
23	B	602	CLA	O2A-CGA-CBA	2.53	119.54	111.83
31	d	408	LHG	O8-C23-C24	2.53	119.54	111.83
23	b	611	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
29	D	407	PL9	C51-C49-C50	2.53	120.40	114.59
25	d	405	BCR	C38-C26-C25	-2.53	121.73	124.48
25	a	409	BCR	C15-C16-C17	-2.52	118.35	123.52
23	b	602	CLA	C2A-C1A-CHA	-2.52	119.49	123.87
23	b	606	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
26	a	412	SQD	O9-S-C6	2.52	110.52	106.76
23	B	601	CLA	CAC-C3C-C4C	2.52	128.07	124.79
23	B	607	CLA	C4-C3-C5	2.52	119.60	115.23
23	B	613	CLA	CHD-C4C-NC	2.52	128.14	124.23
23	A	405	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
23	d	404	CLA	C1-C2-C3	-2.52	122.07	126.20
23	C	509	CLA	C4-C3-C5	2.52	119.60	115.23
23	c	506	CLA	CMB-C2B-C1B	2.51	129.25	125.42
26	A	410	SQD	O48-C23-O10	-2.51	117.34	123.63
23	C	513	CLA	C1-C2-C3	-2.51	122.08	126.20
23	b	603	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
23	b	606	CLA	O2A-CGA-CBA	2.51	119.49	111.83
33	J	101	LMG	O8-C28-O10	-2.51	117.35	123.63
23	B	603	CLA	CHD-C4C-NC	2.51	128.12	124.23
23	b	615	CLA	CAC-C3C-C4C	2.51	128.05	124.79
25	H	101	BCR	C2-C1-C6	2.51	114.08	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
35	D	403	LMT	O1B-C4'-C5'	-2.51	102.90	109.48
23	c	506	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
33	Z	102	LMG	C9-C8-C7	-2.50	105.95	111.78
23	d	403	CLA	CAA-C2A-C3A	-2.50	106.23	113.00
25	T	101	BCR	C1-C6-C7	2.50	122.44	115.65
34	c	522	HTG	O5-C1-C2	2.50	113.77	110.32
23	C	513	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
25	k	101	BCR	C10-C11-C12	-2.50	115.96	123.20
23	C	510	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
33	j	101	LMG	O8-C28-C29	2.50	119.45	111.83
25	h	101	BCR	C16-C15-C14	-2.50	118.41	123.52
23	B	615	CLA	CAC-C3C-C4C	2.49	128.04	124.79
25	C	515	BCR	C11-C10-C9	-2.49	123.78	127.28
33	c	520	LMG	O8-C28-O10	-2.49	117.39	123.63
23	B	602	CLA	CED-O2D-CGD	2.49	121.57	115.92
25	C	515	BCR	C20-C21-C22	-2.49	123.78	127.28
23	b	616	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
23	b	608	CLA	CBC-CAC-C3C	-2.49	105.66	112.42
23	c	501	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	C	506	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
23	B	613	CLA	CED-O2D-CGD	2.49	121.57	115.92
23	B	607	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	C	514	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
25	B	619	BCR	C37-C22-C21	-2.49	118.78	122.82
25	B	619	BCR	C7-C8-C9	-2.49	122.56	126.23
25	B	618	BCR	C10-C11-C12	-2.49	116.00	123.20
23	c	503	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
33	Z	102	LMG	O6-C1-C2	2.48	115.47	110.37
23	b	610	CLA	C4B-C3B-C2B	-2.48	104.21	107.30
23	B	606	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
25	c	515	BCR	C37-C22-C23	2.48	121.88	118.09
23	c	505	CLA	CED-O2D-CGD	2.48	121.55	115.92
23	D	405	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
23	C	502	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
24	a	406	PHO	C1A-C2A-C3A	-2.48	100.48	102.84
25	b	617	BCR	C32-C1-C6	-2.47	106.36	110.24
23	C	511	CLA	C4C-C3C-C2C	-2.47	103.30	106.89
23	c	512	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
23	b	612	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
23	C	508	CLA	C3B-C4B-NB	2.47	112.73	110.53
23	a	404	CLA	CMA-C3A-C4A	-2.47	105.14	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	CMC-C2C-C1C	2.47	128.89	125.03
23	b	604	CLA	C4-C3-C5	2.46	119.51	115.23
25	T	101	BCR	C2-C1-C6	2.46	114.02	110.44
23	c	501	CLA	C3B-C4B-NB	2.46	112.73	110.53
23	b	610	CLA	CHD-C4C-NC	2.46	128.05	124.23
23	C	505	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
25	c	514	BCR	C2-C1-C6	2.46	114.02	110.44
29	D	407	PL9	C42-C41-C39	-2.46	105.02	113.19
23	a	408	CLA	CHD-C4C-NC	2.46	128.05	124.23
29	A	414	PL9	C53-C6-C1	2.46	120.32	115.28
23	b	610	CLA	C3B-C4B-NB	2.46	112.73	110.53
23	a	405	CLA	CBC-CAC-C3C	-2.46	105.75	112.42
23	b	613	CLA	CMC-C2C-C1C	2.46	128.88	125.03
36	c	516	DGD	C3G-C2G-C1G	-2.46	106.06	111.78
29	a	414	PL9	C53-C6-C1	2.46	120.31	115.28
23	c	503	CLA	CAC-C3C-C4C	2.46	127.99	124.79
23	c	501	CLA	CHD-C4C-NC	2.46	128.04	124.23
23	d	401	CLA	C2A-C1A-CHA	-2.46	119.61	123.87
23	A	405	CLA	CHC-C1C-C2C	-2.45	119.97	126.95
33	Z	102	LMG	C1-O6-C5	2.45	118.51	113.72
23	d	404	CLA	C3B-C4B-NB	2.45	112.72	110.53
23	c	504	CLA	CBC-CAC-C3C	-2.45	105.78	112.42
35	b	627	LMT	C1'-C2'-C3'	2.45	115.17	110.01
23	B	610	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
23	c	508	CLA	CHD-C4C-NC	2.45	128.03	124.23
23	b	609	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
24	D	401	PHO	O2D-CGD-O1D	-2.45	119.08	123.85
23	C	502	CLA	C4C-C3C-C2C	-2.45	103.33	106.89
23	B	602	CLA	CBC-CAC-C3C	-2.45	105.78	112.42
23	B	607	CLA	CMC-C2C-C1C	2.44	128.85	125.03
23	B	608	CLA	CMB-C2B-C1B	2.44	129.14	125.42
36	h	102	DGD	C3G-O3G-C1D	-2.44	108.56	113.80
23	c	505	CLA	O2A-CGA-CBA	2.44	119.27	111.83
23	C	504	CLA	CHD-C4C-NC	2.44	128.01	124.23
23	b	616	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
23	c	509	CLA	CMB-C2B-C1B	2.44	129.13	125.42
23	a	404	CLA	CHD-C4C-NC	2.44	128.01	124.23
23	B	608	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
33	C	520	LMG	O8-C28-O10	-2.44	117.54	123.63
23	c	508	CLA	C4-C3-C5	2.44	119.45	115.23
23	b	616	CLA	CBC-CAC-C3C	-2.43	105.82	112.42
23	B	602	CLA	C1-C2-C3	-2.43	122.21	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	201	HEC	CHA-C4D-ND	2.43	128.27	123.86
40	V	202	HEC	C2A-C1A-NA	-2.43	107.98	110.32
33	b	620	LMG	O8-C28-O10	-2.43	117.54	123.63
25	a	409	BCR	C8-C7-C6	-2.43	120.50	127.00
23	A	408	CLA	CAC-C3C-C4C	2.43	127.95	124.79
25	C	516	BCR	C3-C4-C5	-2.43	109.72	114.06
23	C	511	CLA	CMC-C2C-C1C	2.43	128.83	125.03
23	C	508	CLA	CHD-C4C-NC	2.43	128.00	124.23
23	B	605	CLA	CHC-C1C-C2C	-2.43	120.05	126.95
26	f	101	SQD	O5-C5-C4	2.43	114.07	109.70
25	T	101	BCR	C35-C13-C12	2.43	121.80	118.09
23	B	602	CLA	CHD-C4C-NC	2.43	127.99	124.23
23	C	514	CLA	O2A-CGA-CBA	2.43	119.23	111.83
23	A	404	CLA	CED-O2D-CGD	2.42	121.42	115.92
35	M	101	LMT	C1-O1'-C1'	-2.42	109.54	113.68
26	a	410	SQD	O48-C23-O10	-2.42	117.56	123.63
23	B	616	CLA	C2A-C1A-CHA	-2.42	119.66	123.87
23	C	514	CLA	CBC-CAC-C3C	-2.42	105.85	112.42
23	c	502	CLA	CAC-C3C-C4C	2.42	127.94	124.79
23	c	510	CLA	C4-C3-C2	-2.42	117.41	123.63
38	E	103	HEM	CHD-C1D-ND	2.42	127.03	124.42
23	B	616	CLA	CAC-C3C-C4C	2.42	127.94	124.79
23	A	406	CLA	C4B-C3B-C2B	-2.42	104.30	107.30
23	B	610	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
25	c	514	BCR	C34-C9-C10	-2.42	118.90	122.82
35	b	627	LMT	O5'-C1'-C2'	2.42	115.34	110.37
23	B	616	CLA	CBC-CAC-C3C	-2.42	105.87	112.42
23	B	601	CLA	C2A-C1A-CHA	-2.41	119.68	123.87
23	b	601	CLA	CAC-C3C-C4C	2.41	127.93	124.79
23	B	613	CLA	CBC-CAC-C3C	-2.41	105.88	112.42
23	C	507	CLA	CGD-CBD-CAD	-2.41	103.04	110.85
29	D	407	PL9	C15-C14-C16	2.41	119.41	115.23
25	C	516	BCR	C16-C17-C18	-2.41	123.90	127.28
23	A	405	CLA	C4C-C3C-C2C	-2.41	103.39	106.89
23	B	605	CLA	C3B-C4B-NB	2.41	112.68	110.53
40	V	202	HEC	CHB-C1B-NB	2.41	128.22	123.86
23	C	509	CLA	CHB-C4A-NA	2.41	127.87	124.40
25	D	406	BCR	C21-C20-C19	-2.41	116.23	123.20
23	d	403	CLA	CAC-C3C-C4C	2.40	127.92	124.79
25	C	516	BCR	C21-C20-C19	-2.40	116.24	123.20
23	b	601	CLA	CMB-C2B-C1B	2.40	129.08	125.42
40	v	201	HEC	O2D-CGD-CBD	2.40	121.59	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	101	SQD	O47-C7-O49	-2.40	118.09	123.70
23	b	606	CLA	CMB-C2B-C1B	2.40	129.07	125.42
23	b	613	CLA	CMB-C2B-C1B	2.40	129.07	125.42
40	V	202	HEC	CBA-CAA-C2A	-2.40	105.90	112.53
23	c	505	CLA	C1-O2A-CGA	2.40	122.46	116.65
23	b	610	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
23	B	601	CLA	C4-C3-C5	2.40	119.39	115.23
23	b	601	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
23	a	405	CLA	C1-O2A-CGA	2.40	122.45	116.65
25	C	515	BCR	C38-C26-C25	-2.40	121.87	124.48
23	c	505	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
23	D	404	CLA	CAA-C2A-C3A	-2.39	106.53	113.00
23	C	511	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
33	j	101	LMG	O7-C10-O9	-2.39	118.11	123.70
23	C	507	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
23	c	510	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
25	c	515	BCR	C32-C1-C6	-2.39	106.50	110.24
23	B	606	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
23	B	611	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
23	c	508	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
23	C	514	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
23	c	512	CLA	C1-O2A-CGA	2.39	122.43	116.65
23	b	605	CLA	C1-C2-C3	-2.39	122.29	126.20
23	c	505	CLA	C4-C3-C5	2.39	119.37	115.23
23	c	510	CLA	CAC-C3C-C4C	2.38	127.89	124.79
23	a	408	CLA	C4-C3-C5	2.38	119.36	115.23
26	A	410	SQD	O9-S-C6	2.38	110.31	106.76
33	a	416	LMG	O8-C28-C29	2.38	119.09	111.83
23	C	511	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
25	y	101	BCR	C28-C27-C26	-2.38	109.81	114.06
25	B	619	BCR	C10-C11-C12	-2.38	116.31	123.20
25	a	409	BCR	C33-C5-C6	-2.38	121.89	124.48
34	B	622	HTG	C1'-S1-C1	2.38	105.58	100.45
23	c	513	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
23	B	608	CLA	CMC-C2C-C1C	2.38	128.75	125.03
40	v	201	HEC	C2A-C1A-NA	-2.38	108.03	110.32
38	E	103	HEM	C4B-C3B-C2B	-2.37	105.10	107.28
23	C	502	CLA	C4-C3-C5	2.37	119.35	115.23
36	H	102	DGD	C2G-O2G-C1B	-2.37	112.11	117.80
23	b	611	CLA	CMC-C2C-C1C	2.37	128.74	125.03
23	B	615	CLA	C4-C3-C5	2.37	119.34	115.23
23	b	605	CLA	CAC-C3C-C4C	2.37	127.88	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
23	d	403	CLA	C2A-C1A-CHA	-2.37	119.75	123.87
23	b	616	CLA	C4B-C3B-C2B	-2.37	104.36	107.30
23	b	606	CLA	CMC-C2C-C1C	2.37	128.73	125.03
26	L	101	SQD	C1-C2-C3	-2.37	105.03	110.01
24	D	401	PHO	CMC-C2C-C1C	2.37	128.99	124.73
36	c	516	DGD	C6D-O5D-C1E	-2.37	108.72	113.80
23	B	607	CLA	CAA-CBA-CGA	2.37	119.92	113.21
23	B	613	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
23	b	614	CLA	CBC-CAC-C3C	-2.36	106.01	112.42
23	C	514	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
23	b	602	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
33	z	101	LMG	C8-O7-C10	-2.36	112.14	117.80
23	c	507	CLA	O2A-CGA-CBA	2.36	119.04	111.83
23	B	614	CLA	C2A-C1A-CHA	-2.36	119.77	123.87
40	v	201	HEC	C4B-NB-C1B	2.36	109.67	105.82
23	C	507	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
36	c	518	DGD	O1G-C1A-C2A	2.36	119.02	111.83
23	b	601	CLA	C2A-C1A-CHA	-2.36	119.78	123.87
23	c	509	CLA	CMC-C2C-C1C	2.36	128.72	125.03
23	d	403	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
23	B	610	CLA	CHB-C4A-NA	2.35	127.80	124.40
23	B	612	CLA	CMB-C2B-C1B	2.35	129.00	125.42
29	a	414	PL9	C7-C8-C9	-2.35	122.78	126.83
36	C	517	DGD	C4E-C3E-C2E	-2.35	106.70	110.83
24	D	401	PHO	C4A-C3A-C2A	-2.35	100.60	102.84
23	B	611	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
23	c	513	CLA	CHC-C1C-C2C	-2.35	120.26	126.95
23	B	612	CLA	C11-C12-C13	-2.35	108.15	115.97
40	v	201	HEC	CHD-C1D-ND	2.35	128.12	123.86
23	a	408	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
31	A	416	LHG	C5-O7-C7	-2.35	112.17	117.80
26	L	101	SQD	O47-C7-O49	-2.35	118.22	123.70
23	C	503	CLA	CMC-C2C-C1C	2.35	128.70	125.03
26	f	101	SQD	C4-C3-C2	-2.35	106.71	110.83
25	y	101	BCR	C40-C30-C25	-2.35	106.56	110.24
23	B	610	CLA	C4-C3-C5	2.35	119.30	115.23
23	A	406	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
23	A	404	CLA	CHD-C4C-NC	2.34	127.86	124.23
25	t	101	BCR	C20-C21-C22	-2.34	123.99	127.28
23	b	612	CLA	CMC-C2C-C1C	2.34	128.69	125.03
23	a	408	CLA	CMA-C3A-C4A	-2.34	105.48	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	413	SQD	C46-C45-C44	-2.34	106.33	111.78
23	c	506	CLA	C2A-C1A-CHA	-2.34	119.81	123.87
23	b	601	CLA	CBC-CAC-C3C	-2.34	106.08	112.42
36	h	102	DGD	O1G-C1A-O1A	-2.34	117.78	123.63
23	b	615	CLA	O2A-CGA-CBA	2.34	118.96	111.83
23	b	609	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
23	C	511	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
23	C	507	CLA	C4C-C3C-C2C	-2.33	103.49	106.89
23	B	616	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
25	b	617	BCR	C24-C23-C22	-2.33	122.78	126.23
23	b	606	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
23	A	408	CLA	O2A-CGA-CBA	2.33	118.95	111.83
23	C	502	CLA	CMB-C2B-C1B	2.33	128.97	125.42
23	B	605	CLA	C4-C3-C5	2.33	119.28	115.23
24	A	407	PHO	CMA-C3A-C4A	-2.33	109.59	114.61
23	c	510	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
23	D	405	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
35	D	403	LMT	C1-O1'-C1'	-2.33	109.70	113.68
23	d	404	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
23	D	405	CLA	O2A-CGA-CBA	2.33	118.94	111.83
23	B	609	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
25	b	619	BCR	C21-C20-C19	-2.33	116.46	123.20
40	V	202	HEC	C4B-NB-C1B	2.32	109.61	105.82
23	a	404	CLA	CAC-C3C-C4C	2.32	127.81	124.79
23	c	502	CLA	CMC-C2C-C1C	2.32	128.66	125.03
23	b	602	CLA	CBC-CAC-C3C	-2.32	106.12	112.42
25	k	101	BCR	C39-C30-C25	-2.32	106.60	110.24
23	B	616	CLA	C4-C3-C5	2.32	119.26	115.23
23	C	503	CLA	CBC-CAC-C3C	-2.32	106.13	112.42
23	b	601	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
25	Y	101	BCR	C40-C30-C25	-2.32	106.61	110.24
38	E	103	HEM	O2A-CGA-CBA	2.32	121.32	114.00
25	c	515	BCR	C11-C10-C9	-2.32	124.03	127.28
25	a	409	BCR	C38-C26-C25	-2.32	121.96	124.48
23	C	505	CLA	CAC-C3C-C4C	2.32	127.80	124.79
31	d	408	LHG	O8-C23-O10	-2.31	117.84	123.63
29	a	414	PL9	C51-C49-C50	2.31	119.91	114.59
23	d	404	CLA	CBC-CAC-C3C	-2.31	106.15	112.42
23	d	404	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
33	j	101	LMG	O8-C28-O10	-2.31	117.84	123.63
36	c	518	DGD	O3G-C3G-C2G	-2.31	105.20	110.82
23	c	504	CLA	C4-C3-C5	2.31	119.24	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
23	c	508	CLA	CMC-C2C-C1C	2.31	128.64	125.03
23	B	615	CLA	O2A-CGA-CBA	2.31	118.87	111.83
23	A	405	CLA	C1-C2-C3	-2.31	122.42	126.20
23	B	608	CLA	CHB-C4A-NA	2.31	127.73	124.40
23	b	602	CLA	CMB-C2B-C1B	2.31	128.93	125.42
23	c	507	CLA	CMC-C2C-C1C	2.31	128.64	125.03
29	d	406	PL9	C53-C6-C1	2.30	120.00	115.28
40	v	201	HEC	CHB-C1B-NB	2.30	128.04	123.86
36	C	517	DGD	O1G-C1A-O1A	-2.30	117.86	123.63
23	c	503	CLA	CBC-CAC-C3C	-2.30	106.17	112.42
25	H	101	BCR	C7-C6-C5	2.30	126.86	121.56
23	a	405	CLA	O2A-CGA-CBA	2.30	118.86	111.83
23	b	601	CLA	CMC-C2C-C1C	2.30	128.63	125.03
36	c	518	DGD	O2G-C1B-C2B	2.30	116.46	111.48
23	B	602	CLA	C1-O2A-CGA	2.30	122.22	116.65
31	D	408	LHG	O8-C23-C24	2.30	118.85	111.83
38	e	103	HEM	C4C-NC-C1C	2.30	109.57	105.82
23	b	606	CLA	C1-O2A-CGA	2.30	122.21	116.65
23	b	606	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
26	A	410	SQD	O47-C7-O49	-2.30	118.34	123.70
25	a	409	BCR	C37-C22-C21	-2.29	119.10	122.82
24	A	407	PHO	C4-C3-C5	2.29	119.21	115.23
23	C	505	CLA	C4-C3-C5	2.29	119.21	115.23
23	B	604	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
23	C	508	CLA	C6-C7-C8	-2.29	108.35	115.97
23	d	401	CLA	CAA-CBA-CGA	2.29	119.71	113.21
33	C	501	LMG	O8-C28-C29	2.29	118.82	111.83
23	B	605	CLA	CAC-C3C-C4C	2.29	127.76	124.79
23	C	512	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
23	A	405	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
23	C	504	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
25	B	619	BCR	C2-C3-C4	-2.28	106.27	111.28
29	A	414	PL9	C51-C49-C50	2.28	119.83	114.59
23	A	406	CLA	CHB-C4A-NA	2.28	127.69	124.40
35	B	631	LMT	O1'-C1'-C2'	2.28	111.73	108.27
23	d	404	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
23	C	512	CLA	C11-C10-C8	-2.28	108.39	115.97
25	t	101	BCR	C16-C15-C14	-2.28	118.86	123.52
31	d	407	LHG	O7-C7-O9	-2.28	118.38	123.70
23	c	507	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
23	C	509	CLA	CAA-C2A-C3A	-2.27	106.85	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	620	LMG	C4-C3-C2	-2.27	106.84	110.83
25	H	101	BCR	C2-C3-C4	-2.27	106.28	111.28
23	C	511	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
23	d	404	CLA	C1-O2A-CGA	2.27	122.15	116.65
23	c	512	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
25	b	619	BCR	C37-C22-C23	2.27	121.56	118.09
23	B	612	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
23	b	616	CLA	C3B-C4B-NB	2.27	112.56	110.53
23	C	513	CLA	CHB-C4A-NA	2.27	127.67	124.40
23	B	612	CLA	CHD-C4C-NC	2.27	127.75	124.23
23	a	404	CLA	CMC-C2C-C1C	2.27	128.58	125.03
23	d	404	CLA	C4-C3-C5	2.27	119.16	115.23
23	a	405	CLA	CAC-C3C-C4C	2.26	127.73	124.79
23	C	506	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
25	c	515	BCR	C20-C21-C22	-2.26	124.10	127.28
25	y	101	BCR	C11-C10-C9	-2.26	124.10	127.28
23	B	605	CLA	O2A-CGA-CBA	2.26	118.73	111.83
23	B	609	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
23	A	405	CLA	C4-C3-C5	2.26	119.15	115.23
23	B	609	CLA	CBC-CAC-C3C	-2.26	106.29	112.42
23	c	510	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
23	C	503	CLA	O2A-CGA-CBA	2.26	118.73	111.83
35	D	403	LMT	C1B-O5B-C5B	-2.26	109.31	113.72
23	b	602	CLA	C4-C3-C5	2.26	119.15	115.23
29	D	407	PL9	C17-C18-C19	-2.26	122.46	127.62
23	C	503	CLA	C2A-C1A-CHA	-2.26	119.95	123.87
23	b	616	CLA	CMC-C2C-C1C	2.25	128.56	125.03
38	E	103	HEM	CMD-C2D-C1D	2.25	128.56	125.03
23	C	502	CLA	C2A-C1A-CHA	-2.25	119.96	123.87
26	a	410	SQD	C3-C4-C5	2.25	114.32	110.23
25	c	515	BCR	C40-C30-C25	-2.25	106.71	110.24
33	Z	101	LMG	C4-C3-C2	2.25	114.78	110.83
25	c	515	BCR	C15-C16-C17	-2.25	118.91	123.52
23	A	404	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
23	C	502	CLA	OBD-CAD-C3D	-2.25	123.16	128.42
23	a	404	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
23	C	503	CLA	C4-C3-C5	2.25	119.13	115.23
25	T	101	BCR	C16-C15-C14	2.25	128.12	123.52
23	a	405	CLA	C4-C3-C5	2.25	119.13	115.23
23	c	501	CLA	CBC-CAC-C3C	-2.25	106.32	112.42
23	b	613	CLA	CHB-C4A-NA	2.25	127.64	124.40
23	B	611	CLA	CAC-C3C-C4C	2.25	127.71	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
23	B	607	CLA	O2A-CGA-CBA	2.24	118.68	111.83
25	B	617	BCR	C28-C27-C26	-2.24	110.05	114.06
36	C	519	DGD	O6D-C1D-O3G	-2.24	104.75	110.04
23	C	513	CLA	CAC-C3C-C4C	2.24	127.70	124.79
23	A	404	CLA	CMA-C3A-C2A	-2.24	105.32	113.98
31	D	409	LHG	O7-C7-O9	-2.24	118.47	123.70
23	b	608	CLA	CAC-C3C-C4C	2.24	127.70	124.79
23	b	606	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
25	y	101	BCR	C16-C15-C14	-2.23	118.95	123.52
23	A	404	CLA	C4-C3-C5	2.23	119.11	115.23
23	D	405	CLA	CHB-C4A-NA	2.23	127.62	124.40
25	H	101	BCR	C31-C1-C6	-2.23	106.74	110.24
23	a	405	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
23	b	607	CLA	CHD-C4C-NC	2.23	127.69	124.23
23	b	608	CLA	C4-C3-C5	2.23	119.10	115.23
25	t	101	BCR	C29-C28-C27	-2.23	106.37	111.28
23	B	609	CLA	CED-O2D-CGD	2.23	120.97	115.92
40	V	202	HEC	CHD-C1D-ND	2.23	127.90	123.86
35	b	627	LMT	C3'-C4'-C5'	-2.23	105.99	110.93
25	k	101	BCR	C36-C18-C19	2.23	121.49	118.09
23	C	510	CLA	C1-O2A-CGA	2.23	122.05	116.65
23	B	615	CLA	C1-O2A-CGA	2.23	122.04	116.65
29	d	406	PL9	C27-C28-C29	-2.23	122.53	127.62
23	B	614	CLA	CMC-C2C-C1C	2.23	128.51	125.03
25	B	617	BCR	C29-C30-C25	2.23	113.67	110.44
29	d	406	PL9	C30-C29-C31	2.23	119.09	115.23
23	c	513	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
23	C	504	CLA	CBC-CAC-C3C	-2.23	106.39	112.42
23	B	604	CLA	CGD-CBD-CAD	-2.22	103.64	110.85
23	c	509	CLA	C4-C3-C5	2.22	119.09	115.23
23	b	610	CLA	C4-C3-C2	-2.22	117.91	123.63
25	A	409	BCR	C31-C1-C6	-2.22	106.75	110.24
23	b	616	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
23	B	611	CLA	CMB-C2B-C1B	2.22	128.80	125.42
25	T	101	BCR	C37-C22-C23	2.22	121.48	118.09
23	c	510	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
31	E	101	LHG	O8-C23-O10	-2.22	118.07	123.63
23	C	508	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
25	Y	101	BCR	C36-C18-C19	2.21	121.47	118.09
25	b	618	BCR	C20-C21-C22	-2.21	124.17	127.28
23	c	504	CLA	CHB-C4A-NA	2.21	127.59	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CBC-CAC-C3C	-2.21	106.43	112.42
23	C	512	CLA	CHB-C4A-NA	2.21	127.59	124.40
23	C	513	CLA	CMC-C2C-C1C	2.21	128.48	125.03
23	B	611	CLA	CED-O2D-CGD	2.21	120.92	115.92
23	c	505	CLA	C2A-C1A-CHA	-2.21	120.04	123.87
24	a	406	PHO	CBC-CAC-C3C	-2.21	109.72	112.87
24	a	406	PHO	CBA-CAA-C2A	-2.21	107.28	113.78
24	D	401	PHO	C1-O2A-CGA	2.20	121.98	116.65
23	B	605	CLA	CHB-C4A-NA	2.20	127.58	124.40
34	B	622	HTG	O2-C2-C3	-2.20	105.19	110.38
25	H	101	BCR	C16-C15-C14	-2.20	119.02	123.52
29	D	407	PL9	C25-C24-C26	2.20	119.05	115.23
23	C	508	CLA	CMC-C2C-C1C	2.20	128.47	125.03
25	D	406	BCR	C10-C11-C12	-2.20	116.83	123.20
23	b	609	CLA	C7-C6-C5	-2.20	107.40	113.26
38	e	103	HEM	CHA-C1A-NA	2.20	127.85	123.86
29	a	414	PL9	C40-C39-C41	2.20	119.04	115.23
24	D	401	PHO	CBA-CAA-C2A	-2.20	107.30	113.78
23	c	511	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
35	I	101	LMT	O1'-C1'-C2'	2.20	111.61	108.27
24	A	407	PHO	O2A-CGA-O1A	-2.19	118.14	123.63
33	B	621	LMG	C7-O1-C1	-2.19	109.10	113.80
35	m	102	LMT	O1B-C1B-C2B	2.19	113.48	108.09
23	B	610	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
23	B	613	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
23	c	501	CLA	CMC-C2C-C1C	2.19	128.46	125.03
23	B	614	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
36	c	517	DGD	O5D-C1E-C2E	2.19	111.60	108.27
29	A	414	PL9	C47-C48-C49	-2.19	120.34	127.64
23	a	405	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
23	B	603	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
25	d	405	BCR	C38-C26-C27	2.18	118.25	113.60
26	D	413	SQD	O5-C1-C2	-2.18	105.88	110.37
34	B	624	HTG	C1-C2-C3	2.18	114.82	110.55
23	b	616	CLA	C11-C12-C13	-2.18	108.71	115.97
40	v	201	HEC	O2A-CGA-CBA	2.18	120.90	114.00
25	B	619	BCR	C29-C30-C25	2.18	113.61	110.44
24	A	407	PHO	CED-O2D-CGD	2.18	120.86	115.92
36	C	517	DGD	O3G-C3G-C2G	-2.18	105.51	110.82
23	b	614	CLA	C4-C3-C5	2.18	119.01	115.23
23	C	509	CLA	CMB-C2B-C1B	2.18	128.74	125.42
23	B	616	CLA	C1-C2-C3	-2.18	122.62	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C35-C13-C12	2.18	121.42	118.09
23	a	404	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
23	c	510	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
23	c	512	CLA	CMA-C3A-C4A	-2.18	105.92	111.77
34	b	622	HTG	C1-O5-C5	2.18	116.47	112.56
23	C	513	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
29	a	414	PL9	C45-C44-C46	2.17	119.00	115.23
23	c	504	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
23	B	602	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
24	a	407	PHO	CBA-CAA-C2A	-2.17	107.38	113.78
23	C	505	CLA	OBD-CAD-C3D	-2.17	123.34	128.42
33	J	101	LMG	O7-C10-O9	-2.17	118.63	123.70
25	a	409	BCR	C2-C1-C6	2.17	113.59	110.44
25	c	514	BCR	C21-C20-C19	-2.17	116.91	123.20
35	M	103	LMT	O5'-C5'-C4'	2.17	114.21	109.72
35	a	417	LMT	C1B-O1B-C4'	-2.17	112.84	117.98
23	c	507	CLA	CHB-C4A-NA	2.17	127.53	124.40
31	d	407	LHG	C5-O7-C7	-2.17	112.61	117.80
25	C	515	BCR	C11-C12-C13	-2.17	120.42	126.36
23	c	506	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	D	406	BCR	C30-C25-C24	2.17	121.52	115.65
25	h	101	BCR	C37-C22-C23	2.16	121.39	118.09
25	B	618	BCR	C16-C17-C18	-2.16	124.24	127.28
23	c	502	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	c	507	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
23	a	408	CLA	CBC-CAC-C3C	-2.16	106.56	112.42
23	c	509	CLA	CHD-C4C-NC	2.16	127.58	124.23
23	C	505	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
25	k	101	BCR	C34-C9-C8	2.15	121.38	118.09
23	d	401	CLA	CHB-C4A-NA	2.15	127.51	124.40
25	h	101	BCR	C20-C21-C22	-2.15	124.26	127.28
25	c	514	BCR	C3-C4-C5	-2.15	110.22	114.06
23	b	603	CLA	CBC-CAC-C3C	-2.15	106.59	112.42
23	c	513	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
25	h	101	BCR	C37-C22-C21	-2.15	119.33	122.82
23	d	401	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
23	A	405	CLA	O2A-CGA-CBA	2.15	118.38	111.83
25	T	101	BCR	C10-C11-C12	-2.14	116.99	123.20
23	c	506	CLA	CBC-CAC-C3C	-2.14	106.61	112.42
29	a	414	PL9	C17-C18-C19	-2.14	122.72	127.62
26	B	620	SQD	O48-C46-C45	2.14	114.57	108.40
24	a	406	PHO	O2A-CGA-O1A	-2.14	118.27	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
23	a	405	CLA	CHB-C4A-NA	2.14	127.49	124.40
23	B	611	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
23	C	512	CLA	CBC-CAC-C3C	-2.14	106.62	112.42
29	d	406	PL9	C45-C44-C46	2.14	118.94	115.23
31	l	101	LHG	O8-C23-O10	-2.14	118.28	123.63
25	B	619	BCR	C37-C22-C23	2.14	121.35	118.09
34	b	623	HTG	C1-O5-C5	2.14	116.39	112.56
38	E	103	HEM	CHA-C1A-NA	2.14	127.73	123.86
36	C	517	DGD	O1G-C1A-C2A	2.14	118.35	111.83
35	m	102	LMT	C1B-O5B-C5B	2.14	117.89	113.72
29	D	407	PL9	C45-C44-C46	2.14	118.93	115.23
25	b	618	BCR	C15-C16-C17	-2.13	119.15	123.52
33	c	520	LMG	C9-C8-C7	-2.13	106.81	111.78
29	d	406	PL9	C36-C37-C38	-2.13	101.46	112.02
26	A	412	SQD	C46-C45-C44	-2.13	106.81	111.78
23	B	606	CLA	CMC-C2C-C1C	2.13	128.37	125.03
36	c	516	DGD	O2G-C1B-O1B	-2.13	118.72	123.70
23	B	601	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
23	B	601	CLA	CHB-C4A-NA	2.13	127.47	124.40
33	c	519	LMG	O8-C28-O10	-2.13	118.31	123.63
23	B	612	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
23	b	607	CLA	CMC-C2C-C1C	2.13	128.35	125.03
23	C	504	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
26	D	413	SQD	O48-C23-O10	-2.12	118.32	123.63
23	C	510	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
23	B	608	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
25	a	409	BCR	C28-C27-C26	-2.12	110.28	114.06
23	d	403	CLA	CHD-C4C-NC	2.12	127.52	124.23
36	C	519	DGD	O6E-C1E-O5D	-2.12	105.04	110.04
23	C	511	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
26	B	620	SQD	O5-C1-C2	-2.12	106.02	110.37
23	C	510	CLA	C11-C12-C13	-2.12	108.93	115.97
35	D	402	LMT	O5B-C5B-C4B	2.12	113.51	109.70
25	K	102	BCR	C11-C10-C9	-2.12	124.31	127.28
34	V	203	HTG	C1-O5-C5	2.12	115.02	112.19
23	A	406	CLA	CMA-C3A-C4A	-2.11	106.09	111.77
36	H	102	DGD	O1G-C1A-O1A	-2.11	118.34	123.63
23	b	602	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
35	e	102	LMT	O1B-C1B-C2B	2.11	113.29	108.09
23	c	509	CLA	C6-C5-C3	-2.11	108.32	113.47
31	E	101	LHG	O7-C7-O9	-2.11	118.77	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
36	c	517	DGD	O2G-C1B-O1B	-2.11	118.77	123.70
23	b	613	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	B	607	CLA	C1-O2A-CGA	2.11	121.76	116.65
25	C	515	BCR	C21-C20-C19	-2.11	117.09	123.20
23	A	406	CLA	C4-C3-C5	2.11	118.89	115.23
23	b	613	CLA	CAC-C3C-C4C	2.11	127.53	124.79
23	b	616	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
23	B	615	CLA	CHA-C1A-NA	-2.11	121.62	126.39
23	C	510	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	c	502	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
38	E	103	HEM	C4D-ND-C1D	2.11	107.70	105.21
23	c	502	CLA	CHB-C4A-NA	2.11	127.44	124.40
29	D	407	PL9	C2-C1-C6	2.11	121.50	119.00
23	B	606	CLA	C1-O2A-CGA	2.11	121.75	116.65
23	C	510	CLA	CMB-C2B-C1B	2.10	128.62	125.42
25	T	101	BCR	C21-C20-C19	-2.10	117.10	123.20
35	D	403	LMT	C3B-C4B-C5B	2.10	114.05	110.23
23	C	506	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
23	A	404	CLA	CHB-C4A-NA	2.10	127.43	124.40
23	B	613	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
23	B	601	CLA	CBC-CAC-C3C	-2.10	106.73	112.42
23	B	602	CLA	C11-C12-C13	-2.10	108.98	115.97
23	D	404	CLA	C4-C3-C2	-2.10	118.23	123.63
23	B	606	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
25	h	101	BCR	C29-C30-C25	2.10	113.49	110.44
23	c	504	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	b	617	BCR	C11-C10-C9	-2.10	124.34	127.28
38	E	103	HEM	O2D-CGD-CBD	2.10	120.62	114.00
40	v	201	HEC	CBA-CAA-C2A	-2.10	106.74	112.53
23	A	405	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
23	b	614	CLA	C2A-C1A-CHA	-2.10	120.23	123.87
38	E	103	HEM	CBA-CAA-C2A	-2.10	106.74	112.53
23	d	403	CLA	CHA-C1A-NA	-2.09	121.65	126.39
23	C	510	CLA	C4-C3-C5	2.09	118.86	115.23
25	Y	101	BCR	C21-C20-C19	-2.09	117.13	123.20
23	a	404	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
23	b	603	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
34	C	522	HTG	O5-C1-C2	2.09	113.20	110.32
29	a	414	PL9	C12-C13-C14	-2.09	122.84	127.62
23	b	610	CLA	C11-C12-C13	-2.09	109.02	115.97
23	C	505	CLA	O2A-CGA-CBA	2.09	118.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	BCR	C7-C8-C9	-2.09	123.15	126.23
25	h	101	BCR	C15-C14-C13	-2.08	124.35	127.28
25	t	101	BCR	C28-C27-C26	-2.08	110.34	114.06
34	B	627	HTG	C1-O5-C5	2.08	116.30	112.56
33	B	621	LMG	O8-C28-O10	-2.08	118.42	123.63
23	B	607	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	K	102	BCR	C10-C11-C12	-2.08	117.17	123.20
35	B	630	LMT	C1'-O5'-C5'	2.08	117.79	113.72
25	b	617	BCR	C38-C26-C25	-2.08	122.21	124.48
33	J	101	LMG	C8-O7-C10	-2.08	112.82	117.80
29	D	407	PL9	C30-C29-C31	2.08	118.84	115.23
23	d	404	CLA	CMA-C3A-C2A	-2.08	105.95	113.98
36	h	102	DGD	C3B-C2B-C1B	-2.08	106.08	113.69
26	B	620	SQD	O48-C23-O10	-2.08	118.43	123.63
36	c	518	DGD	O6D-C1D-O3G	-2.08	105.14	110.04
36	c	517	DGD	C1D-O6D-C5D	2.07	117.77	113.72
34	b	628	HTG	O5-C1-C2	2.07	113.17	110.32
25	b	619	BCR	C20-C21-C22	-2.07	124.37	127.28
23	C	507	CLA	CED-O2D-CGD	2.07	120.61	115.92
23	b	604	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
23	B	609	CLA	C7-C6-C5	-2.07	107.76	113.26
23	c	503	CLA	C2A-C1A-CHA	-2.06	120.28	123.87
23	D	404	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
25	b	617	BCR	C15-C16-C17	-2.06	119.30	123.52
23	C	512	CLA	C2A-C1A-CHA	-2.06	120.29	123.87
23	a	405	CLA	CMC-C2C-C1C	2.06	128.25	125.03
38	e	103	HEM	CBD-CAD-C3D	-2.06	106.84	112.53
23	A	404	CLA	CMB-C2B-C1B	2.06	128.56	125.42
25	Y	101	BCR	C28-C27-C26	-2.06	110.38	114.06
23	B	605	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
23	C	511	CLA	C1-O2A-CGA	2.06	121.63	116.65
23	B	603	CLA	CHB-C1B-C2B	-2.06	121.46	127.43
23	B	602	CLA	CHB-C4A-NA	2.06	127.37	124.40
23	c	510	CLA	CHB-C4A-NA	2.06	127.37	124.40
23	b	613	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
25	C	516	BCR	C36-C18-C19	2.05	121.23	118.09
40	V	202	HEC	CHB-C1B-C2B	-2.05	121.46	127.43
24	a	407	PHO	O2A-CGA-CBA	2.05	118.10	111.83
23	B	601	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
25	Y	101	BCR	C29-C28-C27	-2.05	106.76	111.28
25	b	618	BCR	C21-C20-C19	-2.05	117.25	123.20
36	c	518	DGD	O5D-C6D-C5D	-2.05	104.80	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CMB-C2B-C1B	2.05	128.54	125.42
25	K	102	BCR	C38-C26-C25	-2.05	122.25	124.48
33	c	519	LMG	O7-C10-O9	-2.05	118.92	123.70
38	E	103	HEM	C4C-NC-C1C	2.05	109.16	105.82
29	a	414	PL9	C37-C36-C34	-2.05	106.40	113.19
23	B	614	CLA	CHC-C1C-NC	2.05	127.39	124.31
36	c	518	DGD	C3G-C2G-C1G	-2.05	107.01	111.78
25	B	618	BCR	C36-C18-C17	-2.05	119.50	122.82
23	A	405	CLA	C11-C10-C8	-2.05	109.17	115.97
23	b	616	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
25	T	101	BCR	C34-C9-C8	2.05	121.21	118.09
29	D	407	PL9	C32-C33-C34	-2.04	122.94	127.62
36	c	517	DGD	O1G-C1A-O1A	-2.04	118.52	123.63
23	a	408	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
25	y	101	BCR	C35-C13-C12	2.04	121.21	118.09
23	A	408	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
23	b	610	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
40	V	202	HEC	CMD-C2D-C1D	2.04	128.52	125.42
33	C	501	LMG	O7-C10-O9	-2.04	118.94	123.70
36	H	102	DGD	O6E-C5E-C6E	2.04	111.49	106.44
23	A	406	CLA	CAC-C3C-C4C	2.04	127.44	124.79
23	b	607	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
23	B	614	CLA	CHB-C4A-NA	2.04	127.34	124.40
23	d	401	CLA	CMB-C2B-C1B	2.04	128.52	125.42
25	b	618	BCR	C37-C22-C21	-2.04	119.52	122.82
35	e	102	LMT	C1B-C2B-C3B	2.04	114.29	110.01
25	t	101	BCR	C36-C18-C19	2.03	121.20	118.09
36	C	519	DGD	C3G-C2G-C1G	-2.03	107.04	111.78
25	b	617	BCR	C37-C22-C21	-2.03	119.52	122.82
25	b	619	BCR	C28-C27-C26	-2.03	110.43	114.06
26	a	412	SQD	O48-C23-O10	-2.03	118.55	123.63
23	B	613	CLA	CMB-C2B-C3B	2.03	131.32	126.55
23	d	404	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
23	b	615	CLA	C2A-C1A-CHA	-2.03	120.35	123.87
26	A	410	SQD	O9-S-O7	-2.03	107.23	113.82
23	a	408	CLA	CHB-C4A-NA	2.03	127.33	124.40
25	t	101	BCR	C37-C22-C21	-2.03	119.53	122.82
23	d	404	CLA	CHB-C4A-NA	2.03	127.33	124.40
25	c	514	BCR	C36-C18-C19	2.03	121.18	118.09
36	c	516	DGD	O6D-C1D-O3G	-2.03	105.26	110.04
25	T	101	BCR	C3-C4-C5	-2.03	110.44	114.06
26	B	620	SQD	O5-C5-C4	2.03	113.35	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C6-C7-C8	-2.03	109.23	115.97
23	b	607	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
23	C	508	CLA	C4B-C3B-C2B	-2.02	104.79	107.30
36	C	518	DGD	O6E-C5E-C6E	2.02	111.45	106.44
23	c	506	CLA	CMC-C2C-C1C	2.02	128.19	125.03
23	C	505	CLA	CHB-C1B-NB	-2.02	121.02	124.05
23	C	508	CLA	CHB-C4A-NA	2.02	127.32	124.40
25	Y	101	BCR	C1-C6-C7	2.02	121.13	115.65
23	d	403	CLA	CHB-C4A-NA	2.02	127.31	124.40
23	B	613	CLA	C7-C6-C5	-2.02	107.89	113.26
35	I	101	LMT	O5'-C1'-C2'	2.02	114.51	110.37
34	V	203	HTG	C1-C2-C3	2.01	112.58	109.64
23	C	506	CLA	CHA-C1A-NA	-2.01	121.83	126.39
29	D	407	PL9	C45-C44-C43	-2.01	118.46	123.63
25	B	619	BCR	C16-C17-C18	-2.01	124.46	127.28
26	L	101	SQD	O48-C23-O10	-2.01	118.60	123.63
23	b	603	CLA	CAC-C3C-C4C	2.01	127.40	124.79
23	b	610	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
23	b	602	CLA	C7-C6-C5	-2.01	107.91	113.26
36	H	102	DGD	C3G-O3G-C1D	-2.01	109.49	113.80
23	C	502	CLA	CAA-C2A-C3A	-2.01	107.58	113.00
23	c	504	CLA	OBD-CAD-C3D	-2.01	123.73	128.42
23	B	603	CLA	C1-C2-C3	-2.01	122.91	126.20
23	d	401	CLA	CMC-C2C-C1C	2.01	128.17	125.03
23	b	606	CLA	CHB-C1B-C2B	-2.01	121.61	127.43
25	y	101	BCR	C36-C18-C19	2.00	121.15	118.09
23	d	401	CLA	C4C-C3C-C2C	-2.00	103.97	106.89
23	C	505	CLA	CHB-C4A-NA	2.00	127.29	124.40
23	C	504	CLA	CHC-C1C-NC	2.00	127.33	124.31
23	C	511	CLA	CAA-C2A-C3A	-2.00	107.59	113.00
23	b	611	CLA	CMB-C2B-C1B	2.00	128.47	125.42
23	C	513	CLA	C11-C12-C13	-2.00	109.31	115.97
31	D	409	LHG	C6-C5-C4	-2.00	107.12	111.78
29	A	414	PL9	C47-C46-C44	-2.00	106.55	113.19
23	b	611	CLA	C7-C6-C5	-2.00	107.93	113.26
33	z	101	LMG	C7-O1-C1	-2.00	109.51	113.80
31	A	416	LHG	O4-P-O5	2.00	121.75	112.44

All (66) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND

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Mol	Chain	Res	Type	Atom
23	A	405	CLA	ND
23	A	406	CLA	ND
23	A	408	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	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	C	502	CLA	ND
23	C	503	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	404	CLA	ND
23	D	405	CLA	ND
23	a	404	CLA	ND
23	a	408	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

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Mol	Chain	Res	Type	Atom
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	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	c	513	CLA	ND
23	d	401	CLA	ND
23	d	403	CLA	ND
23	d	404	CLA	ND

All (1318) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	C3A-C2A-CAA-CBA
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	C2B-C3B-CAB-CBB
23	B	616	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	508	CLA	C2B-C3B-CAB-CBB
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	510	CLA	CHA-CBD-CGD-O2D
23	C	514	CLA	C2B-C3B-CAB-CBB
23	C	514	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	a	405	CLA	C4B-C3B-CAB-CBB
23	a	408	CLA	C2B-C3B-CAB-CBB
23	a	408	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4-C3-C5-C6
23	b	607	CLA	C4B-C3B-CAB-CBB
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	C2-C1-O2A-CGA
23	c	512	CLA	CHA-CBD-CGD-O2D
23	d	404	CLA	C2B-C3B-CAB-CBB
23	d	404	CLA	C4B-C3B-CAB-CBB
25	D	406	BCR	C7-C8-C9-C10
25	D	406	BCR	C21-C22-C23-C24
25	D	406	BCR	C37-C22-C23-C24
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	d	405	BCR	C7-C8-C9-C10
25	d	405	BCR	C21-C22-C23-C24
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
26	D	413	SQD	O49-C7-O47-C45
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	101	SQD	O49-C7-O47-C45
26	L	101	SQD	C5-C6-S-O7
26	L	101	SQD	C5-C6-S-O8
26	L	101	SQD	C5-C6-S-O9
26	a	412	SQD	O6-C44-C45-O47
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	A	411	GOL	O1-C1-C2-C3
27	B	625	GOL	O1-C1-C2-C3
27	B	626	GOL	C1-C2-C3-O3
27	C	523	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
27	C	523	GOL	O1-C1-C2-C3
27	a	411	GOL	C1-C2-C3-O3
27	d	402	GOL	O1-C1-C2-C3
29	d	406	PL9	C39-C41-C42-C43
31	A	416	LHG	C4-O6-P-O5
31	A	417	LHG	O1-C1-C2-C3
31	A	417	LHG	C3-O3-P-O4
31	A	417	LHG	C4-O6-P-O3
31	A	417	LHG	C4-O6-P-O4
31	D	408	LHG	C3-O3-P-O4
31	D	408	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
31	D	408	LHG	C4-O6-P-O4
31	D	409	LHG	C4-O6-P-O4
31	E	101	LHG	O1-C1-C2-C3
31	E	101	LHG	C1-C2-C3-O3
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	d	407	LHG	O1-C1-C2-C3
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C3-O3-P-O5
31	d	408	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O3
31	d	408	LHG	C4-O6-P-O4
31	d	409	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
31	l	101	LHG	C4-O6-P-O3
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
33	C	501	LMG	C11-C10-O7-C8
33	Z	102	LMG	C2-C1-O1-C7
33	Z	102	LMG	O9-C10-O7-C8
33	Z	102	LMG	C11-C10-O7-C8
33	a	416	LMG	O9-C10-O7-C8
33	c	520	LMG	C11-C10-O7-C8
33	z	101	LMG	C11-C10-O7-C8
34	B	623	HTG	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
34	B	624	HTG	O5-C1-S1-C1'
35	B	629	LMT	C2'-C1'-O1'-C1
35	B	629	LMT	O5'-C1'-O1'-C1
35	B	631	LMT	C2'-C1'-O1'-C1
35	B	631	LMT	O5'-C1'-O1'-C1
35	D	402	LMT	C2'-C1'-O1'-C1
35	D	402	LMT	O5'-C1'-O1'-C1
35	D	403	LMT	C3'-C4'-O1B-C1B
35	I	101	LMT	C2'-C1'-O1'-C1
35	I	101	LMT	O5'-C1'-O1'-C1
35	M	103	LMT	C2'-C1'-O1'-C1
35	b	621	LMT	O5'-C1'-O1'-C1
35	b	627	LMT	O5'-C1'-O1'-C1
38	E	103	HEM	C2C-C3C-CAC-CBC
38	E	103	HEM	C4C-C3C-CAC-CBC
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	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
35	I	101	LMT	C3'-C4'-O1B-C1B
33	c	520	LMG	O9-C10-O7-C8
33	z	101	LMG	O9-C10-O7-C8
23	A	408	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	C	514	CLA	CBD-CGD-O2D-CED
26	L	101	SQD	C8-C7-O47-C45
33	a	416	LMG	C11-C10-O7-C8
23	B	603	CLA	C4-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	D	405	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	c	504	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
29	A	414	PL9	C15-C14-C16-C17
29	A	414	PL9	C25-C24-C26-C27
23	B	603	CLA	C2-C3-C5-C6
23	B	614	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	D	405	CLA	C2-C3-C5-C6
23	b	604	CLA	C2-C3-C5-C6
23	c	504	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
29	A	414	PL9	C13-C14-C16-C17
29	A	414	PL9	C23-C24-C26-C27
23	C	504	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	C3-C5-C6-C7
33	c	520	LMG	O6-C5-C6-O5
33	C	501	LMG	O9-C10-O7-C8
35	D	403	LMT	C4'-C5'-C6'-O6'
23	b	616	CLA	C3-C5-C6-C7
23	c	506	CLA	C3-C5-C6-C7
23	c	501	CLA	CBD-CGD-O2D-CED
31	D	408	LHG	O2-C2-C3-O3
31	E	101	LHG	O2-C2-C3-O3
31	d	408	LHG	O2-C2-C3-O3
34	B	624	HTG	O5-C5-C6-O6
33	Z	101	LMG	O6-C5-C6-O5
23	d	401	CLA	CBD-CGD-O2D-CED
35	I	101	LMT	O5B-C5B-C6B-O6B
23	a	405	CLA	CBD-CGD-O2D-CED
34	c	521	HTG	S1-C1'-C2'-C3'
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	b	614	CLA	C2-C3-C5-C6
34	b	625	HTG	O5-C5-C6-O6
29	A	414	PL9	C14-C16-C17-C18
29	D	407	PL9	C39-C41-C42-C43
35	M	103	LMT	O5'-C5'-C6'-O6'
35	B	630	LMT	O5'-C1'-O1'-C1
35	E	102	LMT	O5'-C1'-O1'-C1
35	M	103	LMT	O5'-C1'-O1'-C1
35	a	417	LMT	O5'-C1'-O1'-C1
35	e	102	LMT	O5'-C1'-O1'-C1
23	C	502	CLA	CBD-CGD-O2D-CED
35	D	403	LMT	O5'-C5'-C6'-O6'
35	D	403	LMT	O5B-C5B-C6B-O6B
23	c	512	CLA	C3-C5-C6-C7
35	D	403	LMT	C4B-C5B-C6B-O6B
31	D	408	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
23	A	408	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CBA-CGA-O2A-C1
31	D	409	LHG	C24-C23-O8-C6
34	d	411	HTG	C4-C5-C6-O6
35	E	102	LMT	C4'-C5'-C6'-O6'
23	C	508	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	d	404	CLA	C4-C3-C5-C6
23	d	404	CLA	C2-C3-C5-C6
23	B	601	CLA	C11-C10-C8-C9
23	B	605	CLA	C6-C7-C8-C9
23	B	616	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	c	502	CLA	C14-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C9
33	c	520	LMG	C4-C5-C6-O5
35	B	630	LMT	C2'-C1'-O1'-C1
35	E	102	LMT	C2'-C1'-O1'-C1
35	a	417	LMT	C2'-C1'-O1'-C1
35	e	102	LMT	C2'-C1'-O1'-C1
33	j	101	LMG	C10-C11-C12-C13
25	D	406	BCR	C7-C8-C9-C34
25	H	101	BCR	C7-C8-C9-C34
25	d	405	BCR	C7-C8-C9-C34
25	d	405	BCR	C37-C22-C23-C24
34	b	628	HTG	S1-C1'-C2'-C3'
25	H	101	BCR	C7-C8-C9-C10
23	C	511	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	O1A-CGA-O2A-C1
34	B	623	HTG	C4-C5-C6-O6
26	A	410	SQD	C8-C7-O47-C45
23	A	405	CLA	C15-C16-C17-C18
23	C	508	CLA	C5-C6-C7-C8
33	J	101	LMG	O6-C5-C6-O5
23	C	502	CLA	C15-C16-C17-C18
34	b	623	HTG	O5-C5-C6-O6
23	A	408	CLA	C12-C13-C15-C16
26	A	412	SQD	C26-C27-C28-C29
25	T	101	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
35	B	631	LMT	O1'-C1-C2-C3
23	C	514	CLA	O1D-CGD-O2D-CED
23	b	606	CLA	C10-C11-C12-C13
33	Z	102	LMG	C10-C11-C12-C13
33	c	520	LMG	C10-C11-C12-C13
23	A	408	CLA	O1A-CGA-O2A-C1
23	a	408	CLA	CBA-CGA-O2A-C1
23	B	601	CLA	C5-C6-C7-C8
23	B	614	CLA	C5-C6-C7-C8
35	I	101	LMT	O1'-C1-C2-C3
35	B	631	LMT	C4'-C5'-C6'-O6'
23	b	606	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
34	b	628	HTG	O5-C5-C6-O6
34	B	624	HTG	C4-C5-C6-O6
36	C	518	DGD	C1A-C2A-C3A-C4A
31	D	409	LHG	O10-C23-O8-C6
31	D	408	LHG	C32-C33-C34-C35
23	B	601	CLA	C15-C16-C17-C18
23	B	605	CLA	C5-C6-C7-C8
23	B	606	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	C	506	CLA	C8-C10-C11-C12
23	a	404	CLA	C15-C16-C17-C18
23	a	408	CLA	C5-C6-C7-C8
23	b	611	CLA	C15-C16-C17-C18
23	b	616	CLA	C5-C6-C7-C8
23	c	502	CLA	C15-C16-C17-C18
23	d	404	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	C13-C15-C16-C17
26	A	410	SQD	O49-C7-O47-C45
35	B	631	LMT	O5'-C5'-C6'-O6'
35	I	101	LMT	C4B-C5B-C6B-O6B
23	b	605	CLA	C8-C10-C11-C12
36	c	516	DGD	O6D-C5D-C6D-O5D
23	C	504	CLA	O1D-CGD-O2D-CED
23	b	601	CLA	C8-C10-C11-C12
23	c	510	CLA	C10-C11-C12-C13
23	D	405	CLA	C3-C5-C6-C7
23	B	616	CLA	C10-C11-C12-C13
31	d	408	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	B	602	CLA	C15-C16-C17-C18
23	b	604	CLA	CBD-CGD-O2D-CED
36	C	517	DGD	O6D-C5D-C6D-O5D
26	D	413	SQD	C7-C8-C9-C10
23	C	511	CLA	C5-C6-C7-C8
23	c	507	CLA	C8-C10-C11-C12
23	B	604	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
36	C	517	DGD	C4D-C5D-C6D-O5D
23	b	614	CLA	C3-C5-C6-C7
33	b	620	LMG	C11-C10-O7-C8
35	D	402	LMT	C1-C2-C3-C4
23	c	501	CLA	O1D-CGD-O2D-CED
33	b	620	LMG	O9-C10-O7-C8
35	b	621	LMT	C2'-C1'-O1'-C1
35	b	627	LMT	C2'-C1'-O1'-C1
35	m	102	LMT	C2'-C1'-O1'-C1
36	C	517	DGD	C2E-C1E-O5D-C6D
36	C	518	DGD	C2E-C1E-O5D-C6D
35	E	102	LMT	O5'-C5'-C6'-O6'
34	B	623	HTG	O5-C5-C6-O6
34	d	411	HTG	O5-C5-C6-O6
25	K	102	BCR	C7-C8-C9-C34
31	E	101	LHG	C11-C10-C9-C8
23	c	507	CLA	C2A-CAA-CBA-CGA
36	c	516	DGD	C4D-C5D-C6D-O5D
27	B	625	GOL	C1-C2-C3-O3
27	b	624	GOL	O1-C1-C2-C3
31	A	416	LHG	O1-C1-C2-C3
23	a	408	CLA	O1A-CGA-O2A-C1
23	d	404	CLA	C3-C5-C6-C7
23	c	512	CLA	C13-C15-C16-C17
26	B	620	SQD	O5-C1-O6-C44
33	Z	102	LMG	O6-C1-O1-C7
35	m	102	LMT	O5'-C1'-O1'-C1
36	C	517	DGD	O6E-C1E-O5D-C6D
23	b	614	CLA	C15-C16-C17-C18
23	b	615	CLA	C13-C15-C16-C17
23	B	601	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C15-C16-C17-C18
23	a	404	CLA	CBD-CGD-O2D-CED
26	A	410	SQD	C11-C10-C9-C8
23	b	601	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C16-C17-C18-C20
23	d	404	CLA	O1A-CGA-O2A-C1
34	C	522	HTG	O5-C5-C6-O6
26	A	410	SQD	C9-C10-C11-C12
35	b	627	LMT	C2-C3-C4-C5
26	a	410	SQD	C11-C12-C13-C14
31	d	409	LHG	C32-C33-C34-C35
33	B	621	LMG	C17-C18-C19-C20
35	e	102	LMT	C3-C4-C5-C6
35	m	102	LMT	C11-C10-C9-C8
36	C	517	DGD	CAA-CBA-CCA-CDA
26	A	412	SQD	C18-C19-C20-C21
26	L	101	SQD	C24-C25-C26-C27
26	a	410	SQD	C9-C10-C11-C12
33	Z	101	LMG	C16-C17-C18-C19
33	a	416	LMG	C31-C32-C33-C34
33	b	620	LMG	C38-C39-C40-C41
33	Z	101	LMG	C17-C18-C19-C20
27	A	411	GOL	O1-C1-C2-O2
27	B	625	GOL	O1-C1-C2-O2
27	B	626	GOL	O2-C2-C3-O3
27	d	402	GOL	O1-C1-C2-O2
31	d	407	LHG	O1-C1-C2-O2
35	B	631	LMT	C2-C1-O1'-C1'
35	b	627	LMT	C2-C1-O1'-C1'
26	L	101	SQD	C14-C15-C16-C17
33	c	519	LMG	C33-C34-C35-C36
36	C	518	DGD	C7B-C8B-C9B-CAB
23	d	401	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C4B-C3B-CAB-CBB
23	b	616	CLA	C4B-C3B-CAB-CBB
26	a	410	SQD	C13-C14-C15-C16
23	B	608	CLA	C16-C17-C18-C19
31	d	408	LHG	C13-C14-C15-C16
31	d	409	LHG	C34-C35-C36-C37
36	C	518	DGD	C9A-CAA-CBA-CCA
36	H	102	DGD	CAB-CBB-CCB-CDB
26	D	413	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C15-C16-C17-C18
31	A	417	LHG	C23-C24-C25-C26
23	B	605	CLA	C8-C10-C11-C12
26	f	101	SQD	C28-C29-C30-C31
31	A	417	LHG	C17-C18-C19-C20
31	E	101	LHG	C24-C25-C26-C27
36	c	517	DGD	C7A-C8A-C9A-CAA
31	D	409	LHG	C29-C30-C31-C32
23	c	509	CLA	C5-C6-C7-C8
33	c	519	LMG	C4-C5-C6-O5
34	b	625	HTG	C3'-C4'-C5'-C6'
23	B	608	CLA	C16-C17-C18-C20
33	C	501	LMG	C37-C38-C39-C40
35	B	630	LMT	C2-C3-C4-C5
31	d	409	LHG	C24-C23-O8-C6
33	C	520	LMG	C12-C13-C14-C15
33	a	416	LMG	C30-C31-C32-C33
23	c	509	CLA	C3-C5-C6-C7
23	C	502	CLA	O1D-CGD-O2D-CED
23	a	405	CLA	O1D-CGD-O2D-CED
26	a	412	SQD	C10-C11-C12-C13
31	d	408	LHG	C14-C15-C16-C17
31	l	101	LHG	C27-C28-C29-C30
33	B	621	LMG	C36-C37-C38-C39
33	C	520	LMG	C11-C12-C13-C14
36	H	102	DGD	CCA-CDA-CEA-CFA
34	C	522	HTG	S1-C1'-C2'-C3'
33	J	101	LMG	C30-C31-C32-C33
26	a	412	SQD	C25-C26-C27-C28
35	B	629	LMT	C5-C6-C7-C8
33	B	621	LMG	C28-C29-C30-C31
23	B	601	CLA	O1A-CGA-O2A-C1
23	C	506	CLA	C2B-C3B-CAB-CBB
23	a	405	CLA	C2B-C3B-CAB-CBB
23	b	607	CLA	C2B-C3B-CAB-CBB
23	b	616	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C2B-C3B-CAB-CBB
33	B	621	LMG	C11-C10-O7-C8
36	c	516	DGD	C5A-C6A-C7A-C8A
36	H	102	DGD	CBA-CCA-CDA-CEA
33	C	520	LMG	C28-C29-C30-C31
26	A	412	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	D	413	SQD	C24-C25-C26-C27
35	b	621	LMT	C3-C4-C5-C6
31	d	409	LHG	O10-C23-O8-C6
26	A	412	SQD	C16-C17-C18-C19
35	b	627	LMT	C3-C4-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
26	a	410	SQD	C29-C30-C31-C32
26	A	410	SQD	C15-C16-C17-C18
26	L	101	SQD	C26-C27-C28-C29
33	z	101	LMG	C18-C19-C20-C21
34	B	622	HTG	C1'-C2'-C3'-C4'
23	b	601	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	C6-C7-C8-C9
33	b	620	LMG	C14-C15-C16-C17
26	D	413	SQD	C32-C33-C34-C35
36	C	518	DGD	CCB-CDB-CEB-CFB
36	C	518	DGD	O6E-C1E-O5D-C6D
26	f	101	SQD	C25-C26-C27-C28
31	D	408	LHG	C13-C14-C15-C16
26	B	620	SQD	C33-C34-C35-C36
33	j	101	LMG	C29-C30-C31-C32
31	A	417	LHG	C13-C14-C15-C16
31	A	417	LHG	C25-C26-C27-C28
36	H	102	DGD	C6A-C7A-C8A-C9A
26	L	101	SQD	C27-C28-C29-C30
26	a	412	SQD	C27-C28-C29-C30
33	a	416	LMG	C35-C36-C37-C38
23	B	610	CLA	C16-C17-C18-C19
23	B	601	CLA	C10-C11-C12-C13
26	L	101	SQD	C13-C14-C15-C16
26	a	412	SQD	C24-C25-C26-C27
33	j	101	LMG	C38-C39-C40-C41
26	D	413	SQD	C11-C10-C9-C8
23	b	606	CLA	C8-C10-C11-C12
25	Y	101	BCR	C37-C22-C23-C24
25	y	101	BCR	C37-C22-C23-C24
31	D	409	LHG	C13-C14-C15-C16
31	d	408	LHG	C16-C17-C18-C19
23	b	605	CLA	C3-C5-C6-C7
25	y	101	BCR	C21-C22-C23-C24
33	b	620	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
23	B	610	CLA	C16-C17-C18-C20
23	c	502	CLA	C16-C17-C18-C20
26	a	410	SQD	C30-C31-C32-C33
33	J	101	LMG	C36-C37-C38-C39
23	c	505	CLA	C4-C3-C5-C6
29	D	407	PL9	C15-C14-C16-C17
23	c	505	CLA	C2-C3-C5-C6
23	b	611	CLA	C8-C10-C11-C12
31	A	416	LHG	C32-C33-C34-C35
33	Z	101	LMG	C4-C5-C6-O5
23	c	513	CLA	C10-C11-C12-C13
31	D	409	LHG	C15-C16-C17-C18
33	J	101	LMG	C20-C21-C22-C23
34	B	624	HTG	C3'-C4'-C5'-C6'
33	B	621	LMG	O9-C10-O7-C8
33	J	101	LMG	C34-C35-C36-C37
23	C	509	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	C	507	CLA	C16-C17-C18-C19
31	l	101	LHG	C14-C15-C16-C17
34	b	628	HTG	C1'-C2'-C3'-C4'
36	c	516	DGD	O6E-C5E-C6E-O5E
26	B	620	SQD	C18-C19-C20-C21
36	H	102	DGD	CBB-CCB-CDB-CEB
33	Z	102	LMG	O6-C5-C6-O5
34	B	627	HTG	O5-C5-C6-O6
36	C	517	DGD	O6E-C5E-C6E-O5E
23	C	503	CLA	C3-C5-C6-C7
23	b	601	CLA	C3-C5-C6-C7
23	b	608	CLA	C3-C5-C6-C7
35	B	629	LMT	C11-C10-C9-C8
35	e	102	LMT	C5-C6-C7-C8
31	d	407	LHG	C25-C26-C27-C28
36	C	519	DGD	CAA-CBA-CCA-CDA
23	C	510	CLA	C2-C1-O2A-CGA
34	b	625	HTG	C4-C5-C6-O6
33	c	520	LMG	C37-C38-C39-C40
23	B	605	CLA	C4-C3-C5-C6
23	B	615	CLA	C2-C3-C5-C6
29	D	407	PL9	C13-C14-C16-C17
23	c	512	CLA	C10-C11-C12-C13
33	C	520	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	Z	102	LMG	C19-C20-C21-C22
23	A	404	CLA	C2A-CAA-CBA-CGA
23	B	610	CLA	C2A-CAA-CBA-CGA
31	e	101	LHG	C26-C27-C28-C29
26	a	410	SQD	C27-C28-C29-C30
31	A	417	LHG	C24-C25-C26-C27
33	c	519	LMG	C34-C35-C36-C37
35	E	102	LMT	C5-C6-C7-C8
35	b	627	LMT	C11-C10-C9-C8
23	B	615	CLA	C16-C17-C18-C20
27	a	411	GOL	O2-C2-C3-O3
31	A	416	LHG	O1-C1-C2-O2
31	E	101	LHG	O1-C1-C2-O2
23	b	601	CLA	O1A-CGA-O2A-C1
33	B	621	LMG	C32-C33-C34-C35
36	C	518	DGD	CCA-CDA-CEA-CFA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
36	c	516	DGD	O6E-C1E-O5D-C6D
31	d	408	LHG	C30-C31-C32-C33
36	C	517	DGD	C3B-C4B-C5B-C6B
31	A	416	LHG	C25-C26-C27-C28
31	d	407	LHG	C34-C35-C36-C37
23	c	506	CLA	C13-C15-C16-C17
33	j	101	LMG	O6-C5-C6-O5
35	I	101	LMT	O5'-C5'-C6'-O6'
31	d	407	LHG	C32-C33-C34-C35
23	B	610	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	b	614	CLA	C12-C13-C15-C16
23	d	403	CLA	C11-C12-C13-C15
23	a	404	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
26	B	620	SQD	C24-C23-O48-C46
23	b	608	CLA	C13-C15-C16-C17
31	l	101	LHG	C12-C13-C14-C15
23	C	514	CLA	C4-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
33	B	621	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
35	b	621	LMT	C4-C5-C6-C7
31	A	416	LHG	C18-C19-C20-C21
23	B	604	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C10-C8-C9
31	l	101	LHG	C16-C17-C18-C19
23	c	502	CLA	C16-C17-C18-C19
35	m	102	LMT	C7-C8-C9-C10
36	C	518	DGD	C8A-C9A-CAA-CBA
23	c	508	CLA	C5-C6-C7-C8
34	c	522	HTG	O5-C5-C6-O6
26	L	101	SQD	C44-C45-C46-O48
26	a	412	SQD	O6-C44-C45-C46
31	D	409	LHG	C4-C5-C6-O8
35	B	629	LMT	C4'-C5'-C6'-O6'
36	c	517	DGD	C9A-CAA-CBA-CCA
36	h	102	DGD	CBB-CCB-CDB-CEB
31	A	417	LHG	C12-C13-C14-C15
33	j	101	LMG	C21-C22-C23-C24
23	B	602	CLA	C13-C15-C16-C17
33	a	416	LMG	C39-C40-C41-C42
23	A	406	CLA	C2C-C3C-CAC-CBC
31	d	408	LHG	C9-C10-C11-C12
35	B	629	LMT	C7-C8-C9-C10
36	c	517	DGD	C1B-C2B-C3B-C4B
23	C	506	CLA	C4-C3-C5-C6
23	C	507	CLA	C2-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
23	b	613	CLA	C5-C6-C7-C8
23	d	404	CLA	C5-C6-C7-C8
23	B	615	CLA	C16-C17-C18-C19
31	d	409	LHG	C33-C34-C35-C36
31	l	101	LHG	C34-C35-C36-C37
25	K	102	BCR	C7-C8-C9-C10
23	B	615	CLA	C13-C15-C16-C17
23	c	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	CBD-CGD-O2D-CED
26	a	410	SQD	C34-C35-C36-C37
31	D	408	LHG	C28-C29-C30-C31
33	C	520	LMG	C37-C38-C39-C40
31	d	407	LHG	C33-C34-C35-C36
33	J	101	LMG	C14-C15-C16-C17
36	h	102	DGD	C5B-C6B-C7B-C8B
31	D	409	LHG	C28-C29-C30-C31
33	c	519	LMG	C31-C32-C33-C34
34	B	623	HTG	C2'-C3'-C4'-C5'
26	B	620	SQD	O10-C23-O48-C46
33	C	520	LMG	C15-C16-C17-C18
23	D	405	CLA	C8-C10-C11-C12
35	B	631	LMT	C7-C8-C9-C10
36	c	517	DGD	CBA-CCA-CDA-CEA
23	c	511	CLA	CBA-CGA-O2A-C1
26	a	410	SQD	C10-C11-C12-C13
26	f	101	SQD	C31-C32-C33-C34
35	a	417	LMT	C4-C5-C6-C7
35	M	103	LMT	C4'-C5'-C6'-O6'
23	C	511	CLA	C4-C3-C5-C6
23	B	604	CLA	C2-C3-C5-C6
23	a	404	CLA	O1D-CGD-O2D-CED
31	A	416	LHG	C29-C30-C31-C32
31	E	101	LHG	C25-C26-C27-C28
33	Z	101	LMG	C18-C19-C20-C21
35	D	402	LMT	C3-C4-C5-C6
36	c	518	DGD	CAB-CBB-CCB-CDB
26	f	101	SQD	O6-C44-C45-O47
33	a	416	LMG	O7-C8-C9-O8
36	C	519	DGD	CBA-CCA-CDA-CEA
31	D	408	LHG	C17-C18-C19-C20
23	a	404	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C3-C5-C6-C7
33	c	519	LMG	C21-C22-C23-C24
35	D	402	LMT	C5-C6-C7-C8
23	C	512	CLA	CBA-CGA-O2A-C1
23	b	611	CLA	CBA-CGA-O2A-C1
26	a	412	SQD	C24-C23-O48-C46
23	B	601	CLA	CAA-CBA-CGA-O2A
35	a	417	LMT	C11-C10-C9-C8
31	l	101	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
23	b	612	CLA	C10-C11-C12-C13
23	b	602	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
29	a	414	PL9	C20-C19-C21-C22
34	b	628	HTG	C3'-C4'-C5'-C6'
33	C	520	LMG	C36-C37-C38-C39
31	A	417	LHG	O1-C1-C2-O2
23	A	408	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
23	B	615	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C12-C13-C14
35	M	103	LMT	C6-C7-C8-C9
23	A	406	CLA	C4B-C3B-CAB-CBB
23	A	408	CLA	C4B-C3B-CAB-CBB
23	B	607	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
23	d	403	CLA	C4B-C3B-CAB-CBB
35	B	630	LMT	C6-C7-C8-C9
36	c	516	DGD	C2A-C1A-O1G-C1G
31	e	101	LHG	C11-C12-C13-C14
36	c	517	DGD	C2E-C1E-O5D-C6D
23	B	613	CLA	C15-C16-C17-C18
35	e	102	LMT	C4'-C5'-C6'-O6'
34	B	623	HTG	C3'-C4'-C5'-C6'
34	c	521	HTG	C4-C5-C6-O6
23	B	604	CLA	C6-C7-C8-C10
23	B	614	CLA	C12-C13-C15-C16
23	B	615	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	a	408	CLA	C11-C10-C8-C7
23	b	604	CLA	C11-C10-C8-C7
23	b	615	CLA	C12-C13-C15-C16
23	c	502	CLA	C12-C13-C15-C16
23	d	404	CLA	C11-C10-C8-C7
23	B	611	CLA	C13-C15-C16-C17
36	C	519	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
26	A	410	SQD	C12-C13-C14-C15
33	B	621	LMG	C37-C38-C39-C40
23	c	511	CLA	O1A-CGA-O2A-C1
23	C	507	CLA	C3A-C2A-CAA-CBA
29	a	414	PL9	C45-C44-C46-C47
36	h	102	DGD	O2G-C1B-C2B-C3B
36	H	102	DGD	C7B-C8B-C9B-CAB
23	D	405	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C24-C23-O8-C6
25	b	619	BCR	C37-C22-C23-C24
24	A	407	PHO	C2C-C3C-CAC-CBC
33	B	621	LMG	C14-C15-C16-C17
33	j	101	LMG	C35-C36-C37-C38
36	c	517	DGD	CAA-CBA-CCA-CDA
35	E	102	LMT	C9-C10-C11-C12
34	B	622	HTG	C2'-C3'-C4'-C5'
36	c	517	DGD	C9B-CAB-CBB-CCB
23	B	601	CLA	C2A-CAA-CBA-CGA
26	A	410	SQD	O6-C44-C45-C46
29	a	414	PL9	C14-C16-C17-C18
31	E	101	LHG	C4-C5-C6-O8
31	e	101	LHG	C4-C5-C6-O8
33	b	620	LMG	O1-C7-C8-C9
26	f	101	SQD	C34-C35-C36-C37
33	Z	102	LMG	C17-C18-C19-C20
36	c	518	DGD	CBA-CCA-CDA-CEA
23	b	603	CLA	C13-C15-C16-C17
35	B	629	LMT	O5'-C5'-C6'-O6'
29	d	406	PL9	C15-C14-C16-C17
36	c	517	DGD	C7B-C8B-C9B-CAB
23	C	512	CLA	O1A-CGA-O2A-C1
31	e	101	LHG	C14-C15-C16-C17
25	D	406	BCR	C23-C24-C25-C30
25	b	617	BCR	C1-C6-C7-C8
31	D	409	LHG	C2-C3-O3-P
36	h	102	DGD	CDA-CEA-CFA-CGA
36	C	519	DGD	CDA-CEA-CFA-CGA
33	B	621	LMG	C33-C34-C35-C36
36	c	517	DGD	C2B-C3B-C4B-C5B
36	c	516	DGD	CDB-CEB-CFB-CGB
23	b	615	CLA	C5-C6-C7-C8
26	A	410	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
26	B	620	SQD	O47-C45-C46-O48
26	L	101	SQD	O47-C45-C46-O48
31	D	409	LHG	O7-C5-C6-O8
33	b	620	LMG	O1-C7-C8-O7
29	A	414	PL9	C4-C3-C7-C8
29	a	414	PL9	C4-C3-C7-C8
33	Z	101	LMG	C33-C34-C35-C36
36	C	517	DGD	C8A-C9A-CAA-CBA
36	C	517	DGD	C9A-CAA-CBA-CCA
24	D	401	PHO	C4-C3-C5-C6
31	d	409	LHG	C30-C31-C32-C33
24	D	401	PHO	C2-C3-C5-C6
29	a	414	PL9	C18-C19-C21-C22
29	a	414	PL9	C43-C44-C46-C47
36	H	102	DGD	C9B-CAB-CBB-CCB
33	C	520	LMG	C10-C11-C12-C13
23	C	503	CLA	C14-C13-C15-C16
24	a	407	PHO	C2C-C3C-CAC-CBC
36	c	517	DGD	O6E-C1E-O5D-C6D
23	B	604	CLA	C13-C15-C16-C17
33	a	416	LMG	C20-C21-C22-C23
34	b	628	HTG	C2'-C3'-C4'-C5'
23	C	512	CLA	C3-C5-C6-C7
25	k	101	BCR	C9-C10-C11-C12
29	d	406	PL9	C13-C14-C16-C17
23	B	612	CLA	C10-C11-C12-C13
23	C	507	CLA	C8-C10-C11-C12
24	a	407	PHO	C8-C10-C11-C12
26	A	412	SQD	C15-C16-C17-C18
33	C	520	LMG	C16-C17-C18-C19
36	h	102	DGD	C9A-CAA-CBA-CCA
23	b	611	CLA	O1A-CGA-O2A-C1
23	b	611	CLA	C3-C5-C6-C7
26	L	101	SQD	C24-C23-O48-C46
31	d	407	LHG	C24-C23-O8-C6
33	a	416	LMG	C29-C28-O8-C9
33	C	520	LMG	C13-C14-C15-C16
33	Z	102	LMG	C11-C12-C13-C14
23	C	506	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C7
23	b	616	CLA	C11-C12-C13-C15
23	A	406	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	B	611	CLA	C8-C10-C11-C12
23	c	506	CLA	C15-C16-C17-C18
23	d	401	CLA	C15-C16-C17-C18
25	Y	101	BCR	C21-C22-C23-C24
23	D	405	CLA	O1A-CGA-O2A-C1
26	a	412	SQD	O10-C23-O48-C46
33	Z	101	LMG	C8-C7-O1-C1
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	517	DGD	C5D-C6D-O5D-C1E
23	c	512	CLA	C15-C16-C17-C18
29	A	414	PL9	C30-C29-C31-C32
31	D	408	LHG	O10-C23-O8-C6
36	C	519	DGD	O1A-C1A-O1G-C1G
36	c	516	DGD	O1A-C1A-O1G-C1G
38	e	103	HEM	C2B-C3B-CAB-CBB
31	d	408	LHG	C28-C29-C30-C31
23	C	510	CLA	CBD-CGD-O2D-CED
23	A	408	CLA	C8-C10-C11-C12
23	b	603	CLA	C10-C11-C12-C13
26	B	620	SQD	C46-C45-O47-C7
26	L	101	SQD	C46-C45-O47-C7
23	B	604	CLA	C2C-C3C-CAC-CBC
23	A	404	CLA	C13-C15-C16-C17
23	C	507	CLA	C13-C15-C16-C17
36	C	519	DGD	O6E-C5E-C6E-O5E
36	h	102	DGD	C9B-CAB-CBB-CCB
23	a	408	CLA	C16-C17-C18-C20
31	e	101	LHG	C9-C10-C11-C12
33	a	416	LMG	C36-C37-C38-C39
31	d	407	LHG	O10-C23-O8-C6
23	C	510	CLA	C3-C5-C6-C7
23	C	508	CLA	C13-C15-C16-C17
35	e	102	LMT	C2B-C1B-O1B-C4'
26	L	101	SQD	C12-C13-C14-C15
36	C	519	DGD	O6D-C1D-O3G-C3G
26	A	412	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	f	101	SQD	C44-C45-C46-O48
29	a	414	PL9	C9-C11-C12-C13
23	b	604	CLA	C13-C15-C16-C17
23	b	602	CLA	C10-C11-C12-C13
23	b	601	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	414	PL9	C2-C3-C7-C8
31	A	416	LHG	C24-C25-C26-C27
23	B	604	CLA	C3-C5-C6-C7
31	A	417	LHG	C14-C15-C16-C17
31	d	408	LHG	C26-C27-C28-C29
26	a	410	SQD	O6-C44-C45-O47
26	f	101	SQD	O47-C45-C46-O48
23	b	603	CLA	C11-C10-C8-C9
23	b	609	CLA	C6-C7-C8-C9
23	c	509	CLA	C14-C13-C15-C16
23	A	405	CLA	C2C-C3C-CAC-CBC
33	b	620	LMG	C35-C36-C37-C38
34	b	623	HTG	C4-C5-C6-O6
31	D	409	LHG	C17-C18-C19-C20
26	A	412	SQD	C8-C7-O47-C45
23	B	616	CLA	C2-C1-O2A-CGA
36	c	516	DGD	C2E-C1E-O5D-C6D
23	A	406	CLA	C16-C17-C18-C19
36	h	102	DGD	CBA-CCA-CDA-CEA
29	A	414	PL9	C45-C44-C46-C47
23	C	513	CLA	C3-C5-C6-C7
31	d	408	LHG	O10-C23-O8-C6
33	a	416	LMG	O10-C28-O8-C9
23	b	602	CLA	C2A-CAA-CBA-CGA
31	d	409	LHG	C9-C10-C11-C12
26	L	101	SQD	O10-C23-O48-C46
31	A	416	LHG	C11-C12-C13-C14
31	A	416	LHG	C33-C34-C35-C36
33	B	621	LMG	O6-C5-C6-O5
35	E	102	LMT	O1'-C1-C2-C3
26	A	410	SQD	C18-C19-C20-C21
36	H	102	DGD	CCB-CDB-CEB-CFB
23	C	513	CLA	C4B-C3B-CAB-CBB
23	b	601	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB
23	c	512	CLA	CBA-CGA-O2A-C1
31	d	408	LHG	C24-C23-O8-C6
31	E	101	LHG	C23-C24-C25-C26
29	D	407	PL9	C45-C44-C46-C47
23	B	608	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	d	401	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	b	601	CLA	C2-C3-C5-C6
35	e	102	LMT	C4-C5-C6-C7
26	D	413	SQD	C27-C28-C29-C30
31	l	101	LHG	O6-C4-C5-C6
23	c	509	CLA	CBD-CGD-O2D-CED
26	A	412	SQD	O49-C7-O47-C45
23	B	606	CLA	C10-C11-C12-C13
23	c	509	CLA	C13-C15-C16-C17
23	A	406	CLA	C12-C13-C15-C16
23	B	604	CLA	C11-C12-C13-C15
23	B	605	CLA	C6-C7-C8-C10
23	C	514	CLA	C6-C7-C8-C10
23	c	509	CLA	C12-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C10
36	h	102	DGD	C4B-C5B-C6B-C7B
23	A	408	CLA	C16-C17-C18-C19
36	c	516	DGD	CDA-CEA-CFA-CGA
31	E	101	LHG	C15-C16-C17-C18
31	E	101	LHG	C10-C11-C12-C13
23	b	605	CLA	O1A-CGA-O2A-C1
31	d	409	LHG	C29-C30-C31-C32
40	V	202	HEC	C4C-C3C-CAC-CBC
33	j	101	LMG	C19-C20-C21-C22
23	C	514	CLA	C2-C3-C5-C6
29	A	414	PL9	C28-C29-C31-C32
23	A	405	CLA	C13-C15-C16-C17
23	a	408	CLA	C11-C10-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	b	614	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C12-C13-C14
23	b	609	CLA	O1A-CGA-O2A-C1
23	c	508	CLA	C16-C17-C18-C19
31	D	408	LHG	C33-C34-C35-C36
35	M	103	LMT	O5B-C5B-C6B-O6B
33	j	101	LMG	C16-C17-C18-C19
31	d	409	LHG	C26-C27-C28-C29
34	B	622	HTG	C3'-C4'-C5'-C6'
34	c	521	HTG	C3'-C4'-C5'-C6'
31	E	101	LHG	O7-C5-C6-O8
31	e	101	LHG	O7-C5-C6-O8
35	M	103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
35	m	102	LMT	C9-C10-C11-C12
26	f	101	SQD	O6-C44-C45-C46
33	a	416	LMG	C7-C8-C9-O8
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	O1A-CGA-O2A-C1
36	c	518	DGD	O1A-C1A-O1G-C1G
33	Z	101	LMG	C37-C38-C39-C40
36	h	102	DGD	CAB-CBB-CCB-CDB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	512	CLA	CHA-CBD-CGD-O1D
25	t	101	BCR	C15-C16-C17-C18
31	A	417	LHG	C3-O3-P-O6
31	A	417	LHG	C4-O6-P-O5
31	D	408	LHG	C4-O6-P-O5
31	E	101	LHG	C4-O6-P-O5
31	d	408	LHG	C4-O6-P-O5
31	d	409	LHG	C4-O6-P-O3
31	d	409	LHG	C4-O6-P-O5
40	V	202	HEC	C2C-C3C-CAC-CBC
34	B	623	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
33	Z	102	LMG	C15-C16-C17-C18
23	A	406	CLA	C2B-C3B-CAB-CBB
23	B	602	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	b	601	CLA	C2B-C3B-CAB-CBB
35	B	629	LMT	C3-C4-C5-C6
23	B	605	CLA	C2-C3-C5-C6
29	A	414	PL9	C43-C44-C46-C47
31	d	407	LHG	C11-C12-C13-C14
23	b	613	CLA	O1D-CGD-O2D-CED
35	D	402	LMT	O1'-C1-C2-C3
23	b	615	CLA	C16-C17-C18-C20
35	D	403	LMT	C5-C6-C7-C8
31	l	101	LHG	C9-C10-C11-C12
33	j	101	LMG	C14-C15-C16-C17
31	D	409	LHG	C30-C31-C32-C33
23	C	507	CLA	C5-C6-C7-C8
29	d	406	PL9	C9-C11-C12-C13
33	c	519	LMG	C29-C30-C31-C32
35	D	403	LMT	C6-C7-C8-C9
23	b	605	CLA	CBA-CGA-O2A-C1
23	A	408	CLA	C6-C7-C8-C9
23	B	610	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	505	CLA	C11-C12-C13-C14
23	A	408	CLA	C6-C7-C8-C10
23	b	603	CLA	C6-C7-C8-C10
23	b	614	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C12-C13-C15
23	c	510	CLA	O1A-CGA-O2A-C1
23	B	604	CLA	C4C-C3C-CAC-CBC
31	D	409	LHG	C10-C11-C12-C13
33	C	501	LMG	C12-C13-C14-C15
23	b	604	CLA	O1D-CGD-O2D-CED
31	e	101	LHG	C24-C25-C26-C27
23	A	406	CLA	C4C-C3C-CAC-CBC
36	C	519	DGD	C2D-C1D-O3G-C3G
23	b	612	CLA	C13-C15-C16-C17
29	a	414	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
31	d	407	LHG	C24-C25-C26-C27
23	a	408	CLA	C16-C17-C18-C19
34	b	623	HTG	S1-C1'-C2'-C3'
33	b	620	LMG	C22-C23-C24-C25
23	b	616	CLA	O1A-CGA-O2A-C1
35	b	621	LMT	C11-C10-C9-C8
23	b	601	CLA	CAA-CBA-CGA-O2A
36	H	102	DGD	O2G-C1B-C2B-C3B
23	b	609	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
33	z	101	LMG	C10-C11-C12-C13
23	d	404	CLA	C16-C17-C18-C20
36	H	102	DGD	C4A-C5A-C6A-C7A
26	D	413	SQD	C23-C24-C25-C26
35	e	102	LMT	O5B-C1B-O1B-C4'
29	a	414	PL9	C39-C41-C42-C43
23	C	507	CLA	C3-C5-C6-C7
23	A	405	CLA	C16-C17-C18-C20
23	a	408	CLA	C15-C16-C17-C18
23	B	602	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
25	a	409	BCR	C19-C20-C21-C22
35	D	403	LMT	C2-C3-C4-C5
33	a	416	LMG	C10-C11-C12-C13
33	b	620	LMG	C37-C38-C39-C40
23	C	503	CLA	C10-C11-C12-C13
23	b	613	CLA	O1A-CGA-O2A-C1
29	D	407	PL9	C43-C44-C46-C47
35	B	629	LMT	C4-C5-C6-C7
29	a	414	PL9	C2-C3-C7-C8
23	A	406	CLA	C16-C17-C18-C20
23	a	404	CLA	C16-C17-C18-C19
26	A	410	SQD	C16-C17-C18-C19
33	c	519	LMG	C28-C29-C30-C31
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	CBA-CGA-O2A-C1
31	d	407	LHG	C7-C8-C9-C10
36	c	518	DGD	CCB-CDB-CEB-CFB
23	C	514	CLA	O1A-CGA-O2A-C1
31	A	417	LHG	C16-C17-C18-C19
23	C	513	CLA	CBA-CGA-O2A-C1
23	C	514	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	c	518	DGD	C2A-C1A-O1G-C1G
23	C	506	CLA	C5-C6-C7-C8
23	b	616	CLA	C4-C3-C5-C6
33	c	519	LMG	O6-C5-C6-O5
31	A	417	LHG	C30-C31-C32-C33
35	e	102	LMT	C1-C2-C3-C4
23	c	508	CLA	C16-C17-C18-C20
23	B	615	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C12-C13-C15
23	d	404	CLA	C12-C13-C15-C16
34	b	625	HTG	C1'-C2'-C3'-C4'
36	C	518	DGD	CDA-CEA-CFA-CGA
33	c	519	LMG	C35-C36-C37-C38
33	c	520	LMG	C36-C37-C38-C39
23	C	513	CLA	O1A-CGA-O2A-C1
26	f	101	SQD	C29-C30-C31-C32
23	A	406	CLA	C3A-C2A-CAA-CBA
23	b	608	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
26	L	101	SQD	O5-C1-O6-C44
23	D	404	CLA	C2C-C3C-CAC-CBC
23	b	609	CLA	C13-C15-C16-C17
35	M	103	LMT	O5B-C1B-O1B-C4'
35	M	103	LMT	C4B-C5B-C6B-O6B
35	E	102	LMT	C3-C4-C5-C6
23	c	510	CLA	C4-C3-C5-C6
29	D	407	PL9	C35-C34-C36-C37
26	L	101	SQD	C10-C11-C12-C13
35	m	102	LMT	C6-C7-C8-C9
33	J	101	LMG	C19-C20-C21-C22
31	A	417	LHG	C11-C12-C13-C14
26	a	412	SQD	C12-C13-C14-C15
36	H	102	DGD	C6B-C7B-C8B-C9B
23	B	602	CLA	C11-C12-C13-C14
23	C	502	CLA	C11-C12-C13-C14
23	C	510	CLA	C6-C7-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	B	613	CLA	C13-C15-C16-C17
23	B	612	CLA	CBA-CGA-O2A-C1
40	v	201	HEC	CAD-CBD-CGD-O2D
33	C	501	LMG	O8-C28-C29-C30
23	c	510	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	z	101	LMG	C12-C13-C14-C15
23	a	405	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
33	C	501	LMG	C14-C15-C16-C17
23	A	408	CLA	C2B-C3B-CAB-CBB
23	B	603	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C2B-C3B-CAB-CBB
23	b	603	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C1-C6-C7-C8
25	D	406	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C30
24	D	401	PHO	CBA-CGA-O2A-C1
36	h	102	DGD	O1B-C1B-C2B-C3B
31	d	409	LHG	C2-C3-O3-P
35	E	102	LMT	C2B-C1B-O1B-C4'
38	E	103	HEM	CAD-CBD-CGD-O1D
29	a	414	PL9	C15-C14-C16-C17
36	C	517	DGD	CCA-CDA-CEA-CFA
23	b	616	CLA	C2-C3-C5-C6
23	B	601	CLA	CAA-CBA-CGA-O1A
26	B	620	SQD	C11-C10-C9-C8
31	l	101	LHG	C24-C25-C26-C27
23	b	604	CLA	C10-C11-C12-C13
23	A	404	CLA	C11-C12-C13-C15
23	B	616	CLA	C11-C12-C13-C15
23	c	510	CLA	C6-C7-C8-C10
36	C	519	DGD	C9B-CAB-CBB-CCB
31	A	416	LHG	C28-C29-C30-C31
33	b	620	LMG	C19-C20-C21-C22
35	M	103	LMT	C2B-C1B-O1B-C4'
38	e	103	HEM	CAA-CBA-CGA-O2A
29	D	407	PL9	C33-C34-C36-C37
31	d	407	LHG	C17-C18-C19-C20
35	M	101	LMT	C2-C3-C4-C5
26	D	413	SQD	C29-C30-C31-C32
31	l	101	LHG	C13-C14-C15-C16
40	v	201	HEC	CAD-CBD-CGD-O1D
33	z	101	LMG	O6-C1-O1-C7
23	C	510	CLA	O1D-CGD-O2D-CED
29	d	406	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
38	e	103	HEM	CAA-CBA-CGA-O1A
34	b	628	HTG	C4-C5-C6-O6
29	D	407	PL9	C28-C29-C31-C32
31	D	408	LHG	C9-C10-C11-C12
33	j	101	LMG	C15-C16-C17-C18
33	j	101	LMG	C28-C29-C30-C31
35	I	101	LMT	C5'-C4'-O1B-C1B
26	a	410	SQD	O6-C44-C45-C46
29	d	406	PL9	C34-C36-C37-C38
33	c	519	LMG	C30-C31-C32-C33
35	M	101	LMT	O5'-C5'-C6'-O6'
35	m	102	LMT	O5'-C5'-C6'-O6'
26	D	413	SQD	C28-C29-C30-C31
23	b	615	CLA	C16-C17-C18-C19
23	a	405	CLA	C13-C15-C16-C17
31	D	409	LHG	O6-C4-C5-O7
31	A	417	LHG	C32-C33-C34-C35
34	b	622	HTG	C2'-C3'-C4'-C5'
23	B	603	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
36	C	518	DGD	C4A-C5A-C6A-C7A
31	d	409	LHG	C31-C32-C33-C34
23	d	404	CLA	C16-C17-C18-C19
24	D	401	PHO	CHA-CBD-CGD-O1D
23	C	508	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C3-C5-C6-C7
26	B	620	SQD	C34-C35-C36-C37
23	b	613	CLA	CBA-CGA-O2A-C1
26	a	410	SQD	C31-C32-C33-C34
31	l	101	LHG	C32-C33-C34-C35
23	B	607	CLA	C4-C3-C5-C6
29	D	407	PL9	C30-C29-C31-C32
23	c	509	CLA	O1D-CGD-O2D-CED
23	D	405	CLA	C10-C11-C12-C13
23	b	607	CLA	C13-C15-C16-C17
23	B	602	CLA	C11-C12-C13-C15
36	C	519	DGD	C8B-C9B-CAB-CBB
38	E	103	HEM	CAD-CBD-CGD-O2D
25	y	101	BCR	C9-C10-C11-C12
35	E	102	LMT	O5B-C1B-O1B-C4'
23	B	604	CLA	C11-C12-C13-C14
23	C	511	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	c	504	CLA	C11-C12-C13-C14
23	d	401	CLA	C11-C12-C13-C14
24	D	401	PHO	O1A-CGA-O2A-C1
23	B	603	CLA	CBD-CGD-O2D-CED
26	A	412	SQD	C5-C6-S-O8
26	B	620	SQD	C45-C44-O6-C1
36	C	517	DGD	C5D-C6D-O5D-C1E
36	C	518	DGD	C2G-C3G-O3G-C1D
36	c	516	DGD	C5D-C6D-O5D-C1E
36	h	102	DGD	C2G-C3G-O3G-C1D
33	b	620	LMG	C33-C34-C35-C36
23	B	613	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	c	511	CLA	C2-C1-O2A-CGA
23	b	606	CLA	CBD-CGD-O2D-CED
33	a	416	LMG	C21-C22-C23-C24
23	B	612	CLA	C3A-C2A-CAA-CBA
23	b	609	CLA	C3A-C2A-CAA-CBA
23	A	405	CLA	C4C-C3C-CAC-CBC
23	b	603	CLA	CBA-CGA-O2A-C1
26	L	101	SQD	C11-C10-C9-C8
23	B	609	CLA	O1A-CGA-O2A-C1
34	d	411	HTG	C1'-C2'-C3'-C4'
23	a	405	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C19
40	V	202	HEC	CAD-CBD-CGD-O1D
35	I	101	LMT	C1-C2-C3-C4
33	j	101	LMG	C36-C37-C38-C39
33	C	501	LMG	C29-C30-C31-C32
36	C	517	DGD	C7A-C8A-C9A-CAA
34	b	625	HTG	C4'-C5'-C6'-C7'
38	e	103	HEM	CAD-CBD-CGD-O1D
33	c	519	LMG	C32-C33-C34-C35
23	B	612	CLA	O1A-CGA-O2A-C1
33	Z	102	LMG	C18-C19-C20-C21
23	b	611	CLA	C13-C15-C16-C17
33	a	416	LMG	C29-C30-C31-C32
36	c	516	DGD	C6B-C7B-C8B-C9B
33	C	501	LMG	C16-C17-C18-C19
23	d	404	CLA	C10-C11-C12-C13
38	e	103	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	D	404	CLA	C16-C17-C18-C20
23	b	607	CLA	C16-C17-C18-C20
36	C	519	DGD	C6B-C7B-C8B-C9B
31	d	408	LHG	C35-C36-C37-C38
23	B	609	CLA	C13-C15-C16-C17
40	V	202	HEC	CAD-CBD-CGD-O2D
33	Z	102	LMG	O1-C7-C8-O7
23	b	603	CLA	O1A-CGA-O2A-C1
23	A	406	CLA	C14-C13-C15-C16
23	B	605	CLA	C14-C13-C15-C16
23	B	611	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
23	a	404	CLA	C16-C17-C18-C20
31	l	101	LHG	O7-C7-C8-C9
26	B	620	SQD	C16-C17-C18-C19
35	M	103	LMT	C1-C2-C3-C4
31	d	408	LHG	C25-C26-C27-C28
23	B	606	CLA	C11-C10-C8-C7
23	C	505	CLA	C6-C7-C8-C10
23	C	511	CLA	C6-C7-C8-C10
23	D	405	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C12-C13-C15
23	d	401	CLA	C11-C12-C13-C15
31	l	101	LHG	C35-C36-C37-C38
23	B	607	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
23	d	403	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C5-C6-C7-C8
25	C	516	BCR	C1-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C26
23	B	613	CLA	CAA-CBA-CGA-O2A
31	e	101	LHG	O8-C23-C24-C25
33	C	520	LMG	O8-C28-C29-C30
26	A	412	SQD	C30-C31-C32-C33
23	B	608	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
23	b	610	CLA	C2-C1-O2A-CGA
36	C	519	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C16-C17-C18-C20
34	b	622	HTG	C4'-C5'-C6'-C7'
23	B	612	CLA	CAA-CBA-CGA-O2A
23	C	511	CLA	CAA-CBA-CGA-O2A
26	a	412	SQD	O48-C23-C24-C25
26	L	101	SQD	C29-C30-C31-C32
36	C	517	DGD	CDB-CEB-CFB-CGB
36	H	102	DGD	CDB-CEB-CFB-CGB
26	L	101	SQD	C18-C19-C20-C21
33	C	520	LMG	O7-C10-C11-C12
36	c	517	DGD	O1B-C1B-O2G-C2G
23	c	507	CLA	C5-C6-C7-C8
34	b	625	HTG	C2'-C1'-S1-C1
34	c	521	HTG	C2'-C1'-S1-C1
23	c	503	CLA	C2A-CAA-CBA-CGA
26	A	410	SQD	C13-C14-C15-C16
23	b	613	CLA	CAA-CBA-CGA-O2A
35	B	630	LMT	C4-C5-C6-C7
35	b	621	LMT	C6-C7-C8-C9
36	C	519	DGD	CCB-CDB-CEB-CFB
36	c	517	DGD	CBB-CCB-CDB-CEB
23	b	612	CLA	CAA-CBA-CGA-O2A
26	f	101	SQD	O47-C7-C8-C9
33	Z	102	LMG	O7-C10-C11-C12
23	A	406	CLA	O1A-CGA-O2A-C1
38	e	103	HEM	CAD-CBD-CGD-O2D
35	I	101	LMT	C4-C5-C6-C7
35	B	630	LMT	C3-C4-C5-C6
33	J	101	LMG	O7-C10-C11-C12
29	a	414	PL9	C13-C14-C16-C17
38	E	103	HEM	CAA-CBA-CGA-O1A
33	C	501	LMG	C17-C18-C19-C20
36	h	102	DGD	CAA-CBA-CCA-CDA
34	c	521	HTG	C2'-C3'-C4'-C5'
23	c	510	CLA	CAA-CBA-CGA-O2A
33	c	519	LMG	O7-C10-C11-C12
33	C	520	LMG	C32-C33-C34-C35
33	B	621	LMG	O1-C7-C8-C9
23	c	513	CLA	C4B-C3B-CAB-CBB
31	A	417	LHG	O7-C7-C8-C9
29	a	414	PL9	C31-C32-C33-C34
25	b	619	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C8-C10-C11-C12
23	A	406	CLA	CBA-CGA-O2A-C1
31	d	408	LHG	C17-C18-C19-C20
35	B	629	LMT	C3'-C4'-O1B-C1B
31	l	101	LHG	C28-C29-C30-C31
31	E	101	LHG	C12-C13-C14-C15
35	D	403	LMT	C5'-C4'-O1B-C1B
23	c	512	CLA	C2-C1-O2A-CGA
23	d	403	CLA	C2-C1-O2A-CGA
31	d	409	LHG	O8-C23-C24-C25
23	B	601	CLA	C11-C10-C8-C7
23	B	615	CLA	C6-C7-C8-C10
23	b	616	CLA	C12-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C15
29	a	414	PL9	C23-C24-C26-C27
23	B	610	CLA	C13-C15-C16-C17
26	L	101	SQD	O48-C23-C24-C25
34	B	627	HTG	C2'-C3'-C4'-C5'
35	E	102	LMT	C6-C7-C8-C9
23	B	603	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C16-C17-C18-C20
38	E	103	HEM	CAA-CBA-CGA-O2A
35	B	630	LMT	C4'-C5'-C6'-O6'
36	C	519	DGD	C3B-C4B-C5B-C6B
23	B	602	CLA	C4-C3-C5-C6
33	C	520	LMG	O9-C10-C11-C12
36	C	519	DGD	C1B-C2B-C3B-C4B
36	h	102	DGD	C6A-C7A-C8A-C9A
36	H	102	DGD	C2B-C3B-C4B-C5B
23	b	612	CLA	CAA-CBA-CGA-O1A
26	a	412	SQD	O10-C23-C24-C25
33	C	520	LMG	O10-C28-C29-C30
31	l	101	LHG	O6-C4-C5-O7
26	A	412	SQD	O5-C1-O6-C44
26	a	410	SQD	C26-C27-C28-C29
26	f	101	SQD	O49-C7-C8-C9
23	A	404	CLA	C11-C12-C13-C14
23	C	505	CLA	C6-C7-C8-C9
23	C	509	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
31	l	101	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	J	101	LMG	O9-C10-C11-C12
23	B	607	CLA	C2-C3-C5-C6
36	h	102	DGD	CDB-CEB-CFB-CGB
23	B	613	CLA	CAA-CBA-CGA-O1A
31	e	101	LHG	O10-C23-C24-C25
23	B	612	CLA	C13-C15-C16-C17
27	B	625	GOL	O2-C2-C3-O3
36	C	518	DGD	CBA-CCA-CDA-CEA
23	C	511	CLA	CAA-CBA-CGA-O1A
23	b	616	CLA	C10-C11-C12-C13
23	B	612	CLA	CAA-CBA-CGA-O1A
33	Z	102	LMG	O9-C10-C11-C12
36	C	517	DGD	O2G-C1B-C2B-C3B
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	C2A-CAA-CBA-CGA
24	A	407	PHO	C16-C17-C18-C19
31	E	101	LHG	C26-C27-C28-C29
33	Z	102	LMG	C7-C8-C9-O8
26	A	412	SQD	C28-C29-C30-C31
23	b	613	CLA	CAA-CBA-CGA-O1A
29	D	407	PL9	C11-C12-C13-C14
29	D	407	PL9	C36-C37-C38-C39
35	b	621	LMT	C3'-C4'-O1B-C1B
23	c	510	CLA	C13-C15-C16-C17
31	A	417	LHG	O9-C7-C8-C9
33	c	519	LMG	O9-C10-C11-C12
23	B	615	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
23	C	511	CLA	C13-C15-C16-C17
36	H	102	DGD	C5B-C6B-C7B-C8B
23	C	513	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
31	d	407	LHG	C18-C19-C20-C21
36	c	516	DGD	CCB-CDB-CEB-CFB
23	B	616	CLA	C6-C7-C8-C10
23	b	602	CLA	CAA-CBA-CGA-O2A
26	A	410	SQD	O47-C7-C8-C9
35	D	403	LMT	C3-C4-C5-C6
23	C	506	CLA	CAA-CBA-CGA-O2A
23	c	512	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	e	101	LHG	C23-C24-C25-C26

There are no ring outliers.

151 monomers are involved in 343 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	405	CLA	2	0
29	D	407	PL9	3	0
33	c	520	LMG	1	0
23	B	605	CLA	6	0
31	D	409	LHG	4	0
23	B	612	CLA	1	0
23	b	602	CLA	1	0
23	B	616	CLA	6	0
23	C	502	CLA	3	0
23	b	613	CLA	3	0
33	j	101	LMG	2	0
34	C	521	HTG	1	0
33	Z	101	LMG	2	0
26	A	412	SQD	3	0
33	B	621	LMG	1	0
23	c	511	CLA	3	0
33	C	501	LMG	7	0
27	a	411	GOL	1	0
36	c	516	DGD	3	0
36	C	518	DGD	2	0
33	c	519	LMG	1	0
23	c	501	CLA	3	0
33	J	101	LMG	3	0
23	C	512	CLA	2	0
23	c	504	CLA	2	0
23	C	509	CLA	3	0
33	Z	102	LMG	1	0
23	d	403	CLA	4	0
36	c	518	DGD	3	0
23	c	512	CLA	6	0
23	c	508	CLA	7	0
34	c	521	HTG	1	0
25	B	619	BCR	3	0
23	b	601	CLA	2	0
23	c	509	CLA	5	0
23	b	603	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	505	CLA	1	0
23	B	611	CLA	2	0
23	c	503	CLA	3	0
23	B	608	CLA	1	0
25	K	102	BCR	1	0
25	C	516	BCR	3	0
34	b	625	HTG	1	0
34	b	628	HTG	1	0
26	D	413	SQD	1	0
24	a	407	PHO	3	0
23	b	608	CLA	2	0
23	B	615	CLA	3	0
23	A	404	CLA	2	0
24	D	401	PHO	1	0
33	a	416	LMG	4	0
23	C	506	CLA	8	0
27	B	626	GOL	1	0
26	A	410	SQD	3	0
38	e	103	HEM	3	0
25	y	101	BCR	1	0
36	C	519	DGD	1	0
23	b	616	CLA	3	0
25	k	101	BCR	2	0
35	D	403	LMT	2	0
31	A	416	LHG	3	0
34	c	522	HTG	1	0
35	M	101	LMT	2	0
25	C	515	BCR	2	0
23	b	604	CLA	5	0
25	d	405	BCR	5	0
25	c	514	BCR	6	0
23	a	408	CLA	3	0
35	B	630	LMT	3	0
34	d	411	HTG	1	0
23	A	405	CLA	2	0
27	C	523	GOL	1	0
23	B	604	CLA	4	0
25	B	617	BCR	1	0
25	H	101	BCR	3	0
23	B	614	CLA	4	0
23	a	404	CLA	4	0
23	C	513	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	407	PHO	2	0
23	c	506	CLA	5	0
27	B	625	GOL	1	0
34	b	622	HTG	2	0
25	T	101	BCR	5	0
23	B	613	CLA	2	0
26	L	101	SQD	5	0
25	t	101	BCR	3	0
23	B	602	CLA	5	0
23	D	404	CLA	3	0
23	c	507	CLA	4	0
23	b	611	CLA	1	0
26	B	620	SQD	2	0
31	A	417	LHG	2	0
23	B	609	CLA	4	0
23	c	510	CLA	3	0
23	C	508	CLA	5	0
23	b	614	CLA	3	0
35	b	621	LMT	1	0
35	I	101	LMT	1	0
35	M	103	LMT	1	0
36	H	102	DGD	1	0
25	b	618	BCR	3	0
38	E	103	HEM	3	0
23	B	606	CLA	3	0
34	B	622	HTG	4	0
35	E	102	LMT	1	0
36	c	517	DGD	3	0
23	C	504	CLA	5	0
25	b	617	BCR	2	0
23	b	615	CLA	3	0
25	h	101	BCR	5	0
31	E	101	LHG	1	0
23	b	610	CLA	1	0
23	A	406	CLA	2	0
23	b	605	CLA	7	0
31	e	101	LHG	2	0
31	d	409	LHG	7	0
24	a	406	PHO	1	0
25	A	409	BCR	1	0
23	B	603	CLA	1	0
23	b	609	CLA	5	0

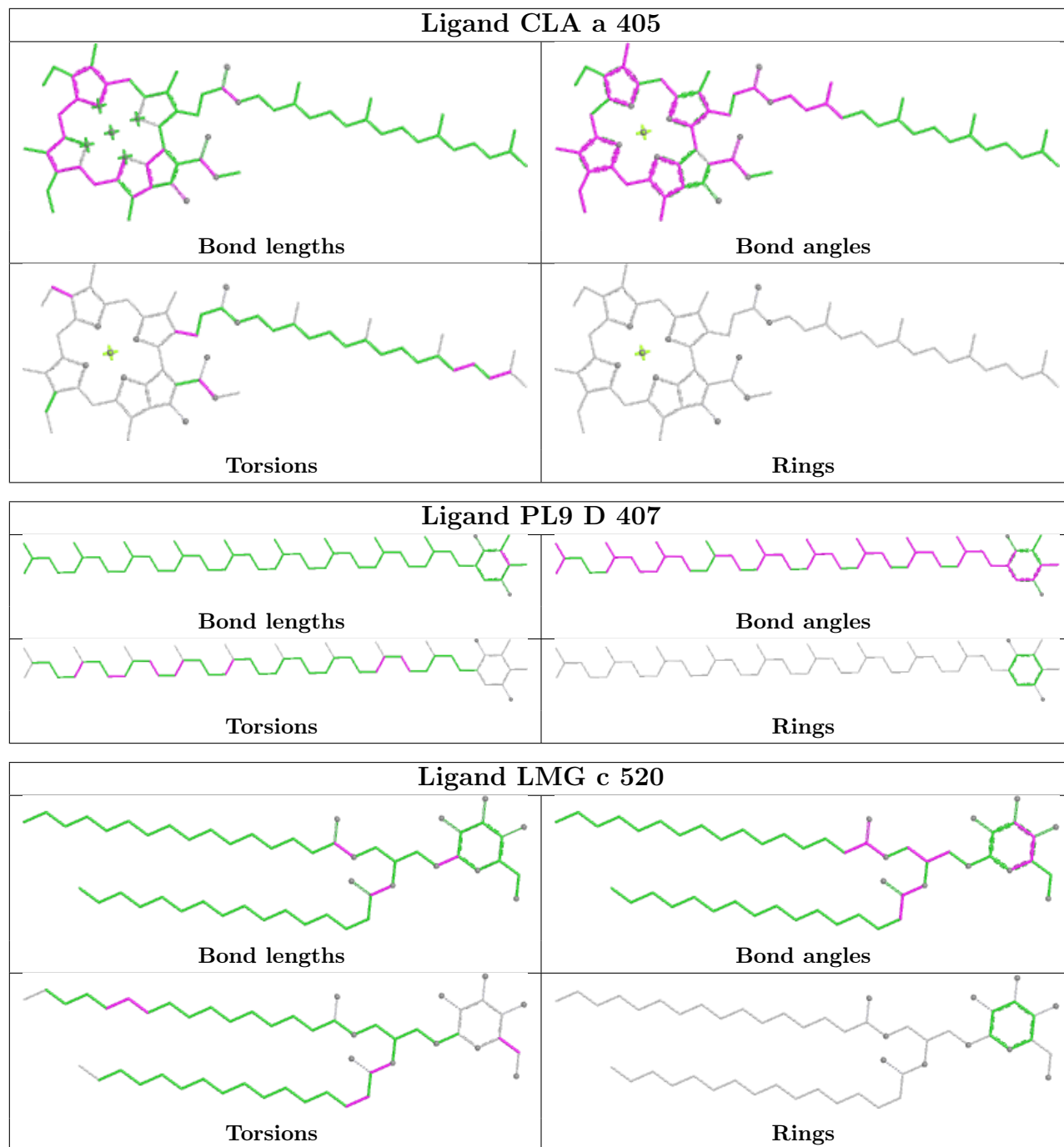
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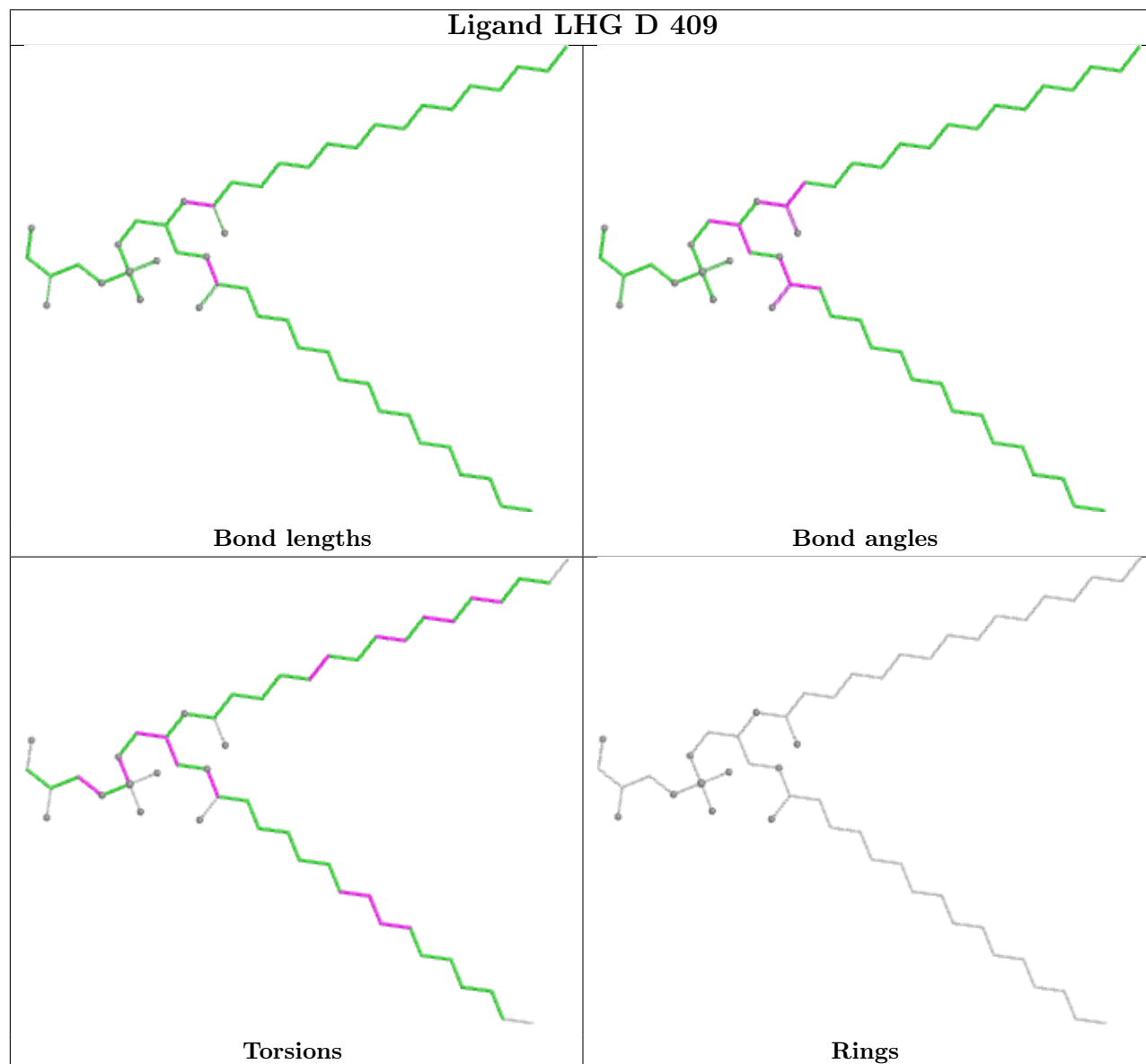
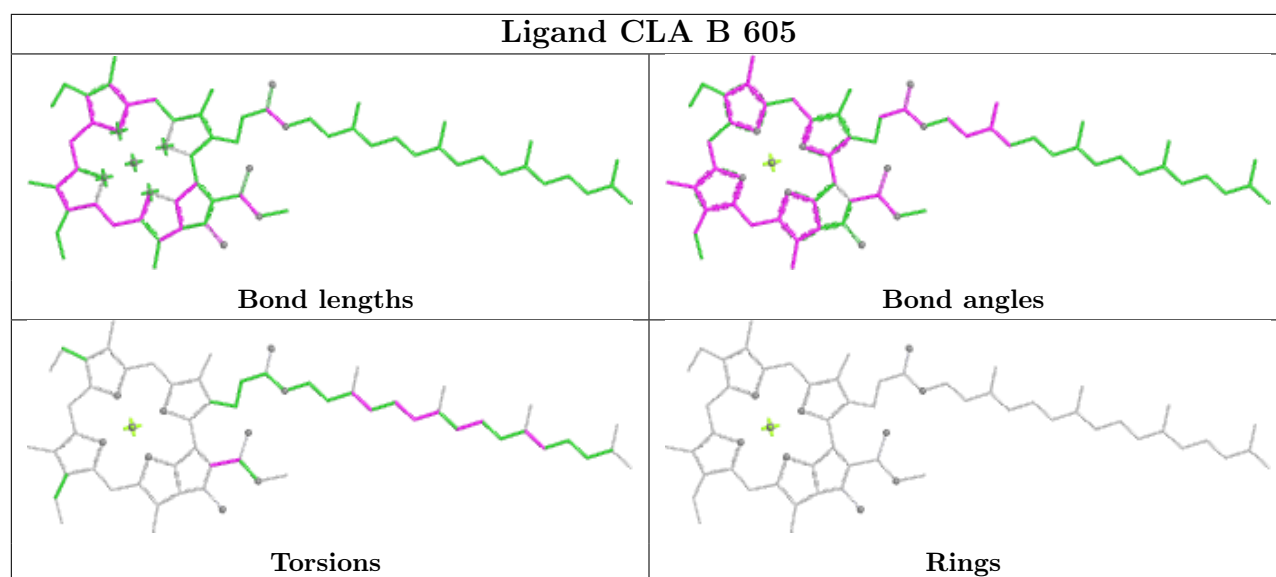
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	505	CLA	5	0
23	C	507	CLA	9	0
33	z	101	LMG	1	0
25	D	406	BCR	2	0
25	Y	101	BCR	2	0
29	A	414	PL9	6	0
23	B	607	CLA	1	0
23	C	503	CLA	2	0
23	C	510	CLA	1	0
23	d	404	CLA	4	0
25	B	618	BCR	4	0
35	D	402	LMT	2	0
23	b	612	CLA	4	0
34	B	623	HTG	2	0
25	c	515	BCR	4	0
31	D	408	LHG	2	0
36	C	517	DGD	5	0
26	a	410	SQD	4	0
23	d	401	CLA	4	0
23	B	610	CLA	1	0
23	c	513	CLA	7	0
31	d	408	LHG	3	0
23	c	502	CLA	3	0
35	B	629	LMT	1	0
33	b	620	LMG	1	0
23	B	601	CLA	2	0
23	A	408	CLA	6	0
23	C	514	CLA	7	0
25	b	619	BCR	2	0
25	a	409	BCR	1	0
29	a	414	PL9	4	0

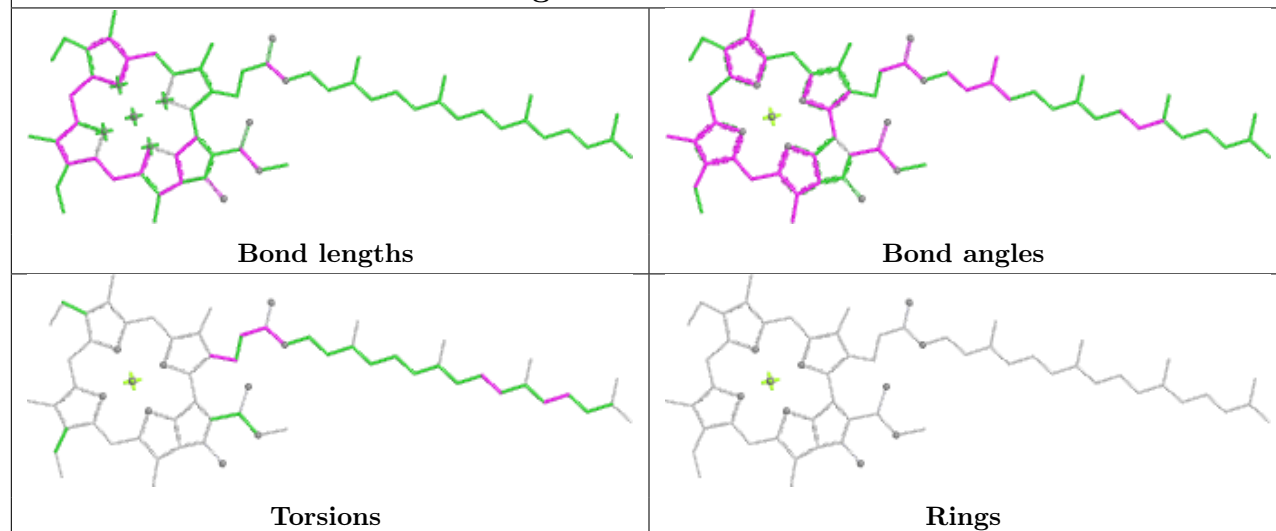
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

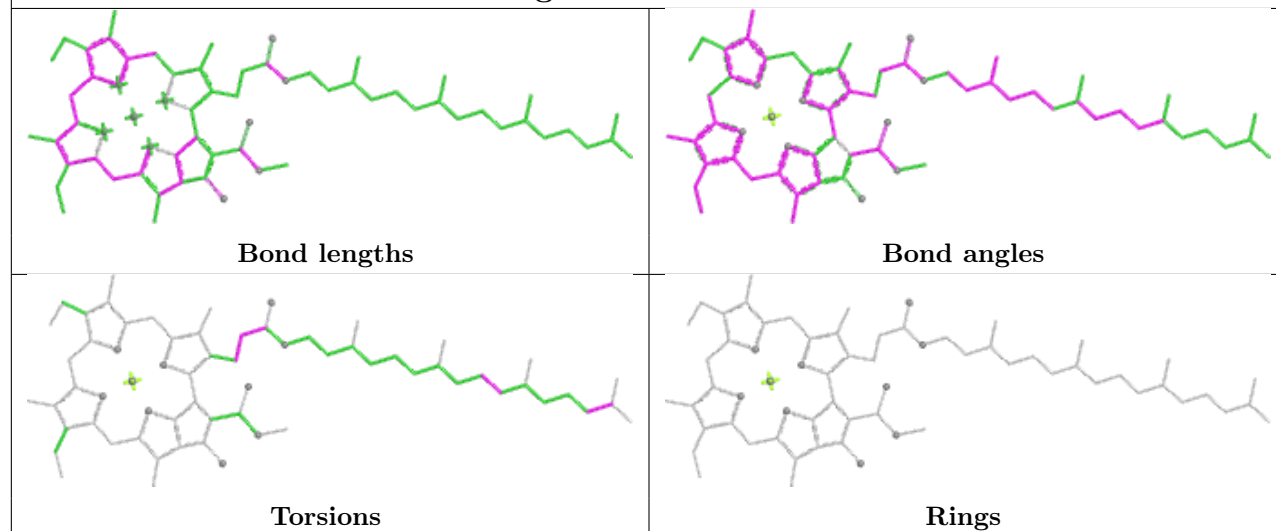




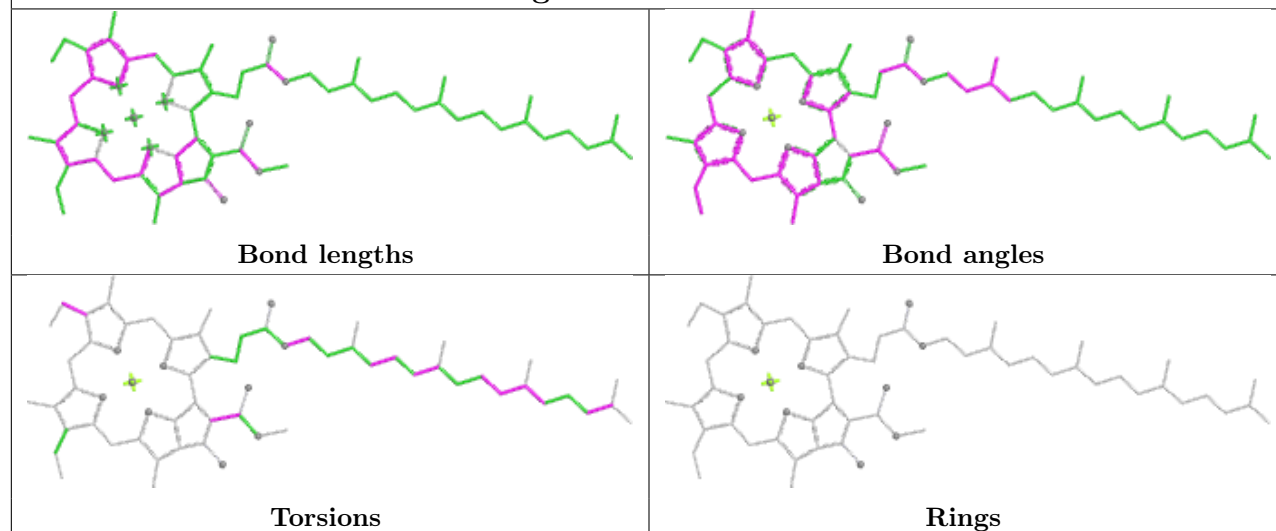
Ligand CLA B 612

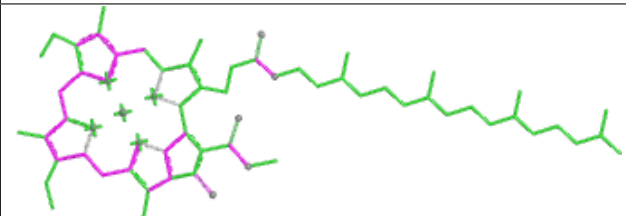
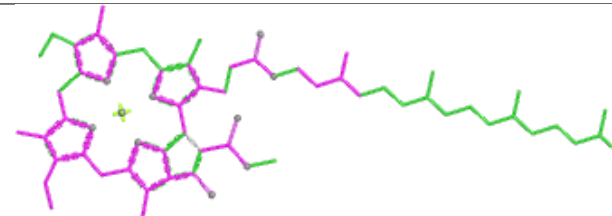
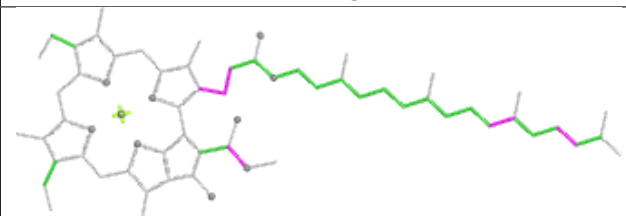
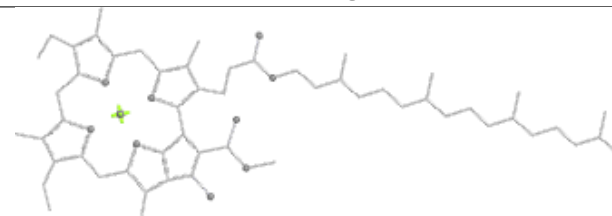


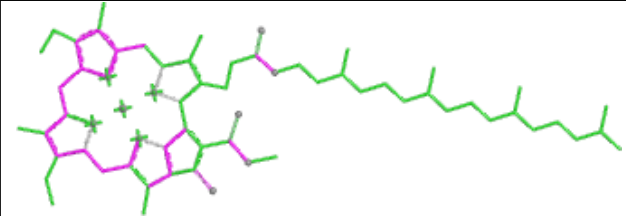
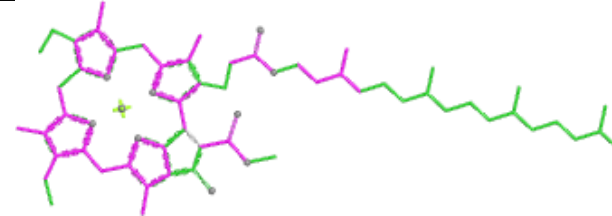
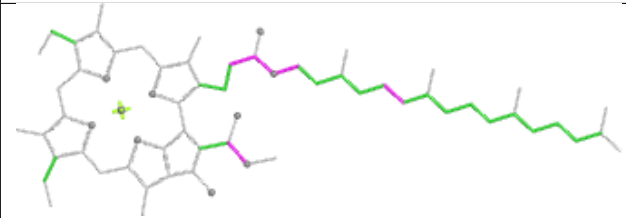
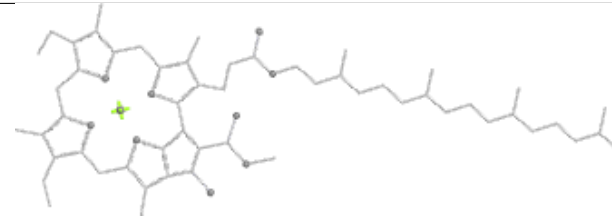
Ligand CLA b 602

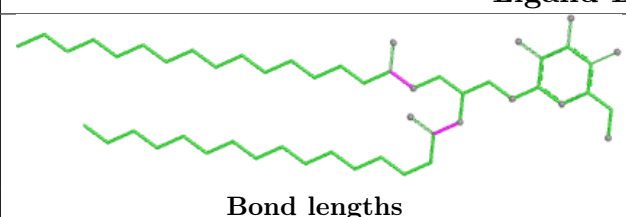
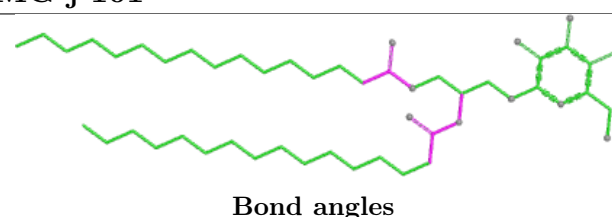
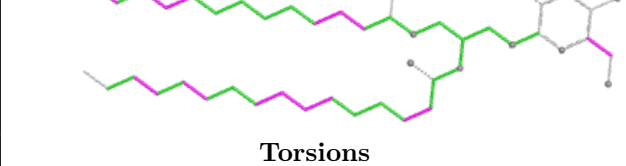


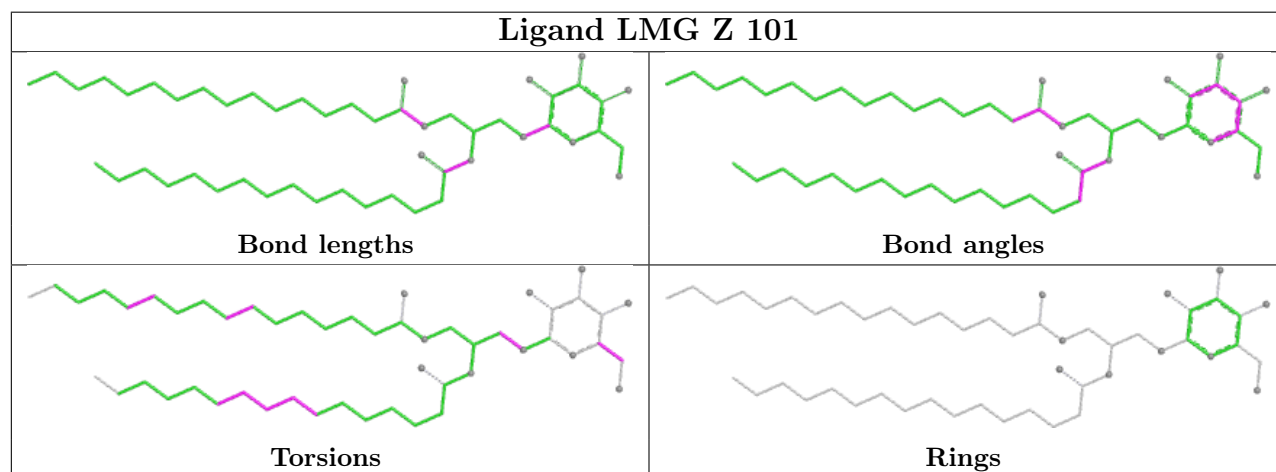
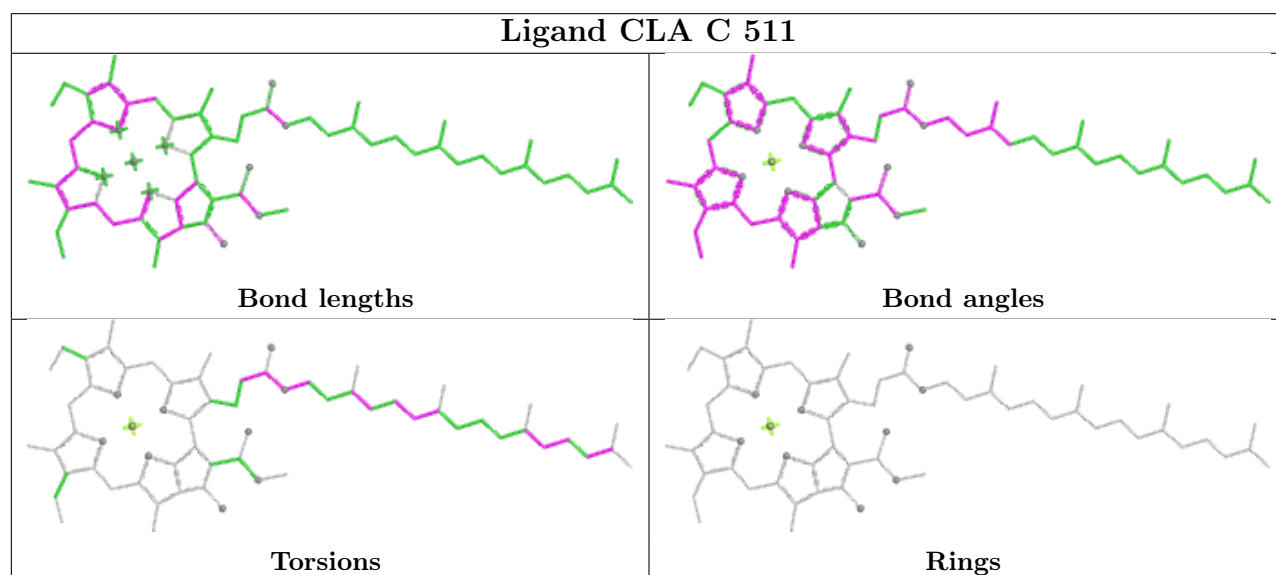
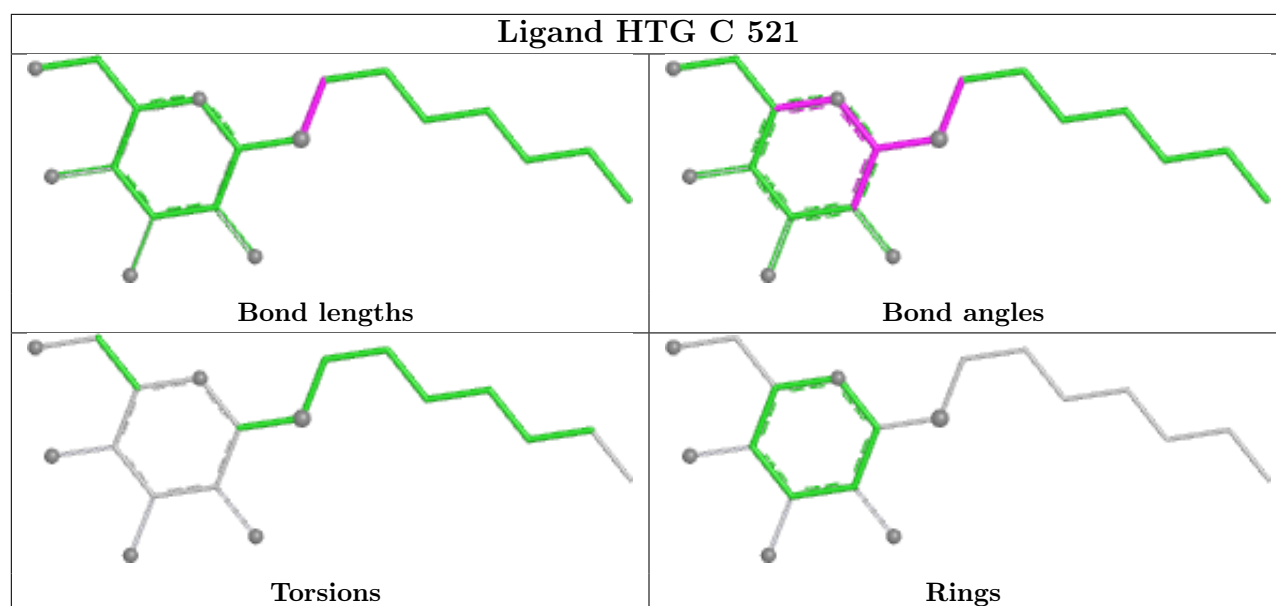
Ligand CLA B 616

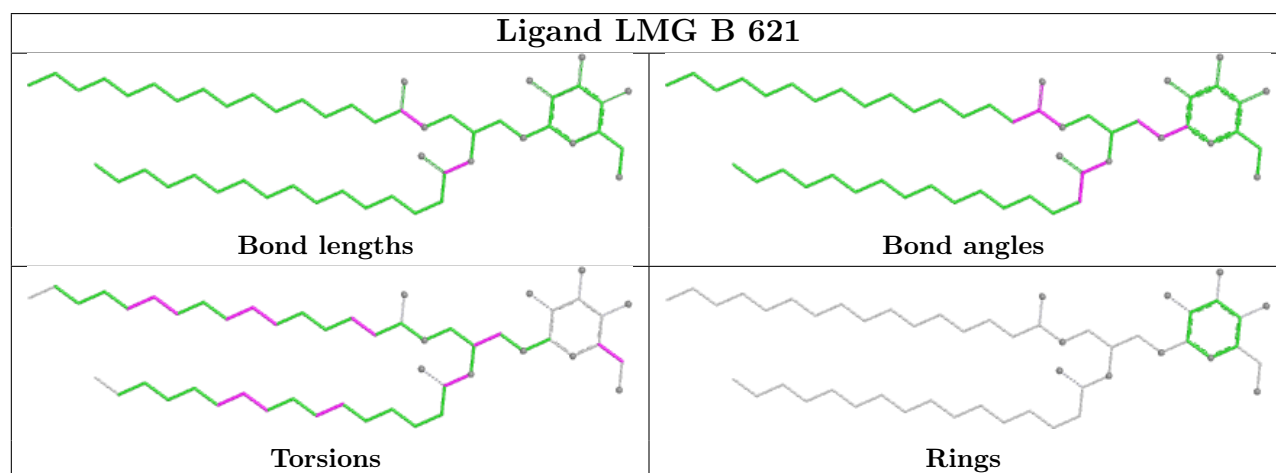
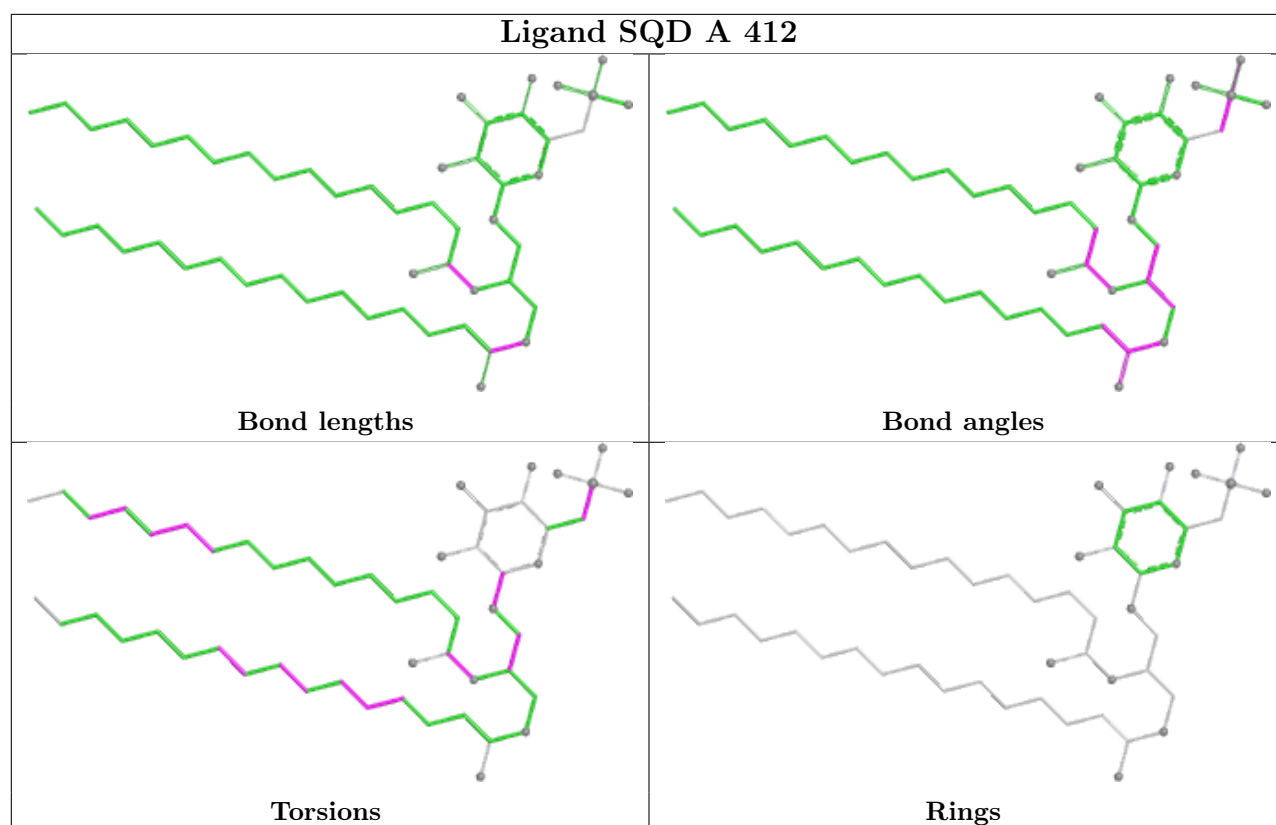


Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

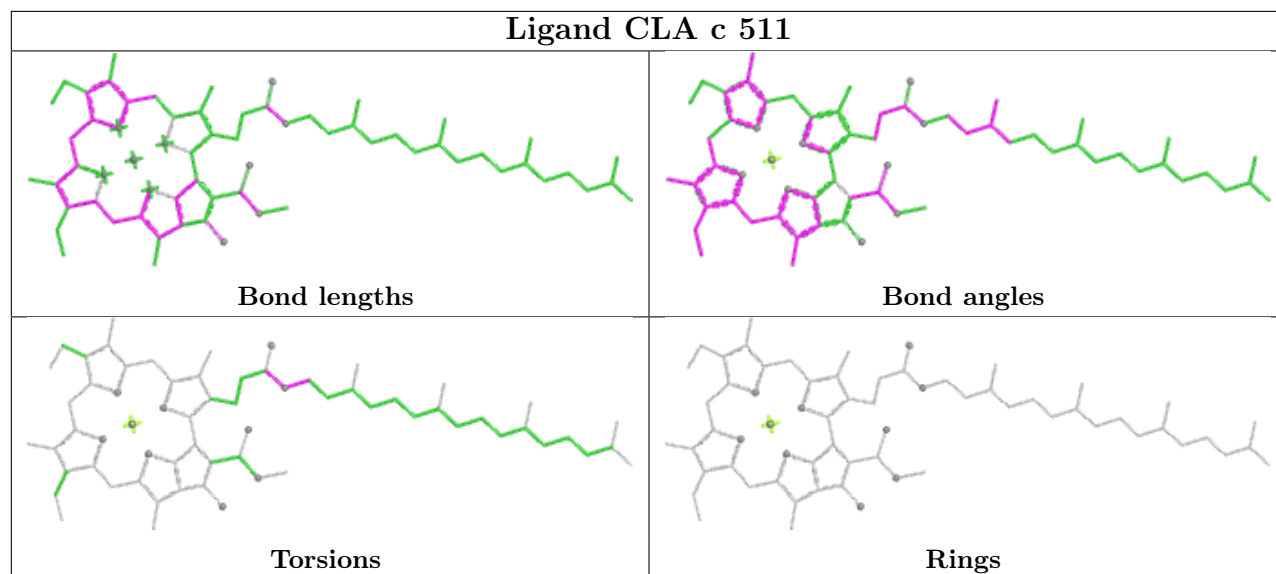
Ligand CLA b 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

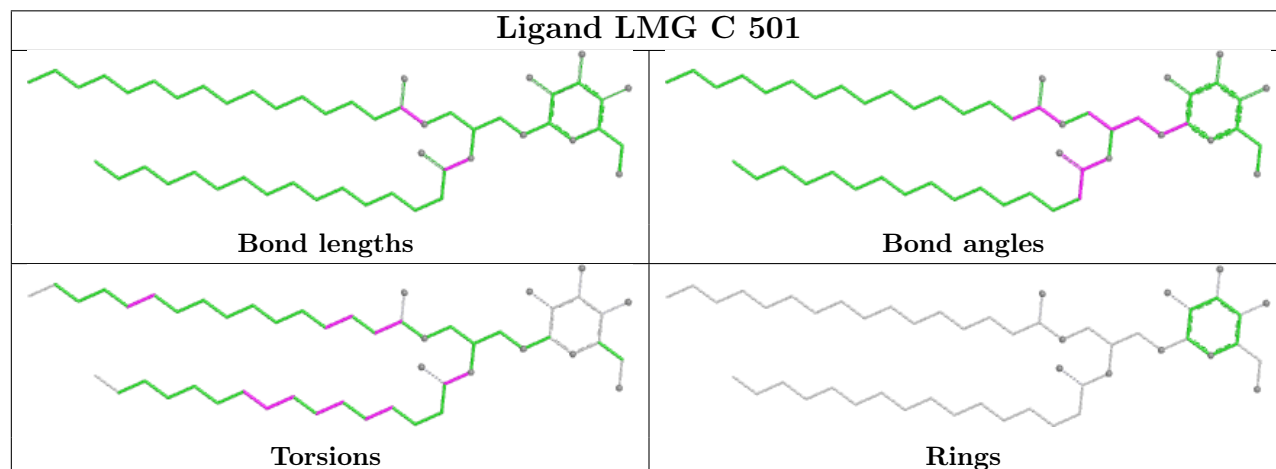


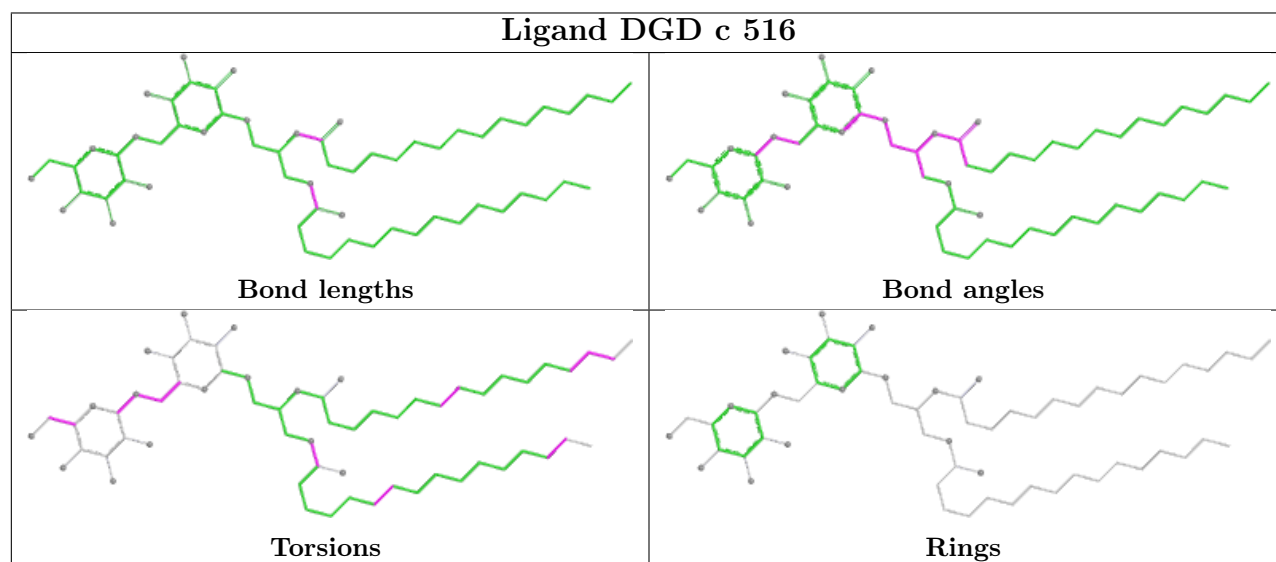
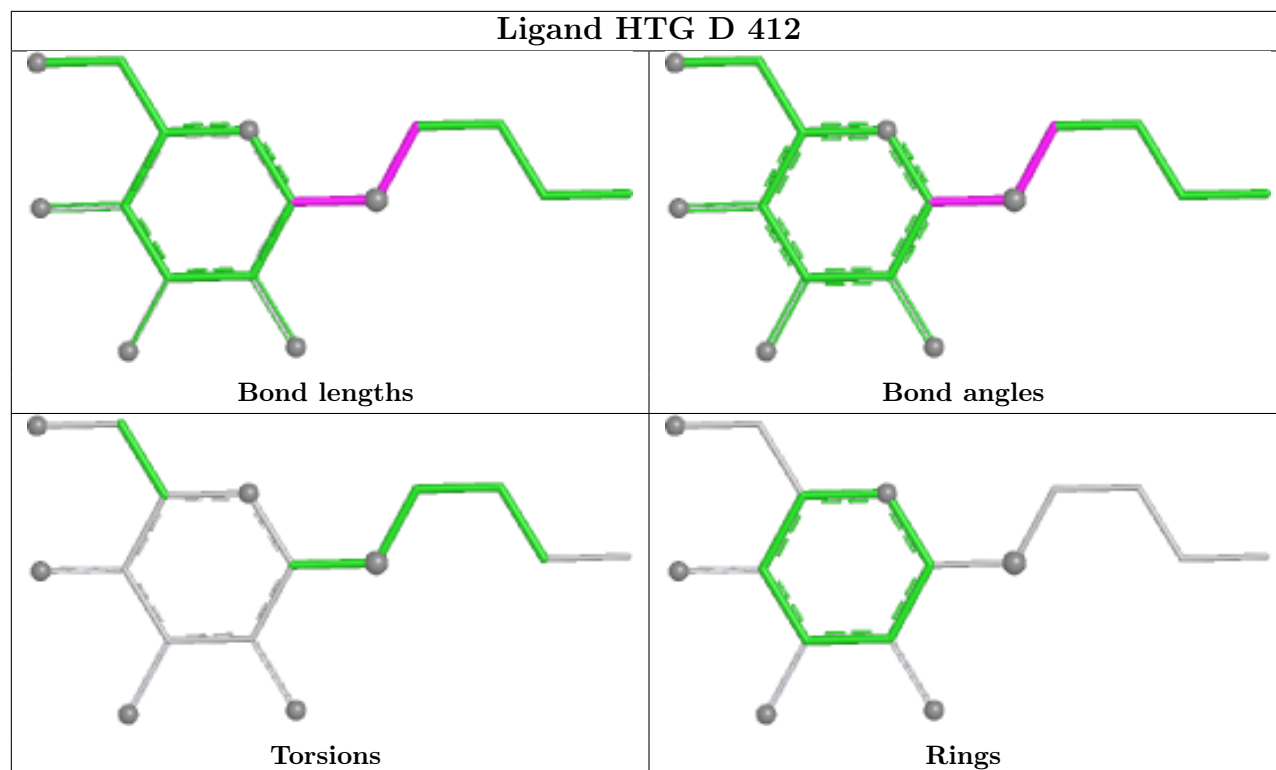


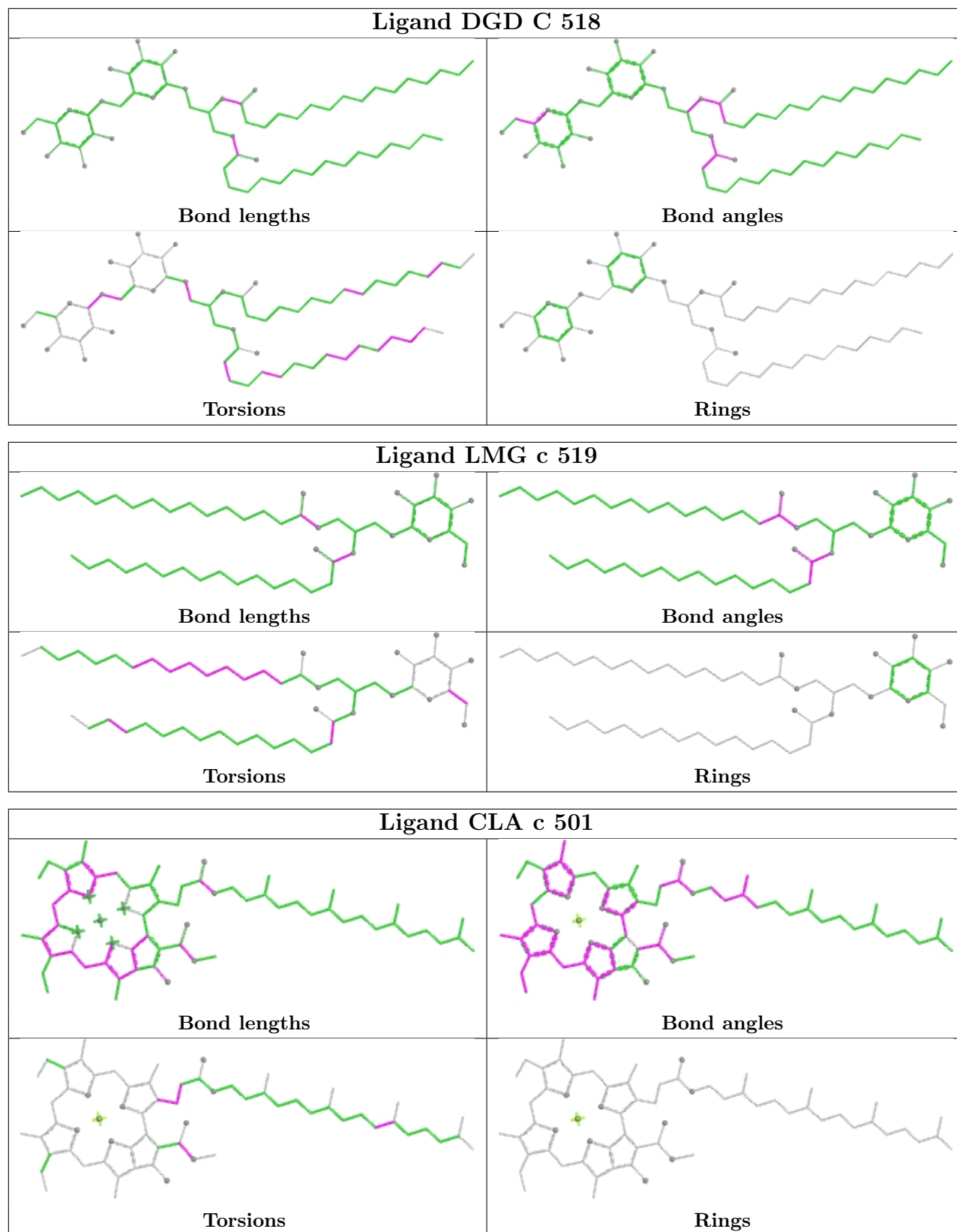
Ligand CLA c 511



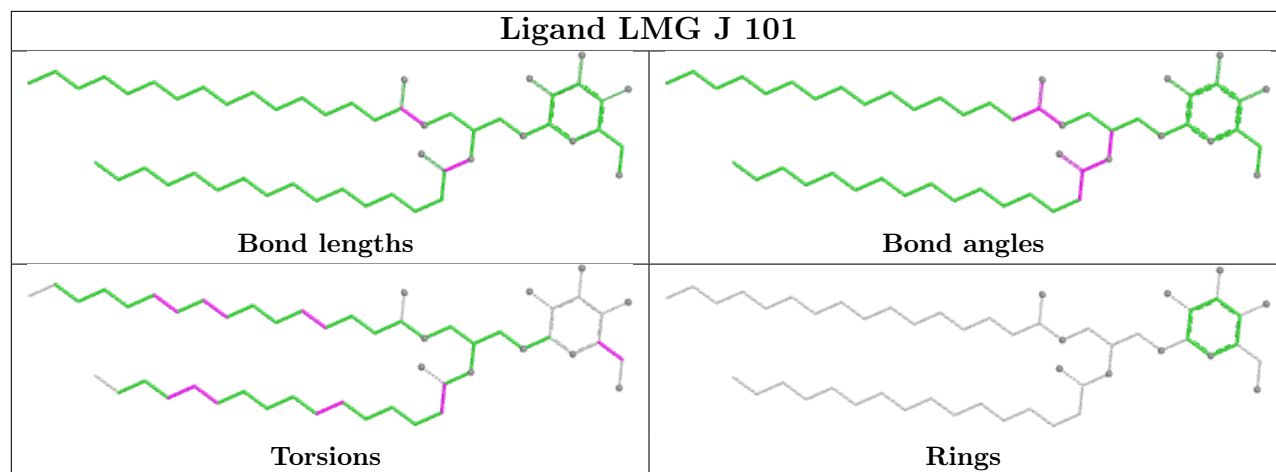
Ligand LMG C 501



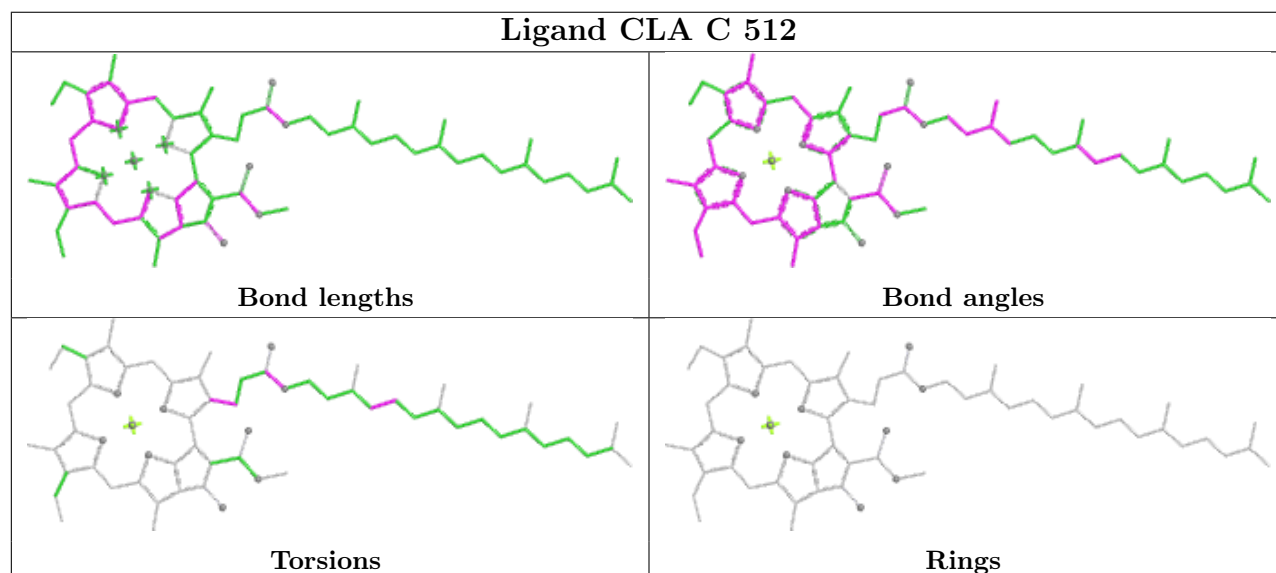




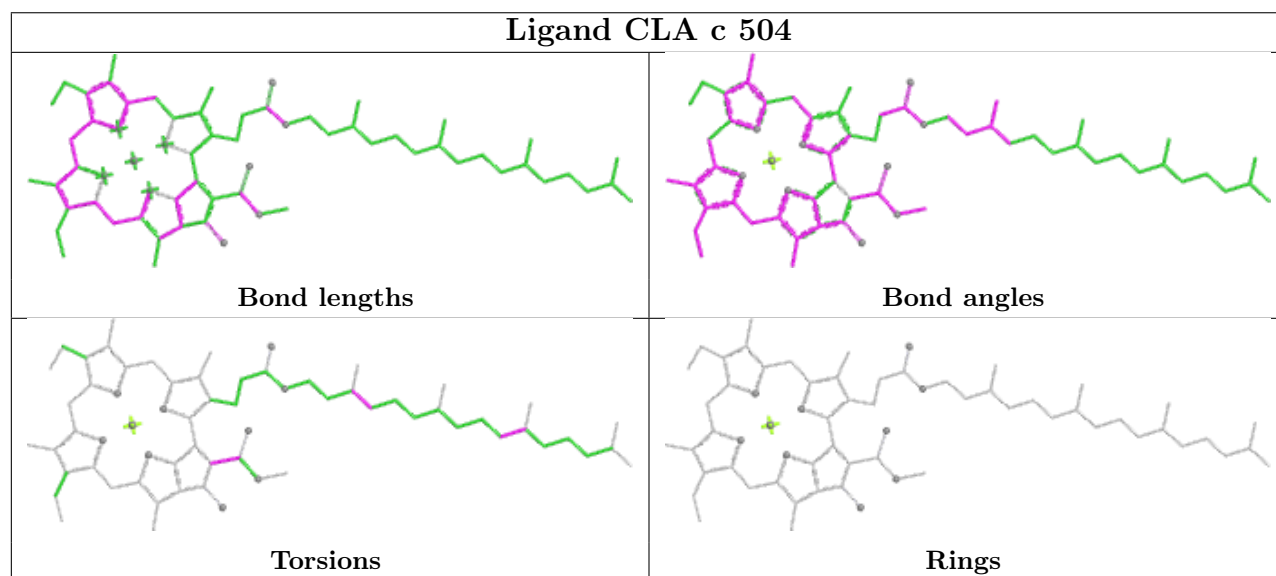
Ligand LMG J 101



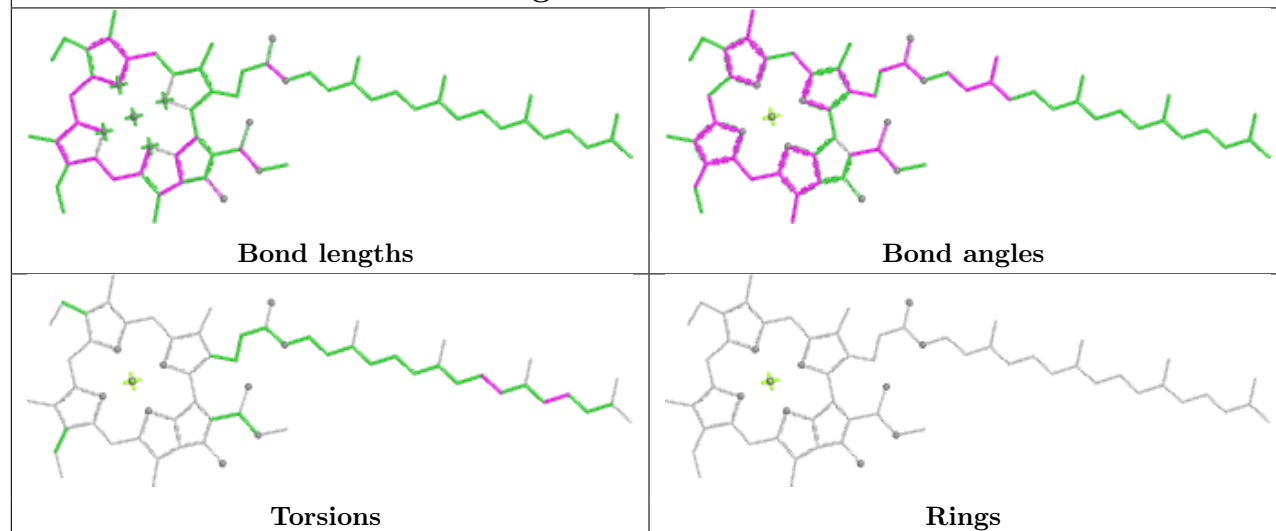
Ligand CLA C 512



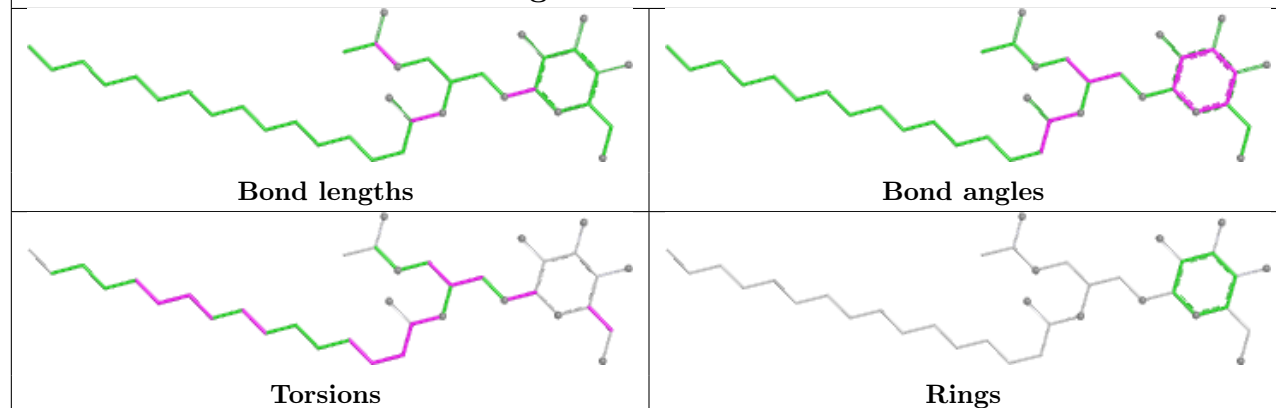
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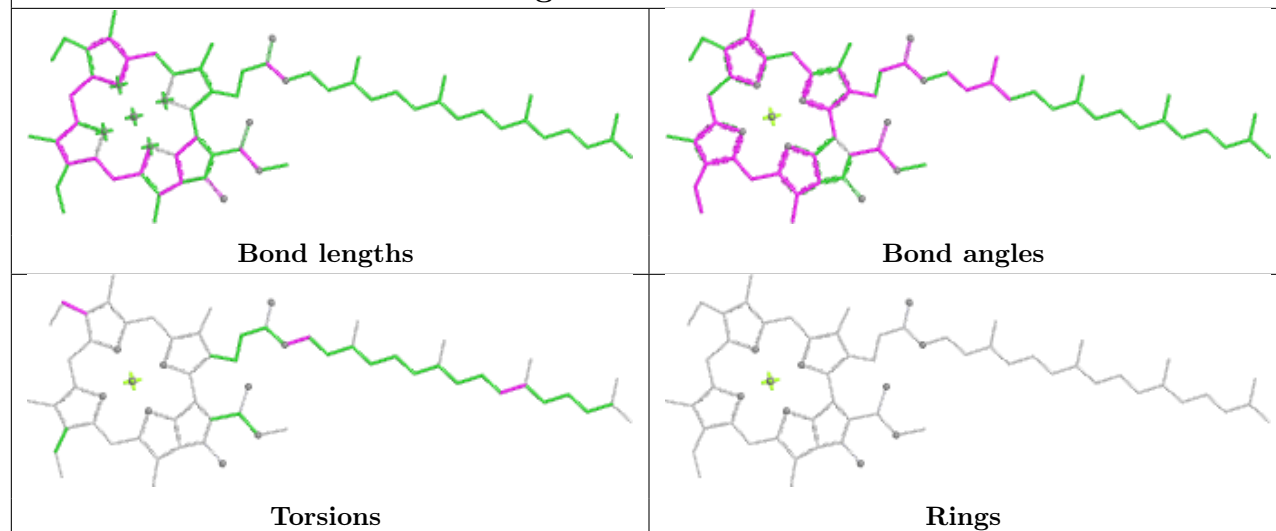
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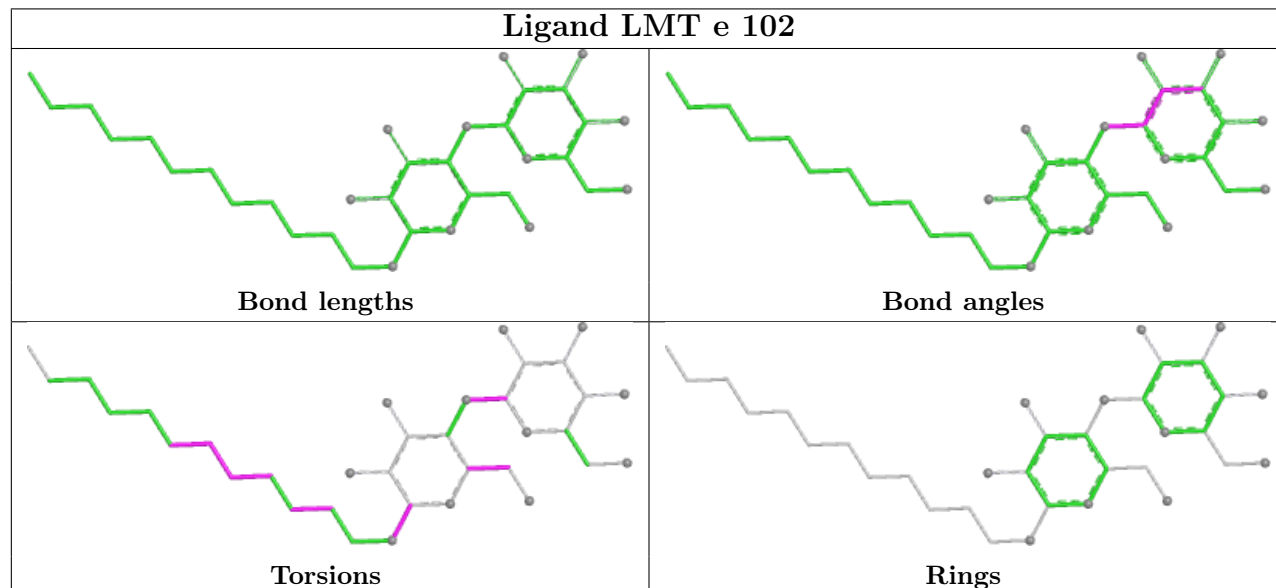
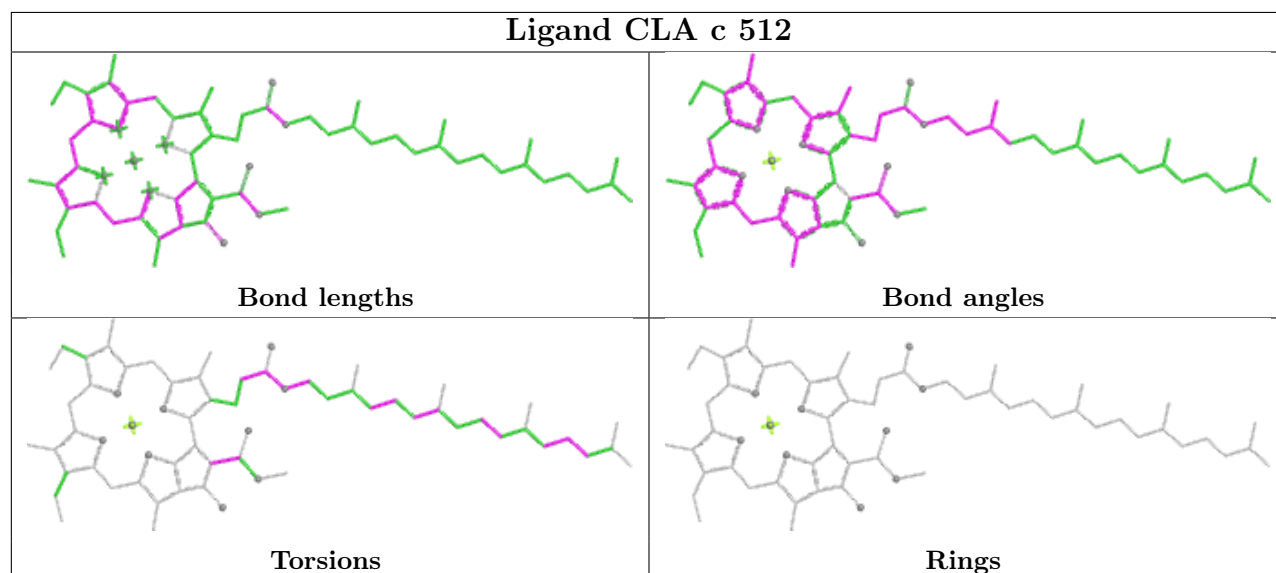
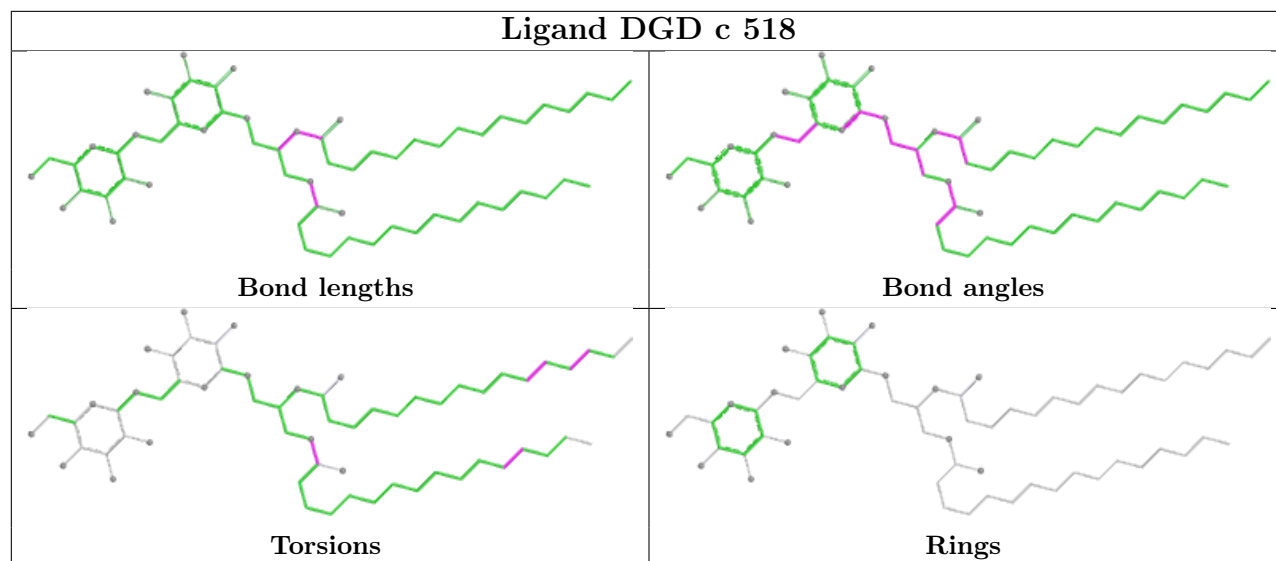


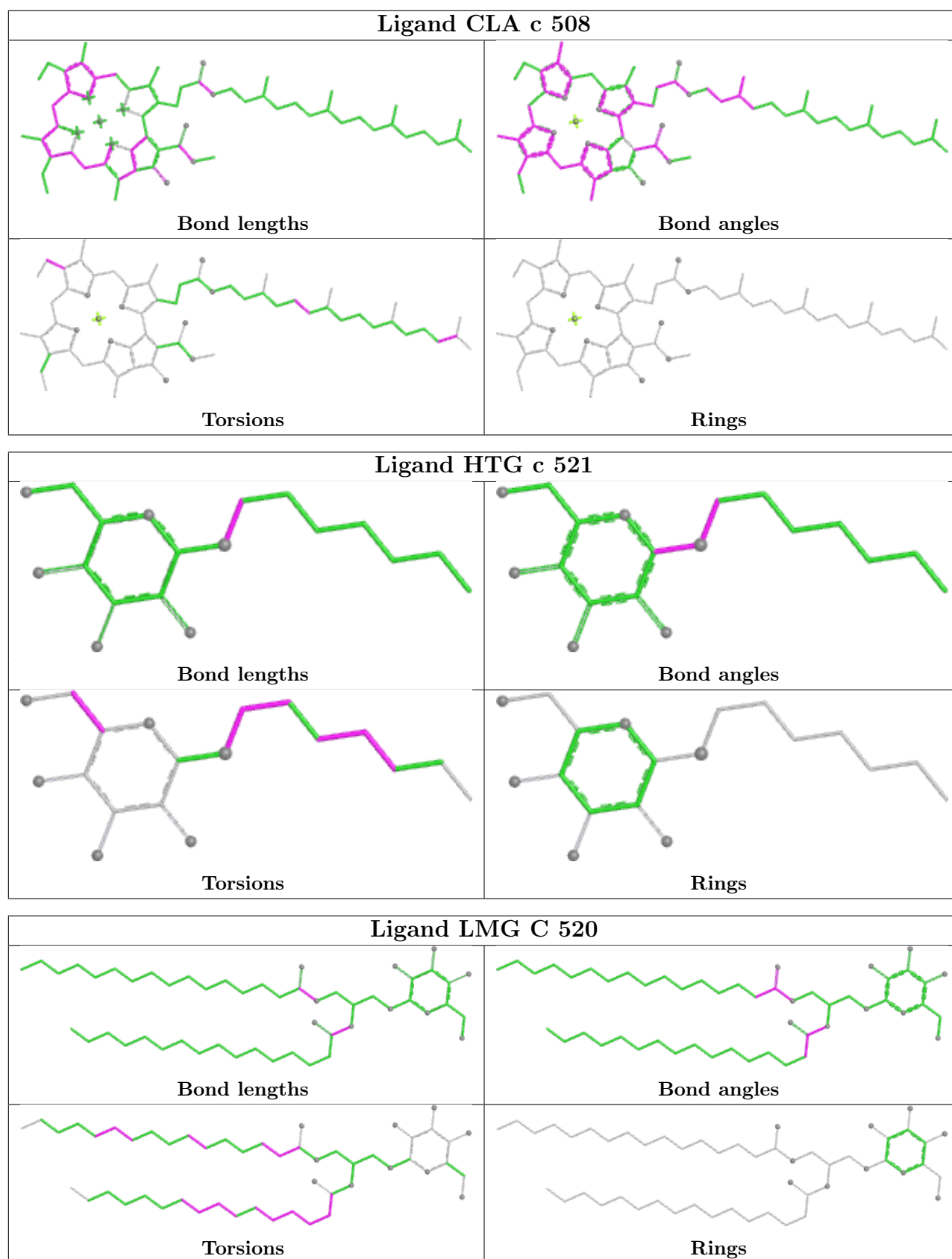
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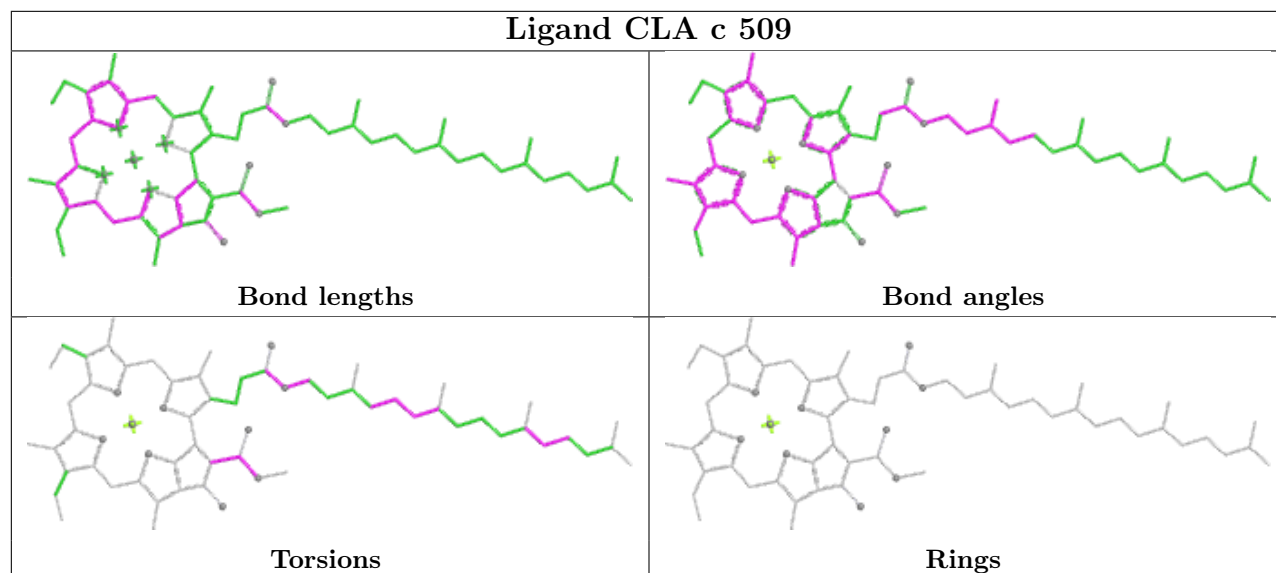
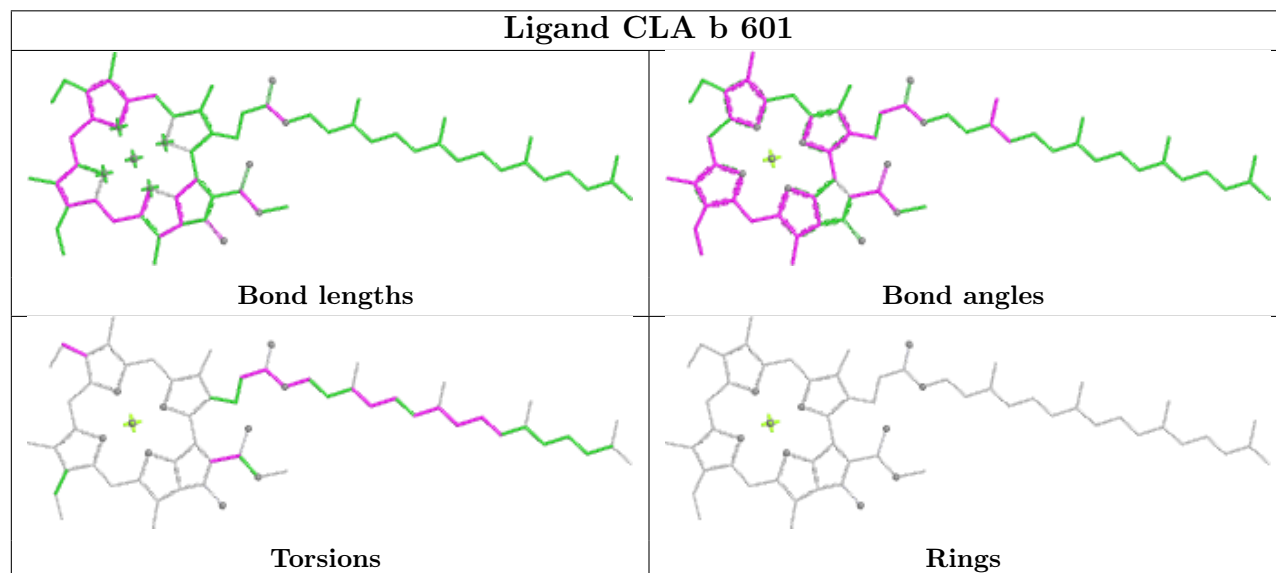
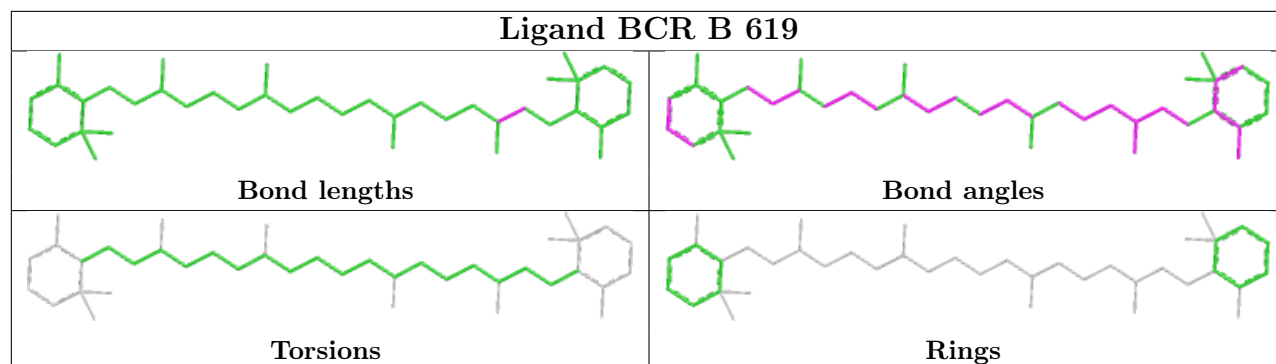


Ligand CLA d 403

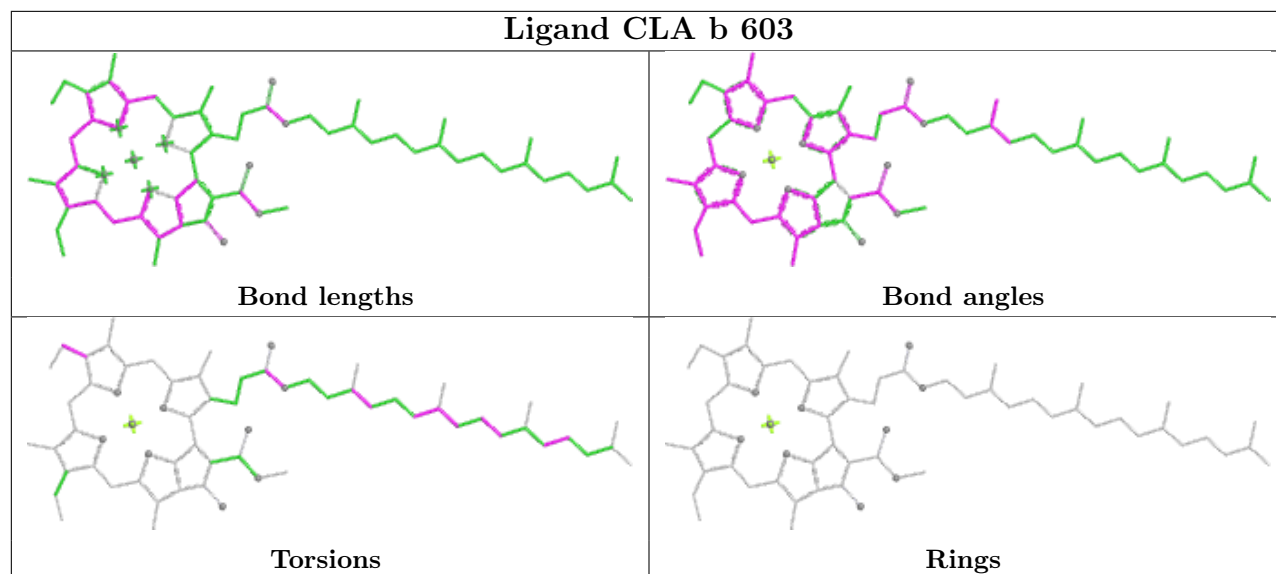




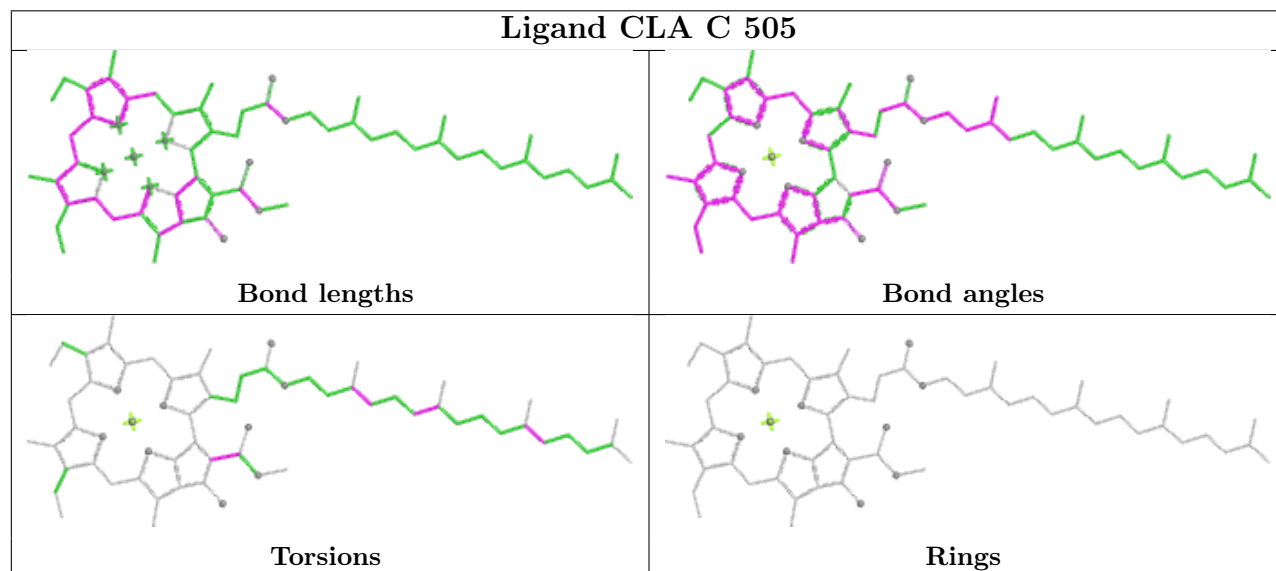




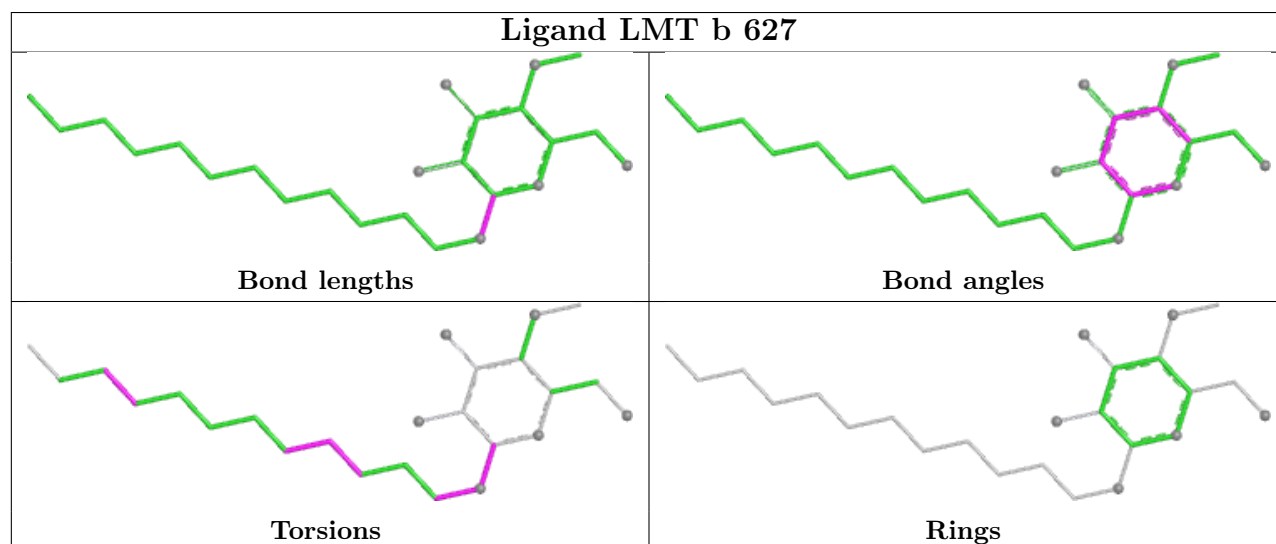
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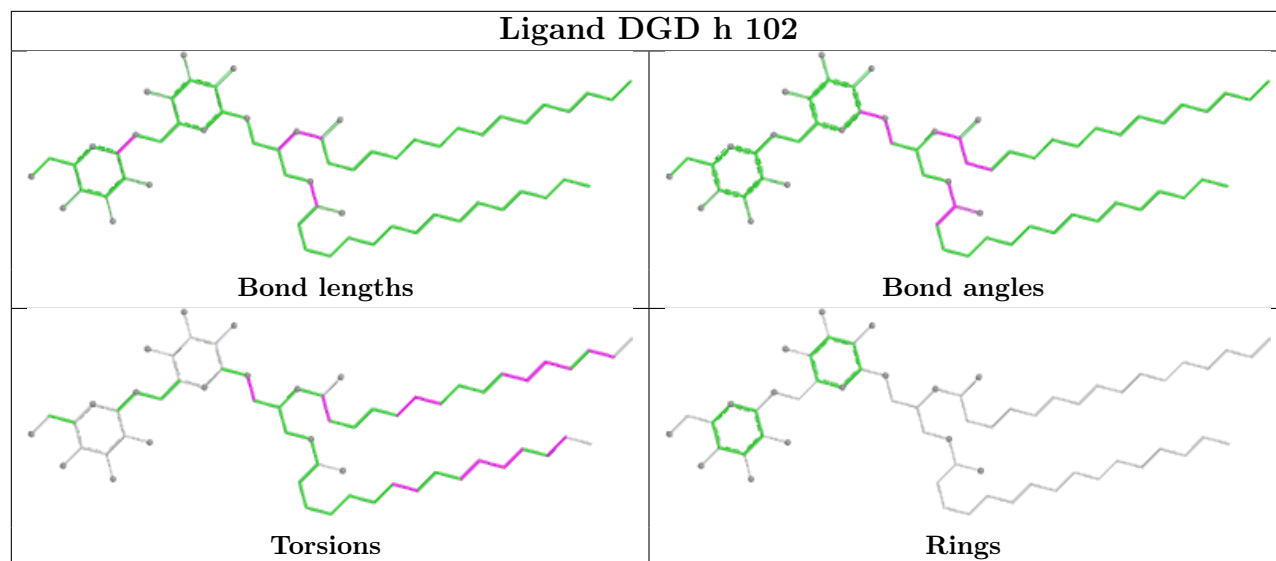
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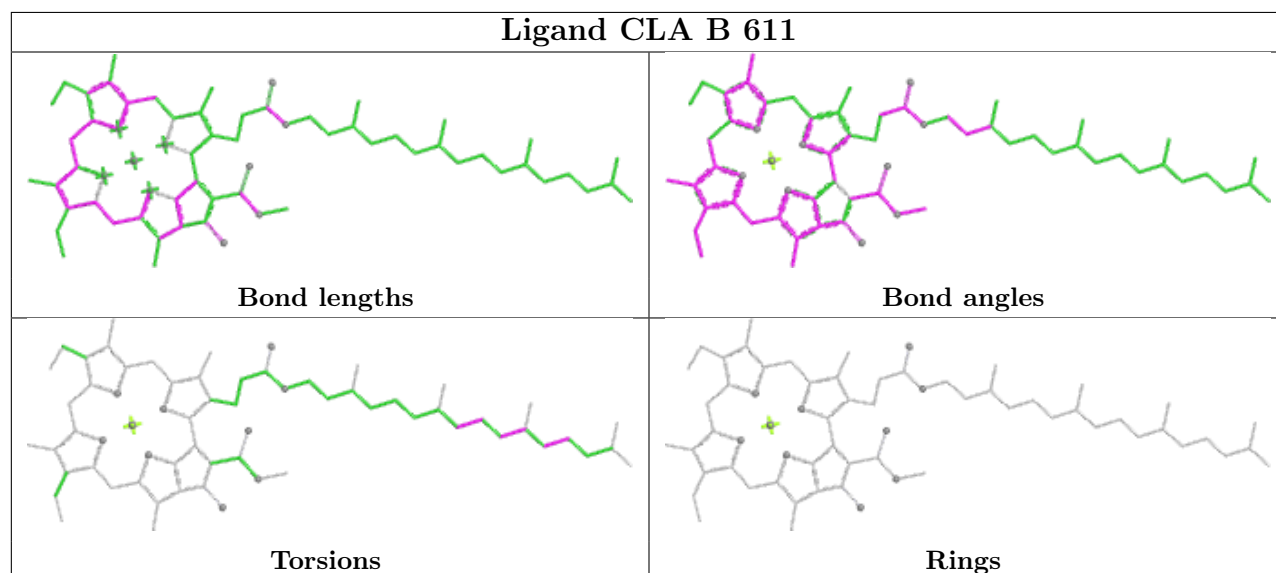
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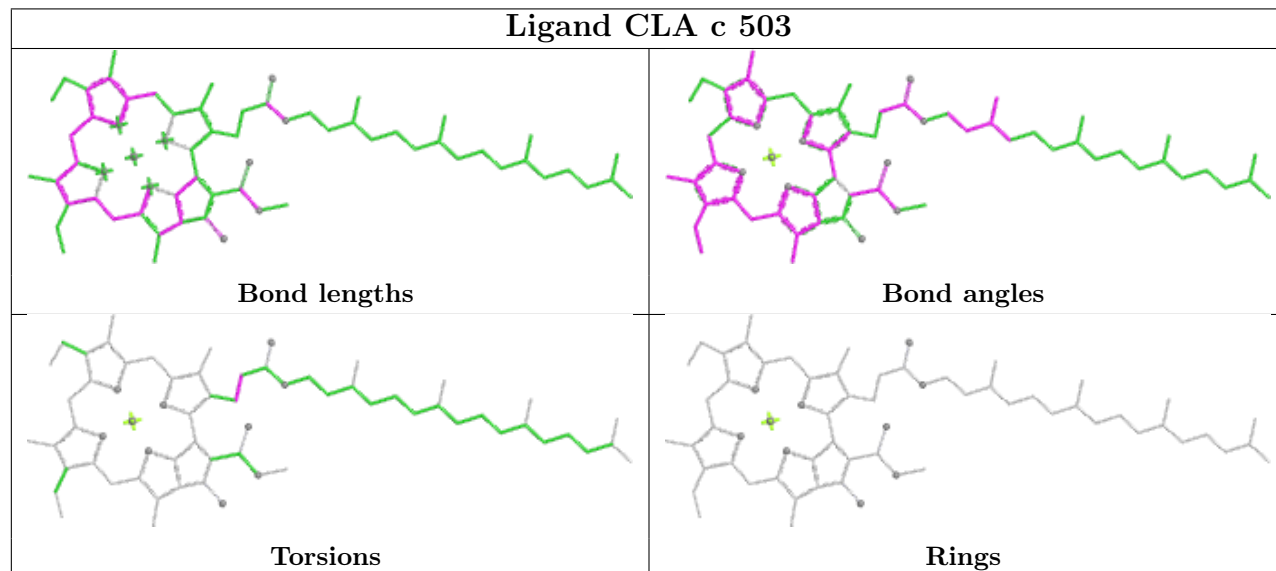
Ligand DGD h 102

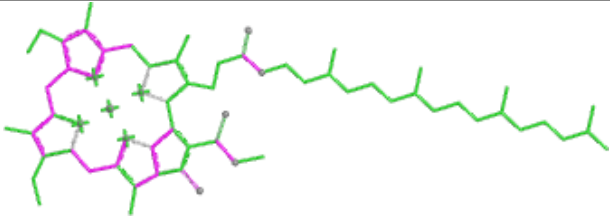
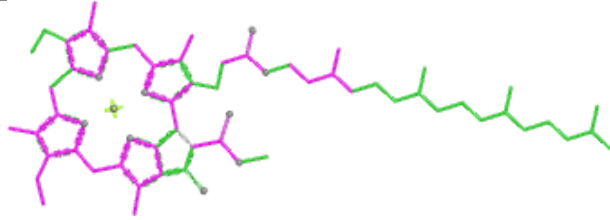
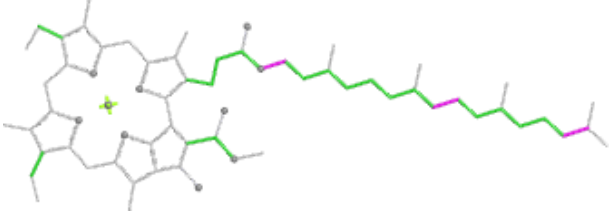
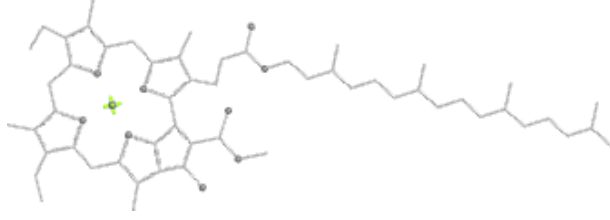
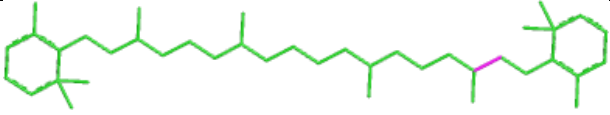
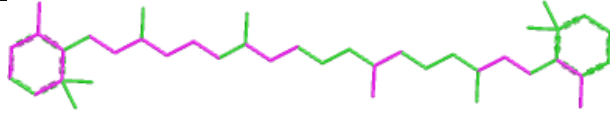
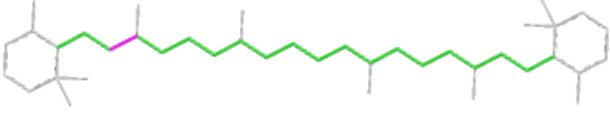
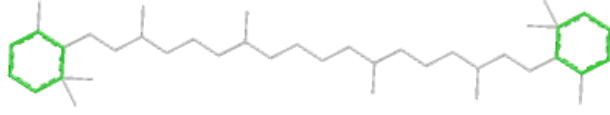
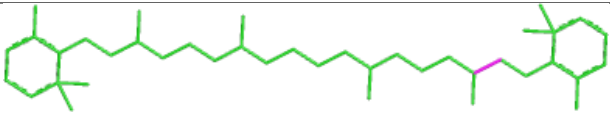
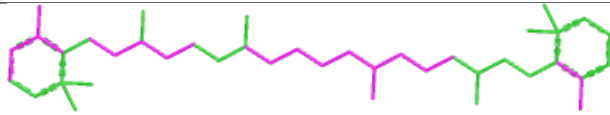
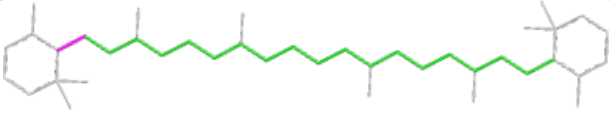
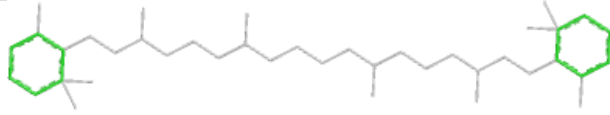


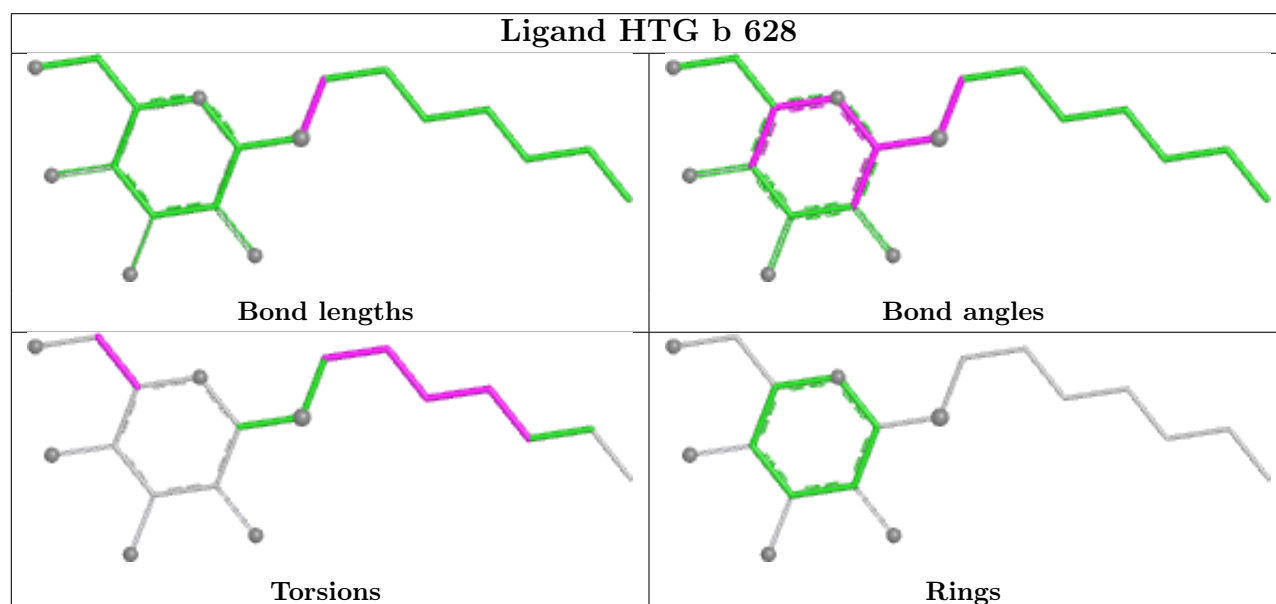
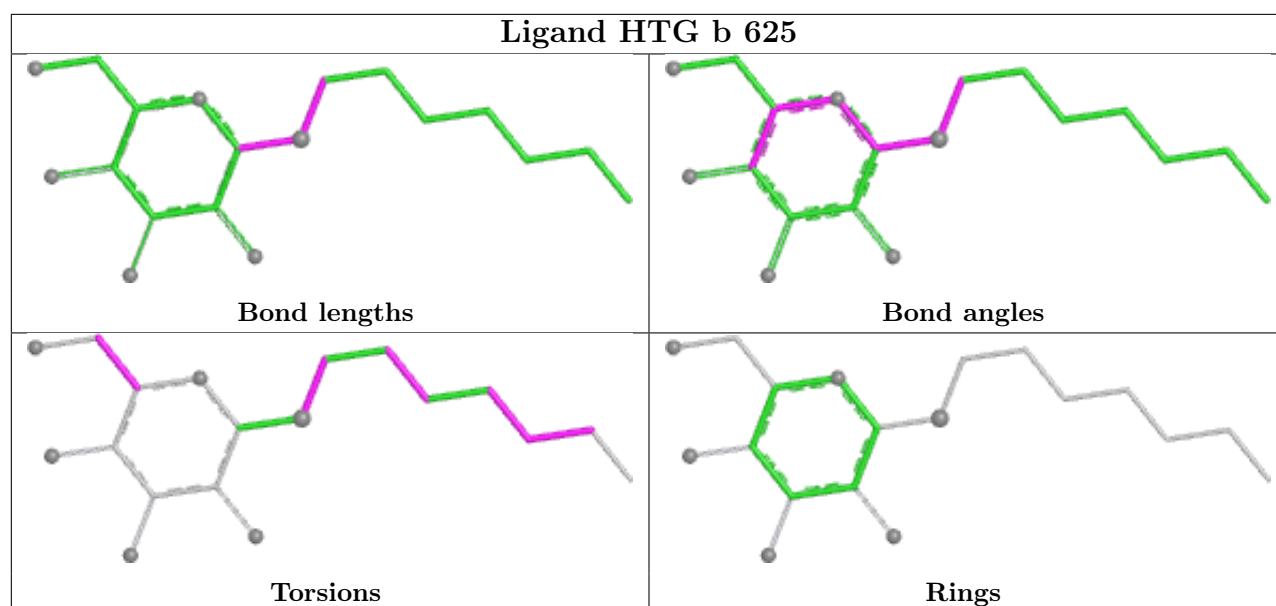
Ligand CLA B 611

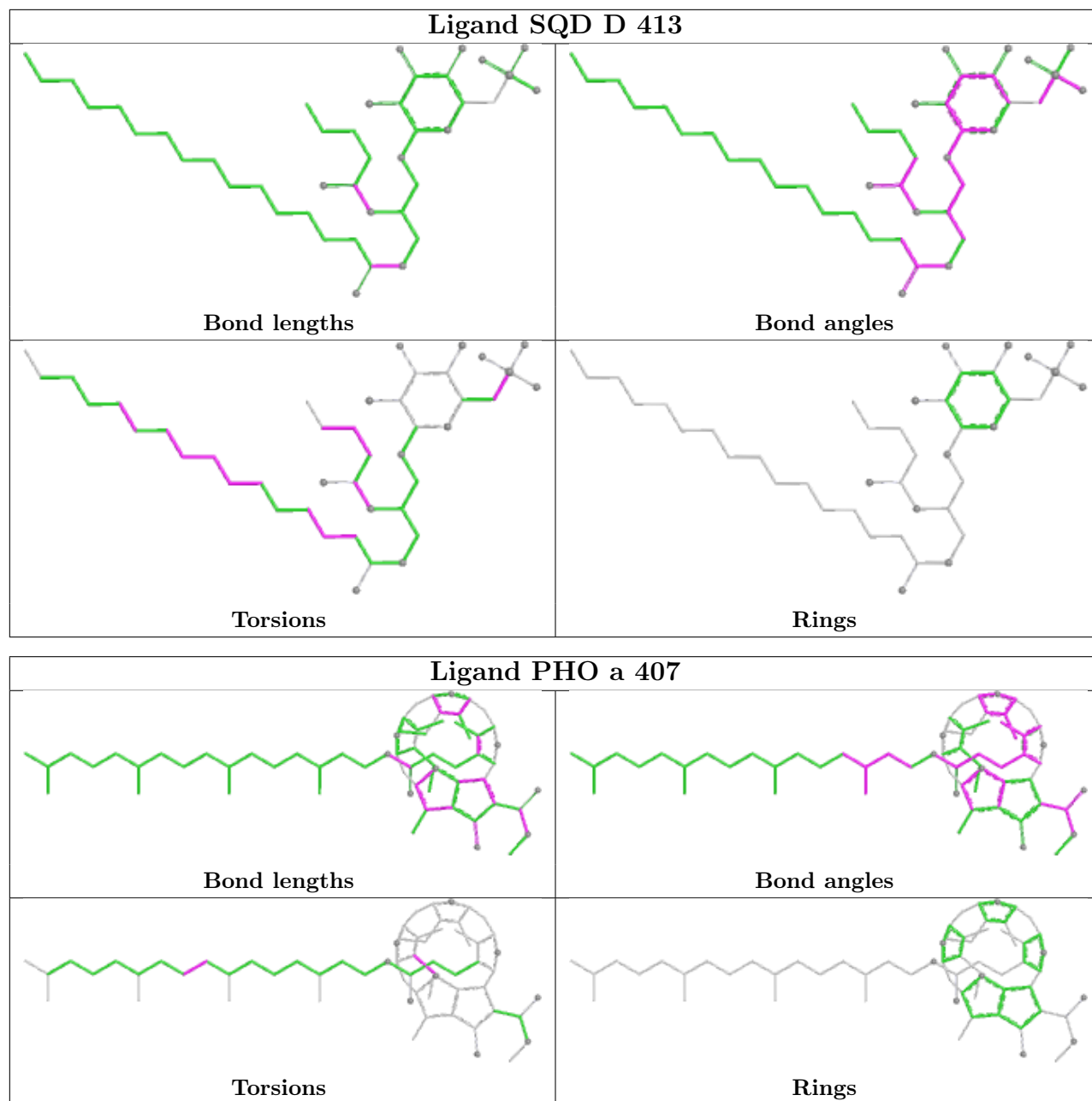


Ligand CLA c 503

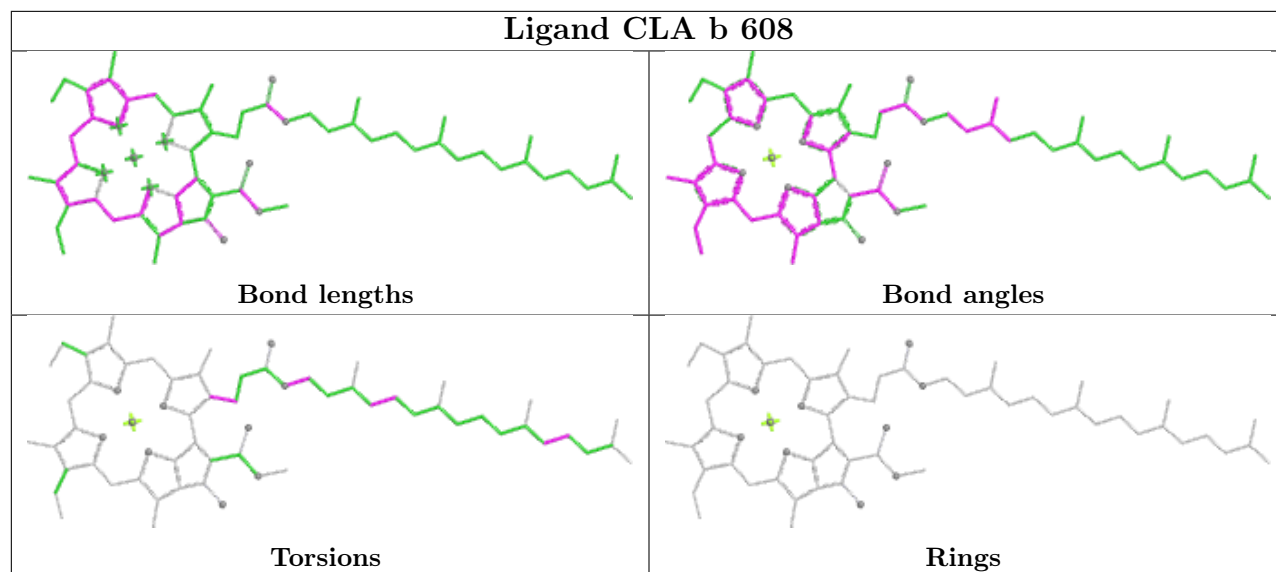


Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

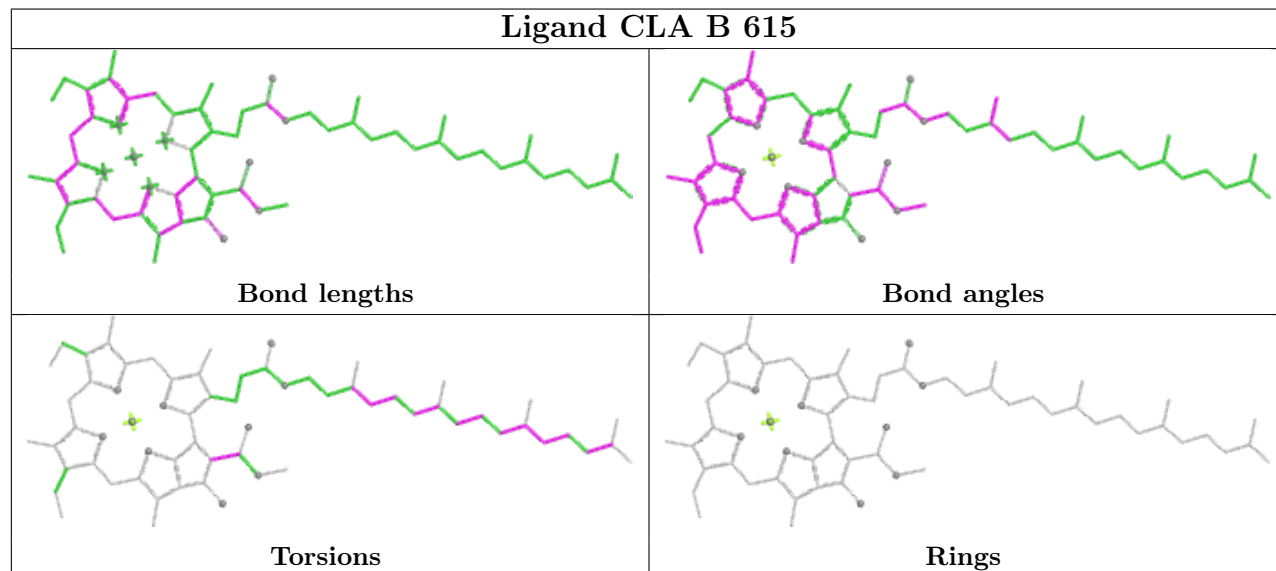




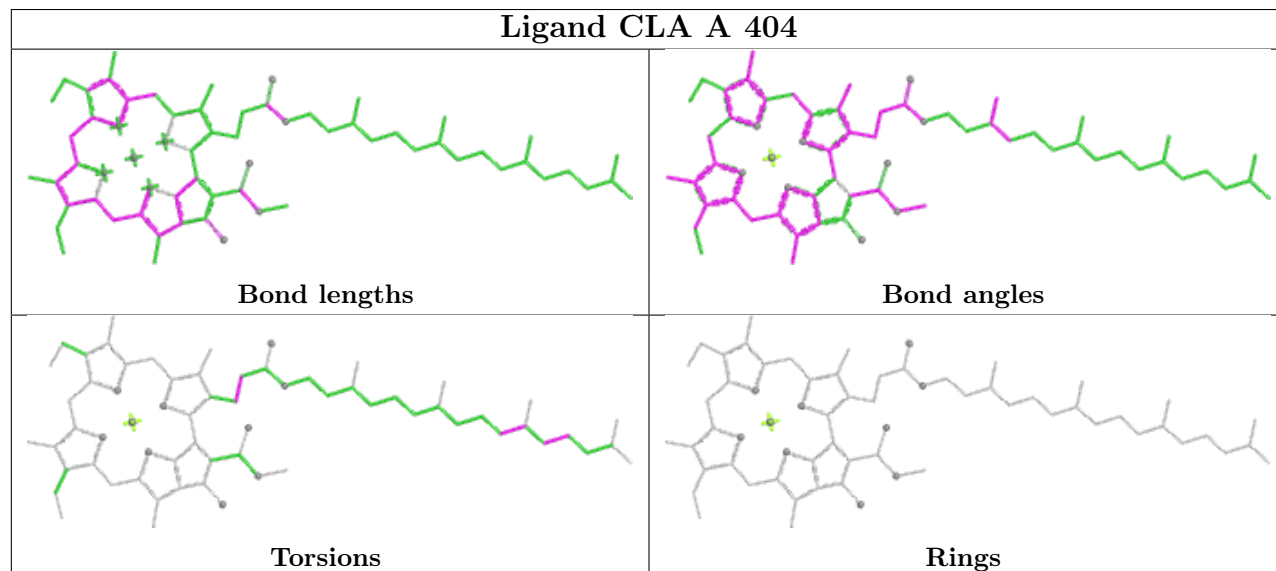
Ligand CLA b 608

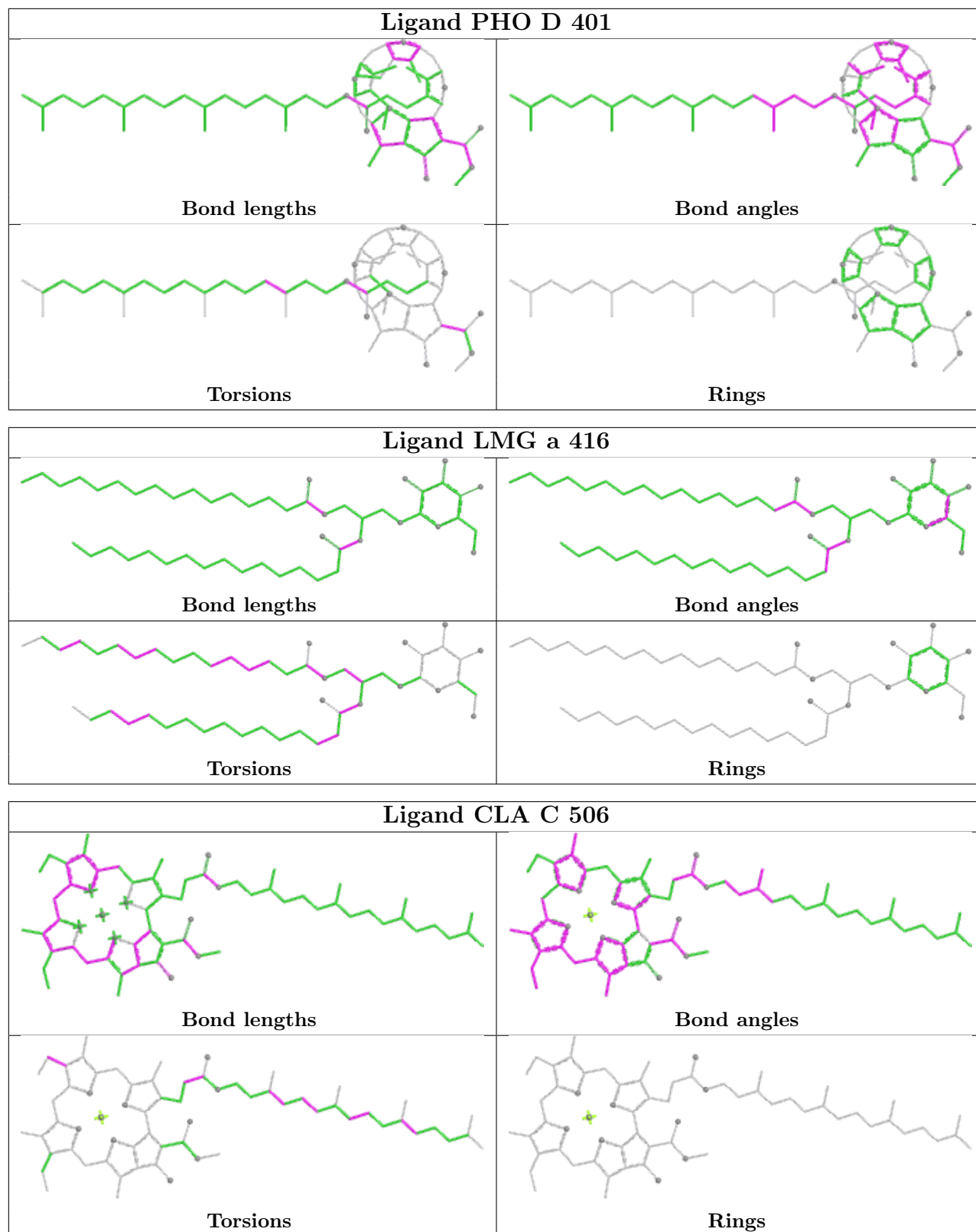


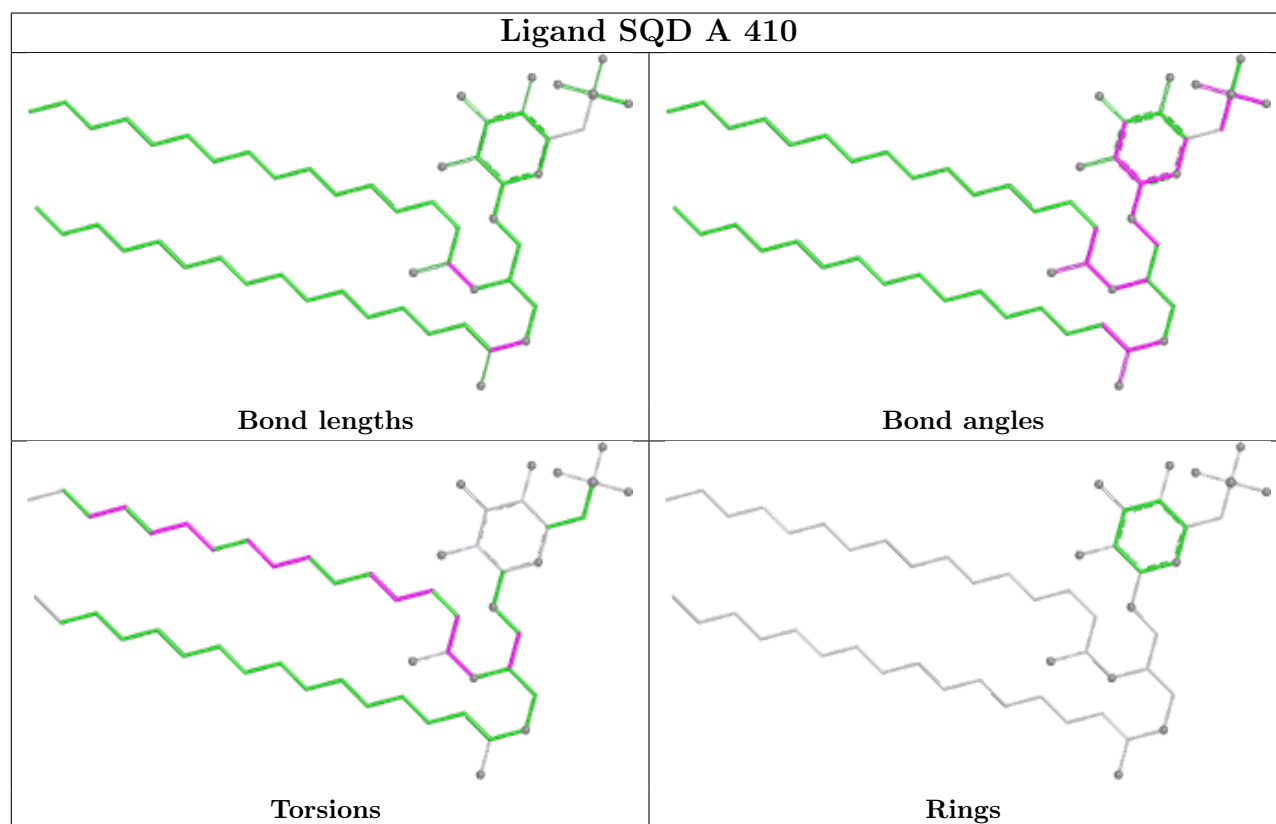
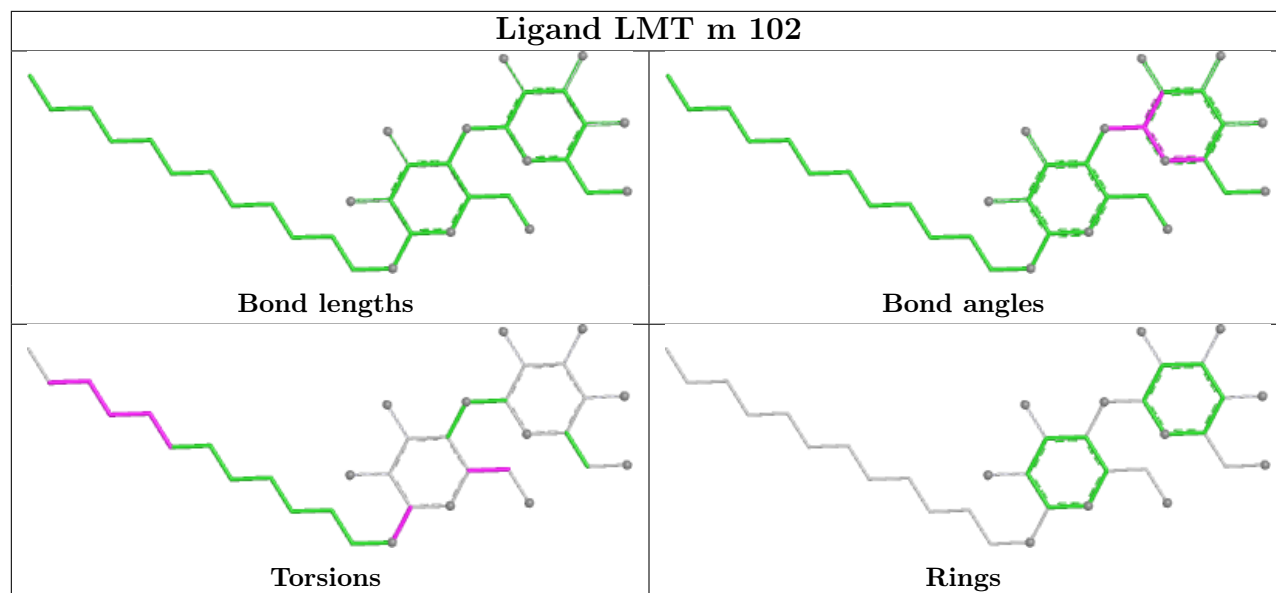
Ligand CLA B 615



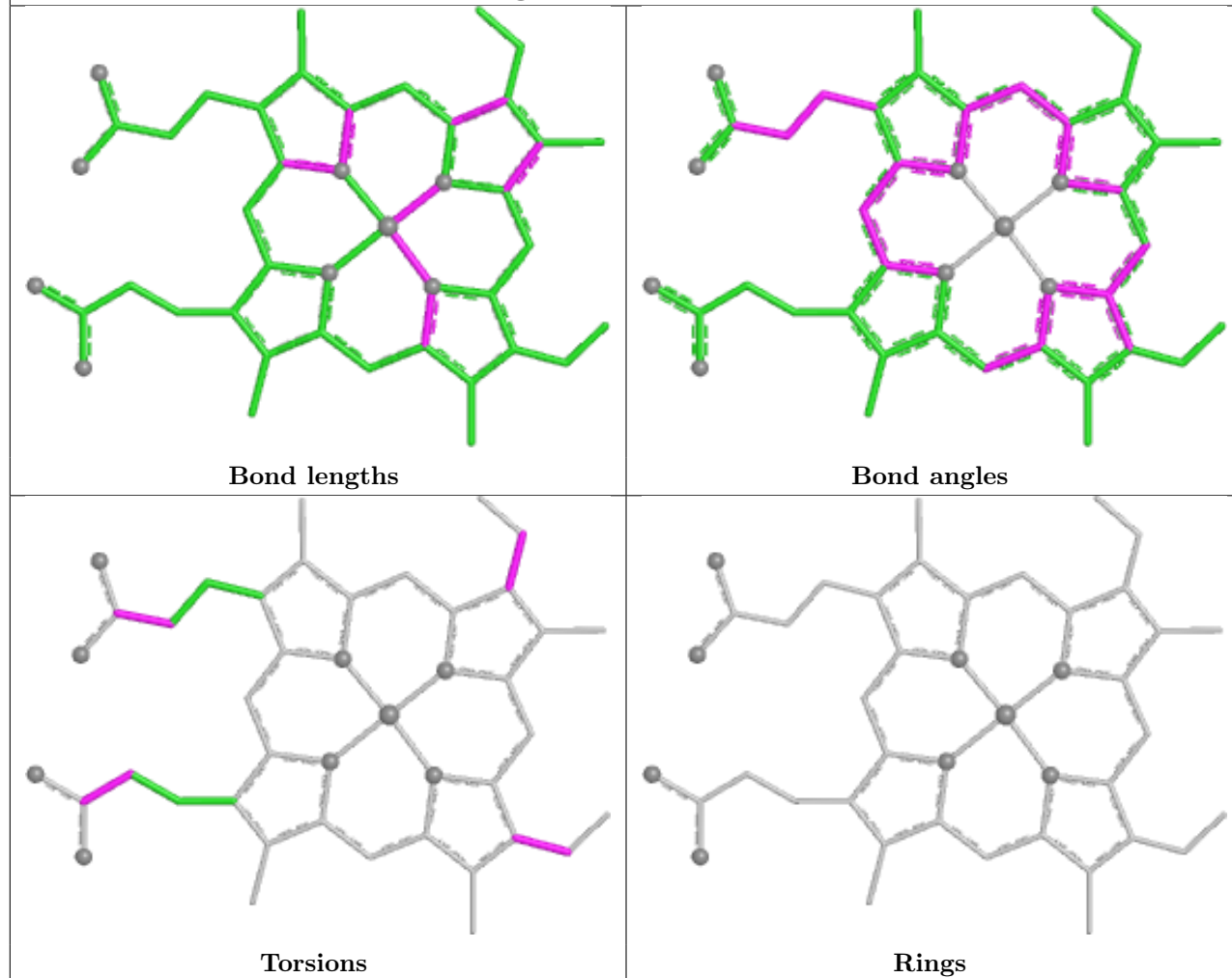
Ligand CLA A 404



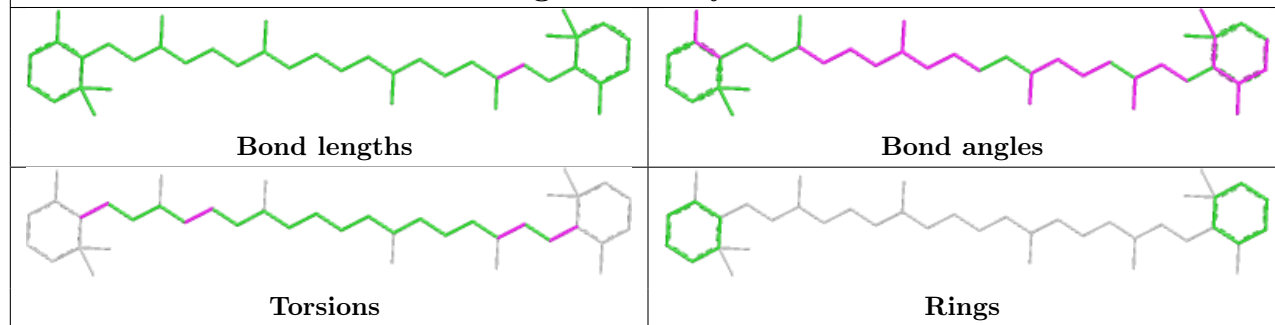


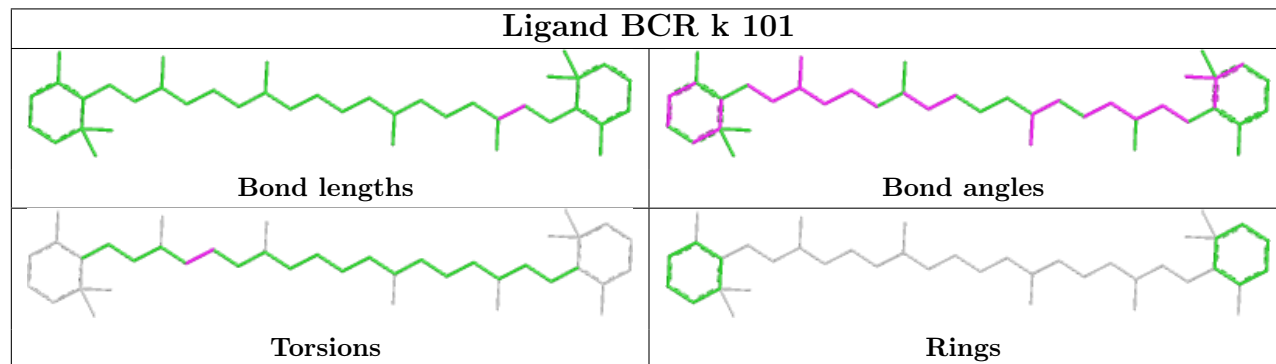
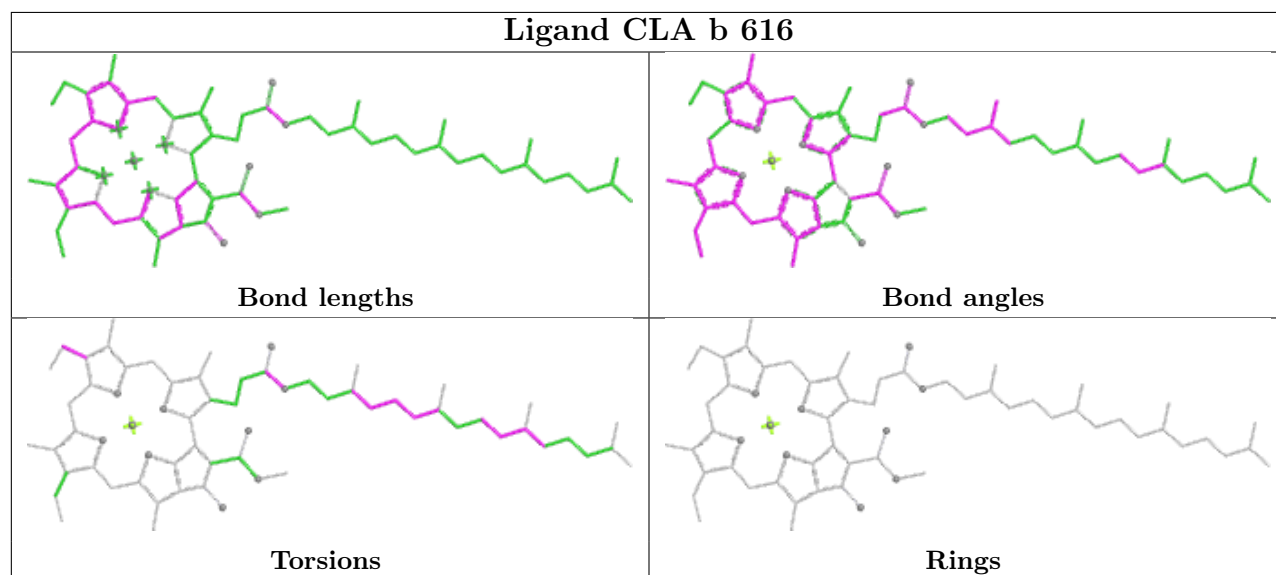
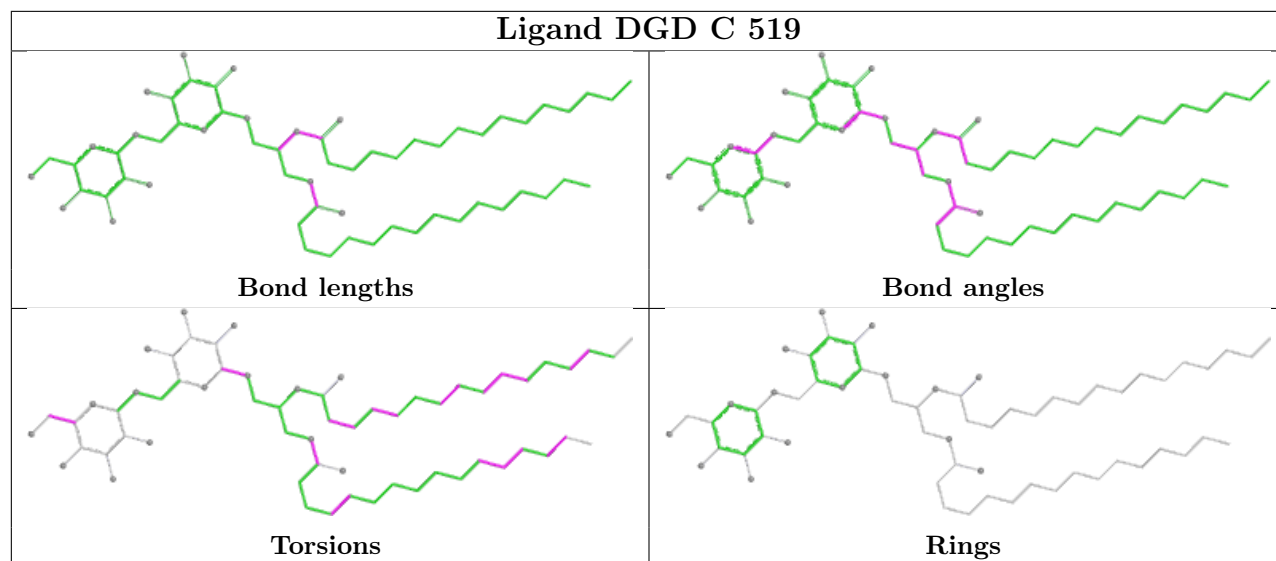


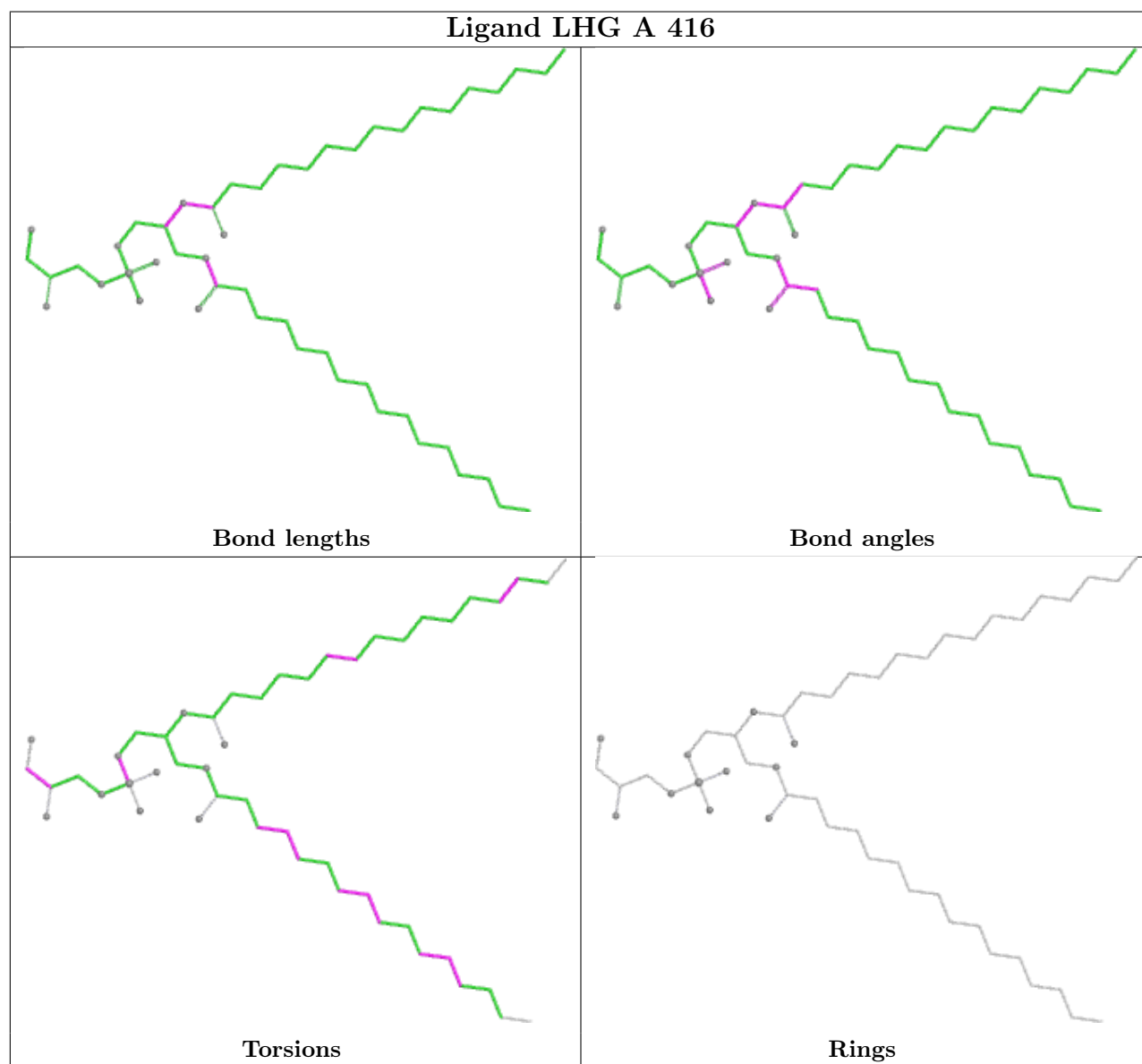
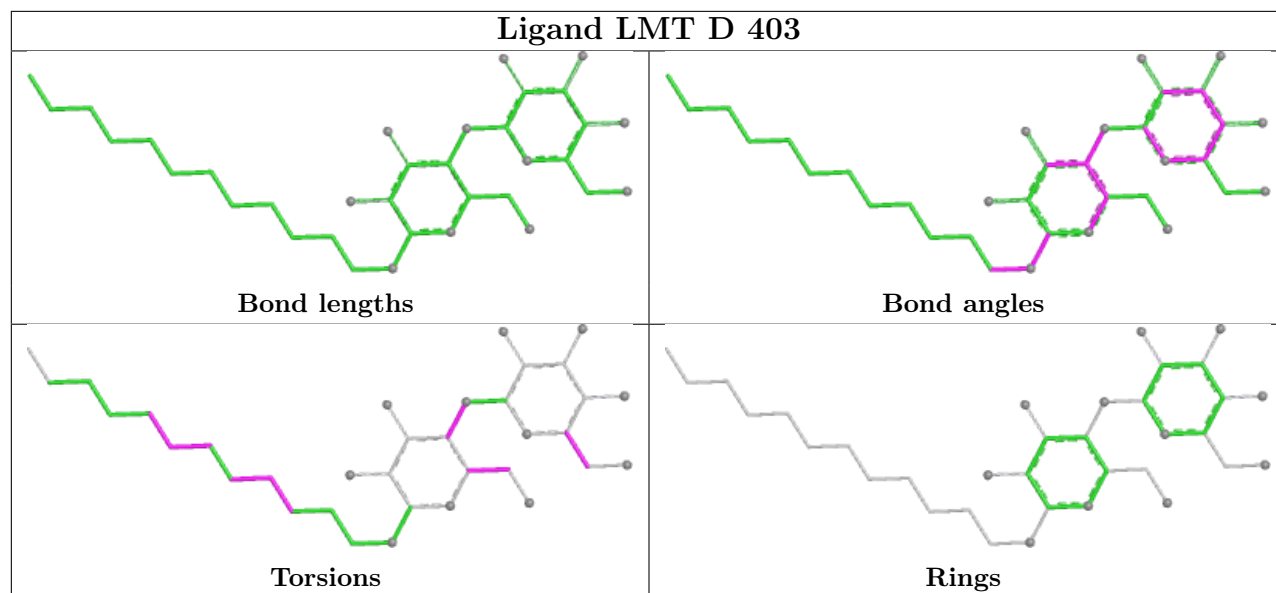
Ligand HEM e 103

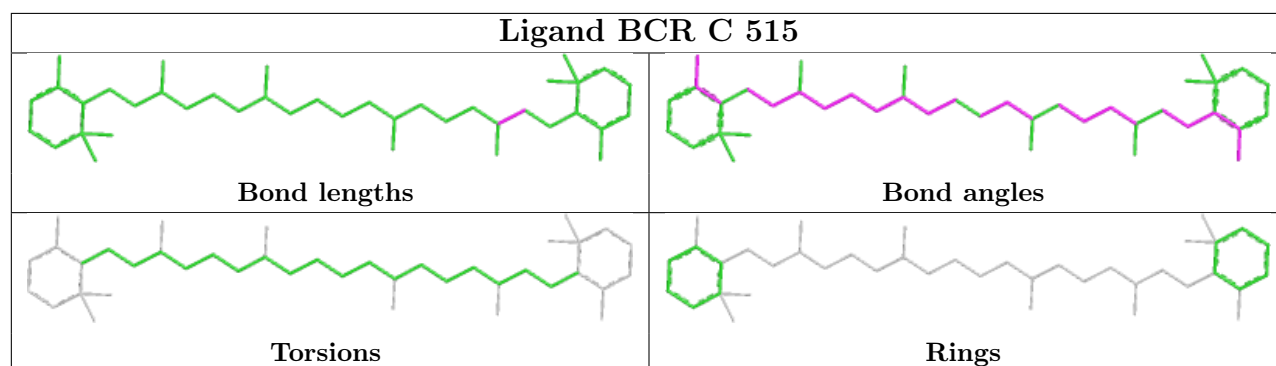
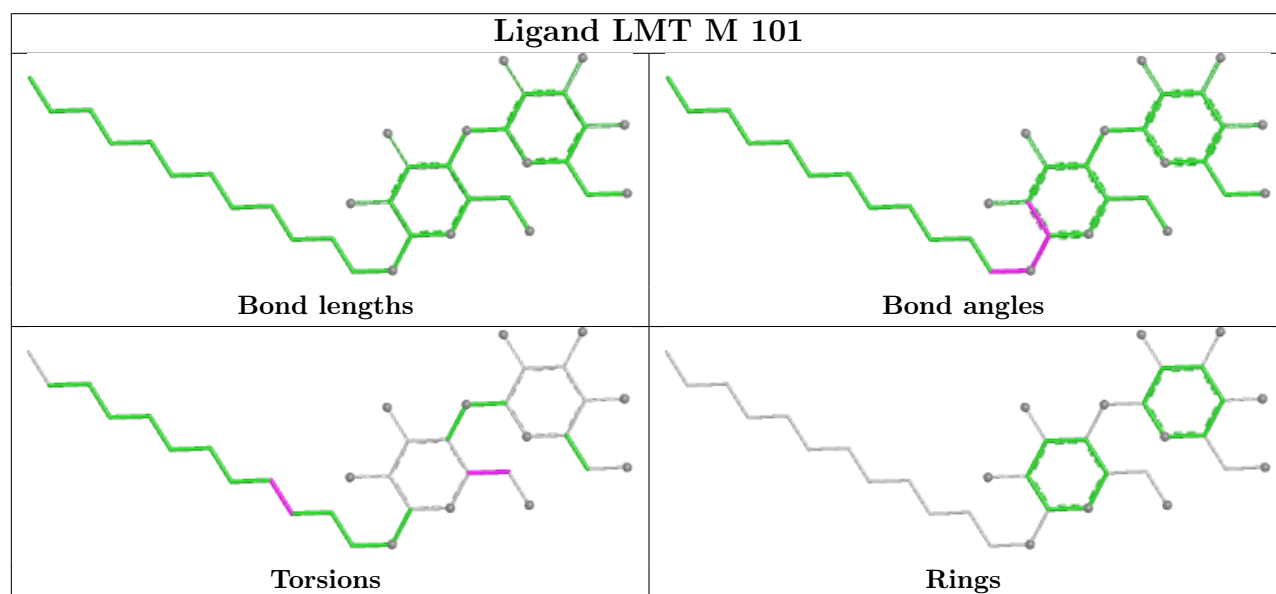
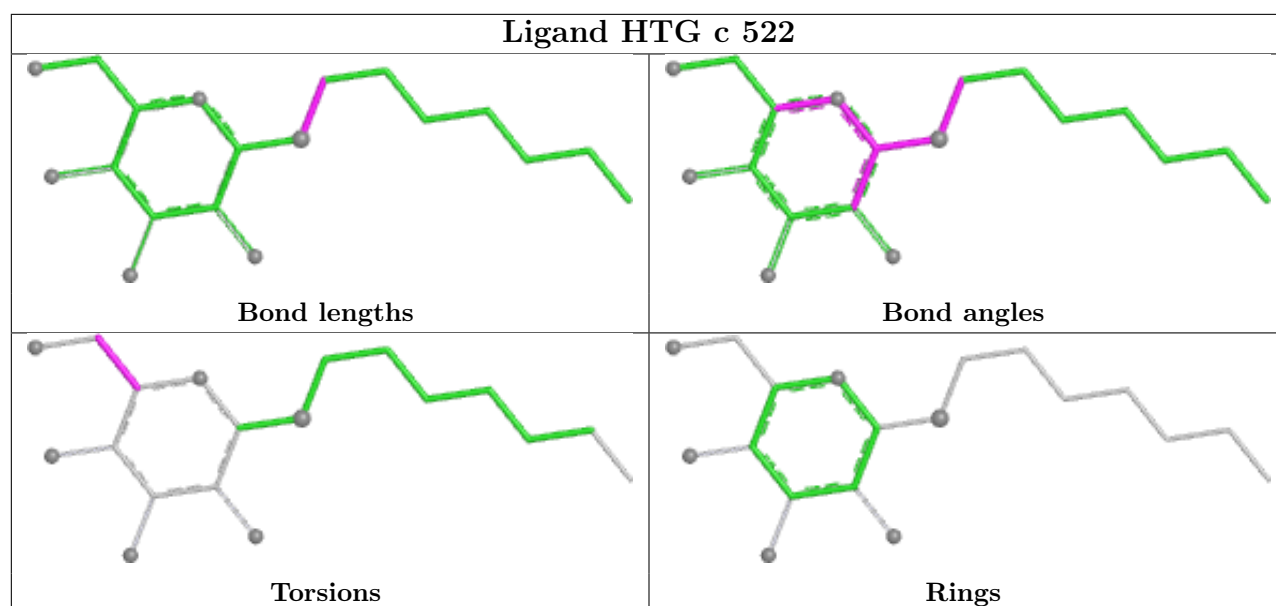


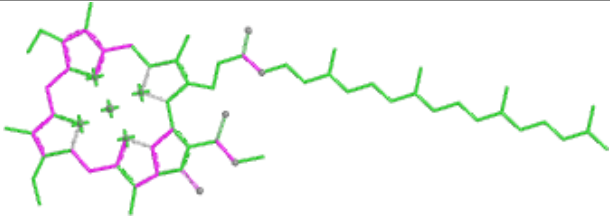
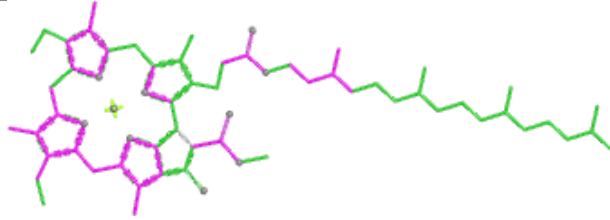
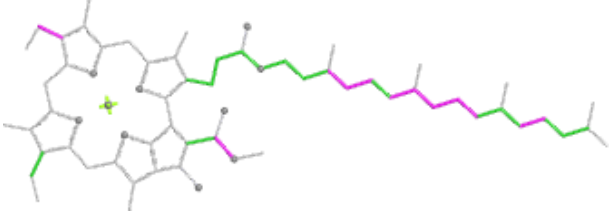
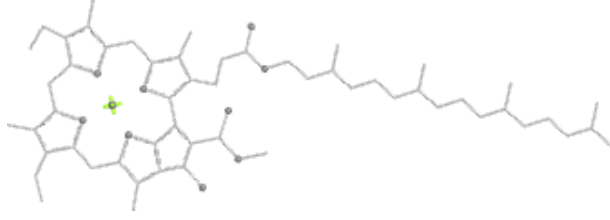
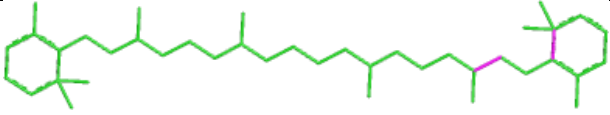
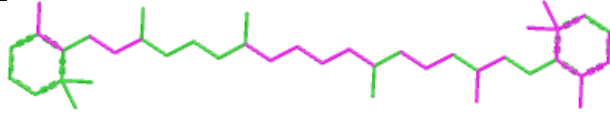
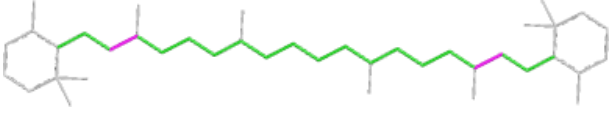
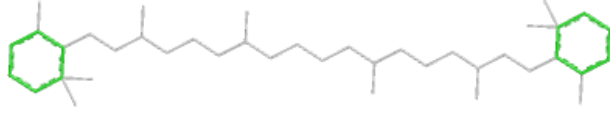
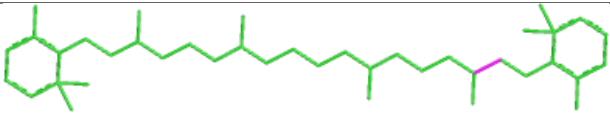
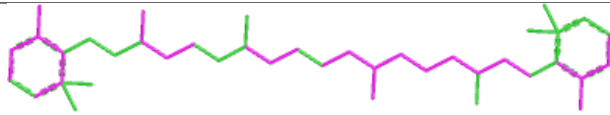
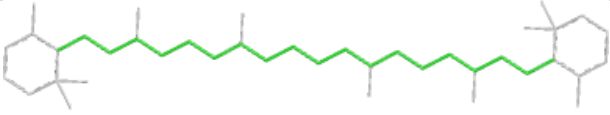
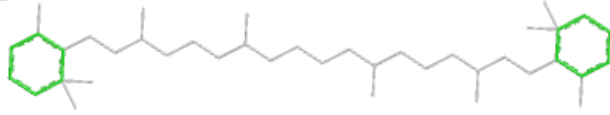
Ligand BCR y 101



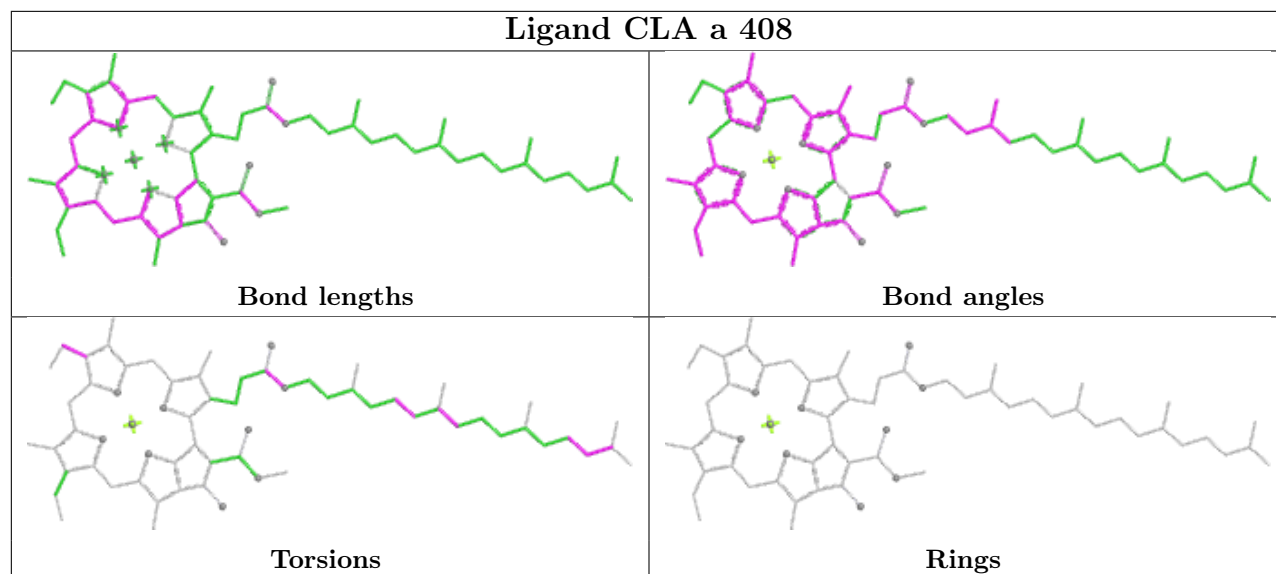




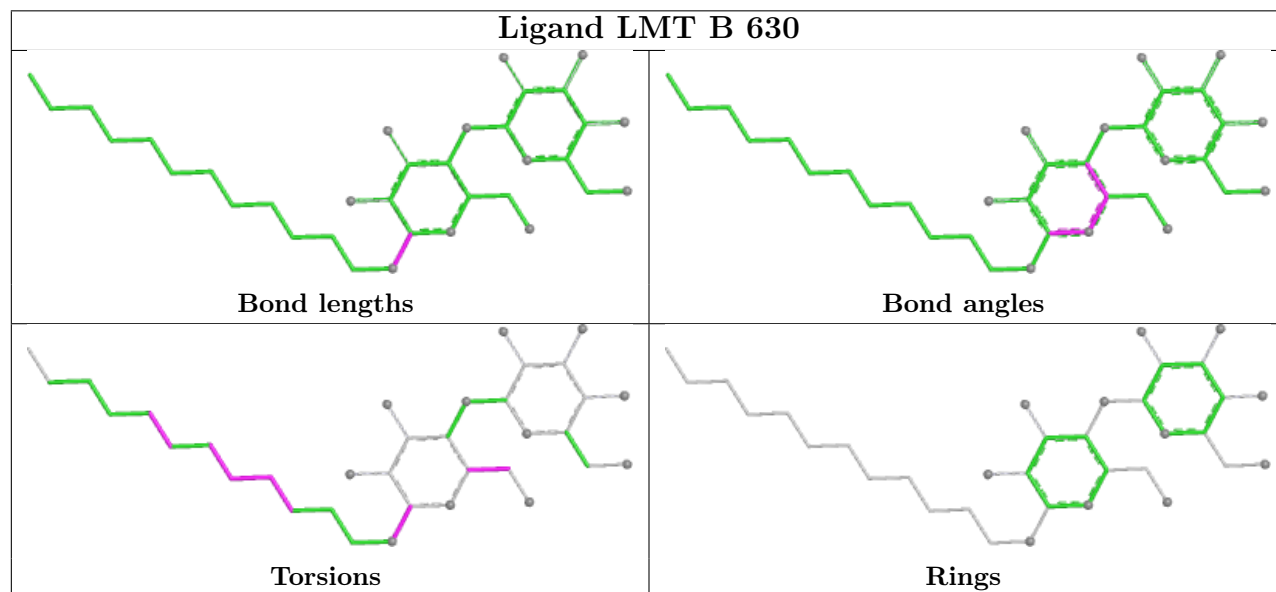


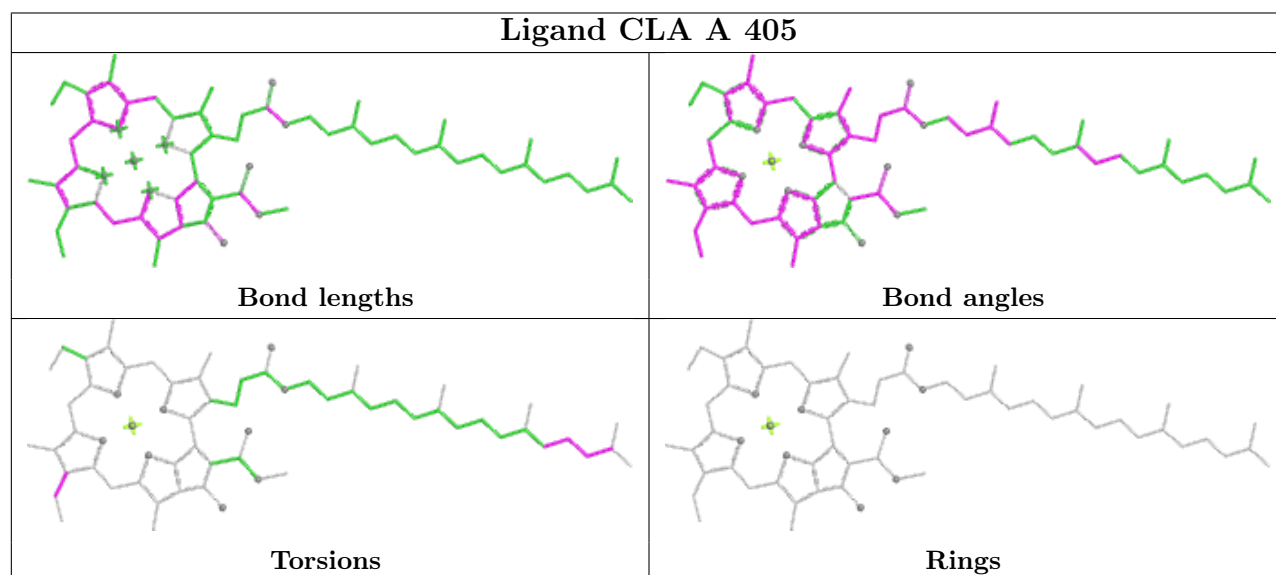
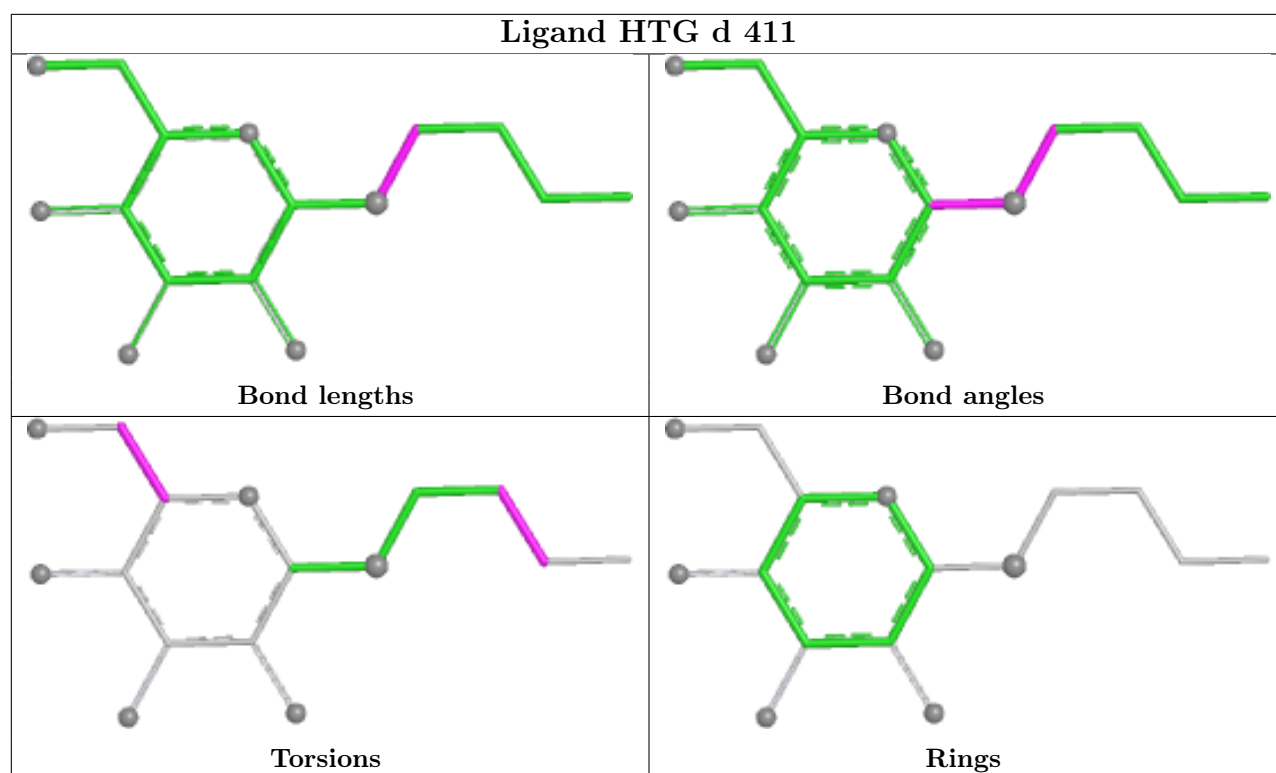
Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

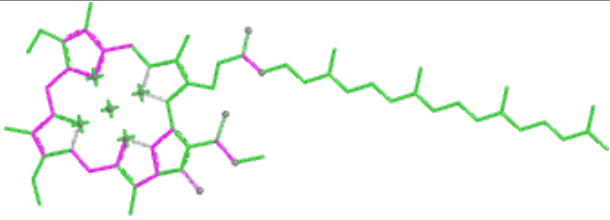
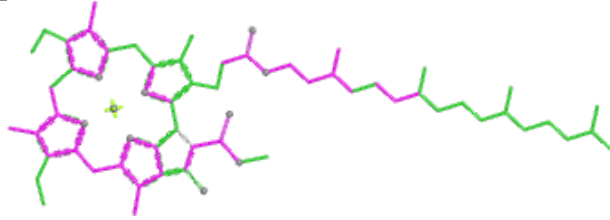
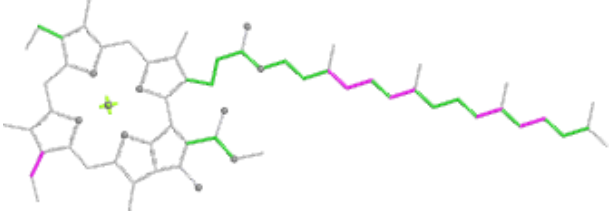
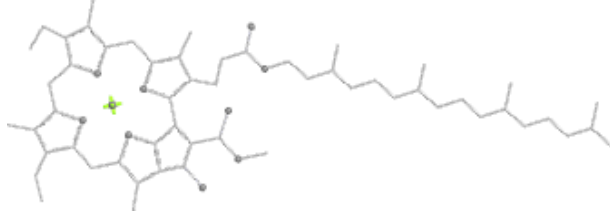
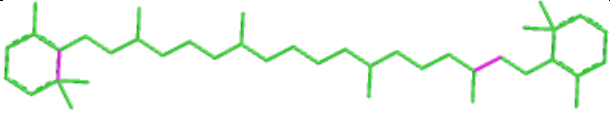
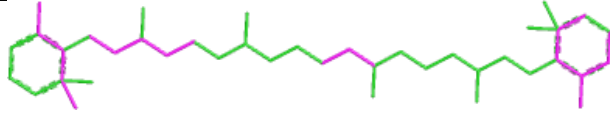
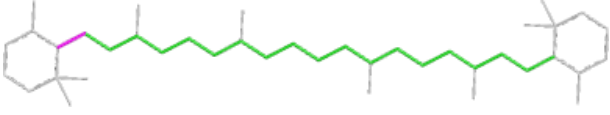
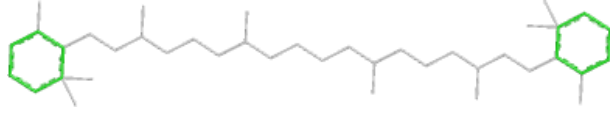
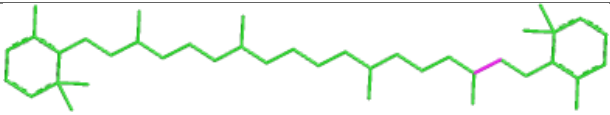
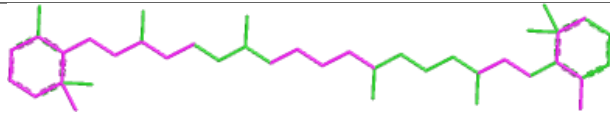
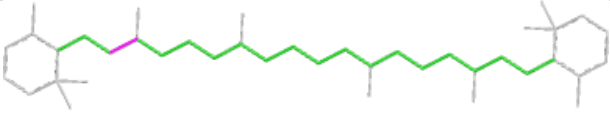
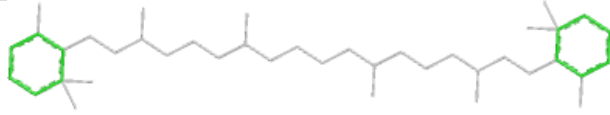
Ligand CLA a 408



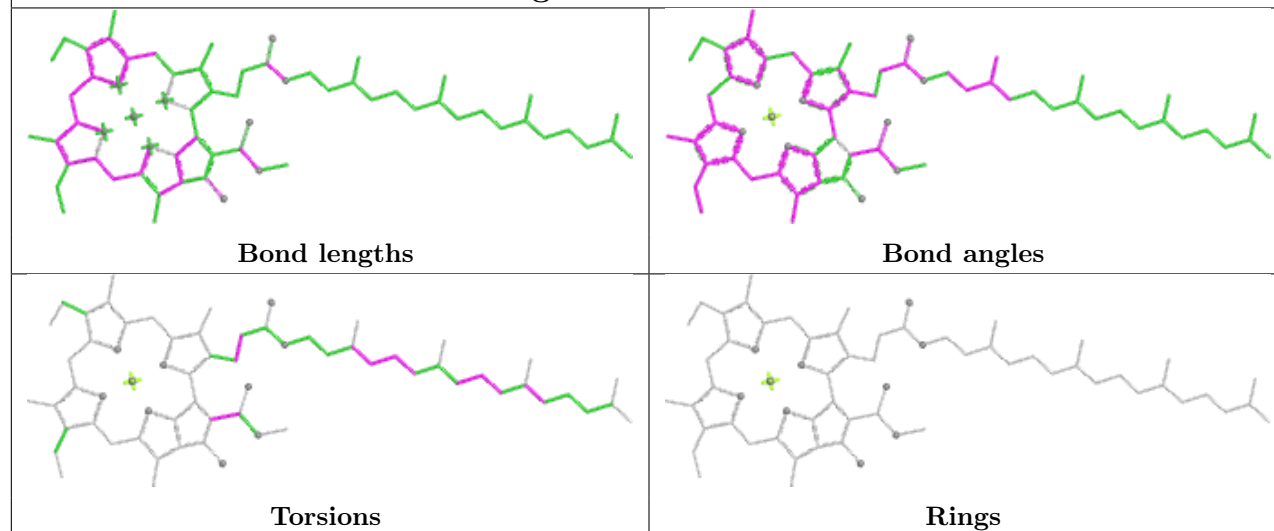
Ligand LMT B 630



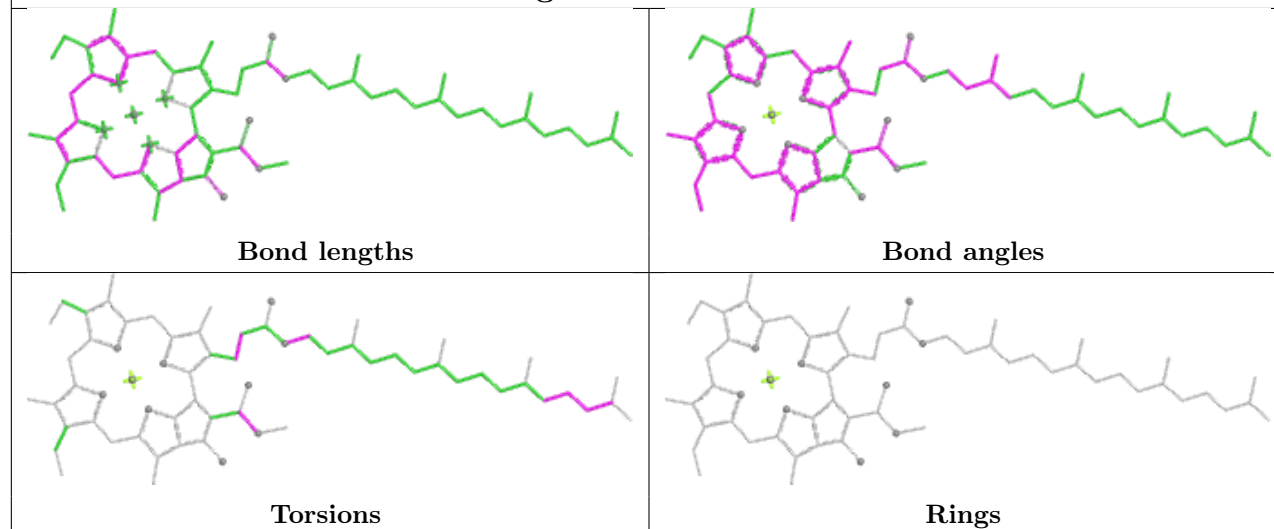


Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

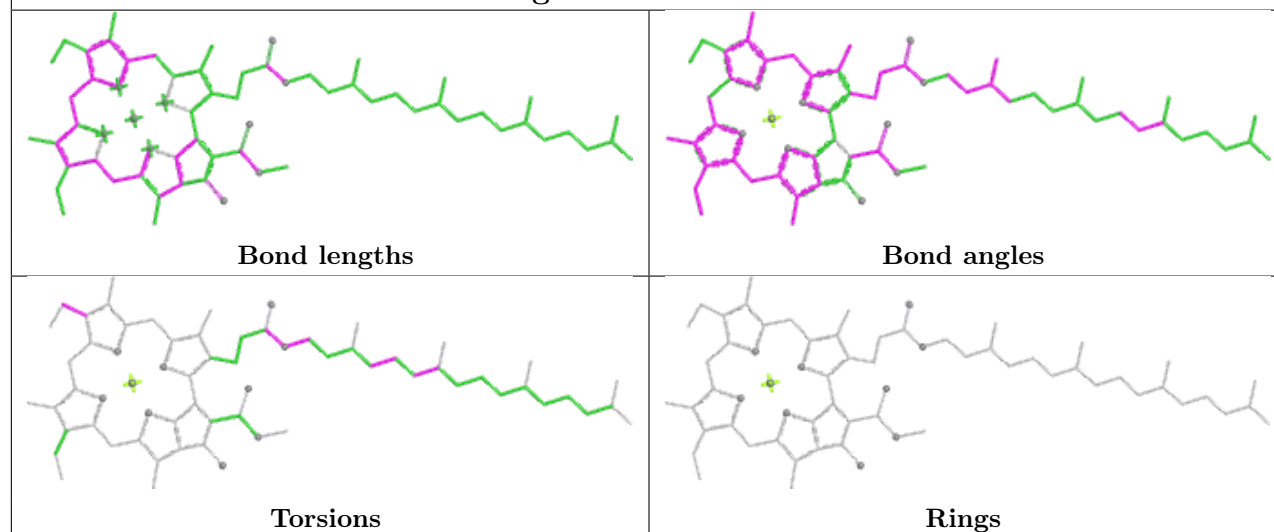
Ligand CLA B 614

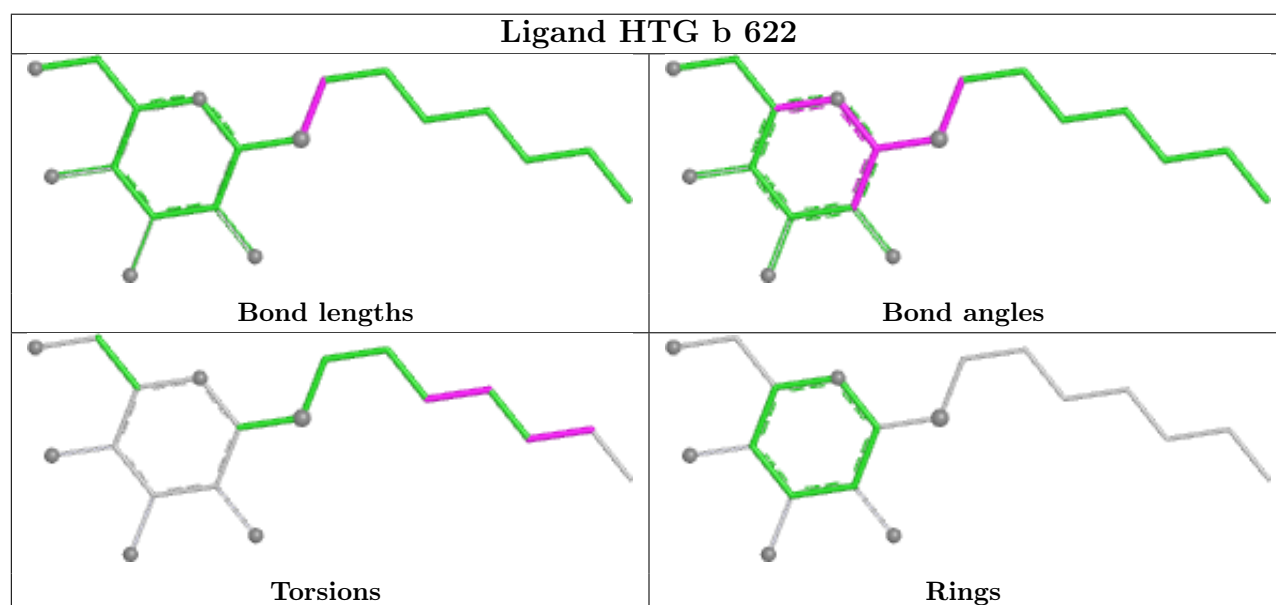
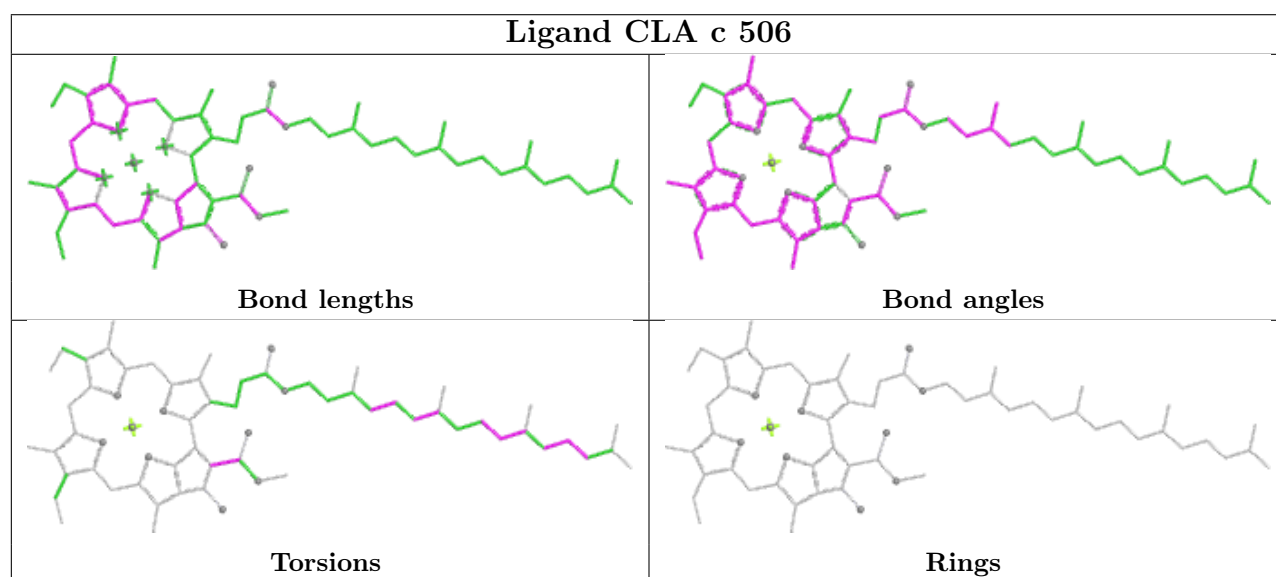
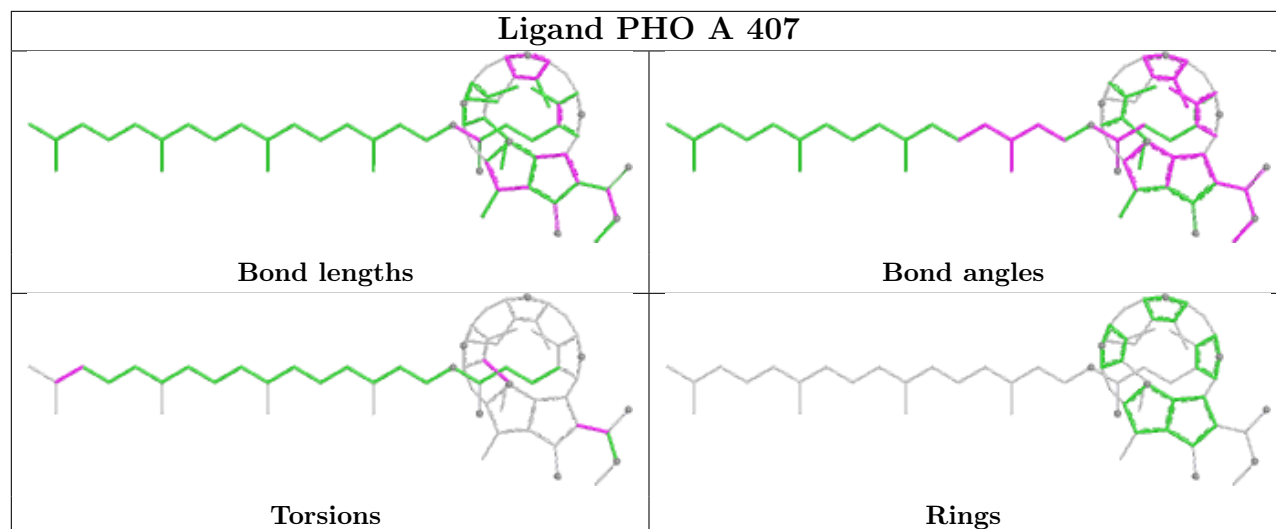


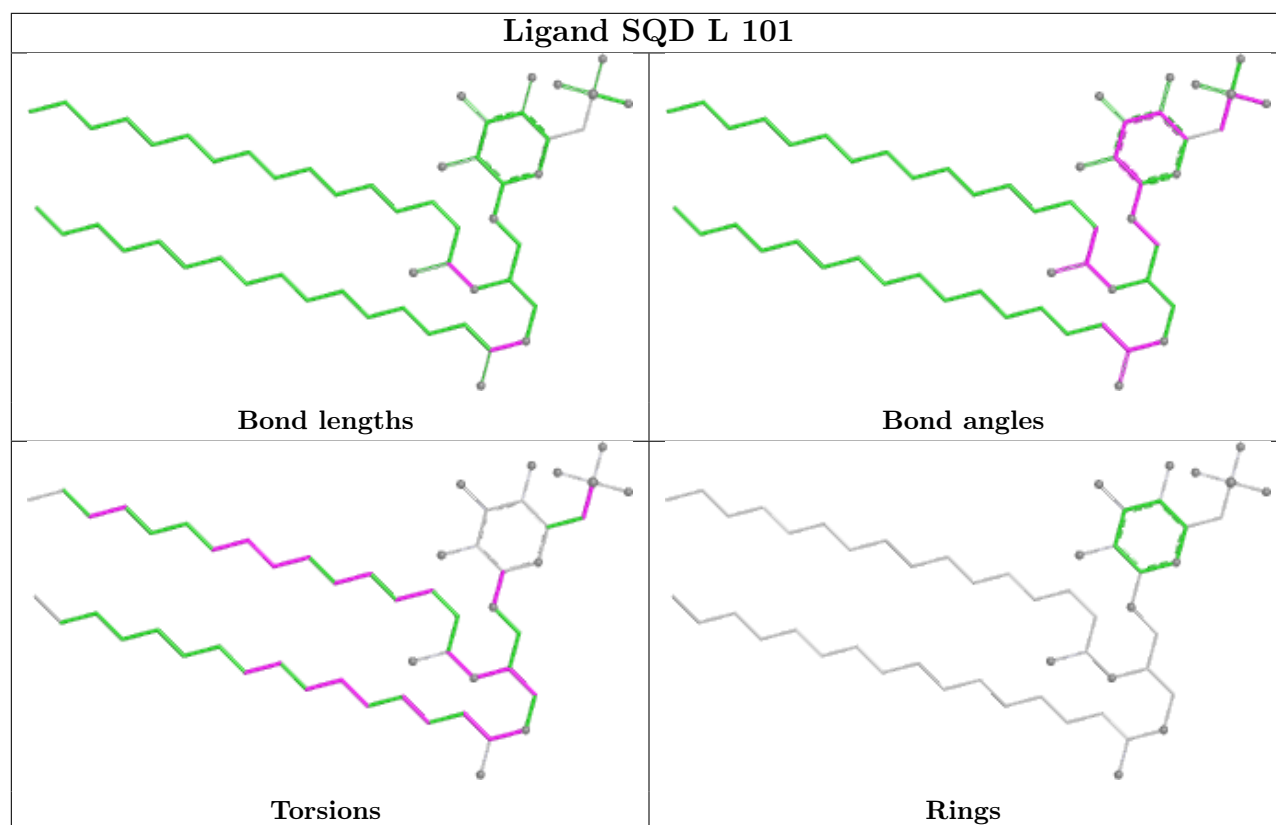
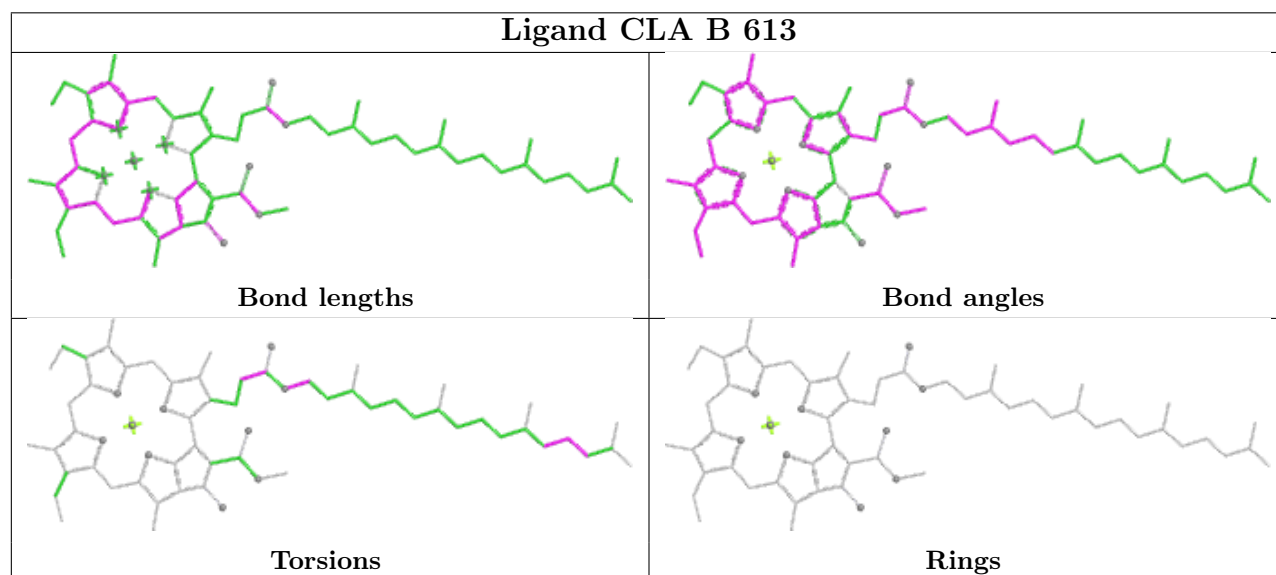
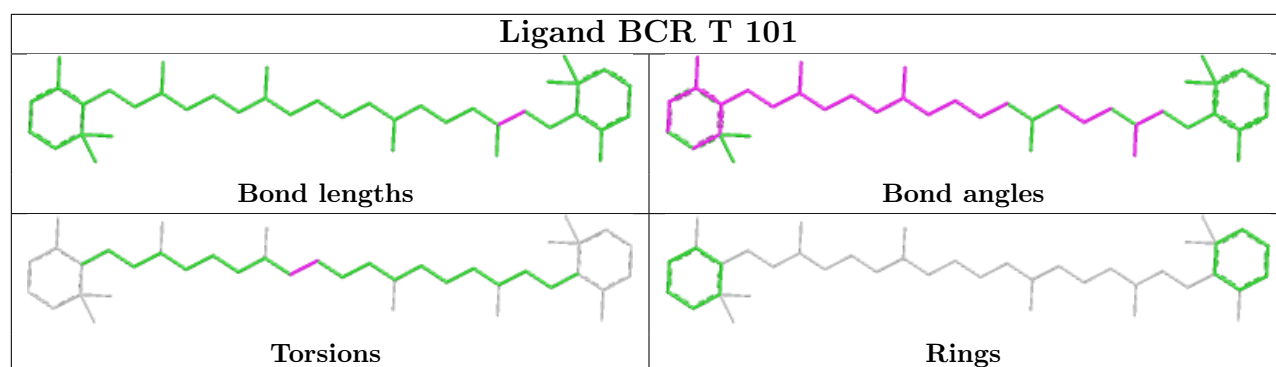
Ligand CLA a 404



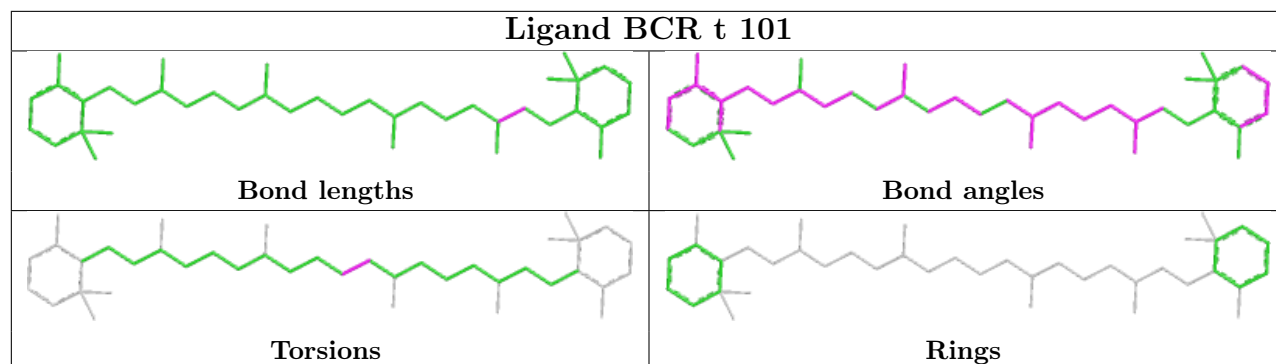
Ligand CLA C 513



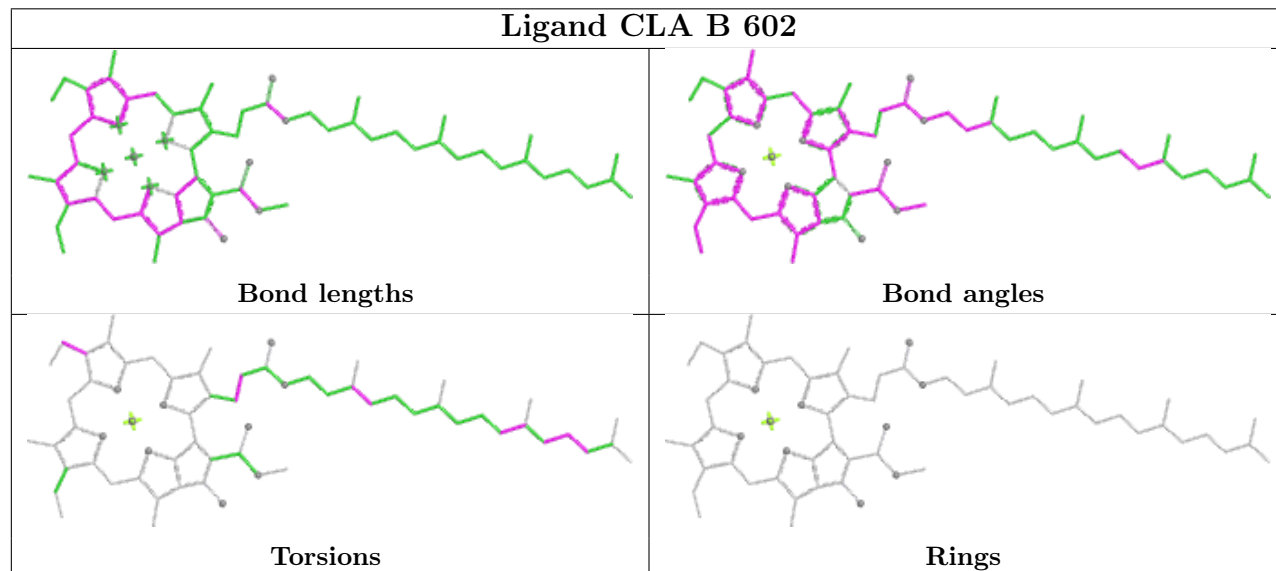




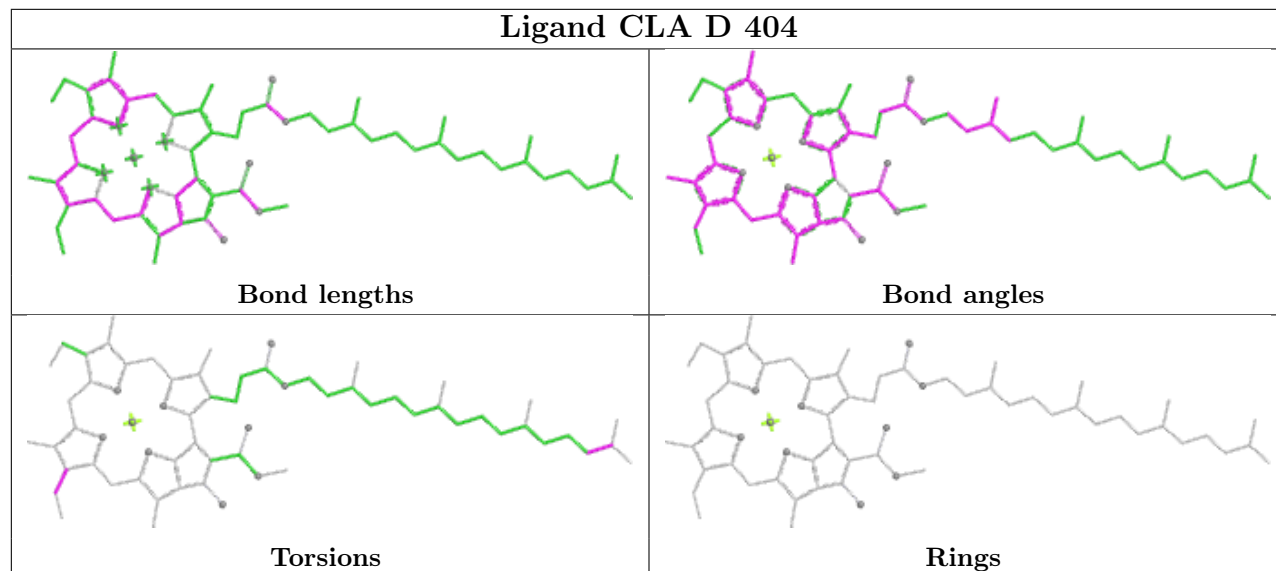
Ligand BCR t 101



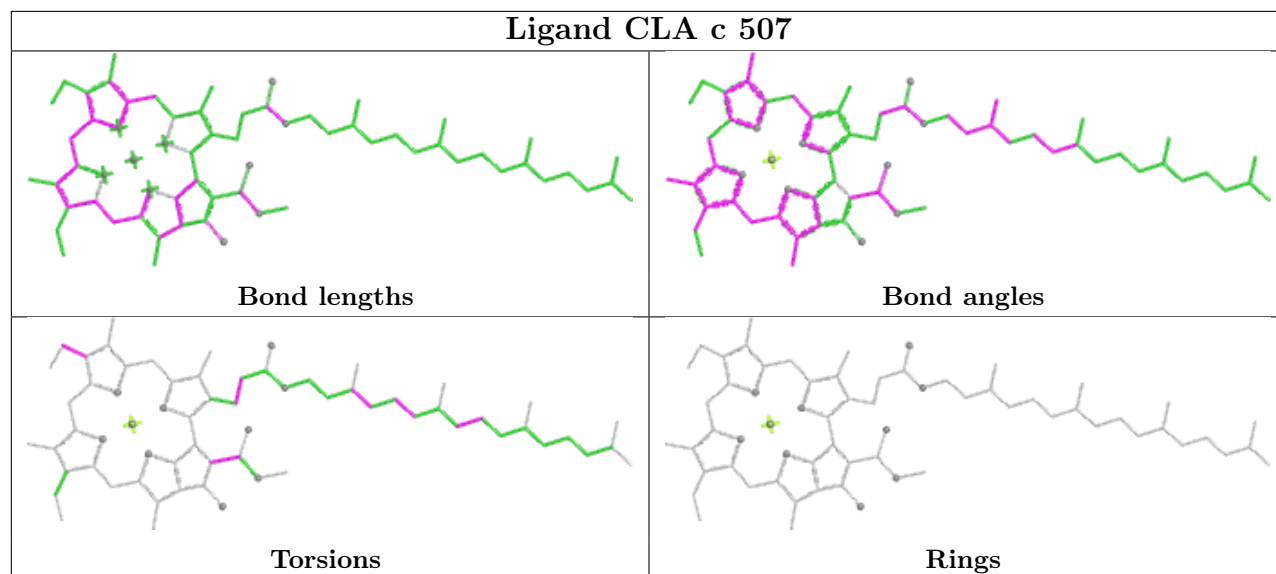
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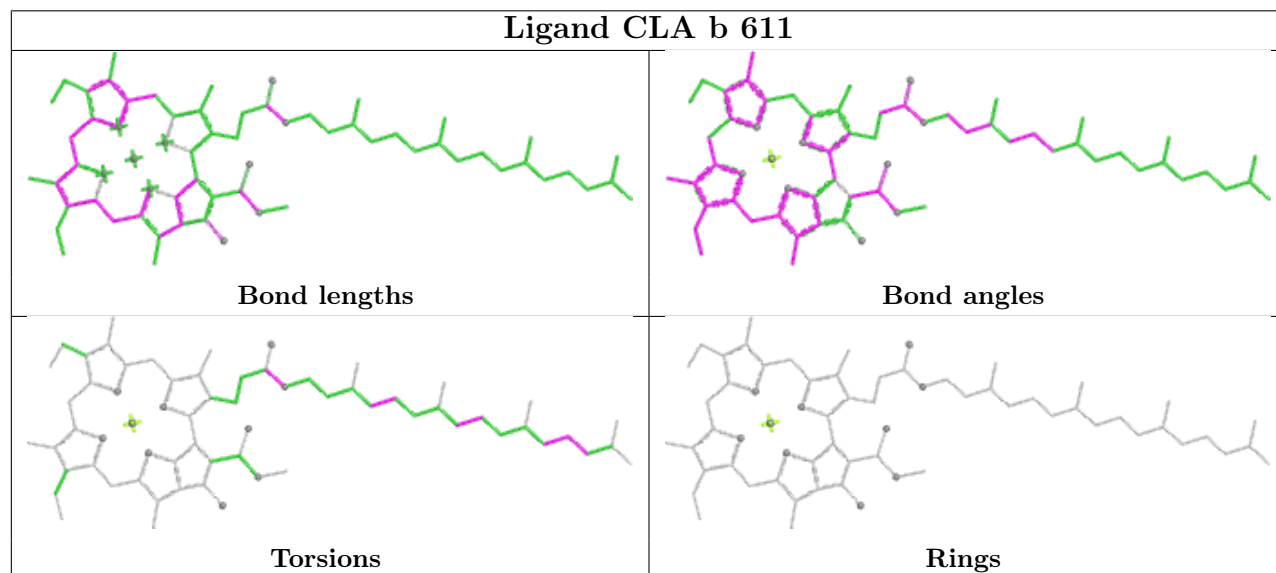
Ligand CLA D 404

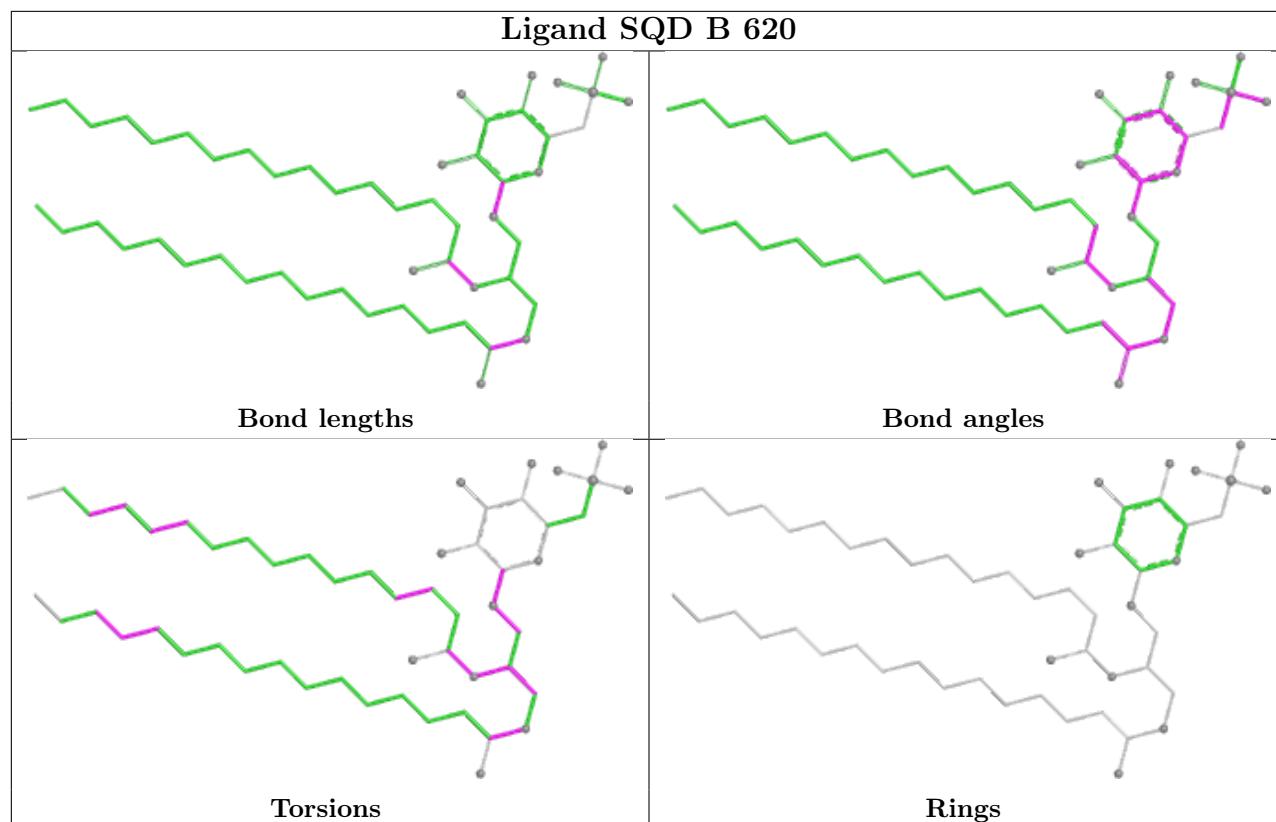


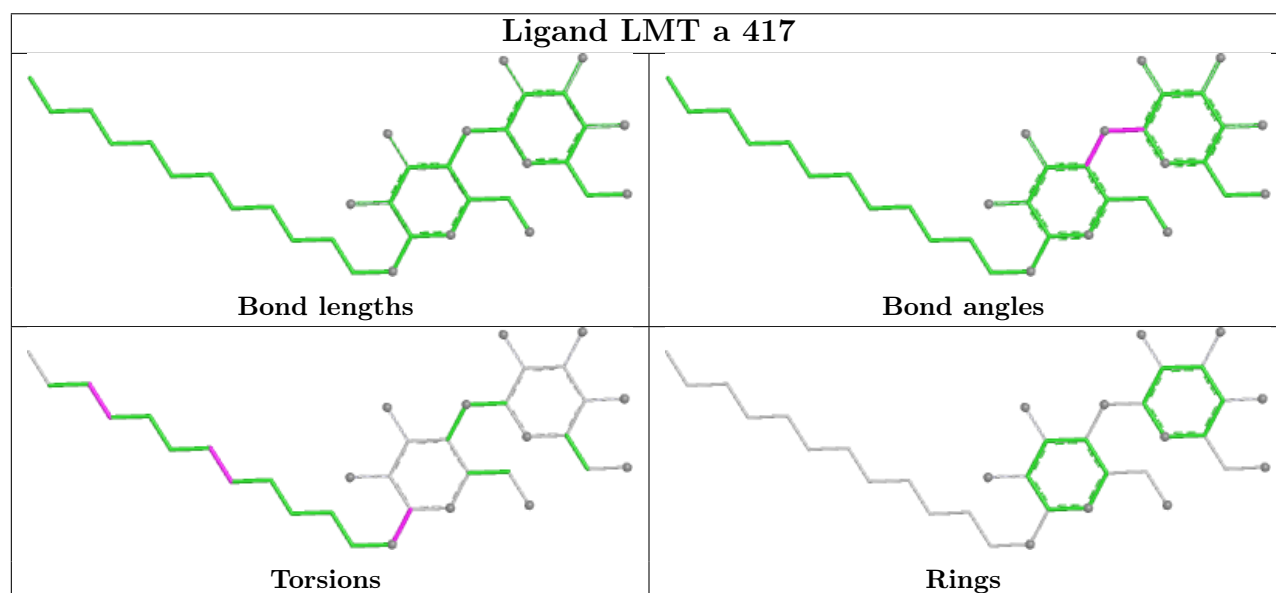
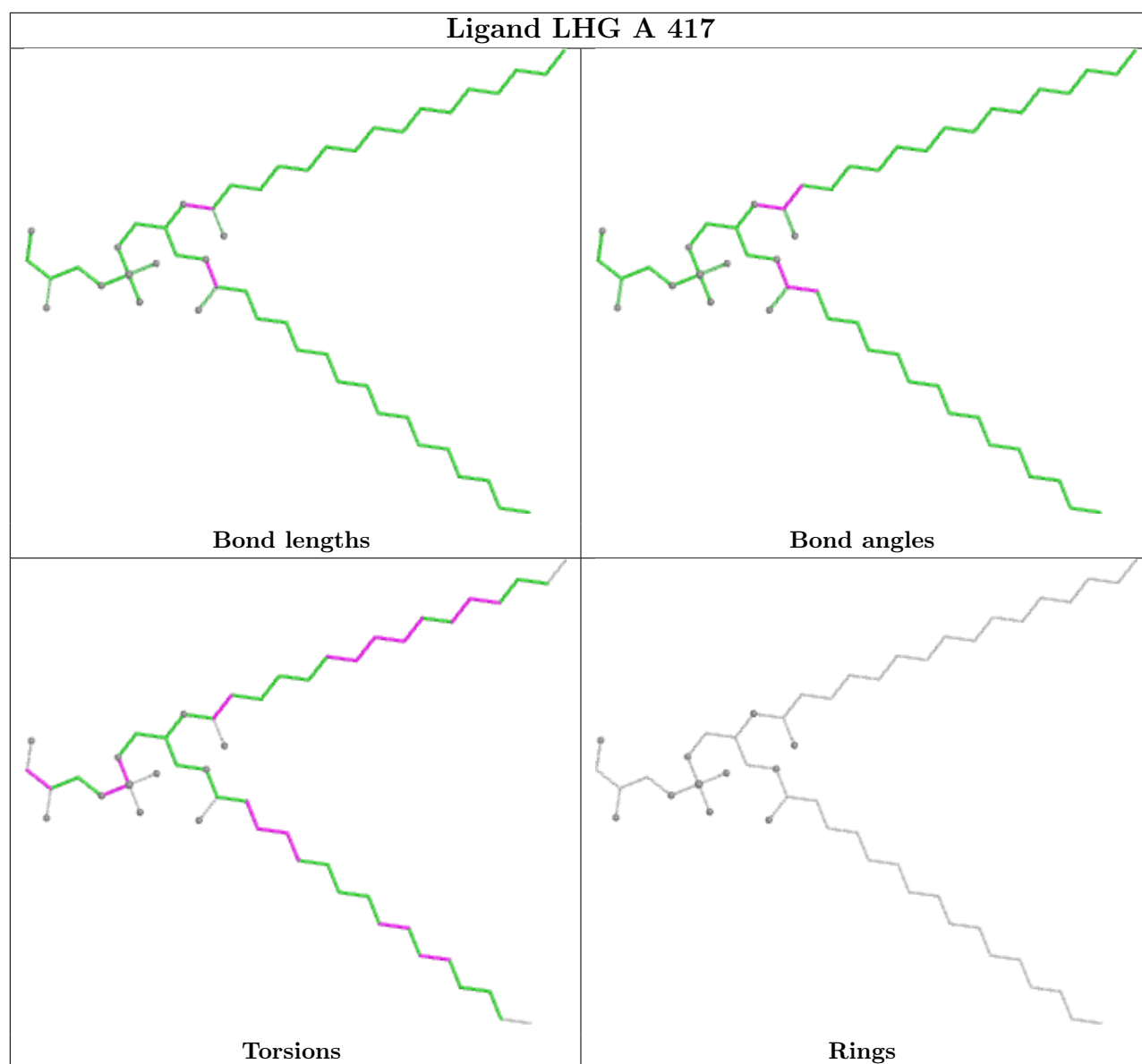
Ligand CLA c 507



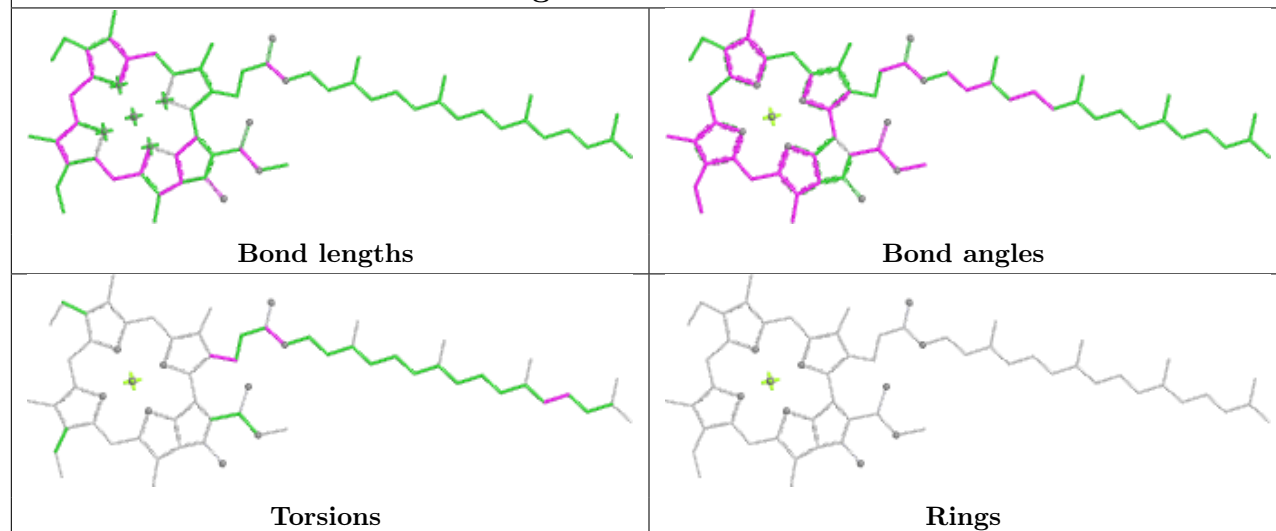
Ligand CLA b 611



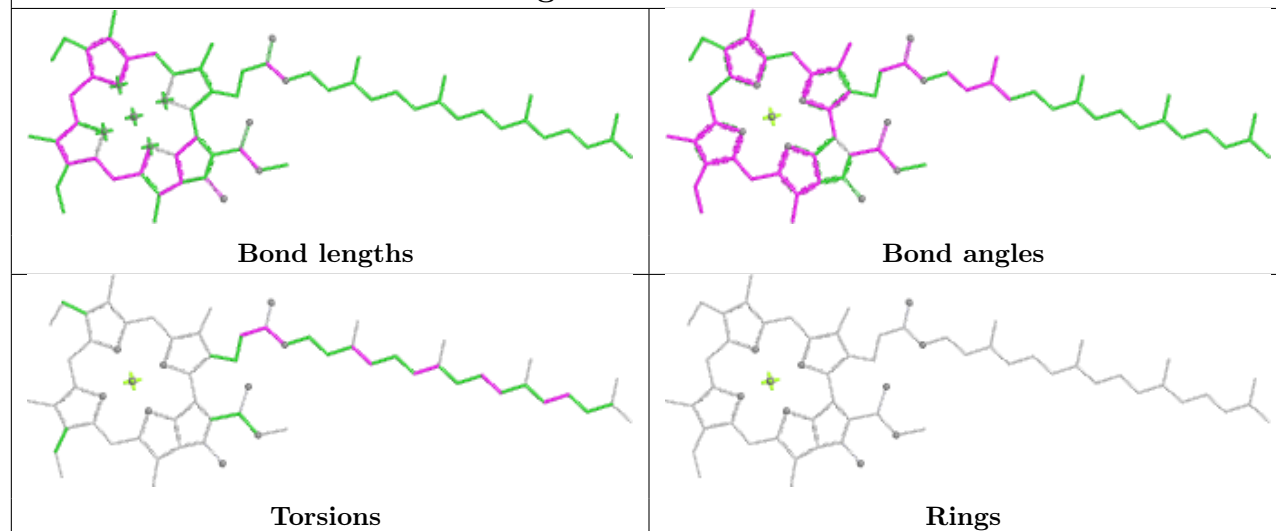




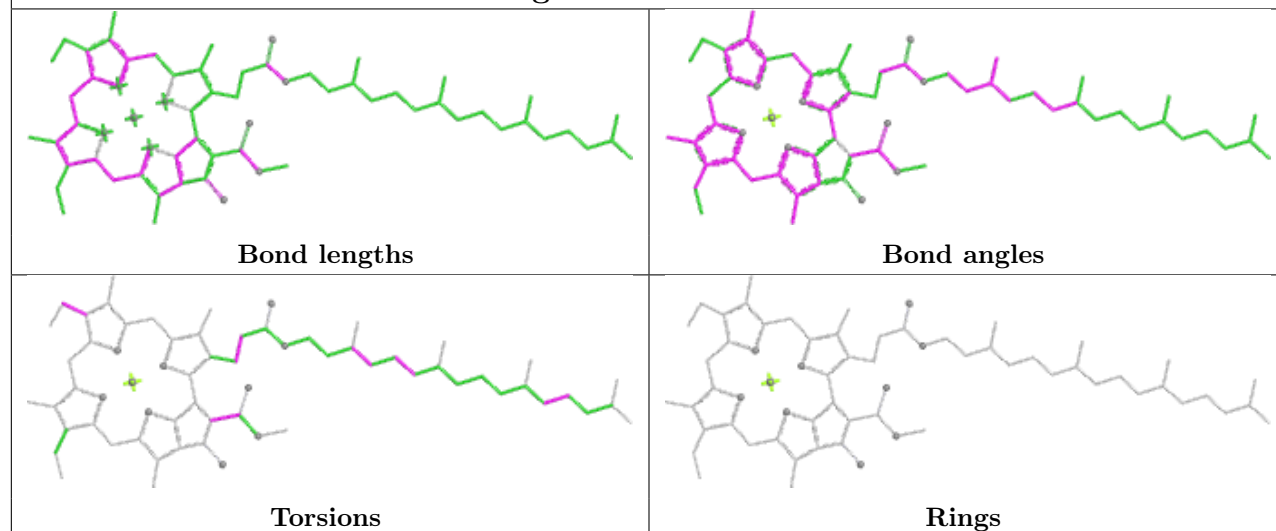
Ligand CLA B 609

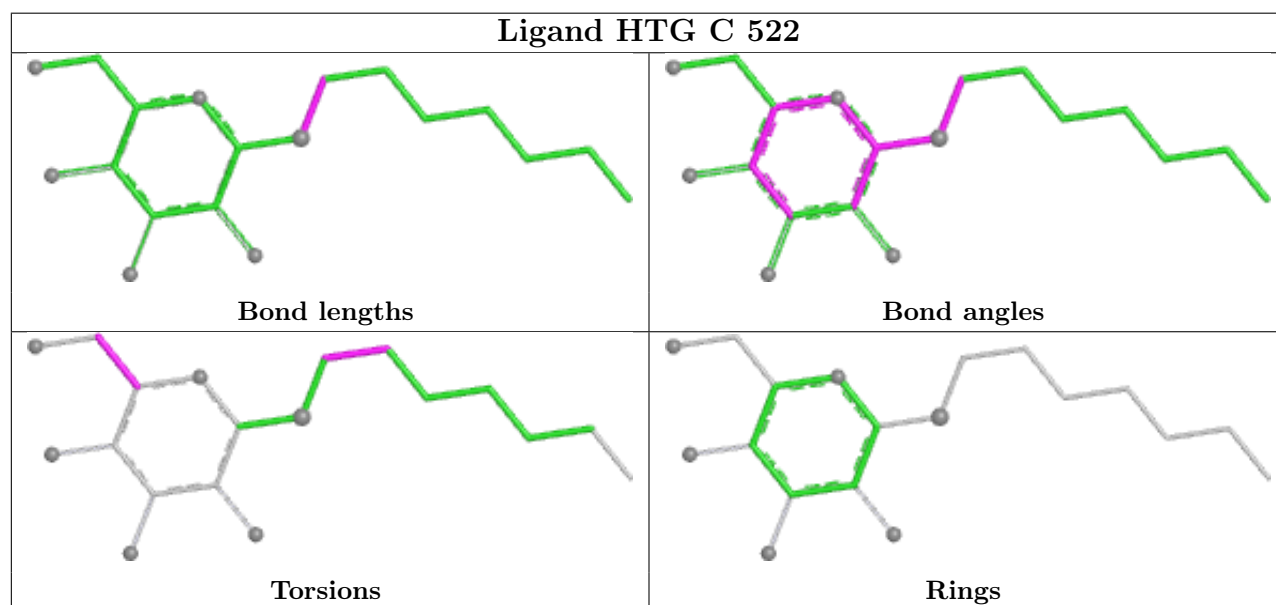
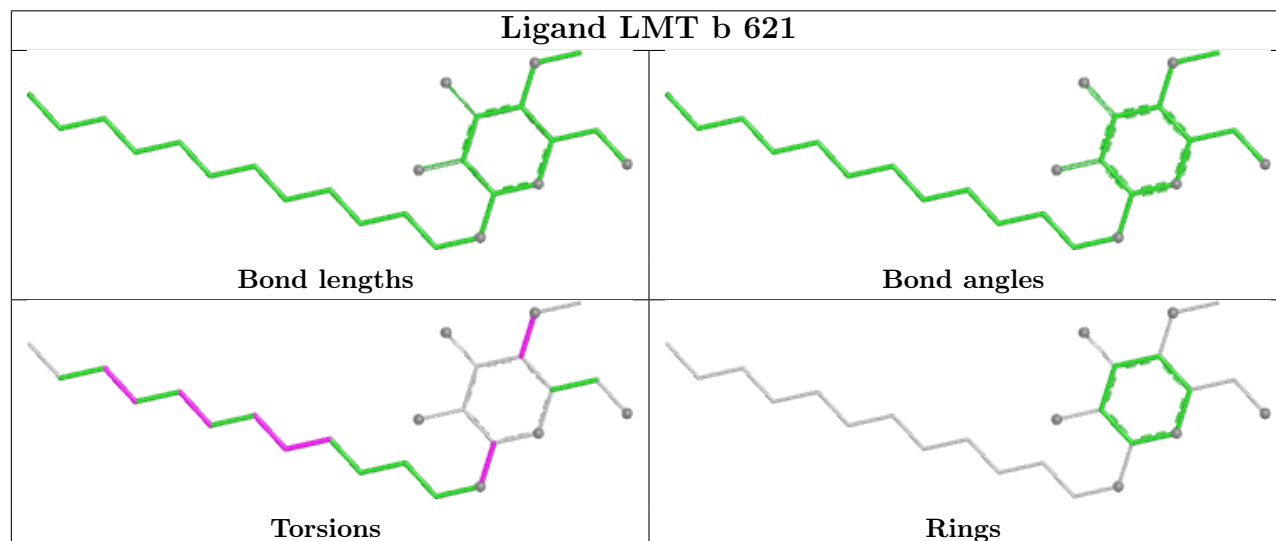
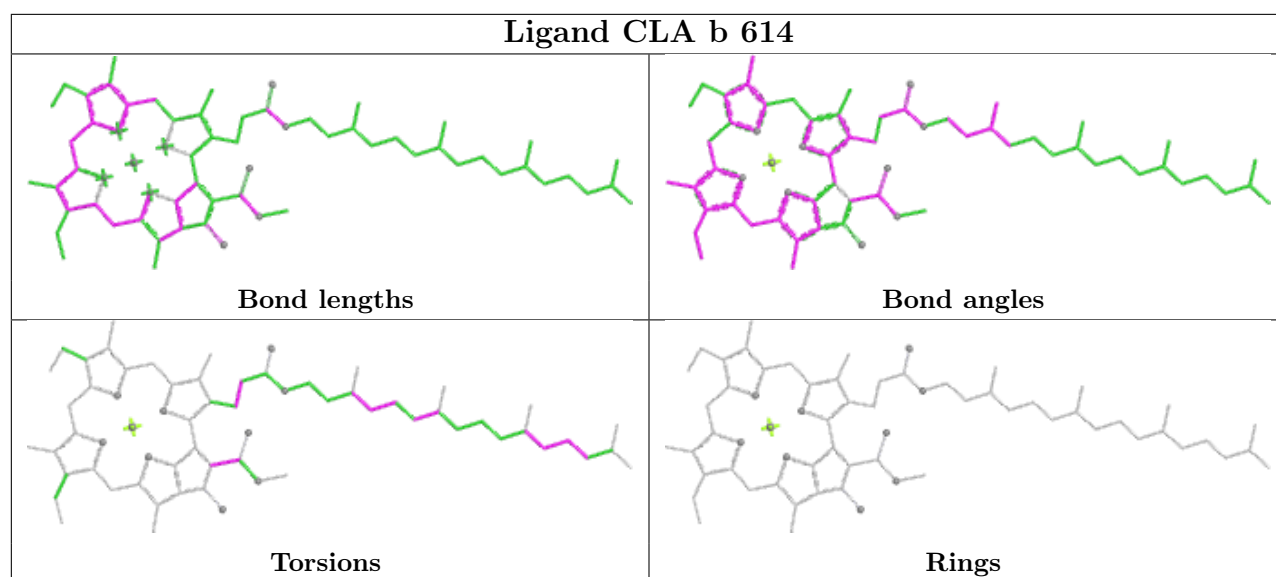


Ligand CLA c 510

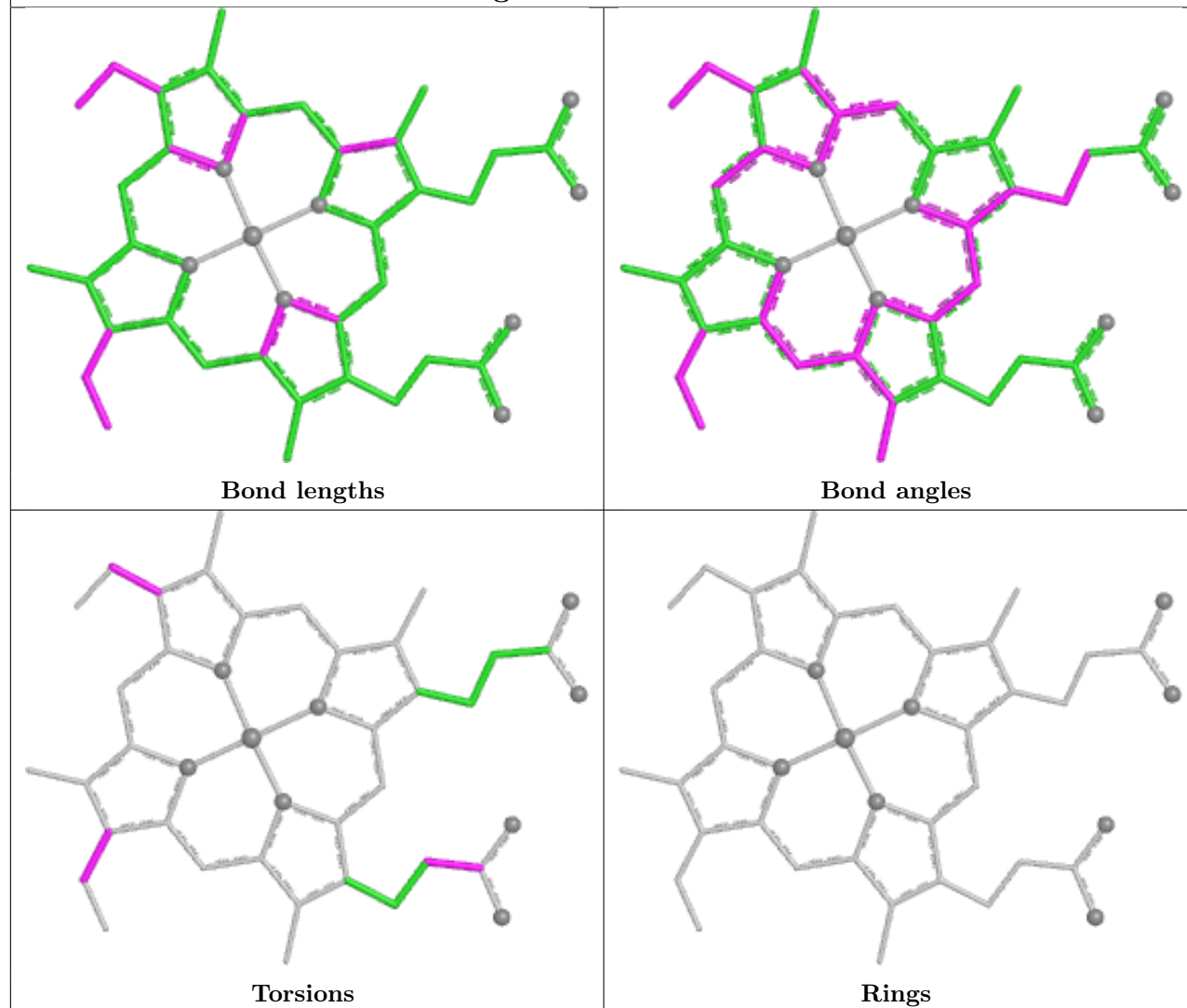


Ligand CLA C 508

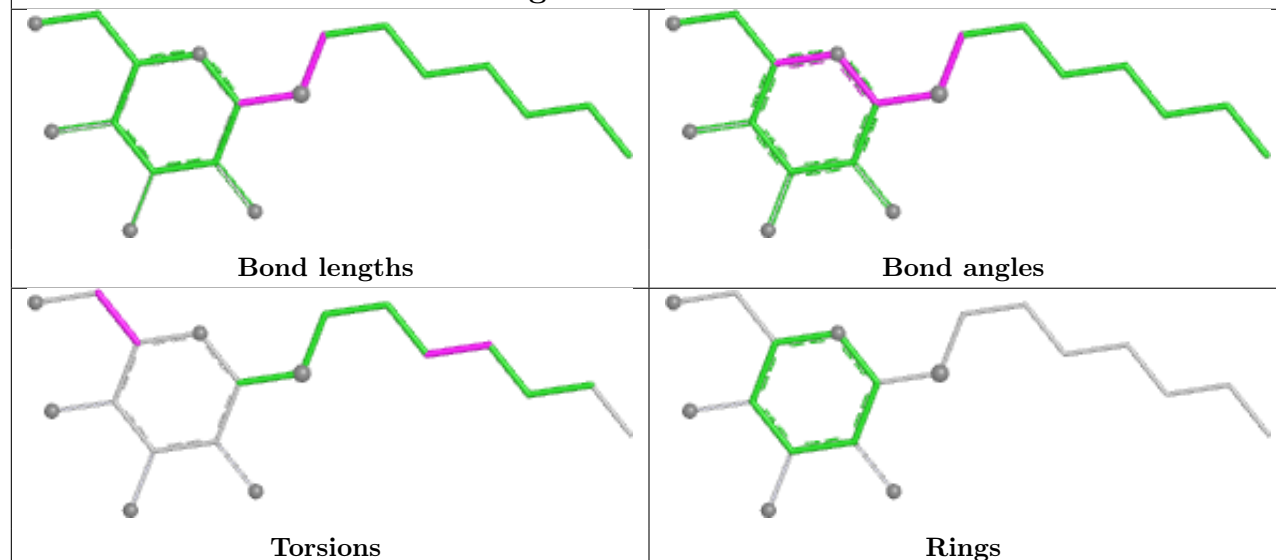


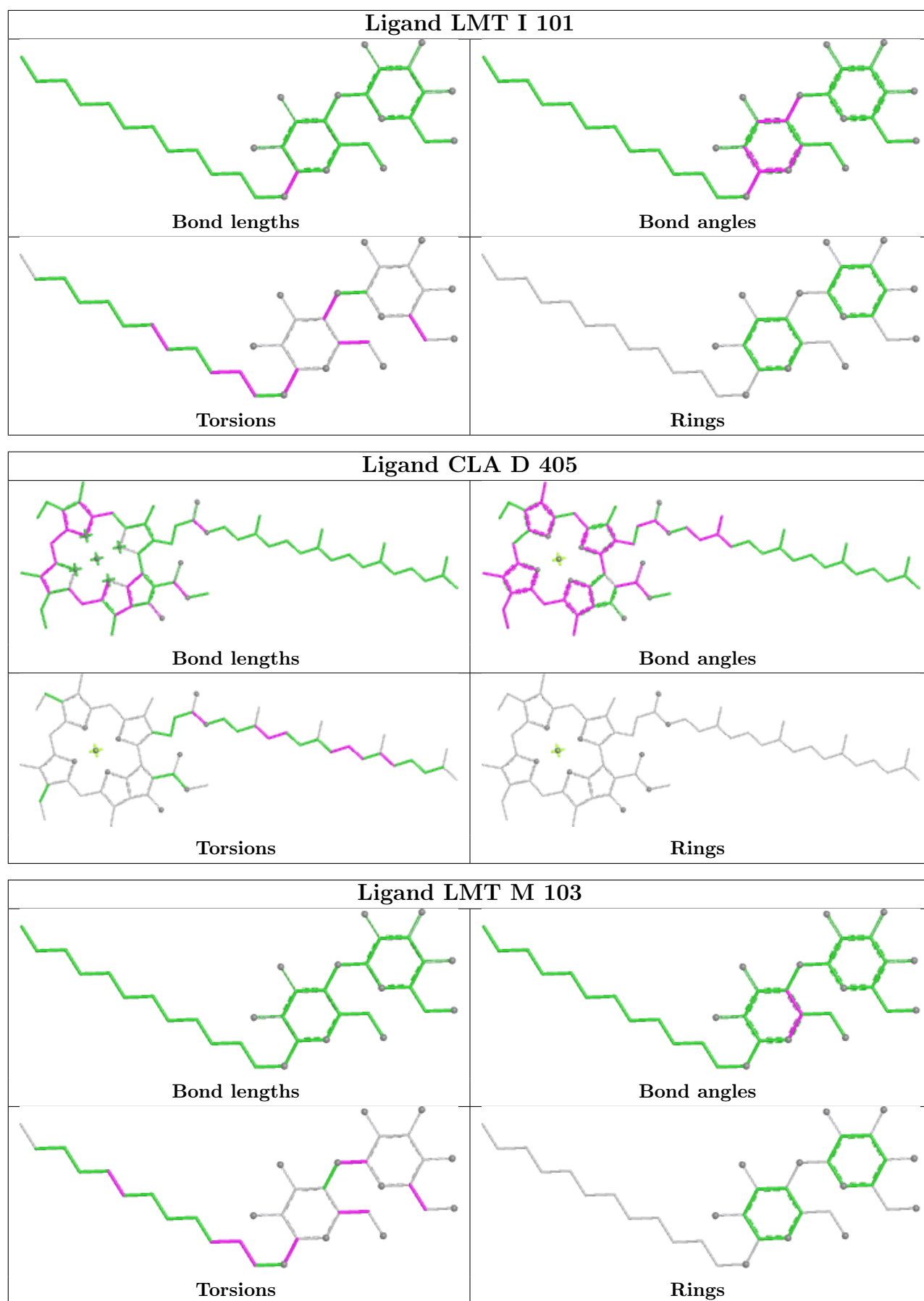


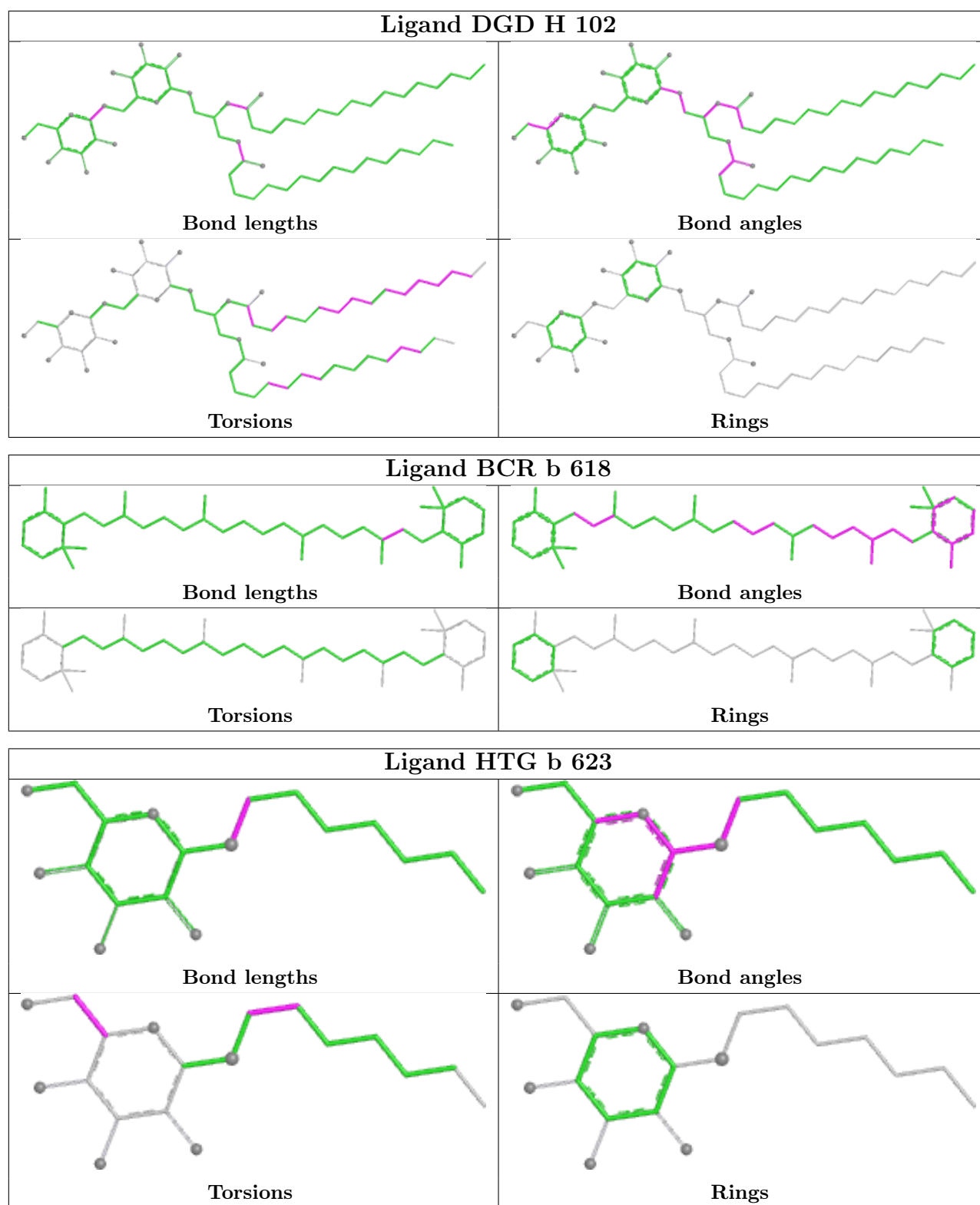
Ligand HEC V 202

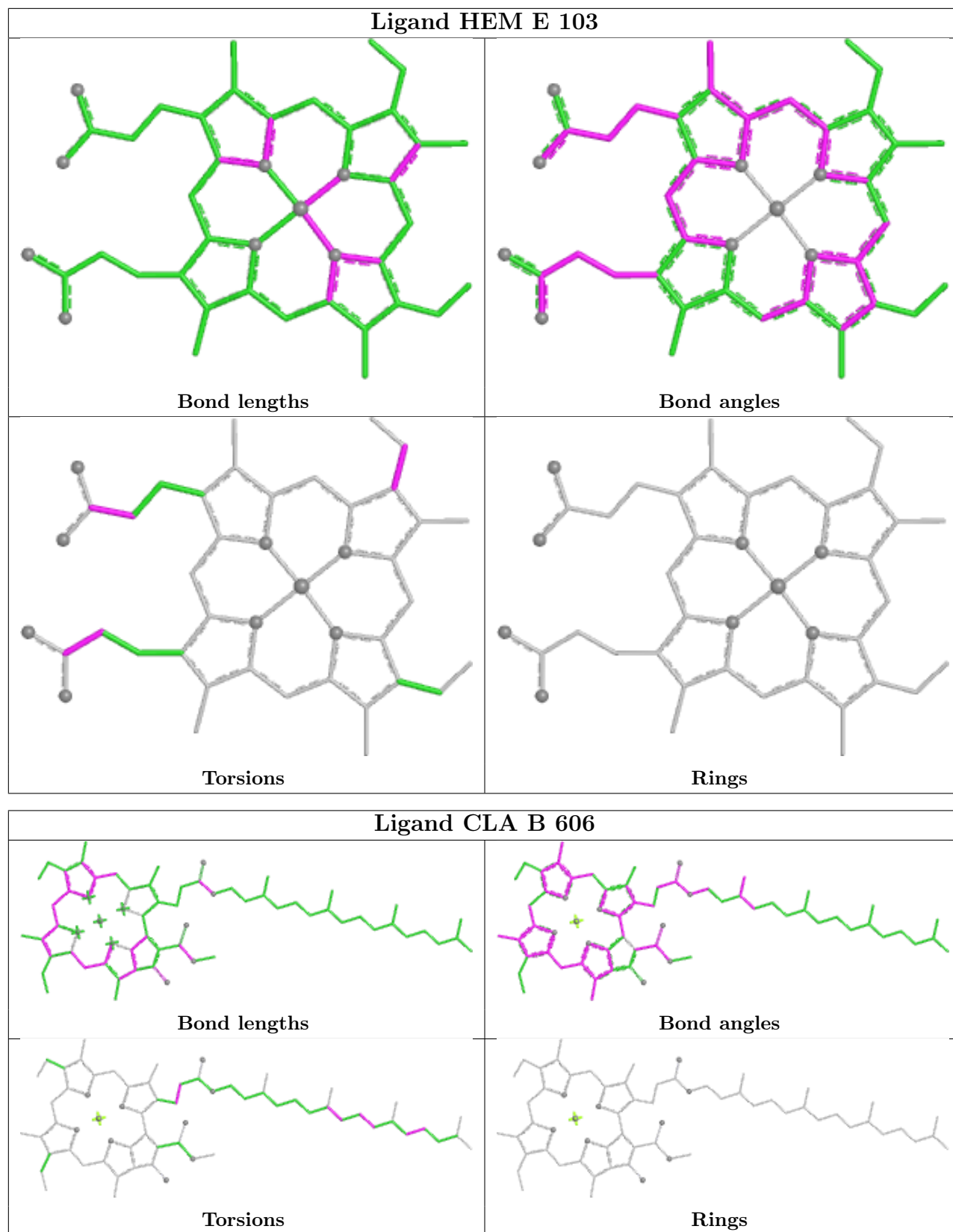


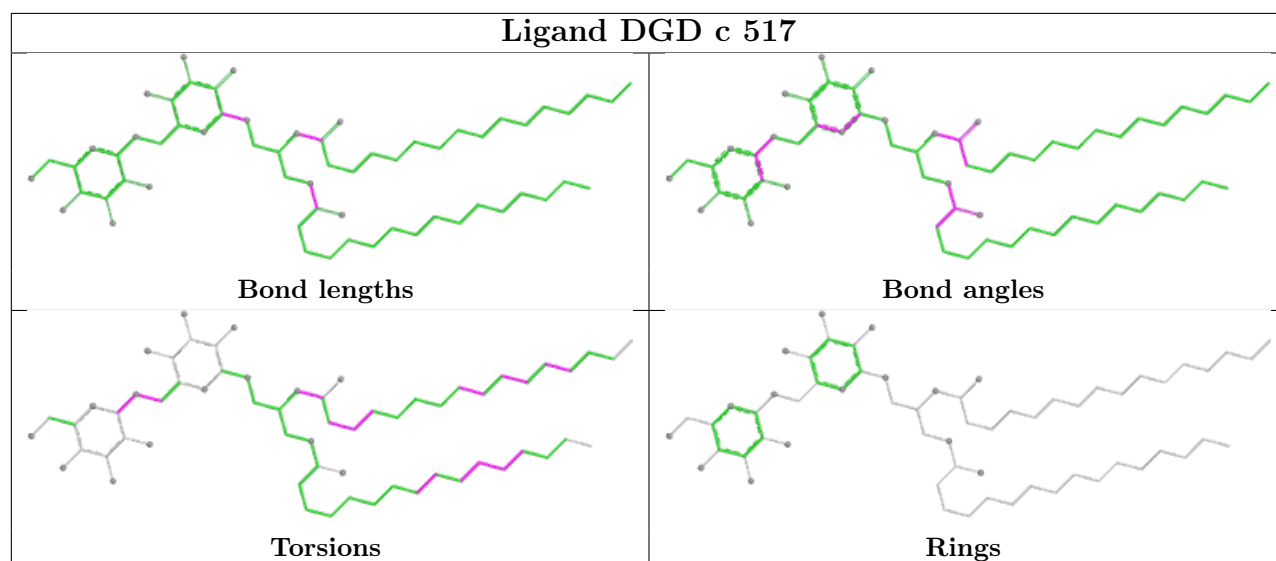
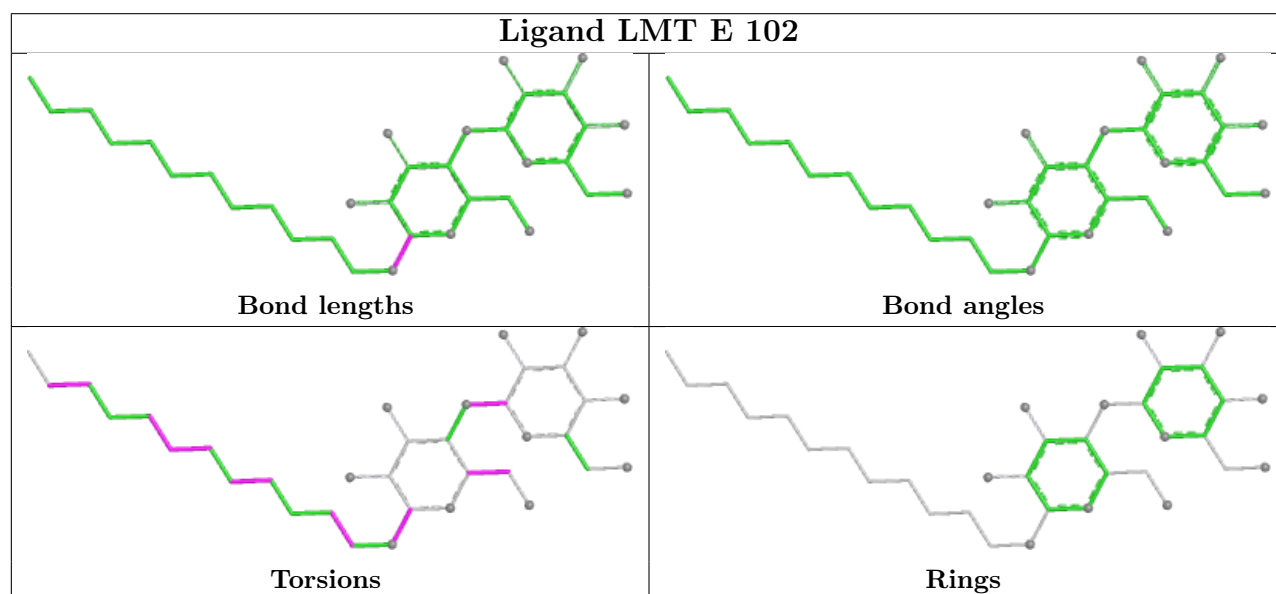
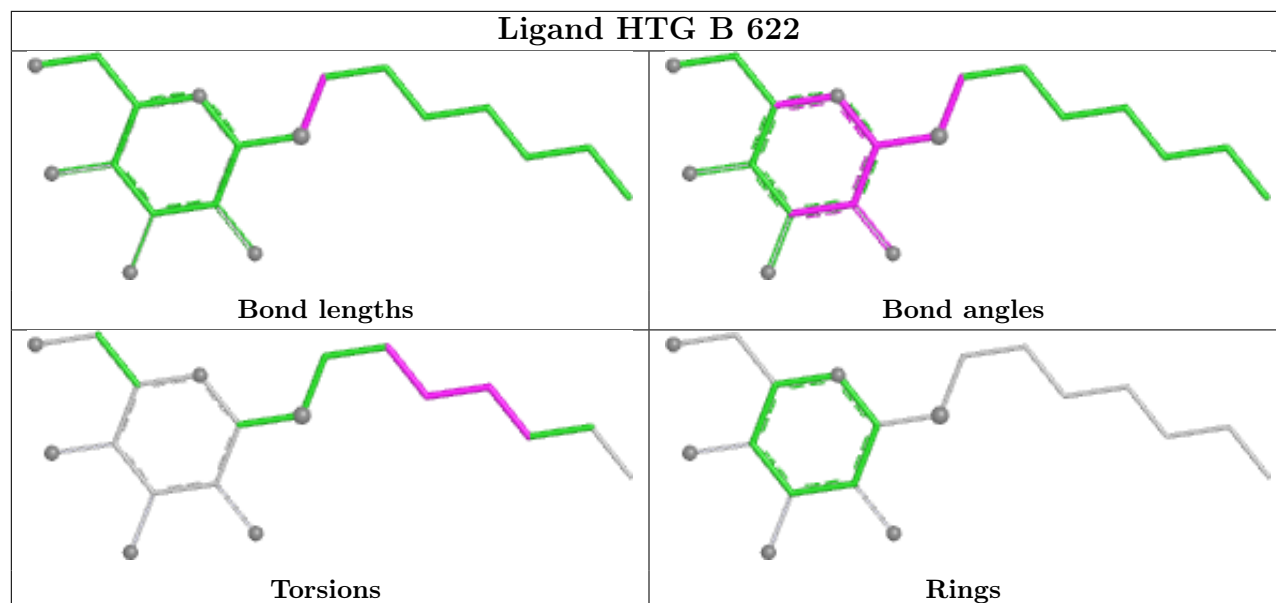
Ligand HTG B 627

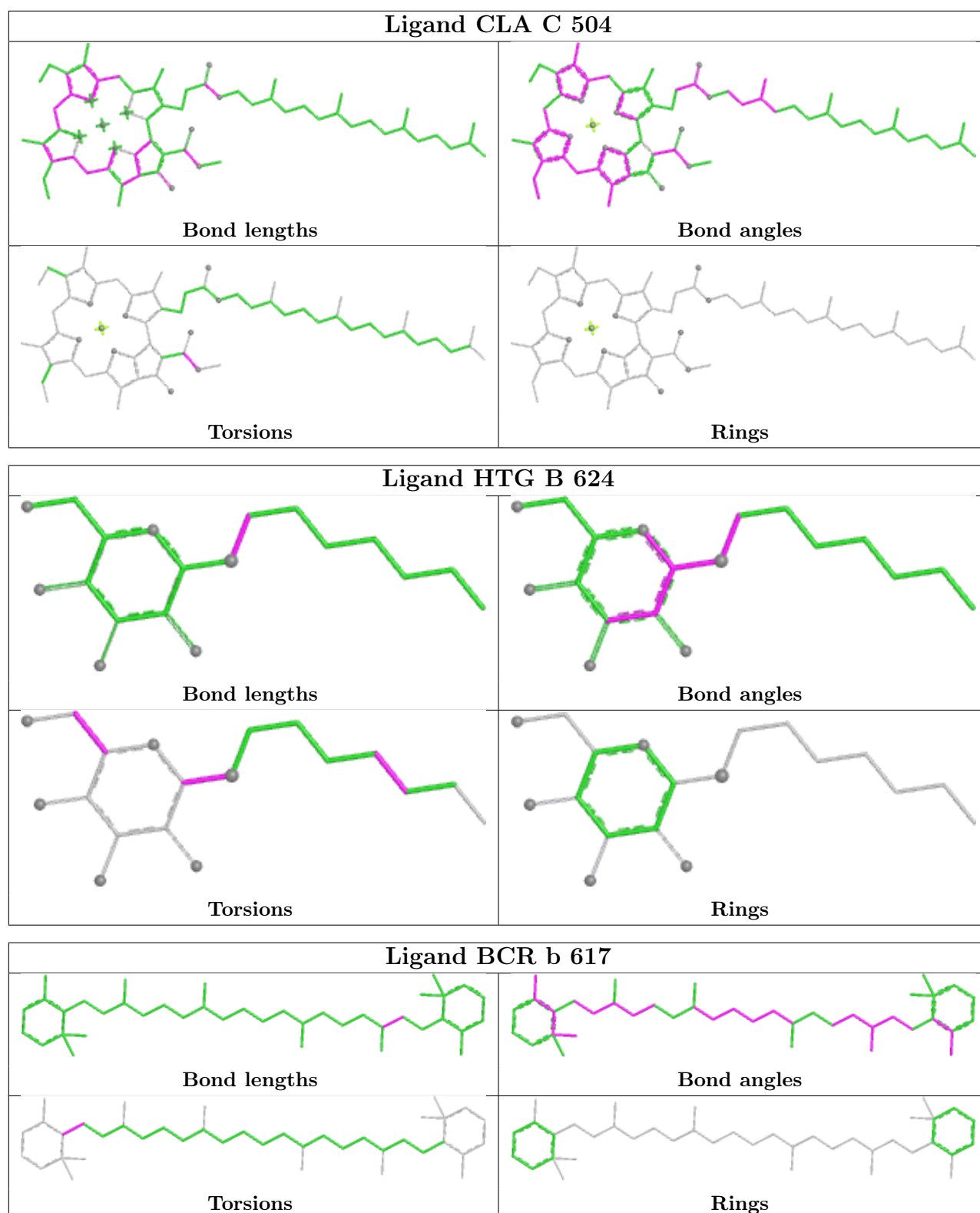


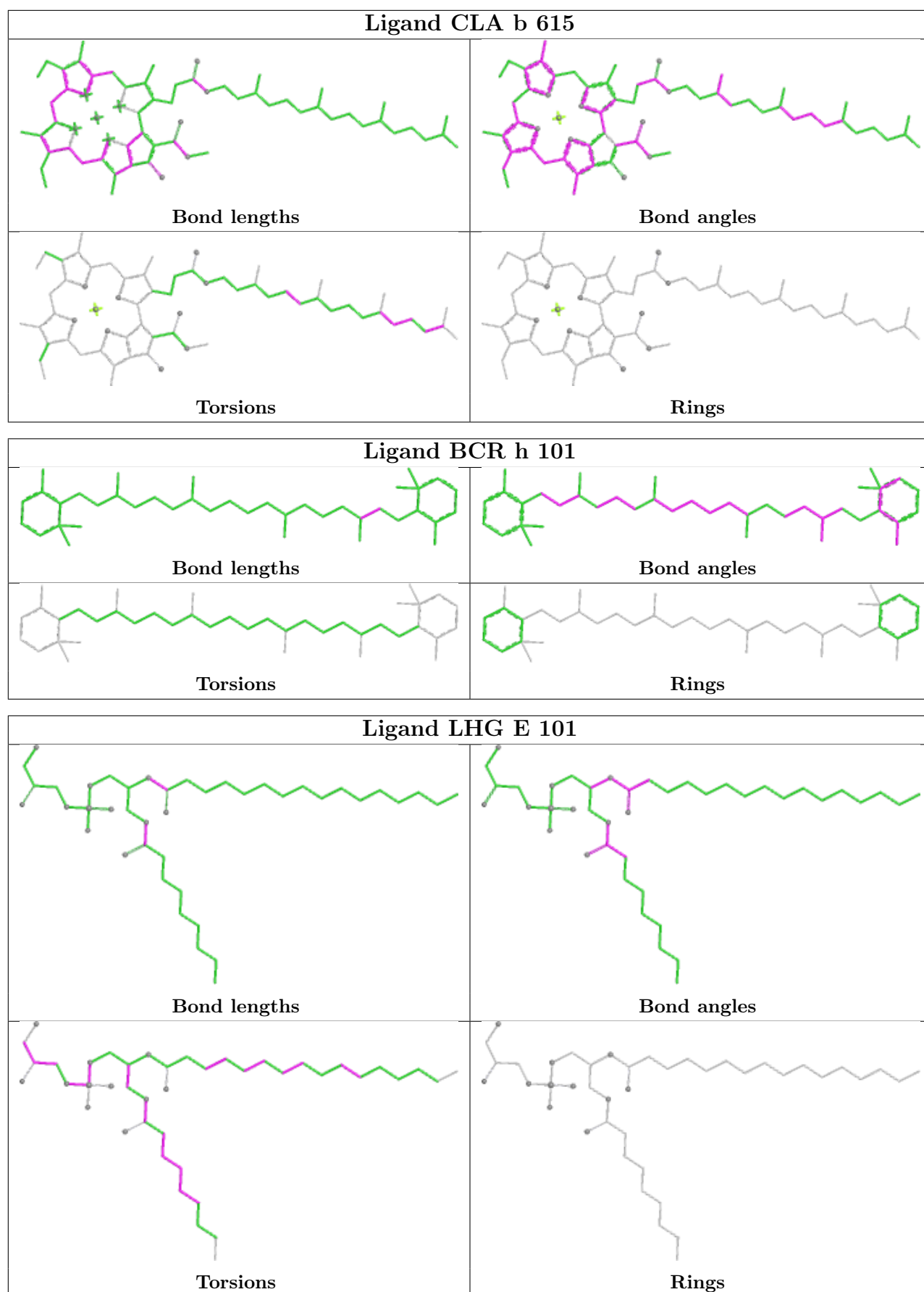




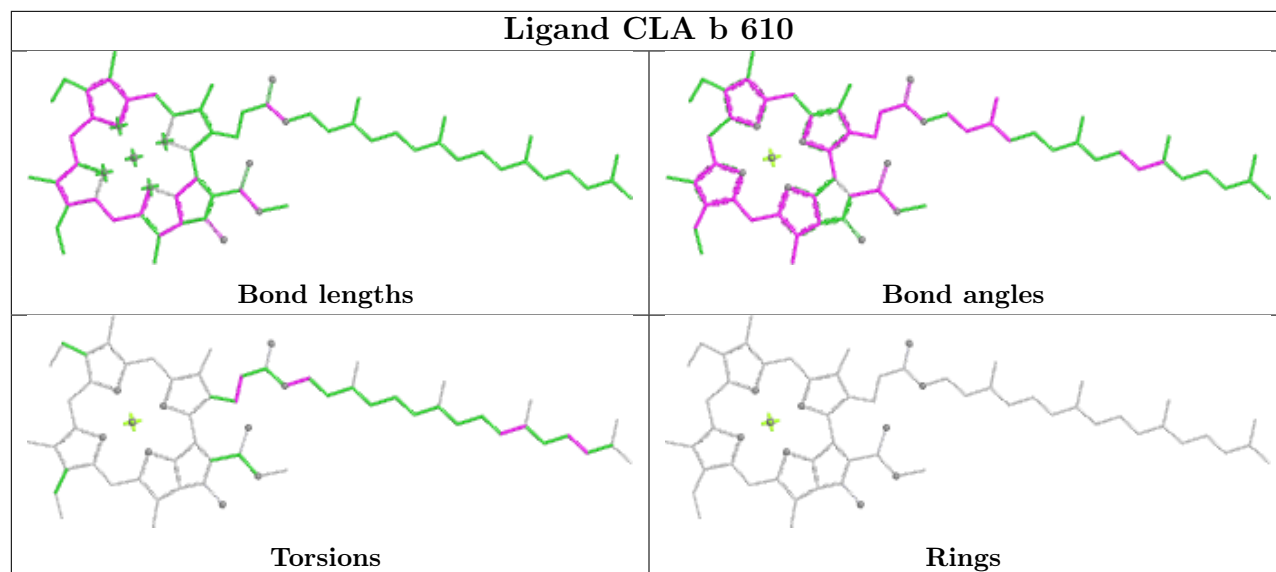




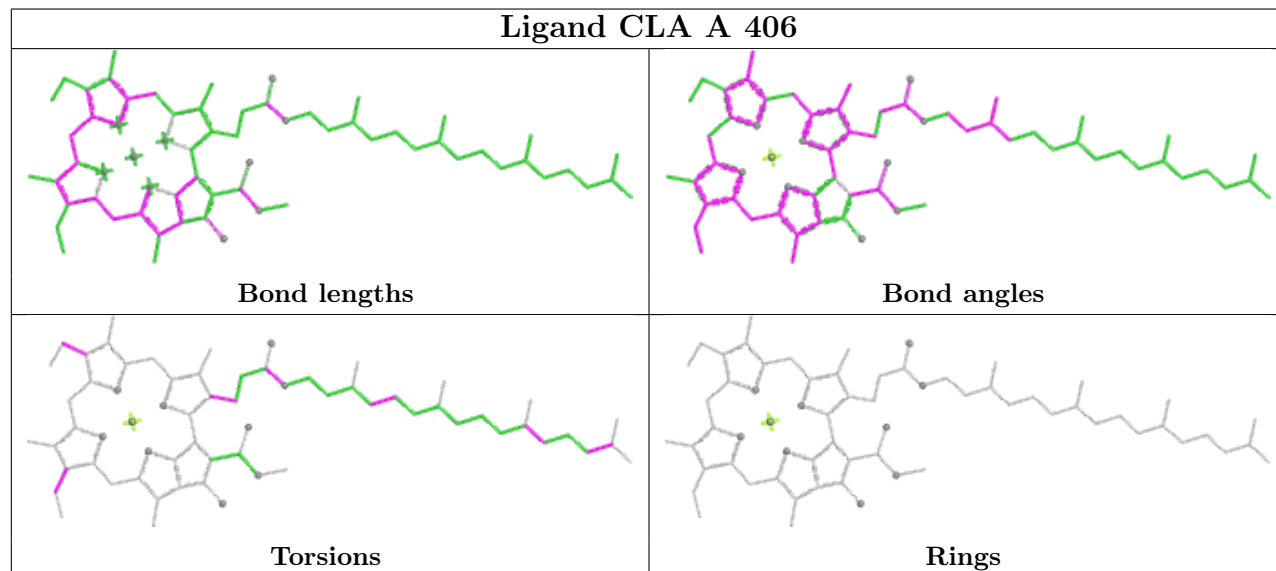




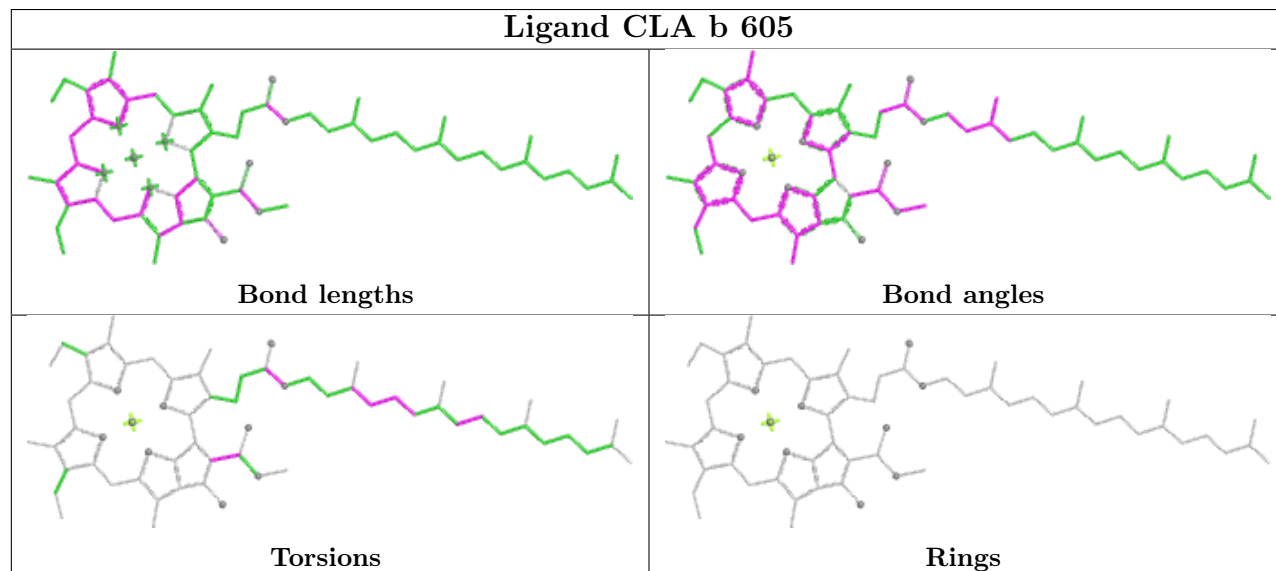
Ligand CLA b 610

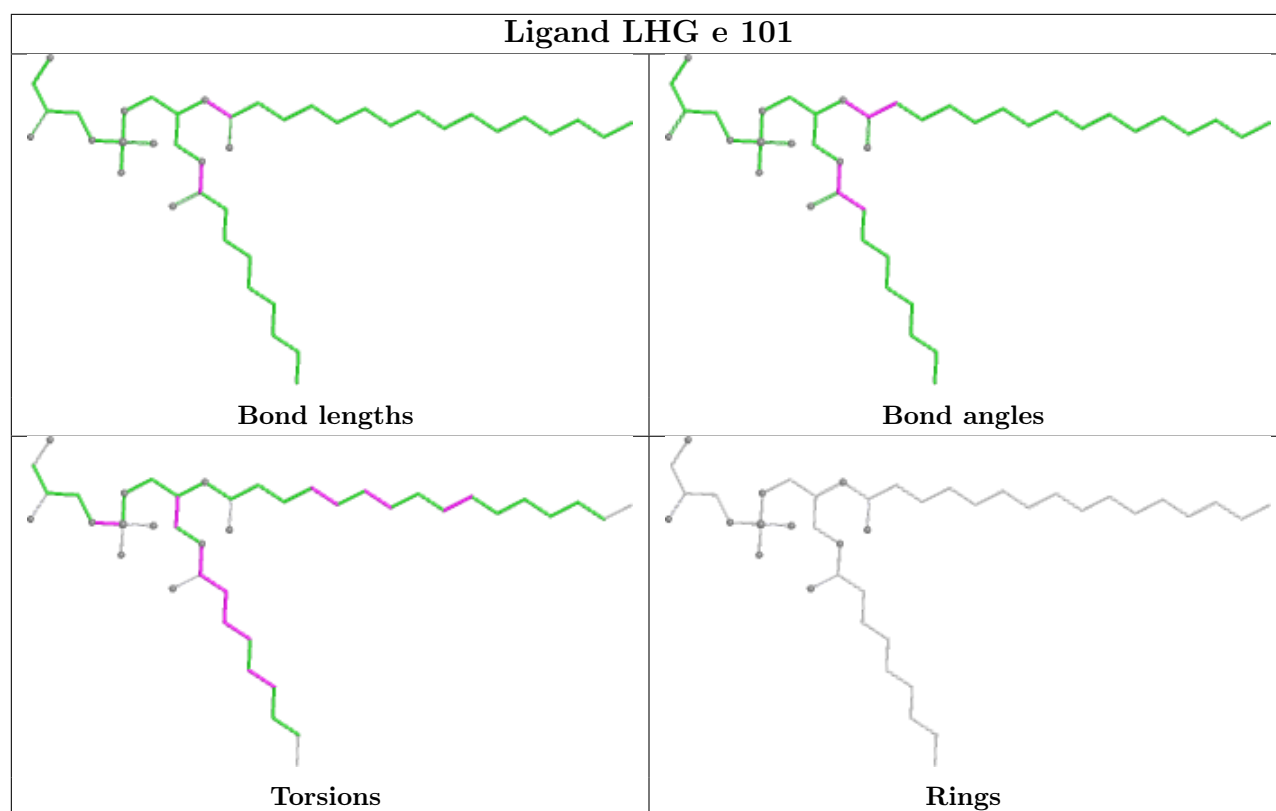


Ligand CLA A 406

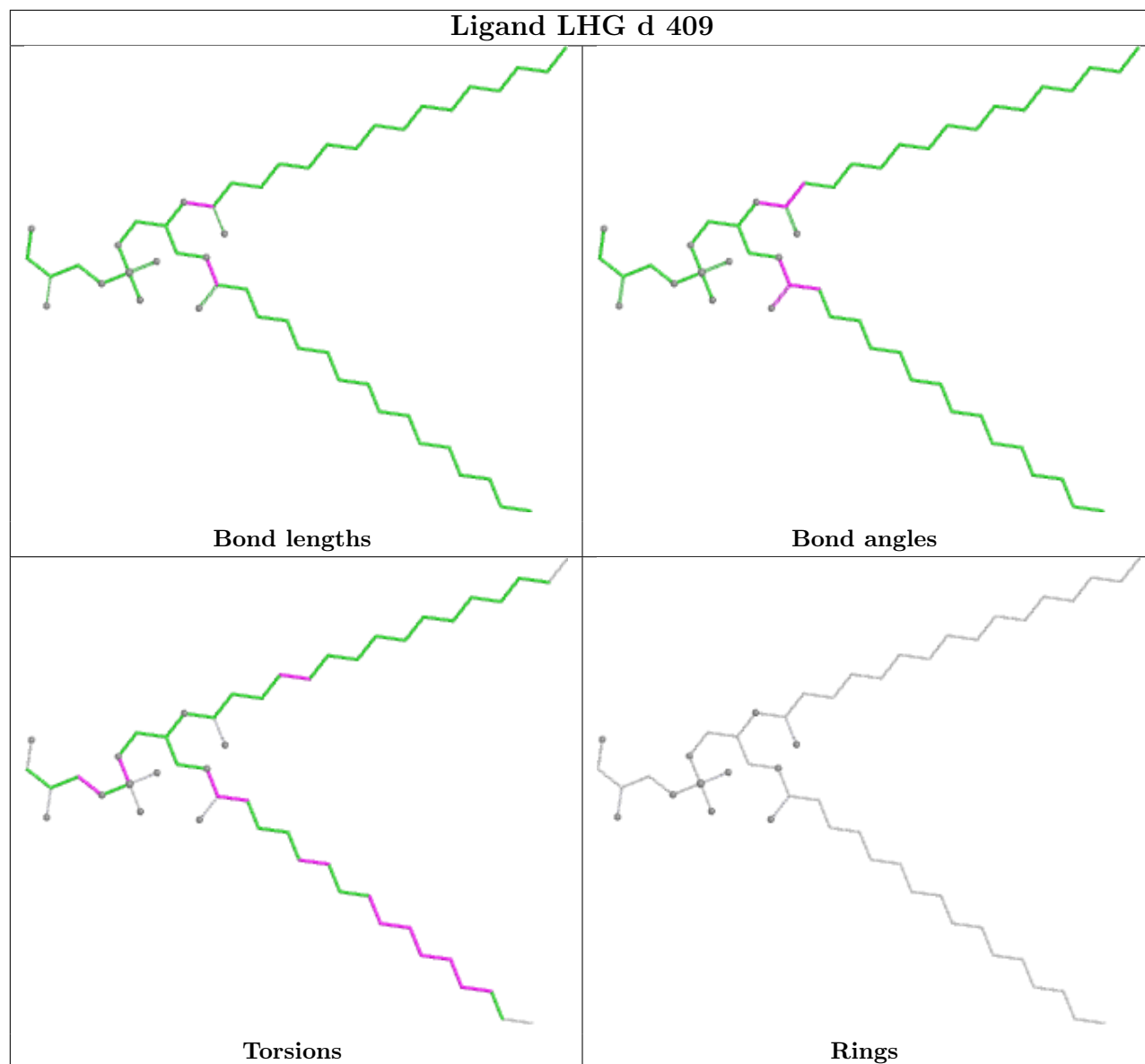


Ligand CLA b 605

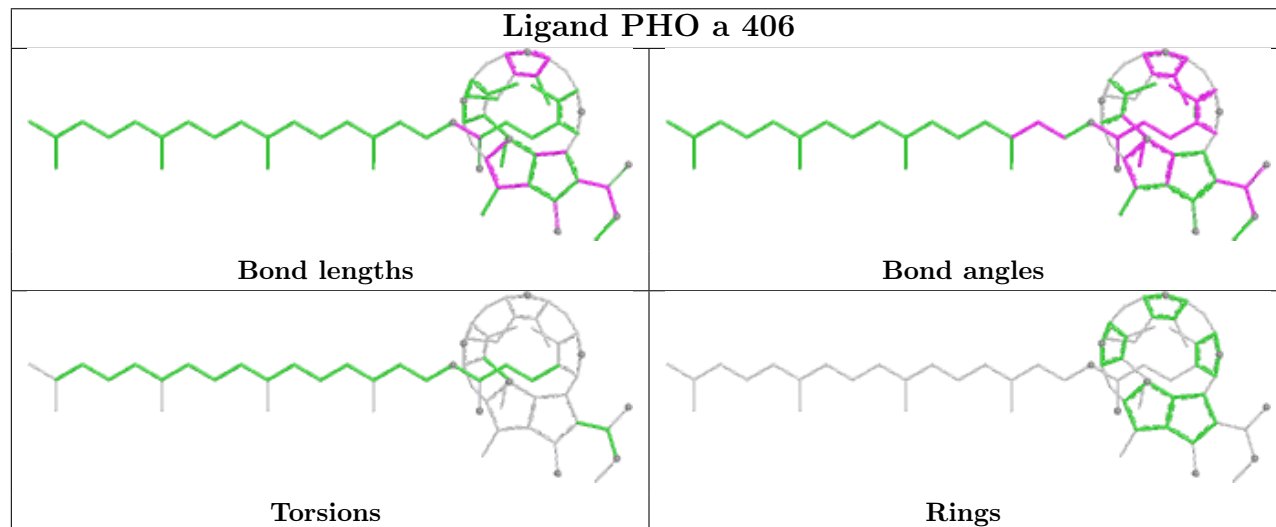




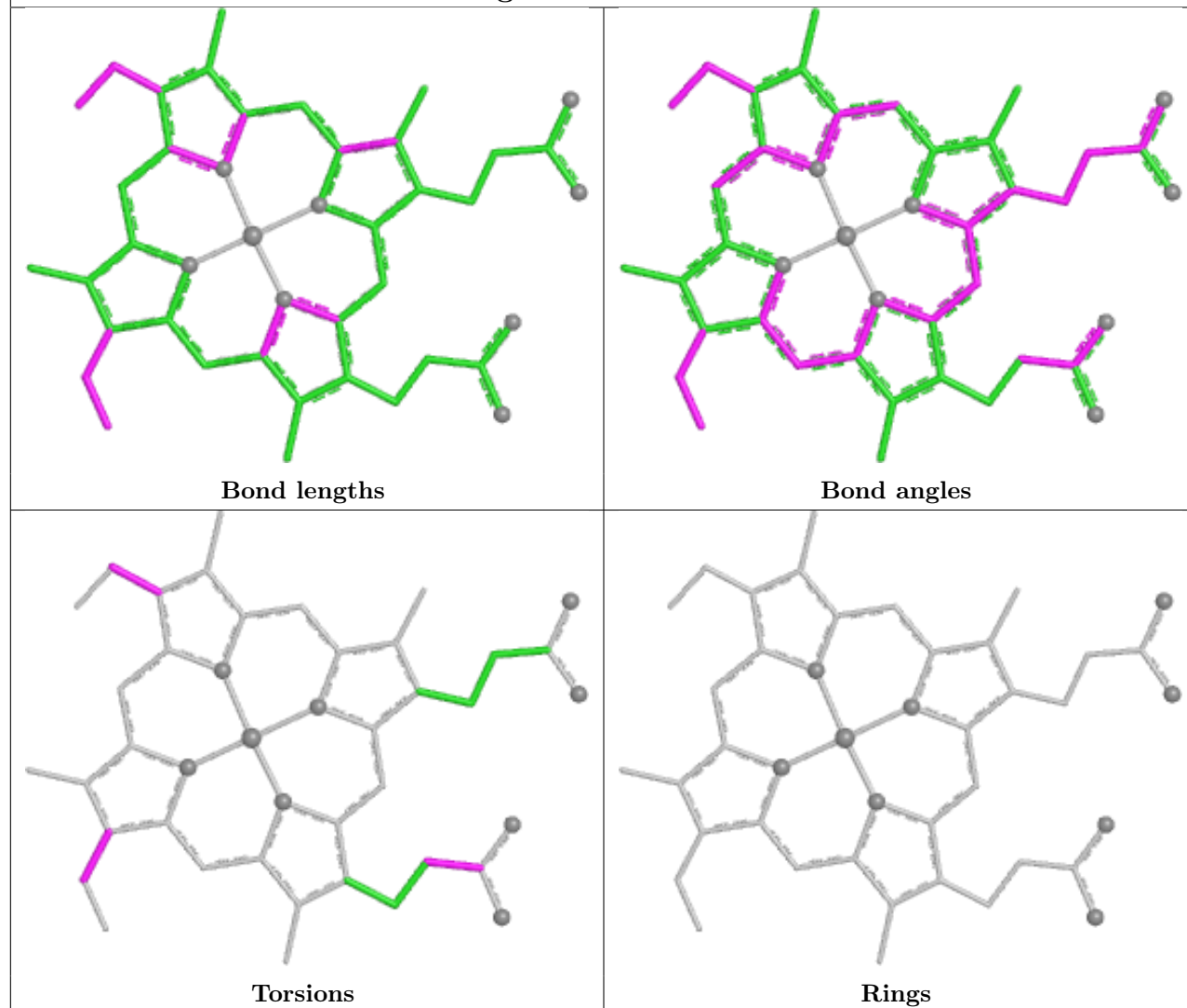
Ligand LHG d 409



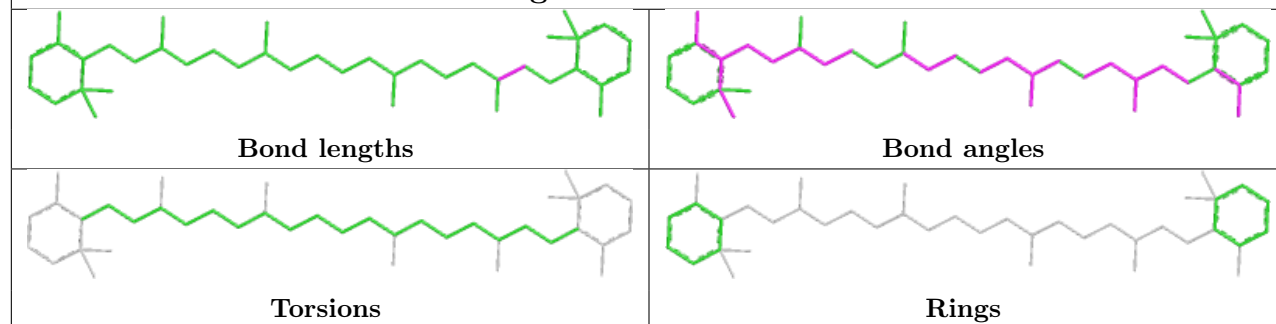
Ligand PHO a 406

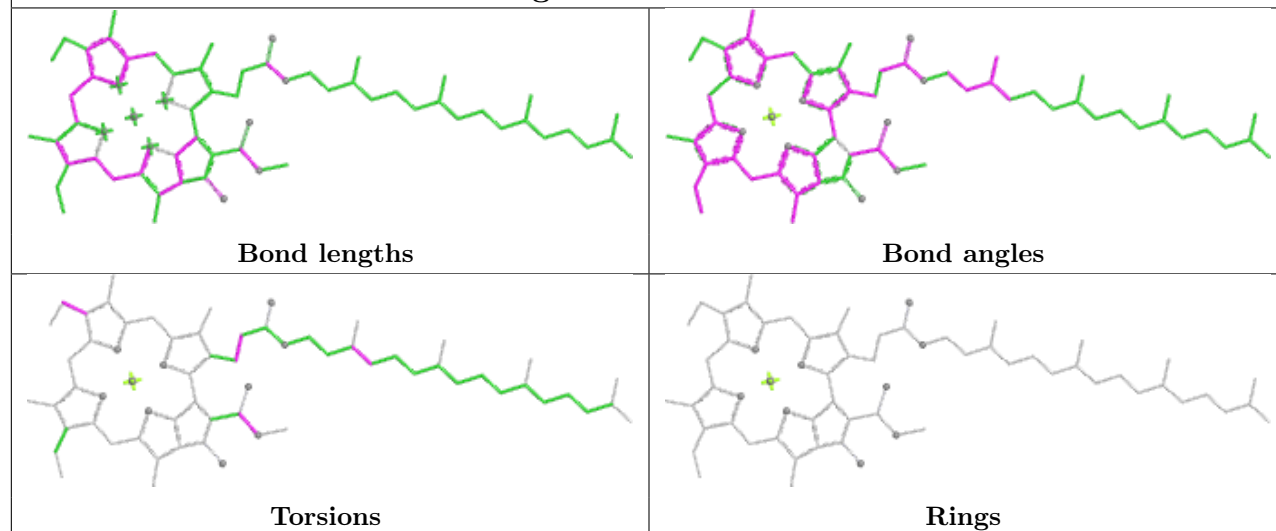
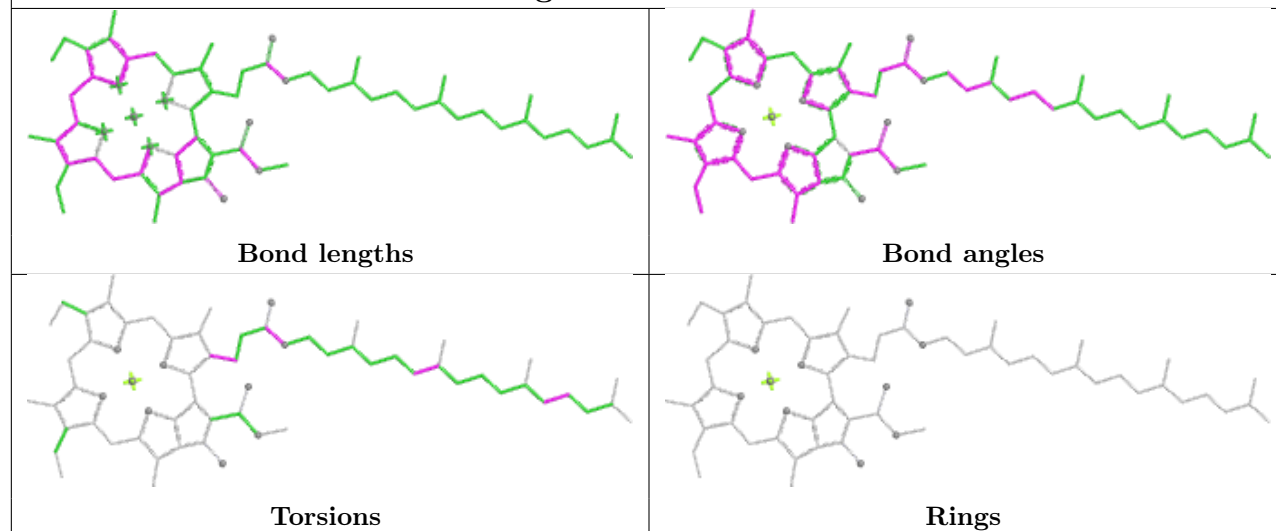
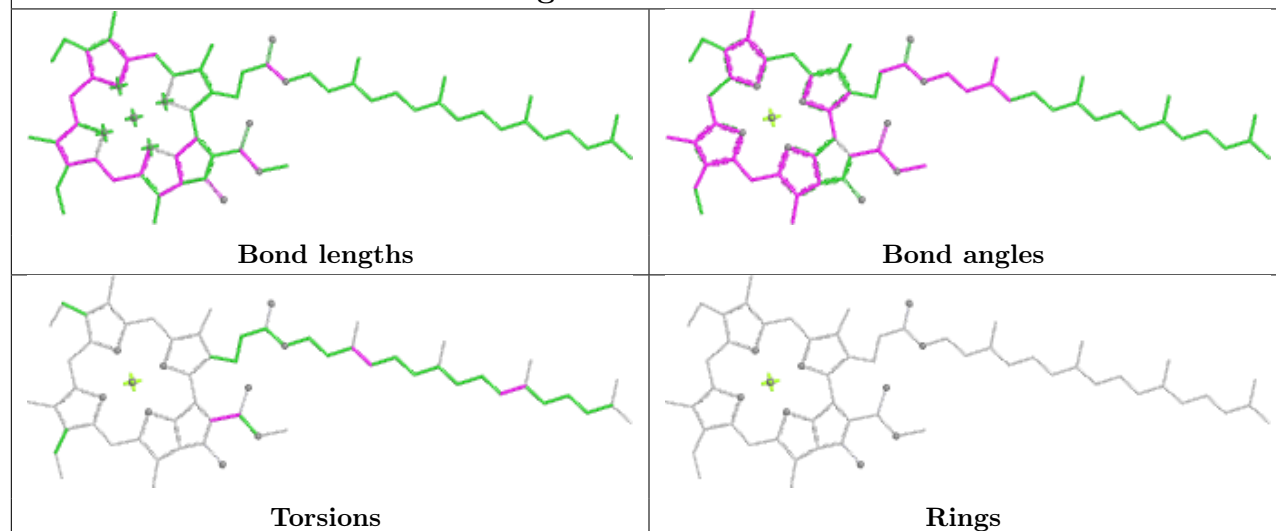


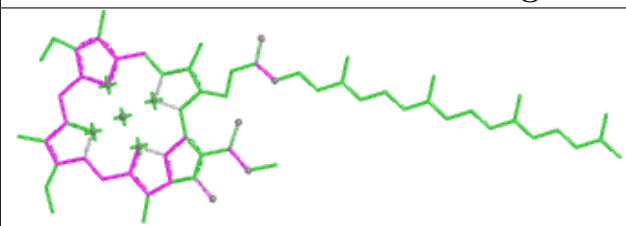
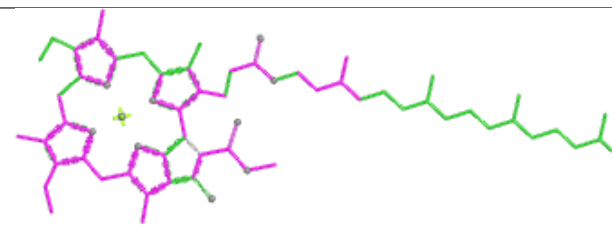
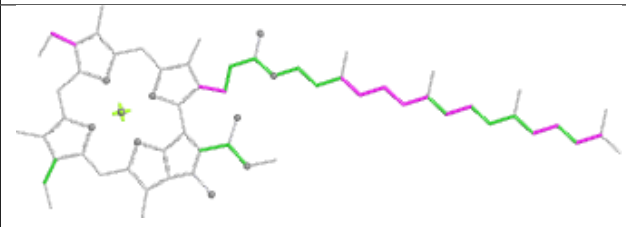
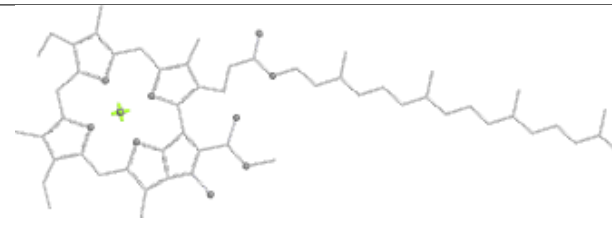
Ligand HEC v 201

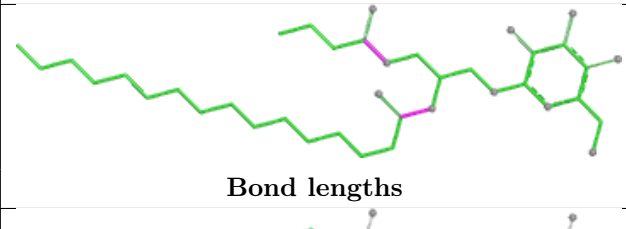
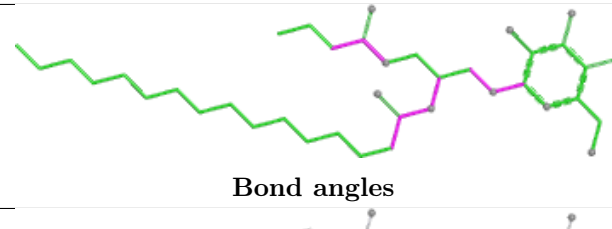
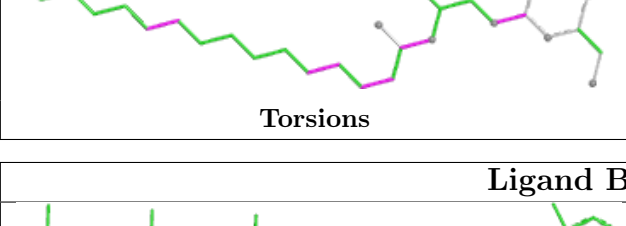
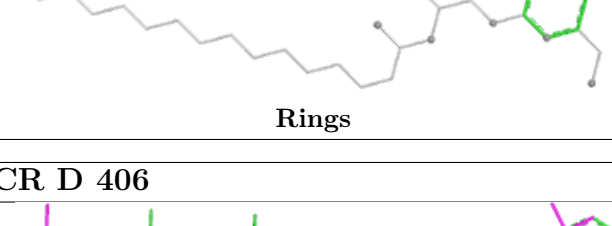


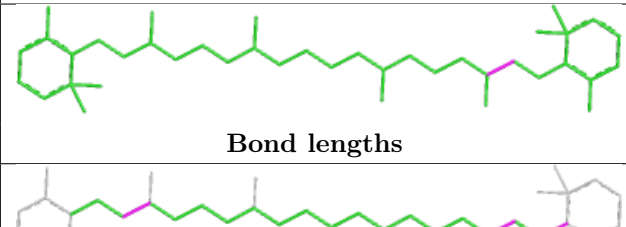
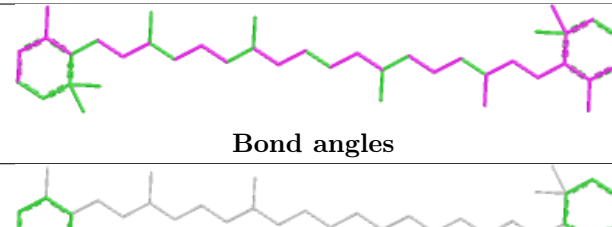
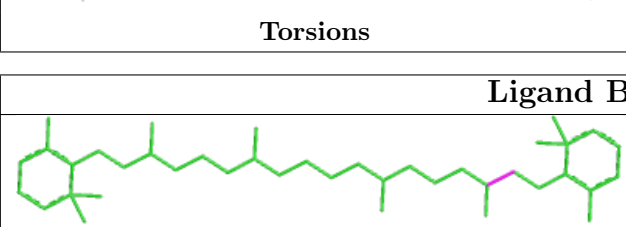
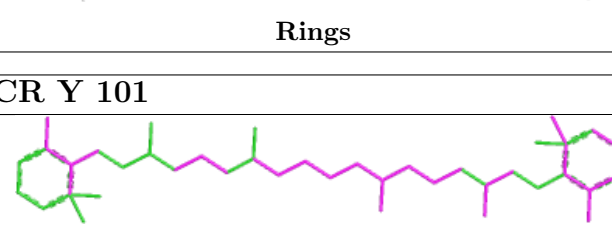
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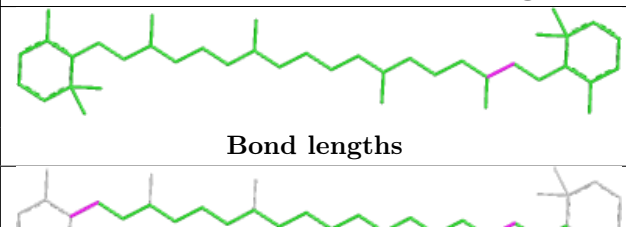
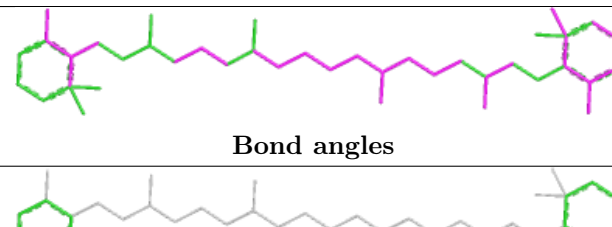


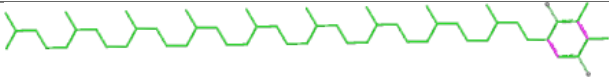
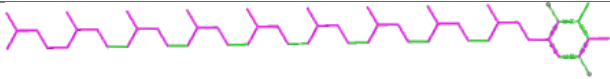
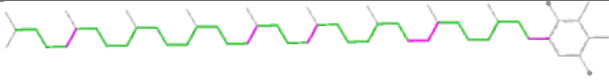
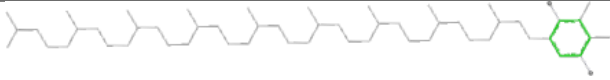
Ligand CLA B 603**Ligand CLA b 609****Ligand CLA c 505**

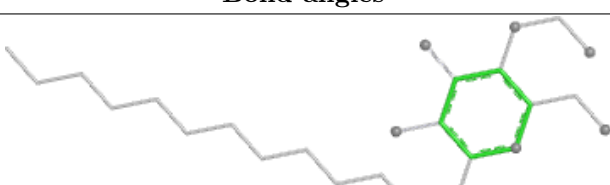
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

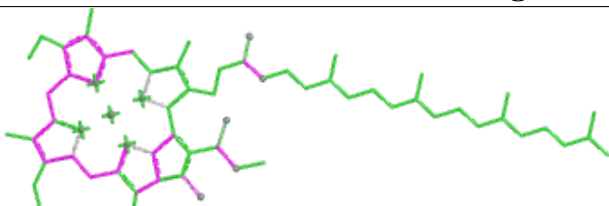
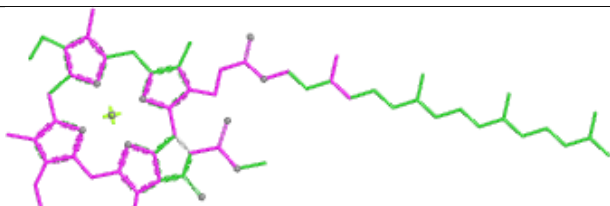
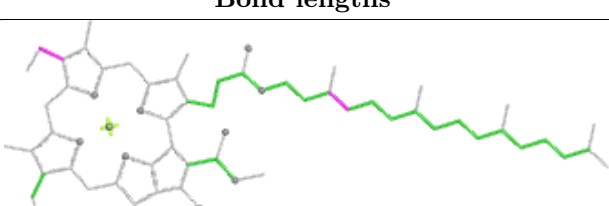
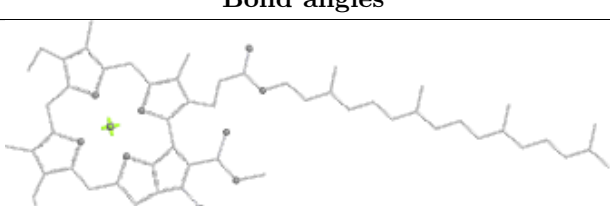
Ligand LMG z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

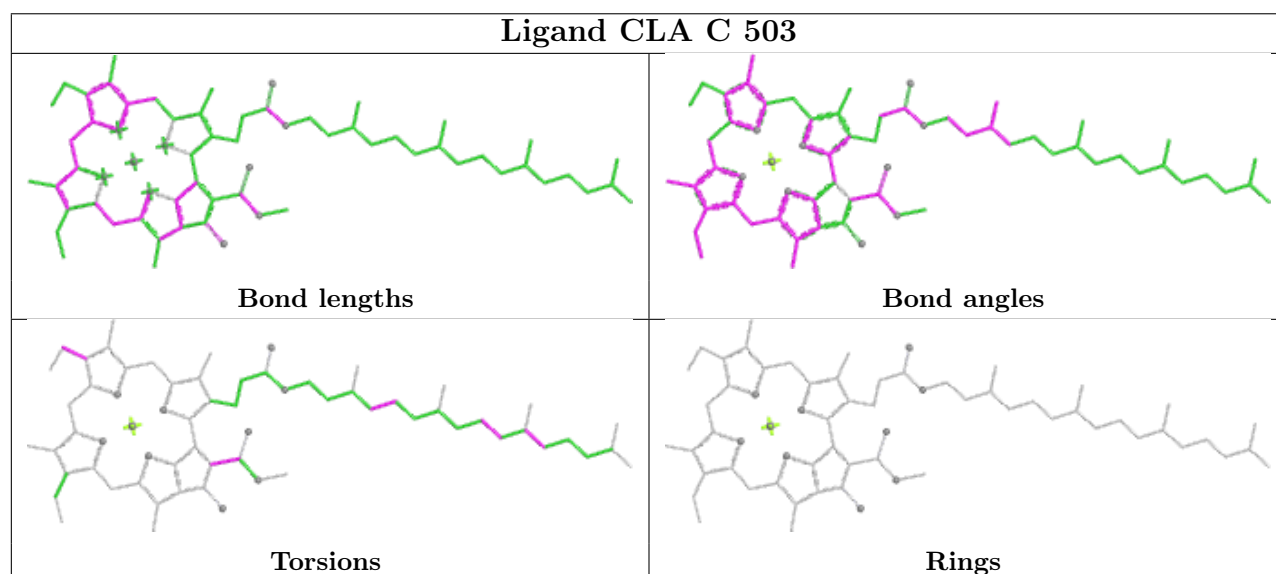
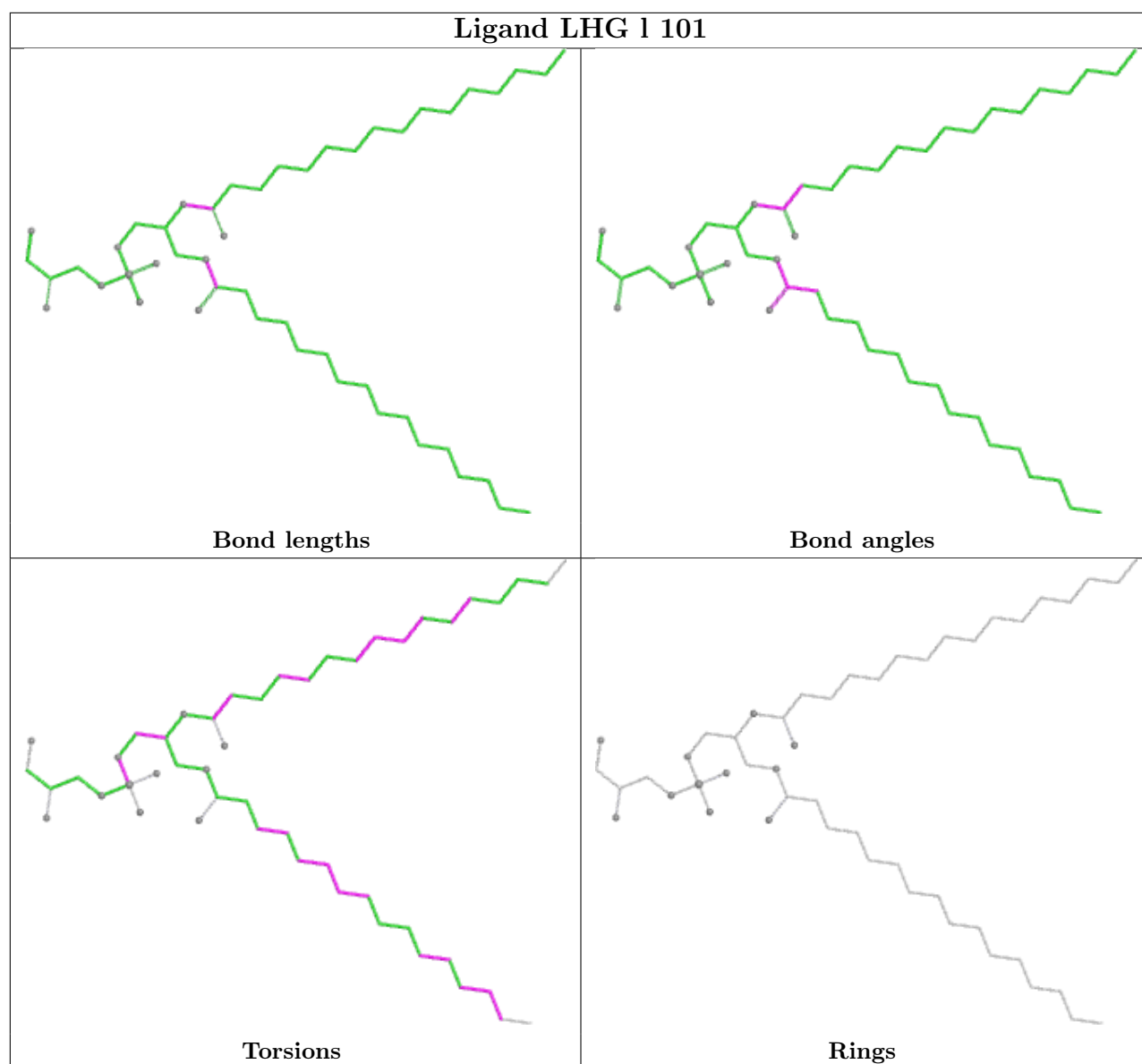
Ligand BCR D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

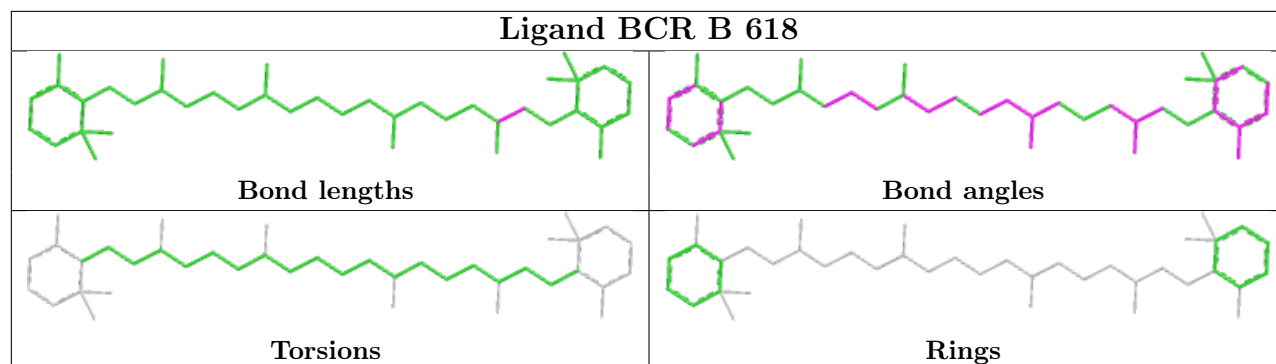
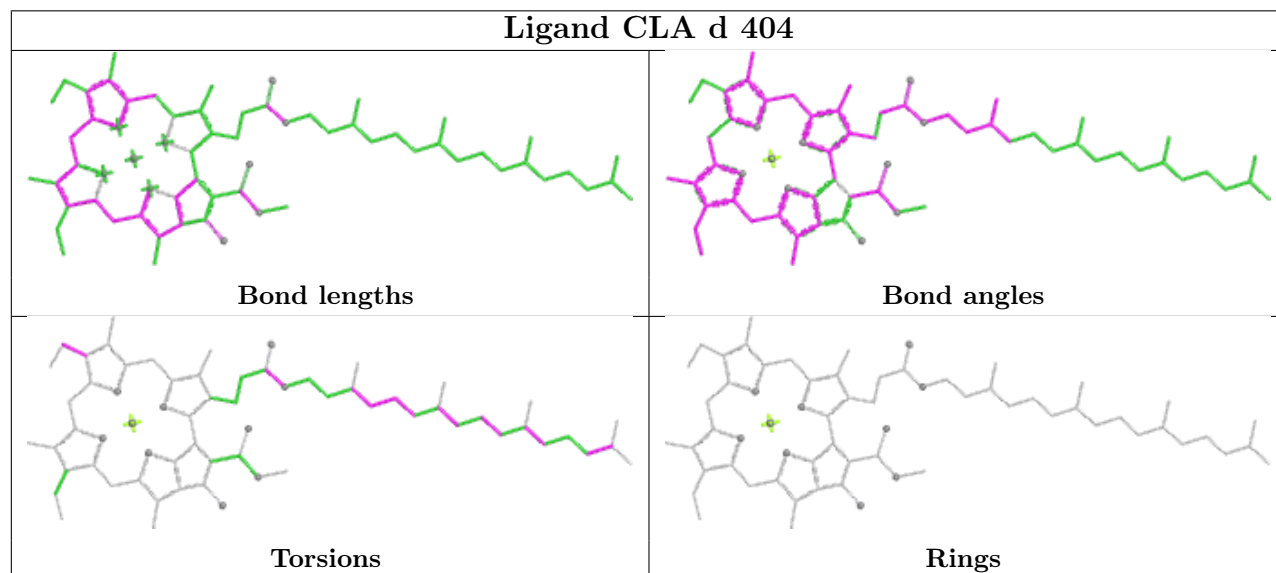
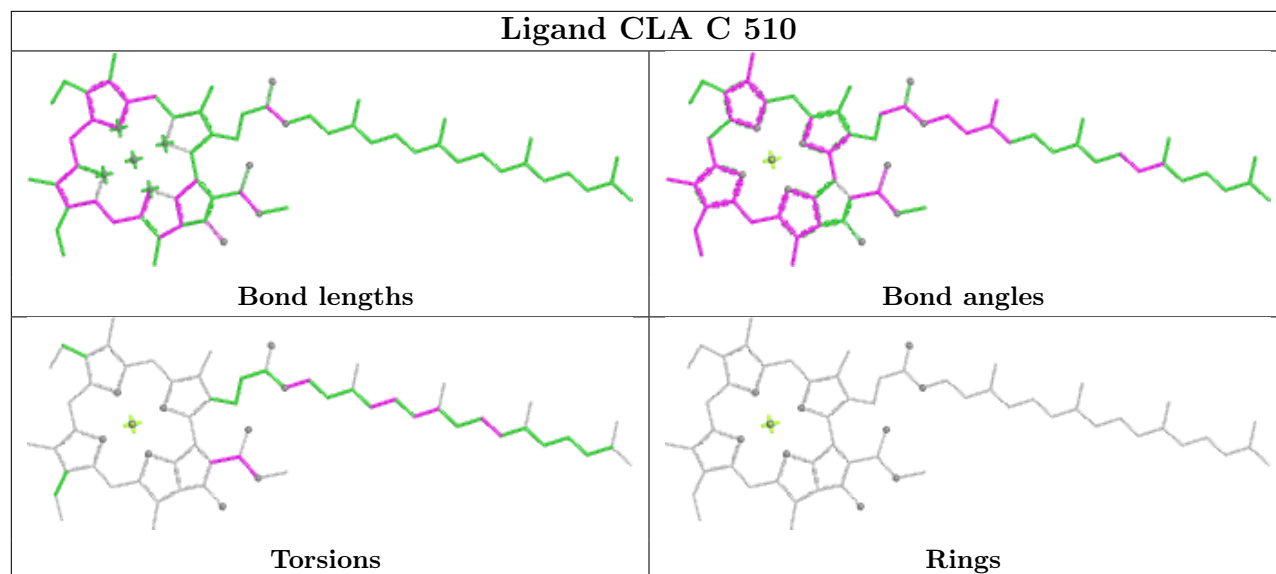
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

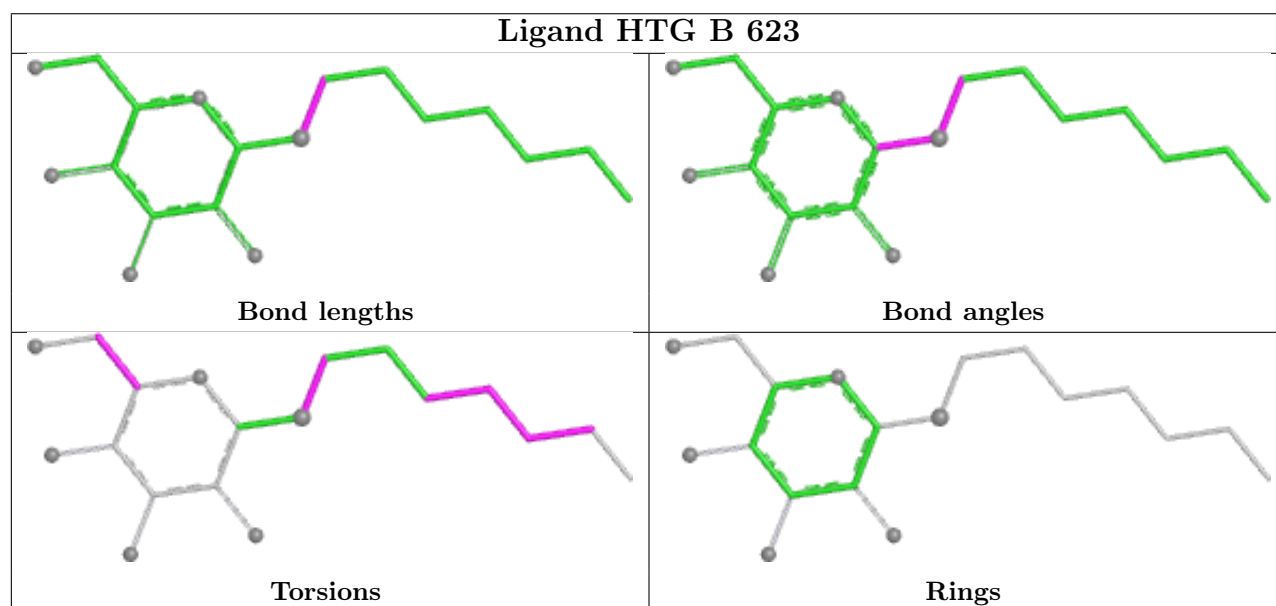
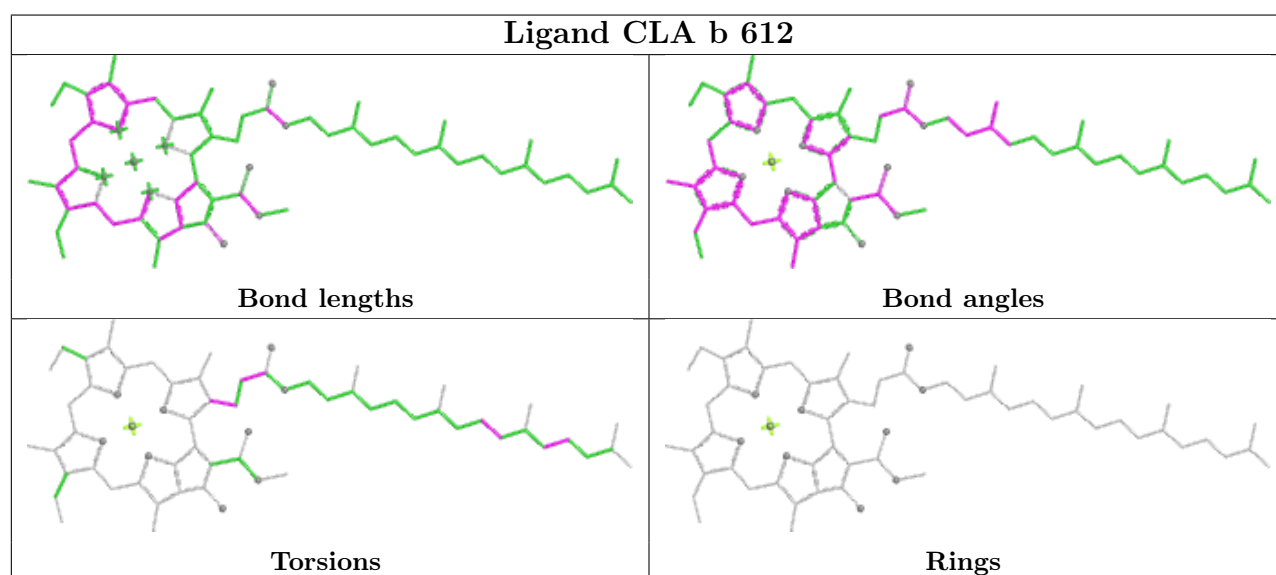
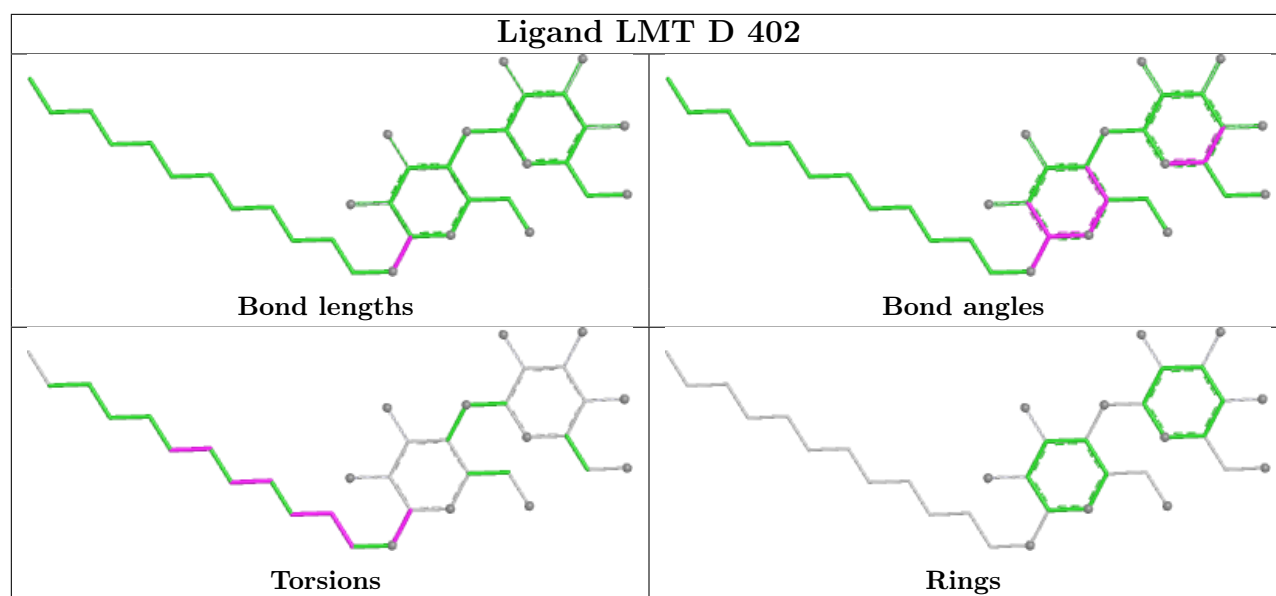
Ligand PL9 A 414	
 Bond lengths	 Bond angles
 Torsions	 Rings

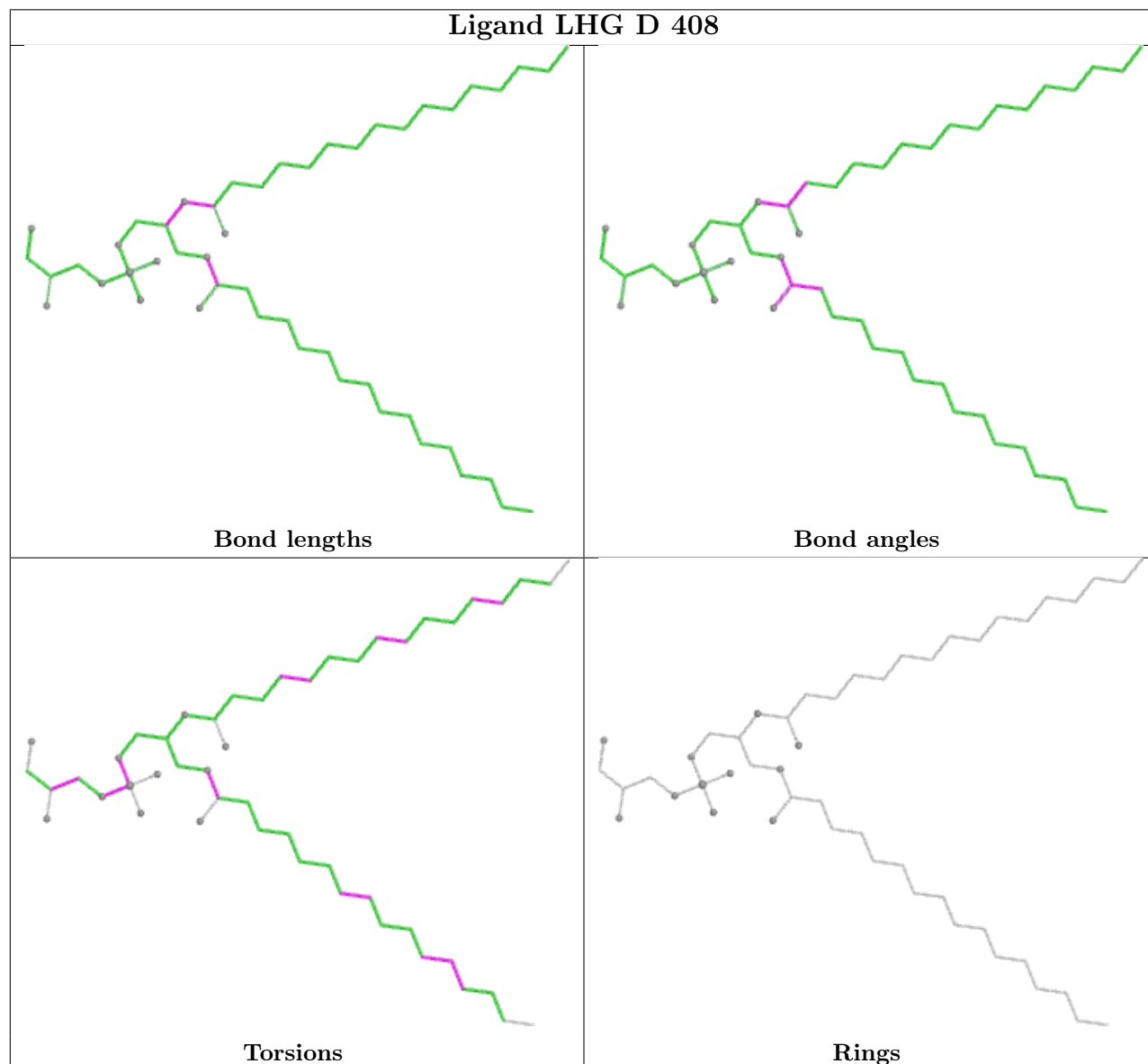
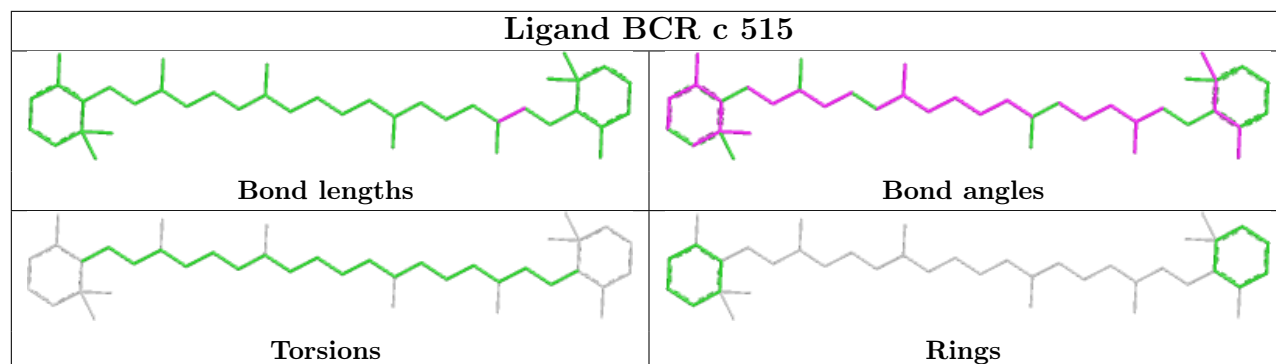
Ligand LMT B 631	
 Bond lengths	 Bond angles
 Torsions	 Rings

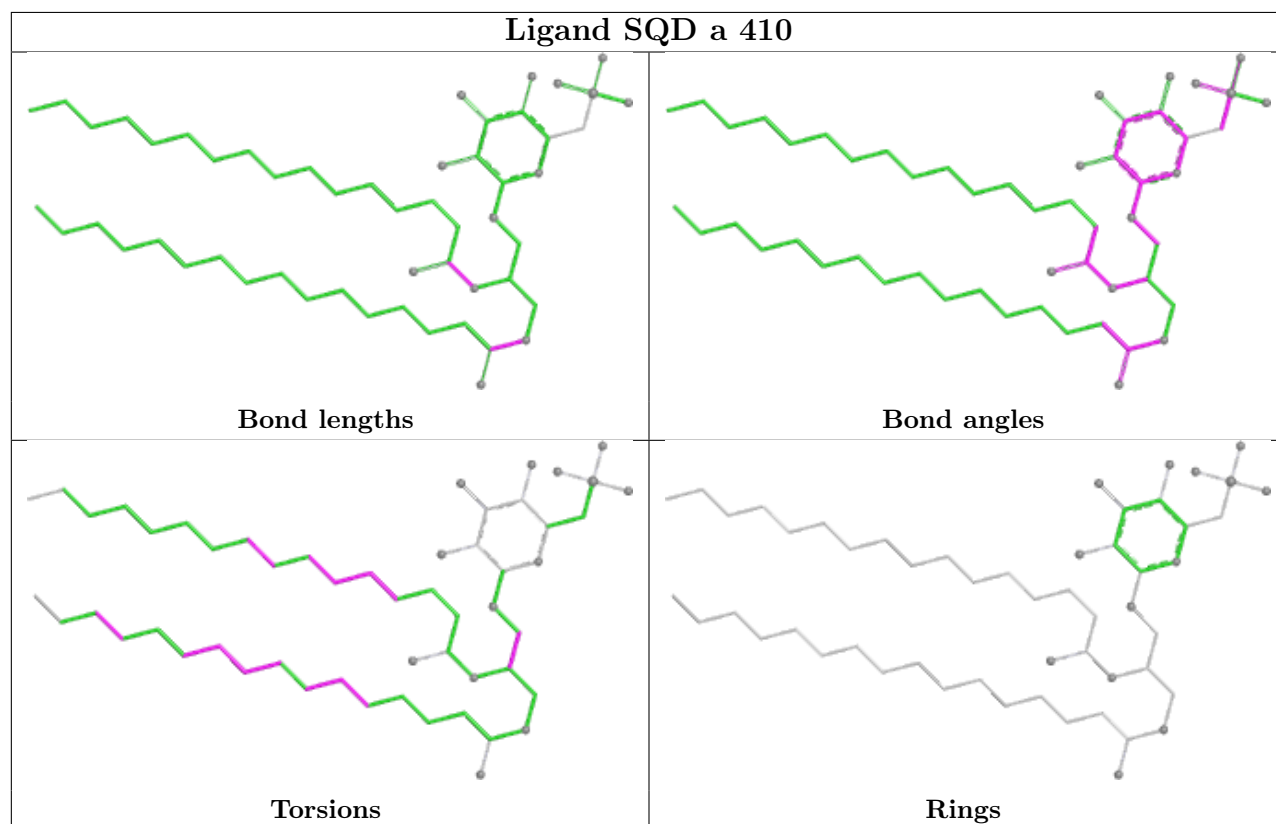
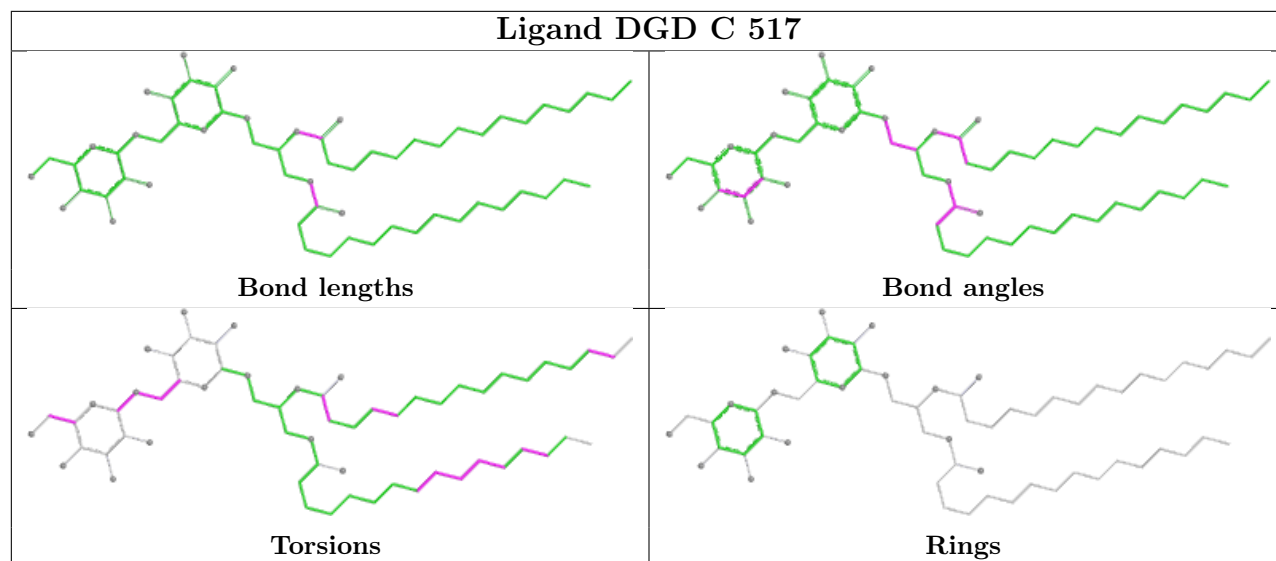
Ligand CLA B 607	
 Bond lengths	 Bond angles
 Torsions	 Rings



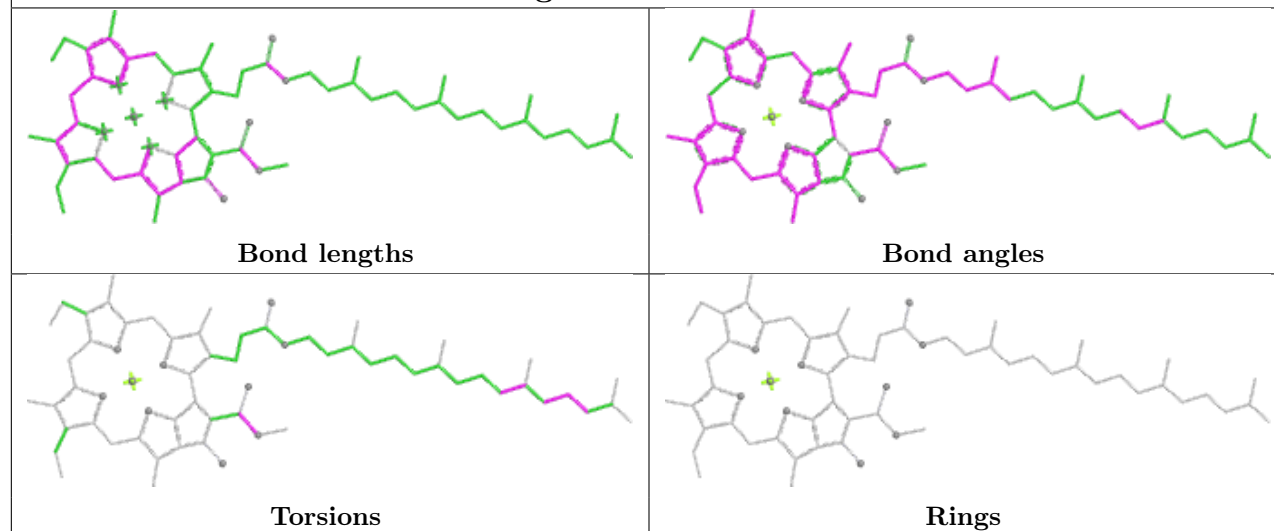




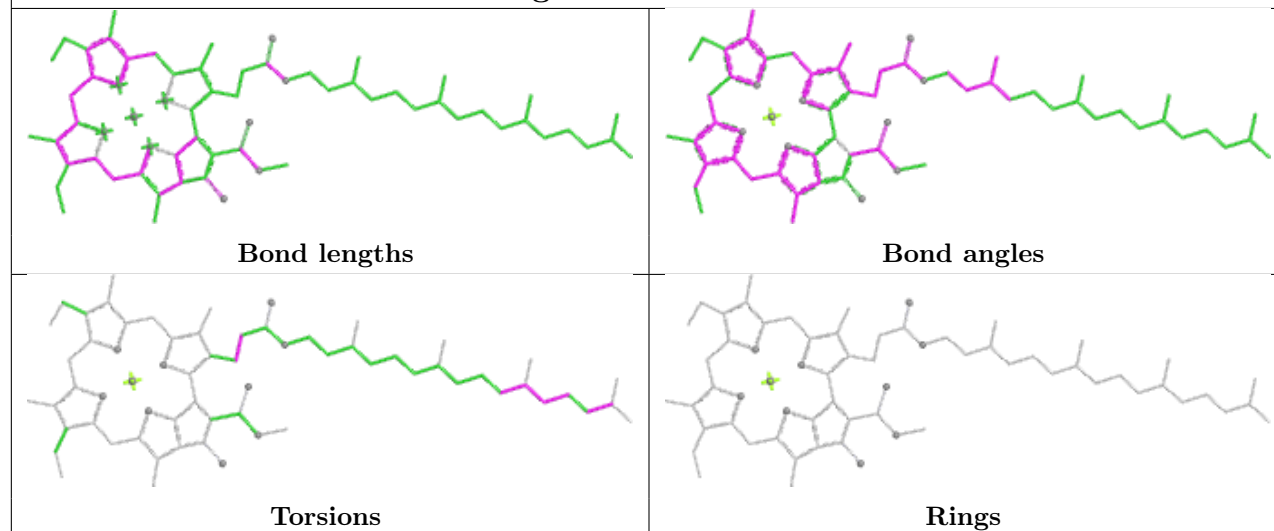




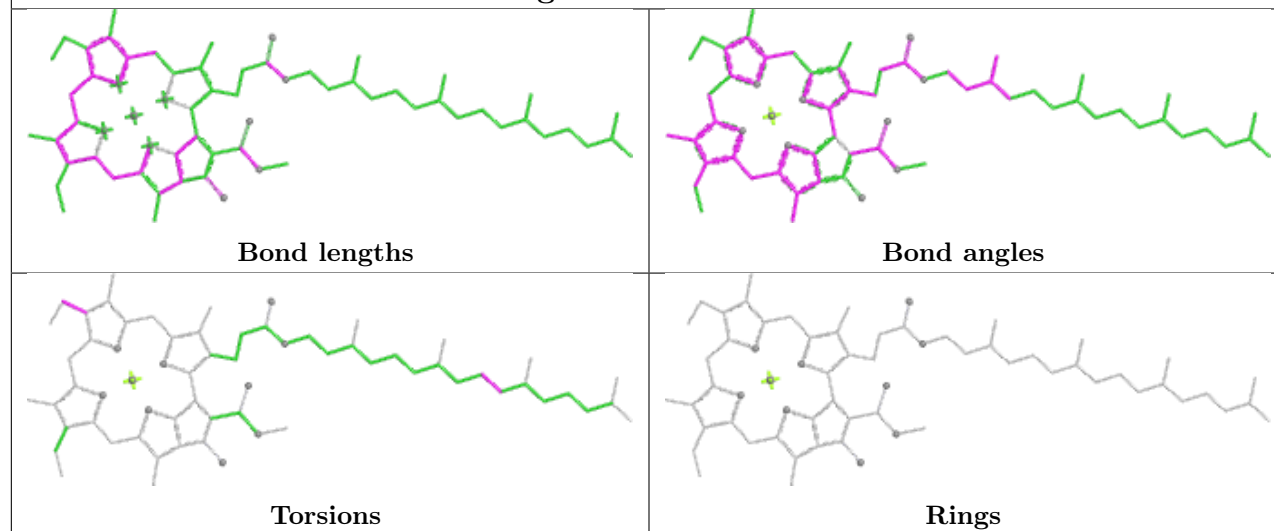
Ligand CLA d 401

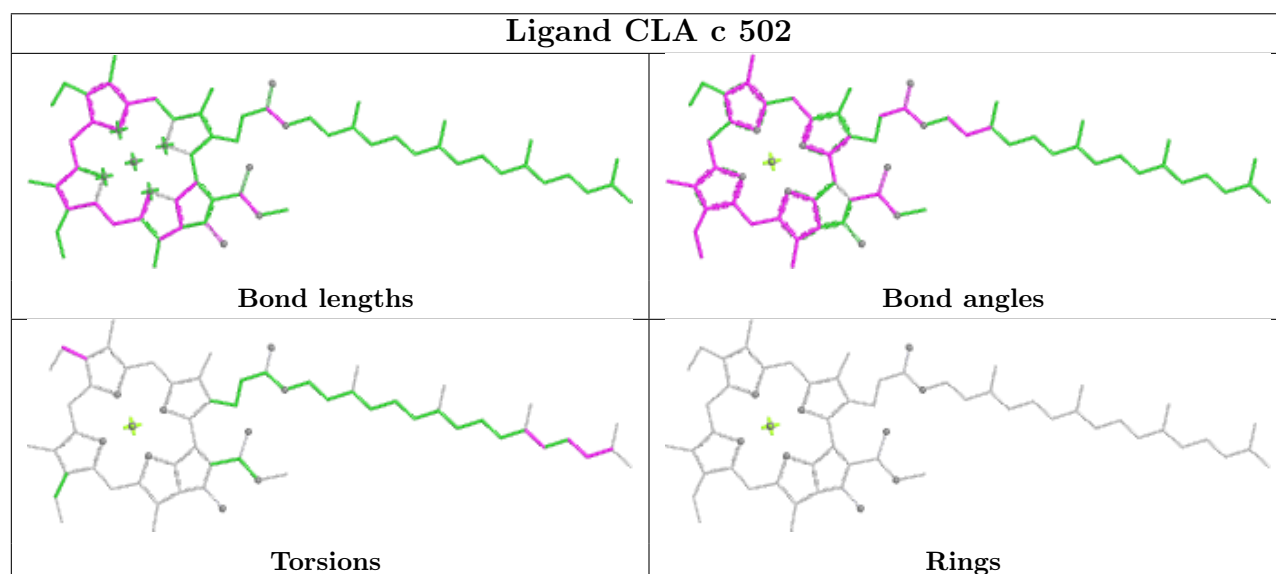
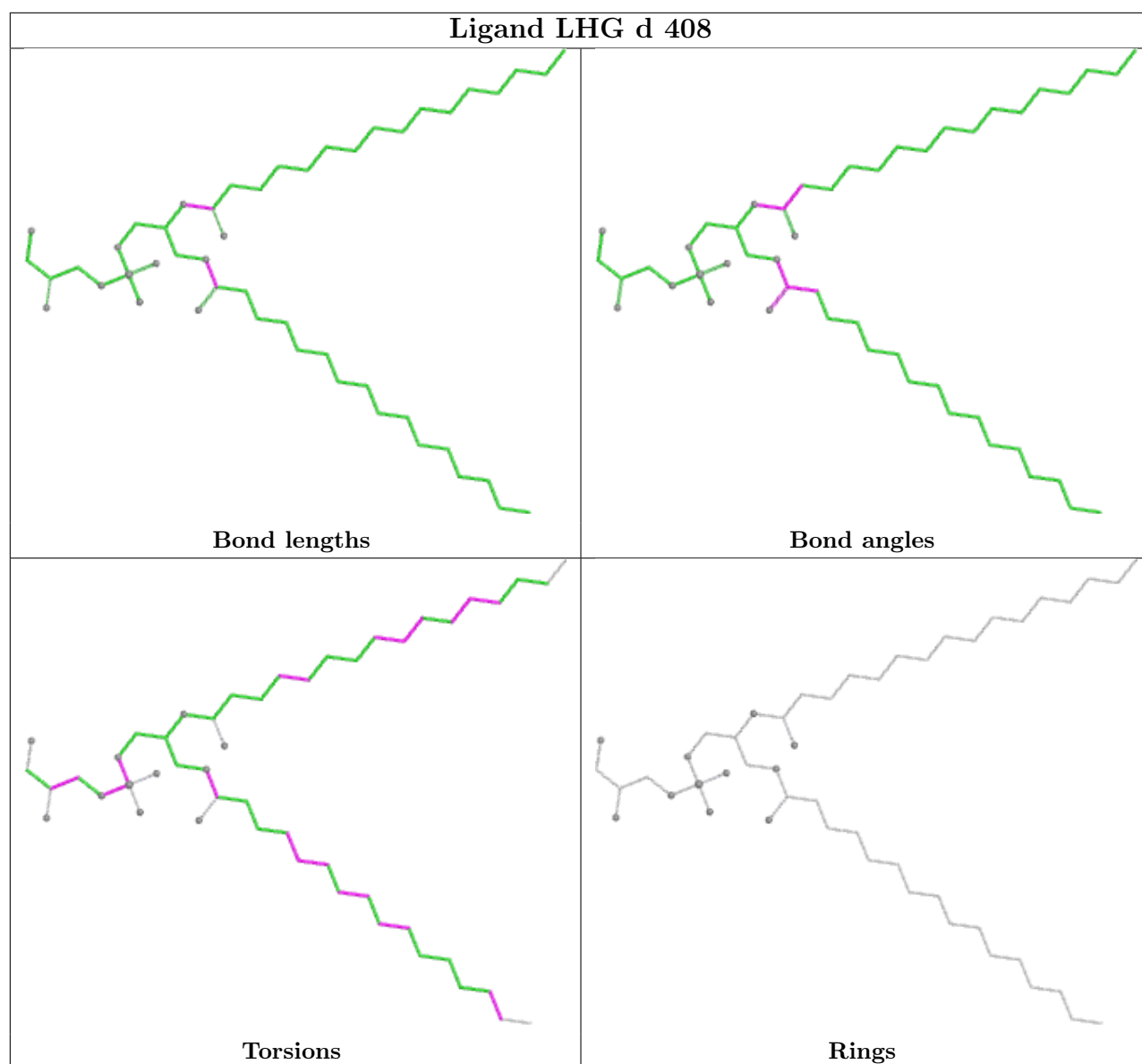


Ligand CLA B 610

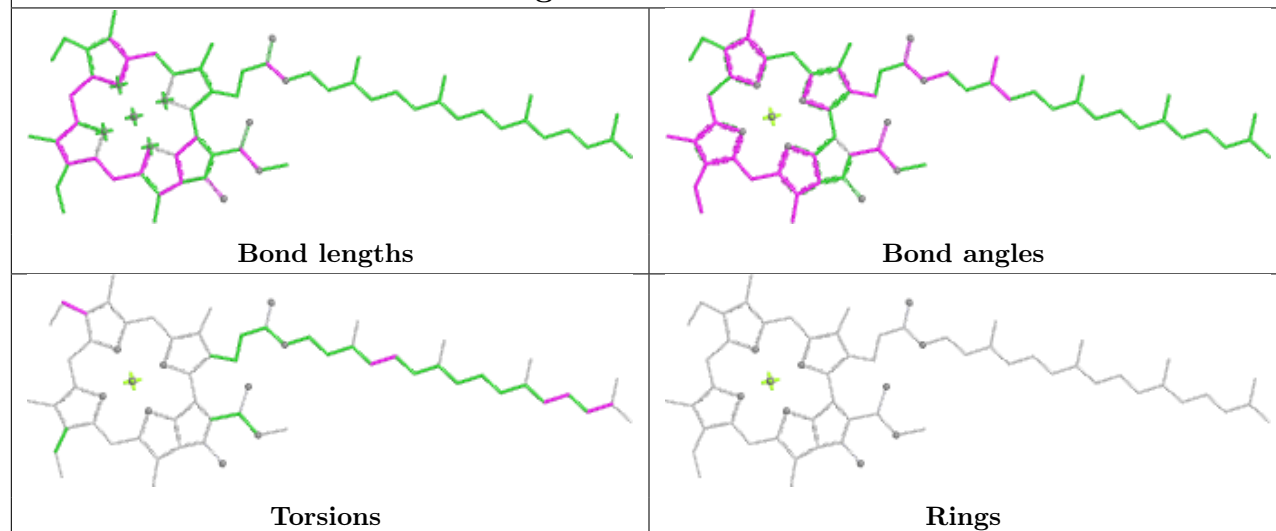


Ligand CLA c 513

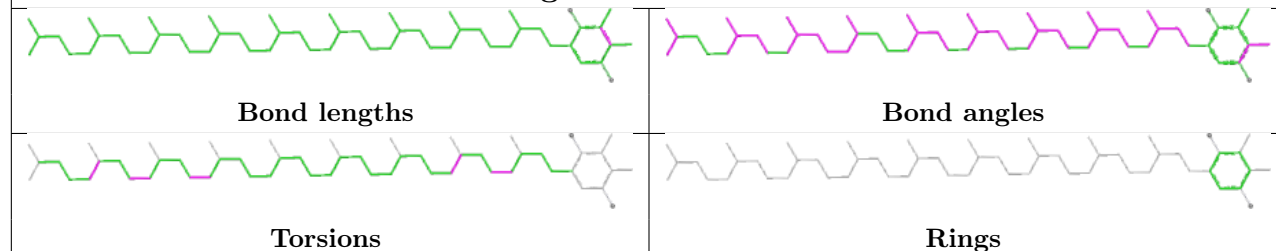




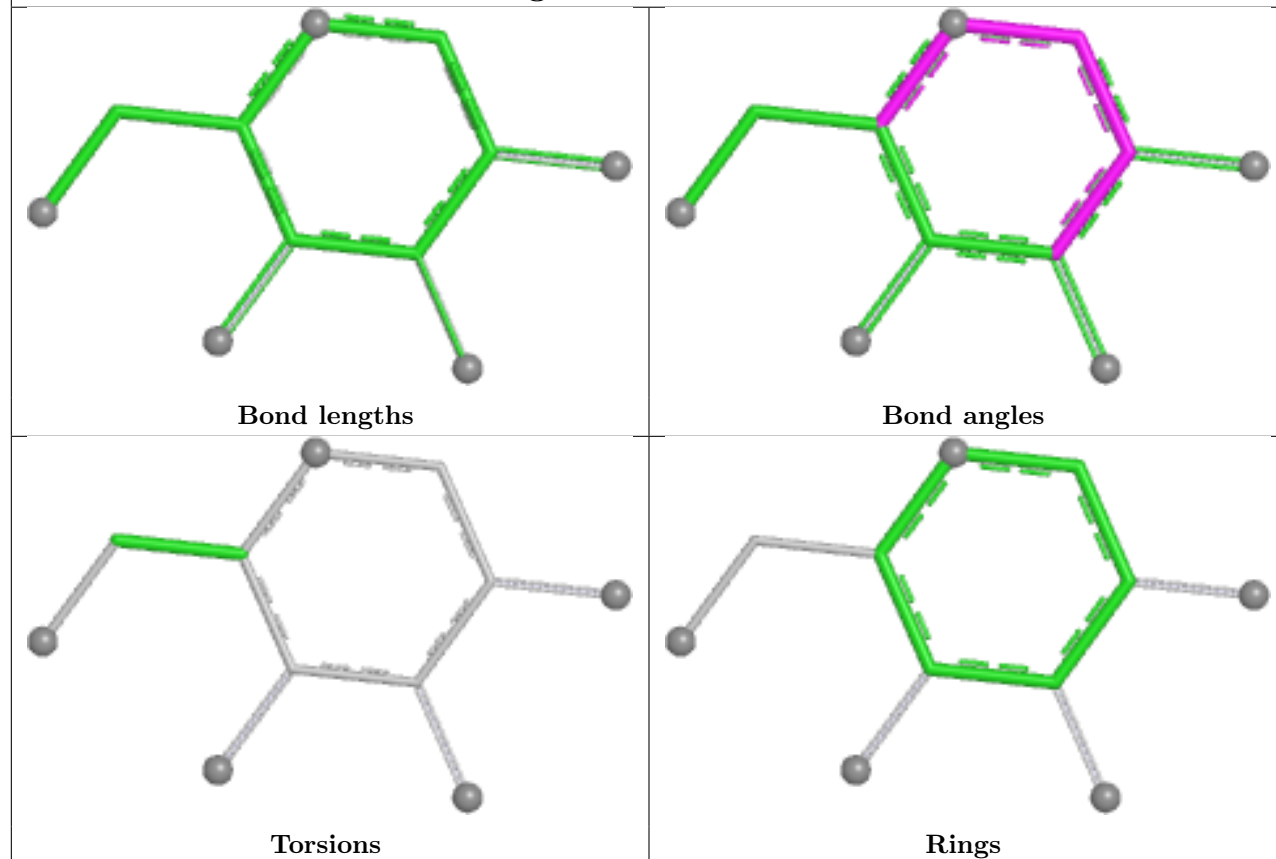
Ligand CLA b 607

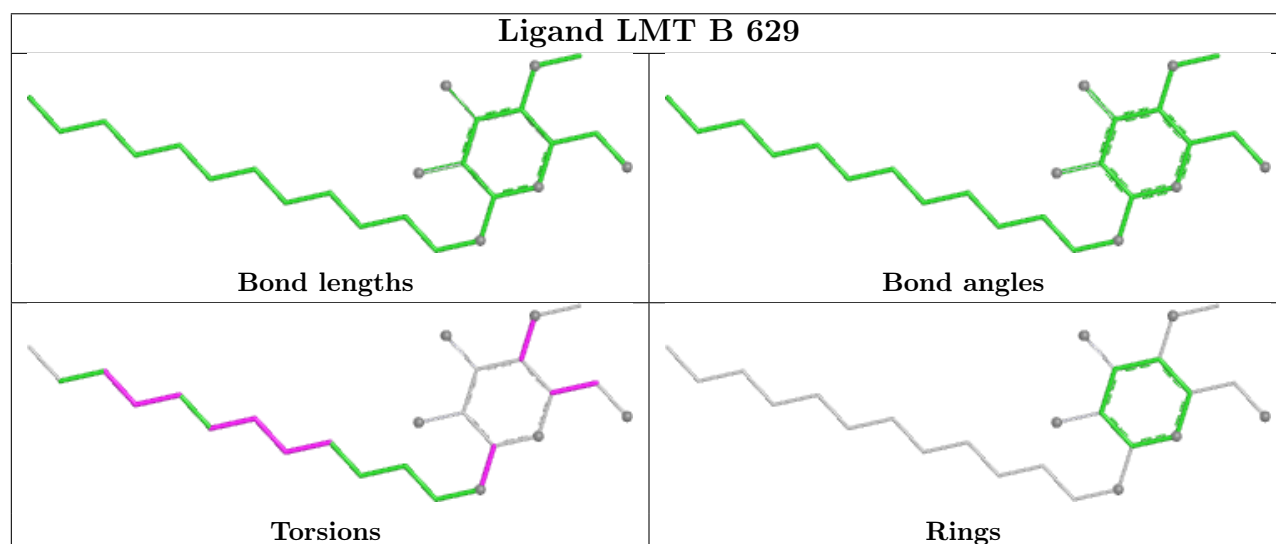
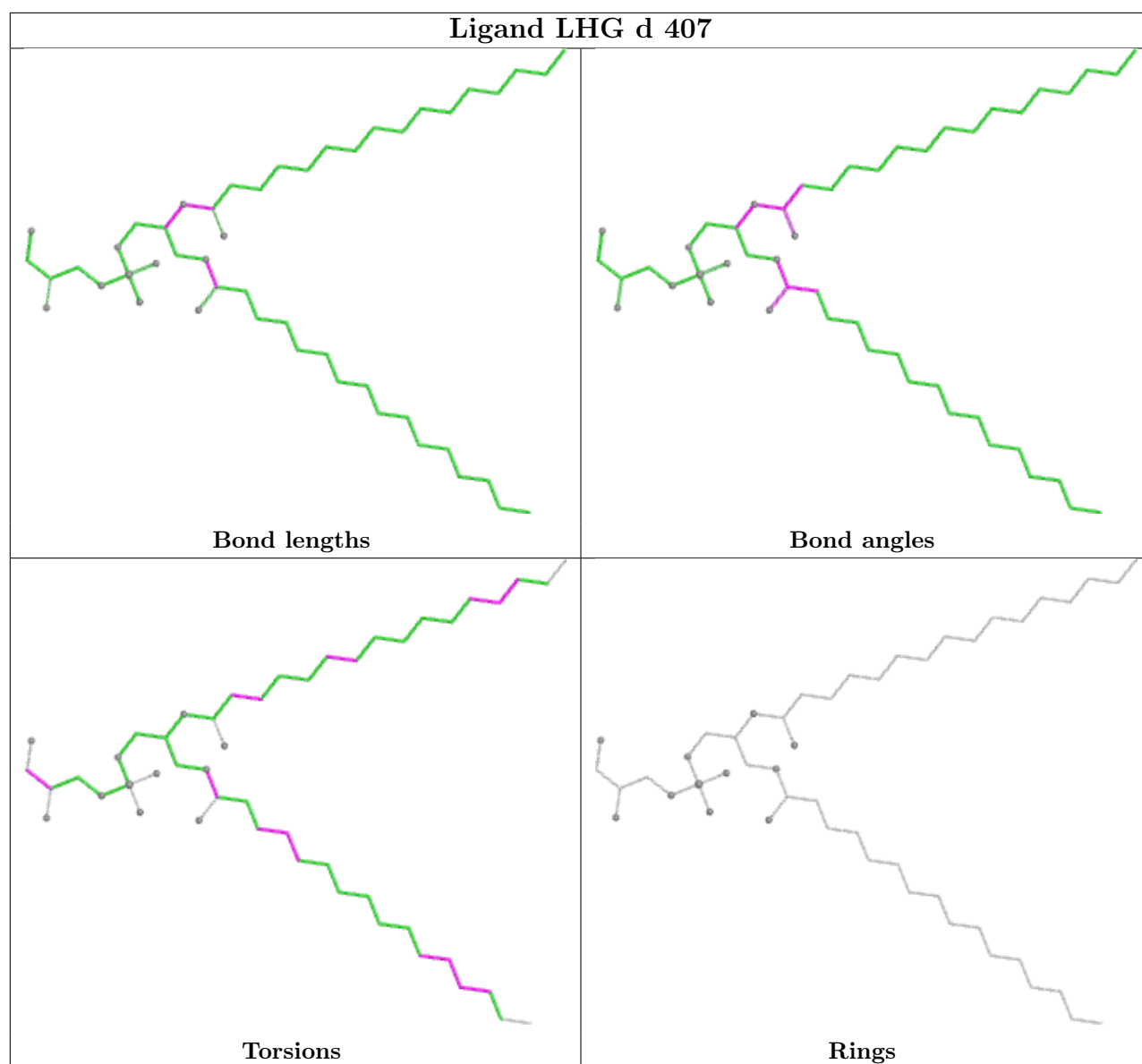


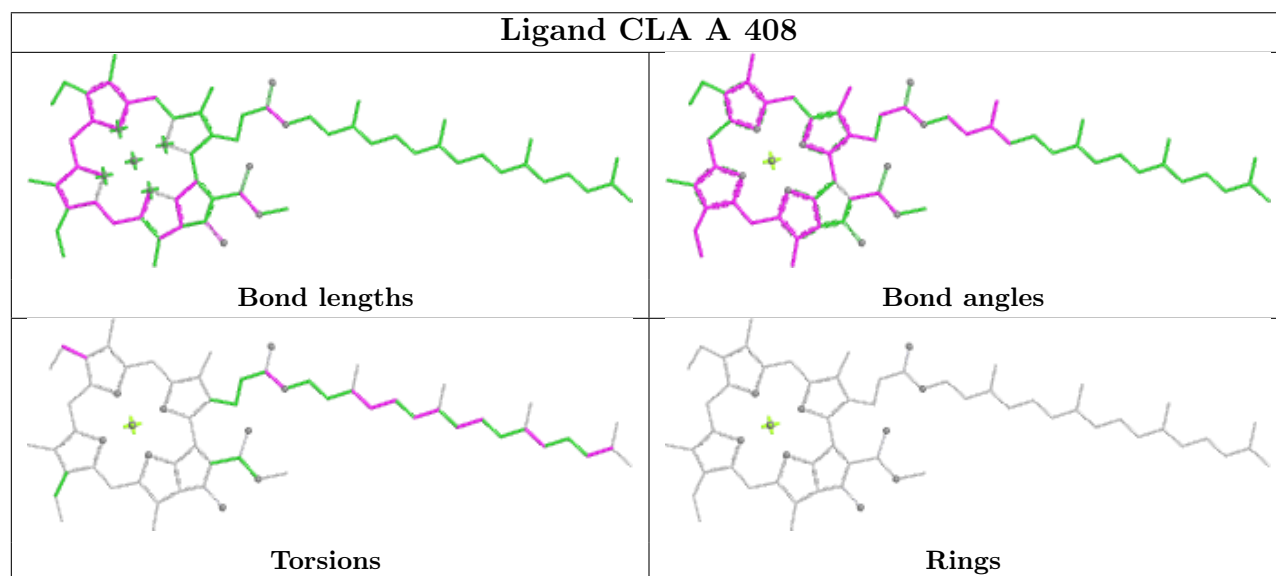
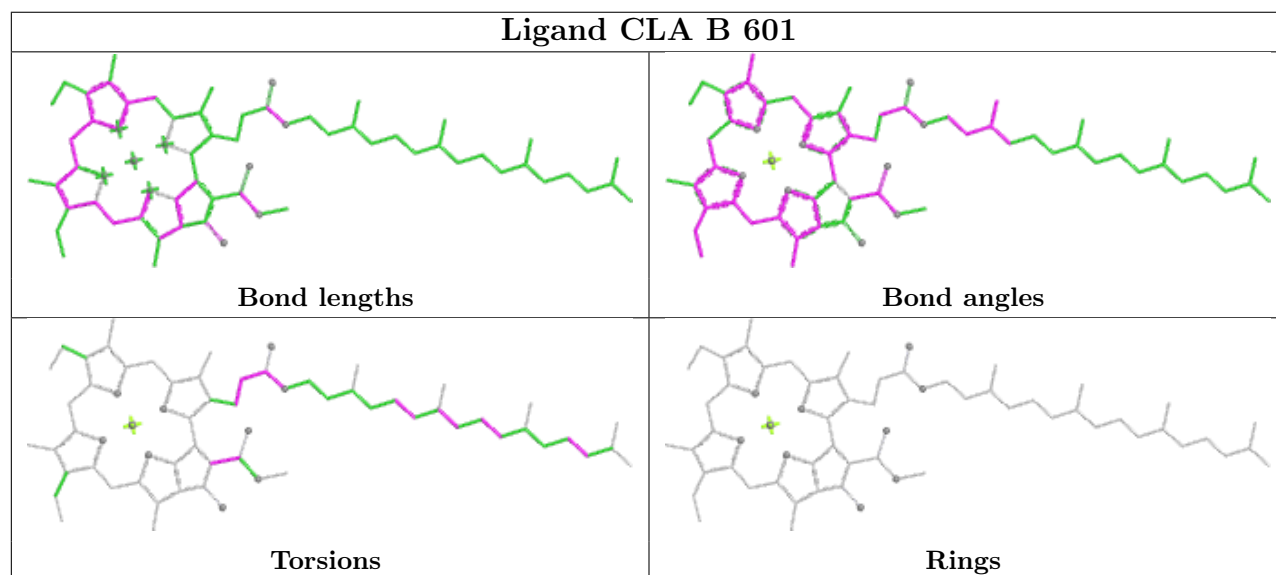
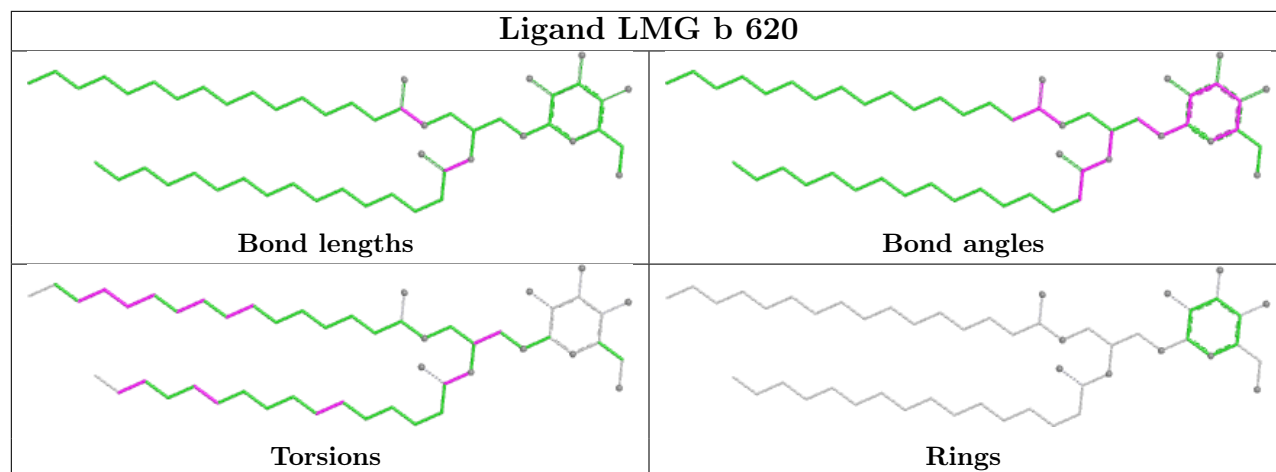
Ligand PL9 d 406

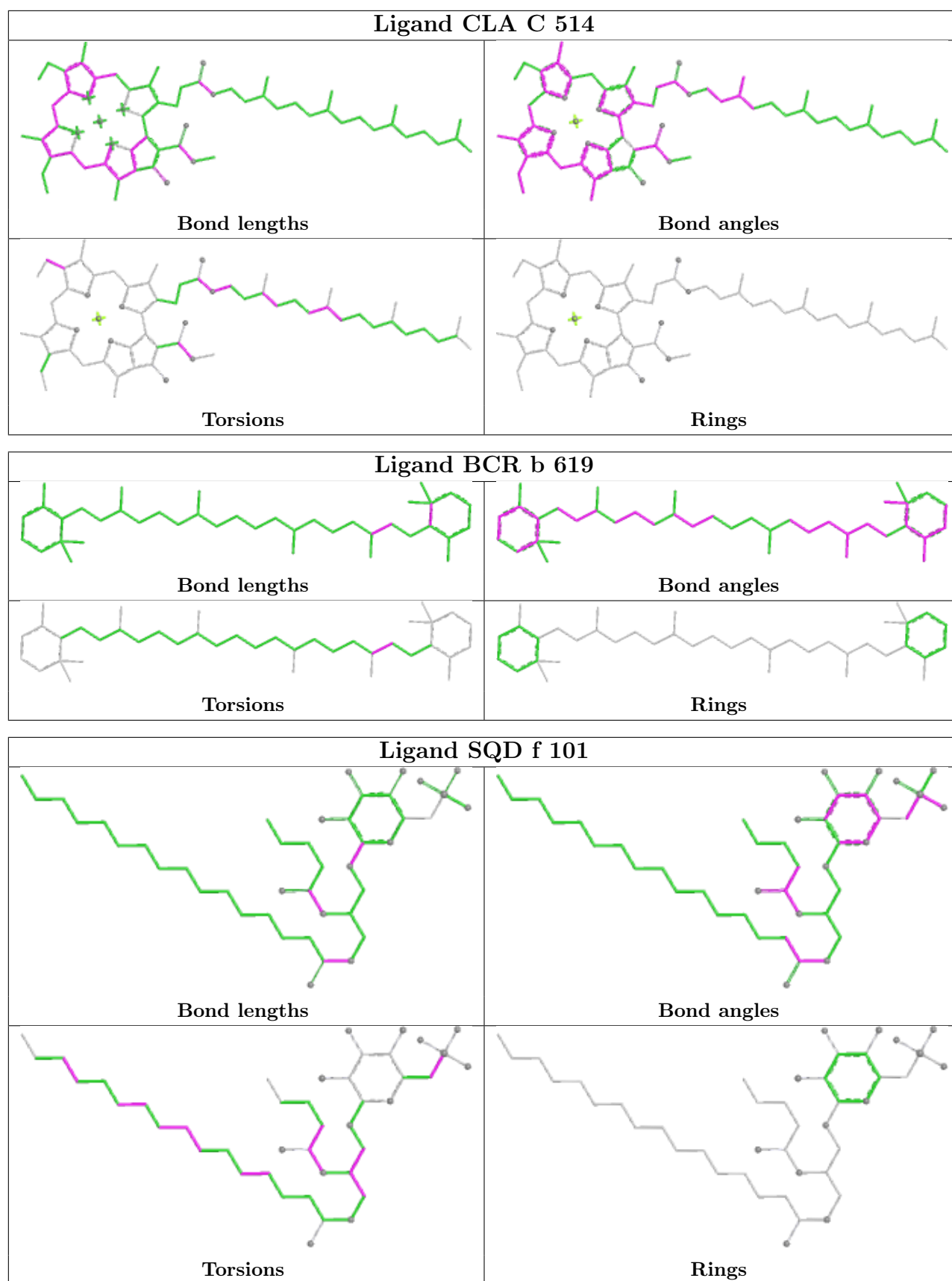


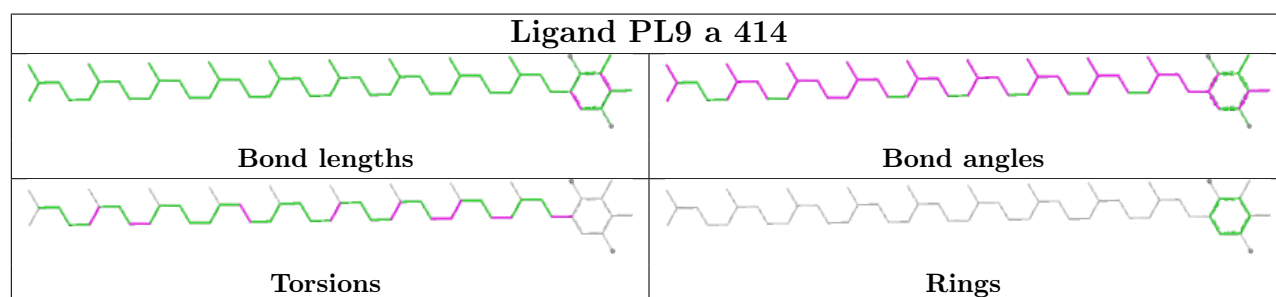
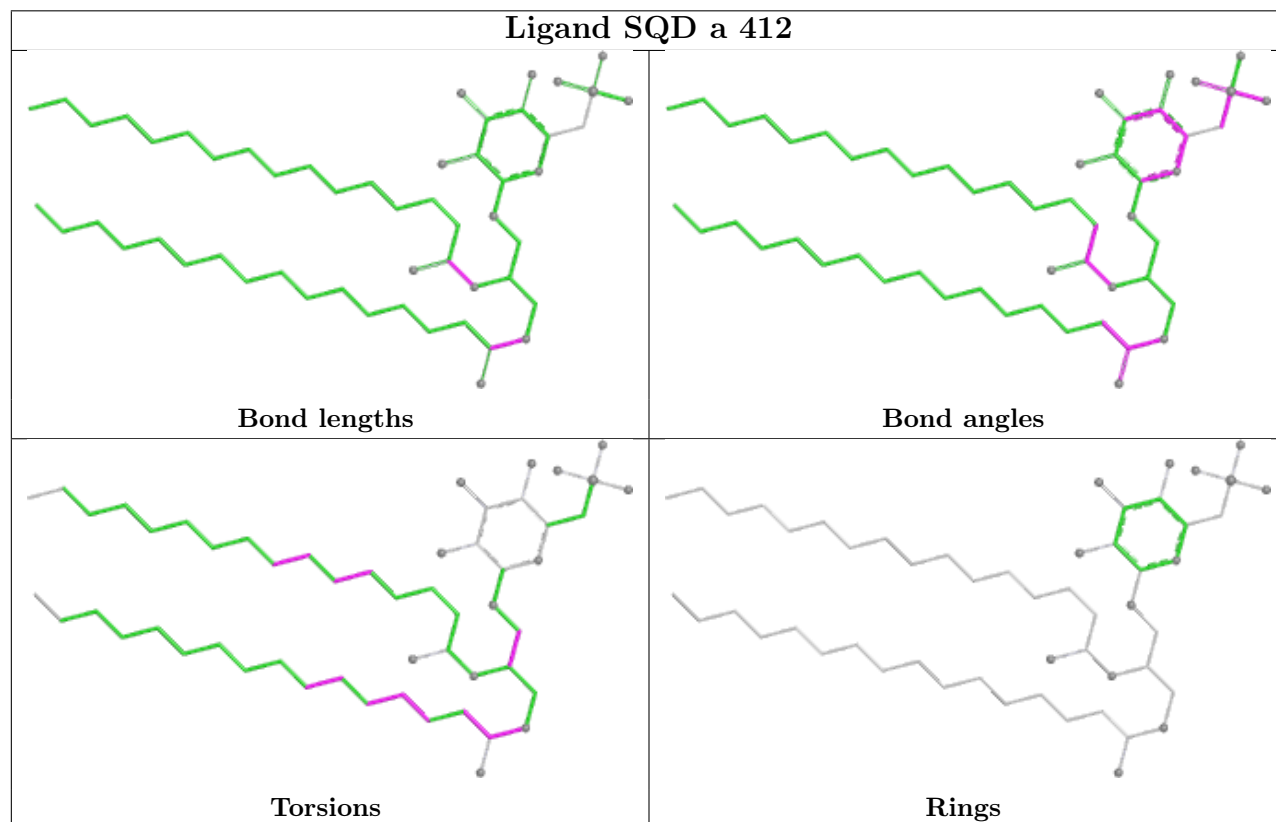
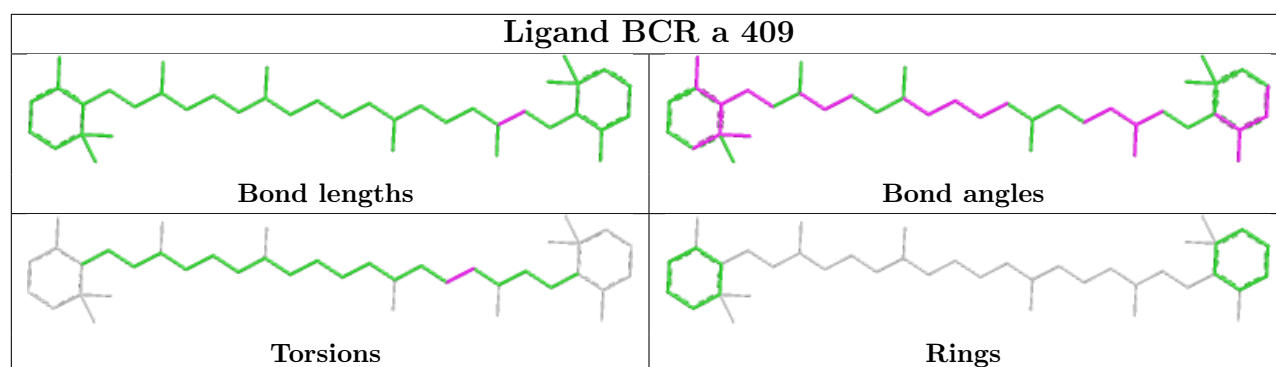
Ligand HTG V 203

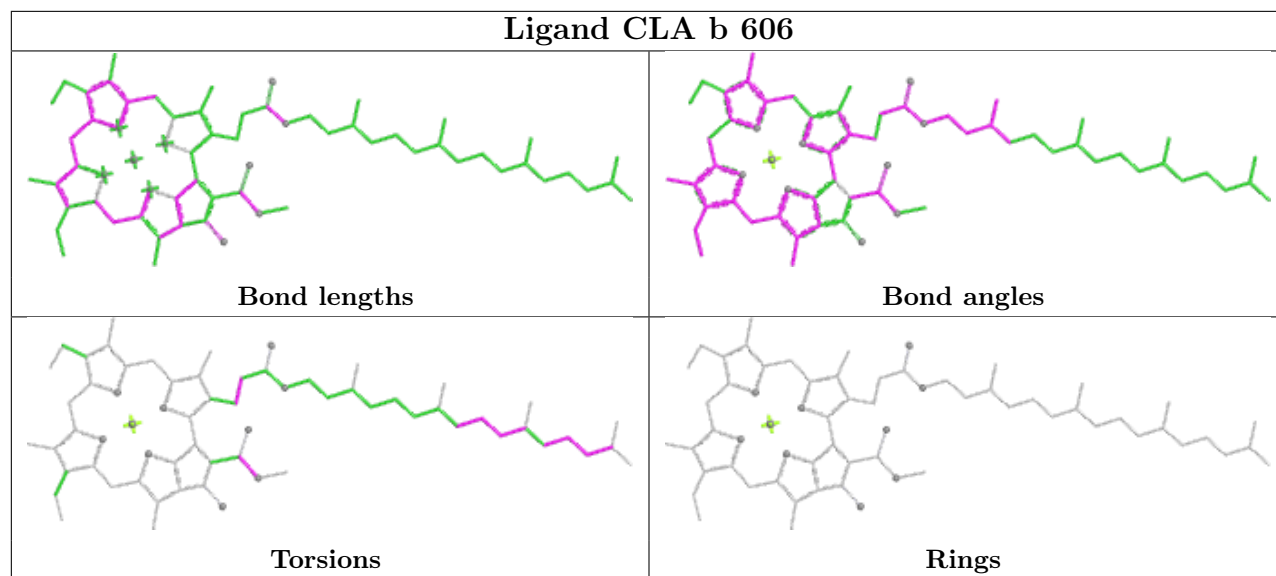












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-1.12	0 100 100	20, 31, 53, 100	3 (0%)
1	a	334/344 (97%)	-1.11	0 100 100	22, 33, 62, 108	5 (1%)
2	B	504/505 (99%)	-1.08	0 100 100	17, 36, 65, 109	8 (1%)
2	b	504/505 (99%)	-1.03	0 100 100	20, 37, 74, 118	4 (0%)
3	C	451/455 (99%)	-1.01	0 100 100	24, 45, 67, 117	4 (0%)
3	c	455/455 (100%)	-0.99	0 100 100	27, 48, 69, 109	5 (1%)
4	D	342/342 (100%)	-1.12	0 100 100	18, 32, 53, 108	1 (0%)
4	d	341/342 (99%)	-1.14	0 100 100	20, 36, 54, 123	1 (0%)
5	E	81/84 (96%)	-0.87	0 100 100	35, 54, 82, 120	1 (1%)
5	e	79/84 (94%)	-0.85	0 100 100	42, 58, 97, 120	0
6	F	34/44 (77%)	-0.97	0 100 100	38, 46, 78, 92	0
6	f	31/44 (70%)	-0.87	0 100 100	44, 50, 86, 122	0
7	H	64/65 (98%)	-0.85	1 (1%) 70 67	26, 47, 68, 101	1 (1%)
7	h	65/65 (100%)	-0.97	0 100 100	37, 51, 74, 141	0
8	I	37/38 (97%)	-0.88	0 100 100	37, 46, 88, 130	0
8	i	37/38 (97%)	-0.78	0 100 100	38, 46, 93, 135	0
9	J	38/39 (97%)	-0.98	0 100 100	32, 52, 106, 147	0
9	j	39/39 (100%)	-0.81	0 100 100	40, 51, 107, 129	0
10	K	37/37 (100%)	-1.05	0 100 100	44, 53, 76, 91	0
10	k	37/37 (100%)	-1.06	0 100 100	47, 54, 78, 93	0
11	L	36/37 (97%)	-1.16	0 100 100	15, 26, 89, 129	1 (2%)
11	l	36/37 (97%)	-1.12	0 100 100	17, 28, 87, 128	1 (2%)
12	M	32/36 (88%)	-1.12	0 100 100	16, 29, 49, 117	1 (3%)
12	m	33/36 (91%)	-1.09	0 100 100	24, 29, 72, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.99	0 100 100	22, 45, 100, 157	5 (2%)
13	o	243/244 (99%)	-1.00	0 100 100	24, 46, 99, 144	2 (0%)
14	T	29/32 (90%)	-1.11	0 100 100	23, 28, 60, 96	0
14	t	29/32 (90%)	-1.12	0 100 100	23, 29, 61, 97	0
15	U	96/104 (92%)	-1.08	0 100 100	31, 40, 66, 84	0
15	u	97/104 (93%)	-1.14	0 100 100	32, 43, 68, 101	0
16	V	137/137 (100%)	-1.02	0 100 100	29, 43, 70, 100	0
16	v	137/137 (100%)	-1.02	0 100 100	34, 50, 74, 101	0
17	X	38/40 (95%)	-0.77	0 100 100	44, 56, 82, 110	0
17	x	38/40 (95%)	-0.55	0 100 100	47, 58, 83, 112	0
18	Y	29/30 (96%)	-0.50	0 100 100	56, 71, 112, 114	0
18	y	29/30 (96%)	-0.77	0 100 100	58, 70, 110, 114	0
19	Z	62/62 (100%)	-0.80	0 100 100	57, 72, 117, 152	0
19	z	62/62 (100%)	-0.55	0 100 100	60, 74, 117, 153	0
20	R	34/34 (100%)	0.41	0 100 100	89, 108, 128, 135	0
All	All	5284/5384 (98%)	-1.01	1 (0%) 100 100	15, 41, 82, 157	43 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.1

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
8	FME	I	1	10/11	0.97	0.04	31,47,56,62	0
14	FME	T	1	10/11	0.97	0.05	18,32,46,47	0
14	FME	t	1	10/11	0.97	0.04	21,32,41,71	0
8	FME	i	1	10/11	0.98	0.03	37,49,57,62	0
12	FME	m	1	10/11	0.98	0.04	30,42,63,78	0
12	FME	M	1	10/11	0.98	0.06	18,38,70,79	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	A	415	28/-	0.65	0.14	67,87,108,112	0
30	UNL	i	101	40/-	0.67	0.13	48,88,140,147	0
35	LMT	E	102	35/35	0.68	0.14	78,120,147,150	0
30	UNL	m	101	10/-	0.69	0.12	40,50,55,56	0
34	HTG	B	624	19/19	0.71	0.10	57,104,140,144	0
30	UNL	J	102	10/-	0.72	0.15	55,64,89,90	0
34	HTG	D	412	16/19	0.73	0.10	48,115,128,130	0
35	LMT	B	630	35/35	0.73	0.12	33,105,126,134	0
35	LMT	D	402	35/35	0.73	0.11	31,97,113,115	0
33	LMG	Z	101	51/55	0.73	0.11	46,105,140,150	0
34	HTG	B	623	19/19	0.75	0.14	60,84,110,115	0
34	HTG	b	622	19/19	0.75	0.14	74,95,125,130	0
34	HTG	c	521	19/19	0.75	0.10	68,112,134,140	0
30	UNL	a	415	30/-	0.76	0.11	72,90,111,118	0
30	UNL	K	101	34/-	0.77	0.10	55,96,114,125	0
35	LMT	a	417	35/35	0.77	0.11	78,114,130,131	0
35	LMT	e	102	35/35	0.77	0.12	76,134,147,156	0
26	SQD	f	101	43/54	0.78	0.11	85,111,157,164	0
30	UNL	D	411	40/-	0.78	0.11	40,77,117,122	0
35	LMT	I	101	35/35	0.79	0.10	74,108,131,141	0
35	LMT	D	403	35/35	0.79	0.09	48,91,116,117	0
35	LMT	b	621	25/35	0.79	0.10	60,99,144,148	0
34	HTG	C	521	19/19	0.79	0.10	66,101,116,120	0
35	LMT	M	103	35/35	0.80	0.10	40,120,148,154	0
34	HTG	c	522	19/19	0.80	0.11	79,124,142,146	0
30	UNL	M	102	10/-	0.80	0.10	33,52,59,69	0
34	HTG	V	203	11/19	0.80	0.09	71,92,107,108	0
33	LMG	c	520	51/55	0.81	0.09	51,102,132,138	0
34	HTG	b	623	19/19	0.81	0.10	71,109,141,169	0
34	HTG	d	411	16/19	0.81	0.11	81,112,121,122	0
30	UNL	I	102	40/-	0.82	0.11	40,85,135,142	0
30	UNL	b	629	36/-	0.83	0.09	49,80,131,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	b	626	33/-	0.83	0.10	44,78,131,135	0
30	UNL	c	525	32/-	0.84	0.10	71,97,113,119	0
30	UNL	B	628	33/-	0.84	0.10	29,76,136,139	0
30	UNL	j	102	10/-	0.84	0.11	60,75,88,89	0
34	HTG	C	522	19/19	0.84	0.09	58,139,157,179	0
29	PL9	A	414	55/55	0.85	0.13	41,88,105,119	0
35	LMT	M	101	35/35	0.85	0.08	39,80,103,109	0
33	LMG	Z	102	37/55	0.85	0.10	47,97,129,137	0
26	SQD	a	412	54/54	0.86	0.08	44,73,125,133	0
31	LHG	E	101	42/49	0.86	0.09	41,93,108,124	0
31	LHG	e	101	42/49	0.86	0.09	81,118,142,148	0
35	LMT	m	102	35/35	0.86	0.09	34,78,102,109	0
35	LMT	B	629	25/35	0.87	0.10	34,68,124,125	0
27	GOL	a	411	6/6	0.87	0.11	52,60,62,66	0
26	SQD	A	412	54/54	0.87	0.07	39,65,102,118	0
29	PL9	a	414	55/55	0.87	0.12	57,93,112,120	0
34	HTG	b	628	19/19	0.88	0.10	34,65,115,119	0
26	SQD	B	620	54/54	0.89	0.08	41,73,108,113	0
27	GOL	b	624	6/6	0.89	0.08	58,76,78,86	0
34	HTG	B	627	19/19	0.89	0.07	45,63,74,75	0
27	GOL	d	402	6/6	0.89	0.21	33,50,65,68	0
33	LMG	z	101	39/55	0.89	0.10	63,112,140,147	0
33	LMG	C	501	51/55	0.90	0.08	35,74,98,102	0
26	SQD	D	413	43/54	0.90	0.09	64,97,112,116	0
30	UNL	D	410	17/-	0.90	0.08	44,56,91,100	0
30	UNL	x	101	18/-	0.90	0.09	44,63,91,92	0
26	SQD	L	101	54/54	0.90	0.07	47,71,116,121	0
27	GOL	B	626	6/6	0.90	0.12	38,51,55,62	0
25	BCR	D	406	40/40	0.91	0.07	32,42,87,90	0
33	LMG	a	416	51/55	0.91	0.07	41,77,102,118	0
33	LMG	c	519	51/55	0.91	0.08	43,77,114,124	0
35	LMT	b	627	25/35	0.91	0.08	29,61,134,139	0
27	GOL	C	523	6/6	0.91	0.10	44,54,59,60	0
25	BCR	y	101	40/40	0.91	0.07	44,54,70,72	0
35	LMT	B	631	26/35	0.92	0.08	52,80,105,109	0
23	CLA	b	601	65/65	0.92	0.07	43,69,99,126	0
27	GOL	A	411	6/6	0.92	0.07	50,58,65,79	0
33	LMG	C	520	51/55	0.92	0.08	37,69,104,121	0
34	HTG	B	622	19/19	0.93	0.07	34,61,127,132	0
25	BCR	d	405	40/40	0.93	0.07	40,50,74,81	0
23	CLA	c	513	65/65	0.93	0.07	52,73,115,119	0
23	CLA	B	601	65/65	0.93	0.07	39,57,88,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LMG	J	101	51/55	0.93	0.07	30,51,88,99	0
33	LMG	j	101	51/55	0.93	0.07	37,53,102,123	0
27	GOL	B	625	6/6	0.93	0.09	48,76,85,89	0
36	DGD	c	517	62/66	0.93	0.06	38,53,112,129	0
37	CA	V	201	1/1	0.93	0.05	93,93,93,93	0
26	SQD	a	410	54/54	0.94	0.07	41,64,98,105	0
25	BCR	K	102	40/40	0.94	0.07	39,47,62,65	0
25	BCR	Y	101	40/40	0.94	0.07	37,49,59,62	0
23	CLA	c	504	65/65	0.94	0.07	37,50,89,111	0
30	UNL	d	410	17/-	0.94	0.06	42,57,85,90	0
33	LMG	b	620	51/55	0.94	0.06	29,50,88,106	0
23	CLA	C	514	65/65	0.94	0.07	46,64,87,95	0
34	HTG	b	625	19/19	0.94	0.06	43,56,83,93	0
26	SQD	A	410	54/54	0.94	0.07	38,62,99,105	0
25	BCR	B	619	40/40	0.94	0.06	28,42,63,67	0
25	BCR	C	515	40/40	0.94	0.07	46,61,72,73	0
23	CLA	C	507	65/65	0.94	0.07	39,55,102,106	0
36	DGD	c	516	62/66	0.94	0.06	33,43,73,95	0
25	BCR	H	101	40/40	0.94	0.06	33,42,63,67	0
30	UNL	X	101	18/-	0.94	0.08	40,53,83,90	0
29	PL9	d	406	55/55	0.95	0.06	23,30,41,58	0
25	BCR	k	101	40/40	0.95	0.07	47,55,79,81	0
25	BCR	t	101	40/40	0.95	0.05	19,42,59,62	0
23	CLA	b	616	65/65	0.95	0.07	31,46,98,105	0
23	CLA	C	513	65/65	0.95	0.07	43,59,94,101	0
23	CLA	c	506	65/65	0.95	0.06	44,58,90,111	0
23	CLA	c	507	65/65	0.95	0.07	41,53,65,68	0
25	BCR	T	101	40/40	0.95	0.05	20,36,45,53	0
31	LHG	A	416	49/49	0.95	0.06	26,44,61,77	0
31	LHG	D	409	49/49	0.95	0.07	29,47,107,124	0
23	CLA	C	505	65/65	0.95	0.06	30,41,79,104	0
36	DGD	C	518	62/66	0.95	0.06	29,46,103,110	0
25	BCR	c	514	40/40	0.95	0.06	52,65,76,79	0
33	LMG	B	621	51/55	0.95	0.06	32,49,79,105	0
36	DGD	c	518	62/66	0.95	0.05	36,46,77,96	0
23	CLA	B	606	65/65	0.95	0.06	26,35,76,99	0
37	CA	c	523	1/1	0.95	0.07	68,68,68,68	0
25	BCR	b	617	40/40	0.96	0.04	20,34,41,44	0
25	BCR	b	618	40/40	0.96	0.04	21,34,49,55	0
25	BCR	b	619	40/40	0.96	0.05	32,45,61,69	0
31	LHG	d	407	49/49	0.96	0.06	25,44,72,87	0
31	LHG	d	409	49/49	0.96	0.07	33,50,98,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	PL9	D	407	55/55	0.96	0.05	20,31,45,54	0
31	LHG	l	101	49/49	0.96	0.05	25,38,55,60	0
23	CLA	B	614	65/65	0.96	0.06	21,31,82,100	0
25	BCR	c	515	40/40	0.96	0.05	37,52,65,75	0
23	CLA	B	616	65/65	0.96	0.07	30,45,113,124	0
25	BCR	h	101	40/40	0.96	0.06	39,50,64,77	0
23	CLA	c	508	65/65	0.96	0.06	35,48,107,118	0
23	CLA	c	511	65/65	0.96	0.07	43,56,74,82	0
23	CLA	c	512	65/65	0.96	0.06	48,64,90,96	0
23	CLA	D	405	65/65	0.96	0.07	31,46,99,111	0
23	CLA	d	404	65/65	0.96	0.07	38,48,98,109	0
24	PHO	a	407	64/64	0.96	0.05	28,35,50,52	0
25	BCR	A	409	40/40	0.96	0.05	22,34,46,49	0
25	BCR	B	618	40/40	0.96	0.04	21,36,54,69	0
23	CLA	a	405	65/65	0.96	0.06	27,36,105,111	0
23	CLA	a	408	65/65	0.96	0.08	28,40,107,115	0
36	DGD	C	517	62/66	0.96	0.05	27,36,81,92	0
25	BCR	C	516	40/40	0.96	0.05	36,48,66,73	0
36	DGD	C	519	62/66	0.96	0.05	28,44,71,95	0
23	CLA	B	602	65/65	0.96	0.05	29,37,55,67	0
23	CLA	b	606	65/65	0.96	0.05	27,42,77,106	0
23	CLA	A	408	65/65	0.96	0.06	26,36,101,109	0
23	CLA	c	501	65/65	0.96	0.05	38,49,64,71	0
23	CLA	C	509	65/65	0.96	0.06	30,43,102,115	0
23	CLA	b	608	65/65	0.97	0.04	32,41,60,68	0
25	BCR	a	409	40/40	0.97	0.04	24,35,45,49	0
23	CLA	b	609	65/65	0.97	0.05	36,44,63,82	0
23	CLA	b	611	65/65	0.97	0.04	25,34,49,61	0
23	CLA	b	612	65/65	0.97	0.05	25,35,48,59	0
23	CLA	b	614	65/65	0.97	0.05	23,34,76,89	0
23	CLA	b	615	65/65	0.97	0.05	29,40,66,81	0
23	CLA	B	609	65/65	0.97	0.05	29,39,53,63	0
23	CLA	C	506	65/65	0.97	0.05	31,40,71,78	0
23	CLA	c	502	65/65	0.97	0.05	37,48,68,73	0
23	CLA	c	503	65/65	0.97	0.05	40,51,63,78	0
23	CLA	B	610	65/65	0.97	0.06	27,36,52,69	0
23	CLA	c	505	65/65	0.97	0.05	32,45,68,86	0
23	CLA	C	508	65/65	0.97	0.05	36,47,60,70	0
23	CLA	B	611	65/65	0.97	0.04	23,30,41,45	0
23	CLA	C	510	65/65	0.97	0.06	36,47,67,69	0
31	LHG	A	417	49/49	0.97	0.05	23,37,55,66	0
31	LHG	D	408	49/49	0.97	0.06	22,34,51,68	0

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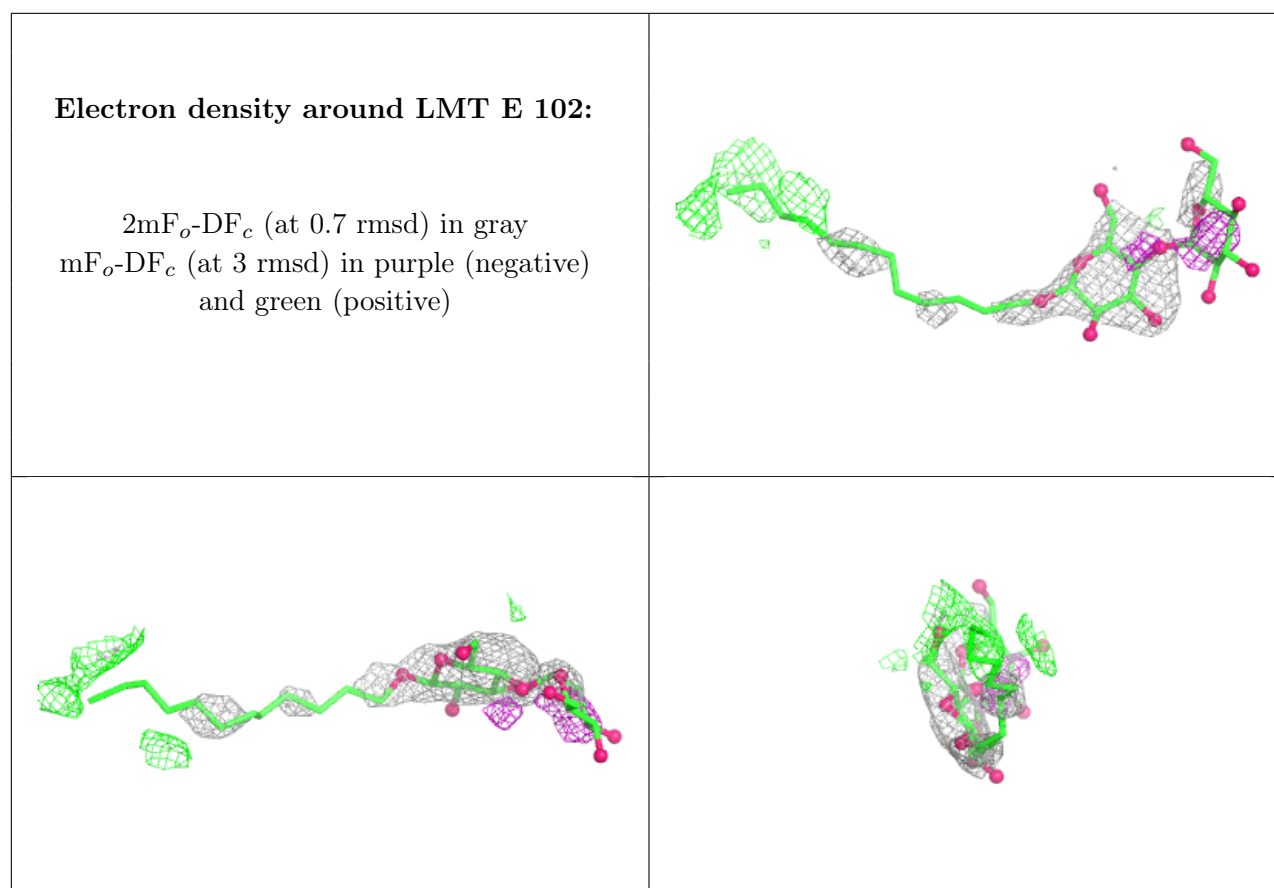
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	509	65/65	0.97	0.06	43,52,66,73	0
23	CLA	c	510	65/65	0.97	0.05	39,47,62,66	0
23	CLA	C	511	65/65	0.97	0.04	33,44,57,61	0
31	LHG	d	408	49/49	0.97	0.05	24,35,53,70	0
23	CLA	C	512	65/65	0.97	0.06	36,52,73,84	0
23	CLA	B	613	65/65	0.97	0.04	21,29,68,78	0
23	CLA	B	603	65/65	0.97	0.05	26,39,52,57	0
24	PHO	A	407	64/64	0.97	0.05	23,31,46,51	0
23	CLA	D	404	65/65	0.97	0.05	20,26,46,52	0
23	CLA	B	615	65/65	0.97	0.04	27,34,61,68	0
25	BCR	B	617	40/40	0.97	0.04	22,31,46,49	0
23	CLA	A	406	65/65	0.97	0.05	22,29,80,89	0
23	CLA	C	502	65/65	0.97	0.05	34,41,60,77	0
23	CLA	C	503	65/65	0.97	0.06	31,42,55,73	0
36	DGD	H	102	62/66	0.97	0.05	26,40,58,66	0
23	CLA	b	602	65/65	0.97	0.05	32,44,60,68	0
23	CLA	b	603	65/65	0.97	0.05	30,40,53,74	0
23	CLA	b	604	65/65	0.97	0.05	23,31,85,96	0
36	DGD	h	102	62/66	0.97	0.05	31,46,62,73	0
23	CLA	C	504	65/65	0.97	0.05	36,44,65,75	0
23	CLA	b	607	65/65	0.97	0.05	20,31,53,63	0
23	CLA	B	604	65/65	0.98	0.05	21,29,92,104	0
23	CLA	B	612	65/65	0.98	0.05	24,29,42,51	0
23	CLA	B	605	65/65	0.98	0.04	22,30,44,48	0
23	CLA	b	605	65/65	0.98	0.05	24,34,52,97	0
23	CLA	d	401	65/65	0.98	0.04	23,26,48,75	0
23	CLA	d	403	65/65	0.98	0.05	25,29,49,62	0
23	CLA	A	405	65/65	0.98	0.04	19,23,41,47	0
23	CLA	B	607	65/65	0.98	0.04	18,27,54,66	0
24	PHO	D	401	64/64	0.98	0.04	21,27,35,45	0
24	PHO	a	406	64/64	0.98	0.04	22,31,40,51	0
23	CLA	a	404	65/65	0.98	0.05	25,30,50,60	0
23	CLA	B	608	65/65	0.98	0.03	27,37,51,55	0
23	CLA	b	610	65/65	0.98	0.04	30,42,51,60	0
22	CL	a	403	1/1	0.98	0.04	34,34,34,34	0
23	CLA	A	404	65/65	0.98	0.04	20,23,41,58	0
37	CA	O	301	1/1	0.98	0.05	87,87,87,87	0
23	CLA	b	613	65/65	0.98	0.04	22,33,67,78	0
32	BCT	a	418	4/4	0.98	0.04	45,52,54,59	0
37	CA	o	301	1/1	0.98	0.02	85,85,85,85	0
38	HEM	E	103	43/43	0.98	0.06	40,54,66,73	0
38	HEM	e	103	43/43	0.98	0.07	48,73,98,105	0

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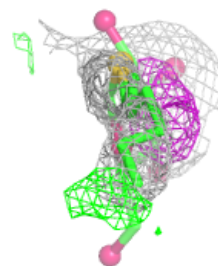
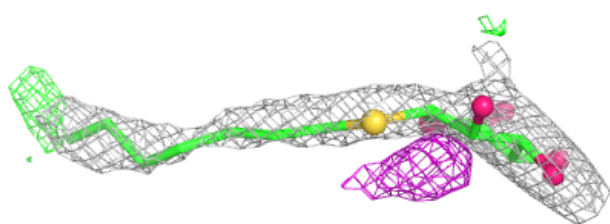
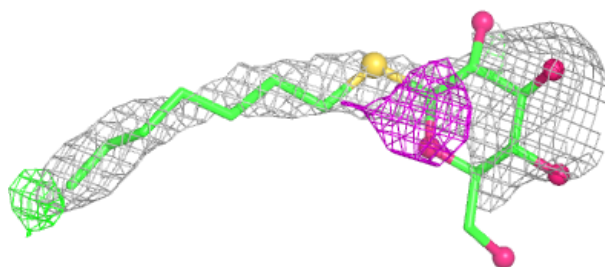
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
39	MG	j	103	1/1	0.98	0.07	51,51,51,51	0
40	HEC	v	201	43/43	0.98	0.05	40,50,59,66	0
22	CL	A	402	1/1	0.99	0.06	24,24,24,24	0
22	CL	A	403	1/1	0.99	0.01	27,27,27,27	0
37	CA	c	524	1/1	0.99	0.05	66,66,66,66	0
32	BCT	A	418	4/4	0.99	0.04	34,39,47,65	0
22	CL	a	402	1/1	0.99	0.04	31,31,31,31	0
21	FE2	A	401	1/1	0.99	0.03	42,42,42,42	0
39	MG	J	103	1/1	0.99	0.08	39,39,39,39	0
37	CA	C	524	1/1	0.99	0.08	62,62,62,62	0
40	HEC	V	202	43/43	0.99	0.04	30,33,44,53	0
21	FE2	a	401	1/1	0.99	0.05	45,45,45,45	0
28	OEX	a	413	10/10	1.00	0.02	27,34,45,53	0
28	OEX	A	413	10/10	1.00	0.02	22,30,43,45	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.

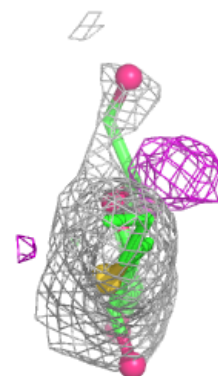
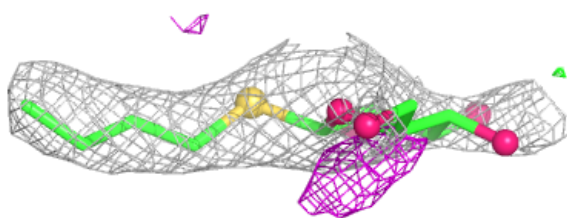
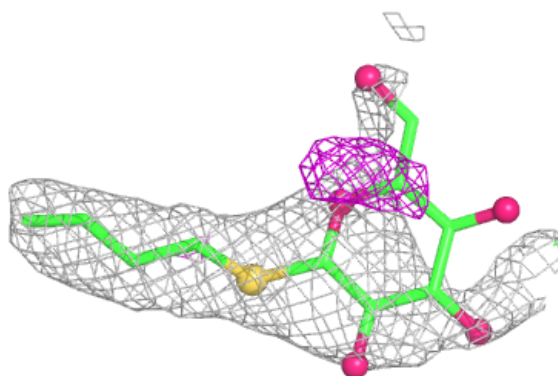


Electron density around HTG B 624:

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

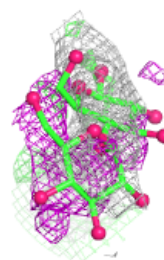
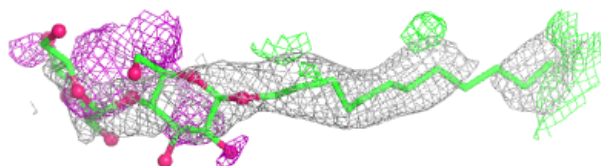
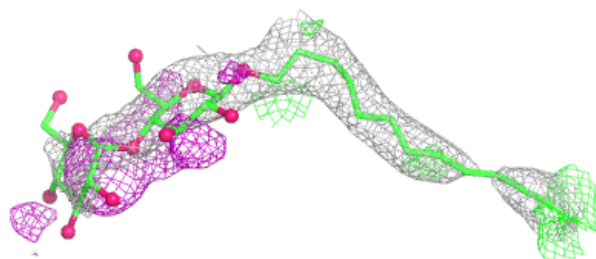
**Electron density around HTG D 412:**

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

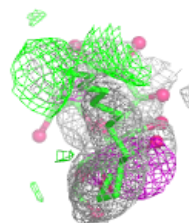
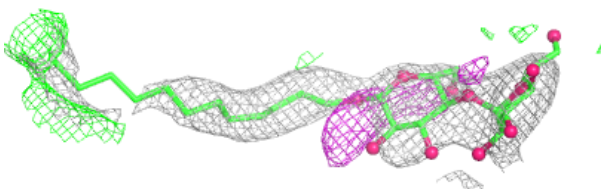
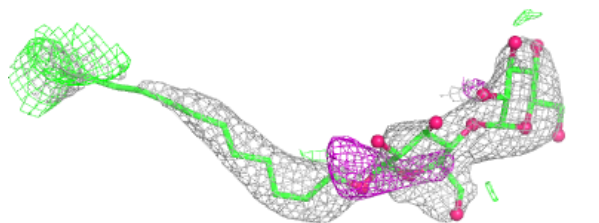


Electron density around LMT B 630:

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

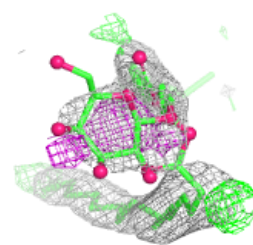
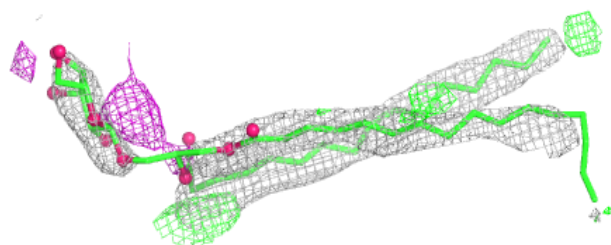
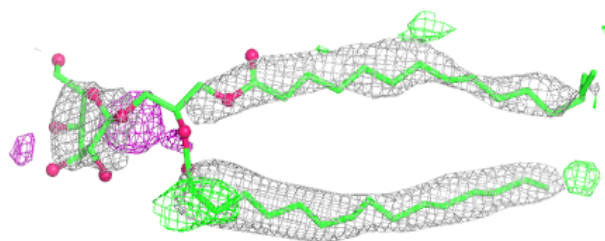
**Electron density around LMT D 402:**

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

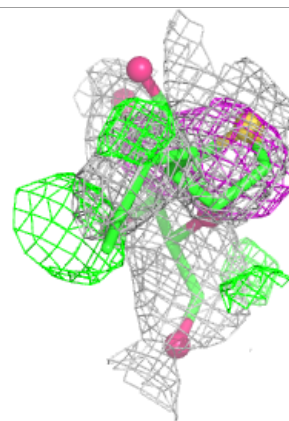
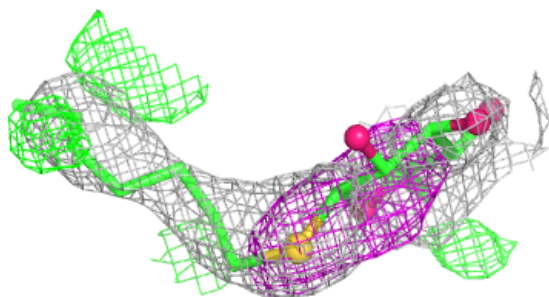
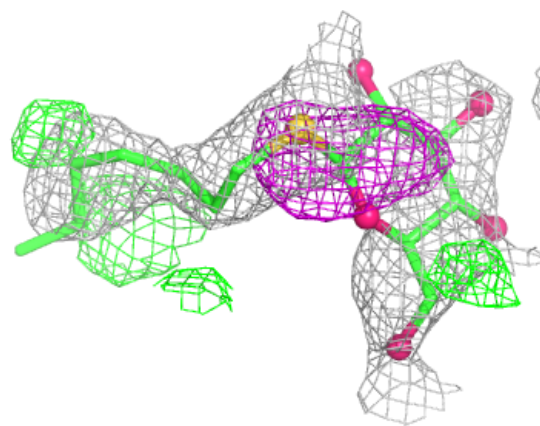


Electron density around LMG Z 101:

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

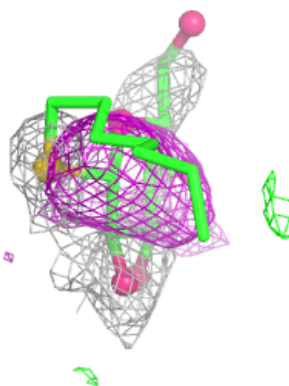
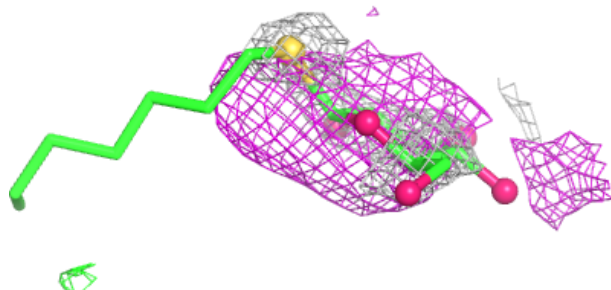
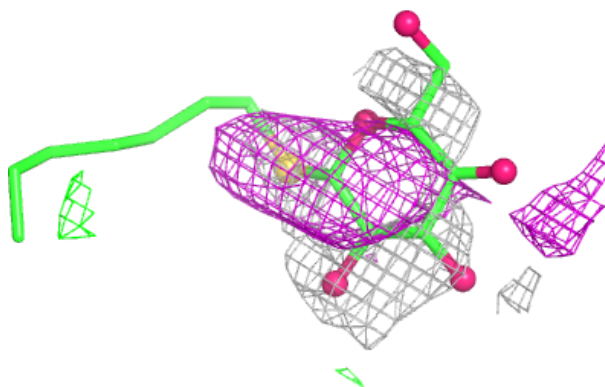
**Electron density around HTG B 623:**

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

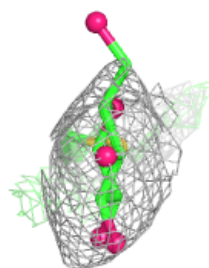
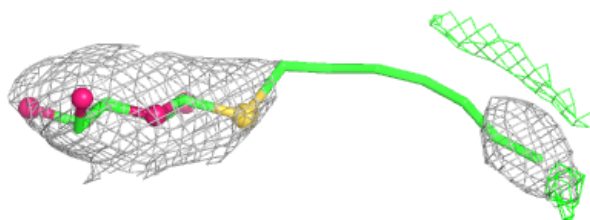
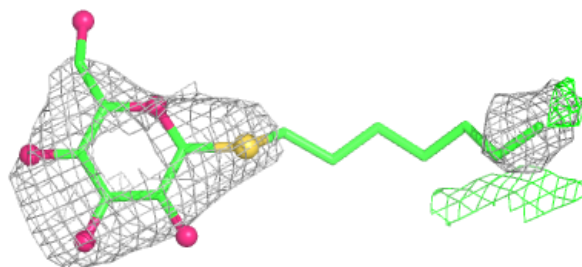


Electron density around HTG b 622:

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

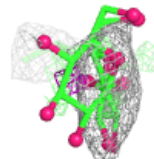
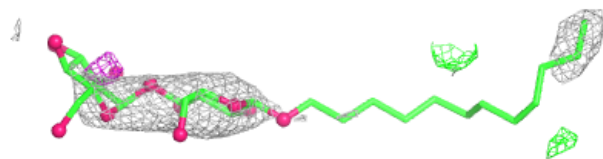
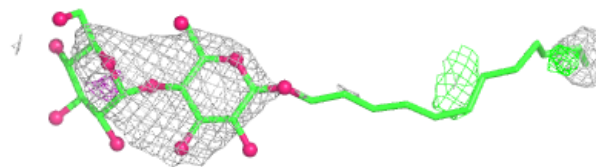
**Electron density around HTG c 521:**

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

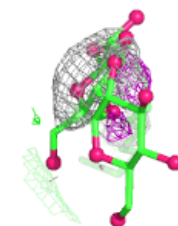
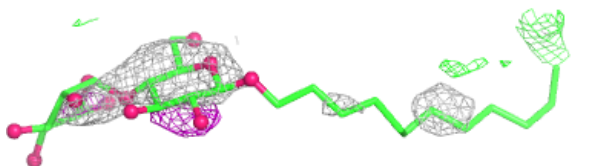
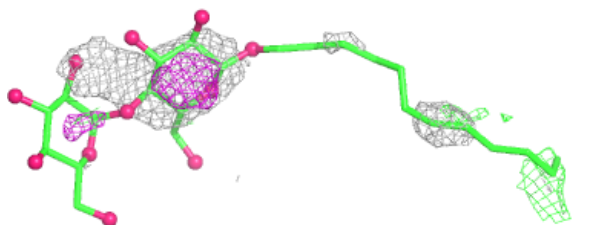


Electron density around LMT a 417:

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

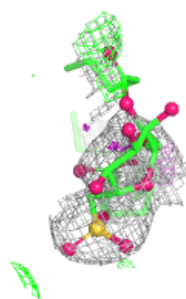
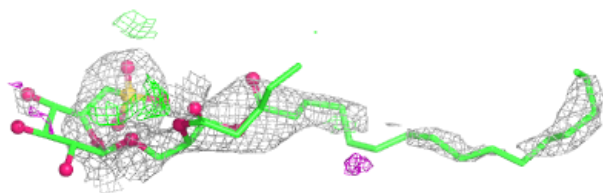
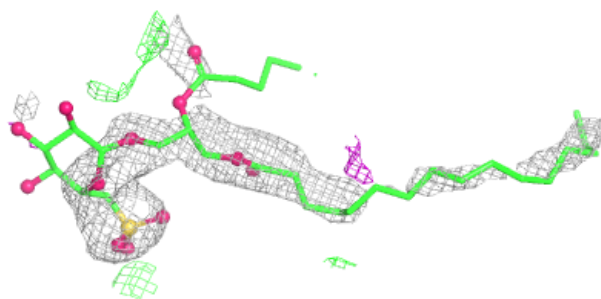
**Electron density around LMT e 102:**

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

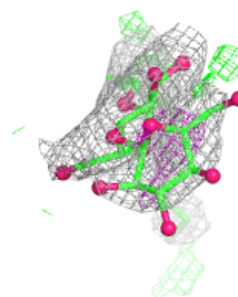
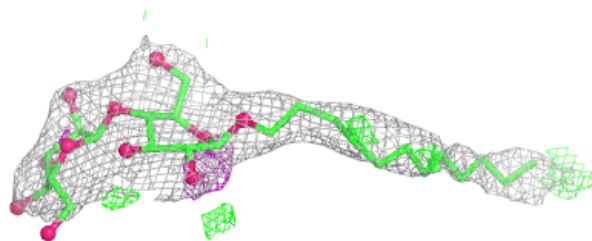
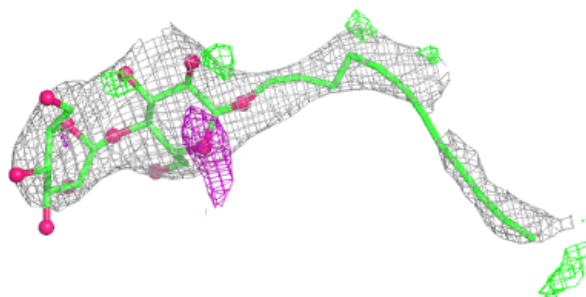


Electron density around SQD f 101:

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

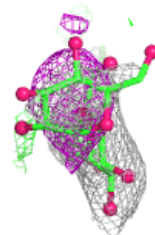
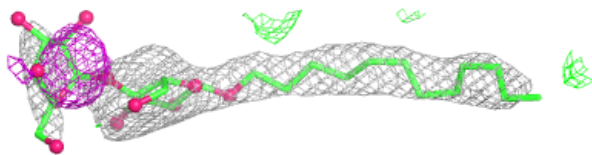
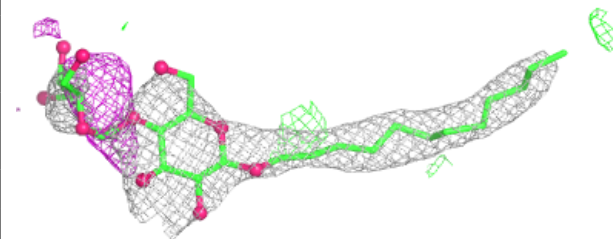
**Electron density around LMT I 101:**

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

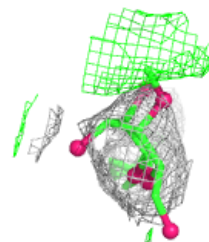
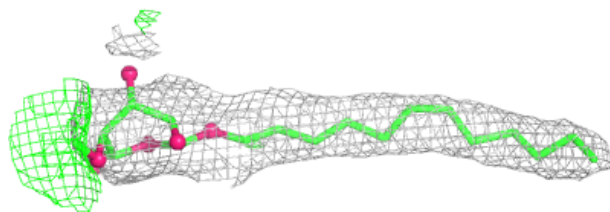
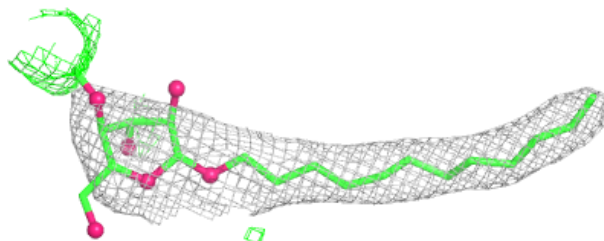


Electron density around LMT D 403:

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

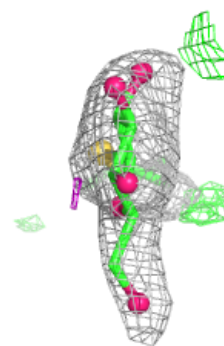
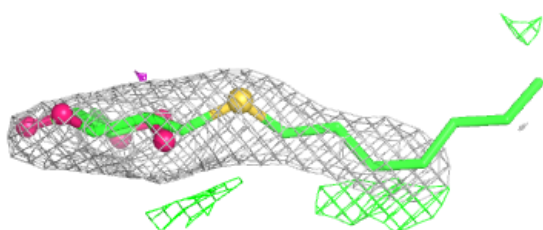
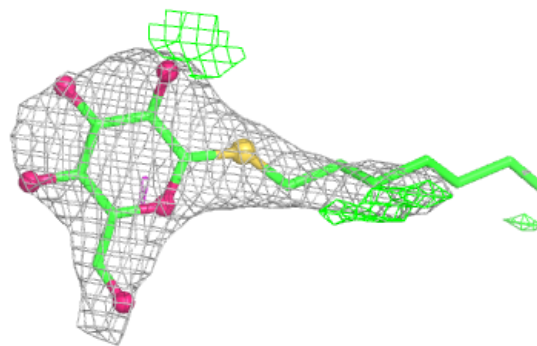
**Electron density around LMT b 621:**

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

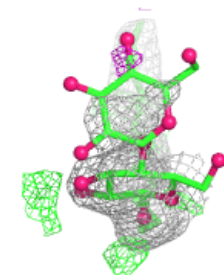
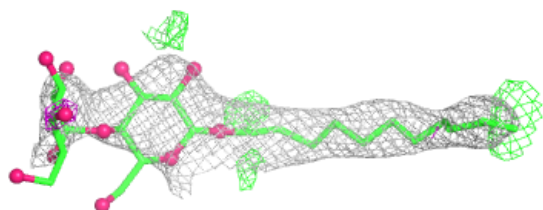
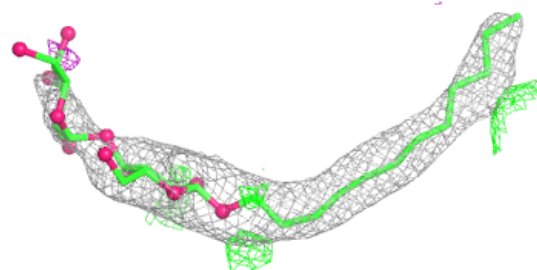


Electron density around HTG C 521:

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

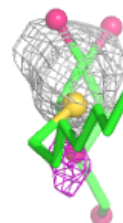
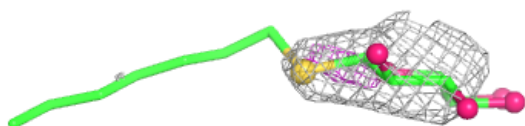
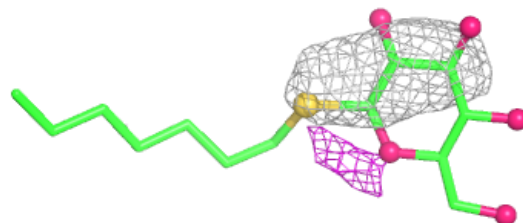
**Electron density around LMT M 103:**

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



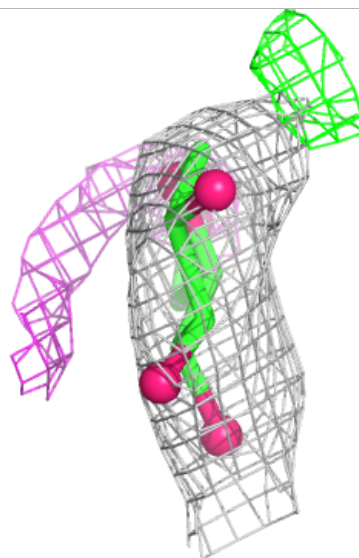
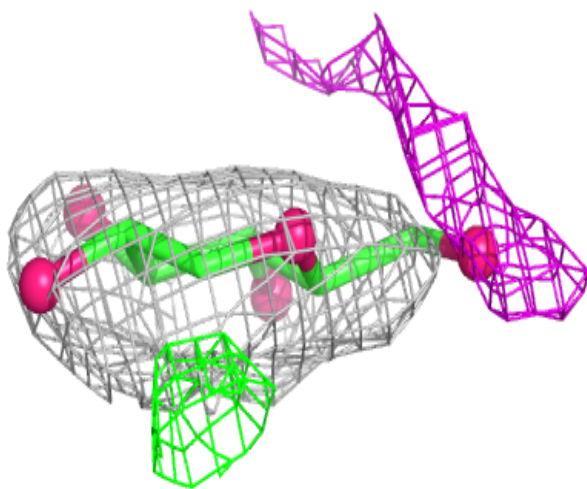
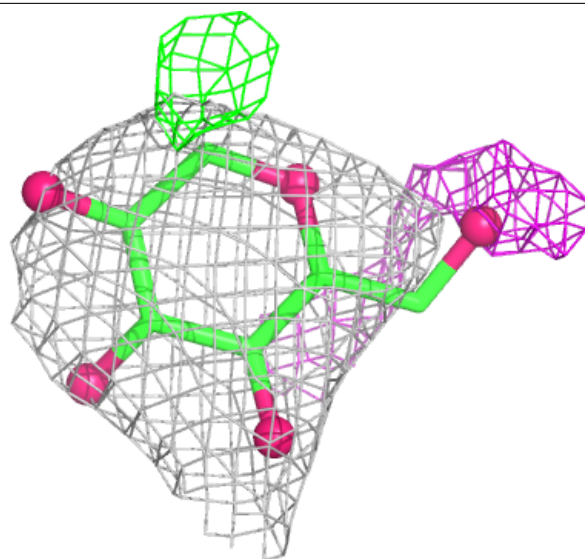
Electron density around HTG c 522:

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



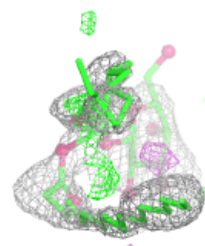
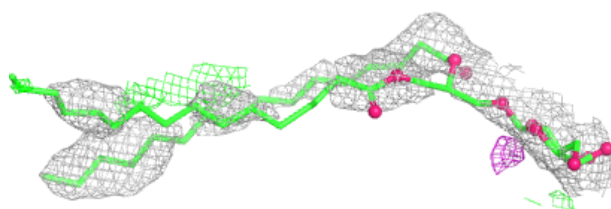
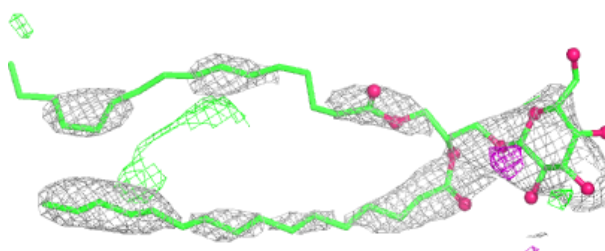
Electron density around HTG V 203:

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

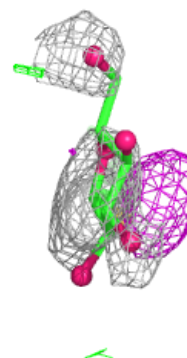
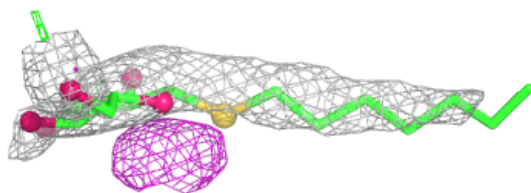
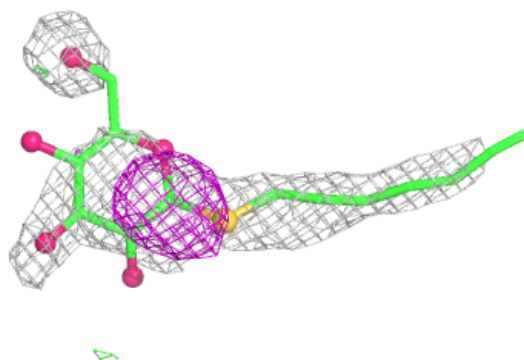


Electron density around LMG c 520:

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

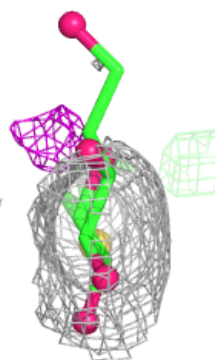
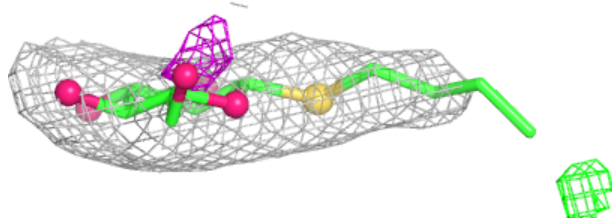
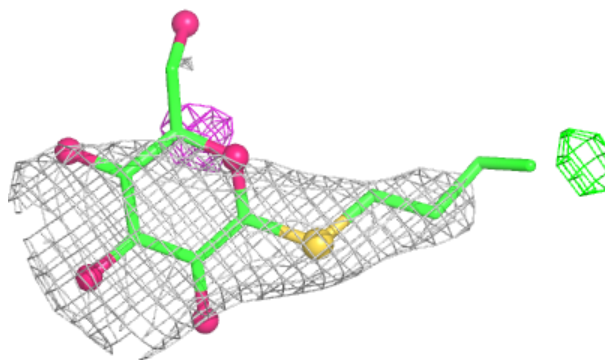
**Electron density around HTG b 623:**

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

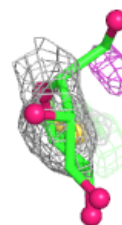
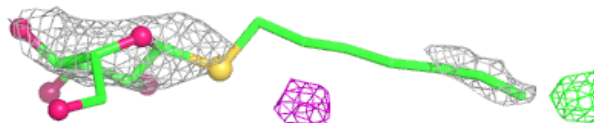
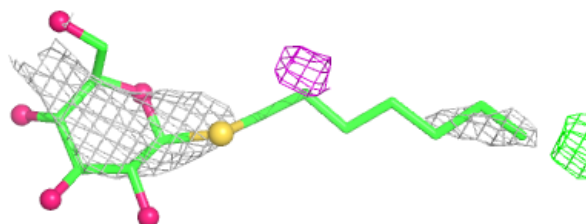


Electron density around HTG d 411:

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

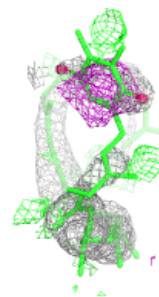
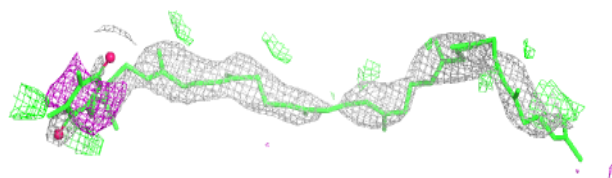
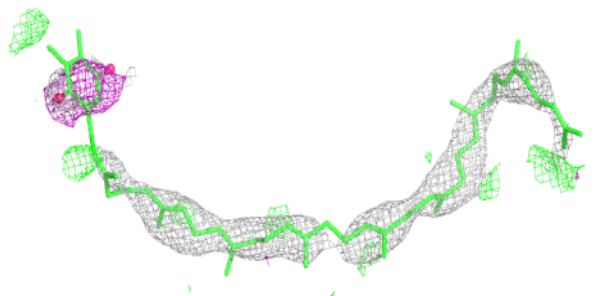
**Electron density around HTG C 522:**

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

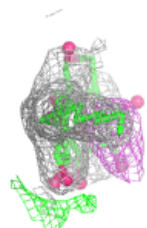
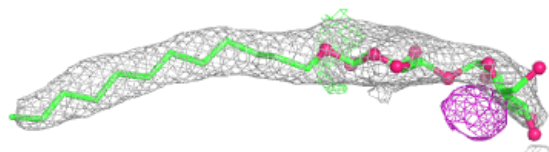
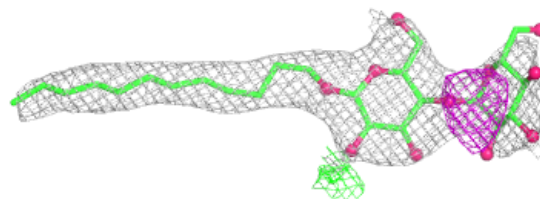


Electron density around PL9 A 414:

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

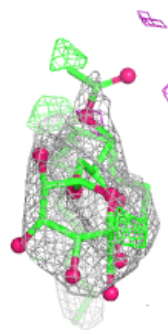
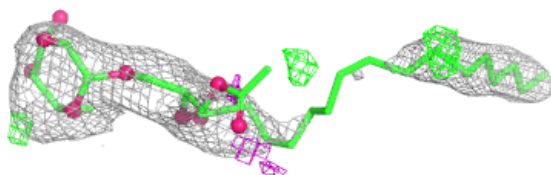
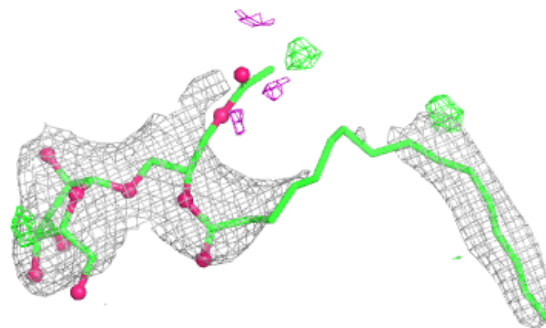
**Electron density around LMT M 101:**

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

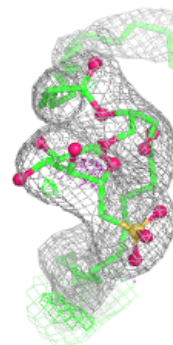
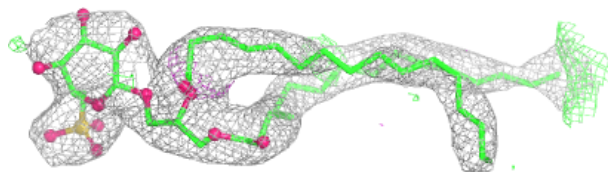
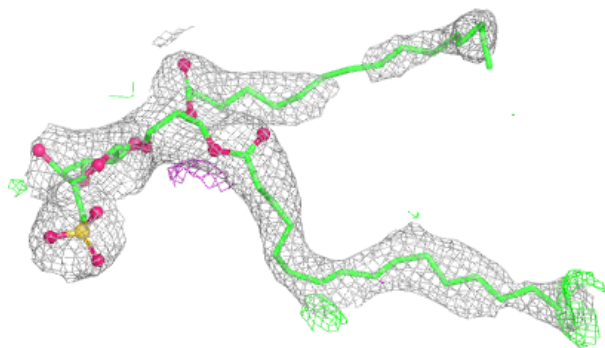


Electron density around LMG Z 102:

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

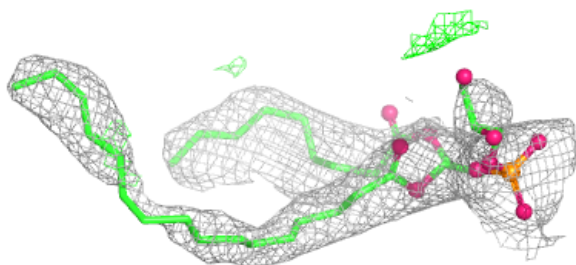
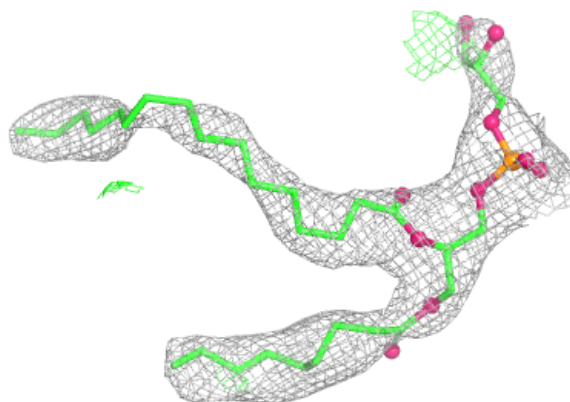
**Electron density around SQD a 412:**

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

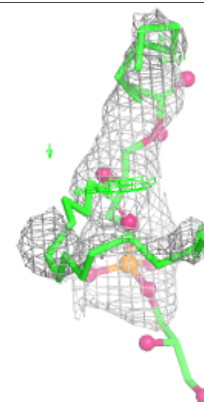
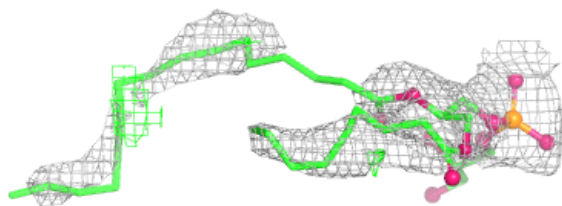
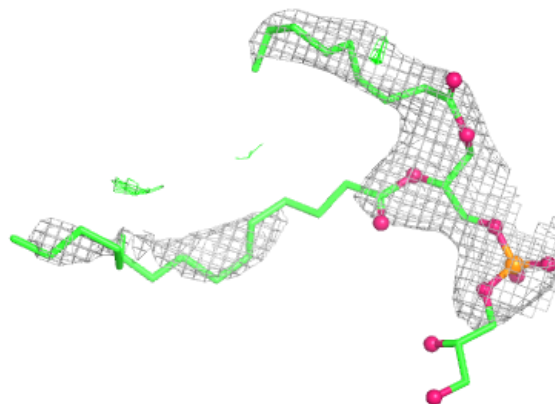


Electron density around LHG E 101:

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

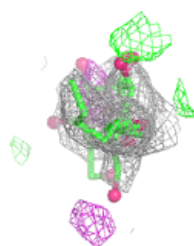
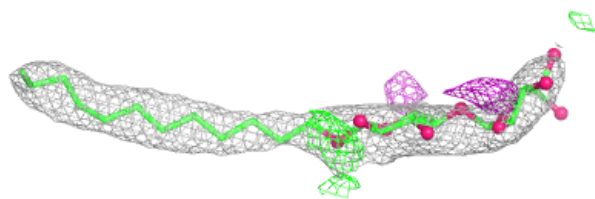
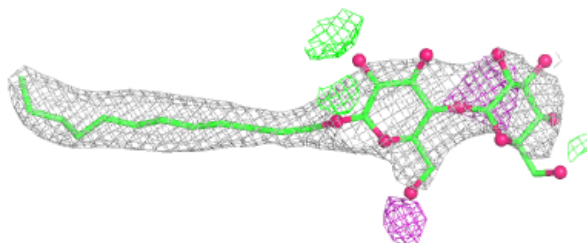
**Electron density around LHG e 101:**

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

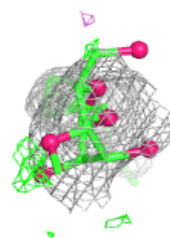
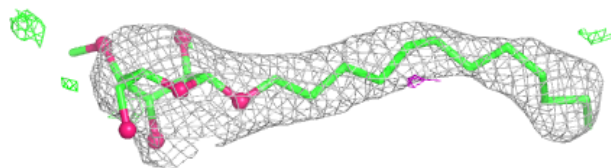
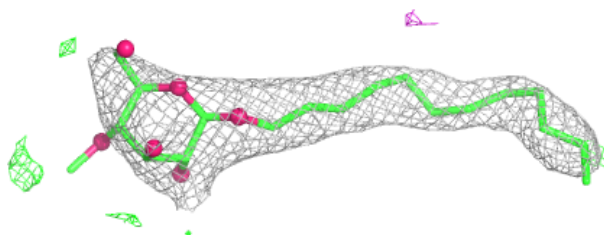


Electron density around LMT m 102:

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

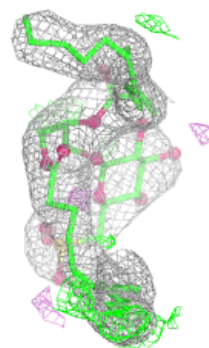
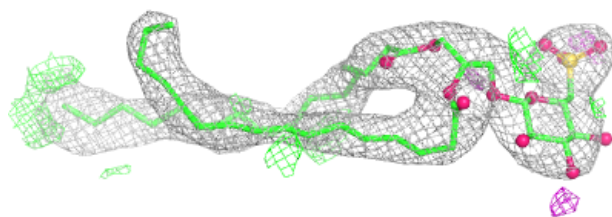
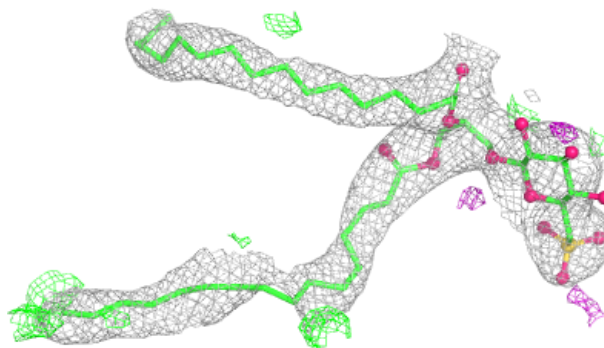
**Electron density around LMT B 629:**

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

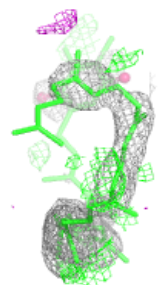
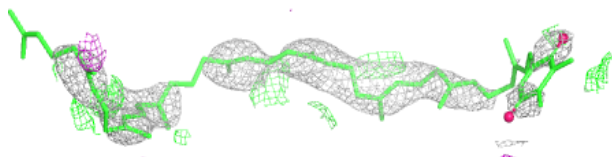
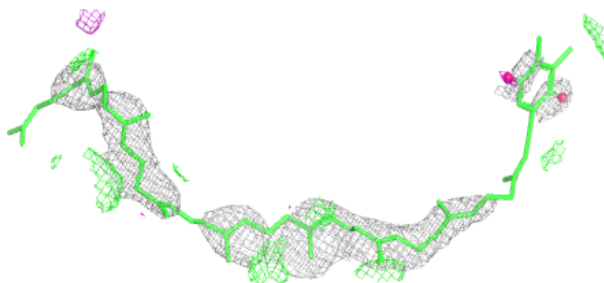


Electron density around SQD A 412:

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

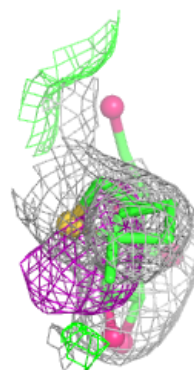
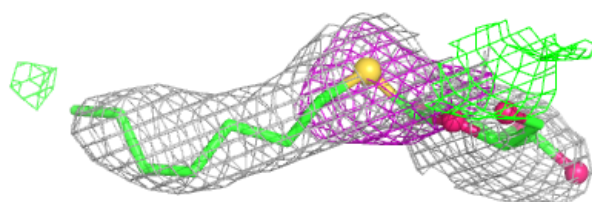
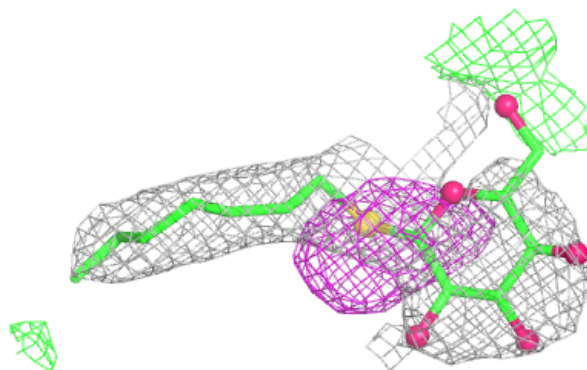
**Electron density around PL9 a 414:**

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

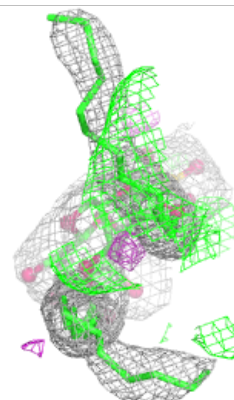
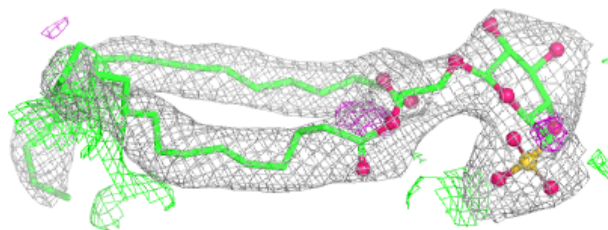
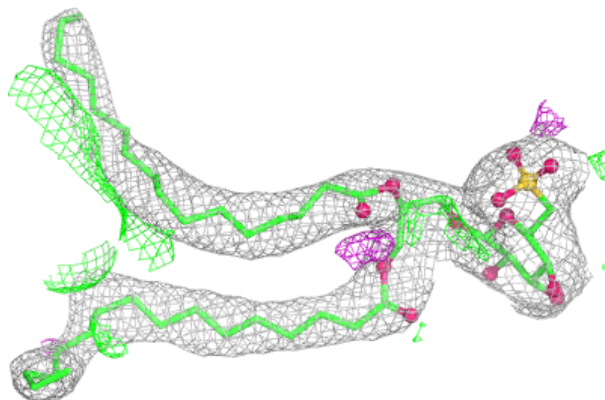


Electron density around HTG b 628:

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

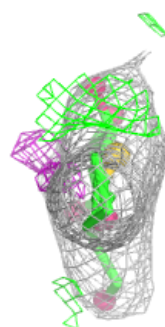
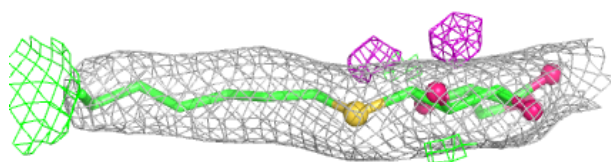
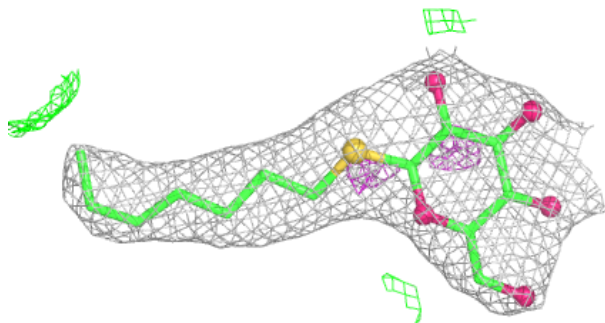
**Electron density around SQD B 620:**

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

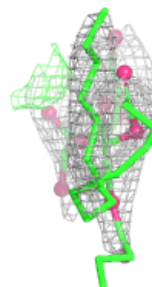
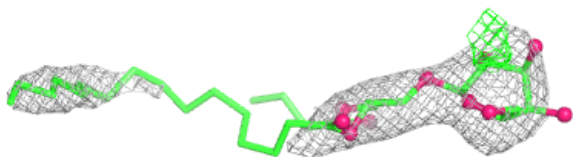
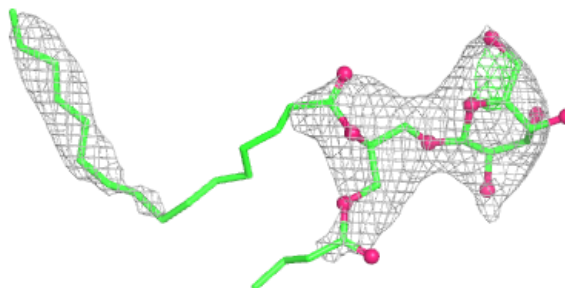


Electron density around HTG B 627:

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

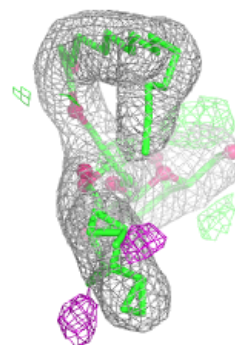
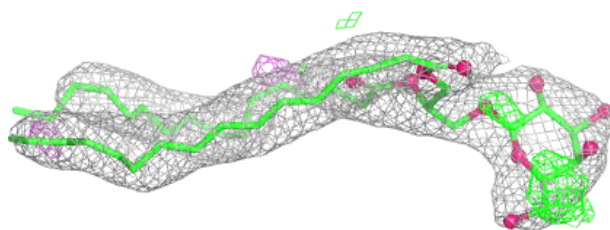
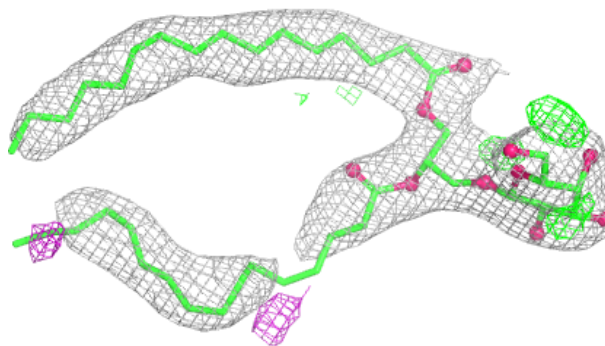
**Electron density around LMG z 101:**

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

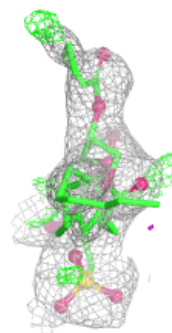
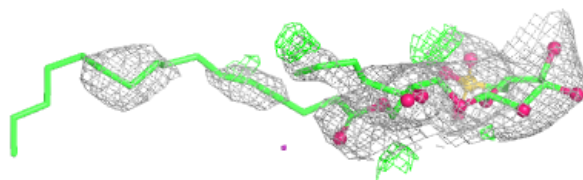
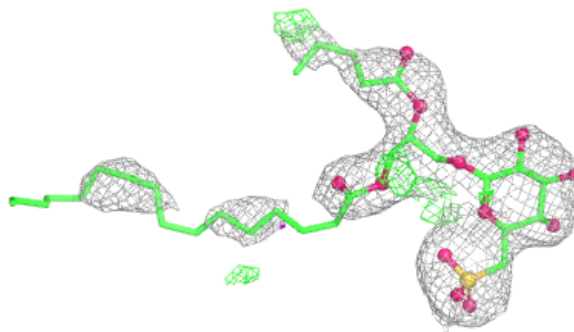


Electron density around LMG C 501:

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

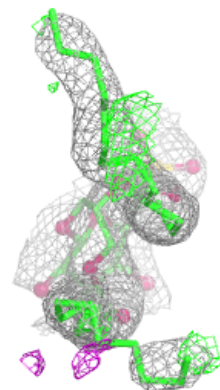
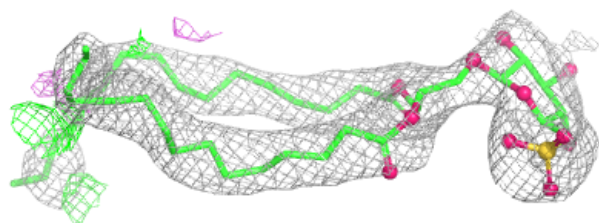
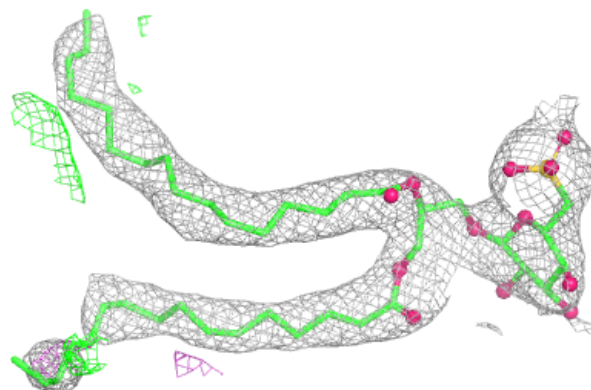
**Electron density around SQD D 413:**

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

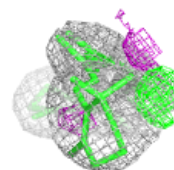
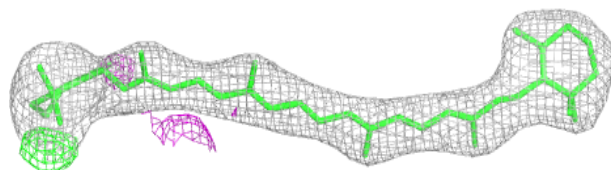
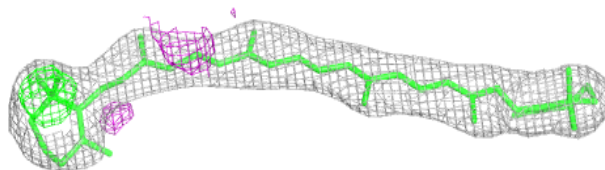


Electron density around SQD L 101:

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

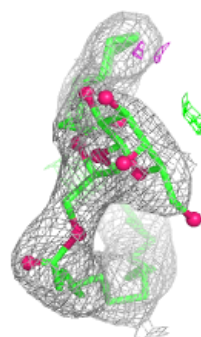
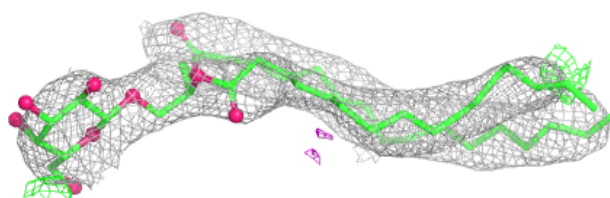
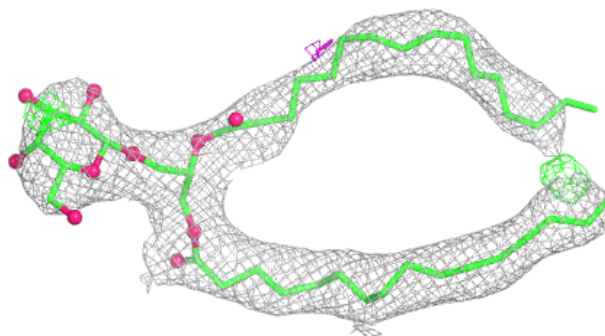
**Electron density around BCR D 406:**

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

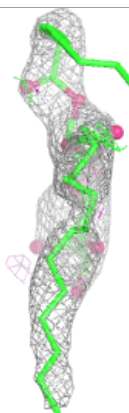
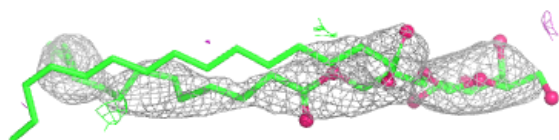
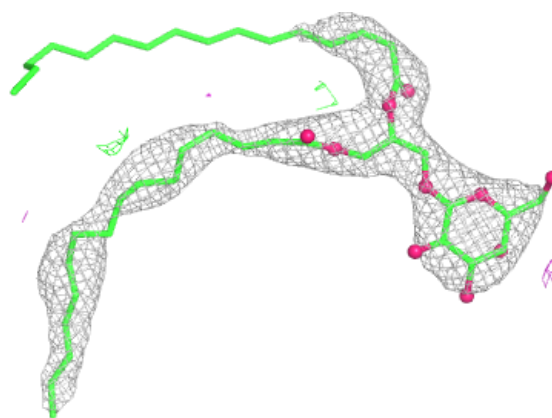


Electron density around LMG a 416:

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

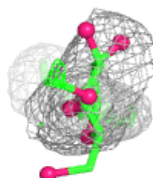
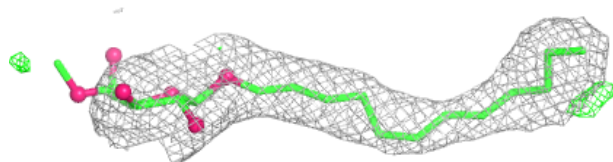
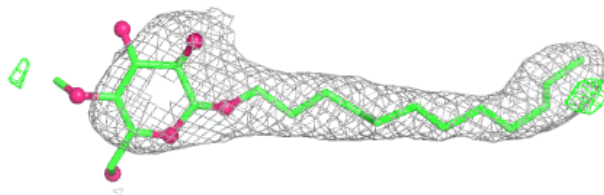
**Electron density around LMG c 519:**

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

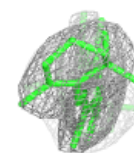
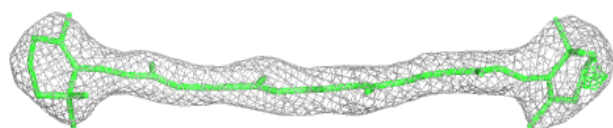
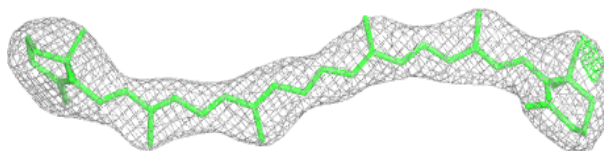


Electron density around LMT b 627:

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

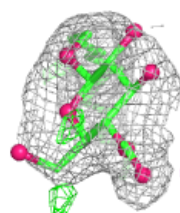
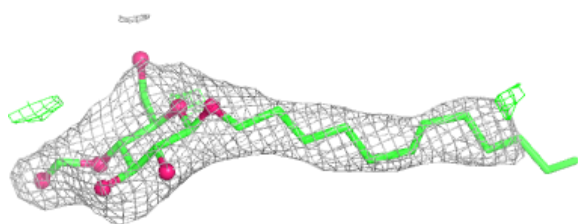
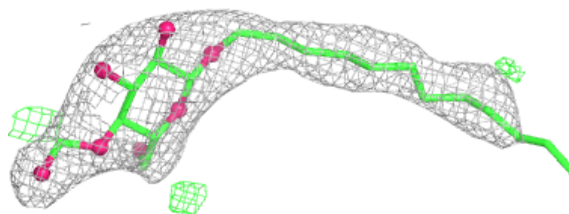
**Electron density around BCR y 101:**

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

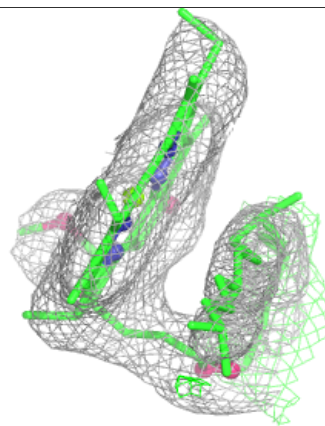
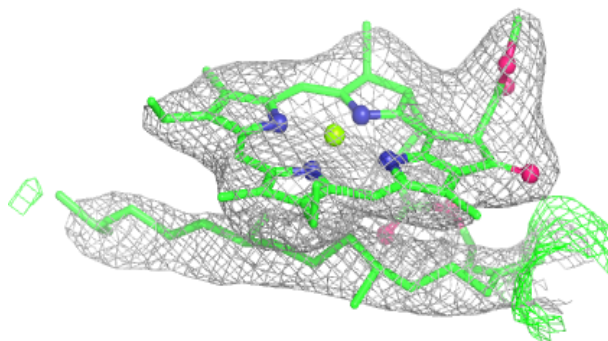
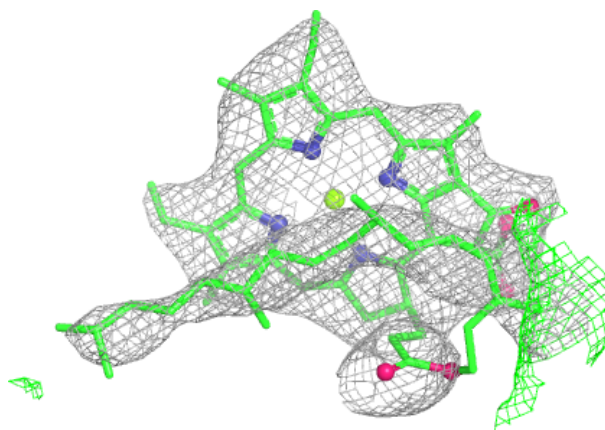


Electron density around LMT B 631:

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

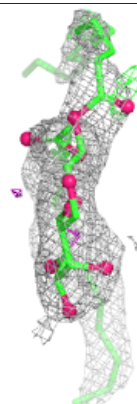
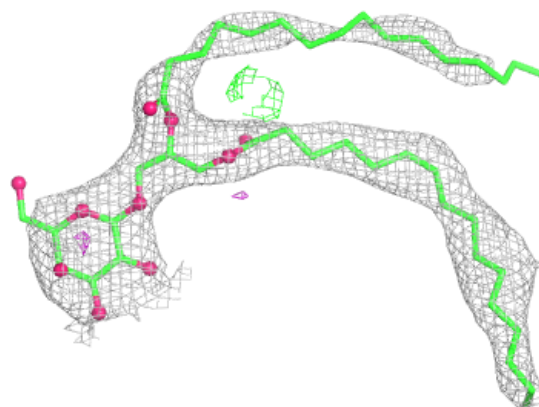
**Electron density around CLA b 601:**

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

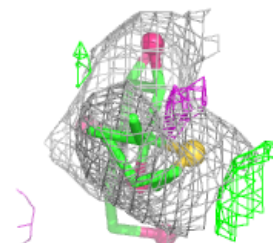
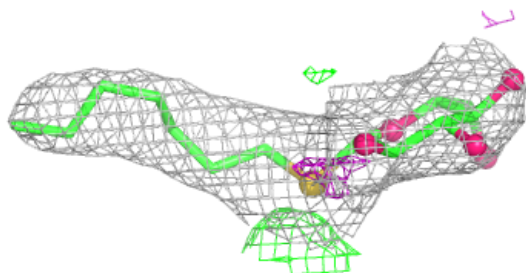
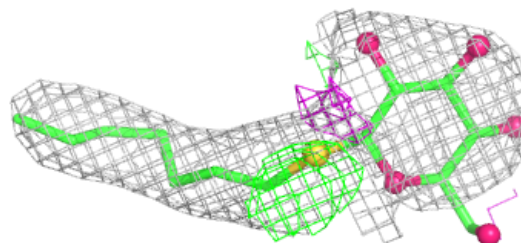


Electron density around LMG C 520:

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

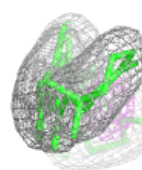
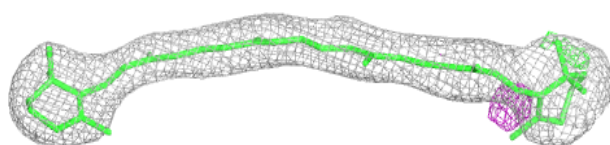
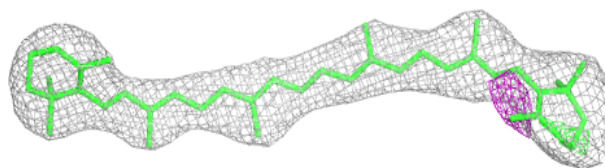
**Electron density around HTG B 622:**

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

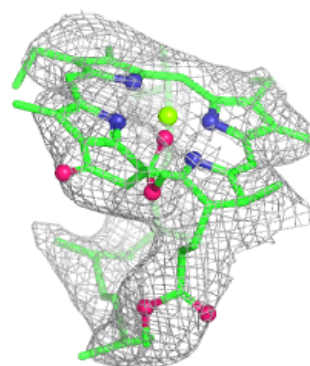
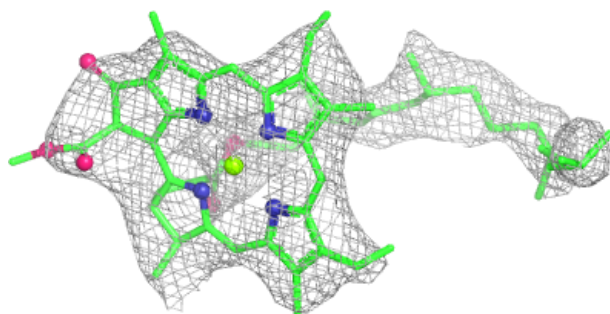
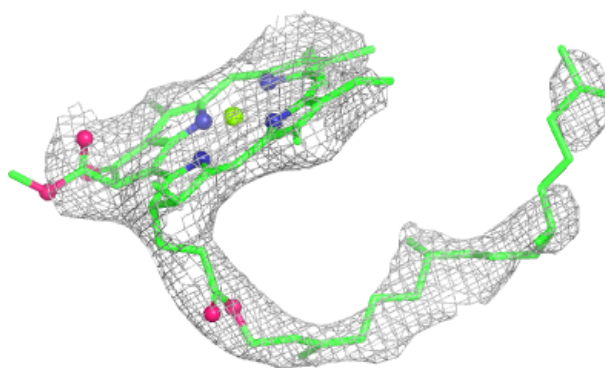


Electron density around BCR d 405:

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

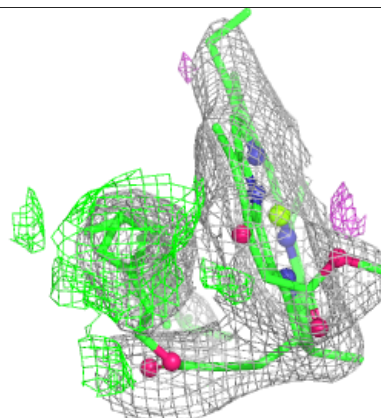
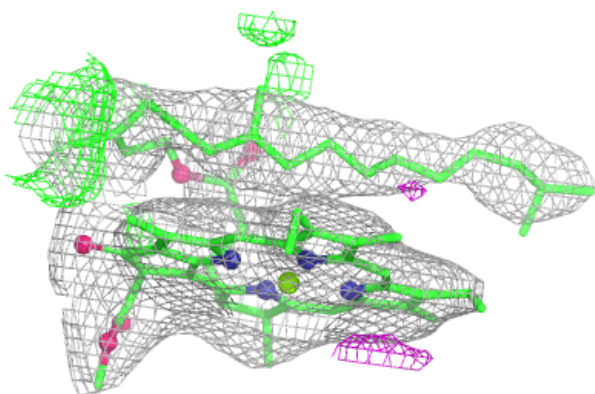
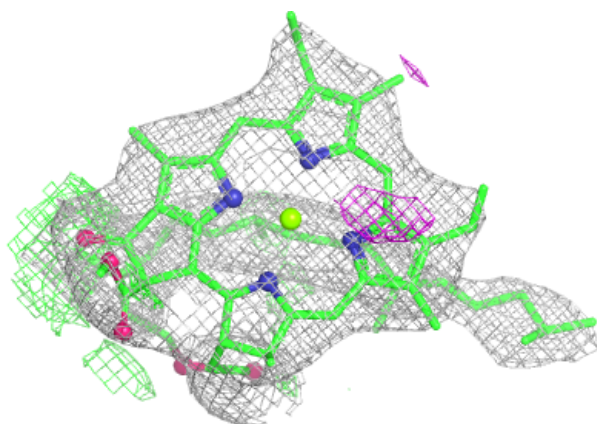
**Electron density around CLA c 513:**

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

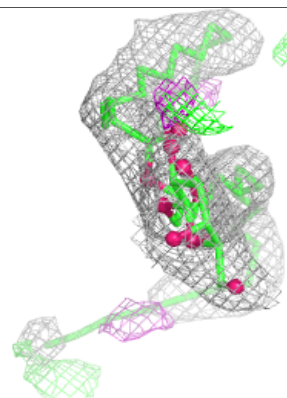
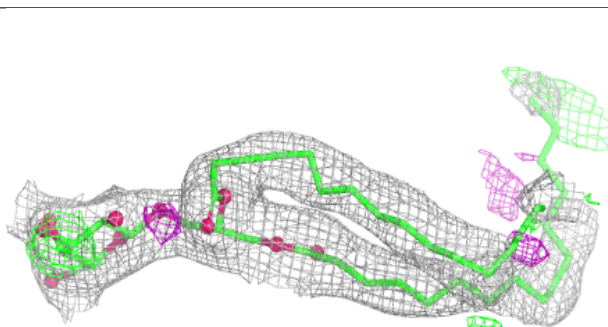
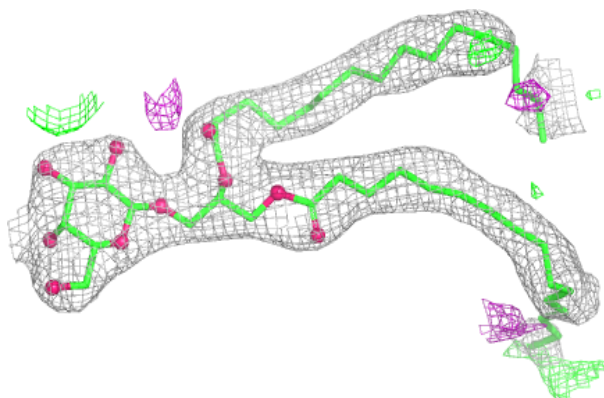


Electron density around CLA B 601:

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

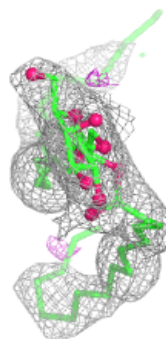
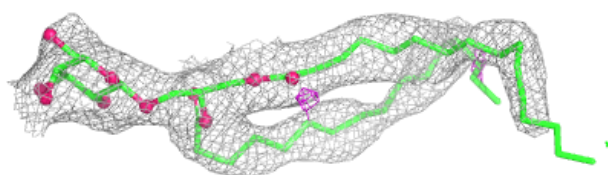
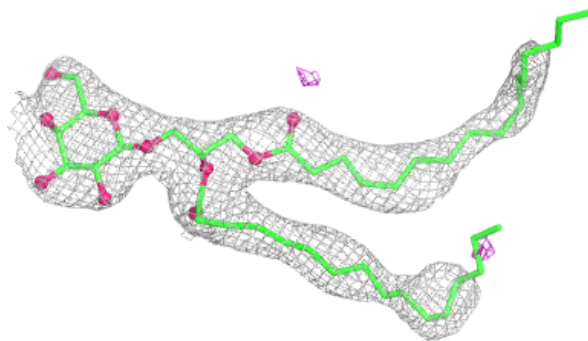
**Electron density around LMG J 101:**

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

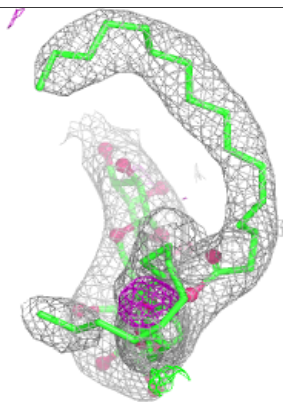
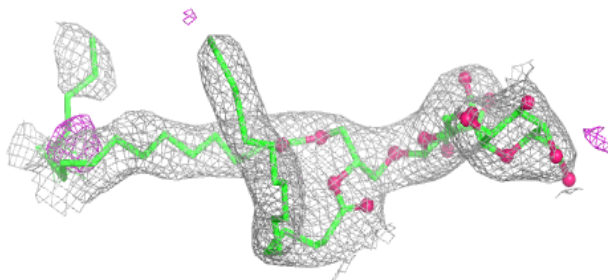
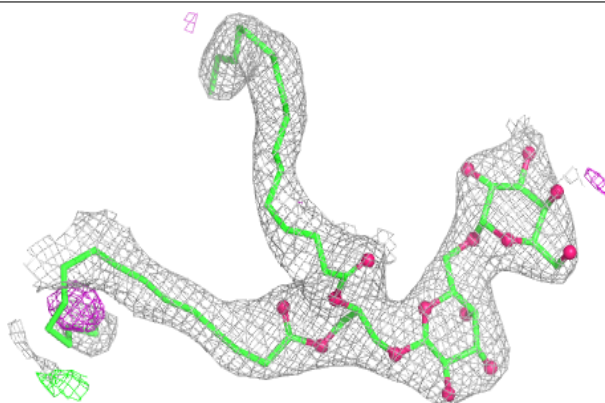


Electron density around LMG j 101:

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

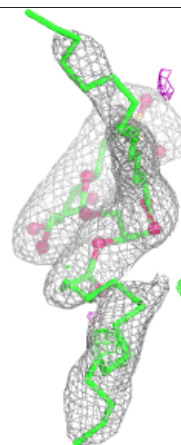
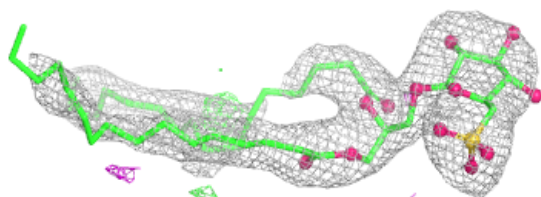
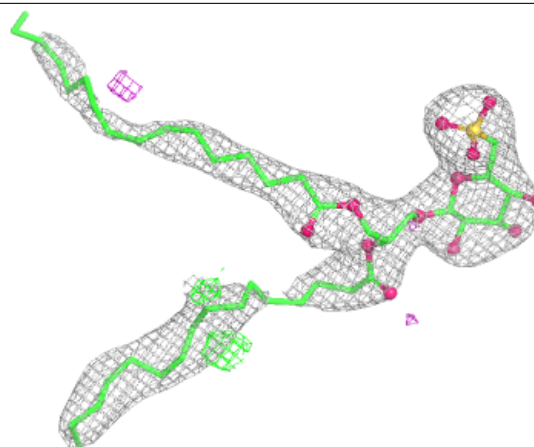
**Electron density around DGD c 517:**

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

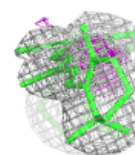
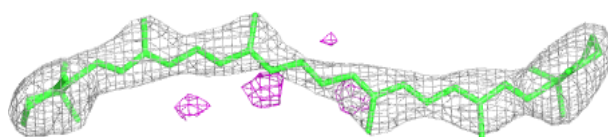
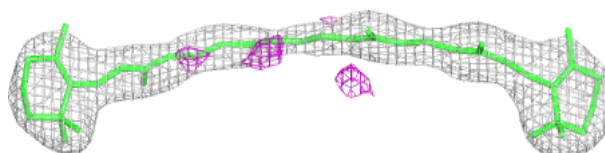


Electron density around SQD a 410:

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

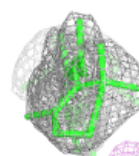
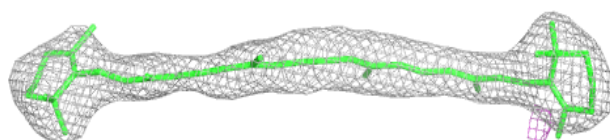
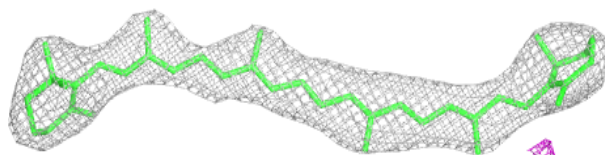
**Electron density around BCR K 102:**

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

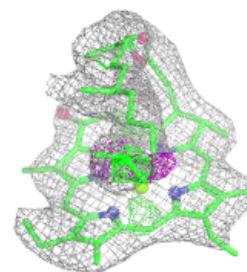
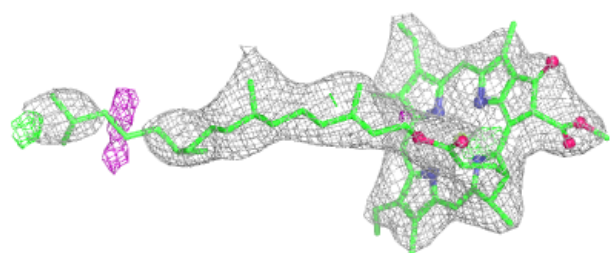
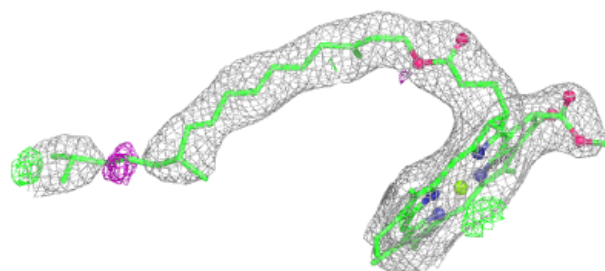


Electron density around BCR Y 101:

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

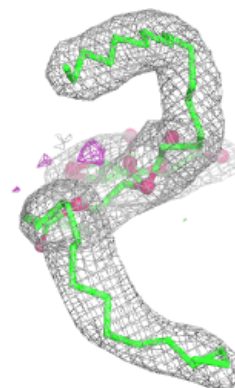
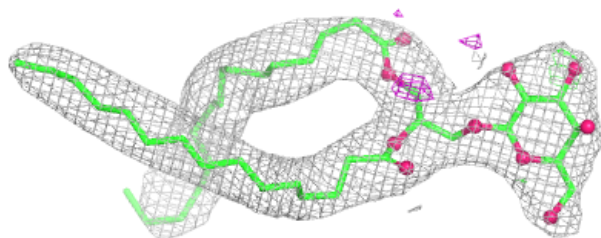
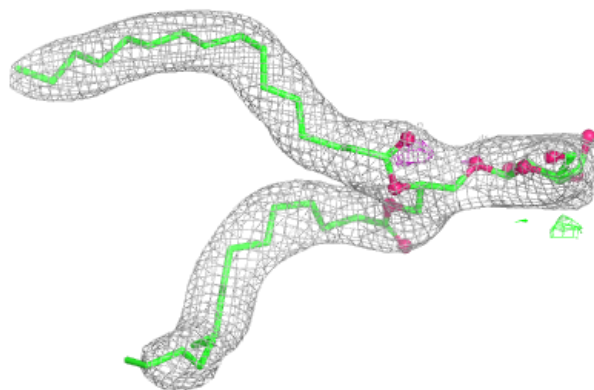
**Electron density around CLA c 504:**

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

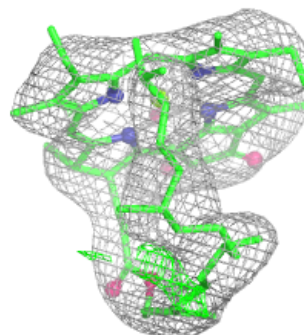
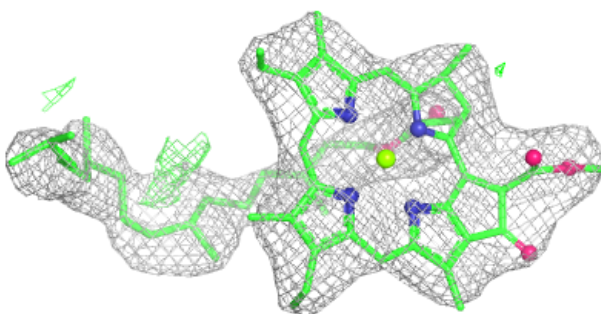
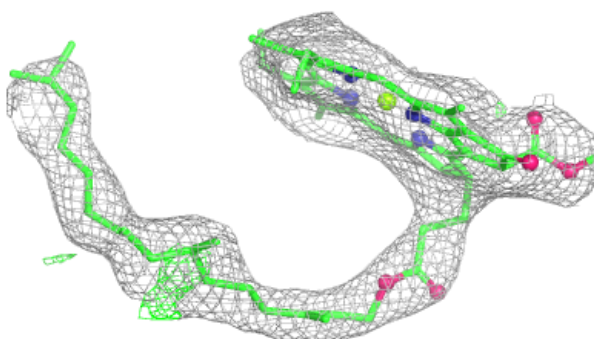


Electron density around LMG b 620:

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

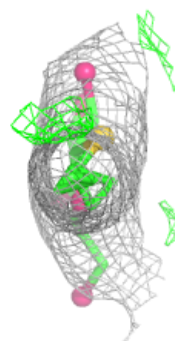
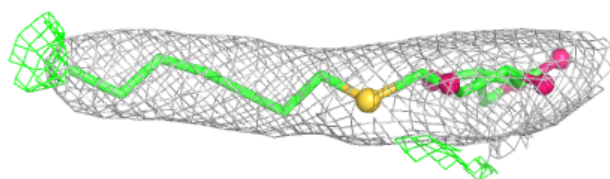
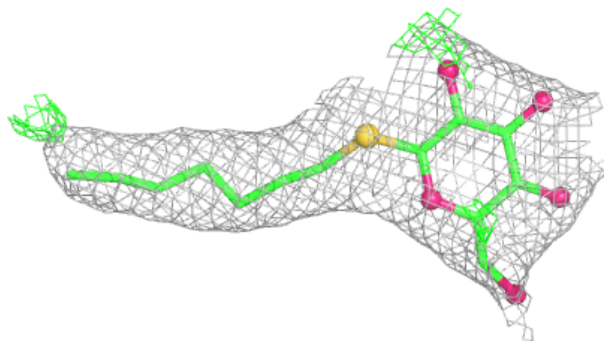
**Electron density around CLA C 514:**

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

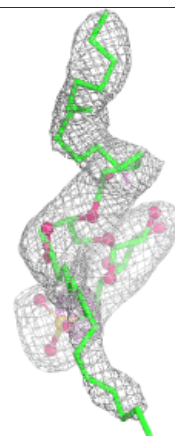
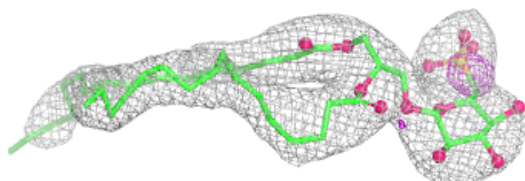
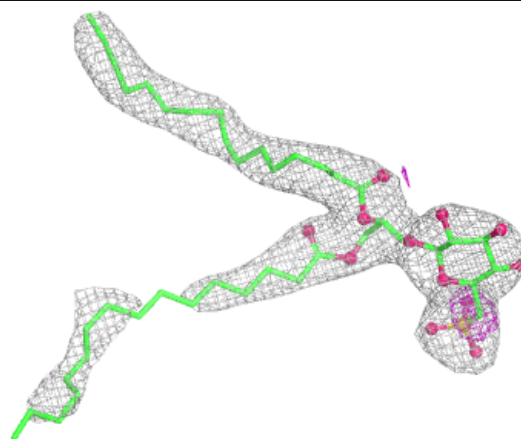


Electron density around HTG b 625:

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

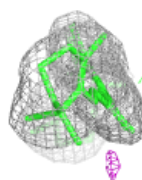
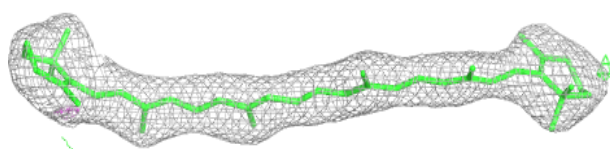
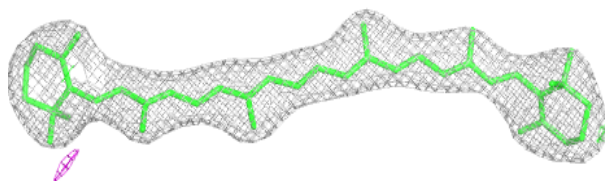
**Electron density around SQD A 410:**

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

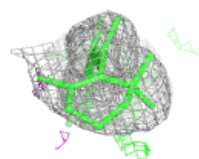
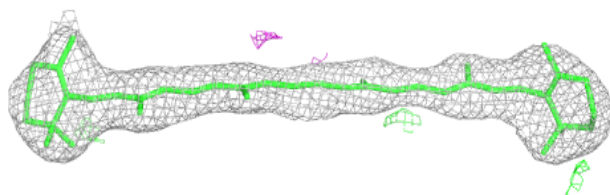
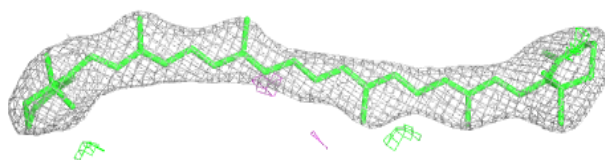


Electron density around BCR B 619:

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

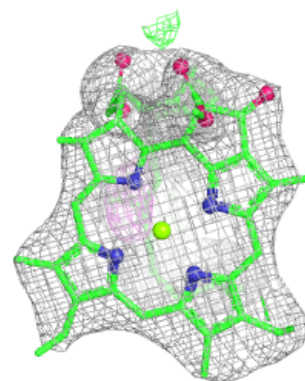
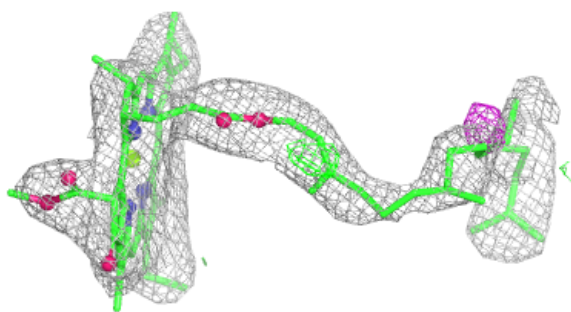
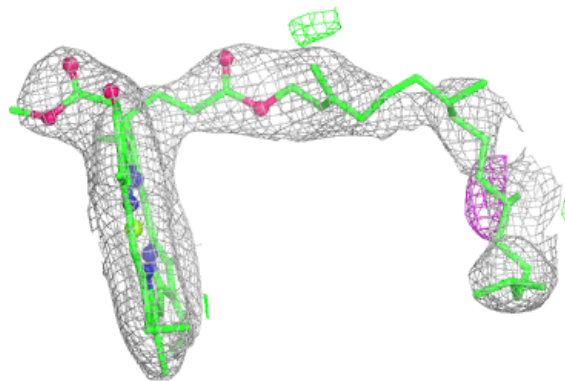
**Electron density around BCR C 515:**

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

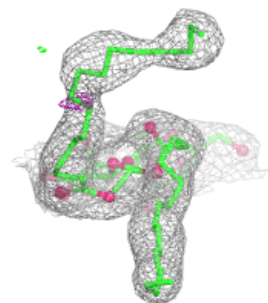
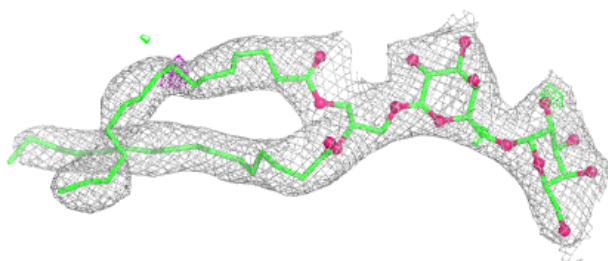
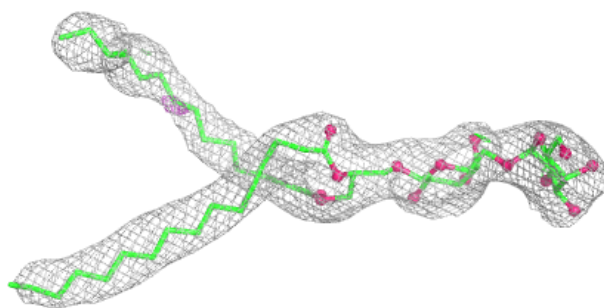


Electron density around CLA C 507:

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

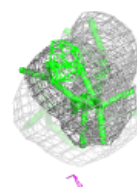
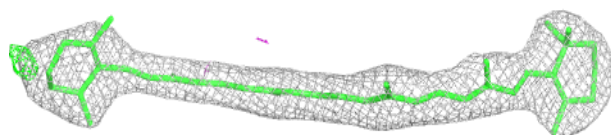
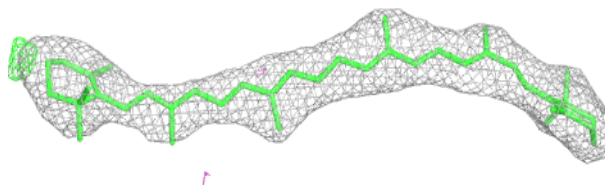
**Electron density around DGD c 516:**

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

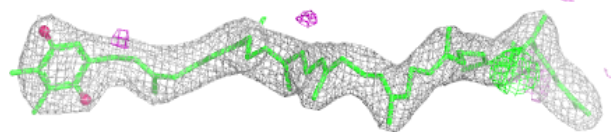
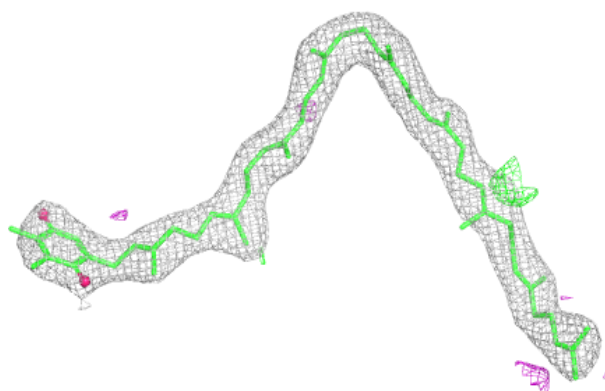


Electron density around BCR H 101:

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

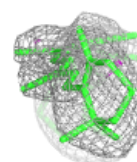
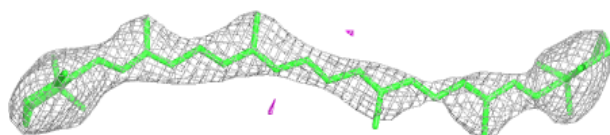
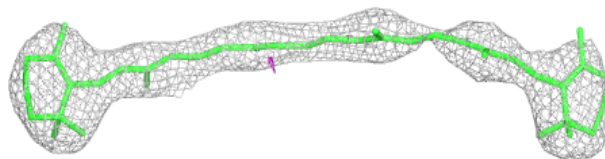
**Electron density around PL9 d 406:**

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

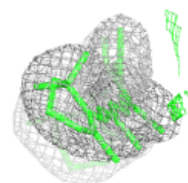
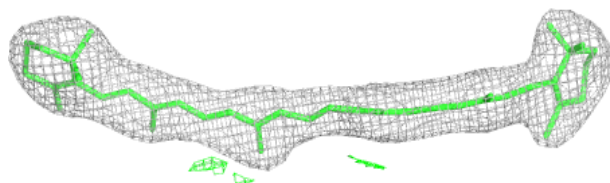
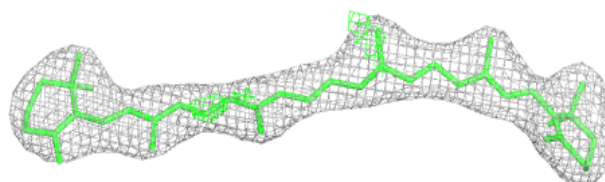


Electron density around BCR k 101:

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

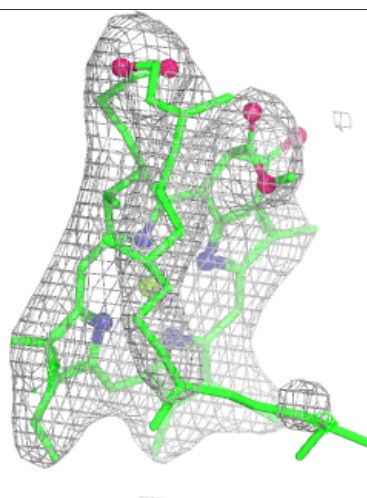
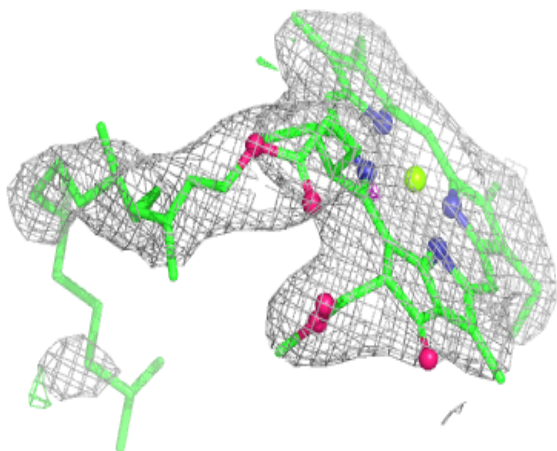
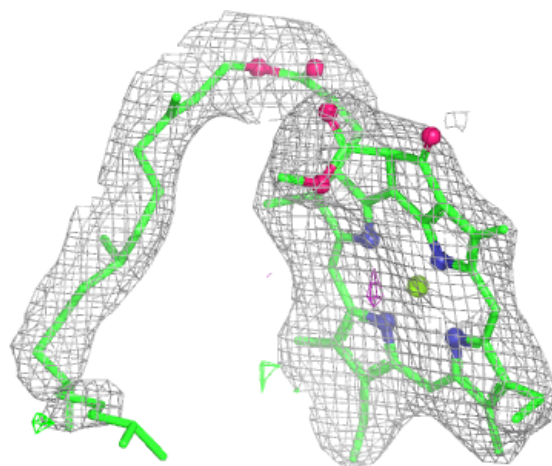
**Electron density around BCR t 101:**

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



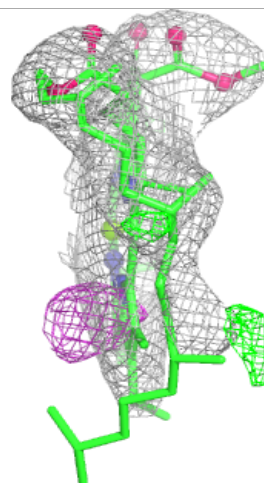
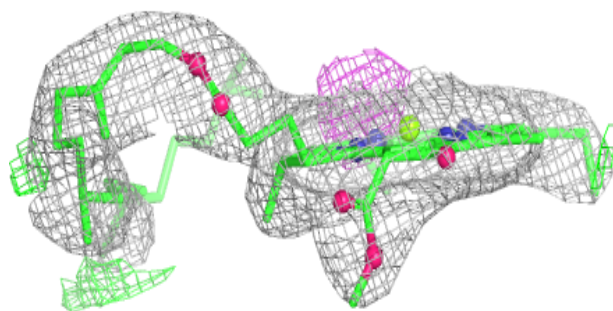
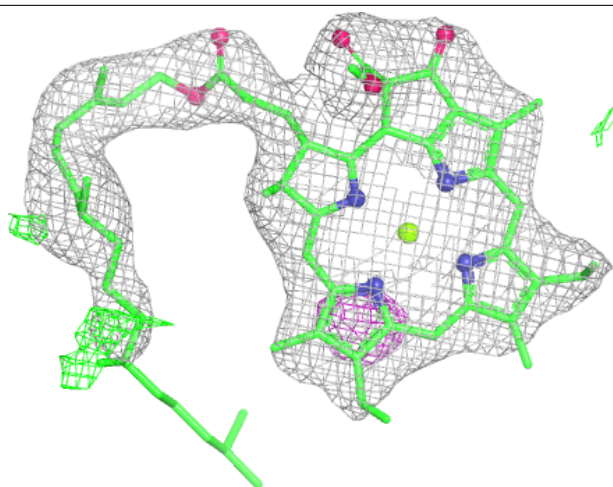
Electron density around CLA b 616:

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



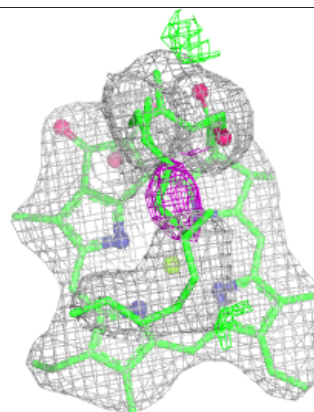
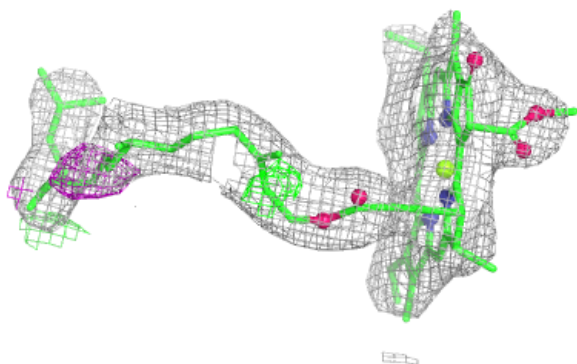
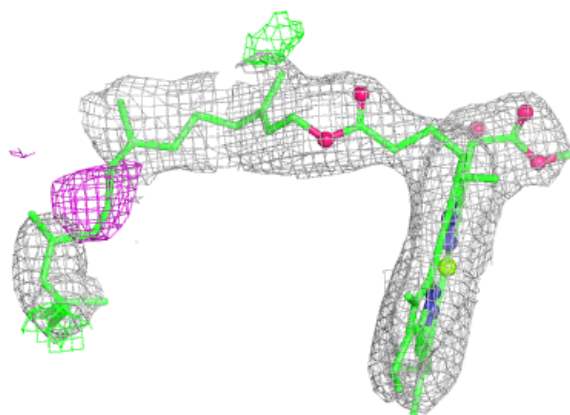
Electron density around CLA C 513:

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



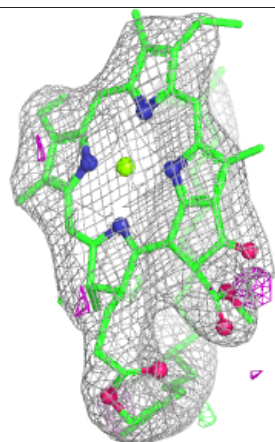
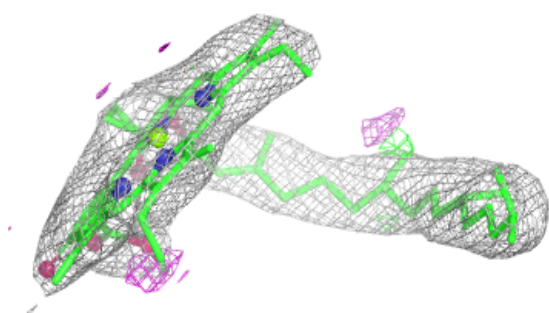
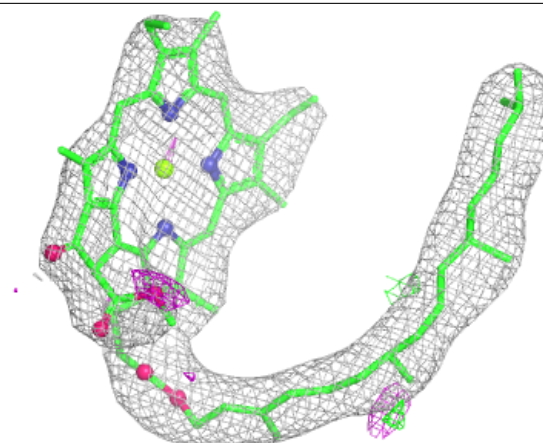
Electron density around CLA c 506:

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

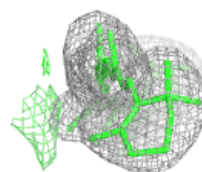
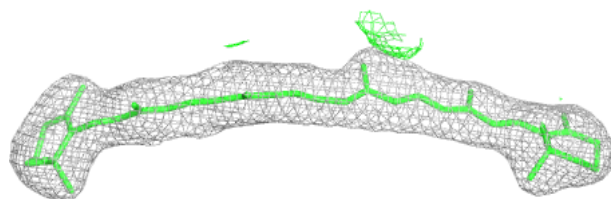
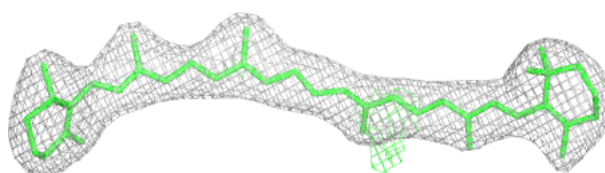


Electron density around CLA c 507:

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

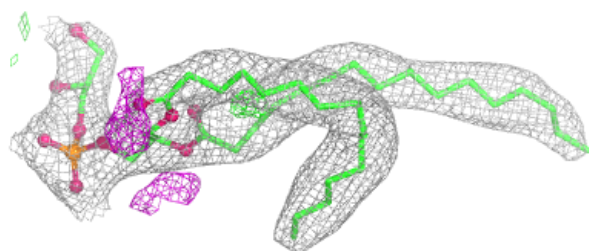
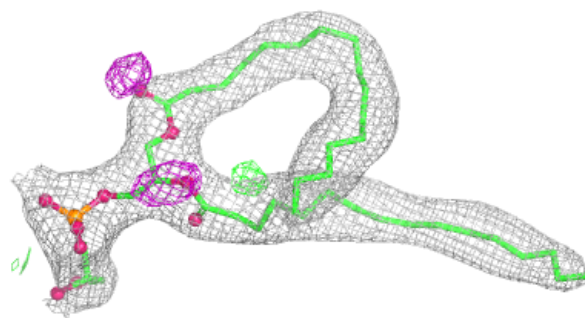
**Electron density around BCR T 101:**

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

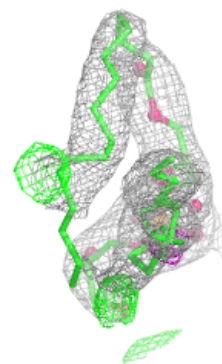
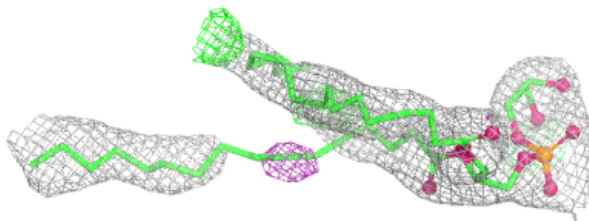
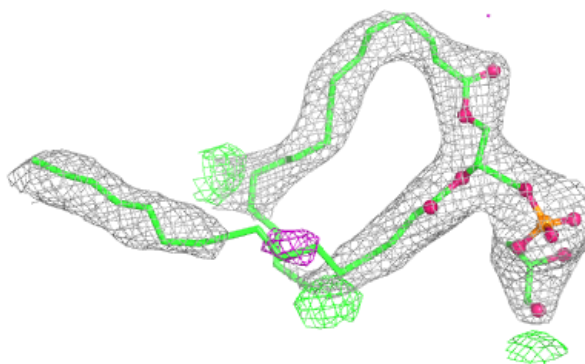


Electron density around LHG A 416:

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

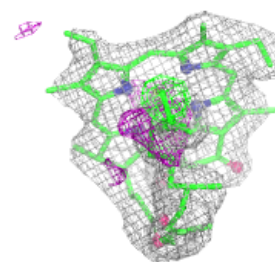
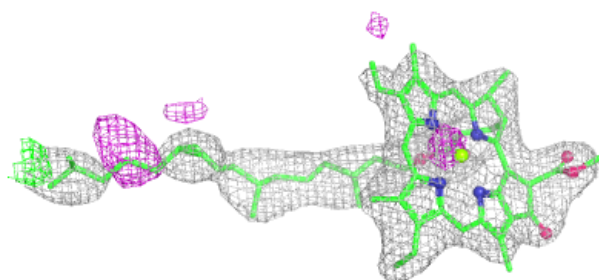
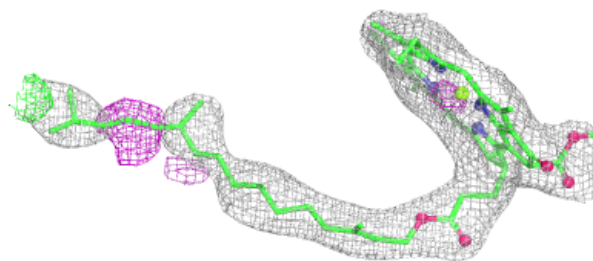
**Electron density around LHG D 409:**

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



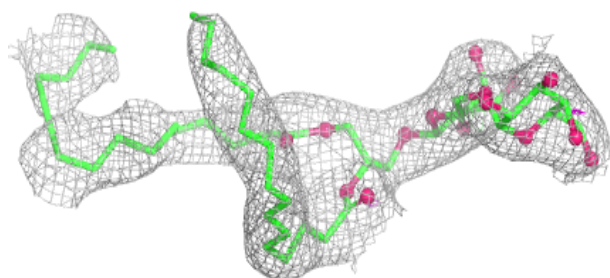
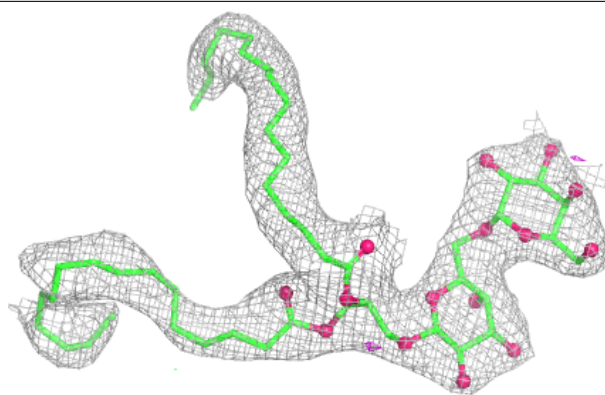
Electron density around CLA C 505:

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

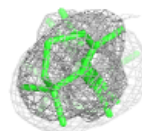
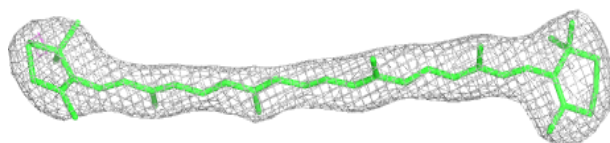
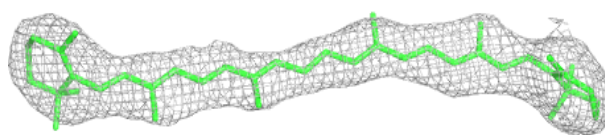


Electron density around DGD C 518:

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

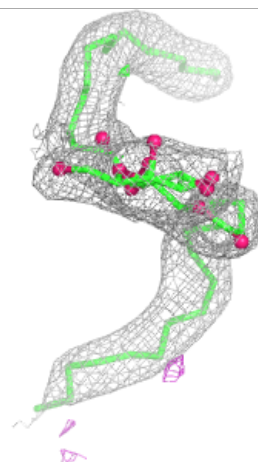
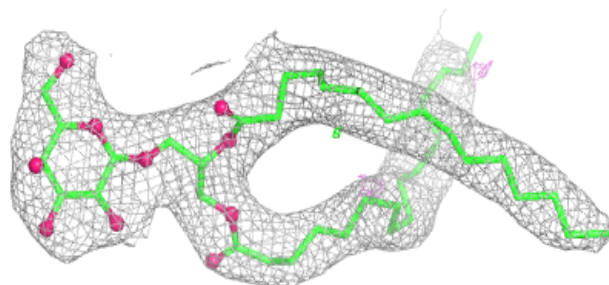
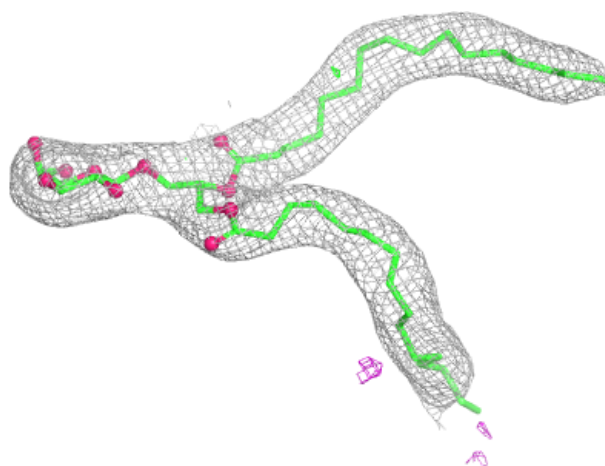
**Electron density around BCR c 514:**

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



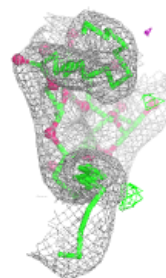
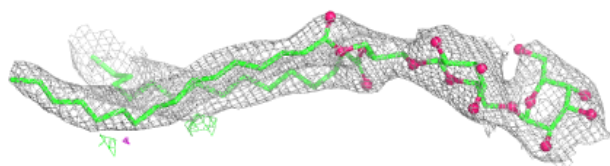
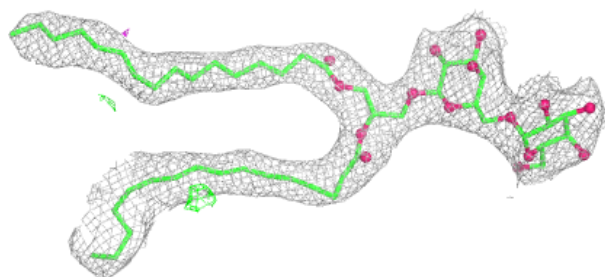
Electron density around LMG B 621:

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

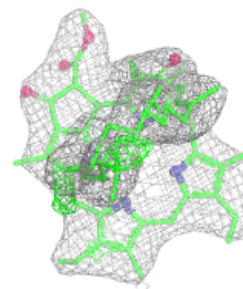
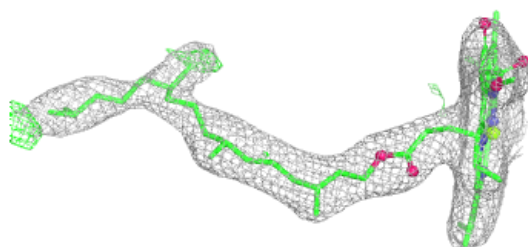
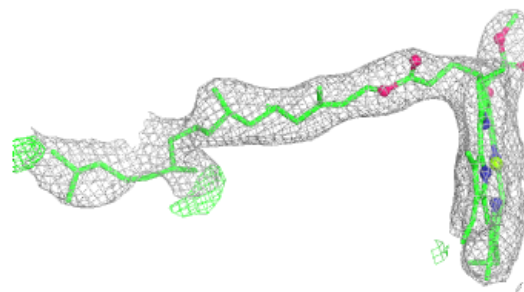


Electron density around DGD c 518:

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

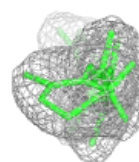
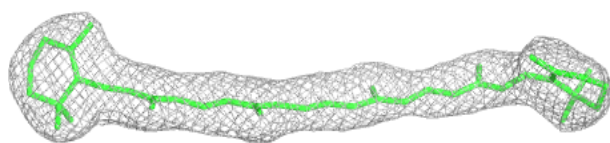
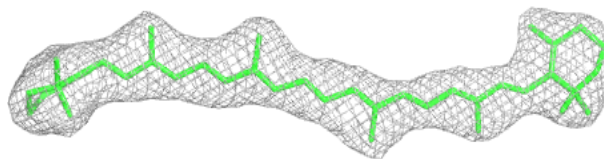
**Electron density around CLA B 606:**

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

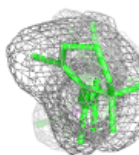
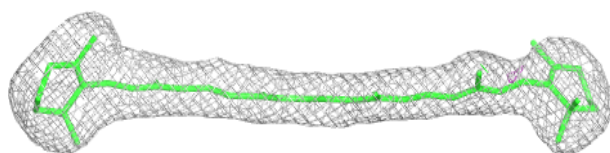
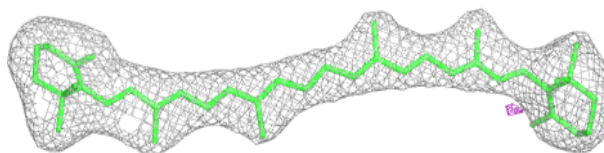


Electron density around BCR b 617:

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

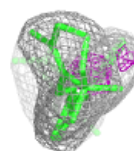
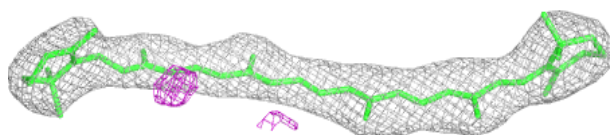
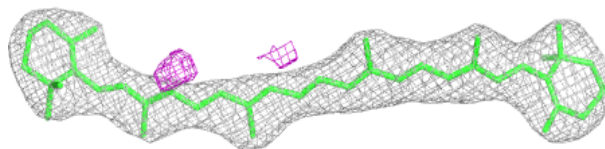
**Electron density around BCR b 618:**

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

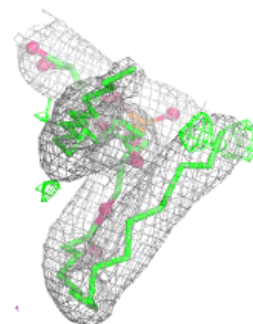
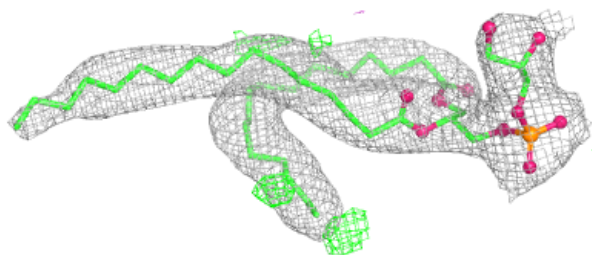
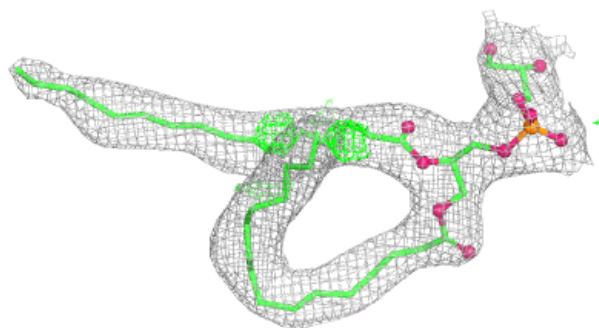


Electron density around BCR b 619:

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

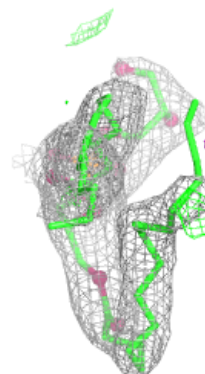
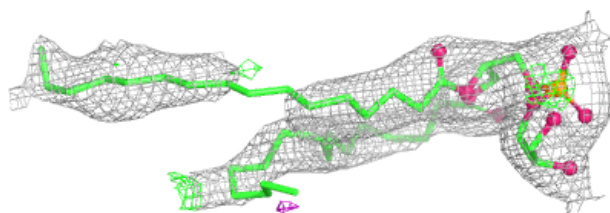
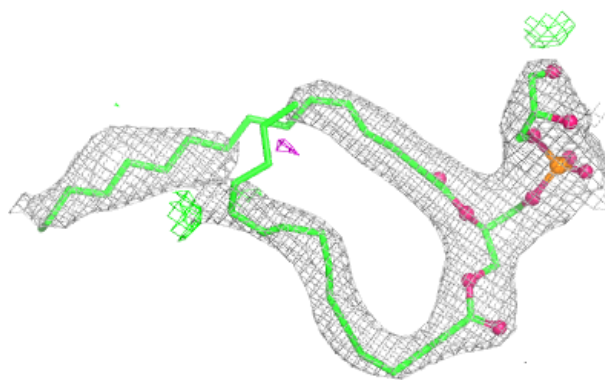
**Electron density around LHG d 407:**

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

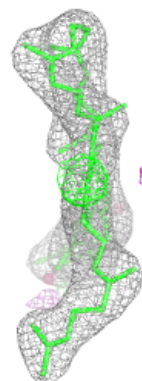
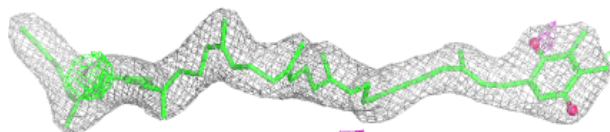
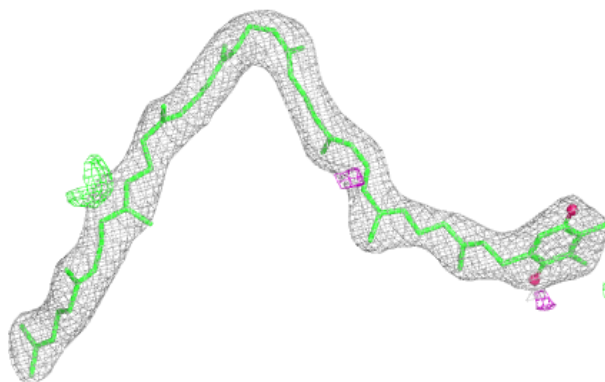


Electron density around LHG d 409:

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

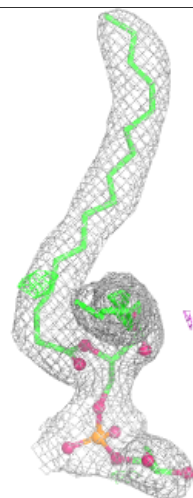
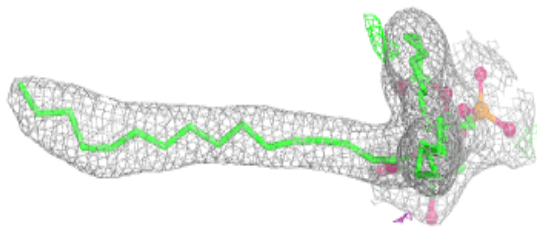
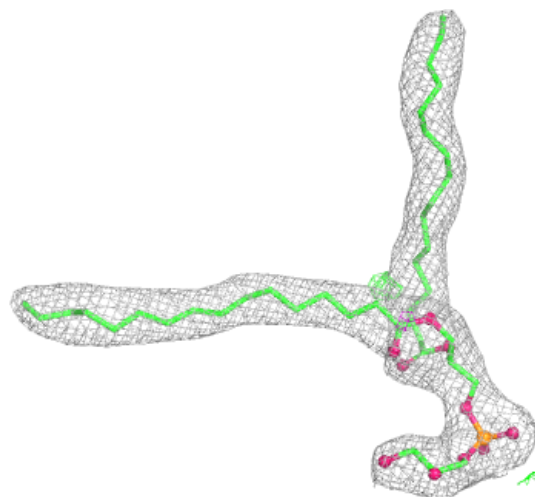
**Electron density around PL9 D 407:**

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



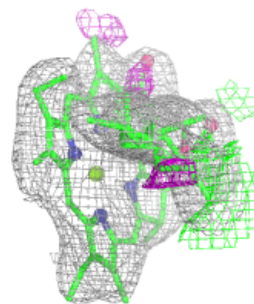
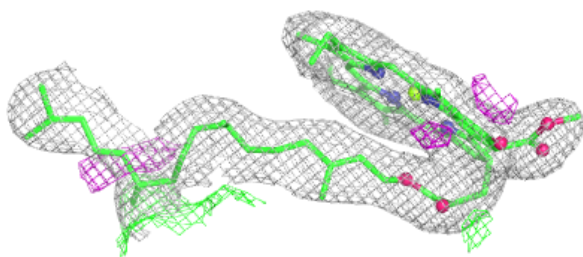
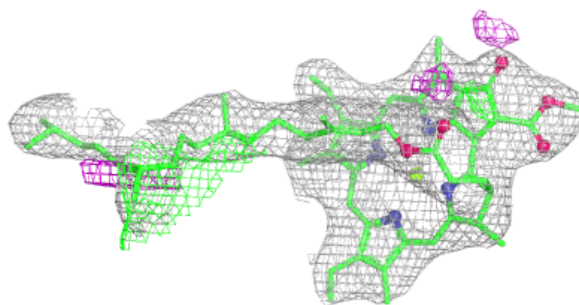
Electron density around LHG 1 101:

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

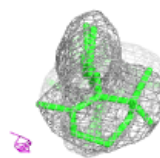
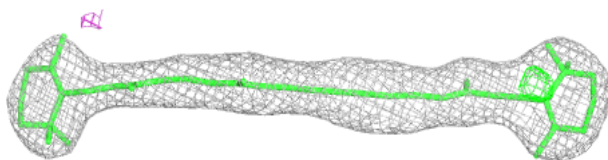
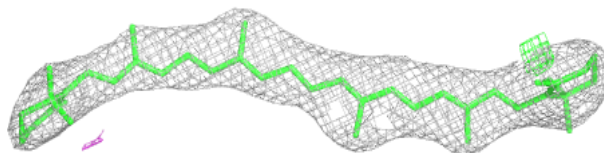


Electron density around CLA B 614:

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

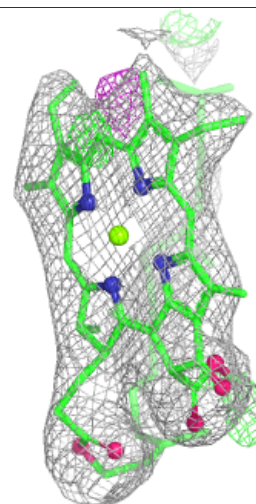
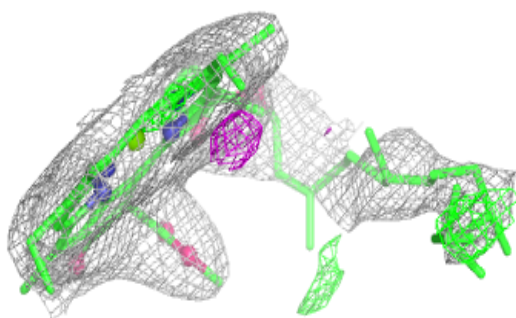
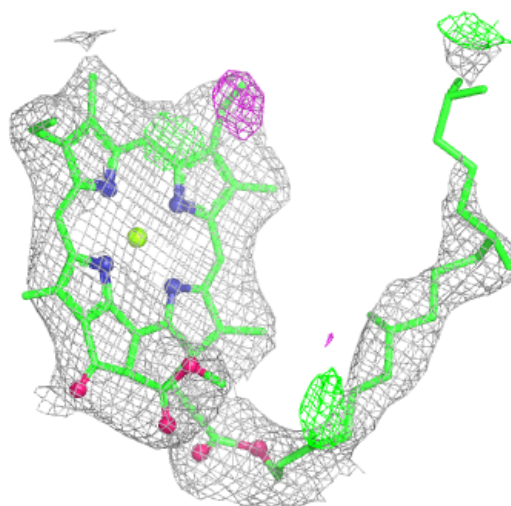
**Electron density around BCR c 515:**

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



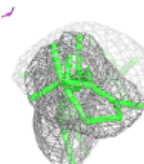
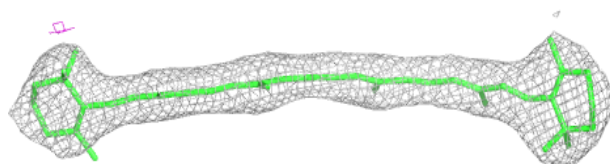
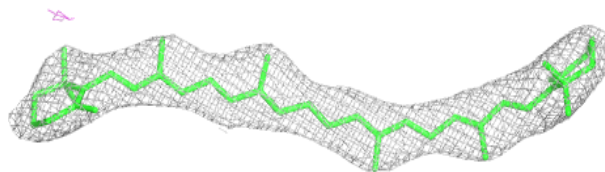
Electron density around CLA B 616:

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

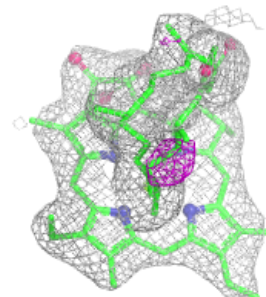
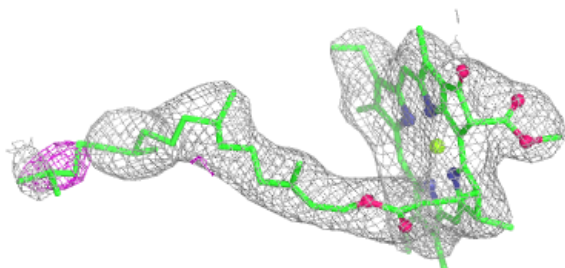
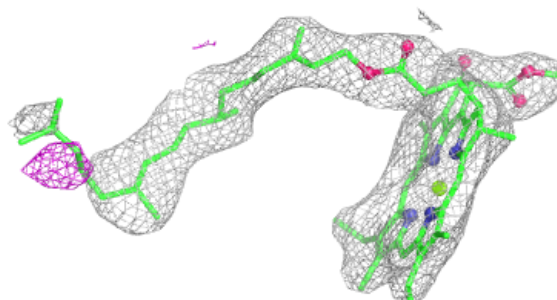


Electron density around BCR h 101:

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

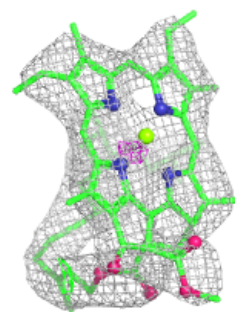
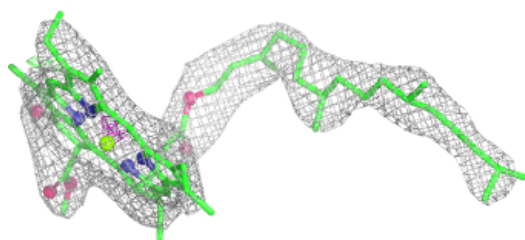
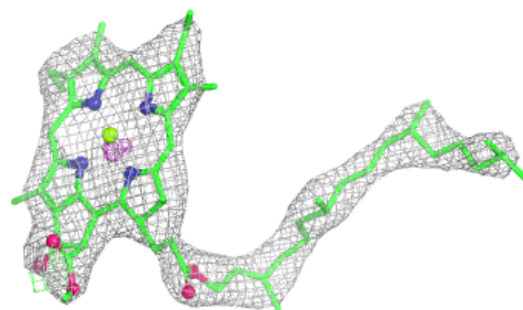
**Electron density around CLA c 508:**

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



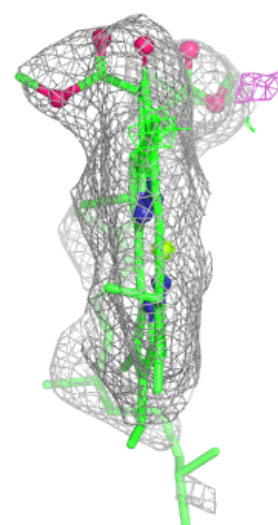
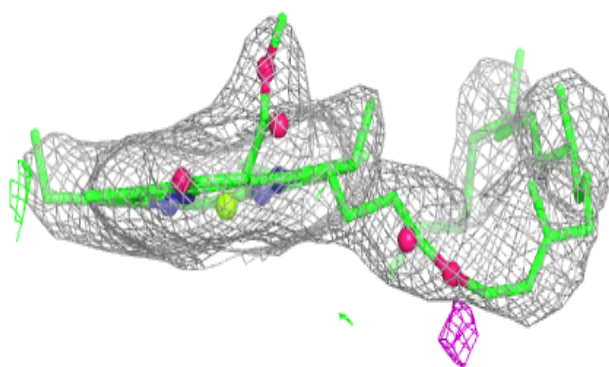
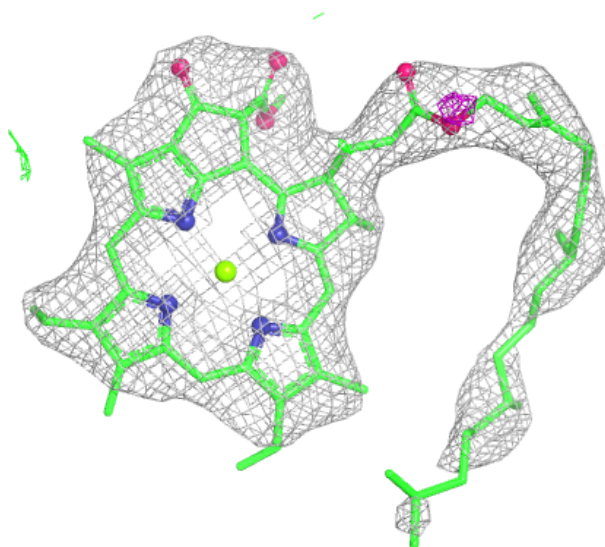
Electron density around CLA c 511:

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



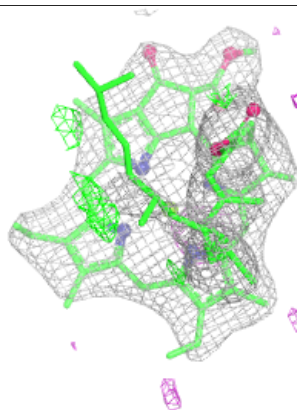
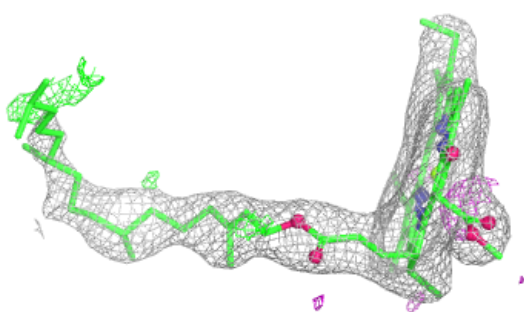
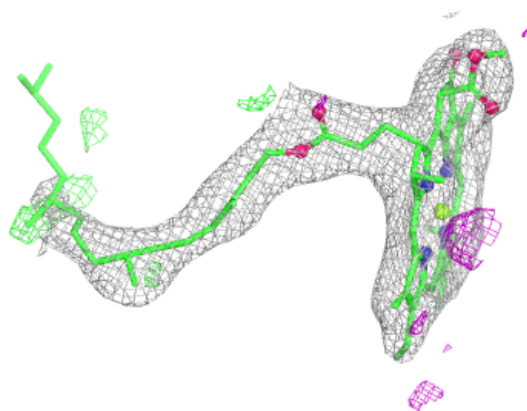
Electron density around CLA c 512:

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

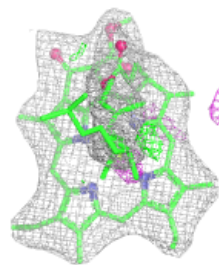
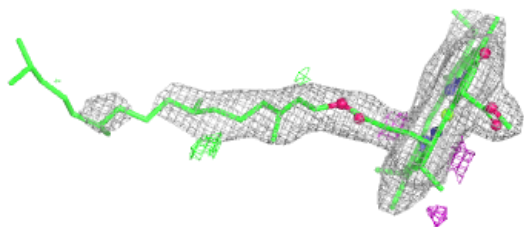
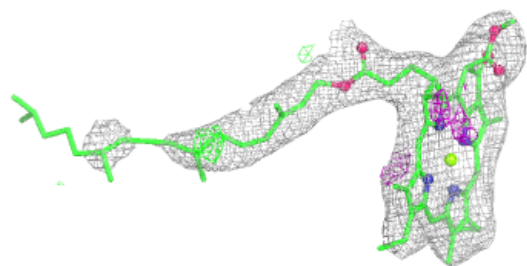


Electron density around CLA D 405:

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

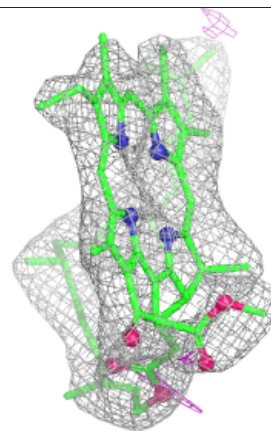
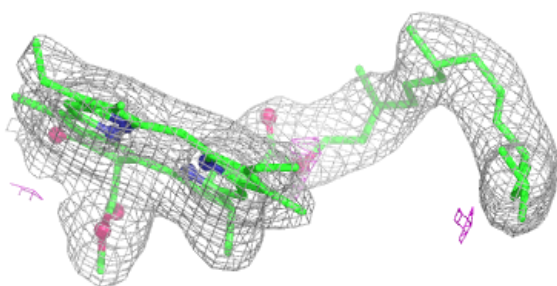
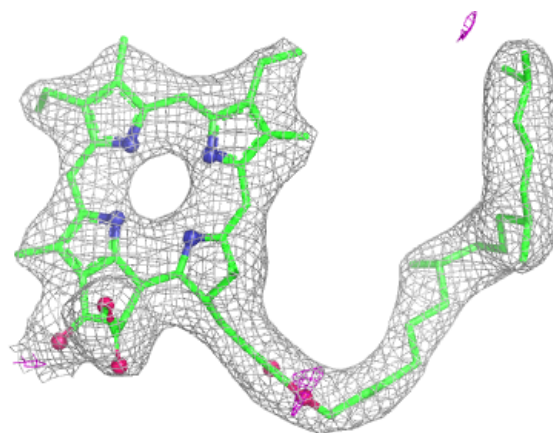
**Electron density around CLA d 404:**

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

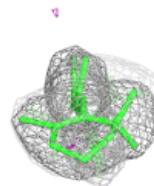
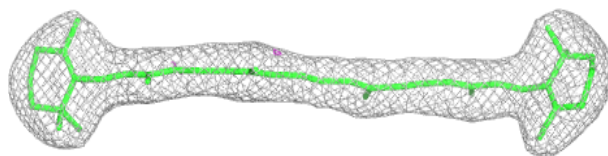
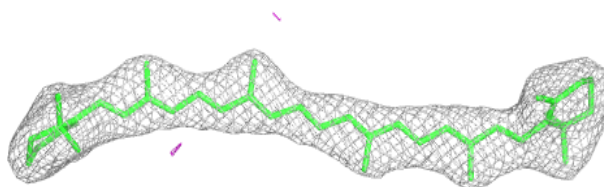


Electron density around PHO a 407:

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

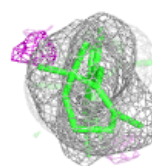
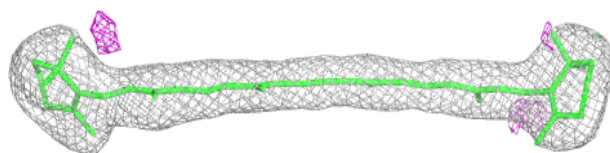
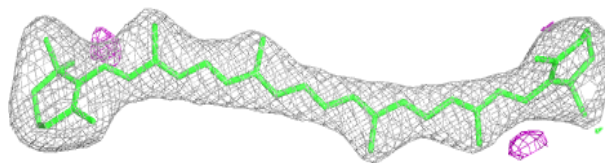
**Electron density around BCR A 409:**

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

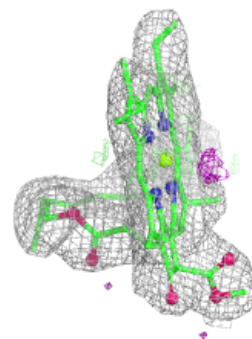
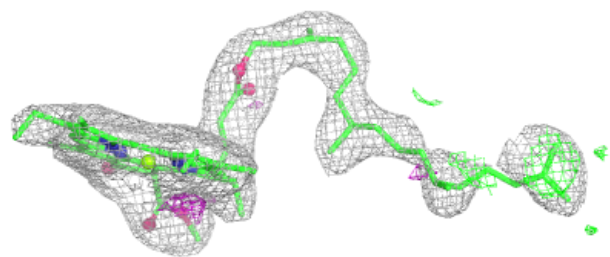
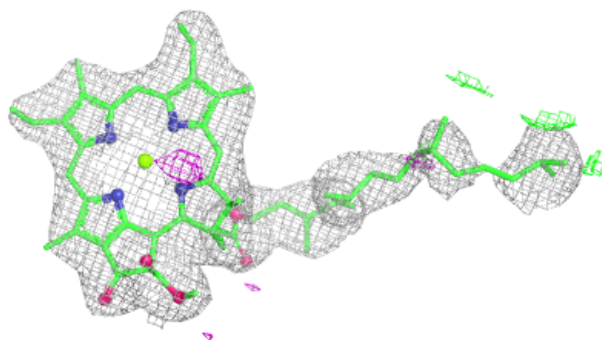


Electron density around BCR B 618:

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

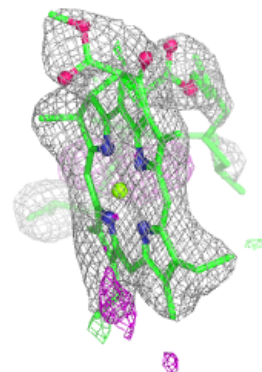
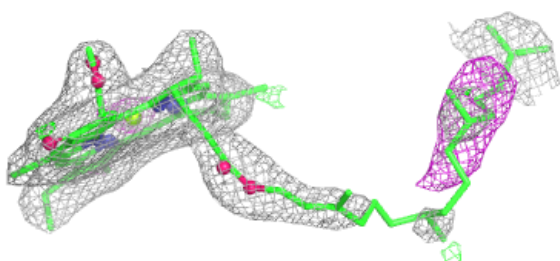
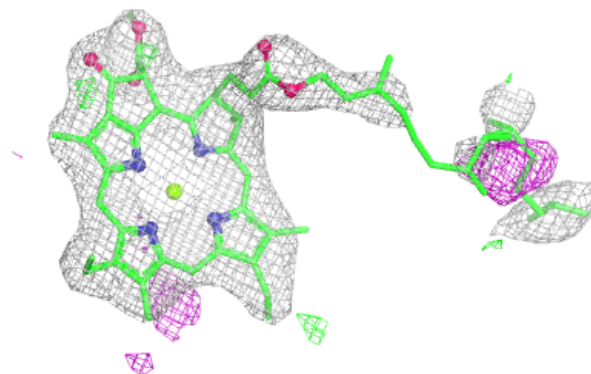
**Electron density around CLA a 405:**

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

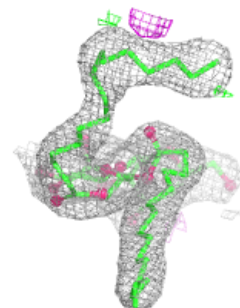
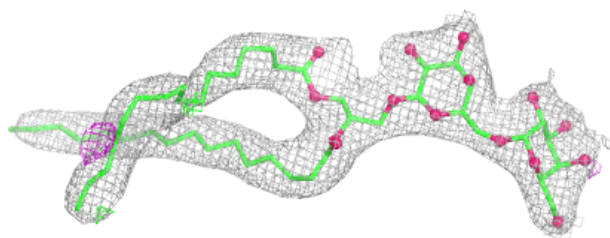
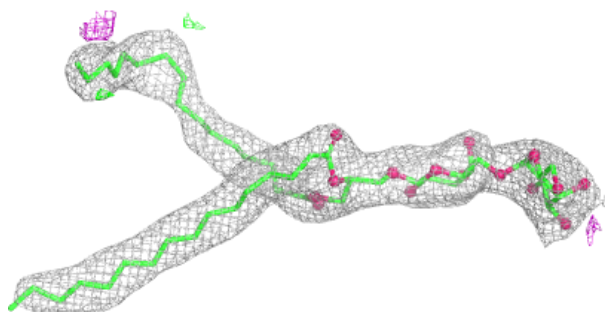


Electron density around CLA a 408:

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

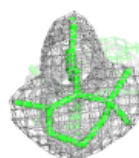
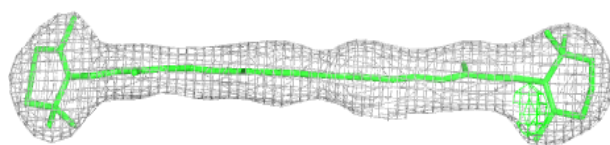
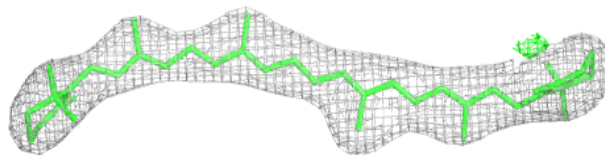
**Electron density around DGD C 517:**

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

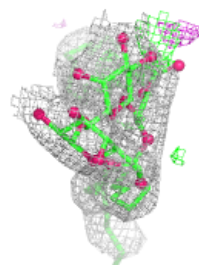
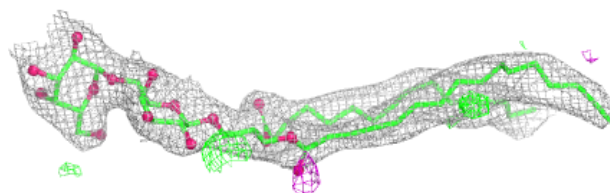
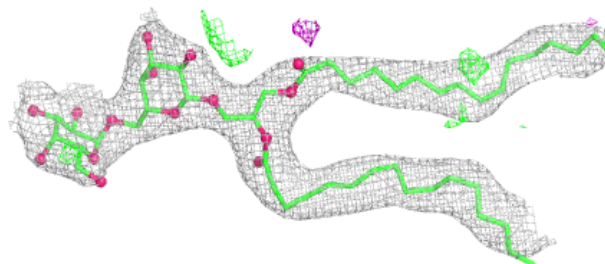


Electron density around BCR C 516:

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

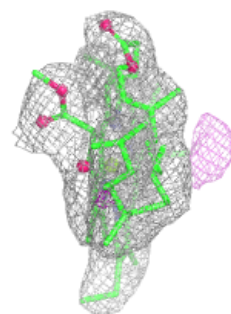
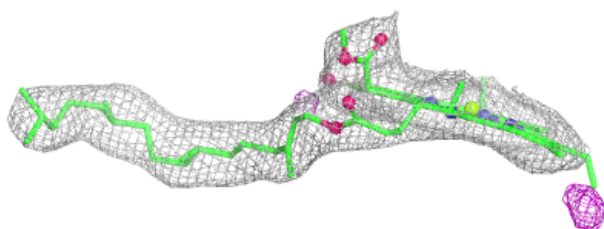
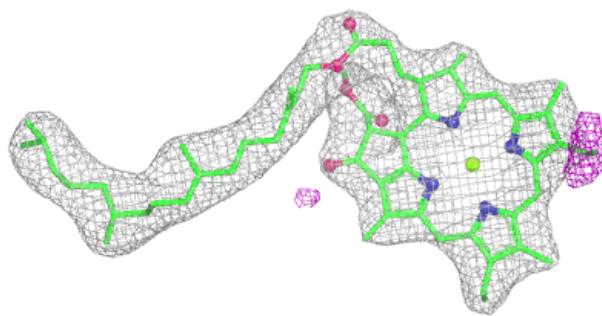
**Electron density around DGD C 519:**

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

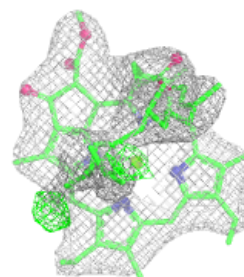
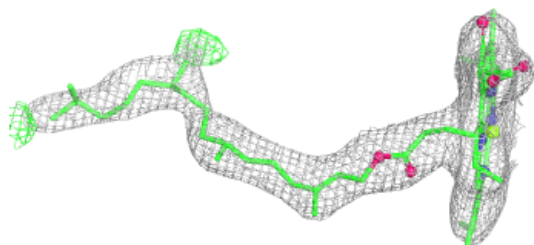
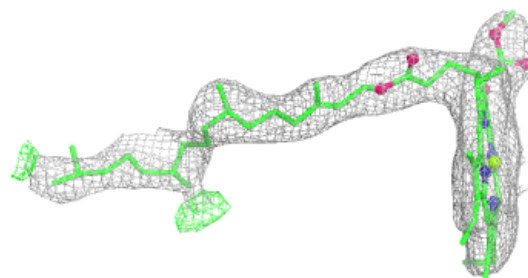


Electron density around CLA B 602:

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

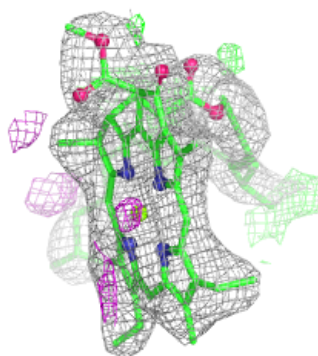
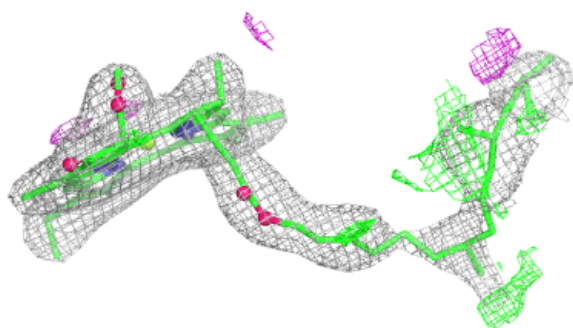
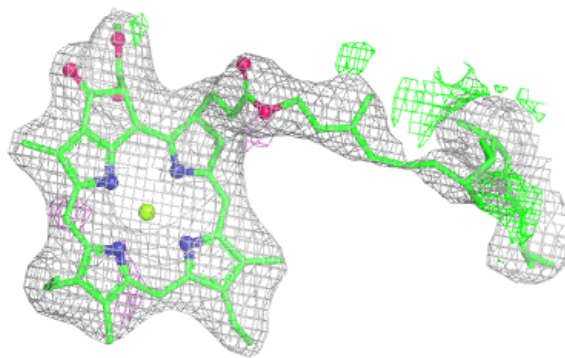
**Electron density around CLA b 606:**

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

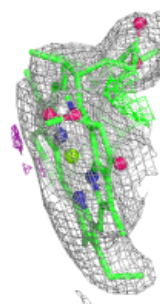
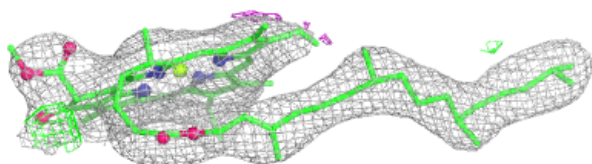
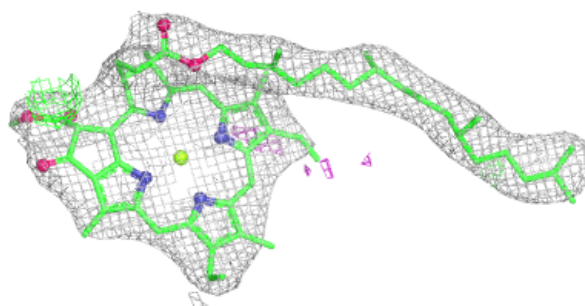


Electron density around CLA A 408:

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

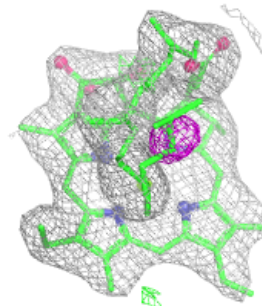
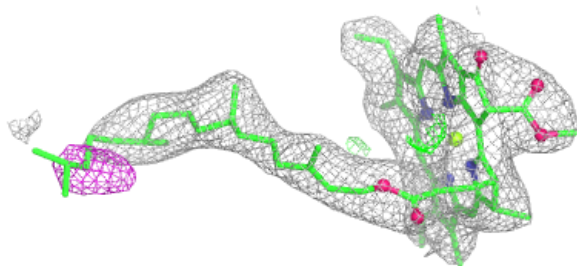
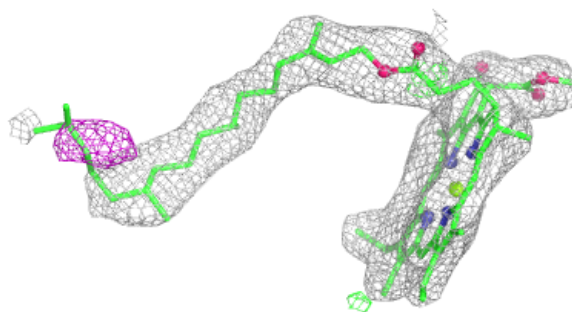
**Electron density around CLA c 501:**

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

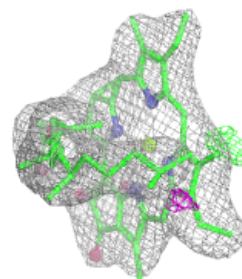
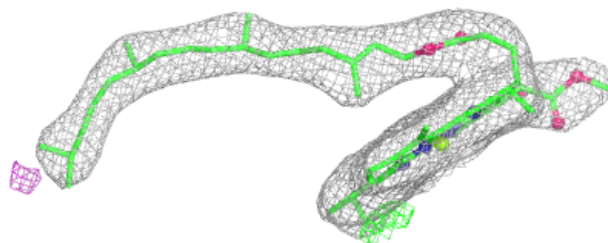
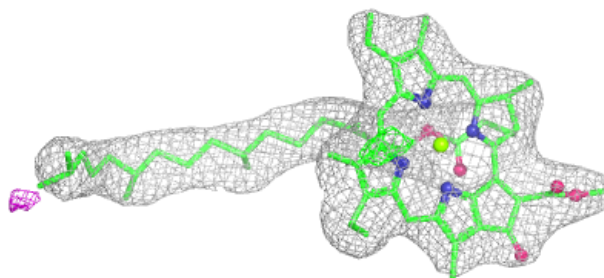


Electron density around CLA C 509:

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

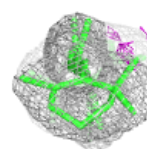
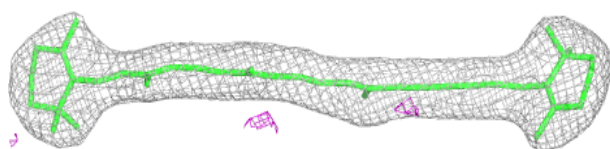
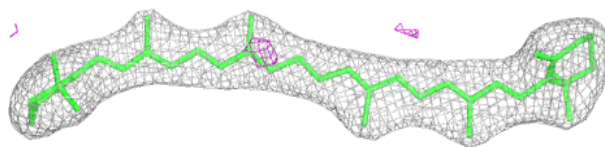
**Electron density around CLA b 608:**

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

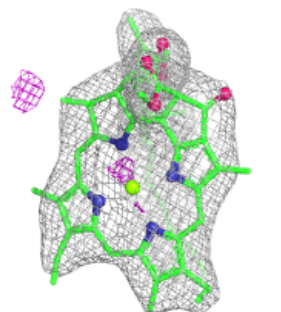
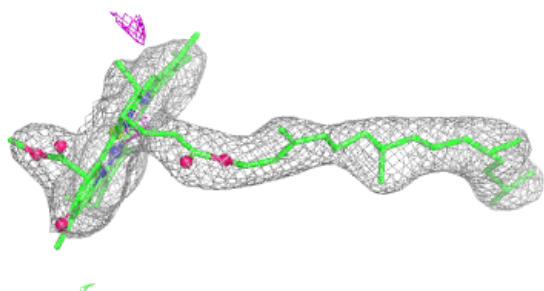
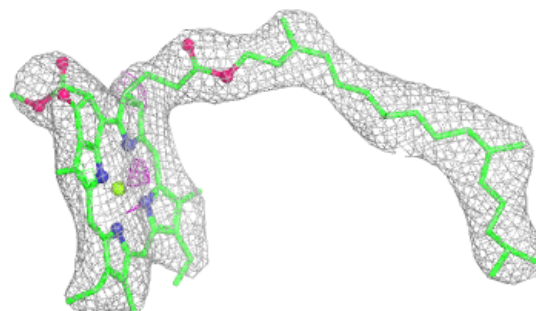


Electron density around BCR a 409:

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

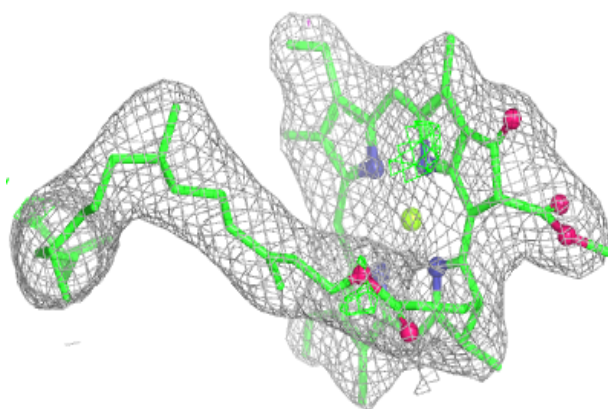
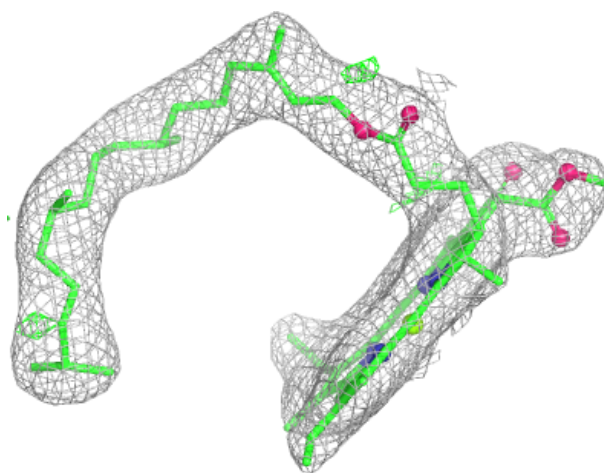
**Electron density around CLA b 609:**

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



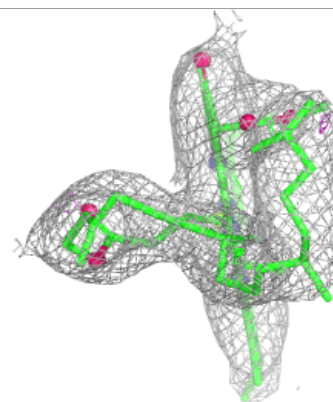
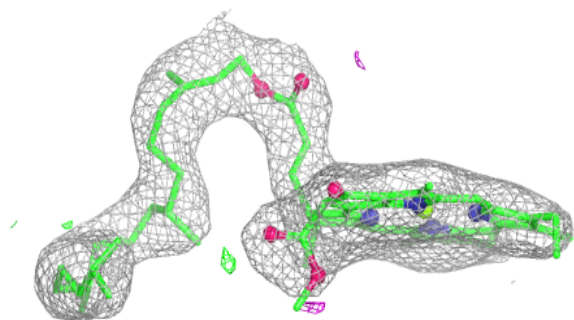
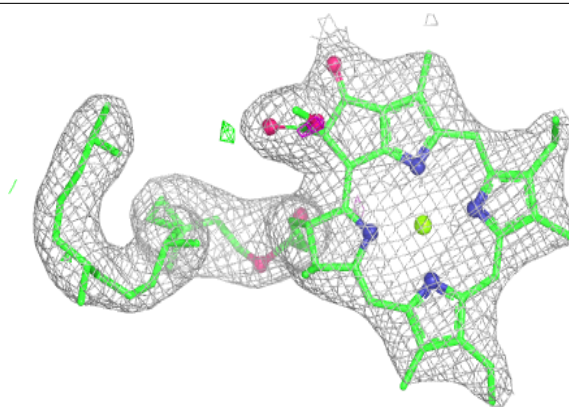
Electron density around CLA b 611:

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

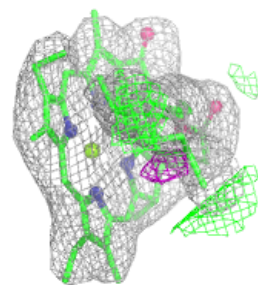
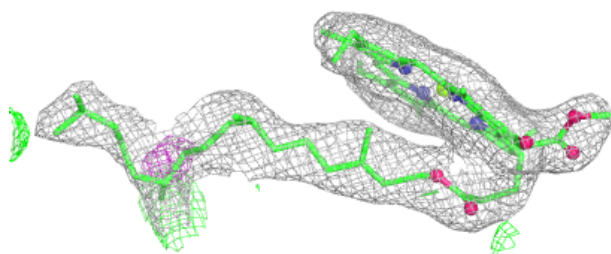
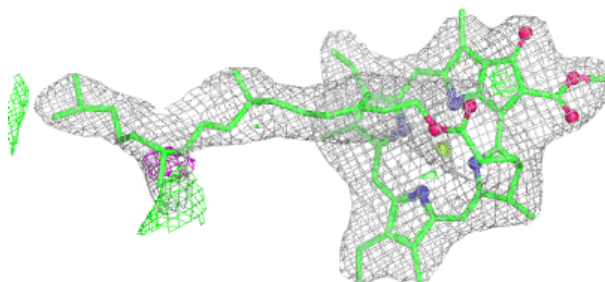


Electron density around CLA b 612:

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

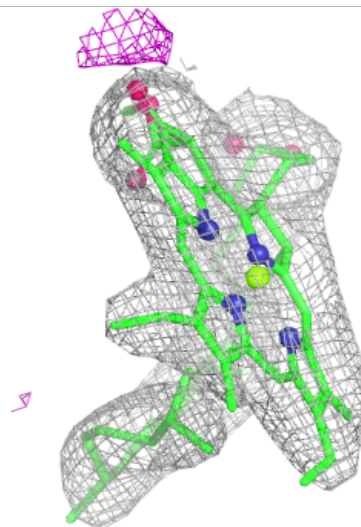
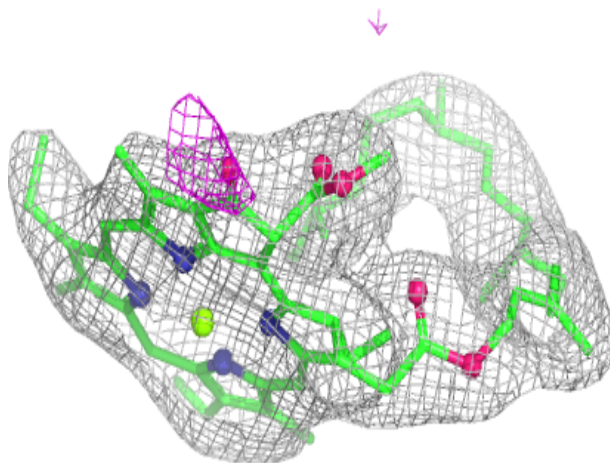
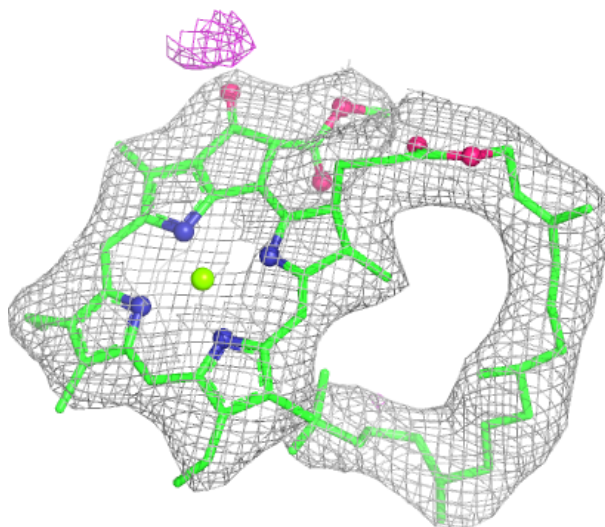
**Electron density around CLA b 614:**

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



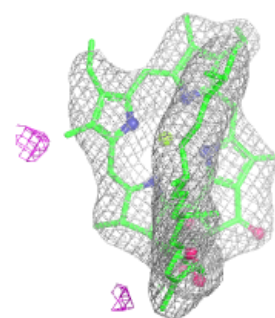
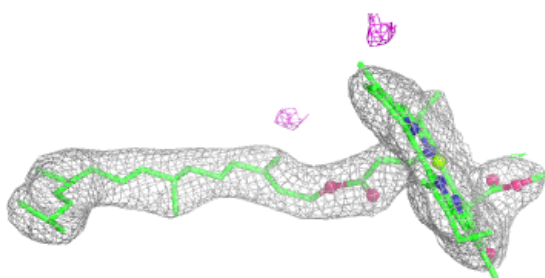
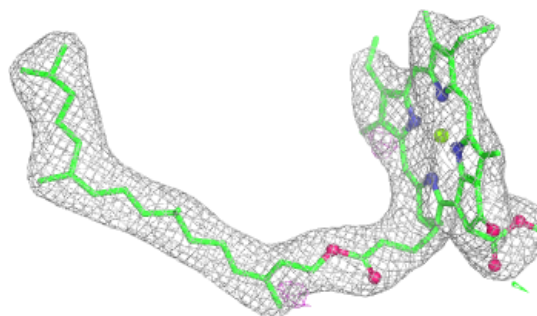
Electron density around CLA b 615:

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

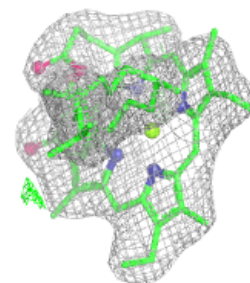
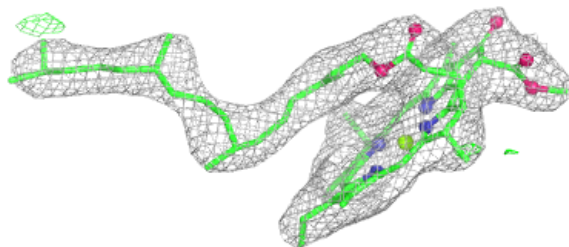
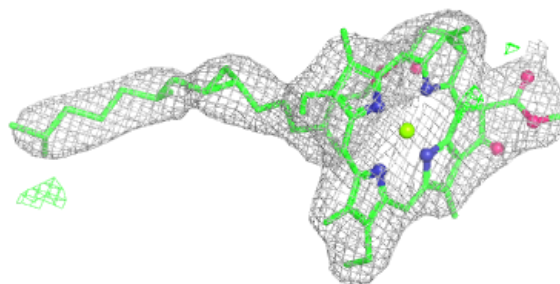


Electron density around CLA B 609:

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

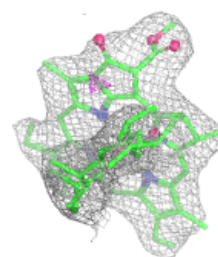
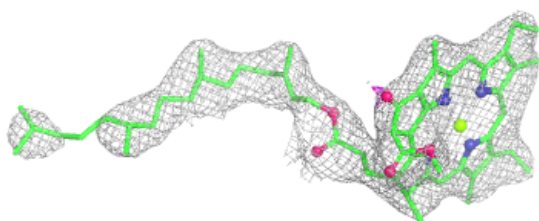
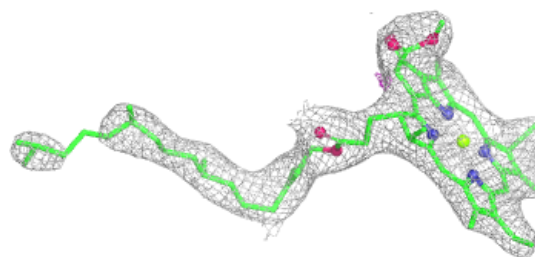
**Electron density around CLA C 506:**

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



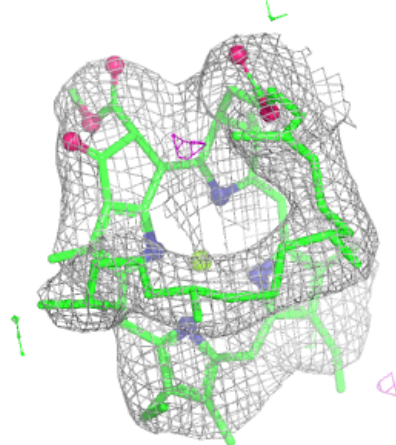
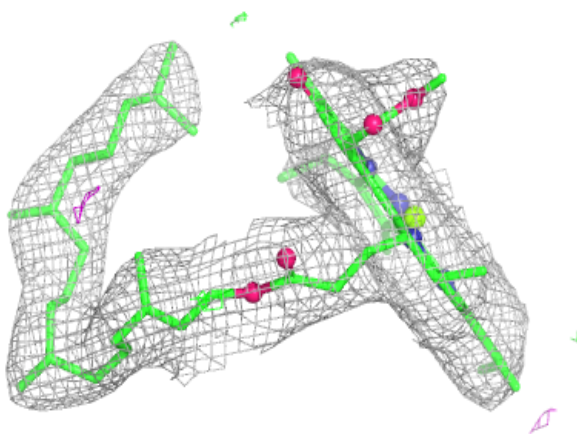
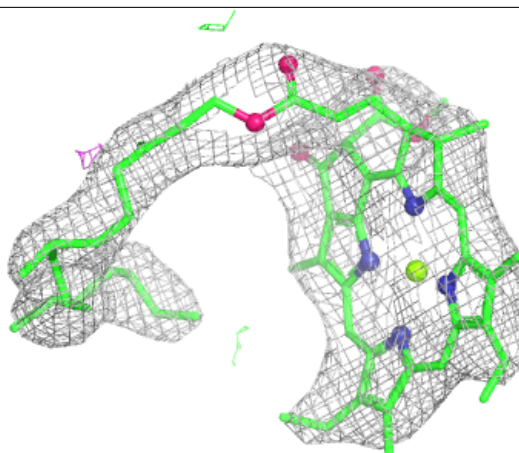
Electron density around CLA c 502:

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



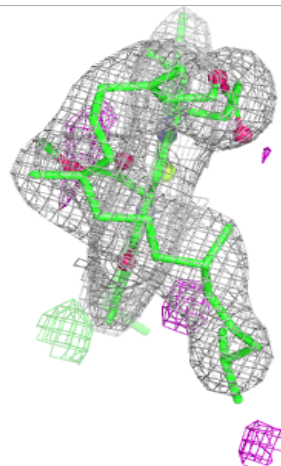
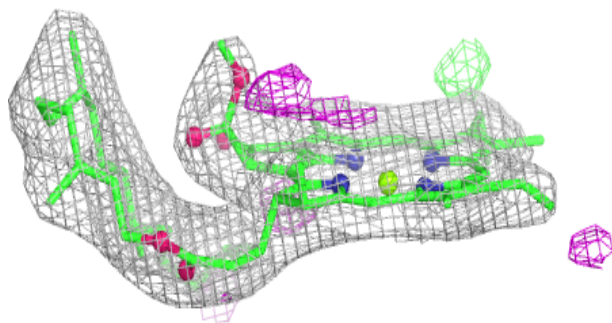
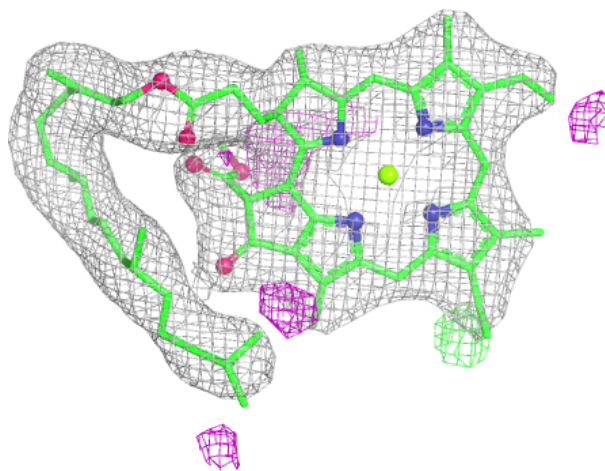
Electron density around CLA c 503:

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



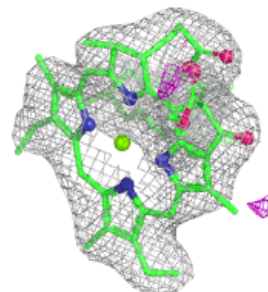
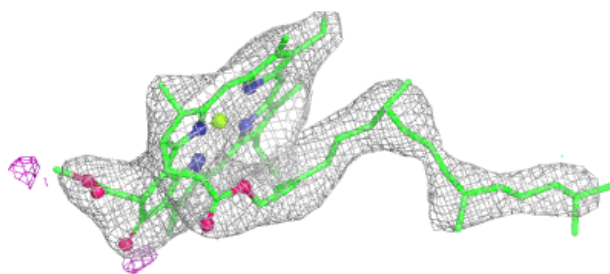
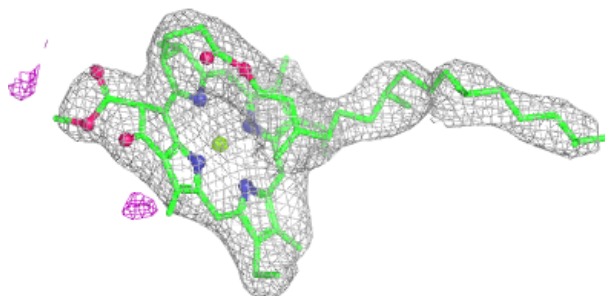
Electron density around CLA B 610:

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

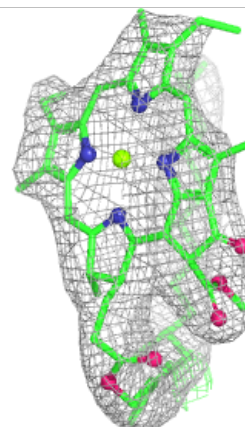
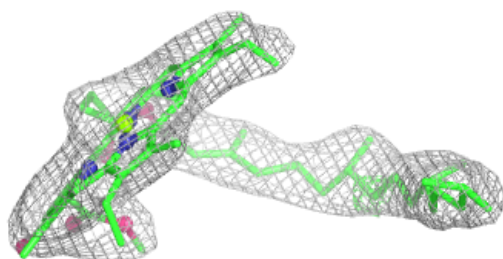
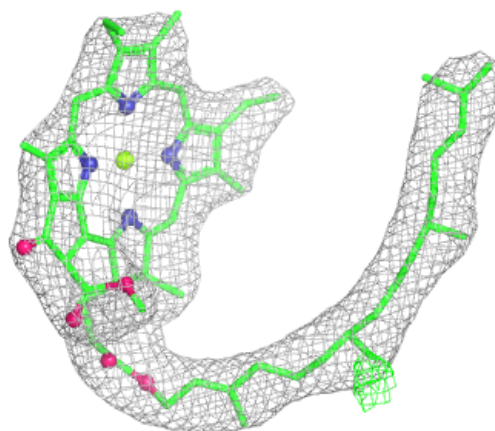


Electron density around CLA c 505:

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

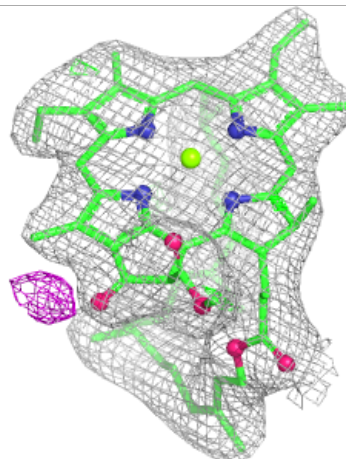
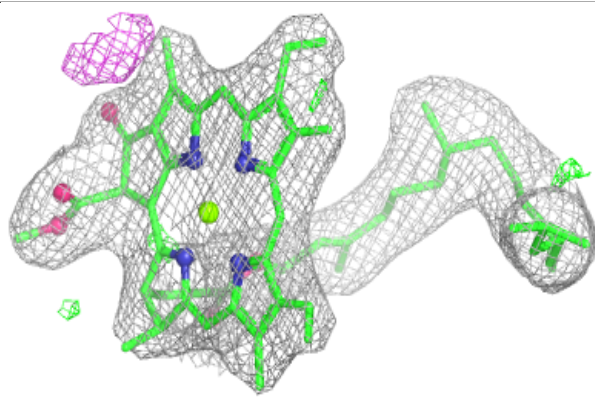
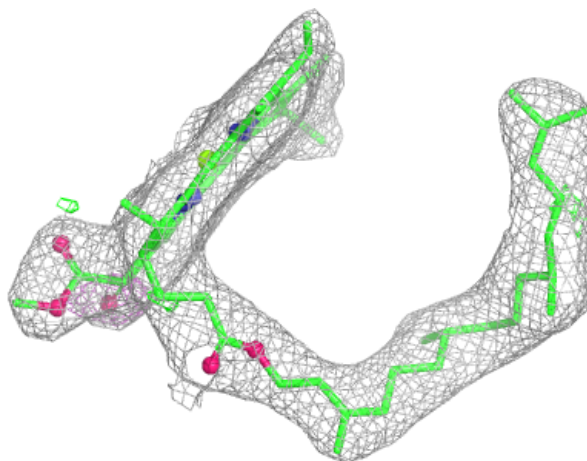
**Electron density around CLA C 508:**

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



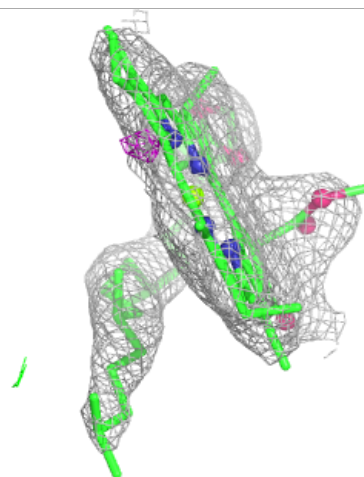
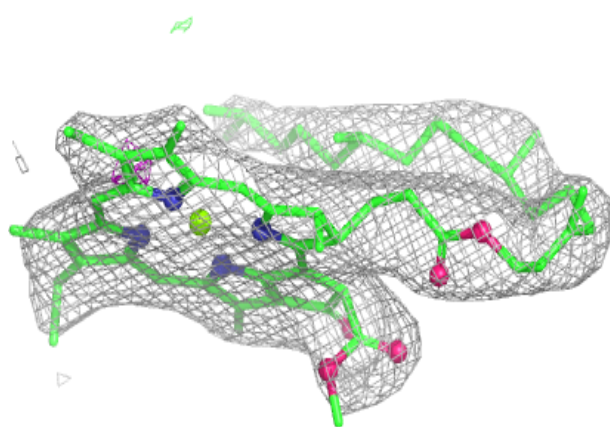
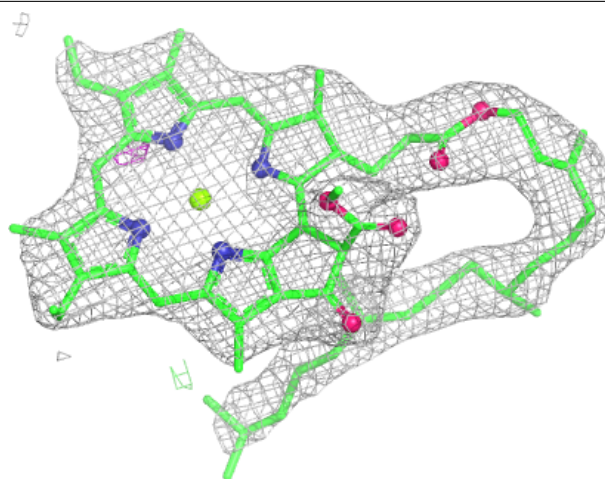
Electron density around CLA B 611:

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



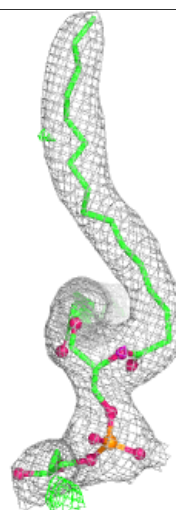
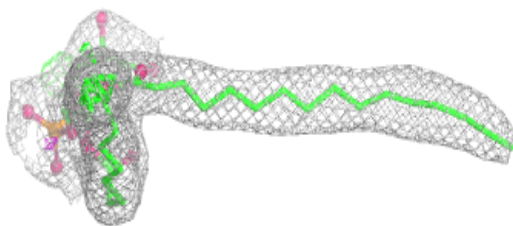
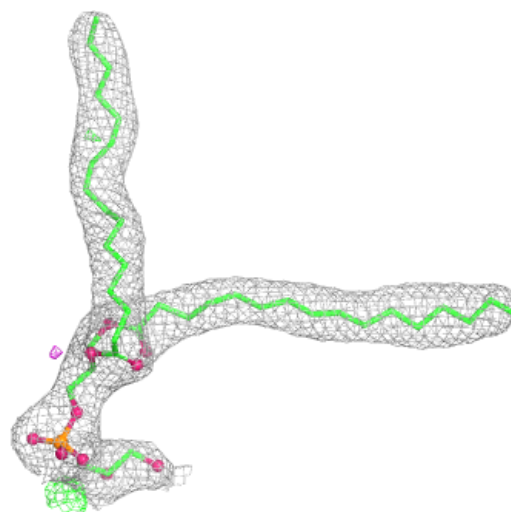
Electron density around CLA C 510:

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



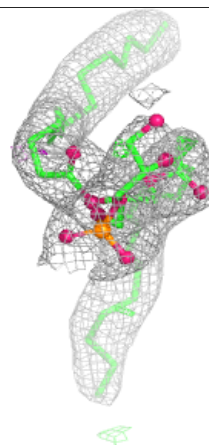
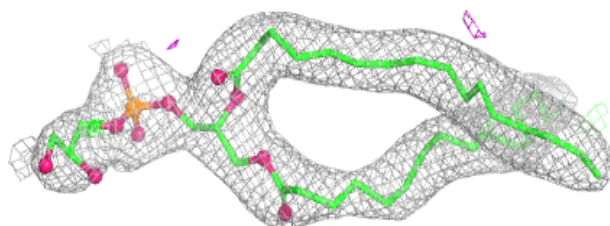
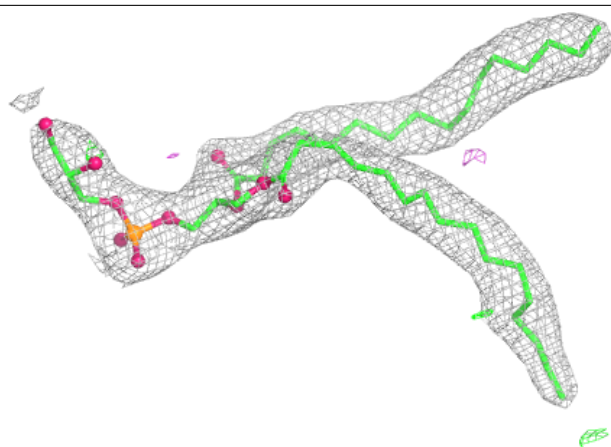
Electron density around LHG A 417:

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



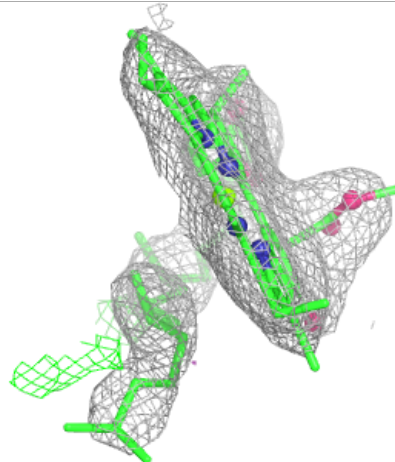
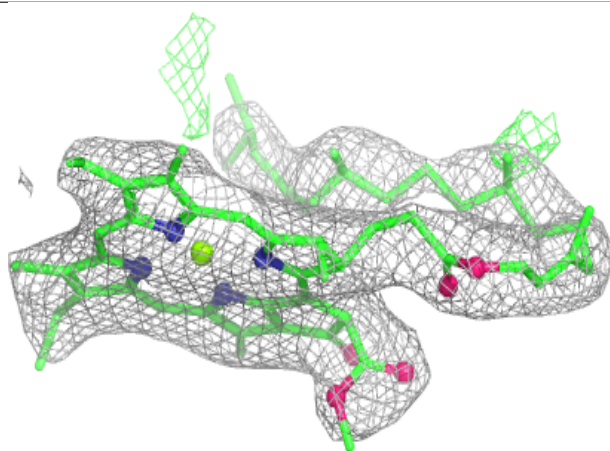
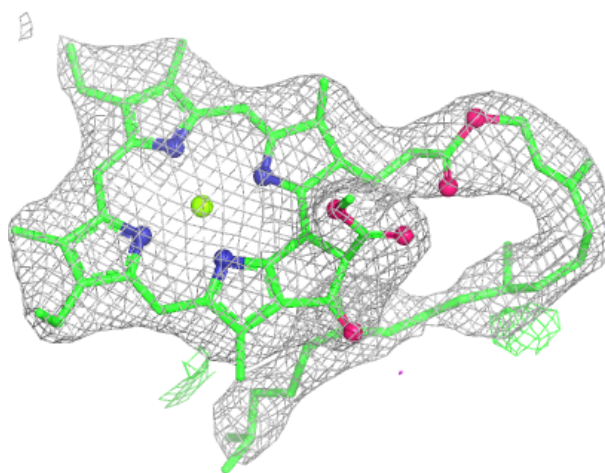
Electron density around LHG D 408:

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



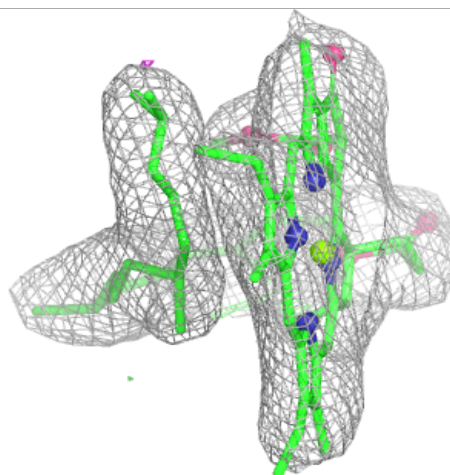
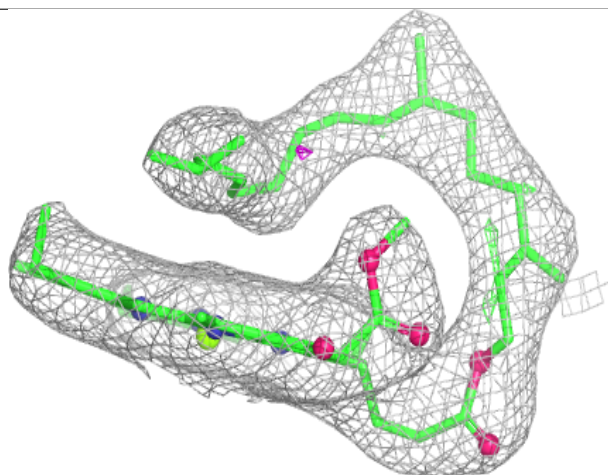
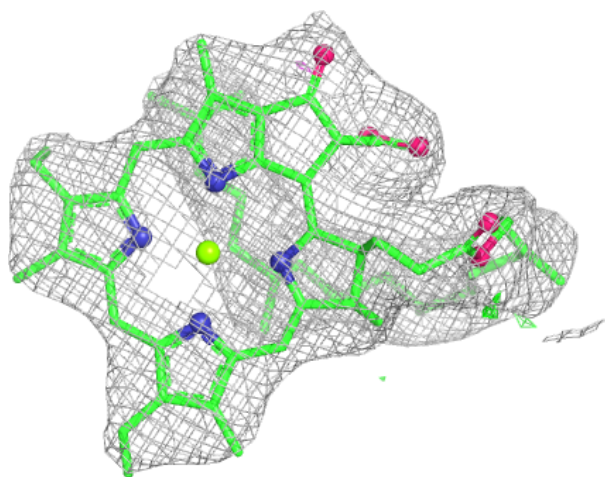
Electron density around CLA c 509:

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



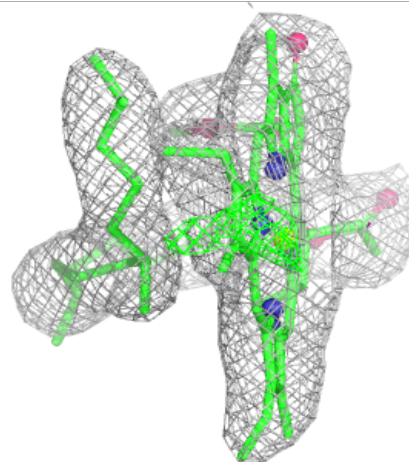
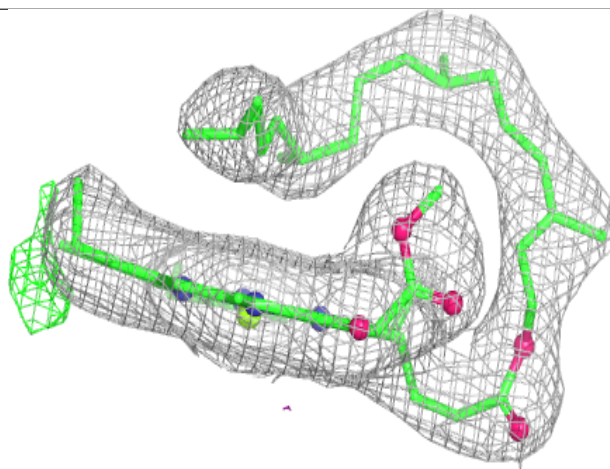
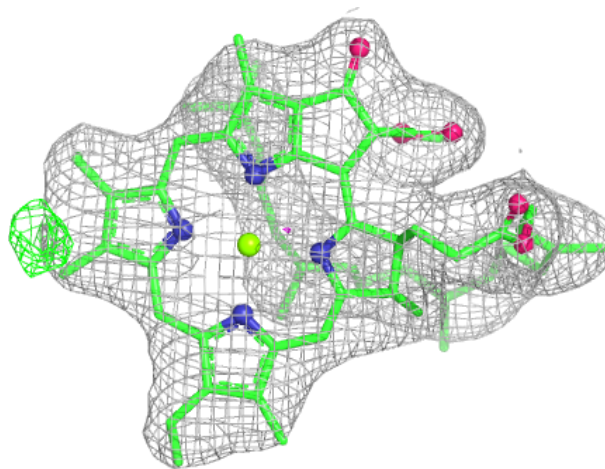
Electron density around CLA c 510:

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



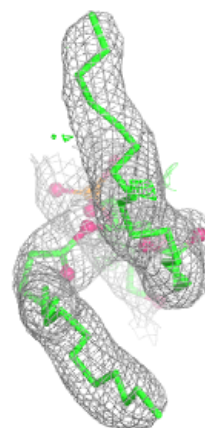
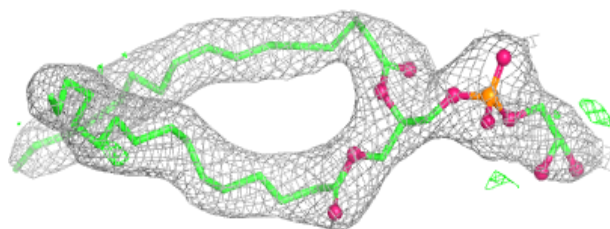
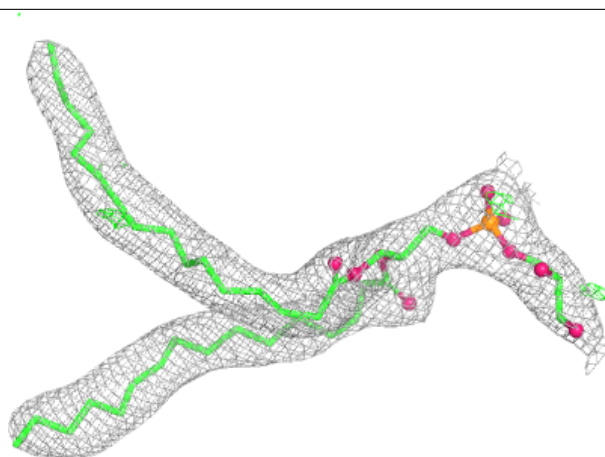
Electron density around CLA C 511:

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



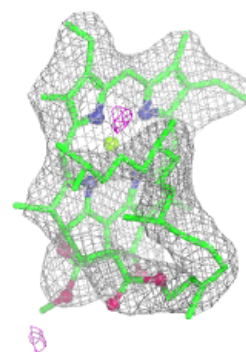
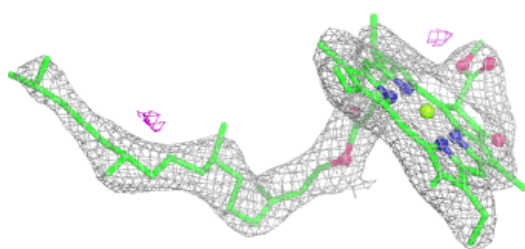
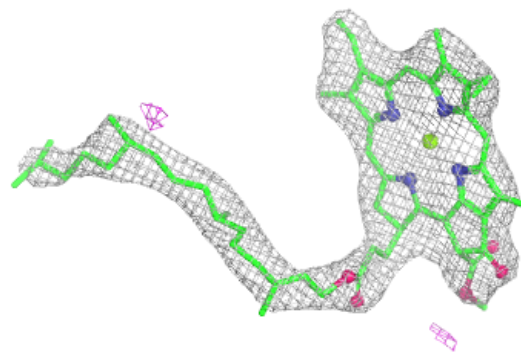
Electron density around LHG d 408:

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



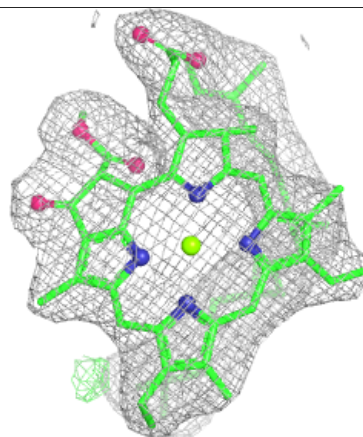
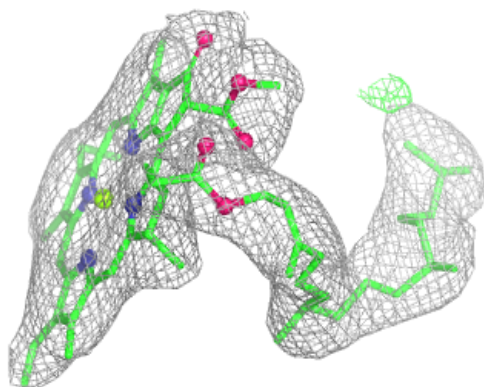
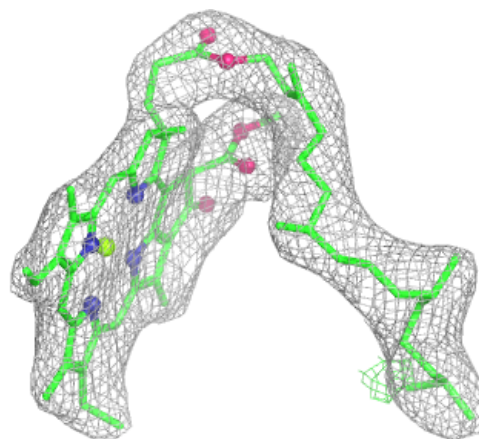
Electron density around CLA C 512:

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



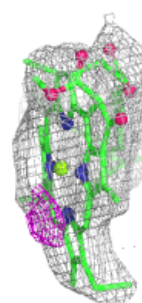
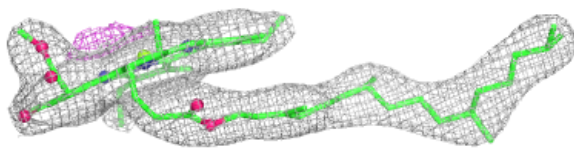
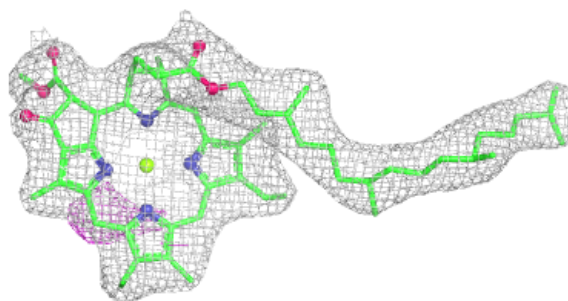
Electron density around CLA B 613:

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

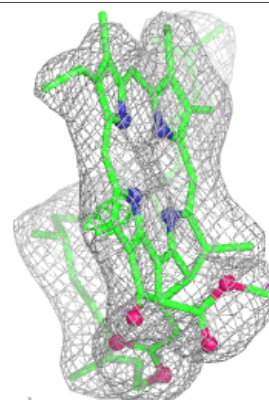
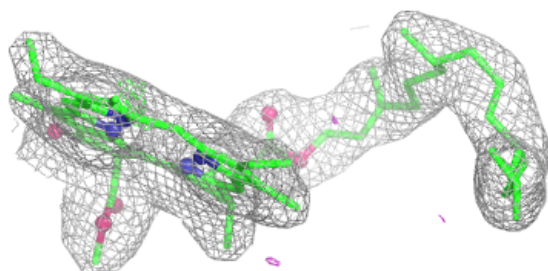
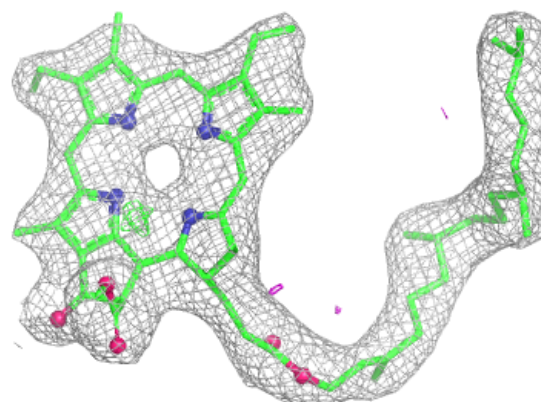


Electron density around CLA B 603:

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

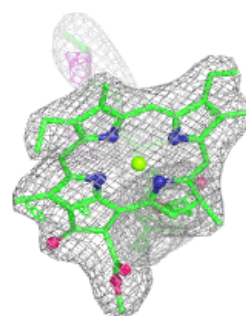
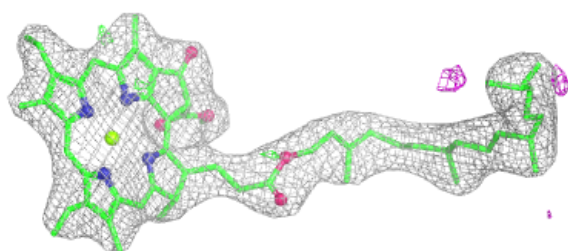
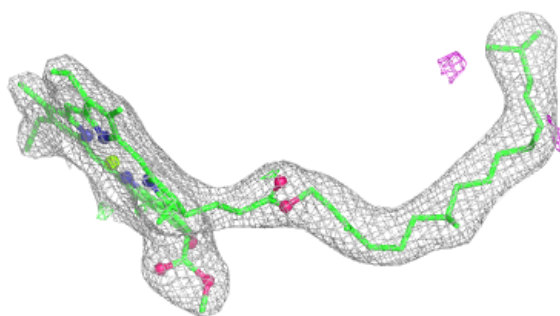
**Electron density around PHO A 407:**

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



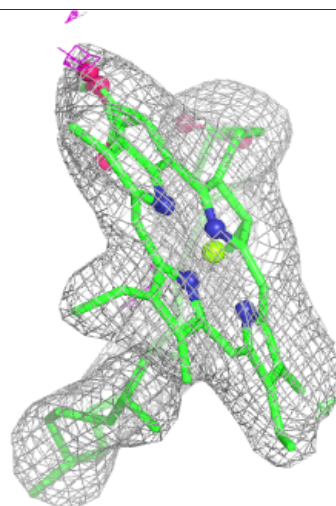
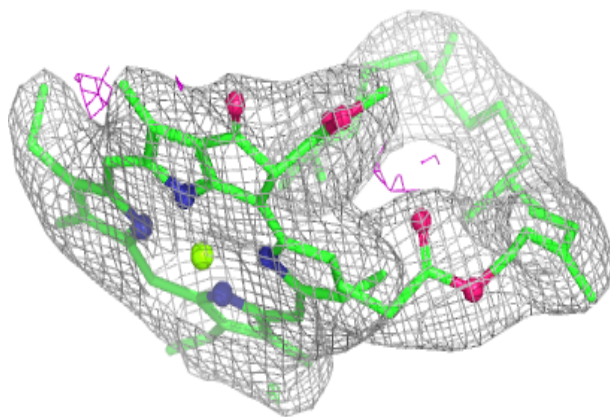
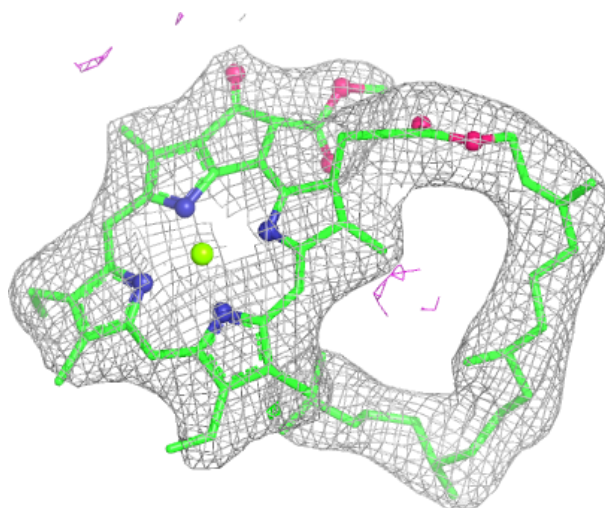
Electron density around CLA D 404:

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



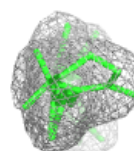
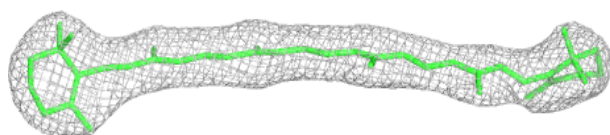
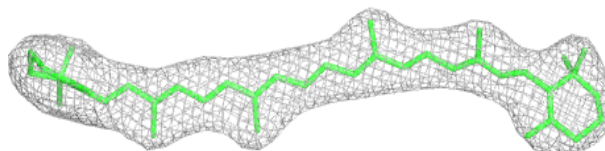
Electron density around CLA B 615:

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

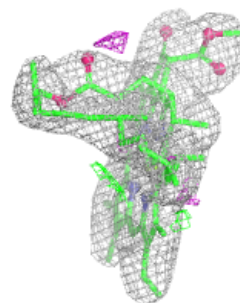
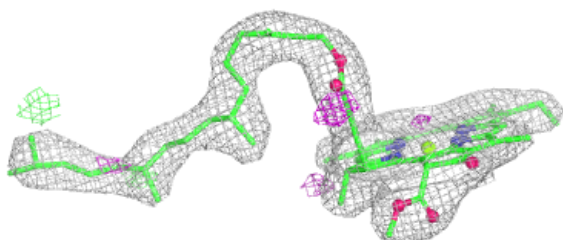
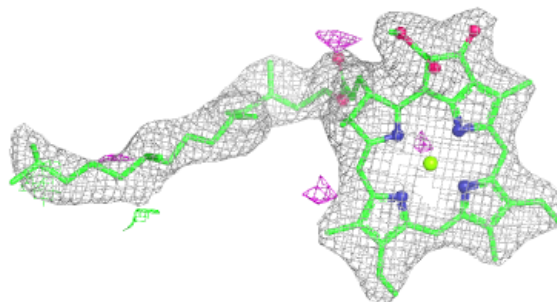


Electron density around BCR B 617:

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

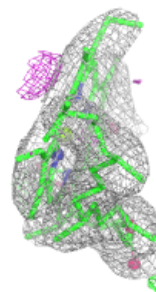
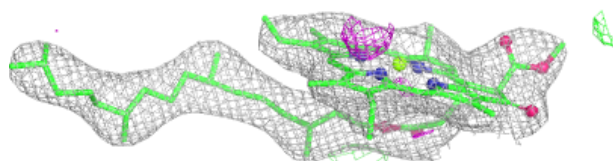
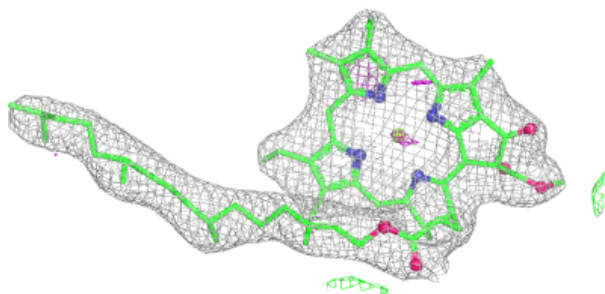
**Electron density around CLA A 406:**

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

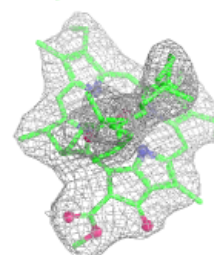
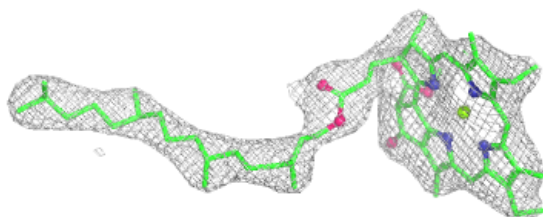
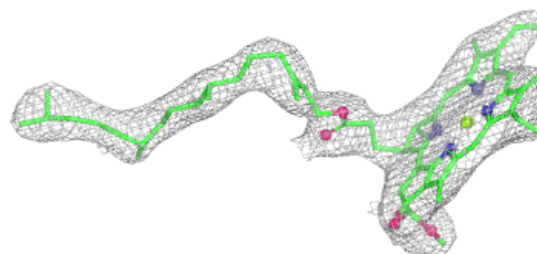


Electron density around CLA C 502:

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

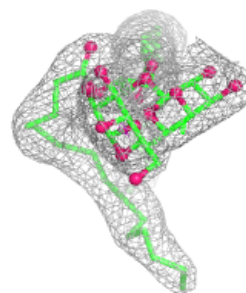
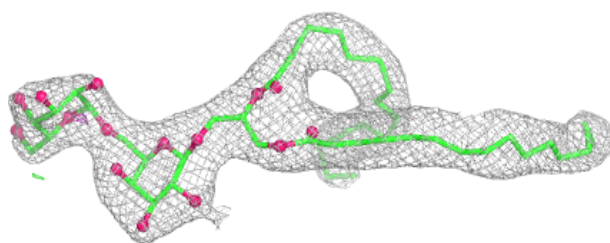
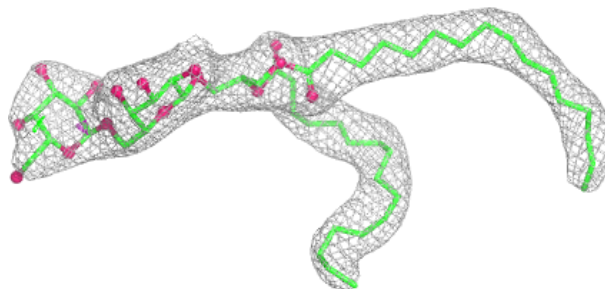
**Electron density around CLA C 503:**

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

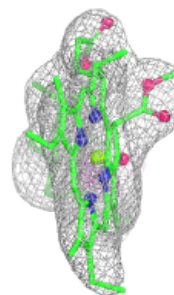
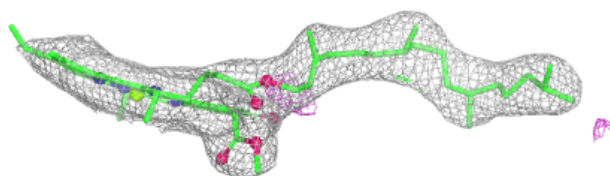
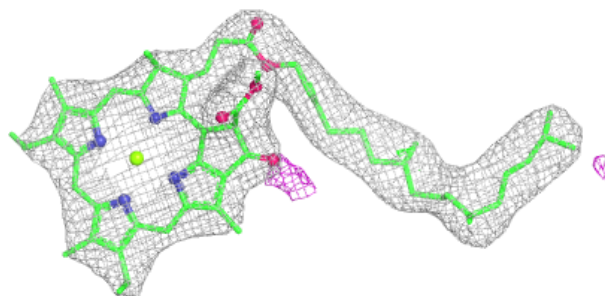


Electron density around DGD H 102:

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

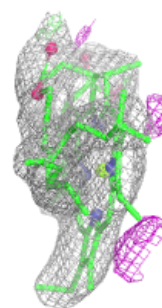
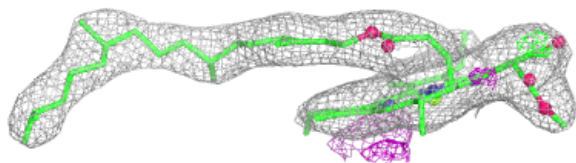
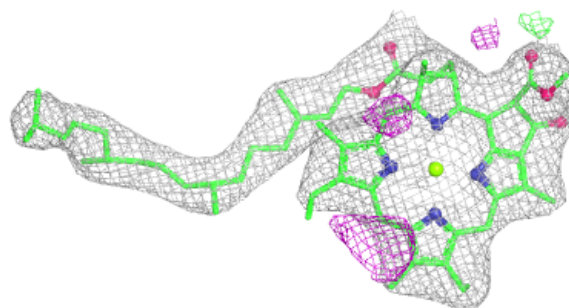
**Electron density around CLA b 602:**

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

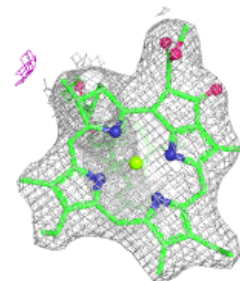
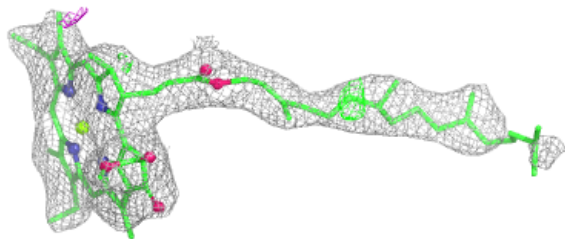
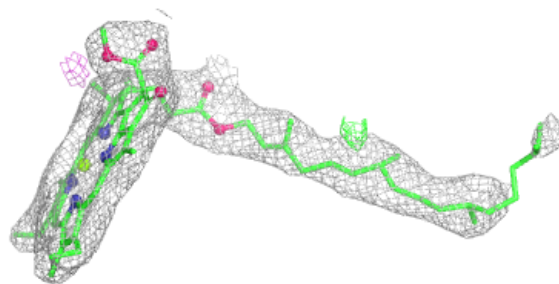


Electron density around CLA b 603:

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

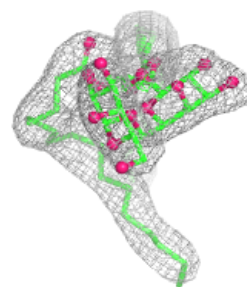
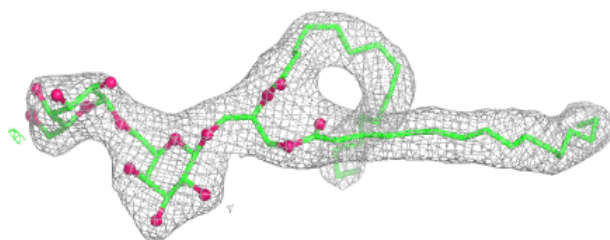
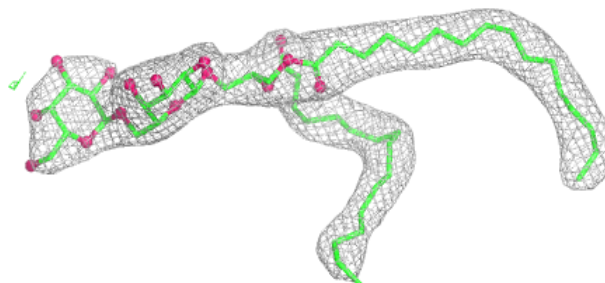
**Electron density around CLA b 604:**

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

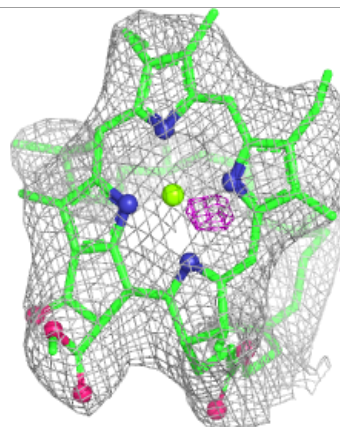
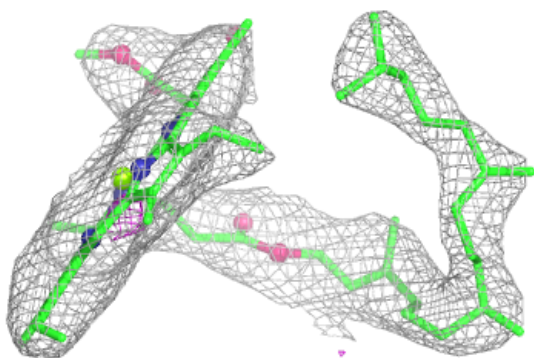
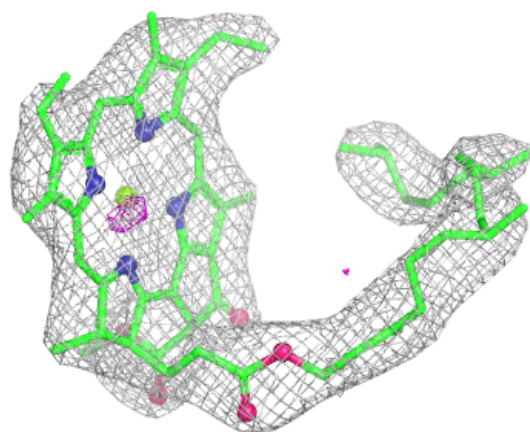


Electron density around DGD h 102:

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

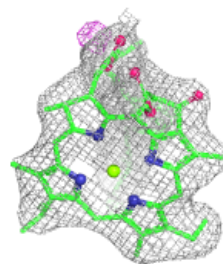
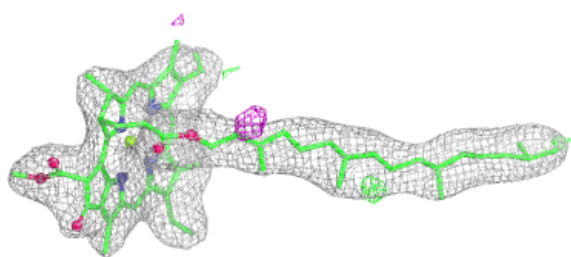
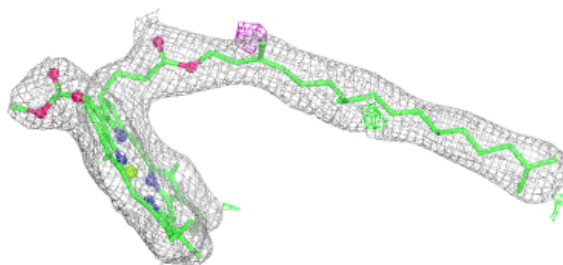
**Electron density around CLA C 504:**

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

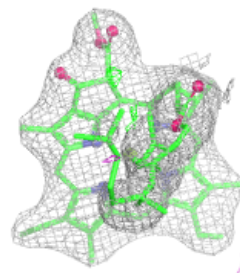
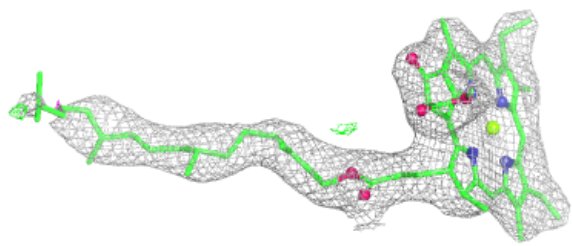
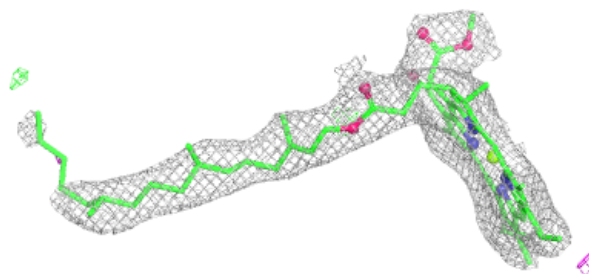


Electron density around CLA b 607:

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

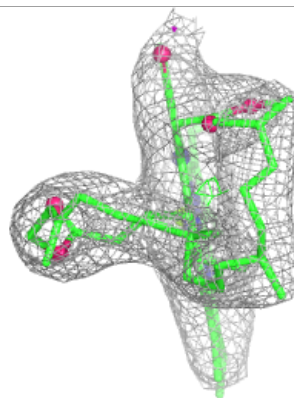
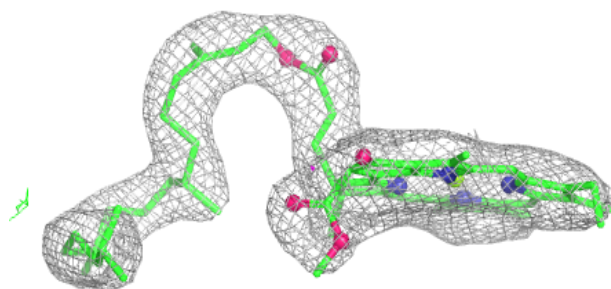
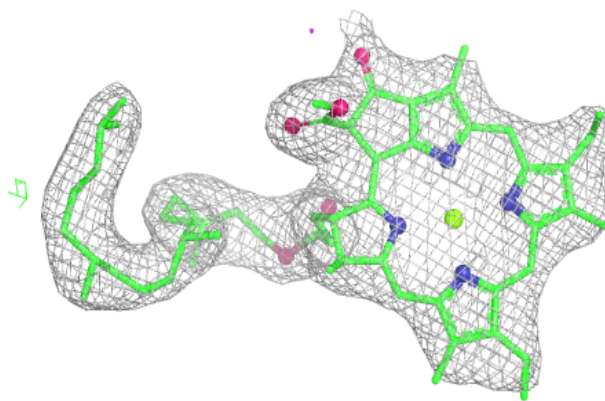
**Electron density around CLA B 604:**

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

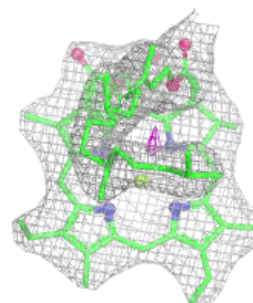
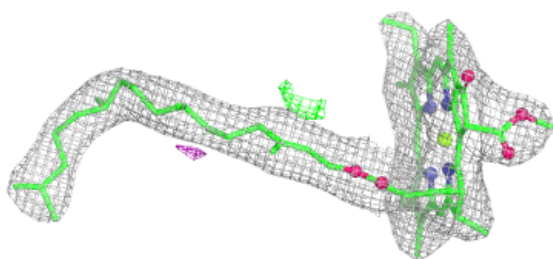
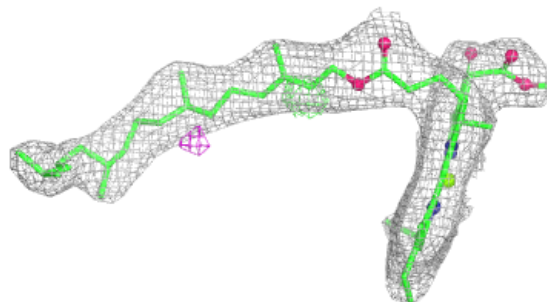


Electron density around CLA B 612:

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

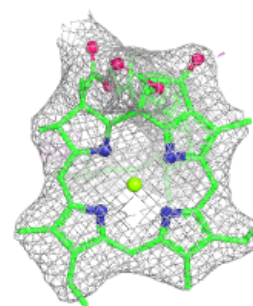
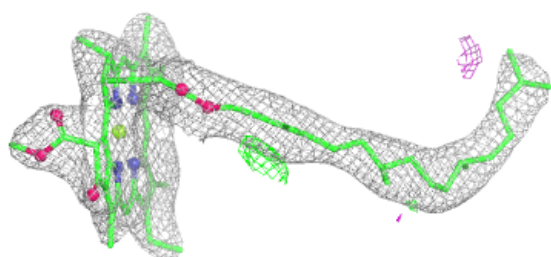
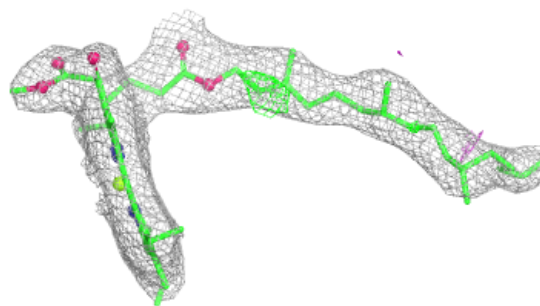
**Electron density around CLA B 605:**

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

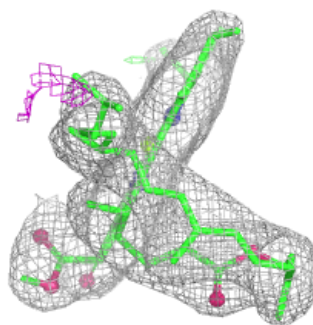
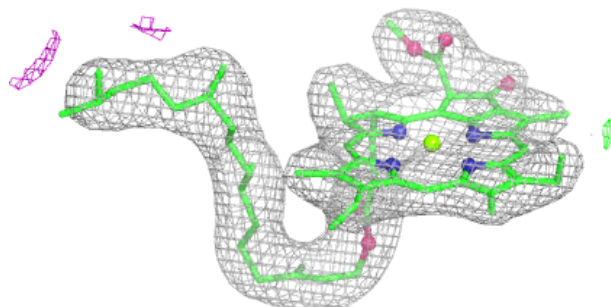
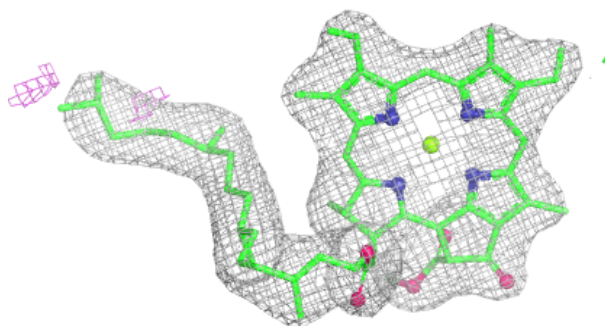


Electron density around CLA b 605:

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

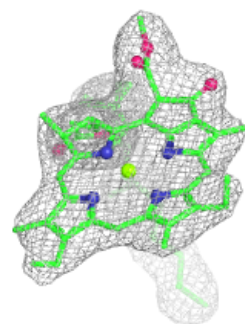
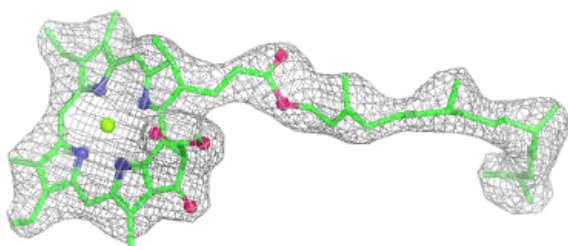
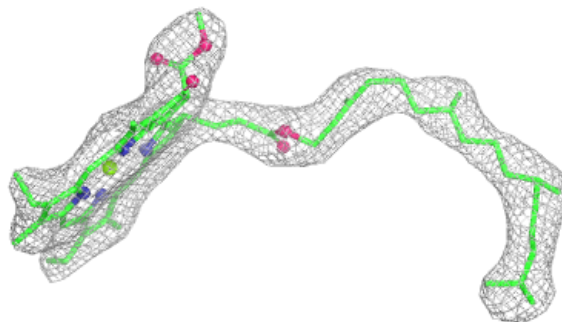
**Electron density around CLA d 401:**

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

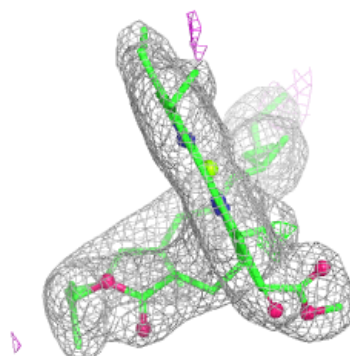
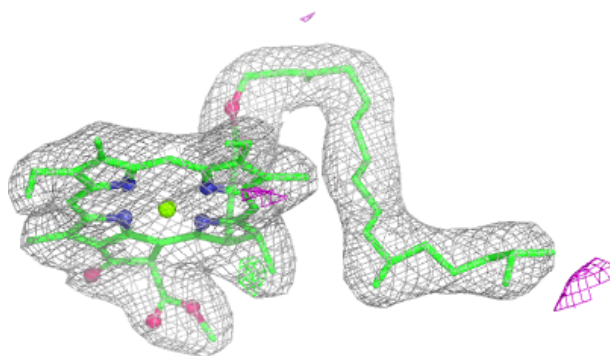
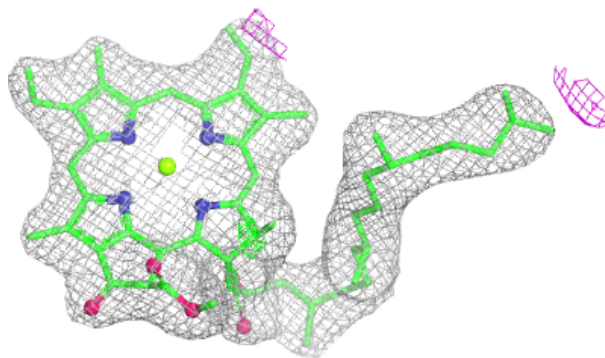


Electron density around CLA d 403:

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

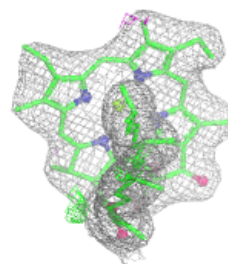
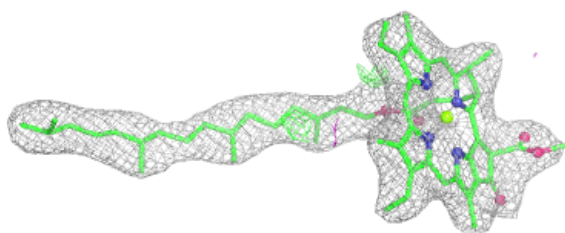
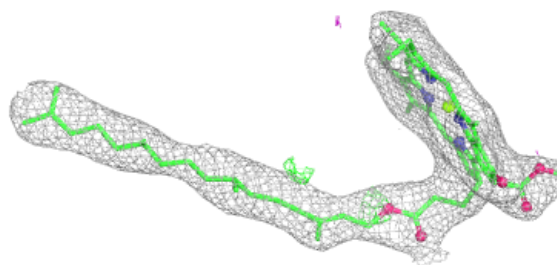
**Electron density around CLA A 405:**

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



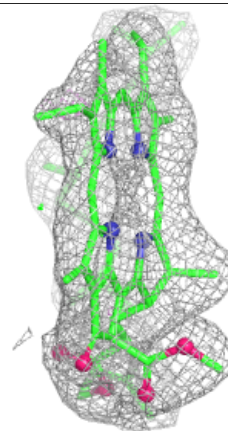
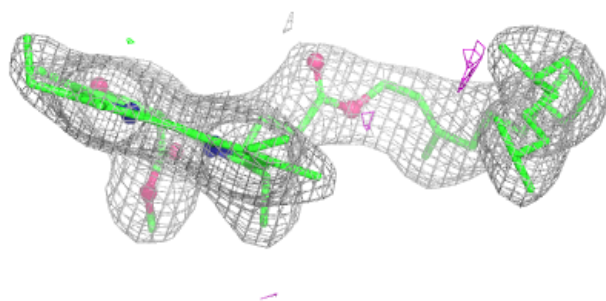
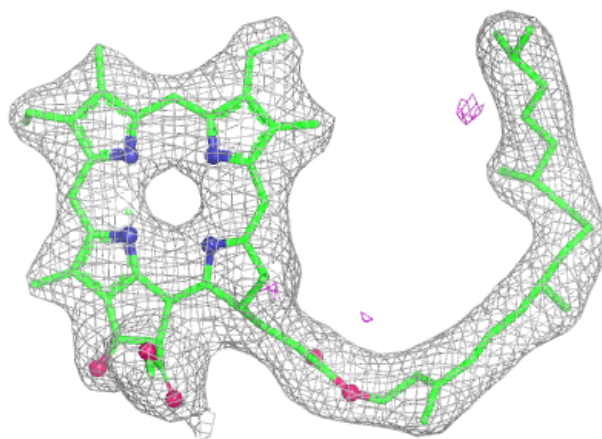
Electron density around CLA B 607:

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



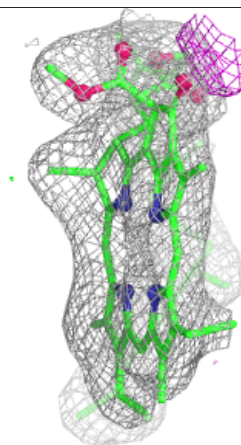
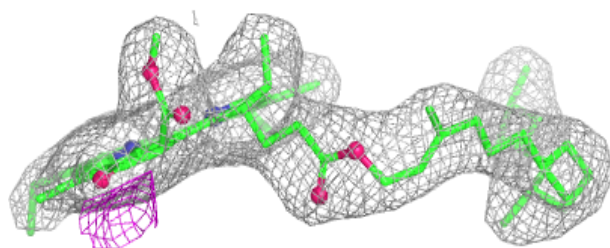
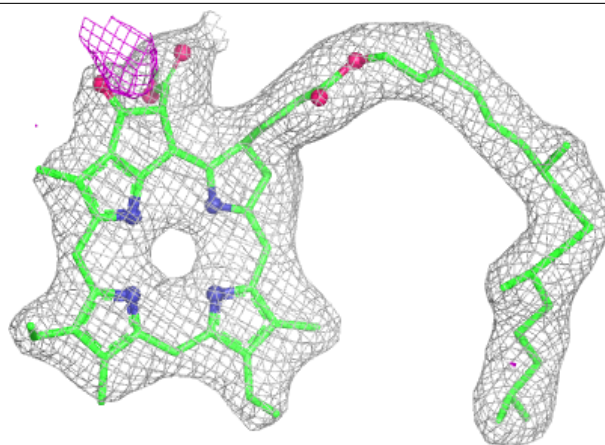
Electron density around PHO D 401:

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



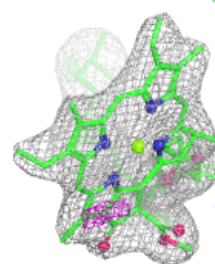
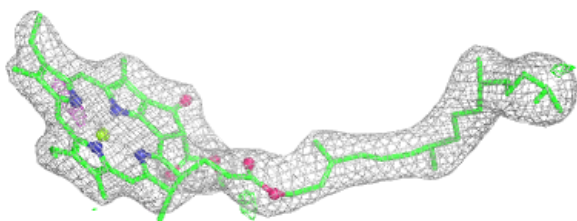
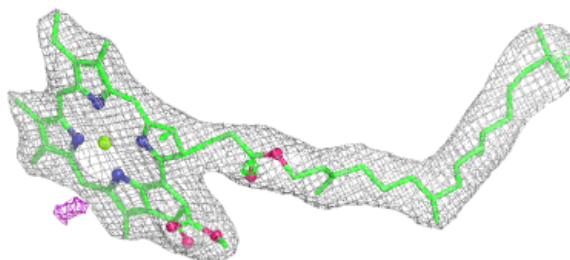
Electron density around PHO a 406:

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

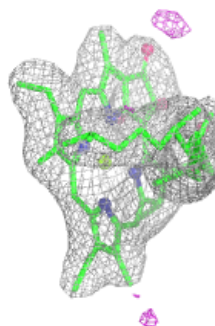
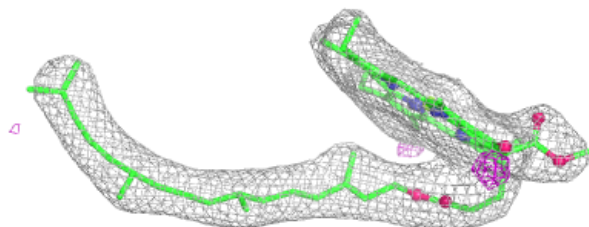
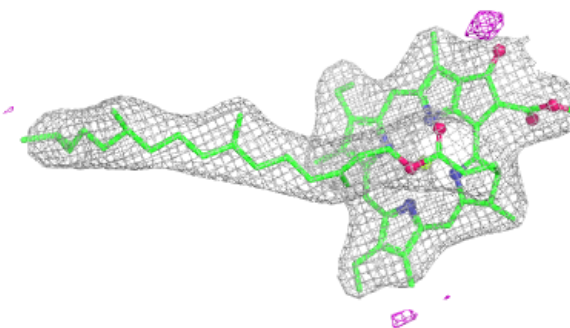


Electron density around CLA a 404:

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

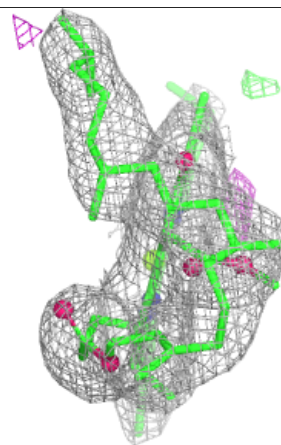
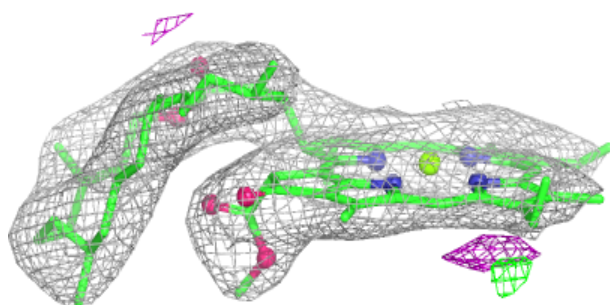
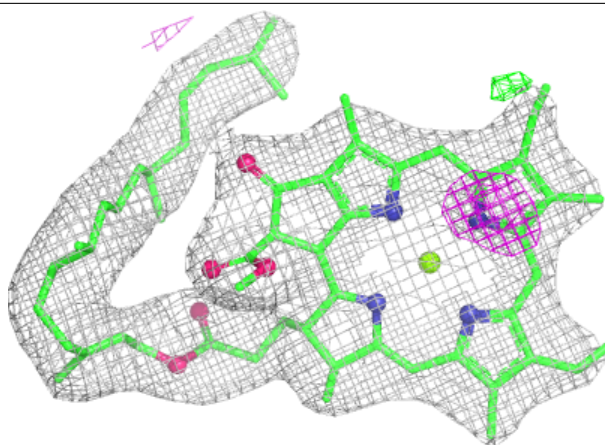
**Electron density around CLA B 608:**

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



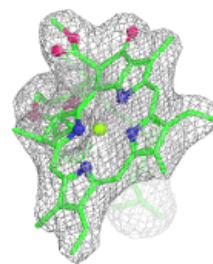
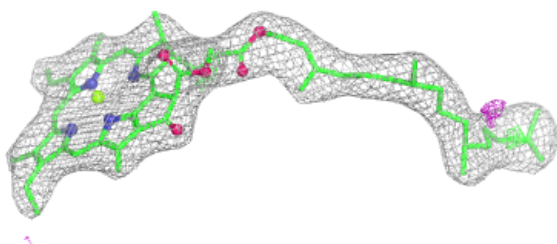
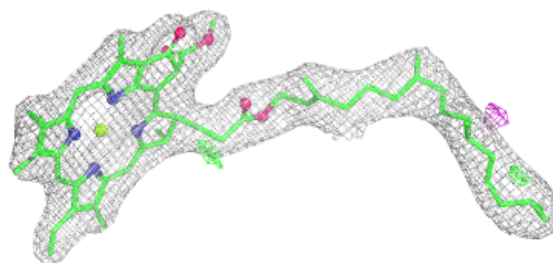
Electron density around CLA b 610:

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



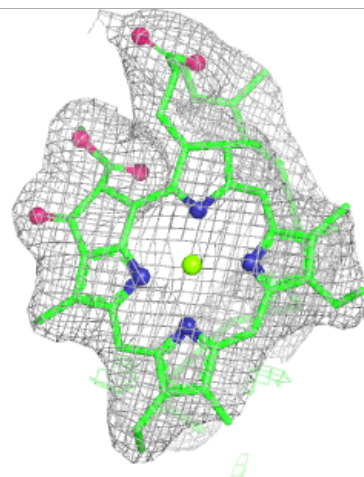
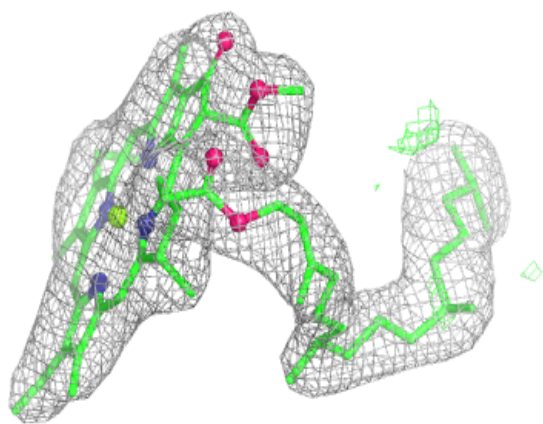
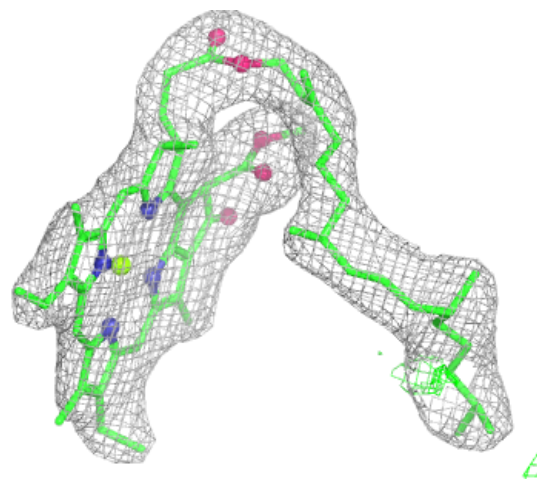
Electron density around CLA A 404:

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



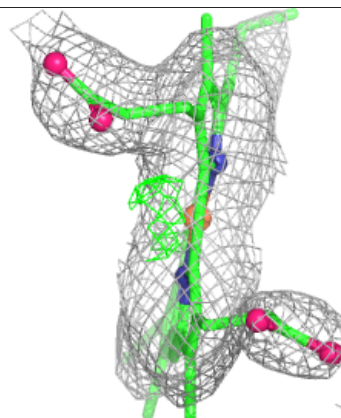
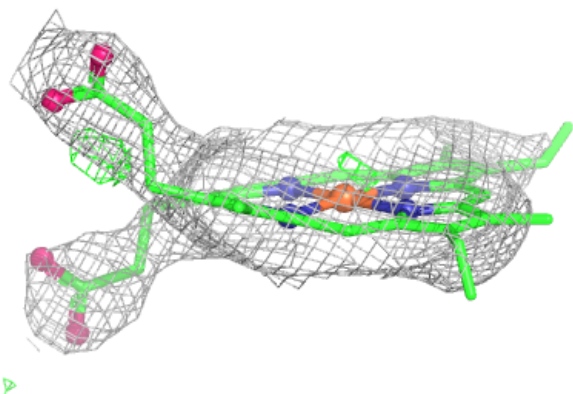
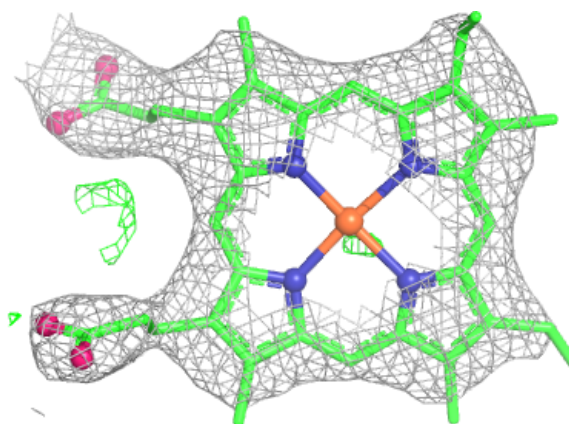
Electron density around CLA b 613:

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



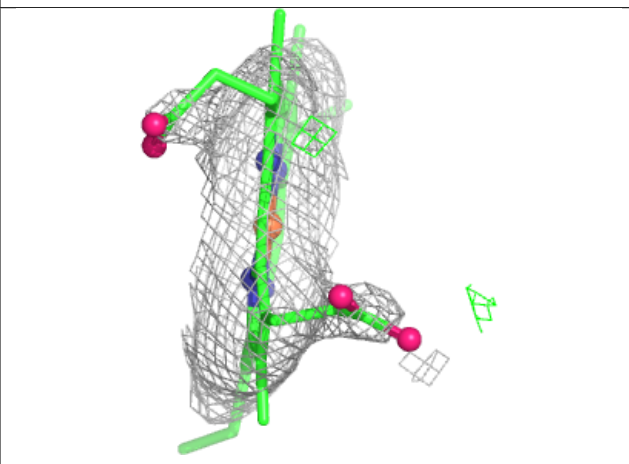
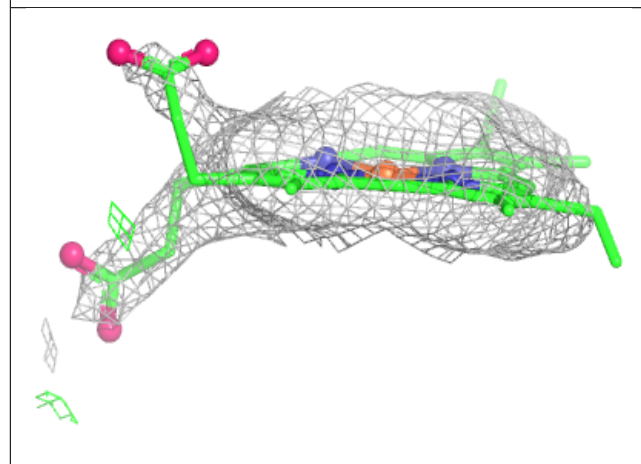
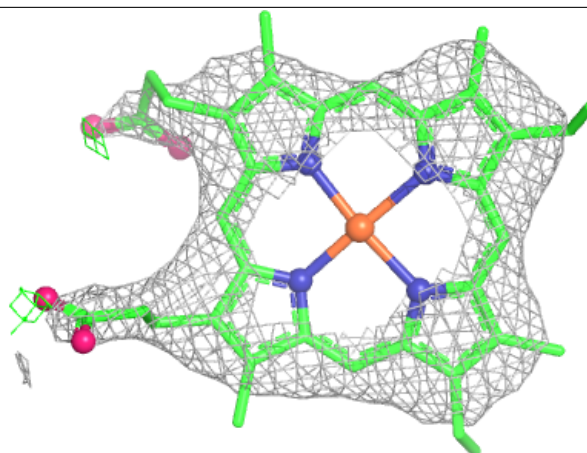
Electron density around HEM E 103:

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



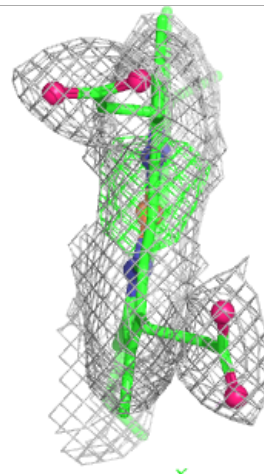
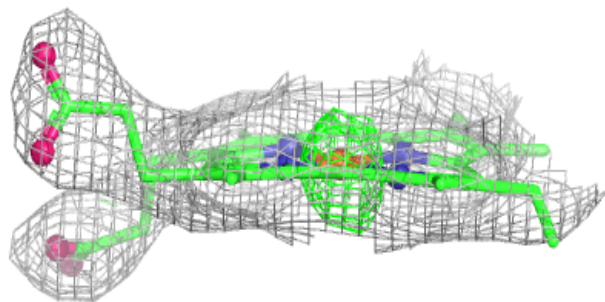
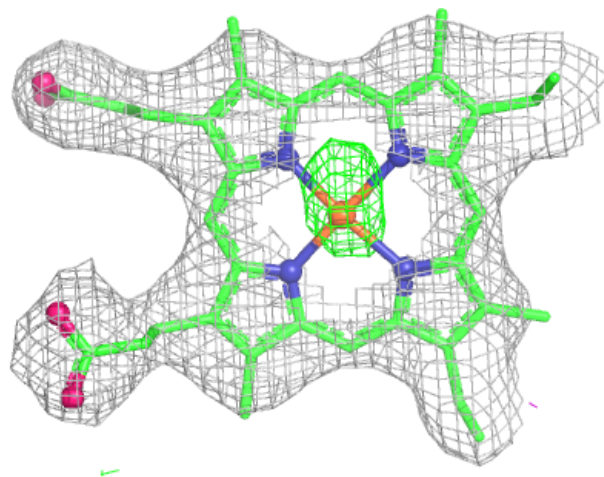
Electron density around HEM e 103:

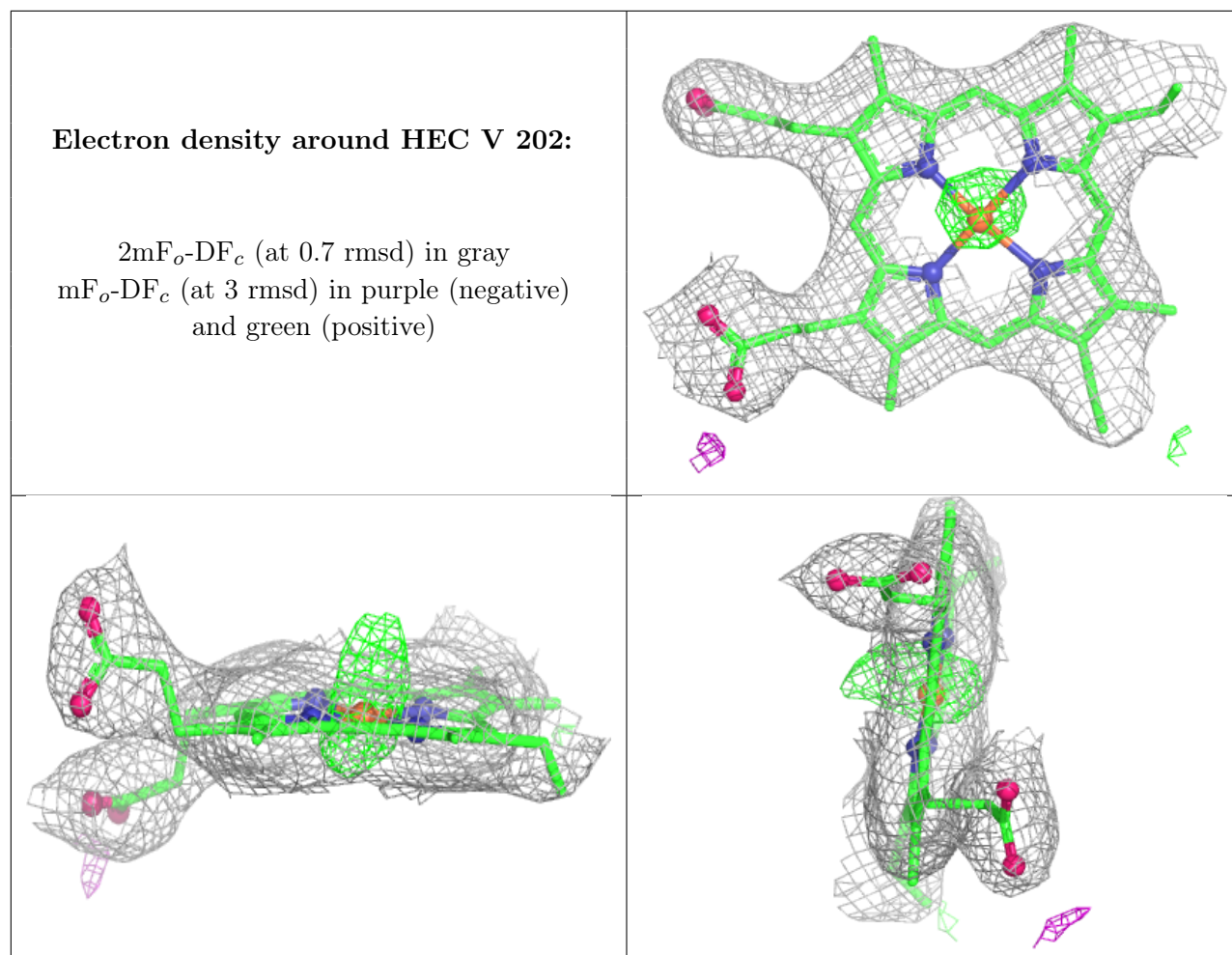
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.